



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2021 – 12:07 PM EDT

PDB ID : 4P9H  
Title : Crystal structure of 8ANC195 Fab in complex with gp120 of 93TH057 HIV-1 and soluble CD4 D1D2  
Authors : Scharf, L.; Bjorkman, P.J.  
Deposited on : 2014-04-04  
Resolution : 3.00 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](mailto: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.

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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 : 2.22  
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) : 2.22

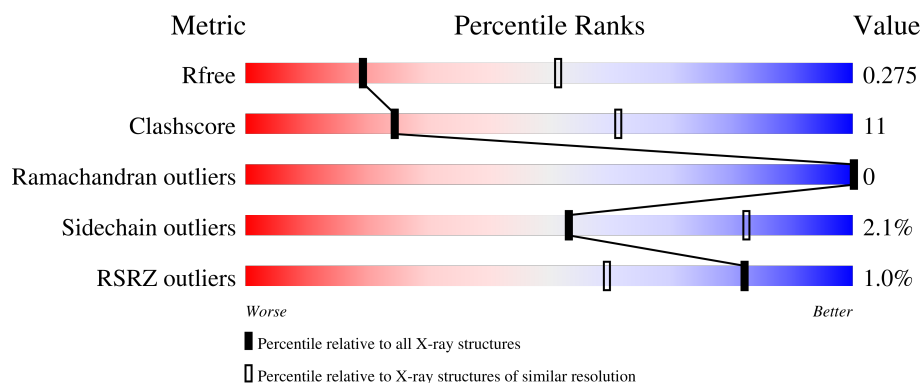
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	C	192	<div> <div>2%</div> <div>68% 18% 13%</div> </div>
2	G	361	<div> <div>80% 13% 6%</div> </div>
3	H	244	<div> <div>66% 23% 12%</div> </div>
4	L	215	<div> <div>2%</div> <div>80% 19%</div> </div>
5	A	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	2	 50% 50%
6	B	10	 80% 20%
7	D	4	 75% 25%
8	E	5	 100%
9	I	4	 100%

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7371 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 T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	167	Total	C	N	O	S	0	0	0
			1225	763	207	251	4			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	THR	LYS	conflict	UNP P01730
C	183	ILE	-	expression tag	UNP P01730
C	184	ASP	-	expression tag	UNP P01730
C	185	GLY	-	expression tag	UNP P01730
C	186	ARG	-	expression tag	UNP P01730
C	187	HIS	-	expression tag	UNP P01730
C	188	HIS	-	expression tag	UNP P01730
C	189	HIS	-	expression tag	UNP P01730
C	190	HIS	-	expression tag	UNP P01730
C	191	HIS	-	expression tag	UNP P01730
C	192	HIS	-	expression tag	UNP P01730

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	338	Total	C	N	O	S	0	0	0
			2616	1639	453	500	24			

There are 284 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	65	CYS	VAL	conflict	UNP Q0ED31
G	88	GLN	ASN	conflict	UNP Q0ED31
G	115	CYS	SER	conflict	UNP Q0ED31
G	124	GLY	-	expression tag	UNP Q0ED31
G	198	GLY	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	199	SER	-	expression tag	UNP Q0ED31
G	200	VAL	-	expression tag	UNP Q0ED31
G	201	ILE	-	expression tag	UNP Q0ED31
G	202	LYS	-	expression tag	UNP Q0ED31
G	203	GLN	-	expression tag	UNP Q0ED31
G	204	ALA	-	expression tag	UNP Q0ED31
G	205	CYS	-	expression tag	UNP Q0ED31
G	206	PRO	-	expression tag	UNP Q0ED31
G	207	LYS	-	expression tag	UNP Q0ED31
G	208	ILE	-	expression tag	UNP Q0ED31
G	209	SER	-	expression tag	UNP Q0ED31
G	210	PHE	-	expression tag	UNP Q0ED31
G	211	ASP	-	expression tag	UNP Q0ED31
G	212	PRO	-	expression tag	UNP Q0ED31
G	213	ILE	-	expression tag	UNP Q0ED31
G	214	PRO	-	expression tag	UNP Q0ED31
G	215	ILE	-	expression tag	UNP Q0ED31
G	216	HIS	-	expression tag	UNP Q0ED31
G	217	TYR	-	expression tag	UNP Q0ED31
G	218	CYS	-	expression tag	UNP Q0ED31
G	219	THR	-	expression tag	UNP Q0ED31
G	220	PRO	-	expression tag	UNP Q0ED31
G	221	ALA	-	expression tag	UNP Q0ED31
G	222	GLY	-	expression tag	UNP Q0ED31
G	223	TYR	-	expression tag	UNP Q0ED31
G	224	VAL	-	expression tag	UNP Q0ED31
G	225	ILE	-	expression tag	UNP Q0ED31
G	226	LEU	-	expression tag	UNP Q0ED31
G	227	LYS	-	expression tag	UNP Q0ED31
G	228	CYS	-	expression tag	UNP Q0ED31
G	229	ASN	-	expression tag	UNP Q0ED31
G	230	ASP	-	expression tag	UNP Q0ED31
G	231	LYS	-	expression tag	UNP Q0ED31
G	232	ASN	-	expression tag	UNP Q0ED31
G	233	PHE	-	expression tag	UNP Q0ED31
G	234	ASN	-	expression tag	UNP Q0ED31
G	235	GLY	-	expression tag	UNP Q0ED31
G	236	THR	-	expression tag	UNP Q0ED31
G	237	GLY	-	expression tag	UNP Q0ED31
G	238	PRO	-	expression tag	UNP Q0ED31
G	239	CYS	-	expression tag	UNP Q0ED31
G	240	LYS	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	241	ASN	-	expression tag	UNP Q0ED31
G	242	VAL	-	expression tag	UNP Q0ED31
G	243	SER	-	expression tag	UNP Q0ED31
G	244	SER	-	expression tag	UNP Q0ED31
G	245	VAL	-	expression tag	UNP Q0ED31
G	246	GLN	-	expression tag	UNP Q0ED31
G	247	CYS	-	expression tag	UNP Q0ED31
G	248	THR	-	expression tag	UNP Q0ED31
G	249	HIS	-	expression tag	UNP Q0ED31
G	250	GLY	-	expression tag	UNP Q0ED31
G	251	ILE	-	expression tag	UNP Q0ED31
G	252	LYS	-	expression tag	UNP Q0ED31
G	253	PRO	-	expression tag	UNP Q0ED31
G	254	VAL	-	expression tag	UNP Q0ED31
G	255	VAL	-	expression tag	UNP Q0ED31
G	256	SER	-	expression tag	UNP Q0ED31
G	257	THR	-	expression tag	UNP Q0ED31
G	258	GLN	-	expression tag	UNP Q0ED31
G	259	LEU	-	expression tag	UNP Q0ED31
G	260	LEU	-	expression tag	UNP Q0ED31
G	261	LEU	-	expression tag	UNP Q0ED31
G	262	ASN	-	expression tag	UNP Q0ED31
G	263	GLY	-	expression tag	UNP Q0ED31
G	264	SER	-	expression tag	UNP Q0ED31
G	265	LEU	-	expression tag	UNP Q0ED31
G	266	ALA	-	expression tag	UNP Q0ED31
G	267	GLU	-	expression tag	UNP Q0ED31
G	268	GLU	-	expression tag	UNP Q0ED31
G	269	GLU	-	expression tag	UNP Q0ED31
G	270	ILE	-	expression tag	UNP Q0ED31
G	271	ILE	-	expression tag	UNP Q0ED31
G	272	ILE	-	expression tag	UNP Q0ED31
G	273	ARG	-	expression tag	UNP Q0ED31
G	274	SER	-	expression tag	UNP Q0ED31
G	275	GLU	-	expression tag	UNP Q0ED31
G	276	ASN	-	expression tag	UNP Q0ED31
G	277	LEU	-	expression tag	UNP Q0ED31
G	278	THR	-	expression tag	UNP Q0ED31
G	279	ASN	-	expression tag	UNP Q0ED31
G	280	ASN	-	expression tag	UNP Q0ED31
G	281	ALA	-	expression tag	UNP Q0ED31
G	282	LYS	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	283	THR	-	expression tag	UNP Q0ED31
G	284	ILE	-	expression tag	UNP Q0ED31
G	285	ILE	-	expression tag	UNP Q0ED31
G	286	VAL	-	expression tag	UNP Q0ED31
G	287	HIS	-	expression tag	UNP Q0ED31
G	288	LEU	-	expression tag	UNP Q0ED31
G	289	GLN	-	expression tag	UNP Q0ED31
G	290	LYS	-	expression tag	UNP Q0ED31
G	291	SER	-	expression tag	UNP Q0ED31
G	292	VAL	-	expression tag	UNP Q0ED31
G	293	GLU	-	expression tag	UNP Q0ED31
G	294	ILE	-	expression tag	UNP Q0ED31
G	295	ASN	-	expression tag	UNP Q0ED31
G	296	CYS	-	expression tag	UNP Q0ED31
G	297	THR	-	expression tag	UNP Q0ED31
G	298	ARG	-	expression tag	UNP Q0ED31
G	299	PRO	-	expression tag	UNP Q0ED31
G	300	SER	-	expression tag	UNP Q0ED31
G	301	ASN	-	expression tag	UNP Q0ED31
G	318	GLY	-	expression tag	UNP Q0ED31
G	319	GLY	-	expression tag	UNP Q0ED31
G	320	SER	-	expression tag	UNP Q0ED31
G	321	GLY	-	expression tag	UNP Q0ED31
G	322	SER	-	expression tag	UNP Q0ED31
G	323	GLY	-	expression tag	UNP Q0ED31
G	324	GLY	-	expression tag	UNP Q0ED31
G	325	ASP	-	expression tag	UNP Q0ED31
G	326	ILE	-	expression tag	UNP Q0ED31
G	327	ARG	-	expression tag	UNP Q0ED31
G	328	LYS	-	expression tag	UNP Q0ED31
G	329	ALA	-	expression tag	UNP Q0ED31
G	330	TYR	-	expression tag	UNP Q0ED31
G	331	CYS	-	expression tag	UNP Q0ED31
G	332	GLU	-	expression tag	UNP Q0ED31
G	333	ILE	-	expression tag	UNP Q0ED31
G	334	GLN	-	expression tag	UNP Q0ED31
G	335	GLY	-	expression tag	UNP Q0ED31
G	336	THR	-	expression tag	UNP Q0ED31
G	337	LYS	-	expression tag	UNP Q0ED31
G	338	TRP	-	expression tag	UNP Q0ED31
G	339	ASN	-	expression tag	UNP Q0ED31
G	340	LYS	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	341	VAL	-	expression tag	UNP Q0ED31
G	342	LEU	-	expression tag	UNP Q0ED31
G	343	LYS	-	expression tag	UNP Q0ED31
G	344	GLN	-	expression tag	UNP Q0ED31
G	345	VAL	-	expression tag	UNP Q0ED31
G	346	THR	-	expression tag	UNP Q0ED31
G	347	GLU	-	expression tag	UNP Q0ED31
G	348	LYS	-	expression tag	UNP Q0ED31
G	349	LEU	-	expression tag	UNP Q0ED31
G	350	LYS	-	expression tag	UNP Q0ED31
G	351	GLU	-	expression tag	UNP Q0ED31
G	352	HIS	-	expression tag	UNP Q0ED31
G	353	PHE	-	expression tag	UNP Q0ED31
G	354	ASN	-	expression tag	UNP Q0ED31
G	355	ASN	-	expression tag	UNP Q0ED31
G	357	LYS	-	expression tag	UNP Q0ED31
G	358	THR	-	expression tag	UNP Q0ED31
G	359	ILE	-	expression tag	UNP Q0ED31
G	360	ILE	-	expression tag	UNP Q0ED31
G	361	PHE	-	expression tag	UNP Q0ED31
G	362	GLN	-	expression tag	UNP Q0ED31
G	363	PRO	-	expression tag	UNP Q0ED31
G	364	PRO	-	expression tag	UNP Q0ED31
G	365	SER	-	expression tag	UNP Q0ED31
G	366	GLY	-	expression tag	UNP Q0ED31
G	367	GLY	-	expression tag	UNP Q0ED31
G	368	ASP	-	expression tag	UNP Q0ED31
G	369	LEU	-	expression tag	UNP Q0ED31
G	370	GLU	-	expression tag	UNP Q0ED31
G	371	ILE	-	expression tag	UNP Q0ED31
G	372	THR	-	expression tag	UNP Q0ED31
G	373	MET	-	expression tag	UNP Q0ED31
G	374	HIS	-	expression tag	UNP Q0ED31
G	375	HIS	-	expression tag	UNP Q0ED31
G	376	PHE	-	expression tag	UNP Q0ED31
G	377	ASN	-	expression tag	UNP Q0ED31
G	378	CYS	-	expression tag	UNP Q0ED31
G	379	ARG	-	expression tag	UNP Q0ED31
G	380	GLY	-	expression tag	UNP Q0ED31
G	381	GLU	-	expression tag	UNP Q0ED31
G	382	PHE	-	expression tag	UNP Q0ED31
G	383	PHE	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	384	TYR	-	expression tag	UNP Q0ED31
G	385	CYS	-	expression tag	UNP Q0ED31
G	386	ASN	-	expression tag	UNP Q0ED31
G	387	THR	-	expression tag	UNP Q0ED31
G	388	THR	-	expression tag	UNP Q0ED31
G	389	GLN	-	expression tag	UNP Q0ED31
G	390	LEU	-	expression tag	UNP Q0ED31
G	391	PHE	-	expression tag	UNP Q0ED31
G	392	GLN	-	expression tag	UNP Q0ED31
G	393	ASN	-	expression tag	UNP Q0ED31
G	394	THR	-	expression tag	UNP Q0ED31
G	395	CYS	-	expression tag	UNP Q0ED31
G	402	ILE	-	expression tag	UNP Q0ED31
G	403	GLY	-	expression tag	UNP Q0ED31
G	404	ASN	-	expression tag	UNP Q0ED31
G	405	GLU	-	expression tag	UNP Q0ED31
G	406	THR	-	expression tag	UNP Q0ED31
G	407	MET	-	expression tag	UNP Q0ED31
G	408	LYS	-	expression tag	UNP Q0ED31
G	409	GLY	-	expression tag	UNP Q0ED31
G	410	CYS	-	expression tag	UNP Q0ED31
G	411	ASN	-	expression tag	UNP Q0ED31
G	412	GLY	-	expression tag	UNP Q0ED31
G	413	THR	-	expression tag	UNP Q0ED31
G	414	ILE	-	expression tag	UNP Q0ED31
G	415	THR	-	expression tag	UNP Q0ED31
G	416	LEU	-	expression tag	UNP Q0ED31
G	417	PRO	-	expression tag	UNP Q0ED31
G	418	CYS	-	expression tag	UNP Q0ED31
G	419	LYS	-	expression tag	UNP Q0ED31
G	420	ILE	-	expression tag	UNP Q0ED31
G	421	LYS	-	expression tag	UNP Q0ED31
G	422	GLN	-	expression tag	UNP Q0ED31
G	423	ILE	-	expression tag	UNP Q0ED31
G	424	ILE	-	expression tag	UNP Q0ED31
G	425	ASN	-	expression tag	UNP Q0ED31
G	426	MET	-	expression tag	UNP Q0ED31
G	427	TRP	-	expression tag	UNP Q0ED31
G	428	GLN	-	expression tag	UNP Q0ED31
G	429	GLY	-	expression tag	UNP Q0ED31
G	430	THR	-	expression tag	UNP Q0ED31
G	431	GLY	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	432	GLN	-	expression tag	UNP Q0ED31
G	433	ALA	-	expression tag	UNP Q0ED31
G	434	MET	-	expression tag	UNP Q0ED31
G	435	TYR	-	expression tag	UNP Q0ED31
G	436	ALA	-	expression tag	UNP Q0ED31
G	437	PRO	-	expression tag	UNP Q0ED31
G	438	PRO	-	expression tag	UNP Q0ED31
G	439	ILE	-	expression tag	UNP Q0ED31
G	440	ASP	-	expression tag	UNP Q0ED31
G	441	GLY	-	expression tag	UNP Q0ED31
G	442	LYS	-	expression tag	UNP Q0ED31
G	443	ILE	-	expression tag	UNP Q0ED31
G	444	ASN	-	expression tag	UNP Q0ED31
G	445	CYS	-	expression tag	UNP Q0ED31
G	446	VAL	-	expression tag	UNP Q0ED31
G	447	SER	-	expression tag	UNP Q0ED31
G	448	GLN	-	expression tag	UNP Q0ED31
G	449	ILE	-	expression tag	UNP Q0ED31
G	450	THR	-	expression tag	UNP Q0ED31
G	451	GLY	-	expression tag	UNP Q0ED31
G	452	ILE	-	expression tag	UNP Q0ED31
G	453	LEU	-	expression tag	UNP Q0ED31
G	454	LEU	-	expression tag	UNP Q0ED31
G	455	THR	-	expression tag	UNP Q0ED31
G	456	ARG	-	expression tag	UNP Q0ED31
G	457	ASP	-	expression tag	UNP Q0ED31
G	458	GLY	-	expression tag	UNP Q0ED31
G	459	GLY	-	expression tag	UNP Q0ED31
G	460	ALA	-	expression tag	UNP Q0ED31
G	461	ASN	-	expression tag	UNP Q0ED31
G	462	ASN	-	expression tag	UNP Q0ED31
G	463	THR	-	expression tag	UNP Q0ED31
G	464	SER	-	expression tag	UNP Q0ED31
G	465	ASN	-	expression tag	UNP Q0ED31
G	466	GLU	-	expression tag	UNP Q0ED31
G	467	THR	-	expression tag	UNP Q0ED31
G	468	PHE	-	expression tag	UNP Q0ED31
G	469	ARG	-	expression tag	UNP Q0ED31
G	470	PRO	-	expression tag	UNP Q0ED31
G	471	GLY	-	expression tag	UNP Q0ED31
G	472	GLY	-	expression tag	UNP Q0ED31
G	473	GLY	-	expression tag	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	474	ASN	-	expression tag	UNP Q0ED31
G	475	ILE	-	expression tag	UNP Q0ED31
G	476	LYS	-	expression tag	UNP Q0ED31
G	477	ASP	-	expression tag	UNP Q0ED31
G	478	ASN	-	expression tag	UNP Q0ED31
G	479	TRP	-	expression tag	UNP Q0ED31
G	480	ARG	-	expression tag	UNP Q0ED31
G	481	SER	-	expression tag	UNP Q0ED31
G	482	GLU	-	expression tag	UNP Q0ED31
G	483	LEU	-	expression tag	UNP Q0ED31
G	484	TYR	-	expression tag	UNP Q0ED31
G	485	LYS	-	expression tag	UNP Q0ED31
G	486	TYR	-	expression tag	UNP Q0ED31
G	487	LYS	-	expression tag	UNP Q0ED31
G	488	VAL	-	expression tag	UNP Q0ED31
G	489	VAL	-	expression tag	UNP Q0ED31
G	490	GLN	-	expression tag	UNP Q0ED31
G	491	ILE	-	expression tag	UNP Q0ED31
G	492	GLU	-	expression tag	UNP Q0ED31
G	493	GLY	-	expression tag	UNP Q0ED31
G	494	SER	-	expression tag	UNP Q0ED31
G	495	HIS	-	expression tag	UNP Q0ED31
G	496	HIS	-	expression tag	UNP Q0ED31
G	497	HIS	-	expression tag	UNP Q0ED31
G	498	HIS	-	expression tag	UNP Q0ED31
G	499	HIS	-	expression tag	UNP Q0ED31
G	500	HIS	-	expression tag	UNP Q0ED31

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1573	1000	262	306	5			

- Molecule 4 is a protein called Fab light chain.

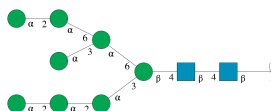
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1549	969	263	312	5			

- Molecule 5 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
5	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



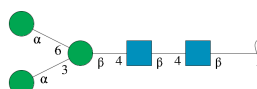
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	B	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
7	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



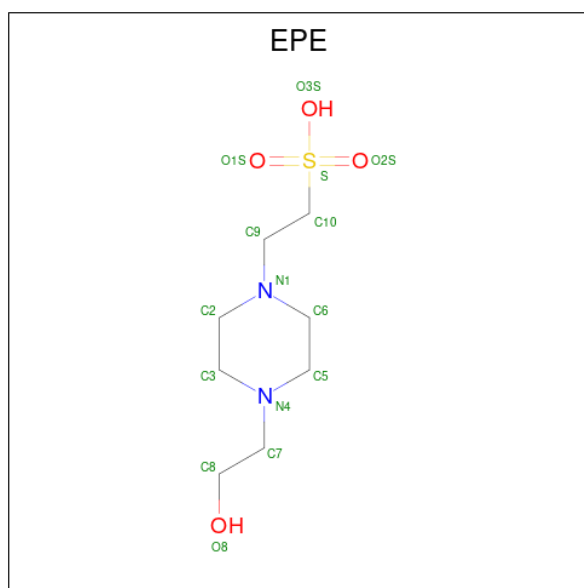
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	E	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



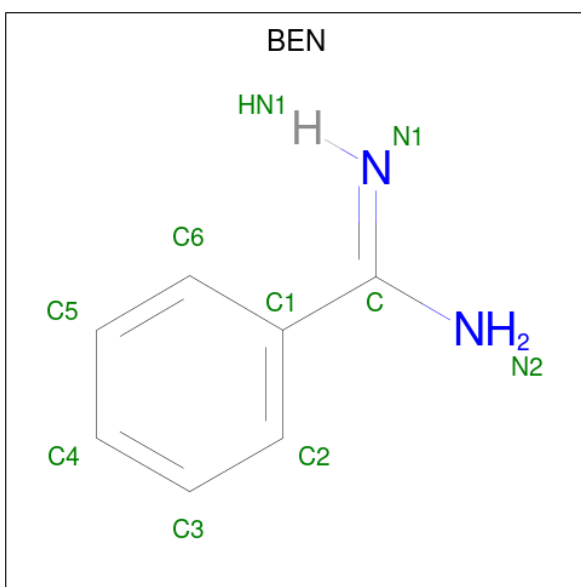
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 10 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



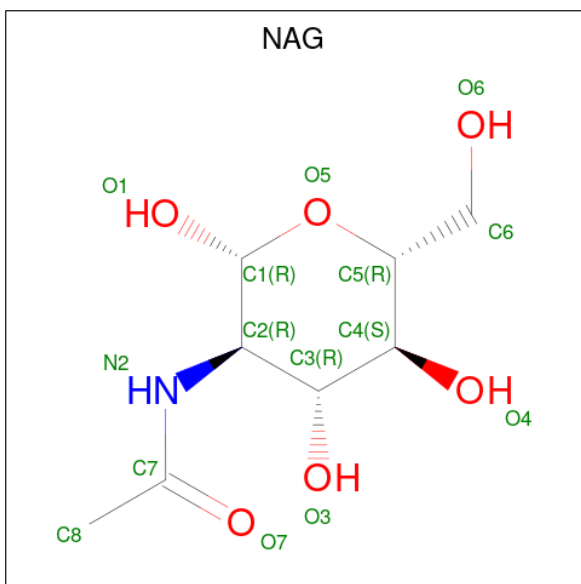
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 11 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	G	1	Total	C	N	0	0
			9	7	2		
11	G	1	Total	C	N	0	0
			9	7	2		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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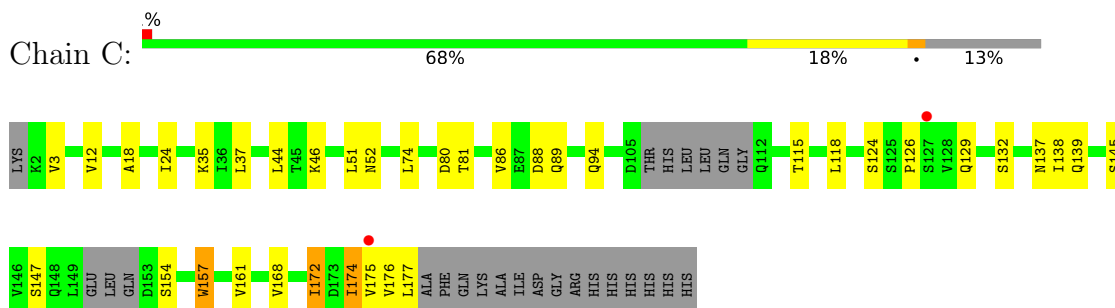
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	1	Total	C	N	O	0	0
			14	8	1	5		
12	H	1	Total	C	N	O	0	0
			14	8	1	5		

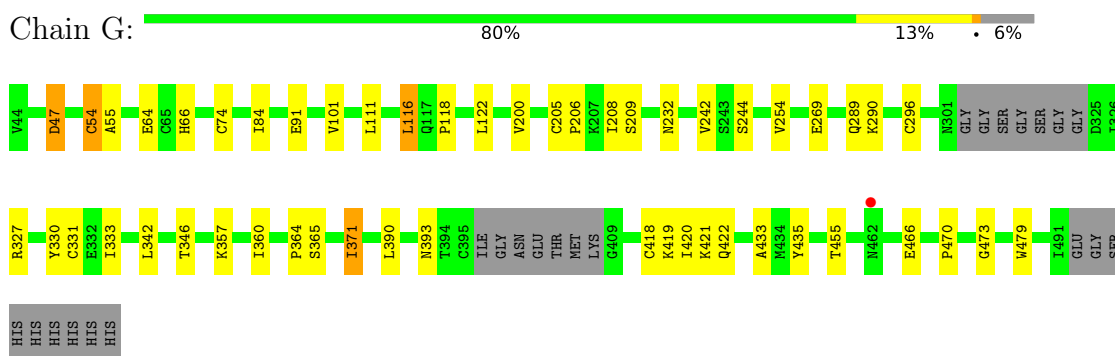
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

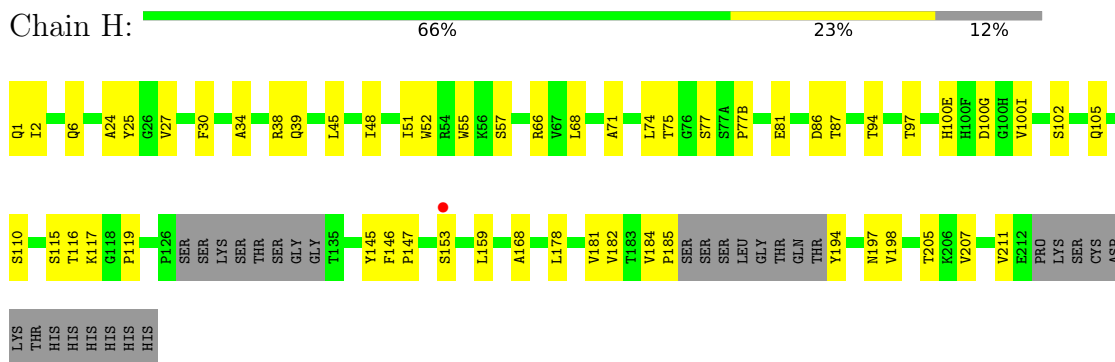
- Molecule 1: T-cell surface glycoprotein CD4



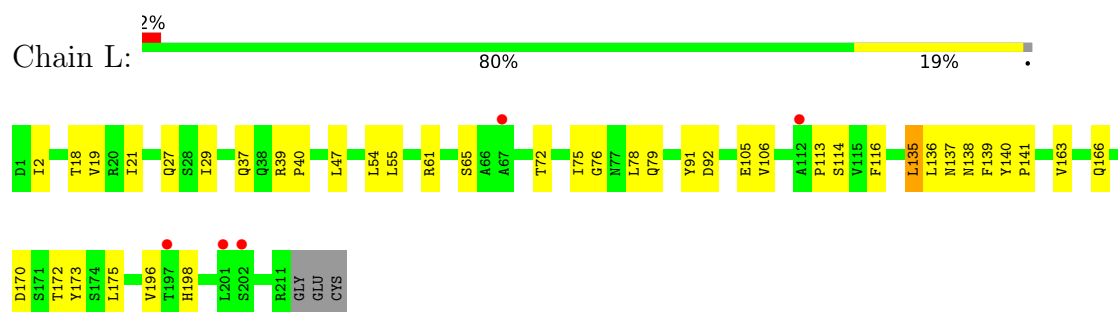
- Molecule 2: Envelope glycoprotein gp160



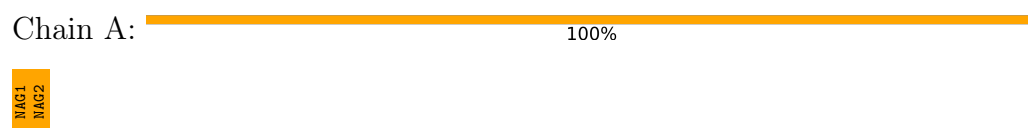
- Molecule 3: Fab heavy chain



- Molecule 4: Fab light chain



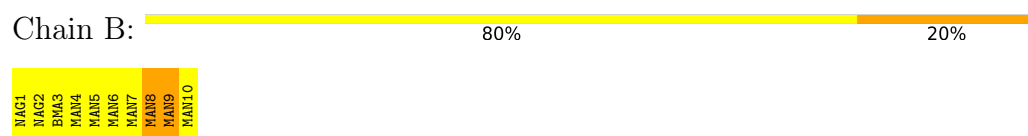
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



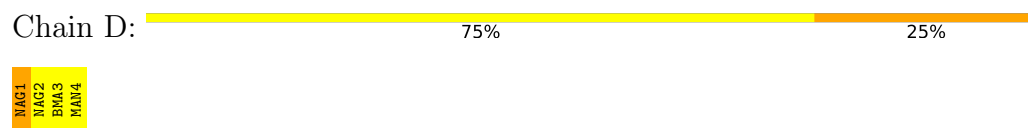
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



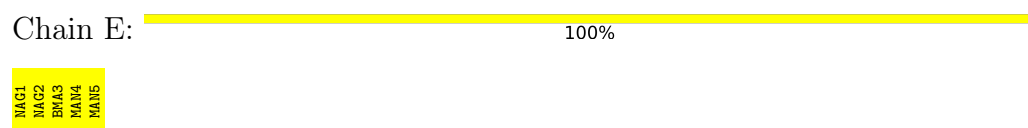
- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

100%

MAG1  
MAG2  
BMA3  
MAN4

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.53Å 132.49Å 142.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 3.00 39.22 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.22-3.00) 97.6 (39.22-2.65)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.272 0.242 , 0.275	Depositor DCC
$R_{free}$ test set	2000 reflections (5.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BEN, NAG, MAN, BMA, EPE

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	C	0.37	0/1241	0.57	1/1686 (0.1%)
2	G	0.43	0/2672	0.54	0/3637
3	H	0.39	0/1615	0.49	0/2214
4	L	0.34	0/1583	0.50	0/2165
All	All	0.39	0/7111	0.52	1/9702 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1225	0	1162	36	0
2	G	2616	0	2495	39	0
3	H	1573	0	1491	37	0
4	L	1549	0	1434	47	0
5	A	28	0	25	2	0
5	F	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	116	0	97	3	0
7	D	50	0	43	1	0
8	E	61	0	52	0	0
9	I	50	0	43	0	0
10	G	15	0	18	1	0
11	G	18	0	15	1	0
12	G	28	0	26	0	0
12	H	14	0	13	0	0
All	All	7371	0	6939	156	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 11.

All (156) 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:G:419:LYS:HE3	2:G:421:LYS:HD2	1.36	1.07
1:C:175:VAL:HG12	1:C:176:VAL:H	1.17	1.05
1:C:175:VAL:HG12	1:C:176:VAL:N	1.73	0.95
2:G:419:LYS:CE	2:G:421:LYS:HD3	1.98	0.94
2:G:419:LYS:HE3	2:G:421:LYS:CD	1.97	0.94
2:G:419:LYS:CE	2:G:421:LYS:CD	2.45	0.93
1:C:175:VAL:CG1	1:C:176:VAL:H	1.81	0.93
2:G:419:LYS:HE2	2:G:421:LYS:HD3	1.48	0.91
1:C:176:VAL:HG12	1:C:177:LEU:N	1.85	0.91
4:L:61:ARG:NH1	4:L:79:GLN:HG3	1.86	0.91
1:C:176:VAL:HG12	1:C:177:LEU:H	1.37	0.90
1:C:154:SER:OG	1:C:176:VAL:HG23	1.77	0.85
2:G:419:LYS:CE	2:G:421:LYS:HD2	2.09	0.82
2:G:419:LYS:HE2	2:G:421:LYS:CD	2.10	0.81
4:L:105:GLU:HG2	4:L:166:GLN:OE1	1.79	0.81
4:L:105:GLU:HG3	4:L:173:TYR:OH	1.81	0.79
1:C:176:VAL:CG1	1:C:177:LEU:H	1.95	0.79
4:L:105:GLU:OE2	4:L:106:VAL:O	2.00	0.78
3:H:1:GLN:HG2	3:H:2:ILE:H	1.48	0.78
1:C:86:VAL:HG13	1:C:89:GLN:HB2	1.66	0.77
3:H:159:LEU:HD21	3:H:182:VAL:HG11	1.68	0.75
1:C:154:SER:OG	1:C:176:VAL:CG2	2.37	0.73
3:H:1:GLN:CG	3:H:2:ILE:H	2.02	0.72
1:C:52:ASN:ND2	2:G:365:SER:O	2.23	0.72
4:L:105:GLU:OE2	4:L:166:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:54:CYS:SG	2:G:55:ALA:N	2.66	0.68
1:C:154:SER:CB	1:C:176:VAL:HG23	2.24	0.68
3:H:87:THR:HG23	3:H:110:SER:HA	1.76	0.67
4:L:137:ASN:O	4:L:139:PHE:HD1	1.78	0.67
2:G:422:GLN:HB3	2:G:435:TYR:O	1.95	0.67
4:L:61:ARG:HH11	4:L:79:GLN:HG3	1.59	0.66
4:L:61:ARG:HH12	4:L:79:GLN:HB2	1.59	0.66
5:A:1:NAG:O6	5:A:2:NAG:C7	2.46	0.64
1:C:175:VAL:CG1	1:C:176:VAL:N	2.42	0.63
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.80	0.63
3:H:119:PRO:HB3	3:H:145:TYR:HB3	1.80	0.63
4:L:136:LEU:HD22	4:L:175:LEU:HD22	1.82	0.61
1:C:86:VAL:HG22	1:C:86:VAL:O	1.99	0.61
1:C:157:TRP:HB3	1:C:172:ILE:CD1	2.31	0.61
4:L:61:ARG:HH12	4:L:79:GLN:HG3	1.65	0.61
4:L:105:GLU:OE2	4:L:140:TYR:CE2	2.53	0.61
4:L:137:ASN:O	4:L:139:PHE:CD1	2.55	0.60
4:L:61:ARG:NH1	4:L:79:GLN:CG	2.64	0.59
1:C:174:ILE:HG22	1:C:175:VAL:H	1.66	0.59
3:H:119:PRO:HD2	3:H:205:THR:HG21	1.84	0.59
4:L:61:ARG:HH12	4:L:79:GLN:CG	2.16	0.59
1:C:154:SER:CB	1:C:176:VAL:CG2	2.80	0.59
1:C:37:LEU:HD11	1:C:44:LEU:HD11	1.86	0.58
4:L:105:GLU:OE2	4:L:140:TYR:HE2	1.87	0.57
4:L:170:ASP:HB2	4:L:172:THR:HG22	1.86	0.56
3:H:198:VAL:HB	3:H:207:VAL:HG23	1.88	0.56
4:L:61:ARG:HH12	4:L:79:GLN:CB	2.19	0.56
4:L:138:ASN:HB3	4:L:172:THR:HG21	1.88	0.55
2:G:84:ILE:HG13	2:G:244:SER:HB3	1.87	0.55
2:G:371:ILE:HD11	2:G:473:GLY:CA	2.36	0.55
1:C:3:VAL:HG22	1:C:94:GLN:HB3	1.88	0.55
2:G:327:ARG:HG2	2:G:420:ILE:O	2.07	0.54
1:C:80:ASP:OD1	1:C:81:THR:N	2.39	0.54
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.41	0.53
2:G:122:LEU:HD13	2:G:200:VAL:HG22	1.90	0.53
3:H:1:GLN:HG2	3:H:2:ILE:N	2.21	0.53
1:C:46:LYS:HD3	1:C:52:ASN:O	2.08	0.53
4:L:78:LEU:O	4:L:79:GLN:HG2	2.09	0.52
3:H:181:VAL:HG11	4:L:135:LEU:HD22	1.90	0.52
3:H:97:THR:HA	3:H:100(E):HIS:CD2	2.44	0.52
4:L:136:LEU:HD11	4:L:196:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:51:ILE:HD13	3:H:71:ALA:HB3	1.92	0.52
1:C:35:LYS:NZ	2:G:455:THR:HG22	2.24	0.51
2:G:66:HIS:CD2	2:G:111:LEU:HD21	2.44	0.51
3:H:1:GLN:CG	3:H:2:ILE:N	2.73	0.51
3:H:38:ARG:HB3	3:H:48:ILE:HD11	1.92	0.51
2:G:296:CYS:HA	2:G:331:CYS:HA	1.92	0.51
4:L:54:LEU:HD23	4:L:55:LEU:O	2.11	0.51
4:L:116:PHE:HB2	4:L:135:LEU:HD23	1.93	0.51
4:L:78:LEU:C	4:L:79:GLN:HG2	2.31	0.50
1:C:46:LYS:O	2:G:365:SER:OG	2.29	0.50
2:G:342:LEU:O	2:G:346:THR:HG23	2.12	0.50
2:G:208:ILE:HG13	2:G:209:SER:N	2.27	0.50
4:L:135:LEU:C	4:L:136:LEU:HD12	2.31	0.49
4:L:140:TYR:CD1	4:L:141:PRO:HA	2.46	0.49
4:L:136:LEU:HD12	4:L:136:LEU:N	2.28	0.49
2:G:333:ILE:HD12	2:G:390:LEU:HD21	1.93	0.49
3:H:6:GLN:O	3:H:105:GLN:NE2	2.46	0.49
2:G:371:ILE:HD11	2:G:473:GLY:N	2.28	0.48
1:C:12:VAL:HG12	1:C:74:LEU:HD21	1.96	0.48
2:G:330:TYR:OH	5:F:2:NAG:H81	2.13	0.48
3:H:74:LEU:HD12	3:H:77(B):PRO:HA	1.96	0.48
4:L:136:LEU:N	4:L:136:LEU:CD1	2.76	0.47
3:H:57:SER:HB3	6:B:8:MAN:H2	1.95	0.47
4:L:65:SER:HB3	4:L:72:THR:HG23	1.94	0.47
2:G:357:LYS:HE3	2:G:466:GLU:HG2	1.95	0.47
3:H:94:THR:HG22	3:H:102:SER:HB2	1.96	0.47
3:H:117:LYS:N	3:H:146:PHE:O	2.39	0.47
2:G:118:PRO:HB3	2:G:433:ALA:HB1	1.96	0.47
3:H:68:LEU:HA	6:B:9:MAN:H62	1.96	0.46
1:C:132:SER:HA	1:C:157:TRP:CD1	2.50	0.46
3:H:34:ALA:HB2	3:H:52:TRP:CD1	2.50	0.46
4:L:138:ASN:HA	4:L:173:TYR:O	2.15	0.46
2:G:205:CYS:N	2:G:206:PRO:HD3	2.31	0.46
2:G:64:GLU:OE1	2:G:66:HIS:HB2	2.16	0.45
2:G:327:ARG:HH11	10:G:601:EPE:H102	1.80	0.45
4:L:114:SER:HB2	4:L:137:ASN:HB3	1.99	0.45
3:H:168:ALA:HA	3:H:178:LEU:HB3	1.98	0.45
3:H:100(I):VAL:HG12	4:L:91:TYR:HB2	1.99	0.45
3:H:153:SER:HB3	3:H:197:ASN:HB2	1.99	0.45
1:C:157:TRP:HB3	1:C:172:ILE:HD12	1.98	0.45
3:H:57:SER:OG	6:B:9:MAN:O6	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:25:TYR:CE2	3:H:77(B):PRO:HG3	2.52	0.45
4:L:170:ASP:CB	4:L:172:THR:HG22	2.46	0.45
1:C:18:ALA:HA	1:C:89:GLN:HE22	1.83	0.44
4:L:113:PRO:HD3	4:L:198:HIS:ND1	2.32	0.44
1:C:154:SER:HB3	1:C:176:VAL:CG2	2.46	0.44
2:G:331:CYS:SG	2:G:418:CYS:SG	3.16	0.44
2:G:360:ILE:HA	2:G:393:ASN:HD21	1.83	0.44
2:G:47:ASP:OD1	2:G:47:ASP:N	2.51	0.43
4:L:163:VAL:HG22	4:L:175:LEU:HD12	2.00	0.43
2:G:91:GLU:HB3	2:G:242:VAL:HG21	2.00	0.43
2:G:101:VAL:HG13	2:G:479:TRP:HB2	1.99	0.43
4:L:2:ILE:HD12	4:L:27:GLN:HG2	2.00	0.43
4:L:65:SER:HB3	4:L:72:THR:CG2	2.49	0.43
3:H:184:VAL:CG1	3:H:185:PRO:HD2	2.49	0.43
4:L:37:GLN:HB2	4:L:47:LEU:HD11	2.00	0.43
1:C:176:VAL:CG1	1:C:177:LEU:N	2.52	0.43
1:C:161:VAL:HB	1:C:168:VAL:HG13	2.01	0.43
4:L:105:GLU:CG	4:L:166:GLN:OE1	2.59	0.42
3:H:75:THR:HG23	3:H:77:SER:H	1.83	0.42
4:L:140:TYR:CD1	4:L:141:PRO:CA	3.03	0.42
3:H:30:PHE:HB2	3:H:55:TRP:CH2	2.53	0.42
3:H:116:THR:HB	3:H:147:PRO:HD3	2.02	0.42
3:H:194:TYR:O	3:H:211:VAL:HG12	2.20	0.42
1:C:132:SER:HB2	1:C:157:TRP:CE2	2.55	0.42
1:C:137:ASN:C	1:C:138:ILE:HD12	2.40	0.42
2:G:232:ASN:ND2	2:G:269:GLU:OE2	2.52	0.42
4:L:61:ARG:HB2	4:L:76:GLY:O	2.20	0.42
2:G:364:PRO:HD3	2:G:470:PRO:HG2	2.02	0.42
5:A:1:NAG:HO6	5:A:2:NAG:C7	2.33	0.42
3:H:68:LEU:HB3	3:H:81:GLU:HB3	2.00	0.42
1:C:86:VAL:CG1	1:C:89:GLN:HB2	2.44	0.41
1:C:118:LEU:CD2	1:C:126:PRO:HB3	2.50	0.41
4:L:18:THR:HA	4:L:75:ILE:O	2.20	0.41
4:L:139:PHE:N	4:L:172:THR:OG1	2.53	0.41
1:C:138:ILE:HD12	1:C:138:ILE:N	2.35	0.41
2:G:254:VAL:HG13	7:D:1:NAG:H81	2.02	0.41
4:L:61:ARG:NH1	4:L:79:GLN:HB2	2.33	0.41
3:H:34:ALA:HB2	3:H:52:TRP:HD1	1.85	0.41
4:L:19:VAL:HG12	4:L:21:ILE:HG13	2.03	0.41
2:G:116:LEU:HD12	2:G:116:LEU:HA	1.95	0.41
3:H:24:ALA:HB1	3:H:27:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:68:LEU:HD13	3:H:68:LEU:C	2.41	0.41
4:L:29:ILE:HG23	4:L:92:ASP:HB2	2.02	0.41
1:C:129:GLN:HA	1:C:138:ILE:O	2.21	0.40
4:L:39:ARG:CG	4:L:40:PRO:HD2	2.51	0.40
2:G:74:CYS:O	11:G:602:BEN:N1	2.54	0.40
2:G:289:GLN:HG3	2:G:290:LYS:N	2.37	0.40
1:C:124:SER:C	1:C:126:PRO:HD3	2.42	0.40
3:H:184:VAL:HG13	3:H:185:PRO:HD2	2.03	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	C	161/192 (84%)	153 (95%)	8 (5%)	0	100	100
2	G	332/361 (92%)	315 (95%)	17 (5%)	0	100	100
3	H	209/244 (86%)	207 (99%)	2 (1%)	0	100	100
4	L	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
All	All	912/1012 (90%)	882 (97%)	30 (3%)	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	C	136/173 (79%)	127 (93%)	9 (7%)	16	49
2	G	293/318 (92%)	289 (99%)	4 (1%)	67	88
3	H	173/210 (82%)	171 (99%)	2 (1%)	71	90
4	L	162/182 (89%)	161 (99%)	1 (1%)	86	95
All	All	764/883 (86%)	748 (98%)	16 (2%)	53	82

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	24	ILE
1	C	51	LEU
1	C	115	THR
1	C	139	GLN
1	C	145	SER
1	C	147	SER
1	C	157	TRP
1	C	172	ILE
1	C	174	ILE
2	G	47	ASP
2	G	54	CYS
2	G	116	LEU
2	G	371	ILE
3	H	100(G)	ASP
3	H	115	SER
4	L	135	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
2	G	229	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

27 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	A	1	5,1	14,14,15	1.29	3 (21%)	17,19,21	1.85	3 (17%)
5	NAG	A	2	5	14,14,15	1.37	2 (14%)	17,19,21	1.77	3 (17%)
6	NAG	B	1	2,6	14,14,15	1.45	3 (21%)	17,19,21	0.90	0
6	MAN	B	10	6	11,11,12	1.34	2 (18%)	15,15,17	0.70	0
6	NAG	B	2	6	14,14,15	1.36	3 (21%)	17,19,21	1.01	0
6	BMA	B	3	6	11,11,12	1.45	2 (18%)	15,15,17	1.27	1 (6%)
6	MAN	B	4	6	11,11,12	1.56	2 (18%)	15,15,17	1.04	1 (6%)
6	MAN	B	5	6	11,11,12	1.35	2 (18%)	15,15,17	1.50	1 (6%)
6	MAN	B	6	6	11,11,12	1.42	2 (18%)	15,15,17	0.71	0
6	MAN	B	7	6	11,11,12	1.45	2 (18%)	15,15,17	1.00	2 (13%)
6	MAN	B	8	6	11,11,12	1.71	2 (18%)	15,15,17	1.50	3 (20%)
6	MAN	B	9	6	11,11,12	1.22	2 (18%)	15,15,17	1.01	0
7	NAG	D	1	2,7	14,14,15	1.44	3 (21%)	17,19,21	0.98	1 (5%)
7	NAG	D	2	7	14,14,15	1.40	4 (28%)	17,19,21	1.24	3 (17%)
7	BMA	D	3	7	11,11,12	1.30	1 (9%)	15,15,17	1.76	1 (6%)
7	MAN	D	4	7	11,11,12	1.37	2 (18%)	15,15,17	0.96	0
8	NAG	E	1	2,8	14,14,15	1.51	5 (35%)	17,19,21	1.67	5 (29%)
8	NAG	E	2	8	14,14,15	1.47	2 (14%)	17,19,21	3.24	5 (29%)
8	BMA	E	3	8	11,11,12	1.43	2 (18%)	15,15,17	1.16	2 (13%)
8	MAN	E	4	8	11,11,12	1.87	3 (27%)	15,15,17	2.58	4 (26%)
8	MAN	E	5	8	11,11,12	1.91	3 (27%)	15,15,17	2.10	2 (13%)
5	NAG	F	1	2,5	14,14,15	1.27	3 (21%)	17,19,21	1.71	3 (17%)
5	NAG	F	2	5	14,14,15	1.51	4 (28%)	17,19,21	0.84	0
9	NAG	I	1	2,9	14,14,15	1.42	4 (28%)	17,19,21	1.20	1 (5%)
9	NAG	I	2	9	14,14,15	1.44	4 (28%)	17,19,21	1.06	2 (11%)
9	BMA	I	3	9	11,11,12	1.38	2 (18%)	15,15,17	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	I	4	9	11,11,12	1.42	2 (18%)	15,15,17	0.96	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	A	2	5	-	0/6/23/26	0/1/1/1
6	NAG	B	1	2,6	-	2/6/23/26	0/1/1/1
6	MAN	B	10	6	-	0/2/19/22	0/1/1/1
6	NAG	B	2	6	-	0/6/23/26	0/1/1/1
6	BMA	B	3	6	-	0/2/19/22	0/1/1/1
6	MAN	B	4	6	-	0/2/19/22	0/1/1/1
6	MAN	B	5	6	-	2/2/19/22	0/1/1/1
6	MAN	B	6	6	-	0/2/19/22	0/1/1/1
6	MAN	B	7	6	-	0/2/19/22	0/1/1/1
6	MAN	B	8	6	-	2/2/19/22	0/1/1/1
6	MAN	B	9	6	-	2/2/19/22	0/1/1/1
7	NAG	D	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	D	2	7	-	2/6/23/26	0/1/1/1
7	BMA	D	3	7	-	2/2/19/22	0/1/1/1
7	MAN	D	4	7	-	2/2/19/22	0/1/1/1
8	NAG	E	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	E	2	8	-	4/6/23/26	0/1/1/1
8	BMA	E	3	8	-	2/2/19/22	0/1/1/1
8	MAN	E	4	8	-	0/2/19/22	0/1/1/1
8	MAN	E	5	8	-	0/2/19/22	0/1/1/1
5	NAG	F	1	2,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
9	NAG	I	1	2,9	-	1/6/23/26	0/1/1/1
9	NAG	I	2	9	-	1/6/23/26	0/1/1/1
9	BMA	I	3	9	-	1/2/19/22	0/1/1/1
9	MAN	I	4	9	-	2/2/19/22	0/1/1/1

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	5	MAN	O5-C1	5.13	1.51	1.43
8	E	4	MAN	O5-C1	4.34	1.50	1.43
6	B	8	MAN	O5-C1	3.90	1.49	1.43
6	B	4	MAN	O5-C1	3.63	1.49	1.43
9	I	4	MAN	O5-C1	3.36	1.49	1.43
9	I	3	BMA	O5-C1	3.31	1.49	1.43
6	B	7	MAN	C2-C3	-3.19	1.47	1.52
7	D	3	BMA	O5-C1	3.11	1.48	1.43
8	E	4	MAN	C2-C3	-3.05	1.48	1.52
6	B	6	MAN	O5-C1	3.04	1.48	1.43
6	B	3	BMA	O5-C1	3.01	1.48	1.43
6	B	3	BMA	C2-C3	-2.94	1.48	1.52
6	B	8	MAN	C2-C3	-2.93	1.48	1.52
6	B	10	MAN	O5-C1	2.89	1.48	1.43
6	B	6	MAN	C2-C3	-2.86	1.48	1.52
8	E	3	BMA	C2-C3	-2.85	1.48	1.52
6	B	4	MAN	C2-C3	-2.83	1.48	1.52
7	D	4	MAN	O5-C1	2.82	1.48	1.43
7	D	4	MAN	C2-C3	-2.77	1.48	1.52
6	B	5	MAN	O5-C1	2.75	1.48	1.43
8	E	3	BMA	O5-C1	2.69	1.48	1.43
6	B	7	MAN	O5-C1	2.64	1.47	1.43
8	E	2	NAG	C7-N2	2.64	1.43	1.34
8	E	1	NAG	C3-C2	-2.60	1.47	1.52
5	A	2	NAG	C7-N2	2.58	1.43	1.34
5	F	1	NAG	C7-N2	2.49	1.42	1.34
5	F	2	NAG	O5-C1	2.47	1.47	1.43
6	B	9	MAN	O5-C1	2.46	1.47	1.43
5	A	1	NAG	C6-C5	-2.44	1.43	1.51
6	B	5	MAN	C2-C3	-2.41	1.49	1.52
5	F	2	NAG	O7-C7	2.40	1.28	1.23
5	A	1	NAG	C7-N2	2.38	1.42	1.34
6	B	2	NAG	C7-N2	2.38	1.42	1.34
6	B	1	NAG	C7-N2	2.38	1.42	1.34
9	I	2	NAG	C7-N2	2.35	1.42	1.34
8	E	1	NAG	C1-C2	-2.33	1.48	1.52
9	I	2	NAG	O7-C7	2.33	1.28	1.23
7	D	2	NAG	C7-N2	2.30	1.42	1.34
9	I	4	MAN	C2-C3	-2.29	1.49	1.52
5	A	2	NAG	O7-C7	2.29	1.28	1.23
7	D	1	NAG	O7-C7	2.27	1.28	1.23
9	I	1	NAG	O7-C7	2.27	1.28	1.23
8	E	5	MAN	C2-C3	-2.24	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	10	MAN	C2-C3	-2.23	1.49	1.52
5	F	1	NAG	C6-C5	-2.23	1.44	1.51
9	I	2	NAG	O5-C1	2.20	1.47	1.43
5	A	1	NAG	O7-C7	2.20	1.28	1.23
9	I	1	NAG	C6-C5	-2.20	1.44	1.51
8	E	1	NAG	C7-N2	2.19	1.41	1.34
5	F	2	NAG	O5-C5	2.19	1.47	1.43
7	D	1	NAG	C6-C5	-2.18	1.44	1.51
5	F	2	NAG	C7-N2	2.18	1.41	1.34
9	I	1	NAG	C7-N2	2.15	1.41	1.34
7	D	2	NAG	O7-C7	2.14	1.28	1.23
6	B	1	NAG	O7-C7	2.14	1.28	1.23
9	I	3	BMA	C2-C3	-2.14	1.49	1.52
8	E	1	NAG	O7-C7	2.14	1.28	1.23
8	E	4	MAN	O5-C5	2.13	1.47	1.43
6	B	1	NAG	O5-C1	2.12	1.47	1.43
7	D	1	NAG	C3-C2	-2.12	1.48	1.52
7	D	2	NAG	O5-C1	2.11	1.47	1.43
6	B	2	NAG	O7-C7	2.10	1.28	1.23
5	F	1	NAG	O7-C7	2.09	1.28	1.23
6	B	2	NAG	O5-C1	2.08	1.47	1.43
6	B	9	MAN	C2-C3	-2.08	1.49	1.52
8	E	5	MAN	O5-C5	2.06	1.47	1.43
8	E	1	NAG	C6-C5	-2.04	1.45	1.51
8	E	2	NAG	O5-C1	2.03	1.47	1.43
9	I	1	NAG	O5-C1	2.02	1.46	1.43
9	I	2	NAG	C6-C5	-2.02	1.45	1.51
7	D	2	NAG	O5-C5	2.00	1.47	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	2	NAG	C2-N2-C7	8.23	134.63	122.90
8	E	2	NAG	C8-C7-N2	7.94	129.55	116.10
8	E	4	MAN	C1-O5-C5	6.17	120.56	112.19
7	D	3	BMA	C1-O5-C5	-5.94	104.14	112.19
8	E	4	MAN	C1-C2-C3	5.82	116.82	109.67
8	E	5	MAN	C1-O5-C5	5.62	119.81	112.19
8	E	5	MAN	C1-C2-C3	5.19	116.05	109.67
6	B	5	MAN	C1-C2-C3	4.66	115.39	109.67
5	A	1	NAG	C1-O5-C5	-4.65	105.89	112.19
8	E	2	NAG	O7-C7-N2	-4.52	113.64	121.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2	NAG	C1-O5-C5	4.38	118.12	112.19
5	F	1	NAG	O5-C5-C6	-3.82	101.21	107.20
5	A	2	NAG	C8-C7-N2	3.62	122.23	116.10
9	I	1	NAG	C1-O5-C5	-3.53	107.41	112.19
5	F	1	NAG	O5-C1-C2	-3.31	106.06	111.29
5	F	1	NAG	C8-C7-N2	3.30	121.69	116.10
6	B	3	BMA	C1-O5-C5	-3.07	108.03	112.19
5	A	1	NAG	C1-C2-N2	-2.97	105.41	110.49
6	B	8	MAN	C1-O5-C5	2.95	116.19	112.19
8	E	1	NAG	C1-C2-N2	-2.93	105.48	110.49
8	E	1	NAG	C3-C4-C5	2.84	115.31	110.24
9	I	2	NAG	C1-O5-C5	-2.83	108.35	112.19
5	A	2	NAG	O5-C1-C2	2.83	115.76	111.29
7	D	1	NAG	C2-N2-C7	-2.82	118.88	122.90
8	E	2	NAG	O7-C7-C8	-2.82	116.81	122.06
9	I	4	MAN	C1-C2-C3	2.67	112.94	109.67
8	E	3	BMA	C1-O5-C5	-2.61	108.66	112.19
8	E	1	NAG	C8-C7-N2	2.60	120.50	116.10
5	A	1	NAG	O4-C4-C5	-2.59	102.87	109.30
7	D	2	NAG	O5-C1-C2	-2.52	107.31	111.29
6	B	8	MAN	O2-C2-C3	-2.48	105.16	110.14
8	E	4	MAN	O3-C3-C2	-2.41	105.37	109.99
8	E	1	NAG	C2-N2-C7	-2.35	119.55	122.90
8	E	2	NAG	C3-C4-C5	2.27	114.30	110.24
6	B	4	MAN	C1-O5-C5	2.23	115.22	112.19
6	B	7	MAN	C1-C2-C3	2.20	112.38	109.67
8	E	4	MAN	O5-C1-C2	2.15	114.09	110.77
8	E	1	NAG	O3-C3-C2	-2.14	105.03	109.47
6	B	7	MAN	O3-C3-C2	-2.14	105.90	109.99
6	B	8	MAN	O2-C2-C1	2.14	113.52	109.15
7	D	2	NAG	C1-O5-C5	-2.12	109.31	112.19
7	D	2	NAG	C4-C3-C2	2.11	114.10	111.02
8	E	3	BMA	C3-C4-C5	-2.08	106.52	110.24
9	I	2	NAG	C1-C2-N2	-2.03	107.02	110.49

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	E	2	NAG	C3-C2-N2-C7
6	B	1	NAG	O5-C5-C6-O6
6	B	8	MAN	O5-C5-C6-O6

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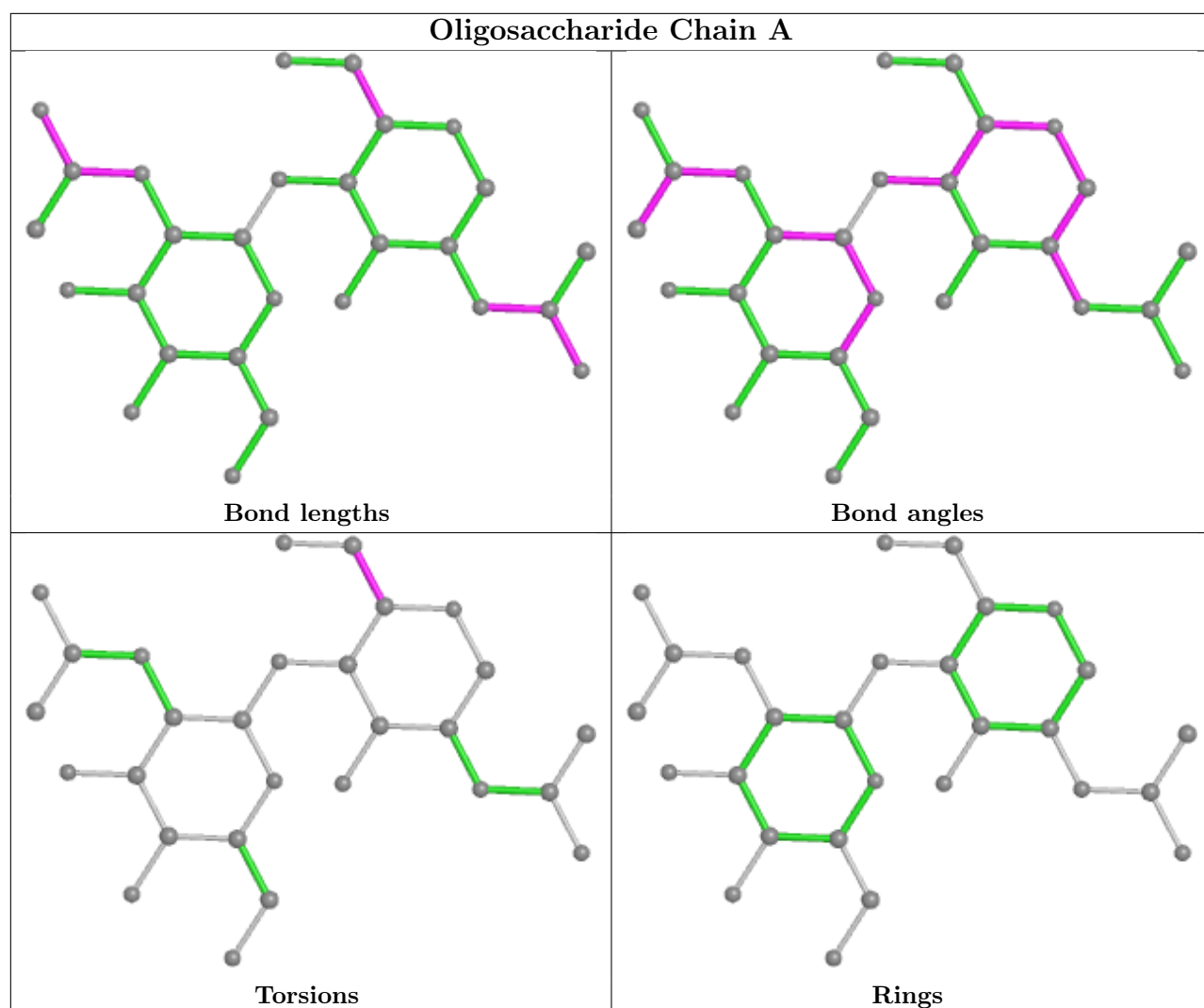
Mol	Chain	Res	Type	Atoms
6	B	8	MAN	C4-C5-C6-O6
5	A	1	NAG	O5-C5-C6-O6
6	B	9	MAN	O5-C5-C6-O6
7	D	3	BMA	O5-C5-C6-O6
9	I	4	MAN	C4-C5-C6-O6
6	B	1	NAG	C4-C5-C6-O6
6	B	9	MAN	C4-C5-C6-O6
5	F	1	NAG	C8-C7-N2-C2
5	F	1	NAG	O7-C7-N2-C2
8	E	2	NAG	C8-C7-N2-C2
8	E	2	NAG	O7-C7-N2-C2
6	B	5	MAN	O5-C5-C6-O6
7	D	2	NAG	O5-C5-C6-O6
8	E	3	BMA	O5-C5-C6-O6
8	E	1	NAG	O5-C5-C6-O6
7	D	3	BMA	C4-C5-C6-O6
6	B	5	MAN	C4-C5-C6-O6
7	D	2	NAG	C4-C5-C6-O6
7	D	4	MAN	C4-C5-C6-O6
9	I	4	MAN	O5-C5-C6-O6
5	A	1	NAG	C4-C5-C6-O6
8	E	3	BMA	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
8	E	2	NAG	O5-C5-C6-O6
7	D	4	MAN	O5-C5-C6-O6
9	I	3	BMA	C4-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
8	E	1	NAG	C4-C5-C6-O6

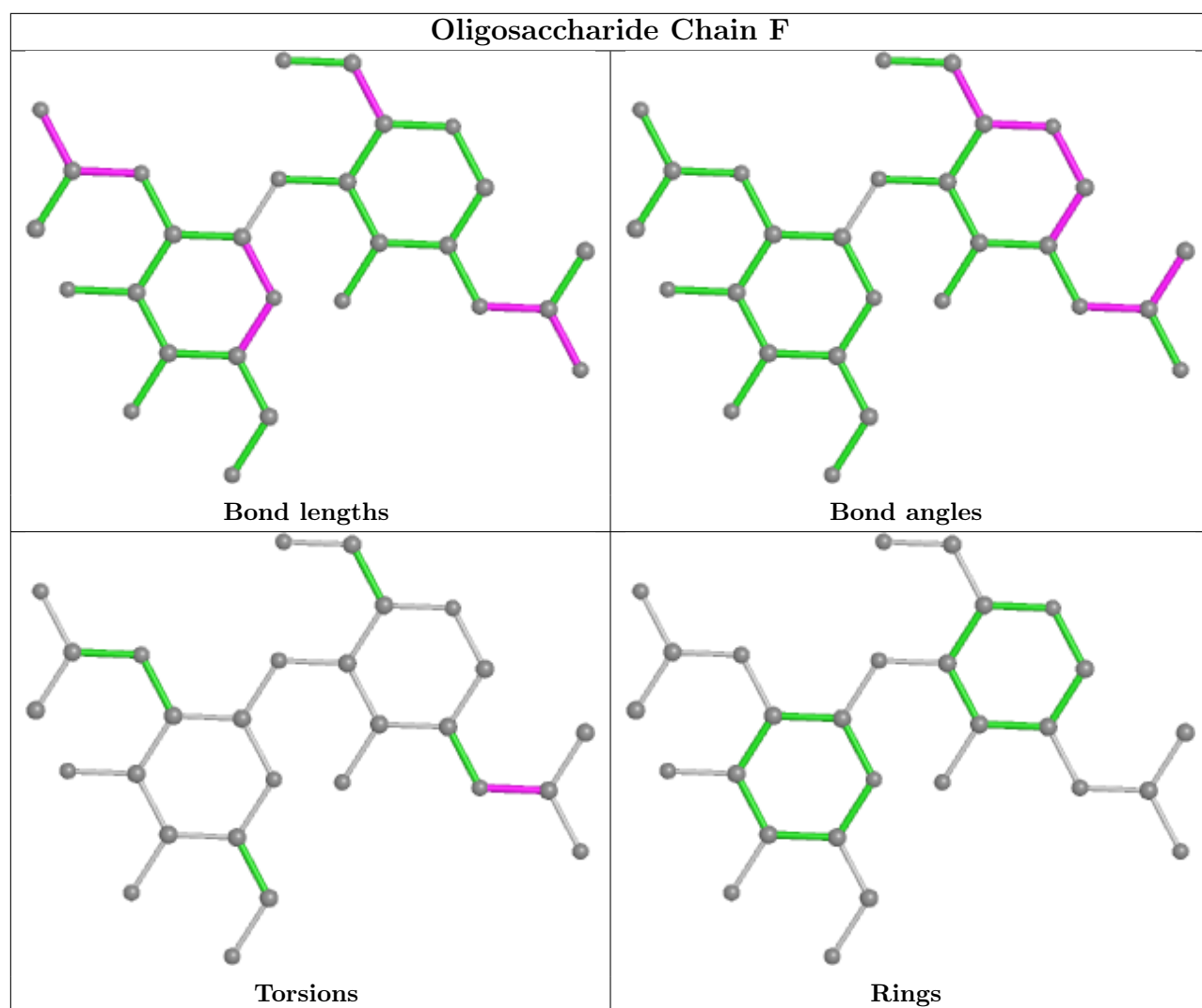
There are no ring outliers.

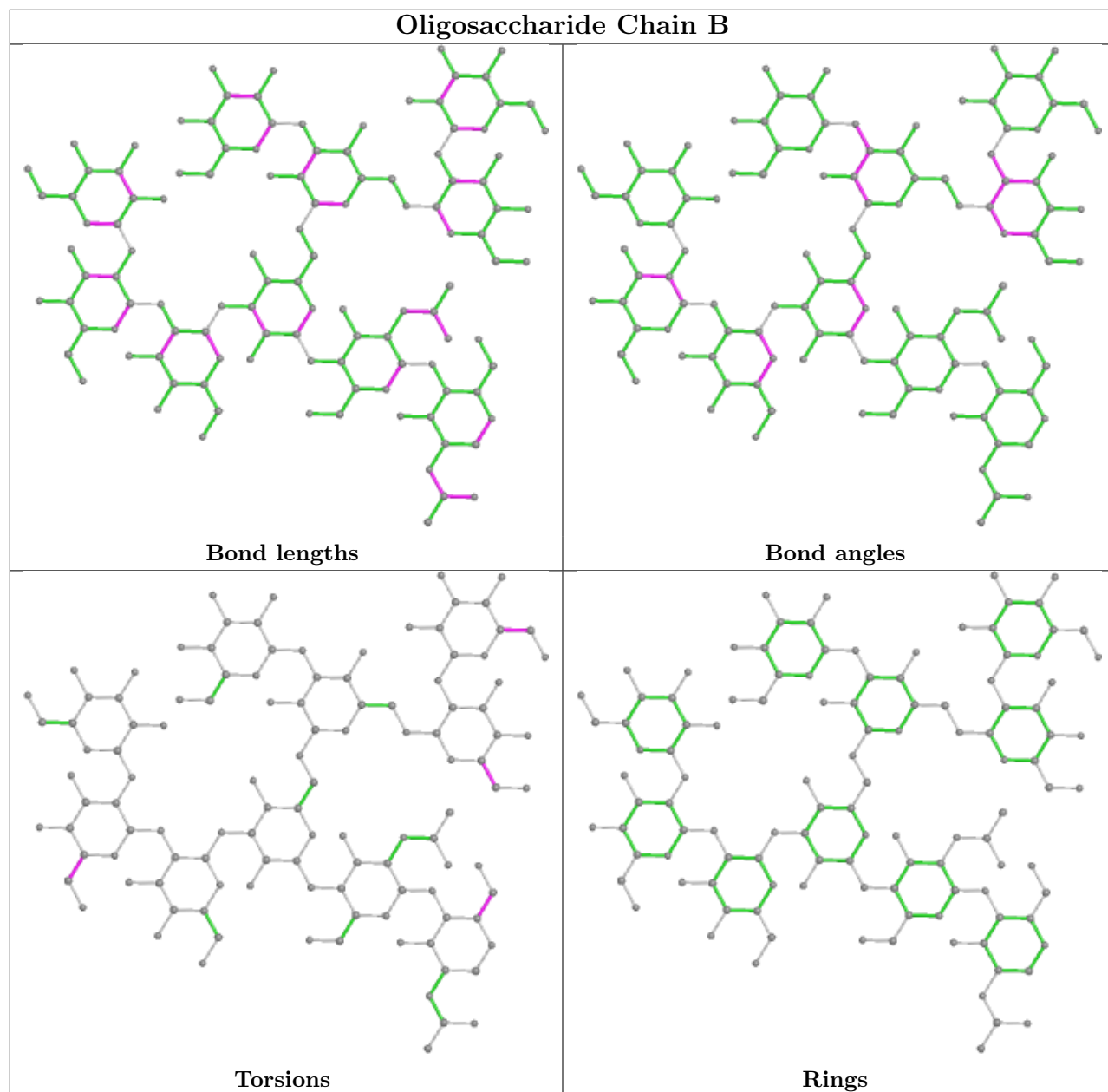
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	NAG	1	0
6	B	8	MAN	1	0
7	D	1	NAG	1	0
5	A	1	NAG	2	0
5	A	2	NAG	2	0
6	B	9	MAN	2	0

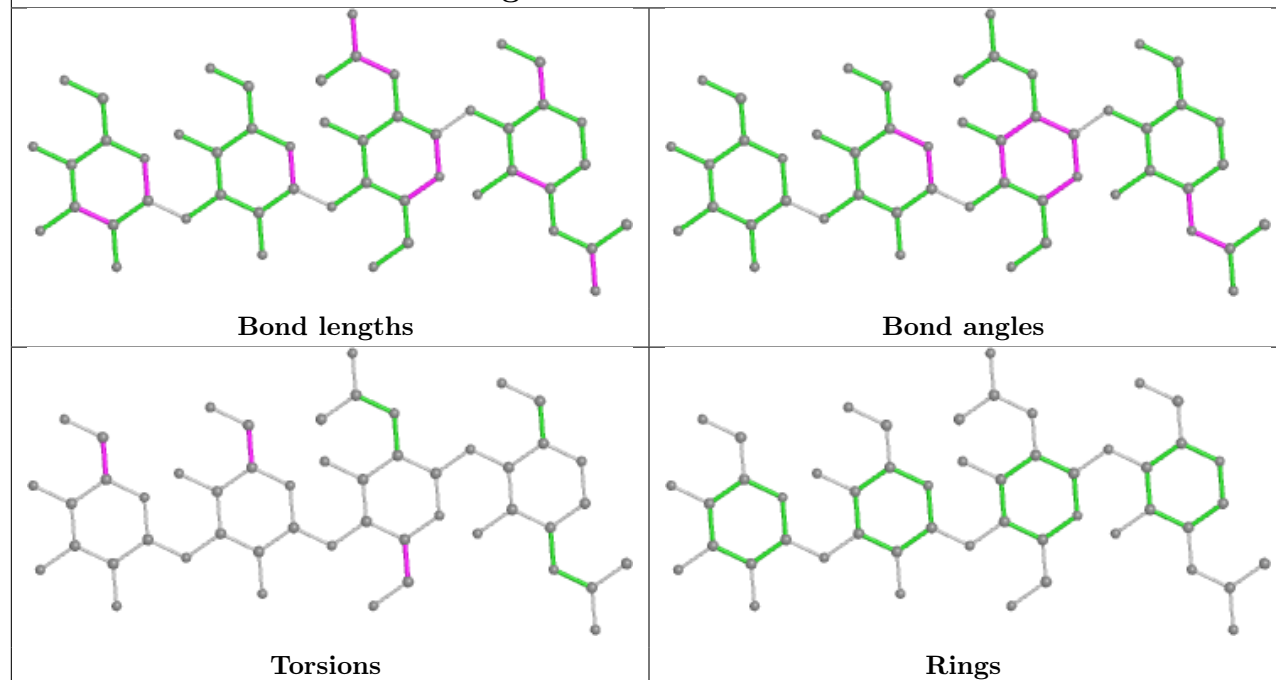
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



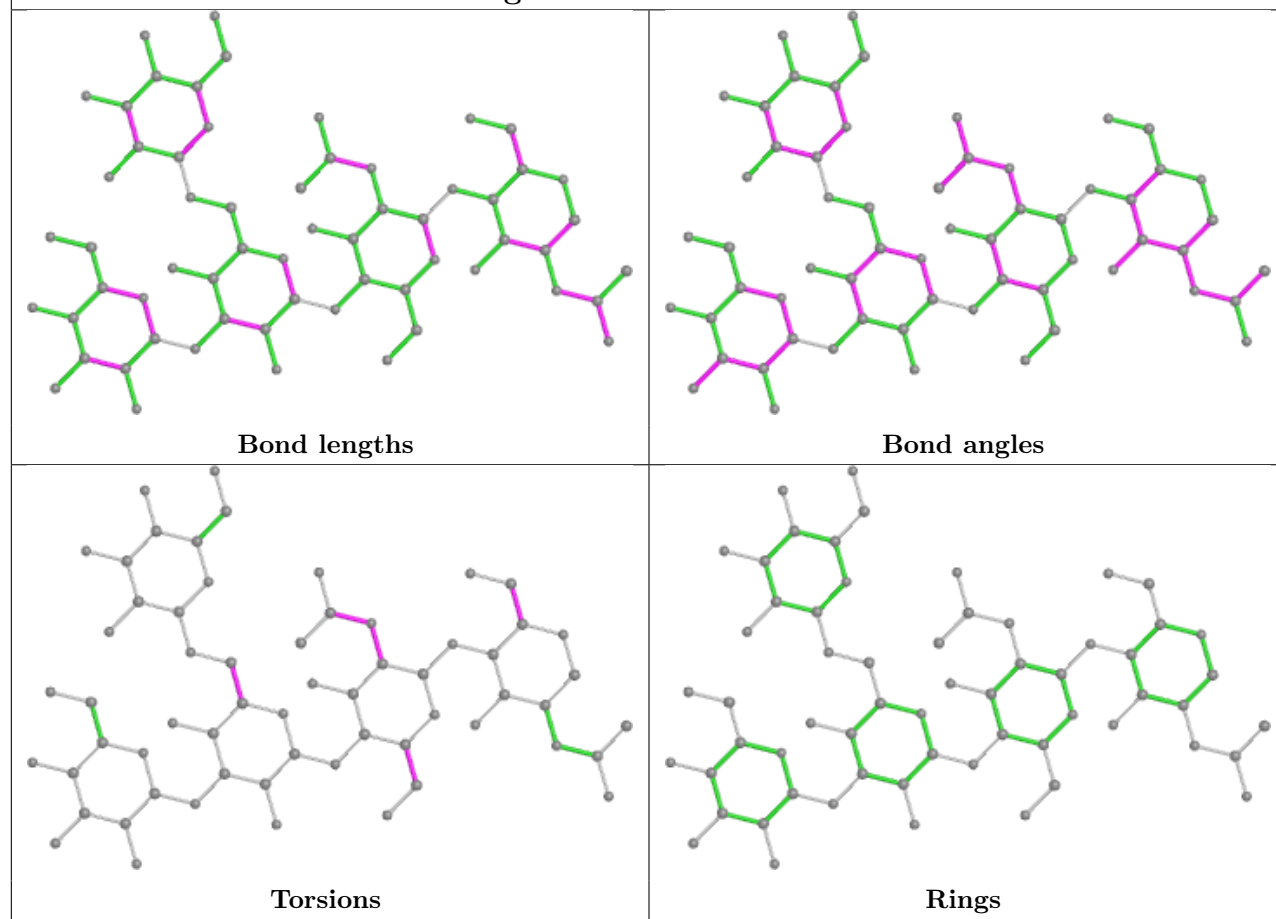


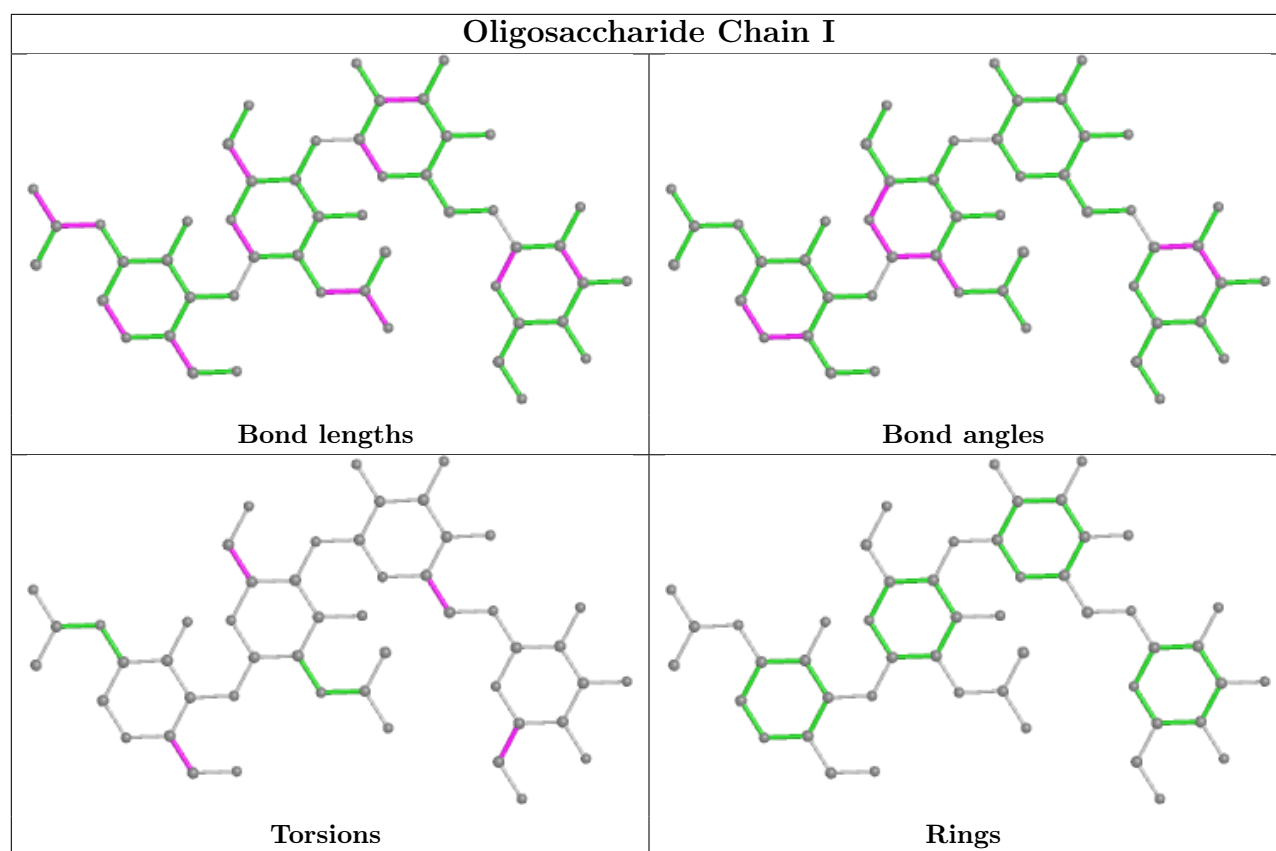


## Oligosaccharide Chain D



## Oligosaccharide Chain E





## 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
10	EPE	G	601	-	15,15,15	1.23	2 (13%)	18,20,20	1.26	3 (16%)
11	BEN	G	602	-	9,9,9	1.30	1 (11%)	7,11,11	0.97	0
12	NAG	H	1001	3	14,14,15	1.48	4 (28%)	17,19,21	1.04	0
12	NAG	G	626	2	14,14,15	1.43	4 (28%)	17,19,21	1.55	1 (5%)
11	BEN	G	603	-	9,9,9	1.39	2 (22%)	7,11,11	0.69	0
12	NAG	G	614	2	14,14,15	1.46	3 (21%)	17,19,21	0.84	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
10	EPE	G	601	-	-	5/9/19/19	0/1/1/1
11	BEN	G	602	-	-	0/4/4/4	0/1/1/1
12	NAG	H	1001	3	-	2/6/23/26	0/1/1/1
12	NAG	G	626	2	-	2/6/23/26	0/1/1/1
11	BEN	G	603	-	-	0/4/4/4	0/1/1/1
12	NAG	G	614	2	-	1/6/23/26	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	603	BEN	C-N2	3.29	1.42	1.33
11	G	602	BEN	C-N1	3.11	1.41	1.28
12	H	1001	NAG	O5-C1	2.50	1.47	1.43
12	G	614	NAG	C7-N2	2.46	1.42	1.34
12	H	1001	NAG	C7-N2	2.39	1.42	1.34
12	G	614	NAG	O5-C1	2.37	1.47	1.43
12	G	626	NAG	O5-C1	2.37	1.47	1.43
12	G	626	NAG	C7-N2	2.35	1.42	1.34
12	G	614	NAG	O7-C7	2.27	1.28	1.23
12	H	1001	NAG	O7-C7	2.22	1.28	1.23
10	G	601	EPE	C2-N1	-2.17	1.40	1.46
10	G	601	EPE	O1S-S	2.12	1.51	1.45
12	H	1001	NAG	O5-C5	2.12	1.47	1.43
11	G	603	BEN	C1-C	2.06	1.51	1.47
12	G	626	NAG	O5-C5	2.01	1.47	1.43
12	G	626	NAG	C6-C5	-2.00	1.45	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	G	626	NAG	C1-O5-C5	-5.39	104.89	112.19
10	G	601	EPE	O1S-S-C10	2.85	110.34	106.92
10	G	601	EPE	O2S-S-C10	2.14	109.49	106.92
10	G	601	EPE	O3S-S-O2S	-2.05	106.27	111.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	G	601	EPE	S-C10-C9-N1
12	H	1001	NAG	C4-C5-C6-O6
12	G	626	NAG	O5-C5-C6-O6
12	H	1001	NAG	O5-C5-C6-O6
12	G	626	NAG	C4-C5-C6-O6
10	G	601	EPE	C9-C10-S-O3S
10	G	601	EPE	N4-C7-C8-O8
10	G	601	EPE	C9-C10-S-O1S
10	G	601	EPE	C9-C10-S-O2S
12	G	614	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	G	601	EPE	1	0
11	G	602	BEN	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 [i](#)

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	167/192 (86%)	-0.13	2 (1%) 79 54	42, 74, 105, 120	0
2	G	338/361 (93%)	-0.34	1 (0%) 94 84	28, 47, 75, 136	0
3	H	215/244 (88%)	-0.30	1 (0%) 91 75	41, 60, 108, 113	0
4	L	212/215 (98%)	-0.20	5 (2%) 59 30	50, 77, 110, 155	0
All	All	932/1012 (92%)	-0.26	9 (0%) 82 59	28, 61, 106, 155	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	462	ASN	3.2
1	C	127	SER	2.9
4	L	202	SER	2.7
4	L	112	ALA	2.6
1	C	175	VAL	2.4
4	L	201	LEU	2.3
4	L	197	THR	2.2
3	H	153	SER	2.1
4	L	67	ALA	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](#)

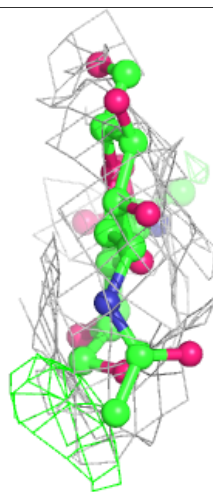
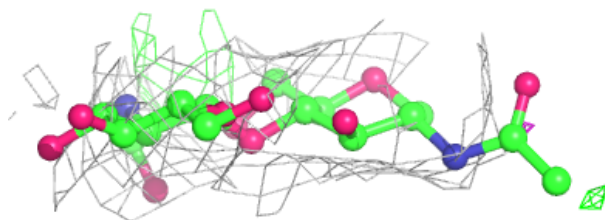
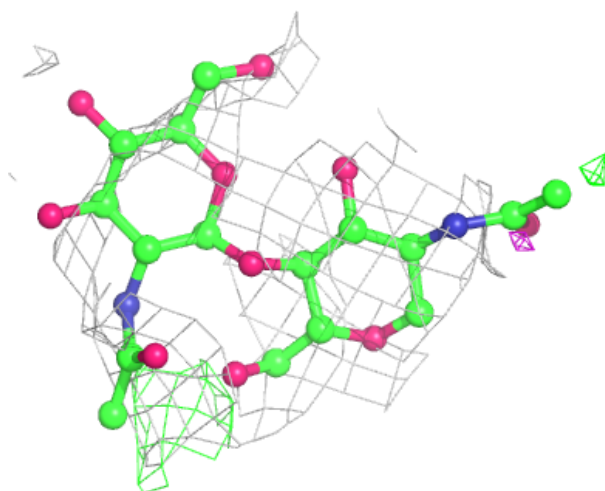
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	MAN	E	5	11/12	0.55	0.30	98,115,126,129	0
5	NAG	F	2	14/15	0.65	0.33	122,136,140,141	0
5	NAG	A	2	14/15	0.71	0.32	118,129,132,133	0
5	NAG	A	1	14/15	0.72	0.20	106,114,125,127	0
9	MAN	I	4	11/12	0.73	0.32	118,125,131,131	0
9	BMA	I	3	11/12	0.78	0.24	127,131,133,138	0
7	BMA	D	3	11/12	0.80	0.25	100,115,120,123	0
7	MAN	D	4	11/12	0.82	0.28	86,119,124,129	0
6	MAN	B	8	11/12	0.82	0.20	66,80,86,94	11
6	MAN	B	10	11/12	0.85	0.35	88,97,104,105	0
8	MAN	E	4	11/12	0.86	0.24	81,88,98,101	11
8	BMA	E	3	11/12	0.88	0.14	83,92,105,106	0
6	MAN	B	9	11/12	0.89	0.22	53,63,65,68	11
6	BMA	B	3	11/12	0.89	0.17	63,66,72,76	0
5	NAG	F	1	14/15	0.89	0.20	83,94,106,117	0
9	NAG	I	2	14/15	0.90	0.24	103,117,127,129	0
6	MAN	B	4	11/12	0.90	0.20	71,78,87,100	0
6	MAN	B	7	11/12	0.90	0.14	60,72,78,81	0
8	NAG	E	1	14/15	0.91	0.19	46,57,77,98	0
6	MAN	B	6	11/12	0.91	0.19	65,69,74,74	0
9	NAG	I	1	14/15	0.91	0.19	58,68,78,93	0
7	NAG	D	2	14/15	0.92	0.19	66,82,92,98	0
7	NAG	D	1	14/15	0.93	0.25	56,72,105,131	0
6	MAN	B	5	11/12	0.93	0.21	65,69,79,81	0
6	NAG	B	2	14/15	0.93	0.20	51,56,65,82	0
8	NAG	E	2	14/15	0.94	0.18	58,66,76,78	0
6	NAG	B	1	14/15	0.94	0.23	46,50,59,67	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.

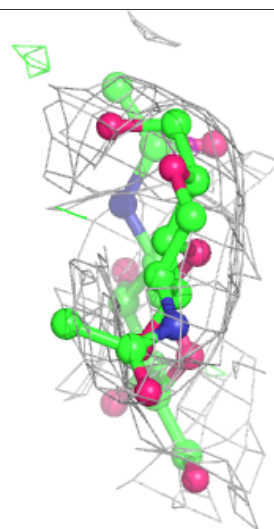
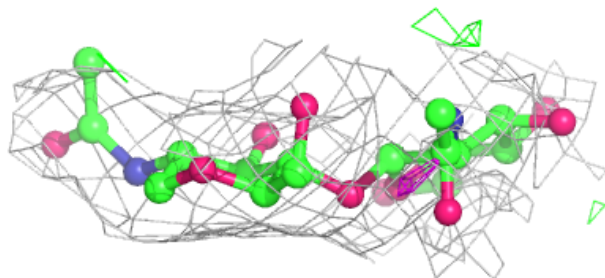
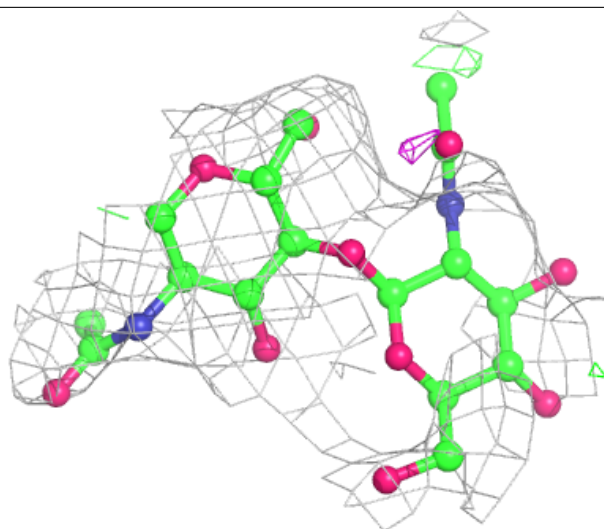
**Electron density around Chain A:**

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



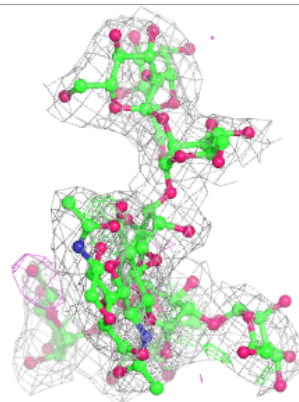
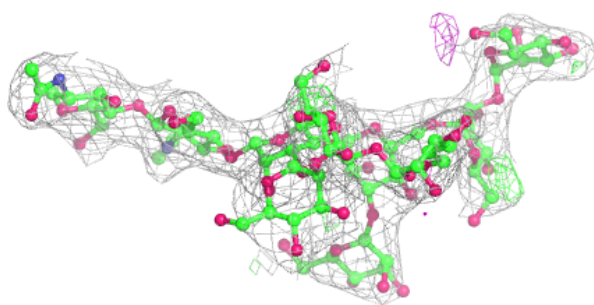
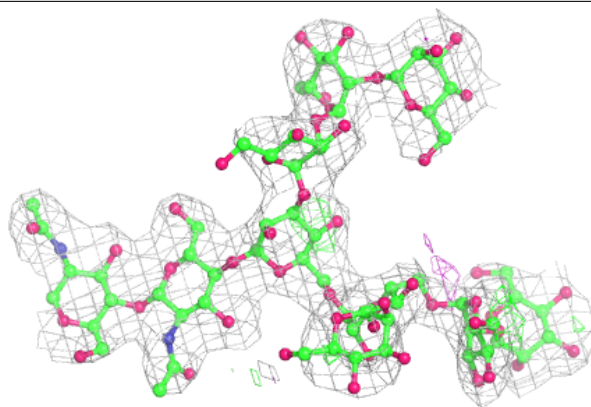
**Electron density around Chain F:**

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

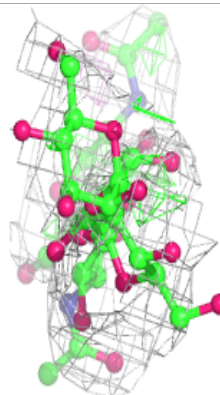
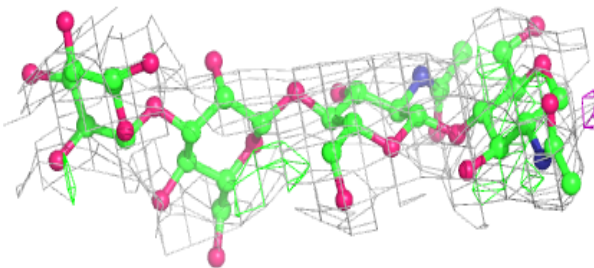
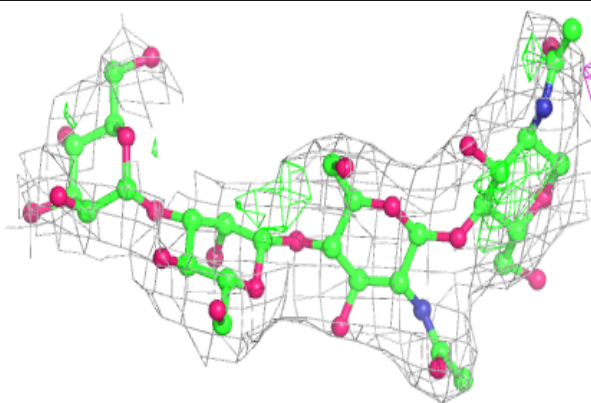


**Electron density around Chain B:**

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

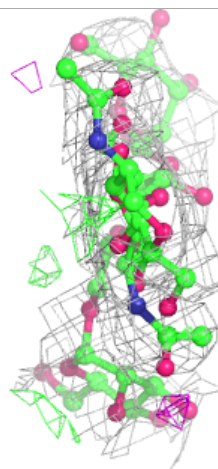
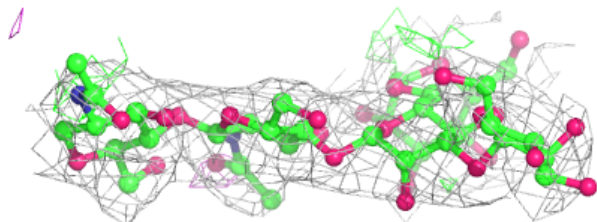
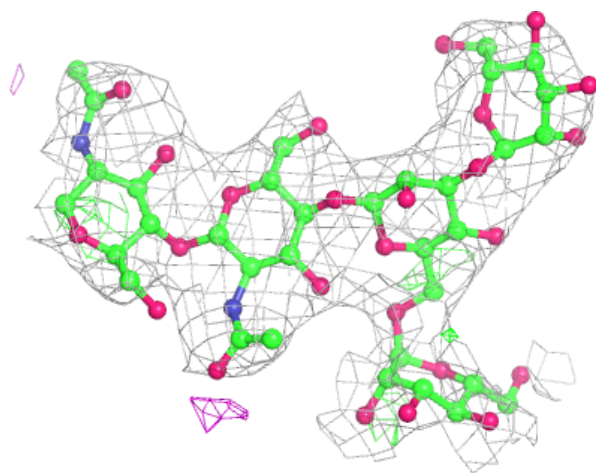
**Electron density around Chain D:**

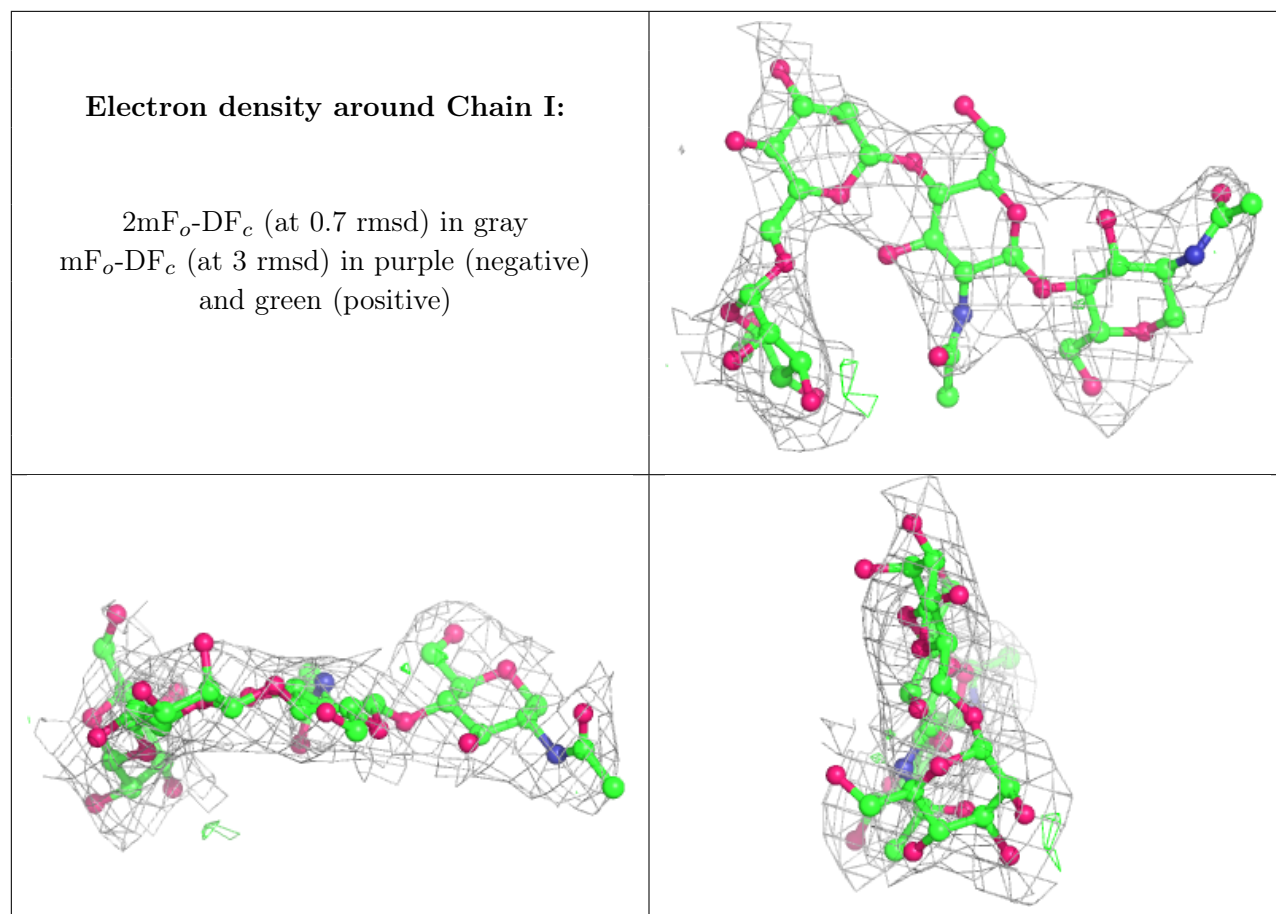
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain E:**

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





## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
12	NAG	G	626	14/15	0.76	0.30	110,120,134,145	0
12	NAG	H	1001	14/15	0.76	0.27	90,108,112,113	0
12	NAG	G	614	14/15	0.78	0.30	100,105,116,120	0
11	BEN	G	603	9/9	0.88	0.28	40,43,52,55	9
11	BEN	G	602	9/9	0.91	0.33	33,38,43,45	9
10	EPE	G	601	15/15	0.94	0.23	37,45,63,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.