wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:47 AM UTC

PDB ID	:	8EJI / pdb_00008eji
EMDB ID	:	EMD-28183
Title	:	Lassa virus glycoprotein complex (Josiah) bound to 19.7E Fab
Authors	:	Perrett, H.R.; Ward, A.B.
Deposited on	:	2022-09-16
Resolution	:	3.81 Å(reported)
Based on initial model	:	7SGD

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
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:

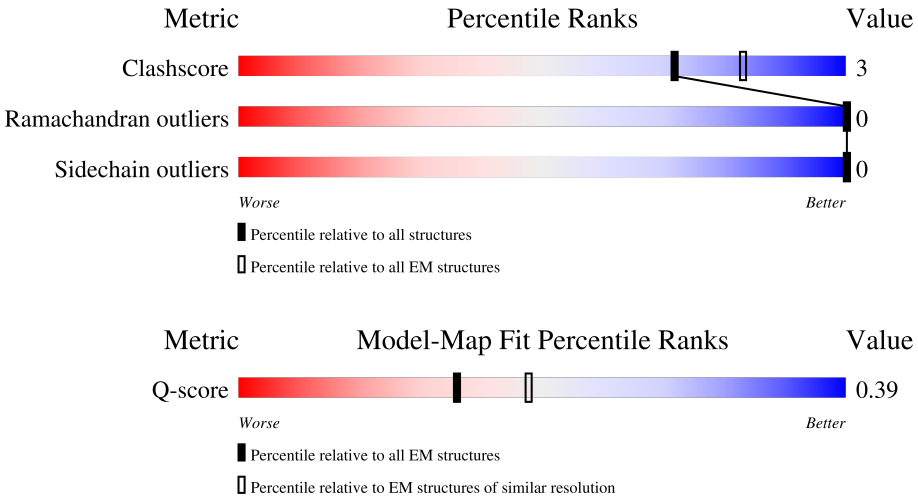
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.81 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.



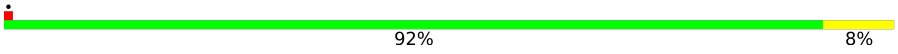
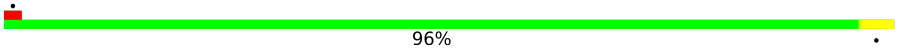
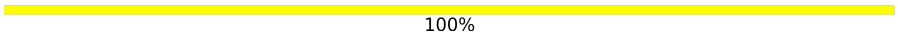
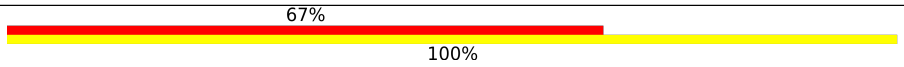
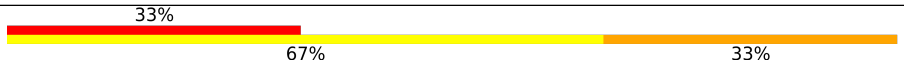
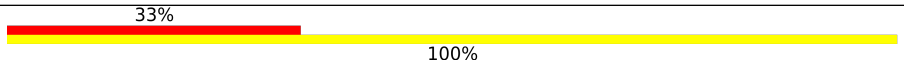
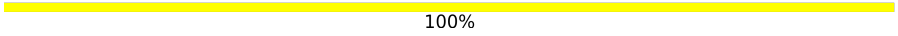
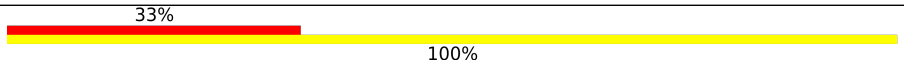
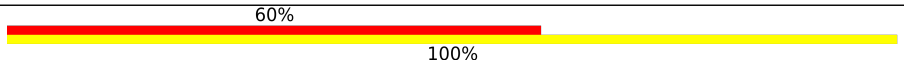
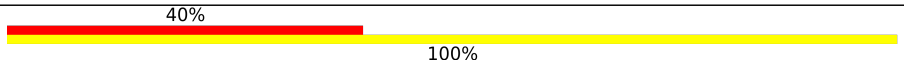
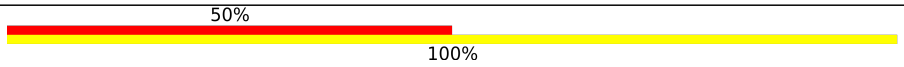
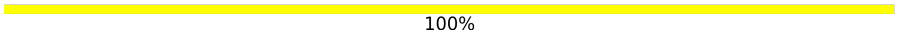
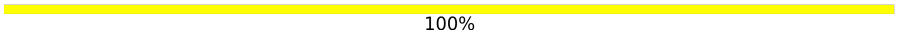
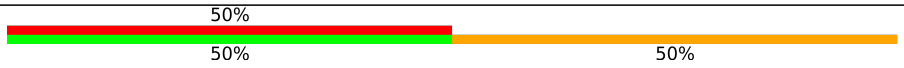
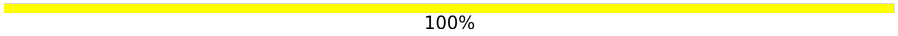
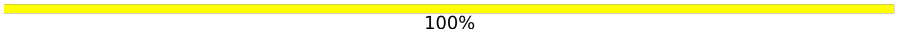
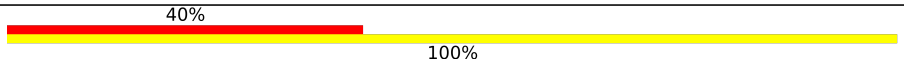
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9193 (3.31 - 4.31)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	259	69% 5% 26%
1	B	259	64% 10% 27%
1	C	259	63% 10% 27%
2	a	406	35% 61%

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Mol	Chain	Length	Quality of chain
2	b	406	
2	c	406	
3	H	119	
4	L	107	
5	D	3	
5	F	3	
5	K	3	
5	N	3	
5	O	3	
5	T	3	
6	E	5	
7	G	5	
7	M	5	
8	I	2	
8	P	2	
8	Q	2	
8	S	2	
8	U	2	
8	V	2	
8	X	2	
9	J	5	
10	R	6	
10	W	6	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 11023 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Glycoprotein G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	191	Total	C	N	O	S	0	0
			1516	956	254	290	16		
1	B	190	Total	C	N	O	S	0	0
			1504	947	253	288	16		
1	C	190	Total	C	N	O	S	0	0
			1504	947	253	288	16		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	CYS	ARG	engineered mutation	UNP P08669
A	258	ARG	LEU	engineered mutation	UNP P08669
A	259	ARG	LEU	engineered mutation	UNP P08669
B	207	CYS	ARG	engineered mutation	UNP P08669
B	258	ARG	LEU	engineered mutation	UNP P08669
B	259	ARG	LEU	engineered mutation	UNP P08669
C	207	CYS	ARG	engineered mutation	UNP P08669
C	258	ARG	LEU	engineered mutation	UNP P08669
C	259	ARG	LEU	engineered mutation	UNP P08669

- Molecule 2 is a protein called Glycoprotein G2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	159	Total	C	N	O	S	0	0
			1286	810	217	245	14		
2	b	150	Total	C	N	O	S	0	0
			1223	774	207	228	14		
2	c	151	Total	C	N	O	S	0	0
			1232	779	208	231	14		

There are 729 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	329	PRO	GLU	engineered mutation	UNP P08669
a	360	CYS	GLY	engineered mutation	UNP P08669
a	425	GLY	-	expression tag	UNP P08669
a	426	SER	-	expression tag	UNP P08669
a	427	GLY	-	expression tag	UNP P08669
a	428	GLY	-	expression tag	UNP P08669
a	429	SER	-	expression tag	UNP P08669
a	430	GLY	-	expression tag	UNP P08669
a	431	GLY	-	expression tag	UNP P08669
a	432	SER	-	expression tag	UNP P08669
a	433	GLY	-	expression tag	UNP P08669
a	434	GLY	-	expression tag	UNP P08669
a	435	SER	-	expression tag	UNP P08669
a	436	GLY	-	expression tag	UNP P08669
a	437	GLY	-	expression tag	UNP P08669
a	438	SER	-	expression tag	UNP P08669
a	439	GLU	-	expression tag	UNP P08669
a	440	LYS	-	expression tag	UNP P08669
a	441	ALA	-	expression tag	UNP P08669
a	442	ALA	-	expression tag	UNP P08669
a	443	LYS	-	expression tag	UNP P08669
a	444	ALA	-	expression tag	UNP P08669
a	445	GLU	-	expression tag	UNP P08669
a	446	GLU	-	expression tag	UNP P08669
a	447	ALA	-	expression tag	UNP P08669
a	448	ALA	-	expression tag	UNP P08669
a	449	ARG	-	expression tag	UNP P08669
a	450	LYS	-	expression tag	UNP P08669
a	451	MET	-	expression tag	UNP P08669
a	452	GLU	-	expression tag	UNP P08669
a	453	GLU	-	expression tag	UNP P08669
a	454	LEU	-	expression tag	UNP P08669
a	455	PHE	-	expression tag	UNP P08669
a	456	LYS	-	expression tag	UNP P08669
a	457	LYS	-	expression tag	UNP P08669
a	458	HIS	-	expression tag	UNP P08669
a	459	LYS	-	expression tag	UNP P08669
a	460	ILE	-	expression tag	UNP P08669
a	461	VAL	-	expression tag	UNP P08669
a	462	ALA	-	expression tag	UNP P08669
a	463	VAL	-	expression tag	UNP P08669
a	464	LEU	-	expression tag	UNP P08669
a	465	ARG	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	466	ALA	-	expression tag	UNP P08669
a	467	ASN	-	expression tag	UNP P08669
a	468	SER	-	expression tag	UNP P08669
a	469	VAL	-	expression tag	UNP P08669
a	470	GLU	-	expression tag	UNP P08669
a	471	GLU	-	expression tag	UNP P08669
a	472	ALA	-	expression tag	UNP P08669
a	473	ILE	-	expression tag	UNP P08669
a	474	GLU	-	expression tag	UNP P08669
a	475	LYS	-	expression tag	UNP P08669
a	476	ALA	-	expression tag	UNP P08669
a	477	VAL	-	expression tag	UNP P08669
a	478	ALA	-	expression tag	UNP P08669
a	479	VAL	-	expression tag	UNP P08669
a	480	PHE	-	expression tag	UNP P08669
a	481	ALA	-	expression tag	UNP P08669
a	482	GLY	-	expression tag	UNP P08669
a	483	GLY	-	expression tag	UNP P08669
a	484	VAL	-	expression tag	UNP P08669
a	485	HIS	-	expression tag	UNP P08669
a	486	LEU	-	expression tag	UNP P08669
a	487	ILE	-	expression tag	UNP P08669
a	488	GLU	-	expression tag	UNP P08669
a	489	ILE	-	expression tag	UNP P08669
a	490	THR	-	expression tag	UNP P08669
a	491	PHE	-	expression tag	UNP P08669
a	492	THR	-	expression tag	UNP P08669
a	493	VAL	-	expression tag	UNP P08669
a	494	PRO	-	expression tag	UNP P08669
a	495	ASP	-	expression tag	UNP P08669
a	496	ALA	-	expression tag	UNP P08669
a	497	ASP	-	expression tag	UNP P08669
a	498	THR	-	expression tag	UNP P08669
a	499	VAL	-	expression tag	UNP P08669
a	500	ILE	-	expression tag	UNP P08669
a	501	LYS	-	expression tag	UNP P08669
a	502	ALA	-	expression tag	UNP P08669
a	503	LEU	-	expression tag	UNP P08669
a	504	SER	-	expression tag	UNP P08669
a	505	VAL	-	expression tag	UNP P08669
a	506	LEU	-	expression tag	UNP P08669
a	507	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
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a	509	LYS	-	expression tag	UNP P08669
a	510	GLY	-	expression tag	UNP P08669
a	511	ALA	-	expression tag	UNP P08669
a	512	ILE	-	expression tag	UNP P08669
a	513	ILE	-	expression tag	UNP P08669
a	514	GLY	-	expression tag	UNP P08669
a	515	ALA	-	expression tag	UNP P08669
a	516	GLY	-	expression tag	UNP P08669
a	517	THR	-	expression tag	UNP P08669
a	518	VAL	-	expression tag	UNP P08669
a	519	THR	-	expression tag	UNP P08669
a	520	SER	-	expression tag	UNP P08669
a	521	VAL	-	expression tag	UNP P08669
a	522	GLU	-	expression tag	UNP P08669
a	523	GLN	-	expression tag	UNP P08669
a	524	CYS	-	expression tag	UNP P08669
a	525	ARG	-	expression tag	UNP P08669
a	526	LYS	-	expression tag	UNP P08669
a	527	ALA	-	expression tag	UNP P08669
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a	529	GLU	-	expression tag	UNP P08669
a	530	SER	-	expression tag	UNP P08669
a	531	GLY	-	expression tag	UNP P08669
a	532	ALA	-	expression tag	UNP P08669
a	533	GLU	-	expression tag	UNP P08669
a	534	PHE	-	expression tag	UNP P08669
a	535	ILE	-	expression tag	UNP P08669
a	536	VAL	-	expression tag	UNP P08669
a	537	SER	-	expression tag	UNP P08669
a	538	PRO	-	expression tag	UNP P08669
a	539	HIS	-	expression tag	UNP P08669
a	540	LEU	-	expression tag	UNP P08669
a	541	ASP	-	expression tag	UNP P08669
a	542	GLU	-	expression tag	UNP P08669
a	543	GLU	-	expression tag	UNP P08669
a	544	ILE	-	expression tag	UNP P08669
a	545	SER	-	expression tag	UNP P08669
a	546	GLN	-	expression tag	UNP P08669
a	547	PHE	-	expression tag	UNP P08669
a	548	CYS	-	expression tag	UNP P08669
a	549	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
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a	551	LYS	-	expression tag	UNP P08669
a	552	GLY	-	expression tag	UNP P08669
a	553	VAL	-	expression tag	UNP P08669
a	554	PHE	-	expression tag	UNP P08669
a	555	TYR	-	expression tag	UNP P08669
a	556	MET	-	expression tag	UNP P08669
a	557	PRO	-	expression tag	UNP P08669
a	558	GLY	-	expression tag	UNP P08669
a	559	VAL	-	expression tag	UNP P08669
a	560	MET	-	expression tag	UNP P08669
a	561	THR	-	expression tag	UNP P08669
a	562	PRO	-	expression tag	UNP P08669
a	563	THR	-	expression tag	UNP P08669
a	564	GLU	-	expression tag	UNP P08669
a	565	LEU	-	expression tag	UNP P08669
a	566	VAL	-	expression tag	UNP P08669
a	567	LYS	-	expression tag	UNP P08669
a	568	ALA	-	expression tag	UNP P08669
a	569	MET	-	expression tag	UNP P08669
a	570	LYS	-	expression tag	UNP P08669
a	571	LEU	-	expression tag	UNP P08669
a	572	GLY	-	expression tag	UNP P08669
a	573	HIS	-	expression tag	UNP P08669
a	574	ASP	-	expression tag	UNP P08669
a	575	ILE	-	expression tag	UNP P08669
a	576	LEU	-	expression tag	UNP P08669
a	577	LYS	-	expression tag	UNP P08669
a	578	LEU	-	expression tag	UNP P08669
a	579	PHE	-	expression tag	UNP P08669
a	580	PRO	-	expression tag	UNP P08669
a	581	GLY	-	expression tag	UNP P08669
a	582	GLU	-	expression tag	UNP P08669
a	583	VAL	-	expression tag	UNP P08669
a	584	VAL	-	expression tag	UNP P08669
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a	587	GLU	-	expression tag	UNP P08669
a	588	PHE	-	expression tag	UNP P08669
a	589	VAL	-	expression tag	UNP P08669
a	590	LYS	-	expression tag	UNP P08669
a	591	ALA	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
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a	593	LYS	-	expression tag	UNP P08669
a	594	GLY	-	expression tag	UNP P08669
a	595	PRO	-	expression tag	UNP P08669
a	596	PHE	-	expression tag	UNP P08669
a	597	PRO	-	expression tag	UNP P08669
a	598	ASN	-	expression tag	UNP P08669
a	599	VAL	-	expression tag	UNP P08669
a	600	LYS	-	expression tag	UNP P08669
a	601	PHE	-	expression tag	UNP P08669
a	602	VAL	-	expression tag	UNP P08669
a	603	PRO	-	expression tag	UNP P08669
a	604	THR	-	expression tag	UNP P08669
a	605	GLY	-	expression tag	UNP P08669
a	606	GLY	-	expression tag	UNP P08669
a	607	VAL	-	expression tag	UNP P08669
a	608	ASP	-	expression tag	UNP P08669
a	609	LEU	-	expression tag	UNP P08669
a	610	ASP	-	expression tag	UNP P08669
a	611	ASN	-	expression tag	UNP P08669
a	612	VAL	-	expression tag	UNP P08669
a	613	CYS	-	expression tag	UNP P08669
a	614	GLU	-	expression tag	UNP P08669
a	615	TRP	-	expression tag	UNP P08669
a	616	PHE	-	expression tag	UNP P08669
a	617	ASP	-	expression tag	UNP P08669
a	618	ALA	-	expression tag	UNP P08669
a	619	GLY	-	expression tag	UNP P08669
a	620	VAL	-	expression tag	UNP P08669
a	621	LEU	-	expression tag	UNP P08669
a	622	ALA	-	expression tag	UNP P08669
a	623	VAL	-	expression tag	UNP P08669
a	624	GLY	-	expression tag	UNP P08669
a	625	VAL	-	expression tag	UNP P08669
a	626	GLY	-	expression tag	UNP P08669
a	627	ASP	-	expression tag	UNP P08669
a	628	ALA	-	expression tag	UNP P08669
a	629	LEU	-	expression tag	UNP P08669
a	630	VAL	-	expression tag	UNP P08669
a	631	GLU	-	expression tag	UNP P08669
a	632	GLY	-	expression tag	UNP P08669
a	633	ASP	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
a	634	PRO	-	expression tag	UNP P08669
a	635	ASP	-	expression tag	UNP P08669
a	636	GLU	-	expression tag	UNP P08669
a	637	VAL	-	expression tag	UNP P08669
a	638	ARG	-	expression tag	UNP P08669
a	639	GLU	-	expression tag	UNP P08669
a	640	LYS	-	expression tag	UNP P08669
a	641	ALA	-	expression tag	UNP P08669
a	642	LYS	-	expression tag	UNP P08669
a	643	GLU	-	expression tag	UNP P08669
a	644	PHE	-	expression tag	UNP P08669
a	645	VAL	-	expression tag	UNP P08669
a	646	GLU	-	expression tag	UNP P08669
a	647	LYS	-	expression tag	UNP P08669
a	648	ILE	-	expression tag	UNP P08669
a	649	ARG	-	expression tag	UNP P08669
a	650	GLY	-	expression tag	UNP P08669
a	651	CYS	-	expression tag	UNP P08669
a	652	THR	-	expression tag	UNP P08669
a	653	GLU	-	expression tag	UNP P08669
a	654	GLY	-	expression tag	UNP P08669
a	655	SER	-	expression tag	UNP P08669
a	656	LEU	-	expression tag	UNP P08669
a	657	GLU	-	expression tag	UNP P08669
a	658	TRP	-	expression tag	UNP P08669
a	659	SER	-	expression tag	UNP P08669
a	660	HIS	-	expression tag	UNP P08669
a	661	PRO	-	expression tag	UNP P08669
a	662	GLN	-	expression tag	UNP P08669
a	663	PHE	-	expression tag	UNP P08669
a	664	GLU	-	expression tag	UNP P08669
a	665	LYS	-	expression tag	UNP P08669
b	329	PRO	GLU	engineered mutation	UNP P08669
b	360	CYS	GLY	engineered mutation	UNP P08669
b	425	GLY	-	expression tag	UNP P08669
b	426	SER	-	expression tag	UNP P08669
b	427	GLY	-	expression tag	UNP P08669
b	428	GLY	-	expression tag	UNP P08669
b	429	SER	-	expression tag	UNP P08669
b	430	GLY	-	expression tag	UNP P08669
b	431	GLY	-	expression tag	UNP P08669
b	432	SER	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	433	GLY	-	expression tag	UNP P08669
b	434	GLY	-	expression tag	UNP P08669
b	435	SER	-	expression tag	UNP P08669
b	436	GLY	-	expression tag	UNP P08669
b	437	GLY	-	expression tag	UNP P08669
b	438	SER	-	expression tag	UNP P08669
b	439	GLU	-	expression tag	UNP P08669
b	440	LYS	-	expression tag	UNP P08669
b	441	ALA	-	expression tag	UNP P08669
b	442	ALA	-	expression tag	UNP P08669
b	443	LYS	-	expression tag	UNP P08669
b	444	ALA	-	expression tag	UNP P08669
b	445	GLU	-	expression tag	UNP P08669
b	446	GLU	-	expression tag	UNP P08669
b	447	ALA	-	expression tag	UNP P08669
b	448	ALA	-	expression tag	UNP P08669
b	449	ARG	-	expression tag	UNP P08669
b	450	LYS	-	expression tag	UNP P08669
b	451	MET	-	expression tag	UNP P08669
b	452	GLU	-	expression tag	UNP P08669
b	453	GLU	-	expression tag	UNP P08669
b	454	LEU	-	expression tag	UNP P08669
b	455	PHE	-	expression tag	UNP P08669
b	456	LYS	-	expression tag	UNP P08669
b	457	LYS	-	expression tag	UNP P08669
b	458	HIS	-	expression tag	UNP P08669
b	459	LYS	-	expression tag	UNP P08669
b	460	ILE	-	expression tag	UNP P08669
b	461	VAL	-	expression tag	UNP P08669
b	462	ALA	-	expression tag	UNP P08669
b	463	VAL	-	expression tag	UNP P08669
b	464	LEU	-	expression tag	UNP P08669
b	465	ARG	-	expression tag	UNP P08669
b	466	ALA	-	expression tag	UNP P08669
b	467	ASN	-	expression tag	UNP P08669
b	468	SER	-	expression tag	UNP P08669
b	469	VAL	-	expression tag	UNP P08669
b	470	GLU	-	expression tag	UNP P08669
b	471	GLU	-	expression tag	UNP P08669
b	472	ALA	-	expression tag	UNP P08669
b	473	ILE	-	expression tag	UNP P08669
b	474	GLU	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	475	LYS	-	expression tag	UNP P08669
b	476	ALA	-	expression tag	UNP P08669
b	477	VAL	-	expression tag	UNP P08669
b	478	ALA	-	expression tag	UNP P08669
b	479	VAL	-	expression tag	UNP P08669
b	480	PHE	-	expression tag	UNP P08669
b	481	ALA	-	expression tag	UNP P08669
b	482	GLY	-	expression tag	UNP P08669
b	483	GLY	-	expression tag	UNP P08669
b	484	VAL	-	expression tag	UNP P08669
b	485	HIS	-	expression tag	UNP P08669
b	486	LEU	-	expression tag	UNP P08669
b	487	ILE	-	expression tag	UNP P08669
b	488	GLU	-	expression tag	UNP P08669
b	489	ILE	-	expression tag	UNP P08669
b	490	THR	-	expression tag	UNP P08669
b	491	PHE	-	expression tag	UNP P08669
b	492	THR	-	expression tag	UNP P08669
b	493	VAL	-	expression tag	UNP P08669
b	494	PRO	-	expression tag	UNP P08669
b	495	ASP	-	expression tag	UNP P08669
b	496	ALA	-	expression tag	UNP P08669
b	497	ASP	-	expression tag	UNP P08669
b	498	THR	-	expression tag	UNP P08669
b	499	VAL	-	expression tag	UNP P08669
b	500	ILE	-	expression tag	UNP P08669
b	501	LYS	-	expression tag	UNP P08669
b	502	ALA	-	expression tag	UNP P08669
b	503	LEU	-	expression tag	UNP P08669
b	504	SER	-	expression tag	UNP P08669
b	505	VAL	-	expression tag	UNP P08669
b	506	LEU	-	expression tag	UNP P08669
b	507	LYS	-	expression tag	UNP P08669
b	508	GLU	-	expression tag	UNP P08669
b	509	LYS	-	expression tag	UNP P08669
b	510	GLY	-	expression tag	UNP P08669
b	511	ALA	-	expression tag	UNP P08669
b	512	ILE	-	expression tag	UNP P08669
b	513	ILE	-	expression tag	UNP P08669
b	514	GLY	-	expression tag	UNP P08669
b	515	ALA	-	expression tag	UNP P08669
b	516	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	517	THR	-	expression tag	UNP P08669
b	518	VAL	-	expression tag	UNP P08669
b	519	THR	-	expression tag	UNP P08669
b	520	SER	-	expression tag	UNP P08669
b	521	VAL	-	expression tag	UNP P08669
b	522	GLU	-	expression tag	UNP P08669
b	523	GLN	-	expression tag	UNP P08669
b	524	CYS	-	expression tag	UNP P08669
b	525	ARG	-	expression tag	UNP P08669
b	526	LYS	-	expression tag	UNP P08669
b	527	ALA	-	expression tag	UNP P08669
b	528	VAL	-	expression tag	UNP P08669
b	529	GLU	-	expression tag	UNP P08669
b	530	SER	-	expression tag	UNP P08669
b	531	GLY	-	expression tag	UNP P08669
b	532	ALA	-	expression tag	UNP P08669
b	533	GLU	-	expression tag	UNP P08669
b	534	PHE	-	expression tag	UNP P08669
b	535	ILE	-	expression tag	UNP P08669
b	536	VAL	-	expression tag	UNP P08669
b	537	SER	-	expression tag	UNP P08669
b	538	PRO	-	expression tag	UNP P08669
b	539	HIS	-	expression tag	UNP P08669
b	540	LEU	-	expression tag	UNP P08669
b	541	ASP	-	expression tag	UNP P08669
b	542	GLU	-	expression tag	UNP P08669
b	543	GLU	-	expression tag	UNP P08669
b	544	ILE	-	expression tag	UNP P08669
b	545	SER	-	expression tag	UNP P08669
b	546	GLN	-	expression tag	UNP P08669
b	547	PHE	-	expression tag	UNP P08669
b	548	CYS	-	expression tag	UNP P08669
b	549	LYS	-	expression tag	UNP P08669
b	550	GLU	-	expression tag	UNP P08669
b	551	LYS	-	expression tag	UNP P08669
b	552	GLY	-	expression tag	UNP P08669
b	553	VAL	-	expression tag	UNP P08669
b	554	PHE	-	expression tag	UNP P08669
b	555	TYR	-	expression tag	UNP P08669
b	556	MET	-	expression tag	UNP P08669
b	557	PRO	-	expression tag	UNP P08669
b	558	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	559	VAL	-	expression tag	UNP P08669
b	560	MET	-	expression tag	UNP P08669
b	561	THR	-	expression tag	UNP P08669
b	562	PRO	-	expression tag	UNP P08669
b	563	THR	-	expression tag	UNP P08669
b	564	GLU	-	expression tag	UNP P08669
b	565	LEU	-	expression tag	UNP P08669
b	566	VAL	-	expression tag	UNP P08669
b	567	LYS	-	expression tag	UNP P08669
b	568	ALA	-	expression tag	UNP P08669
b	569	MET	-	expression tag	UNP P08669
b	570	LYS	-	expression tag	UNP P08669
b	571	LEU	-	expression tag	UNP P08669
b	572	GLY	-	expression tag	UNP P08669
b	573	HIS	-	expression tag	UNP P08669
b	574	ASP	-	expression tag	UNP P08669
b	575	ILE	-	expression tag	UNP P08669
b	576	LEU	-	expression tag	UNP P08669
b	577	LYS	-	expression tag	UNP P08669
b	578	LEU	-	expression tag	UNP P08669
b	579	PHE	-	expression tag	UNP P08669
b	580	PRO	-	expression tag	UNP P08669
b	581	GLY	-	expression tag	UNP P08669
b	582	GLU	-	expression tag	UNP P08669
b	583	VAL	-	expression tag	UNP P08669
b	584	VAL	-	expression tag	UNP P08669
b	585	GLY	-	expression tag	UNP P08669
b	586	PRO	-	expression tag	UNP P08669
b	587	GLU	-	expression tag	UNP P08669
b	588	PHE	-	expression tag	UNP P08669
b	589	VAL	-	expression tag	UNP P08669
b	590	LYS	-	expression tag	UNP P08669
b	591	ALA	-	expression tag	UNP P08669
b	592	MET	-	expression tag	UNP P08669
b	593	LYS	-	expression tag	UNP P08669
b	594	GLY	-	expression tag	UNP P08669
b	595	PRO	-	expression tag	UNP P08669
b	596	PHE	-	expression tag	UNP P08669
b	597	PRO	-	expression tag	UNP P08669
b	598	ASN	-	expression tag	UNP P08669
b	599	VAL	-	expression tag	UNP P08669
b	600	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	601	PHE	-	expression tag	UNP P08669
b	602	VAL	-	expression tag	UNP P08669
b	603	PRO	-	expression tag	UNP P08669
b	604	THR	-	expression tag	UNP P08669
b	605	GLY	-	expression tag	UNP P08669
b	606	GLY	-	expression tag	UNP P08669
b	607	VAL	-	expression tag	UNP P08669
b	608	ASP	-	expression tag	UNP P08669
b	609	LEU	-	expression tag	UNP P08669
b	610	ASP	-	expression tag	UNP P08669
b	611	ASN	-	expression tag	UNP P08669
b	612	VAL	-	expression tag	UNP P08669
b	613	CYS	-	expression tag	UNP P08669
b	614	GLU	-	expression tag	UNP P08669
b	615	TRP	-	expression tag	UNP P08669
b	616	PHE	-	expression tag	UNP P08669
b	617	ASP	-	expression tag	UNP P08669
b	618	ALA	-	expression tag	UNP P08669
b	619	GLY	-	expression tag	UNP P08669
b	620	VAL	-	expression tag	UNP P08669
b	621	LEU	-	expression tag	UNP P08669
b	622	ALA	-	expression tag	UNP P08669
b	623	VAL	-	expression tag	UNP P08669
b	624	GLY	-	expression tag	UNP P08669
b	625	VAL	-	expression tag	UNP P08669
b	626	GLY	-	expression tag	UNP P08669
b	627	ASP	-	expression tag	UNP P08669
b	628	ALA	-	expression tag	UNP P08669
b	629	LEU	-	expression tag	UNP P08669
b	630	VAL	-	expression tag	UNP P08669
b	631	GLU	-	expression tag	UNP P08669
b	632	GLY	-	expression tag	UNP P08669
b	633	ASP	-	expression tag	UNP P08669
b	634	PRO	-	expression tag	UNP P08669
b	635	ASP	-	expression tag	UNP P08669
b	636	GLU	-	expression tag	UNP P08669
b	637	VAL	-	expression tag	UNP P08669
b	638	ARG	-	expression tag	UNP P08669
b	639	GLU	-	expression tag	UNP P08669
b	640	LYS	-	expression tag	UNP P08669
b	641	ALA	-	expression tag	UNP P08669
b	642	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
b	643	GLU	-	expression tag	UNP P08669
b	644	PHE	-	expression tag	UNP P08669
b	645	VAL	-	expression tag	UNP P08669
b	646	GLU	-	expression tag	UNP P08669
b	647	LYS	-	expression tag	UNP P08669
b	648	ILE	-	expression tag	UNP P08669
b	649	ARG	-	expression tag	UNP P08669
b	650	GLY	-	expression tag	UNP P08669
b	651	CYS	-	expression tag	UNP P08669
b	652	THR	-	expression tag	UNP P08669
b	653	GLU	-	expression tag	UNP P08669
b	654	GLY	-	expression tag	UNP P08669
b	655	SER	-	expression tag	UNP P08669
b	656	LEU	-	expression tag	UNP P08669
b	657	GLU	-	expression tag	UNP P08669
b	658	TRP	-	expression tag	UNP P08669
b	659	SER	-	expression tag	UNP P08669
b	660	HIS	-	expression tag	UNP P08669
b	661	PRO	-	expression tag	UNP P08669
b	662	GLN	-	expression tag	UNP P08669
b	663	PHE	-	expression tag	UNP P08669
b	664	GLU	-	expression tag	UNP P08669
b	665	LYS	-	expression tag	UNP P08669
c	329	PRO	GLU	engineered mutation	UNP P08669
c	360	CYS	GLY	engineered mutation	UNP P08669
c	425	GLY	-	expression tag	UNP P08669
c	426	SER	-	expression tag	UNP P08669
c	427	GLY	-	expression tag	UNP P08669
c	428	GLY	-	expression tag	UNP P08669
c	429	SER	-	expression tag	UNP P08669
c	430	GLY	-	expression tag	UNP P08669
c	431	GLY	-	expression tag	UNP P08669
c	432	SER	-	expression tag	UNP P08669
c	433	GLY	-	expression tag	UNP P08669
c	434	GLY	-	expression tag	UNP P08669
c	435	SER	-	expression tag	UNP P08669
c	436	GLY	-	expression tag	UNP P08669
c	437	GLY	-	expression tag	UNP P08669
c	438	SER	-	expression tag	UNP P08669
c	439	GLU	-	expression tag	UNP P08669
c	440	LYS	-	expression tag	UNP P08669
c	441	ALA	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	442	ALA	-	expression tag	UNP P08669
c	443	LYS	-	expression tag	UNP P08669
c	444	ALA	-	expression tag	UNP P08669
c	445	GLU	-	expression tag	UNP P08669
c	446	GLU	-	expression tag	UNP P08669
c	447	ALA	-	expression tag	UNP P08669
c	448	ALA	-	expression tag	UNP P08669
c	449	ARG	-	expression tag	UNP P08669
c	450	LYS	-	expression tag	UNP P08669
c	451	MET	-	expression tag	UNP P08669
c	452	GLU	-	expression tag	UNP P08669
c	453	GLU	-	expression tag	UNP P08669
c	454	LEU	-	expression tag	UNP P08669
c	455	PHE	-	expression tag	UNP P08669
c	456	LYS	-	expression tag	UNP P08669
c	457	LYS	-	expression tag	UNP P08669
c	458	HIS	-	expression tag	UNP P08669
c	459	LYS	-	expression tag	UNP P08669
c	460	ILE	-	expression tag	UNP P08669
c	461	VAL	-	expression tag	UNP P08669
c	462	ALA	-	expression tag	UNP P08669
c	463	VAL	-	expression tag	UNP P08669
c	464	LEU	-	expression tag	UNP P08669
c	465	ARG	-	expression tag	UNP P08669
c	466	ALA	-	expression tag	UNP P08669
c	467	ASN	-	expression tag	UNP P08669
c	468	SER	-	expression tag	UNP P08669
c	469	VAL	-	expression tag	UNP P08669
c	470	GLU	-	expression tag	UNP P08669
c	471	GLU	-	expression tag	UNP P08669
c	472	ALA	-	expression tag	UNP P08669
c	473	ILE	-	expression tag	UNP P08669
c	474	GLU	-	expression tag	UNP P08669
c	475	LYS	-	expression tag	UNP P08669
c	476	ALA	-	expression tag	UNP P08669
c	477	VAL	-	expression tag	UNP P08669
c	478	ALA	-	expression tag	UNP P08669
c	479	VAL	-	expression tag	UNP P08669
c	480	PHE	-	expression tag	UNP P08669
c	481	ALA	-	expression tag	UNP P08669
c	482	GLY	-	expression tag	UNP P08669
c	483	GLY	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	484	VAL	-	expression tag	UNP P08669
c	485	HIS	-	expression tag	UNP P08669
c	486	LEU	-	expression tag	UNP P08669
c	487	ILE	-	expression tag	UNP P08669
c	488	GLU	-	expression tag	UNP P08669
c	489	ILE	-	expression tag	UNP P08669
c	490	THR	-	expression tag	UNP P08669
c	491	PHE	-	expression tag	UNP P08669
c	492	THR	-	expression tag	UNP P08669
c	493	VAL	-	expression tag	UNP P08669
c	494	PRO	-	expression tag	UNP P08669
c	495	ASP	-	expression tag	UNP P08669
c	496	ALA	-	expression tag	UNP P08669
c	497	ASP	-	expression tag	UNP P08669
c	498	THR	-	expression tag	UNP P08669
c	499	VAL	-	expression tag	UNP P08669
c	500	ILE	-	expression tag	UNP P08669
c	501	LYS	-	expression tag	UNP P08669
c	502	ALA	-	expression tag	UNP P08669
c	503	LEU	-	expression tag	UNP P08669
c	504	SER	-	expression tag	UNP P08669
c	505	VAL	-	expression tag	UNP P08669
c	506	LEU	-	expression tag	UNP P08669
c	507	LYS	-	expression tag	UNP P08669
c	508	GLU	-	expression tag	UNP P08669
c	509	LYS	-	expression tag	UNP P08669
c	510	GLY	-	expression tag	UNP P08669
c	511	ALA	-	expression tag	UNP P08669
c	512	ILE	-	expression tag	UNP P08669
c	513	ILE	-	expression tag	UNP P08669
c	514	GLY	-	expression tag	UNP P08669
c	515	ALA	-	expression tag	UNP P08669
c	516	GLY	-	expression tag	UNP P08669
c	517	THR	-	expression tag	UNP P08669
c	518	VAL	-	expression tag	UNP P08669
c	519	THR	-	expression tag	UNP P08669
c	520	SER	-	expression tag	UNP P08669
c	521	VAL	-	expression tag	UNP P08669
c	522	GLU	-	expression tag	UNP P08669
c	523	GLN	-	expression tag	UNP P08669
c	524	CYS	-	expression tag	UNP P08669
c	525	ARG	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	526	LYS	-	expression tag	UNP P08669
c	527	ALA	-	expression tag	UNP P08669
c	528	VAL	-	expression tag	UNP P08669
c	529	GLU	-	expression tag	UNP P08669
c	530	SER	-	expression tag	UNP P08669
c	531	GLY	-	expression tag	UNP P08669
c	532	ALA	-	expression tag	UNP P08669
c	533	GLU	-	expression tag	UNP P08669
c	534	PHE	-	expression tag	UNP P08669
c	535	ILE	-	expression tag	UNP P08669
c	536	VAL	-	expression tag	UNP P08669
c	537	SER	-	expression tag	UNP P08669
c	538	PRO	-	expression tag	UNP P08669
c	539	HIS	-	expression tag	UNP P08669
c	540	LEU	-	expression tag	UNP P08669
c	541	ASP	-	expression tag	UNP P08669
c	542	GLU	-	expression tag	UNP P08669
c	543	GLU	-	expression tag	UNP P08669
c	544	ILE	-	expression tag	UNP P08669
c	545	SER	-	expression tag	UNP P08669
c	546	GLN	-	expression tag	UNP P08669
c	547	PHE	-	expression tag	UNP P08669
c	548	CYS	-	expression tag	UNP P08669
c	549	LYS	-	expression tag	UNP P08669
c	550	GLU	-	expression tag	UNP P08669
c	551	LYS	-	expression tag	UNP P08669
c	552	GLY	-	expression tag	UNP P08669
c	553	VAL	-	expression tag	UNP P08669
c	554	PHE	-	expression tag	UNP P08669
c	555	TYR	-	expression tag	UNP P08669
c	556	MET	-	expression tag	UNP P08669
c	557	PRO	-	expression tag	UNP P08669
c	558	GLY	-	expression tag	UNP P08669
c	559	VAL	-	expression tag	UNP P08669
c	560	MET	-	expression tag	UNP P08669
c	561	THR	-	expression tag	UNP P08669
c	562	PRO	-	expression tag	UNP P08669
c	563	THR	-	expression tag	UNP P08669
c	564	GLU	-	expression tag	UNP P08669
c	565	LEU	-	expression tag	UNP P08669
c	566	VAL	-	expression tag	UNP P08669
c	567	LYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	568	ALA	-	expression tag	UNP P08669
c	569	MET	-	expression tag	UNP P08669
c	570	LYS	-	expression tag	UNP P08669
c	571	LEU	-	expression tag	UNP P08669
c	572	GLY	-	expression tag	UNP P08669
c	573	HIS	-	expression tag	UNP P08669
c	574	ASP	-	expression tag	UNP P08669
c	575	ILE	-	expression tag	UNP P08669
c	576	LEU	-	expression tag	UNP P08669
c	577	LYS	-	expression tag	UNP P08669
c	578	LEU	-	expression tag	UNP P08669
c	579	PHE	-	expression tag	UNP P08669
c	580	PRO	-	expression tag	UNP P08669
c	581	GLY	-	expression tag	UNP P08669
c	582	GLU	-	expression tag	UNP P08669
c	583	VAL	-	expression tag	UNP P08669
c	584	VAL	-	expression tag	UNP P08669
c	585	GLY	-	expression tag	UNP P08669
c	586	PRO	-	expression tag	UNP P08669
c	587	GLU	-	expression tag	UNP P08669
c	588	PHE	-	expression tag	UNP P08669
c	589	VAL	-	expression tag	UNP P08669
c	590	LYS	-	expression tag	UNP P08669
c	591	ALA	-	expression tag	UNP P08669
c	592	MET	-	expression tag	UNP P08669
c	593	LYS	-	expression tag	UNP P08669
c	594	GLY	-	expression tag	UNP P08669
c	595	PRO	-	expression tag	UNP P08669
c	596	PHE	-	expression tag	UNP P08669
c	597	PRO	-	expression tag	UNP P08669
c	598	ASN	-	expression tag	UNP P08669
c	599	VAL	-	expression tag	UNP P08669
c	600	LYS	-	expression tag	UNP P08669
c	601	PHE	-	expression tag	UNP P08669
c	602	VAL	-	expression tag	UNP P08669
c	603	PRO	-	expression tag	UNP P08669
c	604	THR	-	expression tag	UNP P08669
c	605	GLY	-	expression tag	UNP P08669
c	606	GLY	-	expression tag	UNP P08669
c	607	VAL	-	expression tag	UNP P08669
c	608	ASP	-	expression tag	UNP P08669
c	609	LEU	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	610	ASP	-	expression tag	UNP P08669
c	611	ASN	-	expression tag	UNP P08669
c	612	VAL	-	expression tag	UNP P08669
c	613	CYS	-	expression tag	UNP P08669
c	614	GLU	-	expression tag	UNP P08669
c	615	TRP	-	expression tag	UNP P08669
c	616	PHE	-	expression tag	UNP P08669
c	617	ASP	-	expression tag	UNP P08669
c	618	ALA	-	expression tag	UNP P08669
c	619	GLY	-	expression tag	UNP P08669
c	620	VAL	-	expression tag	UNP P08669
c	621	LEU	-	expression tag	UNP P08669
c	622	ALA	-	expression tag	UNP P08669
c	623	VAL	-	expression tag	UNP P08669
c	624	GLY	-	expression tag	UNP P08669
c	625	VAL	-	expression tag	UNP P08669
c	626	GLY	-	expression tag	UNP P08669
c	627	ASP	-	expression tag	UNP P08669
c	628	ALA	-	expression tag	UNP P08669
c	629	LEU	-	expression tag	UNP P08669
c	630	VAL	-	expression tag	UNP P08669
c	631	GLU	-	expression tag	UNP P08669
c	632	GLY	-	expression tag	UNP P08669
c	633	ASP	-	expression tag	UNP P08669
c	634	PRO	-	expression tag	UNP P08669
c	635	ASP	-	expression tag	UNP P08669
c	636	GLU	-	expression tag	UNP P08669
c	637	VAL	-	expression tag	UNP P08669
c	638	ARG	-	expression tag	UNP P08669
c	639	GLU	-	expression tag	UNP P08669
c	640	LYS	-	expression tag	UNP P08669
c	641	ALA	-	expression tag	UNP P08669
c	642	LYS	-	expression tag	UNP P08669
c	643	GLU	-	expression tag	UNP P08669
c	644	PHE	-	expression tag	UNP P08669
c	645	VAL	-	expression tag	UNP P08669
c	646	GLU	-	expression tag	UNP P08669
c	647	LYS	-	expression tag	UNP P08669
c	648	ILE	-	expression tag	UNP P08669
c	649	ARG	-	expression tag	UNP P08669
c	650	GLY	-	expression tag	UNP P08669
c	651	CYS	-	expression tag	UNP P08669

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Chain	Residue	Modelled	Actual	Comment	Reference
c	652	THR	-	expression tag	UNP P08669
c	653	GLU	-	expression tag	UNP P08669
c	654	GLY	-	expression tag	UNP P08669
c	655	SER	-	expression tag	UNP P08669
c	656	LEU	-	expression tag	UNP P08669
c	657	GLU	-	expression tag	UNP P08669
c	658	TRP	-	expression tag	UNP P08669
c	659	SER	-	expression tag	UNP P08669
c	660	HIS	-	expression tag	UNP P08669
c	661	PRO	-	expression tag	UNP P08669
c	662	GLN	-	expression tag	UNP P08669
c	663	PHE	-	expression tag	UNP P08669
c	664	GLU	-	expression tag	UNP P08669
c	665	LYS	-	expression tag	UNP P08669

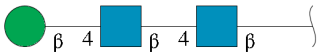
- Molecule 3 is a protein called 19.7E Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	119	Total	C	N	O	S	0	0
			923	586	161	172	4		

- Molecule 4 is a protein called 19.7E Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	107	Total	C	N	O	S	0	0
			821	515	137	166	3		

- 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.



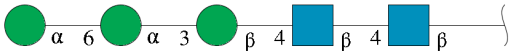
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	3	Total	C	N	O	0	0
			39	22	2	15		
5	F	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		

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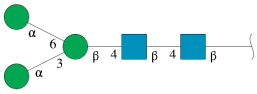
Mol	Chain	Residues	Atoms				AltConf	Trace
5	N	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-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.



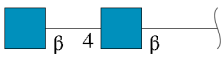
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 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.



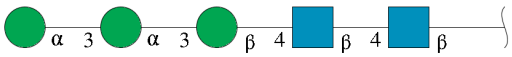
Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	5	Total	C	N	O	0	0
			61	34	2	25		
7	M	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



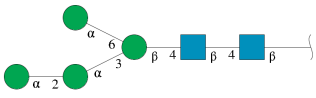
Mol	Chain	Residues	Atoms				AltConf	Trace
8	I	2	Total	C	N	O	0	0
			28	16	2	10		
8	P	2	Total	C	N	O	0	0
			28	16	2	10		
8	Q	2	Total	C	N	O	0	0
			28	16	2	10		
8	S	2	Total	C	N	O	0	0
			28	16	2	10		
8	U	2	Total	C	N	O	0	0
			28	16	2	10		
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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.



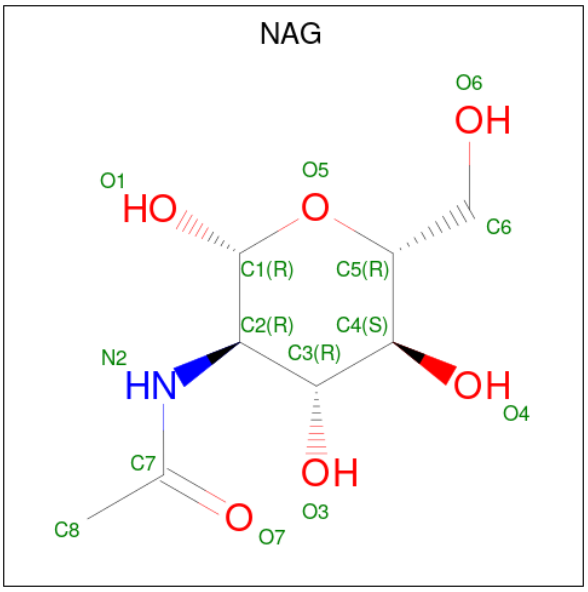
Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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				AltConf	Trace
10	R	6	Total	C	N	O	0	0
			72	40	2	30		
10	W	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
11	a	1	Total	C	N	O	0
			14	8	1	5	
11	a	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	B	1	Total	C	N	O	0
			14	8	1	5	
11	b	1	Total	C	N	O	0
			14	8	1	5	
11	b	1	Total	C	N	O	0
			14	8	1	5	
11	C	1	Total	C	N	O	0
			14	8	1	5	
11	C	1	Total	C	N	O	0
			14	8	1	5	
11	C	1	Total	C	N	O	0
			14	8	1	5	
11	C	1	Total	C	N	O	0
			14	8	1	5	
11	c	1	Total	C	N	O	0
			14	8	1	5	
11	c	1	Total	C	N	O	0
			14	8	1	5	

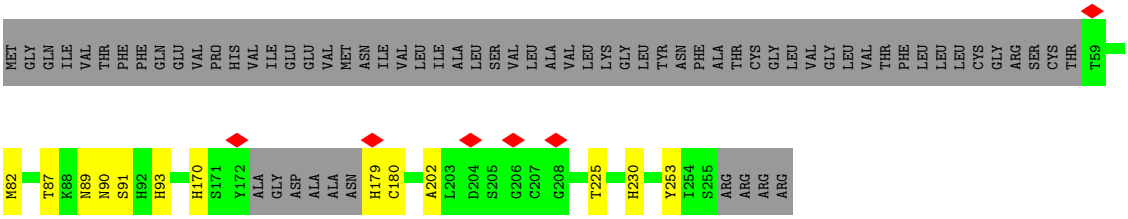
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Glycoprotein G1

Chain A:

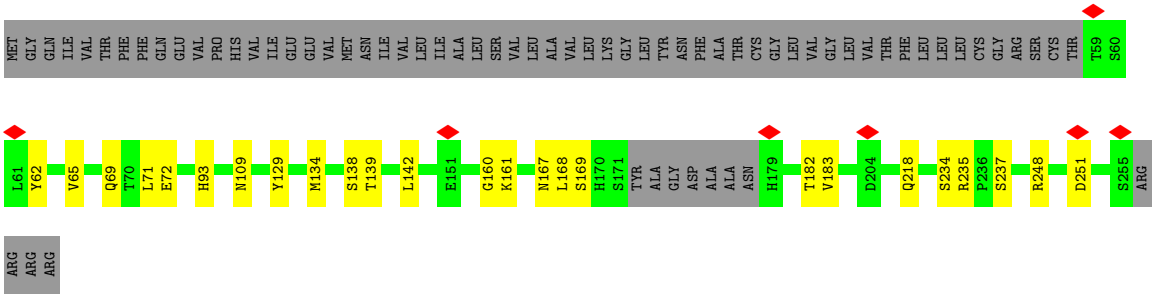




• Molecule 1: Glycoprotein G1

Chain B:

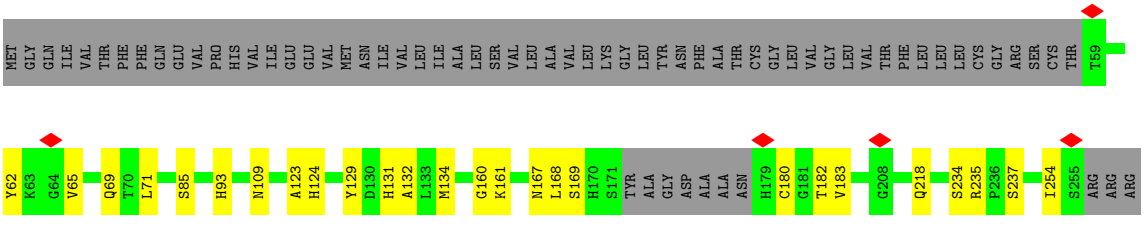




• Molecule 1: Glycoprotein G1

Chain C:

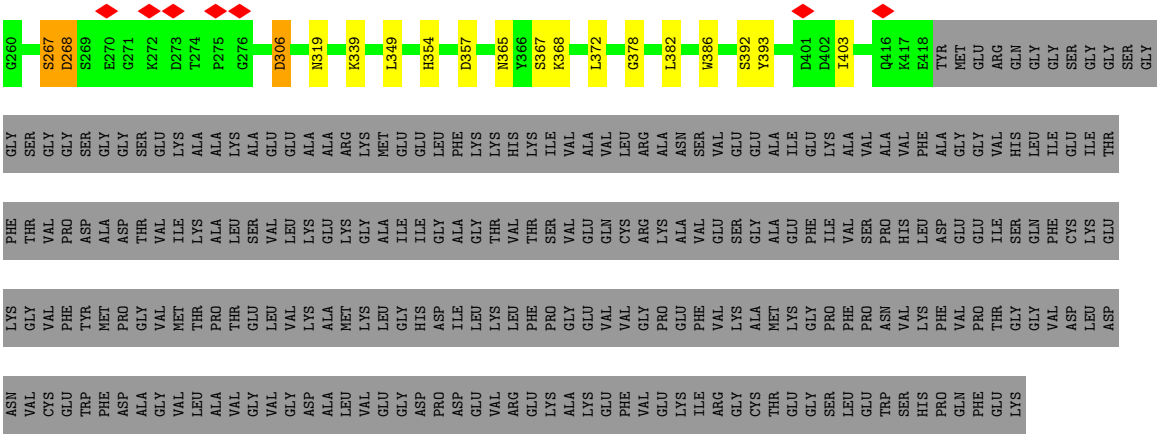




• Molecule 2: Glycoprotein G2

Chain a:

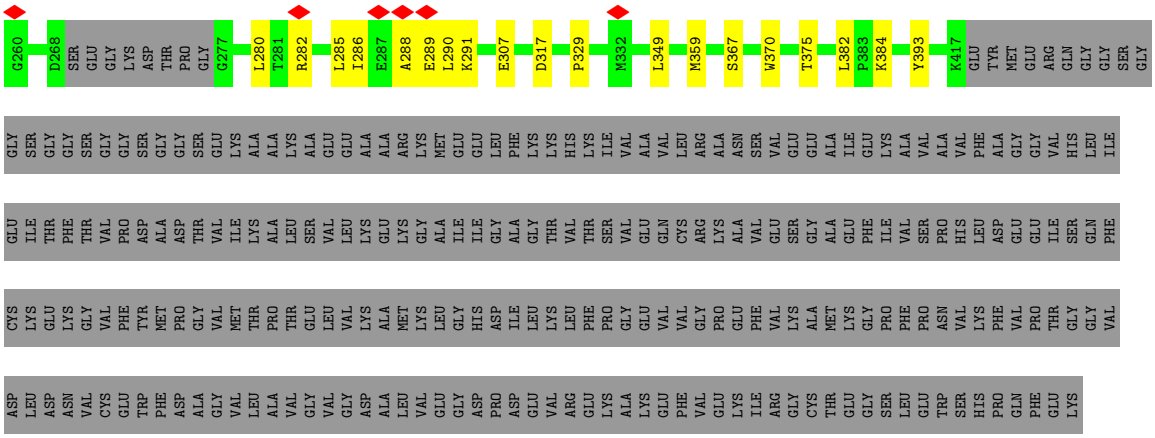




• Molecule 2: Glycoprotein G2

Chain b:

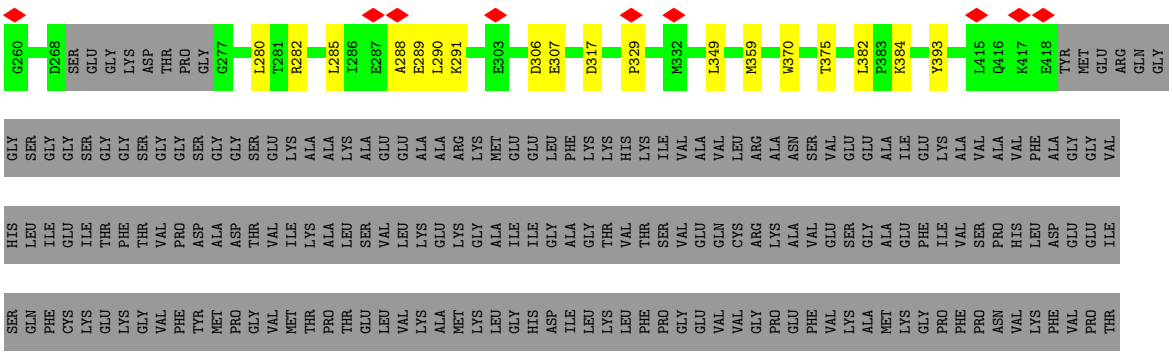


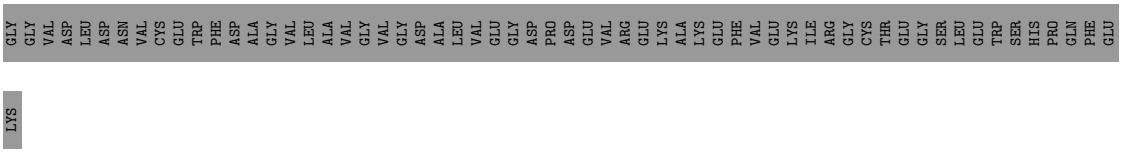


• Molecule 2: Glycoprotein G2

Chain c:

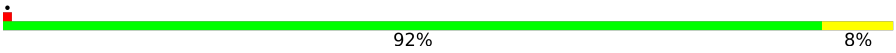






• Molecule 3: 19.7E Fab heavy chain

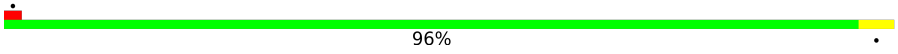
Chain H:

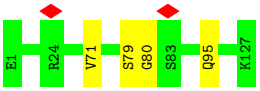




• Molecule 4: 19.7E Fab light chain

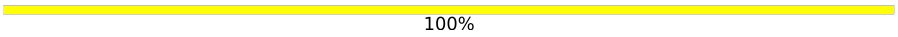
Chain L:





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

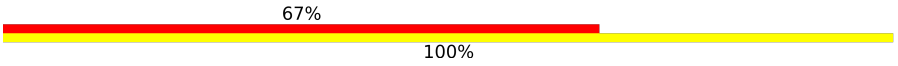
Chain D:





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

Chain F:





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

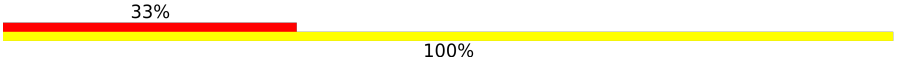
Chain K:





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

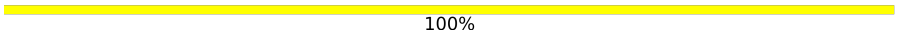
Chain N:





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

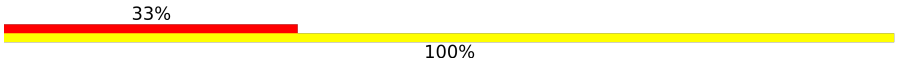
Chain O:





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

Chain T:

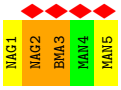




• Molecule 6: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

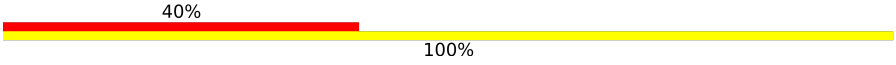
Chain G:





• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

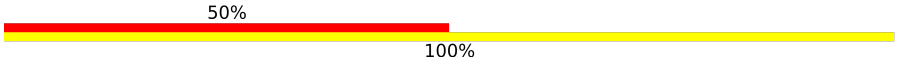
Chain M:





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

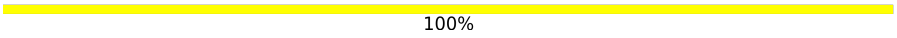
Chain I:





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

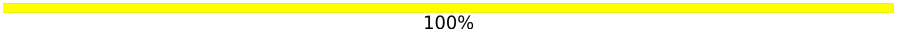
Chain P:





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

Chain Q:





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

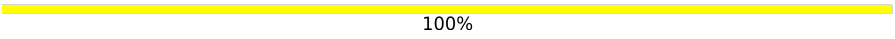
Chain S:





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

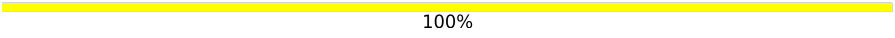
Chain U:





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

Chain V:





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

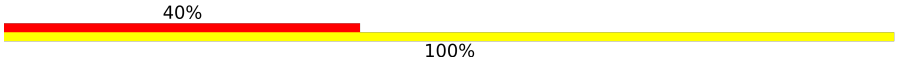
Chain X:





• Molecule 9: alpha-D-mannopyranose-(1-3)-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

Chain J:

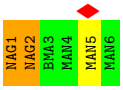




• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

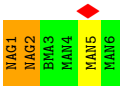




• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70071	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.2	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.062	Depositor
Minimum map value	-0.489	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	313.5, 313.5, 313.5	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.14	3/1551 (0.2%)	1.24	6/2102 (0.3%)
1	B	1.08	1/1538 (0.1%)	1.27	8/2084 (0.4%)
1	C	1.08	1/1538 (0.1%)	1.27	10/2084 (0.5%)
2	a	1.10	3/1313 (0.2%)	1.29	12/1774 (0.7%)
2	b	1.08	0/1248	1.27	6/1685 (0.4%)
2	c	1.08	0/1257	1.27	6/1697 (0.4%)
3	H	1.09	1/946 (0.1%)	1.24	4/1282 (0.3%)
4	L	1.13	0/839	1.20	4/1140 (0.4%)
All	All	1.10	9/10230 (0.1%)	1.26	56/13848 (0.4%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170	HIS	CB-CG	-6.45	1.41	1.50
1	A	93	HIS	CB-CG	-6.09	1.41	1.50
2	a	354	HIS	CB-CG	-5.96	1.41	1.50
2	a	372	LEU	CB-CG	-5.38	1.42	1.53
3	H	40	HIS	CB-CG	-5.25	1.42	1.50

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	a	382	LEU	N-CA-C	-8.34	99.24	109.83
2	a	267	SER	CB-CA-C	-7.49	107.05	117.23
2	c	370	TRP	CB-CA-C	-7.32	98.41	110.85
2	b	370	TRP	CB-CA-C	-7.29	98.45	110.85
2	c	382	LEU	N-CA-C	-7.14	99.00	109.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1516	0	1438	4	0
1	B	1504	0	1428	23	0
1	C	1504	0	1428	19	0
2	a	1286	0	1237	5	0
2	b	1223	0	1182	15	0
2	c	1232	0	1188	10	0
3	H	923	0	902	3	0
4	L	821	0	798	1	0
5	D	39	0	34	0	0
5	F	39	0	34	0	0
5	K	39	0	34	1	0
5	N	39	0	34	0	0
5	O	39	0	34	0	0
5	T	39	0	34	0	0
6	E	61	0	52	1	0
7	G	61	0	52	0	0
7	M	61	0	52	0	0
8	I	28	0	25	0	0
8	P	28	0	25	0	0
8	Q	28	0	25	0	0
8	S	28	0	25	1	0
8	U	28	0	25	0	0
8	V	28	0	25	0	0
8	X	28	0	25	1	0
9	J	61	0	52	0	0
10	R	72	0	61	9	0
10	W	72	0	61	7	0
11	B	56	0	52	0	0
11	C	56	0	52	0	0
11	a	28	0	26	0	0
11	b	28	0	26	0	0
11	c	28	0	26	0	0
All	All	11023	0	10492	72	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 3.

The worst 5 of 72 close contacts within the same asymmetric unit are listed below, sorted by their

clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ARG:HB2	10:R:1:NAG:H62	1.63	0.79
2:c:285:LEU:HD12	2:c:290:LEU:HA	1.74	0.69
1:B:235:ARG:HG3	10:R:2:NAG:O5	1.94	0.67
1:C:234:SER:HA	10:W:2:NAG:H5	1.81	0.63
1:B:234:SER:HA	10:R:2:NAG:H5	1.84	0.59

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 PDB entries followed by that with respect to all EM entries.

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	187/259 (72%)	179 (96%)	8 (4%)	0	100	100
1	B	186/259 (72%)	173 (93%)	13 (7%)	0	100	100
1	C	186/259 (72%)	173 (93%)	13 (7%)	0	100	100
2	a	157/406 (39%)	150 (96%)	7 (4%)	0	100	100
2	b	146/406 (36%)	144 (99%)	2 (1%)	0	100	100
2	c	147/406 (36%)	144 (98%)	3 (2%)	0	100	100
3	H	117/119 (98%)	117 (100%)	0	0	100	100
4	L	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
All	All	1231/2221 (55%)	1181 (96%)	50 (4%)	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 PDB entries followed by that with respect to all EM entries.

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	172/228 (75%)	172 (100%)	0	100	100
1	B	171/228 (75%)	171 (100%)	0	100	100
1	C	171/228 (75%)	171 (100%)	0	100	100
2	a	143/337 (42%)	143 (100%)	0	100	100
2	b	136/337 (40%)	136 (100%)	0	100	100
2	c	137/337 (41%)	137 (100%)	0	100	100
3	H	102/102 (100%)	102 (100%)	0	100	100
4	L	93/93 (100%)	93 (100%)	0	100	100
All	All	1125/1890 (60%)	1125 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	405	GLN
3	H	3	GLN
2	c	405	GLN
2	c	302	ASN
2	c	319	ASN

5.3.3 RNA (i)

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)

64 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	D	1	1,5	14,14,15	1.90	2 (14%)	17,19,21	1.25	2 (11%)
5	NAG	D	2	5	14,14,15	1.93	5 (35%)	17,19,21	0.99	1 (5%)
5	BMA	D	3	5	11,11,12	1.81	4 (36%)	15,15,17	0.67	0
6	NAG	E	1	1,6	14,14,15	2.09	4 (28%)	17,19,21	1.29	3 (17%)
6	NAG	E	2	6	14,14,15	0.43	0	17,19,21	1.31	1 (5%)
6	BMA	E	3	6	11,11,12	0.75	0	15,15,17	1.71	1 (6%)
6	MAN	E	4	6	11,11,12	0.84	0	15,15,17	0.90	0
6	MAN	E	5	6	11,11,12	1.88	5 (45%)	15,15,17	0.72	0
5	NAG	F	1	1,5	14,14,15	2.17	5 (35%)	17,19,21	2.47	5 (29%)
5	NAG	F	2	5	14,14,15	2.04	6 (42%)	17,19,21	0.92	1 (5%)
5	BMA	F	3	5	11,11,12	1.84	5 (45%)	15,15,17	0.73	0
7	NAG	G	1	7,1	14,14,15	1.96	4 (28%)	17,19,21	1.06	1 (5%)
7	NAG	G	2	7	14,14,15	1.77	3 (21%)	17,19,21	0.98	2 (11%)
7	BMA	G	3	7	11,11,12	1.38	1 (9%)	15,15,17	0.59	0
7	MAN	G	4	7	11,11,12	1.89	5 (45%)	15,15,17	0.70	0
7	MAN	G	5	7	11,11,12	1.84	5 (45%)	15,15,17	0.72	0
8	NAG	I	1	1,8	14,14,15	2.15	5 (35%)	17,19,21	1.68	4 (23%)
8	NAG	I	2	8	14,14,15	2.02	4 (28%)	17,19,21	0.84	0
9	NAG	J	1	9,1	14,14,15	1.94	3 (21%)	17,19,21	1.15	3 (17%)
9	NAG	J	2	9	14,14,15	1.76	4 (28%)	17,19,21	1.01	2 (11%)
9	BMA	J	3	9	11,11,12	0.62	0	15,15,17	1.06	1 (6%)
9	MAN	J	4	9	11,11,12	0.74	0	15,15,17	0.90	1 (6%)
9	MAN	J	5	9	11,11,12	1.92	5 (45%)	15,15,17	0.69	0
5	NAG	K	1	1,5	14,14,15	1.94	4 (28%)	17,19,21	1.34	3 (17%)
5	NAG	K	2	5	14,14,15	1.95	5 (35%)	17,19,21	1.00	2 (11%)
5	BMA	K	3	5	11,11,12	1.84	4 (36%)	15,15,17	0.66	0
7	NAG	M	1	7,2	14,14,15	1.87	2 (14%)	17,19,21	1.01	0
7	NAG	M	2	7	14,14,15	1.71	3 (21%)	17,19,21	1.11	2 (11%)
7	BMA	M	3	7	11,11,12	1.32	2 (18%)	15,15,17	0.61	0
7	MAN	M	4	7	11,11,12	1.84	4 (36%)	15,15,17	0.63	0
7	MAN	M	5	7	11,11,12	1.80	4 (36%)	15,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	N	1	5,2	14,14,15	2.06	6 (42%)	17,19,21	1.20	2 (11%)
5	NAG	N	2	5	14,14,15	1.88	5 (35%)	17,19,21	0.86	0
5	BMA	N	3	5	11,11,12	1.83	4 (36%)	15,15,17	0.70	0
5	NAG	O	1	1,5	14,14,15	1.80	3 (21%)	17,19,21	1.56	6 (35%)
5	NAG	O	2	5	14,14,15	1.91	4 (28%)	17,19,21	0.93	0
5	BMA	O	3	5	11,11,12	1.74	4 (36%)	15,15,17	0.78	0
8	NAG	P	1	1,8	14,14,15	1.95	5 (35%)	17,19,21	1.30	2 (11%)
8	NAG	P	2	8	14,14,15	1.97	5 (35%)	17,19,21	0.88	1 (5%)
8	NAG	Q	1	1,8	14,14,15	2.00	5 (35%)	17,19,21	1.13	1 (5%)
8	NAG	Q	2	8	14,14,15	1.97	5 (35%)	17,19,21	0.94	0
10	NAG	R	1	10,2	14,14,15	0.45	0	17,19,21	1.50	3 (17%)
10	NAG	R	2	10	14,14,15	0.29	0	17,19,21	1.09	2 (11%)
10	BMA	R	3	10	11,11,12	0.40	0	15,15,17	0.83	0
10	MAN	R	4	10	11,11,12	0.42	0	15,15,17	0.87	0
10	MAN	R	5	10	11,11,12	1.84	5 (45%)	15,15,17	0.64	0
10	MAN	R	6	10	11,11,12	0.23	0	15,15,17	0.64	0
8	NAG	S	1	8,2	14,14,15	2.21	6 (42%)	17,19,21	1.37	3 (17%)
8	NAG	S	2	8	14,14,15	0.32	0	17,19,21	0.69	0
5	NAG	T	1	1,5	14,14,15	1.81	3 (21%)	17,19,21	1.56	6 (35%)
5	NAG	T	2	5	14,14,15	1.91	3 (21%)	17,19,21	0.93	0
5	BMA	T	3	5	11,11,12	1.74	4 (36%)	15,15,17	0.78	0
8	NAG	U	1	1,8	14,14,15	1.95	5 (35%)	17,19,21	1.30	3 (17%)
8	NAG	U	2	8	14,14,15	1.98	5 (35%)	17,19,21	0.88	1 (5%)
8	NAG	V	1	1,8	14,14,15	2.00	5 (35%)	17,19,21	1.13	1 (5%)
8	NAG	V	2	8	14,14,15	1.98	5 (35%)	17,19,21	0.93	0
10	NAG	W	1	10,2	14,14,15	0.44	0	17,19,21	1.60	4 (23%)
10	NAG	W	2	10	14,14,15	0.30	0	17,19,21	1.05	2 (11%)
10	BMA	W	3	10	11,11,12	0.40	0	15,15,17	0.84	0
10	MAN	W	4	10	11,11,12	0.42	0	15,15,17	0.84	0
10	MAN	W	5	10	11,11,12	1.83	5 (45%)	15,15,17	0.64	0
10	MAN	W	6	10	11,11,12	0.22	0	15,15,17	0.64	0
8	NAG	X	1	8,2	14,14,15	2.21	6 (42%)	17,19,21	1.36	3 (17%)
8	NAG	X	2	8	14,14,15	0.33	0	17,19,21	0.69	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
5	NAG	D	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
5	BMA	D	3	5	-	1/2/19/22	0/1/1/1
6	NAG	E	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	1/2/19/22	0/1/1/1
6	MAN	E	4	6	-	2/2/19/22	0/1/1/1
6	MAN	E	5	6	-	1/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	1/2/19/22	0/1/1/1
7	NAG	G	1	7,1	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	0/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	0/2/19/22	0/1/1/1
7	MAN	G	5	7	-	1/2/19/22	0/1/1/1
8	NAG	I	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	I	2	8	-	1/6/23/26	0/1/1/1
9	NAG	J	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	J	2	9	-	0/6/23/26	0/1/1/1
9	BMA	J	3	9	-	1/2/19/22	0/1/1/1
9	MAN	J	4	9	-	1/2/19/22	0/1/1/1
9	MAN	J	5	9	-	2/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
7	NAG	M	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	M	2	7	-	0/6/23/26	0/1/1/1
7	BMA	M	3	7	-	0/2/19/22	0/1/1/1
7	MAN	M	4	7	-	1/2/19/22	0/1/1/1
7	MAN	M	5	7	-	1/2/19/22	0/1/1/1
5	NAG	N	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	BMA	N	3	5	-	0/2/19/22	0/1/1/1
5	NAG	O	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
8	NAG	P	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	P	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Q	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	Q	2	8	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	R	1	10,2	-	2/6/23/26	0/1/1/1
10	NAG	R	2	10	-	3/6/23/26	0/1/1/1
10	BMA	R	3	10	-	0/2/19/22	0/1/1/1
10	MAN	R	4	10	-	0/2/19/22	0/1/1/1
10	MAN	R	5	10	-	1/2/19/22	0/1/1/1
10	MAN	R	6	10	-	1/2/19/22	0/1/1/1
8	NAG	S	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	S	2	8	-	2/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	0/6/23/26	0/1/1/1
5	BMA	T	3	5	-	1/2/19/22	0/1/1/1
8	NAG	U	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	U	2	8	-	2/6/23/26	0/1/1/1
8	NAG	V	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	V	2	8	-	1/6/23/26	0/1/1/1
10	NAG	W	1	10,2	-	2/6/23/26	0/1/1/1
10	NAG	W	2	10	-	3/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1
10	MAN	W	5	10	-	1/2/19/22	0/1/1/1
10	MAN	W	6	10	-	1/2/19/22	0/1/1/1
8	NAG	X	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1

The worst 5 of 201 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1	NAG	C1-C2	5.53	1.59	1.52
5	D	1	NAG	C1-C2	5.52	1.59	1.52
9	J	1	NAG	C1-C2	5.45	1.59	1.52
5	N	1	NAG	C1-C2	5.34	1.59	1.52
8	S	1	NAG	C1-C2	5.26	1.59	1.52

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1	NAG	C8-C7-N2	7.51	128.58	116.12
6	E	3	BMA	O3-C3-C4	4.70	121.46	110.38
5	F	1	NAG	O7-C7-N2	-4.61	113.84	121.98
6	E	2	NAG	O5-C1-C2	-4.60	104.18	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	R	1	NAG	O4-C4-C3	3.43	118.46	110.38

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	S	2	NAG	C8-C7-N2-C2
8	S	2	NAG	O7-C7-N2-C2
8	X	2	NAG	C8-C7-N2-C2
8	X	2	NAG	O7-C7-N2-C2
10	R	1	NAG	C8-C7-N2-C2

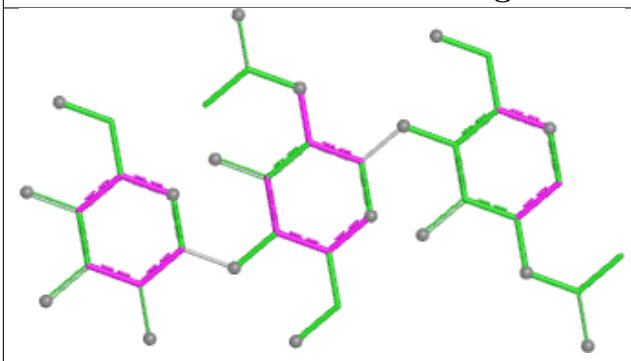
There are no ring outliers.

9 monomers are involved in 20 short contacts:

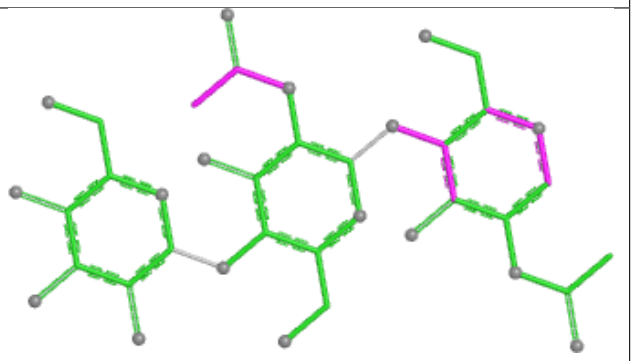
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
8	S	1	NAG	1	0
10	W	2	NAG	4	0
6	E	3	BMA	1	0
10	R	1	NAG	5	0
8	X	1	NAG	1	0
10	R	2	NAG	5	0
6	E	2	NAG	1	0
10	W	1	NAG	4	0

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

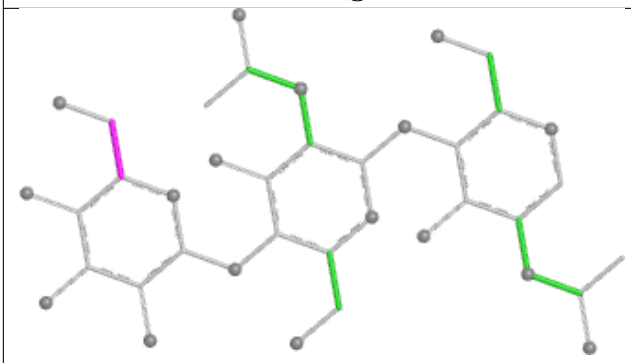
Oligosaccharide Chain D



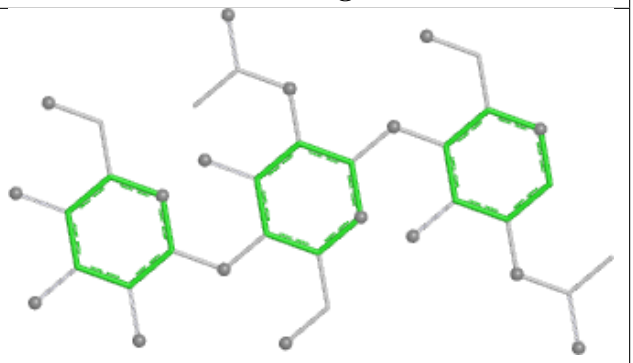
Bond lengths



Bond angles

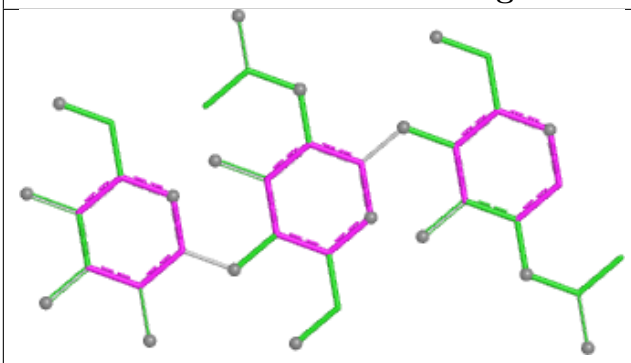


Torsions

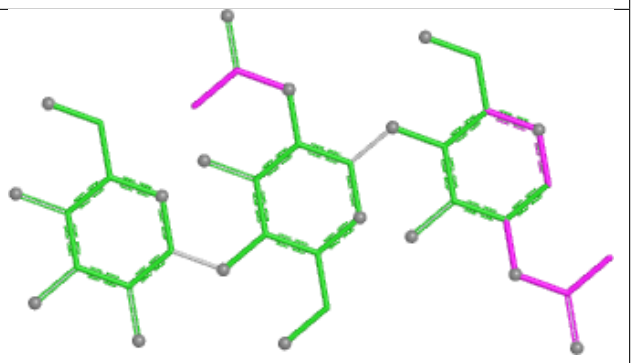


Rings

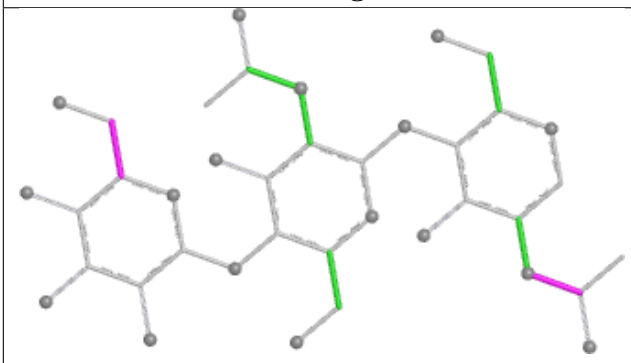
Oligosaccharide Chain F



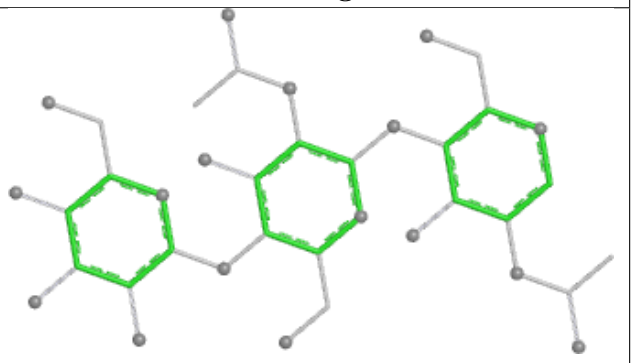
Bond lengths



Bond angles

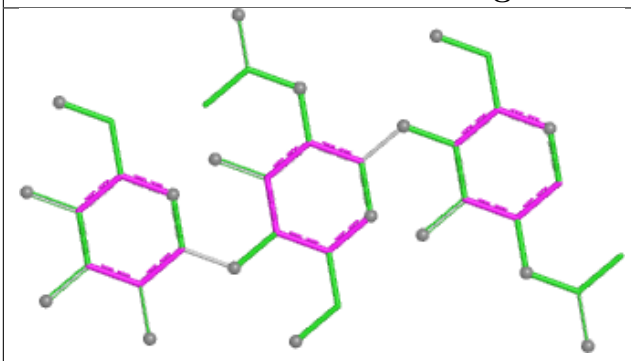


Torsions

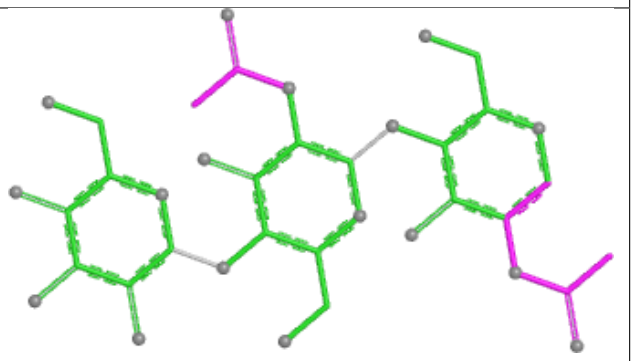


Rings

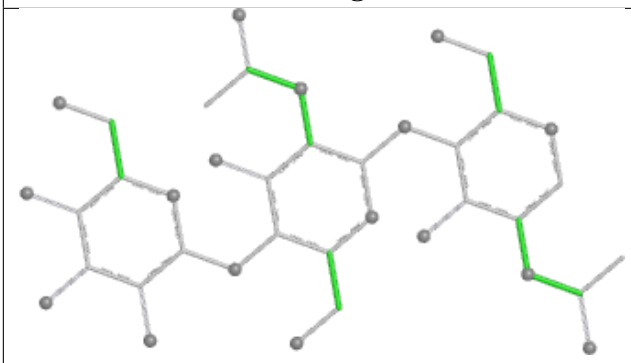
Oligosaccharide Chain K



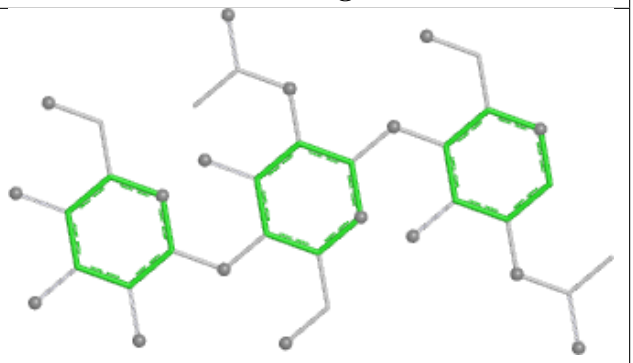
Bond lengths



Bond angles

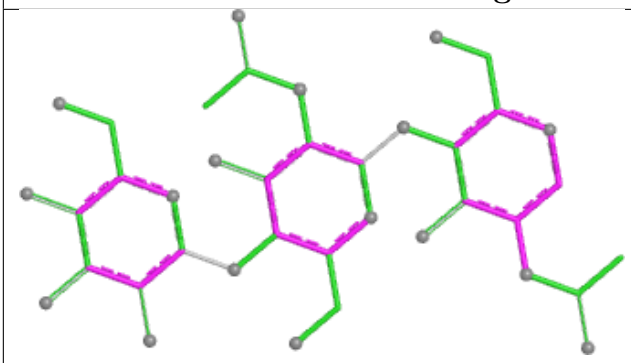


Torsions

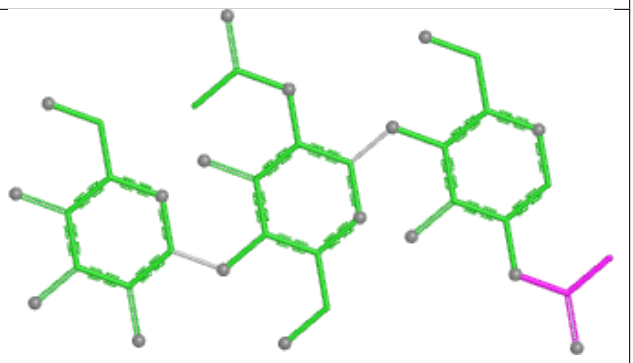


Rings

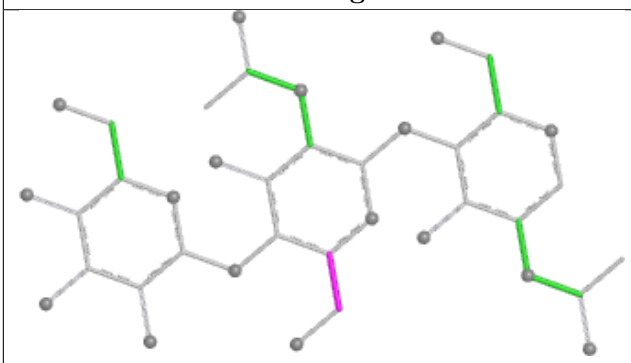
Oligosaccharide Chain N



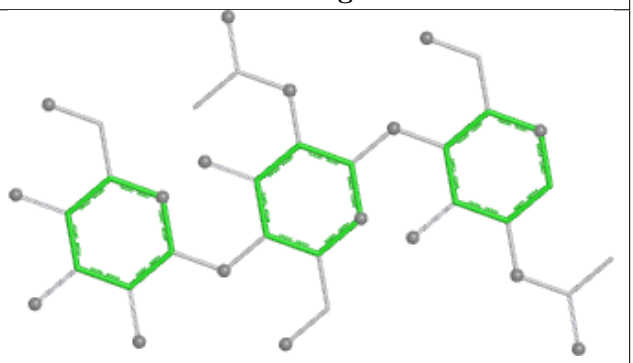
Bond lengths



Bond angles

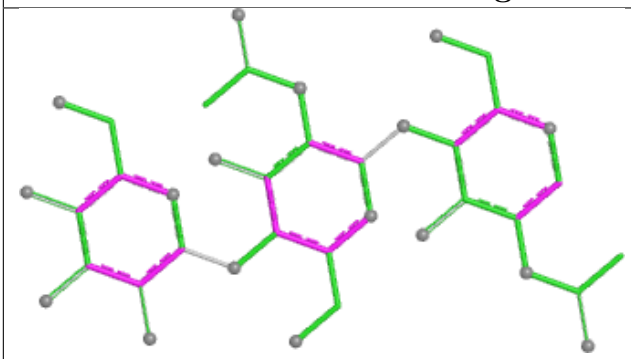


Torsions

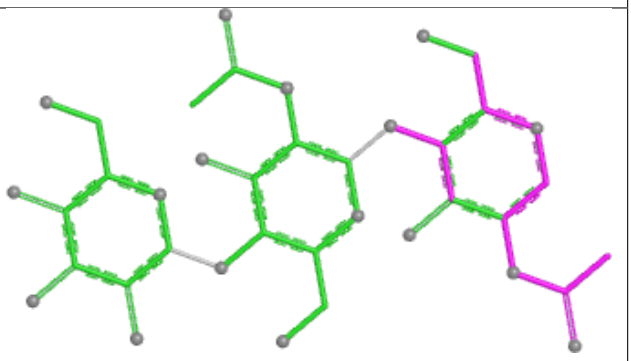


Rings

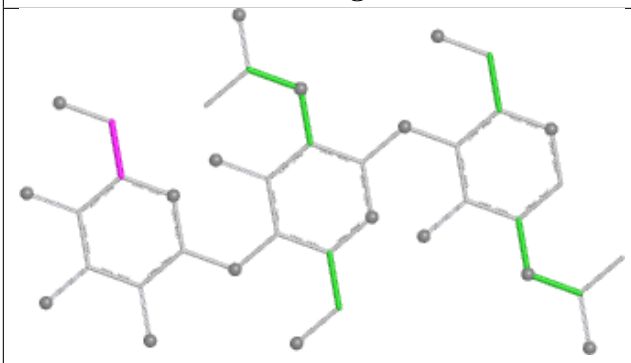
Oligosaccharide Chain O



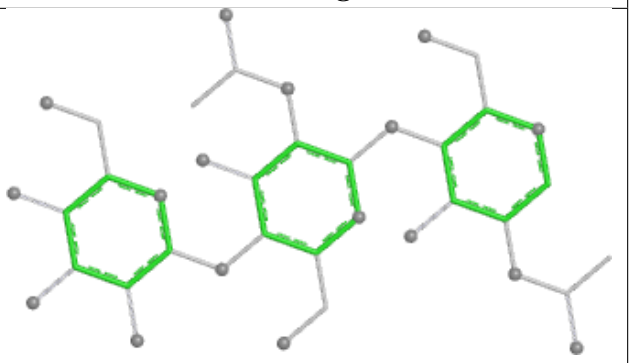
Bond lengths



Bond angles

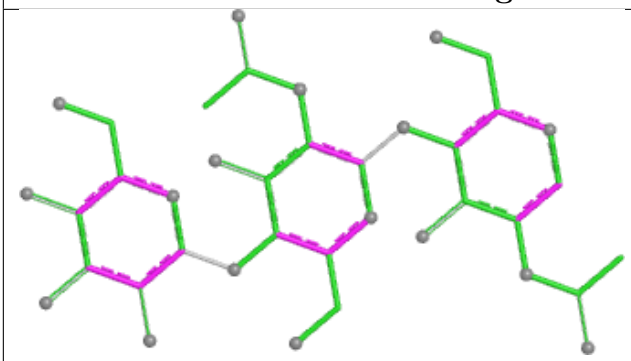


Torsions

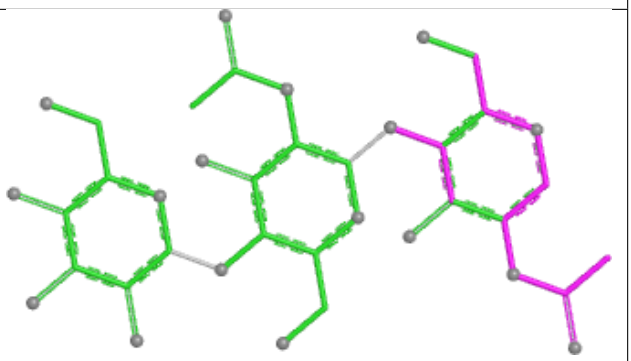


Rings

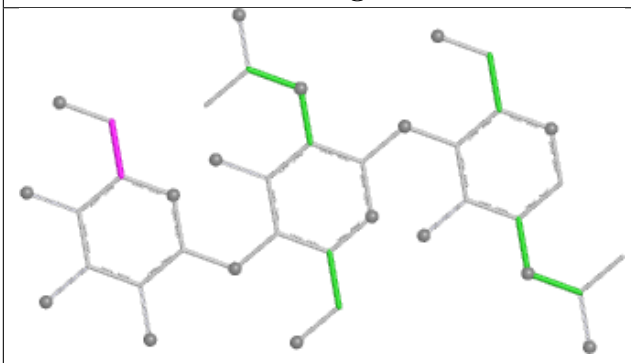
Oligosaccharide Chain T



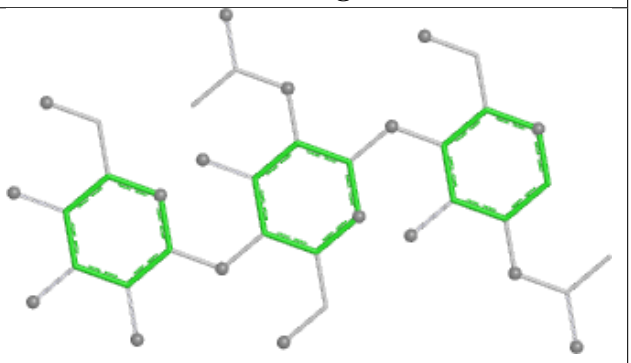
Bond lengths



Bond angles

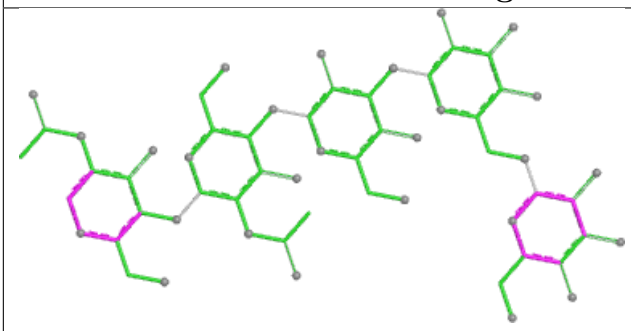


Torsions

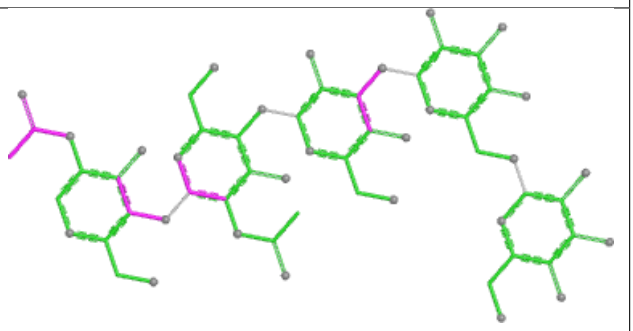


Rings

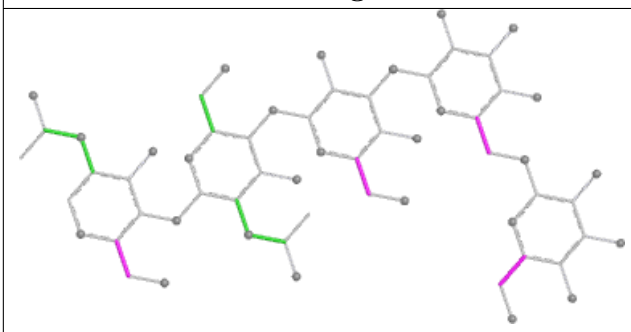
Oligosaccharide Chain E



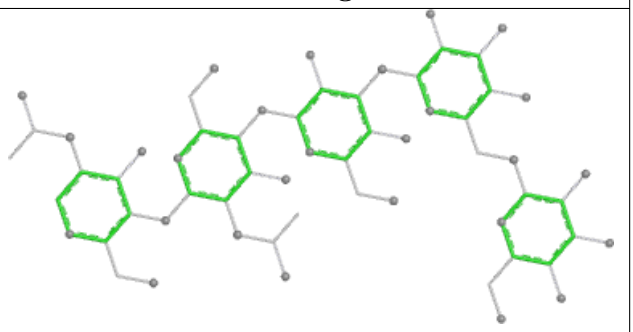
Bond lengths



Bond angles

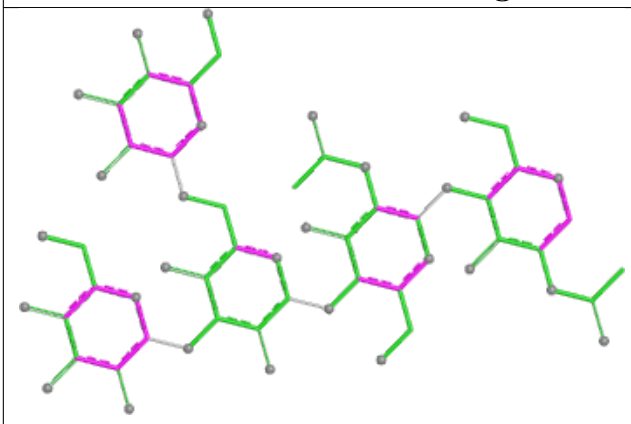


Torsions

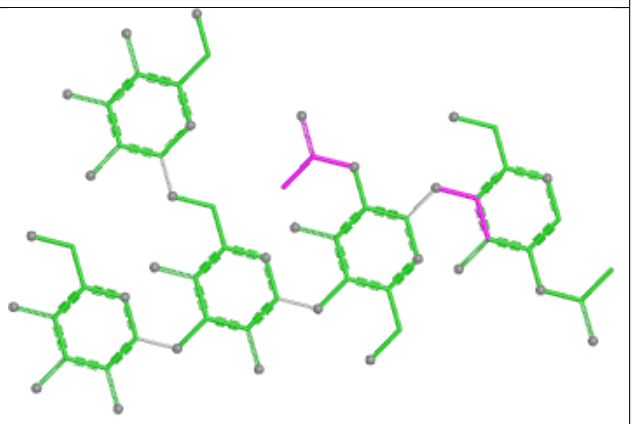


Rings

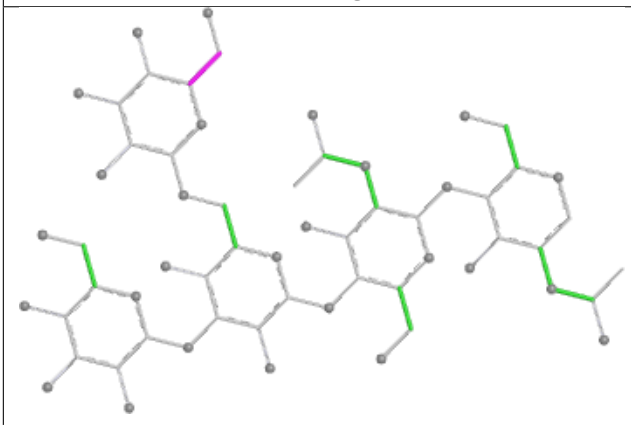
Oligosaccharide Chain G



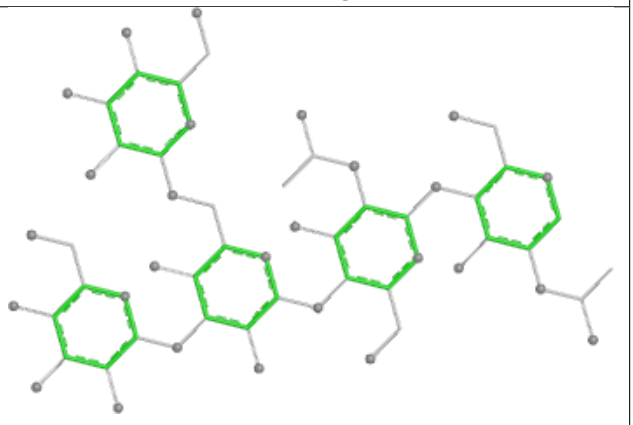
Bond lengths



Bond angles

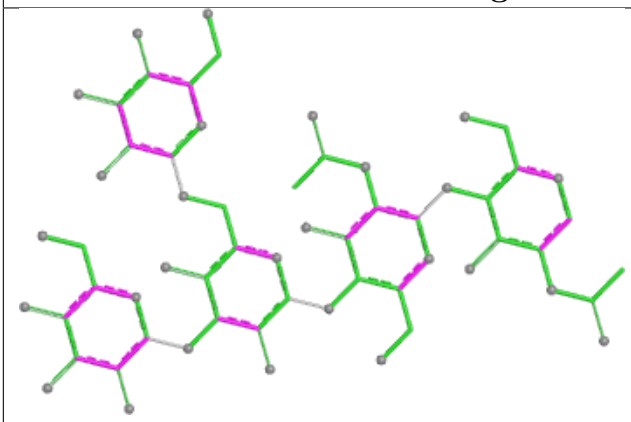


Torsions

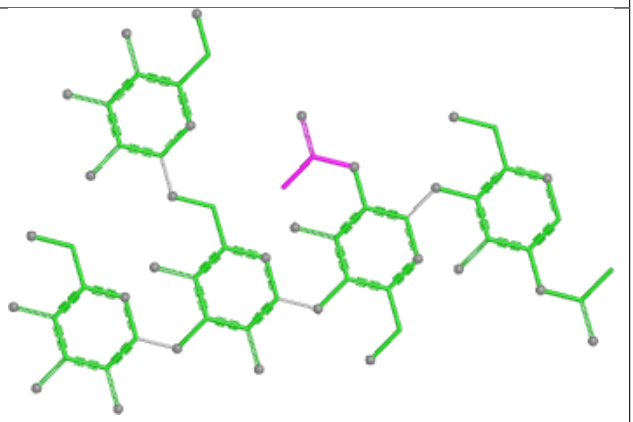


Rings

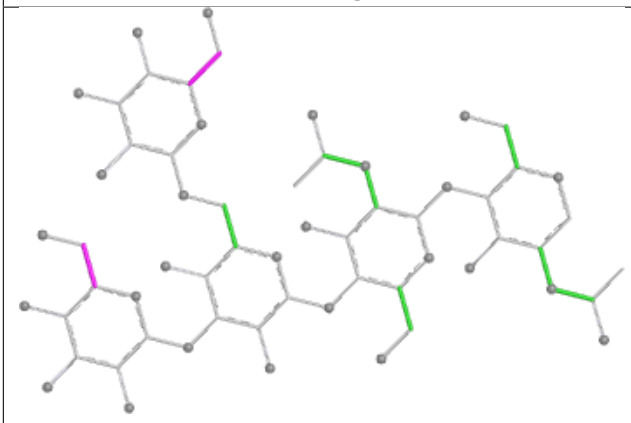
Oligosaccharide Chain M



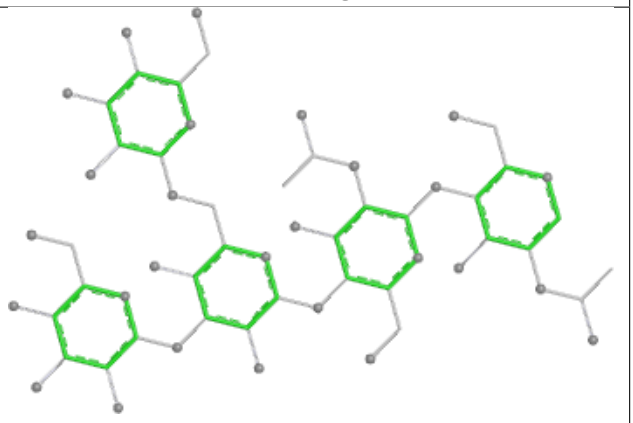
Bond lengths



Bond angles

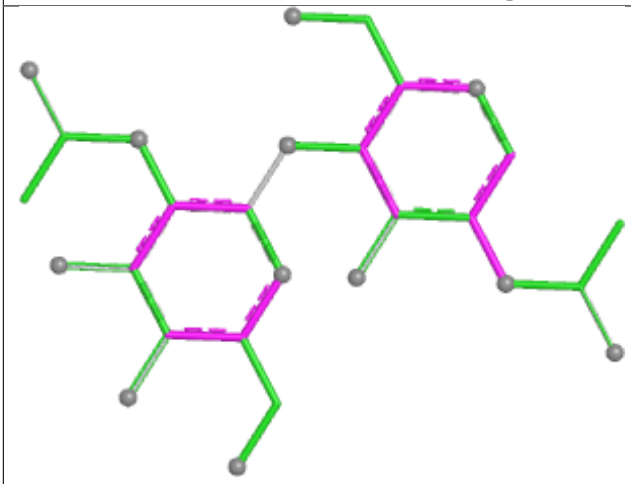


Torsions

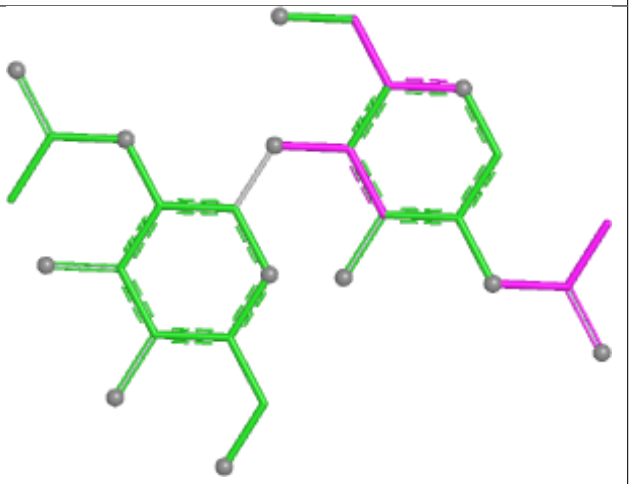


Rings

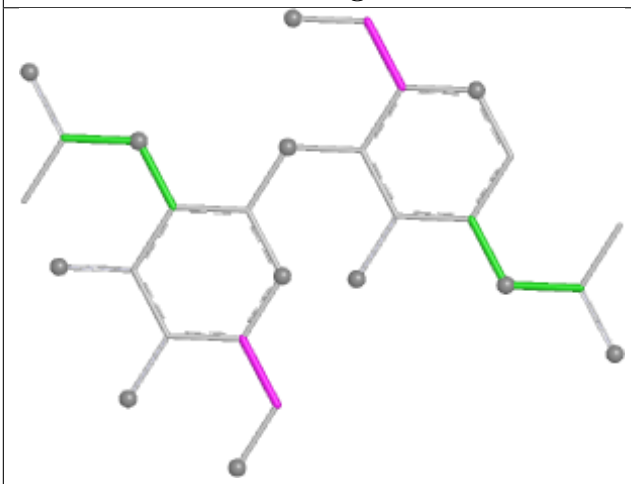
Oligosaccharide Chain I



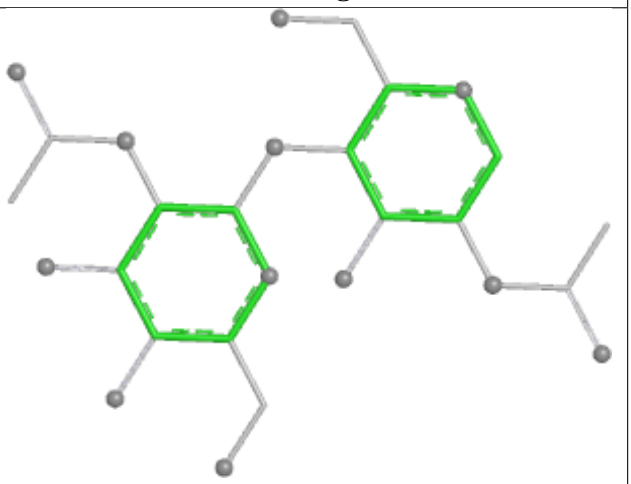
Bond lengths



Bond angles

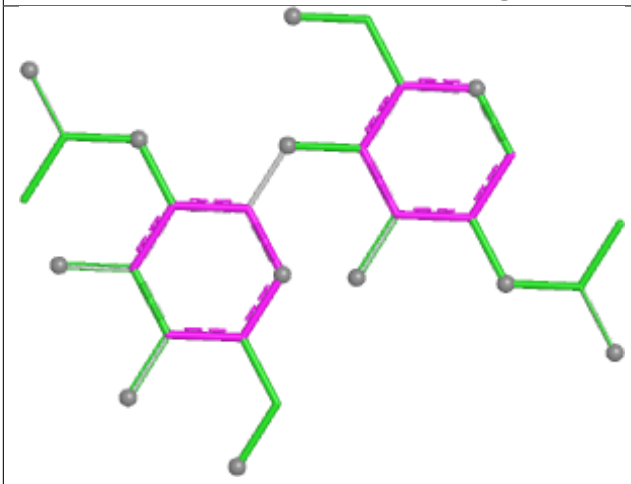


Torsions

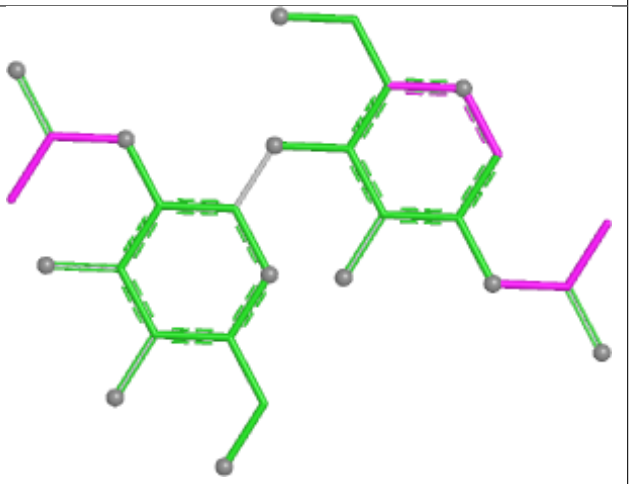


Rings

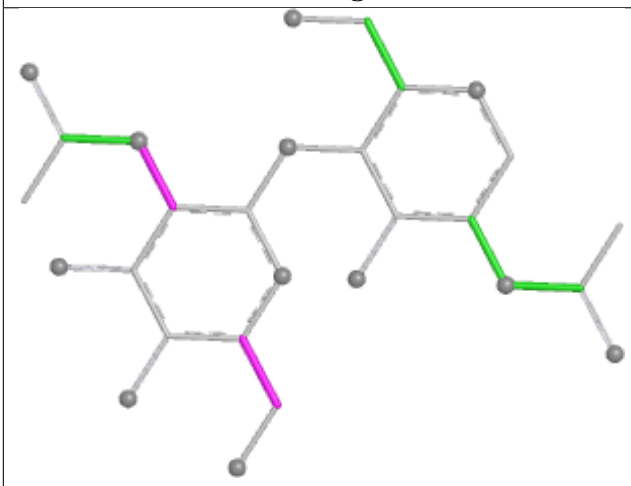
Oligosaccharide Chain P



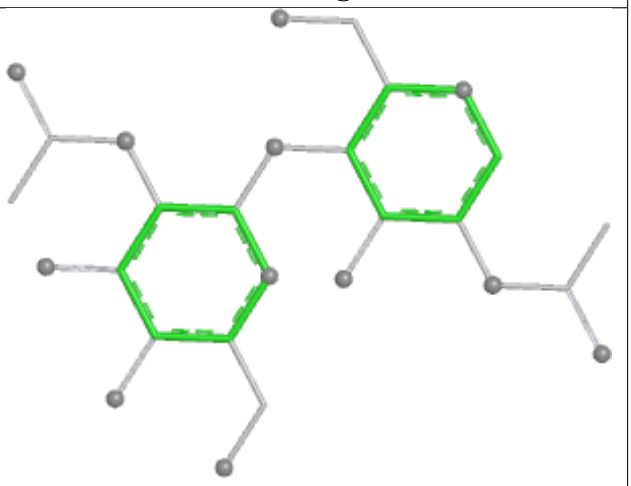
Bond lengths



Bond angles

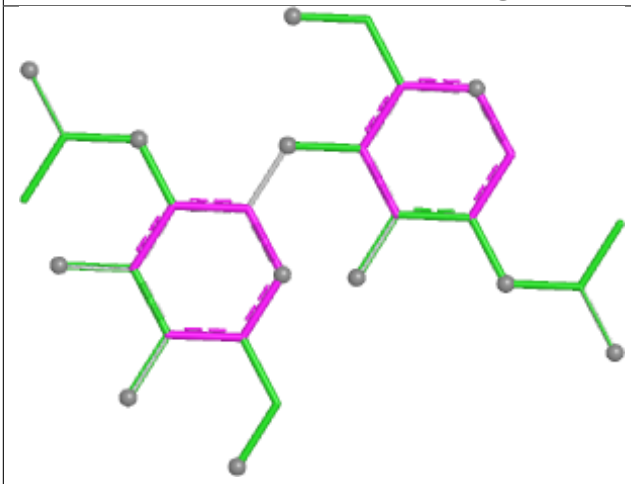


Torsions

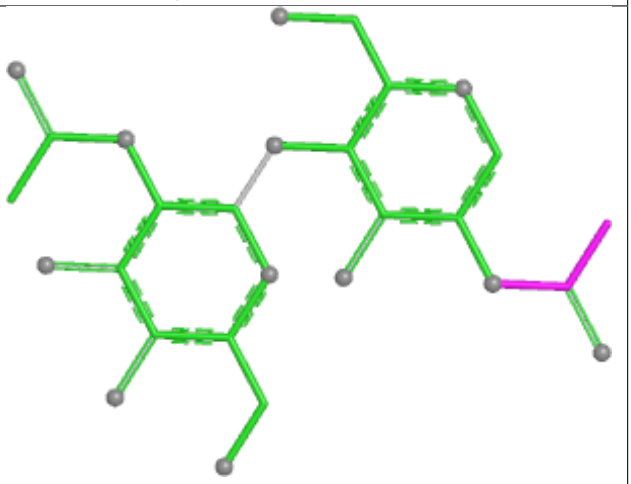


Rings

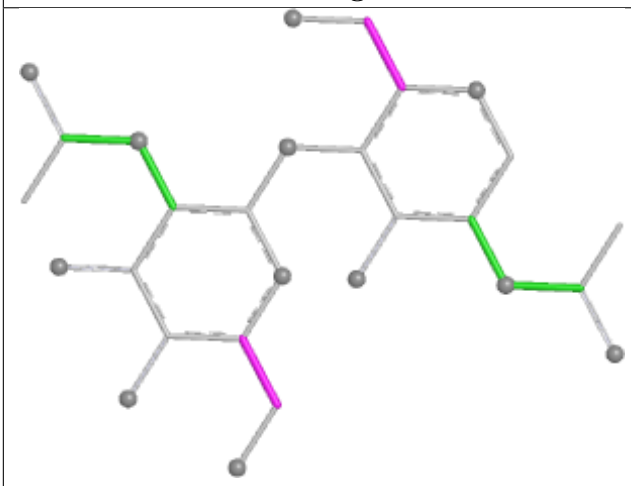
Oligosaccharide Chain Q



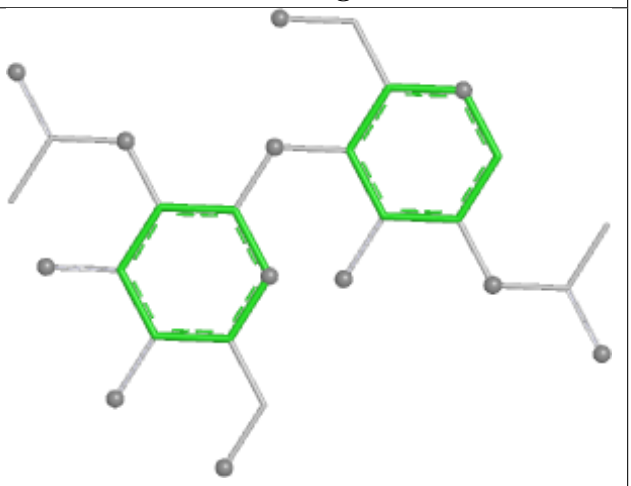
Bond lengths



Bond angles

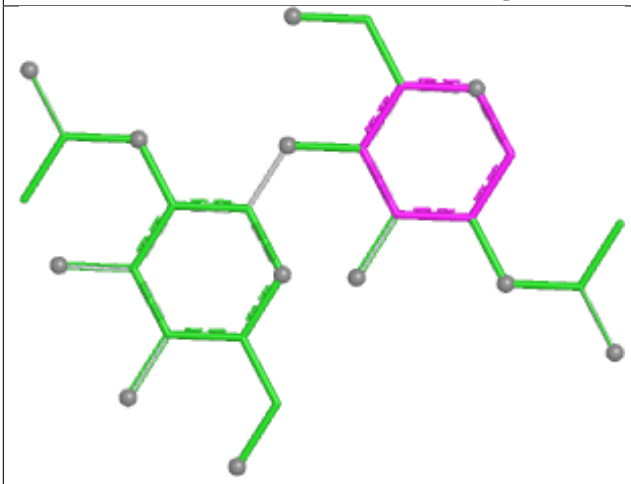


Torsions

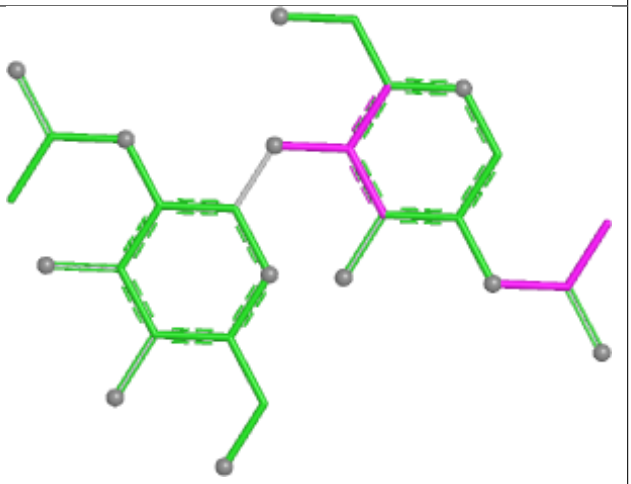


Rings

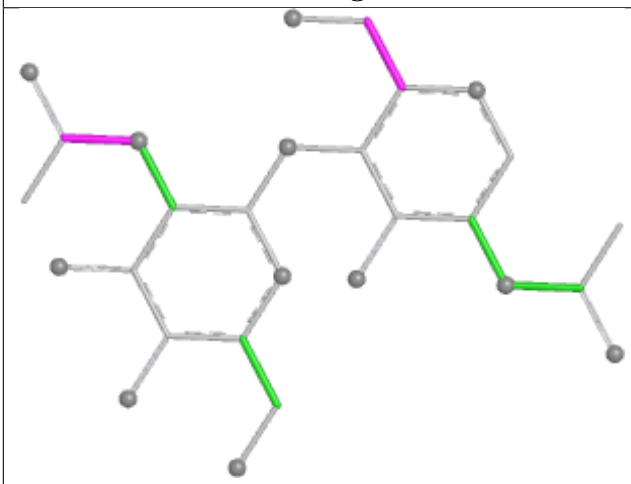
Oligosaccharide Chain S



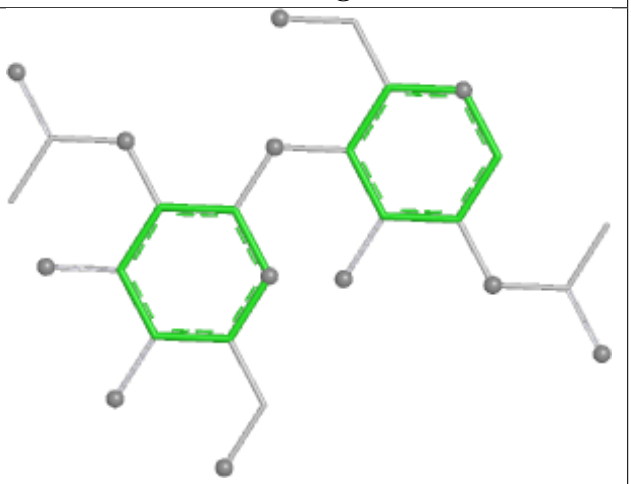
Bond lengths



Bond angles

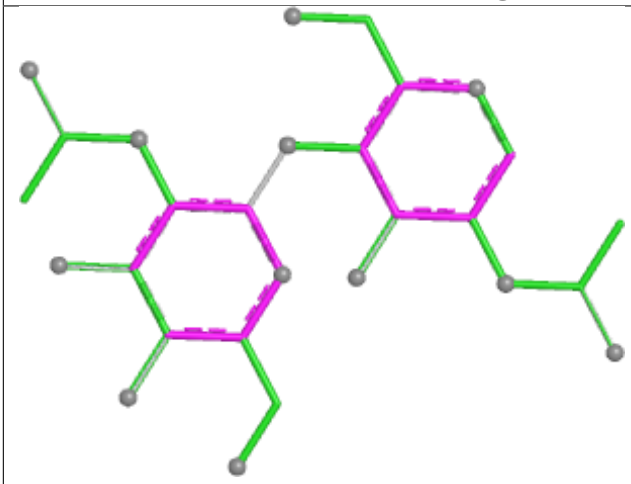


Torsions

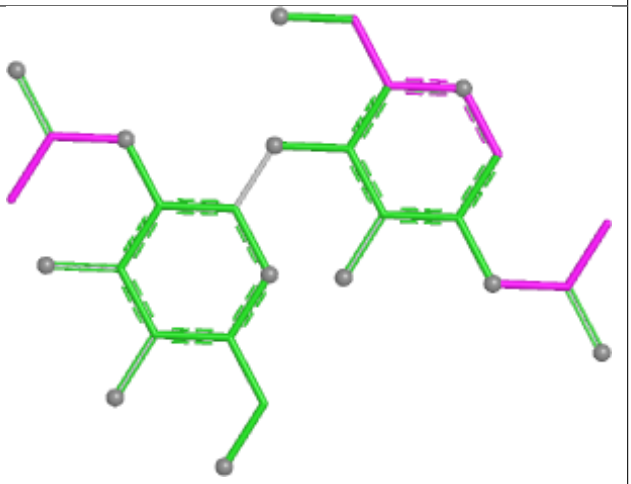


Rings

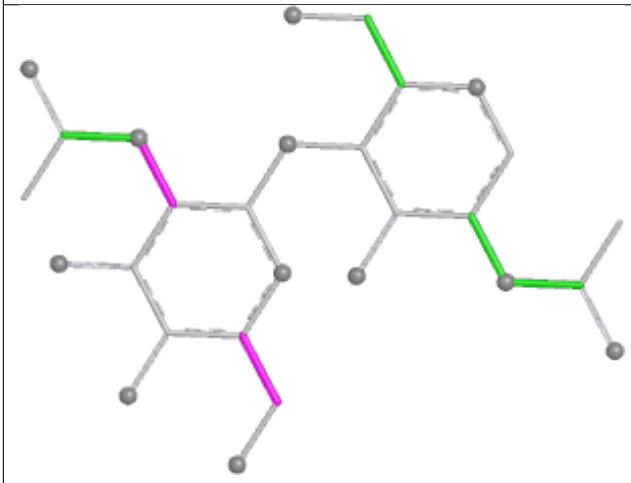
Oligosaccharide Chain U



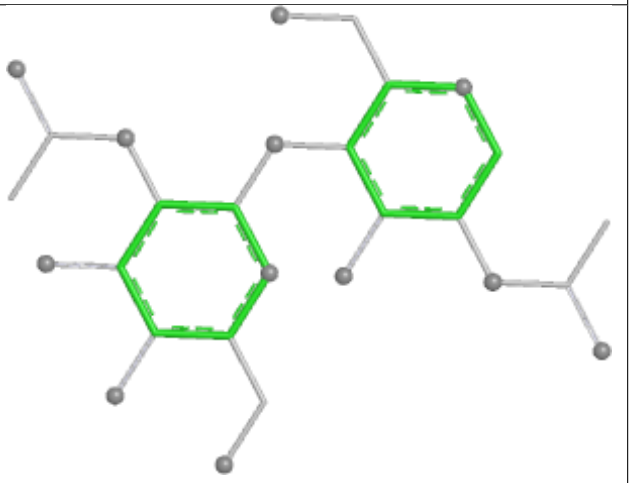
Bond lengths



Bond angles

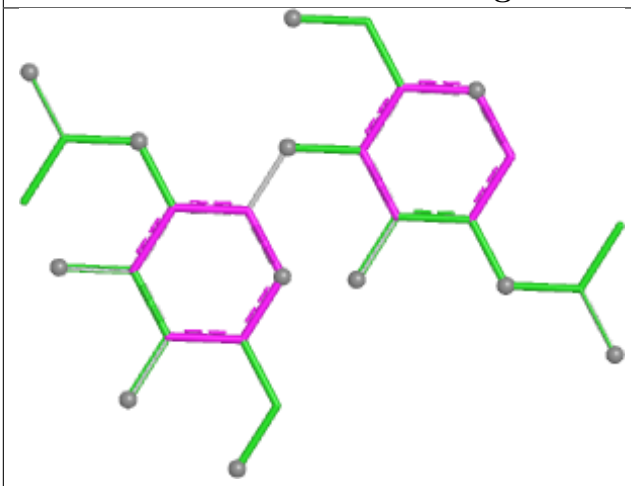


Torsions

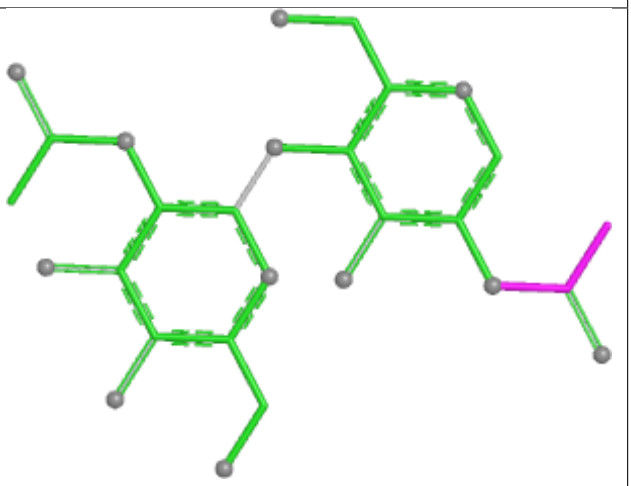


Rings

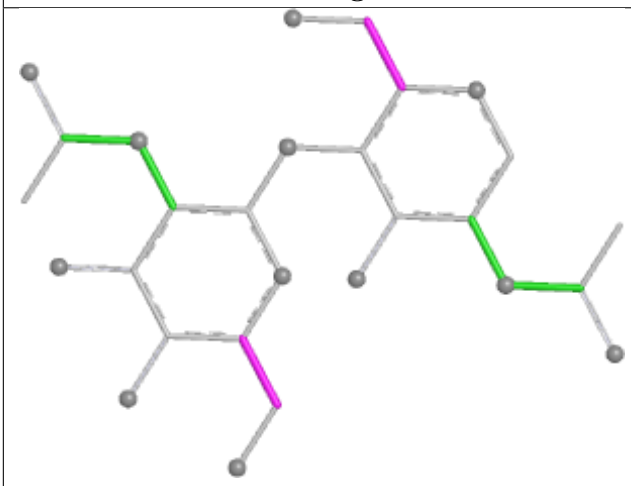
Oligosaccharide Chain V



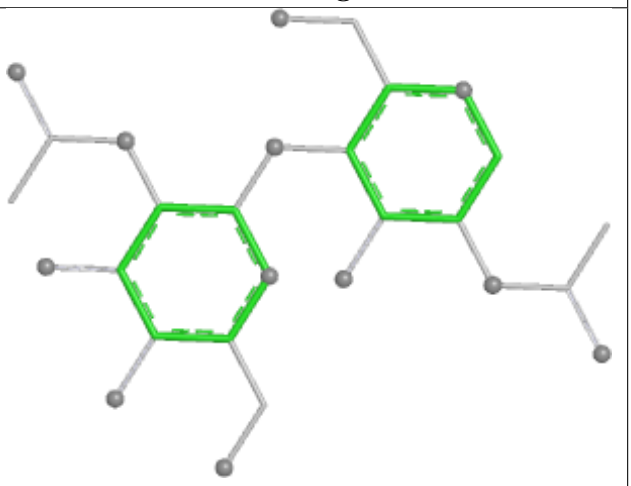
Bond lengths



Bond angles

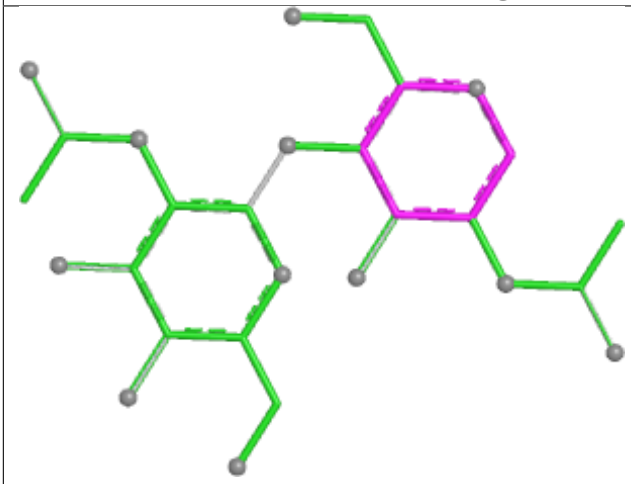


Torsions

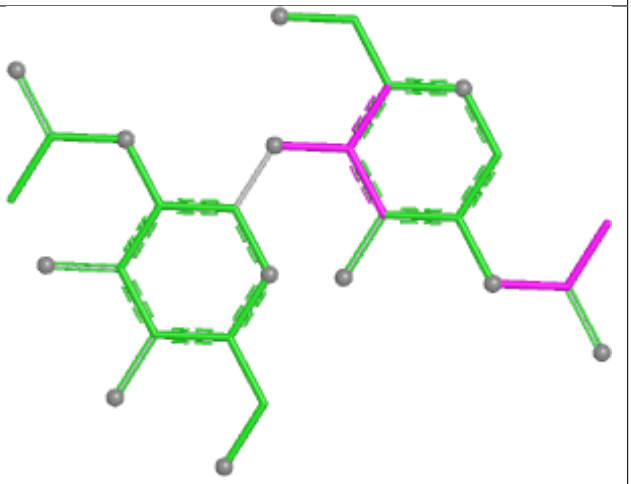


Rings

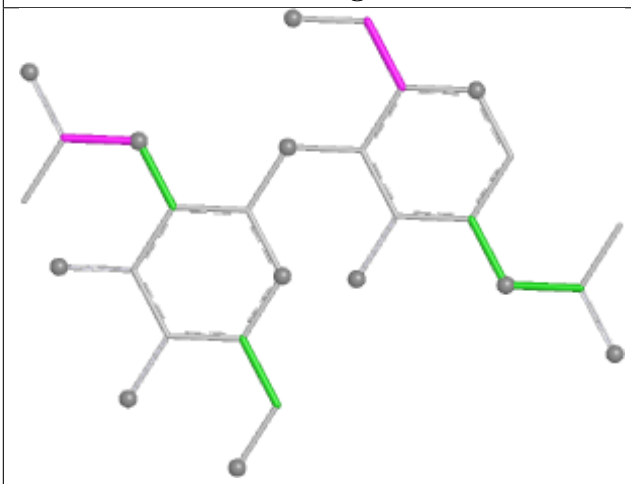
Oligosaccharide Chain X



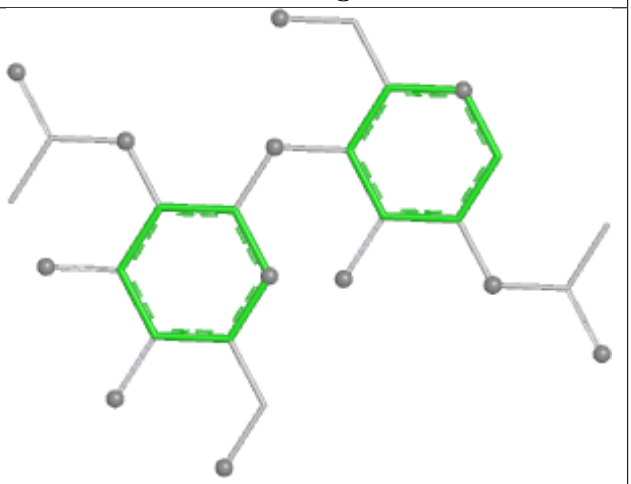
Bond lengths



Bond angles

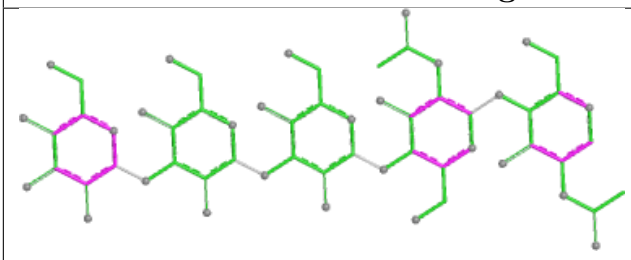


Torsions

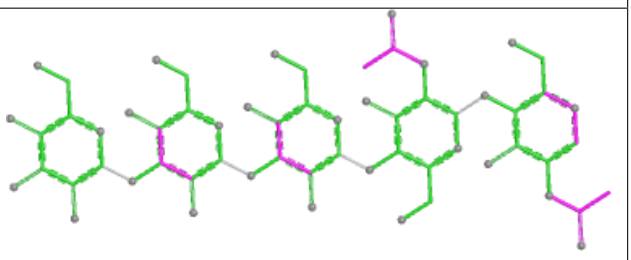


Rings

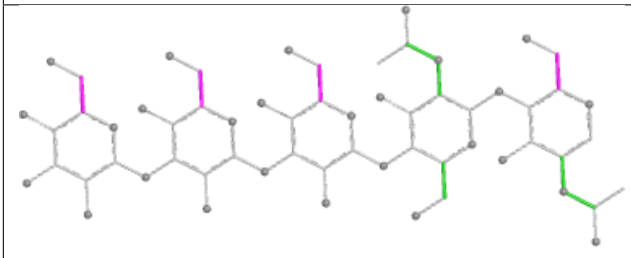
Oligosaccharide Chain J



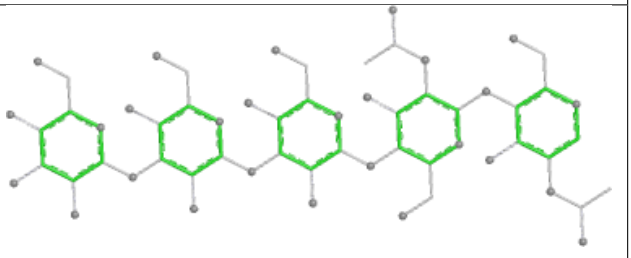
Bond lengths



Bond angles

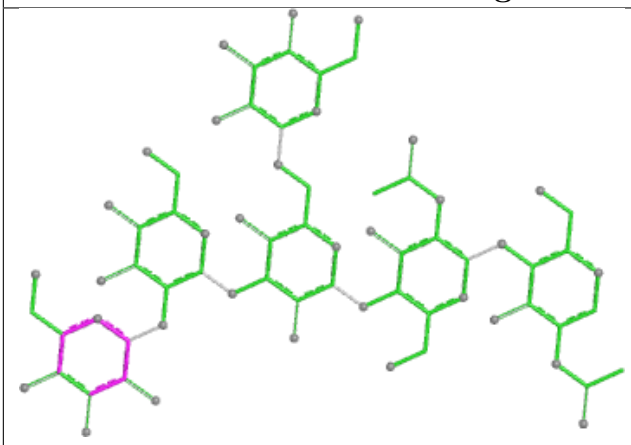


Torsions

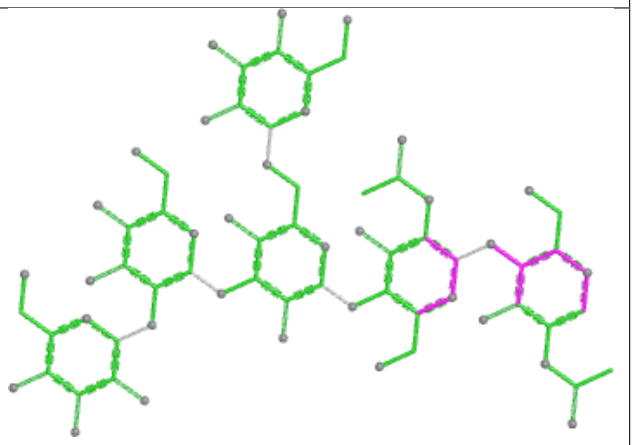


Rings

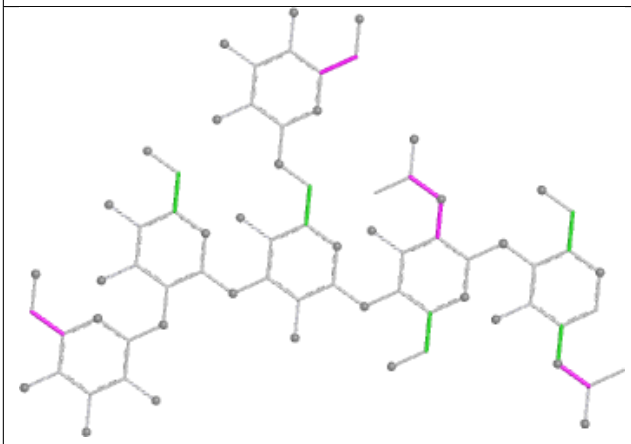
Oligosaccharide Chain R



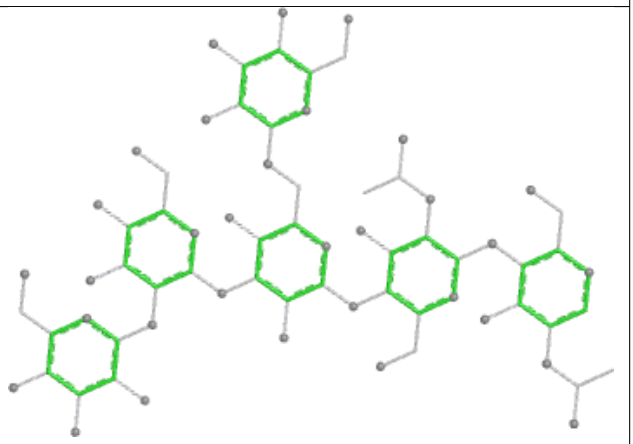
Bond lengths



Bond angles

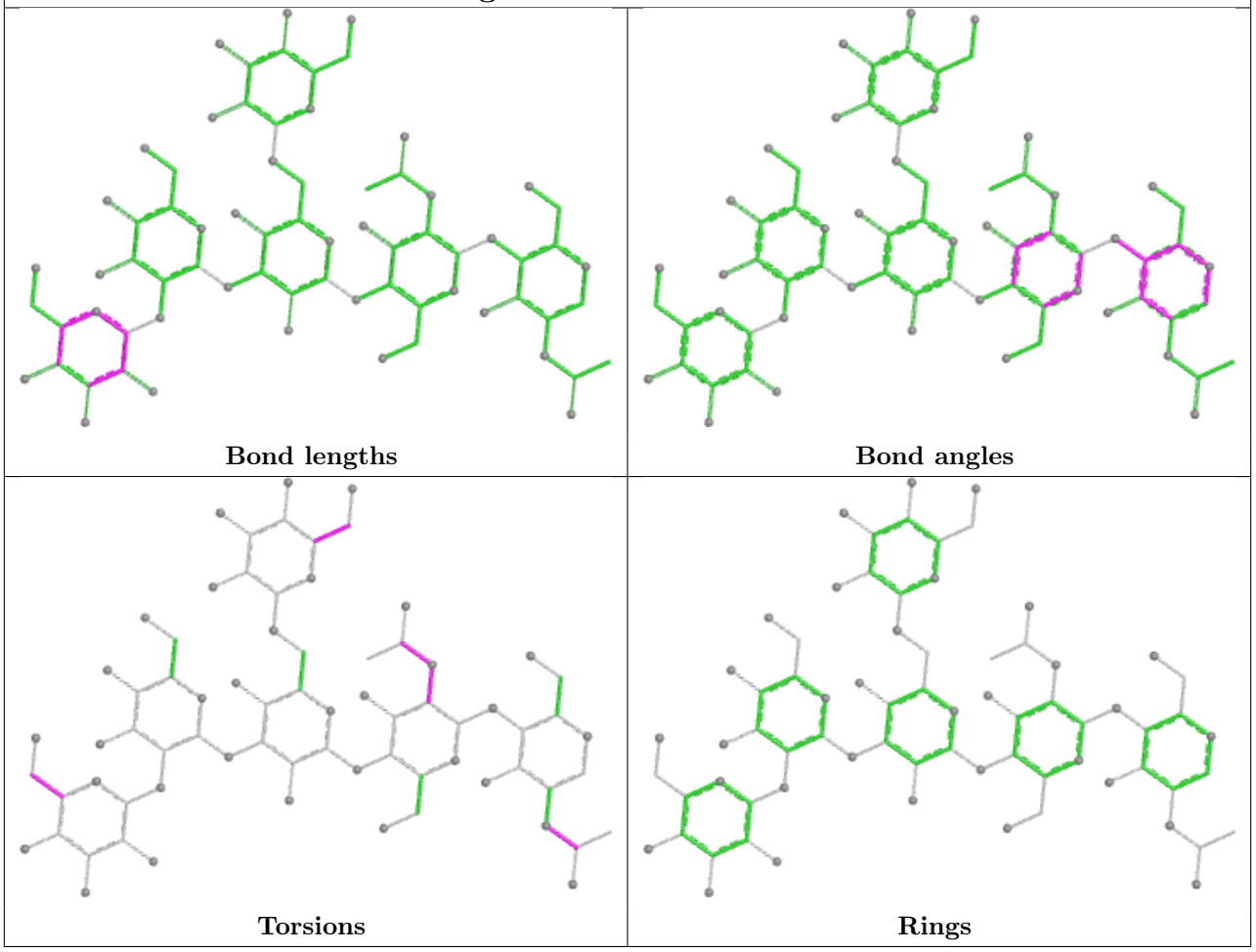


Torsions



Rings

Oligosaccharide Chain W



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
11	NAG	a	702	2	14,14,15	2.26	5 (35%)	17,19,21	0.98	1 (5%)
11	NAG	B	301	1	14,14,15	2.11	3 (21%)	17,19,21	0.98	2 (11%)
11	NAG	b	701	2	14,14,15	2.21	6 (42%)	17,19,21	1.17	2 (11%)
11	NAG	B	302	1	14,14,15	2.24	6 (42%)	17,19,21	2.41	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	c	701	2	14,14,15	2.20	6 (42%)	17,19,21	1.17	2 (11%)
11	NAG	C	304	1	14,14,15	2.06	5 (35%)	17,19,21	1.00	0
11	NAG	c	702	2	14,14,15	2.24	5 (35%)	17,19,21	0.98	0
11	NAG	C	302	1	14,14,15	2.24	6 (42%)	17,19,21	2.41	4 (23%)
11	NAG	B	304	1	14,14,15	2.07	5 (35%)	17,19,21	1.00	0
11	NAG	C	301	1	14,14,15	2.11	4 (28%)	17,19,21	0.99	2 (11%)
11	NAG	b	702	2	14,14,15	2.24	5 (35%)	17,19,21	0.99	0
11	NAG	B	303	1	14,14,15	2.28	5 (35%)	17,19,21	0.93	0
11	NAG	a	701	2	14,14,15	2.26	6 (42%)	17,19,21	1.02	1 (5%)
11	NAG	C	303	1	14,14,15	2.28	5 (35%)	17,19,21	0.92	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
11	NAG	a	702	2	-	0/6/23/26	0/1/1/1
11	NAG	B	301	1	-	1/6/23/26	0/1/1/1
11	NAG	b	701	2	-	0/6/23/26	0/1/1/1
11	NAG	B	302	1	-	4/6/23/26	0/1/1/1
11	NAG	c	701	2	-	0/6/23/26	0/1/1/1
11	NAG	C	304	1	-	0/6/23/26	0/1/1/1
11	NAG	c	702	2	-	0/6/23/26	0/1/1/1
11	NAG	C	302	1	-	4/6/23/26	0/1/1/1
11	NAG	B	304	1	-	0/6/23/26	0/1/1/1
11	NAG	C	301	1	-	1/6/23/26	0/1/1/1
11	NAG	b	702	2	-	0/6/23/26	0/1/1/1
11	NAG	B	303	1	-	0/6/23/26	0/1/1/1
11	NAG	a	701	2	-	0/6/23/26	0/1/1/1
11	NAG	C	303	1	-	0/6/23/26	0/1/1/1

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	303	NAG	C1-C2	6.23	1.60	1.52
11	C	303	NAG	C1-C2	6.21	1.60	1.52
11	a	701	NAG	C1-C2	6.15	1.60	1.52
11	B	302	NAG	C1-C2	6.10	1.60	1.52
11	C	302	NAG	C1-C2	6.09	1.60	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	302	NAG	C8-C7-N2	7.60	128.72	116.12
11	B	302	NAG	C8-C7-N2	7.58	128.70	116.12
11	C	302	NAG	O7-C7-N2	-4.42	114.17	121.98
11	B	302	NAG	O7-C7-N2	-4.39	114.22	121.98
11	B	302	NAG	O7-C7-C8	-2.79	117.08	122.05

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	302	NAG	C8-C7-N2-C2
11	B	302	NAG	O7-C7-N2-C2
11	C	302	NAG	C8-C7-N2-C2
11	C	302	NAG	O7-C7-N2-C2
11	B	302	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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.

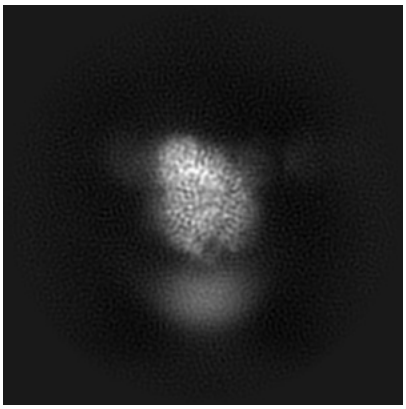
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28183. These allow visual inspection of the internal detail of the map and identification of artifacts.

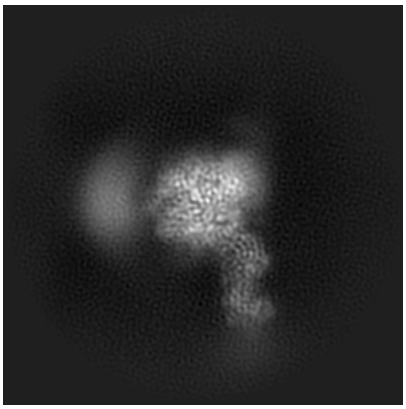
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

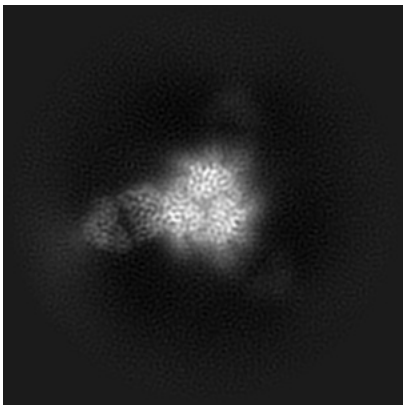
6.1.1 Primary map



X

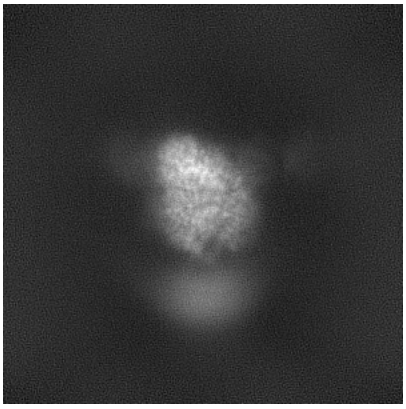


Y

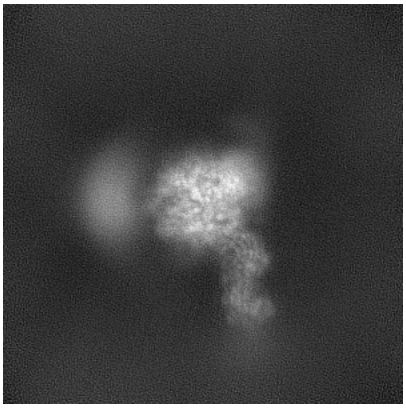


Z

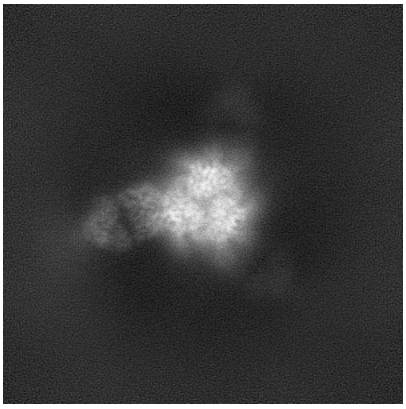
6.1.2 Raw map



X



Y

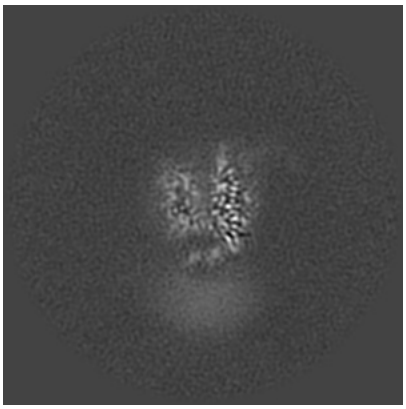


Z

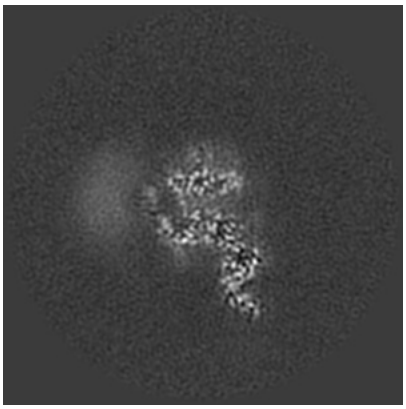
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

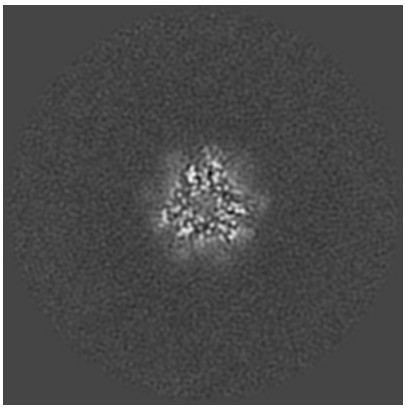
6.2.1 Primary map



X Index: 150

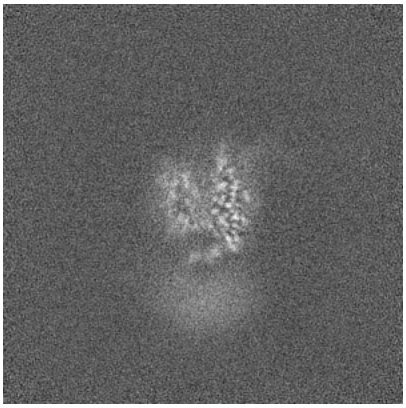


Y Index: 150

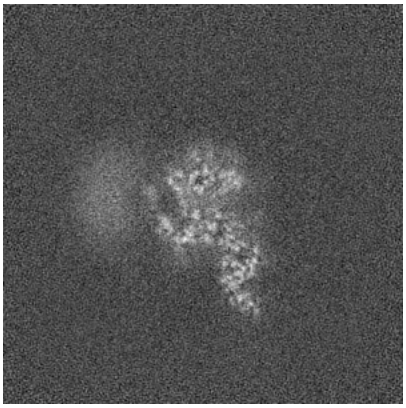


Z Index: 150

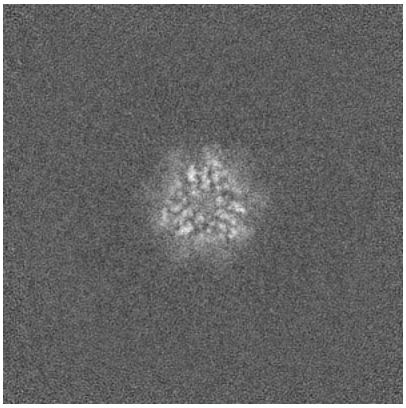
6.2.2 Raw map



X Index: 150



Y Index: 150

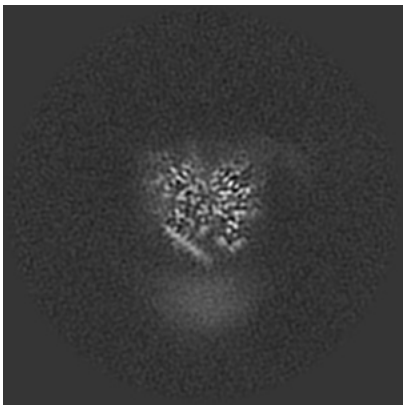


Z Index: 150

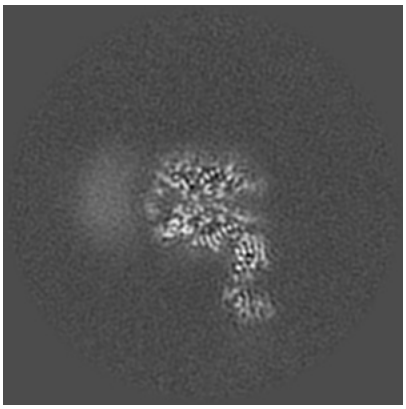
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

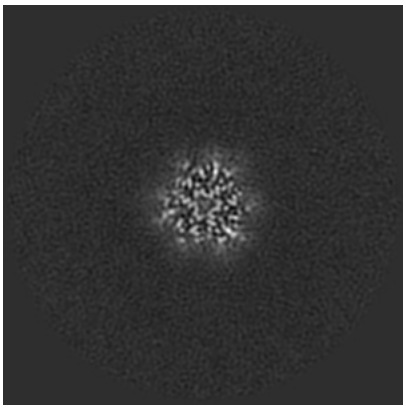
6.3.1 Primary map



X Index: 160

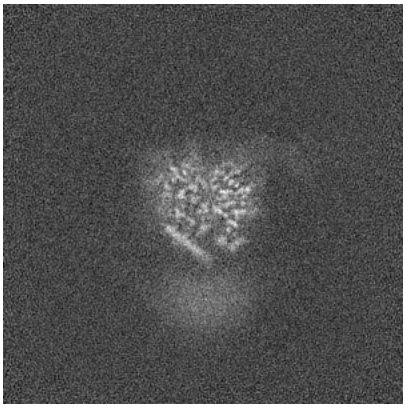


Y Index: 142

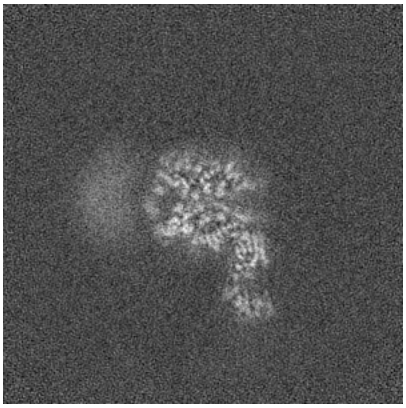


Z Index: 144

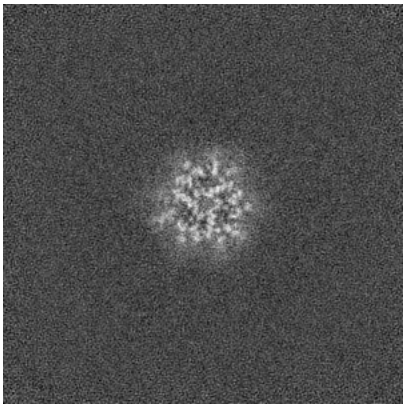
6.3.2 Raw map



X Index: 160



Y Index: 142

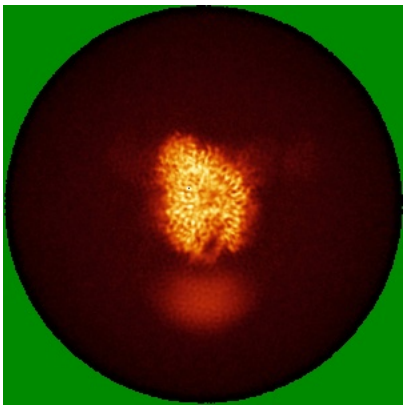


Z Index: 145

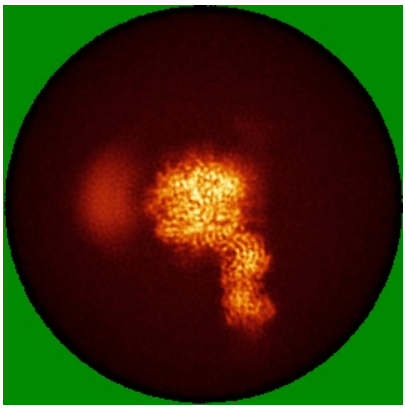
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

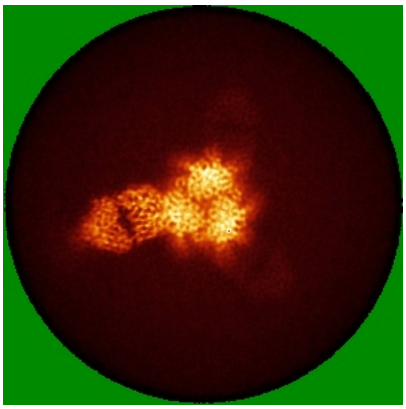
6.4.1 Primary map



X

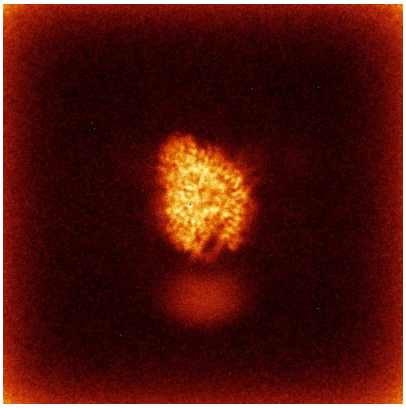


Y

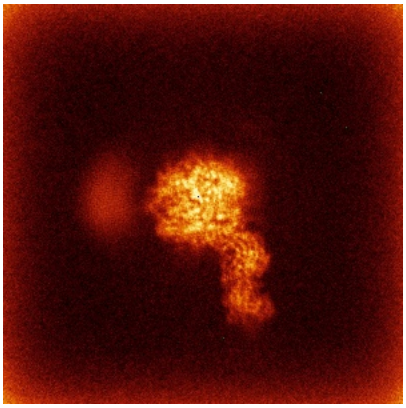


Z

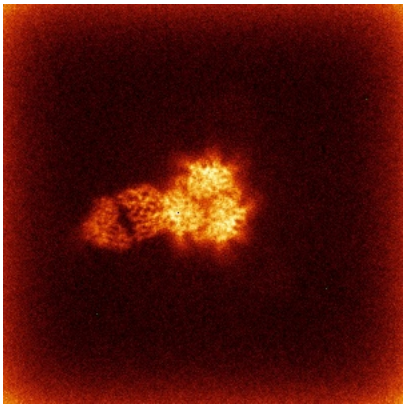
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

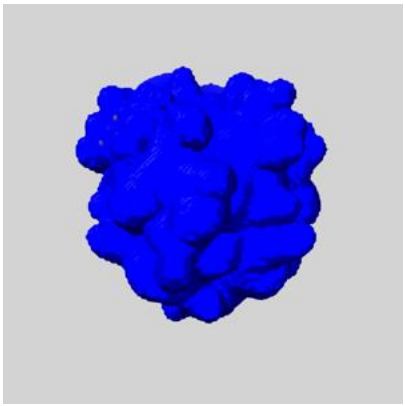
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

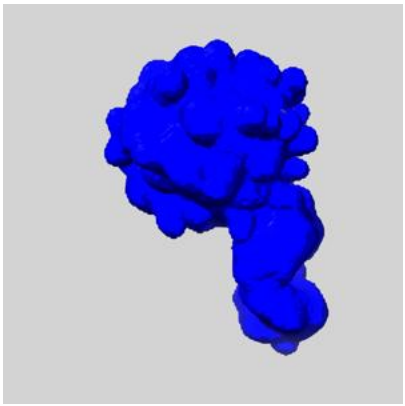
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

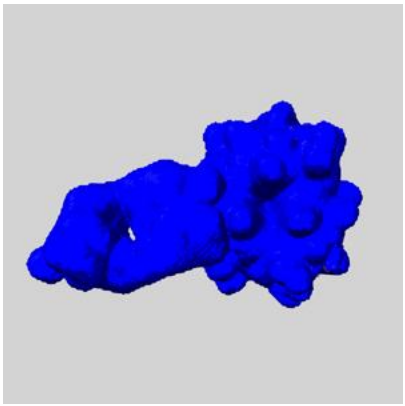
6.6.1 emd_28183_msk_1.map (i)



X



Y

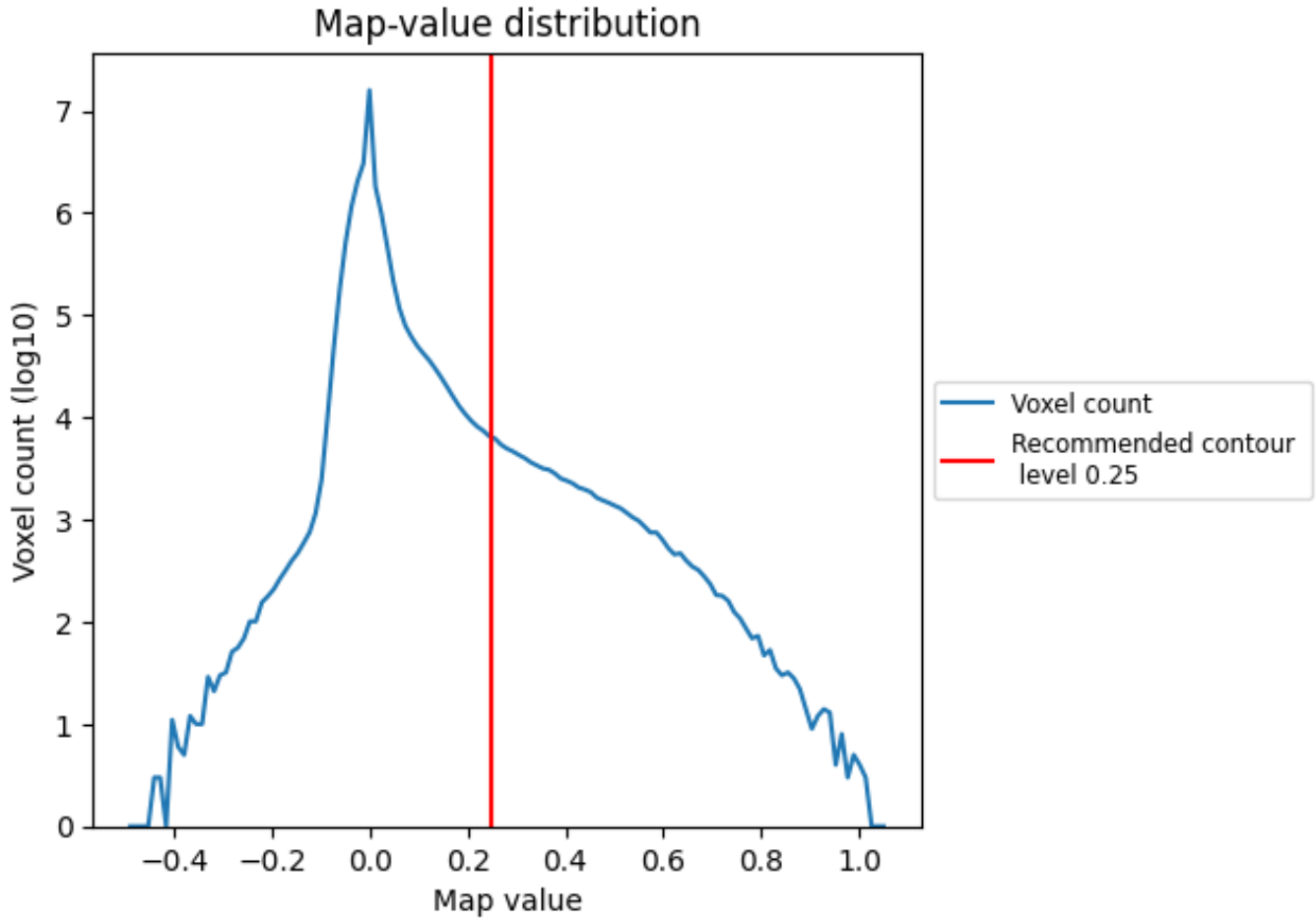


Z

7 Map analysis

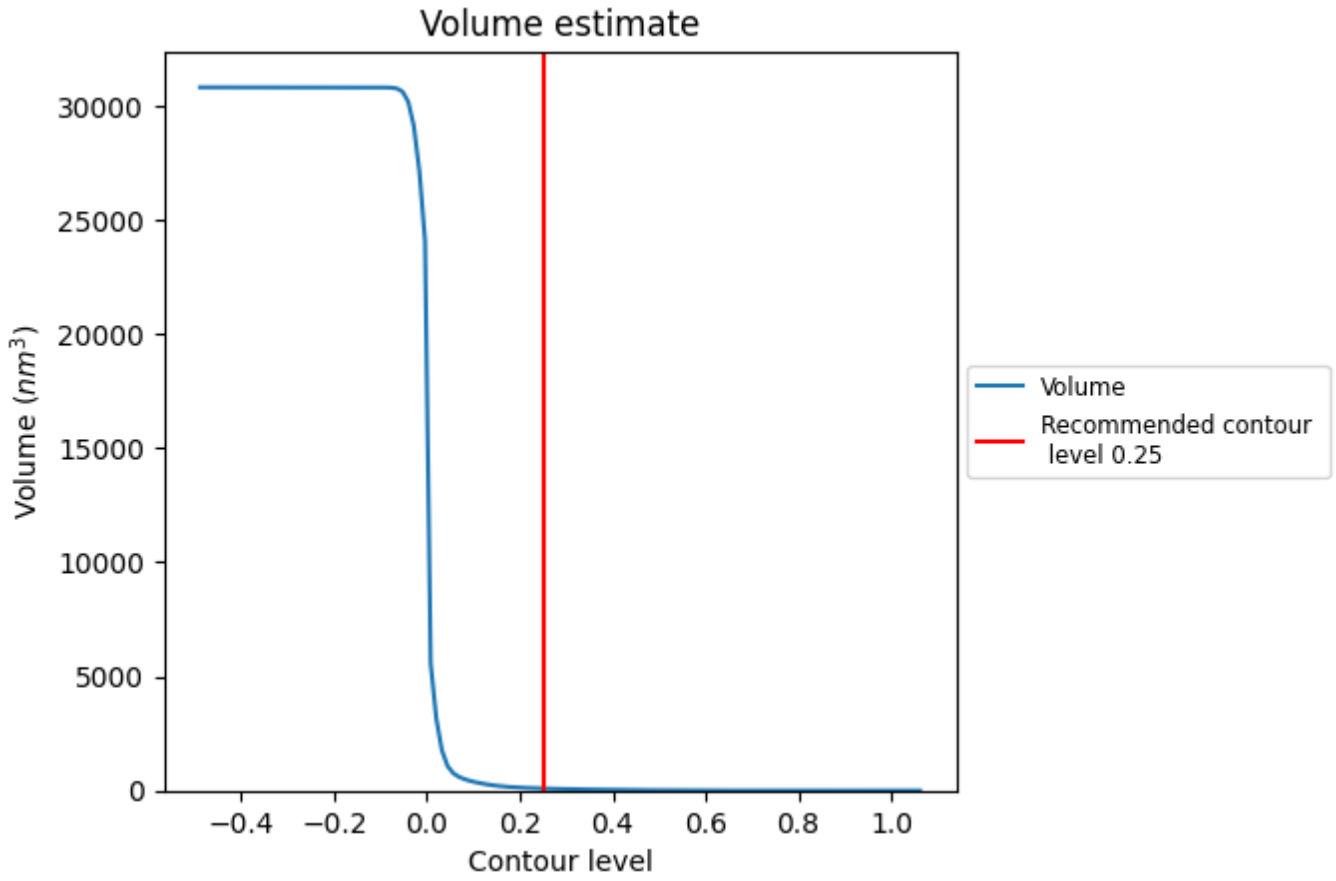
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

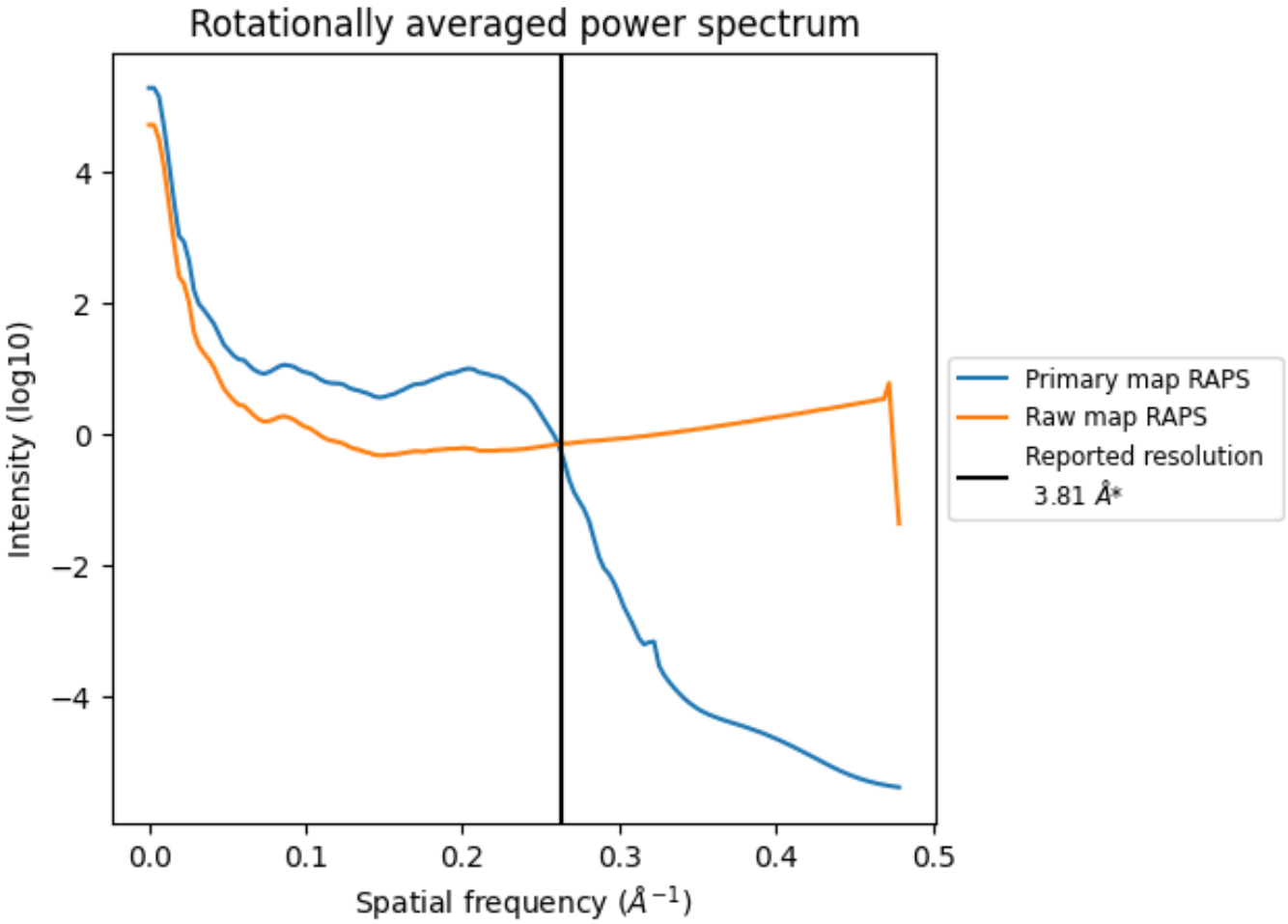
7.2 Volume estimate (i)



The volume at the recommended contour level is 91 nm^3; this corresponds to an approximate mass of 82 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

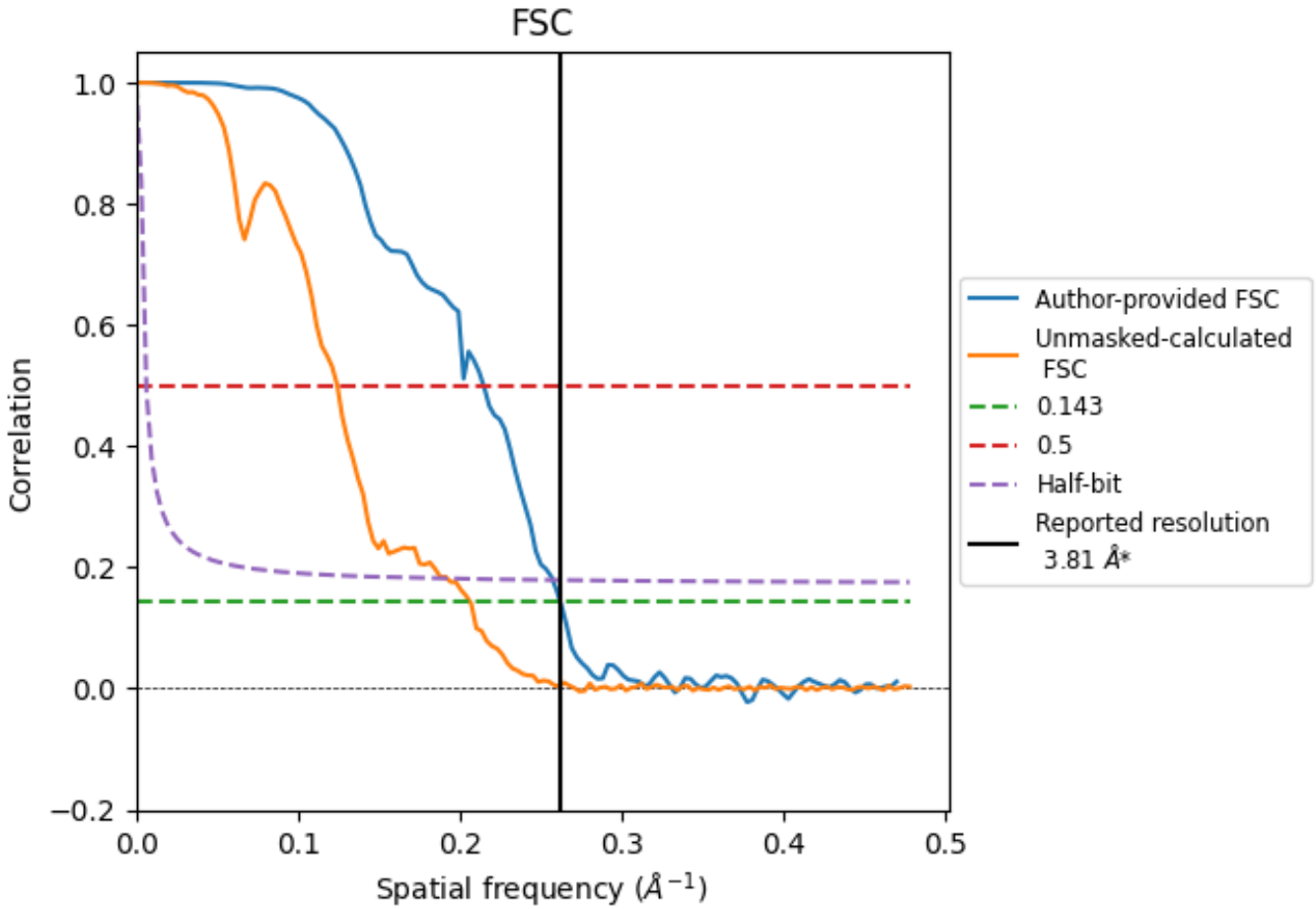


*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.81	-	-
Author-provided FSC curve	3.81	4.65	3.88
Unmasked-calculated*	4.84	8.03	5.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.84 differs from the reported value 3.81 by more than 10 %

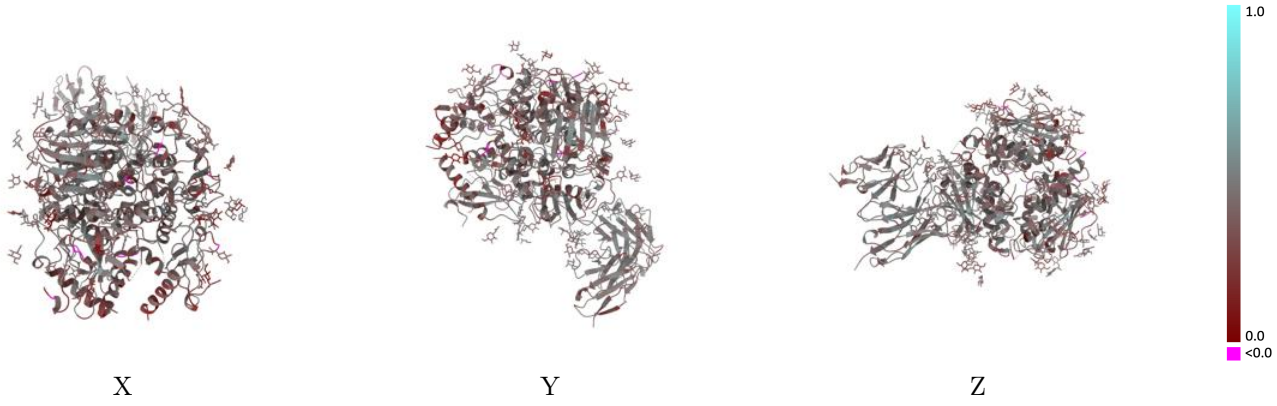
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28183 and PDB model 8EJI. Per-residue inclusion information can be found in section 3 on page 26.

9.1 Map-model overlay

This section was not generated.

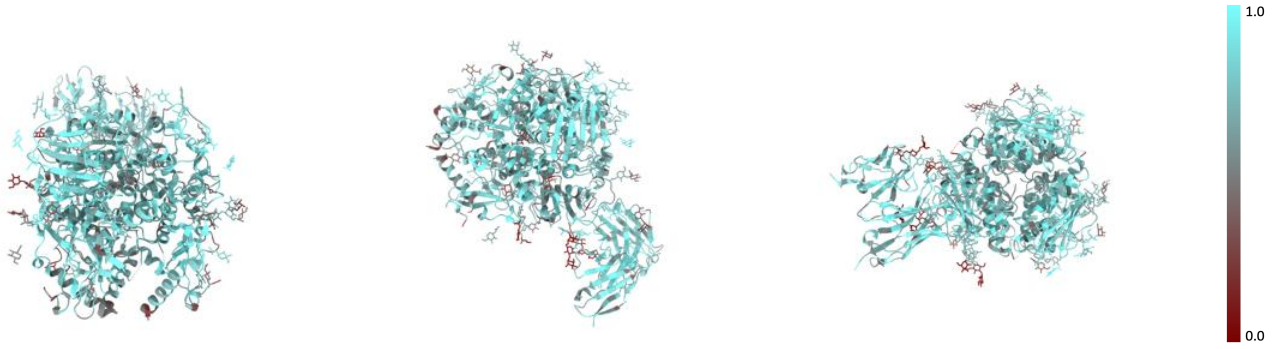
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

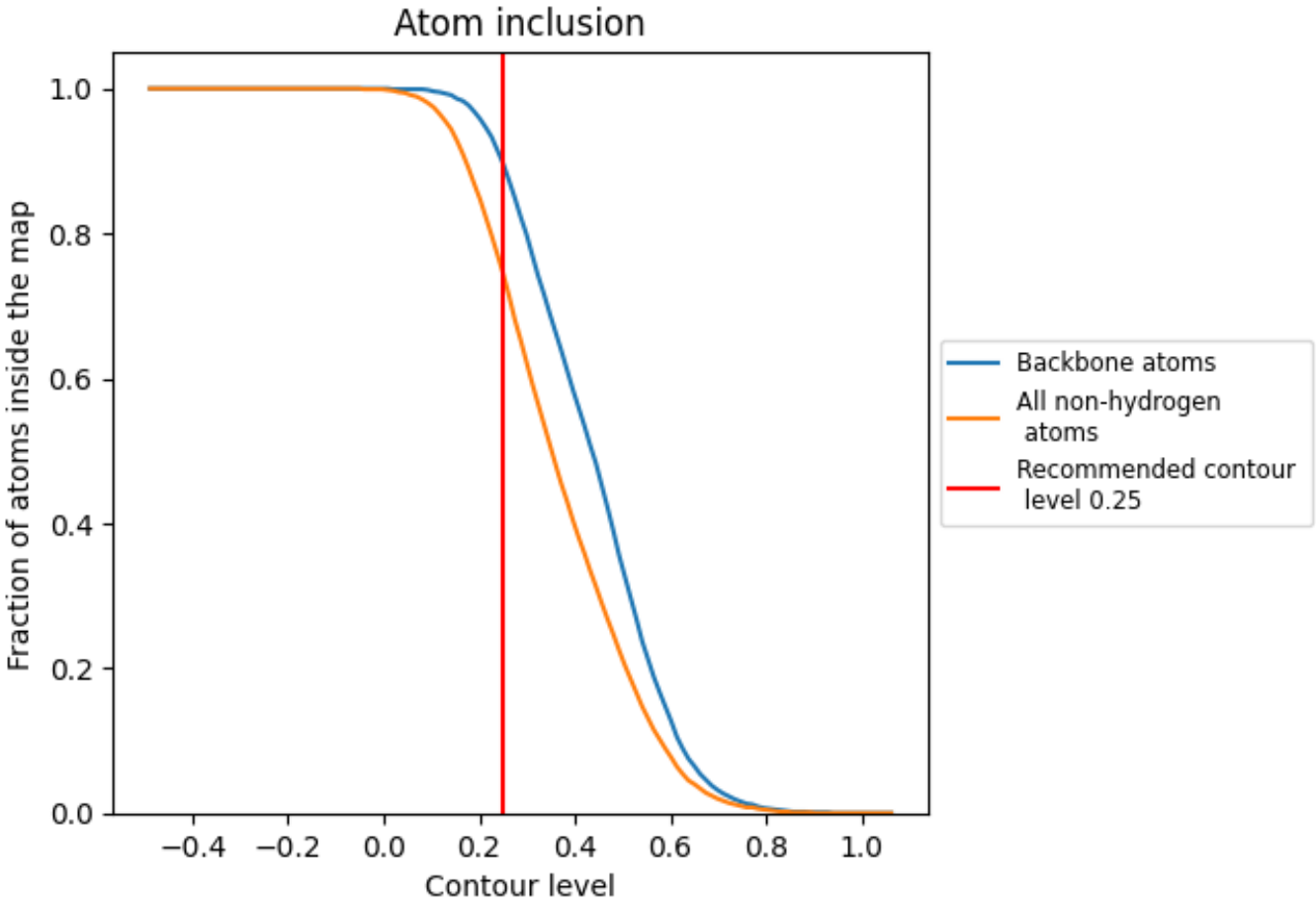
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.3900
A	0.7740	0.4130
B	0.7780	0.3860
C	0.7700	0.3800
D	0.7180	0.3960
E	0.2460	0.4130
F	0.3080	0.3490
G	0.4100	0.4200
H	0.8000	0.4410
I	0.5000	0.3320
J	0.6230	0.4290
K	0.4870	0.3610
L	0.7560	0.4220
M	0.5080	0.4100
N	0.4620	0.3420
O	0.6920	0.3940
P	0.7860	0.4600
Q	0.6430	0.3320
R	0.5830	0.2960
S	0.5000	0.2190
T	0.6150	0.3950
U	0.7500	0.3430
V	0.6070	0.2960
W	0.5280	0.2600
X	0.5360	0.1330
a	0.7240	0.3860
b	0.7480	0.3710
c	0.7480	0.3630

