Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:18 PM UTC

PDB ID	:	7YIW / pdb_00007yiw
Title	:	The Crystal Structure of Human Tissue Nonspecific Alkaline Phosphatase (ALPL) at Acidic pH
Authors	:	Yu, Y.T.; Yao, D.Q.; Zhang, Q.; Rao, B.; Xia, Y.; Lu, Y.; Qin, A.; Cao, Y.
Deposited on	:	2022-07-18
Resolution	:	2.89 Å(reported)

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

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

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

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

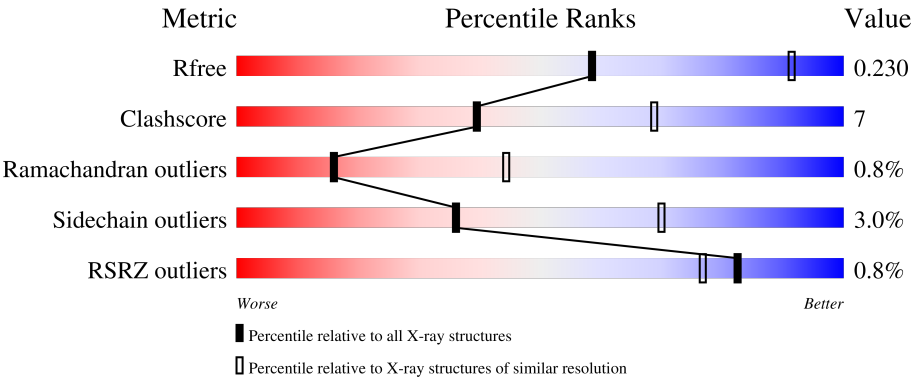
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	503	81% 15%
1	B	503	78% 17%
1	C	503	78% 17%
1	D	503	81% 14%
1	E	503	76% 19%

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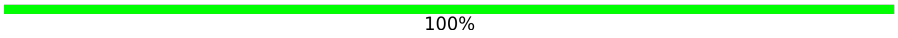
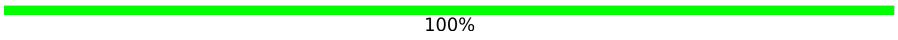
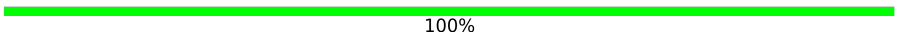
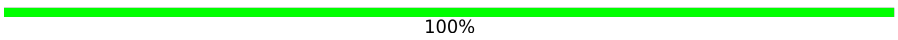
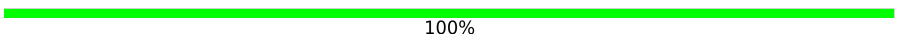
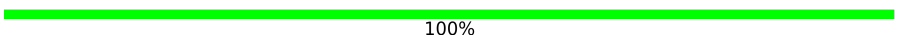
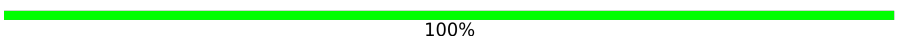
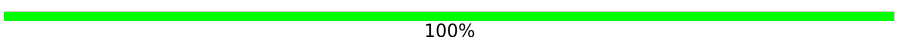
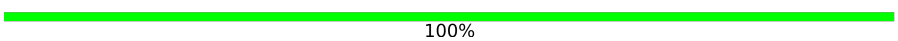
Mol	Chain	Length	Quality of chain
1	F	503	
1	G	503	
1	H	503	
2	1	2	
2	8	2	
2	BA	2	
2	IA	2	
2	K	2	
2	LA	2	
2	N	2	
2	SA	2	
2	U	2	
2	VA	2	
2	X	2	
2	e	2	
2	h	2	
2	o	2	
2	r	2	
2	y	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 30683 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alkaline phosphatase, tissue-nonspecific isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	D	482	Total	C	N	O	S	0	0	0
			3738	2339	663	717	19			
1	C	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	B	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	G	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	H	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			
1	F	483	Total	C	N	O	S	0	0	0
			3743	2342	664	718	19			
1	E	484	Total	C	N	O	S	0	0	0
			3748	2345	665	719	19			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P05186
A	0	LYS	-	expression tag	UNP P05186
A	1	THR	-	expression tag	UNP P05186
A	2	ILE	-	expression tag	UNP P05186
A	3	ILE	-	expression tag	UNP P05186
A	4	ALA	-	expression tag	UNP P05186
A	5	LEU	-	expression tag	UNP P05186
A	6	SER	-	expression tag	UNP P05186
A	7	TYR	-	expression tag	UNP P05186
A	8	ILE	-	expression tag	UNP P05186
A	9	PHE	-	expression tag	UNP P05186
A	10	CYS	-	expression tag	UNP P05186
A	11	LEU	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
A	12	VAL	-	expression tag	UNP P05186
A	13	PHE	-	expression tag	UNP P05186
A	14	ALA	-	expression tag	UNP P05186
A	15	GLY	-	expression tag	UNP P05186
A	16	ARG	-	expression tag	UNP P05186
A	17	ALA	-	expression tag	UNP P05186
A	501	ALA	-	expression tag	UNP P05186
D	-1	MET	-	initiating methionine	UNP P05186
D	0	LYS	-	expression tag	UNP P05186
D	1	THR	-	expression tag	UNP P05186
D	2	ILE	-	expression tag	UNP P05186
D	3	ILE	-	expression tag	UNP P05186
D	4	ALA	-	expression tag	UNP P05186
D	5	LEU	-	expression tag	UNP P05186
D	6	SER	-	expression tag	UNP P05186
D	7	TYR	-	expression tag	UNP P05186
D	8	ILE	-	expression tag	UNP P05186
D	9	PHE	-	expression tag	UNP P05186
D	10	CYS	-	expression tag	UNP P05186
D	11	LEU	-	expression tag	UNP P05186
D	12	VAL	-	expression tag	UNP P05186
D	13	PHE	-	expression tag	UNP P05186
D	14	ALA	-	expression tag	UNP P05186
D	15	GLY	-	expression tag	UNP P05186
D	16	ARG	-	expression tag	UNP P05186
D	17	ALA	-	expression tag	UNP P05186
D	501	ALA	-	expression tag	UNP P05186
C	-1	MET	-	initiating methionine	UNP P05186
C	0	LYS	-	expression tag	UNP P05186
C	1	THR	-	expression tag	UNP P05186
C	2	ILE	-	expression tag	UNP P05186
C	3	ILE	-	expression tag	UNP P05186
C	4	ALA	-	expression tag	UNP P05186
C	5	LEU	-	expression tag	UNP P05186
C	6	SER	-	expression tag	UNP P05186
C	7	TYR	-	expression tag	UNP P05186
C	8	ILE	-	expression tag	UNP P05186
C	9	PHE	-	expression tag	UNP P05186
C	10	CYS	-	expression tag	UNP P05186
C	11	LEU	-	expression tag	UNP P05186
C	12	VAL	-	expression tag	UNP P05186
C	13	PHE	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	ALA	-	expression tag	UNP P05186
C	15	GLY	-	expression tag	UNP P05186
C	16	ARG	-	expression tag	UNP P05186
C	17	ALA	-	expression tag	UNP P05186
C	501	ALA	-	expression tag	UNP P05186
B	-1	MET	-	initiating methionine	UNP P05186
B	0	LYS	-	expression tag	UNP P05186
B	1	THR	-	expression tag	UNP P05186
B	2	ILE	-	expression tag	UNP P05186
B	3	ILE	-	expression tag	UNP P05186
B	4	ALA	-	expression tag	UNP P05186
B	5	LEU	-	expression tag	UNP P05186
B	6	SER	-	expression tag	UNP P05186
B	7	TYR	-	expression tag	UNP P05186
B	8	ILE	-	expression tag	UNP P05186
B	9	PHE	-	expression tag	UNP P05186
B	10	CYS	-	expression tag	UNP P05186
B	11	LEU	-	expression tag	UNP P05186
B	12	VAL	-	expression tag	UNP P05186
B	13	PHE	-	expression tag	UNP P05186
B	14	ALA	-	expression tag	UNP P05186
B	15	GLY	-	expression tag	UNP P05186
B	16	ARG	-	expression tag	UNP P05186
B	17	ALA	-	expression tag	UNP P05186
B	501	ALA	-	expression tag	UNP P05186
G	-1	MET	-	initiating methionine	UNP P05186
G	0	LYS	-	expression tag	UNP P05186
G	1	THR	-	expression tag	UNP P05186
G	2	ILE	-	expression tag	UNP P05186
G	3	ILE	-	expression tag	UNP P05186
G	4	ALA	-	expression tag	UNP P05186
G	5	LEU	-	expression tag	UNP P05186
G	6	SER	-	expression tag	UNP P05186
G	7	TYR	-	expression tag	UNP P05186
G	8	ILE	-	expression tag	UNP P05186
G	9	PHE	-	expression tag	UNP P05186
G	10	CYS	-	expression tag	UNP P05186
G	11	LEU	-	expression tag	UNP P05186
G	12	VAL	-	expression tag	UNP P05186
G	13	PHE	-	expression tag	UNP P05186
G	14	ALA	-	expression tag	UNP P05186
G	15	GLY	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
G	16	ARG	-	expression tag	UNP P05186
G	17	ALA	-	expression tag	UNP P05186
G	501	ALA	-	expression tag	UNP P05186
H	-1	MET	-	initiating methionine	UNP P05186
H	0	LYS	-	expression tag	UNP P05186
H	1	THR	-	expression tag	UNP P05186
H	2	ILE	-	expression tag	UNP P05186
H	3	ILE	-	expression tag	UNP P05186
H	4	ALA	-	expression tag	UNP P05186
H	5	LEU	-	expression tag	UNP P05186
H	6	SER	-	expression tag	UNP P05186
H	7	TYR	-	expression tag	UNP P05186
H	8	ILE	-	expression tag	UNP P05186
H	9	PHE	-	expression tag	UNP P05186
H	10	CYS	-	expression tag	UNP P05186
H	11	LEU	-	expression tag	UNP P05186
H	12	VAL	-	expression tag	UNP P05186
H	13	PHE	-	expression tag	UNP P05186
H	14	ALA	-	expression tag	UNP P05186
H	15	GLY	-	expression tag	UNP P05186
H	16	ARG	-	expression tag	UNP P05186
H	17	ALA	-	expression tag	UNP P05186
H	501	ALA	-	expression tag	UNP P05186
F	-1	MET	-	initiating methionine	UNP P05186
F	0	LYS	-	expression tag	UNP P05186
F	1	THR	-	expression tag	UNP P05186
F	2	ILE	-	expression tag	UNP P05186
F	3	ILE	-	expression tag	UNP P05186
F	4	ALA	-	expression tag	UNP P05186
F	5	LEU	-	expression tag	UNP P05186
F	6	SER	-	expression tag	UNP P05186
F	7	TYR	-	expression tag	UNP P05186
F	8	ILE	-	expression tag	UNP P05186
F	9	PHE	-	expression tag	UNP P05186
F	10	CYS	-	expression tag	UNP P05186
F	11	LEU	-	expression tag	UNP P05186
F	12	VAL	-	expression tag	UNP P05186
F	13	PHE	-	expression tag	UNP P05186
F	14	ALA	-	expression tag	UNP P05186
F	15	GLY	-	expression tag	UNP P05186
F	16	ARG	-	expression tag	UNP P05186
F	17	ALA	-	expression tag	UNP P05186

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Chain	Residue	Modelled	Actual	Comment	Reference
F	501	ALA	-	expression tag	UNP P05186
E	-1	MET	-	initiating methionine	UNP P05186
E	0	LYS	-	expression tag	UNP P05186
E	1	THR	-	expression tag	UNP P05186
E	2	ILE	-	expression tag	UNP P05186
E	3	ILE	-	expression tag	UNP P05186
E	4	ALA	-	expression tag	UNP P05186
E	5	LEU	-	expression tag	UNP P05186
E	6	SER	-	expression tag	UNP P05186
E	7	TYR	-	expression tag	UNP P05186
E	8	ILE	-	expression tag	UNP P05186
E	9	PHE	-	expression tag	UNP P05186
E	10	CYS	-	expression tag	UNP P05186
E	11	LEU	-	expression tag	UNP P05186
E	12	VAL	-	expression tag	UNP P05186
E	13	PHE	-	expression tag	UNP P05186
E	14	ALA	-	expression tag	UNP P05186
E	15	GLY	-	expression tag	UNP P05186
E	16	ARG	-	expression tag	UNP P05186
E	17	ALA	-	expression tag	UNP P05186
E	501	ALA	-	expression tag	UNP P05186

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	U	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	X	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	h	2	Total	C	N	O	0	0	0
			28	16	2	10			

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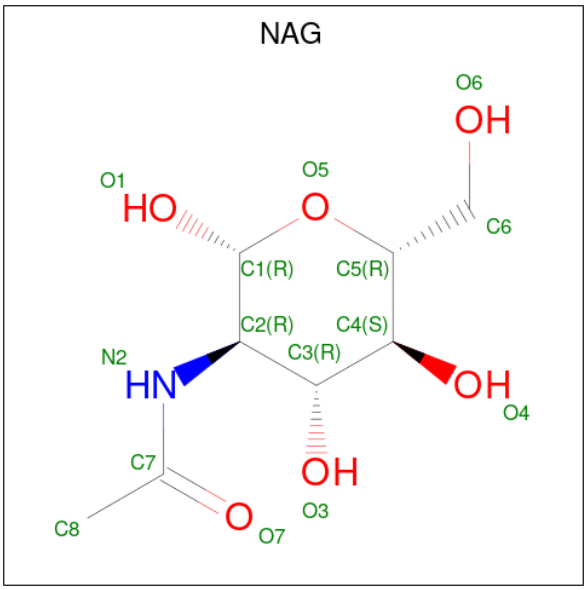
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	o	2	Total C N O 28 16 2 10	0	0	0
2	r	2	Total C N O 28 16 2 10	0	0	0
2	y	2	Total C N O 28 16 2 10	0	0	0
2	1	2	Total C N O 28 16 2 10	0	0	0
2	8	2	Total C N O 28 16 2 10	0	0	0
2	BA	2	Total C N O 28 16 2 10	0	0	0
2	IA	2	Total C N O 28 16 2 10	0	0	0
2	LA	2	Total C N O 28 16 2 10	0	0	0
2	SA	2	Total C N O 28 16 2 10	0	0	0
2	VA	2	Total C N O 28 16 2 10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	G	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	H	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	H	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Zn 2 2	0	0
5	D	2	Total Zn 2 2	0	0
5	C	2	Total Zn 2 2	0	0
5	B	2	Total Zn 2 2	0	0
5	G	2	Total Zn 2 2	0	0
5	H	2	Total Zn 2 2	0	0
5	F	2	Total Zn 2 2	0	0
5	E	2	Total Zn 2 2	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	D	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0
6	B	1	Total Ca 1 1	0	0
6	G	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Ca 1 1	0	0
6	F	1	Total Ca 1 1	0	0
6	E	1	Total Ca 1 1	0	0

- Molecule 7 is water.

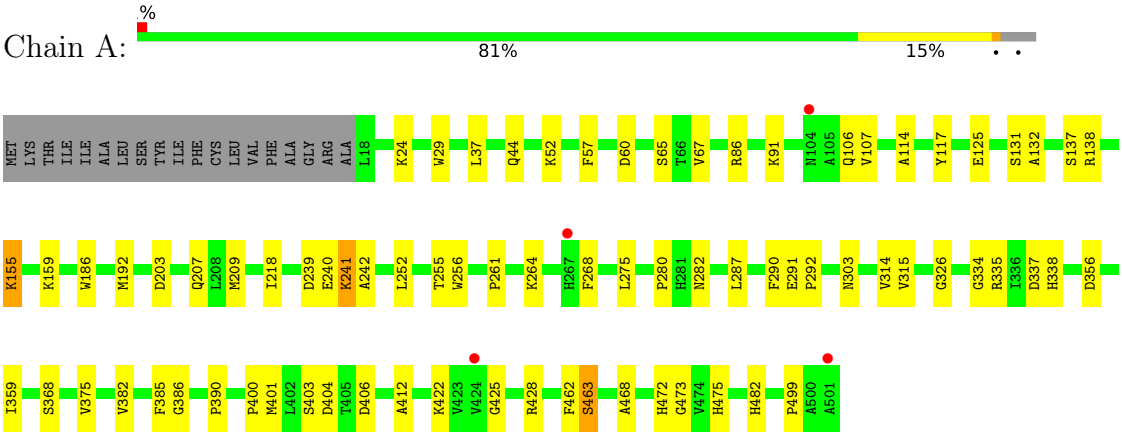
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total O 2 2	0	0
7	B	4	Total O 4 4	0	0
7	G	2	Total O 2 2	0	0
7	H	1	Total O 1 1	0	0
7	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

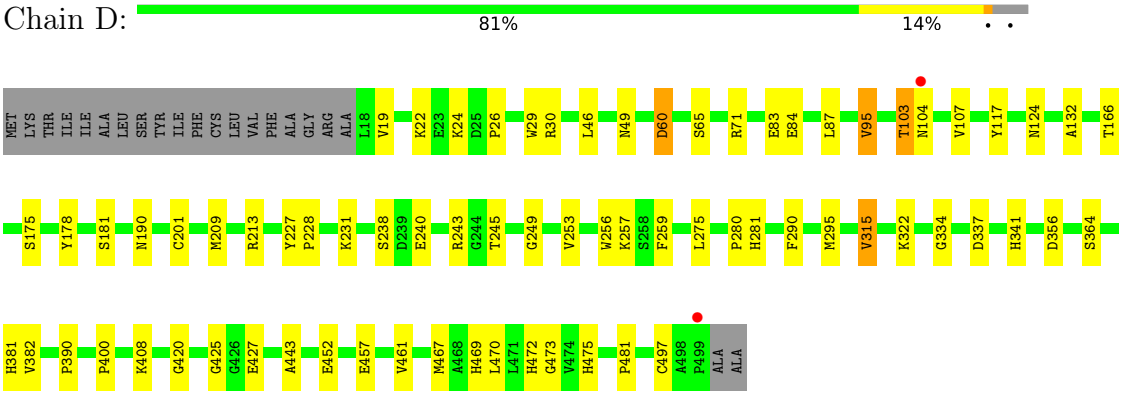
• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain A:



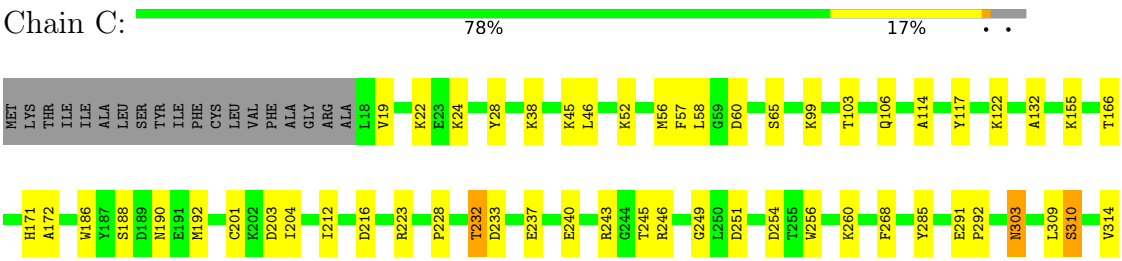
• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

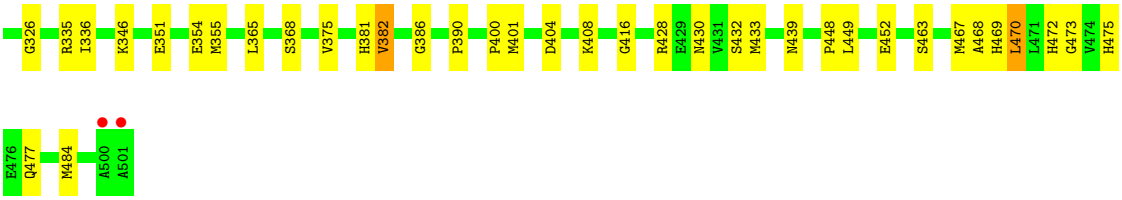
Chain D:



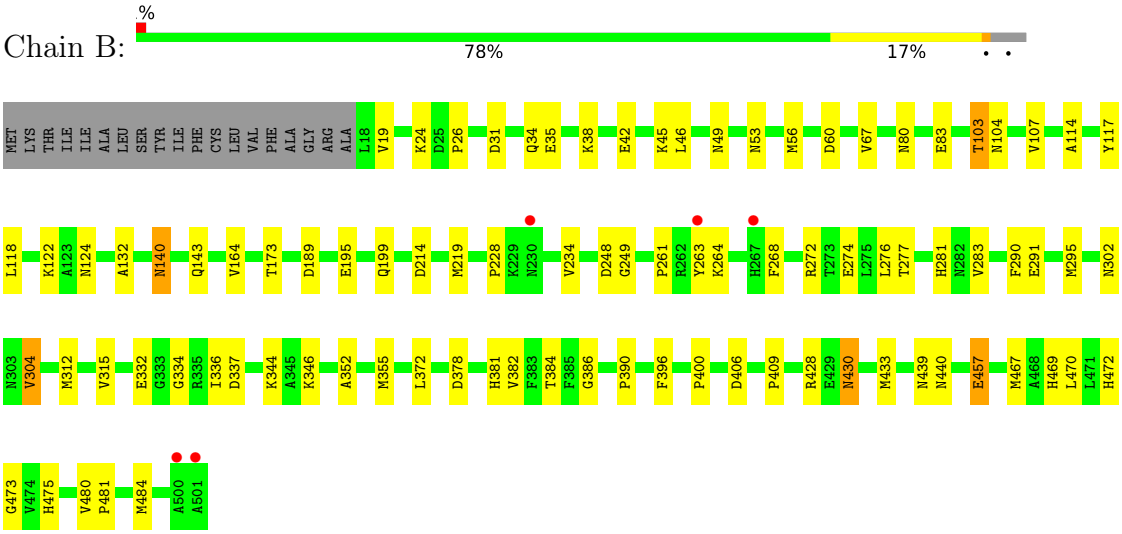
• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

Chain C:

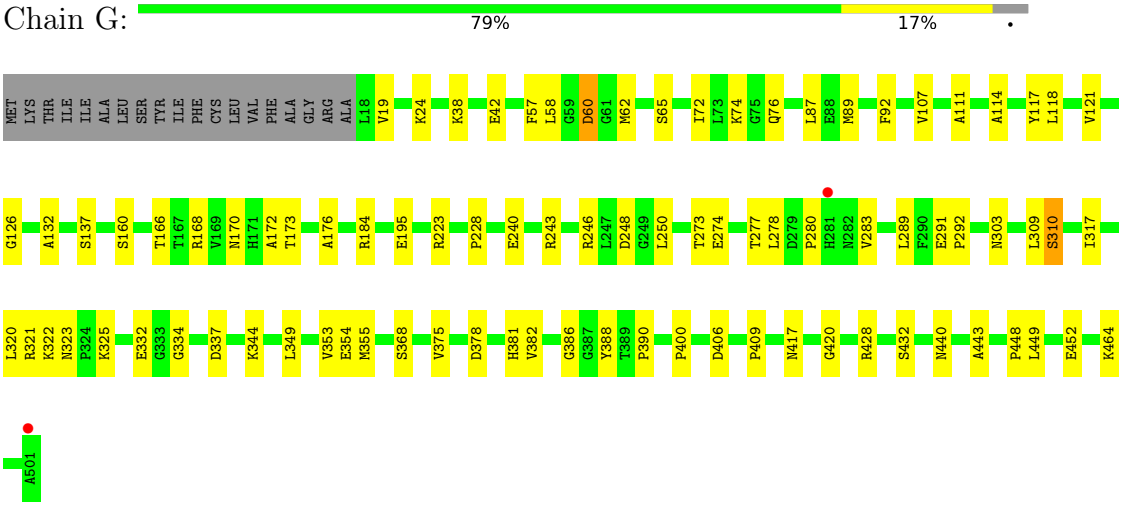




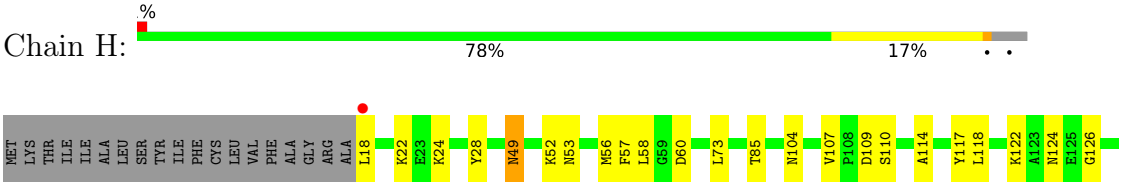
• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

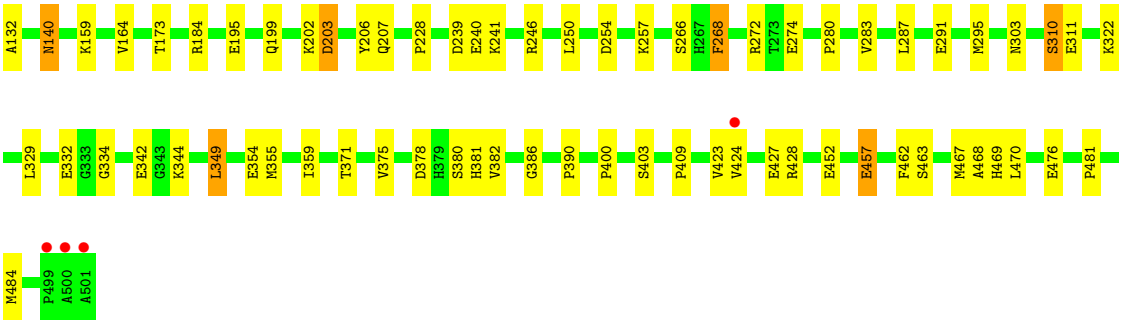


• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

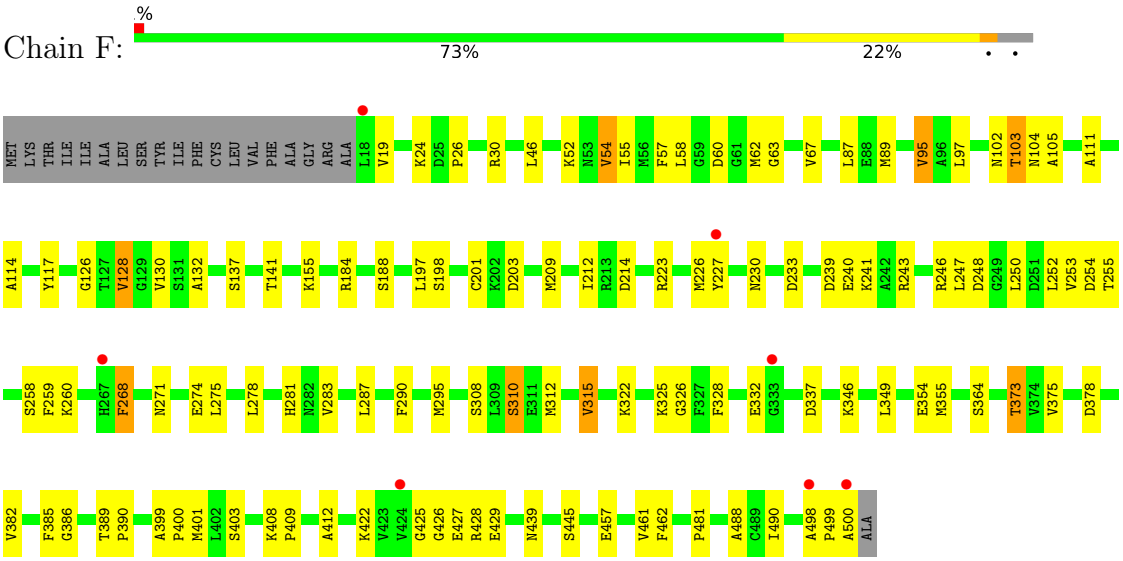


• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

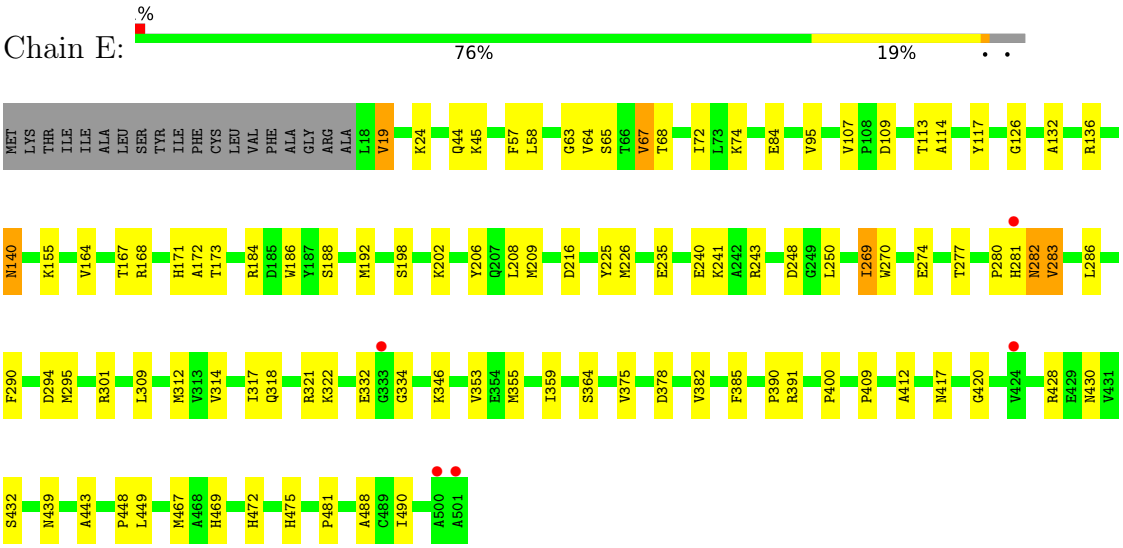




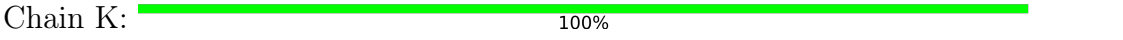
• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme



• Molecule 1: Alkaline phosphatase, tissue-nonspecific isozyme

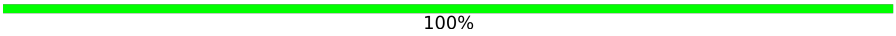


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



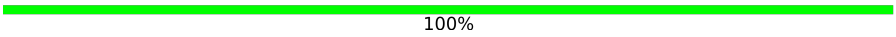
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain U:

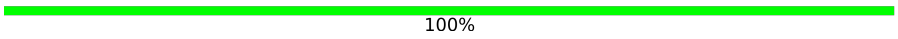


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

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

Chain e:



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

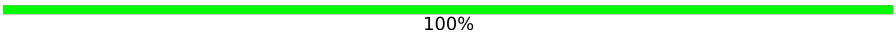
Chain h:

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

Chain o:

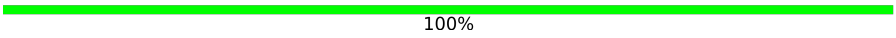
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



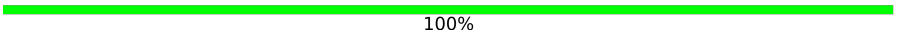
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y:



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

Chain 1:

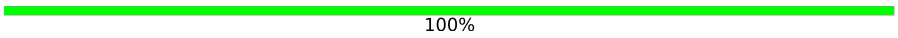


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8:

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

Chain BA:



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

Chain IA:

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

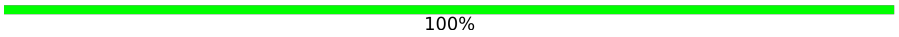
Chain LA:

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

Chain SA:

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

Chain VA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	159.36Å 166.53Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.96 – 2.89 48.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.96-2.89) 99.8 (48.96-2.89)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.201 , 0.230 0.201 , 0.230	Depositor DCC
R_{free} test set	2003 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	47.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30683	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, MG, 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	0.10	0/3834	0.32	0/5201
1	B	0.10	0/3834	0.32	0/5201
1	C	0.11	0/3834	0.31	0/5201
1	D	0.10	0/3824	0.33	0/5187
1	E	0.12	0/3834	0.33	0/5201
1	F	0.13	0/3829	0.34	0/5194
1	G	0.10	0/3834	0.31	0/5201
1	H	0.12	0/3834	0.32	0/5201
All	All	0.11	0/30657	0.32	0/41587

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3748	0	3628	41	0
1	B	3748	0	3629	61	0
1	C	3748	0	3629	53	0
1	D	3738	0	3619	43	0
1	E	3748	0	3628	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3743	0	3624	71	0
1	G	3748	0	3629	51	0
1	H	3748	0	3629	53	0
2	1	28	0	25	0	0
2	8	28	0	25	1	0
2	BA	28	0	25	0	0
2	IA	28	0	25	2	0
2	K	28	0	25	0	0
2	LA	28	0	25	1	0
2	N	28	0	25	0	0
2	SA	28	0	25	1	0
2	U	28	0	25	0	0
2	VA	28	0	25	0	0
2	X	28	0	25	1	0
2	e	28	0	25	0	0
2	h	28	0	25	1	0
2	o	28	0	25	1	0
2	r	28	0	25	0	0
2	y	28	0	25	0	0
3	A	28	0	26	0	0
3	B	28	0	26	1	0
3	C	28	0	26	1	0
3	D	28	0	26	0	0
3	E	28	0	26	2	0
3	F	28	0	26	1	0
3	G	28	0	26	1	0
3	H	28	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0
5	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	B	4	0	0	0	0
7	D	2	0	0	0	0
7	F	1	0	0	0	0
7	G	2	0	0	0	0
7	H	1	0	0	0	0
All	All	30683	0	29623	403	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 7.

All (403) 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:F:239:ASP:OD1	1:F:241:LYS:HD2	1.68	0.94
1:F:246:ARG:HH11	1:F:252:LEU:HD11	1.38	0.88
1:E:109:ASP:OD2	1:E:184:ARG:NH1	2.10	0.83
1:C:390:PRO:HD3	1:C:400:PRO:HG3	1.60	0.82
1:F:268:PHE:HD1	1:F:287:LEU:HD12	1.48	0.78
1:F:132:ALA:HB3	1:E:24:LYS:HA	1.67	0.77
1:G:107:VAL:HG21	1:H:386:GLY:HA2	1.69	0.75
1:A:472:HIS:H	1:A:475:HIS:HE1	1.36	0.74
1:F:386:GLY:HA2	1:E:107:VAL:HG21	1.70	0.74
1:G:240:GLU:HG2	1:G:243:ARG:HE	1.53	0.73
1:D:275:LEU:HD11	1:D:315:VAL:HG21	1.69	0.73
1:B:390:PRO:HD3	1:B:400:PRO:HG3	1.70	0.73
1:G:132:ALA:HB3	1:H:24:LYS:HA	1.69	0.73
1:E:390:PRO:HD3	1:E:400:PRO:HG3	1.71	0.73
1:C:463:SER:HB3	1:C:468:ALA:HB1	1.69	0.73
1:G:390:PRO:HD3	1:G:400:PRO:HG3	1.72	0.71
1:H:240:GLU:OE1	1:H:240:GLU:N	2.24	0.70
1:D:24:LYS:HA	1:C:132:ALA:HB3	1.72	0.70
1:G:60:ASP:HB3	1:G:337:ASP:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLY:HA2	1:B:107:VAL:HG21	1.74	0.69
1:E:281:HIS:HA	1:E:322:LYS:HE2	1.74	0.69
1:F:57:PHE:HB2	1:F:375:VAL:HG22	1.74	0.68
1:G:24:LYS:HA	1:H:132:ALA:HB3	1.74	0.68
1:C:473:GLY:H	1:C:475:HIS:CE1	2.11	0.68
1:B:473:GLY:H	1:B:475:HIS:CE1	2.12	0.67
1:D:473:GLY:H	1:D:475:HIS:CE1	2.13	0.66
1:A:107:VAL:HG21	1:B:386:GLY:HA2	1.78	0.66
1:F:87:LEU:HD13	1:F:89:MET:HE3	1.78	0.65
1:C:56:MET:HE2	1:C:484:MET:HE1	1.78	0.65
1:B:56:MET:HE3	1:B:484:MET:HE1	1.78	0.65
1:E:248:ASP:HB3	1:E:250:LEU:HG	1.78	0.65
1:C:346:LYS:HD3	1:C:439:ASN:HA	1.77	0.65
1:B:346:LYS:HD3	1:B:439:ASN:HA	1.78	0.65
1:G:448:PRO:O	1:H:403:SER:OG	2.15	0.65
1:H:467:MET:HE3	1:H:470:LEU:HD11	1.79	0.64
1:E:283:VAL:O	1:E:322:LYS:NZ	2.31	0.64
1:D:467:MET:HE3	1:D:470:LEU:HD11	1.81	0.63
1:D:390:PRO:HD3	1:D:400:PRO:HG3	1.80	0.63
1:C:408:LYS:NZ	1:C:428:ARG:O	2.31	0.63
1:G:283:VAL:O	1:G:322:LYS:NZ	2.31	0.62
1:G:246:ARG:NH2	1:G:248:ASP:OD2	2.32	0.62
1:F:390:PRO:HD3	1:F:400:PRO:HG3	1.80	0.62
1:C:430:ASN:HB3	1:C:433:MET:HE2	1.80	0.62
1:F:102:ASN:HB2	1:F:105:ALA:HB3	1.81	0.62
1:H:110:SER:HB2	1:H:184:ARG:HH12	1.65	0.61
1:F:403:SER:OG	1:E:448:PRO:O	2.18	0.61
1:A:24:LYS:HA	1:B:132:ALA:HB3	1.82	0.61
1:F:57:PHE:HB3	1:F:355:MET:HE3	1.82	0.61
1:D:472:HIS:H	1:D:475:HIS:HE1	1.47	0.61
1:B:290:PHE:HB2	1:B:295:MET:HE3	1.81	0.61
1:H:310:SER:OG	1:H:354:GLU:OE2	2.19	0.61
1:F:310:SER:OG	1:F:354:GLU:OE2	2.19	0.61
1:D:60:ASP:HB2	1:D:334:GLY:HA2	1.82	0.61
1:F:346:LYS:HD3	1:F:439:ASN:HA	1.83	0.61
1:C:408:LYS:HG2	2:h:1:NAG:H82	1.84	0.60
1:H:390:PRO:HD3	1:H:400:PRO:HG3	1.83	0.60
1:D:83:GLU:OE2	1:C:106:GLN:HB2	2.02	0.60
1:H:56:MET:HB2	1:H:484:MET:HE1	1.83	0.60
1:F:226:MET:HA	1:F:252:LEU:HD12	1.84	0.60
1:F:278:LEU:HD13	1:F:283:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:HIS:HD2	1:B:34:GLN:HE21	1.50	0.59
1:H:274:GLU:OE2	2:8:1:NAG:H62	2.03	0.59
1:C:228:PRO:HB3	1:C:249:GLY:HA2	1.85	0.59
1:G:248:ASP:HB3	1:G:250:LEU:H	1.67	0.59
1:A:473:GLY:H	1:A:475:HIS:CE1	2.21	0.59
1:H:375:VAL:HB	1:H:462:PHE:HB2	1.84	0.59
1:A:261:PRO:HB2	1:A:264:LYS:HG3	1.85	0.59
1:G:386:GLY:HA2	1:H:107:VAL:HG21	1.85	0.59
1:F:248:ASP:HB3	1:F:250:LEU:HD13	1.83	0.59
1:H:380:SER:OG	1:H:381:HIS:N	2.36	0.58
1:F:274:GLU:OE2	2:IA:1:NAG:H62	2.03	0.58
1:A:132:ALA:HB3	1:B:24:LYS:HA	1.86	0.58
1:F:55:ILE:HB	1:F:373:THR:HG23	1.85	0.58
1:F:268:PHE:CD1	1:F:287:LEU:HD12	2.34	0.58
1:F:408:LYS:HG2	2:LA:1:NAG:H82	1.87	0.57
1:A:106:GLN:HB2	1:B:83:GLU:OE2	2.05	0.57
1:H:140:ASN:N	1:H:140:ASN:OD1	2.37	0.57
1:F:255:THR:HG22	1:F:259:PHE:CE1	2.39	0.57
1:F:290:PHE:HB2	1:F:295:MET:HE3	1.86	0.57
1:G:332:GLU:OE2	1:G:334:GLY:HA2	2.04	0.56
1:E:274:GLU:OE2	2:SA:1:NAG:H62	2.05	0.56
1:A:406:ASP:OD2	1:A:428:ARG:HD3	2.05	0.56
1:F:126:GLY:HA2	1:F:184:ARG:HG2	1.88	0.56
1:C:240:GLU:HA	1:C:243:ARG:HG3	1.87	0.56
1:C:251:ASP:OD2	1:C:254:ASP:HB2	2.05	0.56
1:C:467:MET:HB3	1:C:470:LEU:HD22	1.87	0.56
1:E:409:PRO:O	1:E:428:ARG:NH2	2.38	0.56
1:E:346:LYS:HD3	1:E:439:ASN:HA	1.88	0.56
1:D:22:LYS:NZ	1:B:80:ASN:OD1	2.36	0.55
1:F:97:LEU:HG	1:E:95:VAL:HG11	1.89	0.55
1:F:46:LEU:HD13	1:E:44:GLN:HG2	1.89	0.55
1:A:57:PHE:HB2	1:A:375:VAL:HG22	1.88	0.55
1:H:104:ASN:HB2	1:H:124:ASN:HA	1.89	0.55
1:F:214:ASP:OD1	1:F:214:ASP:N	2.38	0.55
1:F:223:ARG:NH1	1:F:233:ASP:OD2	2.33	0.55
1:B:291:GLU:HG3	1:B:295:MET:HA	1.87	0.55
1:G:310:SER:OG	1:G:354:GLU:OE2	2.25	0.54
1:A:218:ILE:HB	1:A:287:LEU:HD12	1.90	0.54
1:H:122:LYS:NZ	1:H:476:GLU:OE1	2.36	0.54
1:A:356:ASP:HA	1:A:359:ILE:HD12	1.90	0.54
1:C:57:PHE:HB2	1:C:375:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:409:PRO:O	1:H:428:ARG:NH2	2.41	0.54
1:B:481:PRO:HA	1:B:484:MET:HE3	1.89	0.54
1:C:223:ARG:NH1	1:C:233:ASP:OD2	2.42	0.53
1:A:209:MET:SD	1:A:256:TRP:HB2	2.48	0.53
1:A:60:ASP:HB2	1:A:334:GLY:HA2	1.90	0.53
1:B:140:ASN:OD1	1:B:140:ASN:N	2.37	0.53
1:A:65:SER:HA	1:B:457:GLU:HB3	1.90	0.53
1:E:84:GLU:OE1	1:E:391:ARG:NH2	2.33	0.53
1:F:155:LYS:NZ	1:F:214:ASP:O	2.38	0.53
1:E:208:LEU:HD23	1:E:226:MET:HE1	1.89	0.52
1:H:240:GLU:H	1:H:240:GLU:CD	2.15	0.52
1:F:24:LYS:HA	1:E:132:ALA:HB3	1.90	0.52
1:G:65:SER:HA	1:H:457:GLU:HB3	1.91	0.52
1:G:349:LEU:O	1:G:353:VAL:HG23	2.09	0.52
1:E:117:TYR:HE2	1:E:378:ASP:HB3	1.74	0.52
1:E:202:LYS:HD3	1:E:206:TYR:CE1	2.45	0.52
1:G:118:LEU:HD12	1:G:176:ALA:HB3	1.91	0.52
1:D:104:ASN:HB2	1:D:124:ASN:HA	1.92	0.52
1:F:254:ASP:O	1:F:258:SER:OG	2.27	0.52
1:F:275:LEU:HD11	1:F:315:VAL:HG21	1.91	0.52
1:F:378:ASP:OD1	1:F:378:ASP:N	2.41	0.52
1:D:427:GLU:HA	1:D:427:GLU:OE1	2.11	0.51
1:C:314:VAL:HG13	1:C:365:LEU:HD11	1.93	0.51
1:H:60:ASP:HB2	1:H:334:GLY:HA2	1.92	0.51
1:F:54:VAL:HG12	1:F:328:PHE:HD2	1.76	0.51
1:F:209:MET:HG3	1:F:252:LEU:HB3	1.92	0.51
1:D:337:ASP:OD1	1:D:381:HIS:NE2	2.40	0.51
1:B:173:THR:HG21	1:B:332:GLU:HG3	1.92	0.51
1:G:228:PRO:HA	1:G:246:ARG:HB2	1.92	0.51
1:H:53:ASN:HB2	1:H:371:THR:HG23	1.92	0.51
1:F:60:ASP:OD2	1:F:332:GLU:OE2	2.27	0.51
1:A:114:ALA:HA	1:A:117:TYR:CZ	2.46	0.51
1:H:202:LYS:HD3	1:H:206:TYR:CE1	2.46	0.51
1:E:317:ILE:O	1:E:321:ARG:HG3	2.11	0.51
1:D:49:ASN:OD1	1:B:281:HIS:NE2	2.43	0.51
1:B:60:ASP:HB2	1:B:334:GLY:HA2	1.92	0.51
1:H:342:GLU:HB3	1:H:344:LYS:HE3	1.93	0.51
1:G:57:PHE:HB2	1:G:375:VAL:HG22	1.93	0.51
1:D:46:LEU:HB3	1:D:469:HIS:CE1	2.46	0.51
1:D:87:LEU:HB3	1:D:356:ASP:OD2	2.11	0.50
1:C:473:GLY:H	1:C:475:HIS:HE1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:THR:HG22	1:F:259:PHE:HE1	1.76	0.50
1:A:155:LYS:NZ	1:A:159:LYS:O	2.44	0.50
1:D:281:HIS:NE2	1:B:49:ASN:OD1	2.34	0.50
1:C:166:THR:HG23	1:C:309:LEU:HD13	1.92	0.50
1:B:346:LYS:HG3	1:B:396:PHE:CZ	2.46	0.50
1:B:195:GLU:O	1:B:199:GLN:HG3	2.12	0.50
1:H:173:THR:HG21	1:H:332:GLU:HG3	1.93	0.50
1:C:228:PRO:HA	1:C:246:ARG:HB2	1.93	0.50
1:D:213:ARG:HD3	1:D:259:PHE:CD2	2.47	0.50
1:B:261:PRO:HB2	1:B:263:TYR:CE1	2.47	0.50
1:G:57:PHE:HB3	1:G:355:MET:HE3	1.94	0.50
1:F:111:ALA:HB1	1:F:128:VAL:HG12	1.93	0.50
1:E:57:PHE:HB2	1:E:375:VAL:HG22	1.93	0.50
1:G:166:THR:HG23	1:G:309:LEU:HD13	1.95	0.49
1:G:280:PRO:O	1:G:322:LYS:NZ	2.44	0.49
1:E:309:LEU:HA	1:E:312:MET:HE2	1.94	0.49
1:E:472:HIS:H	1:E:475:HIS:HE1	1.60	0.49
1:A:44:GLN:HE22	1:B:467:MET:HE1	1.77	0.49
1:D:132:ALA:HB3	1:C:24:LYS:HA	1.93	0.49
1:B:46:LEU:HB3	1:B:469:HIS:CE1	2.47	0.49
1:B:480:VAL:HG12	1:B:484:MET:HE2	1.95	0.49
1:G:38:LYS:O	1:G:42:GLU:HG3	2.12	0.49
1:C:171:HIS:CG	1:C:172:ALA:N	2.81	0.49
1:F:114:ALA:HA	1:F:117:TYR:CZ	2.48	0.49
1:D:84:GLU:H	1:D:84:GLU:CD	2.20	0.49
3:B:602:NAG:H83	3:B:602:NAG:H3	1.93	0.49
1:F:457:GLU:HB2	1:E:65:SER:HA	1.93	0.49
1:H:463:SER:HB3	1:H:468:ALA:HB1	1.95	0.48
1:E:417:ASN:HB2	1:E:449:LEU:HD12	1.94	0.48
1:F:239:ASP:OD1	1:F:240:GLU:N	2.46	0.48
1:H:164:VAL:HG23	1:H:329:LEU:HD11	1.95	0.48
1:F:117:TYR:HA	1:F:481:PRO:HD3	1.94	0.48
1:C:472:HIS:H	1:C:475:HIS:HE1	1.60	0.48
1:G:173:THR:HG21	1:G:332:GLU:HG3	1.95	0.48
1:E:209:MET:HE2	1:E:226:MET:HE3	1.95	0.48
1:E:430:ASN:OD1	1:E:432:SER:OG	2.31	0.48
1:D:473:GLY:H	1:D:475:HIS:HE1	1.60	0.48
1:B:406:ASP:OD2	1:B:428:ARG:NH1	2.47	0.48
1:B:472:HIS:H	1:B:475:HIS:HE1	1.62	0.48
1:F:63:GLY:O	1:F:67:VAL:HG13	2.14	0.48
1:C:46:LEU:HD13	1:C:469:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:GLY:O	1:E:67:VAL:HG13	2.13	0.48
1:F:488:ALA:HB3	1:F:490:ILE:HG12	1.96	0.47
1:C:401:MET:SD	1:C:401:MET:N	2.87	0.47
1:B:114:ALA:O	1:B:118:LEU:HB2	2.14	0.47
1:D:240:GLU:OE1	1:D:243:ARG:NH1	2.48	0.47
1:G:223:ARG:HA	1:G:289:LEU:HD23	1.96	0.47
1:F:117:TYR:CE2	1:F:378:ASP:HB3	2.49	0.47
1:B:473:GLY:H	1:B:475:HIS:HE1	1.59	0.47
1:E:84:GLU:CD	1:E:84:GLU:H	2.22	0.47
1:D:253:VAL:HG12	1:D:257:LYS:HE3	1.96	0.47
1:G:388:TYR:HA	1:H:107:VAL:HB	1.96	0.47
1:B:219:MET:HG2	1:B:290:PHE:HE2	1.80	0.47
1:F:498:ALA:O	1:F:500:ALA:N	2.48	0.47
1:H:73:LEU:HD22	1:H:349:LEU:HB3	1.97	0.47
1:D:95:VAL:HA	1:D:461:VAL:O	2.15	0.46
1:D:227:TYR:HB3	1:D:231:LYS:HD3	1.97	0.46
1:B:302:ASN:OD1	1:B:304:VAL:HG13	2.16	0.46
1:A:186:TRP:CG	1:A:192:MET:HG2	2.50	0.46
1:A:463:SER:HB3	1:A:468:ALA:HB1	1.98	0.46
1:C:256:TRP:CD1	1:C:260:LYS:HZ3	2.34	0.46
1:E:290:PHE:HB2	1:E:295:MET:HE3	1.96	0.46
1:D:253:VAL:O	1:D:257:LYS:HG3	2.15	0.46
1:B:337:ASP:OD1	1:B:381:HIS:NE2	2.46	0.46
1:G:114:ALA:HA	1:G:117:TYR:CZ	2.50	0.46
1:F:60:ASP:HB3	1:F:337:ASP:HB2	1.97	0.46
1:F:117:TYR:HE2	1:F:378:ASP:HB3	1.80	0.46
1:E:467:MET:HA	1:E:469:HIS:CE1	2.50	0.46
1:F:227:TYR:HE1	1:F:253:VAL:HG21	1.81	0.46
1:D:420:GLY:HA3	1:D:443:ALA:O	2.16	0.46
1:C:291:GLU:HG3	1:C:292:PRO:HD2	1.98	0.46
1:G:117:TYR:CE2	1:G:378:ASP:HB3	2.51	0.46
1:H:272:ARG:NH1	1:H:311:GLU:OE2	2.49	0.46
1:F:155:LYS:HD3	1:F:214:ASP:CG	2.41	0.46
1:F:281:HIS:C	1:F:322:LYS:HZ1	2.24	0.46
1:G:92:PHE:CZ	1:G:464:LYS:HE2	2.51	0.46
1:E:269:ILE:HD13	1:E:286:LEU:HD11	1.97	0.46
1:D:228:PRO:HB3	1:D:249:GLY:HA2	1.99	0.45
1:E:240:GLU:HG2	1:E:243:ARG:HE	1.81	0.45
1:D:71:ARG:HG3	1:D:87:LEU:HG	1.97	0.45
1:G:62:MET:SD	1:G:89:MET:HE1	2.56	0.45
1:H:239:ASP:OD1	1:H:241:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:SER:HB3	1:E:225:TYR:HD1	1.82	0.45
1:D:103:THR:HG21	1:D:132:ALA:HB1	1.99	0.45
1:E:420:GLY:HA3	1:E:443:ALA:O	2.16	0.45
1:D:26:PRO:O	1:D:30:ARG:HG3	2.17	0.45
1:B:117:TYR:HE2	1:B:378:ASP:HB3	1.82	0.45
1:F:239:ASP:OD1	1:F:241:LYS:N	2.49	0.45
1:B:140:ASN:HA	1:B:143:GLN:HE22	1.82	0.45
1:F:271:ASN:OD1	1:F:274:GLU:HG3	2.17	0.45
1:E:301:ARG:O	3:E:602:NAG:H82	2.16	0.45
1:D:290:PHE:HB2	1:D:295:MET:HE3	1.97	0.45
1:C:38:LYS:HA	1:C:38:LYS:HD3	1.82	0.45
1:F:409:PRO:O	1:F:428:ARG:NH2	2.50	0.45
1:A:240:GLU:C	1:A:242:ALA:H	2.25	0.45
1:H:423:VAL:HA	1:H:428:ARG:HA	1.98	0.45
1:F:408:LYS:NZ	1:F:427:GLU:HG3	2.31	0.45
1:G:117:TYR:HE2	1:G:378:ASP:HB3	1.80	0.45
1:A:131:SER:HB3	1:B:26:PRO:HG3	1.99	0.45
1:F:401:MET:SD	1:F:401:MET:N	2.89	0.45
1:C:216:ASP:HA	1:C:285:TYR:HD1	1.80	0.45
1:F:188:SER:HA	1:F:203:ASP:OD2	2.16	0.45
3:E:602:NAG:O7	3:E:602:NAG:O3	2.32	0.45
1:D:107:VAL:HG21	1:C:386:GLY:HA2	2.00	0.44
1:B:31:ASP:O	1:B:35:GLU:HG3	2.18	0.44
1:B:272:ARG:HG2	1:B:276:LEU:HD23	1.98	0.44
1:G:273:THR:O	1:G:277:THR:OG1	2.30	0.44
1:G:317:ILE:O	1:G:321:ARG:HG2	2.17	0.44
1:H:117:TYR:HE2	1:H:378:ASP:HB3	1.82	0.44
1:H:291:GLU:HG3	1:H:295:MET:HA	2.00	0.44
1:F:230:ASN:HA	1:F:243:ARG:HD2	1.98	0.44
1:A:86:ARG:NH1	1:A:91:LYS:HG2	2.33	0.44
1:A:239:ASP:OD1	1:A:241:LYS:N	2.50	0.44
1:D:166:THR:O	1:D:295:MET:HB2	2.17	0.44
1:C:186:TRP:O	1:C:204:ILE:HG13	2.18	0.44
1:B:344:LYS:HD3	1:B:440:ASN:HA	2.00	0.44
1:G:323:ASN:OD1	1:G:325:LYS:HG3	2.18	0.44
1:G:344:LYS:HE2	1:G:440:ASN:HB3	1.99	0.44
1:F:203:ASP:OD1	1:F:203:ASP:N	2.45	0.44
1:D:457:GLU:HB3	1:C:65:SER:HA	2.00	0.44
1:C:52:LYS:O	1:C:326:GLY:HA3	2.18	0.44
1:C:114:ALA:HA	1:C:117:TYR:CZ	2.53	0.44
1:D:381:HIS:ND1	1:D:452:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:HIS:HB3	1:C:452:GLU:OE2	2.17	0.44
1:E:117:TYR:CE2	1:E:378:ASP:HB3	2.53	0.44
1:H:424:VAL:N	1:H:427:GLU:O	2.51	0.44
1:G:291:GLU:HG3	1:G:292:PRO:HD2	1.99	0.44
1:C:60:ASP:O	1:C:336:ILE:HB	2.18	0.44
1:B:274:GLU:OE2	2:o:1:NAG:H62	2.18	0.44
1:E:240:GLU:OE1	1:E:241:LYS:HD2	2.17	0.44
1:A:275:LEU:HD12	1:A:290:PHE:CZ	2.52	0.44
1:B:42:GLU:O	1:B:45:LYS:HG2	2.18	0.44
1:E:173:THR:HG21	1:E:332:GLU:HG3	1.99	0.44
1:A:291:GLU:HG3	1:A:292:PRO:HD2	2.00	0.43
1:D:280:PRO:O	1:D:322:LYS:HE3	2.17	0.43
1:G:303:ASN:ND2	3:G:602:NAG:O7	2.51	0.43
1:F:95:VAL:HA	1:F:461:VAL:O	2.18	0.43
1:F:308:SER:O	1:F:312:MET:HG3	2.18	0.43
1:A:239:ASP:OD1	1:A:241:LYS:HE3	2.18	0.43
1:A:252:LEU:HA	1:A:255:THR:HB	1.99	0.43
1:A:280:PRO:C	1:A:282:ASN:H	2.27	0.43
1:A:390:PRO:HD3	1:A:400:PRO:HG3	2.00	0.43
1:C:448:PRO:O	1:C:449:LEU:HD23	2.18	0.43
1:H:22:LYS:HD2	1:H:28:TYR:CE1	2.52	0.43
1:H:203:ASP:O	1:H:207:GLN:HG3	2.17	0.43
1:A:401:MET:SD	1:A:401:MET:N	2.87	0.43
1:D:175:SER:HA	1:D:178:TYR:CZ	2.53	0.43
1:B:38:LYS:O	1:B:42:GLU:HG3	2.18	0.43
1:H:117:TYR:HA	1:H:481:PRO:HD3	1.99	0.43
1:B:467:MET:HE3	1:B:470:LEU:HD11	1.98	0.43
1:E:68:THR:O	1:E:72:ILE:HG13	2.17	0.43
1:E:117:TYR:HA	1:E:481:PRO:HD3	2.00	0.43
1:C:310:SER:OG	1:C:354:GLU:OE2	2.36	0.43
1:H:355:MET:HE3	1:H:359:ILE:HD11	2.00	0.43
1:H:381:HIS:HB3	1:H:452:GLU:OE2	2.18	0.43
1:E:164:VAL:HG13	1:E:312:MET:HE3	1.99	0.43
1:E:355:MET:O	1:E:359:ILE:HG13	2.19	0.43
1:A:203:ASP:O	1:A:207:GLN:HG3	2.18	0.43
1:E:314:VAL:O	1:E:318:GLN:HG3	2.18	0.43
1:B:214:ASP:OD1	1:B:214:ASP:N	2.52	0.43
1:H:228:PRO:HA	1:H:246:ARG:HB2	2.01	0.43
3:F:601:NAG:O7	3:F:601:NAG:O3	2.36	0.43
1:B:164:VAL:HG13	1:B:312:MET:HE3	2.01	0.43
1:B:264:LYS:HD2	1:B:264:LYS:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:LYS:O	1:F:326:GLY:HA3	2.19	0.43
1:E:385:PHE:HA	1:E:412:ALA:O	2.19	0.43
1:C:45:LYS:HD2	1:C:45:LYS:HA	1.75	0.43
1:C:99:LYS:O	1:C:477:GLN:HB2	2.19	0.43
1:C:232:THR:HG22	1:C:237:GLU:HA	2.01	0.43
1:G:74:LYS:HD2	1:G:87:LEU:HD23	2.01	0.43
1:G:420:GLY:HA3	1:G:443:ALA:O	2.18	0.43
1:E:114:ALA:HA	1:E:117:TYR:CZ	2.54	0.43
1:F:375:VAL:HB	1:F:462:PHE:HB2	2.01	0.42
1:E:168:ARG:HG3	1:E:294:ASP:OD1	2.19	0.42
1:E:355:MET:HE3	1:E:359:ILE:HD11	2.01	0.42
1:B:114:ALA:HA	1:B:117:TYR:CZ	2.54	0.42
1:H:195:GLU:O	1:H:199:GLN:HB2	2.19	0.42
1:G:381:HIS:ND1	1:G:452:GLU:OE1	2.52	0.42
1:H:228:PRO:HD3	1:H:250:LEU:O	2.19	0.42
1:B:430:ASN:ND2	1:B:433:MET:HE2	2.35	0.42
1:F:268:PHE:HA	1:F:287:LEU:O	2.19	0.42
1:G:160:SER:HB3	1:G:320:LEU:HD22	2.01	0.42
1:G:274:GLU:O	1:G:278:LEU:HD13	2.20	0.42
1:E:186:TRP:HB3	1:E:192:MET:HG2	2.00	0.42
1:B:45:LYS:HG2	1:B:45:LYS:H	1.67	0.42
1:B:336:ILE:HD11	1:B:352:ALA:HA	2.00	0.42
1:F:26:PRO:O	1:F:30:ARG:HG3	2.19	0.42
1:B:228:PRO:HB3	1:B:249:GLY:HA2	2.02	0.42
1:G:92:PHE:CE1	1:G:464:LYS:HE2	2.54	0.42
1:H:52:LYS:O	1:H:159:LYS:HE3	2.20	0.42
1:A:52:LYS:O	1:A:326:GLY:HA3	2.20	0.42
1:F:389:THR:HG22	1:F:399:ALA:HA	2.02	0.42
1:A:385:PHE:HA	1:A:412:ALA:O	2.20	0.42
1:C:155:LYS:HG2	1:C:212:ILE:HD11	2.01	0.42
1:C:303:ASN:HD22	3:C:602:NAG:C7	2.30	0.42
1:H:114:ALA:HA	1:H:117:TYR:CZ	2.54	0.42
1:H:257:LYS:HE3	1:H:257:LYS:HB2	1.71	0.42
1:E:467:MET:HE3	1:E:467:MET:HB3	1.94	0.42
1:C:404:ASP:OD1	1:C:404:ASP:N	2.51	0.42
1:B:372:LEU:HD21	1:B:484:MET:HG2	2.01	0.42
1:G:111:ALA:HB2	1:G:172:ALA:HB1	2.02	0.42
1:B:355:MET:HE3	1:B:355:MET:HB3	1.78	0.41
1:F:104:ASN:HB3	1:E:19:VAL:HG22	2.02	0.41
1:E:140:ASN:OD1	1:E:140:ASN:N	2.53	0.41
1:E:280:PRO:O	1:E:282:ASN:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:ASN:OD1	1:C:303:ASN:N	2.50	0.41
1:G:417:ASN:HB2	1:G:449:LEU:HD12	2.02	0.41
1:E:488:ALA:HB3	1:E:490:ILE:HG12	2.03	0.41
1:H:57:PHE:HB2	1:H:375:VAL:HG22	2.01	0.41
1:D:117:TYR:HA	1:D:481:PRO:HD3	2.01	0.41
1:F:103:THR:HG21	1:F:132:ALA:HB2	2.02	0.41
1:F:422:LYS:HD3	1:F:429:GLU:OE2	2.21	0.41
1:B:117:TYR:CE2	1:B:378:ASP:HB3	2.56	0.41
1:G:195:GLU:H	1:G:195:GLU:CD	2.28	0.41
1:E:155:LYS:NZ	1:E:216:ASP:OD1	2.52	0.41
1:C:188:SER:HA	1:C:203:ASP:OD2	2.21	0.41
1:H:268:PHE:HA	1:H:287:LEU:O	2.21	0.41
1:F:62:MET:HE2	1:F:62:MET:HB3	1.84	0.41
2:IA:1:NAG:H61	2:IA:2:NAG:H82	2.02	0.41
1:D:190:ASN:HB2	1:D:245:THR:O	2.20	0.41
1:C:355:MET:HE2	1:C:355:MET:HB3	1.93	0.41
1:B:409:PRO:O	1:B:428:ARG:NH2	2.54	0.41
1:G:72:ILE:O	1:G:76:GLN:HG3	2.20	0.41
1:A:29:TRP:CE2	1:B:122:LYS:HB2	2.56	0.41
1:G:126:GLY:HA2	1:G:184:ARG:HG2	2.03	0.41
1:H:280:PRO:O	1:H:322:LYS:HE2	2.20	0.41
1:A:60:ASP:HB3	1:A:337:ASP:HB2	2.03	0.41
1:D:341:HIS:ND1	1:D:452:GLU:O	2.54	0.41
1:C:190:ASN:HB2	1:C:245:THR:O	2.20	0.41
1:C:192:MET:HE2	1:C:192:MET:HB3	1.97	0.41
1:C:382:VAL:HG23	1:C:416:GLY:H	1.86	0.41
1:G:406:ASP:OD2	1:G:428:ARG:NH1	2.53	0.41
1:H:126:GLY:HA2	1:H:184:ARG:HG2	2.03	0.41
1:F:246:ARG:NH1	1:F:252:LEU:HD11	2.20	0.41
1:E:74:LYS:HD2	1:E:353:VAL:HG13	2.02	0.41
1:E:235:GLU:HG3	1:E:270:TRP:HZ3	1.86	0.41
1:D:29:TRP:CE2	1:C:122:LYS:HB2	2.55	0.41
1:D:408:LYS:HG3	2:X:1:NAG:H82	2.03	0.41
1:B:104:ASN:HB2	1:B:124:ASN:HA	2.02	0.41
1:G:168:ARG:HB3	1:G:170:ASN:OD1	2.20	0.41
1:H:114:ALA:O	1:H:118:LEU:HB2	2.21	0.41
1:B:103:THR:HG21	1:B:132:ALA:HB1	2.02	0.40
1:G:409:PRO:O	1:G:428:ARG:NH2	2.54	0.40
1:A:138:ARG:HD3	1:A:138:ARG:HA	1.75	0.40
1:A:192:MET:HE2	1:A:203:ASP:HB3	2.04	0.40
1:A:335:ARG:HD2	1:A:338:HIS:ND1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:MET:SD	1:D:256:TRP:HB2	2.61	0.40
1:H:49:ASN:OD1	1:H:49:ASN:N	2.54	0.40
1:F:385:PHE:HA	1:F:412:ALA:O	2.21	0.40
1:E:113:THR:OG1	1:E:378:ASP:HB2	2.20	0.40
1:G:114:ALA:HA	1:G:117:TYR:CE2	2.56	0.40
1:C:22:LYS:HD2	1:C:28:TYR:CE1	2.57	0.40
1:C:335:ARG:HB2	1:C:351:GLU:OE1	2.22	0.40
1:B:189:ASP:OD2	1:B:248:ASP:N	2.54	0.40
1:B:378:ASP:OD1	1:B:378:ASP:N	2.49	0.40
1:E:126:GLY:HA3	1:E:136:ARG:HD2	2.03	0.40
1:E:171:HIS:CG	1:E:172:ALA:H	2.40	0.40
1:A:375:VAL:HB	1:A:462:PHE:HB2	2.02	0.40
1:B:195:GLU:CD	1:B:195:GLU:H	2.29	0.40
1:H:467:MET:HA	1:H:469:HIS:CE1	2.56	0.40
1:E:167:THR:HG23	1:E:334:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	482/503 (96%)	464 (96%)	13 (3%)	5 (1%)	12	39
1	B	482/503 (96%)	459 (95%)	19 (4%)	4 (1%)	16	44
1	C	482/503 (96%)	460 (95%)	19 (4%)	3 (1%)	21	51
1	D	480/503 (95%)	460 (96%)	16 (3%)	4 (1%)	16	44
1	E	482/503 (96%)	454 (94%)	25 (5%)	3 (1%)	21	51
1	F	481/503 (96%)	451 (94%)	24 (5%)	6 (1%)	10	34
1	G	482/503 (96%)	464 (96%)	16 (3%)	2 (0%)	30	59
1	H	482/503 (96%)	461 (96%)	19 (4%)	2 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3853/4024 (96%)	3673 (95%)	151 (4%)	29 (1%)	16 44

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	497	CYS
1	A	268	PHE
1	E	282	ASN
1	C	268	PHE
1	H	268	PHE
1	A	241	LYS
1	C	19	VAL
1	B	268	PHE
1	F	268	PHE
1	A	425	GLY
1	D	19	VAL
1	B	430	ASN
1	F	499	PRO
1	E	19	VAL
1	G	19	VAL
1	F	19	VAL
1	D	425	GLY
1	B	382	VAL
1	F	426	GLY
1	A	382	VAL
1	D	382	VAL
1	C	382	VAL
1	B	19	VAL
1	G	382	VAL
1	F	382	VAL
1	F	425	GLY
1	H	382	VAL
1	E	382	VAL
1	A	499	PRO

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	398/413 (96%)	385 (97%)	13 (3%)	33	67
1	B	398/413 (96%)	387 (97%)	11 (3%)	38	72
1	C	398/413 (96%)	389 (98%)	9 (2%)	44	76
1	D	398/413 (96%)	389 (98%)	9 (2%)	44	76
1	E	398/413 (96%)	388 (98%)	10 (2%)	42	74
1	F	398/413 (96%)	377 (95%)	21 (5%)	20	52
1	G	398/413 (96%)	391 (98%)	7 (2%)	51	80
1	H	398/413 (96%)	384 (96%)	14 (4%)	32	66
All	All	3184/3304 (96%)	3090 (97%)	94 (3%)	36	70

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	67	VAL
1	A	125	GLU
1	A	137	SER
1	A	155	LYS
1	A	303	ASN
1	A	314	VAL
1	A	315	VAL
1	A	368	SER
1	A	403	SER
1	A	404	ASP
1	A	422	LYS
1	A	463	SER
1	D	60	ASP
1	D	65	SER
1	D	95	VAL
1	D	103	THR
1	D	181	SER
1	D	201	CYS
1	D	238	SER
1	D	315	VAL
1	D	364	SER
1	C	58	LEU
1	C	103	THR
1	C	201	CYS

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Mol	Chain	Res	Type
1	C	232	THR
1	C	303	ASN
1	C	310	SER
1	C	368	SER
1	C	432	SER
1	C	470	LEU
1	B	53	ASN
1	B	67	VAL
1	B	103	THR
1	B	140	ASN
1	B	234	VAL
1	B	277	THR
1	B	283	VAL
1	B	304	VAL
1	B	315	VAL
1	B	384	THR
1	B	457	GLU
1	G	58	LEU
1	G	60	ASP
1	G	121	VAL
1	G	137	SER
1	G	310	SER
1	G	368	SER
1	G	432	SER
1	H	18	LEU
1	H	49	ASN
1	H	58	LEU
1	H	85	THR
1	H	109	ASP
1	H	140	ASN
1	H	203	ASP
1	H	254	ASP
1	H	266	SER
1	H	283	VAL
1	H	303	ASN
1	H	310	SER
1	H	349	LEU
1	H	457	GLU
1	F	54	VAL
1	F	58	LEU
1	F	95	VAL
1	F	103	THR

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Mol	Chain	Res	Type
1	F	128	VAL
1	F	130	VAL
1	F	137	SER
1	F	141	THR
1	F	197	LEU
1	F	198	SER
1	F	201	CYS
1	F	212	ILE
1	F	247	LEU
1	F	260	LYS
1	F	310	SER
1	F	315	VAL
1	F	325	LYS
1	F	349	LEU
1	F	364	SER
1	F	373	THR
1	F	445	SER
1	E	45	LYS
1	E	58	LEU
1	E	64	VAL
1	E	67	VAL
1	E	140	ASN
1	E	198	SER
1	E	269	ILE
1	E	277	THR
1	E	283	VAL
1	E	364	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44	GLN
1	A	106	GLN
1	A	230	ASN
1	A	267	HIS
1	A	475	HIS
1	A	482	HIS
1	D	53	ASN
1	D	78	HIS
1	D	124	ASN
1	D	145	ASN

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Mol	Chain	Res	Type
1	D	475	HIS
1	D	482	HIS
1	D	493	ASN
1	C	34	GLN
1	C	44	GLN
1	C	102	ASN
1	C	210	HIS
1	C	361	GLN
1	C	475	HIS
1	C	478	ASN
1	B	32	GLN
1	B	143	GLN
1	B	199	GLN
1	B	211	ASN
1	B	296	GLN
1	B	475	HIS
1	G	53	ASN
1	G	379	HIS
1	F	32	GLN
1	F	44	GLN
1	F	171	HIS
1	F	211	ASN
1	F	282	ASN
1	F	451	HIS
1	F	469	HIS
1	E	171	HIS
1	E	267	HIS
1	E	318	GLN

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)

32 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	$\#\|Z\| > 2$
2	NAG	1	1	1,2	14,14,15	0.38	0	17,19,21	0.77	0
2	NAG	1	2	2	14,14,15	0.42	0	17,19,21	0.52	0
2	NAG	8	1	1,2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	8	2	2	14,14,15	0.31	0	17,19,21	0.44	0
2	NAG	BA	1	1,2	14,14,15	0.29	0	17,19,21	0.73	0
2	NAG	BA	2	2	14,14,15	0.36	0	17,19,21	0.61	0
2	NAG	IA	1	1,2	14,14,15	0.24	0	17,19,21	0.62	1 (5%)
2	NAG	IA	2	2	14,14,15	0.36	0	17,19,21	0.48	0
2	NAG	K	1	1,2	14,14,15	0.29	0	17,19,21	0.39	0
2	NAG	K	2	2	14,14,15	0.27	0	17,19,21	0.44	0
2	NAG	LA	1	1,2	14,14,15	0.28	0	17,19,21	0.80	1 (5%)
2	NAG	LA	2	2	14,14,15	0.37	0	17,19,21	0.78	0
2	NAG	N	1	1,2	14,14,15	0.33	0	17,19,21	0.71	0
2	NAG	N	2	2	14,14,15	0.50	0	17,19,21	0.50	0
2	NAG	SA	1	1,2	14,14,15	0.49	0	17,19,21	0.77	0
2	NAG	SA	2	2	14,14,15	0.30	0	17,19,21	0.38	0
2	NAG	U	1	1,2	14,14,15	0.20	0	17,19,21	0.46	0
2	NAG	U	2	2	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	VA	1	1,2	14,14,15	0.28	0	17,19,21	0.60	0
2	NAG	VA	2	2	14,14,15	0.34	0	17,19,21	0.48	0
2	NAG	X	1	1,2	14,14,15	0.23	0	17,19,21	0.59	0
2	NAG	X	2	2	14,14,15	0.20	0	17,19,21	0.72	0
2	NAG	e	1	1,2	14,14,15	0.21	0	17,19,21	0.52	0
2	NAG	e	2	2	14,14,15	0.28	0	17,19,21	0.48	0
2	NAG	h	1	1,2	14,14,15	0.24	0	17,19,21	0.59	0
2	NAG	h	2	2	14,14,15	0.31	0	17,19,21	0.35	0
2	NAG	o	1	1,2	14,14,15	0.27	0	17,19,21	0.47	0
2	NAG	o	2	2	14,14,15	0.27	0	17,19,21	0.41	0
2	NAG	r	1	1,2	14,14,15	0.30	0	17,19,21	0.61	0
2	NAG	r	2	2	14,14,15	0.39	0	17,19,21	0.54	0
2	NAG	y	1	1,2	14,14,15	0.29	0	17,19,21	0.46	0
2	NAG	y	2	2	14,14,15	0.37	0	17,19,21	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	1	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	1	2	2	-	3/6/23/26	0/1/1/1
2	NAG	8	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	8	2	2	-	0/6/23/26	0/1/1/1
2	NAG	BA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	IA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	IA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
2	NAG	LA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	LA	2	2	-	3/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	SA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	SA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	U	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	U	2	2	-	0/6/23/26	0/1/1/1
2	NAG	VA	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	VA	2	2	-	2/6/23/26	0/1/1/1
2	NAG	X	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	X	2	2	-	3/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	0/6/23/26	0/1/1/1
2	NAG	h	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	NAG	o	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	o	2	2	-	2/6/23/26	0/1/1/1
2	NAG	r	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	r	2	2	-	4/6/23/26	0/1/1/1
2	NAG	y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	y	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	LA	1	NAG	C1-O5-C5	2.31	115.28	112.19
2	IA	1	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (35) torsion outliers are listed below:

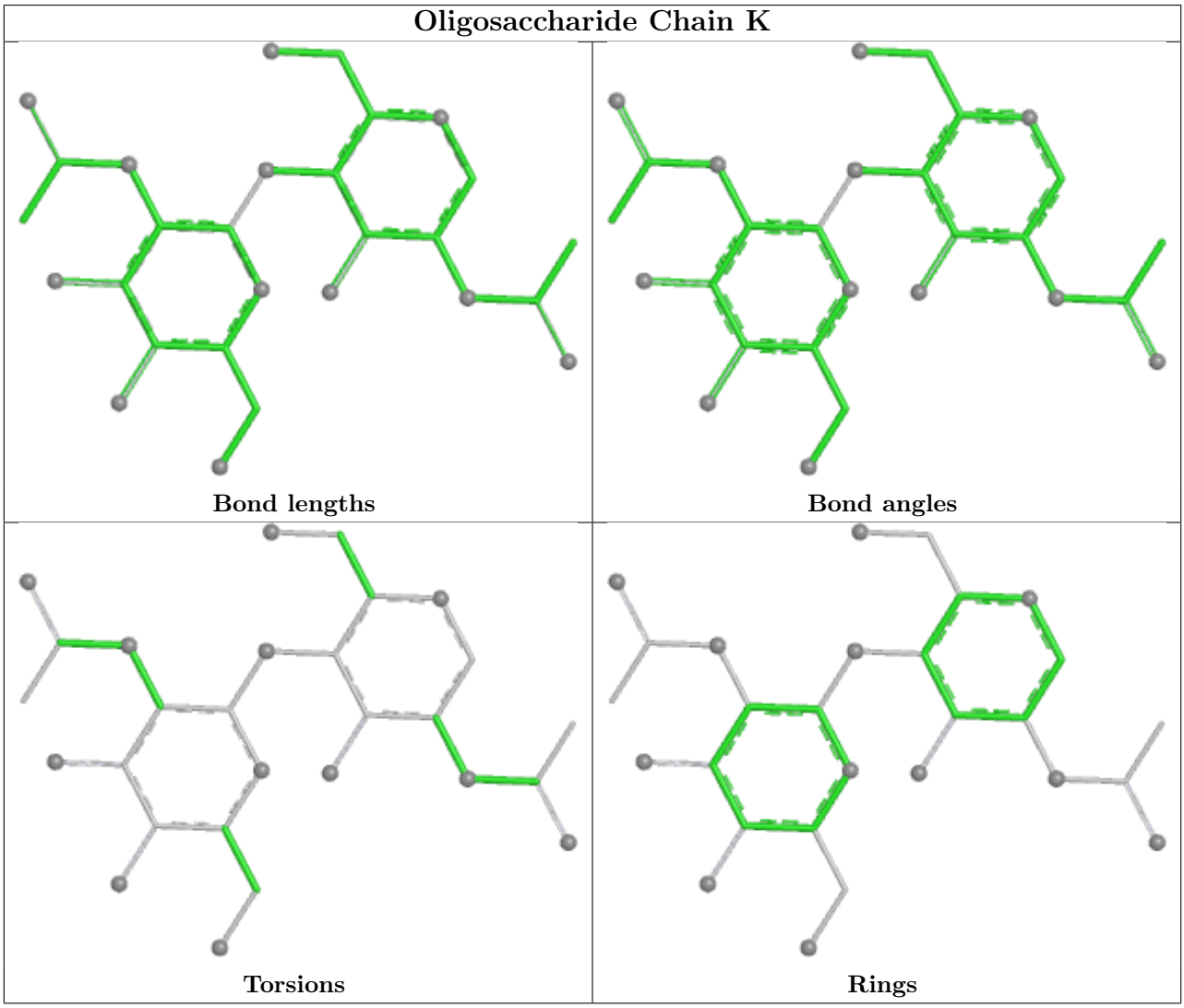
Mol	Chain	Res	Type	Atoms
2	LA	2	NAG	C1-C2-N2-C7
2	BA	1	NAG	O5-C5-C6-O6
2	IA	2	NAG	O5-C5-C6-O6
2	SA	2	NAG	O5-C5-C6-O6
2	LA	2	NAG	O5-C5-C6-O6
2	BA	1	NAG	C4-C5-C6-O6
2	IA	2	NAG	C4-C5-C6-O6
2	h	2	NAG	O5-C5-C6-O6
2	h	2	NAG	C4-C5-C6-O6
2	o	2	NAG	O5-C5-C6-O6
2	SA	2	NAG	C4-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	o	2	NAG	C4-C5-C6-O6
2	LA	2	NAG	C4-C5-C6-O6
2	VA	2	NAG	O5-C5-C6-O6
2	h	1	NAG	C4-C5-C6-O6
2	h	1	NAG	O5-C5-C6-O6
2	r	1	NAG	O5-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	1	2	NAG	O5-C5-C6-O6
2	r	2	NAG	C4-C5-C6-O6
2	X	2	NAG	C1-C2-N2-C7
2	1	2	NAG	C1-C2-N2-C7
2	BA	2	NAG	C1-C2-N2-C7
2	VA	2	NAG	C4-C5-C6-O6
2	r	2	NAG	C3-C2-N2-C7
2	VA	1	NAG	C4-C5-C6-O6
2	r	1	NAG	C4-C5-C6-O6
2	r	2	NAG	O5-C5-C6-O6
2	X	2	NAG	C4-C5-C6-O6
2	r	2	NAG	C1-C2-N2-C7
2	X	2	NAG	C3-C2-N2-C7
2	1	2	NAG	C3-C2-N2-C7
2	BA	2	NAG	C3-C2-N2-C7
2	VA	1	NAG	O5-C5-C6-O6

There are no ring outliers.

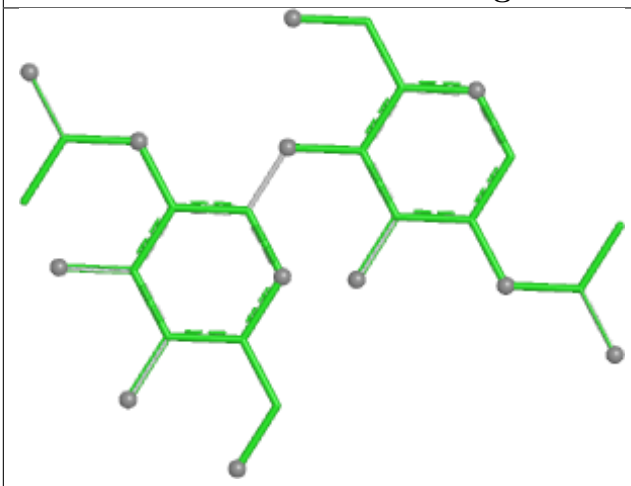
8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	o	1	NAG	1	0
2	X	1	NAG	1	0
2	LA	1	NAG	1	0
2	8	1	NAG	1	0
2	SA	1	NAG	1	0
2	IA	2	NAG	1	0
2	h	1	NAG	1	0
2	IA	1	NAG	2	0

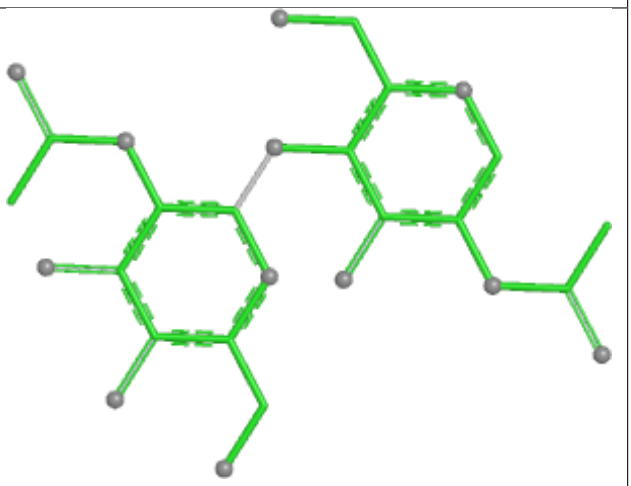
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



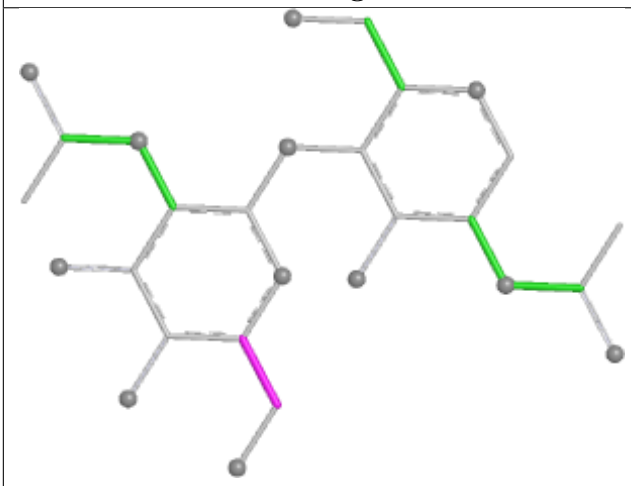
Oligosaccharide Chain N



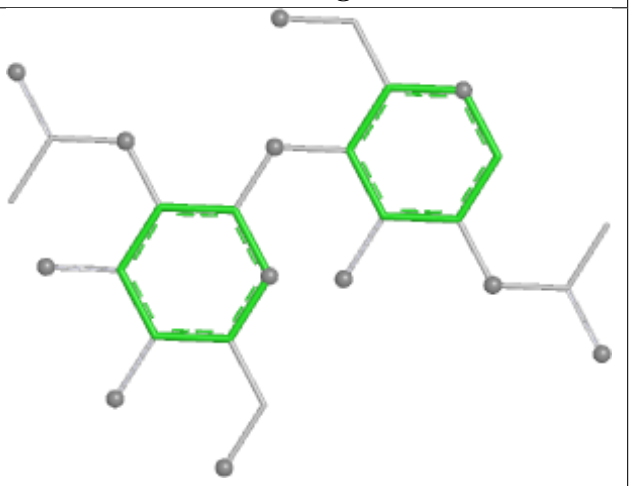
Bond lengths



Bond angles

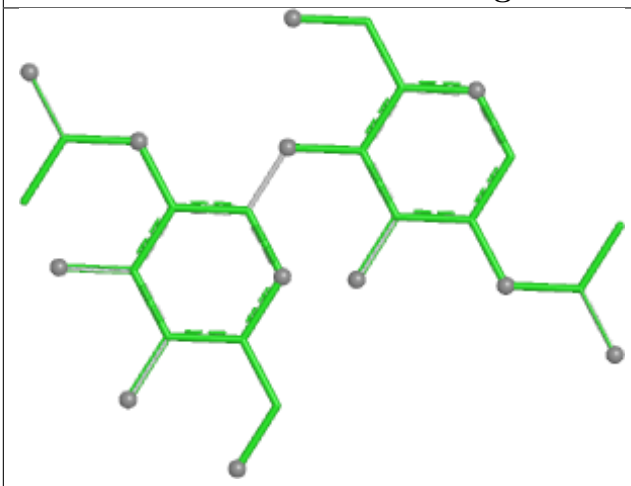


Torsions

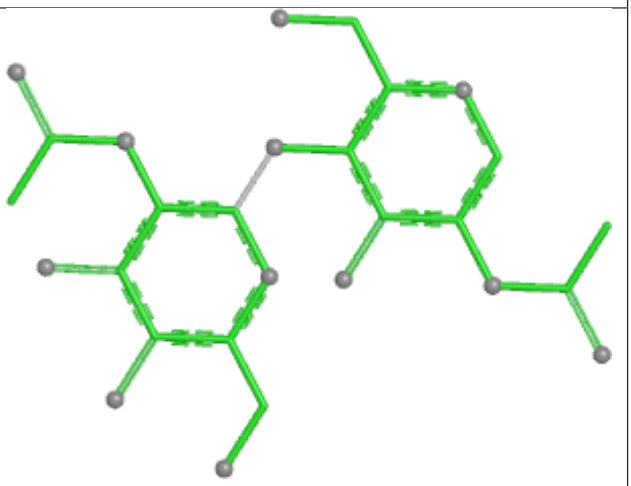


Rings

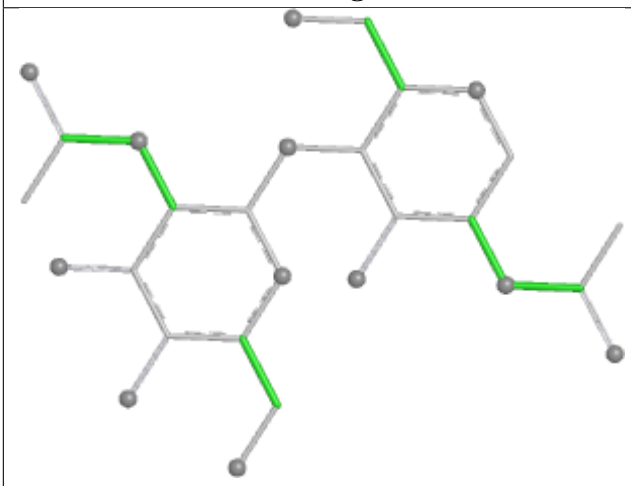
Oligosaccharide Chain U



Bond lengths



Bond angles



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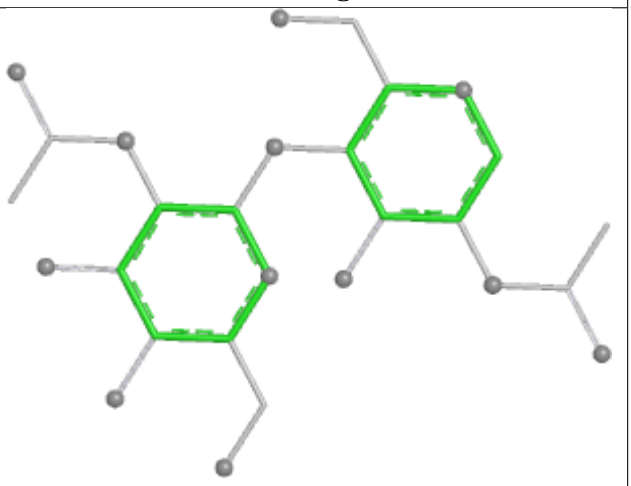
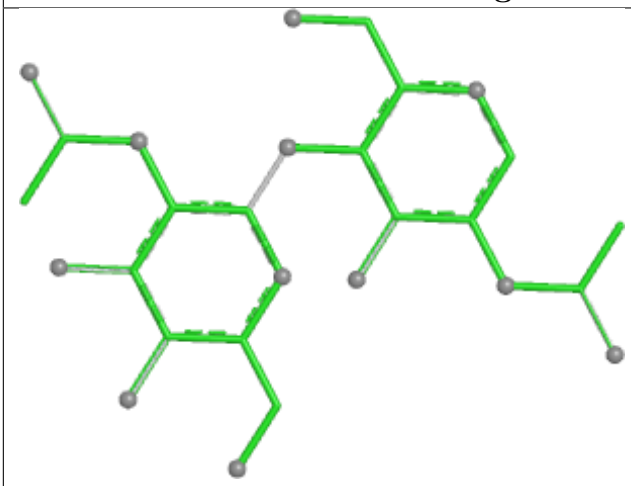
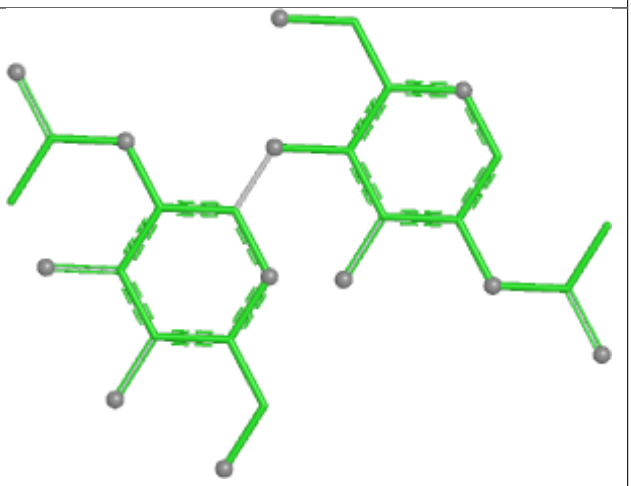


Rings

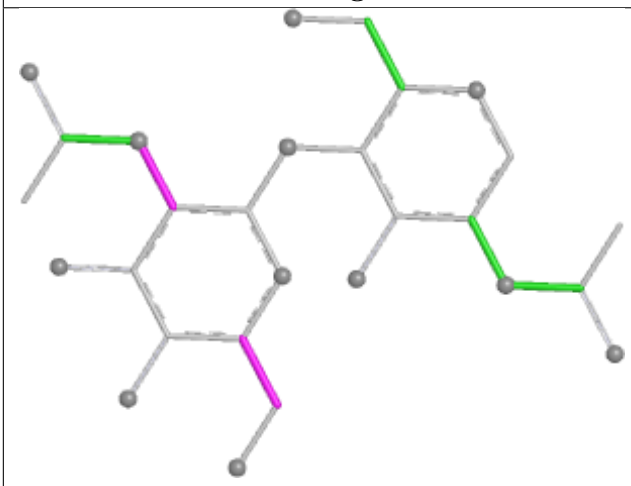
Oligosaccharide Chain X



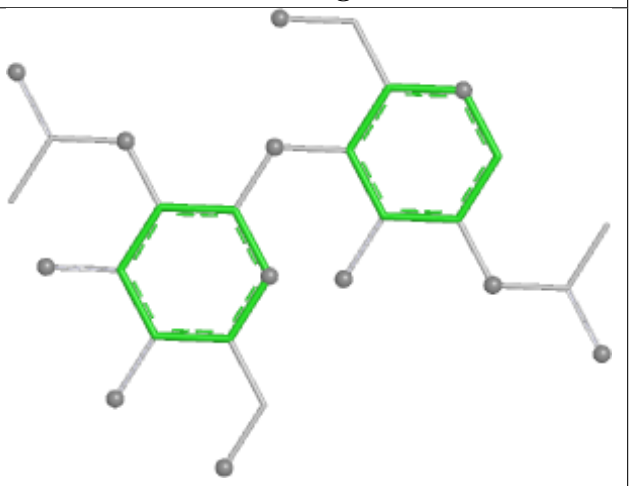
Bond lengths



Bond angles

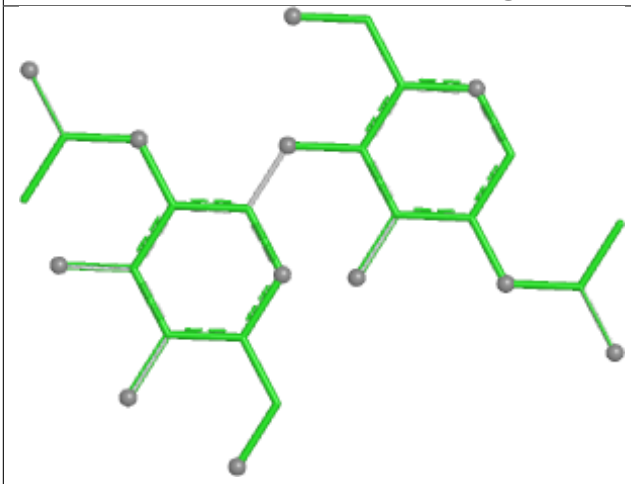


Torsions

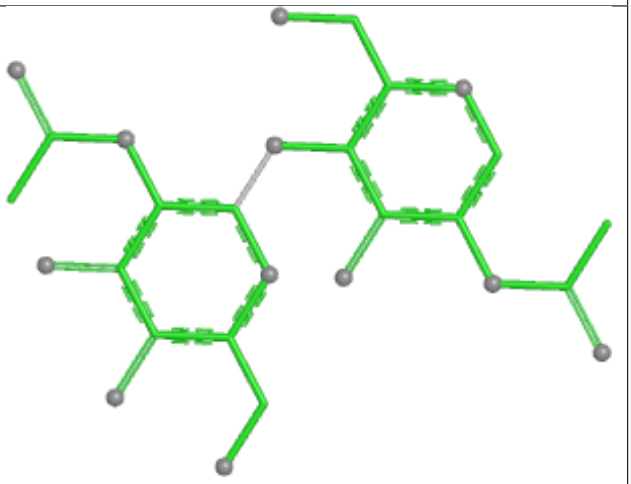


Rings

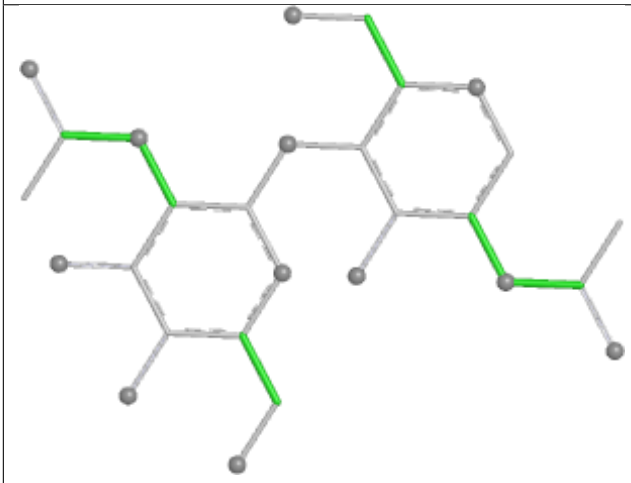
Oligosaccharide Chain e



Bond lengths



Bond angles



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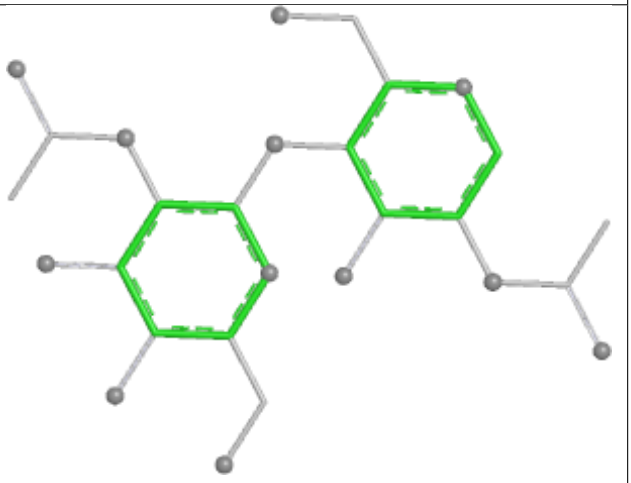
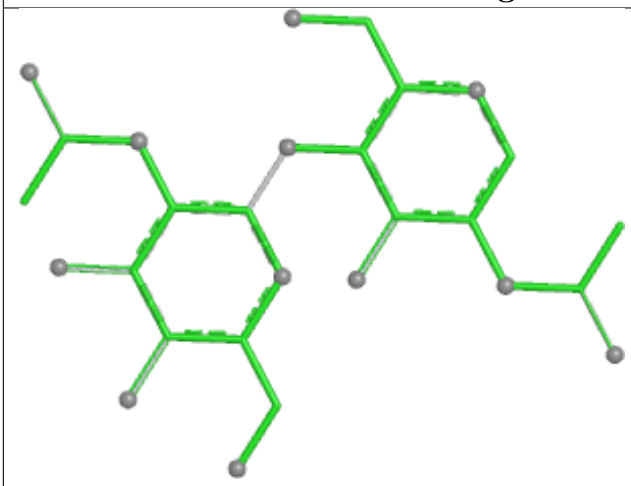


Rings

Oligosaccharide Chain h



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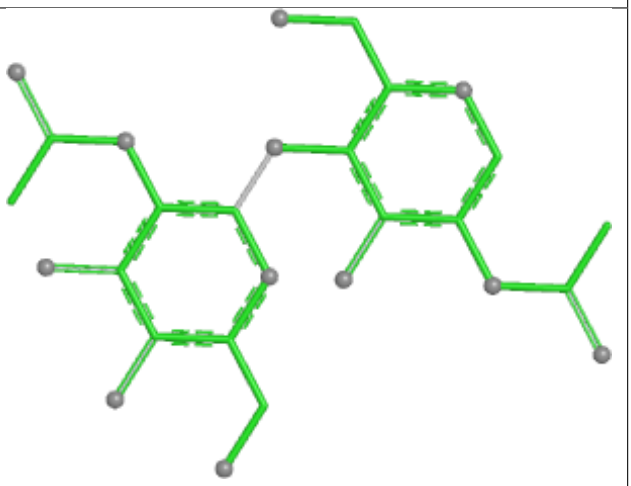
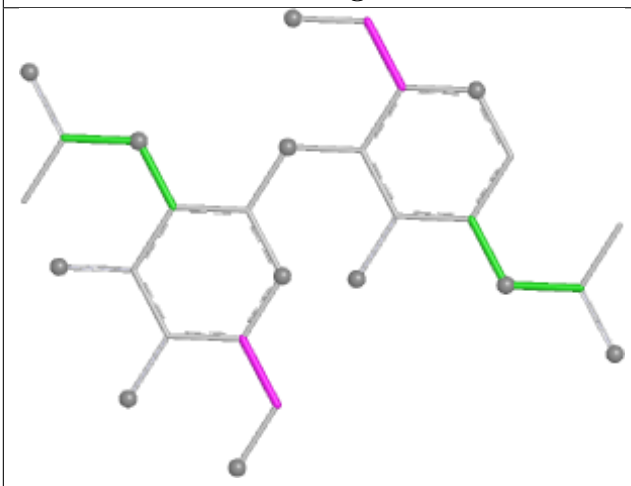


Bond angles



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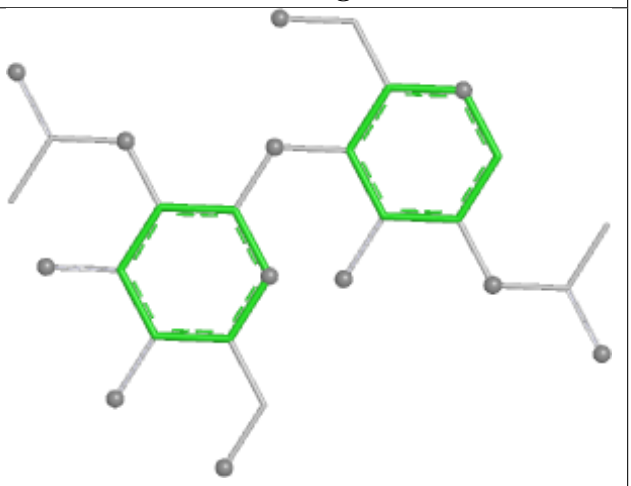
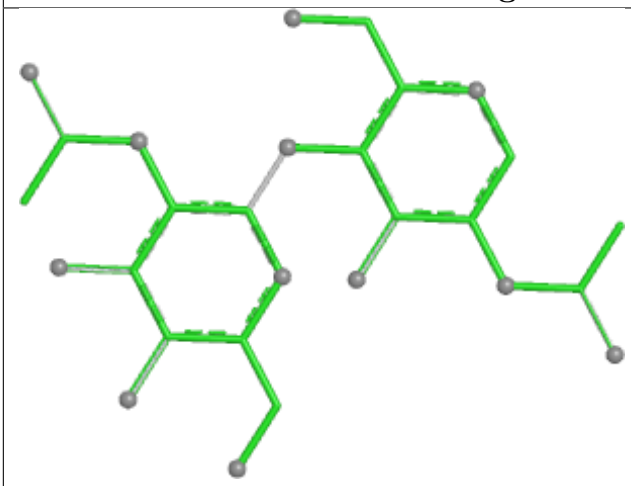


Rings

Oligosaccharide Chain o



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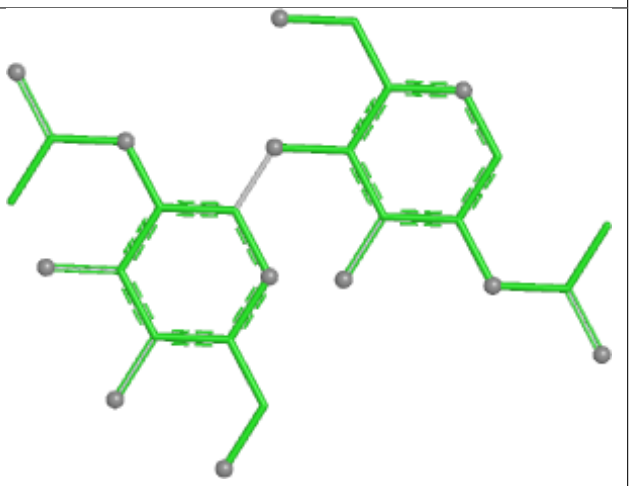

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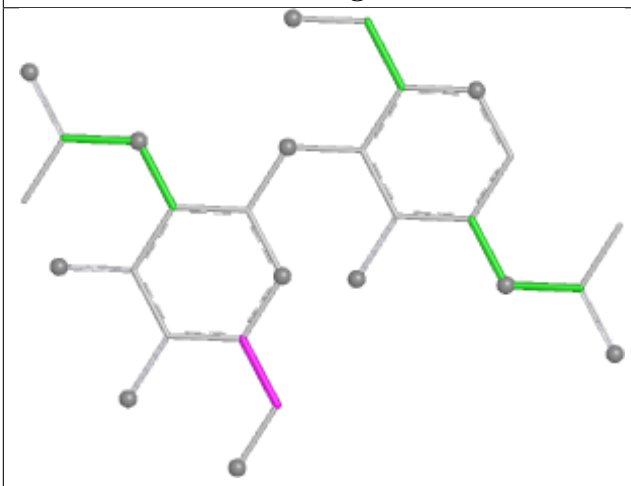

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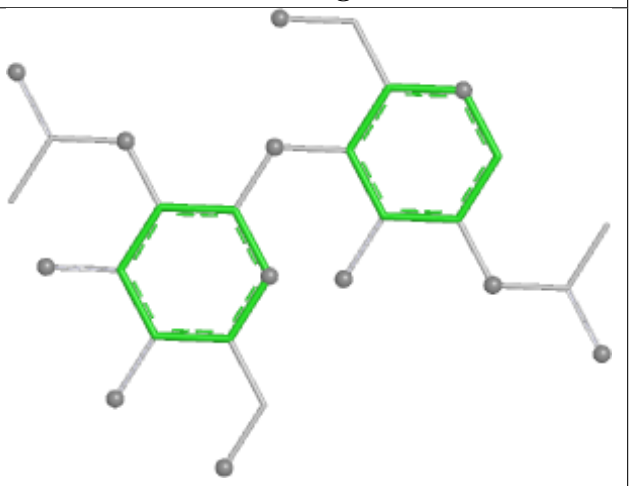
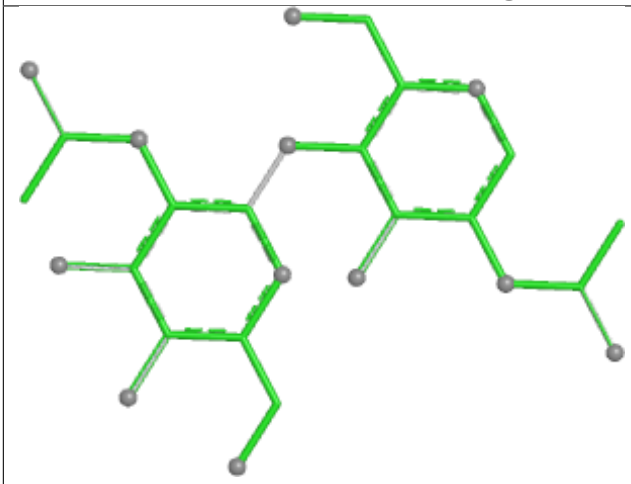


Rings

Oligosaccharide Chain r



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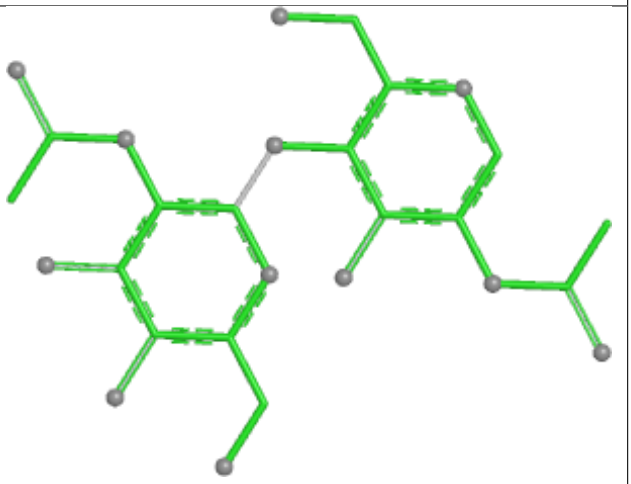

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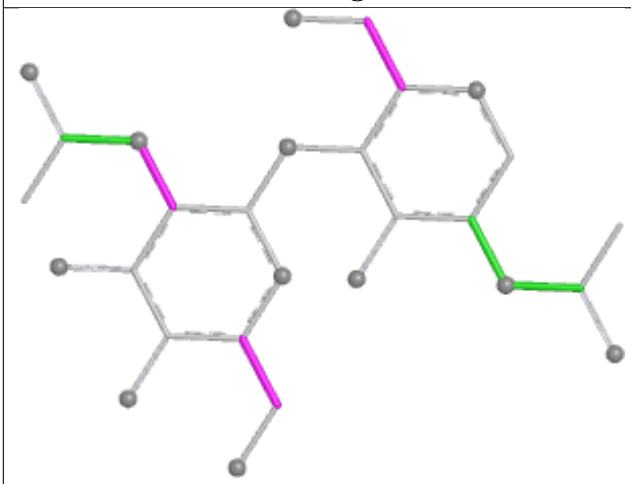

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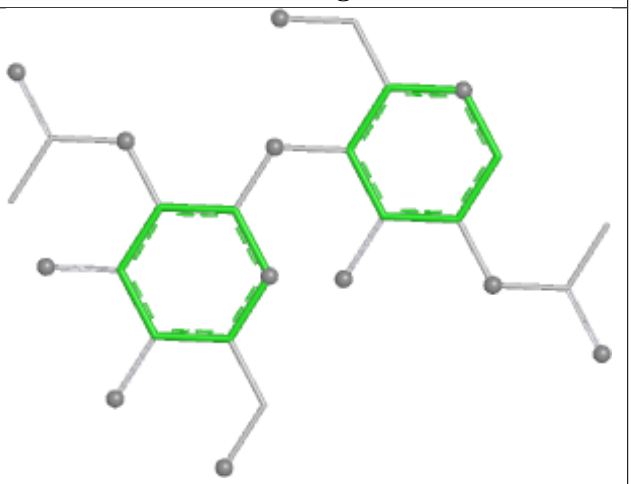
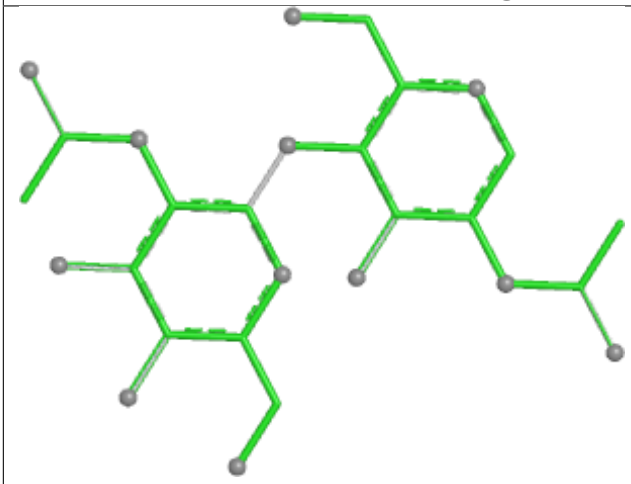


Rings

Oligosaccharide Chain y



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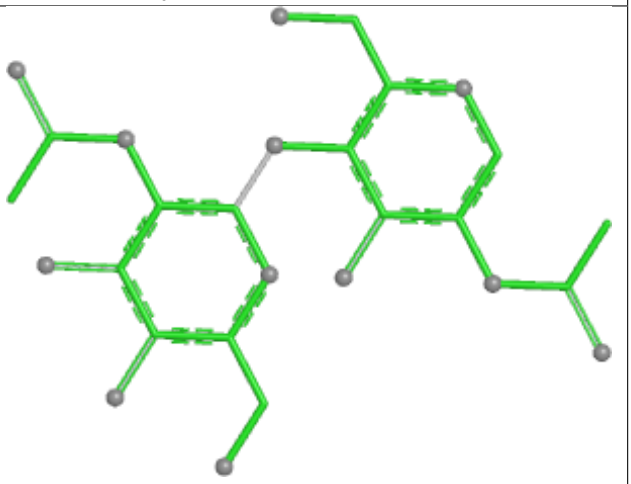

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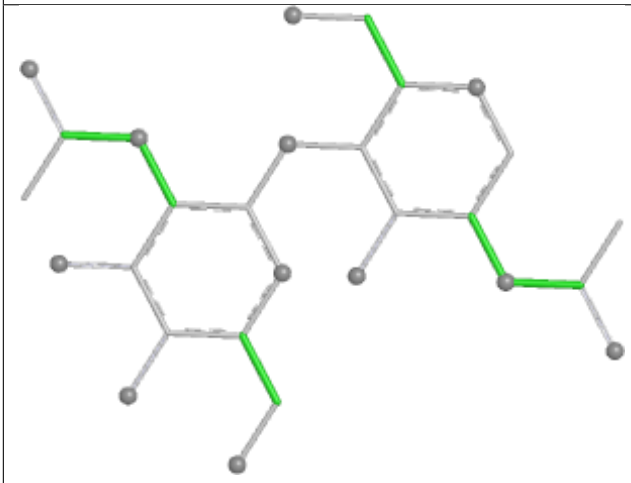

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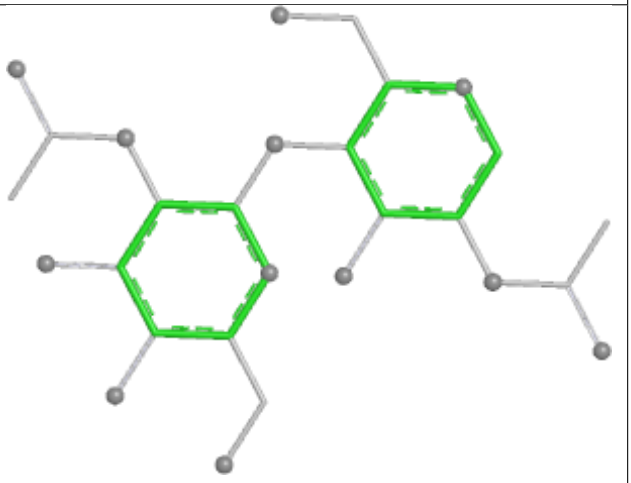
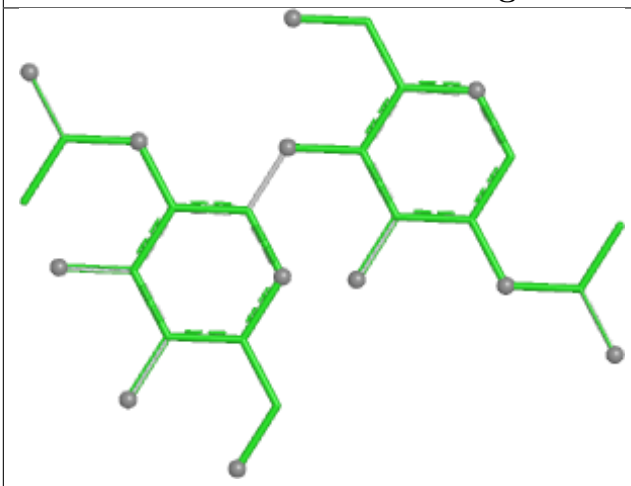


Rings

Oligosaccharide Chain 1



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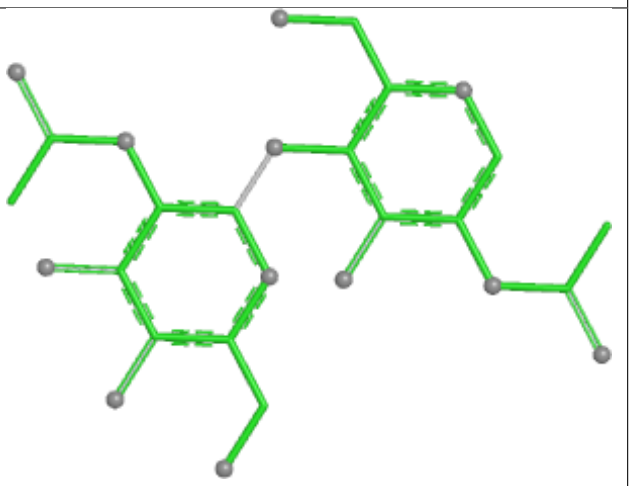

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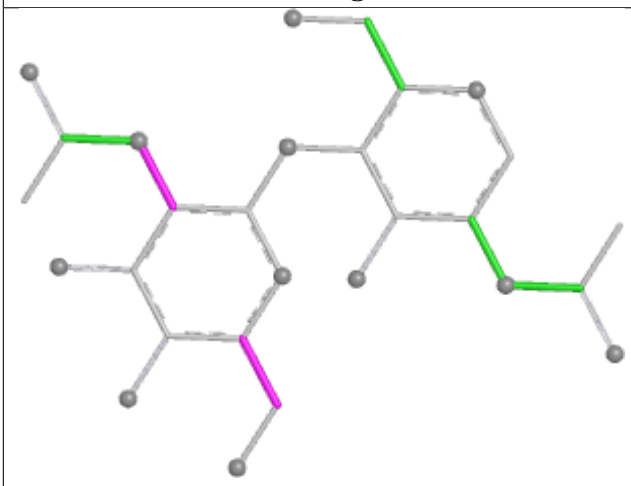

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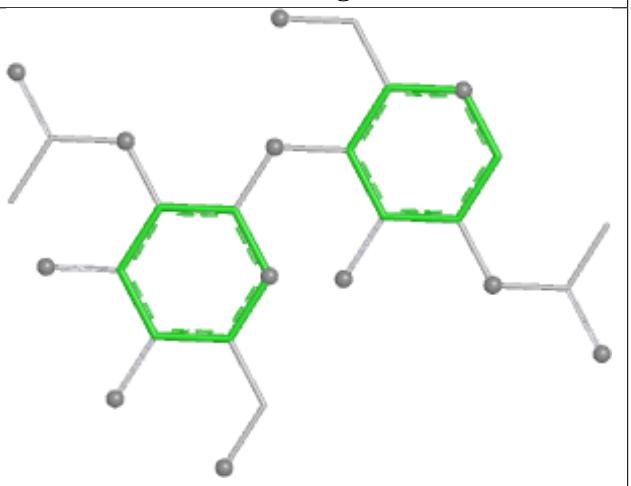
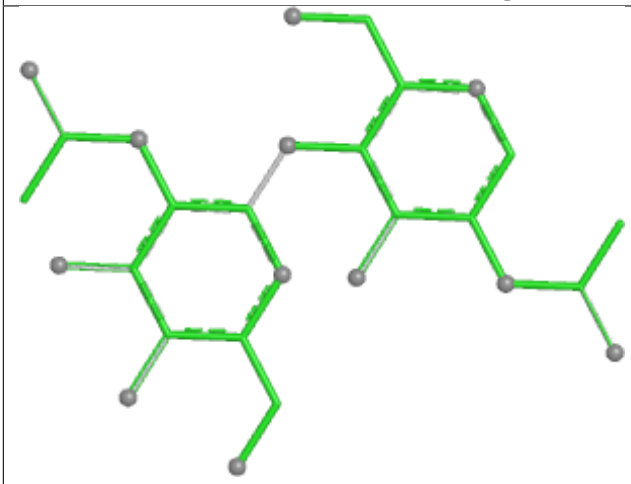


Rings

Oligosaccharide Chain 8



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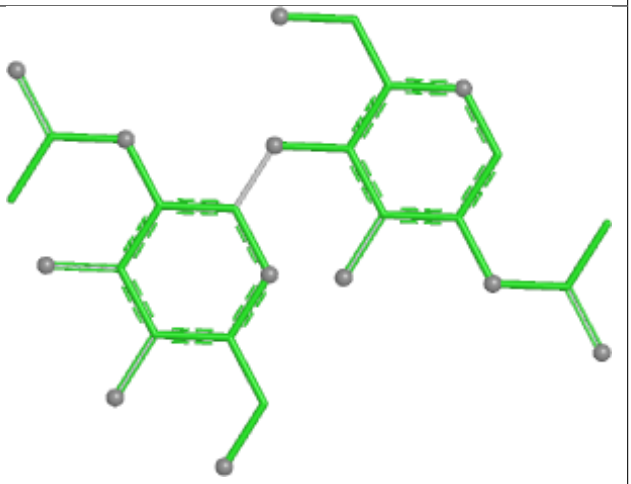

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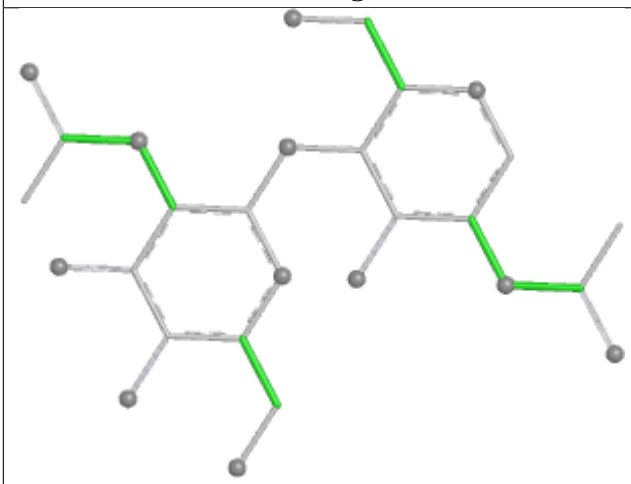

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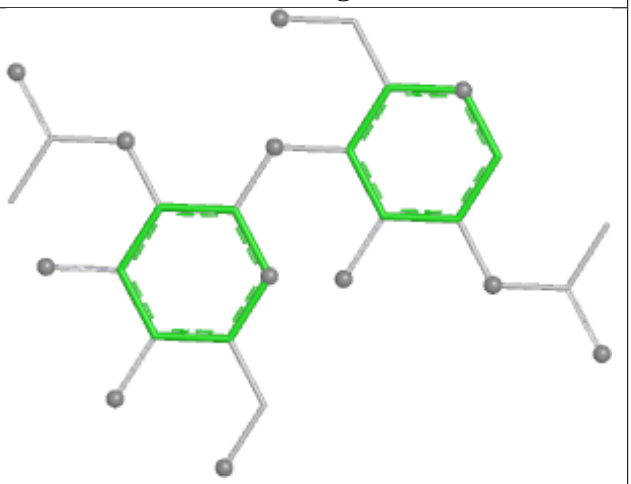
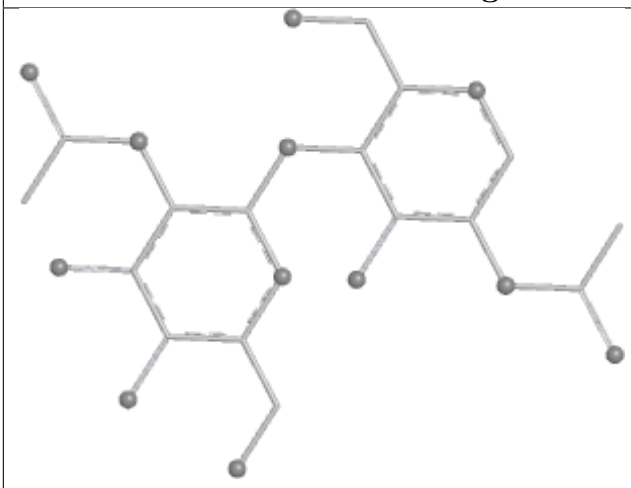


Rings

Oligosaccharide Chain BA



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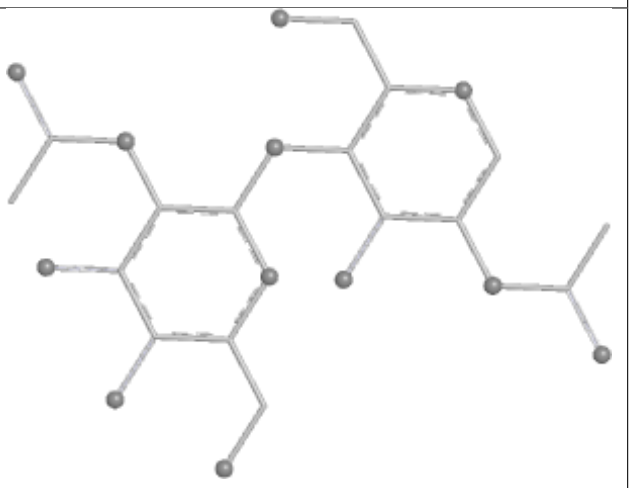

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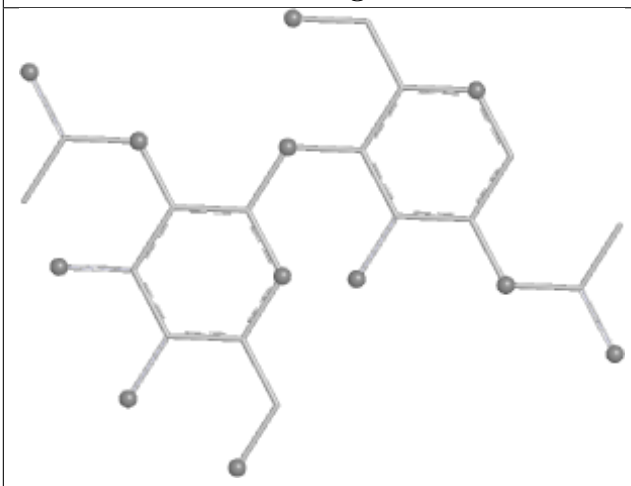

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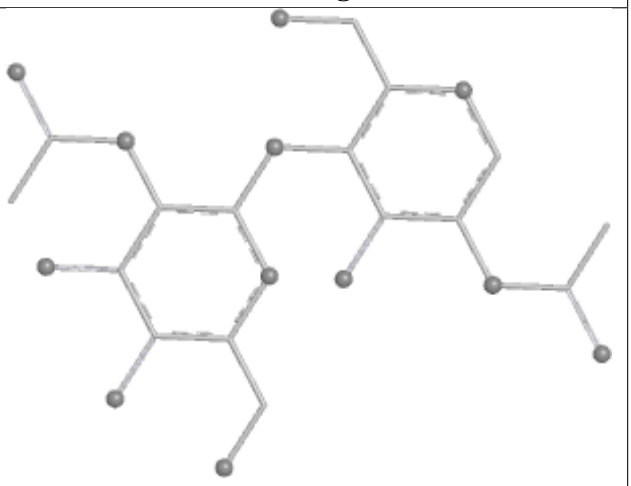
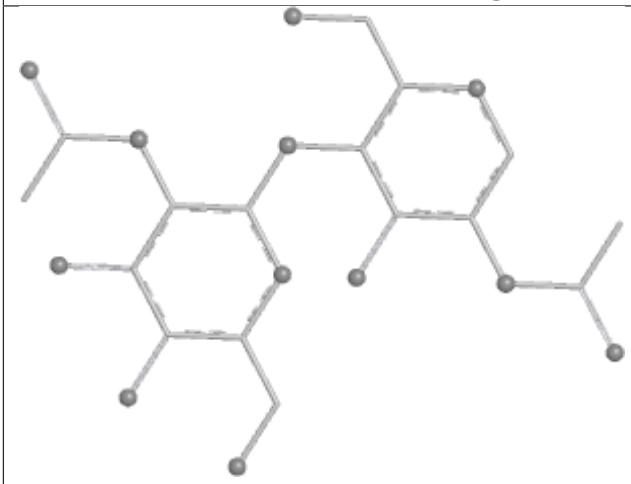


Rings

Oligosaccharide Chain IA



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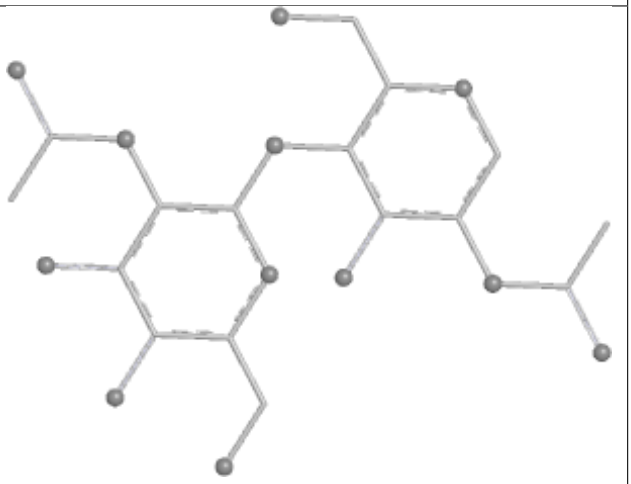
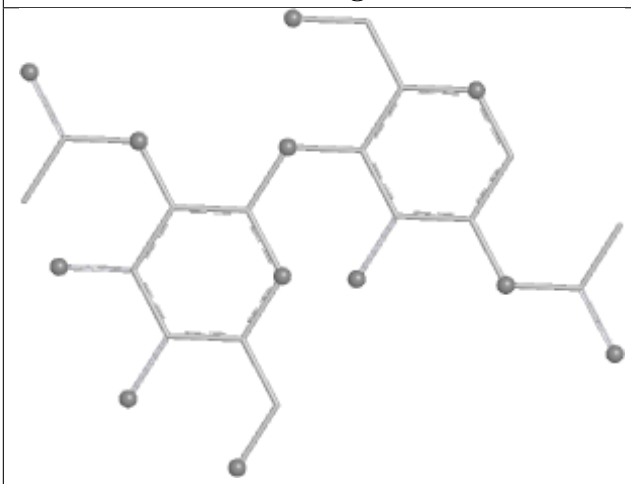


Bond angles



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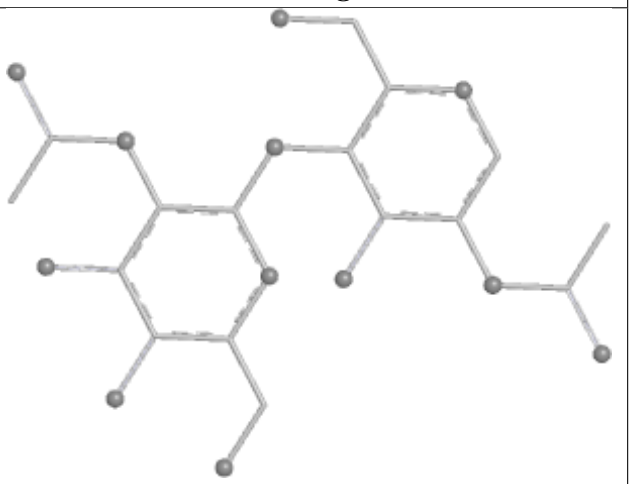
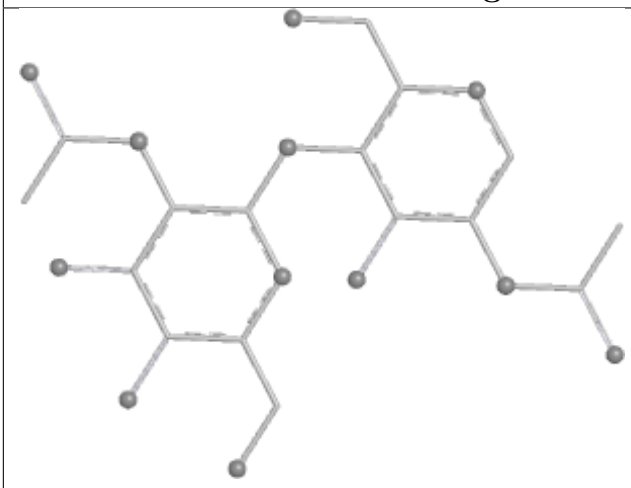
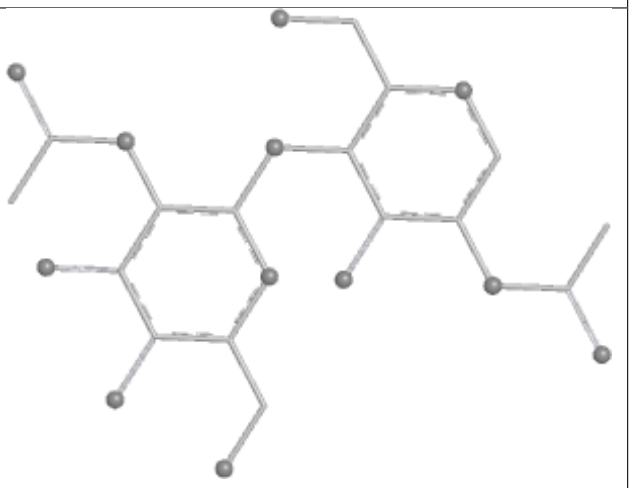


Rings

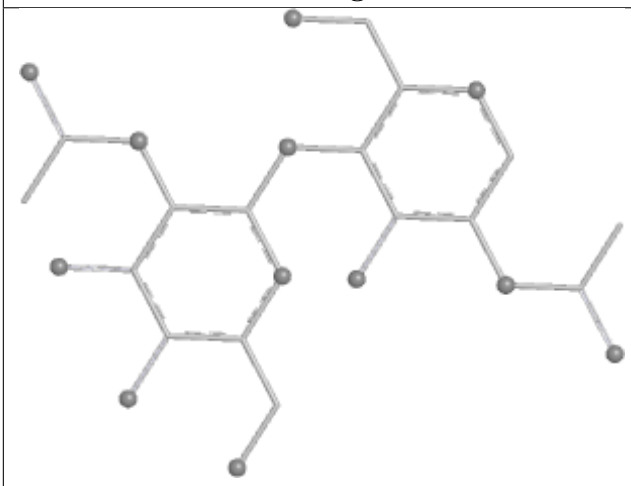
Oligosaccharide Chain LA



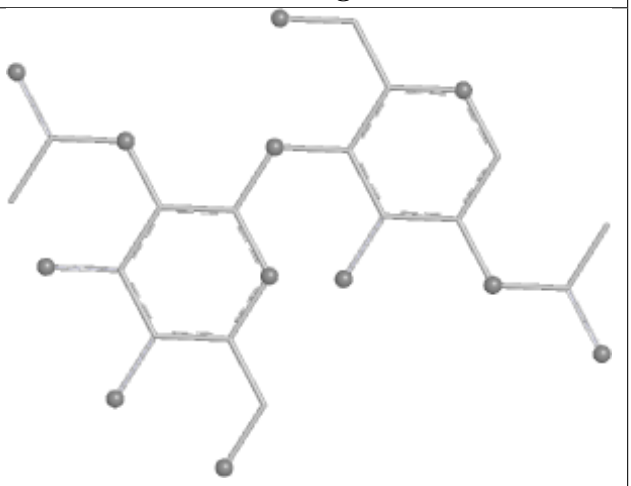
Bond lengths



Bond angles

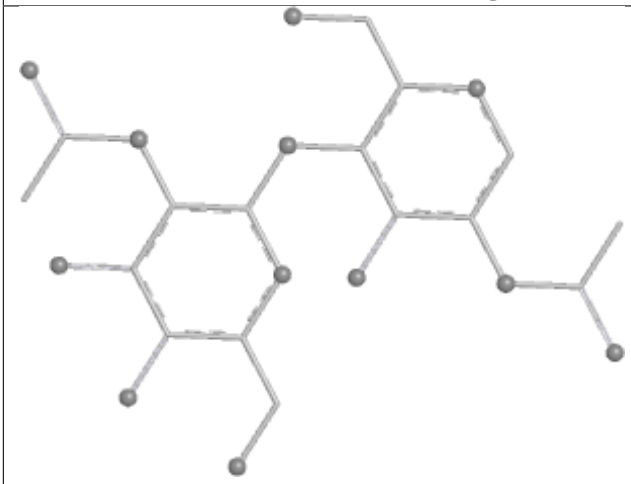


Torsions

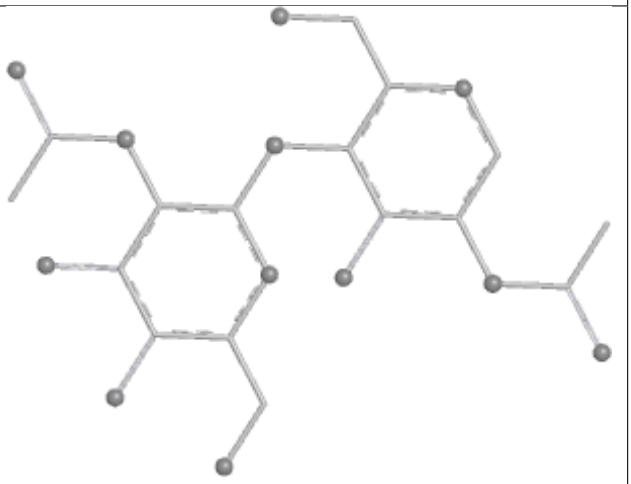


Rings

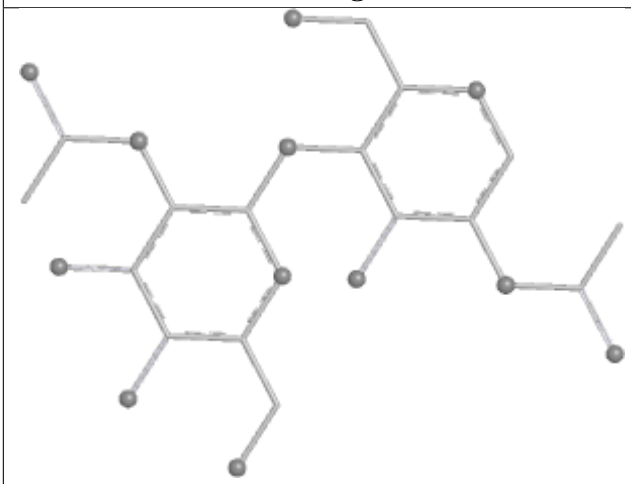
Oligosaccharide Chain SA



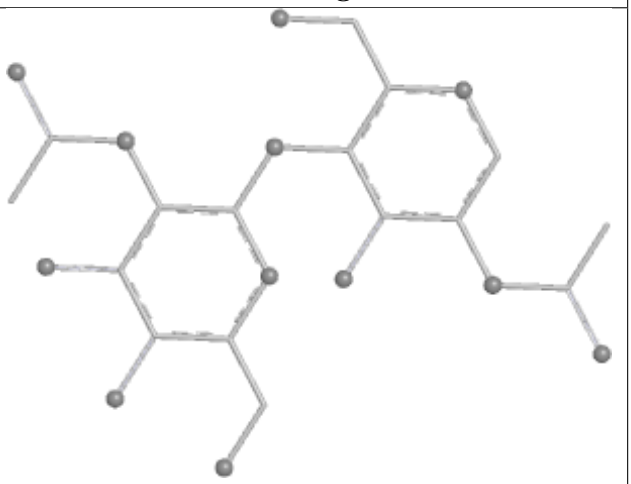
Bond lengths



Bond angles

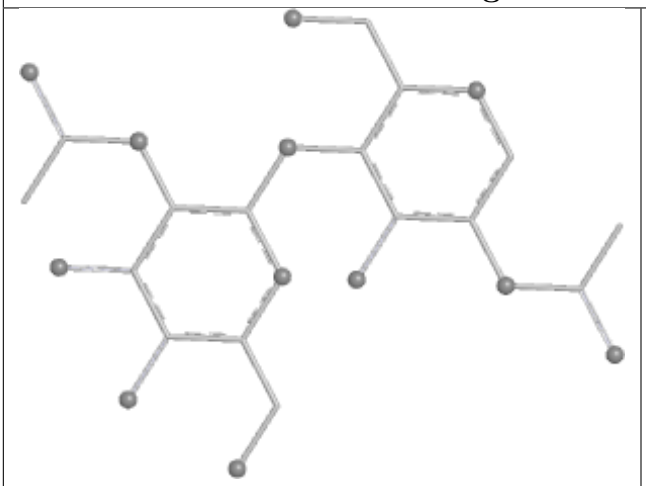


Torsions

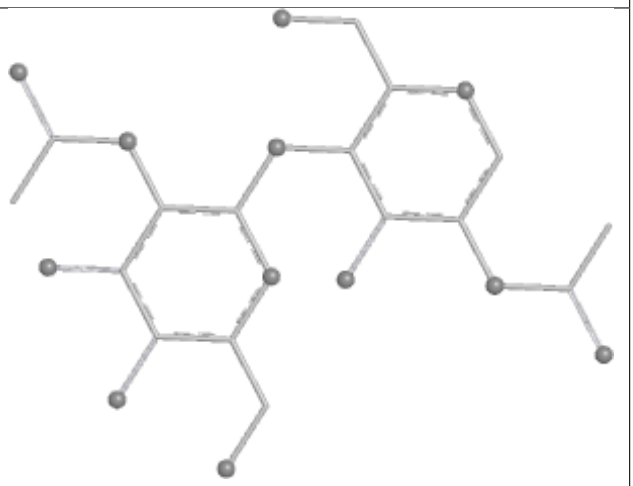


Rings

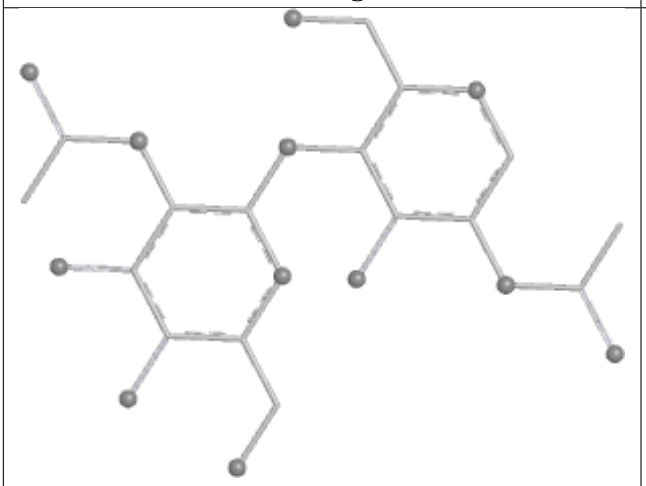
Oligosaccharide Chain VA



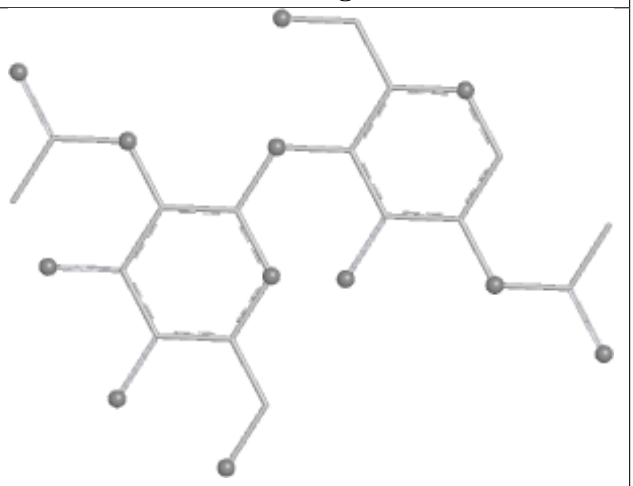
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 48 ligands modelled in this entry, 32 are monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
3	NAG	H	602	1	14,14,15	0.32	0	17,19,21	0.62	1 (5%)
3	NAG	A	602	1	14,14,15	0.31	0	17,19,21	0.61	0
3	NAG	E	601	1	14,14,15	0.65	1 (7%)	17,19,21	0.73	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	D	601	1	14,14,15	0.31	0	17,19,21	0.56	0
3	NAG	D	602	1	14,14,15	0.55	0	17,19,21	0.61	0
3	NAG	C	601	1	14,14,15	0.35	0	17,19,21	0.56	0
3	NAG	F	601	1	14,14,15	0.46	0	17,19,21	0.38	0
3	NAG	E	602	1	14,14,15	0.68	1 (7%)	17,19,21	0.43	0
3	NAG	C	602	1	14,14,15	0.30	0	17,19,21	0.41	0
3	NAG	B	601	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	H	601	1	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	G	601	1	14,14,15	0.62	1 (7%)	17,19,21	0.68	1 (5%)
3	NAG	G	602	1	14,14,15	0.54	0	17,19,21	0.81	1 (5%)
3	NAG	A	601	1	14,14,15	0.31	0	17,19,21	0.43	0
3	NAG	F	602	1	14,14,15	0.37	0	17,19,21	0.59	0
3	NAG	B	602	1	14,14,15	0.34	0	17,19,21	1.44	2 (11%)

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
3	NAG	H	602	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	1	-	1/6/23/26	0/1/1/1
3	NAG	E	601	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	1	-	0/6/23/26	0/1/1/1
3	NAG	D	602	1	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1	-	1/6/23/26	0/1/1/1
3	NAG	F	601	1	-	3/6/23/26	0/1/1/1
3	NAG	E	602	1	-	1/6/23/26	0/1/1/1
3	NAG	C	602	1	-	3/6/23/26	0/1/1/1
3	NAG	B	601	1	-	1/6/23/26	0/1/1/1
3	NAG	H	601	1	-	2/6/23/26	0/1/1/1
3	NAG	G	601	1	-	3/6/23/26	0/1/1/1
3	NAG	G	602	1	-	4/6/23/26	0/1/1/1
3	NAG	A	601	1	-	0/6/23/26	0/1/1/1
3	NAG	F	602	1	-	2/6/23/26	0/1/1/1
3	NAG	B	602	1	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	NAG	C1-C2	2.33	1.55	1.52
3	E	601	NAG	C1-C2	2.17	1.55	1.52
3	G	601	NAG	C1-C2	2.07	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	NAG	C2-N2-C7	4.79	129.32	122.90
3	G	602	NAG	C1-O5-C5	2.66	115.75	112.19
3	E	601	NAG	C1-O5-C5	2.54	115.59	112.19
3	B	602	NAG	C1-C2-N2	2.51	114.38	110.43
3	G	601	NAG	C1-O5-C5	2.26	115.22	112.19
3	H	602	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	C4-C5-C6-O6
3	G	601	NAG	C4-C5-C6-O6
3	F	601	NAG	O5-C5-C6-O6
3	F	602	NAG	O5-C5-C6-O6
3	E	601	NAG	O5-C5-C6-O6
3	F	602	NAG	C4-C5-C6-O6
3	H	601	NAG	O5-C5-C6-O6
3	G	601	NAG	O5-C5-C6-O6
3	C	602	NAG	C8-C7-N2-C2
3	C	602	NAG	O7-C7-N2-C2
3	B	602	NAG	C8-C7-N2-C2
3	B	602	NAG	O7-C7-N2-C2
3	H	602	NAG	O5-C5-C6-O6
3	G	602	NAG	O5-C5-C6-O6
3	F	601	NAG	C4-C5-C6-O6
3	H	601	NAG	C4-C5-C6-O6
3	C	601	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6
3	C	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	G	602	NAG	C4-C5-C6-O6
3	B	602	NAG	C1-C2-N2-C7
3	B	602	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	E	602	NAG	C3-C2-N2-C7
3	G	602	NAG	C1-C2-N2-C7
3	G	601	NAG	C3-C2-N2-C7
3	G	602	NAG	C3-C2-N2-C7
3	F	601	NAG	C3-C2-N2-C7
3	H	602	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	601	NAG	1	0
3	E	602	NAG	2	0
3	C	602	NAG	1	0
3	G	602	NAG	1	0
3	B	602	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	484/503 (96%)	-0.27	4 (0%)	82	77	22, 32, 50, 70	0
1	B	484/503 (96%)	-0.14	5 (1%)	79	73	21, 35, 57, 95	0
1	C	484/503 (96%)	-0.16	2 (0%)	88	85	22, 35, 59, 72	0
1	D	482/503 (95%)	-0.29	2 (0%)	88	85	20, 31, 49, 74	0
1	E	484/503 (96%)	-0.04	5 (1%)	79	73	25, 43, 63, 82	0
1	F	483/503 (96%)	0.11	7 (1%)	73	65	27, 48, 74, 109	0
1	G	484/503 (96%)	-0.10	2 (0%)	88	85	26, 40, 57, 79	0
1	H	484/503 (96%)	-0.06	5 (1%)	79	73	26, 42, 65, 96	0
All	All	3869/4024 (96%)	-0.12	32 (0%)	82	77	20, 38, 63, 109	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	501	ALA	4.8
1	B	500	ALA	4.4
1	C	501	ALA	3.9
1	G	501	ALA	3.9
1	B	501	ALA	3.8
1	H	500	ALA	3.7
1	A	501	ALA	3.4
1	H	501	ALA	3.3
1	F	500	ALA	3.1
1	B	230	ASN	3.0
1	H	499	PRO	3.0
1	A	424	VAL	2.8
1	D	104	ASN	2.7
1	D	499	PRO	2.7
1	E	333	GLY	2.7
1	H	18	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	281	HIS	2.5
1	E	424	VAL	2.5
1	F	18	LEU	2.5
1	B	267	HIS	2.5
1	B	263	TYR	2.4
1	A	104	ASN	2.3
1	F	267	HIS	2.3
1	E	500	ALA	2.3
1	F	424	VAL	2.2
1	H	424	VAL	2.2
1	A	267	HIS	2.2
1	F	333	GLY	2.2
1	C	500	ALA	2.1
1	F	498	ALA	2.1
1	E	281	HIS	2.0
1	F	227	TYR	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	U	2	14/15	0.63	0.14	48,69,78,80	0
2	NAG	N	2	14/15	0.74	0.13	74,78,88,88	0
2	NAG	X	2	14/15	0.76	0.12	73,80,84,86	0
2	NAG	K	2	14/15	0.80	0.12	55,70,80,80	0
2	NAG	X	1	14/15	0.81	0.11	50,60,68,75	0
2	NAG	U	1	14/15	0.84	0.11	31,50,59,66	0
2	NAG	N	1	14/15	0.86	0.11	42,57,72,77	0
2	NAG	K	1	14/15	0.91	0.08	40,50,60,67	0
2	NAG	e	1	14/15	-	-	49,54,64,73	0
2	NAG	e	2	14/15	-	-	71,81,90,90	0
2	NAG	h	1	14/15	-	-	60,68,72,78	0
2	NAG	h	2	14/15	-	-	74,83,90,91	0

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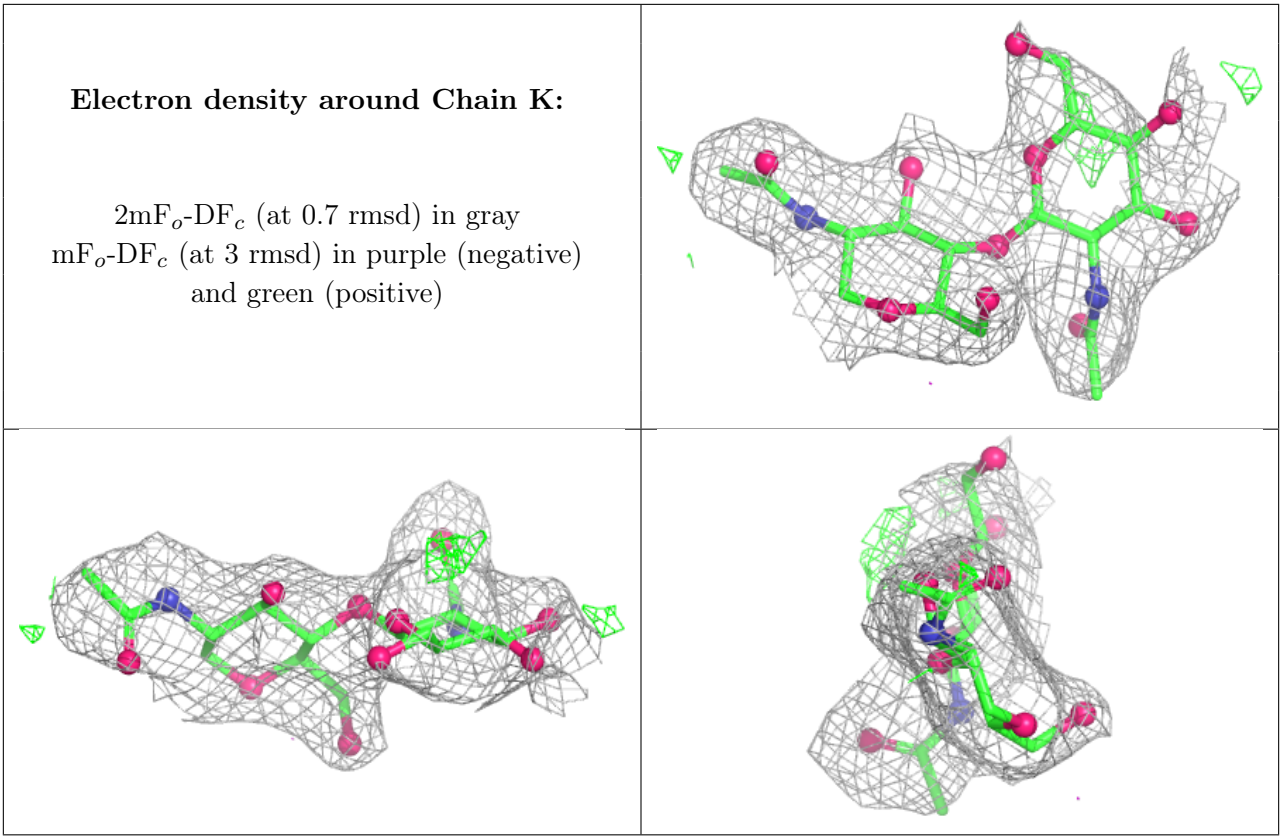
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	o	1	14/15	-	-	48,52,62,68	0
2	NAG	o	2	14/15	-	-	60,72,83,84	0
2	NAG	r	1	14/15	-	-	43,57,68,72	0
2	NAG	r	2	14/15	-	-	74,81,88,88	0
2	NAG	y	1	14/15	-	-	53,68,74,85	0
2	NAG	y	2	14/15	-	-	72,94,102,103	0
2	NAG	1	1	14/15	-	-	51,66,75,77	0
2	NAG	1	2	14/15	-	-	67,86,89,90	0
2	NAG	8	1	14/15	-	-	48,62,77,86	0
2	NAG	8	2	14/15	-	-	77,89,96,100	0
2	NAG	BA	1	14/15	-	-	37,58,76,77	0
2	NAG	BA	2	14/15	-	-	88,95,100,101	0
2	NAG	IA	1	14/15	-	-	63,71,78,86	0
2	NAG	IA	2	14/15	-	-	78,91,98,99	0
2	NAG	LA	1	14/15	-	-	52,59,71,72	0
2	NAG	LA	2	14/15	-	-	73,79,83,85	0
2	NAG	SA	1	14/15	-	-	54,64,71,72	0
2	NAG	SA	2	14/15	-	-	56,76,83,84	0
2	NAG	VA	1	14/15	-	-	53,69,76,80	0
2	NAG	VA	2	14/15	-	-	77,86,90,90	0

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

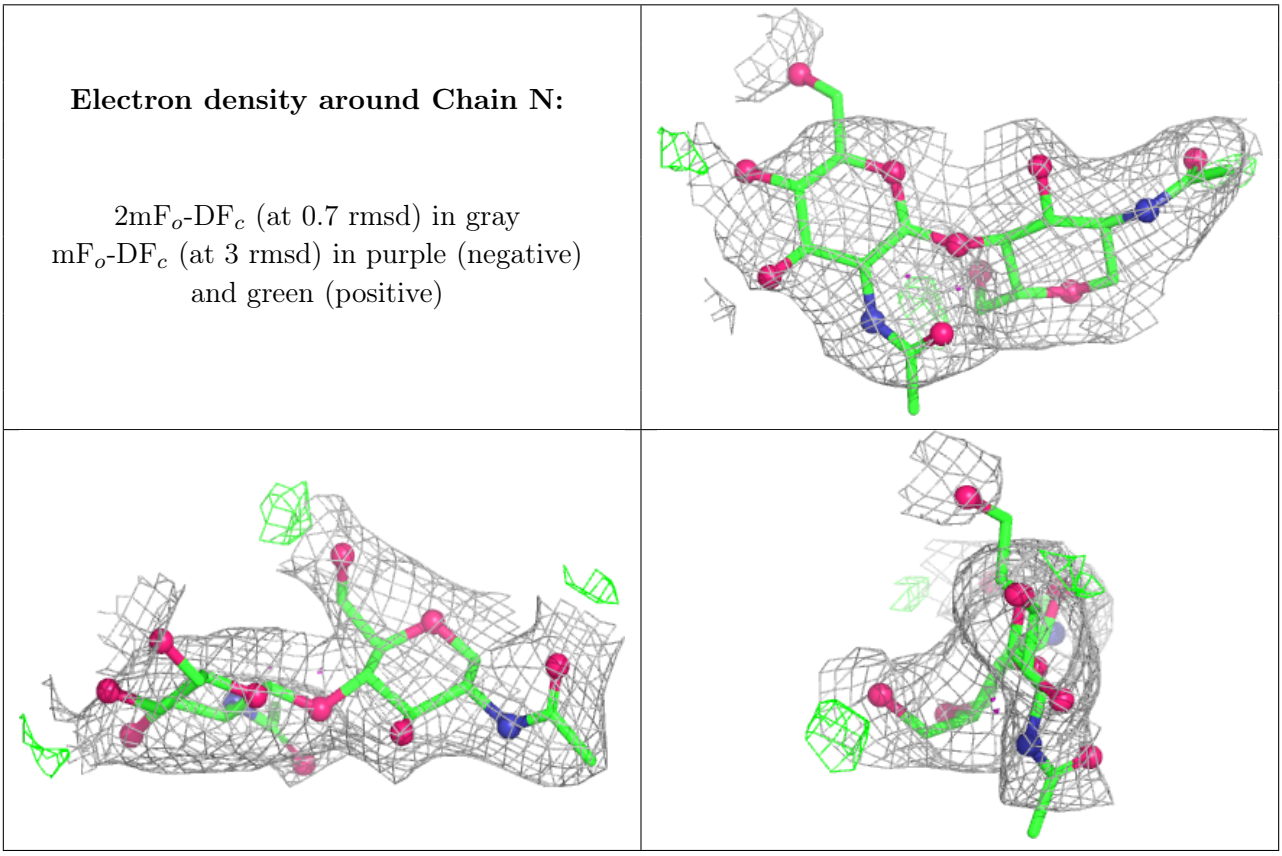
Electron density around Chain K:

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



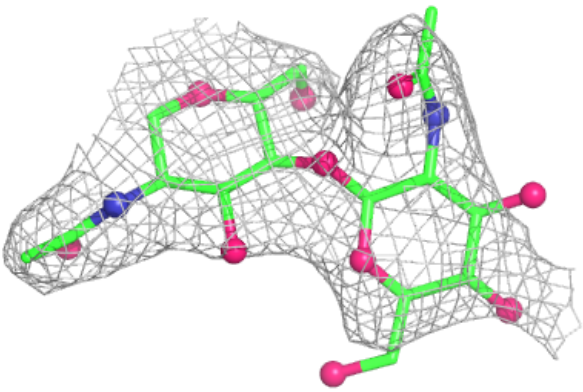
Electron density around Chain N:

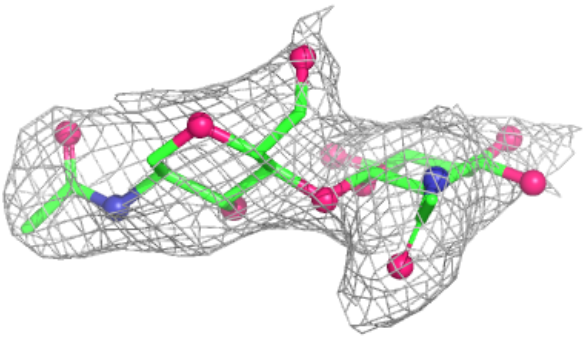
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

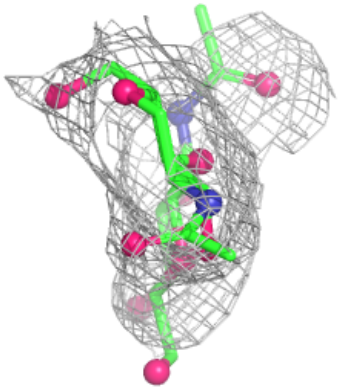


Electron density around Chain U:

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

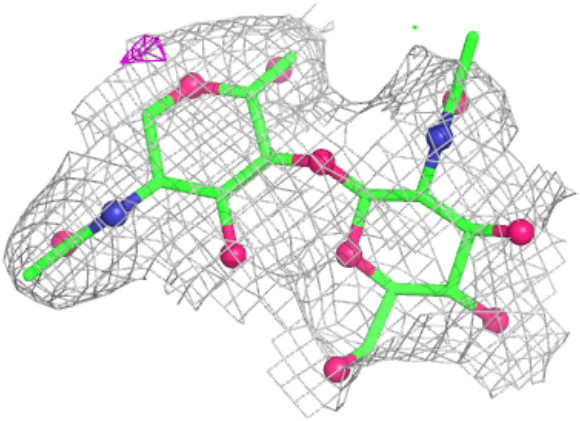


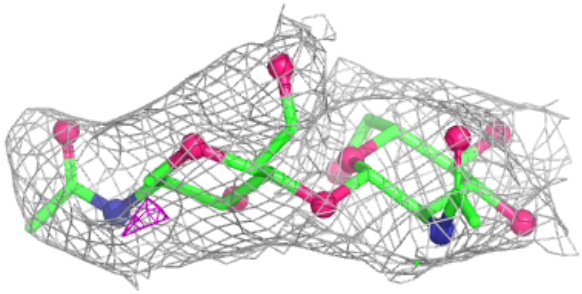


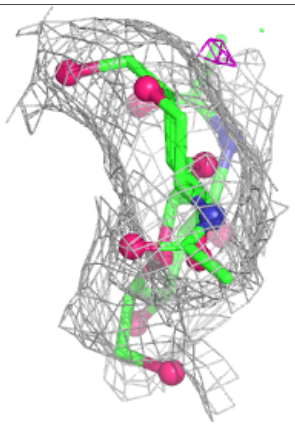


Electron density around Chain X:

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

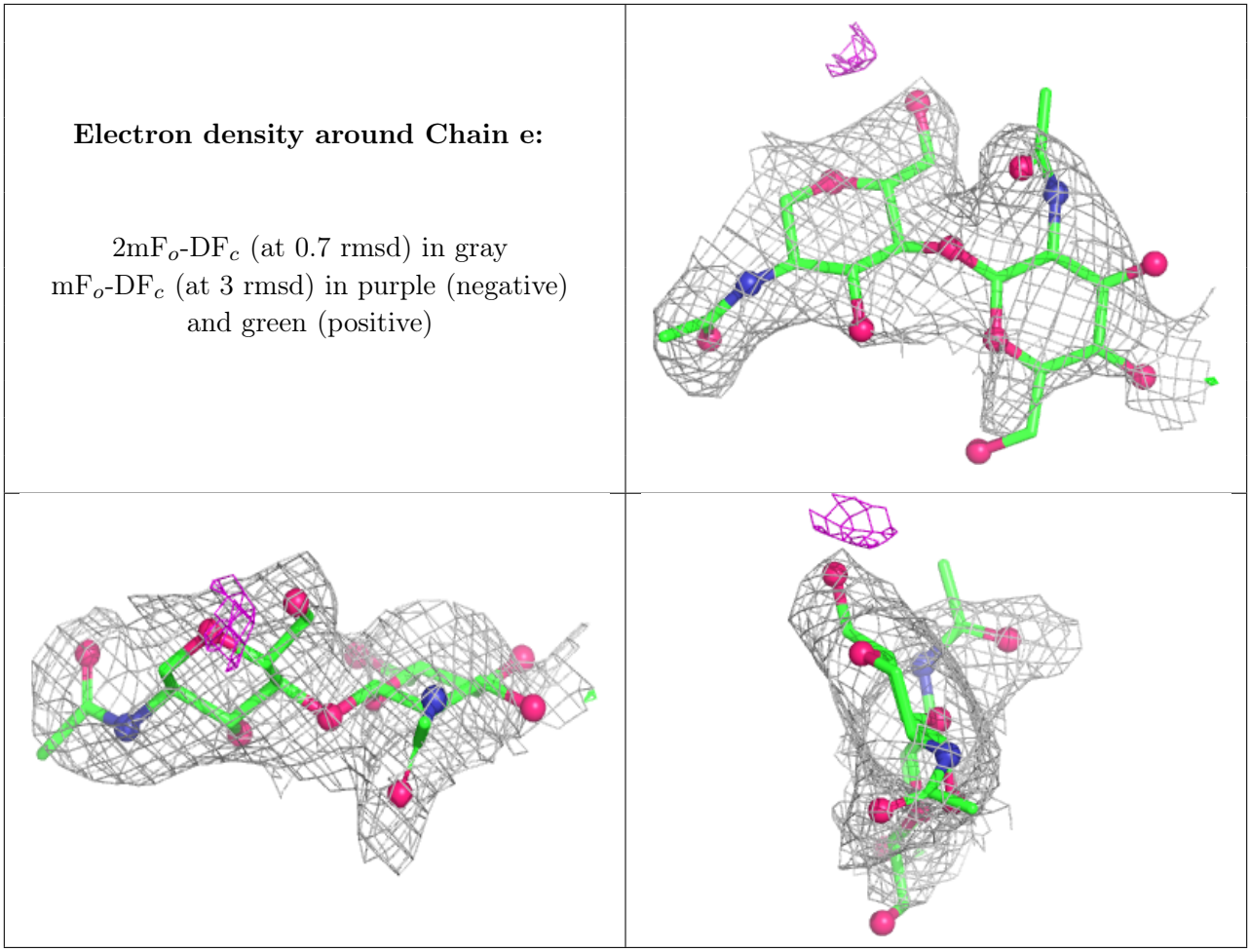






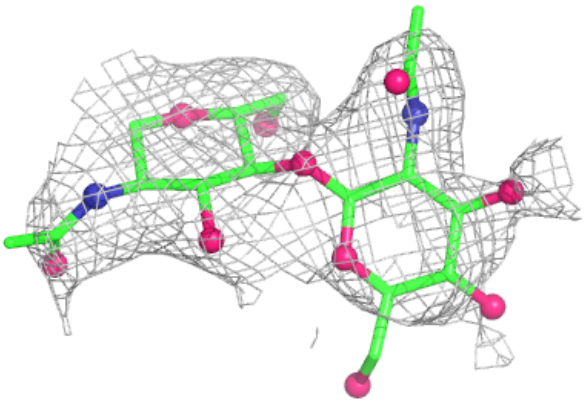
Electron density around Chain e:

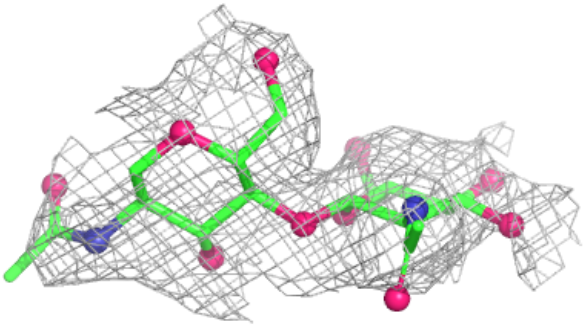
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

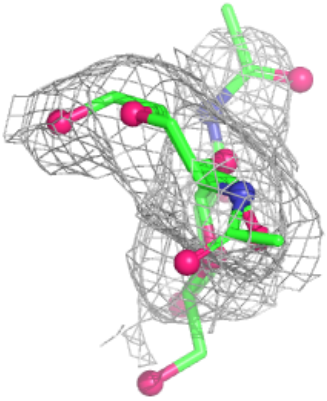


Electron density around Chain h:

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

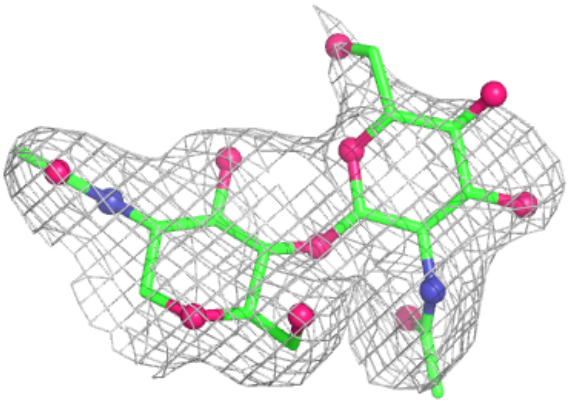


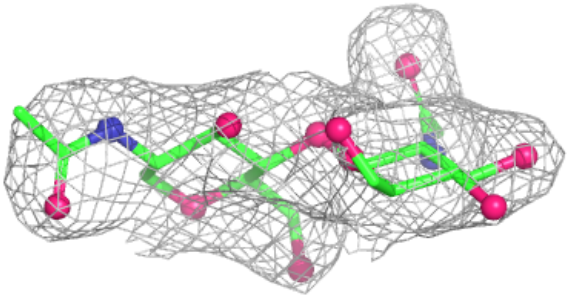


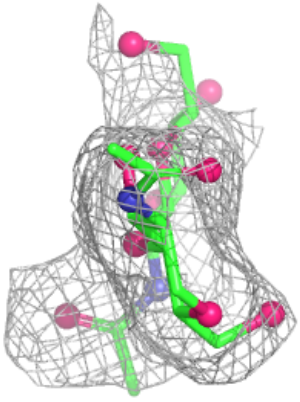


Electron density around Chain o:

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

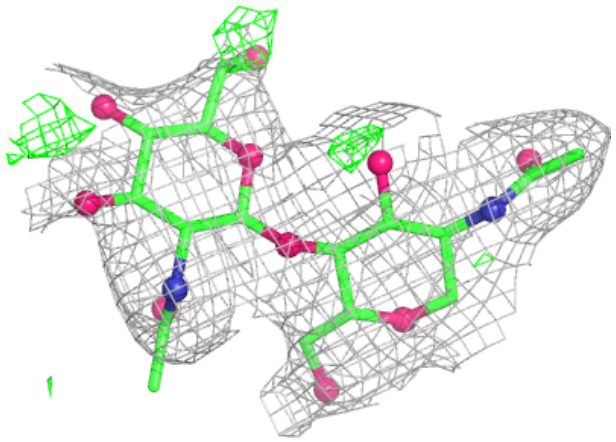


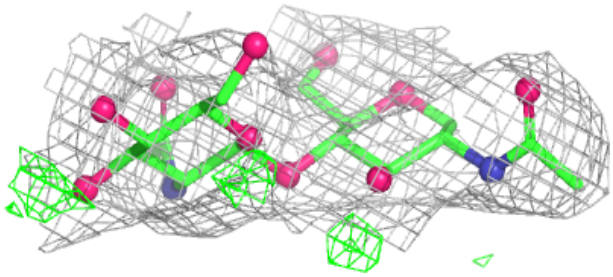




Electron density around Chain r:

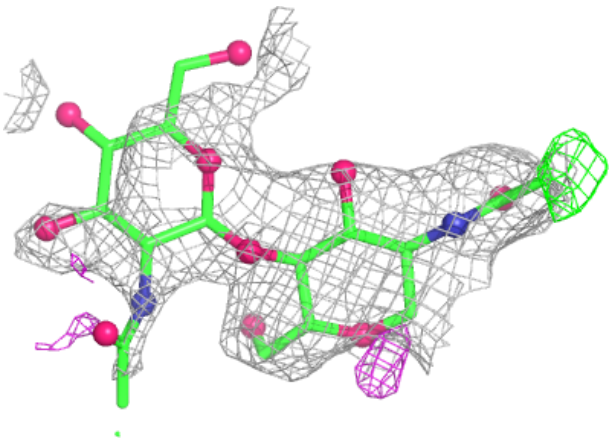
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

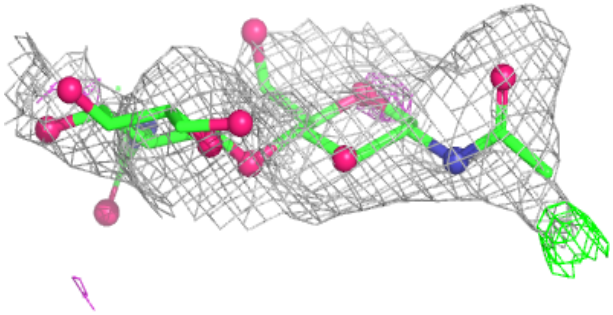


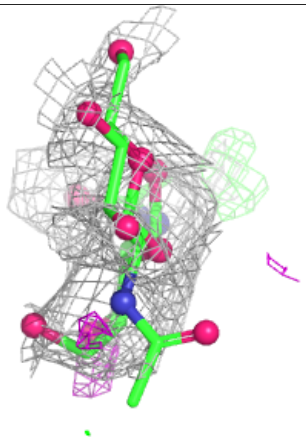


Electron density around Chain y:

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

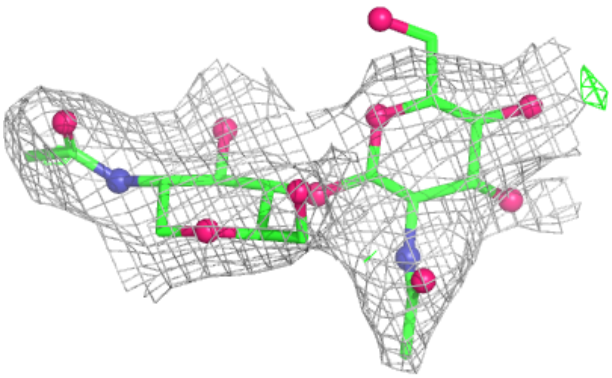


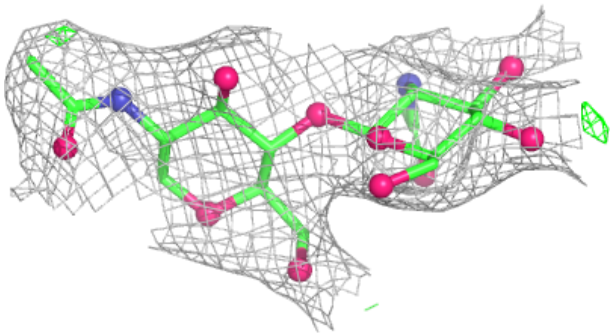


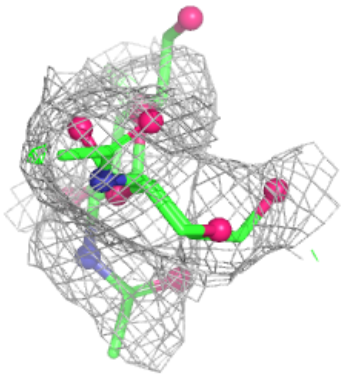


Electron density around Chain 1:

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

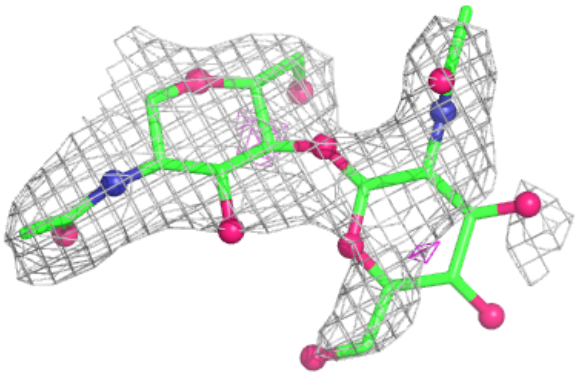


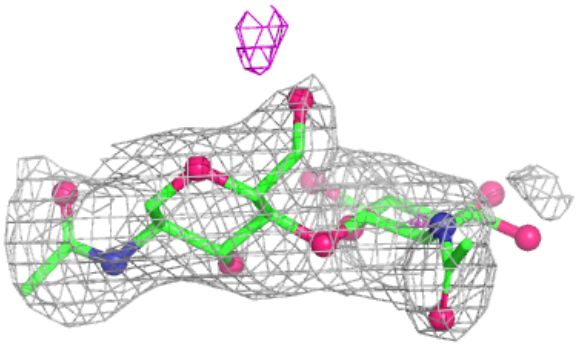


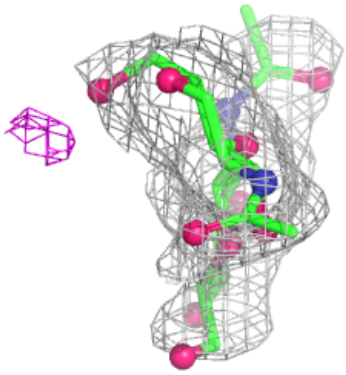


Electron density around Chain 8:

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

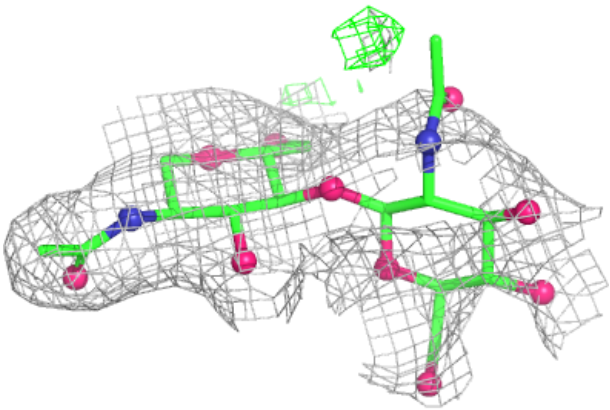


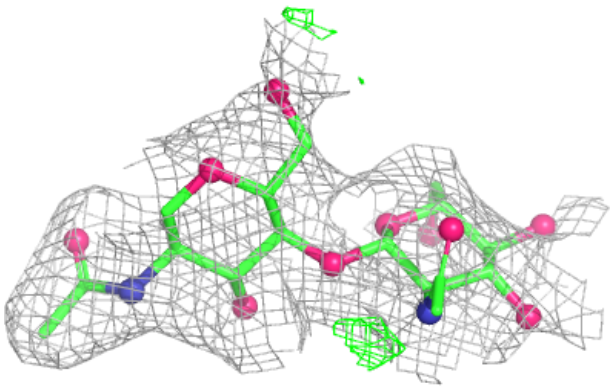


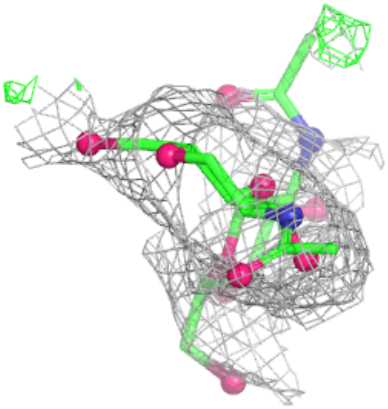


Electron density around Chain BA:

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

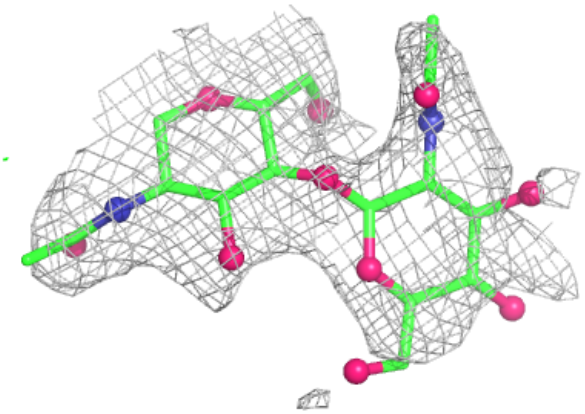


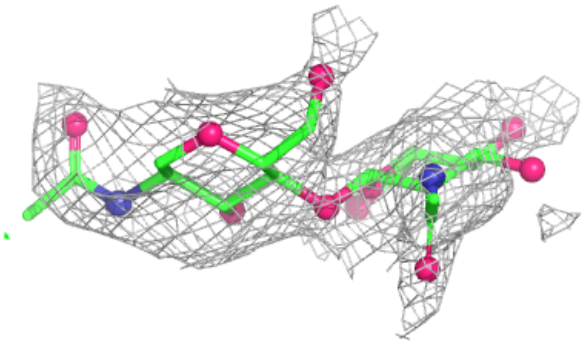


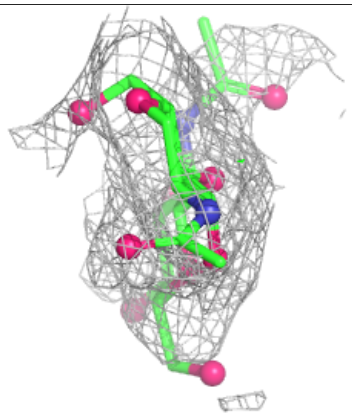


Electron density around Chain IA:

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

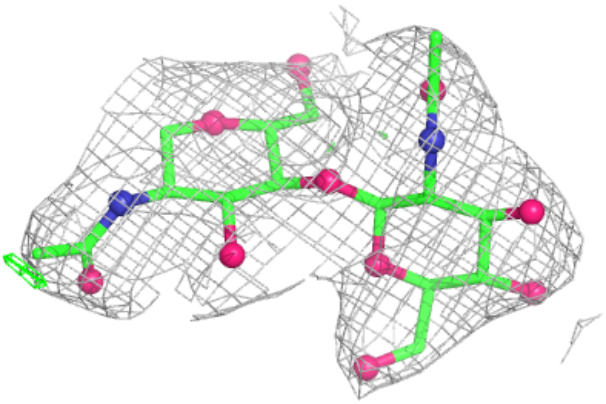


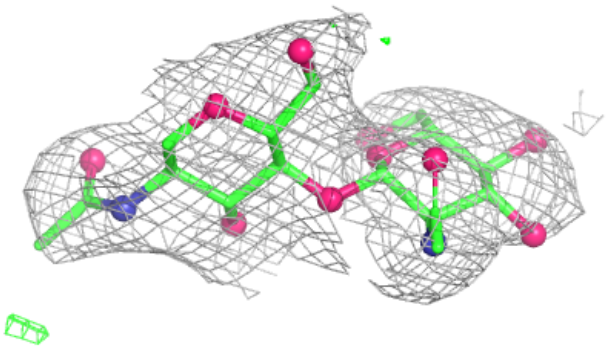


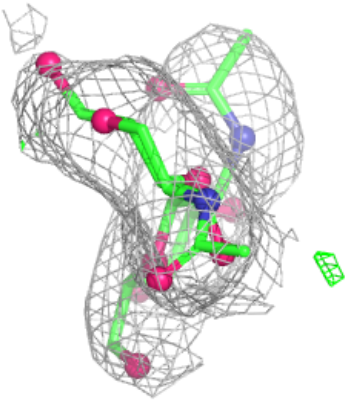


Electron density around Chain LA:

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

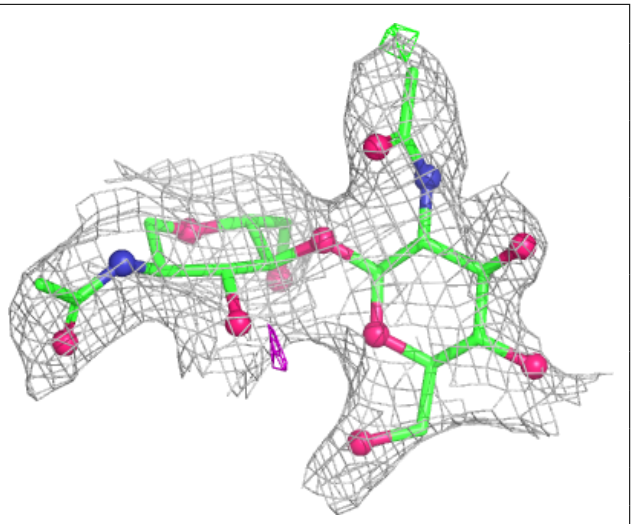


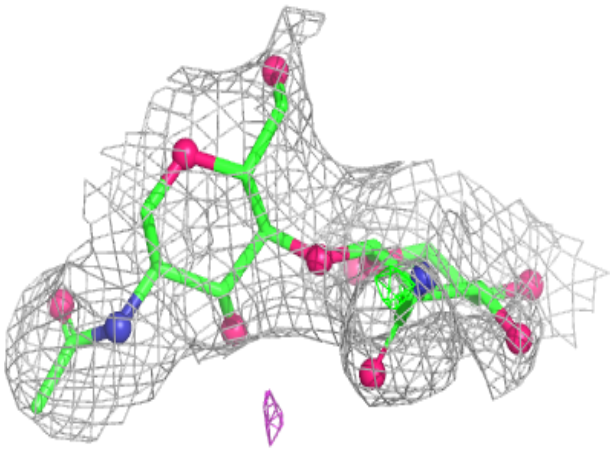


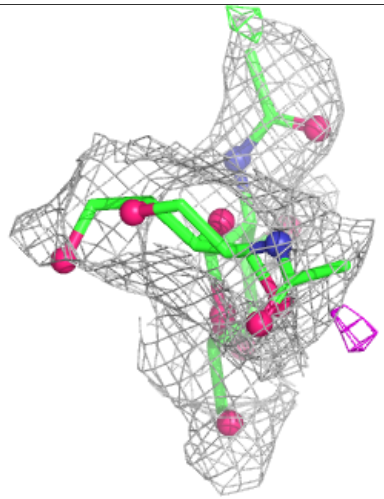


Electron density around Chain SA:

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

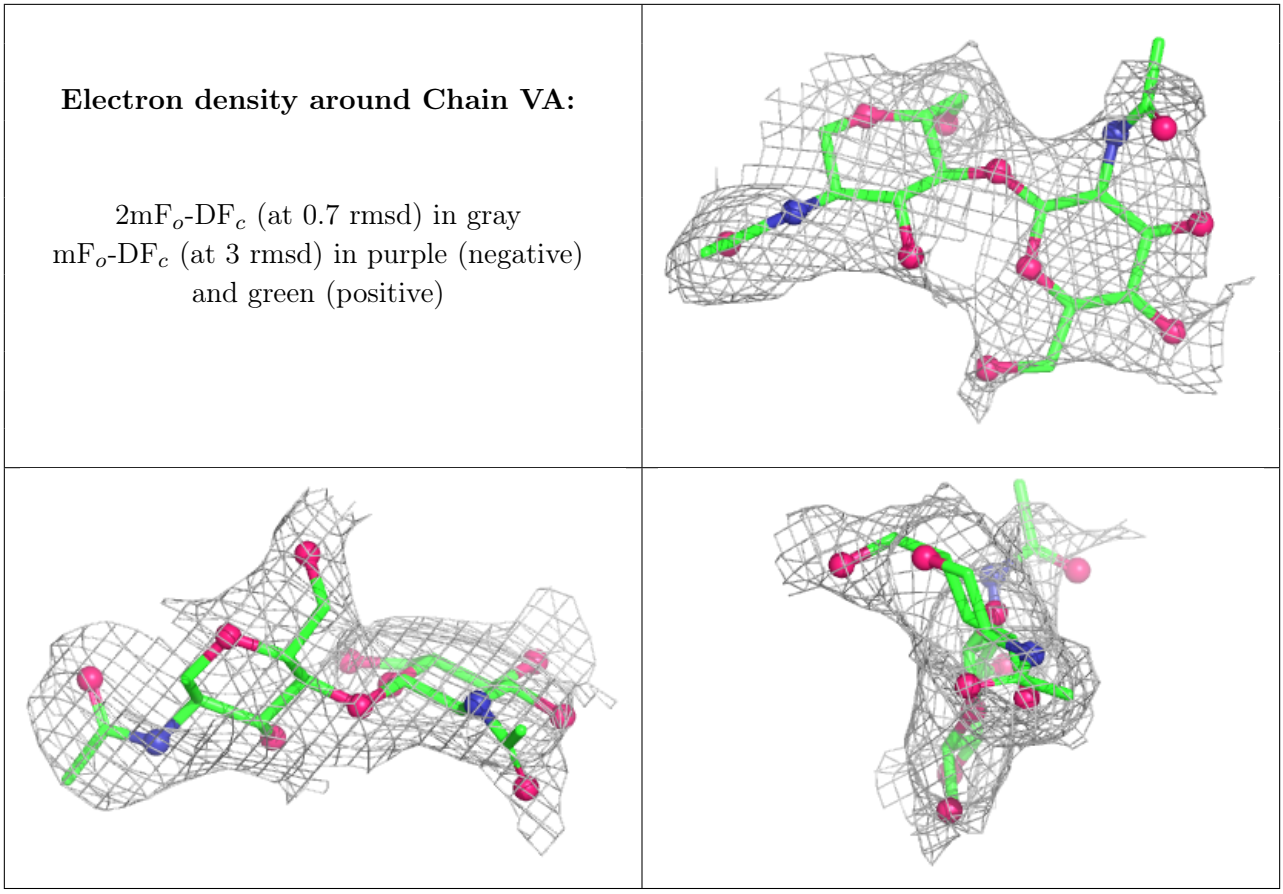






Electron density around Chain VA:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	E	602	14/15	0.17	0.22	85,96,103,105	0
3	NAG	H	601	14/15	0.45	0.20	63,88,92,95	0
3	NAG	B	601	14/15	0.53	0.19	71,80,87,92	0
3	NAG	D	602	14/15	0.55	0.18	48,65,73,74	0
3	NAG	H	602	14/15	0.58	0.16	58,74,82,83	0
3	NAG	A	601	14/15	0.59	0.15	54,71,78,78	0
3	NAG	F	602	14/15	0.63	0.17	65,73,84,85	0
3	NAG	A	602	14/15	0.64	0.16	53,65,75,79	0
3	NAG	F	601	14/15	0.64	0.16	85,95,106,106	0
3	NAG	C	601	14/15	0.68	0.15	78,83,90,91	0
3	NAG	C	602	14/15	0.69	0.12	59,70,80,81	0
3	NAG	G	602	14/15	0.71	0.17	60,67,77,79	0
3	NAG	G	601	14/15	0.71	0.14	79,88,95,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	D	601	14/15	0.72	0.14	56,69,76,79	0
3	NAG	E	601	14/15	0.74	0.13	67,73,83,85	0
3	NAG	B	602	14/15	0.74	0.14	54,62,67,68	0
4	MG	H	603	1/1	0.74	0.12	59,59,59,59	0
4	MG	B	603	1/1	0.86	0.12	51,51,51,51	0
4	MG	G	603	1/1	0.89	0.07	51,51,51,51	0
4	MG	F	603	1/1	0.89	0.10	60,60,60,60	0
6	CA	H	605	1/1	0.91	0.08	50,50,50,50	0
5	ZN	B	606	1/1	0.92	0.12	80,80,80,80	0
5	ZN	C	604	1/1	0.93	0.05	35,35,35,35	0
4	MG	C	603	1/1	0.94	0.08	43,43,43,43	0
6	CA	G	605	1/1	0.94	0.07	40,40,40,40	0
5	ZN	C	606	1/1	0.94	0.12	71,71,71,71	0
4	MG	E	603	1/1	0.95	0.07	50,50,50,50	0
6	CA	D	605	1/1	0.95	0.04	37,37,37,37	0
6	CA	F	605	1/1	0.95	0.06	61,61,61,61	0
6	CA	A	605	1/1	0.96	0.06	42,42,42,42	0
5	ZN	A	606	1/1	0.96	0.08	68,68,68,68	0
6	CA	C	605	1/1	0.96	0.07	43,43,43,43	0
5	ZN	B	604	1/1	0.96	0.22	69,69,69,69	0
4	MG	D	603	1/1	0.96	0.07	44,44,44,44	0
5	ZN	H	604	1/1	0.96	0.07	43,43,43,43	0
6	CA	E	605	1/1	0.96	0.04	53,53,53,53	0
5	ZN	E	606	1/1	0.97	0.06	62,62,62,62	0
5	ZN	D	606	1/1	0.97	0.05	67,67,67,67	0
4	MG	A	603	1/1	0.97	0.15	41,41,41,41	0
5	ZN	F	606	1/1	0.97	0.11	75,75,75,75	0
5	ZN	G	606	1/1	0.98	0.06	68,68,68,68	0
6	CA	B	605	1/1	0.98	0.05	42,42,42,42	0
5	ZN	E	604	1/1	0.98	0.11	43,43,43,43	0
5	ZN	A	604	1/1	0.98	0.04	29,29,29,29	0
5	ZN	H	606	1/1	0.98	0.04	73,73,73,73	0
5	ZN	F	604	1/1	0.98	0.04	41,41,41,41	0
5	ZN	G	604	1/1	0.99	0.05	34,34,34,34	0
5	ZN	D	604	1/1	0.99	0.04	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.