Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 06:01 PM EDT

PDB ID	:	6M8P
Title	:	Human ERAP1 bound to phosphinic pseudotripeptide inhibitor DG013
Authors	:	Maben, Z.; Stern, L.J.
Deposited on	:	2018-08-22
Resolution	:	3.31 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 (i) 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 (i)) were used in the production of this report:

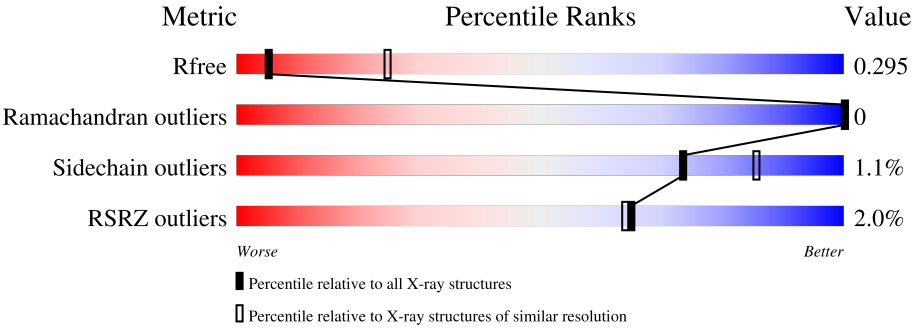
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	899	95%
1	B	899	95%
1	C	899	95%
1	D	899	95%
1	E	899	95%
1	F	899	95%

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Mol	Chain	Length	Quality of chain
1	G	899	95%
1	H	899	95%
1	I	899	95%
1	J	899	95%
1	K	899	.% 95%
1	L	899	95%
1	M	899	95%
1	N	899	2% 95%
1	O	899	2% 95%
1	P	899	3% 95%
1	Q	899	2% 95%
1	R	899	3% 95%
1	S	899	6% 95%
1	T	899	7% 95%
1	U	899	6% 95%
1	V	899	8% 95%
2	0	3	100%
2	1	3	33% 67%
2	2	3	100%
2	3	3	33% 67%
2	4	3	100%
2	5	3	33% 67%
2	6	3	100%
2	7	3	33% 67%
2	8	3	100%

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Mol	Chain	Length	Quality of chain
2	9	3	33% 67%
2	AA	3	100%
2	BA	3	33% 67%
2	CA	3	100%
2	DA	3	33% 67%
2	W	3	100%
2	X	3	33% 67%
2	Y	3	100%
2	Z	3	33% 67%
2	a	3	100%
2	b	3	33% 67%
2	c	3	100%
2	d	3	33% 67%
2	e	3	100%
2	f	3	33% 67%
2	g	3	100%
2	h	3	33% 67%
2	i	3	100%
2	j	3	33% 67%
2	k	3	100%
2	l	3	33% 67%
2	m	3	100%
2	n	3	33% 67%
2	o	3	100%
2	p	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	q	3	100%
2	r	3	33% 67%
2	s	3	100%
2	t	3	33% 67%
2	u	3	100%
2	v	3	33% 67%
2	w	3	100%
2	x	3	33% 67%
2	y	3	100%
2	z	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	1	2	-	-	-	X
2	NAG	3	2	-	-	-	X
2	BMA	3	3	-	-	-	X
2	BMA	5	3	-	-	-	X
2	NAG	7	2	-	-	-	X
2	BMA	7	3	-	-	-	X
2	NAG	8	2	-	-	-	X
2	NAG	9	2	-	-	-	X
2	BMA	9	3	-	-	-	X
2	BMA	AA	3	-	-	-	X
2	NAG	BA	2	-	-	-	X
2	BMA	BA	3	-	-	-	X
2	NAG	DA	1	-	-	-	X
2	NAG	DA	2	-	-	-	X
2	BMA	DA	3	-	-	-	X
2	NAG	X	2	-	-	-	X
2	NAG	Z	2	-	-	-	X
2	BMA	Z	3	-	-	-	X
2	NAG	b	2	-	-	-	X
2	NAG	d	2	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BMA	d	3	-	-	-	X
2	NAG	f	2	-	-	-	X
2	BMA	f	3	-	-	-	X
2	NAG	h	1	-	-	-	X
2	NAG	h	2	-	-	-	X
2	BMA	h	3	-	-	-	X
2	NAG	j	2	-	-	-	X
2	BMA	j	3	-	-	-	X
2	NAG	l	2	-	-	-	X
2	BMA	l	3	-	-	-	X
2	NAG	n	2	-	-	-	X
2	BMA	n	3	-	-	-	X
2	NAG	p	2	-	-	-	X
2	BMA	p	3	-	-	-	X
2	BMA	q	3	-	-	-	X
2	BMA	r	3	-	-	-	X
2	NAG	t	2	-	-	-	X
2	BMA	t	3	-	-	-	X
2	NAG	v	2	-	-	-	X
2	BMA	v	3	-	-	-	X
2	NAG	x	2	-	-	-	X
2	BMA	x	3	-	-	-	X
2	NAG	z	2	-	-	-	X
2	BMA	z	3	-	-	-	X
5	SO4	Q	1007	-	-	-	X
5	SO4	Q	1014	-	-	-	X
5	SO4	R	1007	-	-	-	X
5	SO4	R	1008	-	-	-	X
5	SO4	S	1009	-	-	-	X
5	SO4	T	1016	-	-	-	X
5	SO4	U	1006	-	-	-	X
5	SO4	U	1017	-	-	-	X
5	SO4	V	1007	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 155927 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 Endoplasmic reticulum aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	861	6888	4448	1137	1269	34	0	4	0
1	B	861	6888	4448	1137	1269	34	0	4	0
1	C	861	6890	4449	1138	1269	34	0	4	0
1	D	861	6891	4449	1137	1271	34	0	4	0
1	E	861	6888	4448	1137	1269	34	0	4	0
1	F	861	6891	4449	1137	1271	34	0	4	0
1	G	861	6888	4448	1137	1269	34	0	4	0
1	H	861	6888	4448	1137	1269	34	0	4	0
1	I	861	6888	4448	1137	1269	34	0	4	0
1	J	861	6888	4448	1137	1269	34	0	4	0
1	K	861	6888	4448	1137	1269	34	0	4	0
1	L	861	6888	4448	1137	1269	34	0	4	0
1	M	861	6888	4448	1137	1269	34	0	4	0
1	N	861	6888	4448	1137	1269	34	0	4	0
1	O	861	6888	4448	1137	1269	34	0	4	0
1	P	861	6888	4448	1137	1269	34	0	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	861	6888	4448	1137	1269	34	0	4	0
1	R	861	6888	4448	1137	1269	34	0	4	0
1	S	861	6888	4448	1137	1269	34	0	4	0
1	T	861	6888	4448	1137	1269	34	0	4	0
1	U	861	6888	4448	1137	1269	34	0	4	0
1	V	861	6888	4448	1137	1269	34	0	4	0

There are 968 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	HIS	-	expression tag	UNP Q9NZ08
A	27	HIS	-	expression tag	UNP Q9NZ08
A	28	HIS	-	expression tag	UNP Q9NZ08
A	29	HIS	-	expression tag	UNP Q9NZ08
A	30	HIS	-	expression tag	UNP Q9NZ08
A	31	HIS	-	expression tag	UNP Q9NZ08
A	32	HIS	-	expression tag	UNP Q9NZ08
A	33	HIS	-	expression tag	UNP Q9NZ08
A	34	HIS	-	expression tag	UNP Q9NZ08
A	35	HIS	-	expression tag	UNP Q9NZ08
A	38	GLU	-	insertion	UNP Q9NZ08
A	39	ASN	-	insertion	UNP Q9NZ08
A	40	LEU	-	insertion	UNP Q9NZ08
A	41	TYR	-	insertion	UNP Q9NZ08
A	42	PHE	-	insertion	UNP Q9NZ08
A	43	GLN	-	insertion	UNP Q9NZ08
A	?	-	CYS	deletion	UNP Q9NZ08
A	?	-	PRO	deletion	UNP Q9NZ08
A	?	-	THR	deletion	UNP Q9NZ08
A	?	-	ASP	deletion	UNP Q9NZ08
A	?	-	GLY	deletion	UNP Q9NZ08
A	?	-	VAL	deletion	UNP Q9NZ08
A	?	-	LYS	deletion	UNP Q9NZ08
A	?	-	GLY	deletion	UNP Q9NZ08
A	?	-	MET	deletion	UNP Q9NZ08
A	?	-	ASP	deletion	UNP Q9NZ08
A	?	-	GLY	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP Q9NZ08
A	?	-	CYS	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	ARG	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	GLN	deletion	UNP Q9NZ08
A	?	-	HIS	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	SER	deletion	UNP Q9NZ08
A	?	-	HIS	deletion	UNP Q9NZ08
A	?	-	TRP	deletion	UNP Q9NZ08
A	486	GLY	HIS	linker	UNP Q9NZ08
A	487	GLY	GLN	linker	UNP Q9NZ08
A	488	GLY	GLU	linker	UNP Q9NZ08
B	26	HIS	-	expression tag	UNP Q9NZ08
B	27	HIS	-	expression tag	UNP Q9NZ08
B	28	HIS	-	expression tag	UNP Q9NZ08
B	29	HIS	-	expression tag	UNP Q9NZ08
B	30	HIS	-	expression tag	UNP Q9NZ08
B	31	HIS	-	expression tag	UNP Q9NZ08
B	32	HIS	-	expression tag	UNP Q9NZ08
B	33	HIS	-	expression tag	UNP Q9NZ08
B	34	HIS	-	expression tag	UNP Q9NZ08
B	35	HIS	-	expression tag	UNP Q9NZ08
B	38	GLU	-	insertion	UNP Q9NZ08
B	39	ASN	-	insertion	UNP Q9NZ08
B	40	LEU	-	insertion	UNP Q9NZ08
B	41	TYR	-	insertion	UNP Q9NZ08
B	42	PHE	-	insertion	UNP Q9NZ08
B	43	GLN	-	insertion	UNP Q9NZ08
B	?	-	CYS	deletion	UNP Q9NZ08
B	?	-	PRO	deletion	UNP Q9NZ08
B	?	-	THR	deletion	UNP Q9NZ08
B	?	-	ASP	deletion	UNP Q9NZ08
B	?	-	GLY	deletion	UNP Q9NZ08
B	?	-	VAL	deletion	UNP Q9NZ08
B	?	-	LYS	deletion	UNP Q9NZ08
B	?	-	GLY	deletion	UNP Q9NZ08
B	?	-	MET	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q9NZ08
B	?	-	GLY	deletion	UNP Q9NZ08
B	?	-	PHE	deletion	UNP Q9NZ08
B	?	-	CYS	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	ARG	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	GLN	deletion	UNP Q9NZ08
B	?	-	HIS	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	SER	deletion	UNP Q9NZ08
B	?	-	HIS	deletion	UNP Q9NZ08
B	?	-	TRP	deletion	UNP Q9NZ08
B	486	GLY	HIS	linker	UNP Q9NZ08
B	487	GLY	GLN	linker	UNP Q9NZ08
B	488	GLY	GLU	linker	UNP Q9NZ08
C	26	HIS	-	expression tag	UNP Q9NZ08
C	27	HIS	-	expression tag	UNP Q9NZ08
C	28	HIS	-	expression tag	UNP Q9NZ08
C	29	HIS	-	expression tag	UNP Q9NZ08
C	30	HIS	-	expression tag	UNP Q9NZ08
C	31	HIS	-	expression tag	UNP Q9NZ08
C	32	HIS	-	expression tag	UNP Q9NZ08
C	33	HIS	-	expression tag	UNP Q9NZ08
C	34	HIS	-	expression tag	UNP Q9NZ08
C	35	HIS	-	expression tag	UNP Q9NZ08
C	38	GLU	-	insertion	UNP Q9NZ08
C	39	ASN	-	insertion	UNP Q9NZ08
C	40	LEU	-	insertion	UNP Q9NZ08
C	41	TYR	-	insertion	UNP Q9NZ08
C	42	PHE	-	insertion	UNP Q9NZ08
C	43	GLN	-	insertion	UNP Q9NZ08
C	?	-	CYS	deletion	UNP Q9NZ08
C	?	-	PRO	deletion	UNP Q9NZ08
C	?	-	THR	deletion	UNP Q9NZ08
C	?	-	ASP	deletion	UNP Q9NZ08
C	?	-	GLY	deletion	UNP Q9NZ08
C	?	-	VAL	deletion	UNP Q9NZ08
C	?	-	LYS	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q9NZ08
C	?	-	MET	deletion	UNP Q9NZ08
C	?	-	ASP	deletion	UNP Q9NZ08
C	?	-	GLY	deletion	UNP Q9NZ08
C	?	-	PHE	deletion	UNP Q9NZ08
C	?	-	CYS	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	ARG	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	GLN	deletion	UNP Q9NZ08
C	?	-	HIS	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	SER	deletion	UNP Q9NZ08
C	?	-	HIS	deletion	UNP Q9NZ08
C	?	-	TRP	deletion	UNP Q9NZ08
C	486	GLY	HIS	linker	UNP Q9NZ08
C	487	GLY	GLN	linker	UNP Q9NZ08
C	488	GLY	GLU	linker	UNP Q9NZ08
D	26	HIS	-	expression tag	UNP Q9NZ08
D	27	HIS	-	expression tag	UNP Q9NZ08
D	28	HIS	-	expression tag	UNP Q9NZ08
D	29	HIS	-	expression tag	UNP Q9NZ08
D	30	HIS	-	expression tag	UNP Q9NZ08
D	31	HIS	-	expression tag	UNP Q9NZ08
D	32	HIS	-	expression tag	UNP Q9NZ08
D	33	HIS	-	expression tag	UNP Q9NZ08
D	34	HIS	-	expression tag	UNP Q9NZ08
D	35	HIS	-	expression tag	UNP Q9NZ08
D	38	GLU	-	insertion	UNP Q9NZ08
D	39	ASN	-	insertion	UNP Q9NZ08
D	40	LEU	-	insertion	UNP Q9NZ08
D	41	TYR	-	insertion	UNP Q9NZ08
D	42	PHE	-	insertion	UNP Q9NZ08
D	43	GLN	-	insertion	UNP Q9NZ08
D	?	-	CYS	deletion	UNP Q9NZ08
D	?	-	PRO	deletion	UNP Q9NZ08
D	?	-	THR	deletion	UNP Q9NZ08
D	?	-	ASP	deletion	UNP Q9NZ08
D	?	-	GLY	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP Q9NZ08
D	?	-	LYS	deletion	UNP Q9NZ08
D	?	-	GLY	deletion	UNP Q9NZ08
D	?	-	MET	deletion	UNP Q9NZ08
D	?	-	ASP	deletion	UNP Q9NZ08
D	?	-	GLY	deletion	UNP Q9NZ08
D	?	-	PHE	deletion	UNP Q9NZ08
D	?	-	CYS	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	ARG	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	GLN	deletion	UNP Q9NZ08
D	?	-	HIS	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	SER	deletion	UNP Q9NZ08
D	?	-	HIS	deletion	UNP Q9NZ08
D	?	-	TRP	deletion	UNP Q9NZ08
D	486	GLY	HIS	linker	UNP Q9NZ08
D	487	GLY	GLN	linker	UNP Q9NZ08
D	488	GLY	GLU	linker	UNP Q9NZ08
E	26	HIS	-	expression tag	UNP Q9NZ08
E	27	HIS	-	expression tag	UNP Q9NZ08
E	28	HIS	-	expression tag	UNP Q9NZ08
E	29	HIS	-	expression tag	UNP Q9NZ08
E	30	HIS	-	expression tag	UNP Q9NZ08
E	31	HIS	-	expression tag	UNP Q9NZ08
E	32	HIS	-	expression tag	UNP Q9NZ08
E	33	HIS	-	expression tag	UNP Q9NZ08
E	34	HIS	-	expression tag	UNP Q9NZ08
E	35	HIS	-	expression tag	UNP Q9NZ08
E	38	GLU	-	insertion	UNP Q9NZ08
E	39	ASN	-	insertion	UNP Q9NZ08
E	40	LEU	-	insertion	UNP Q9NZ08
E	41	TYR	-	insertion	UNP Q9NZ08
E	42	PHE	-	insertion	UNP Q9NZ08
E	43	GLN	-	insertion	UNP Q9NZ08
E	?	-	CYS	deletion	UNP Q9NZ08
E	?	-	PRO	deletion	UNP Q9NZ08
E	?	-	THR	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASP	deletion	UNP Q9NZ08
E	?	-	GLY	deletion	UNP Q9NZ08
E	?	-	VAL	deletion	UNP Q9NZ08
E	?	-	LYS	deletion	UNP Q9NZ08
E	?	-	GLY	deletion	UNP Q9NZ08
E	?	-	MET	deletion	UNP Q9NZ08
E	?	-	ASP	deletion	UNP Q9NZ08
E	?	-	GLY	deletion	UNP Q9NZ08
E	?	-	PHE	deletion	UNP Q9NZ08
E	?	-	CYS	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	ARG	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	GLN	deletion	UNP Q9NZ08
E	?	-	HIS	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	SER	deletion	UNP Q9NZ08
E	?	-	HIS	deletion	UNP Q9NZ08
E	?	-	TRP	deletion	UNP Q9NZ08
E	486	GLY	HIS	linker	UNP Q9NZ08
E	487	GLY	GLN	linker	UNP Q9NZ08
E	488	GLY	GLU	linker	UNP Q9NZ08
F	26	HIS	-	expression tag	UNP Q9NZ08
F	27	HIS	-	expression tag	UNP Q9NZ08
F	28	HIS	-	expression tag	UNP Q9NZ08
F	29	HIS	-	expression tag	UNP Q9NZ08
F	30	HIS	-	expression tag	UNP Q9NZ08
F	31	HIS	-	expression tag	UNP Q9NZ08
F	32	HIS	-	expression tag	UNP Q9NZ08
F	33	HIS	-	expression tag	UNP Q9NZ08
F	34	HIS	-	expression tag	UNP Q9NZ08
F	35	HIS	-	expression tag	UNP Q9NZ08
F	38	GLU	-	insertion	UNP Q9NZ08
F	39	ASN	-	insertion	UNP Q9NZ08
F	40	LEU	-	insertion	UNP Q9NZ08
F	41	TYR	-	insertion	UNP Q9NZ08
F	42	PHE	-	insertion	UNP Q9NZ08
F	43	GLN	-	insertion	UNP Q9NZ08
F	?	-	CYS	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	PRO	deletion	UNP Q9NZ08
F	?	-	THR	deletion	UNP Q9NZ08
F	?	-	ASP	deletion	UNP Q9NZ08
F	?	-	GLY	deletion	UNP Q9NZ08
F	?	-	VAL	deletion	UNP Q9NZ08
F	?	-	LYS	deletion	UNP Q9NZ08
F	?	-	GLY	deletion	UNP Q9NZ08
F	?	-	MET	deletion	UNP Q9NZ08
F	?	-	ASP	deletion	UNP Q9NZ08
F	?	-	GLY	deletion	UNP Q9NZ08
F	?	-	PHE	deletion	UNP Q9NZ08
F	?	-	CYS	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	ARG	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	GLN	deletion	UNP Q9NZ08
F	?	-	HIS	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	SER	deletion	UNP Q9NZ08
F	?	-	HIS	deletion	UNP Q9NZ08
F	?	-	TRP	deletion	UNP Q9NZ08
F	486	GLY	HIS	linker	UNP Q9NZ08
F	487	GLY	GLN	linker	UNP Q9NZ08
F	488	GLY	GLU	linker	UNP Q9NZ08
G	26	HIS	-	expression tag	UNP Q9NZ08
G	27	HIS	-	expression tag	UNP Q9NZ08
G	28	HIS	-	expression tag	UNP Q9NZ08
G	29	HIS	-	expression tag	UNP Q9NZ08
G	30	HIS	-	expression tag	UNP Q9NZ08
G	31	HIS	-	expression tag	UNP Q9NZ08
G	32	HIS	-	expression tag	UNP Q9NZ08
G	33	HIS	-	expression tag	UNP Q9NZ08
G	34	HIS	-	expression tag	UNP Q9NZ08
G	35	HIS	-	expression tag	UNP Q9NZ08
G	38	GLU	-	insertion	UNP Q9NZ08
G	39	ASN	-	insertion	UNP Q9NZ08
G	40	LEU	-	insertion	UNP Q9NZ08
G	41	TYR	-	insertion	UNP Q9NZ08
G	42	PHE	-	insertion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
G	43	GLN	-	insertion	UNP Q9NZ08
G	?	-	CYS	deletion	UNP Q9NZ08
G	?	-	PRO	deletion	UNP Q9NZ08
G	?	-	THR	deletion	UNP Q9NZ08
G	?	-	ASP	deletion	UNP Q9NZ08
G	?	-	GLY	deletion	UNP Q9NZ08
G	?	-	VAL	deletion	UNP Q9NZ08
G	?	-	LYS	deletion	UNP Q9NZ08
G	?	-	GLY	deletion	UNP Q9NZ08
G	?	-	MET	deletion	UNP Q9NZ08
G	?	-	ASP	deletion	UNP Q9NZ08
G	?	-	GLY	deletion	UNP Q9NZ08
G	?	-	PHE	deletion	UNP Q9NZ08
G	?	-	CYS	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	ARG	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	GLN	deletion	UNP Q9NZ08
G	?	-	HIS	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	SER	deletion	UNP Q9NZ08
G	?	-	HIS	deletion	UNP Q9NZ08
G	?	-	TRP	deletion	UNP Q9NZ08
G	486	GLY	HIS	linker	UNP Q9NZ08
G	487	GLY	GLN	linker	UNP Q9NZ08
G	488	GLY	GLU	linker	UNP Q9NZ08
H	26	HIS	-	expression tag	UNP Q9NZ08
H	27	HIS	-	expression tag	UNP Q9NZ08
H	28	HIS	-	expression tag	UNP Q9NZ08
H	29	HIS	-	expression tag	UNP Q9NZ08
H	30	HIS	-	expression tag	UNP Q9NZ08
H	31	HIS	-	expression tag	UNP Q9NZ08
H	32	HIS	-	expression tag	UNP Q9NZ08
H	33	HIS	-	expression tag	UNP Q9NZ08
H	34	HIS	-	expression tag	UNP Q9NZ08
H	35	HIS	-	expression tag	UNP Q9NZ08
H	38	GLU	-	insertion	UNP Q9NZ08
H	39	ASN	-	insertion	UNP Q9NZ08
H	40	LEU	-	insertion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
H	41	TYR	-	insertion	UNP Q9NZ08
H	42	PHE	-	insertion	UNP Q9NZ08
H	43	GLN	-	insertion	UNP Q9NZ08
H	?	-	CYS	deletion	UNP Q9NZ08
H	?	-	PRO	deletion	UNP Q9NZ08
H	?	-	THR	deletion	UNP Q9NZ08
H	?	-	ASP	deletion	UNP Q9NZ08
H	?	-	GLY	deletion	UNP Q9NZ08
H	?	-	VAL	deletion	UNP Q9NZ08
H	?	-	LYS	deletion	UNP Q9NZ08
H	?	-	GLY	deletion	UNP Q9NZ08
H	?	-	MET	deletion	UNP Q9NZ08
H	?	-	ASP	deletion	UNP Q9NZ08
H	?	-	GLY	deletion	UNP Q9NZ08
H	?	-	PHE	deletion	UNP Q9NZ08
H	?	-	CYS	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	ARG	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	GLN	deletion	UNP Q9NZ08
H	?	-	HIS	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	SER	deletion	UNP Q9NZ08
H	?	-	HIS	deletion	UNP Q9NZ08
H	?	-	TRP	deletion	UNP Q9NZ08
H	486	GLY	HIS	linker	UNP Q9NZ08
H	487	GLY	GLN	linker	UNP Q9NZ08
H	488	GLY	GLU	linker	UNP Q9NZ08
I	26	HIS	-	expression tag	UNP Q9NZ08
I	27	HIS	-	expression tag	UNP Q9NZ08
I	28	HIS	-	expression tag	UNP Q9NZ08
I	29	HIS	-	expression tag	UNP Q9NZ08
I	30	HIS	-	expression tag	UNP Q9NZ08
I	31	HIS	-	expression tag	UNP Q9NZ08
I	32	HIS	-	expression tag	UNP Q9NZ08
I	33	HIS	-	expression tag	UNP Q9NZ08
I	34	HIS	-	expression tag	UNP Q9NZ08
I	35	HIS	-	expression tag	UNP Q9NZ08
I	38	GLU	-	insertion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
I	39	ASN	-	insertion	UNP Q9NZ08
I	40	LEU	-	insertion	UNP Q9NZ08
I	41	TYR	-	insertion	UNP Q9NZ08
I	42	PHE	-	insertion	UNP Q9NZ08
I	43	GLN	-	insertion	UNP Q9NZ08
I	?	-	CYS	deletion	UNP Q9NZ08
I	?	-	PRO	deletion	UNP Q9NZ08
I	?	-	THR	deletion	UNP Q9NZ08
I	?	-	ASP	deletion	UNP Q9NZ08
I	?	-	GLY	deletion	UNP Q9NZ08
I	?	-	VAL	deletion	UNP Q9NZ08
I	?	-	LYS	deletion	UNP Q9NZ08
I	?	-	GLY	deletion	UNP Q9NZ08
I	?	-	MET	deletion	UNP Q9NZ08
I	?	-	ASP	deletion	UNP Q9NZ08
I	?	-	GLY	deletion	UNP Q9NZ08
I	?	-	PHE	deletion	UNP Q9NZ08
I	?	-	CYS	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	ARG	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	GLN	deletion	UNP Q9NZ08
I	?	-	HIS	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	SER	deletion	UNP Q9NZ08
I	?	-	HIS	deletion	UNP Q9NZ08
I	?	-	TRP	deletion	UNP Q9NZ08
I	486	GLY	HIS	linker	UNP Q9NZ08
I	487	GLY	GLN	linker	UNP Q9NZ08
I	488	GLY	GLU	linker	UNP Q9NZ08
J	26	HIS	-	expression tag	UNP Q9NZ08
J	27	HIS	-	expression tag	UNP Q9NZ08
J	28	HIS	-	expression tag	UNP Q9NZ08
J	29	HIS	-	expression tag	UNP Q9NZ08
J	30	HIS	-	expression tag	UNP Q9NZ08
J	31	HIS	-	expression tag	UNP Q9NZ08
J	32	HIS	-	expression tag	UNP Q9NZ08
J	33	HIS	-	expression tag	UNP Q9NZ08
J	34	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
J	35	HIS	-	expression tag	UNP Q9NZ08
J	38	GLU	-	insertion	UNP Q9NZ08
J	39	ASN	-	insertion	UNP Q9NZ08
J	40	LEU	-	insertion	UNP Q9NZ08
J	41	TYR	-	insertion	UNP Q9NZ08
J	42	PHE	-	insertion	UNP Q9NZ08
J	43	GLN	-	insertion	UNP Q9NZ08
J	?	-	CYS	deletion	UNP Q9NZ08
J	?	-	PRO	deletion	UNP Q9NZ08
J	?	-	THR	deletion	UNP Q9NZ08
J	?	-	ASP	deletion	UNP Q9NZ08
J	?	-	GLY	deletion	UNP Q9NZ08
J	?	-	VAL	deletion	UNP Q9NZ08
J	?	-	LYS	deletion	UNP Q9NZ08
J	?	-	GLY	deletion	UNP Q9NZ08
J	?	-	MET	deletion	UNP Q9NZ08
J	?	-	ASP	deletion	UNP Q9NZ08
J	?	-	GLY	deletion	UNP Q9NZ08
J	?	-	PHE	deletion	UNP Q9NZ08
J	?	-	CYS	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	ARG	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	GLN	deletion	UNP Q9NZ08
J	?	-	HIS	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	SER	deletion	UNP Q9NZ08
J	?	-	HIS	deletion	UNP Q9NZ08
J	?	-	TRP	deletion	UNP Q9NZ08
J	486	GLY	HIS	linker	UNP Q9NZ08
J	487	GLY	GLN	linker	UNP Q9NZ08
J	488	GLY	GLU	linker	UNP Q9NZ08
K	26	HIS	-	expression tag	UNP Q9NZ08
K	27	HIS	-	expression tag	UNP Q9NZ08
K	28	HIS	-	expression tag	UNP Q9NZ08
K	29	HIS	-	expression tag	UNP Q9NZ08
K	30	HIS	-	expression tag	UNP Q9NZ08
K	31	HIS	-	expression tag	UNP Q9NZ08
K	32	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
K	33	HIS	-	expression tag	UNP Q9NZ08
K	34	HIS	-	expression tag	UNP Q9NZ08
K	35	HIS	-	expression tag	UNP Q9NZ08
K	38	GLU	-	insertion	UNP Q9NZ08
K	39	ASN	-	insertion	UNP Q9NZ08
K	40	LEU	-	insertion	UNP Q9NZ08
K	41	TYR	-	insertion	UNP Q9NZ08
K	42	PHE	-	insertion	UNP Q9NZ08
K	43	GLN	-	insertion	UNP Q9NZ08
K	?	-	CYS	deletion	UNP Q9NZ08
K	?	-	PRO	deletion	UNP Q9NZ08
K	?	-	THR	deletion	UNP Q9NZ08
K	?	-	ASP	deletion	UNP Q9NZ08
K	?	-	GLY	deletion	UNP Q9NZ08
K	?	-	VAL	deletion	UNP Q9NZ08
K	?	-	LYS	deletion	UNP Q9NZ08
K	?	-	GLY	deletion	UNP Q9NZ08
K	?	-	MET	deletion	UNP Q9NZ08
K	?	-	ASP	deletion	UNP Q9NZ08
K	?	-	GLY	deletion	UNP Q9NZ08
K	?	-	PHE	deletion	UNP Q9NZ08
K	?	-	CYS	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	ARG	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	GLN	deletion	UNP Q9NZ08
K	?	-	HIS	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	SER	deletion	UNP Q9NZ08
K	?	-	HIS	deletion	UNP Q9NZ08
K	?	-	TRP	deletion	UNP Q9NZ08
K	486	GLY	HIS	linker	UNP Q9NZ08
K	487	GLY	GLN	linker	UNP Q9NZ08
K	488	GLY	GLU	linker	UNP Q9NZ08
L	26	HIS	-	expression tag	UNP Q9NZ08
L	27	HIS	-	expression tag	UNP Q9NZ08
L	28	HIS	-	expression tag	UNP Q9NZ08
L	29	HIS	-	expression tag	UNP Q9NZ08
L	30	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
L	31	HIS	-	expression tag	UNP Q9NZ08
L	32	HIS	-	expression tag	UNP Q9NZ08
L	33	HIS	-	expression tag	UNP Q9NZ08
L	34	HIS	-	expression tag	UNP Q9NZ08
L	35	HIS	-	expression tag	UNP Q9NZ08
L	38	GLU	-	insertion	UNP Q9NZ08
L	39	ASN	-	insertion	UNP Q9NZ08
L	40	LEU	-	insertion	UNP Q9NZ08
L	41	TYR	-	insertion	UNP Q9NZ08
L	42	PHE	-	insertion	UNP Q9NZ08
L	43	GLN	-	insertion	UNP Q9NZ08
L	?	-	CYS	deletion	UNP Q9NZ08
L	?	-	PRO	deletion	UNP Q9NZ08
L	?	-	THR	deletion	UNP Q9NZ08
L	?	-	ASP	deletion	UNP Q9NZ08
L	?	-	GLY	deletion	UNP Q9NZ08
L	?	-	VAL	deletion	UNP Q9NZ08
L	?	-	LYS	deletion	UNP Q9NZ08
L	?	-	GLY	deletion	UNP Q9NZ08
L	?	-	MET	deletion	UNP Q9NZ08
L	?	-	ASP	deletion	UNP Q9NZ08
L	?	-	GLY	deletion	UNP Q9NZ08
L	?	-	PHE	deletion	UNP Q9NZ08
L	?	-	CYS	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	ARG	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	GLN	deletion	UNP Q9NZ08
L	?	-	HIS	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	SER	deletion	UNP Q9NZ08
L	?	-	HIS	deletion	UNP Q9NZ08
L	?	-	TRP	deletion	UNP Q9NZ08
L	486	GLY	HIS	linker	UNP Q9NZ08
L	487	GLY	GLN	linker	UNP Q9NZ08
L	488	GLY	GLU	linker	UNP Q9NZ08
M	26	HIS	-	expression tag	UNP Q9NZ08
M	27	HIS	-	expression tag	UNP Q9NZ08
M	28	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
M	29	HIS	-	expression tag	UNP Q9NZ08
M	30	HIS	-	expression tag	UNP Q9NZ08
M	31	HIS	-	expression tag	UNP Q9NZ08
M	32	HIS	-	expression tag	UNP Q9NZ08
M	33	HIS	-	expression tag	UNP Q9NZ08
M	34	HIS	-	expression tag	UNP Q9NZ08
M	35	HIS	-	expression tag	UNP Q9NZ08
M	38	GLU	-	insertion	UNP Q9NZ08
M	39	ASN	-	insertion	UNP Q9NZ08
M	40	LEU	-	insertion	UNP Q9NZ08
M	41	TYR	-	insertion	UNP Q9NZ08
M	42	PHE	-	insertion	UNP Q9NZ08
M	43	GLN	-	insertion	UNP Q9NZ08
M	?	-	CYS	deletion	UNP Q9NZ08
M	?	-	PRO	deletion	UNP Q9NZ08
M	?	-	THR	deletion	UNP Q9NZ08
M	?	-	ASP	deletion	UNP Q9NZ08
M	?	-	GLY	deletion	UNP Q9NZ08
M	?	-	VAL	deletion	UNP Q9NZ08
M	?	-	LYS	deletion	UNP Q9NZ08
M	?	-	GLY	deletion	UNP Q9NZ08
M	?	-	MET	deletion	UNP Q9NZ08
M	?	-	ASP	deletion	UNP Q9NZ08
M	?	-	GLY	deletion	UNP Q9NZ08
M	?	-	PHE	deletion	UNP Q9NZ08
M	?	-	CYS	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	ARG	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	GLN	deletion	UNP Q9NZ08
M	?	-	HIS	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	SER	deletion	UNP Q9NZ08
M	?	-	HIS	deletion	UNP Q9NZ08
M	?	-	TRP	deletion	UNP Q9NZ08
M	486	GLY	HIS	linker	UNP Q9NZ08
M	487	GLY	GLN	linker	UNP Q9NZ08
M	488	GLY	GLU	linker	UNP Q9NZ08
N	26	HIS	-	expression tag	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
N	27	HIS	-	expression tag	UNP Q9NZ08
N	28	HIS	-	expression tag	UNP Q9NZ08
N	29	HIS	-	expression tag	UNP Q9NZ08
N	30	HIS	-	expression tag	UNP Q9NZ08
N	31	HIS	-	expression tag	UNP Q9NZ08
N	32	HIS	-	expression tag	UNP Q9NZ08
N	33	HIS	-	expression tag	UNP Q9NZ08
N	34	HIS	-	expression tag	UNP Q9NZ08
N	35	HIS	-	expression tag	UNP Q9NZ08
N	38	GLU	-	insertion	UNP Q9NZ08
N	39	ASN	-	insertion	UNP Q9NZ08
N	40	LEU	-	insertion	UNP Q9NZ08
N	41	TYR	-	insertion	UNP Q9NZ08
N	42	PHE	-	insertion	UNP Q9NZ08
N	43	GLN	-	insertion	UNP Q9NZ08
N	?	-	CYS	deletion	UNP Q9NZ08
N	?	-	PRO	deletion	UNP Q9NZ08
N	?	-	THR	deletion	UNP Q9NZ08
N	?	-	ASP	deletion	UNP Q9NZ08
N	?	-	GLY	deletion	UNP Q9NZ08
N	?	-	VAL	deletion	UNP Q9NZ08
N	?	-	LYS	deletion	UNP Q9NZ08
N	?	-	GLY	deletion	UNP Q9NZ08
N	?	-	MET	deletion	UNP Q9NZ08
N	?	-	ASP	deletion	UNP Q9NZ08
N	?	-	GLY	deletion	UNP Q9NZ08
N	?	-	PHE	deletion	UNP Q9NZ08
N	?	-	CYS	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	ARG	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	GLN	deletion	UNP Q9NZ08
N	?	-	HIS	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	SER	deletion	UNP Q9NZ08
N	?	-	HIS	deletion	UNP Q9NZ08
N	?	-	TRP	deletion	UNP Q9NZ08
N	486	GLY	HIS	linker	UNP Q9NZ08
N	487	GLY	GLN	linker	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
N	488	GLY	GLU	linker	UNP Q9NZ08
O	26	HIS	-	expression tag	UNP Q9NZ08
O	27	HIS	-	expression tag	UNP Q9NZ08
O	28	HIS	-	expression tag	UNP Q9NZ08
O	29	HIS	-	expression tag	UNP Q9NZ08
O	30	HIS	-	expression tag	UNP Q9NZ08
O	31	HIS	-	expression tag	UNP Q9NZ08
O	32	HIS	-	expression tag	UNP Q9NZ08
O	33	HIS	-	expression tag	UNP Q9NZ08
O	34	HIS	-	expression tag	UNP Q9NZ08
O	35	HIS	-	expression tag	UNP Q9NZ08
O	38	GLU	-	insertion	UNP Q9NZ08
O	39	ASN	-	insertion	UNP Q9NZ08
O	40	LEU	-	insertion	UNP Q9NZ08
O	41	TYR	-	insertion	UNP Q9NZ08
O	42	PHE	-	insertion	UNP Q9NZ08
O	43	GLN	-	insertion	UNP Q9NZ08
O	?	-	CYS	deletion	UNP Q9NZ08
O	?	-	PRO	deletion	UNP Q9NZ08
O	?	-	THR	deletion	UNP Q9NZ08
O	?	-	ASP	deletion	UNP Q9NZ08
O	?	-	GLY	deletion	UNP Q9NZ08
O	?	-	VAL	deletion	UNP Q9NZ08
O	?	-	LYS	deletion	UNP Q9NZ08
O	?	-	GLY	deletion	UNP Q9NZ08
O	?	-	MET	deletion	UNP Q9NZ08
O	?	-	ASP	deletion	UNP Q9NZ08
O	?	-	GLY	deletion	UNP Q9NZ08
O	?	-	PHE	deletion	UNP Q9NZ08
O	?	-	CYS	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	ARG	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	GLN	deletion	UNP Q9NZ08
O	?	-	HIS	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	SER	deletion	UNP Q9NZ08
O	?	-	HIS	deletion	UNP Q9NZ08
O	?	-	TRP	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
O	486	GLY	HIS	linker	UNP Q9NZ08
O	487	GLY	GLN	linker	UNP Q9NZ08
O	488	GLY	GLU	linker	UNP Q9NZ08
P	26	HIS	-	expression tag	UNP Q9NZ08
P	27	HIS	-	expression tag	UNP Q9NZ08
P	28	HIS	-	expression tag	UNP Q9NZ08
P	29	HIS	-	expression tag	UNP Q9NZ08
P	30	HIS	-	expression tag	UNP Q9NZ08
P	31	HIS	-	expression tag	UNP Q9NZ08
P	32	HIS	-	expression tag	UNP Q9NZ08
P	33	HIS	-	expression tag	UNP Q9NZ08
P	34	HIS	-	expression tag	UNP Q9NZ08
P	35	HIS	-	expression tag	UNP Q9NZ08
P	38	GLU	-	insertion	UNP Q9NZ08
P	39	ASN	-	insertion	UNP Q9NZ08
P	40	LEU	-	insertion	UNP Q9NZ08
P	41	TYR	-	insertion	UNP Q9NZ08
P	42	PHE	-	insertion	UNP Q9NZ08
P	43	GLN	-	insertion	UNP Q9NZ08
P	?	-	CYS	deletion	UNP Q9NZ08
P	?	-	PRO	deletion	UNP Q9NZ08
P	?	-	THR	deletion	UNP Q9NZ08
P	?	-	ASP	deletion	UNP Q9NZ08
P	?	-	GLY	deletion	UNP Q9NZ08
P	?	-	VAL	deletion	UNP Q9NZ08
P	?	-	LYS	deletion	UNP Q9NZ08
P	?	-	GLY	deletion	UNP Q9NZ08
P	?	-	MET	deletion	UNP Q9NZ08
P	?	-	ASP	deletion	UNP Q9NZ08
P	?	-	GLY	deletion	UNP Q9NZ08
P	?	-	PHE	deletion	UNP Q9NZ08
P	?	-	CYS	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	ARG	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	GLN	deletion	UNP Q9NZ08
P	?	-	HIS	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08
P	?	-	SER	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	HIS	deletion	UNP Q9NZ08
P	?	-	TRP	deletion	UNP Q9NZ08
P	486	GLY	HIS	linker	UNP Q9NZ08
P	487	GLY	GLN	linker	UNP Q9NZ08
P	488	GLY	GLU	linker	UNP Q9NZ08
Q	26	HIS	-	expression tag	UNP Q9NZ08
Q	27	HIS	-	expression tag	UNP Q9NZ08
Q	28	HIS	-	expression tag	UNP Q9NZ08
Q	29	HIS	-	expression tag	UNP Q9NZ08
Q	30	HIS	-	expression tag	UNP Q9NZ08
Q	31	HIS	-	expression tag	UNP Q9NZ08
Q	32	HIS	-	expression tag	UNP Q9NZ08
Q	33	HIS	-	expression tag	UNP Q9NZ08
Q	34	HIS	-	expression tag	UNP Q9NZ08
Q	35	HIS	-	expression tag	UNP Q9NZ08
Q	38	GLU	-	insertion	UNP Q9NZ08
Q	39	ASN	-	insertion	UNP Q9NZ08
Q	40	LEU	-	insertion	UNP Q9NZ08
Q	41	TYR	-	insertion	UNP Q9NZ08
Q	42	PHE	-	insertion	UNP Q9NZ08
Q	43	GLN	-	insertion	UNP Q9NZ08
Q	?	-	CYS	deletion	UNP Q9NZ08
Q	?	-	PRO	deletion	UNP Q9NZ08
Q	?	-	THR	deletion	UNP Q9NZ08
Q	?	-	ASP	deletion	UNP Q9NZ08
Q	?	-	GLY	deletion	UNP Q9NZ08
Q	?	-	VAL	deletion	UNP Q9NZ08
Q	?	-	LYS	deletion	UNP Q9NZ08
Q	?	-	GLY	deletion	UNP Q9NZ08
Q	?	-	MET	deletion	UNP Q9NZ08
Q	?	-	ASP	deletion	UNP Q9NZ08
Q	?	-	GLY	deletion	UNP Q9NZ08
Q	?	-	PHE	deletion	UNP Q9NZ08
Q	?	-	CYS	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	ARG	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	GLN	deletion	UNP Q9NZ08
Q	?	-	HIS	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	SER	deletion	UNP Q9NZ08
Q	?	-	HIS	deletion	UNP Q9NZ08
Q	?	-	TRP	deletion	UNP Q9NZ08
Q	486	GLY	HIS	linker	UNP Q9NZ08
Q	487	GLY	GLN	linker	UNP Q9NZ08
Q	488	GLY	GLU	linker	UNP Q9NZ08
R	26	HIS	-	expression tag	UNP Q9NZ08
R	27	HIS	-	expression tag	UNP Q9NZ08
R	28	HIS	-	expression tag	UNP Q9NZ08
R	29	HIS	-	expression tag	UNP Q9NZ08
R	30	HIS	-	expression tag	UNP Q9NZ08
R	31	HIS	-	expression tag	UNP Q9NZ08
R	32	HIS	-	expression tag	UNP Q9NZ08
R	33	HIS	-	expression tag	UNP Q9NZ08
R	34	HIS	-	expression tag	UNP Q9NZ08
R	35	HIS	-	expression tag	UNP Q9NZ08
R	38	GLU	-	insertion	UNP Q9NZ08
R	39	ASN	-	insertion	UNP Q9NZ08
R	40	LEU	-	insertion	UNP Q9NZ08
R	41	TYR	-	insertion	UNP Q9NZ08
R	42	PHE	-	insertion	UNP Q9NZ08
R	43	GLN	-	insertion	UNP Q9NZ08
R	?	-	CYS	deletion	UNP Q9NZ08
R	?	-	PRO	deletion	UNP Q9NZ08
R	?	-	THR	deletion	UNP Q9NZ08
R	?	-	ASP	deletion	UNP Q9NZ08
R	?	-	GLY	deletion	UNP Q9NZ08
R	?	-	VAL	deletion	UNP Q9NZ08
R	?	-	LYS	deletion	UNP Q9NZ08
R	?	-	GLY	deletion	UNP Q9NZ08
R	?	-	MET	deletion	UNP Q9NZ08
R	?	-	ASP	deletion	UNP Q9NZ08
R	?	-	GLY	deletion	UNP Q9NZ08
R	?	-	PHE	deletion	UNP Q9NZ08
R	?	-	CYS	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	ARG	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	GLN	deletion	UNP Q9NZ08
R	?	-	HIS	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	SER	deletion	UNP Q9NZ08
R	?	-	HIS	deletion	UNP Q9NZ08
R	?	-	TRP	deletion	UNP Q9NZ08
R	486	GLY	HIS	linker	UNP Q9NZ08
R	487	GLY	GLN	linker	UNP Q9NZ08
R	488	GLY	GLU	linker	UNP Q9NZ08
S	26	HIS	-	expression tag	UNP Q9NZ08
S	27	HIS	-	expression tag	UNP Q9NZ08
S	28	HIS	-	expression tag	UNP Q9NZ08
S	29	HIS	-	expression tag	UNP Q9NZ08
S	30	HIS	-	expression tag	UNP Q9NZ08
S	31	HIS	-	expression tag	UNP Q9NZ08
S	32	HIS	-	expression tag	UNP Q9NZ08
S	33	HIS	-	expression tag	UNP Q9NZ08
S	34	HIS	-	expression tag	UNP Q9NZ08
S	35	HIS	-	expression tag	UNP Q9NZ08
S	38	GLU	-	insertion	UNP Q9NZ08
S	39	ASN	-	insertion	UNP Q9NZ08
S	40	LEU	-	insertion	UNP Q9NZ08
S	41	TYR	-	insertion	UNP Q9NZ08
S	42	PHE	-	insertion	UNP Q9NZ08
S	43	GLN	-	insertion	UNP Q9NZ08
S	?	-	CYS	deletion	UNP Q9NZ08
S	?	-	PRO	deletion	UNP Q9NZ08
S	?	-	THR	deletion	UNP Q9NZ08
S	?	-	ASP	deletion	UNP Q9NZ08
S	?	-	GLY	deletion	UNP Q9NZ08
S	?	-	VAL	deletion	UNP Q9NZ08
S	?	-	LYS	deletion	UNP Q9NZ08
S	?	-	GLY	deletion	UNP Q9NZ08
S	?	-	MET	deletion	UNP Q9NZ08
S	?	-	ASP	deletion	UNP Q9NZ08
S	?	-	GLY	deletion	UNP Q9NZ08
S	?	-	PHE	deletion	UNP Q9NZ08
S	?	-	CYS	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	ARG	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	GLN	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
S	?	-	HIS	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	SER	deletion	UNP Q9NZ08
S	?	-	HIS	deletion	UNP Q9NZ08
S	?	-	TRP	deletion	UNP Q9NZ08
S	486	GLY	HIS	linker	UNP Q9NZ08
S	487	GLY	GLN	linker	UNP Q9NZ08
S	488	GLY	GLU	linker	UNP Q9NZ08
T	26	HIS	-	expression tag	UNP Q9NZ08
T	27	HIS	-	expression tag	UNP Q9NZ08
T	28	HIS	-	expression tag	UNP Q9NZ08
T	29	HIS	-	expression tag	UNP Q9NZ08
T	30	HIS	-	expression tag	UNP Q9NZ08
T	31	HIS	-	expression tag	UNP Q9NZ08
T	32	HIS	-	expression tag	UNP Q9NZ08
T	33	HIS	-	expression tag	UNP Q9NZ08
T	34	HIS	-	expression tag	UNP Q9NZ08
T	35	HIS	-	expression tag	UNP Q9NZ08
T	38	GLU	-	insertion	UNP Q9NZ08
T	39	ASN	-	insertion	UNP Q9NZ08
T	40	LEU	-	insertion	UNP Q9NZ08
T	41	TYR	-	insertion	UNP Q9NZ08
T	42	PHE	-	insertion	UNP Q9NZ08
T	43	GLN	-	insertion	UNP Q9NZ08
T	?	-	CYS	deletion	UNP Q9NZ08
T	?	-	PRO	deletion	UNP Q9NZ08
T	?	-	THR	deletion	UNP Q9NZ08
T	?	-	ASP	deletion	UNP Q9NZ08
T	?	-	GLY	deletion	UNP Q9NZ08
T	?	-	VAL	deletion	UNP Q9NZ08
T	?	-	LYS	deletion	UNP Q9NZ08
T	?	-	GLY	deletion	UNP Q9NZ08
T	?	-	MET	deletion	UNP Q9NZ08
T	?	-	ASP	deletion	UNP Q9NZ08
T	?	-	GLY	deletion	UNP Q9NZ08
T	?	-	PHE	deletion	UNP Q9NZ08
T	?	-	CYS	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	ARG	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	GLN	deletion	UNP Q9NZ08
T	?	-	HIS	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	SER	deletion	UNP Q9NZ08
T	?	-	HIS	deletion	UNP Q9NZ08
T	?	-	TRP	deletion	UNP Q9NZ08
T	486	GLY	HIS	linker	UNP Q9NZ08
T	487	GLY	GLN	linker	UNP Q9NZ08
T	488	GLY	GLU	linker	UNP Q9NZ08
U	26	HIS	-	expression tag	UNP Q9NZ08
U	27	HIS	-	expression tag	UNP Q9NZ08
U	28	HIS	-	expression tag	UNP Q9NZ08
U	29	HIS	-	expression tag	UNP Q9NZ08
U	30	HIS	-	expression tag	UNP Q9NZ08
U	31	HIS	-	expression tag	UNP Q9NZ08
U	32	HIS	-	expression tag	UNP Q9NZ08
U	33	HIS	-	expression tag	UNP Q9NZ08
U	34	HIS	-	expression tag	UNP Q9NZ08
U	35	HIS	-	expression tag	UNP Q9NZ08
U	38	GLU	-	insertion	UNP Q9NZ08
U	39	ASN	-	insertion	UNP Q9NZ08
U	40	LEU	-	insertion	UNP Q9NZ08
U	41	TYR	-	insertion	UNP Q9NZ08
U	42	PHE	-	insertion	UNP Q9NZ08
U	43	GLN	-	insertion	UNP Q9NZ08
U	?	-	CYS	deletion	UNP Q9NZ08
U	?	-	PRO	deletion	UNP Q9NZ08
U	?	-	THR	deletion	UNP Q9NZ08
U	?	-	ASP	deletion	UNP Q9NZ08
U	?	-	GLY	deletion	UNP Q9NZ08
U	?	-	VAL	deletion	UNP Q9NZ08
U	?	-	LYS	deletion	UNP Q9NZ08
U	?	-	GLY	deletion	UNP Q9NZ08
U	?	-	MET	deletion	UNP Q9NZ08
U	?	-	ASP	deletion	UNP Q9NZ08
U	?	-	GLY	deletion	UNP Q9NZ08
U	?	-	PHE	deletion	UNP Q9NZ08
U	?	-	CYS	deletion	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	ARG	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	GLN	deletion	UNP Q9NZ08
U	?	-	HIS	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	HIS	deletion	UNP Q9NZ08
U	?	-	TRP	deletion	UNP Q9NZ08
U	486	GLY	HIS	linker	UNP Q9NZ08
U	487	GLY	GLN	linker	UNP Q9NZ08
U	488	GLY	GLU	linker	UNP Q9NZ08
V	26	HIS	-	expression tag	UNP Q9NZ08
V	27	HIS	-	expression tag	UNP Q9NZ08
V	28	HIS	-	expression tag	UNP Q9NZ08
V	29	HIS	-	expression tag	UNP Q9NZ08
V	30	HIS	-	expression tag	UNP Q9NZ08
V	31	HIS	-	expression tag	UNP Q9NZ08
V	32	HIS	-	expression tag	UNP Q9NZ08
V	33	HIS	-	expression tag	UNP Q9NZ08
V	34	HIS	-	expression tag	UNP Q9NZ08
V	35	HIS	-	expression tag	UNP Q9NZ08
V	38	GLU	-	insertion	UNP Q9NZ08
V	39	ASN	-	insertion	UNP Q9NZ08
V	40	LEU	-	insertion	UNP Q9NZ08
V	41	TYR	-	insertion	UNP Q9NZ08
V	42	PHE	-	insertion	UNP Q9NZ08
V	43	GLN	-	insertion	UNP Q9NZ08
V	?	-	CYS	deletion	UNP Q9NZ08
V	?	-	PRO	deletion	UNP Q9NZ08
V	?	-	THR	deletion	UNP Q9NZ08
V	?	-	ASP	deletion	UNP Q9NZ08
V	?	-	GLY	deletion	UNP Q9NZ08
V	?	-	VAL	deletion	UNP Q9NZ08
V	?	-	LYS	deletion	UNP Q9NZ08
V	?	-	GLY	deletion	UNP Q9NZ08
V	?	-	MET	deletion	UNP Q9NZ08
V	?	-	ASP	deletion	UNP Q9NZ08
V	?	-	GLY	deletion	UNP Q9NZ08

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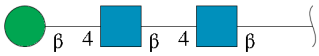
Chain	Residue	Modelled	Actual	Comment	Reference
V	?	-	PHE	deletion	UNP Q9NZ08
V	?	-	CYS	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	ARG	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	GLN	deletion	UNP Q9NZ08
V	?	-	HIS	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	SER	deletion	UNP Q9NZ08
V	?	-	HIS	deletion	UNP Q9NZ08
V	?	-	TRP	deletion	UNP Q9NZ08
V	486	GLY	HIS	linker	UNP Q9NZ08
V	487	GLY	GLN	linker	UNP Q9NZ08
V	488	GLY	GLU	linker	UNP Q9NZ08

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	W	3	39	22	2	15	0	0	0
2	X	3	39	22	2	15	0	0	0
2	Y	3	39	22	2	15	0	0	0
2	Z	3	39	22	2	15	0	0	0
2	a	3	39	22	2	15	0	0	0
2	b	3	39	22	2	15	0	0	0
2	c	3	39	22	2	15	0	0	0
2	d	3	39	22	2	15	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	e	3	39	22	2	15	0	0	0
2	f	3	39	22	2	15	0	0	0
2	g	3	39	22	2	15	0	0	0
2	h	3	39	22	2	15	0	0	0
2	i	3	39	22	2	15	0	0	0
2	j	3	39	22	2	15	0	0	0
2	k	3	39	22	2	15	0	0	0
2	l	3	39	22	2	15	0	0	0
2	m	3	39	22	2	15	0	0	0
2	n	3	39	22	2	15	0	0	0
2	o	3	39	22	2	15	0	0	0
2	p	3	39	22	2	15	0	0	0
2	q	3	39	22	2	15	0	0	0
2	r	3	39	22	2	15	0	0	0
2	s	3	39	22	2	15	0	0	0
2	t	3	39	22	2	15	0	0	0
2	u	3	39	22	2	15	0	0	0
2	v	3	39	22	2	15	0	0	0
2	w	3	39	22	2	15	0	0	0
2	x	3	39	22	2	15	0	0	0
2	y	3	39	22	2	15	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	z	3	39	22	2	15	0	0	0
2	0	3	39	22	2	15	0	0	0
2	1	3	39	22	2	15	0	0	0
2	2	3	39	22	2	15	0	0	0
2	3	3	39	22	2	15	0	0	0
2	4	3	39	22	2	15	0	0	0
2	5	3	39	22	2	15	0	0	0
2	6	3	39	22	2	15	0	0	0
2	7	3	39	22	2	15	0	0	0
2	8	3	39	22	2	15	0	0	0
2	9	3	39	22	2	15	0	0	0
2	AA	3	39	22	2	15	0	0	0
2	BA	3	39	22	2	15	0	0	0
2	CA	3	39	22	2	15	0	0	0
2	DA	3	39	22	2	15	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0
3	D	1	1	1	0	0

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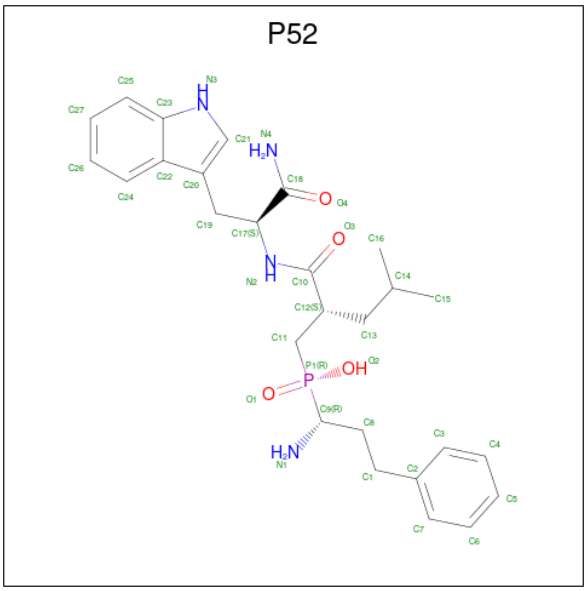
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	E	1	1	1	0	0
3	F	1	1	1	0	0
3	G	1	1	1	0	0
3	H	1	1	1	0	0
3	I	1	1	1	0	0
3	J	1	1	1	0	0
3	K	1	1	1	0	0
3	L	1	1	1	0	0
3	M	1	1	1	0	0
3	N	1	1	1	0	0
3	O	1	1	1	0	0
3	P	1	1	1	0	0
3	Q	1	1	1	0	0
3	R	1	1	1	0	0
3	S	1	1	1	0	0
3	T	1	1	1	0	0
3	U	1	1	1	0	0
3	V	1	1	1	0	0

- Molecule 4 is Nalpha-[(2S)-2-{[[(1R)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]methyl}-4-methylpentanoyl]-L-tryptophanamide (three-letter code: P52) (formula: $C_{27}H_{37}N_4O_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	36	27	4	4	1	0	0
4	B	1	36	27	4	4	1	0	0
4	C	1	36	27	4	4	1	0	0
4	D	1	36	27	4	4	1	0	0
4	E	1	36	27	4	4	1	0	0
4	F	1	36	27	4	4	1	0	0
4	G	1	36	27	4	4	1	0	0
4	H	1	36	27	4	4	1	0	0
4	I	1	36	27	4	4	1	0	0
4	J	1	36	27	4	4	1	0	0
4	K	1	36	27	4	4	1	0	0
4	L	1	36	27	4	4	1	0	0
4	M	1	36	27	4	4	1	0	0
4	N	1	36	27	4	4	1	0	0

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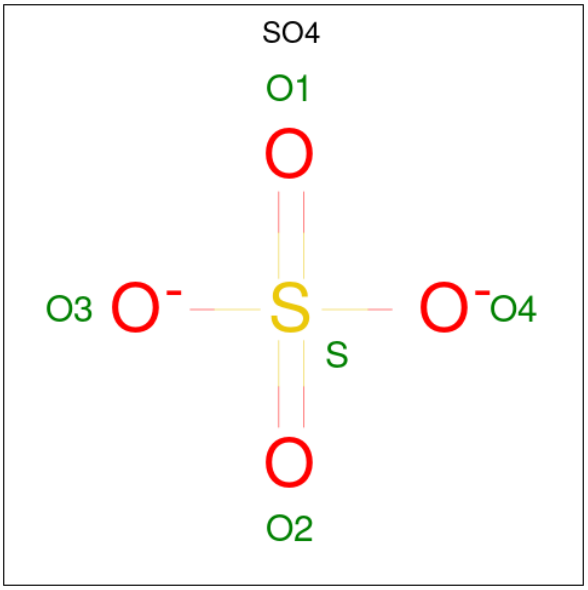
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	O	1	36	27	4	4	1	0	0
4	P	1	36	27	4	4	1	0	0
4	Q	1	36	27	4	4	1	0	0
4	R	1	36	27	4	4	1	0	0
4	S	1	36	27	4	4	1	0	0
4	T	1	36	27	4	4	1	0	0
4	U	1	36	27	4	4	1	0	0
4	V	1	36	27	4	4	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	F	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0
			Total	O	S		
5	G	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	G	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	H	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	I	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	J	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	K	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	L	1	5	4	1		0	0
			Total	O	S			
5	M	1	5	4	1		0	0
			Total	O	S			
5	M	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	M	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0
			Total	O	S		
5	N	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	O	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	P	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	Q	1	5	4	1	0	0
			Total	O	S		
5	Q	1	5	4	1	0	0
			Total	O	S		
5	Q	1	5	4	1	0	0
			Total	O	S		
5	Q	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	R	1	5	4	1	0	0
			Total	O	S		
5	S	1	5	4	1	0	0
			Total	O	S		
5	S	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	S	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	T	1	5	4	1		0	0
			Total	O	S			
5	T	1	5	4	1		0	0
			Total	O	S			
5	T	1	5	4	1		0	0
			Total	O	S			
5	T	1	5	4	1		0	0
			Total	O	S			
5	T	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	U	1	5	4	1		0	0
			Total	O	S			
5	V	1	5	4	1		0	0

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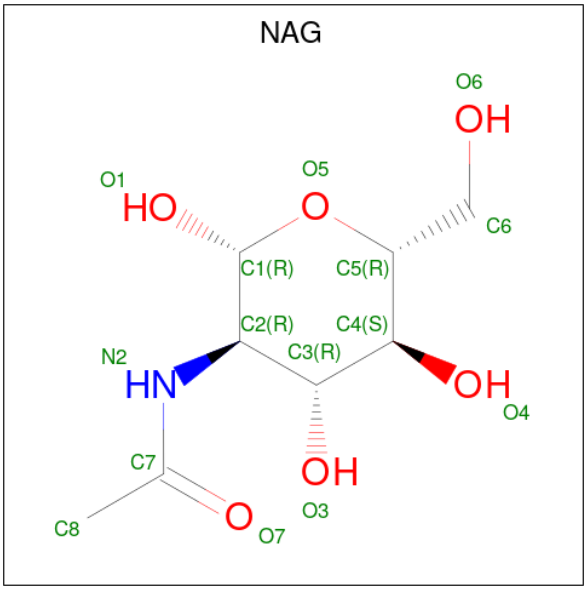
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0
5	V	1	Total O S 5 4 1	0	0

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



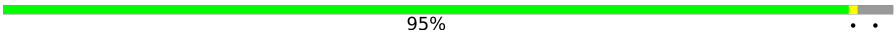
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
6	B	1	14	8	1	5	0	0
6	C	1	14	8	1	5	0	0
6	D	1	14	8	1	5	0	0
6	E	1	14	8	1	5	0	0
6	F	1	14	8	1	5	0	0
6	G	1	14	8	1	5	0	0
6	H	1	14	8	1	5	0	0
6	I	1	14	8	1	5	0	0
6	J	1	14	8	1	5	0	0
6	K	1	14	8	1	5	0	0
6	L	1	14	8	1	5	0	0
6	M	1	14	8	1	5	0	0
6	N	1	14	8	1	5	0	0
6	O	1	14	8	1	5	0	0
6	P	1	14	8	1	5	0	0
6	Q	1	14	8	1	5	0	0
6	R	1	14	8	1	5	0	0
6	S	1	14	8	1	5	0	0
6	T	1	14	8	1	5	0	0
6	U	1	14	8	1	5	0	0
6	V	1	14	8	1	5	0	0

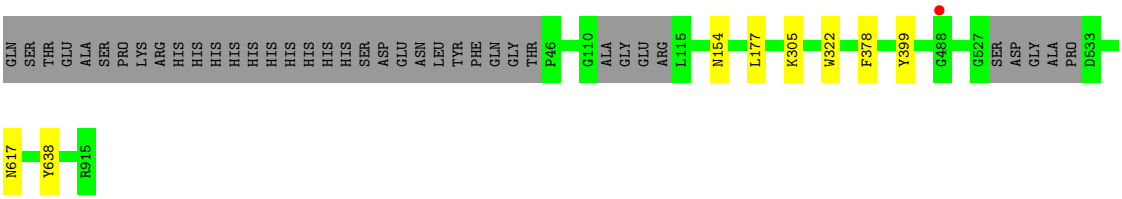
3 Residue-property plots (i)

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: Endoplasmic reticulum aminopeptidase 1

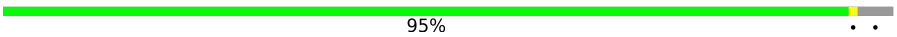
Chain A:

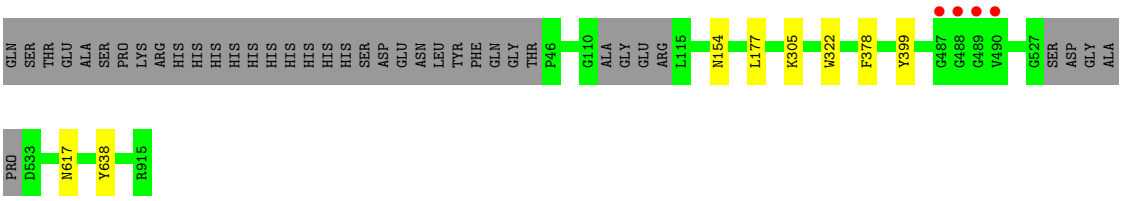




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

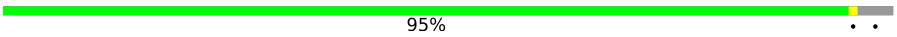
Chain B:

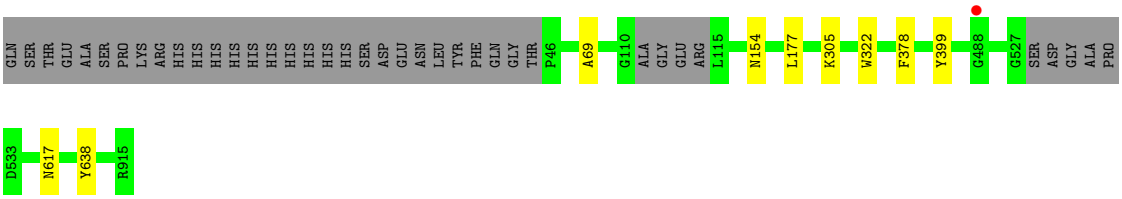




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

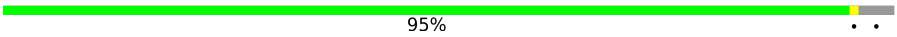
Chain C:

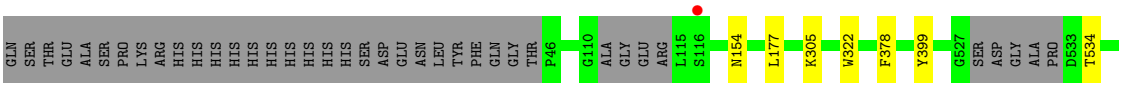




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

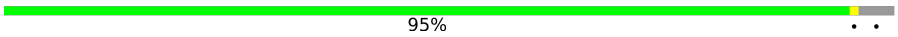
Chain D:

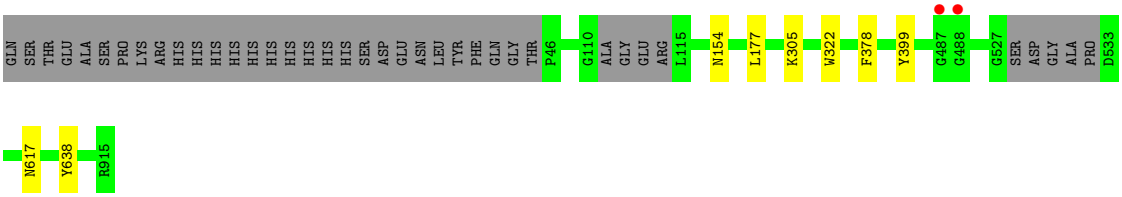




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

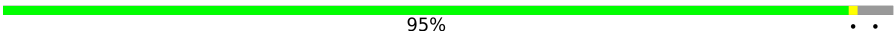
Chain E:

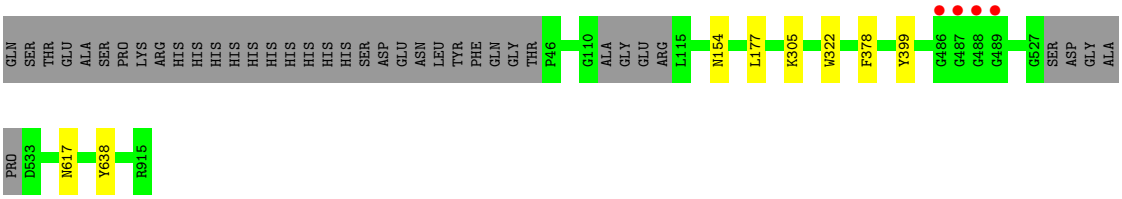




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

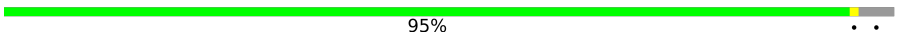
Chain F:

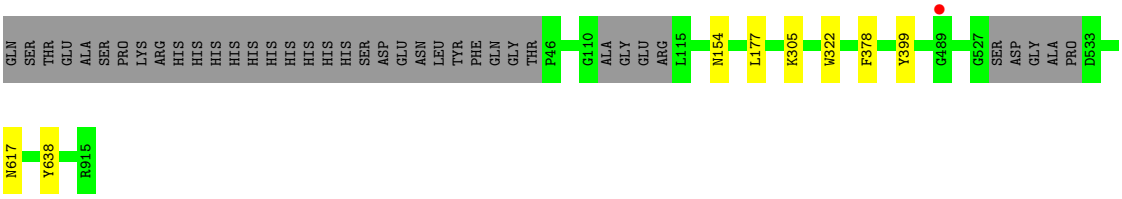




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

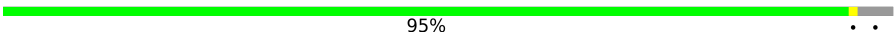
Chain G:

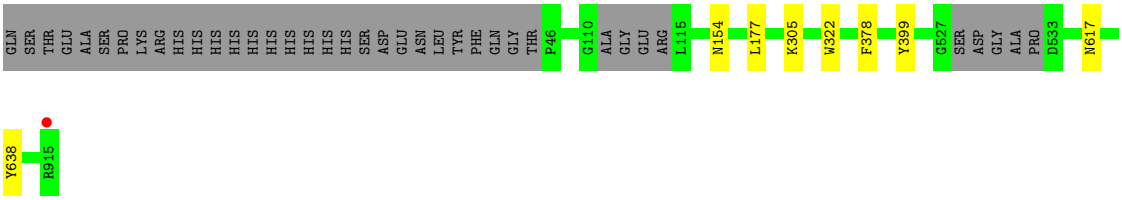




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

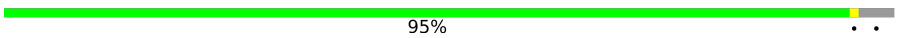
Chain H:

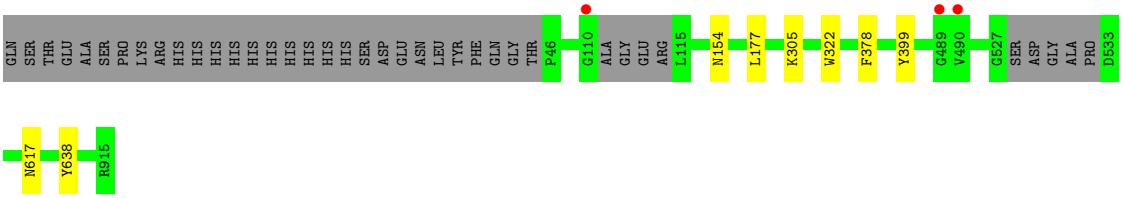




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

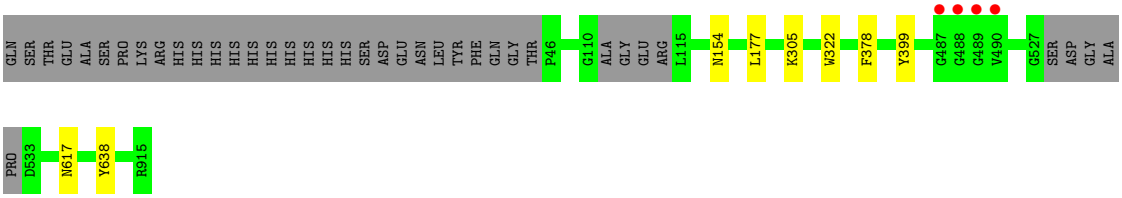
Chain I:





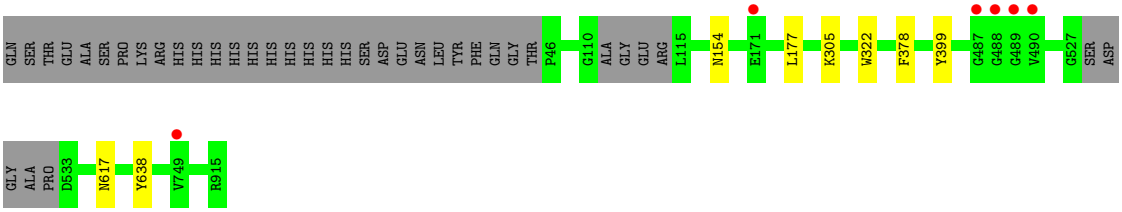
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain J: 95%



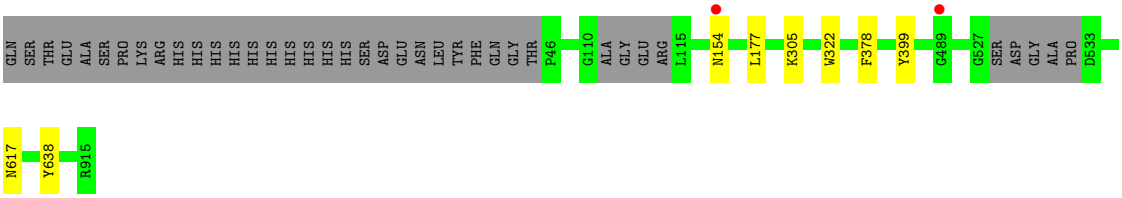
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain K: %
95%



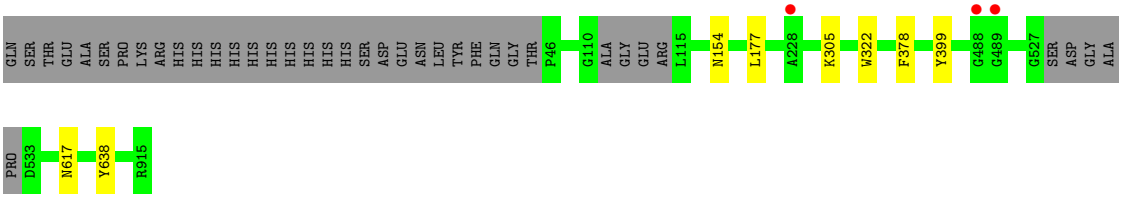
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain L: 95%



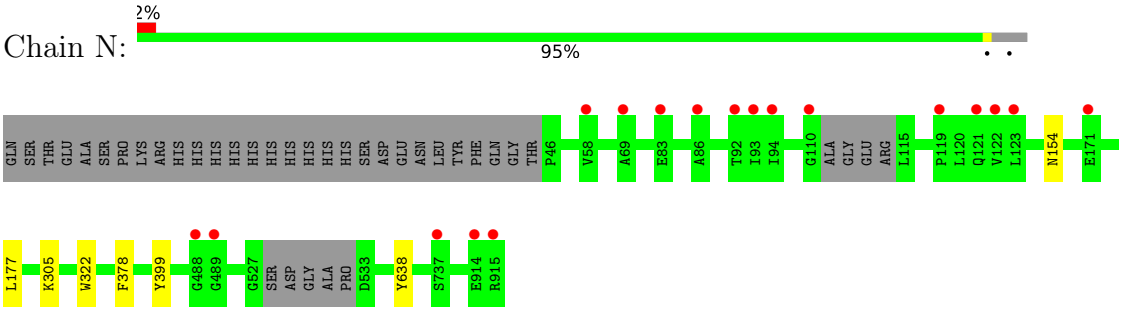
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain M: 95%



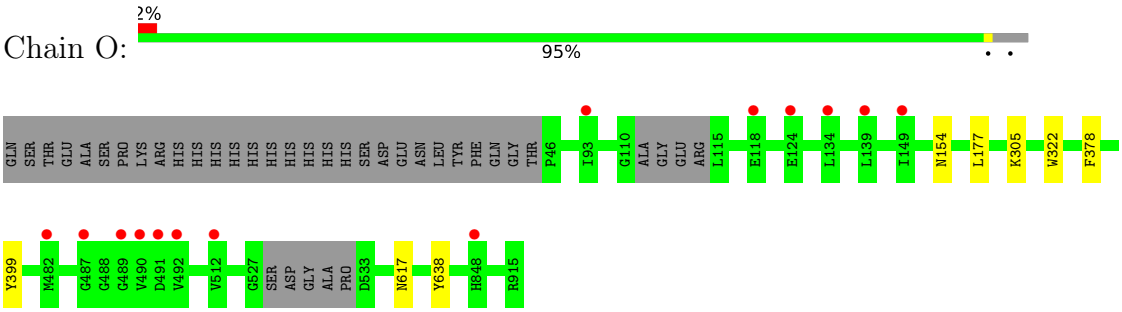
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain N:



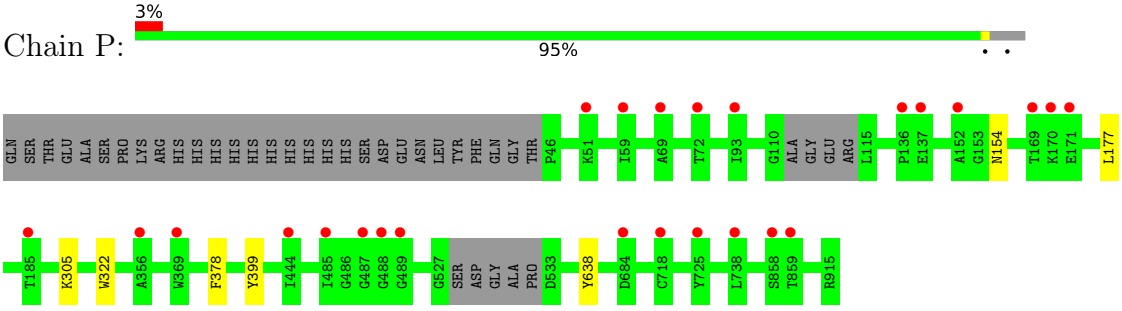
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain O:



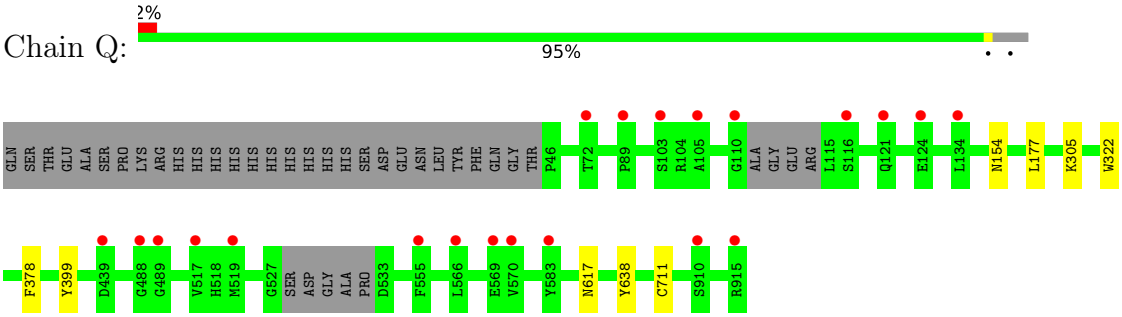
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain P:



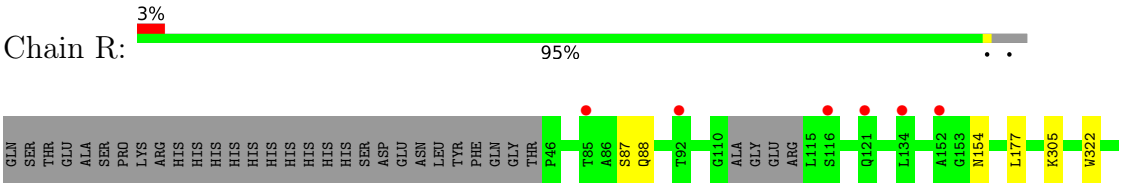
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain Q:



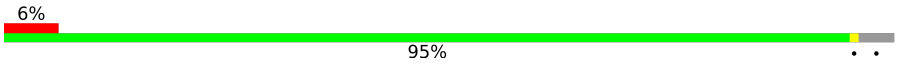
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

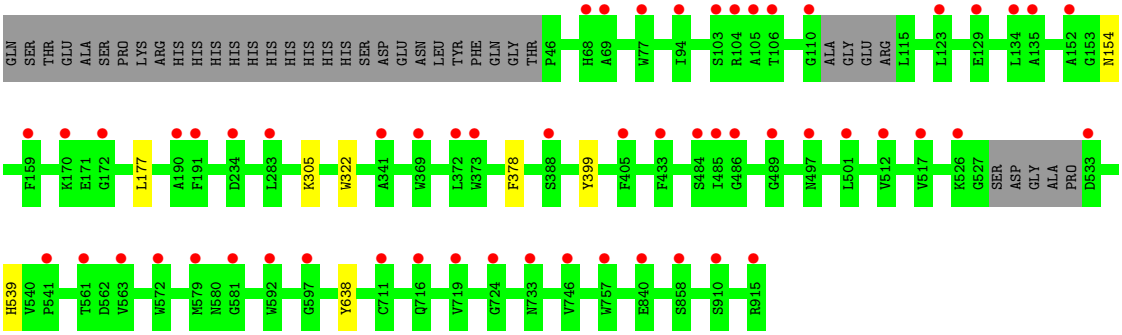
Chain R:



• Molecule 1: Endoplasmic reticulum aminopeptidase 1

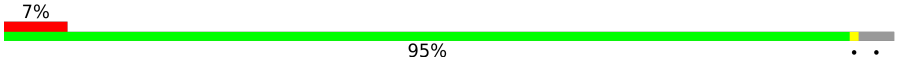
Chain S:

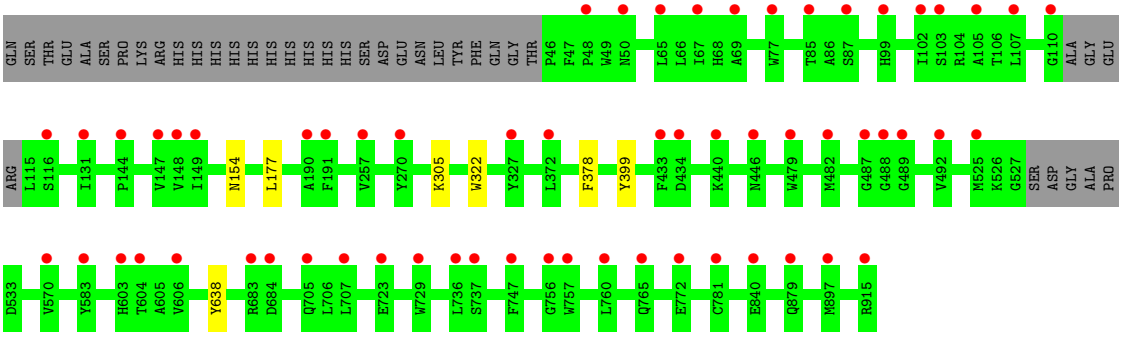




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

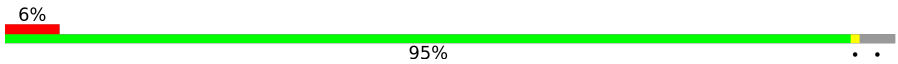
Chain T:

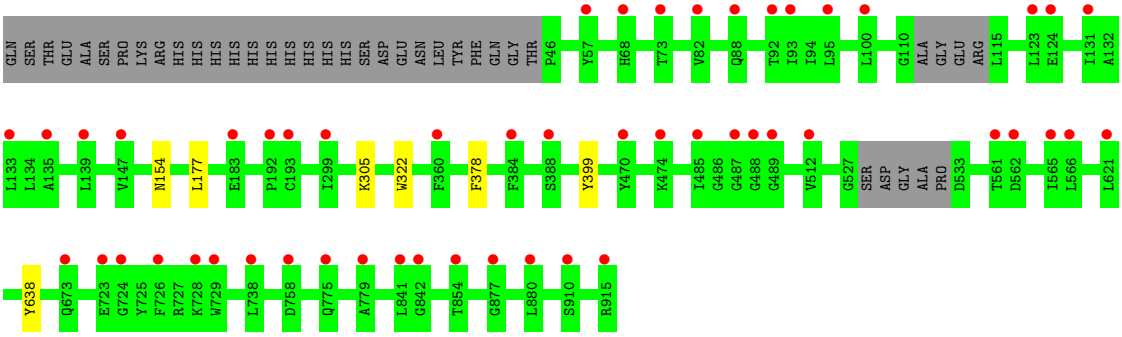




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

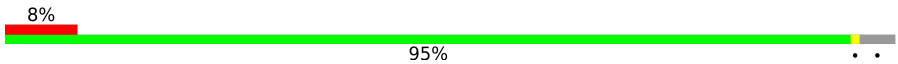
Chain U:

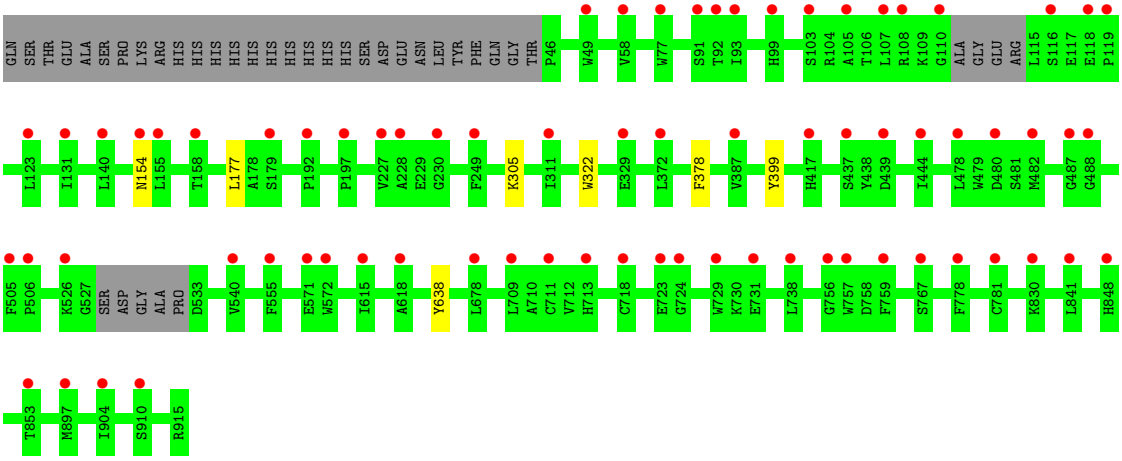




• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain V:





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

Chain W: 100%

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

Chain X: 33% 67%

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

Chain Y: 100%

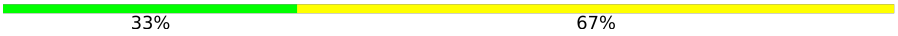
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 33% 67%

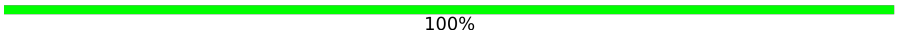
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 100%

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

Chain b: 

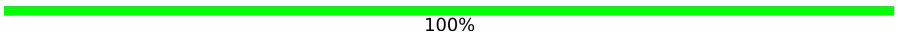
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

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

Chain d:

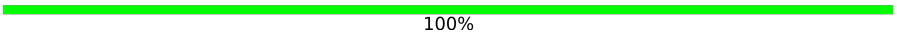
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

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

Chain f:

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

Chain g: 

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

Chain h: 33% 67%

NAG1 NAG2 BMA3

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

Chain i: 100%

NAG1 NAG2 BMA3

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

Chain j: 33% 67%

NAG1 NAG2 BMA3

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

Chain k: 100%

NAG1 NAG2 BMA3

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

Chain l: 33% 67%

NAG1 NAG2 BMA3

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

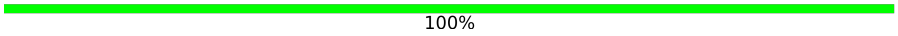
Chain m: 100%

NAG1 NAG2 BMA3

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

Chain n: 33% 67%

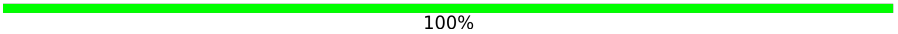
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 

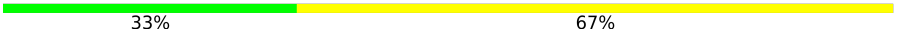
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

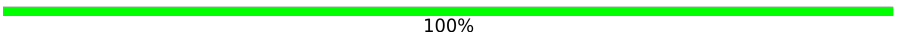
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q: 

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

Chain r: 

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

Chain s: 

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

Chain t:

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

Chain u: 100%

NAG1 NAG2 BMA3

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

Chain v: 33% 67%

NAG1 NAG2 BMA3

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

Chain w: 100%

NAG1 NAG2 BMA3

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

Chain x: 33% 67%

NAG1 NAG2 BMA3

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

Chain y: 100%

NAG1 NAG2 BMA3

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

Chain z: 33% 67%

NAG1 NAG2 BMA3

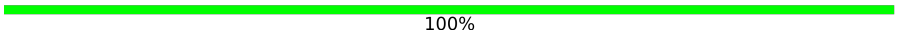
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 0: 100%

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

Chain 1:

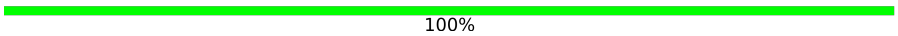
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 2: 

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

Chain 3:

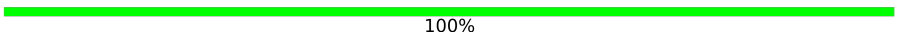
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 

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

Chain 5:

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

Chain 6: 

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

Chain 7: 33% 67%

NAG1 NAG2 BMA3

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

Chain 8: 100%

NAG1 NAG2 BMA3

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

Chain 9: 33% 67%

NAG1 NAG2 BMA3

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

Chain AA: 100%

NAG1 NAG2 BMA3

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

Chain BA: 33% 67%

NAG1 NAG2 BMA3

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

Chain CA: 100%

NAG1 NAG2 BMA3

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

Chain DA: 33% 67%

NAG1
NAG2
BMA3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.79Å 548.68Å 589.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.40 – 3.31 50.11 – 3.31	Depositor EDS
% Data completeness (in resolution range)	74.7 (41.40-3.31) 65.5 (50.11-3.31)	Depositor EDS
R_{merge}	1.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.285 , 0.295 0.286 , 0.295	Depositor DCC
R_{free} test set	2124 reflections (0.47%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , -26.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.70	EDS
Total number of atoms	155927	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN, BMA, P52, 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	0.26	0/7075	0.45	0/9602
1	B	0.26	0/7075	0.45	0/9602
1	C	0.27	1/7077 (0.0%)	0.45	0/9604
1	D	0.26	0/7078	0.45	0/9606
1	E	0.26	0/7075	0.45	0/9602
1	F	0.26	0/7078	0.45	0/9606
1	G	0.27	0/7075	0.45	0/9602
1	H	0.26	0/7075	0.45	0/9602
1	I	0.26	0/7075	0.44	0/9602
1	J	0.26	0/7075	0.44	0/9602
1	K	0.26	0/7075	0.44	0/9602
1	L	0.26	0/7075	0.44	0/9602
1	M	0.26	0/7075	0.44	0/9602
1	N	0.26	0/7075	0.44	0/9602
1	O	0.25	0/7075	0.44	0/9602
1	P	0.26	0/7075	0.44	0/9602
1	Q	0.25	0/7075	0.42	0/9602
1	R	0.26	0/7075	0.44	0/9602
1	S	0.26	0/7075	0.44	0/9602
1	T	0.26	0/7075	0.44	0/9602
1	U	0.26	0/7075	0.44	0/9602
1	V	0.26	0/7075	0.44	0/9602
All	All	0.26	1/155658 (0.0%)	0.44	0/211254

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	ALA	C-N	-5.28	1.22	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
1	B	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
1	C	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	D	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
1	E	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	F	859/899 (96%)	825 (96%)	34 (4%)	0	100	100
1	G	859/899 (96%)	822 (96%)	37 (4%)	0	100	100
1	H	859/899 (96%)	823 (96%)	36 (4%)	0	100	100
1	I	859/899 (96%)	823 (96%)	36 (4%)	0	100	100
1	J	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	K	859/899 (96%)	825 (96%)	34 (4%)	0	100	100
1	L	859/899 (96%)	823 (96%)	36 (4%)	0	100	100
1	M	859/899 (96%)	823 (96%)	36 (4%)	0	100	100
1	N	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	O	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
1	P	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	Q	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	R	859/899 (96%)	822 (96%)	37 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	859/899 (96%)	824 (96%)	35 (4%)	0	100	100
1	T	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
1	U	859/899 (96%)	825 (96%)	34 (4%)	0	100	100
1	V	859/899 (96%)	826 (96%)	33 (4%)	0	100	100
All	All	18898/19778 (96%)	18135 (96%)	763 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	B	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	C	745/799 (93%)	737 (99%)	8 (1%)	73	85
1	D	745/799 (93%)	736 (99%)	9 (1%)	71	84
1	E	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	F	745/799 (93%)	737 (99%)	8 (1%)	73	85
1	G	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	H	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	I	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	J	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	K	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	L	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	M	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	N	744/799 (93%)	737 (99%)	7 (1%)	78	88
1	O	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	P	744/799 (93%)	737 (99%)	7 (1%)	78	88
1	Q	744/799 (93%)	734 (99%)	10 (1%)	69	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	744/799 (93%)	733 (98%)	11 (2%)	65	81
1	S	744/799 (93%)	736 (99%)	8 (1%)	73	85
1	T	744/799 (93%)	737 (99%)	7 (1%)	78	88
1	U	744/799 (93%)	737 (99%)	7 (1%)	78	88
1	V	744/799 (93%)	737 (99%)	7 (1%)	78	88
All	All	16371/17578 (93%)	16194 (99%)	177 (1%)	73	85

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	177	LEU
1	A	305	LYS
1	A	322	TRP
1	A	378	PHE
1	A	399	TYR
1	A	617	ASN
1	A	638	TYR
1	B	154	ASN
1	B	177	LEU
1	B	305	LYS
1	B	322	TRP
1	B	378	PHE
1	B	399	TYR
1	B	617	ASN
1	B	638	TYR
1	C	154	ASN
1	C	177	LEU
1	C	305	LYS
1	C	322	TRP
1	C	378	PHE
1	C	399	TYR
1	C	617	ASN
1	C	638	TYR
1	D	154	ASN
1	D	177	LEU
1	D	305	LYS
1	D	322	TRP
1	D	378	PHE
1	D	399	TYR

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Mol	Chain	Res	Type
1	D	534	THR
1	D	617	ASN
1	D	638	TYR
1	E	154	ASN
1	E	177	LEU
1	E	305	LYS
1	E	322	TRP
1	E	378	PHE
1	E	399	TYR
1	E	617	ASN
1	E	638	TYR
1	F	154	ASN
1	F	177	LEU
1	F	305	LYS
1	F	322	TRP
1	F	378	PHE
1	F	399	TYR
1	F	617	ASN
1	F	638	TYR
1	G	154	ASN
1	G	177	LEU
1	G	305	LYS
1	G	322	TRP
1	G	378	PHE
1	G	399	TYR
1	G	617	ASN
1	G	638	TYR
1	H	154	ASN
1	H	177	LEU
1	H	305	LYS
1	H	322	TRP
1	H	378	PHE
1	H	399	TYR
1	H	617	ASN
1	H	638	TYR
1	I	154	ASN
1	I	177	LEU
1	I	305	LYS
1	I	322	TRP
1	I	378	PHE
1	I	399	TYR
1	I	617	ASN

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Mol	Chain	Res	Type
1	I	638	TYR
1	J	154	ASN
1	J	177	LEU
1	J	305	LYS
1	J	322	TRP
1	J	378	PHE
1	J	399	TYR
1	J	617	ASN
1	J	638	TYR
1	K	154	ASN
1	K	177	LEU
1	K	305	LYS
1	K	322	TRP
1	K	378	PHE
1	K	399	TYR
1	K	617	ASN
1	K	638	TYR
1	L	154	ASN
1	L	177	LEU
1	L	305	LYS
1	L	322	TRP
1	L	378	PHE
1	L	399	TYR
1	L	617	ASN
1	L	638	TYR
1	M	154	ASN
1	M	177	LEU
1	M	305	LYS
1	M	322	TRP
1	M	378	PHE
1	M	399	TYR
1	M	617	ASN
1	M	638	TYR
1	N	154	ASN
1	N	177	LEU
1	N	305	LYS
1	N	322	TRP
1	N	378	PHE
1	N	399	TYR
1	N	638	TYR
1	O	154	ASN
1	O	177	LEU

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Mol	Chain	Res	Type
1	O	305	LYS
1	O	322	TRP
1	O	378	PHE
1	O	399	TYR
1	O	617	ASN
1	O	638	TYR
1	P	154	ASN
1	P	177	LEU
1	P	305	LYS
1	P	322	TRP
1	P	378	PHE
1	P	399	TYR
1	P	638	TYR
1	Q	154	ASN
1	Q	177	LEU
1	Q	305	LYS
1	Q	322	TRP
1	Q	378	PHE
1	Q	399	TYR
1	Q	617	ASN
1	Q	638	TYR
1	Q	711[A]	CYS
1	Q	711[B]	CYS
1	R	87	SER
1	R	88	GLN
1	R	154	ASN
1	R	177	LEU
1	R	305	LYS
1	R	322	TRP
1	R	378	PHE
1	R	399	TYR
1	R	534	THR
1	R	617	ASN
1	R	638	TYR
1	S	154	ASN
1	S	177	LEU
1	S	305	LYS
1	S	322	TRP
1	S	378	PHE
1	S	399	TYR
1	S	539	HIS
1	S	638	TYR

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Mol	Chain	Res	Type
1	T	154	ASN
1	T	177	LEU
1	T	305	LYS
1	T	322	TRP
1	T	378	PHE
1	T	399	TYR
1	T	638	TYR
1	U	154	ASN
1	U	177	LEU
1	U	305	LYS
1	U	322	TRP
1	U	378	PHE
1	U	399	TYR
1	U	638	TYR
1	V	154	ASN
1	V	177	LEU
1	V	305	LYS
1	V	322	TRP
1	V	378	PHE
1	V	399	TYR
1	V	638	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (171) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	130	GLN
1	A	306	GLN
1	A	765	GLN
1	A	826	GLN
1	B	125	HIS
1	B	130	GLN
1	B	306	GLN
1	B	414	ASN
1	B	553	HIS
1	B	617	ASN
1	B	620	GLN
1	B	765	GLN
1	B	826	GLN
1	B	879	GLN
1	C	125	HIS
1	C	130	GLN

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Mol	Chain	Res	Type
1	C	306	GLN
1	C	414	ASN
1	C	765	GLN
1	C	826	GLN
1	D	125	HIS
1	D	306	GLN
1	D	414	ASN
1	D	475	ASN
1	D	603	HIS
1	D	620	GLN
1	D	765	GLN
1	D	826	GLN
1	E	125	HIS
1	E	130	GLN
1	E	306	GLN
1	E	414	ASN
1	E	603	HIS
1	E	620	GLN
1	E	765	GLN
1	E	826	GLN
1	E	856	GLN
1	F	125	HIS
1	F	306	GLN
1	F	414	ASN
1	F	617	ASN
1	F	620	GLN
1	F	765	GLN
1	F	826	GLN
1	G	128	GLN
1	G	306	GLN
1	G	414	ASN
1	G	620	GLN
1	G	765	GLN
1	G	826	GLN
1	H	128	GLN
1	H	306	GLN
1	H	414	ASN
1	H	673	GLN
1	H	765	GLN
1	H	826	GLN
1	H	856	GLN
1	I	125	HIS

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Mol	Chain	Res	Type
1	I	130	GLN
1	I	306	GLN
1	I	414	ASN
1	I	603	HIS
1	I	765	GLN
1	I	790	GLN
1	I	826	GLN
1	J	125	HIS
1	J	306	GLN
1	J	414	ASN
1	J	616	ASN
1	J	620	GLN
1	J	765	GLN
1	J	826	GLN
1	K	125	HIS
1	K	130	GLN
1	K	306	GLN
1	K	414	ASN
1	K	523	HIS
1	K	553	HIS
1	K	603	HIS
1	K	673	GLN
1	K	765	GLN
1	K	826	GLN
1	K	879	GLN
1	L	125	HIS
1	L	306	GLN
1	L	414	ASN
1	L	425	ASN
1	L	475	ASN
1	L	765	GLN
1	L	826	GLN
1	M	128	GLN
1	M	306	GLN
1	M	414	ASN
1	M	446	ASN
1	M	468	HIS
1	M	603	HIS
1	M	765	GLN
1	M	826	GLN
1	N	125	HIS
1	N	130	GLN

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Mol	Chain	Res	Type
1	N	306	GLN
1	N	414	ASN
1	N	603	HIS
1	N	617	ASN
1	N	620	GLN
1	N	765	GLN
1	N	790	GLN
1	N	809	GLN
1	N	826	GLN
1	N	848	HIS
1	O	125	HIS
1	O	130	GLN
1	O	414	ASN
1	O	553	HIS
1	O	765	GLN
1	O	809	GLN
1	O	826	GLN
1	O	856	GLN
1	P	125	HIS
1	P	130	GLN
1	P	306	GLN
1	P	414	ASN
1	P	553	HIS
1	P	617	ASN
1	P	620	GLN
1	P	765	GLN
1	P	826	GLN
1	Q	125	HIS
1	Q	306	GLN
1	Q	414	ASN
1	Q	765	GLN
1	Q	826	GLN
1	Q	879	GLN
1	R	88	GLN
1	R	125	HIS
1	R	306	GLN
1	R	414	ASN
1	R	468	HIS
1	R	617	ASN
1	R	673	GLN
1	R	765	GLN
1	R	826	GLN

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Mol	Chain	Res	Type
1	S	125	HIS
1	S	414	ASN
1	S	620	GLN
1	S	765	GLN
1	S	826	GLN
1	S	856	GLN
1	T	125	HIS
1	T	306	GLN
1	T	414	ASN
1	T	446	ASN
1	T	603	HIS
1	T	765	GLN
1	T	826	GLN
1	U	125	HIS
1	U	130	GLN
1	U	306	GLN
1	U	414	ASN
1	U	475	ASN
1	U	765	GLN
1	U	790	GLN
1	U	826	GLN
1	V	125	HIS
1	V	306	GLN
1	V	414	ASN
1	V	603	HIS
1	V	617	ASN
1	V	765	GLN
1	V	826	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)

132 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	0	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	0	2	2	14,14,15	0.34	0	17,19,21	0.81	0
2	BMA	0	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	1	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	1	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	1	3	2	11,11,12	0.27	0	15,15,17	0.86	0
2	NAG	2	1	1,2	14,14,15	0.31	0	17,19,21	0.77	0
2	NAG	2	2	2	14,14,15	0.33	0	17,19,21	0.80	0
2	BMA	2	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	3	1	2	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
2	NAG	3	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	3	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	4	1	1,2	14,14,15	0.33	0	17,19,21	0.77	0
2	NAG	4	2	2	14,14,15	0.33	0	17,19,21	0.80	0
2	BMA	4	3	2	11,11,12	0.23	0	15,15,17	1.00	0
2	NAG	5	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	5	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	5	3	2	11,11,12	0.28	0	15,15,17	0.86	0
2	NAG	6	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	6	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	6	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	7	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	7	2	2	14,14,15	0.29	0	17,19,21	1.00	1 (5%)
2	BMA	7	3	2	11,11,12	0.25	0	15,15,17	0.86	0
2	NAG	8	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	8	2	2	14,14,15	0.33	0	17,19,21	0.80	0
2	BMA	8	3	2	11,11,12	0.23	0	15,15,17	0.99	0
2	NAG	9	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	9	2	2	14,14,15	0.29	0	17,19,21	1.00	1 (5%)
2	BMA	9	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	AA	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	AA	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	AA	3	2	11,11,12	0.22	0	15,15,17	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	BA	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	BA	2	2	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
2	BMA	BA	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	CA	1	1,2	14,14,15	0.32	0	17,19,21	0.79	0
2	NAG	CA	2	2	14,14,15	0.35	0	17,19,21	0.80	0
2	BMA	CA	3	2	11,11,12	0.21	0	15,15,17	0.99	0
2	NAG	DA	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	DA	2	2	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
2	BMA	DA	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	W	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	W	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	W	3	2	11,11,12	0.23	0	15,15,17	1.00	0
2	NAG	X	1	1,2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	X	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	BMA	X	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	Y	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	Y	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	Y	3	2	11,11,12	0.24	0	15,15,17	1.00	0
2	NAG	Z	1	2	14,14,15	0.31	0	17,19,21	1.02	1 (5%)
2	NAG	Z	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	BMA	Z	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	a	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	a	2	2	14,14,15	0.33	0	17,19,21	0.80	0
2	BMA	a	3	2	11,11,12	0.22	0	15,15,17	0.99	0
2	NAG	b	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	b	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	b	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	c	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	c	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	c	3	2	11,11,12	0.23	0	15,15,17	1.00	0
2	NAG	d	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	d	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	d	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	e	1	1,2	14,14,15	0.33	0	17,19,21	0.77	0
2	NAG	e	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	e	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	f	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	f	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	f	3	2	11,11,12	0.25	0	15,15,17	0.86	0
2	NAG	g	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	g	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	g	3	2	11,11,12	0.23	0	15,15,17	0.99	0
2	NAG	h	1	2	14,14,15	0.33	0	17,19,21	1.01	1 (5%)
2	NAG	h	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	h	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	i	1	1,2	14,14,15	0.31	0	17,19,21	0.78	0
2	NAG	i	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	i	3	2	11,11,12	0.21	0	15,15,17	0.99	0
2	NAG	j	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	j	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	j	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	k	1	1,2	14,14,15	0.33	0	17,19,21	0.77	0
2	NAG	k	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	k	3	2	11,11,12	0.22	0	15,15,17	0.99	0
2	NAG	l	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	l	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	l	3	2	11,11,12	0.27	0	15,15,17	0.86	0
2	NAG	m	1	1,2	14,14,15	0.31	0	17,19,21	0.78	0
2	NAG	m	2	2	14,14,15	0.33	0	17,19,21	0.80	0
2	BMA	m	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	n	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	n	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	BMA	n	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	o	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	o	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	o	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	p	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	p	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	BMA	p	3	2	11,11,12	0.27	0	15,15,17	0.85	0
2	NAG	q	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	q	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	q	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	r	1	2	14,14,15	0.33	0	17,19,21	1.01	1 (5%)
2	NAG	r	2	2	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
2	BMA	r	3	2	11,11,12	0.26	0	15,15,17	0.85	0
2	NAG	s	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	s	2	2	14,14,15	0.33	0	17,19,21	0.79	0
2	BMA	s	3	2	11,11,12	0.22	0	15,15,17	0.99	0
2	NAG	t	1	2	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
2	NAG	t	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BMA	t	3	2	11,11,12	0.27	0	15,15,17	0.86	0
2	NAG	u	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	u	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	u	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	v	1	2	14,14,15	0.33	0	17,19,21	1.01	1 (5%)
2	NAG	v	2	2	14,14,15	0.29	0	17,19,21	0.99	1 (5%)
2	BMA	v	3	2	11,11,12	0.26	0	15,15,17	0.86	0
2	NAG	w	1	1,2	14,14,15	0.32	0	17,19,21	0.78	0
2	NAG	w	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	w	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	x	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	x	2	2	14,14,15	0.28	0	17,19,21	1.00	1 (5%)
2	BMA	x	3	2	11,11,12	0.25	0	15,15,17	0.86	0
2	NAG	y	1	1,2	14,14,15	0.32	0	17,19,21	0.77	0
2	NAG	y	2	2	14,14,15	0.34	0	17,19,21	0.80	0
2	BMA	y	3	2	11,11,12	0.22	0	15,15,17	1.00	0
2	NAG	z	1	2	14,14,15	0.31	0	17,19,21	1.01	1 (5%)
2	NAG	z	2	2	14,14,15	0.29	0	17,19,21	1.01	1 (5%)
2	BMA	z	3	2	11,11,12	0.26	0	15,15,17	0.85	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	0	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	0	2	2	-	2/6/23/26	0/1/1/1
2	BMA	0	3	2	-	1/2/19/22	0/1/1/1
2	NAG	1	1	2	-	2/6/23/26	0/1/1/1
2	NAG	1	2	2	-	2/6/23/26	0/1/1/1
2	BMA	1	3	2	-	1/2/19/22	0/1/1/1
2	NAG	2	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	2	2	2	-	2/6/23/26	0/1/1/1
2	BMA	2	3	2	-	1/2/19/22	0/1/1/1
2	NAG	3	1	2	-	2/6/23/26	0/1/1/1
2	NAG	3	2	2	-	2/6/23/26	0/1/1/1
2	BMA	3	3	2	-	1/2/19/22	0/1/1/1
2	NAG	4	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	4	2	2	-	2/6/23/26	0/1/1/1
2	BMA	4	3	2	-	1/2/19/22	0/1/1/1
2	NAG	5	1	2	-	2/6/23/26	0/1/1/1
2	NAG	5	2	2	-	2/6/23/26	0/1/1/1
2	BMA	5	3	2	-	1/2/19/22	0/1/1/1
2	NAG	6	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	6	2	2	-	2/6/23/26	0/1/1/1
2	BMA	6	3	2	-	1/2/19/22	0/1/1/1
2	NAG	7	1	2	-	2/6/23/26	0/1/1/1
2	NAG	7	2	2	-	2/6/23/26	0/1/1/1
2	BMA	7	3	2	-	1/2/19/22	0/1/1/1
2	NAG	8	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	8	2	2	-	2/6/23/26	0/1/1/1
2	BMA	8	3	2	-	1/2/19/22	0/1/1/1
2	NAG	9	1	2	-	2/6/23/26	0/1/1/1
2	NAG	9	2	2	-	2/6/23/26	0/1/1/1
2	BMA	9	3	2	-	1/2/19/22	0/1/1/1
2	NAG	AA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	AA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	AA	3	2	-	1/2/19/22	0/1/1/1
2	NAG	BA	1	2	-	2/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	BA	3	2	-	1/2/19/22	0/1/1/1
2	NAG	CA	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	CA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	CA	3	2	-	1/2/19/22	0/1/1/1
2	NAG	DA	1	2	-	2/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	2/6/23/26	0/1/1/1
2	BMA	DA	3	2	-	1/2/19/22	0/1/1/1
2	NAG	W	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	W	2	2	-	2/6/23/26	0/1/1/1
2	BMA	W	3	2	-	1/2/19/22	0/1/1/1
2	NAG	X	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	X	2	2	-	2/6/23/26	0/1/1/1
2	BMA	X	3	2	-	1/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	Y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	1/2/19/22	0/1/1/1
2	NAG	Z	1	2	-	2/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	2/6/23/26	0/1/1/1
2	BMA	Z	3	2	-	1/2/19/22	0/1/1/1
2	NAG	a	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	a	2	2	-	2/6/23/26	0/1/1/1
2	BMA	a	3	2	-	1/2/19/22	0/1/1/1
2	NAG	b	1	2	-	2/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	1/2/19/22	0/1/1/1
2	NAG	c	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	c	2	2	-	2/6/23/26	0/1/1/1
2	BMA	c	3	2	-	1/2/19/22	0/1/1/1
2	NAG	d	1	2	-	2/6/23/26	0/1/1/1
2	NAG	d	2	2	-	2/6/23/26	0/1/1/1
2	BMA	d	3	2	-	1/2/19/22	0/1/1/1
2	NAG	e	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	BMA	e	3	2	-	1/2/19/22	0/1/1/1
2	NAG	f	1	2	-	2/6/23/26	0/1/1/1
2	NAG	f	2	2	-	2/6/23/26	0/1/1/1
2	BMA	f	3	2	-	1/2/19/22	0/1/1/1
2	NAG	g	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	g	2	2	-	2/6/23/26	0/1/1/1
2	BMA	g	3	2	-	1/2/19/22	0/1/1/1
2	NAG	h	1	2	-	2/6/23/26	0/1/1/1
2	NAG	h	2	2	-	2/6/23/26	0/1/1/1
2	BMA	h	3	2	-	1/2/19/22	0/1/1/1
2	NAG	i	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	i	2	2	-	2/6/23/26	0/1/1/1
2	BMA	i	3	2	-	1/2/19/22	0/1/1/1
2	NAG	j	1	2	-	2/6/23/26	0/1/1/1
2	NAG	j	2	2	-	2/6/23/26	0/1/1/1
2	BMA	j	3	2	-	1/2/19/22	0/1/1/1
2	NAG	k	1	1,2	-	4/6/23/26	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	w	2	2	-	2/6/23/26	0/1/1/1
2	BMA	w	3	2	-	1/2/19/22	0/1/1/1
2	NAG	x	1	2	-	2/6/23/26	0/1/1/1
2	NAG	x	2	2	-	2/6/23/26	0/1/1/1
2	BMA	x	3	2	-	1/2/19/22	0/1/1/1
2	NAG	y	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	y	2	2	-	2/6/23/26	0/1/1/1
2	BMA	y	3	2	-	1/2/19/22	0/1/1/1
2	NAG	z	1	2	-	2/6/23/26	0/1/1/1
2	NAG	z	2	2	-	2/6/23/26	0/1/1/1
2	BMA	z	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	z	2	NAG	C1-O5-C5	2.25	115.24	112.19
2	X	2	NAG	C1-O5-C5	2.23	115.21	112.19
2	DA	2	NAG	C1-O5-C5	2.22	115.20	112.19
2	t	2	NAG	C1-O5-C5	2.21	115.19	112.19
2	Z	2	NAG	C1-O5-C5	2.20	115.18	112.19
2	x	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	n	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	9	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	r	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	7	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	d	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	p	2	NAG	C1-O5-C5	2.19	115.16	112.19
2	h	2	NAG	C1-O5-C5	2.18	115.14	112.19
2	b	2	NAG	C1-O5-C5	2.18	115.14	112.19
2	BA	2	NAG	C1-O5-C5	2.17	115.14	112.19
2	v	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	f	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	1	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	3	2	NAG	C1-O5-C5	2.17	115.13	112.19
2	j	2	NAG	C1-O5-C5	2.16	115.12	112.19
2	l	2	NAG	C1-O5-C5	2.14	115.10	112.19
2	5	2	NAG	C1-O5-C5	2.14	115.10	112.19
2	X	1	NAG	C1-O5-C5	2.14	115.09	112.19
2	7	1	NAG	C1-O5-C5	2.14	115.08	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	1	NAG	C1-O5-C5	2.13	115.08	112.19
2	t	1	NAG	C1-O5-C5	2.13	115.08	112.19
2	DA	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	1	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	p	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	3	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	5	1	NAG	C1-O5-C5	2.12	115.07	112.19
2	j	1	NAG	C1-O5-C5	2.12	115.06	112.19
2	f	1	NAG	C1-O5-C5	2.11	115.06	112.19
2	d	1	NAG	C1-O5-C5	2.11	115.05	112.19
2	x	1	NAG	C1-O5-C5	2.11	115.05	112.19
2	h	1	NAG	C1-O5-C5	2.10	115.04	112.19
2	BA	1	NAG	C1-O5-C5	2.10	115.04	112.19
2	l	1	NAG	C1-O5-C5	2.10	115.03	112.19
2	n	1	NAG	C1-O5-C5	2.10	115.03	112.19
2	z	1	NAG	C1-O5-C5	2.09	115.02	112.19
2	v	1	NAG	C1-O5-C5	2.08	115.01	112.19
2	r	1	NAG	C1-O5-C5	2.08	115.01	112.19
2	9	1	NAG	C1-O5-C5	2.08	115.01	112.19
2	Z	1	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

All (264) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	W	1	NAG	C8-C7-N2-C2
2	W	1	NAG	O7-C7-N2-C2
2	W	2	NAG	O7-C7-N2-C2
2	X	2	NAG	C3-C2-N2-C7
2	Y	1	NAG	C8-C7-N2-C2
2	Y	1	NAG	O7-C7-N2-C2
2	Y	2	NAG	O7-C7-N2-C2
2	Z	2	NAG	C3-C2-N2-C7
2	a	1	NAG	C8-C7-N2-C2
2	a	1	NAG	O7-C7-N2-C2
2	a	2	NAG	O7-C7-N2-C2
2	b	2	NAG	C3-C2-N2-C7
2	c	1	NAG	C8-C7-N2-C2
2	c	1	NAG	O7-C7-N2-C2
2	c	2	NAG	O7-C7-N2-C2
2	d	2	NAG	C3-C2-N2-C7
2	e	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	e	1	NAG	O7-C7-N2-C2
2	e	2	NAG	O7-C7-N2-C2
2	f	2	NAG	C3-C2-N2-C7
2	g	1	NAG	C8-C7-N2-C2
2	g	1	NAG	O7-C7-N2-C2
2	g	2	NAG	O7-C7-N2-C2
2	h	2	NAG	C3-C2-N2-C7
2	i	1	NAG	C8-C7-N2-C2
2	i	1	NAG	O7-C7-N2-C2
2	i	2	NAG	O7-C7-N2-C2
2	j	2	NAG	C3-C2-N2-C7
2	k	1	NAG	C8-C7-N2-C2
2	k	1	NAG	O7-C7-N2-C2
2	k	2	NAG	O7-C7-N2-C2
2	l	2	NAG	C3-C2-N2-C7
2	m	1	NAG	C8-C7-N2-C2
2	m	1	NAG	O7-C7-N2-C2
2	m	2	NAG	O7-C7-N2-C2
2	n	2	NAG	C3-C2-N2-C7
2	o	1	NAG	C8-C7-N2-C2
2	o	1	NAG	O7-C7-N2-C2
2	o	2	NAG	O7-C7-N2-C2
2	p	2	NAG	C3-C2-N2-C7
2	q	1	NAG	C8-C7-N2-C2
2	q	1	NAG	O7-C7-N2-C2
2	q	2	NAG	O7-C7-N2-C2
2	r	2	NAG	C3-C2-N2-C7
2	s	1	NAG	C8-C7-N2-C2
2	s	1	NAG	O7-C7-N2-C2
2	s	2	NAG	O7-C7-N2-C2
2	t	2	NAG	C3-C2-N2-C7
2	u	1	NAG	C8-C7-N2-C2
2	u	1	NAG	O7-C7-N2-C2
2	u	2	NAG	O7-C7-N2-C2
2	v	2	NAG	C3-C2-N2-C7
2	w	1	NAG	C8-C7-N2-C2
2	w	1	NAG	O7-C7-N2-C2
2	w	2	NAG	O7-C7-N2-C2
2	x	2	NAG	C3-C2-N2-C7
2	y	1	NAG	C8-C7-N2-C2
2	y	1	NAG	O7-C7-N2-C2
2	y	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	z	2	NAG	C3-C2-N2-C7
2	0	1	NAG	C8-C7-N2-C2
2	0	1	NAG	O7-C7-N2-C2
2	0	2	NAG	O7-C7-N2-C2
2	1	2	NAG	C3-C2-N2-C7
2	2	1	NAG	C8-C7-N2-C2
2	2	1	NAG	O7-C7-N2-C2
2	2	2	NAG	O7-C7-N2-C2
2	3	2	NAG	C3-C2-N2-C7
2	4	1	NAG	C8-C7-N2-C2
2	4	1	NAG	O7-C7-N2-C2
2	4	2	NAG	O7-C7-N2-C2
2	5	2	NAG	C3-C2-N2-C7
2	6	1	NAG	C8-C7-N2-C2
2	6	1	NAG	O7-C7-N2-C2
2	6	2	NAG	O7-C7-N2-C2
2	7	2	NAG	C3-C2-N2-C7
2	8	1	NAG	C8-C7-N2-C2
2	8	1	NAG	O7-C7-N2-C2
2	8	2	NAG	O7-C7-N2-C2
2	9	2	NAG	C3-C2-N2-C7
2	AA	1	NAG	C8-C7-N2-C2
2	AA	1	NAG	O7-C7-N2-C2
2	AA	2	NAG	O7-C7-N2-C2
2	BA	2	NAG	C3-C2-N2-C7
2	CA	1	NAG	C8-C7-N2-C2
2	CA	1	NAG	O7-C7-N2-C2
2	CA	2	NAG	O7-C7-N2-C2
2	DA	2	NAG	C3-C2-N2-C7
2	W	2	NAG	C8-C7-N2-C2
2	Y	2	NAG	C8-C7-N2-C2
2	a	2	NAG	C8-C7-N2-C2
2	c	2	NAG	C8-C7-N2-C2
2	e	2	NAG	C8-C7-N2-C2
2	g	2	NAG	C8-C7-N2-C2
2	i	2	NAG	C8-C7-N2-C2
2	k	2	NAG	C8-C7-N2-C2
2	m	2	NAG	C8-C7-N2-C2
2	o	2	NAG	C8-C7-N2-C2
2	q	2	NAG	C8-C7-N2-C2
2	s	2	NAG	C8-C7-N2-C2
2	u	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	w	2	NAG	C8-C7-N2-C2
2	y	2	NAG	C8-C7-N2-C2
2	0	2	NAG	C8-C7-N2-C2
2	2	2	NAG	C8-C7-N2-C2
2	4	2	NAG	C8-C7-N2-C2
2	6	2	NAG	C8-C7-N2-C2
2	8	2	NAG	C8-C7-N2-C2
2	AA	2	NAG	C8-C7-N2-C2
2	CA	2	NAG	C8-C7-N2-C2
2	X	1	NAG	C1-C2-N2-C7
2	Z	1	NAG	C1-C2-N2-C7
2	b	1	NAG	C1-C2-N2-C7
2	d	1	NAG	C1-C2-N2-C7
2	f	1	NAG	C1-C2-N2-C7
2	h	1	NAG	C1-C2-N2-C7
2	j	1	NAG	C1-C2-N2-C7
2	l	1	NAG	C1-C2-N2-C7
2	n	1	NAG	C1-C2-N2-C7
2	p	1	NAG	C1-C2-N2-C7
2	r	1	NAG	C1-C2-N2-C7
2	t	1	NAG	C1-C2-N2-C7
2	v	1	NAG	C1-C2-N2-C7
2	x	1	NAG	C1-C2-N2-C7
2	z	1	NAG	C1-C2-N2-C7
2	1	1	NAG	C1-C2-N2-C7
2	3	1	NAG	C1-C2-N2-C7
2	5	1	NAG	C1-C2-N2-C7
2	7	1	NAG	C1-C2-N2-C7
2	9	1	NAG	C1-C2-N2-C7
2	BA	1	NAG	C1-C2-N2-C7
2	DA	1	NAG	C1-C2-N2-C7
2	a	3	BMA	O5-C5-C6-O6
2	m	3	BMA	O5-C5-C6-O6
2	o	3	BMA	O5-C5-C6-O6
2	q	3	BMA	O5-C5-C6-O6
2	u	3	BMA	O5-C5-C6-O6
2	w	3	BMA	O5-C5-C6-O6
2	y	3	BMA	O5-C5-C6-O6
2	4	3	BMA	O5-C5-C6-O6
2	8	3	BMA	O5-C5-C6-O6
2	AA	3	BMA	O5-C5-C6-O6
2	W	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Y	3	BMA	O5-C5-C6-O6
2	c	3	BMA	O5-C5-C6-O6
2	e	3	BMA	O5-C5-C6-O6
2	g	3	BMA	O5-C5-C6-O6
2	i	3	BMA	O5-C5-C6-O6
2	k	3	BMA	O5-C5-C6-O6
2	s	3	BMA	O5-C5-C6-O6
2	0	3	BMA	O5-C5-C6-O6
2	2	3	BMA	O5-C5-C6-O6
2	6	3	BMA	O5-C5-C6-O6
2	CA	3	BMA	O5-C5-C6-O6
2	X	1	NAG	C3-C2-N2-C7
2	Z	1	NAG	C3-C2-N2-C7
2	b	1	NAG	C3-C2-N2-C7
2	d	1	NAG	C3-C2-N2-C7
2	f	1	NAG	C3-C2-N2-C7
2	h	1	NAG	C3-C2-N2-C7
2	j	1	NAG	C3-C2-N2-C7
2	l	1	NAG	C3-C2-N2-C7
2	n	1	NAG	C3-C2-N2-C7
2	p	1	NAG	C3-C2-N2-C7
2	r	1	NAG	C3-C2-N2-C7
2	t	1	NAG	C3-C2-N2-C7
2	v	1	NAG	C3-C2-N2-C7
2	x	1	NAG	C3-C2-N2-C7
2	z	1	NAG	C3-C2-N2-C7
2	1	1	NAG	C3-C2-N2-C7
2	3	1	NAG	C3-C2-N2-C7
2	5	1	NAG	C3-C2-N2-C7
2	7	1	NAG	C3-C2-N2-C7
2	9	1	NAG	C3-C2-N2-C7
2	BA	1	NAG	C3-C2-N2-C7
2	DA	1	NAG	C3-C2-N2-C7
2	a	1	NAG	C4-C5-C6-O6
2	k	1	NAG	C4-C5-C6-O6
2	2	1	NAG	C4-C5-C6-O6
2	AA	1	NAG	C4-C5-C6-O6
2	CA	1	NAG	C4-C5-C6-O6
2	W	1	NAG	C4-C5-C6-O6
2	Y	1	NAG	C4-C5-C6-O6
2	c	1	NAG	C4-C5-C6-O6
2	e	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	g	1	NAG	C4-C5-C6-O6
2	i	1	NAG	C4-C5-C6-O6
2	m	1	NAG	C4-C5-C6-O6
2	o	1	NAG	C4-C5-C6-O6
2	q	1	NAG	C4-C5-C6-O6
2	s	1	NAG	C4-C5-C6-O6
2	u	1	NAG	C4-C5-C6-O6
2	w	1	NAG	C4-C5-C6-O6
2	y	1	NAG	C4-C5-C6-O6
2	0	1	NAG	C4-C5-C6-O6
2	4	1	NAG	C4-C5-C6-O6
2	6	1	NAG	C4-C5-C6-O6
2	8	1	NAG	C4-C5-C6-O6
2	v	3	BMA	O5-C5-C6-O6
2	d	3	BMA	O5-C5-C6-O6
2	l	3	BMA	O5-C5-C6-O6
2	p	3	BMA	O5-C5-C6-O6
2	z	3	BMA	O5-C5-C6-O6
2	9	3	BMA	O5-C5-C6-O6
2	BA	3	BMA	O5-C5-C6-O6
2	X	3	BMA	O5-C5-C6-O6
2	Z	3	BMA	O5-C5-C6-O6
2	h	3	BMA	O5-C5-C6-O6
2	DA	3	BMA	O5-C5-C6-O6
2	b	3	BMA	O5-C5-C6-O6
2	j	3	BMA	O5-C5-C6-O6
2	n	3	BMA	O5-C5-C6-O6
2	r	3	BMA	O5-C5-C6-O6
2	x	3	BMA	O5-C5-C6-O6
2	3	3	BMA	O5-C5-C6-O6
2	5	3	BMA	O5-C5-C6-O6
2	7	3	BMA	O5-C5-C6-O6
2	f	3	BMA	O5-C5-C6-O6
2	t	3	BMA	O5-C5-C6-O6
2	1	3	BMA	O5-C5-C6-O6
2	a	1	NAG	O5-C5-C6-O6
2	u	1	NAG	O5-C5-C6-O6
2	i	1	NAG	O5-C5-C6-O6
2	Y	1	NAG	O5-C5-C6-O6
2	c	1	NAG	O5-C5-C6-O6
2	e	1	NAG	O5-C5-C6-O6
2	k	1	NAG	O5-C5-C6-O6

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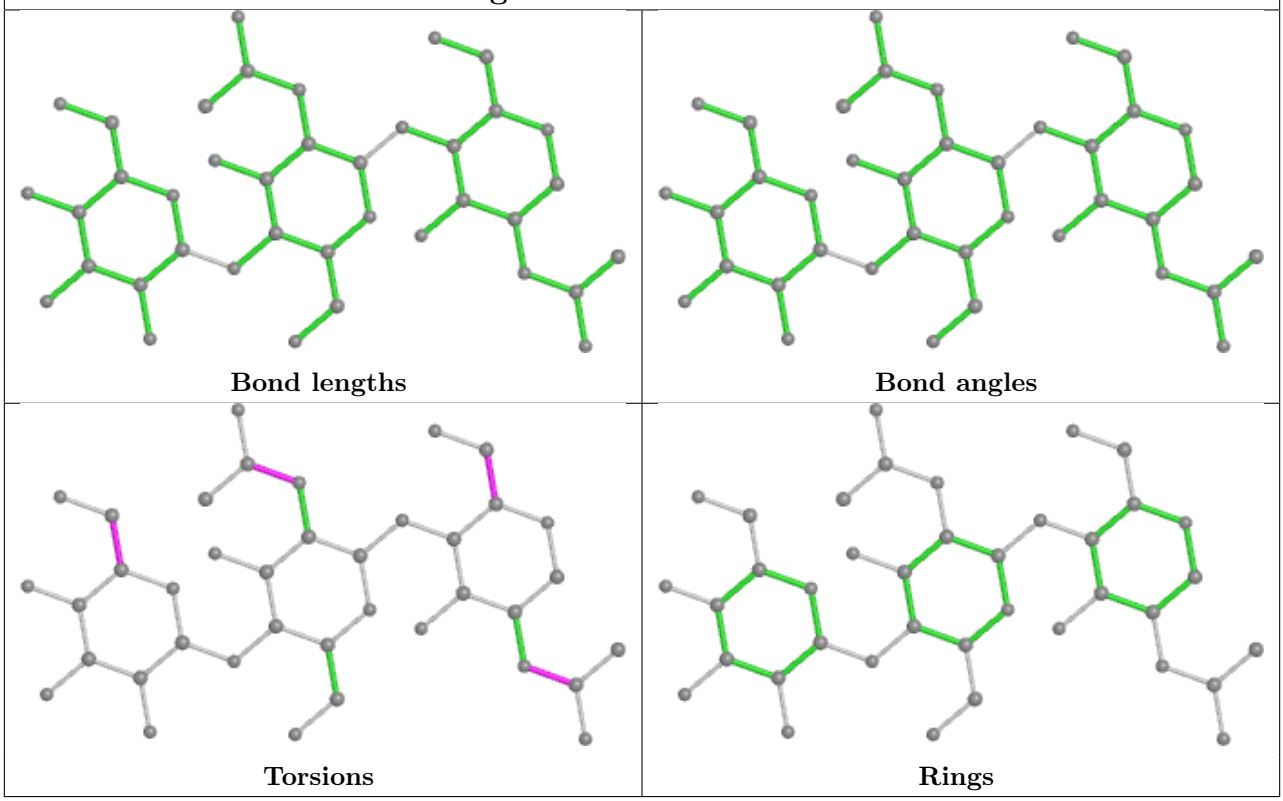
Mol	Chain	Res	Type	Atoms
2	m	1	NAG	O5-C5-C6-O6
2	q	1	NAG	O5-C5-C6-O6
2	s	1	NAG	O5-C5-C6-O6
2	w	1	NAG	O5-C5-C6-O6
2	0	1	NAG	O5-C5-C6-O6
2	2	1	NAG	O5-C5-C6-O6
2	4	1	NAG	O5-C5-C6-O6
2	6	1	NAG	O5-C5-C6-O6
2	8	1	NAG	O5-C5-C6-O6
2	AA	1	NAG	O5-C5-C6-O6
2	CA	1	NAG	O5-C5-C6-O6
2	W	1	NAG	O5-C5-C6-O6
2	g	1	NAG	O5-C5-C6-O6
2	y	1	NAG	O5-C5-C6-O6
2	o	1	NAG	O5-C5-C6-O6
2	X	2	NAG	C1-C2-N2-C7
2	Z	2	NAG	C1-C2-N2-C7
2	b	2	NAG	C1-C2-N2-C7
2	d	2	NAG	C1-C2-N2-C7
2	f	2	NAG	C1-C2-N2-C7
2	h	2	NAG	C1-C2-N2-C7
2	j	2	NAG	C1-C2-N2-C7
2	l	2	NAG	C1-C2-N2-C7
2	n	2	NAG	C1-C2-N2-C7
2	p	2	NAG	C1-C2-N2-C7
2	r	2	NAG	C1-C2-N2-C7
2	t	2	NAG	C1-C2-N2-C7
2	v	2	NAG	C1-C2-N2-C7
2	x	2	NAG	C1-C2-N2-C7
2	z	2	NAG	C1-C2-N2-C7
2	1	2	NAG	C1-C2-N2-C7
2	3	2	NAG	C1-C2-N2-C7
2	5	2	NAG	C1-C2-N2-C7
2	7	2	NAG	C1-C2-N2-C7
2	9	2	NAG	C1-C2-N2-C7
2	BA	2	NAG	C1-C2-N2-C7
2	DA	2	NAG	C1-C2-N2-C7

There are no ring outliers.

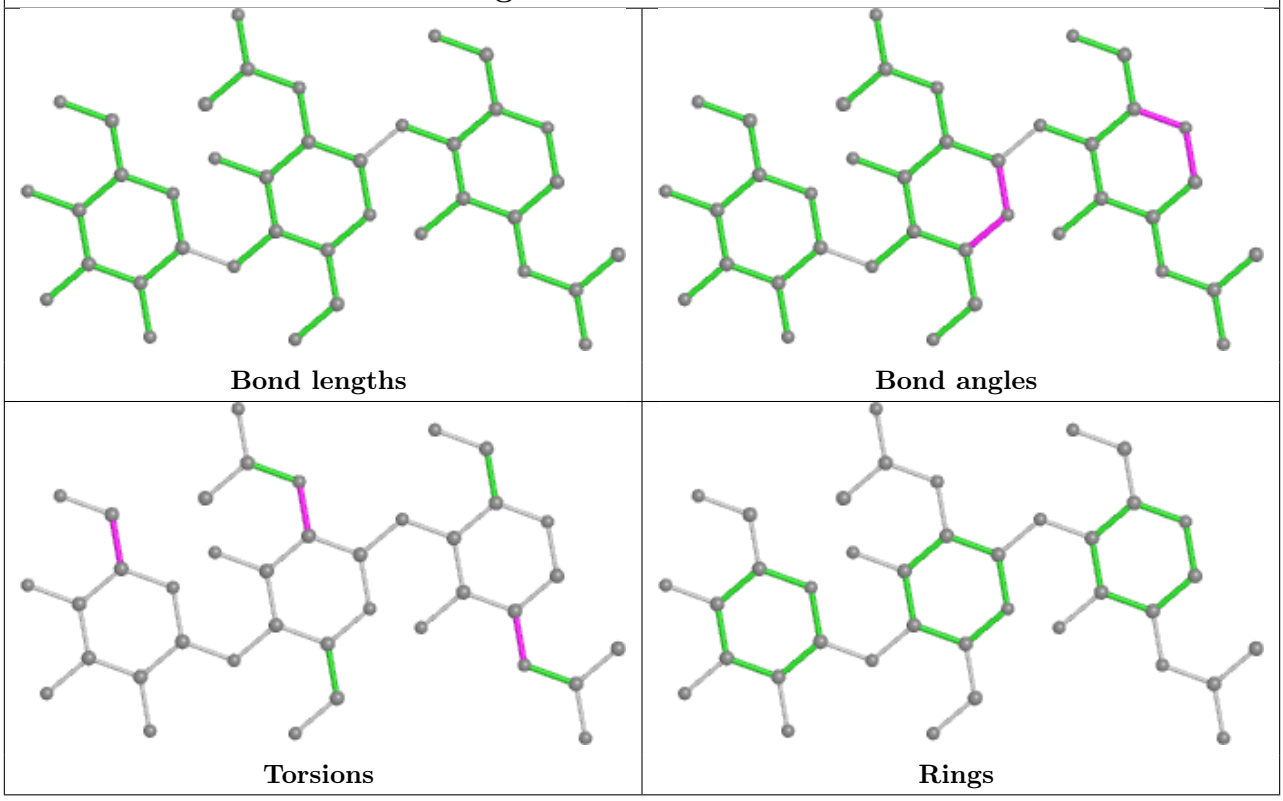
No monomer is involved in short contacts.

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

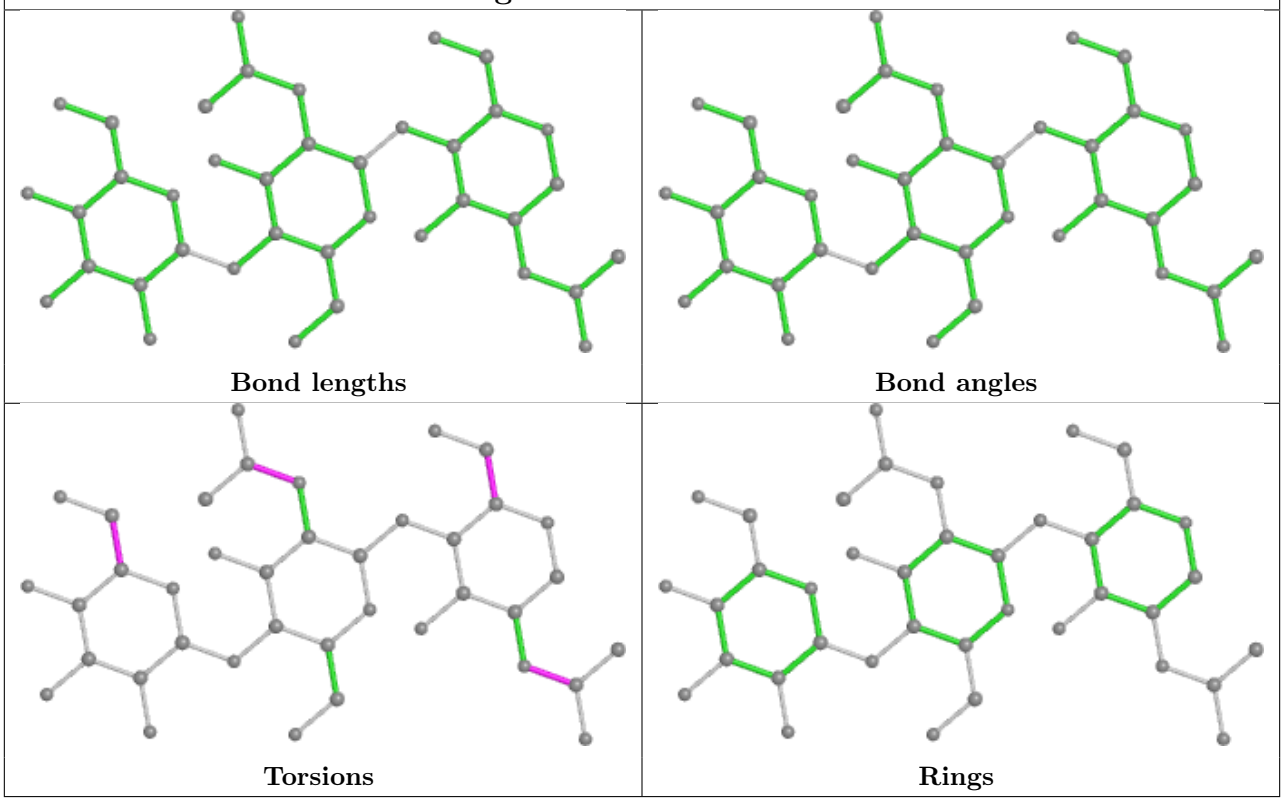
Oligosaccharide Chain W



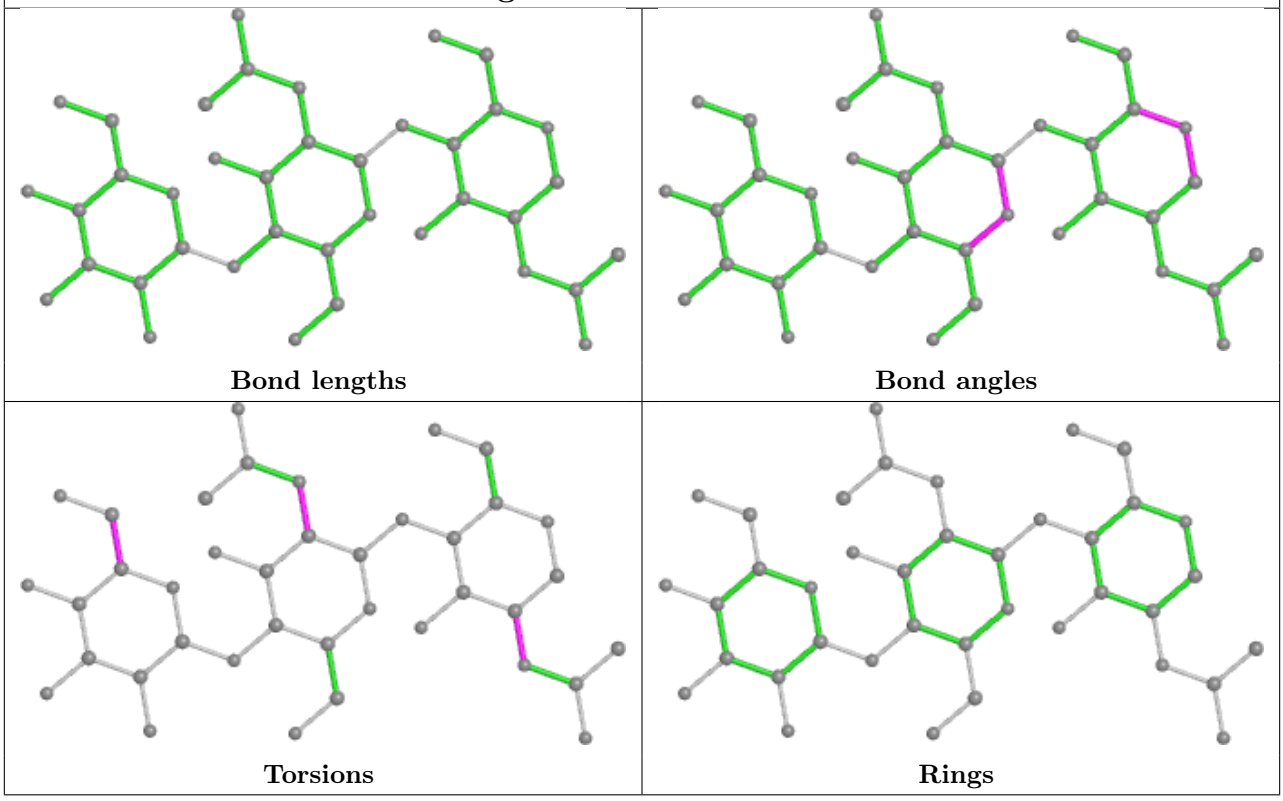
Oligosaccharide Chain X



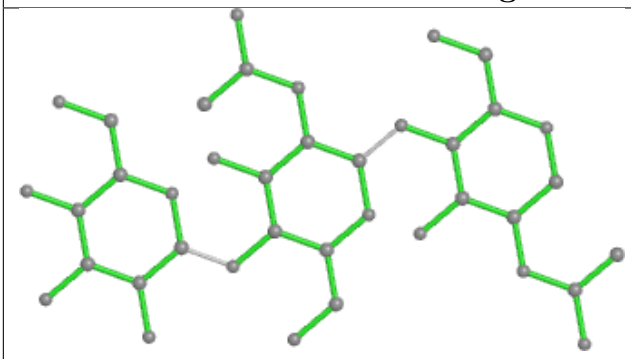
Oligosaccharide Chain Y



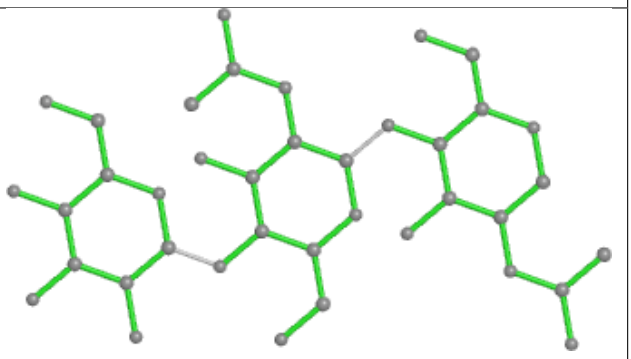
Oligosaccharide Chain Z



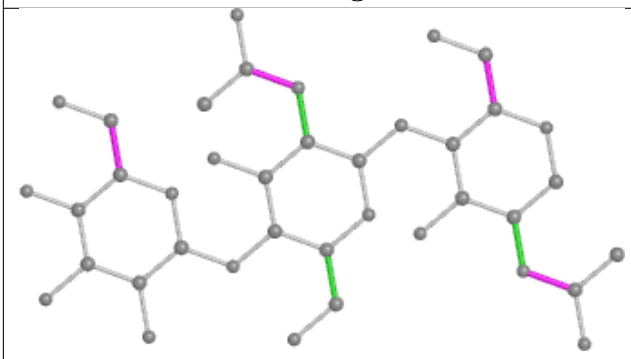
Oligosaccharide Chain a



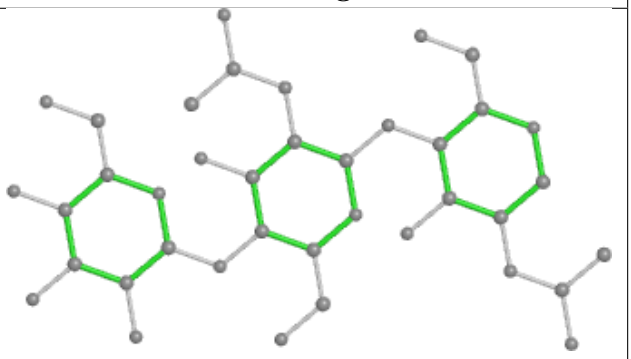
Bond lengths



Bond angles

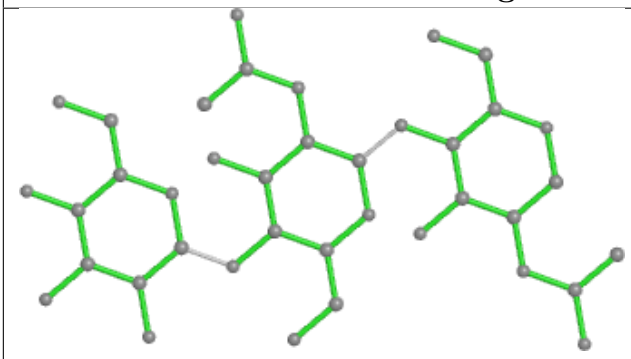


Torsions

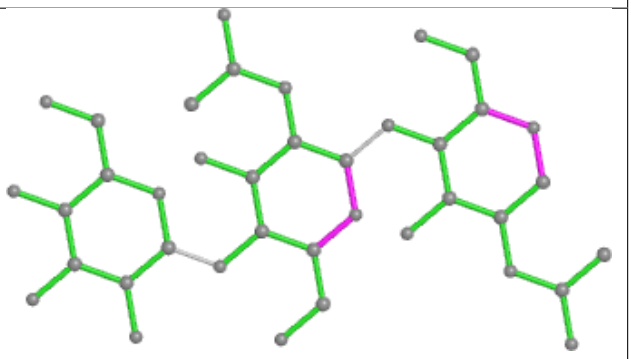


Rings

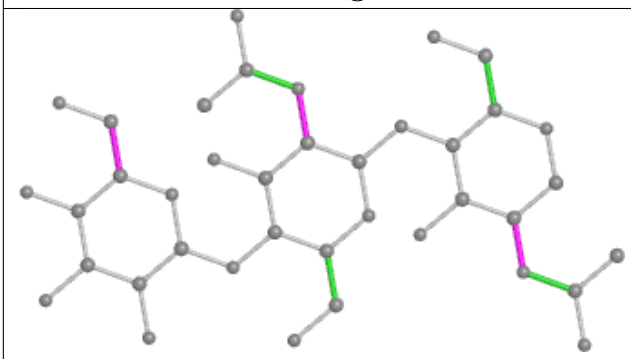
Oligosaccharide Chain b



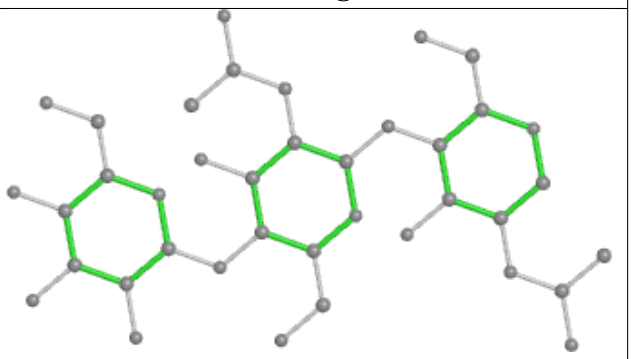
Bond lengths



Bond angles

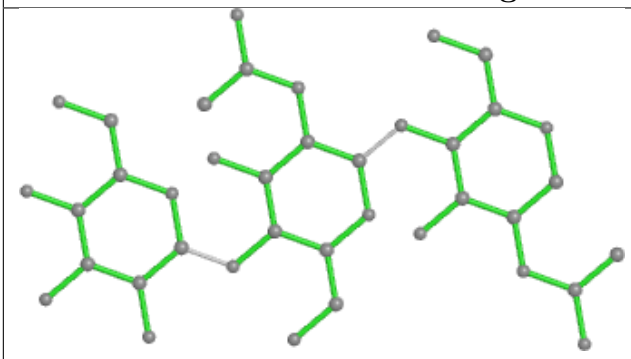


Torsions

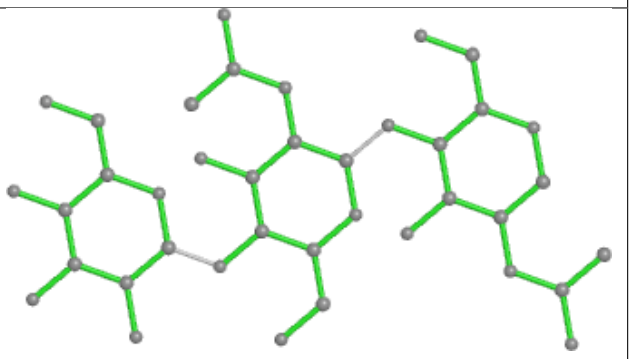


Rings

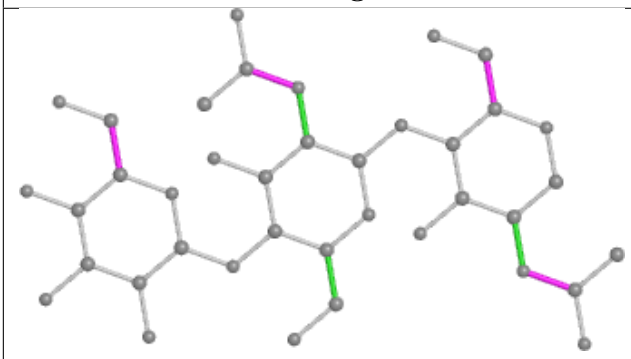
Oligosaccharide Chain c



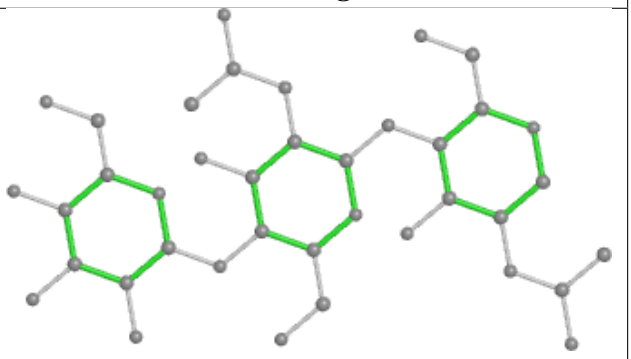
Bond lengths



Bond angles

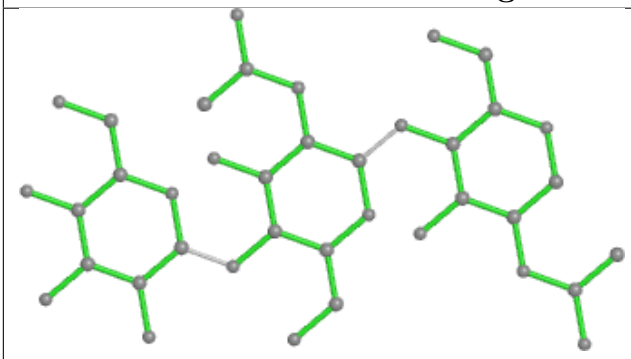


Torsions

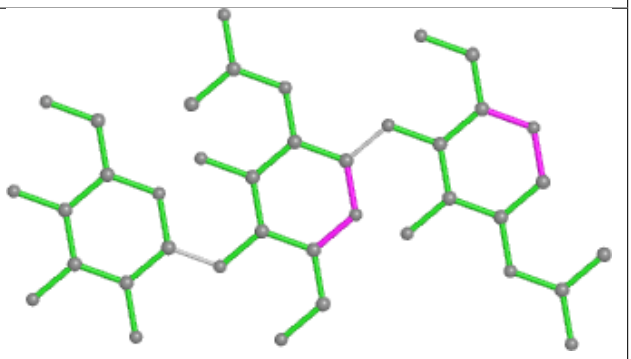


Rings

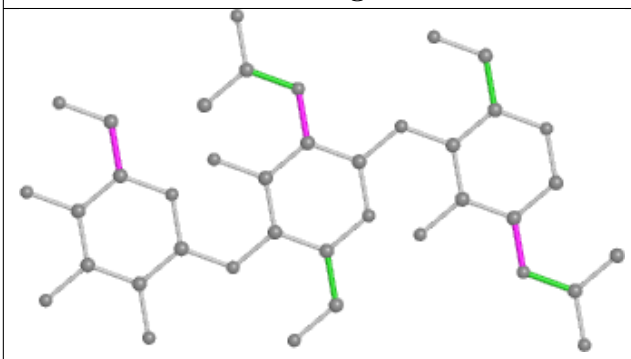
Oligosaccharide Chain d



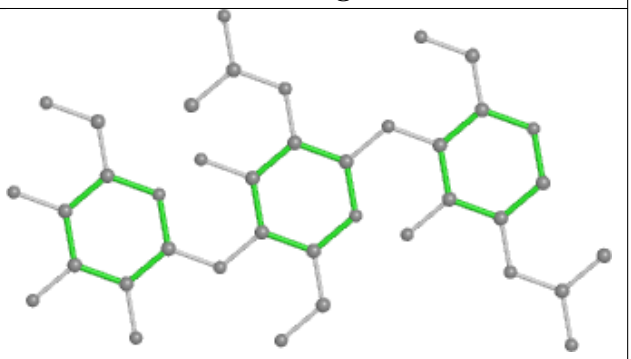
Bond lengths



Bond angles

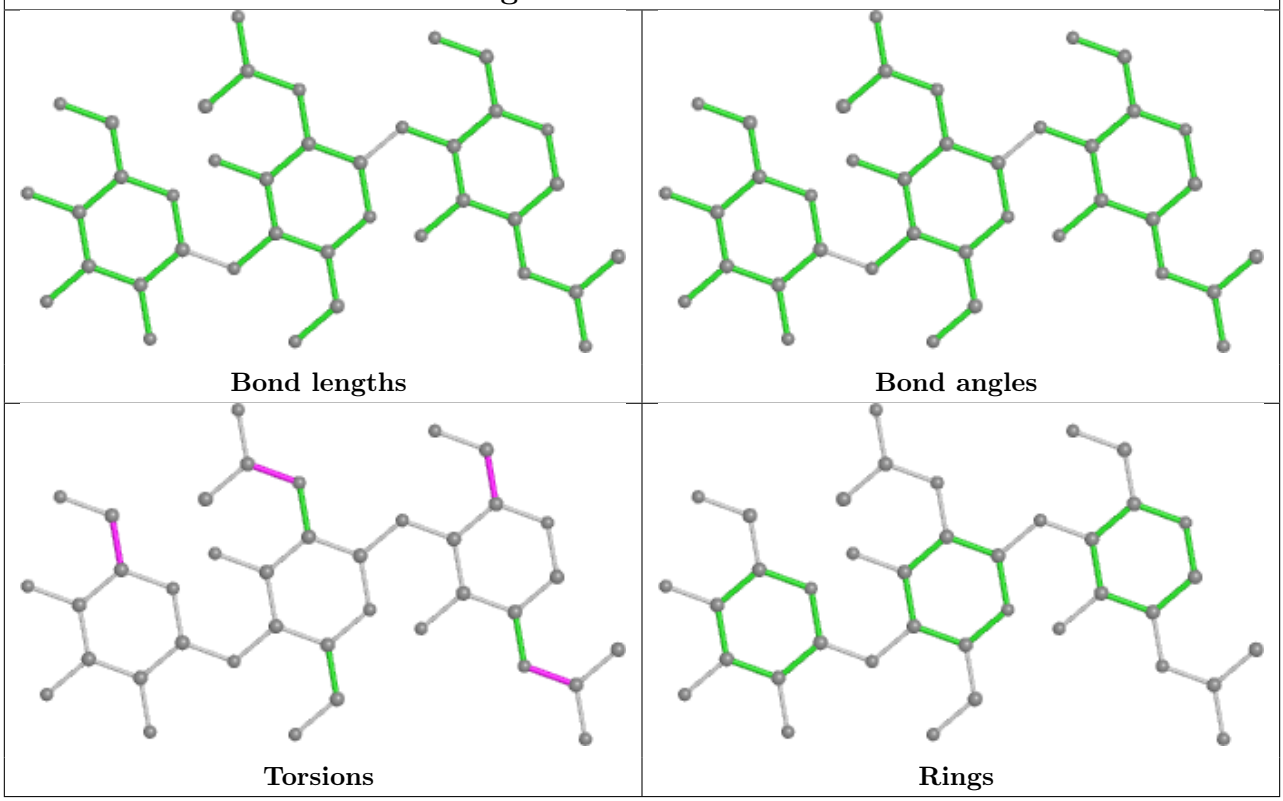


Torsions

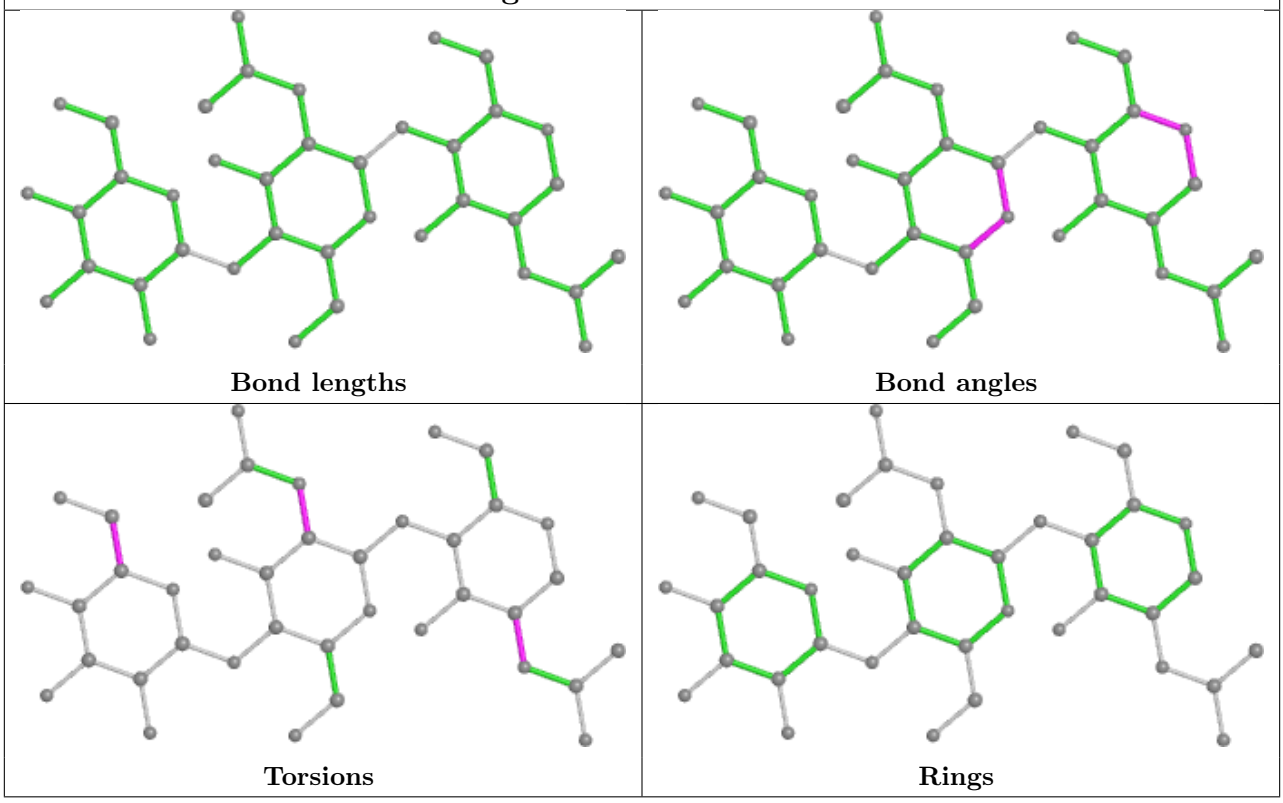


Rings

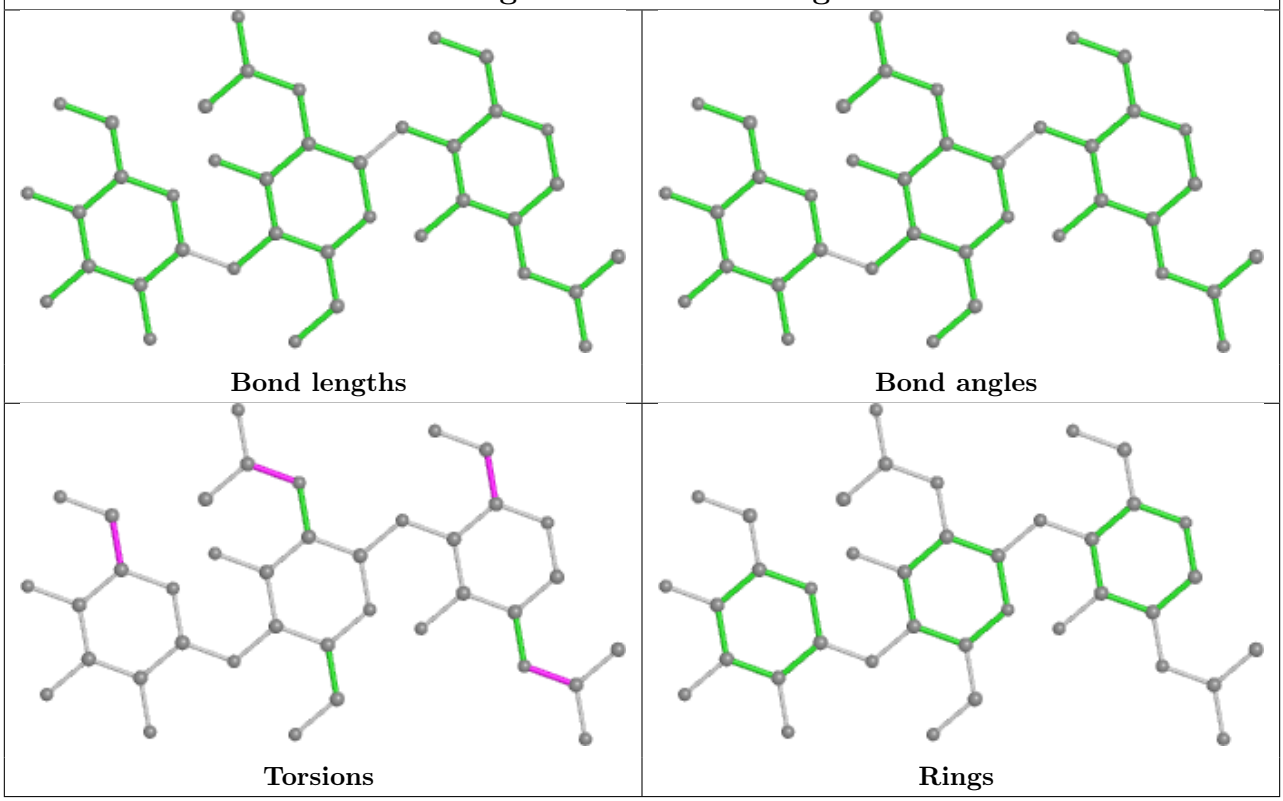
Oligosaccharide Chain e



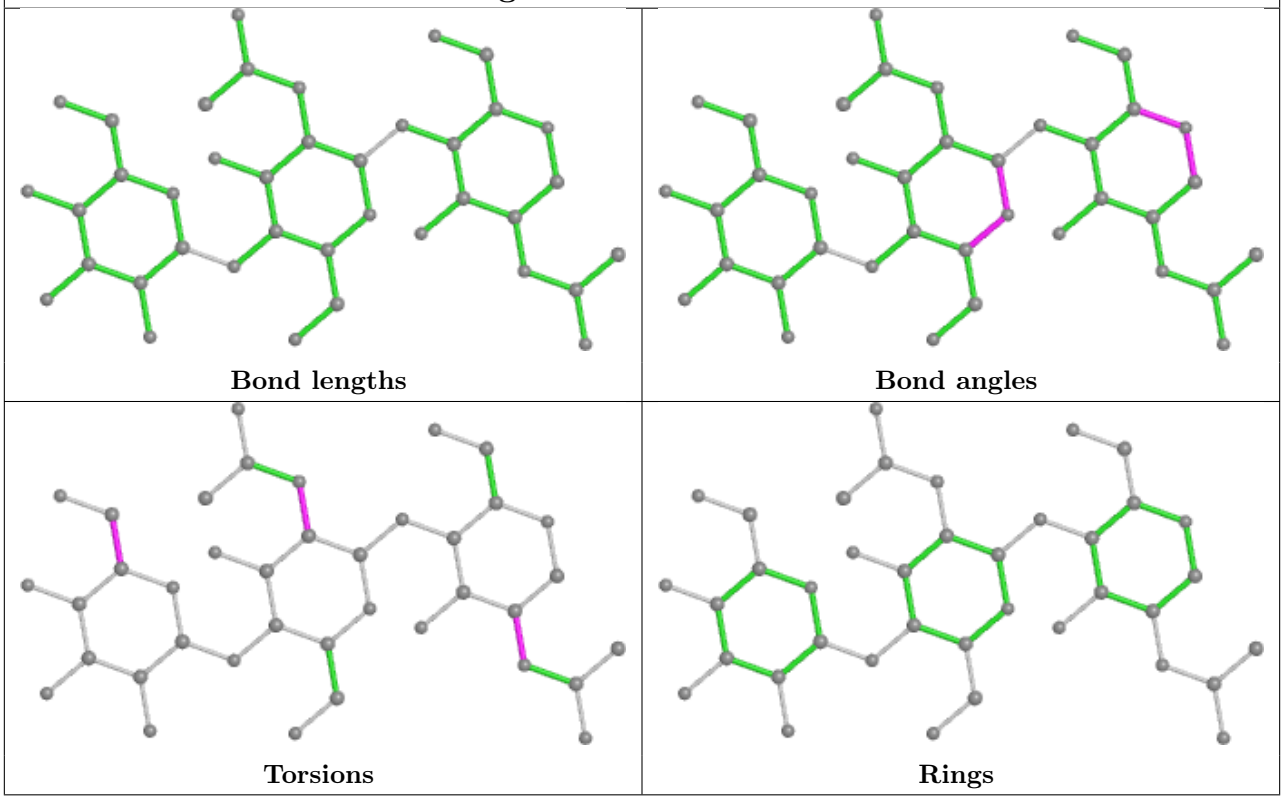
Oligosaccharide Chain f



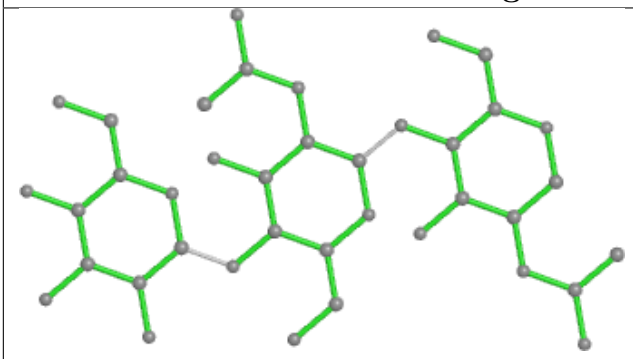
Oligosaccharide Chain g



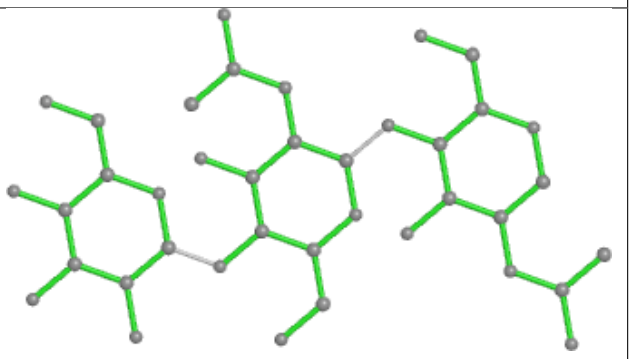
Oligosaccharide Chain h



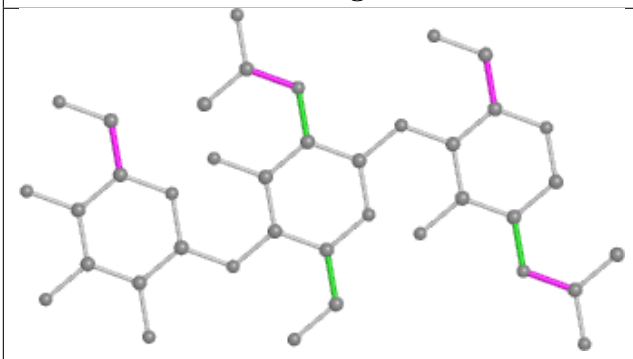
Oligosaccharide Chain i



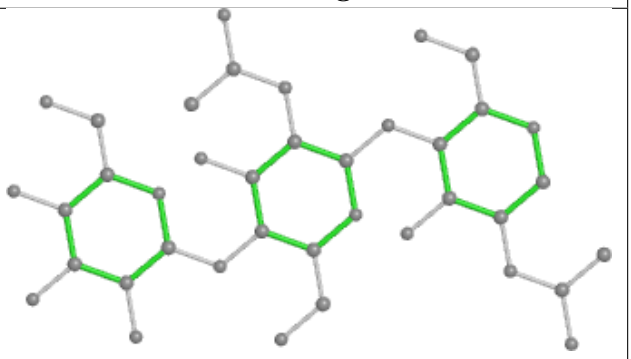
Bond lengths



Bond angles

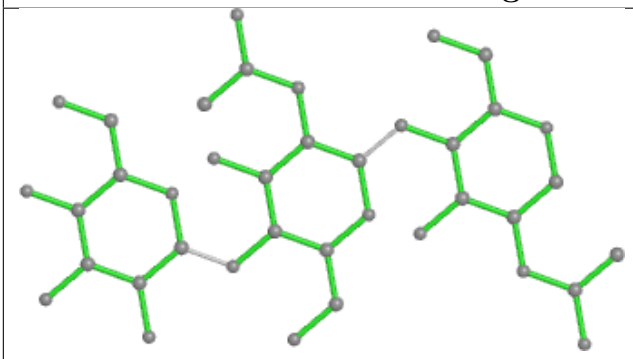


Torsions



Rings

Oligosaccharide Chain j



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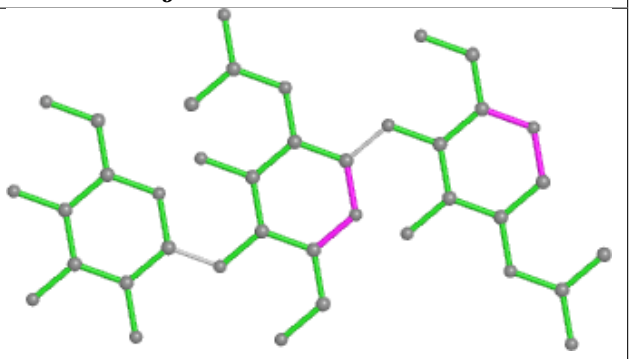

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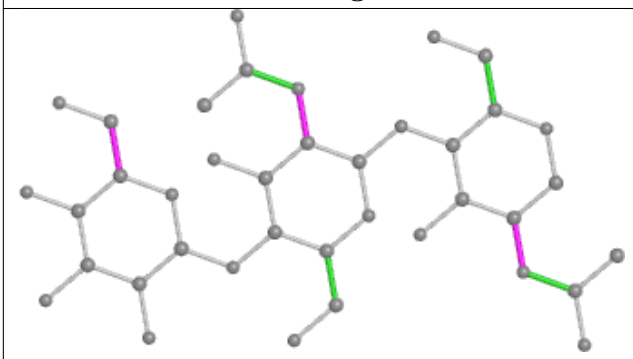

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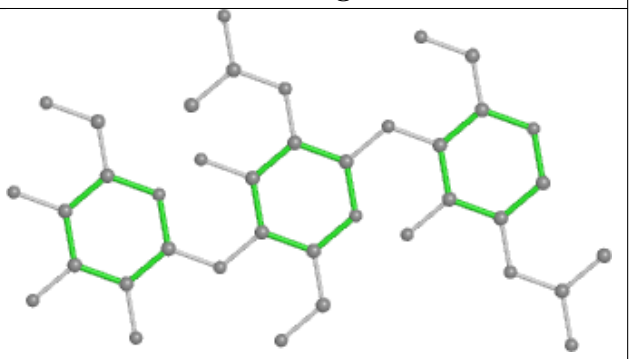
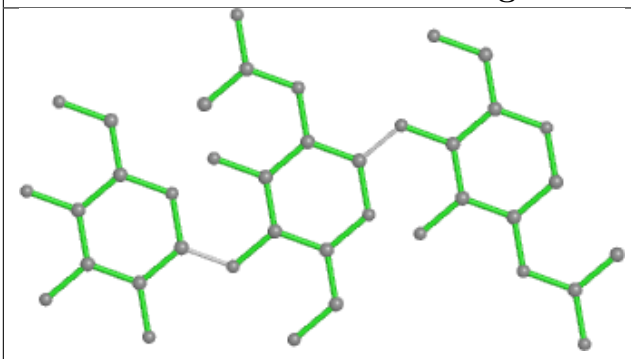


Rings

Oligosaccharide Chain k



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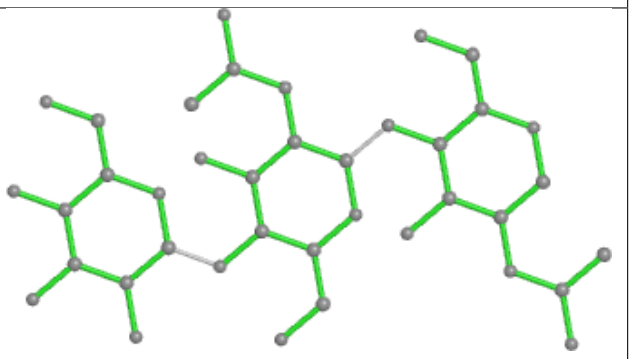
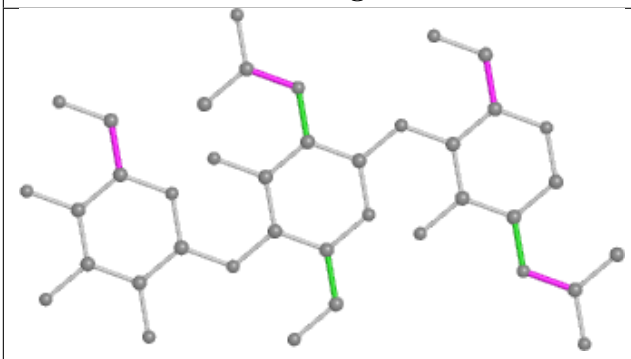


Bond angles



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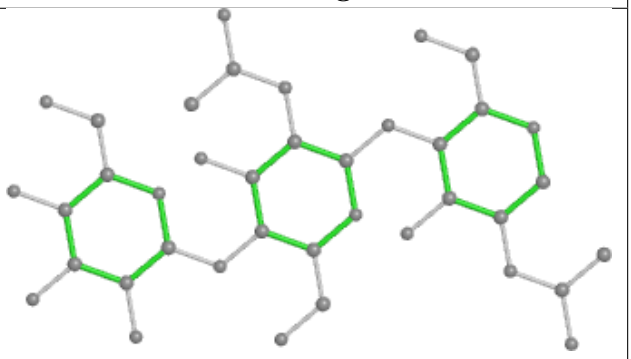
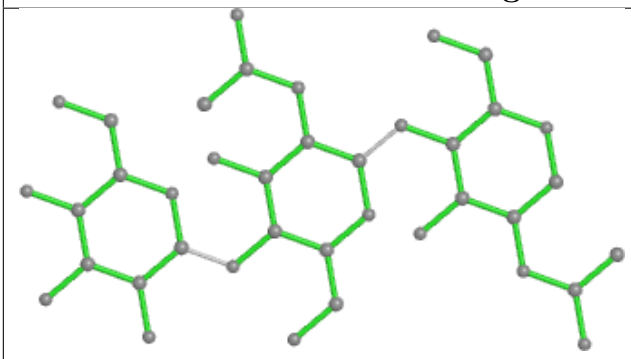


Rings

Oligosaccharide Chain l



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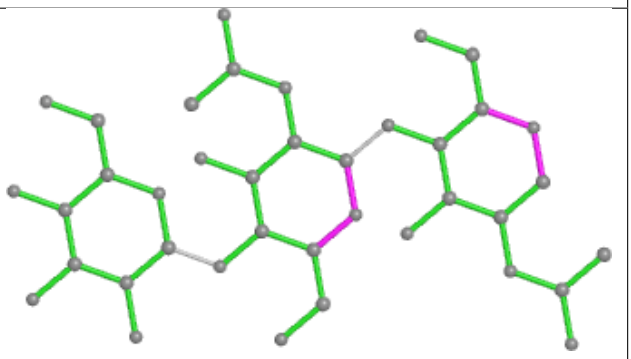

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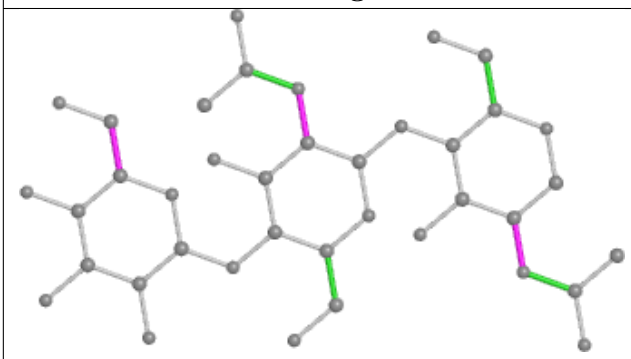

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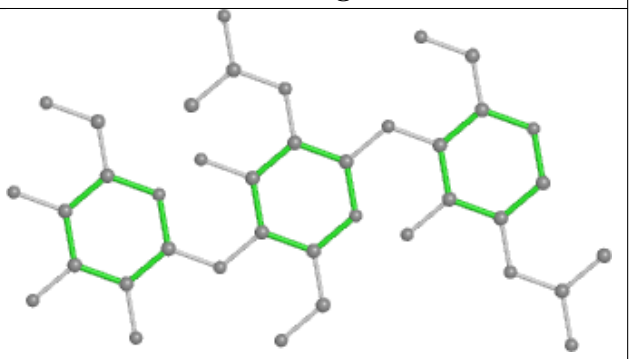
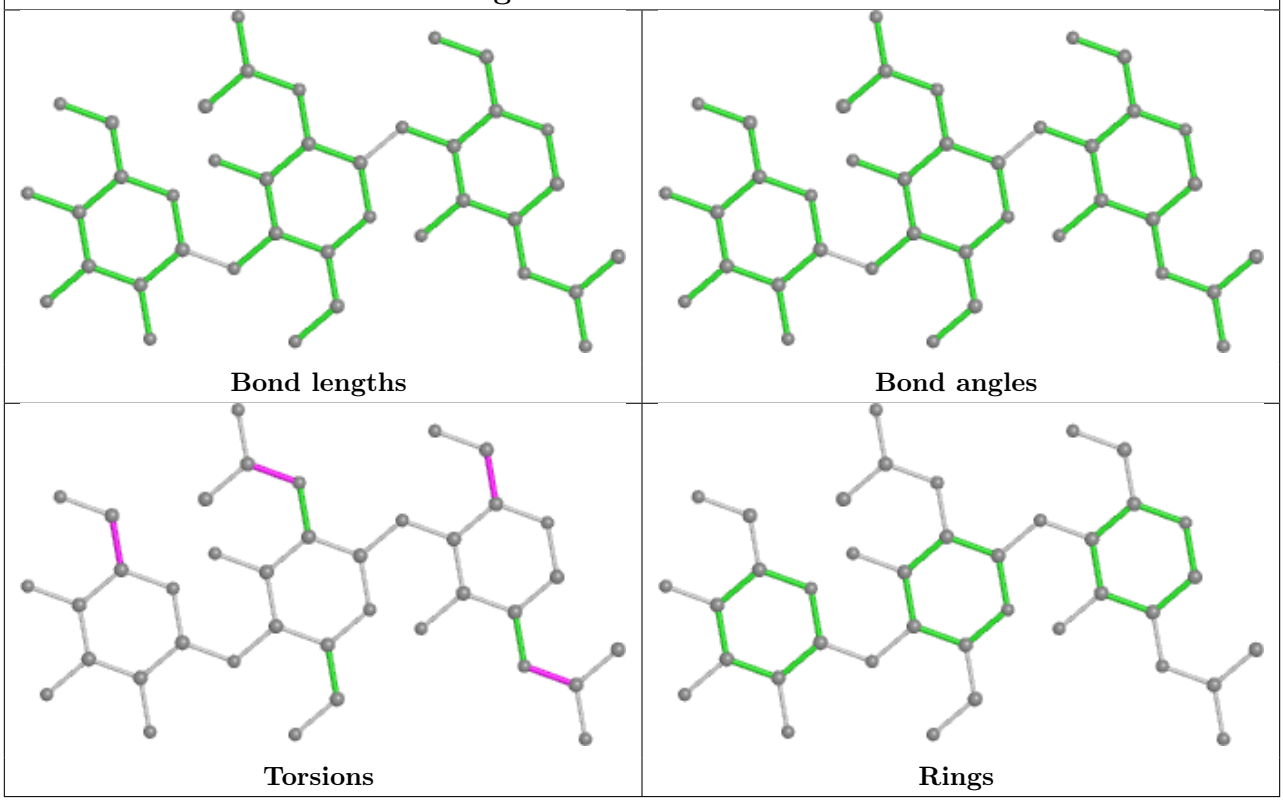


Rings

Oligosaccharide Chain m



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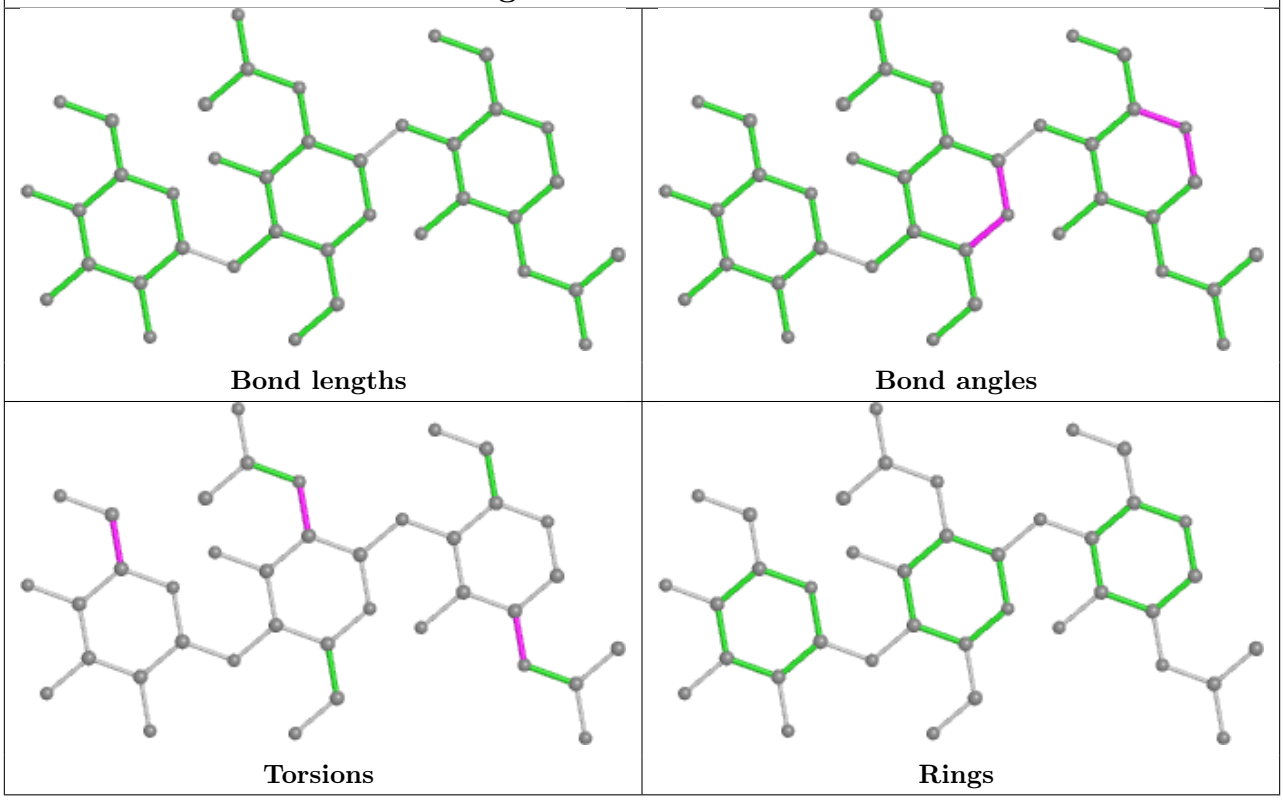

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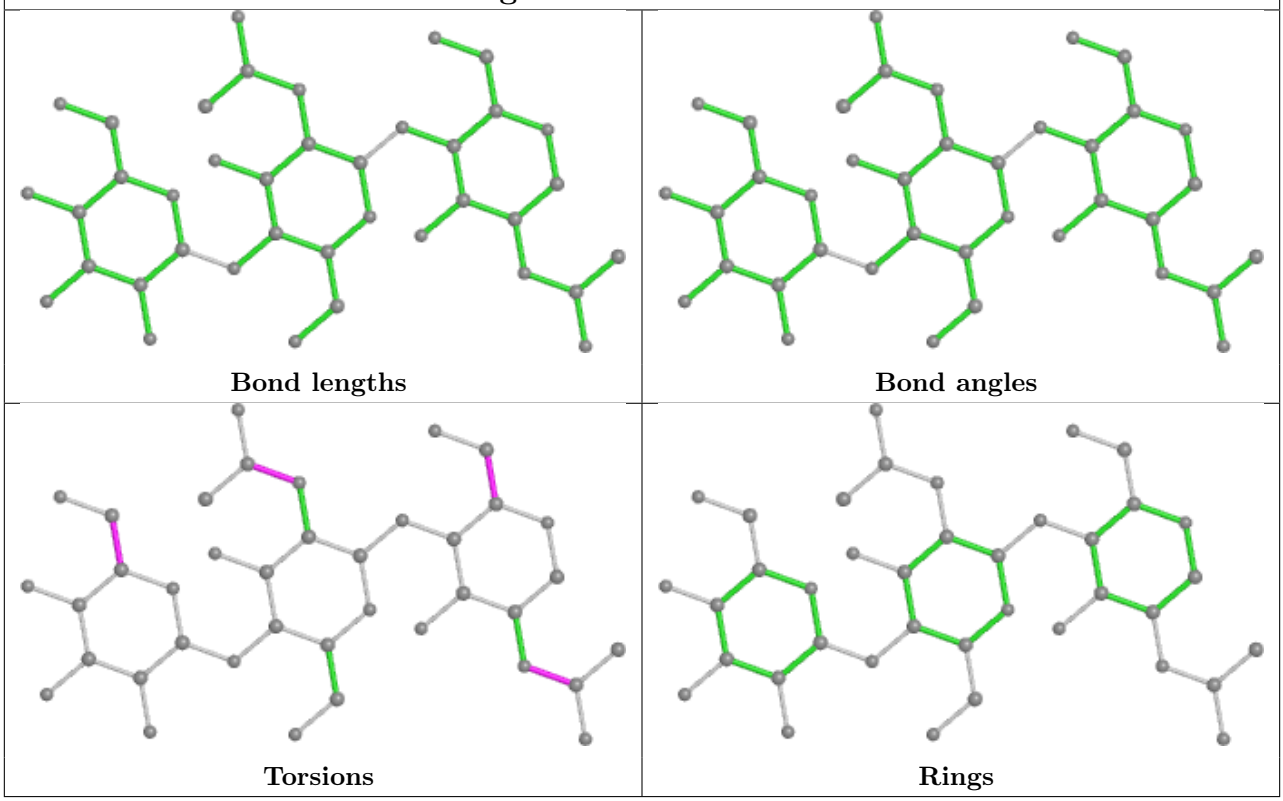

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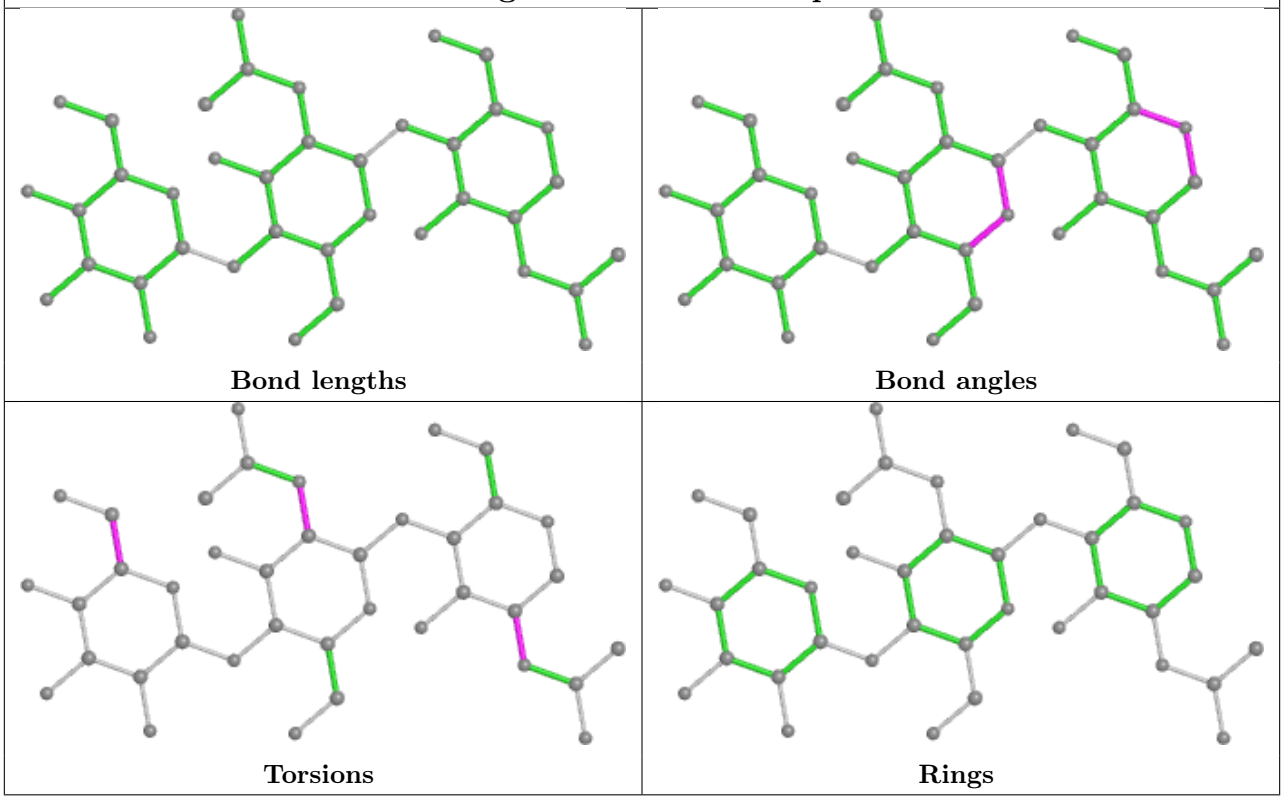

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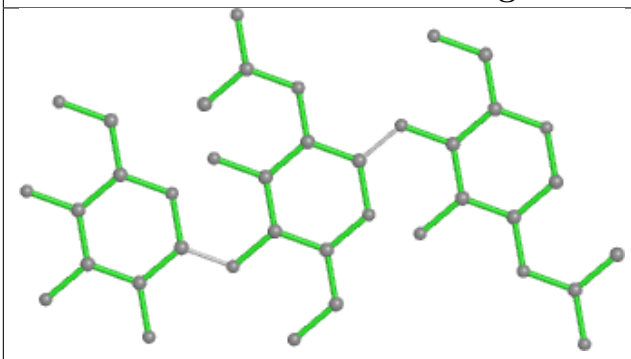

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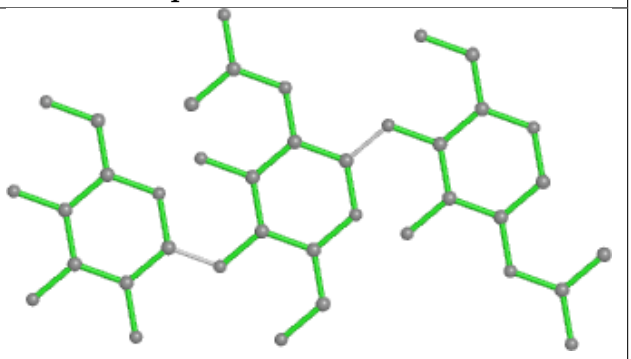
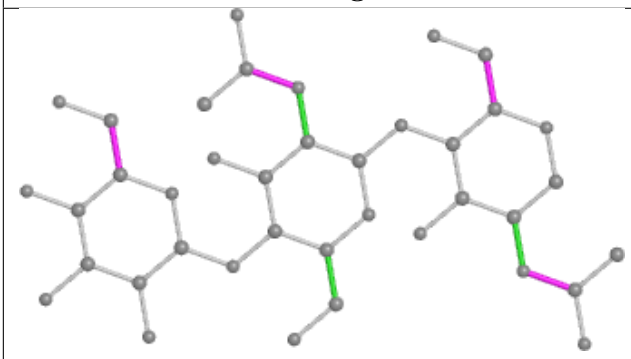
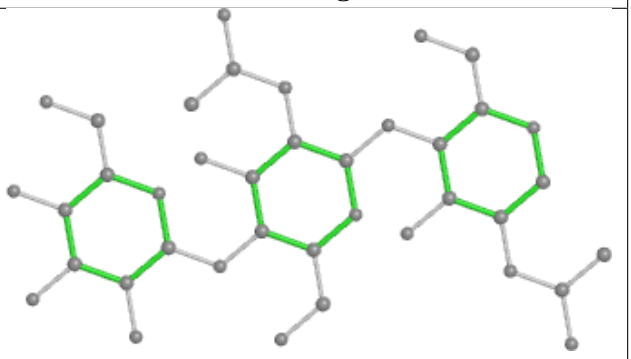


Bond angles

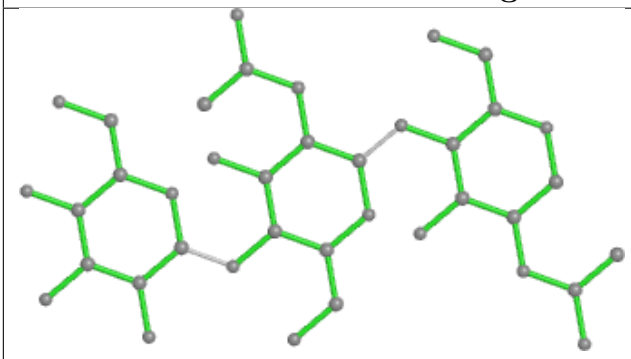


Torsions



Rings

Oligosaccharide Chain r



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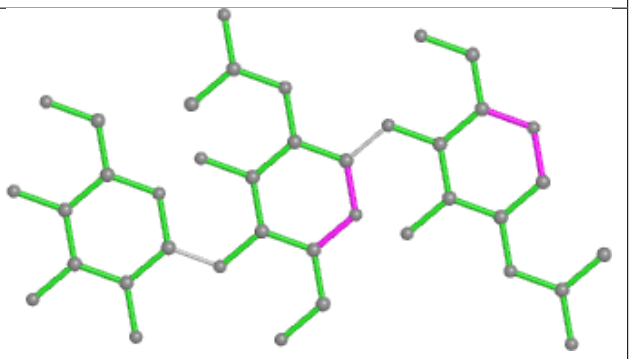

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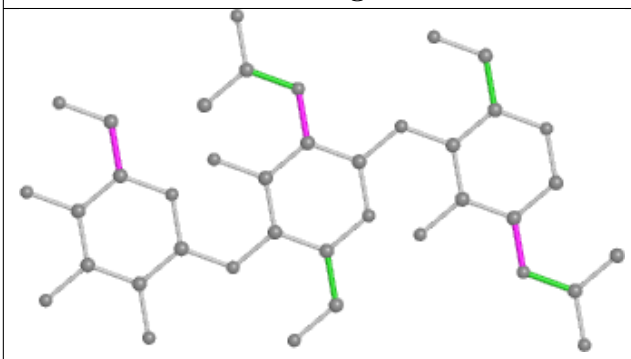

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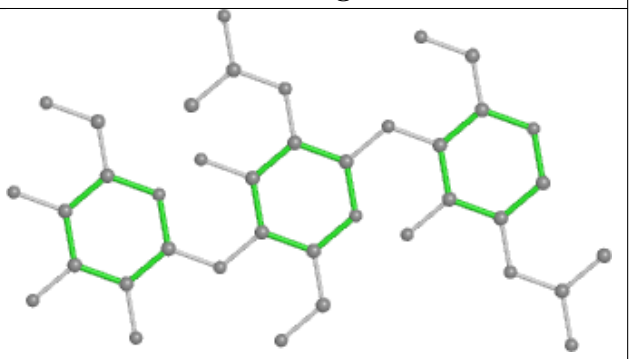

Rings

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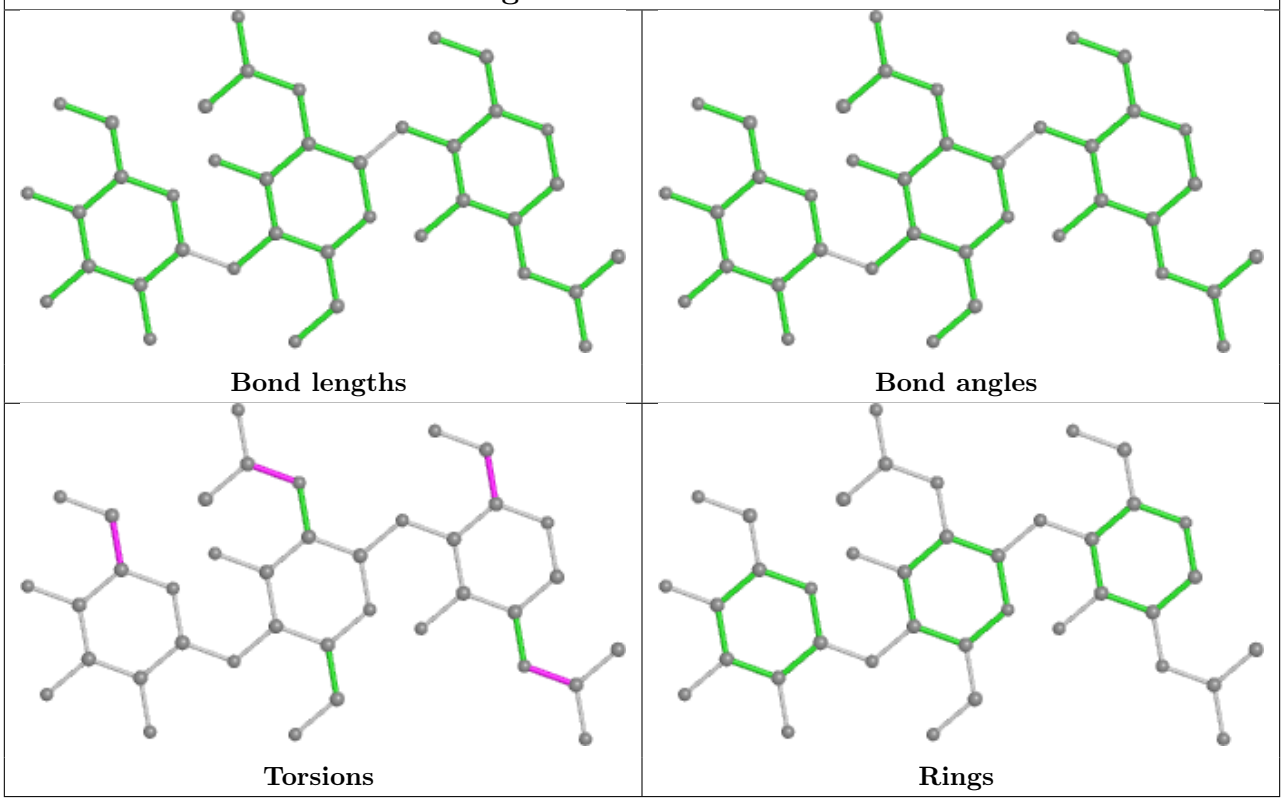

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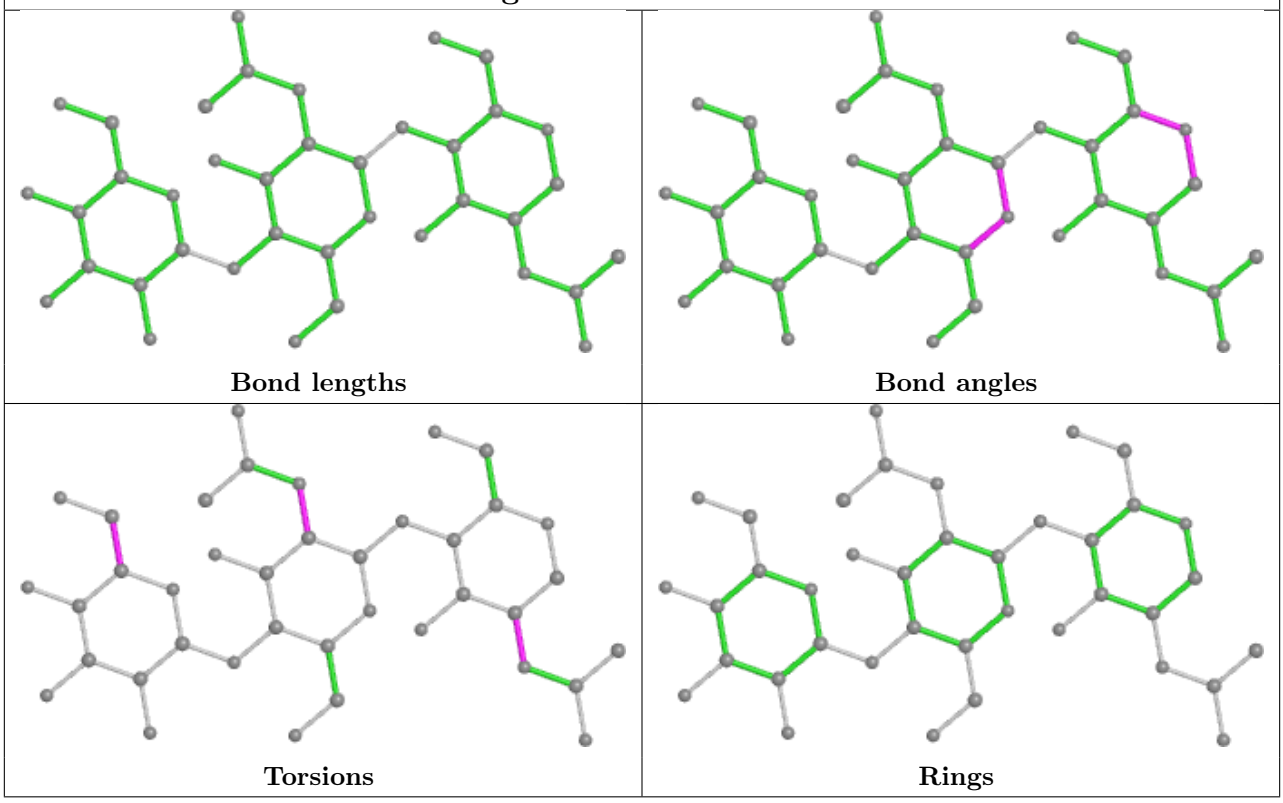
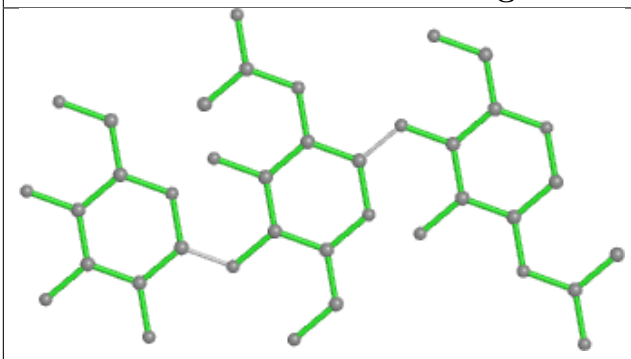


Oligosaccharide Chain u



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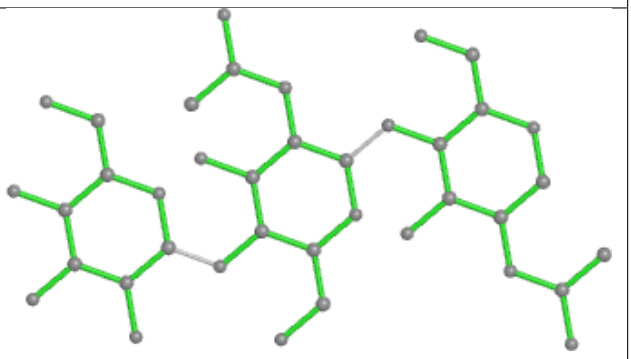
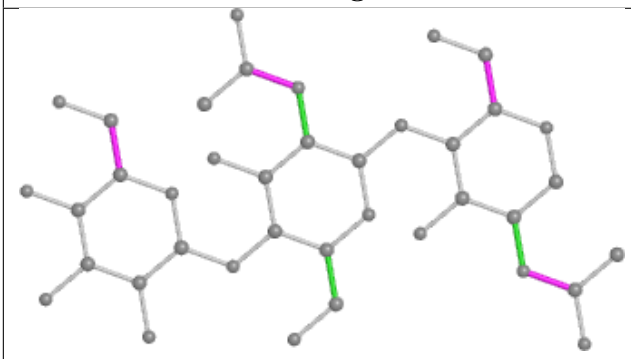


Bond angles



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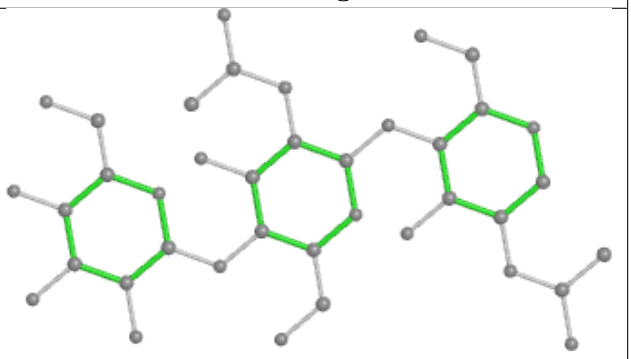
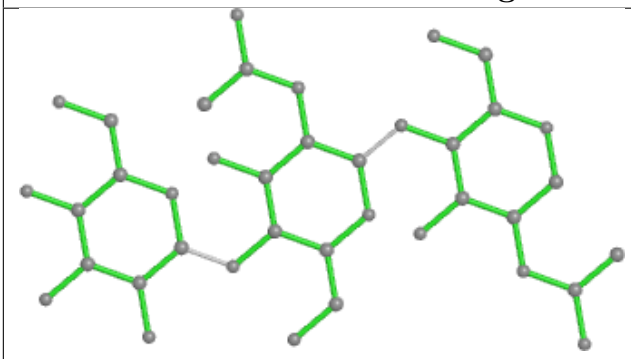


Rings

Oligosaccharide Chain v



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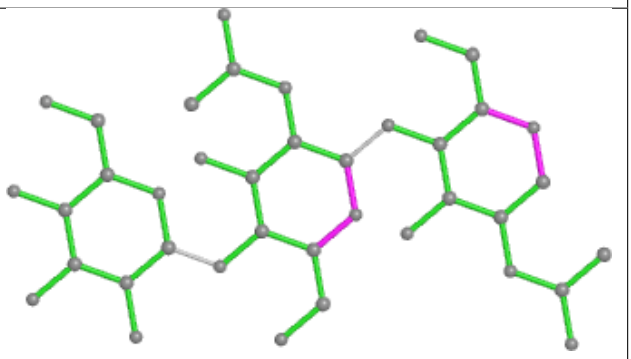

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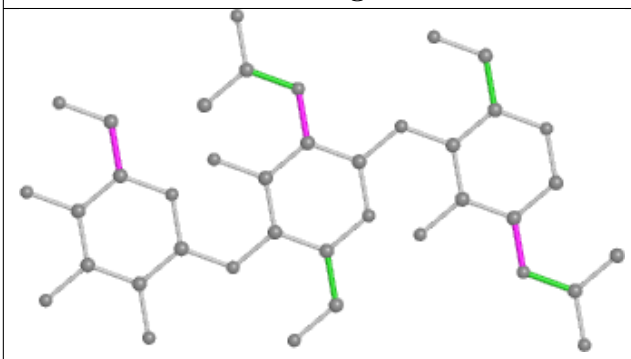

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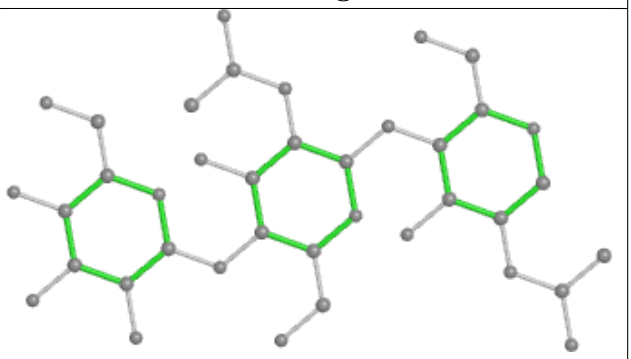
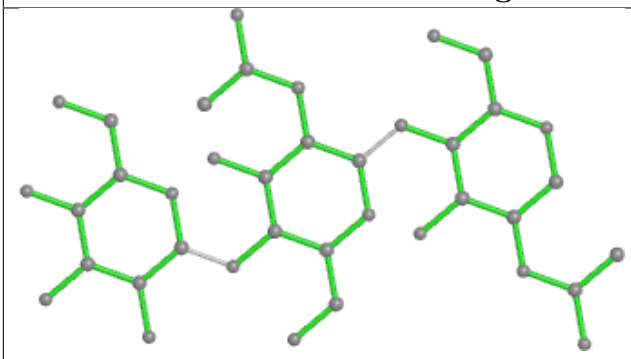


Rings

Oligosaccharide Chain w



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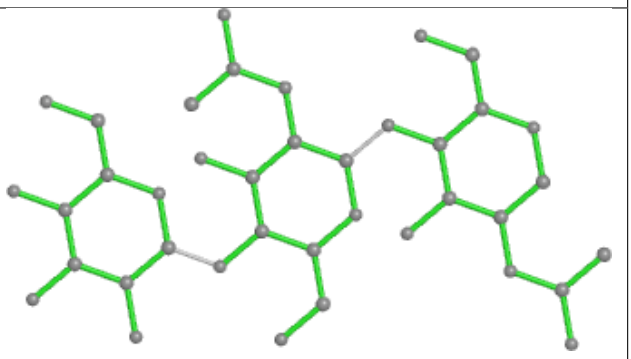
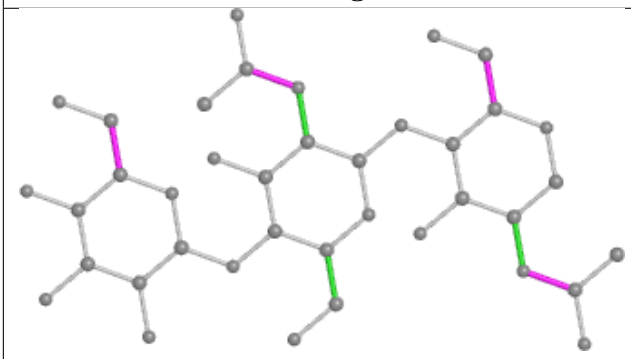


Bond angles



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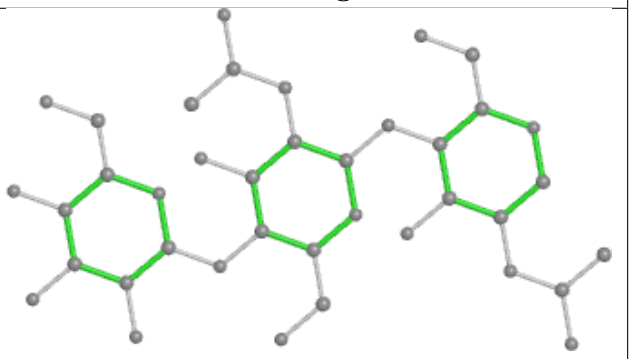
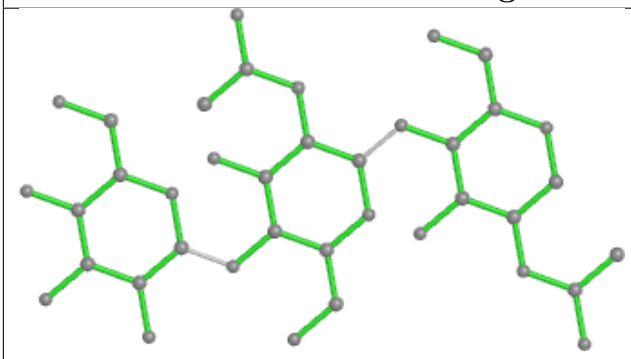


Rings

Oligosaccharide Chain x



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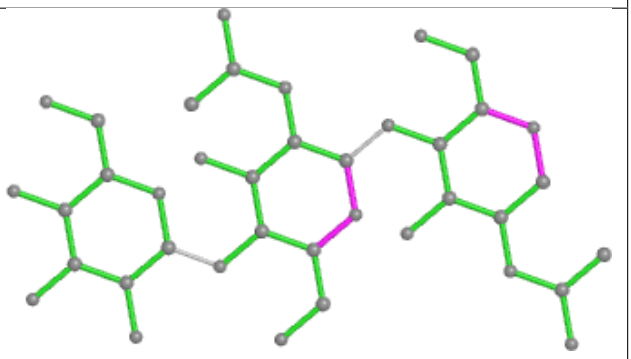
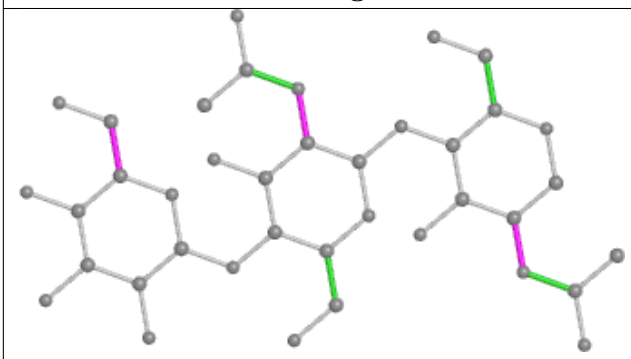


Bond angles



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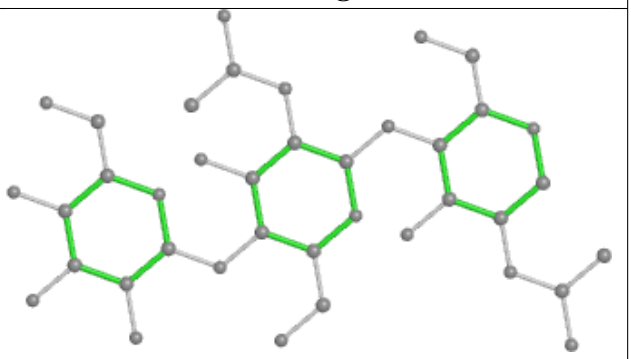
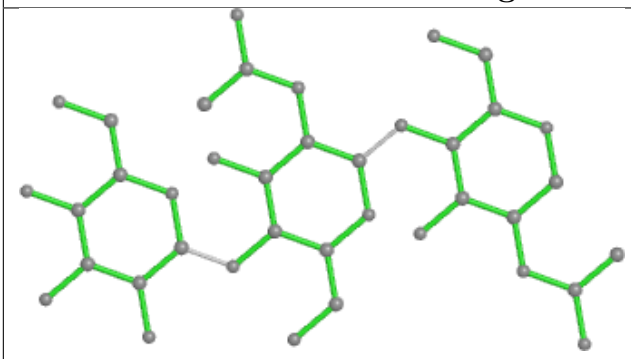


Rings

Oligosaccharide Chain y



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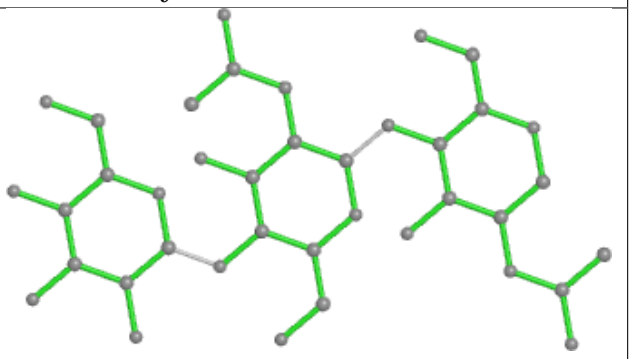

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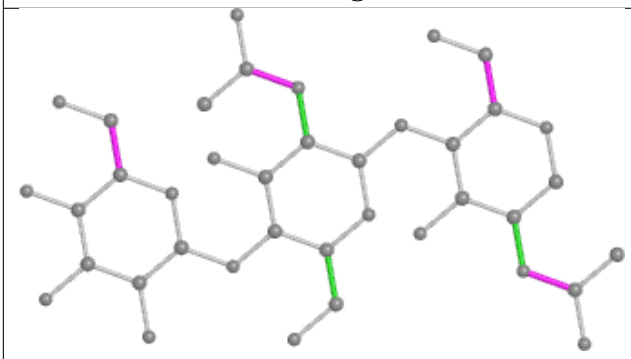

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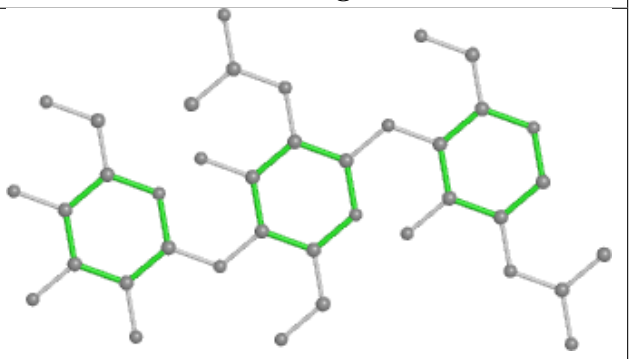
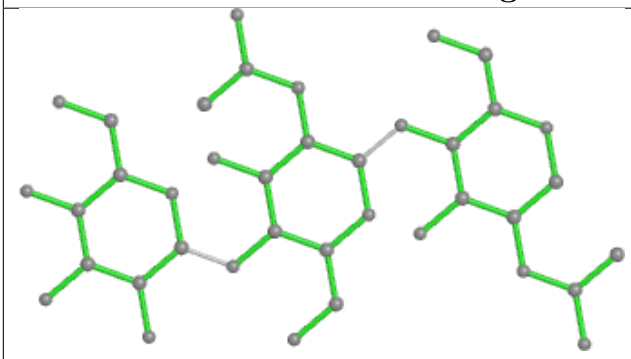
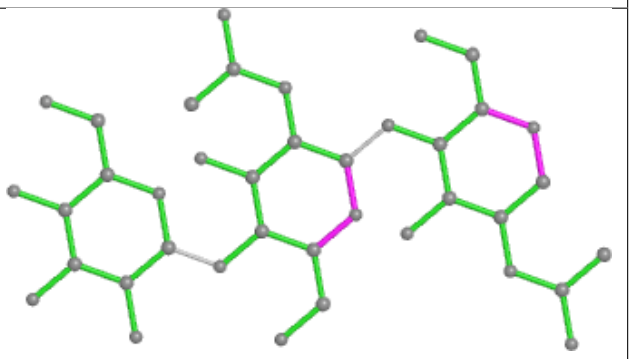


Rings

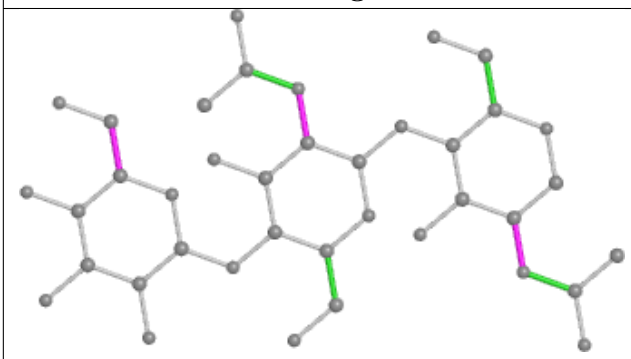
Oligosaccharide Chain z



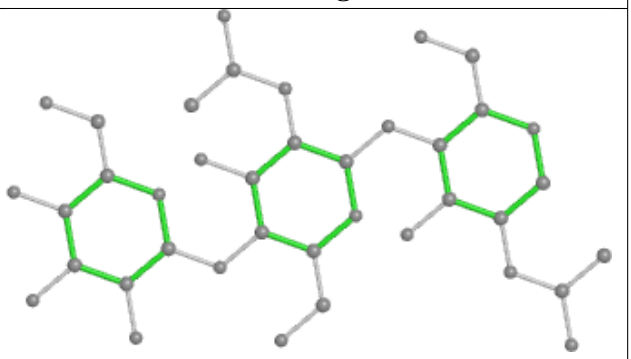
Bond lengths



Bond angles

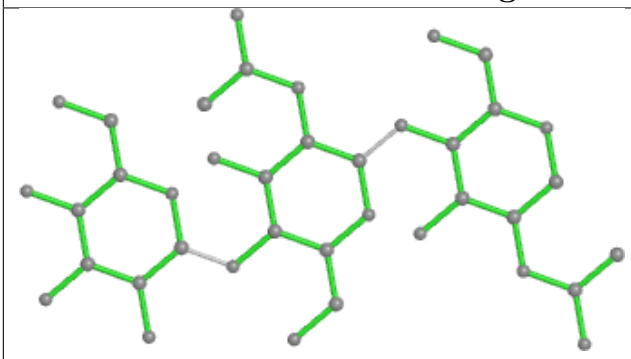


Torsions



Rings

Oligosaccharide Chain 0



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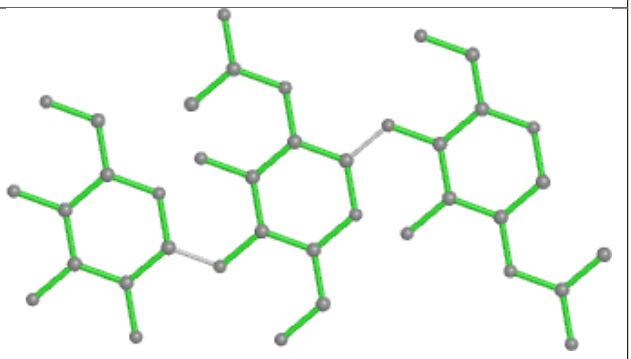

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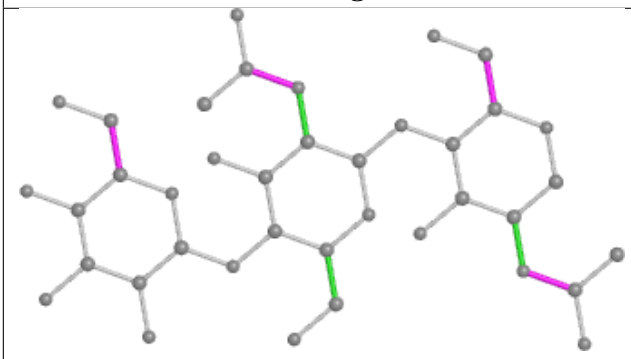

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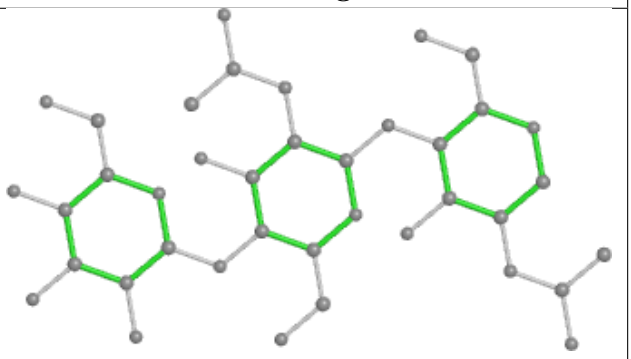
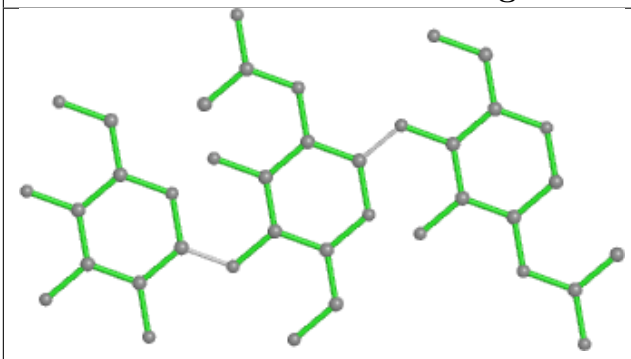


Rings

Oligosaccharide Chain 1



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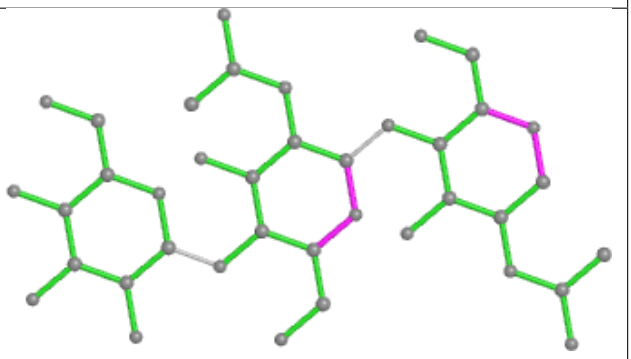

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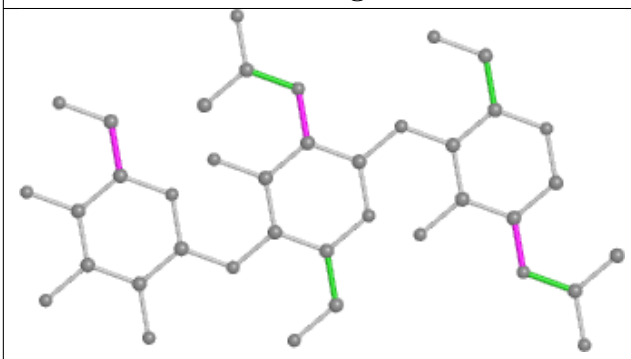

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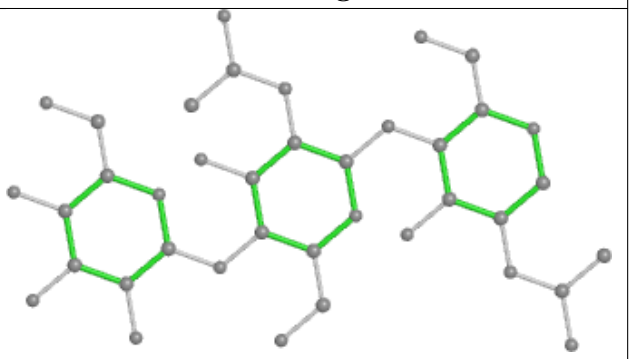
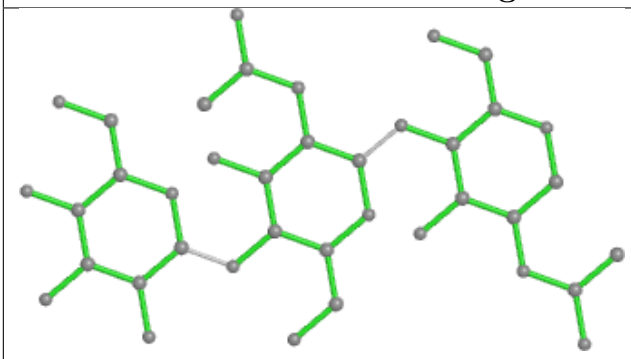


Rings

Oligosaccharide Chain 2



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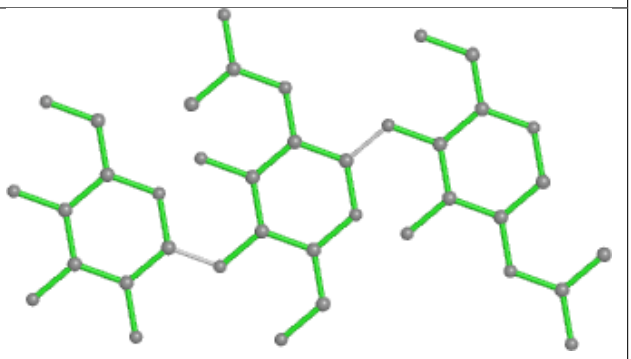

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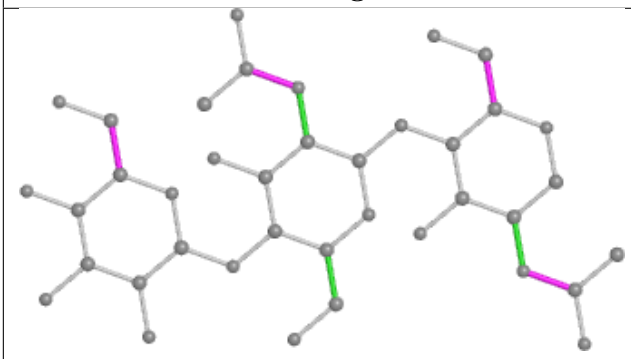

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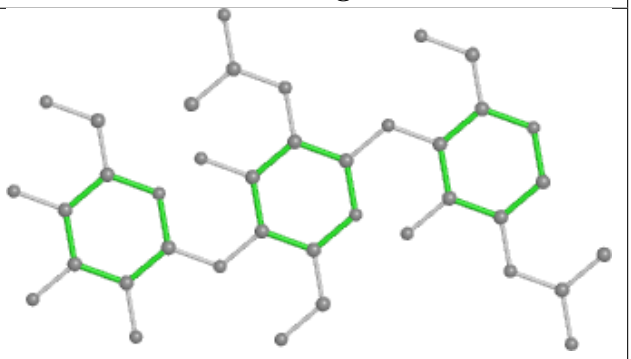
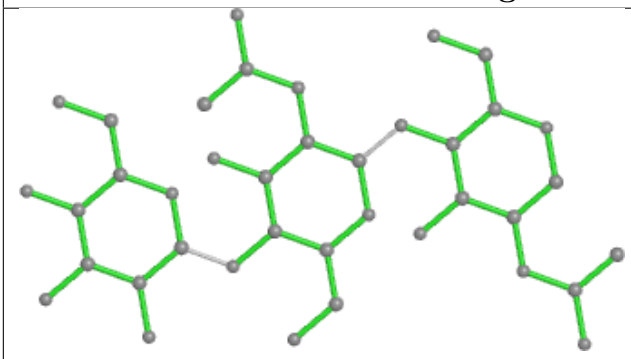


Rings

Oligosaccharide Chain 3



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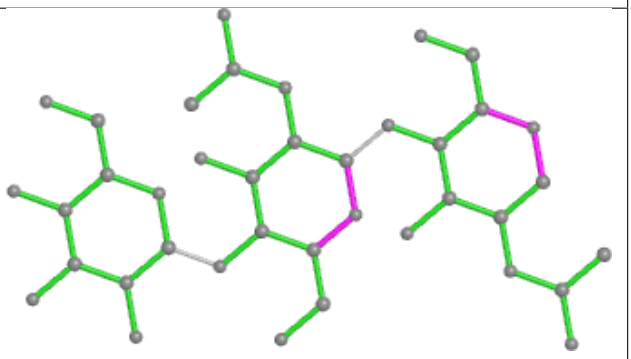

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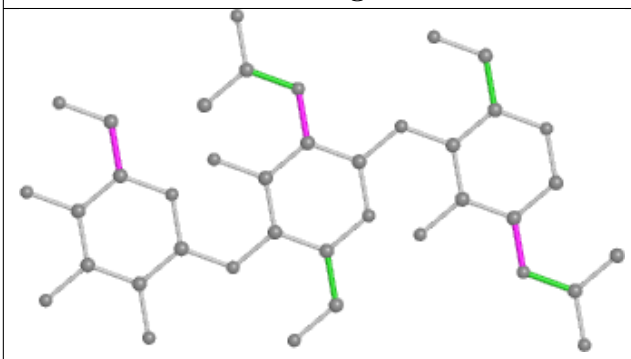

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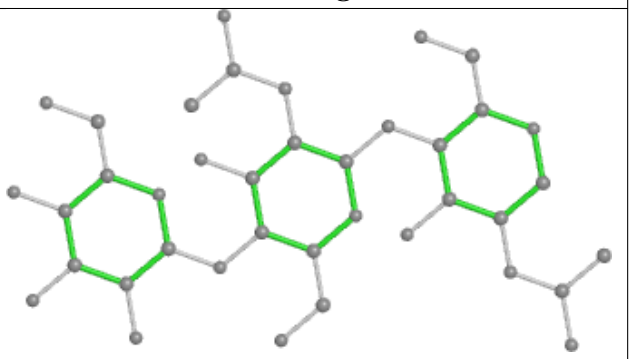
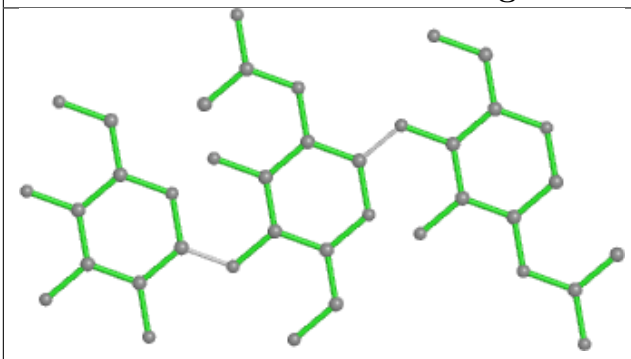


Rings

Oligosaccharide Chain 4



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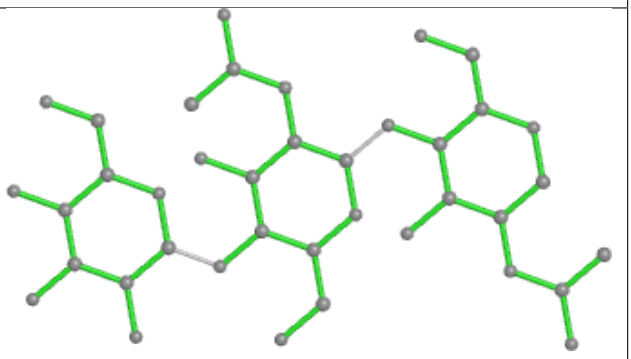

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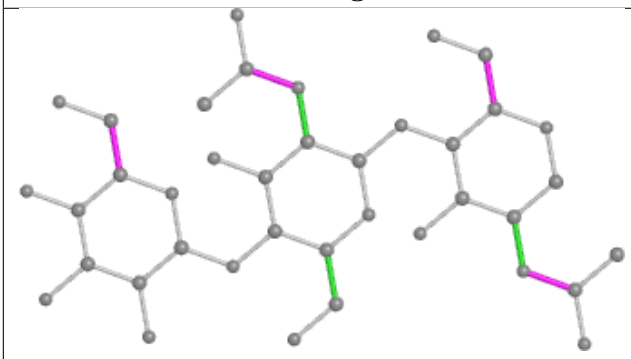

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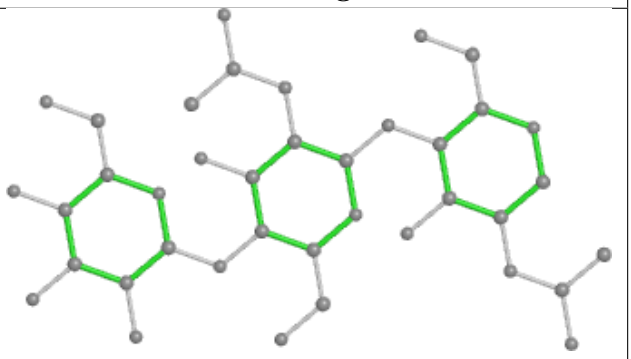
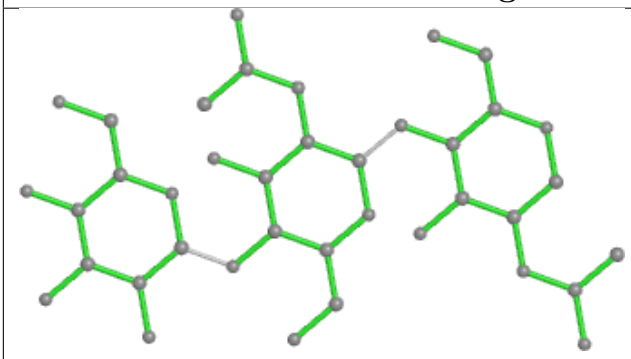


Rings

Oligosaccharide Chain 5



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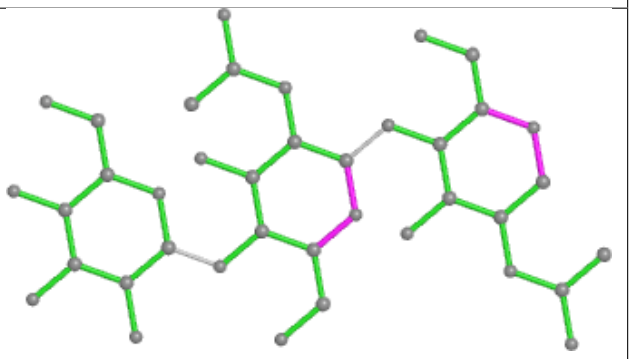

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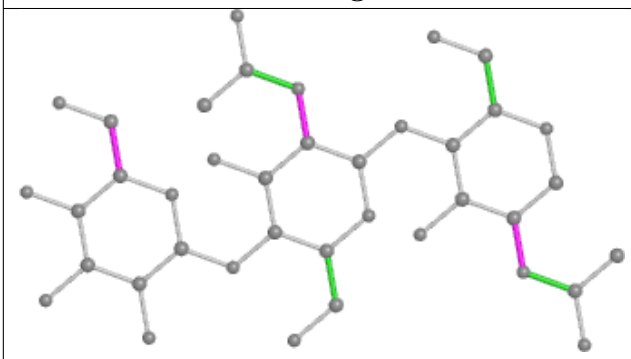

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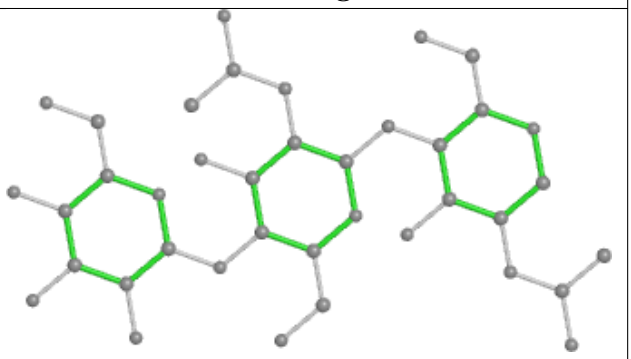
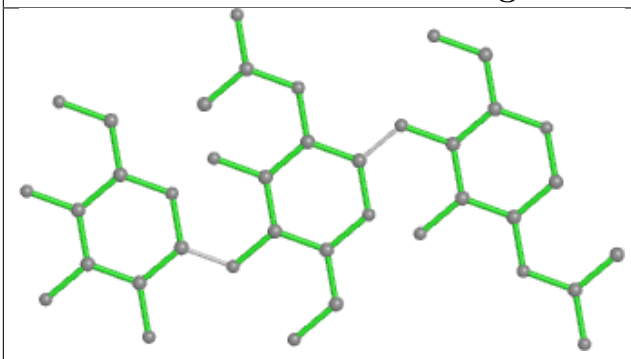


Rings

Oligosaccharide Chain 6



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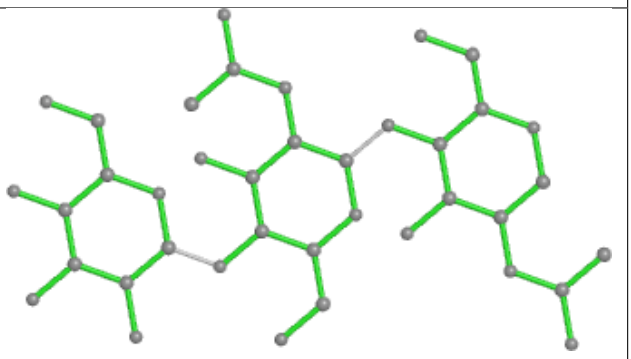

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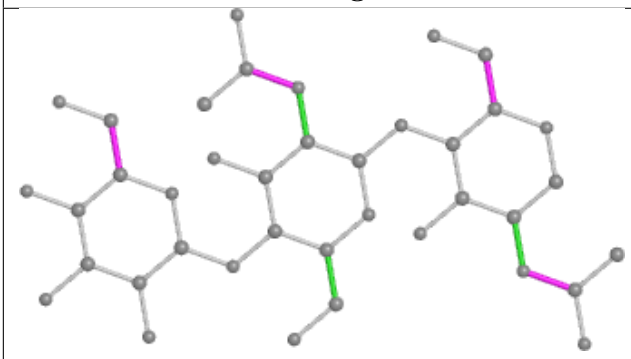

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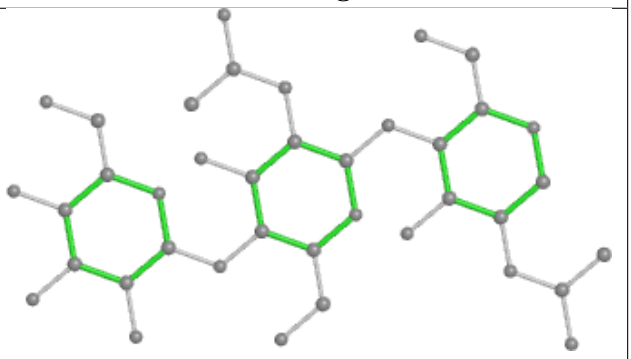
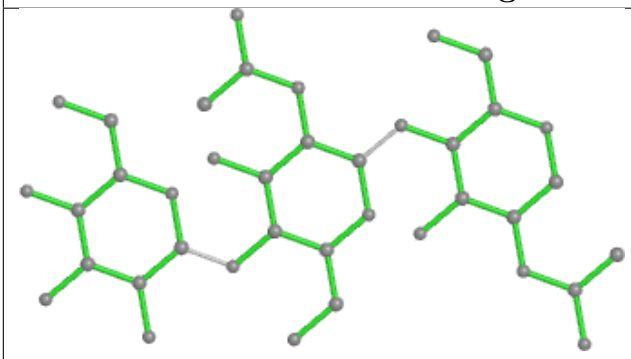


Rings

Oligosaccharide Chain 7



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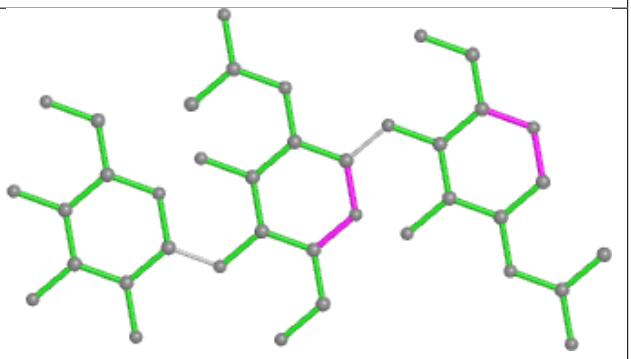

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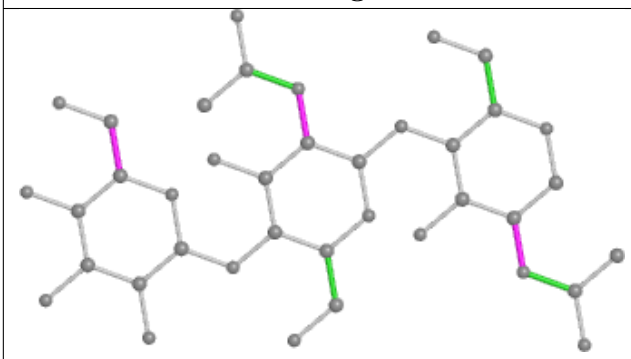

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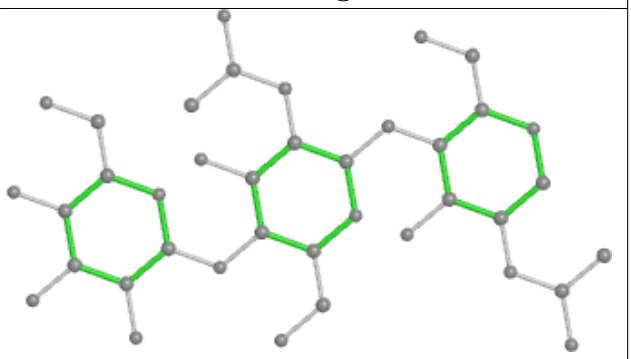
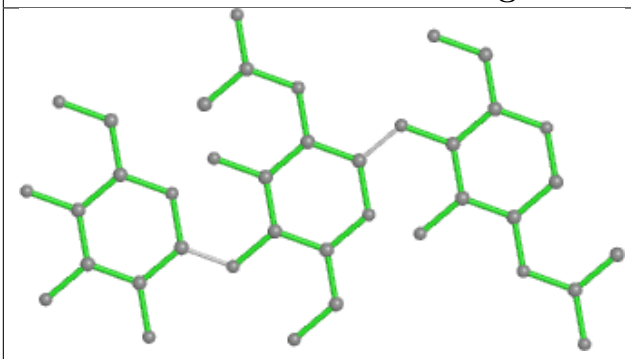


Rings

Oligosaccharide Chain 8



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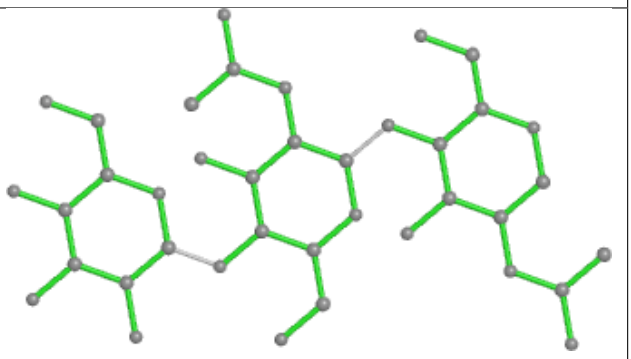

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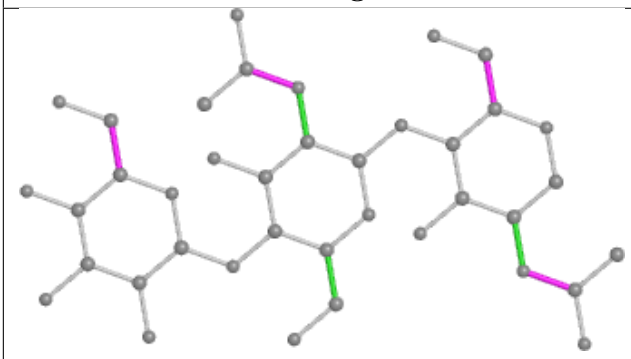

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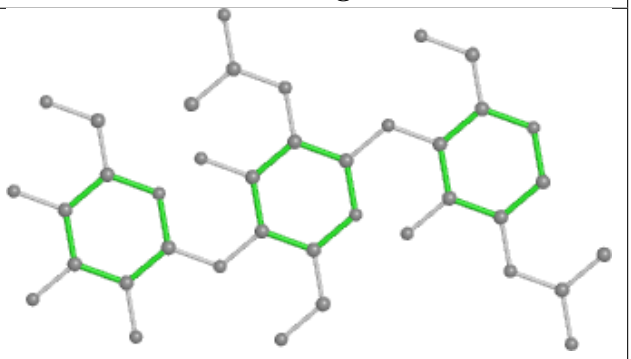
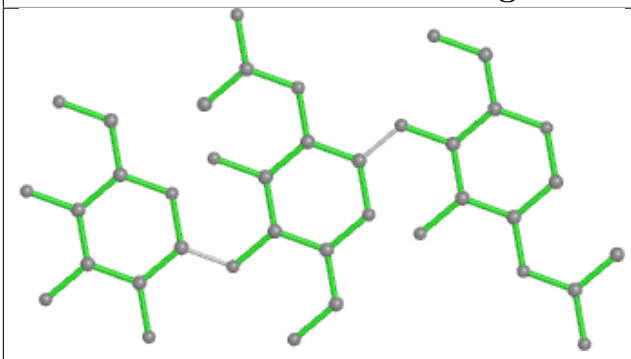


Rings

Oligosaccharide Chain 9



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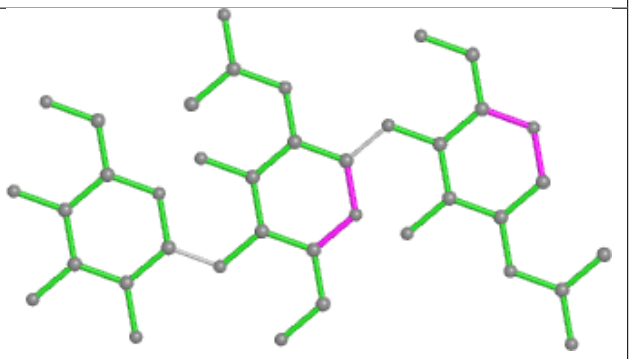

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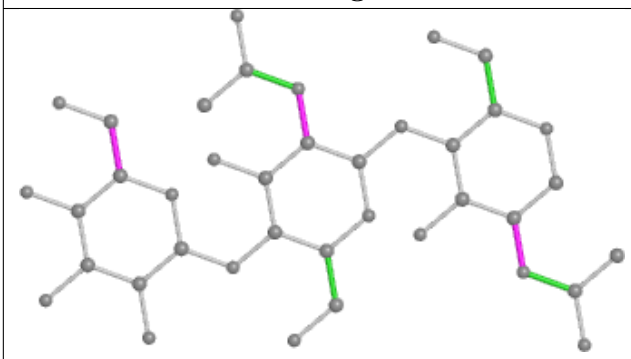

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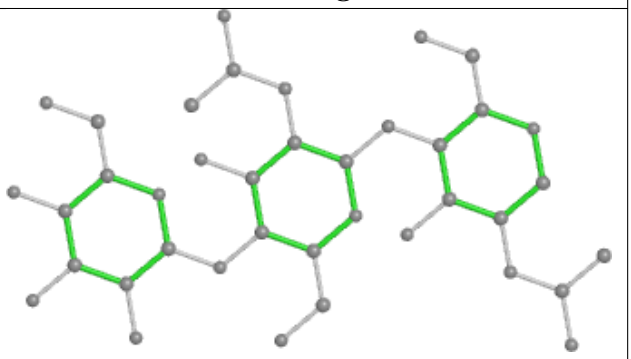
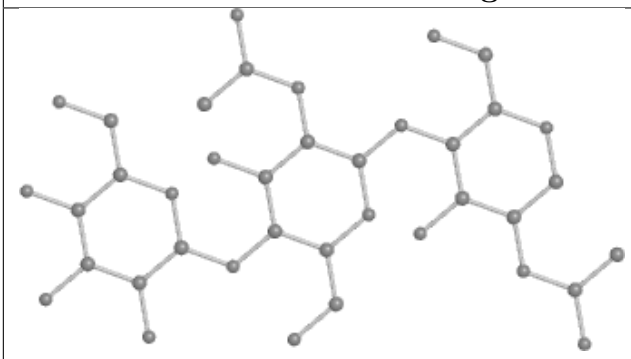


Rings

Oligosaccharide Chain AA



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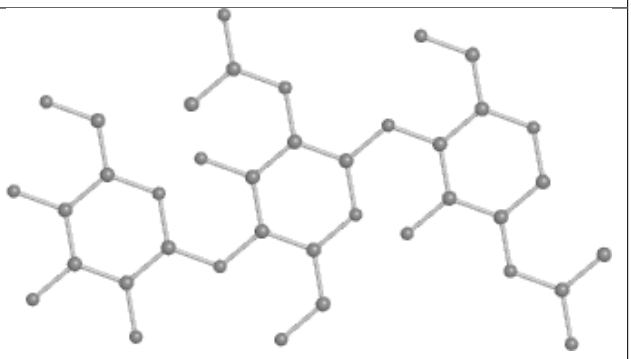
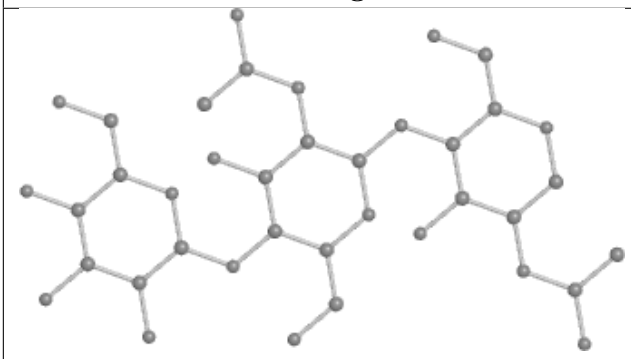


Bond angles



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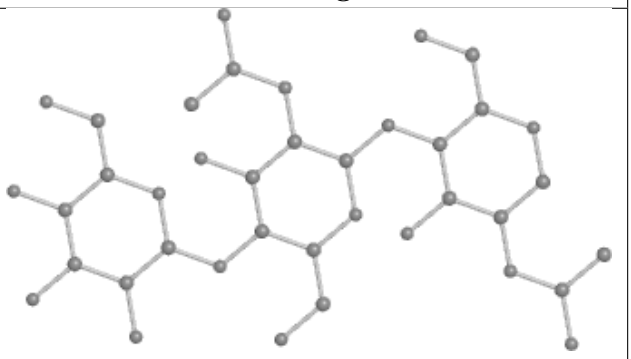
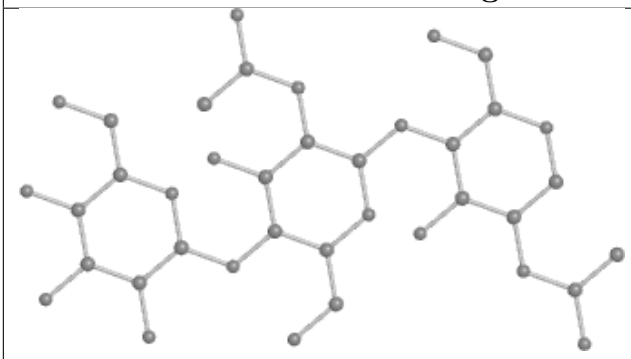


Rings

Oligosaccharide Chain BA



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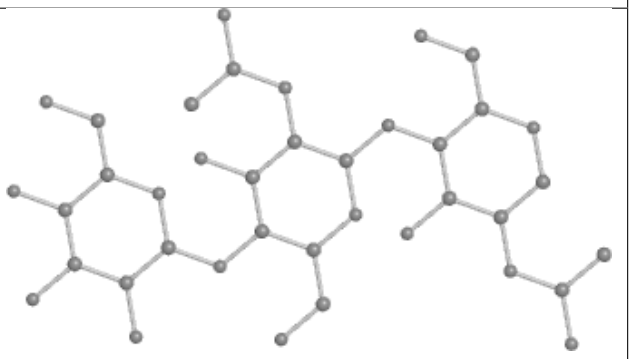
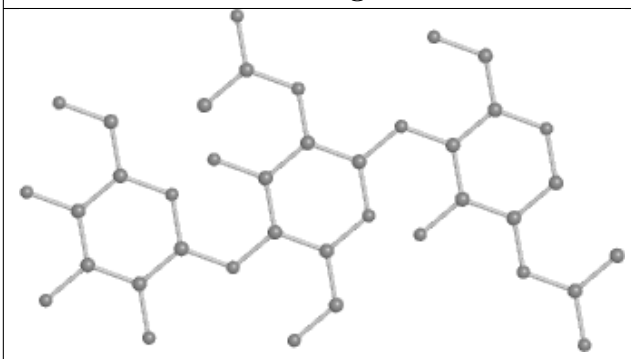


Bond angles



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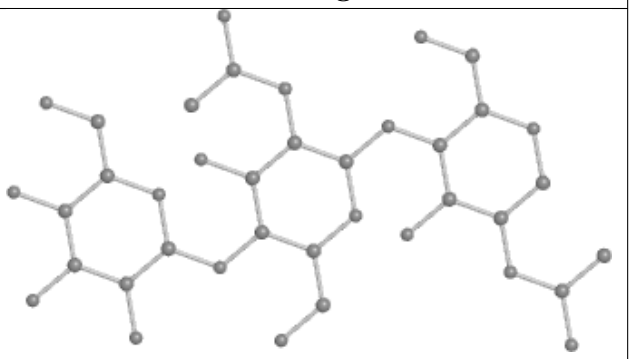
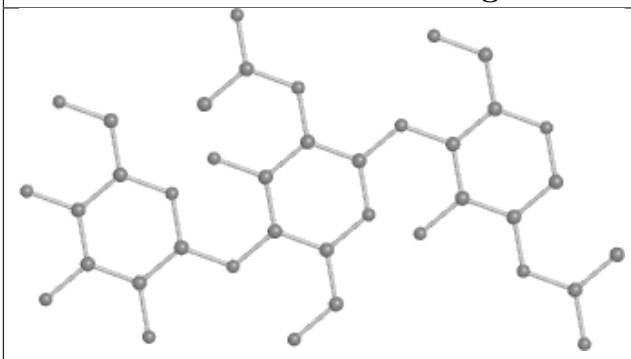
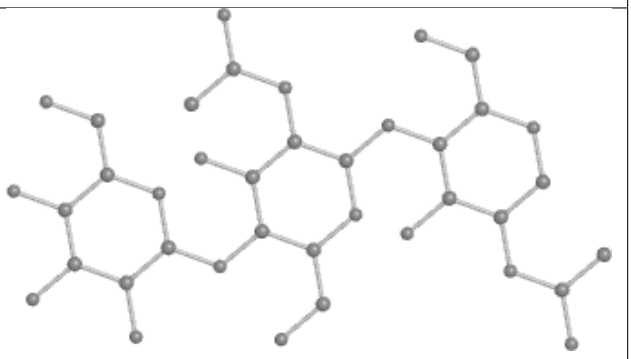


Rings

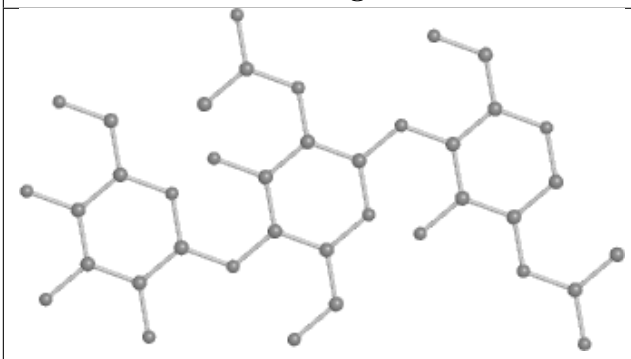
Oligosaccharide Chain CA



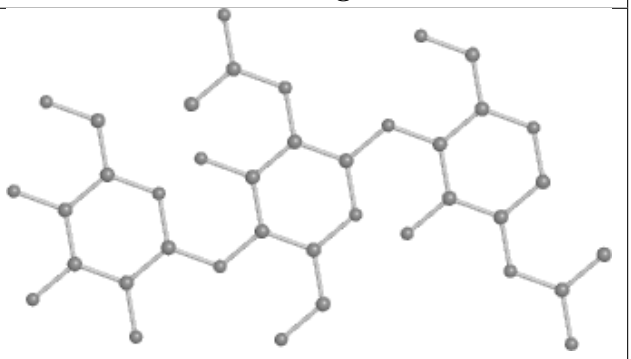
Bond lengths



Bond angles

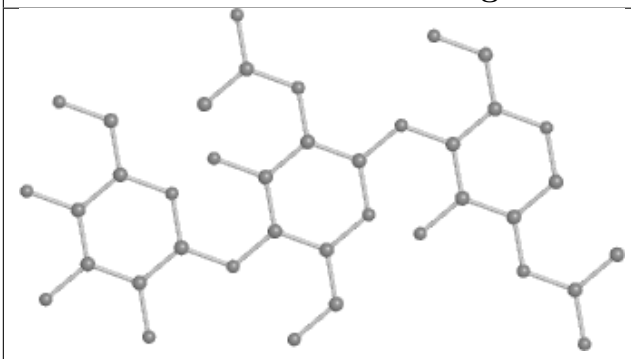


Torsions

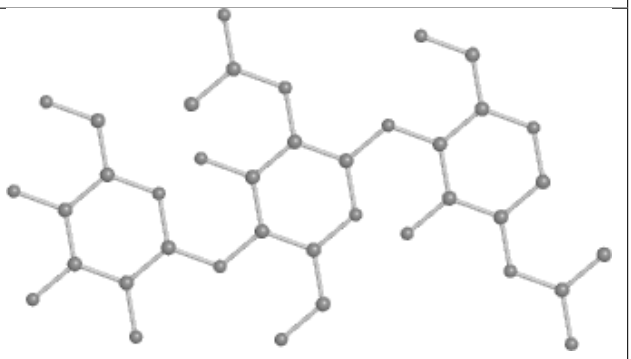


Rings

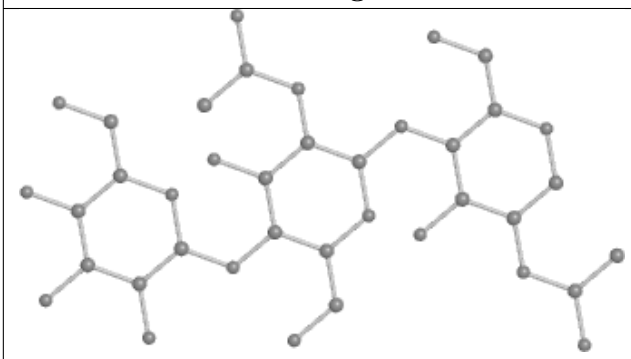
Oligosaccharide Chain DA



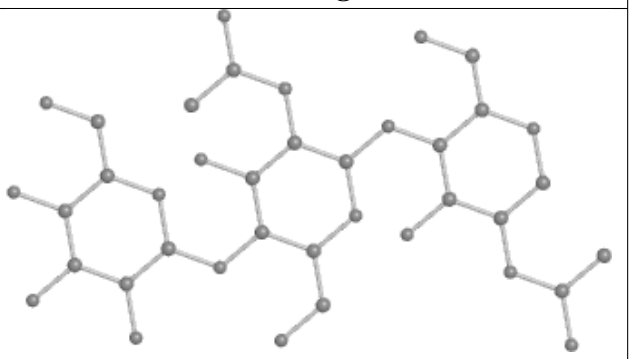
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 375 ligands modelled in this entry, 22 are monoatomic - leaving 353 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	$\#\|Z\| > 2$
5	SO4	N	1016	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	H	1009	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	T	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	K	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	M	1017	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	M	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	H	1001	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	B	1003	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	T	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	H	1003	3	33,38,38	3.53	6 (18%)	38,53,53	1.11	5 (13%)
5	SO4	T	1012	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	H	1004	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	M	1001	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	J	1008	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	V	1006	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	R	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	L	1023	-	14,14,15	0.23	0	17,19,21	0.83	1 (5%)
5	SO4	B	1008	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	U	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	1006	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	Q	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	M	1012	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	G	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	F	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	Q	1022	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	O	1014	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	S	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	I	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1023	-	4,4,4	0.14	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	K	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	U	1010	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	L	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	M	1008	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	F	1010	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	D	1011	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	T	1008	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	Q	1004	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	S	1001	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	K	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	T	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	S	1003	3	33,38,38	3.52	6 (18%)	38,53,53	0.95	3 (7%)
6	NAG	V	1022	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	R	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	I	1012	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	K	1024	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	E	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	H	1008	-	4,4,4	0.16	0	6,6,6	0.11	0
5	SO4	E	1008	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	R	1010	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	P	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1024	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	V	1015	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	S	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	J	1010	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	D	1008	-	4,4,4	0.16	0	6,6,6	0.08	0
5	SO4	P	1014	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	1012	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	R	1012	-	4,4,4	0.14	0	6,6,6	0.07	0
6	NAG	C	1022	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	H	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1006	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	N	1006	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	H	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1009	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	P	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1005	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	O	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	1004	-	4,4,4	0.15	0	6,6,6	0.05	0
4	P52	G	1002	3	33,38,38	3.51	6 (18%)	38,53,53	0.97	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	G	1006	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	M	1011	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	J	1006	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	O	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1006	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	L	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	L	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	U	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	Q	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	H	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	1010	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	E	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	O	1013	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	O	1012	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1006	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	1011	-	4,4,4	0.14	0	6,6,6	0.04	0
6	NAG	E	1023	-	14,14,15	0.24	0	17,19,21	0.83	0
5	SO4	P	1007	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	H	1010	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	Q	1014	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	H	1014	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1010	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	U	1008	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	S	1016	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	V	1005	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	I	1008	-	4,4,4	0.17	0	6,6,6	0.08	0
5	SO4	Q	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	D	1023	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	S	1015	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	T	1003	3	33,38,38	3.53	6 (18%)	38,53,53	1.00	4 (10%)
6	NAG	F	1023	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	G	1007	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	G	1008	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	C	1011	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	Q	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	H	1005	-	4,4,4	0.14	0	6,6,6	0.14	0
6	NAG	I	1023	-	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
5	SO4	L	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	U	1011	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	J	1004	-	4,4,4	0.15	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	P	1022	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	I	1011	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	C	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	M	1005	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	D	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	G	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	1005	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	D	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	I	1006	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	V	1012	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	N	1008	-	4,4,4	0.14	0	6,6,6	0.07	0
4	P52	L	1003	3	33,38,38	3.55	6 (18%)	38,53,53	0.98	2 (5%)
5	SO4	M	1015	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	S	1010	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	R	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	N	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	S	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	E	1003	3	33,38,38	3.51	6 (18%)	38,53,53	1.03	2 (5%)
5	SO4	T	1006	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	U	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	P	1010	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	S	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	L	1012	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1014	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	E	1004	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	N	1011	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	H	1012	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	V	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
6	NAG	N	1023	-	14,14,15	0.23	0	17,19,21	0.84	0
6	NAG	T	1023	-	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	C	1007	-	4,4,4	0.15	0	6,6,6	0.11	0
5	SO4	G	1024	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	S	1005	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	V	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	T	1007	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	V	1007	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	O	1016	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	1012	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	C	1002	3	33,38,38	3.52	6 (18%)	38,53,53	1.02	3 (7%)
5	SO4	M	1007	-	4,4,4	0.15	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	E	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	Q	1002	3	33,38,38	3.50	6 (18%)	38,53,53	1.04	3 (7%)
5	SO4	K	1009	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	R	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	I	1003	3	33,38,38	3.50	6 (18%)	38,53,53	0.97	3 (7%)
5	SO4	P	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	U	1009	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	S	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	1007	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	E	1009	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	U	1001	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	S	1006	-	4,4,4	0.14	0	6,6,6	0.08	0
6	NAG	K	1023	-	14,14,15	0.24	0	17,19,21	0.83	0
5	SO4	O	1010	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	V	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
4	P52	V	1002	3	33,38,38	3.51	6 (18%)	38,53,53	0.99	3 (7%)
4	P52	M	1003	3	33,38,38	3.51	6 (18%)	38,53,53	0.98	3 (7%)
5	SO4	J	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1006	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	H	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	M	1014	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	1015	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	A	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	M	1004	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	F	1009	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	D	1001	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	K	1002	3	33,38,38	3.52	6 (18%)	38,53,53	1.00	3 (7%)
5	SO4	L	1005	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	M	1013	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	H	1016	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	F	1001	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	O	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	Q	1010	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	G	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
4	P52	U	1003	3	33,38,38	3.51	6 (18%)	38,53,53	1.00	4 (10%)
5	SO4	B	1011	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	E	1005	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	F	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	D	1012	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	P52	N	1003	3	33,38,38	3.52	6 (18%)	38,53,53	0.95	2 (5%)
5	SO4	A	1014	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	R	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	K	1007	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	T	1011	-	4,4,4	0.14	0	6,6,6	0.06	0
4	P52	J	1002	3	33,38,38	3.51	6 (18%)	38,53,53	0.99	3 (7%)
5	SO4	C	1006	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	A	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	1007	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	N	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	U	1005	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	C	1014	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1011	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	I	1005	-	4,4,4	0.14	0	6,6,6	0.11	0
6	NAG	R	1023	-	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
5	SO4	C	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	1007	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	Q	1006	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	E	1010	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	U	1015	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	O	1002	3	33,38,38	3.51	6 (18%)	38,53,53	1.00	3 (7%)
5	SO4	K	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	M	1009	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	I	1015	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	Q	1021	-	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
6	NAG	A	1022	1	14,14,15	0.23	0	17,19,21	0.84	1 (5%)
5	SO4	C	1008	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	E	1011	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	P	1006	-	4,4,4	0.13	0	6,6,6	0.06	0
4	P52	R	1002	3	33,38,38	3.52	6 (18%)	38,53,53	1.00	4 (10%)
5	SO4	B	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	O	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	S	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	V	1010	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	U	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	T	1001	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	U	1017	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1007	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	E	1012	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	C	1023	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	K	1016	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1007	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	U	1012	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	F	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	P	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1025	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	T	1005	-	4,4,4	0.14	0	6,6,6	0.15	0
5	SO4	O	1008	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	N	1015	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	S	1011	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	Q	1007	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	F	1016	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	L	1001	-	4,4,4	0.14	0	6,6,6	0.15	0
5	SO4	O	1004	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	I	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	K	1011	-	4,4,4	0.13	0	6,6,6	0.08	0
6	NAG	M	1024	-	14,14,15	0.24	0	17,19,21	0.84	1 (5%)
5	SO4	J	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	1004	-	4,4,4	0.14	0	6,6,6	0.08	0
4	P52	F	1003	3	33,38,38	3.48	6 (18%)	38,53,53	1.00	3 (7%)
5	SO4	N	1012	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	G	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1004	-	4,4,4	0.14	0	6,6,6	0.07	0
4	P52	D	1003	3	33,38,38	3.51	6 (18%)	38,53,53	1.08	4 (10%)
5	SO4	B	1015	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	G	1011	-	4,4,4	0.14	0	6,6,6	0.06	0
6	NAG	J	1022	-	14,14,15	0.22	0	17,19,21	0.83	0
5	SO4	K	1010	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	K	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	I	1001	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	F	1011	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	I	1010	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	N	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	O	1015	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1006	-	4,4,4	0.14	0	6,6,6	0.11	0
5	SO4	N	1005	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	I	1007	-	4,4,4	0.13	0	6,6,6	0.07	0
6	NAG	U	1024	-	14,14,15	0.23	0	17,19,21	0.84	0
5	SO4	D	1006	-	4,4,4	0.14	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	B	1013	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	N	1013	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	P	1008	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	T	1015	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	L	1015	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1009	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	I	1009	-	4,4,4	0.15	0	6,6,6	0.07	0
4	P52	B	1002	3	33,38,38	3.52	6 (18%)	38,53,53	1.03	2 (5%)
5	SO4	N	1009	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	N	1010	-	4,4,4	0.13	0	6,6,6	0.04	0
5	SO4	D	1014	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	J	1005	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	P	1004	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	R	1011	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	G	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	V	1004	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	N	1001	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	E	1015	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	J	1015	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	T	1016	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	1008	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	Q	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	1015	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	R	1008	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	D	1010	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	A	1002	3	33,38,38	3.51	6 (18%)	38,53,53	1.04	3 (7%)
5	SO4	O	1007	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	D	1004	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	Q	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
6	NAG	S	1023	-	14,14,15	0.23	0	17,19,21	0.83	0
5	SO4	V	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	1010	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	J	1012	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	L	1008	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	E	1006	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	P	1011	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	U	1014	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	I	1014	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	P	1009	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	V	1011	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	T	1014	-	4,4,4	0.13	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	U	1007	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	M	1010	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	I	1016	-	4,4,4	0.14	0	6,6,6	0.10	0
6	NAG	H	1023	-	14,14,15	0.22	0	17,19,21	0.83	0
5	SO4	C	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	T	1010	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	J	1003	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	1013	-	4,4,4	0.14	0	6,6,6	0.07	0
6	NAG	O	1023	-	14,14,15	0.23	0	17,19,21	0.84	0
5	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	J	1013	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	H	1011	-	4,4,4	0.14	0	6,6,6	0.05	0
6	NAG	G	1023	-	14,14,15	0.23	0	17,19,21	0.84	0
5	SO4	J	1007	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	C	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	O	1011	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	G	1015	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	M	1016	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	S	1008	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	P	1015	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	J	1011	-	4,4,4	0.14	0	6,6,6	0.05	0
4	P52	P	1002	3	33,38,38	3.53	6 (18%)	38,53,53	0.98	3 (7%)
5	SO4	G	1010	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	A	1008	-	4,4,4	0.14	0	6,6,6	0.10	0
5	SO4	C	1010	-	4,4,4	0.14	0	6,6,6	0.05	0
6	NAG	B	1022	-	14,14,15	0.22	0	17,19,21	0.84	1 (5%)
5	SO4	Q	1011	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	V	1008	-	4,4,4	0.14	0	6,6,6	0.05	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
6	NAG	L	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	S	1023	-	-	5/6/23/26	0/1/1/1
4	P52	E	1003	3	-	11/29/36/36	0/3/3/3
6	NAG	Q	1021	-	-	5/6/23/26	0/1/1/1
6	NAG	V	1022	-	-	5/6/23/26	0/1/1/1
6	NAG	A	1022	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	O	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	K	1023	-	-	5/6/23/26	0/1/1/1
4	P52	J	1002	3	-	11/29/36/36	0/3/3/3
4	P52	V	1002	3	-	10/29/36/36	0/3/3/3
4	P52	M	1003	3	-	11/29/36/36	0/3/3/3
4	P52	C	1002	3	-	9/29/36/36	0/3/3/3
6	NAG	C	1022	-	-	5/6/23/26	0/1/1/1
6	NAG	G	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	I	1023	-	-	5/6/23/26	0/1/1/1
4	P52	R	1002	3	-	10/29/36/36	0/3/3/3
6	NAG	E	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	F	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	N	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	U	1024	-	-	5/6/23/26	0/1/1/1
6	NAG	M	1024	-	-	5/6/23/26	0/1/1/1
6	NAG	T	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	P	1022	-	-	5/6/23/26	0/1/1/1
4	P52	K	1002	3	-	10/29/36/36	0/3/3/3
4	P52	H	1003	3	-	8/29/36/36	0/3/3/3
4	P52	Q	1002	3	-	12/29/36/36	0/3/3/3
4	P52	P	1002	3	-	11/29/36/36	0/3/3/3
4	P52	G	1002	3	-	12/29/36/36	0/3/3/3
4	P52	F	1003	3	-	10/29/36/36	0/3/3/3
4	P52	A	1002	3	-	10/29/36/36	0/3/3/3
6	NAG	D	1023	-	-	5/6/23/26	0/1/1/1
4	P52	D	1003	3	-	11/29/36/36	0/3/3/3
4	P52	I	1003	3	-	12/29/36/36	0/3/3/3
6	NAG	B	1022	-	-	5/6/23/26	0/1/1/1
4	P52	U	1003	3	-	9/29/36/36	0/3/3/3
6	NAG	R	1023	-	-	5/6/23/26	0/1/1/1
4	P52	L	1003	3	-	9/29/36/36	0/3/3/3
6	NAG	H	1023	-	-	5/6/23/26	0/1/1/1
4	P52	N	1003	3	-	9/29/36/36	0/3/3/3
4	P52	B	1002	3	-	9/29/36/36	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P52	T	1003	3	-	10/29/36/36	0/3/3/3
6	NAG	J	1022	-	-	5/6/23/26	0/1/1/1
4	P52	O	1002	3	-	10/29/36/36	0/3/3/3
4	P52	S	1003	3	-	10/29/36/36	0/3/3/3

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1003	P52	P1-C11	16.21	1.95	1.79
4	N	1003	P52	P1-C11	16.09	1.95	1.79
4	T	1003	P52	P1-C11	16.07	1.95	1.79
4	P	1002	P52	P1-C11	16.07	1.95	1.79
4	K	1002	P52	P1-C11	16.06	1.95	1.79
4	C	1002	P52	P1-C11	16.03	1.95	1.79
4	S	1003	P52	P1-C11	16.03	1.95	1.79
4	R	1002	P52	P1-C11	16.03	1.95	1.79
4	H	1003	P52	P1-C11	16.01	1.95	1.79
4	M	1003	P52	P1-C11	16.00	1.95	1.79
4	E	1003	P52	P1-C11	15.99	1.95	1.79
4	D	1003	P52	P1-C11	15.98	1.95	1.79
4	B	1002	P52	P1-C11	15.97	1.95	1.79
4	V	1002	P52	P1-C11	15.97	1.95	1.79
4	J	1002	P52	P1-C11	15.95	1.95	1.79
4	O	1002	P52	P1-C11	15.94	1.95	1.79
4	A	1002	P52	P1-C11	15.94	1.95	1.79
4	U	1003	P52	P1-C11	15.93	1.95	1.79
4	Q	1002	P52	P1-C11	15.92	1.95	1.79
4	G	1002	P52	P1-C11	15.92	1.95	1.79
4	I	1003	P52	P1-C11	15.89	1.94	1.79
4	F	1003	P52	P1-C11	15.82	1.94	1.79
4	H	1003	P52	C10-N2	8.20	1.52	1.34
4	R	1002	P52	C10-N2	8.16	1.52	1.34
4	B	1002	P52	C10-N2	8.14	1.52	1.34
4	P	1002	P52	C10-N2	8.12	1.51	1.34
4	G	1002	P52	C10-N2	8.12	1.51	1.34
4	V	1002	P52	C10-N2	8.12	1.51	1.34
4	C	1002	P52	C10-N2	8.10	1.51	1.34
4	J	1002	P52	C10-N2	8.10	1.51	1.34
4	A	1002	P52	C10-N2	8.10	1.51	1.34
4	E	1003	P52	C10-N2	8.09	1.51	1.34
4	O	1002	P52	C10-N2	8.08	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1003	P52	C10-N2	8.07	1.51	1.34
4	Q	1002	P52	C10-N2	8.07	1.51	1.34
4	M	1003	P52	C10-N2	8.07	1.51	1.34
4	U	1003	P52	C10-N2	8.06	1.51	1.34
4	T	1003	P52	C10-N2	8.06	1.51	1.34
4	L	1003	P52	C10-N2	8.06	1.51	1.34
4	S	1003	P52	C10-N2	8.04	1.51	1.34
4	I	1003	P52	C10-N2	8.01	1.51	1.34
4	K	1002	P52	C10-N2	8.00	1.51	1.34
4	F	1003	P52	C10-N2	7.95	1.51	1.34
4	N	1003	P52	C10-N2	7.94	1.51	1.34
4	G	1002	P52	C18-N4	6.08	1.48	1.32
4	D	1003	P52	C18-N4	6.07	1.48	1.32
4	I	1003	P52	C18-N4	6.03	1.48	1.32
4	J	1002	P52	C18-N4	6.02	1.48	1.32
4	B	1002	P52	C18-N4	6.02	1.48	1.32
4	M	1003	P52	C18-N4	6.01	1.48	1.32
4	C	1002	P52	C18-N4	6.01	1.48	1.32
4	E	1003	P52	C18-N4	6.01	1.48	1.32
4	L	1003	P52	C18-N4	6.01	1.48	1.32
4	K	1002	P52	C18-N4	6.01	1.48	1.32
4	O	1002	P52	C18-N4	6.01	1.48	1.32
4	H	1003	P52	C18-N4	6.00	1.48	1.32
4	N	1003	P52	C18-N4	5.99	1.48	1.32
4	F	1003	P52	C18-N4	5.99	1.48	1.32
4	T	1003	P52	C18-N4	5.99	1.48	1.32
4	S	1003	P52	C18-N4	5.98	1.48	1.32
4	U	1003	P52	C18-N4	5.98	1.48	1.32
4	V	1002	P52	C18-N4	5.98	1.48	1.32
4	Q	1002	P52	C18-N4	5.98	1.48	1.32
4	A	1002	P52	C18-N4	5.98	1.48	1.32
4	P	1002	P52	C18-N4	5.97	1.48	1.32
4	R	1002	P52	C18-N4	5.97	1.48	1.32
4	D	1003	P52	C19-C20	3.14	1.60	1.51
4	Q	1002	P52	C19-C20	3.13	1.60	1.51
4	H	1003	P52	C19-C20	3.13	1.60	1.51
4	P	1002	P52	C19-C20	3.12	1.60	1.51
4	N	1003	P52	C19-C20	3.11	1.59	1.51
4	L	1003	P52	C19-C20	3.11	1.59	1.51
4	C	1002	P52	C19-C20	3.11	1.59	1.51
4	K	1002	P52	C19-C20	3.11	1.59	1.51
4	J	1002	P52	C19-C20	3.10	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002	P52	C19-C20	3.09	1.59	1.51
4	F	1003	P52	C19-C20	3.09	1.59	1.51
4	I	1003	P52	C19-C20	3.09	1.59	1.51
4	M	1003	P52	C19-C20	3.09	1.59	1.51
4	O	1002	P52	C19-C20	3.08	1.59	1.51
4	V	1002	P52	C19-C20	3.08	1.59	1.51
4	U	1003	P52	C19-C20	3.07	1.59	1.51
4	R	1002	P52	C19-C20	3.07	1.59	1.51
4	T	1003	P52	C19-C20	3.06	1.59	1.51
4	S	1003	P52	C19-C20	3.06	1.59	1.51
4	G	1002	P52	C19-C20	3.06	1.59	1.51
4	A	1002	P52	C19-C20	3.05	1.59	1.51
4	E	1003	P52	C19-C20	3.04	1.59	1.51
4	S	1003	P52	C12-C10	2.60	1.56	1.51
4	N	1003	P52	C12-C10	2.59	1.56	1.51
4	A	1002	P52	C12-C10	2.57	1.56	1.51
4	P	1002	P52	C12-C10	2.57	1.56	1.51
4	H	1003	P52	C17-N2	2.54	1.51	1.45
4	B	1002	P52	C17-N2	2.53	1.51	1.45
4	R	1002	P52	C12-C10	2.53	1.56	1.51
4	F	1003	P52	C12-C10	2.51	1.56	1.51
4	L	1003	P52	C12-C10	2.50	1.56	1.51
4	C	1002	P52	C12-C10	2.50	1.56	1.51
4	T	1003	P52	C12-C10	2.50	1.56	1.51
4	R	1002	P52	C17-N2	2.49	1.51	1.45
4	P	1002	P52	C17-N2	2.49	1.51	1.45
4	M	1003	P52	C12-C10	2.49	1.56	1.51
4	J	1002	P52	C12-C10	2.48	1.56	1.51
4	I	1003	P52	C12-C10	2.47	1.56	1.51
4	Q	1002	P52	C17-N2	2.47	1.51	1.45
4	G	1002	P52	C17-N2	2.47	1.51	1.45
4	U	1003	P52	C17-N2	2.47	1.51	1.45
4	V	1002	P52	C17-N2	2.46	1.51	1.45
4	C	1002	P52	C17-N2	2.45	1.51	1.45
4	V	1002	P52	C12-C10	2.45	1.55	1.51
4	H	1003	P52	C12-C10	2.44	1.55	1.51
4	U	1003	P52	C12-C10	2.44	1.55	1.51
4	D	1003	P52	C17-N2	2.44	1.51	1.45
4	I	1003	P52	C17-N2	2.44	1.51	1.45
4	J	1002	P52	C17-N2	2.43	1.51	1.45
4	O	1002	P52	C17-N2	2.43	1.51	1.45
4	Q	1002	P52	C12-C10	2.43	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	1002	P52	C17-N2	2.43	1.51	1.45
4	B	1002	P52	C12-C10	2.42	1.55	1.51
4	L	1003	P52	C17-N2	2.42	1.51	1.45
4	O	1002	P52	C12-C10	2.42	1.55	1.51
4	T	1003	P52	C17-N2	2.42	1.51	1.45
4	M	1003	P52	C17-N2	2.41	1.51	1.45
4	D	1003	P52	C12-C10	2.41	1.55	1.51
4	K	1002	P52	C12-C10	2.41	1.55	1.51
4	G	1002	P52	C12-C10	2.40	1.55	1.51
4	E	1003	P52	C17-N2	2.40	1.50	1.45
4	F	1003	P52	C17-N2	2.40	1.50	1.45
4	E	1003	P52	C12-C10	2.39	1.55	1.51
4	S	1003	P52	C17-N2	2.37	1.50	1.45
4	N	1003	P52	C17-N2	2.35	1.50	1.45
4	A	1002	P52	C17-N2	2.35	1.50	1.45

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1003	P52	O3-C10-C12	-2.97	118.25	122.12
4	H	1003	P52	O3-C10-C12	-2.83	118.43	122.12
4	B	1002	P52	O3-C10-C12	-2.79	118.49	122.12
4	H	1003	P52	C20-C19-C17	2.74	118.80	113.45
4	R	1002	P52	O3-C10-C12	-2.70	118.60	122.12
4	D	1003	P52	O3-C10-C12	-2.63	118.69	122.12
4	D	1003	P52	C20-C19-C17	2.63	118.60	113.45
4	Q	1002	P52	O3-C10-C12	-2.63	118.70	122.12
4	A	1002	P52	O3-C10-C12	-2.63	118.70	122.12
4	E	1003	P52	C12-C10-N2	2.63	120.75	116.21
4	G	1002	P52	O3-C10-C12	-2.57	118.78	122.12
4	N	1003	P52	C20-C19-C17	2.56	118.46	113.45
4	V	1002	P52	O3-C10-C12	-2.55	118.80	122.12
4	K	1002	P52	C20-C19-C17	2.54	118.42	113.45
4	U	1003	P52	O3-C10-C12	-2.53	118.82	122.12
4	C	1002	P52	O3-C10-C12	-2.53	118.83	122.12
4	Q	1002	P52	C20-C19-C17	2.49	118.33	113.45
4	T	1003	P52	O3-C10-C12	-2.49	118.89	122.12
4	O	1002	P52	O3-C10-C12	-2.46	118.92	122.12
4	O	1002	P52	C20-C19-C17	2.45	118.25	113.45
4	H	1003	P52	C19-C17-N2	2.45	115.95	110.79
4	F	1003	P52	C20-C19-C17	2.43	118.21	113.45
4	J	1002	P52	O3-C10-C12	-2.43	118.96	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	1002	P52	O3-C10-C12	-2.42	118.97	122.12
4	F	1003	P52	C19-C17-N2	2.40	115.86	110.79
4	L	1003	P52	O3-C10-C12	-2.39	119.01	122.12
4	C	1002	P52	C20-C19-C17	2.37	118.09	113.45
4	Q	1002	P52	C19-C17-N2	2.35	115.74	110.79
4	H	1003	P52	C17-N2-C10	2.33	126.67	121.67
4	M	1003	P52	O3-C10-C12	-2.33	119.08	122.12
4	U	1003	P52	C20-C19-C17	2.32	117.99	113.45
4	K	1002	P52	C19-C17-N2	2.32	115.67	110.79
4	A	1002	P52	C20-C19-C17	2.30	117.95	113.45
4	N	1003	P52	C19-C17-N2	2.26	115.55	110.79
4	J	1002	P52	C20-C19-C17	2.25	117.85	113.45
4	G	1002	P52	C12-C10-N2	2.23	120.06	116.21
4	S	1003	P52	O3-C10-C12	-2.20	119.26	122.12
4	U	1003	P52	C19-C17-N2	2.18	115.39	110.79
4	T	1003	P52	C20-C19-C17	2.18	117.70	113.45
4	R	1002	P52	C12-C10-N2	2.17	119.97	116.21
4	O	1002	P52	C19-C17-N2	2.17	115.37	110.79
4	P	1002	P52	C20-C19-C17	2.16	117.68	113.45
4	I	1003	P52	O3-C10-C12	-2.16	119.31	122.12
4	V	1002	P52	C20-C19-C17	2.16	117.67	113.45
4	F	1003	P52	O3-C10-C12	-2.16	119.31	122.12
4	M	1003	P52	C20-C19-C17	2.15	117.66	113.45
4	S	1003	P52	C12-C10-N2	2.14	119.91	116.21
4	D	1003	P52	C19-C17-N2	2.14	115.30	110.79
4	S	1003	P52	C20-C19-C17	2.13	117.62	113.45
4	I	1003	P52	C20-C19-C17	2.13	117.62	113.45
4	L	1003	P52	C20-C19-C17	2.13	117.61	113.45
4	A	1002	P52	C12-C10-N2	2.13	119.89	116.21
4	C	1002	P52	C19-C17-N2	2.12	115.25	110.79
4	T	1003	P52	C12-C10-N2	2.11	119.86	116.21
4	B	1002	P52	C19-C17-N2	2.10	115.22	110.79
4	V	1002	P52	C19-C17-N2	2.09	115.19	110.79
4	M	1003	P52	C19-C17-N2	2.09	115.19	110.79
4	K	1002	P52	O3-C10-C12	-2.08	119.42	122.12
4	D	1003	P52	C12-C10-N2	2.07	119.80	116.21
4	I	1003	P52	C19-C17-N2	2.07	115.15	110.79
4	T	1003	P52	C19-C17-N2	2.07	115.15	110.79
4	U	1003	P52	C12-C10-N2	2.06	119.77	116.21
4	P	1002	P52	C19-C17-N2	2.04	115.09	110.79
6	Q	1021	NAG	O5-C5-C6	2.03	110.39	107.20
4	R	1002	P52	C20-C19-C17	2.03	117.42	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1022	NAG	O5-C5-C6	2.03	110.39	107.20
6	M	1024	NAG	O5-C5-C6	2.03	110.39	107.20
4	J	1002	P52	C19-C17-N2	2.02	115.06	110.79
4	R	1002	P52	C19-C17-N2	2.02	115.06	110.79
6	D	1023	NAG	O5-C5-C6	2.02	110.38	107.20
6	F	1023	NAG	O5-C5-C6	2.02	110.37	107.20
6	C	1022	NAG	O5-C5-C6	2.01	110.36	107.20
6	P	1022	NAG	O5-C5-C6	2.01	110.35	107.20
6	R	1023	NAG	O5-C5-C6	2.01	110.35	107.20
4	H	1003	P52	O4-C18-N4	-2.01	119.51	123.00
6	T	1023	NAG	O5-C5-C6	2.00	110.34	107.20
6	L	1023	NAG	O5-C5-C6	2.00	110.34	107.20
6	V	1022	NAG	O5-C5-C6	2.00	110.34	107.20
6	B	1022	NAG	O5-C5-C6	2.00	110.34	107.20
6	I	1023	NAG	O5-C5-C6	2.00	110.34	107.20

There are no chirality outliers.

All (334) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	P52	P1-C11-C12-C10
4	A	1002	P52	P1-C11-C12-C13
4	A	1002	P52	C12-C13-C14-C16
4	B	1002	P52	P1-C11-C12-C13
4	C	1002	P52	P1-C11-C12-C13
4	D	1003	P52	P1-C11-C12-C10
4	D	1003	P52	P1-C11-C12-C13
4	D	1003	P52	N2-C17-C18-N4
4	E	1003	P52	P1-C11-C12-C13
4	E	1003	P52	N2-C17-C18-N4
4	F	1003	P52	P1-C11-C12-C13
4	G	1002	P52	P1-C11-C12-C13
4	H	1003	P52	P1-C11-C12-C13
4	H	1003	P52	C19-C17-N2-C10
4	I	1003	P52	P1-C11-C12-C13
4	J	1002	P52	P1-C11-C12-C13
4	K	1002	P52	P1-C11-C12-C10
4	K	1002	P52	P1-C11-C12-C13
4	L	1003	P52	P1-C11-C12-C10
4	L	1003	P52	P1-C11-C12-C13
4	M	1003	P52	P1-C11-C12-C13
4	N	1003	P52	P1-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
4	O	1002	P52	P1-C11-C12-C10
4	O	1002	P52	P1-C11-C12-C13
4	P	1002	P52	P1-C11-C12-C13
4	Q	1002	P52	P1-C11-C12-C10
4	Q	1002	P52	P1-C11-C12-C13
4	Q	1002	P52	C12-C13-C14-C15
4	R	1002	P52	P1-C11-C12-C13
4	S	1003	P52	P1-C11-C12-C10
4	S	1003	P52	P1-C11-C12-C13
4	T	1003	P52	P1-C11-C12-C13
4	U	1003	P52	P1-C11-C12-C13
4	U	1003	P52	C12-C13-C14-C15
4	U	1003	P52	C12-C13-C14-C16
4	V	1002	P52	P1-C11-C12-C10
4	V	1002	P52	P1-C11-C12-C13
6	A	1022	NAG	C3-C2-N2-C7
6	A	1022	NAG	O7-C7-N2-C2
6	B	1022	NAG	C3-C2-N2-C7
6	B	1022	NAG	O7-C7-N2-C2
6	C	1022	NAG	C3-C2-N2-C7
6	C	1022	NAG	O7-C7-N2-C2
6	D	1023	NAG	C3-C2-N2-C7
6	D	1023	NAG	O7-C7-N2-C2
6	E	1023	NAG	C3-C2-N2-C7
6	E	1023	NAG	O7-C7-N2-C2
6	F	1023	NAG	C3-C2-N2-C7
6	F	1023	NAG	O7-C7-N2-C2
6	G	1023	NAG	C3-C2-N2-C7
6	G	1023	NAG	O7-C7-N2-C2
6	H	1023	NAG	C3-C2-N2-C7
6	H	1023	NAG	O7-C7-N2-C2
6	I	1023	NAG	C3-C2-N2-C7
6	I	1023	NAG	O7-C7-N2-C2
6	J	1022	NAG	C3-C2-N2-C7
6	J	1022	NAG	O7-C7-N2-C2
6	K	1023	NAG	C3-C2-N2-C7
6	K	1023	NAG	O7-C7-N2-C2
6	L	1023	NAG	C3-C2-N2-C7
6	L	1023	NAG	O7-C7-N2-C2
6	M	1024	NAG	C3-C2-N2-C7
6	M	1024	NAG	O7-C7-N2-C2
6	N	1023	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
6	N	1023	NAG	O7-C7-N2-C2
6	O	1023	NAG	C3-C2-N2-C7
6	O	1023	NAG	O7-C7-N2-C2
6	P	1022	NAG	C3-C2-N2-C7
6	P	1022	NAG	O7-C7-N2-C2
6	Q	1021	NAG	C3-C2-N2-C7
6	Q	1021	NAG	O7-C7-N2-C2
6	R	1023	NAG	C3-C2-N2-C7
6	R	1023	NAG	O7-C7-N2-C2
6	S	1023	NAG	C3-C2-N2-C7
6	S	1023	NAG	O7-C7-N2-C2
6	T	1023	NAG	C3-C2-N2-C7
6	T	1023	NAG	O7-C7-N2-C2
6	U	1024	NAG	C3-C2-N2-C7
6	U	1024	NAG	O7-C7-N2-C2
6	V	1022	NAG	C3-C2-N2-C7
6	V	1022	NAG	O7-C7-N2-C2
4	B	1002	P52	C19-C17-N2-C10
4	C	1002	P52	C19-C17-N2-C10
4	K	1002	P52	C19-C17-N2-C10
4	M	1003	P52	C19-C17-N2-C10
4	Q	1002	P52	C19-C17-N2-C10
4	D	1003	P52	C19-C17-N2-C10
4	F	1003	P52	C19-C17-N2-C10
4	I	1003	P52	C19-C17-N2-C10
4	J	1002	P52	C19-C17-N2-C10
4	O	1002	P52	C19-C17-N2-C10
4	P	1002	P52	C19-C17-N2-C10
4	R	1002	P52	C19-C17-N2-C10
4	T	1003	P52	C19-C17-N2-C10
4	U	1003	P52	C19-C17-N2-C10
4	V	1002	P52	C19-C17-N2-C10
4	A	1002	P52	C19-C17-N2-C10
4	L	1003	P52	C19-C17-N2-C10
4	N	1003	P52	C19-C17-N2-C10
6	A	1022	NAG	C8-C7-N2-C2
6	B	1022	NAG	C8-C7-N2-C2
6	C	1022	NAG	C8-C7-N2-C2
6	D	1023	NAG	C8-C7-N2-C2
6	E	1023	NAG	C8-C7-N2-C2
6	F	1023	NAG	C8-C7-N2-C2
6	G	1023	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	H	1023	NAG	C8-C7-N2-C2
6	I	1023	NAG	C8-C7-N2-C2
6	J	1022	NAG	C8-C7-N2-C2
6	K	1023	NAG	C8-C7-N2-C2
6	L	1023	NAG	C8-C7-N2-C2
6	M	1024	NAG	C8-C7-N2-C2
6	N	1023	NAG	C8-C7-N2-C2
6	O	1023	NAG	C8-C7-N2-C2
6	P	1022	NAG	C8-C7-N2-C2
6	Q	1021	NAG	C8-C7-N2-C2
6	R	1023	NAG	C8-C7-N2-C2
6	S	1023	NAG	C8-C7-N2-C2
6	T	1023	NAG	C8-C7-N2-C2
6	U	1024	NAG	C8-C7-N2-C2
6	V	1022	NAG	C8-C7-N2-C2
4	B	1002	P52	C12-C13-C14-C16
4	C	1002	P52	C12-C13-C14-C16
4	D	1003	P52	C12-C13-C14-C16
4	E	1003	P52	C12-C13-C14-C16
4	F	1003	P52	C12-C13-C14-C16
4	G	1002	P52	C12-C13-C14-C16
4	H	1003	P52	C12-C13-C14-C15
4	H	1003	P52	C12-C13-C14-C16
4	I	1003	P52	C12-C13-C14-C16
4	J	1002	P52	C12-C13-C14-C16
4	K	1002	P52	C12-C13-C14-C16
4	L	1003	P52	C12-C13-C14-C16
4	M	1003	P52	C12-C13-C14-C16
4	N	1003	P52	C12-C13-C14-C16
4	O	1002	P52	C12-C13-C14-C16
4	P	1002	P52	C12-C13-C14-C15
4	P	1002	P52	C12-C13-C14-C16
4	Q	1002	P52	C12-C13-C14-C16
4	R	1002	P52	C12-C13-C14-C15
4	R	1002	P52	C12-C13-C14-C16
4	S	1003	P52	C12-C13-C14-C16
4	T	1003	P52	C12-C13-C14-C16
4	V	1002	P52	C12-C13-C14-C16
4	B	1002	P52	C12-C13-C14-C15
4	C	1002	P52	C12-C13-C14-C15
4	D	1003	P52	C12-C13-C14-C15
4	F	1003	P52	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	G	1002	P52	C12-C13-C14-C15
4	I	1003	P52	C12-C13-C14-C15
4	J	1002	P52	C12-C13-C14-C15
4	K	1002	P52	C12-C13-C14-C15
4	M	1003	P52	C12-C13-C14-C15
4	N	1003	P52	C12-C13-C14-C15
4	O	1002	P52	C12-C13-C14-C15
4	S	1003	P52	C12-C13-C14-C15
4	T	1003	P52	C12-C13-C14-C15
4	V	1002	P52	C12-C13-C14-C15
4	S	1003	P52	C19-C17-N2-C10
4	E	1003	P52	C12-C13-C14-C15
4	G	1002	P52	C19-C17-N2-C10
4	E	1003	P52	C19-C17-N2-C10
6	A	1022	NAG	C4-C5-C6-O6
6	B	1022	NAG	C4-C5-C6-O6
6	C	1022	NAG	C4-C5-C6-O6
6	D	1023	NAG	C4-C5-C6-O6
6	E	1023	NAG	C4-C5-C6-O6
6	F	1023	NAG	C4-C5-C6-O6
6	G	1023	NAG	C4-C5-C6-O6
6	H	1023	NAG	C4-C5-C6-O6
6	I	1023	NAG	C4-C5-C6-O6
6	J	1022	NAG	C4-C5-C6-O6
6	K	1023	NAG	C4-C5-C6-O6
6	L	1023	NAG	C4-C5-C6-O6
6	M	1024	NAG	C4-C5-C6-O6
6	N	1023	NAG	C4-C5-C6-O6
6	O	1023	NAG	C4-C5-C6-O6
6	P	1022	NAG	C4-C5-C6-O6
6	Q	1021	NAG	C4-C5-C6-O6
6	R	1023	NAG	C4-C5-C6-O6
6	S	1023	NAG	C4-C5-C6-O6
6	T	1023	NAG	C4-C5-C6-O6
6	U	1024	NAG	C4-C5-C6-O6
6	V	1022	NAG	C4-C5-C6-O6
4	L	1003	P52	C12-C13-C14-C15
4	A	1002	P52	C12-C13-C14-C15
4	D	1003	P52	N2-C17-C18-O4
4	E	1003	P52	N2-C17-C18-O4
4	F	1003	P52	N2-C17-C18-O4
4	F	1003	P52	N2-C17-C18-N4

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Mol	Chain	Res	Type	Atoms
4	G	1002	P52	N2-C17-C18-O4
4	G	1002	P52	N2-C17-C18-N4
4	I	1003	P52	N2-C17-C18-O4
4	I	1003	P52	N2-C17-C18-N4
4	M	1003	P52	N2-C17-C18-N4
4	P	1002	P52	N2-C17-C18-N4
4	Q	1002	P52	N2-C17-C18-O4
4	Q	1002	P52	N2-C17-C18-N4
4	D	1003	P52	C19-C17-C18-O4
4	E	1003	P52	C19-C17-C18-O4
6	E	1023	NAG	O5-C5-C6-O6
6	F	1023	NAG	O5-C5-C6-O6
6	H	1023	NAG	O5-C5-C6-O6
6	I	1023	NAG	O5-C5-C6-O6
6	O	1023	NAG	O5-C5-C6-O6
6	R	1023	NAG	O5-C5-C6-O6
6	A	1022	NAG	O5-C5-C6-O6
6	B	1022	NAG	O5-C5-C6-O6
6	C	1022	NAG	O5-C5-C6-O6
6	D	1023	NAG	O5-C5-C6-O6
6	G	1023	NAG	O5-C5-C6-O6
6	J	1022	NAG	O5-C5-C6-O6
6	K	1023	NAG	O5-C5-C6-O6
6	L	1023	NAG	O5-C5-C6-O6
6	M	1024	NAG	O5-C5-C6-O6
6	N	1023	NAG	O5-C5-C6-O6
6	P	1022	NAG	O5-C5-C6-O6
6	Q	1021	NAG	O5-C5-C6-O6
6	S	1023	NAG	O5-C5-C6-O6
6	T	1023	NAG	O5-C5-C6-O6
6	U	1024	NAG	O5-C5-C6-O6
6	V	1022	NAG	O5-C5-C6-O6
4	J	1002	P52	C2-C1-C8-C9
4	K	1002	P52	C2-C1-C8-C9
4	A	1002	P52	N2-C17-C18-O4
4	A	1002	P52	N2-C17-C18-N4
4	B	1002	P52	N2-C17-C18-O4
4	B	1002	P52	N2-C17-C18-N4
4	C	1002	P52	N2-C17-C18-O4
4	C	1002	P52	N2-C17-C18-N4
4	H	1003	P52	N2-C17-C18-O4
4	H	1003	P52	N2-C17-C18-N4

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Mol	Chain	Res	Type	Atoms
4	J	1002	P52	N2-C17-C18-O4
4	J	1002	P52	N2-C17-C18-N4
4	L	1003	P52	N2-C17-C18-O4
4	L	1003	P52	N2-C17-C18-N4
4	M	1003	P52	N2-C17-C18-O4
4	P	1002	P52	N2-C17-C18-O4
4	R	1002	P52	N2-C17-C18-O4
4	R	1002	P52	N2-C17-C18-N4
4	D	1003	P52	C19-C17-C18-N4
4	E	1003	P52	C19-C17-C18-N4
4	M	1003	P52	C2-C1-C8-C9
4	T	1003	P52	C2-C1-C8-C9
4	E	1003	P52	C18-C17-N2-C10
4	G	1002	P52	C18-C17-N2-C10
4	S	1003	P52	C18-C17-N2-C10
4	O	1002	P52	C1-C8-C9-N1
4	S	1003	P52	C2-C1-C8-C9
4	N	1003	P52	C18-C17-N2-C10
4	K	1002	P52	N2-C17-C18-O4
4	K	1002	P52	N2-C17-C18-N4
4	N	1003	P52	N2-C17-C18-O4
4	N	1003	P52	N2-C17-C18-N4
4	S	1003	P52	N2-C17-C18-O4
4	V	1002	P52	N2-C17-C18-O4
4	V	1002	P52	N2-C17-C18-N4
4	B	1002	P52	P1-C11-C12-C10
4	C	1002	P52	P1-C11-C12-C10
4	E	1003	P52	P1-C11-C12-C10
4	F	1003	P52	P1-C11-C12-C10
4	G	1002	P52	P1-C11-C12-C10
4	H	1003	P52	P1-C11-C12-C10
4	I	1003	P52	P1-C11-C12-C10
4	J	1002	P52	P1-C11-C12-C10
4	M	1003	P52	P1-C11-C12-C10
4	N	1003	P52	P1-C11-C12-C10
4	P	1002	P52	P1-C11-C12-C10
4	R	1002	P52	P1-C11-C12-C10
4	T	1003	P52	P1-C11-C12-C10
4	U	1003	P52	P1-C11-C12-C10
4	L	1003	P52	C18-C17-N2-C10
4	A	1002	P52	C18-C17-N2-C10
4	G	1002	P52	C19-C17-C18-O4

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Mol	Chain	Res	Type	Atoms
4	G	1002	P52	C2-C1-C8-C9
4	O	1002	P52	C2-C1-C8-C9
4	Q	1002	P52	C2-C1-C8-C9
4	U	1003	P52	C2-C1-C8-C9
4	O	1002	P52	C18-C17-N2-C10
4	O	1002	P52	N2-C17-C18-O4
4	T	1003	P52	N2-C17-C18-O4
4	D	1003	P52	C18-C17-N2-C10
4	P	1002	P52	C18-C17-N2-C10
4	T	1003	P52	C18-C17-N2-C10
4	G	1002	P52	C19-C17-C18-N4
4	U	1003	P52	C18-C17-N2-C10
4	F	1003	P52	C18-C17-N2-C10
4	J	1002	P52	C18-C17-N2-C10
4	V	1002	P52	C18-C17-N2-C10
4	A	1002	P52	C17-C19-C20-C21
4	B	1002	P52	C17-C19-C20-C21
4	C	1002	P52	C17-C19-C20-C21
4	D	1003	P52	C17-C19-C20-C21
4	E	1003	P52	C17-C19-C20-C21
4	F	1003	P52	C17-C19-C20-C21
4	G	1002	P52	C17-C19-C20-C21
4	H	1003	P52	C17-C19-C20-C21
4	I	1003	P52	C17-C19-C20-C21
4	J	1002	P52	C17-C19-C20-C21
4	K	1002	P52	C17-C19-C20-C21
4	L	1003	P52	C17-C19-C20-C21
4	M	1003	P52	C17-C19-C20-C21
4	N	1003	P52	C17-C19-C20-C21
4	O	1002	P52	C17-C19-C20-C21
4	P	1002	P52	C17-C19-C20-C21
4	Q	1002	P52	C17-C19-C20-C21
4	R	1002	P52	C17-C19-C20-C21
4	S	1003	P52	C17-C19-C20-C21
4	T	1003	P52	C17-C19-C20-C21
4	U	1003	P52	C17-C19-C20-C21
4	V	1002	P52	C17-C19-C20-C21
4	R	1002	P52	C18-C17-N2-C10
4	I	1003	P52	C18-C17-N2-C10
4	K	1002	P52	C18-C17-N2-C10
4	Q	1002	P52	C18-C17-N2-C10
4	C	1002	P52	C18-C17-N2-C10

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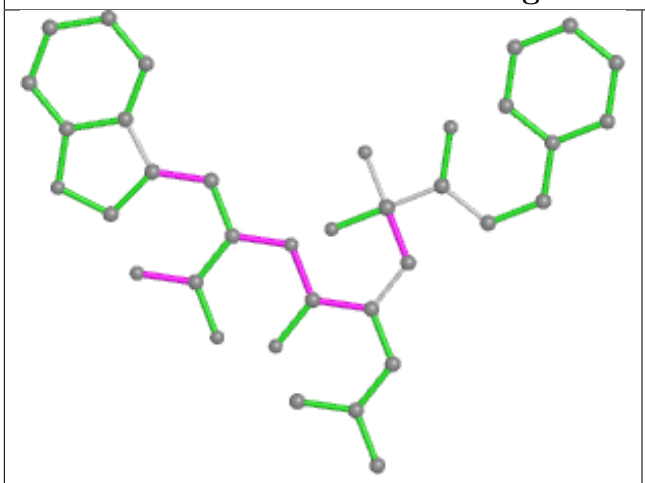
Mol	Chain	Res	Type	Atoms
4	F	1003	P52	C19-C17-C18-O4
4	I	1003	P52	C19-C17-C18-O4
4	I	1003	P52	C19-C17-C18-N4
4	M	1003	P52	C19-C17-C18-O4
4	P	1002	P52	C19-C17-C18-O4
4	Q	1002	P52	C19-C17-C18-O4
4	M	1003	P52	C18-C17-N2-C10
4	A	1002	P52	C1-C8-C9-N1
4	I	1003	P52	C1-C8-C9-N1
4	J	1002	P52	C1-C8-C9-N1
4	P	1002	P52	C1-C8-C9-N1
4	Q	1002	P52	C1-C8-C9-N1
4	R	1002	P52	C1-C8-C9-N1
4	S	1003	P52	C1-C8-C9-N1
4	T	1003	P52	C1-C8-C9-N1
4	U	1003	P52	C1-C8-C9-N1
4	V	1002	P52	C1-C8-C9-N1
4	B	1002	P52	C18-C17-N2-C10

There are no ring outliers.

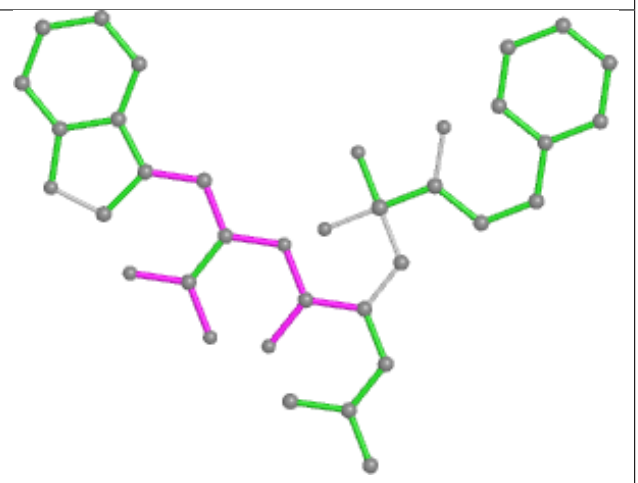
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

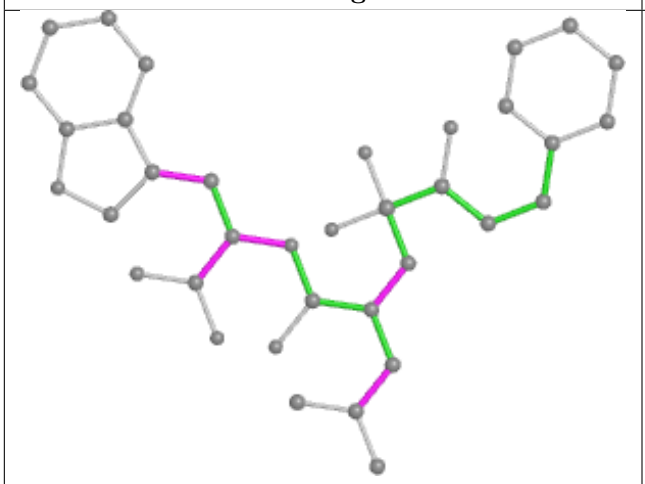
Ligand P52 H 1003



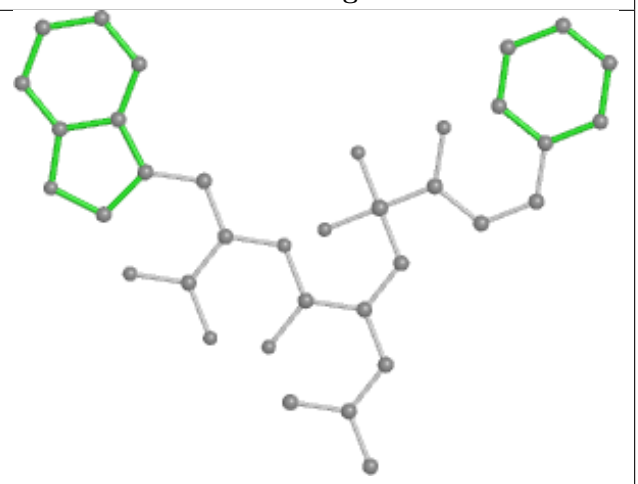
Bond lengths



Bond angles

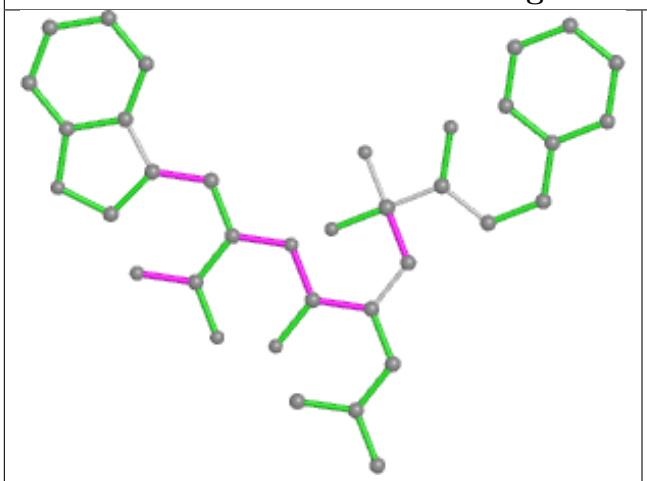


Torsions

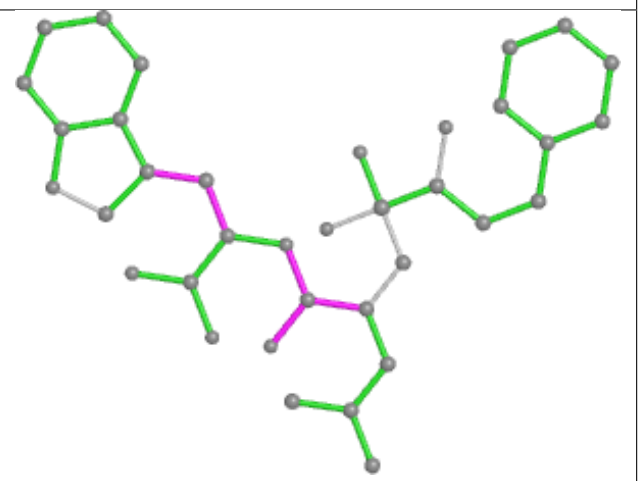


Rings

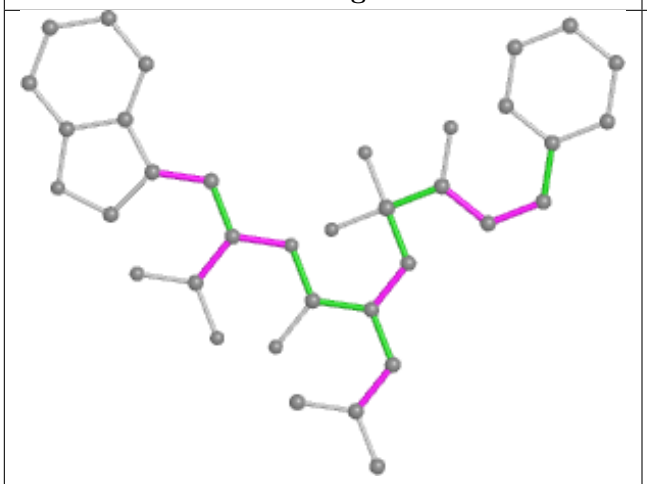
Ligand P52 S 1003



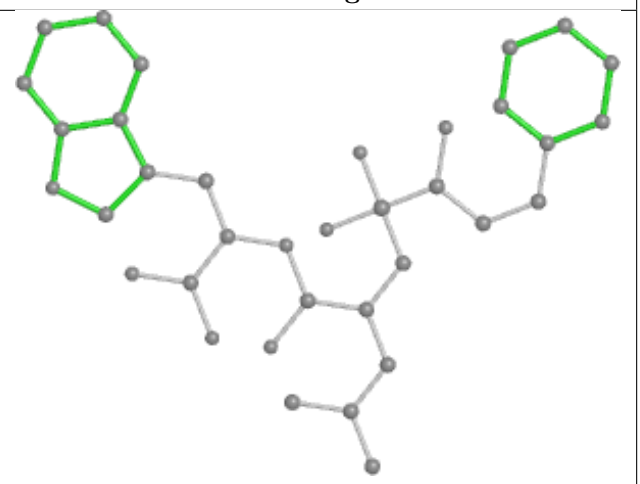
Bond lengths



Bond angles

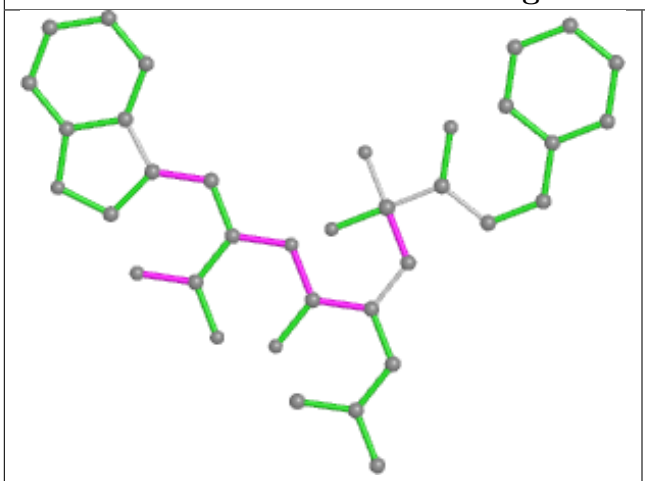


Torsions

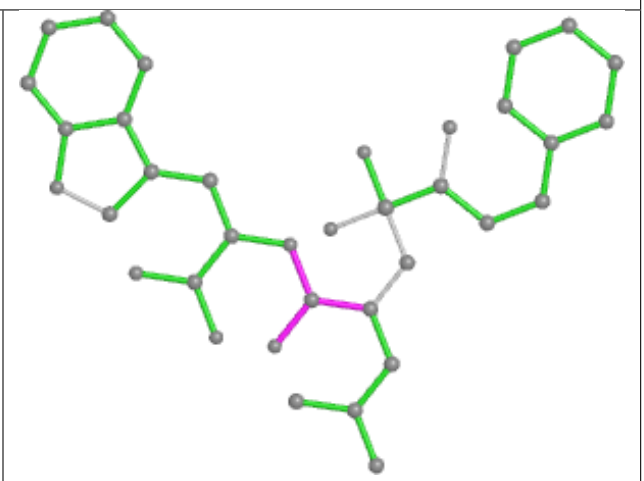


Rings

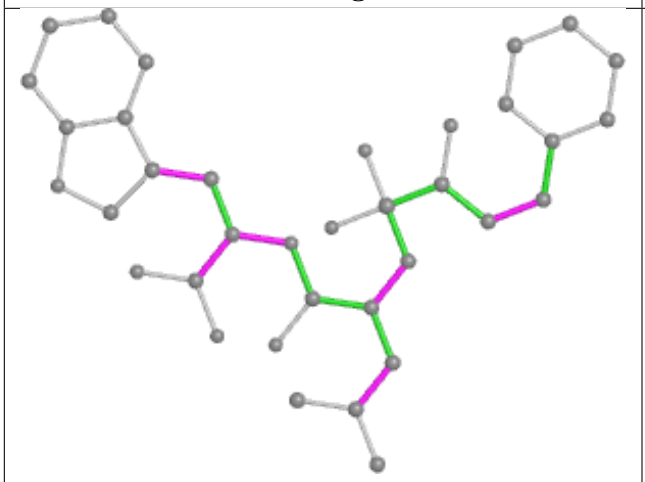
Ligand P52 G 1002



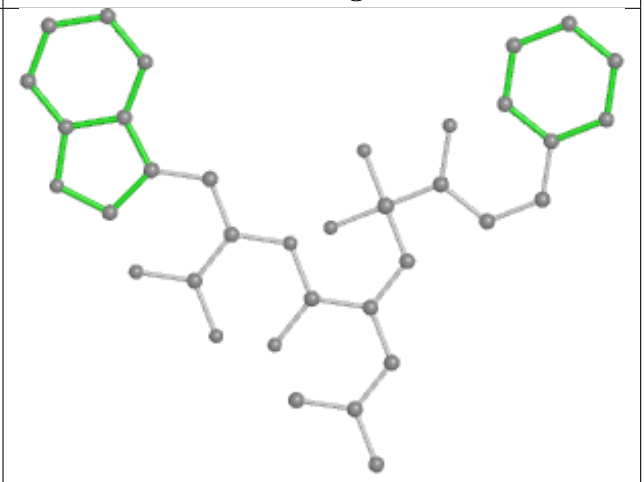
Bond lengths



Bond angles

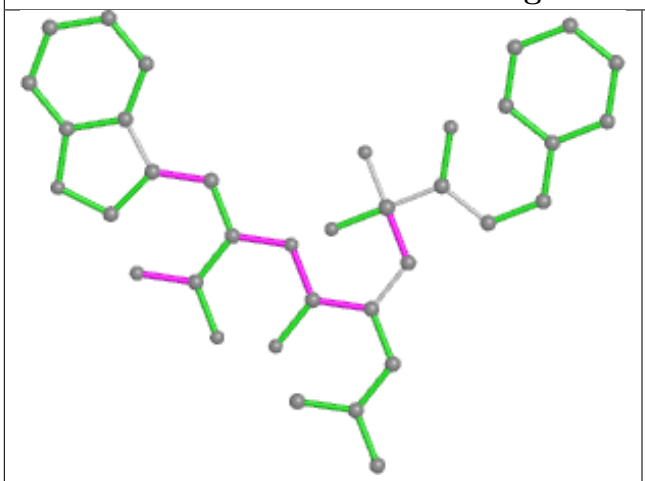


Torsions



Rings

Ligand P52 T 1003



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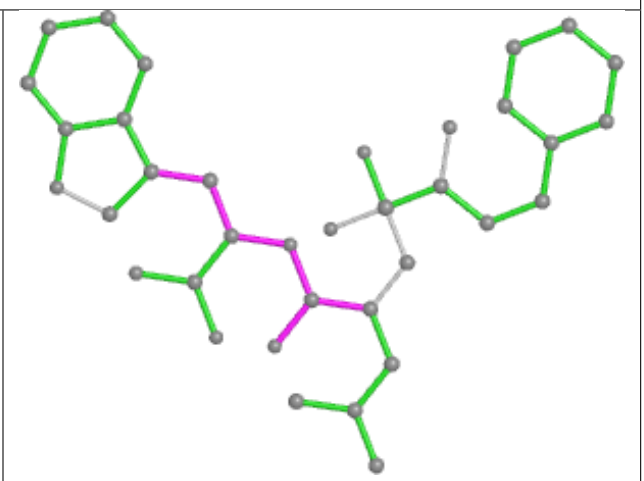

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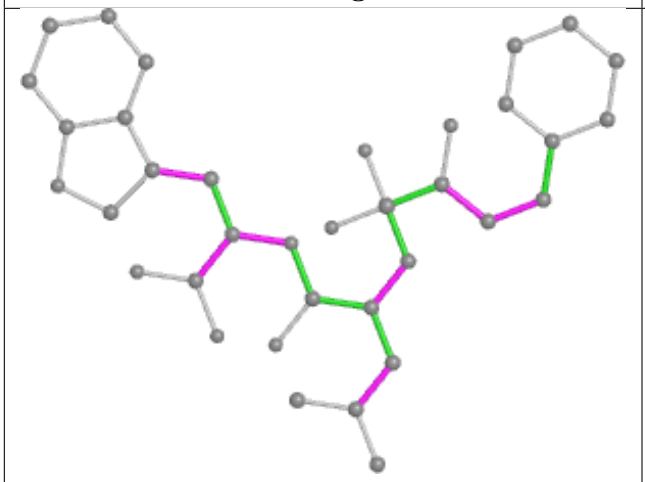

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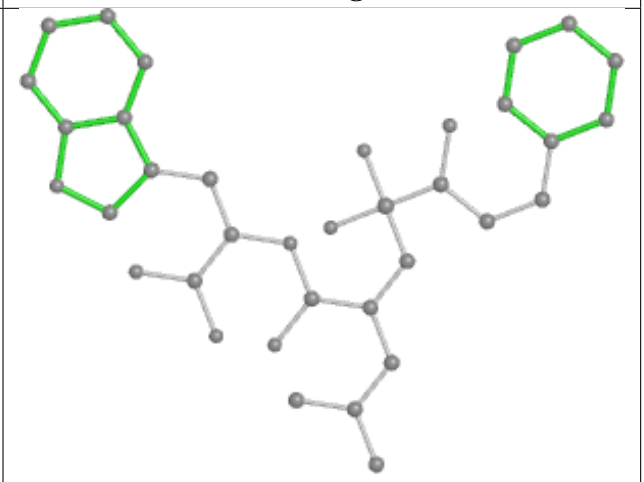
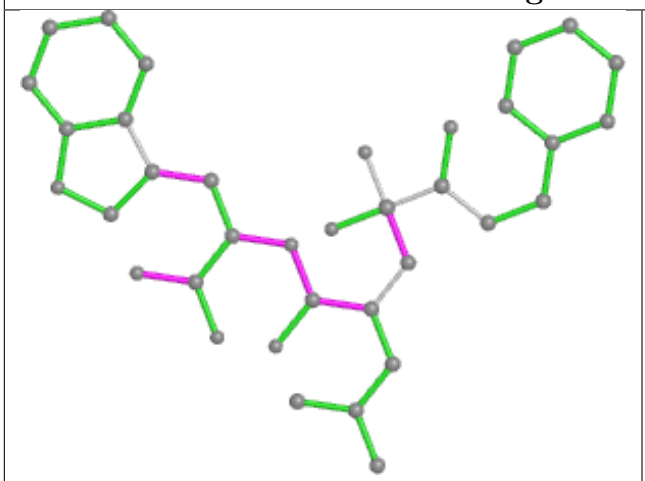


Rings

Ligand P52 L 1003



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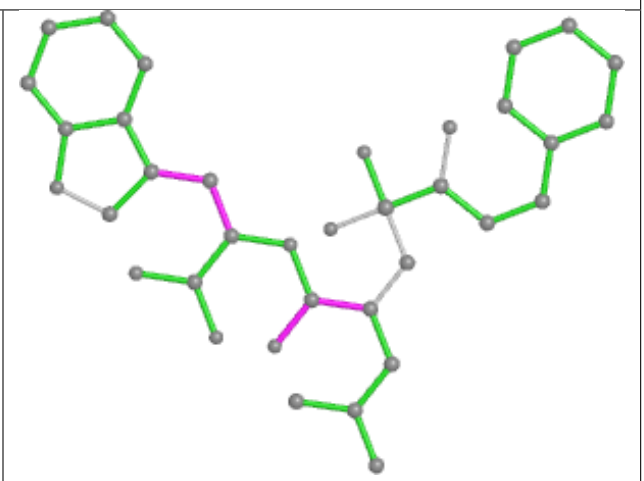

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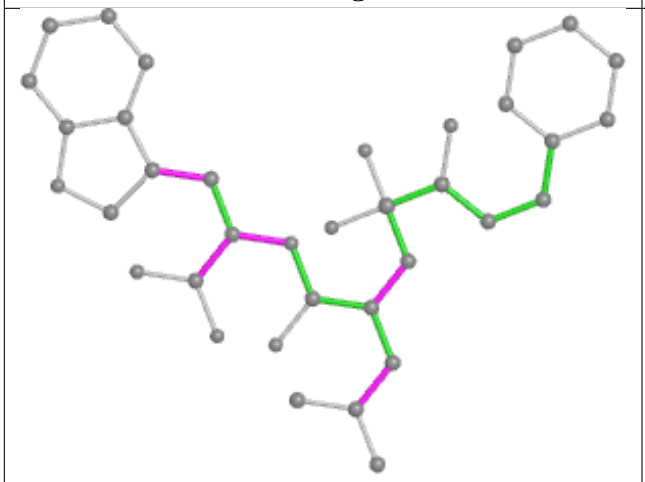

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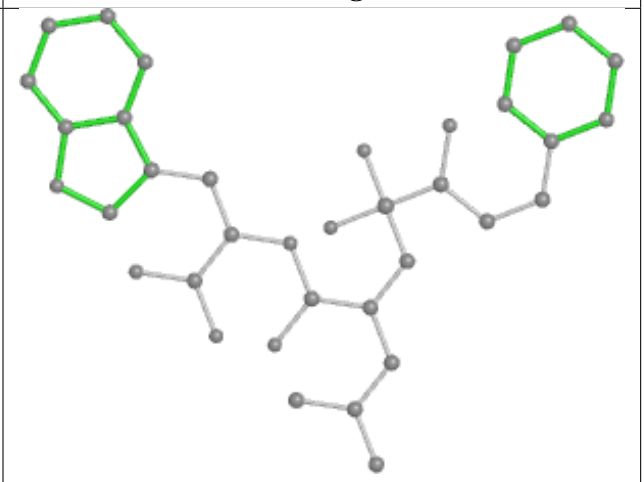
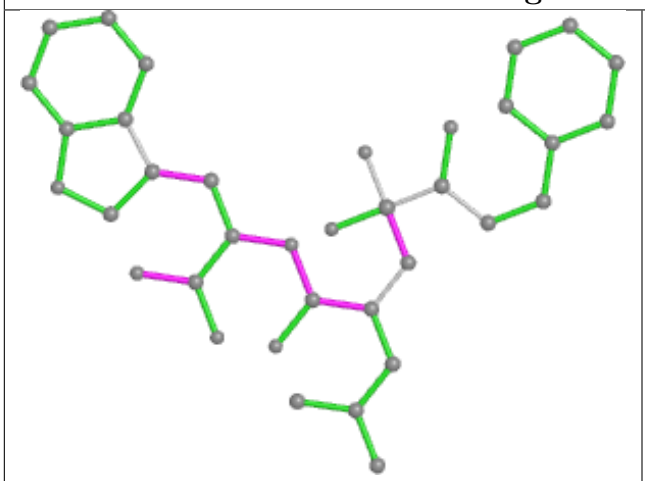


Rings

Ligand P52 E 1003



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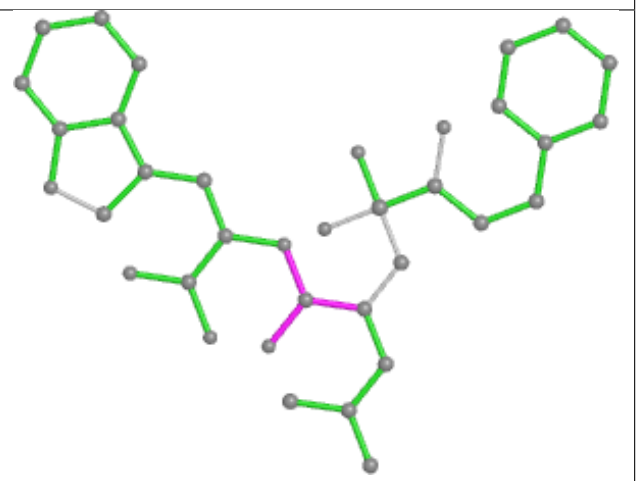

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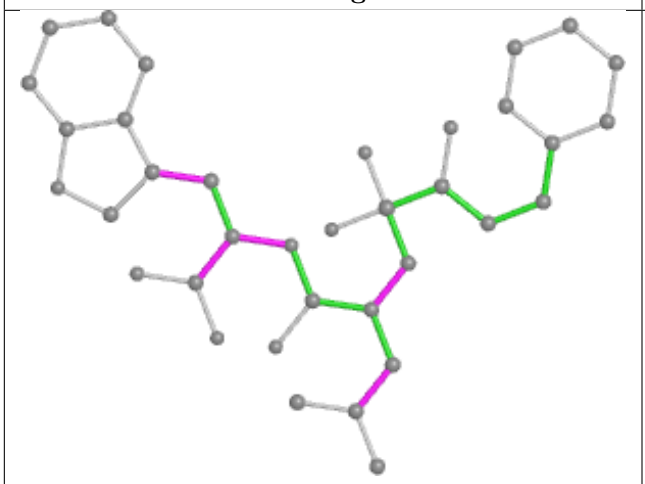

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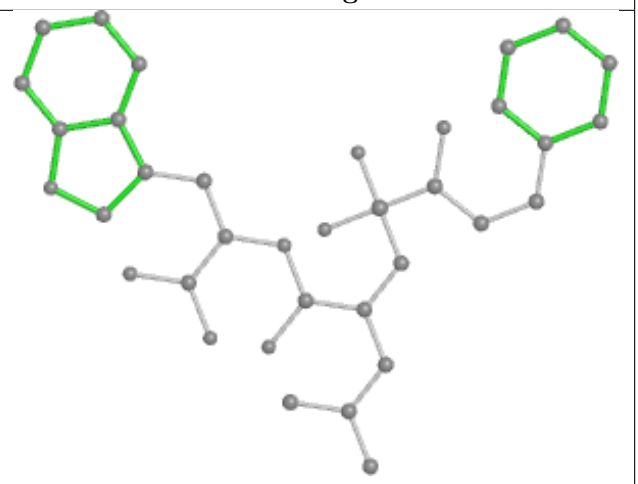
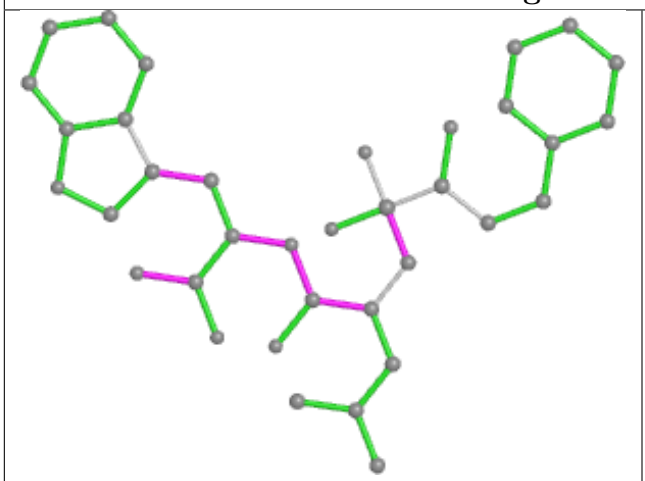


Rings

Ligand P52 C 1002



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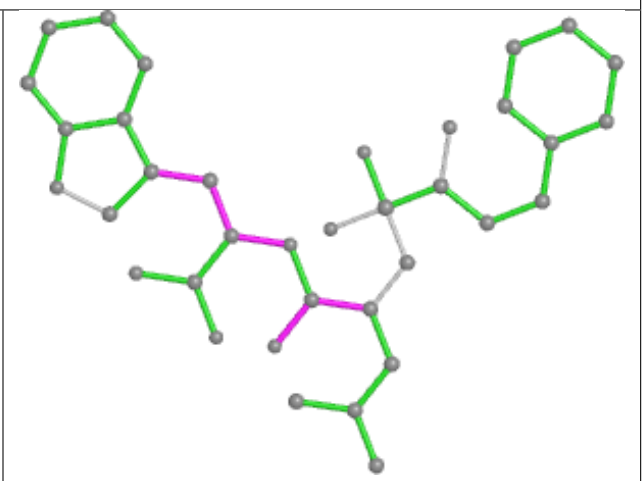

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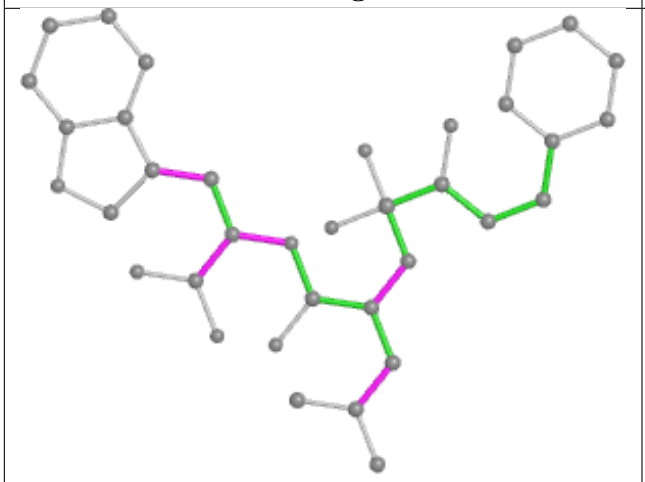

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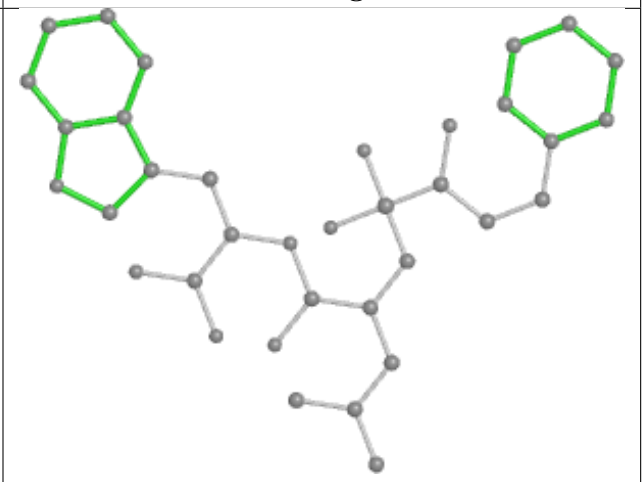

Rings

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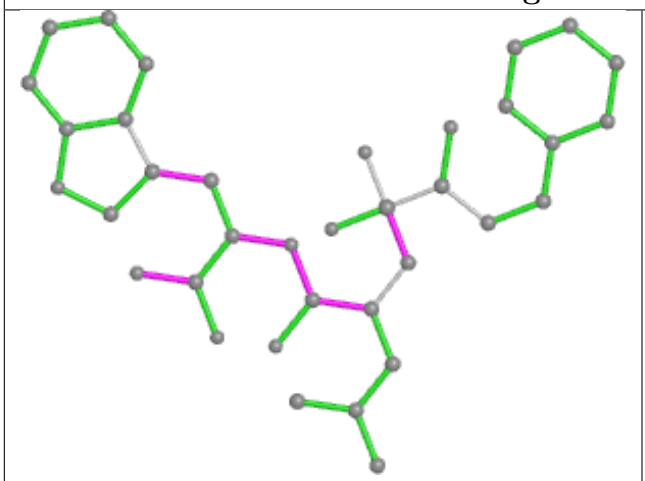

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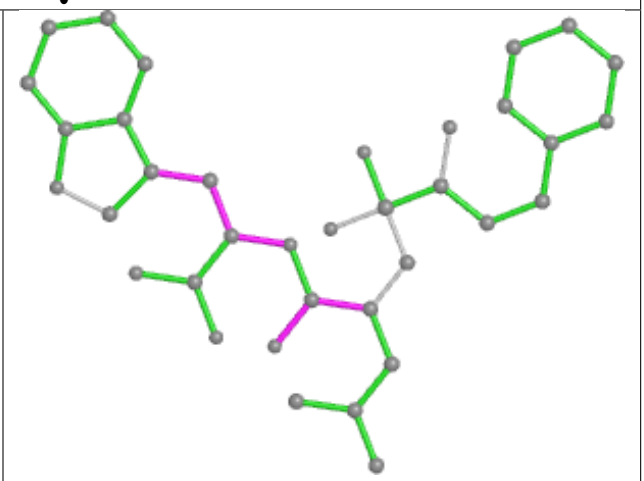

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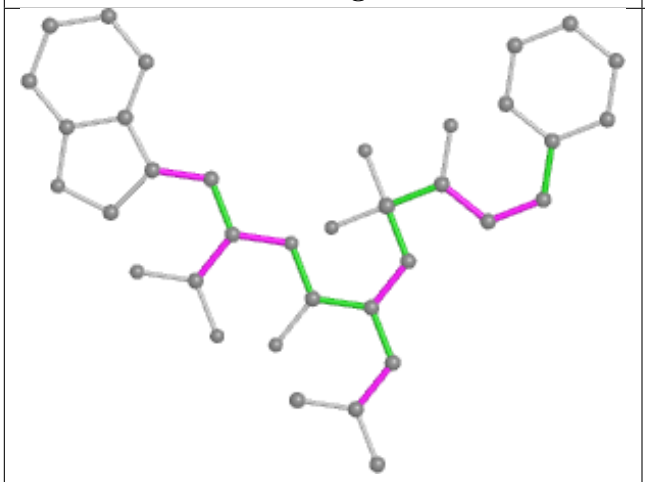

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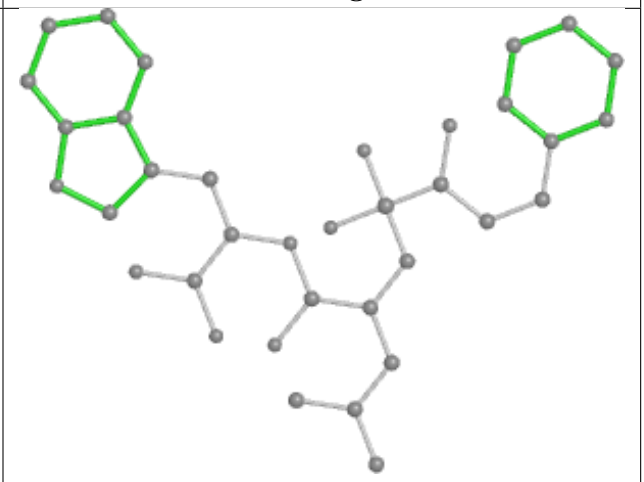
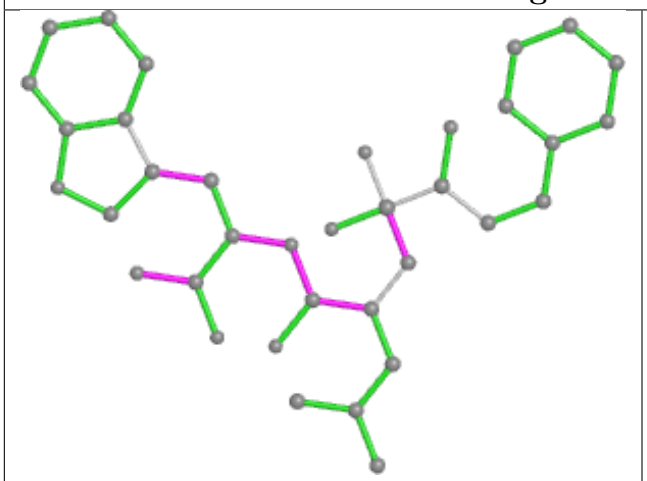


Rings

Ligand P52 I 1003



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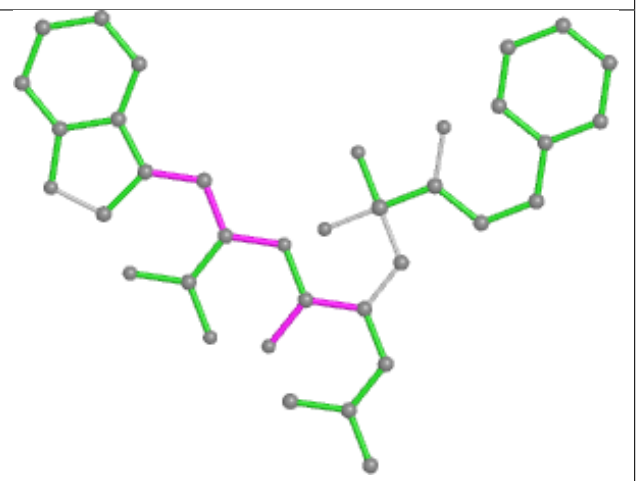

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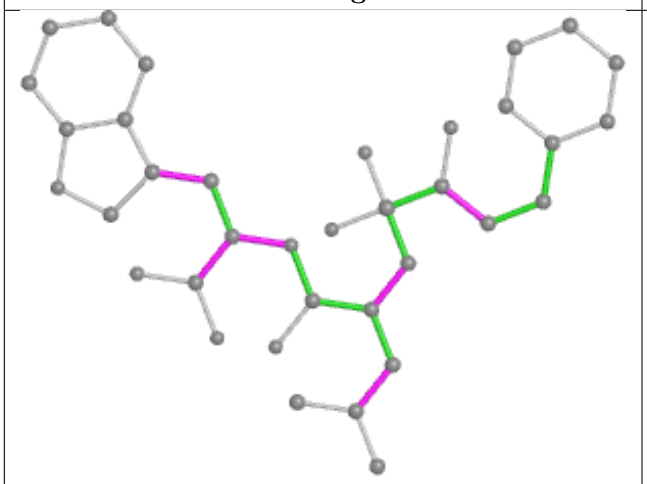

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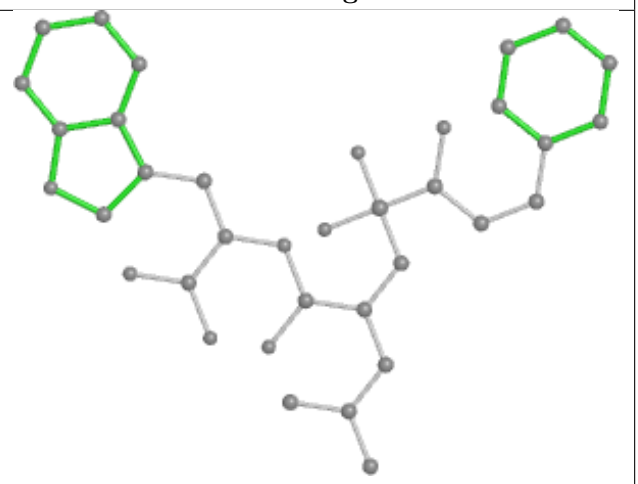
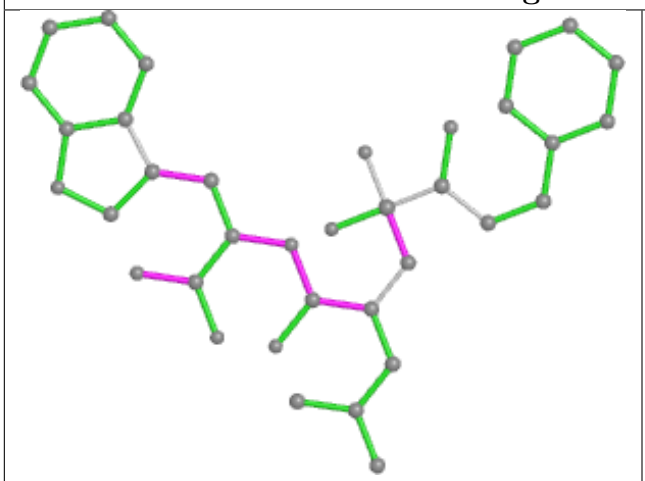


Rings

Ligand P52 V 1002



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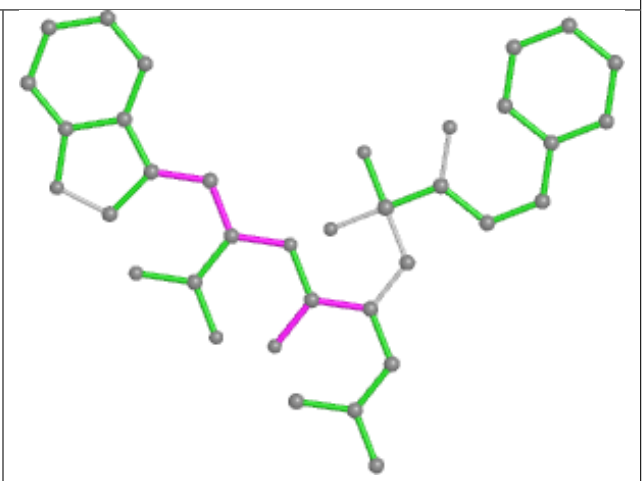

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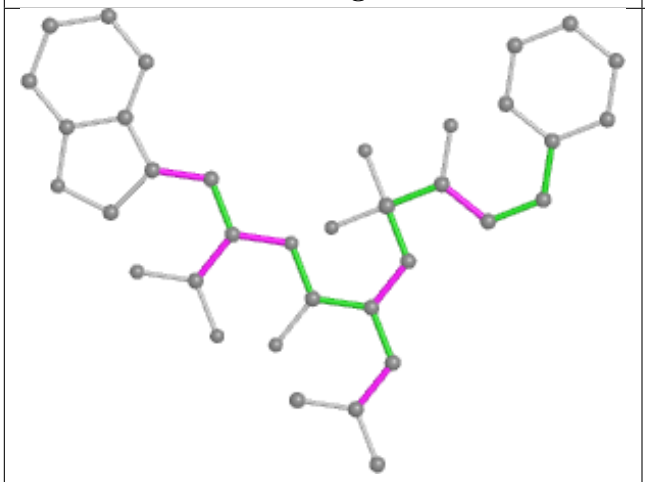

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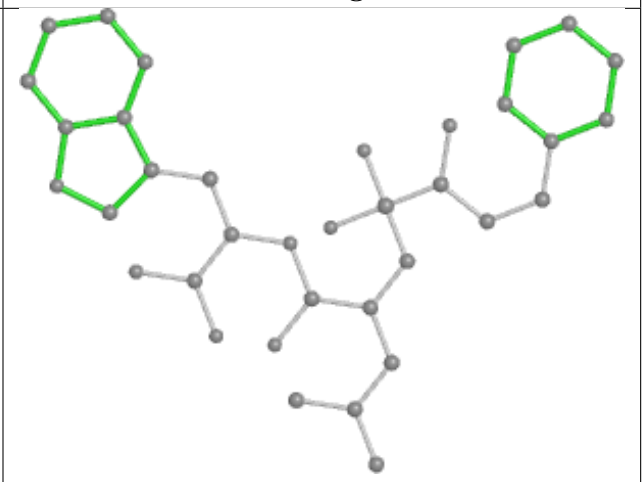
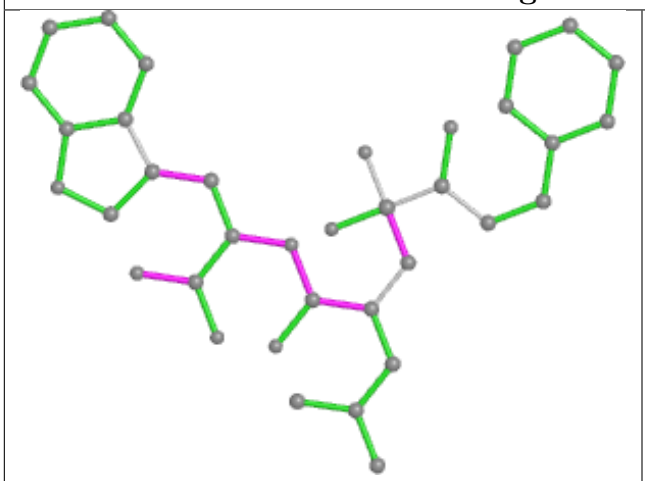


Rings

Ligand P52 M 1003



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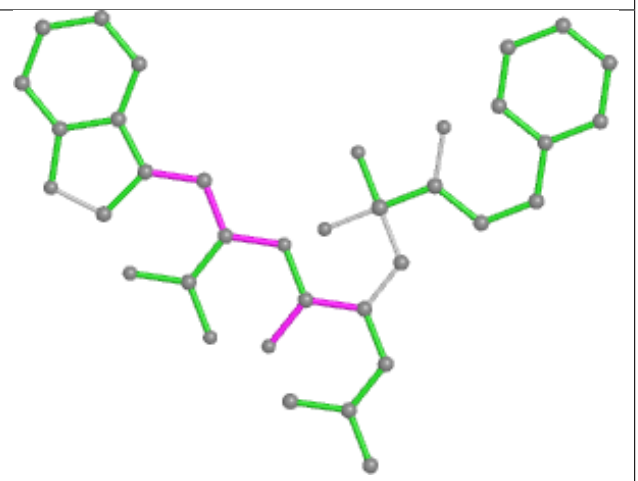

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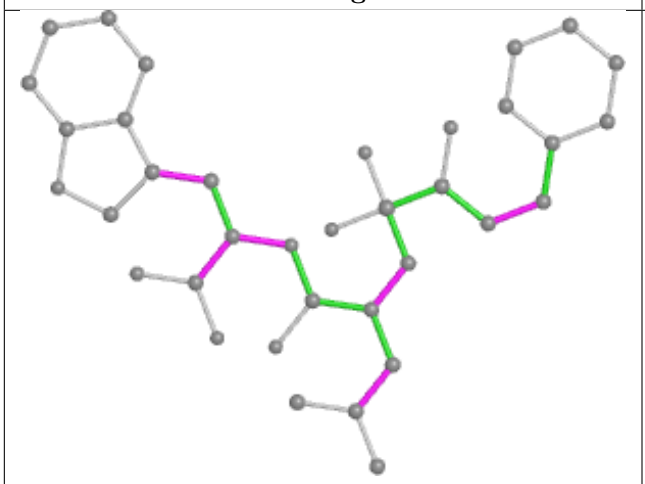

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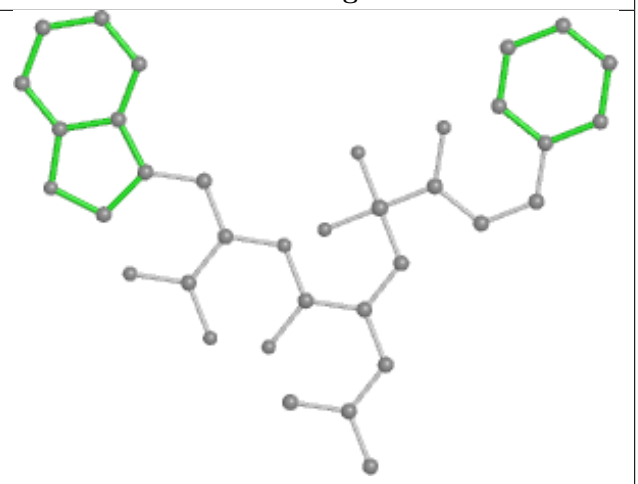

Rings

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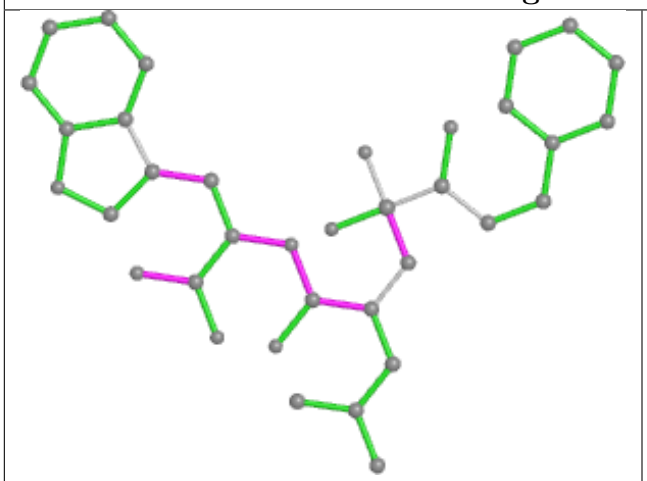

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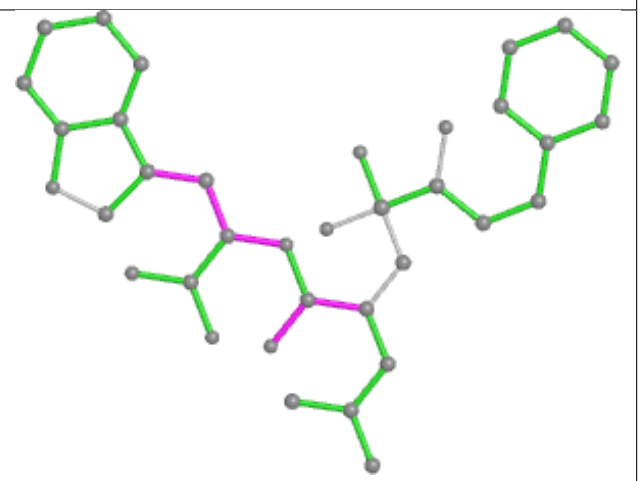

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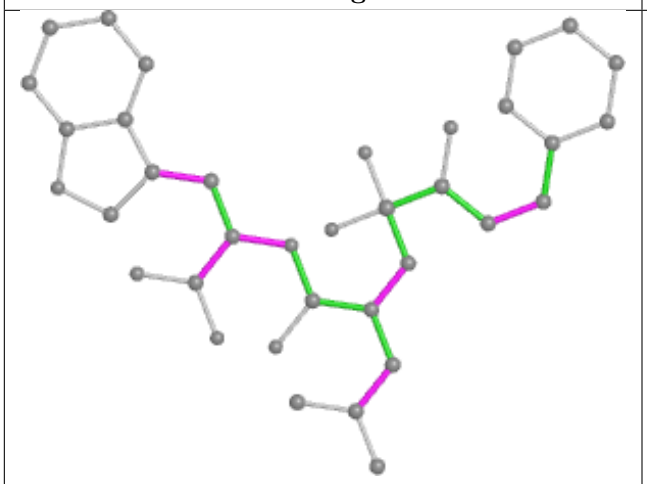

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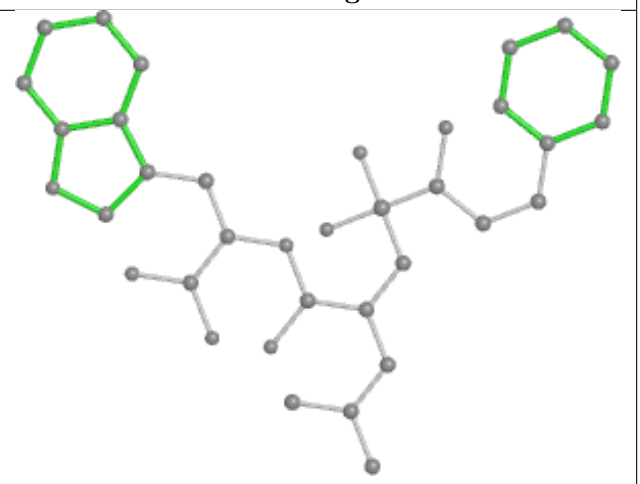
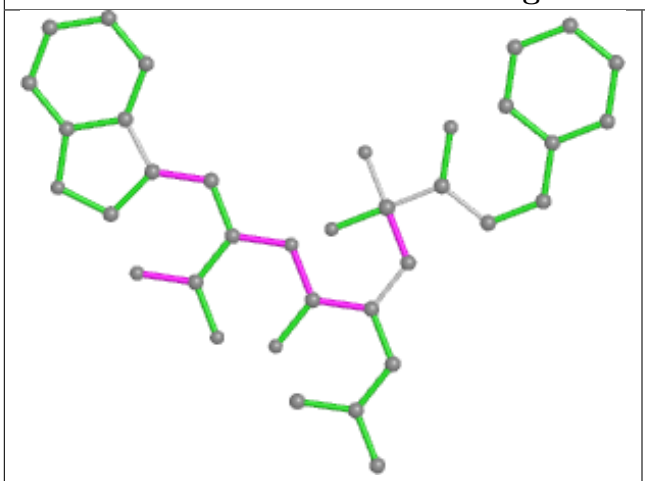


Rings

Ligand P52 U 1003



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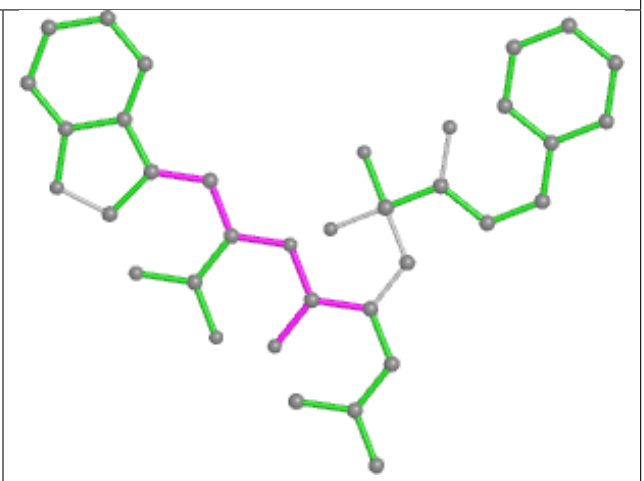

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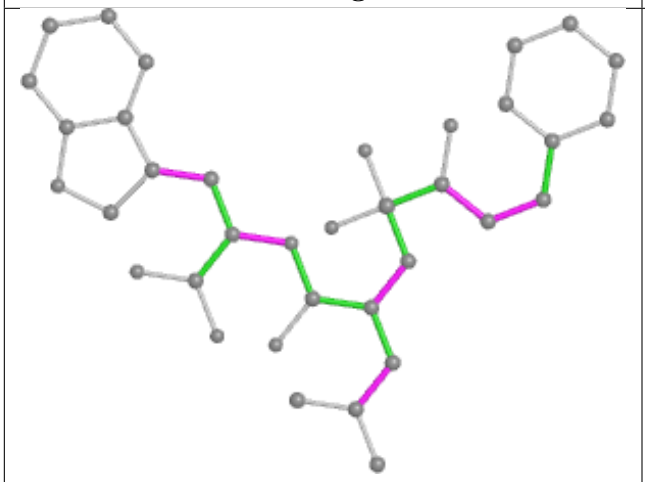

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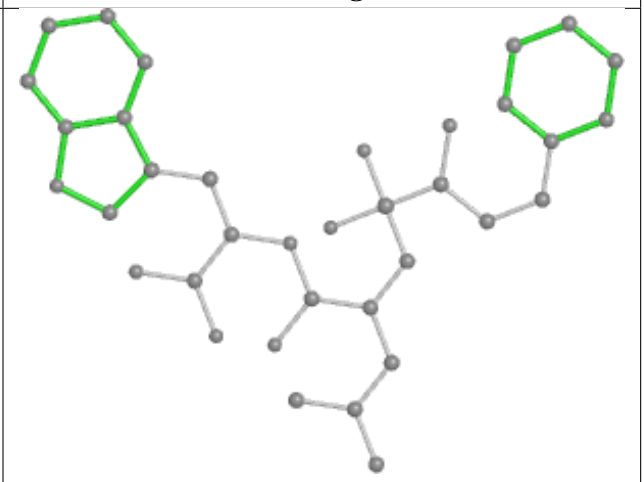
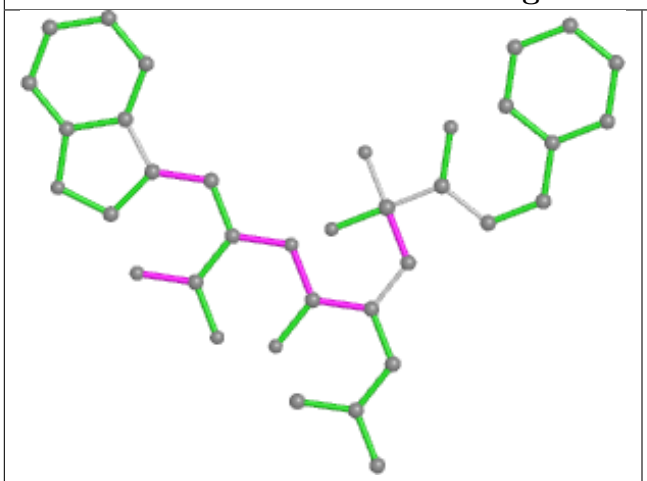


Rings

Ligand P52 N 1003



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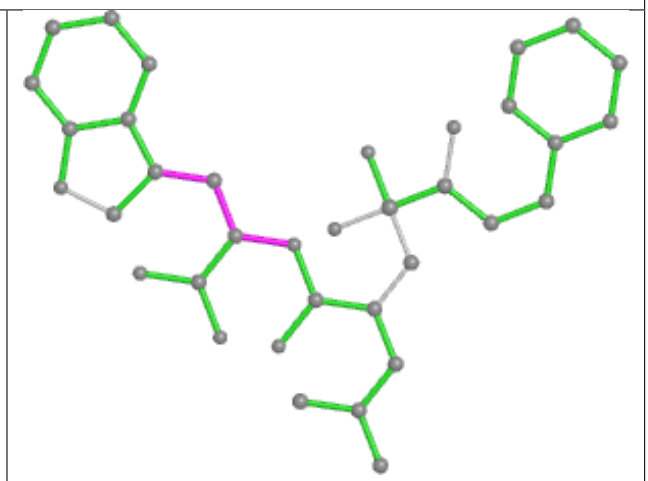

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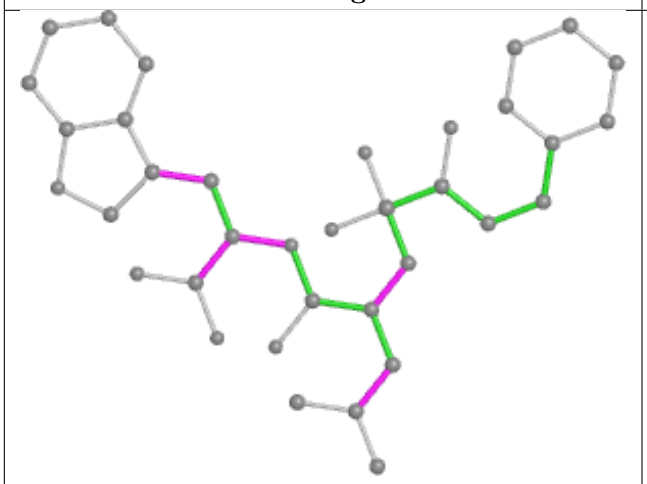

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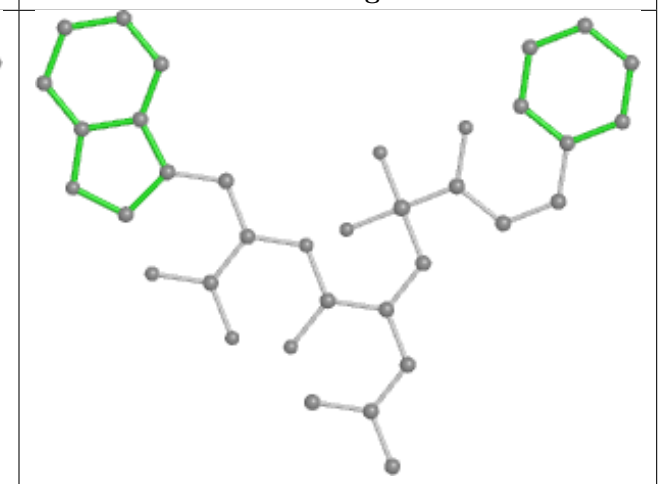

Rings

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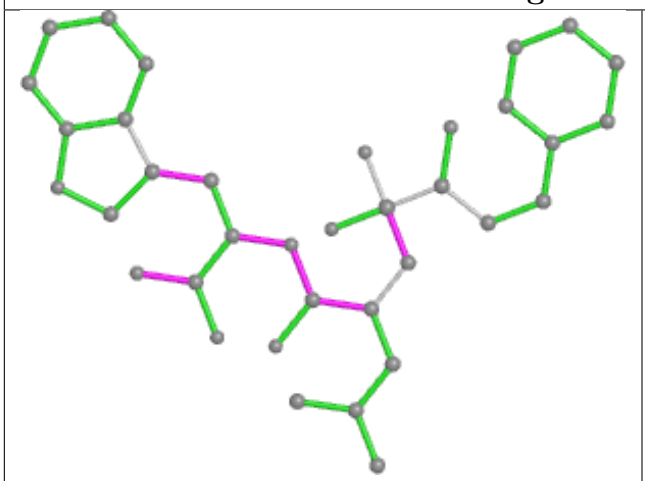

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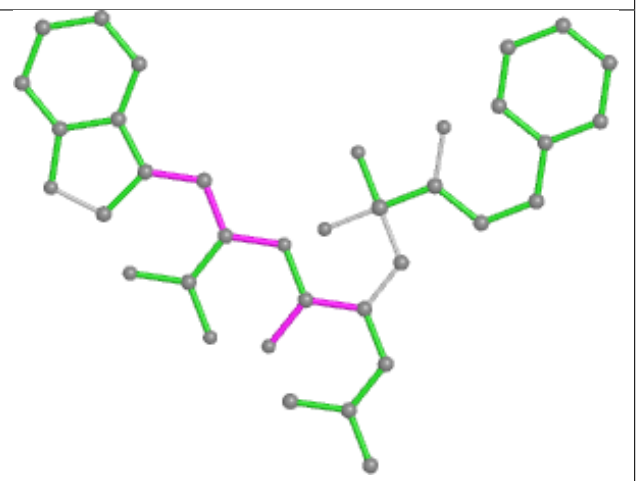

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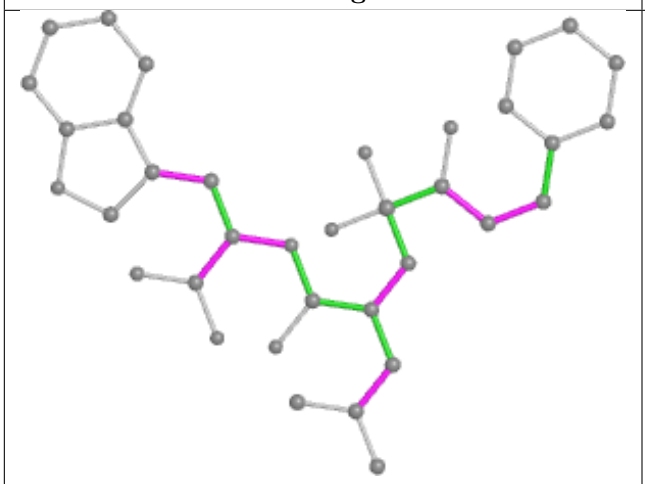

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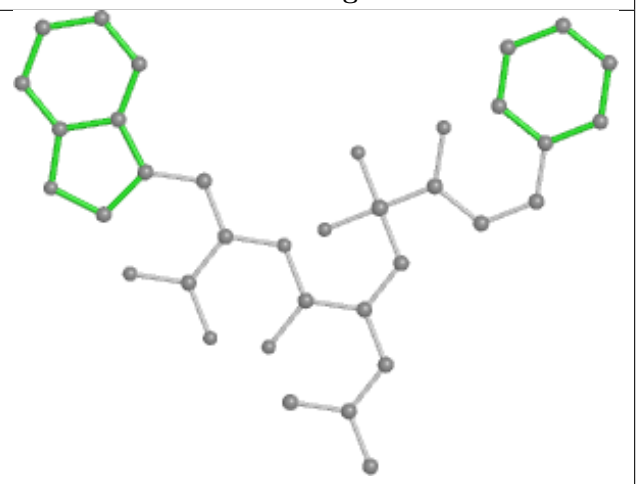
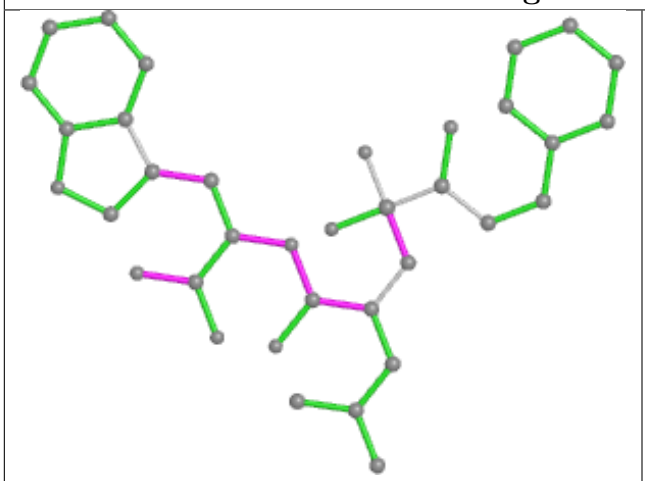


Rings

Ligand P52 O 1002



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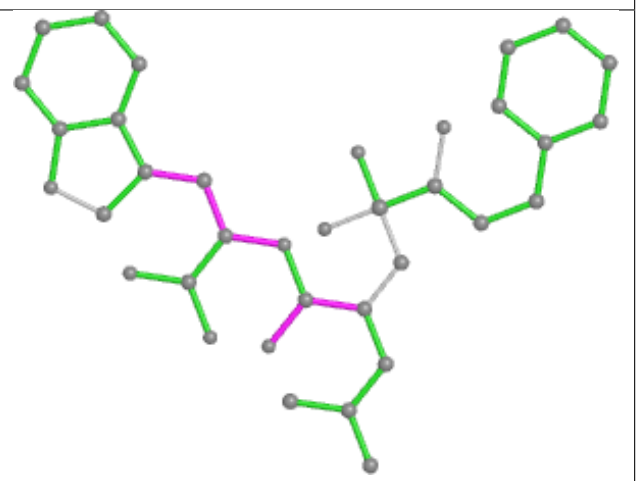
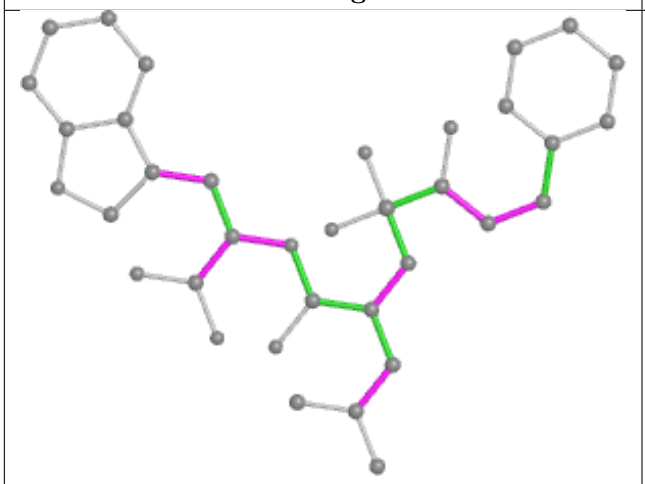
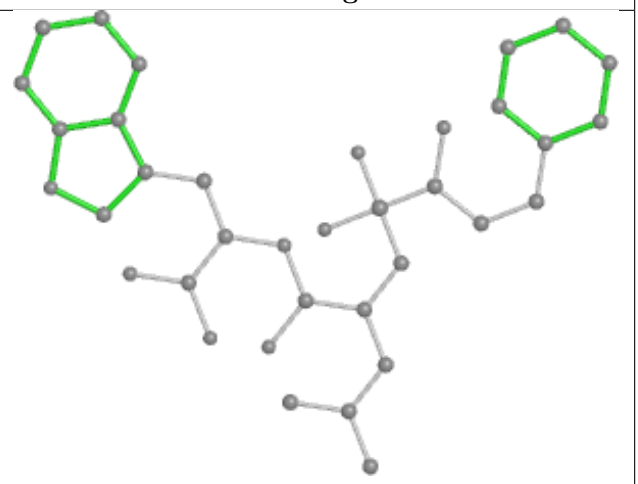


Bond angles

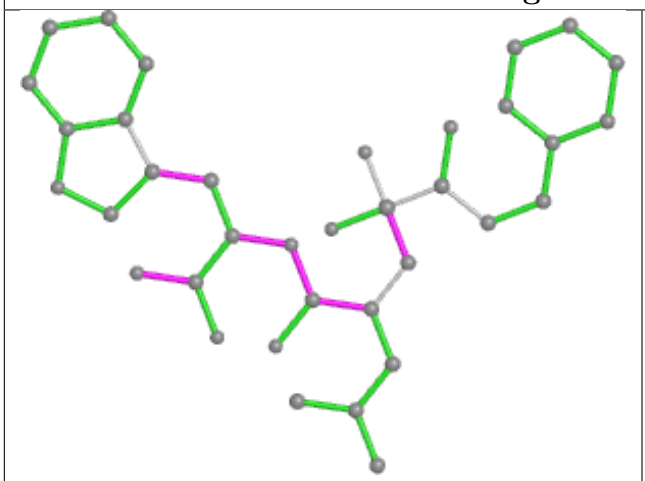


Torsions

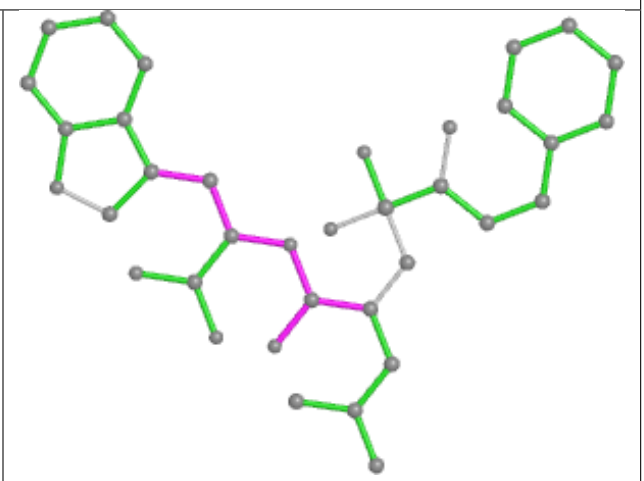


Rings

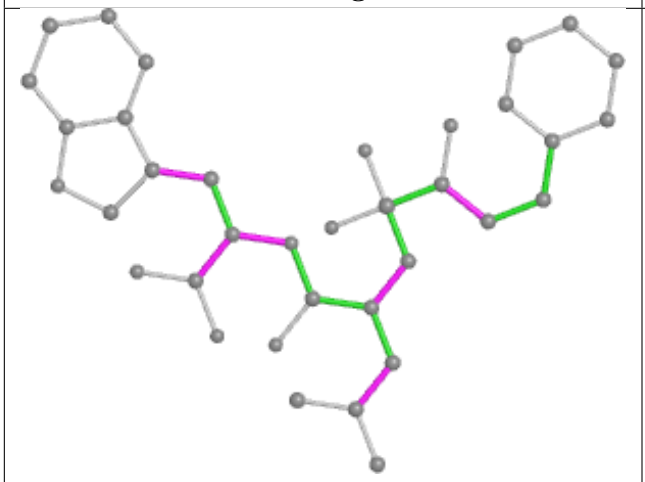
Ligand P52 R 1002



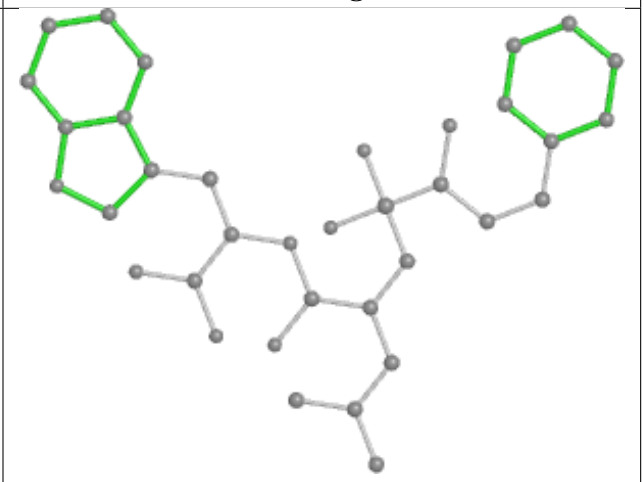
Bond lengths



Bond angles

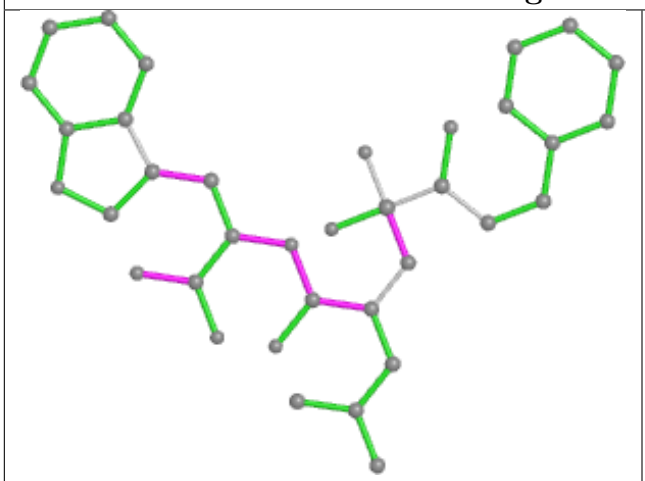


Torsions

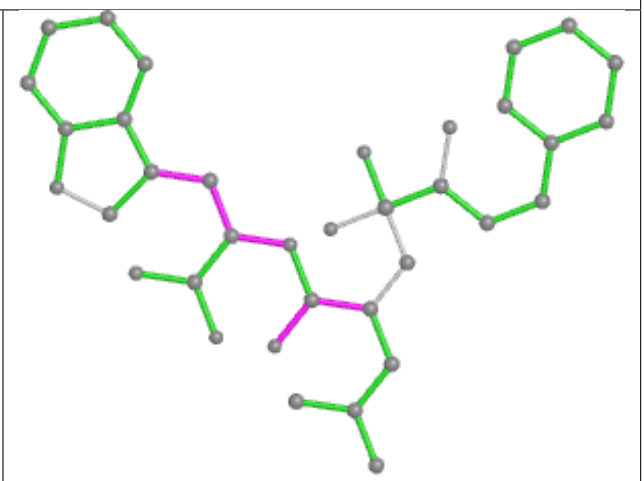


Rings

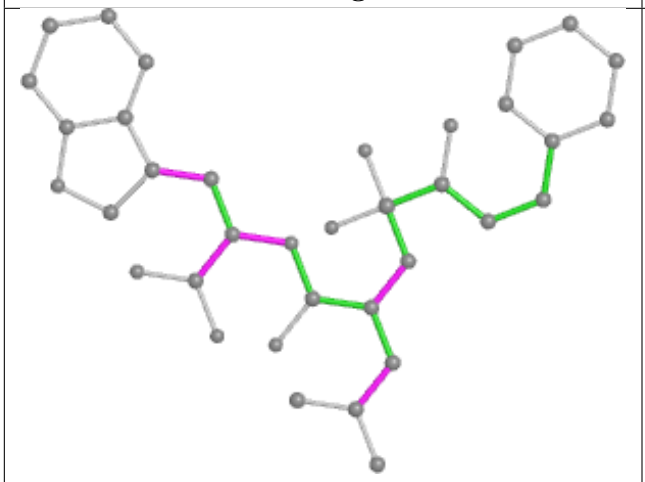
Ligand P52 F 1003



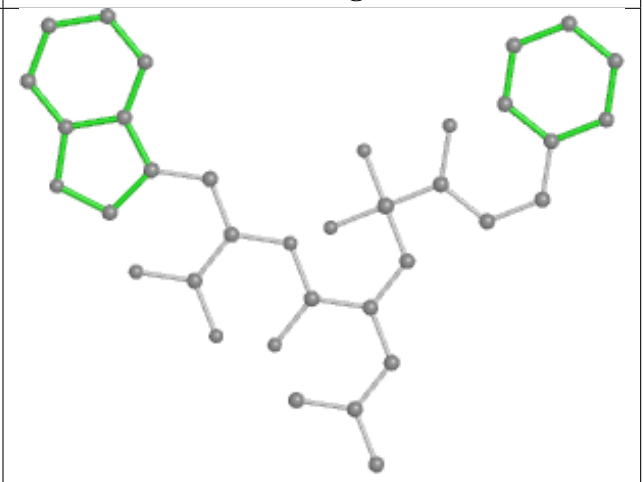
Bond lengths



Bond angles

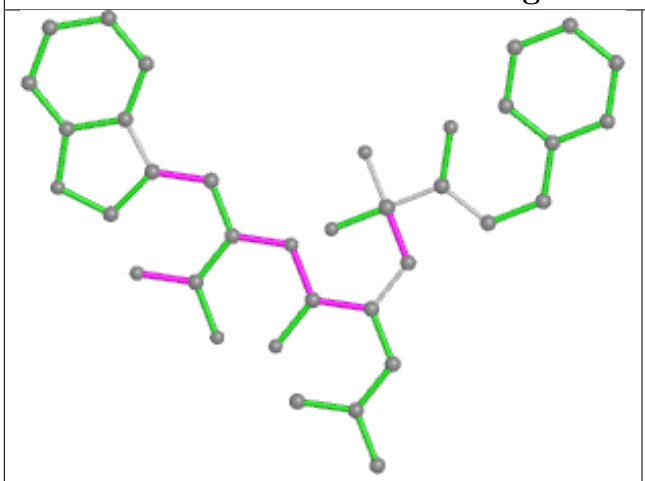


Torsions

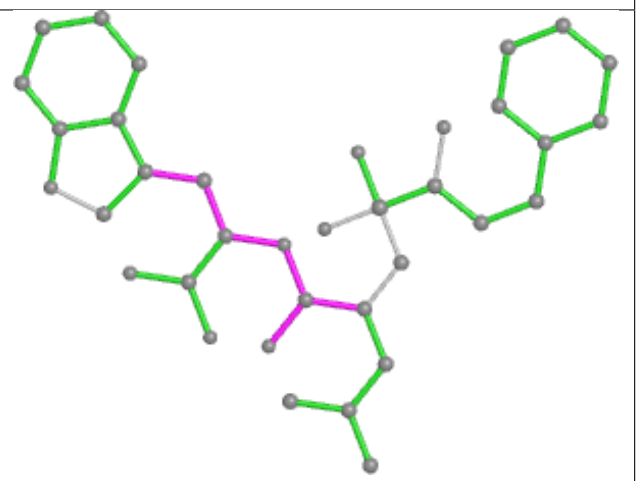


Rings

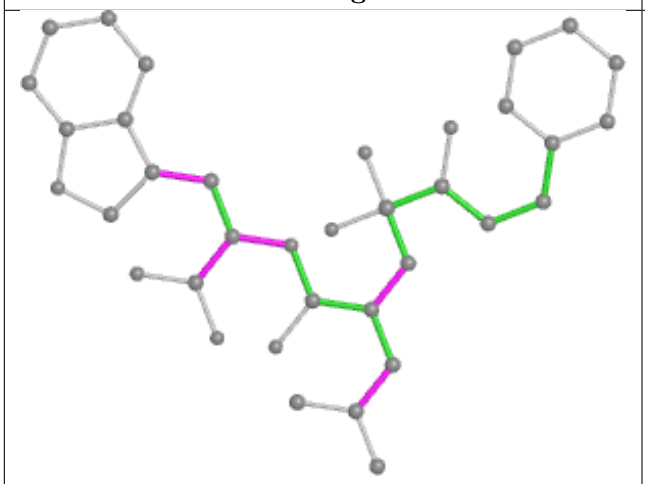
Ligand P52 D 1003



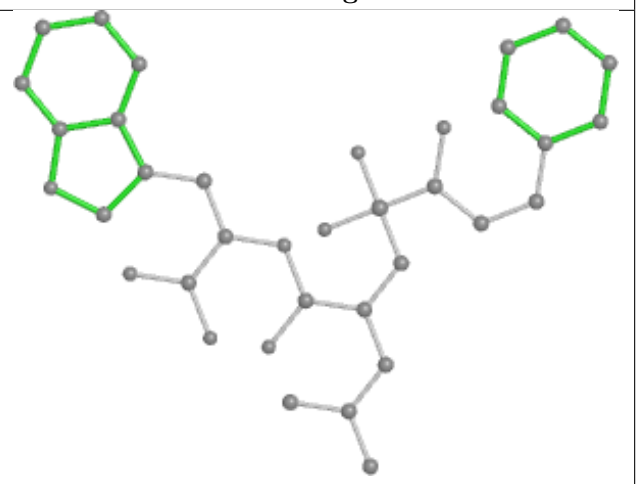
Bond lengths



Bond angles

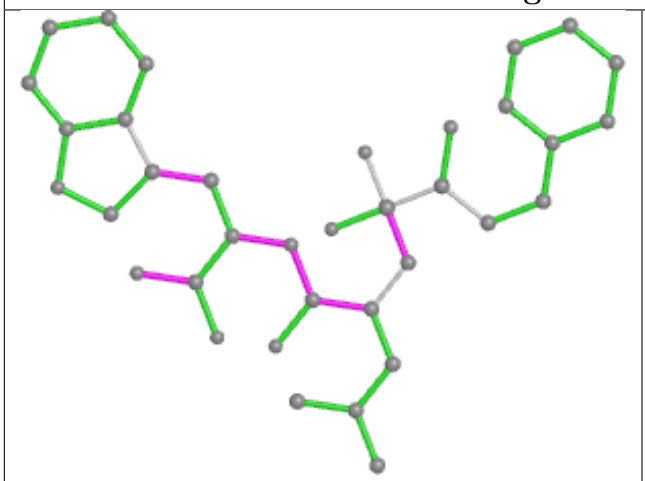


Torsions

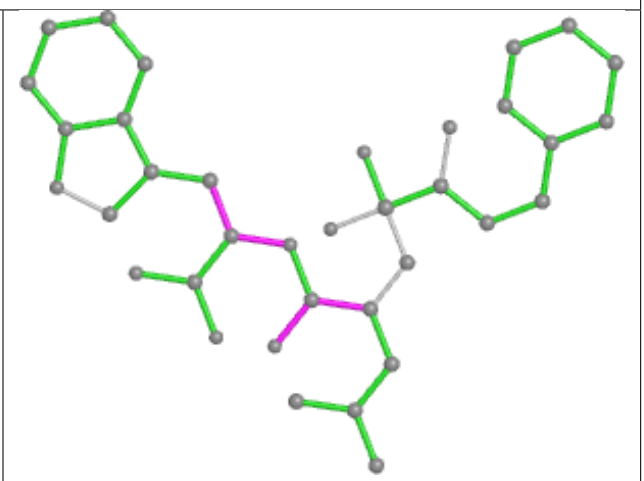


Rings

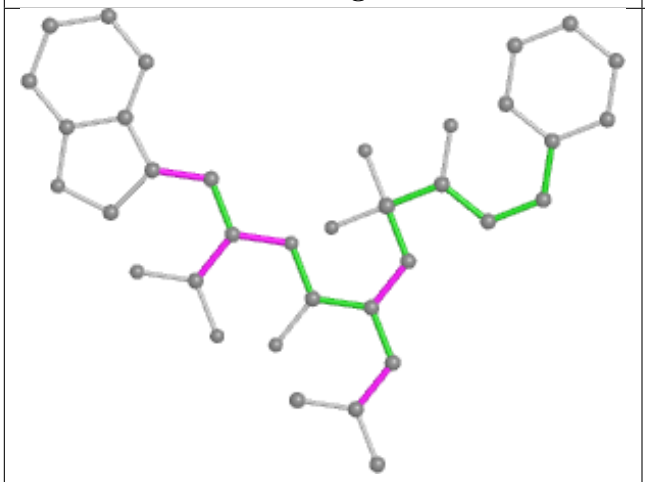
Ligand P52 B 1002



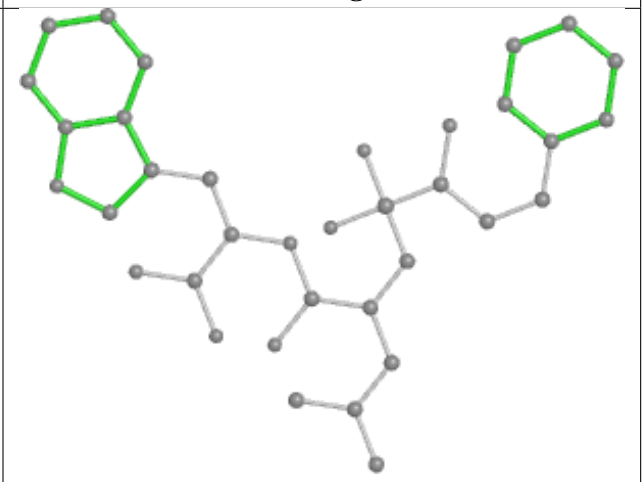
Bond lengths



Bond angles

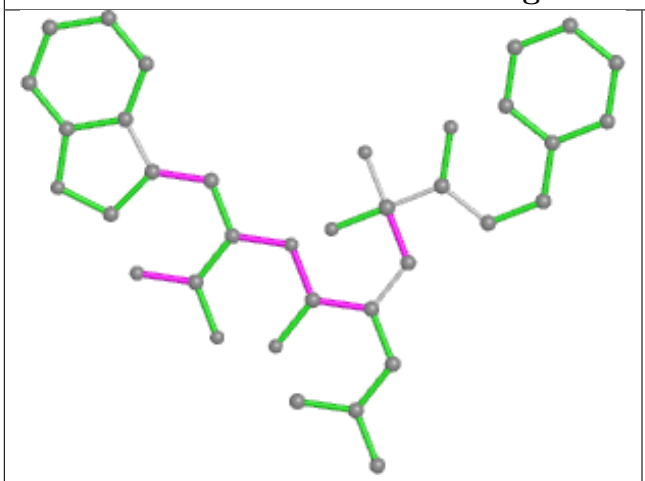


Torsions

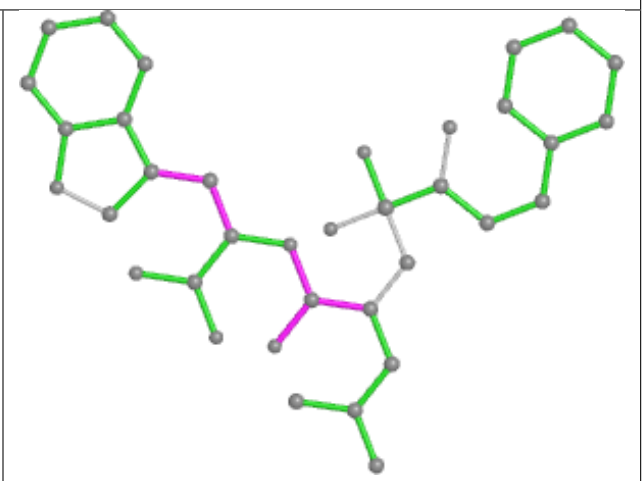


Rings

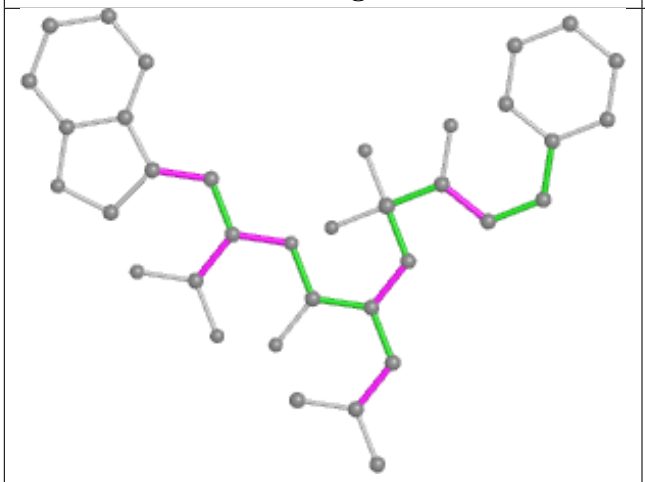
Ligand P52 A 1002



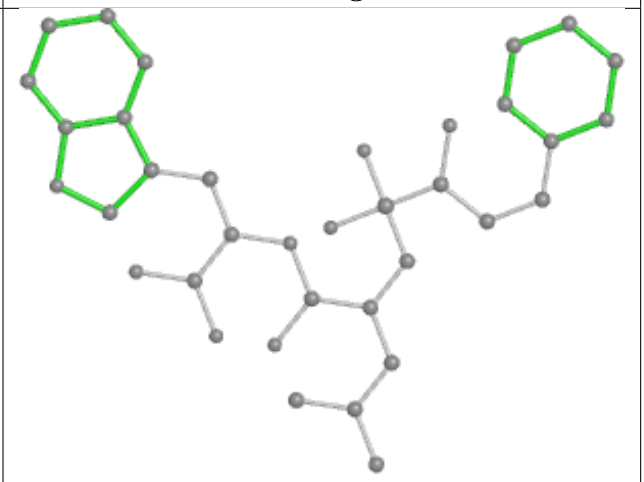
Bond lengths



Bond angles

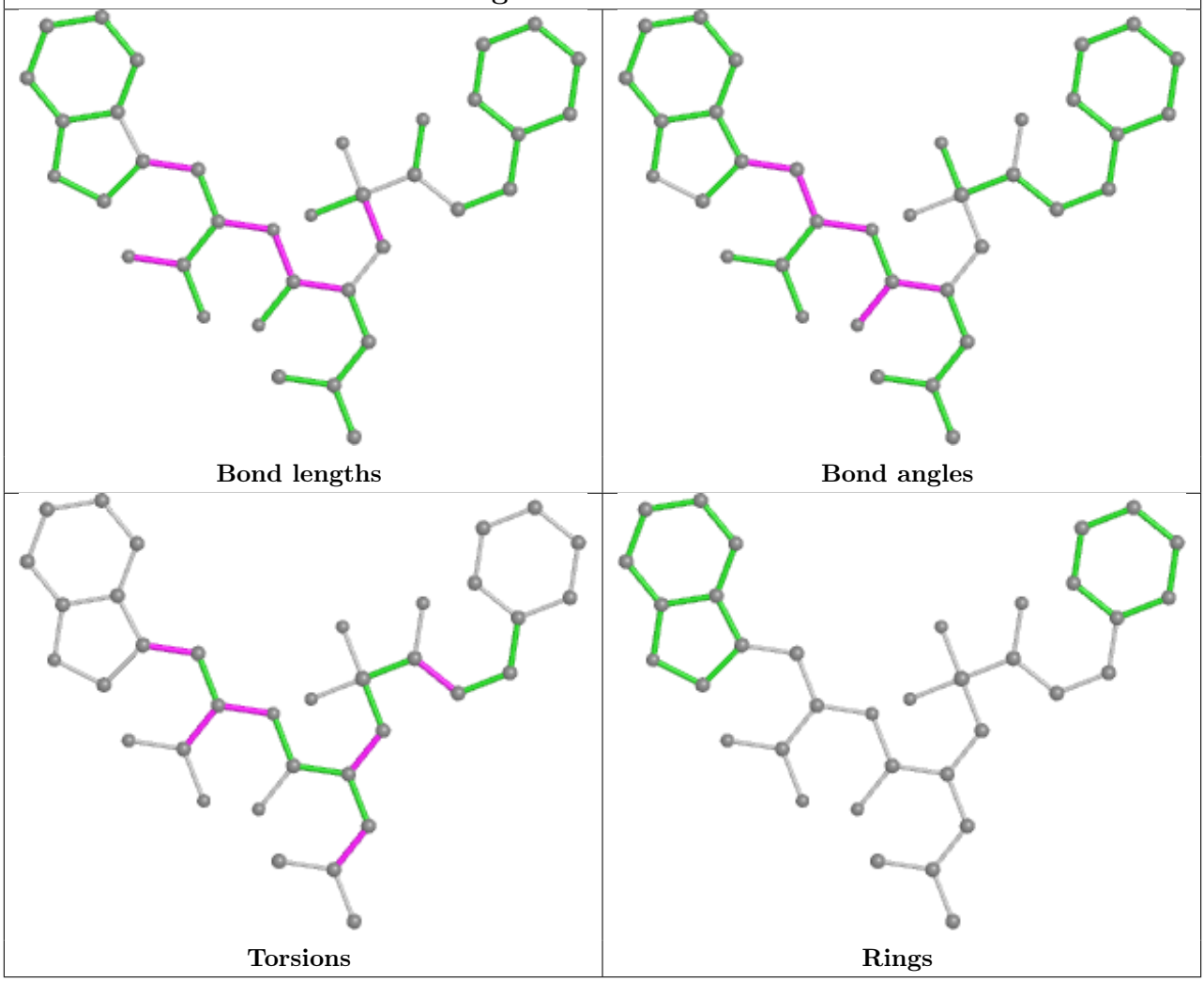


Torsions



Rings

Ligand P52 P 1002



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	861/899 (95%)	-0.16	1 (0%)	95	97	7, 14, 27, 59	0
1	B	861/899 (95%)	-0.08	4 (0%)	91	91	8, 14, 29, 53	0
1	C	861/899 (95%)	-0.10	1 (0%)	95	97	10, 16, 29, 54	0
1	D	861/899 (95%)	-0.09	2 (0%)	95	96	9, 15, 32, 56	0
1	E	861/899 (95%)	-0.11	2 (0%)	95	96	8, 16, 33, 58	0
1	F	861/899 (95%)	-0.07	4 (0%)	91	91	8, 15, 34, 57	0
1	G	861/899 (95%)	-0.06	1 (0%)	95	97	11, 18, 39, 60	0
1	H	861/899 (95%)	-0.06	1 (0%)	95	97	10, 19, 38, 55	0
1	I	861/899 (95%)	0.02	3 (0%)	94	95	21, 31, 40, 68	0
1	J	861/899 (95%)	0.05	4 (0%)	91	91	19, 29, 51, 82	0
1	K	861/899 (95%)	0.09	6 (0%)	87	89	22, 31, 53, 81	0
1	L	861/899 (95%)	0.03	2 (0%)	95	96	16, 28, 50, 68	0
1	M	861/899 (95%)	0.10	3 (0%)	94	95	27, 37, 51, 59	0
1	N	861/899 (95%)	0.31	18 (2%)	63	62	34, 50, 73, 88	0
1	O	861/899 (95%)	0.21	14 (1%)	72	70	29, 42, 67, 89	0
1	P	861/899 (95%)	0.35	25 (2%)	51	51	40, 55, 69, 78	0
1	Q	861/899 (95%)	0.34	21 (2%)	59	57	35, 51, 73, 95	0
1	R	861/899 (95%)	0.41	30 (3%)	44	42	40, 53, 79, 101	0
1	S	861/899 (95%)	0.68	57 (6%)	18	19	61, 74, 85, 94	0
1	T	861/899 (95%)	0.69	61 (7%)	16	17	58, 73, 84, 95	0
1	U	861/899 (95%)	0.66	52 (6%)	21	22	54, 71, 82, 96	0
1	V	861/899 (95%)	0.76	73 (8%)	10	11	59, 79, 89, 100	0
All	All	18942/19778 (95%)	0.18	385 (2%)	65	64	7, 34, 79, 101	0

All (385) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	487	GLY	8.8
1	V	110	GLY	5.0
1	V	718[A]	CYS	4.7
1	Q	915	ARG	4.3
1	T	103	SER	4.3
1	S	724	GLY	4.3
1	Q	566	LEU	4.2
1	K	489	GLY	4.2
1	V	757	TRP	4.2
1	U	910	SER	4.1
1	T	488	GLY	4.0
1	U	487	GLY	3.9
1	T	102	ILE	3.9
1	N	110	GLY	3.9
1	S	69	ALA	3.9
1	J	489	GLY	3.9
1	S	110	GLY	3.9
1	U	915	ARG	3.8
1	V	108	ARG	3.8
1	O	118	GLU	3.7
1	N	488	GLY	3.7
1	U	193	CYS	3.7
1	J	487	GLY	3.7
1	T	879	GLN	3.6
1	N	489	GLY	3.6
1	S	106	THR	3.6
1	S	597	GLY	3.5
1	R	588	GLU	3.5
1	V	192	PRO	3.5
1	O	487	GLY	3.5
1	Q	569	GLU	3.5
1	S	103	SER	3.4
1	U	135	ALA	3.4
1	O	489	GLY	3.4
1	R	915	ARG	3.4
1	Q	489	GLY	3.3
1	U	123	LEU	3.3
1	S	592	TRP	3.3
1	T	110	GLY	3.3
1	F	487	GLY	3.3
1	V	841	LEU	3.3
1	T	446	ASN	3.3
1	Q	910	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	R	486	GLY	3.3
1	R	488	GLY	3.3
1	S	104	ARG	3.3
1	T	489	GLY	3.2
1	Q	570	VAL	3.2
1	J	488	GLY	3.2
1	G	489	GLY	3.2
1	S	581	GLY	3.2
1	I	489	GLY	3.2
1	R	518	HIS	3.2
1	U	93	ILE	3.2
1	U	488	GLY	3.1
1	U	842	GLY	3.1
1	Q	89	PRO	3.1
1	V	724	GLY	3.1
1	V	91	SER	3.1
1	S	541	PRO	3.1
1	S	135	ALA	3.1
1	V	488	GLY	3.1
1	V	480	ASP	3.1
1	S	915	ARG	3.1
1	V	756	GLY	3.1
1	Q	519	MET	3.1
1	T	915	ARG	3.0
1	U	724	GLY	3.0
1	V	904	ILE	3.0
1	V	103	SER	3.0
1	U	147	VAL	3.0
1	T	604	THR	3.0
1	U	841	LEU	3.0
1	T	149	ILE	2.9
1	U	758	ASP	2.9
1	T	99	HIS	2.9
1	V	119	PRO	2.9
1	T	69	ALA	2.9
1	T	433	PHE	2.9
1	T	257	VAL	2.9
1	S	512	VAL	2.9
1	V	116	SER	2.9
1	Q	116	SER	2.9
1	V	118	GLU	2.9
1	U	92	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	V	228	ALA	2.8
1	R	121	GLN	2.8
1	V	778	PHE	2.8
1	S	858	SER	2.8
1	F	488	GLY	2.8
1	T	131	ILE	2.8
1	S	533	ASP	2.8
1	B	487	GLY	2.8
1	S	152	ALA	2.8
1	V	154	ASN	2.8
1	P	485	ILE	2.8
1	U	124	GLU	2.8
1	U	100	LEU	2.8
1	T	757	TRP	2.8
1	N	122	VAL	2.8
1	R	687	ASP	2.8
1	V	77[A]	TRP	2.8
1	V	123	LEU	2.8
1	Q	121	GLN	2.7
1	S	170	LYS	2.7
1	S	517	VAL	2.7
1	V	711[A]	CYS	2.7
1	K	490	VAL	2.7
1	S	190	ALA	2.7
1	S	746	VAL	2.7
1	U	299	ILE	2.7
1	S	572	TRP	2.7
1	R	489	GLY	2.7
1	T	479	TRP	2.7
1	S	373	TRP	2.7
1	D	116	SER	2.7
1	T	684	ASP	2.7
1	U	470	TYR	2.7
1	N	123	LEU	2.7
1	T	144	PRO	2.7
1	Q	134	LEU	2.7
1	B	488	GLY	2.7
1	V	482	MET	2.7
1	V	93	ILE	2.7
1	S	733	ASN	2.7
1	S	486	GLY	2.6
1	V	197	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	U	723	GLU	2.6
1	V	99	HIS	2.6
1	R	492	VAL	2.6
1	L	154	ASN	2.6
1	P	59	ILE	2.6
1	Q	105	ALA	2.6
1	L	489	GLY	2.6
1	P	369	TRP	2.6
1	R	512	VAL	2.6
1	V	230	GLY	2.6
1	I	490	VAL	2.6
1	T	756	GLY	2.6
1	N	58	VAL	2.6
1	U	779	ALA	2.6
1	P	858	SER	2.6
1	S	234	ASP	2.6
1	U	489	GLY	2.6
1	D	915	ARG	2.5
1	O	490	VAL	2.5
1	R	513	ARG	2.5
1	N	915	ARG	2.5
1	S	172	GLY	2.5
1	V	709	LEU	2.5
1	V	179	SER	2.5
1	R	92	THR	2.5
1	U	73	THR	2.5
1	U	854	THR	2.5
1	T	107	LEU	2.5
1	O	93	ILE	2.5
1	V	439	ASP	2.5
1	V	158	THR	2.5
1	P	488	GLY	2.5
1	M	228	ALA	2.5
1	U	82	VAL	2.5
1	P	185	THR	2.5
1	S	561	THR	2.5
1	N	83	GLU	2.5
1	P	718[A]	CYS	2.5
1	T	840	GLU	2.5
1	T	434	ASP	2.5
1	P	725	TYR	2.5
1	U	133	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	136	PRO	2.5
1	V	615	ILE	2.5
1	T	482	MET	2.5
1	A	488	GLY	2.5
1	R	448	LEU	2.5
1	R	913	LEU	2.5
1	Q	439	ASP	2.5
1	R	479	TRP	2.4
1	S	563	VAL	2.4
1	P	487	GLY	2.4
1	H	915	ARG	2.4
1	T	705	GLN	2.4
1	U	183	GLU	2.4
1	Q	110	GLY	2.4
1	T	190	ALA	2.4
1	V	723	GLU	2.4
1	B	489	GLY	2.4
1	S	77[A]	TRP	2.4
1	U	726	PHE	2.4
1	V	58	VAL	2.4
1	P	93	ILE	2.4
1	O	134	LEU	2.4
1	S	372	LEU	2.4
1	P	489	GLY	2.4
1	V	92	THR	2.4
1	R	152	ALA	2.4
1	V	444	ILE	2.4
1	S	283	LEU	2.4
1	F	489	GLY	2.4
1	Q	72	THR	2.4
1	U	192	PRO	2.4
1	V	249	PHE	2.4
1	V	853	THR	2.4
1	T	105	ALA	2.4
1	U	880	LEU	2.4
1	R	897	MET	2.4
1	V	555	PHE	2.4
1	U	95	LEU	2.4
1	R	116	SER	2.4
1	V	105	ALA	2.4
1	U	512	VAL	2.4
1	S	159	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	U	621	LEU	2.4
1	I	110	GLY	2.3
1	N	914	GLU	2.3
1	P	51	LYS	2.3
1	R	593	ASP	2.3
1	S	840	GLU	2.3
1	N	86	ALA	2.3
1	T	87	SER	2.3
1	S	191	PHE	2.3
1	T	747	PHE	2.3
1	S	134	LEU	2.3
1	U	485	ILE	2.3
1	S	68	HIS	2.3
1	T	525	MET	2.3
1	V	848	HIS	2.3
1	P	72	THR	2.3
1	U	673	GLN	2.3
1	S	388	SER	2.3
1	R	597	GLY	2.3
1	V	897	MET	2.3
1	V	478	LEU	2.3
1	R	490	VAL	2.3
1	V	49	TRP	2.3
1	P	69	ALA	2.3
1	E	488	GLY	2.3
1	S	369	TRP	2.3
1	R	589	ASP	2.3
1	V	487	GLY	2.3
1	Q	124	GLU	2.3
1	N	93	ILE	2.3
1	O	848	HIS	2.3
1	N	69	ALA	2.3
1	T	570	VAL	2.3
1	V	729	TRP	2.3
1	M	488	GLY	2.3
1	S	129	GLU	2.3
1	U	561	THR	2.3
1	V	107	LEU	2.3
1	V	437	SER	2.3
1	S	105	ALA	2.3
1	T	77[A]	TRP	2.3
1	T	583	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	V	830	LYS	2.3
1	K	171	GLU	2.3
1	R	741	ASP	2.3
1	V	155	LEU	2.3
1	S	526	LYS	2.3
1	T	67	ILE	2.3
1	N	92	THR	2.2
1	P	169	THR	2.2
1	T	65	LEU	2.2
1	T	148	VAL	2.2
1	V	387	VAL	2.2
1	O	139	LEU	2.2
1	T	707	LEU	2.2
1	P	684	ASP	2.2
1	S	405	PHE	2.2
1	V	311	ILE	2.2
1	T	765	GLN	2.2
1	S	484	SER	2.2
1	T	147	VAL	2.2
1	N	119	PRO	2.2
1	T	440	LYS	2.2
1	V	329	GLU	2.2
1	S	711[A]	CYS	2.2
1	T	372	LEU	2.2
1	T	736	LEU	2.2
1	N	94	ILE	2.2
1	O	149	ILE	2.2
1	O	512	VAL	2.2
1	P	152	ALA	2.2
1	S	341	ALA	2.2
1	U	566	LEU	2.2
1	U	775	GLN	2.2
1	T	191	PHE	2.2
1	T	683	ARG	2.2
1	V	572	TRP	2.2
1	V	767	SER	2.2
1	Q	488	GLY	2.2
1	V	618	ALA	2.2
1	V	526	LYS	2.2
1	K	749	VAL	2.2
1	S	579	MET	2.2
1	Q	103	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	T	116	SER	2.2
1	V	781	CYS	2.2
1	R	473	THR	2.2
1	U	565	ILE	2.2
1	M	489	GLY	2.2
1	V	417	HIS	2.2
1	V	713	HIS	2.2
1	S	501	LEU	2.2
1	B	490	VAL	2.2
1	U	131	ILE	2.2
1	T	85	THR	2.2
1	T	760	LEU	2.1
1	U	88	GLN	2.1
1	V	910	SER	2.1
1	P	171	GLU	2.1
1	V	131	ILE	2.1
1	K	488	GLY	2.1
1	P	356	ALA	2.1
1	T	606	VAL	2.1
1	V	759	PHE	2.1
1	O	124	GLU	2.1
1	E	487	GLY	2.1
1	U	877	GLY	2.1
1	P	738	LEU	2.1
1	T	270	TYR	2.1
1	U	729	TRP	2.1
1	S	485	ILE	2.1
1	V	731	GLU	2.1
1	N	737	SER	2.1
1	P	170	LYS	2.1
1	Q	555	PHE	2.1
1	V	571	GLU	2.1
1	T	781	CYS	2.1
1	T	723	GLU	2.1
1	R	85	THR	2.1
1	S	910	SER	2.1
1	T	327	TYR	2.1
1	U	57	TYR	2.1
1	J	490	VAL	2.1
1	S	719	VAL	2.1
1	K	487	GLY	2.1
1	O	482	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	V	678	LEU	2.1
1	V	738	LEU	2.1
1	V	505	PHE	2.1
1	U	388	SER	2.1
1	Q	517	VAL	2.1
1	V	227	VAL	2.1
1	U	384	PHE	2.1
1	O	492	VAL	2.1
1	U	139	LEU	2.1
1	U	562	ASP	2.1
1	N	121	GLN	2.1
1	S	433	PHE	2.1
1	P	859	THR	2.1
1	T	772	GLU	2.1
1	C	488	GLY	2.1
1	T	487	GLY	2.1
1	T	50	ASN	2.1
1	R	508	ILE	2.1
1	V	372	LEU	2.1
1	O	491	ASP	2.1
1	T	897	MET	2.1
1	U	728	LYS	2.0
1	R	718[A]	CYS	2.0
1	S	757	TRP	2.0
1	T	729	TRP	2.0
1	U	68	HIS	2.0
1	T	492	VAL	2.0
1	U	738	LEU	2.0
1	N	171	GLU	2.0
1	Q	583	TYR	2.0
1	S	123	LEU	2.0
1	F	486	GLY	2.0
1	S	489	GLY	2.0
1	V	506	PRO	2.0
1	T	603	HIS	2.0
1	T	737	SER	2.0
1	P	444	ILE	2.0
1	R	134	LEU	2.0
1	S	94	ILE	2.0
1	S	497	ASN	2.0
1	P	137	GLU	2.0
1	U	474	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	V	140	LEU	2.0
1	U	360	PHE	2.0
1	T	48	PRO	2.0
1	R	516	ASN	2.0
1	S	716	GLN	2.0
1	V	540	VAL	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, 95th 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	BMA	z	3	11/12	0.18	0.87	121,121,121,121	0
2	BMA	DA	3	11/12	0.22	0.69	135,135,135,135	0
2	BMA	t	3	11/12	0.38	1.01	134,134,134,134	0
2	BMA	7	3	11/12	0.42	0.78	139,140,140,140	0
2	NAG	v	2	14/15	0.42	0.65	102,103,103,103	0
2	BMA	r	3	11/12	0.43	0.80	124,124,124,125	0
2	BMA	9	3	11/12	0.43	0.57	119,119,119,119	0
2	BMA	d	3	11/12	0.43	0.46	115,115,115,115	0
2	NAG	t	2	14/15	0.44	0.57	115,115,116,116	0
2	BMA	v	3	11/12	0.45	0.52	113,113,113,113	0
2	BMA	p	3	11/12	0.48	0.61	106,107,107,107	0
2	NAG	r	2	14/15	0.51	0.38	113,113,114,114	0
2	NAG	DA	2	14/15	0.52	0.50	127,128,128,128	0
2	NAG	n	2	14/15	0.53	0.50	110,110,110,110	0
2	BMA	5	3	11/12	0.53	0.51	109,109,109,109	0
2	NAG	l	2	14/15	0.53	0.48	106,107,107,107	0
2	NAG	BA	2	14/15	0.54	0.69	124,124,125,125	0
2	BMA	3	3	11/12	0.54	0.64	120,120,120,121	0
2	NAG	b	2	14/15	0.54	0.44	89,89,89,89	0
2	BMA	h	3	11/12	0.56	0.63	106,106,106,106	0
2	NAG	d	2	14/15	0.57	0.57	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	DA	1	14/15	0.57	0.44	115,115,115,115	0
2	BMA	x	3	11/12	0.58	0.50	122,122,123,123	0
2	BMA	AA	3	11/12	0.58	0.48	79,79,80,80	11
2	NAG	7	2	14/15	0.59	0.63	132,133,133,133	0
2	NAG	z	2	14/15	0.60	0.44	113,114,114,114	0
2	NAG	Z	2	14/15	0.60	0.49	93,93,94,94	0
2	NAG	f	2	14/15	0.60	0.43	97,97,97,97	0
2	BMA	l	3	11/12	0.60	0.57	116,117,117,117	0
2	BMA	n	3	11/12	0.62	0.53	117,117,117,117	0
2	NAG	h	2	14/15	0.64	0.49	94,94,94,94	0
2	BMA	j	3	11/12	0.64	0.42	97,97,97,97	0
2	BMA	Z	3	11/12	0.65	0.44	105,106,106,106	0
2	NAG	9	2	14/15	0.65	0.51	113,113,113,113	0
2	BMA	b	3	11/12	0.65	0.37	94,95,95,95	0
2	NAG	3	2	14/15	0.65	0.73	114,115,115,115	0
2	BMA	8	3	11/12	0.66	0.38	85,85,85,85	11
2	NAG	x	2	14/15	0.66	0.48	114,114,114,114	0
2	NAG	p	2	14/15	0.67	0.51	97,97,98,98	0
2	NAG	9	1	14/15	0.69	0.33	100,100,100,100	0
2	NAG	7	1	14/15	0.70	0.34	108,109,109,109	0
2	NAG	1	2	14/15	0.70	0.63	117,117,117,117	0
2	NAG	j	2	14/15	0.72	0.48	89,90,90,90	0
2	BMA	4	3	11/12	0.72	0.25	66,66,66,66	11
2	BMA	w	3	11/12	0.72	0.30	67,67,67,67	11
2	BMA	BA	3	11/12	0.73	0.70	127,128,128,128	0
2	NAG	BA	1	14/15	0.74	0.31	104,104,105,105	0
2	NAG	5	2	14/15	0.74	0.33	104,104,104,104	0
2	BMA	k	3	11/12	0.74	0.38	54,54,54,54	11
2	BMA	f	3	11/12	0.74	0.44	105,105,106,106	0
2	NAG	h	1	14/15	0.74	0.41	70,70,70,70	0
2	BMA	0	3	11/12	0.74	0.29	74,74,74,74	11
2	NAG	v	1	14/15	0.75	0.24	73,73,74,74	0
2	NAG	1	1	14/15	0.75	0.28	96,96,96,96	0
2	BMA	o	3	11/12	0.76	0.34	65,65,65,65	11
2	NAG	8	2	14/15	0.77	0.48	85,85,85,85	0
2	NAG	X	2	14/15	0.77	0.42	52,52,52,52	0
2	NAG	f	1	14/15	0.77	0.27	71,71,72,72	0
2	BMA	i	3	11/12	0.78	0.30	45,45,46,46	11
2	BMA	u	3	11/12	0.79	0.30	61,61,61,61	11
2	NAG	b	1	14/15	0.79	0.26	64,64,64,65	0
2	BMA	q	3	11/12	0.79	0.43	62,62,62,62	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	2	3	11/12	0.79	0.34	64,64,64,64	11
2	NAG	5	1	14/15	0.80	0.37	91,91,91,92	0
2	BMA	Y	3	11/12	0.80	0.29	38,38,38,38	11
2	BMA	6	3	11/12	0.81	0.25	93,93,93,93	11
2	NAG	Z	1	14/15	0.81	0.26	63,63,64,64	0
2	NAG	z	1	14/15	0.81	0.21	89,90,90,90	0
2	NAG	3	1	14/15	0.81	0.28	93,93,94,94	0
2	BMA	s	3	11/12	0.82	0.32	64,64,64,64	11
2	NAG	x	1	14/15	0.82	0.23	89,89,89,89	0
2	NAG	t	1	14/15	0.82	0.29	84,84,84,84	0
2	NAG	d	1	14/15	0.82	0.23	68,68,69,69	0
2	NAG	r	1	14/15	0.82	0.21	78,78,78,79	0
2	BMA	1	3	11/12	0.82	0.39	120,120,120,120	0
2	NAG	n	1	14/15	0.83	0.27	82,83,83,83	0
2	NAG	l	1	14/15	0.83	0.22	76,76,77,77	0
2	NAG	j	1	14/15	0.83	0.23	66,66,66,67	0
2	BMA	X	3	11/12	0.83	0.31	56,56,56,56	0
2	NAG	4	2	14/15	0.83	0.28	59,59,60,60	0
2	NAG	8	1	14/15	0.83	0.26	77,77,77,77	0
2	NAG	CA	2	14/15	0.83	0.25	88,89,89,89	0
2	BMA	m	3	11/12	0.83	0.36	52,52,53,53	11
2	NAG	s	2	14/15	0.83	0.33	59,60,60,60	0
2	NAG	y	2	14/15	0.83	0.34	54,55,56,56	0
2	BMA	CA	3	11/12	0.84	0.34	86,86,86,86	11
2	NAG	o	2	14/15	0.84	0.30	54,55,55,55	0
2	BMA	e	3	11/12	0.84	0.32	49,49,50,50	11
2	NAG	6	2	14/15	0.84	0.43	96,96,97,97	0
2	NAG	p	1	14/15	0.85	0.27	77,77,78,78	0
2	BMA	y	3	11/12	0.85	0.34	61,61,61,61	11
2	NAG	AA	2	14/15	0.86	0.31	81,81,81,81	0
2	BMA	c	3	11/12	0.86	0.30	49,49,49,49	11
2	BMA	a	3	11/12	0.87	0.24	36,36,36,36	11
2	NAG	2	2	14/15	0.87	0.29	57,57,58,58	0
2	NAG	e	2	14/15	0.87	0.26	44,45,45,45	0
2	BMA	g	3	11/12	0.87	0.21	45,45,45,45	11
2	NAG	u	2	14/15	0.88	0.26	58,58,58,58	0
2	NAG	X	1	14/15	0.89	0.21	39,39,39,39	0
2	NAG	a	2	14/15	0.89	0.21	32,32,33,33	0
2	NAG	CA	1	14/15	0.89	0.33	82,82,82,82	0
2	NAG	c	2	14/15	0.89	0.25	43,43,43,43	0
2	NAG	q	1	14/15	0.90	0.24	39,39,40,40	0
2	NAG	i	2	14/15	0.90	0.21	39,39,40,40	0

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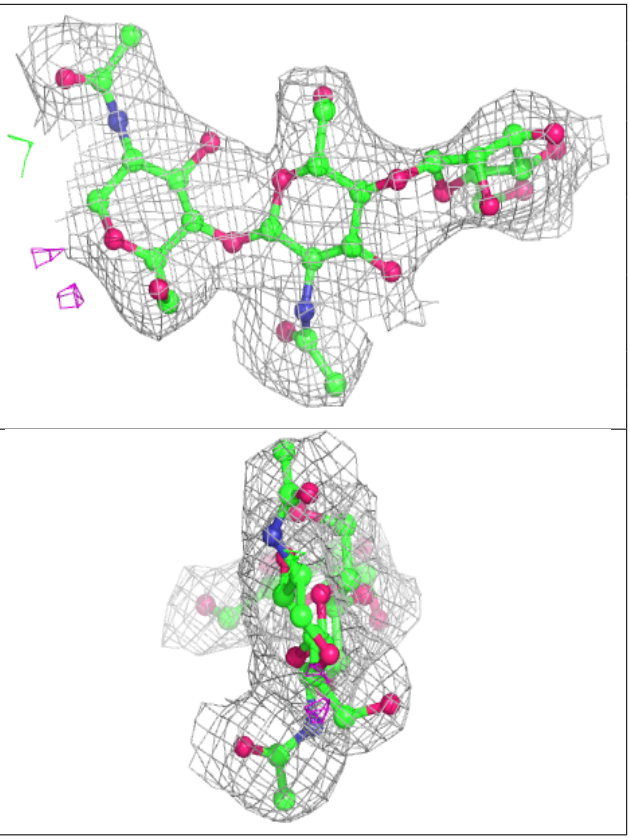
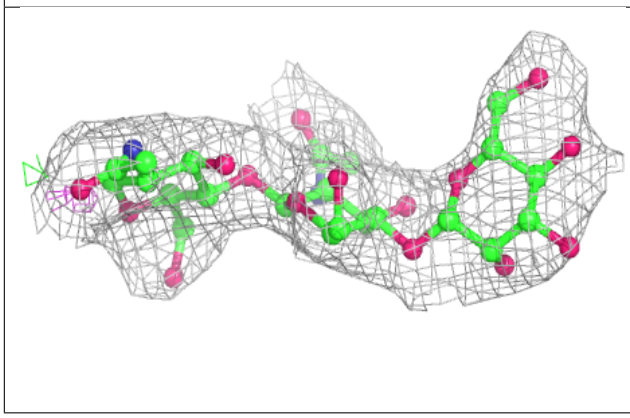
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	g	2	14/15	0.90	0.24	38,38,38,38	0
2	NAG	w	1	14/15	0.91	0.32	60,60,61,61	0
2	NAG	w	2	14/15	0.91	0.25	68,68,68,68	0
2	NAG	Y	2	14/15	0.91	0.18	31,31,31,31	0
2	NAG	2	1	14/15	0.91	0.26	48,48,49,49	0
2	NAG	AA	1	14/15	0.91	0.32	72,73,73,73	0
2	NAG	0	1	14/15	0.91	0.32	62,62,62,62	0
2	NAG	0	2	14/15	0.91	0.21	71,71,72,72	0
2	NAG	m	1	14/15	0.91	0.23	38,38,39,39	0
2	NAG	6	1	14/15	0.92	0.28	81,81,81,81	0
2	BMA	W	3	11/12	0.92	0.28	36,36,36,36	11
2	NAG	o	1	14/15	0.92	0.30	43,43,44,44	0
2	NAG	q	2	14/15	0.92	0.18	50,51,51,51	0
2	NAG	k	2	14/15	0.92	0.30	47,47,48,48	0
2	NAG	4	1	14/15	0.92	0.19	50,51,51,51	0
2	NAG	a	1	14/15	0.93	0.24	22,22,23,23	0
2	NAG	s	1	14/15	0.93	0.22	41,41,42,42	0
2	NAG	W	2	14/15	0.93	0.21	31,31,31,31	0
2	NAG	k	1	14/15	0.93	0.24	38,39,39,39	0
2	NAG	c	1	14/15	0.93	0.25	32,32,33,33	0
2	NAG	y	1	14/15	0.94	0.25	44,45,45,46	0
2	NAG	m	2	14/15	0.94	0.22	50,50,51,51	0
2	NAG	u	1	14/15	0.95	0.27	42,42,43,43	0
2	NAG	i	1	14/15	0.95	0.23	27,27,28,28	0
2	NAG	e	1	14/15	0.95	0.25	28,28,29,29	0
2	NAG	g	1	14/15	0.96	0.18	24,24,24,24	0
2	NAG	W	1	14/15	0.96	0.21	20,20,20,20	0
2	NAG	Y	1	14/15	0.97	0.21	20,21,21,21	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 W:

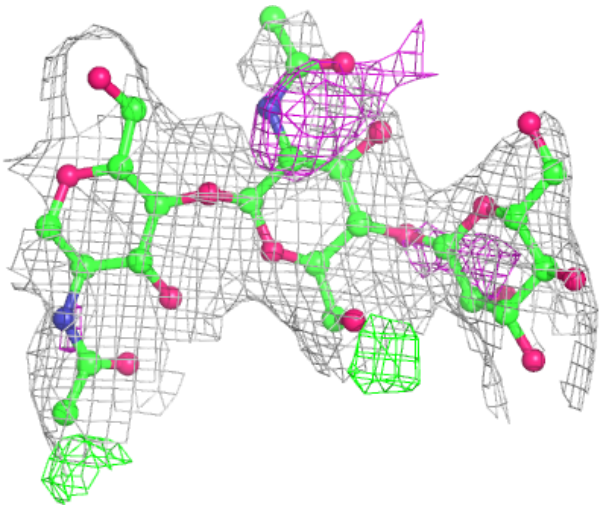
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

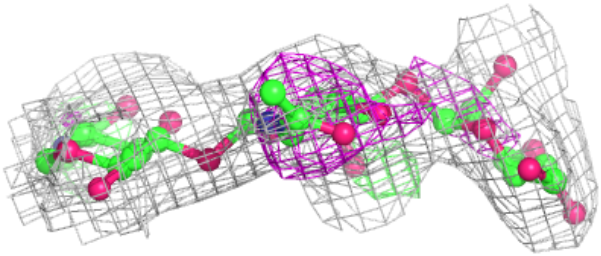


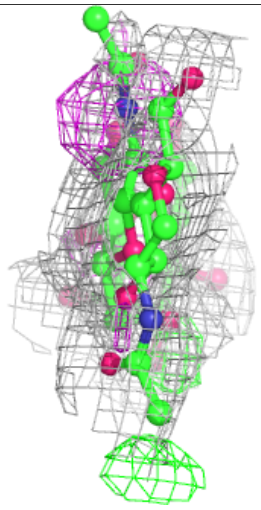


Electron density around Chain X:

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

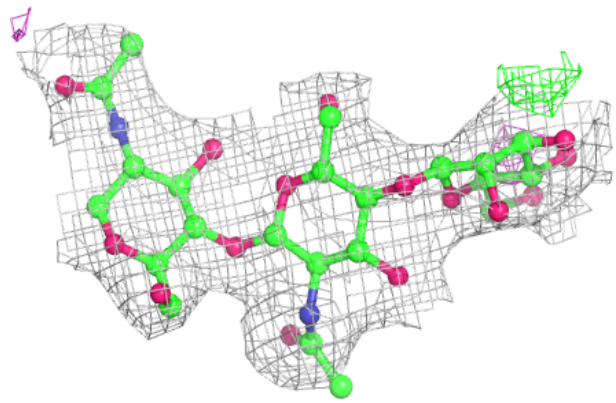


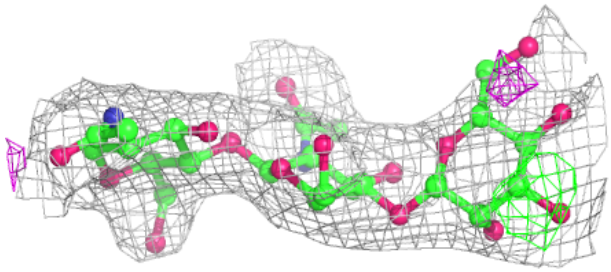


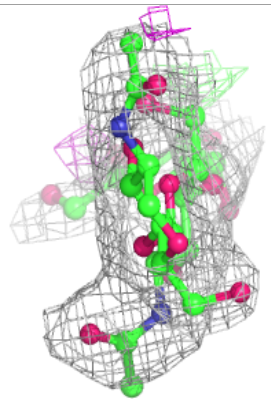


Electron density around Chain Y:

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

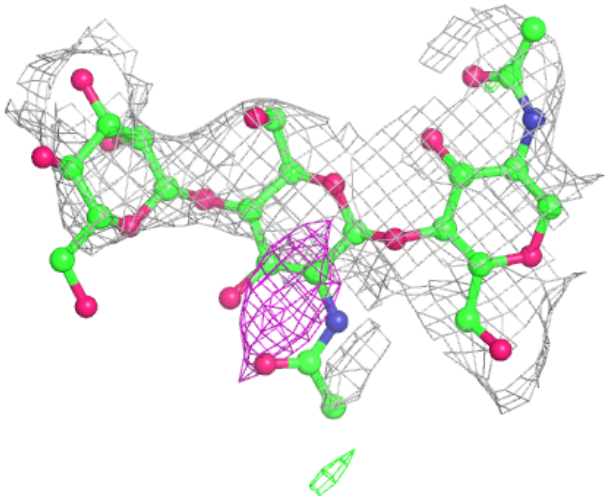


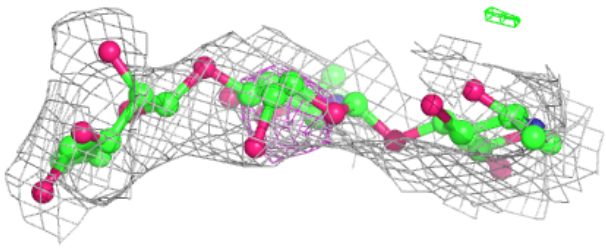


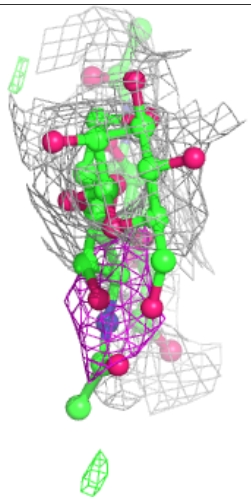


Electron density around Chain Z:

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

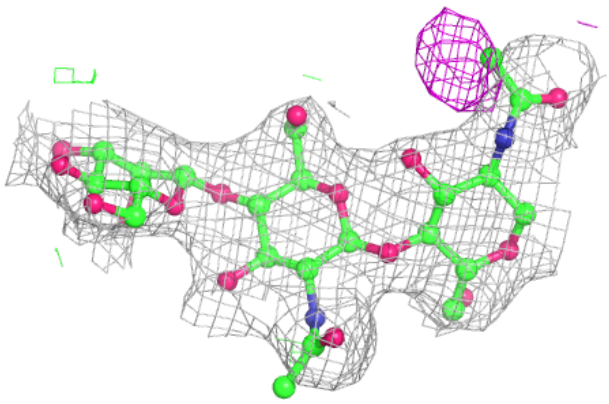


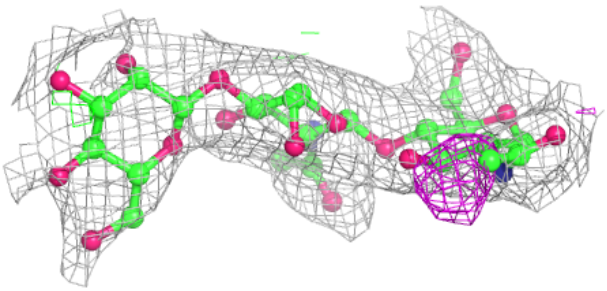


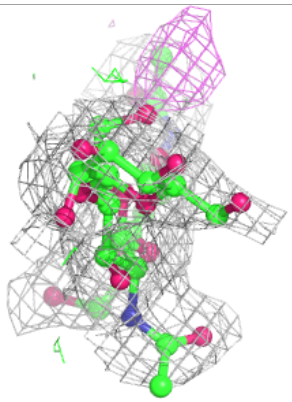


Electron density around Chain a:

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

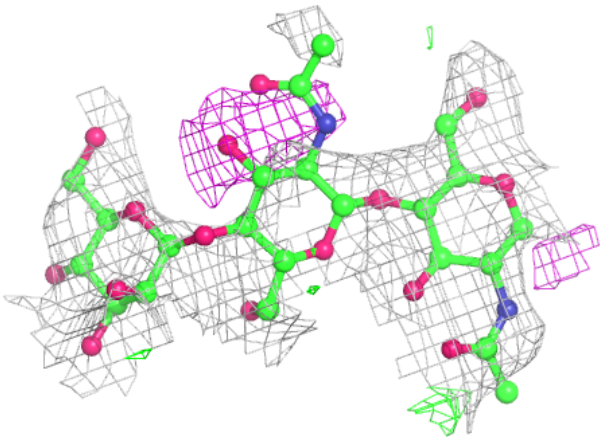


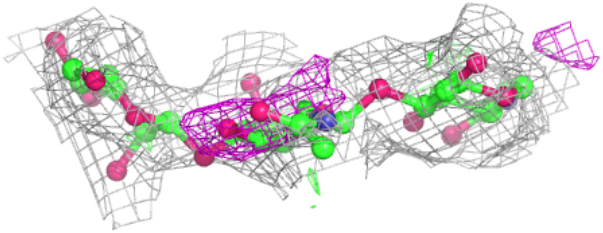


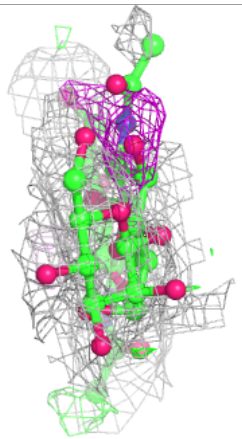


Electron density around Chain b:

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

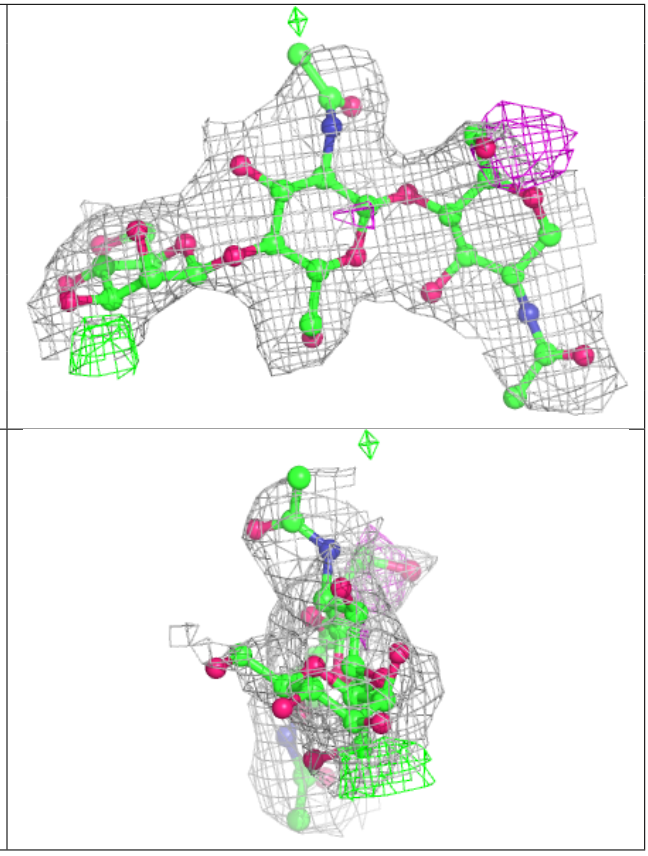


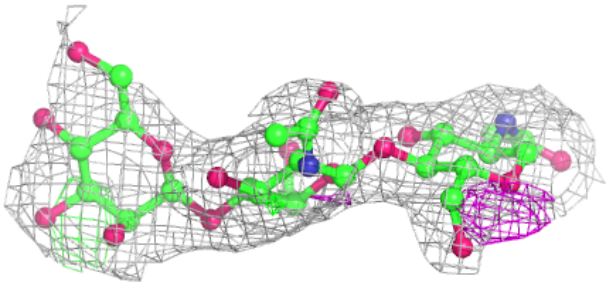




Electron density around Chain c:

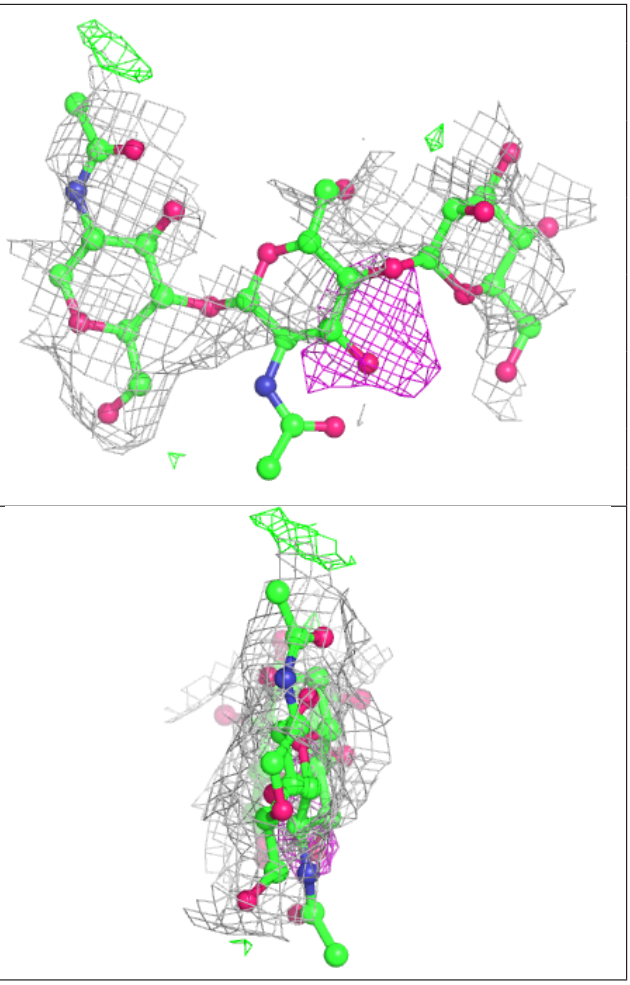
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





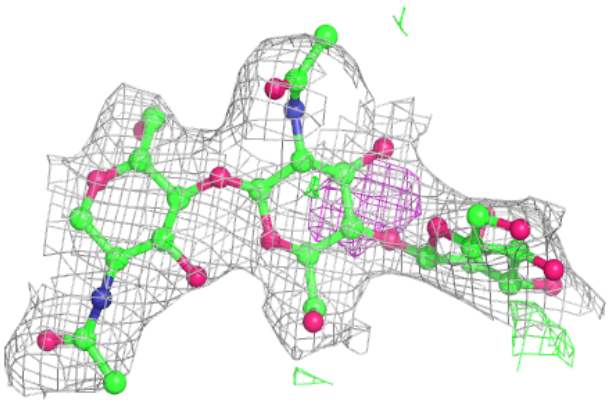
Electron density around Chain d:

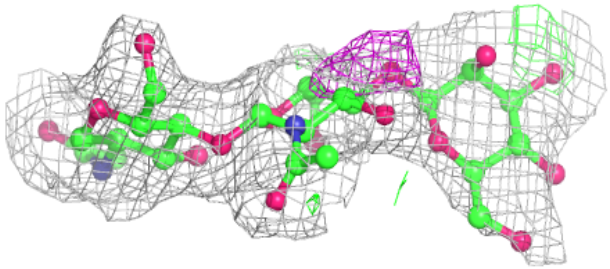
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

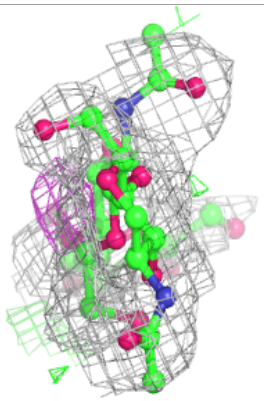


Electron density around Chain e:

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

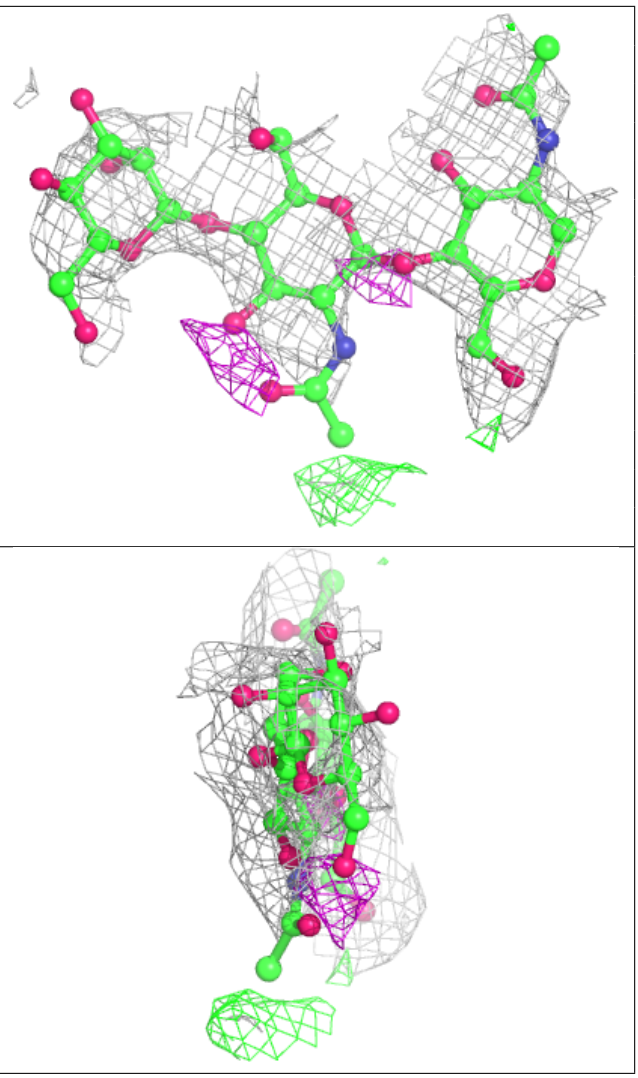






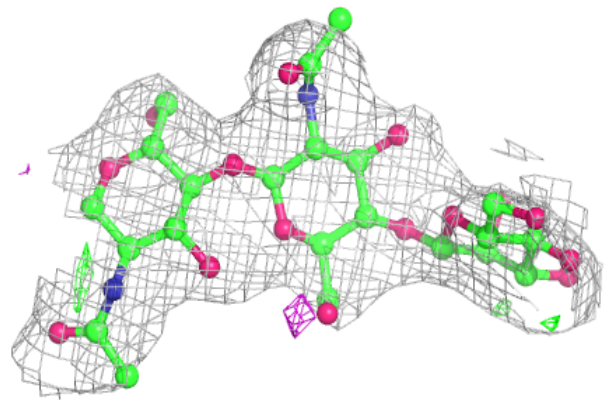
Electron density around Chain f:

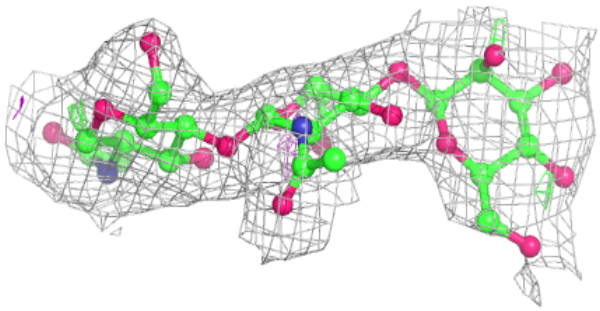
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

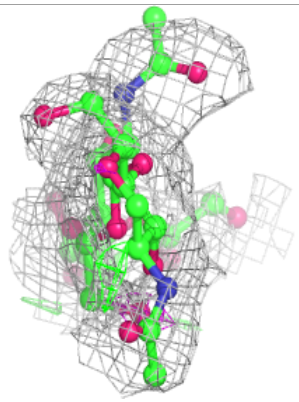


Electron density around Chain g:

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

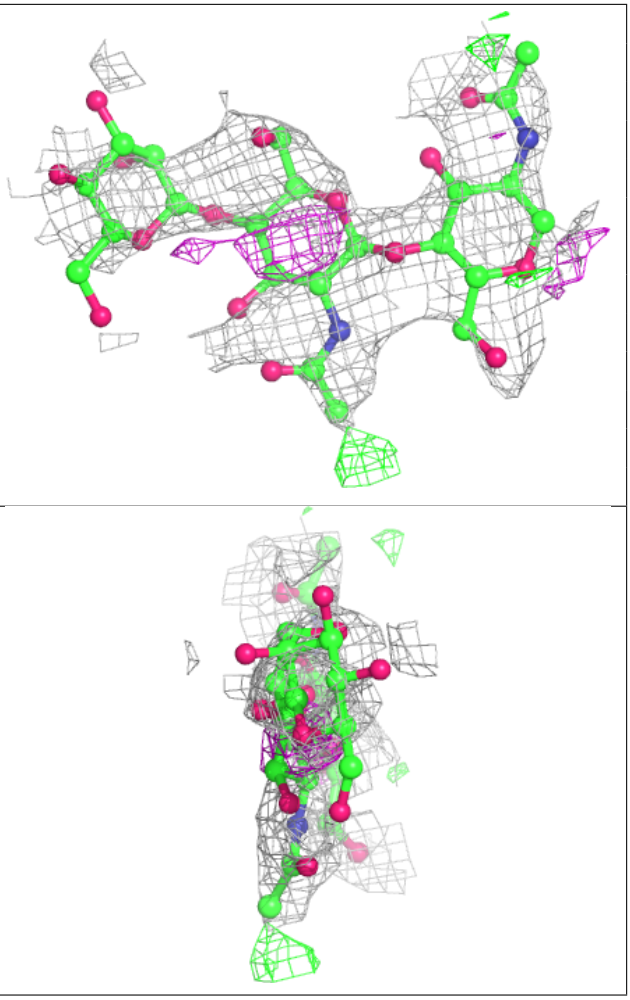






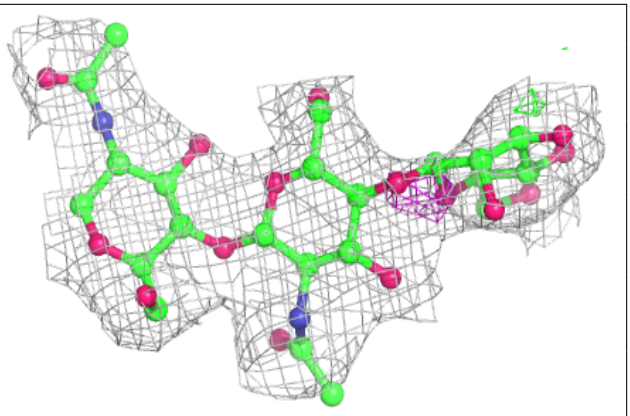
Electron density around Chain h:

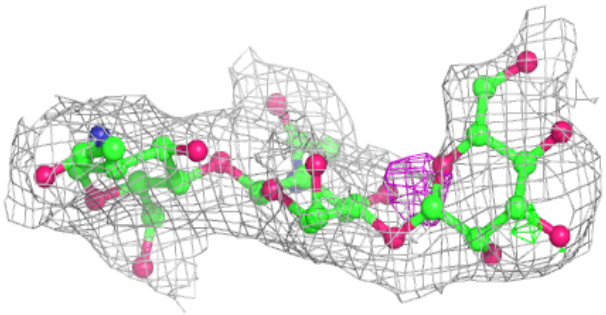
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

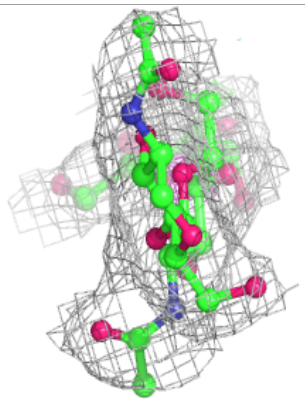


Electron density around Chain i:

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

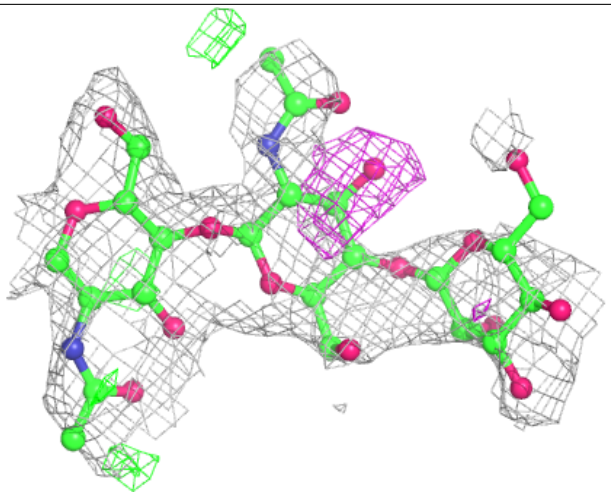


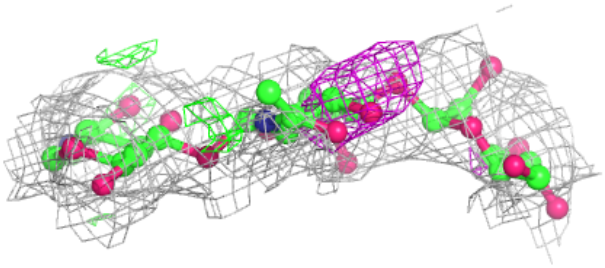


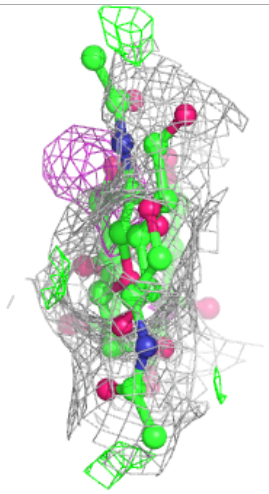


Electron density around Chain j:

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

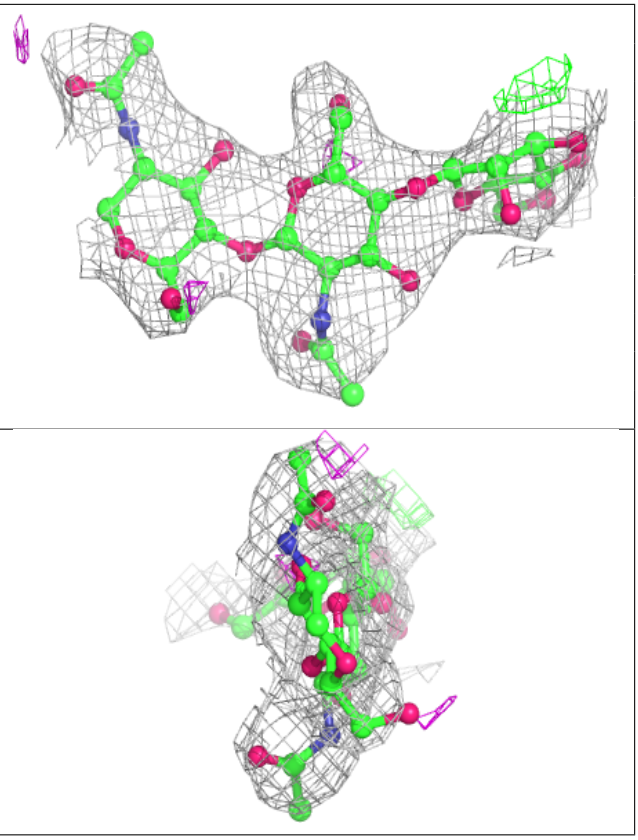






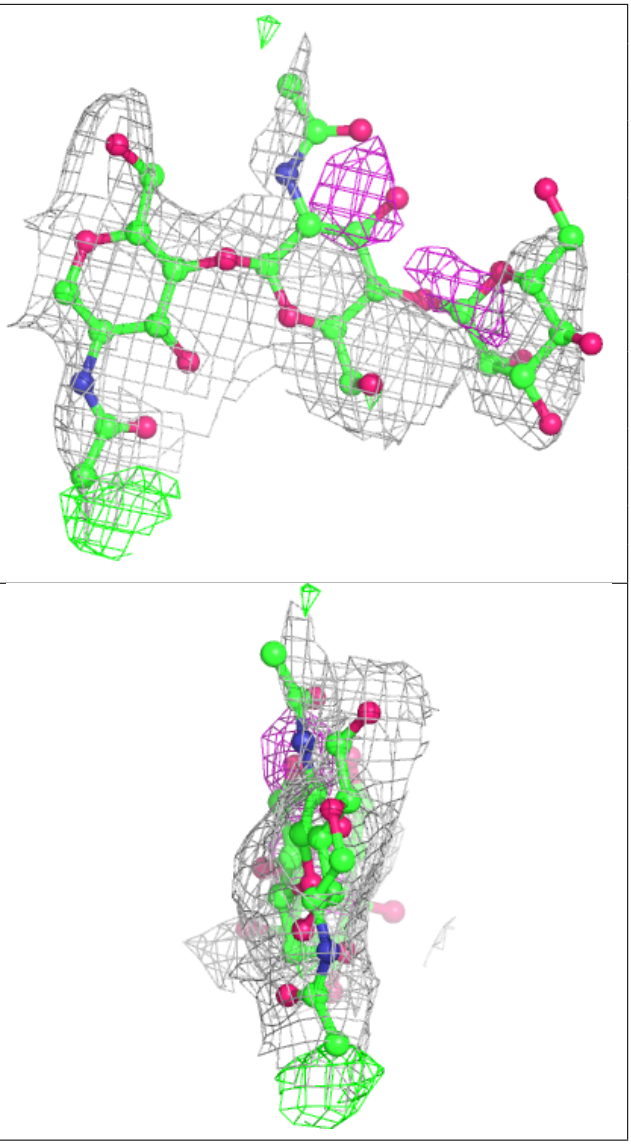
Electron density around Chain k:

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



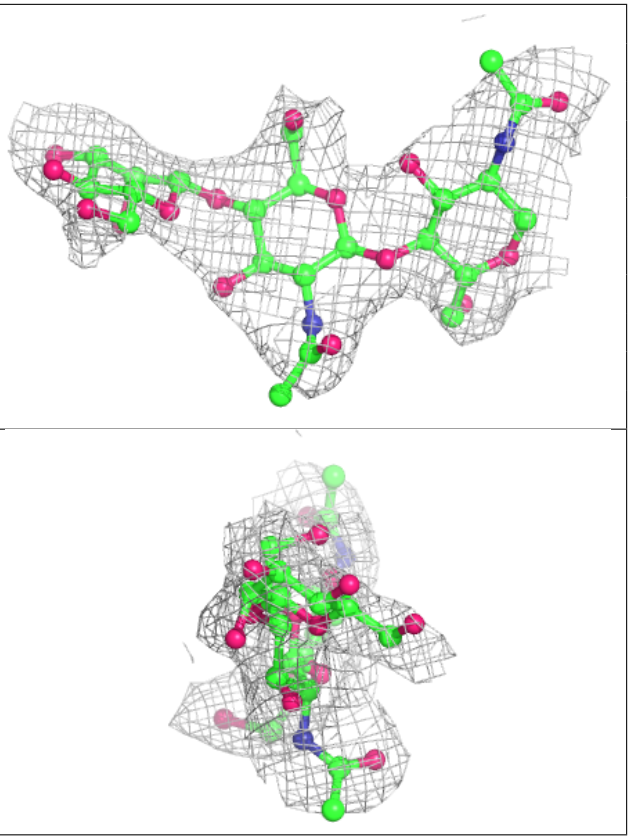
Electron density around Chain l:

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



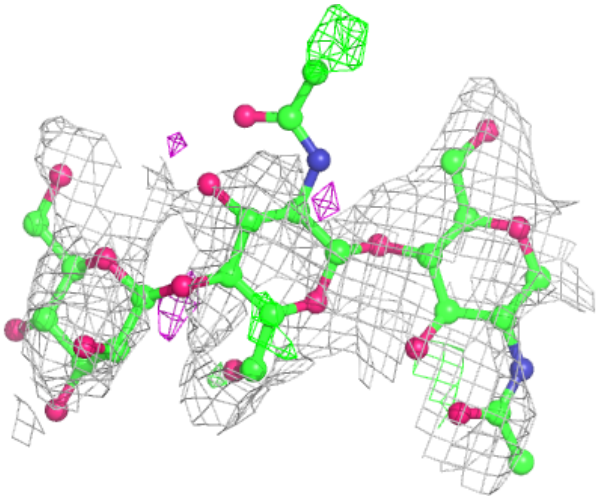
Electron density around Chain m:

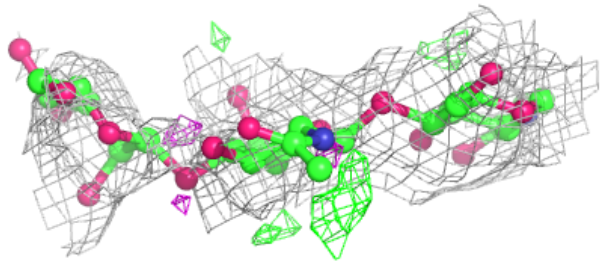
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

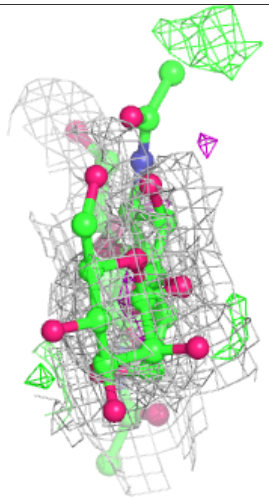


Electron density around Chain n:

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

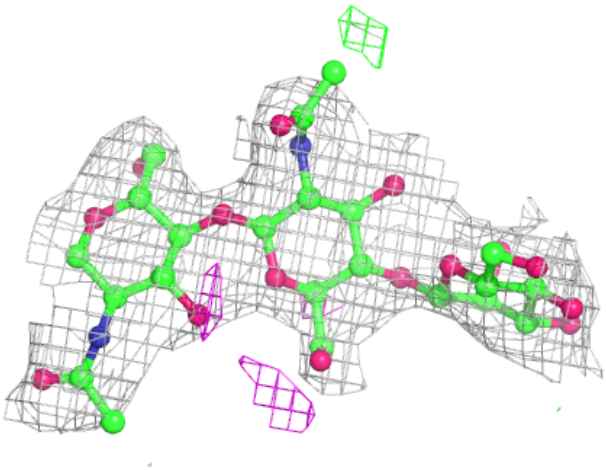


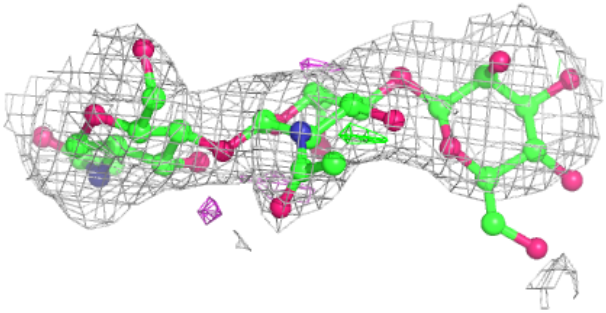


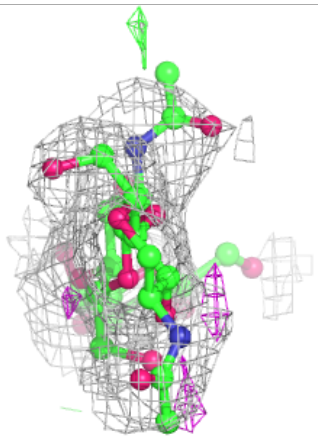


Electron density around Chain o:

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

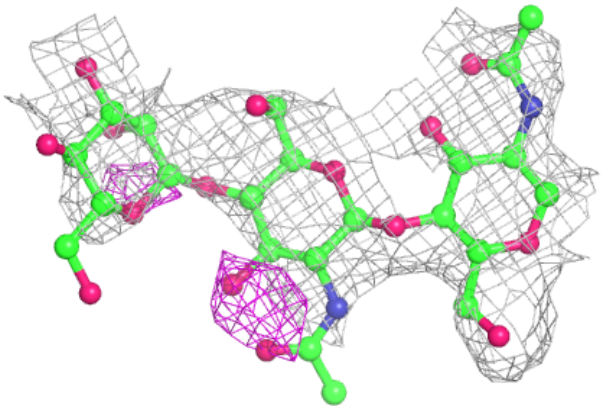


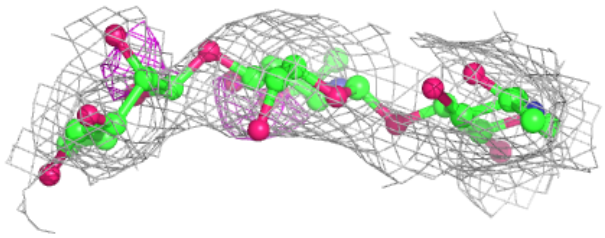


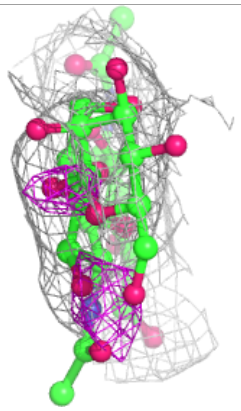


Electron density around Chain p:

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

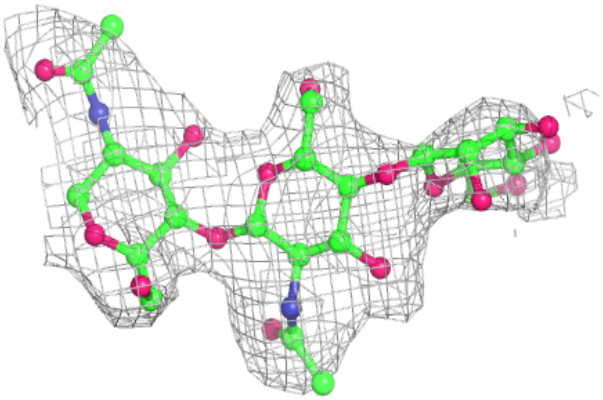


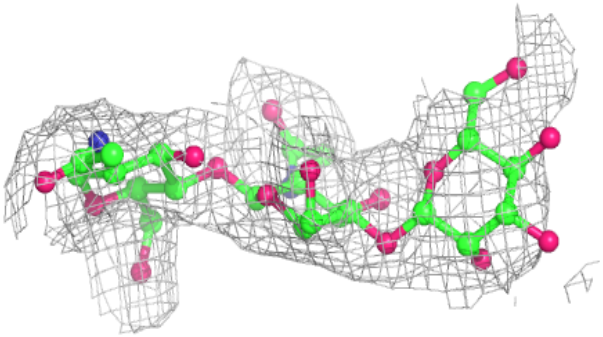


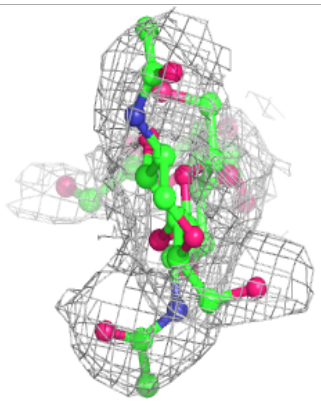


Electron density around Chain q:

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

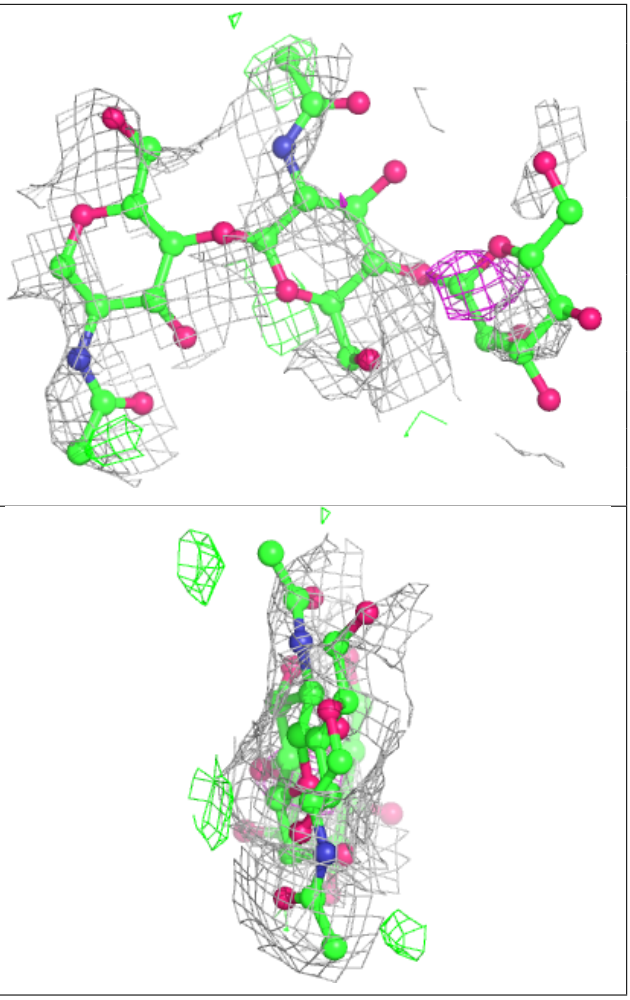






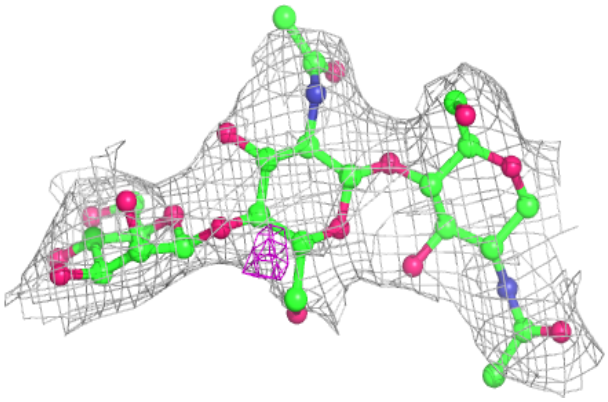
Electron density around Chain r:

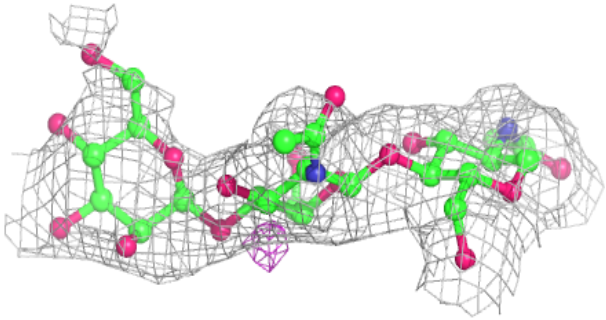
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

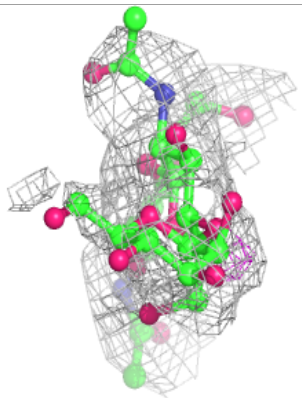


Electron density around Chain s:

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

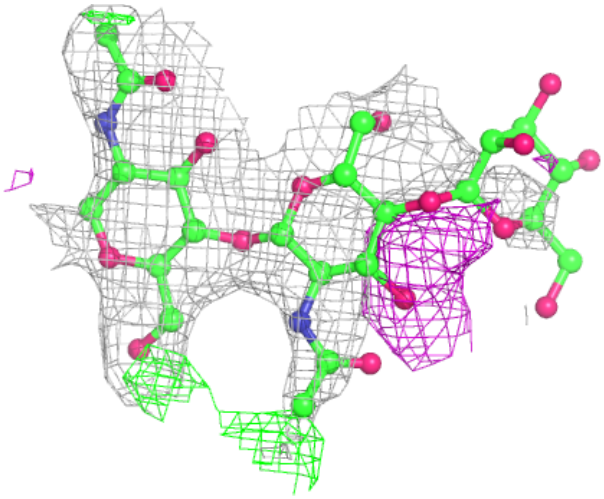


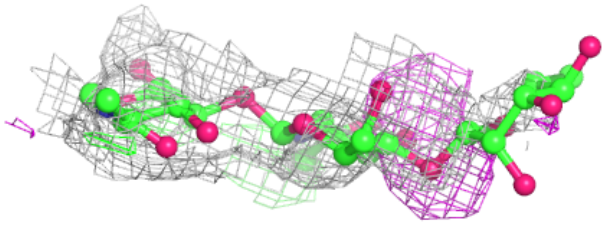


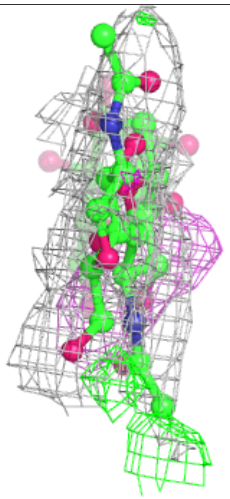


Electron density around Chain t:

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

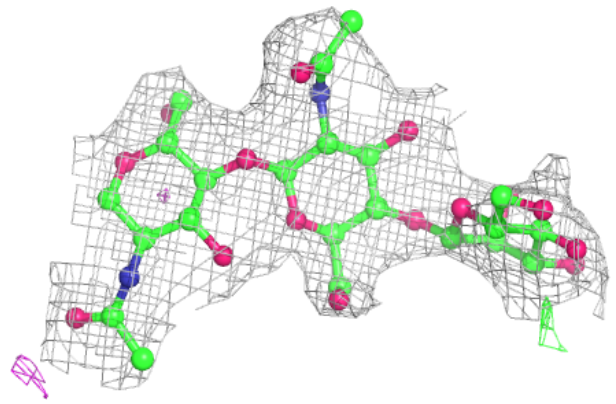


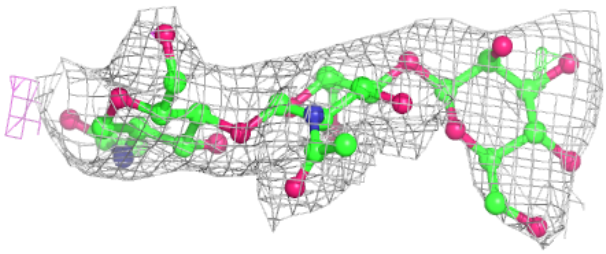


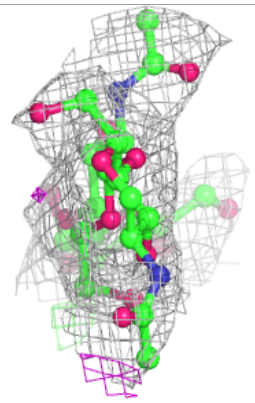


Electron density around Chain u:

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

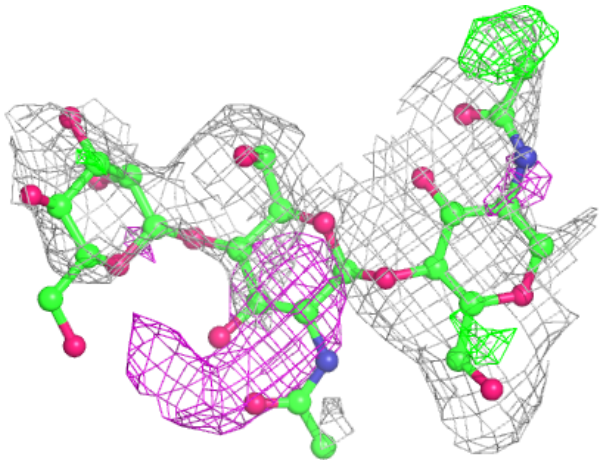


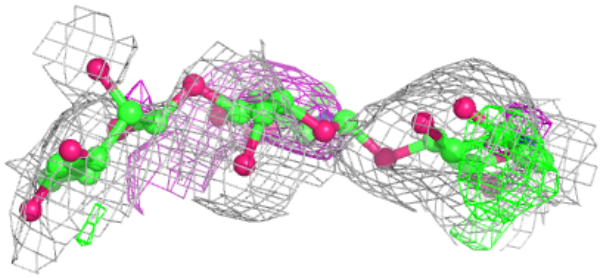


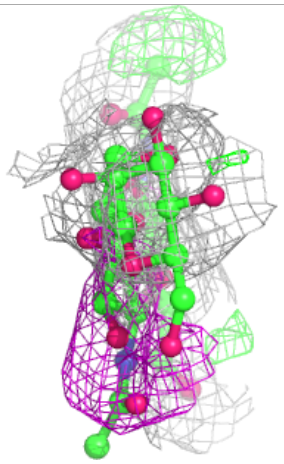


Electron density around Chain v:

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

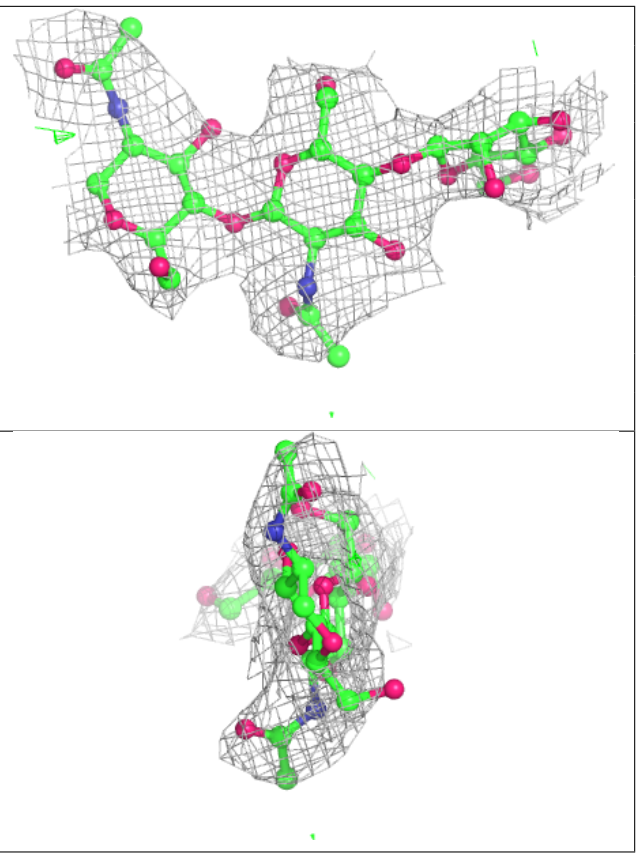


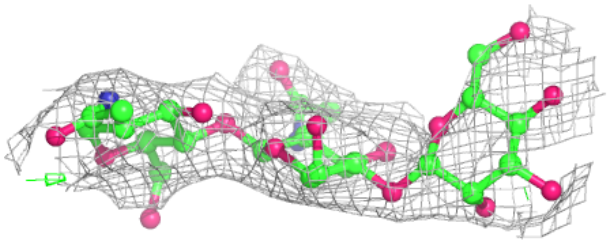




Electron density around Chain w:

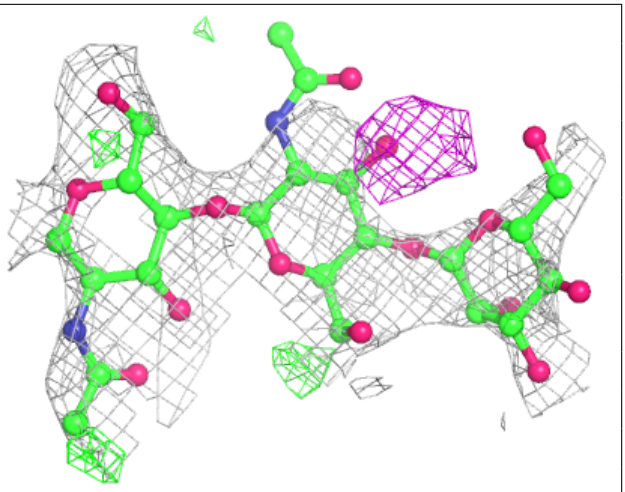
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

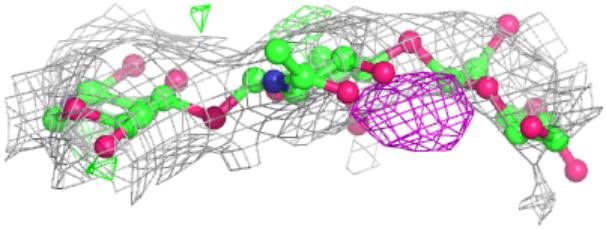


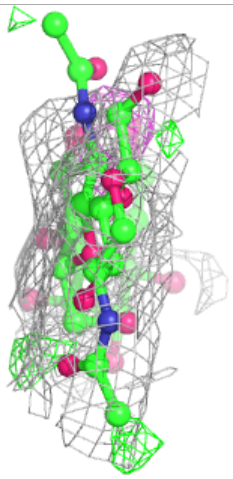


Electron density around Chain x:

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

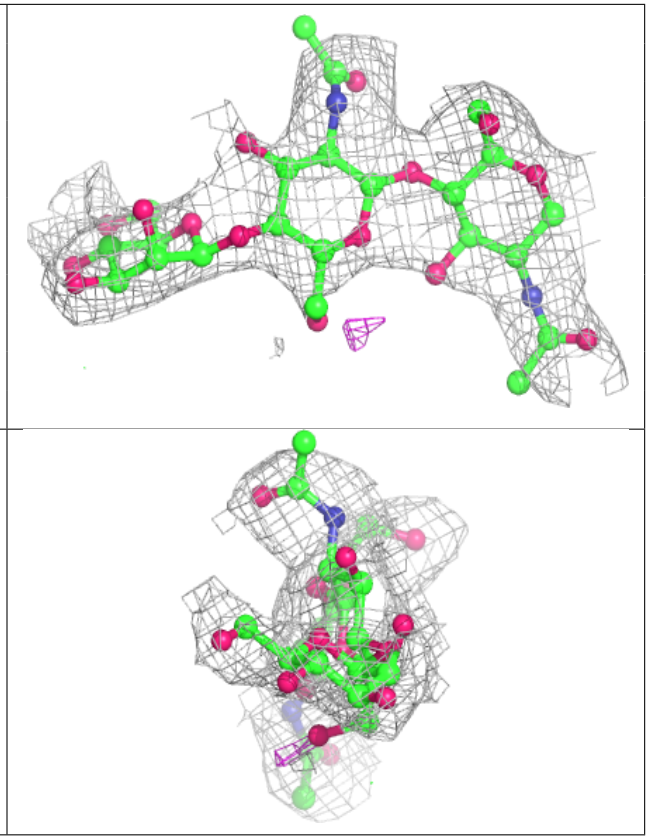






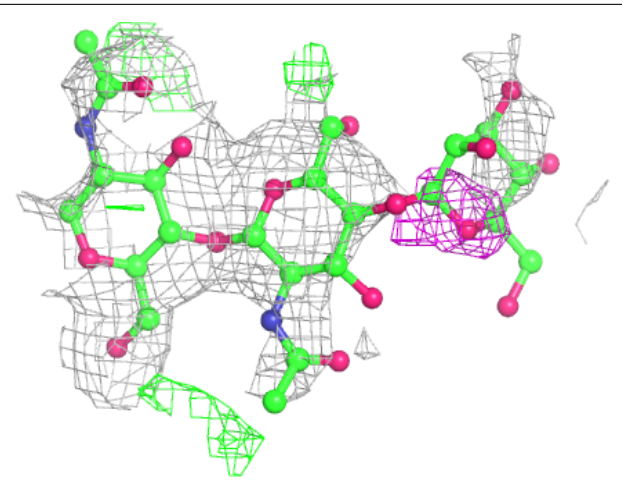
Electron density around Chain y:

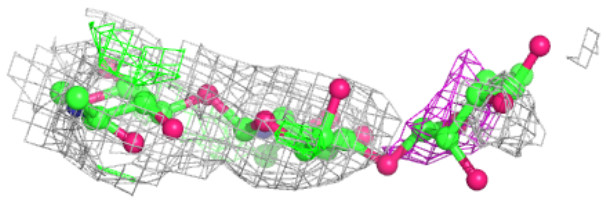
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

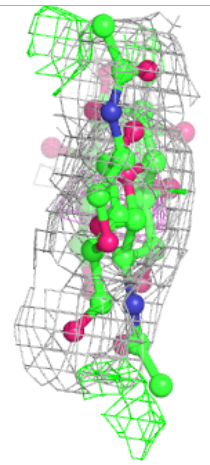


Electron density around Chain z:

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

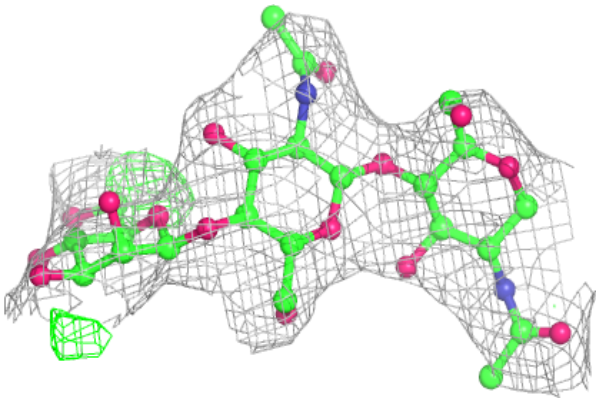


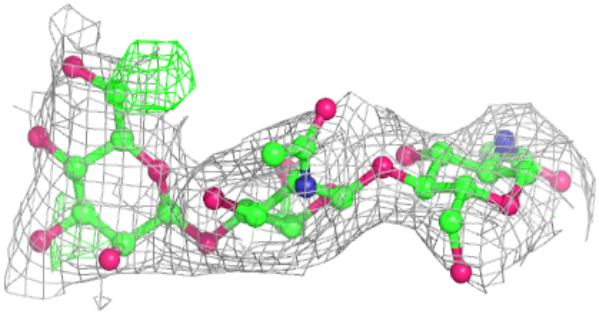


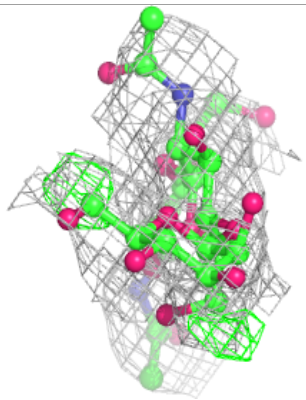


Electron density around Chain 0:

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

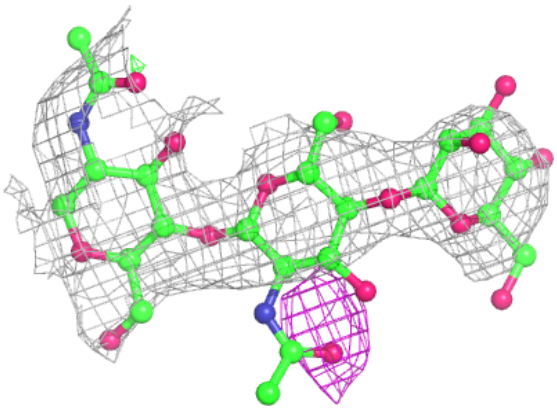


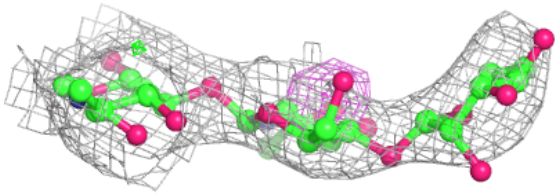


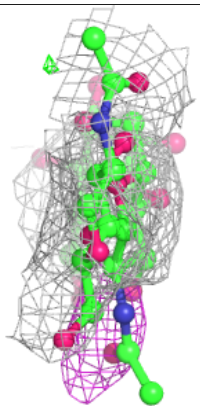


Electron density around Chain 1:

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

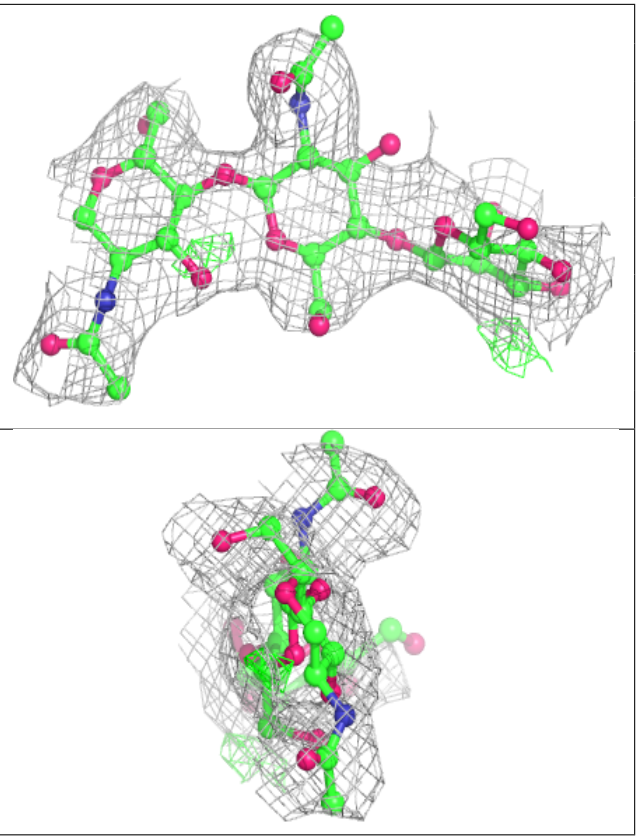






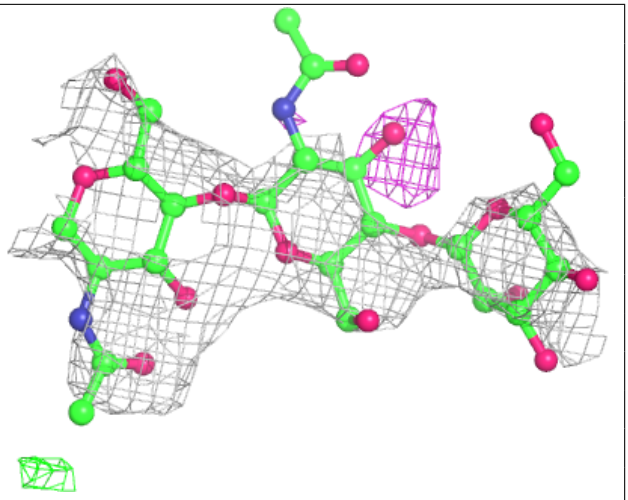
Electron density around Chain 2:

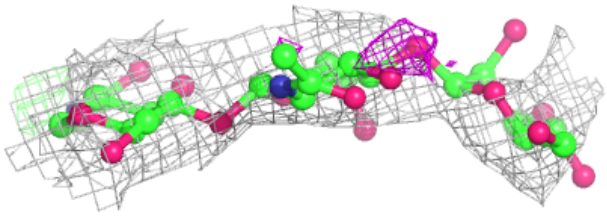
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

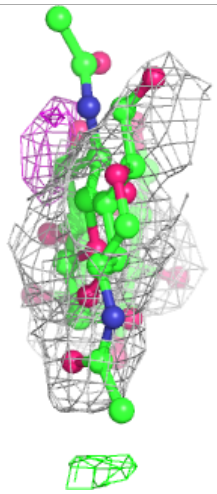


Electron density around Chain 3:

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

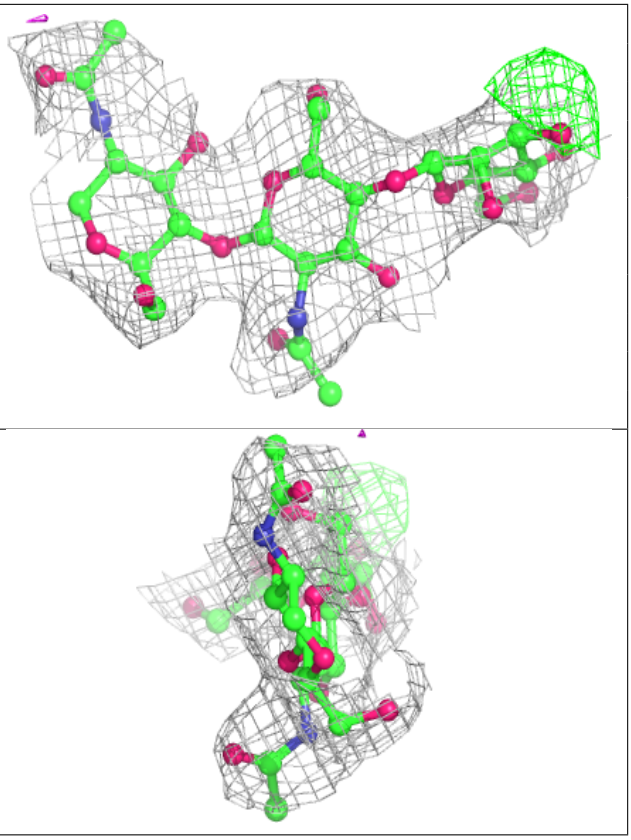


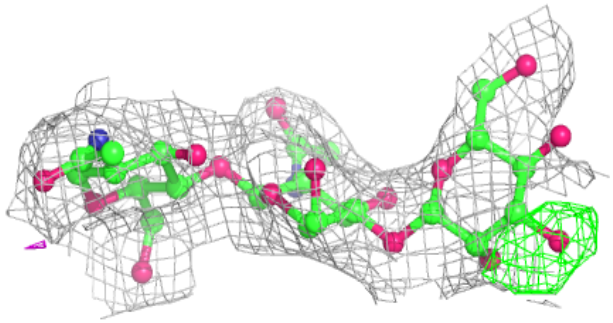




Electron density around Chain 4:

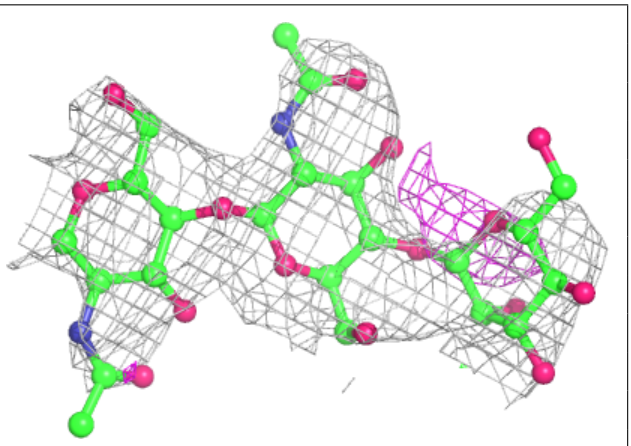
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

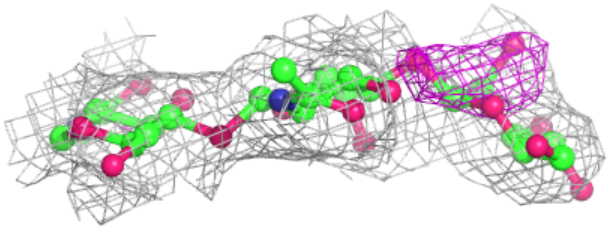


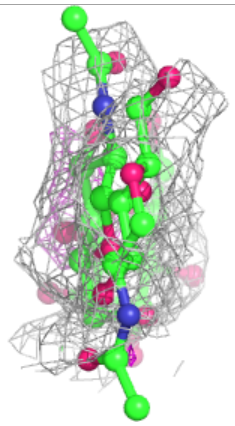


Electron density around Chain 5:

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

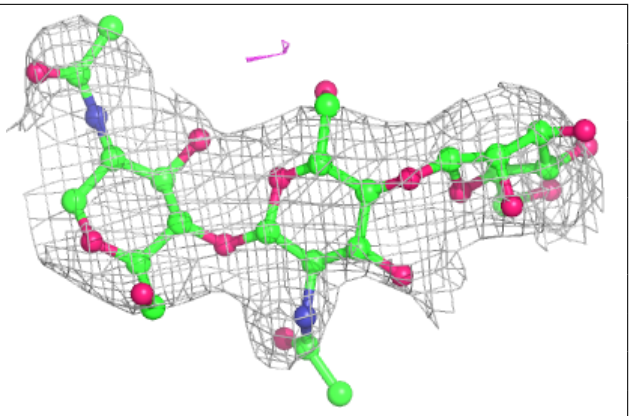


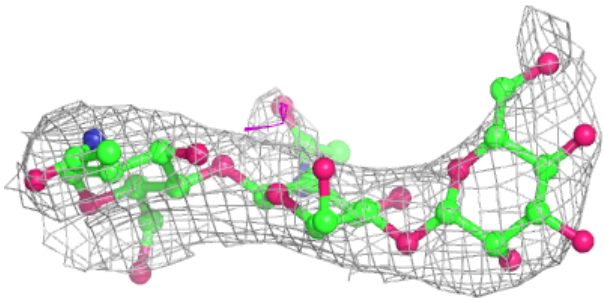


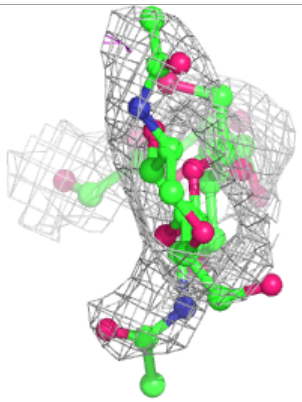


Electron density around Chain 6:

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

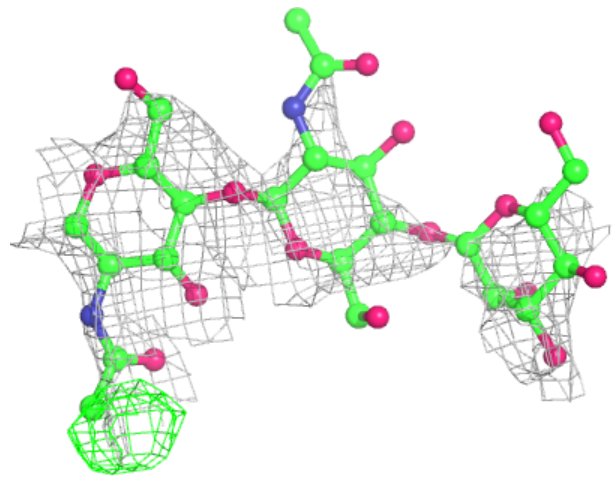


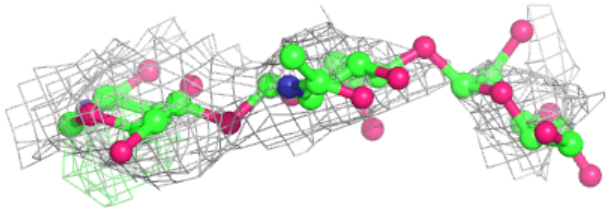


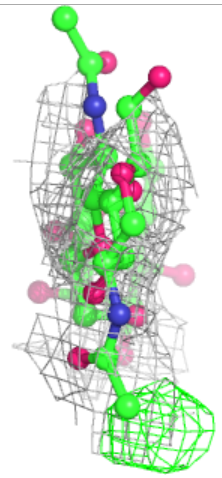


Electron density around Chain 7:

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

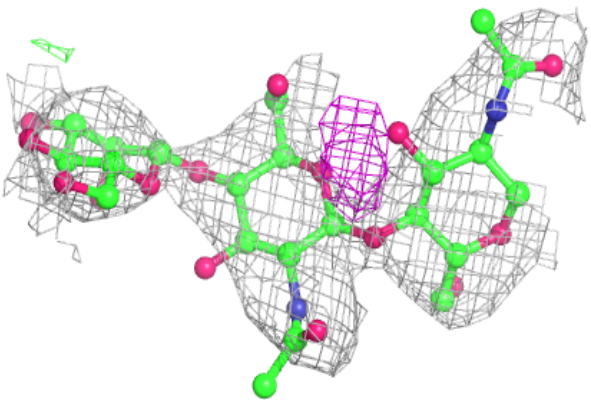


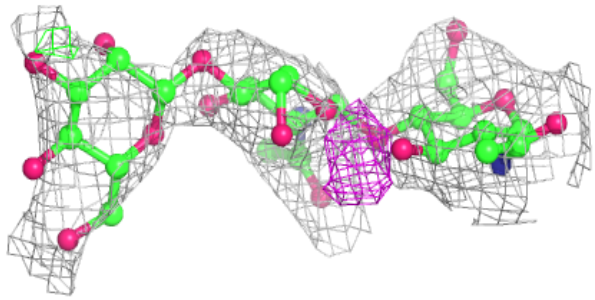


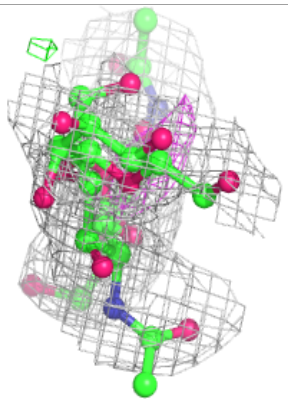


Electron density around Chain 8:

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

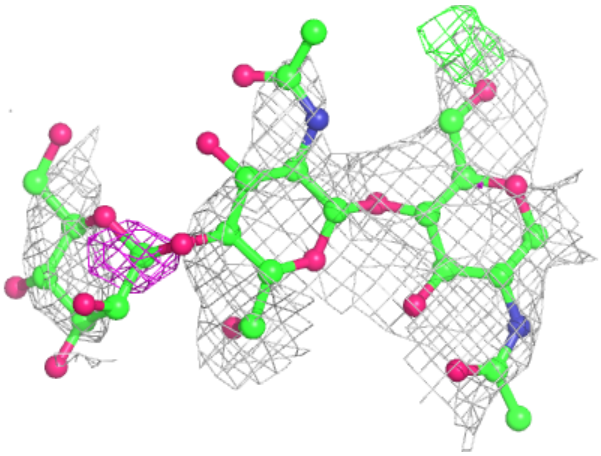


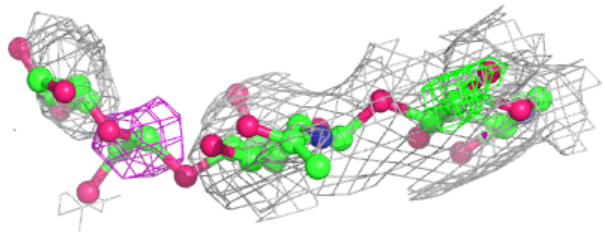


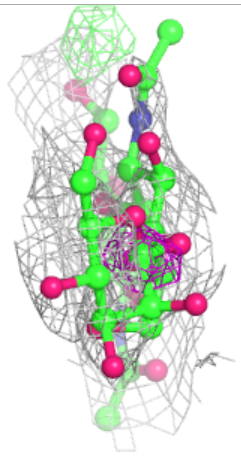


Electron density around Chain 9:

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

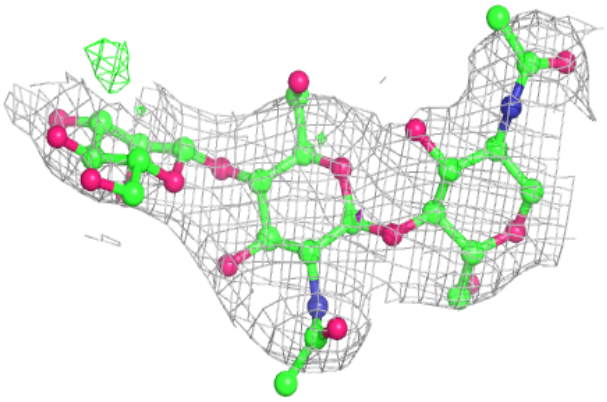


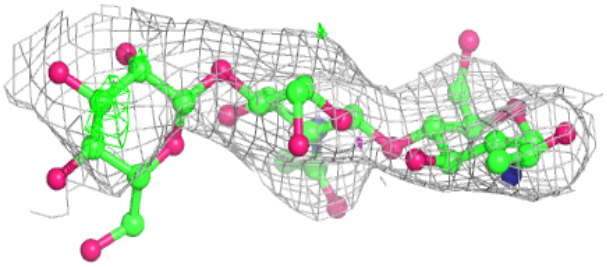


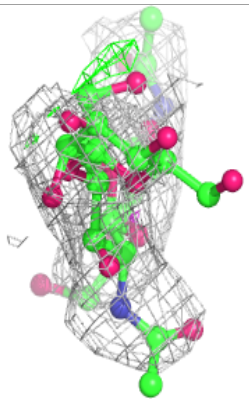


Electron density around Chain AA:

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

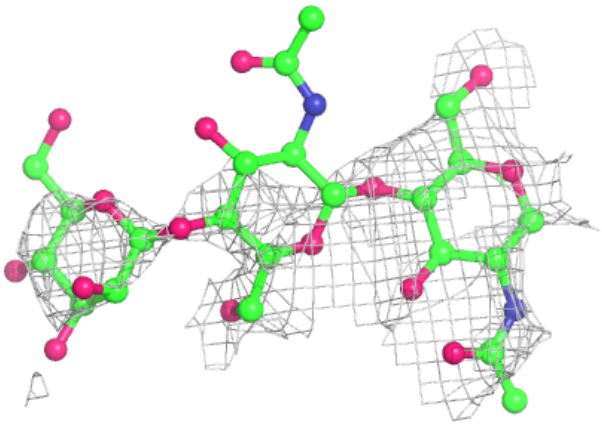


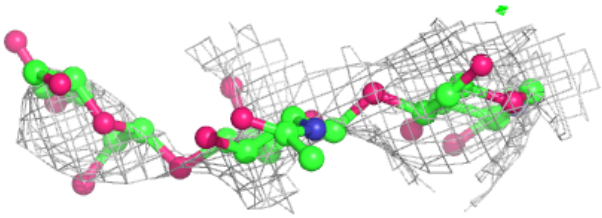


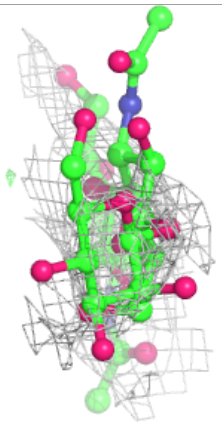


Electron density around Chain BA:

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

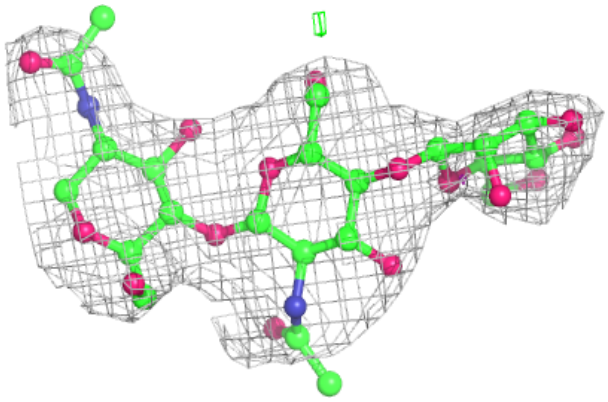


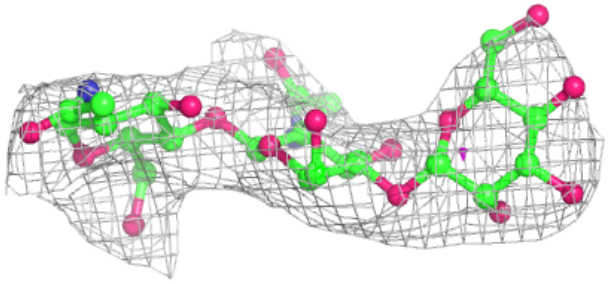


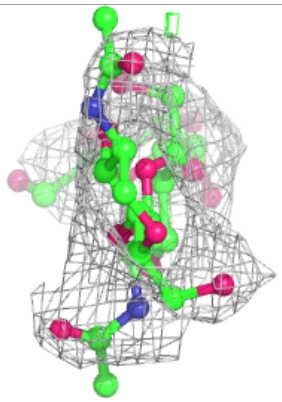


Electron density around Chain CA:

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

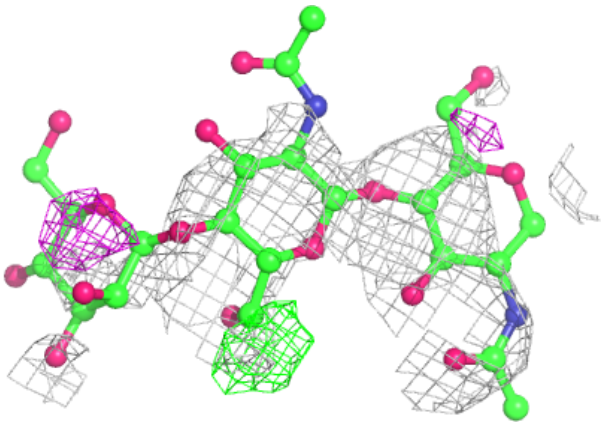


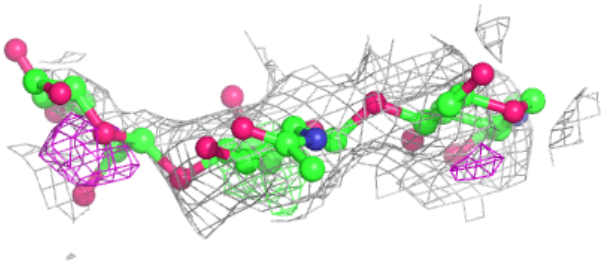


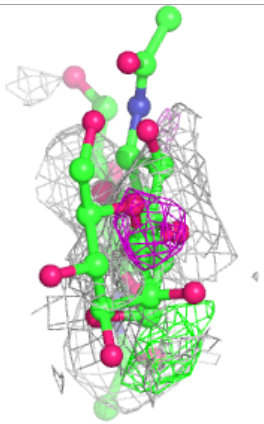


Electron density around Chain DA:

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







6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
5	SO4	R	1008	5/5	0.44	0.67	84,85,85,85	5
5	SO4	P	1013	5/5	0.53	0.36	83,83,84,84	5
5	SO4	S	1016	5/5	0.66	0.28	93,93,94,94	5
5	SO4	U	1017	5/5	0.66	0.56	68,68,68,69	5
5	SO4	Q	1014	5/5	0.67	0.46	74,74,74,74	5
5	SO4	S	1009	5/5	0.69	0.67	97,97,98,98	5
6	NAG	P	1022	14/15	0.69	0.36	70,70,70,70	0
6	NAG	S	1023	14/15	0.71	0.39	79,80,80,80	0
5	SO4	S	1013	5/5	0.73	0.29	90,90,91,91	0
5	SO4	V	1013	5/5	0.73	0.36	88,88,88,88	5
5	SO4	R	1007	5/5	0.74	0.64	91,91,92,92	5
5	SO4	T	1013	5/5	0.74	0.30	98,99,99,99	0
5	SO4	V	1007	5/5	0.76	0.55	75,76,76,76	5
5	SO4	Q	1007	5/5	0.77	0.79	88,88,89,89	5
6	NAG	V	1022	14/15	0.77	0.38	88,88,88,88	0
6	NAG	I	1023	14/15	0.78	0.28	40,41,41,41	0
6	NAG	L	1023	14/15	0.78	0.26	41,41,41,41	0
6	NAG	M	1024	14/15	0.78	0.34	51,51,52,52	0
5	SO4	T	1016	5/5	0.79	0.48	89,89,89,90	5
5	SO4	U	1001	5/5	0.79	0.33	65,65,65,66	5
5	SO4	U	1006	5/5	0.79	0.48	73,73,73,74	5
5	SO4	T	1008	5/5	0.80	0.50	77,78,78,78	5
5	SO4	S	1008	5/5	0.80	0.48	90,90,91,91	5
5	SO4	U	1014	5/5	0.80	0.33	81,82,83,84	5
5	SO4	T	1004	5/5	0.80	0.33	82,82,82,83	5
6	NAG	N	1023	14/15	0.81	0.27	65,66,66,66	0
6	NAG	H	1023	14/15	0.82	0.22	41,41,41,41	0
5	SO4	T	1014	5/5	0.82	0.33	81,81,82,82	5
6	NAG	D	1023	14/15	0.83	0.23	38,38,38,38	0
5	SO4	S	1011	5/5	0.83	0.27	86,86,86,86	5
5	SO4	R	1013	5/5	0.83	0.38	83,83,83,83	5
5	SO4	U	1015	5/5	0.84	0.31	84,84,85,85	5
6	NAG	G	1023	14/15	0.84	0.22	32,33,33,34	0
5	SO4	Q	1008	5/5	0.84	0.29	88,88,88,91	5
6	NAG	Q	1021	14/15	0.84	0.19	66,67,67,67	0
5	SO4	S	1007	5/5	0.84	0.24	81,81,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	U	1024	14/15	0.84	0.33	77,77,78,78	0
5	SO4	K	1015	5/5	0.84	0.41	35,36,36,39	5
5	SO4	R	1011	5/5	0.85	0.30	78,78,78,79	5
5	SO4	U	1016	5/5	0.85	0.42	67,67,68,68	5
5	SO4	O	1013	5/5	0.85	0.27	76,76,76,76	5
5	SO4	P	1014	5/5	0.85	0.44	57,57,58,58	5
5	SO4	V	1012	5/5	0.85	0.36	93,94,94,94	0
5	SO4	Q	1011	5/5	0.85	0.25	72,72,72,73	5
6	NAG	R	1023	14/15	0.86	0.23	71,71,71,71	0
6	NAG	E	1023	14/15	0.86	0.25	39,39,40,40	0
5	SO4	M	1014	5/5	0.86	0.27	55,55,55,56	5
5	SO4	S	1015	5/5	0.86	0.37	76,76,77,78	5
5	SO4	O	1011	5/5	0.87	0.29	57,57,57,61	5
5	SO4	N	1006	5/5	0.87	0.25	60,60,60,61	5
6	NAG	O	1023	14/15	0.87	0.20	50,50,51,51	0
5	SO4	O	1016	5/5	0.87	0.36	54,54,54,55	5
5	SO4	P	1012	5/5	0.87	0.26	63,63,63,63	5
5	SO4	V	1004	5/5	0.87	0.24	78,78,78,78	0
5	SO4	Q	1010	5/5	0.87	0.48	50,51,51,51	5
6	NAG	J	1022	14/15	0.87	0.23	51,52,52,52	0
5	SO4	U	1007	5/5	0.87	0.35	83,83,83,83	0
5	SO4	A	1012	5/5	0.88	0.32	39,40,40,40	5
6	NAG	B	1022	14/15	0.88	0.20	30,31,31,31	0
5	SO4	N	1011	5/5	0.88	0.23	51,52,52,52	5
5	SO4	U	1013	5/5	0.88	0.35	78,78,78,78	5
5	SO4	V	1005	5/5	0.88	0.32	84,84,84,84	5
5	SO4	T	1006	5/5	0.88	0.29	82,82,82,82	5
5	SO4	V	1008	5/5	0.88	0.41	75,75,75,75	5
5	SO4	V	1011	5/5	0.88	0.54	83,84,84,84	5
5	SO4	N	1015	5/5	0.88	0.24	61,61,61,61	5
5	SO4	S	1001	5/5	0.89	0.27	80,80,81,81	0
5	SO4	E	1015	5/5	0.89	0.28	42,42,43,43	5
5	SO4	V	1014	5/5	0.89	0.25	75,75,75,78	5
5	SO4	I	1006	5/5	0.89	0.23	36,36,40,42	5
5	SO4	T	1005	5/5	0.89	0.24	79,79,79,79	0
5	SO4	J	1015	5/5	0.89	0.35	38,39,42,42	5
5	SO4	V	1006	5/5	0.89	0.31	86,86,87,87	0
5	SO4	U	1012	5/5	0.89	0.20	83,83,83,84	0
5	SO4	N	1014	5/5	0.89	0.21	64,64,64,65	5
5	SO4	D	1006	5/5	0.89	0.26	24,24,24,24	5
5	SO4	N	1012	5/5	0.90	0.37	72,72,72,73	5
5	SO4	D	1016	5/5	0.90	0.31	20,20,20,20	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	F	1014	5/5	0.90	0.27	16,16,16,17	5
5	SO4	R	1015	5/5	0.90	0.29	53,53,53,53	5
5	SO4	U	1004	5/5	0.90	0.22	85,86,86,86	0
5	SO4	Q	1012	5/5	0.90	0.25	38,39,39,39	5
5	SO4	V	1010	5/5	0.90	0.35	90,90,90,90	0
5	SO4	S	1004	5/5	0.90	0.18	84,84,84,84	0
5	SO4	U	1009	5/5	0.90	0.40	75,75,75,75	5
5	SO4	S	1006	5/5	0.90	0.34	76,76,76,77	0
5	SO4	P	1015	5/5	0.90	0.27	60,60,60,60	5
5	SO4	T	1007	5/5	0.90	0.20	80,81,81,81	0
5	SO4	P	1010	5/5	0.90	0.20	66,67,67,67	5
5	SO4	T	1011	5/5	0.90	0.18	94,94,94,94	0
5	SO4	P	1005	5/5	0.91	0.21	66,67,67,67	0
5	SO4	L	1013	5/5	0.91	0.21	48,48,50,50	5
4	P52	V	1002	36/36	0.91	0.33	70,72,75,76	0
5	SO4	V	1015	5/5	0.91	0.14	78,79,79,79	5
6	NAG	A	1022	14/15	0.91	0.18	32,33,33,33	0
5	SO4	U	1005	5/5	0.91	0.20	74,74,74,74	0
6	NAG	C	1022	14/15	0.91	0.18	31,31,32,32	0
5	SO4	M	1015	5/5	0.91	0.17	47,47,47,47	5
5	SO4	M	1017	5/5	0.91	0.20	31,31,32,32	5
6	NAG	F	1023	14/15	0.91	0.22	30,30,30,30	0
5	SO4	H	1011	5/5	0.91	0.21	16,17,19,20	5
5	SO4	Q	1003	5/5	0.91	0.21	62,62,63,63	0
5	SO4	H	1015	5/5	0.91	0.23	43,43,44,46	5
3	ZN	U	1002	1/1	0.91	0.11	66,66,66,66	0
5	SO4	N	1013	5/5	0.91	0.23	75,75,75,75	5
5	SO4	I	1013	5/5	0.91	0.23	45,45,45,48	5
5	SO4	J	1012	5/5	0.91	0.21	68,69,69,69	5
5	SO4	E	1013	5/5	0.91	0.21	43,43,43,43	5
5	SO4	O	1012	5/5	0.91	0.40	42,43,43,43	5
5	SO4	K	1014	5/5	0.91	0.28	47,48,48,48	5
5	SO4	O	1014	5/5	0.91	0.19	36,36,36,39	5
5	SO4	O	1015	5/5	0.91	0.41	61,61,62,62	5
6	NAG	T	1023	14/15	0.91	0.27	80,80,81,81	0
5	SO4	C	1014	5/5	0.91	0.30	29,29,30,30	5
5	SO4	T	1015	5/5	0.91	0.21	67,67,67,68	5
5	SO4	H	1014	5/5	0.92	0.33	27,28,28,28	5
5	SO4	T	1012	5/5	0.92	0.38	73,73,73,74	5
5	SO4	P	1004	5/5	0.92	0.20	67,67,67,67	0
4	P52	U	1003	36/36	0.92	0.40	66,67,67,68	0
5	SO4	C	1015	5/5	0.92	0.24	19,20,20,20	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	R	1016	5/5	0.92	0.29	78,79,81,81	5
5	SO4	I	1007	5/5	0.92	0.16	29,30,30,31	5
5	SO4	B	1015	5/5	0.92	0.25	18,18,18,18	5
5	SO4	J	1010	5/5	0.92	0.17	43,44,44,46	0
5	SO4	G	1013	5/5	0.92	0.23	49,49,50,50	5
5	SO4	G	1015	5/5	0.92	0.31	34,34,34,34	5
5	SO4	K	1010	5/5	0.92	0.20	36,36,36,38	5
5	SO4	U	1011	5/5	0.92	0.26	75,75,75,75	5
5	SO4	O	1007	5/5	0.92	0.20	55,56,56,59	5
5	SO4	S	1012	5/5	0.92	0.36	81,81,81,82	0
6	NAG	K	1023	14/15	0.92	0.17	42,42,43,43	0
5	SO4	Q	1009	5/5	0.92	0.22	65,65,65,66	5
5	SO4	K	1012	5/5	0.92	0.11	59,59,60,60	0
5	SO4	K	1013	5/5	0.92	0.32	36,36,37,37	5
5	SO4	T	1001	5/5	0.92	0.21	75,76,76,76	0
5	SO4	V	1003	5/5	0.92	0.20	81,82,82,82	0
5	SO4	H	1006	5/5	0.92	0.25	33,34,35,35	5
5	SO4	Q	1013	5/5	0.92	0.20	66,67,67,67	5
5	SO4	C	1005	5/5	0.92	0.24	23,23,23,24	5
5	SO4	Q	1022	5/5	0.92	0.20	81,81,82,82	5
5	SO4	H	1013	5/5	0.92	0.26	43,43,43,44	5
5	SO4	T	1010	5/5	0.92	0.23	68,68,68,68	5
5	SO4	K	1024	5/5	0.93	0.14	50,51,54,54	0
5	SO4	R	1014	5/5	0.93	0.25	55,55,55,55	5
5	SO4	N	1016	5/5	0.93	0.22	43,44,47,47	5
5	SO4	I	1014	5/5	0.93	0.30	35,35,35,35	5
5	SO4	L	1014	5/5	0.93	0.32	33,33,34,36	5
5	SO4	M	1007	5/5	0.93	0.24	39,39,39,40	0
4	P52	R	1002	36/36	0.93	0.28	45,45,46,47	0
5	SO4	C	1012	5/5	0.93	0.19	38,38,38,39	5
5	SO4	M	1016	5/5	0.93	0.38	41,41,41,41	5
4	P52	T	1003	36/36	0.93	0.35	67,69,71,71	0
5	SO4	F	1006	5/5	0.93	0.23	22,22,22,22	5
5	SO4	V	1009	5/5	0.93	0.13	81,81,81,81	0
5	SO4	B	1013	5/5	0.93	0.25	18,18,18,18	5
5	SO4	P	1006	5/5	0.93	0.16	55,55,55,56	0
5	SO4	R	1006	5/5	0.93	0.23	54,55,55,55	5
5	SO4	F	1015	5/5	0.93	0.26	36,36,36,36	5
4	P52	M	1003	36/36	0.93	0.30	34,35,36,36	0
5	SO4	U	1010	5/5	0.93	0.17	71,72,72,72	0
5	SO4	D	1015	5/5	0.93	0.20	43,43,43,43	5
5	SO4	R	1012	5/5	0.93	0.30	57,57,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	P52	J	1002	36/36	0.94	0.26	22,24,33,35	0
4	P52	L	1003	36/36	0.94	0.30	22,24,28,29	36
5	SO4	R	1004	5/5	0.94	0.16	56,56,56,56	0
5	SO4	T	1009	5/5	0.94	0.21	68,69,69,69	5
5	SO4	R	1005	5/5	0.94	0.34	49,49,49,49	5
5	SO4	K	1016	5/5	0.94	0.27	31,31,31,31	5
4	P52	H	1003	36/36	0.94	0.30	15,16,17,17	0
5	SO4	L	1001	5/5	0.94	0.17	17,17,18,19	0
4	P52	N	1003	36/36	0.94	0.37	44,45,46,49	0
5	SO4	D	1011	5/5	0.94	0.15	24,24,24,24	5
5	SO4	D	1013	5/5	0.94	0.18	40,40,40,40	5
5	SO4	A	1013	5/5	0.94	0.17	25,25,25,25	5
5	SO4	B	1010	5/5	0.94	0.20	18,18,18,18	5
5	SO4	P	1011	5/5	0.94	0.27	66,66,66,66	5
5	SO4	R	1024	5/5	0.94	0.20	83,83,84,84	0
5	SO4	E	1012	5/5	0.94	0.28	17,17,20,21	5
4	P52	P	1002	36/36	0.94	0.32	46,47,49,49	0
5	SO4	B	1014	5/5	0.94	0.24	25,25,26,26	5
5	SO4	N	1010	5/5	0.94	0.21	57,57,57,57	5
5	SO4	I	1016	5/5	0.94	0.20	30,30,30,31	5
5	SO4	Q	1004	5/5	0.94	0.16	46,46,46,47	0
5	SO4	Q	1005	5/5	0.94	0.28	41,42,42,42	5
4	P52	I	1003	36/36	0.94	0.32	28,29,31,31	0
5	SO4	F	1011	5/5	0.94	0.16	25,25,25,25	5
5	SO4	S	1014	5/5	0.94	0.21	69,69,70,70	5
5	SO4	F	1012	5/5	0.94	0.32	15,15,15,15	5
4	P52	S	1003	36/36	0.94	0.37	66,68,69,69	0
5	SO4	C	1010	5/5	0.94	0.16	24,24,25,25	5
5	SO4	O	1005	5/5	0.94	0.30	44,44,46,46	5
5	SO4	G	1005	5/5	0.94	0.24	26,26,27,27	5
5	SO4	M	1005	5/5	0.95	0.20	42,42,42,42	0
5	SO4	M	1006	5/5	0.95	0.21	45,45,45,46	5
4	P52	Q	1002	36/36	0.95	0.30	43,44,45,45	0
5	SO4	S	1010	5/5	0.95	0.27	69,69,69,69	5
5	SO4	M	1012	5/5	0.95	0.16	37,38,38,38	5
5	SO4	M	1013	5/5	0.95	0.24	43,43,43,44	5
5	SO4	A	1005	5/5	0.95	0.21	23,23,23,23	5
5	SO4	I	1012	5/5	0.95	0.27	36,37,37,40	0
5	SO4	F	1013	5/5	0.95	0.16	37,37,37,38	5
5	SO4	D	1014	5/5	0.95	0.18	18,18,18,19	5
5	SO4	N	1001	5/5	0.95	0.21	34,34,37,38	0
5	SO4	N	1005	5/5	0.95	0.19	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	I	1015	5/5	0.95	0.20	42,42,42,47	5
5	SO4	N	1007	5/5	0.95	0.16	56,56,56,57	0
5	SO4	N	1009	5/5	0.95	0.13	41,41,45,45	0
5	SO4	A	1009	5/5	0.95	0.19	17,17,17,17	0
5	SO4	J	1005	5/5	0.95	0.31	31,32,32,32	5
5	SO4	A	1010	5/5	0.95	0.18	21,21,22,22	5
5	SO4	G	1008	5/5	0.95	0.20	20,20,20,21	0
5	SO4	R	1003	5/5	0.95	0.17	65,65,66,66	0
5	SO4	G	1011	5/5	0.95	0.18	22,22,22,23	5
5	SO4	K	1005	5/5	0.95	0.28	36,36,37,37	0
5	SO4	E	1006	5/5	0.95	0.24	22,23,24,24	5
5	SO4	G	1014	5/5	0.95	0.25	11,11,11,12	5
5	SO4	E	1011	5/5	0.95	0.17	19,19,20,20	5
5	SO4	R	1009	5/5	0.95	0.23	53,54,57,57	0
5	SO4	O	1009	5/5	0.95	0.18	34,35,35,37	0
5	SO4	H	1005	5/5	0.95	0.18	40,40,40,40	0
3	ZN	T	1002	1/1	0.95	0.15	57,57,57,57	0
5	SO4	U	1008	5/5	0.95	0.28	81,81,81,81	0
4	P52	B	1002	36/36	0.95	0.25	10,11,12,12	36
5	SO4	E	1014	5/5	0.95	0.16	17,17,18,18	5
4	P52	E	1003	36/36	0.95	0.26	12,12,14,14	0
5	SO4	L	1011	5/5	0.95	0.16	30,31,31,31	5
4	P52	K	1002	36/36	0.95	0.27	27,28,29,29	0
5	SO4	H	1016	5/5	0.95	0.21	13,14,14,14	5
5	SO4	L	1016	5/5	0.95	0.22	23,24,24,24	5
4	P52	A	1002	36/36	0.96	0.29	9,10,10,10	0
3	ZN	I	1002	1/1	0.96	0.19	29,29,29,29	0
5	SO4	C	1013	5/5	0.96	0.17	19,19,19,19	5
4	P52	C	1002	36/36	0.96	0.23	12,13,14,14	0
5	SO4	F	1001	5/5	0.96	0.14	17,17,18,18	0
4	P52	D	1003	36/36	0.96	0.25	17,17,17,17	0
5	SO4	C	1023	5/5	0.96	0.15	20,21,23,24	0
5	SO4	I	1004	5/5	0.96	0.16	29,29,30,33	0
5	SO4	L	1005	5/5	0.96	0.14	45,45,45,45	0
5	SO4	L	1010	5/5	0.96	0.17	28,28,29,29	5
5	SO4	O	1004	5/5	0.96	0.16	39,39,39,39	0
5	SO4	A	1014	5/5	0.96	0.28	26,26,26,26	5
5	SO4	O	1006	5/5	0.96	0.16	36,36,36,37	0
5	SO4	L	1012	5/5	0.96	0.24	31,31,32,34	5
5	SO4	O	1008	5/5	0.96	0.11	63,63,63,67	0
5	SO4	D	1010	5/5	0.96	0.20	11,11,11,12	5
5	SO4	A	1015	5/5	0.96	0.24	16,16,16,17	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	P	1001	1/1	0.96	0.10	44,44,44,44	0
5	SO4	M	1001	5/5	0.96	0.16	26,28,29,30	0
5	SO4	F	1016	5/5	0.96	0.21	18,18,19,19	5
5	SO4	B	1012	5/5	0.96	0.14	27,27,27,27	5
4	P52	F	1003	36/36	0.96	0.27	12,12,12,12	0
5	SO4	M	1010	5/5	0.96	0.12	44,44,44,45	0
5	SO4	M	1011	5/5	0.96	0.17	45,46,46,46	0
4	P52	G	1002	36/36	0.96	0.27	14,15,15,15	0
5	SO4	P	1007	5/5	0.96	0.14	49,49,49,52	0
5	SO4	P	1009	5/5	0.96	0.15	68,68,68,68	0
5	SO4	A	1004	5/5	0.96	0.14	18,18,18,19	0
5	SO4	E	1007	5/5	0.96	0.17	17,18,18,18	0
5	SO4	J	1013	5/5	0.96	0.15	28,28,29,29	5
5	SO4	J	1014	5/5	0.96	0.19	49,49,50,50	5
4	P52	O	1002	36/36	0.96	0.27	32,33,35,35	0
5	SO4	H	1004	5/5	0.96	0.15	23,23,24,24	0
5	SO4	K	1008	5/5	0.96	0.15	42,43,43,43	0
5	SO4	I	1010	5/5	0.97	0.14	36,36,37,40	5
5	SO4	I	1011	5/5	0.97	0.12	25,26,26,28	5
5	SO4	L	1015	5/5	0.97	0.16	42,43,43,45	5
5	SO4	A	1011	5/5	0.97	0.20	14,14,14,14	5
3	ZN	L	1002	1/1	0.97	0.10	26,26,26,26	0
5	SO4	P	1003	5/5	0.97	0.18	51,52,52,53	0
5	SO4	S	1005	5/5	0.97	0.16	67,67,67,68	0
5	SO4	M	1004	5/5	0.97	0.26	41,42,42,43	5
5	SO4	D	1012	5/5	0.97	0.14	20,20,20,20	5
3	ZN	G	1001	1/1	0.97	0.18	16,16,16,16	0
5	SO4	A	1006	5/5	0.97	0.14	16,16,16,16	0
5	SO4	M	1008	5/5	0.97	0.17	27,28,28,31	0
5	SO4	G	1004	5/5	0.97	0.14	25,25,25,25	0
5	SO4	J	1006	5/5	0.97	0.14	25,25,26,26	0
5	SO4	J	1007	5/5	0.97	0.18	29,29,30,32	0
5	SO4	B	1023	5/5	0.97	0.16	16,16,16,16	0
5	SO4	J	1011	5/5	0.97	0.27	32,32,32,34	5
5	SO4	C	1004	5/5	0.97	0.14	20,20,20,20	0
5	SO4	E	1001	5/5	0.97	0.19	16,16,16,16	0
5	SO4	E	1005	5/5	0.97	0.10	32,33,33,33	0
3	ZN	R	1001	1/1	0.97	0.12	43,43,43,43	0
5	SO4	Q	1006	5/5	0.97	0.12	45,45,46,46	0
5	SO4	K	1003	5/5	0.97	0.18	37,37,37,38	0
5	SO4	K	1004	5/5	0.97	0.13	30,30,30,31	0
5	SO4	B	1005	5/5	0.97	0.20	25,25,25,25	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	N	1008	5/5	0.97	0.23	35,35,35,36	0
5	SO4	K	1006	5/5	0.97	0.17	25,25,26,28	0
5	SO4	E	1010	5/5	0.97	0.17	17,18,18,18	5
5	SO4	B	1006	5/5	0.97	0.14	12,12,12,12	0
5	SO4	K	1011	5/5	0.97	0.20	30,30,31,31	5
5	SO4	B	1007	5/5	0.97	0.17	15,15,15,15	0
5	SO4	H	1010	5/5	0.97	0.15	22,24,24,25	0
5	SO4	B	1008	5/5	0.97	0.14	13,13,13,13	0
5	SO4	H	1012	5/5	0.97	0.30	24,24,24,25	5
5	SO4	B	1009	5/5	0.97	0.17	11,11,11,11	0
5	SO4	A	1003	5/5	0.97	0.15	20,20,20,21	0
5	SO4	E	1016	5/5	0.97	0.18	12,12,13,13	5
5	SO4	D	1004	5/5	0.97	0.13	21,21,21,21	0
5	SO4	F	1004	5/5	0.97	0.17	23,23,24,24	0
5	SO4	B	1011	5/5	0.97	0.24	12,12,13,13	5
5	SO4	D	1007	5/5	0.97	0.16	15,15,15,15	0
5	SO4	L	1004	5/5	0.98	0.10	32,32,34,35	0
5	SO4	C	1003	5/5	0.98	0.15	21,21,22,22	0
5	SO4	L	1006	5/5	0.98	0.22	40,40,41,43	5
5	SO4	L	1007	5/5	0.98	0.13	24,24,25,26	0
5	SO4	P	1008	5/5	0.98	0.15	54,55,55,55	0
5	SO4	L	1008	5/5	0.98	0.22	14,14,15,15	0
5	SO4	L	1009	5/5	0.98	0.14	18,18,19,19	0
5	SO4	F	1005	5/5	0.98	0.12	22,22,22,22	0
5	SO4	A	1008	5/5	0.98	0.13	9,9,10,10	0
5	SO4	F	1007	5/5	0.98	0.15	16,16,16,16	0
5	SO4	I	1001	5/5	0.98	0.17	19,20,20,20	0
5	SO4	F	1008	5/5	0.98	0.19	12,12,13,13	0
5	SO4	I	1005	5/5	0.98	0.14	36,36,36,36	0
5	SO4	F	1009	5/5	0.98	0.13	11,11,11,12	0
5	SO4	F	1010	5/5	0.98	0.14	14,14,14,14	0
5	SO4	I	1008	5/5	0.98	0.16	19,20,20,20	0
5	SO4	I	1009	5/5	0.98	0.14	22,22,22,22	0
3	ZN	A	1001	1/1	0.98	0.15	8,8,8,8	0
5	SO4	C	1006	5/5	0.98	0.21	13,13,13,13	0
5	SO4	C	1007	5/5	0.98	0.18	19,19,20,20	0
5	SO4	M	1009	5/5	0.98	0.18	28,28,28,29	0
5	SO4	C	1008	5/5	0.98	0.16	18,18,18,18	0
3	ZN	C	1001	1/1	0.98	0.17	20,20,20,20	0
5	SO4	C	1011	5/5	0.98	0.15	16,16,17,17	5
5	SO4	G	1003	5/5	0.98	0.18	18,18,19,19	0
5	SO4	J	1003	5/5	0.98	0.19	31,31,31,32	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	J	1004	5/5	0.98	0.13	37,37,37,37	0
5	SO4	E	1004	5/5	0.98	0.13	19,20,21,21	0
3	ZN	S	1002	1/1	0.98	0.11	59,59,59,59	0
5	SO4	G	1006	5/5	0.98	0.15	13,14,14,14	0
5	SO4	N	1004	5/5	0.98	0.13	45,46,46,46	0
5	SO4	J	1008	5/5	0.98	0.13	28,30,31,31	0
5	SO4	R	1010	5/5	0.98	0.12	45,45,45,45	0
5	SO4	J	1009	5/5	0.98	0.15	19,19,19,20	0
3	ZN	K	1001	1/1	0.98	0.13	29,29,29,29	0
5	SO4	G	1009	5/5	0.98	0.15	11,11,11,12	0
5	SO4	G	1010	5/5	0.98	0.13	10,10,10,10	5
3	ZN	E	1002	1/1	0.98	0.17	12,12,12,12	0
5	SO4	G	1012	5/5	0.98	0.20	17,18,18,20	5
5	SO4	E	1009	5/5	0.98	0.14	11,11,12,12	0
3	ZN	V	1001	1/1	0.98	0.10	67,67,67,67	0
3	ZN	M	1002	1/1	0.98	0.17	35,35,35,35	0
5	SO4	G	1016	5/5	0.98	0.17	21,21,22,22	5
5	SO4	G	1024	5/5	0.98	0.16	22,22,22,23	0
5	SO4	O	1003	5/5	0.98	0.13	42,43,43,43	0
5	SO4	K	1007	5/5	0.98	0.12	40,41,41,44	0
5	SO4	H	1001	5/5	0.98	0.15	10,10,10,10	0
5	SO4	K	1009	5/5	0.98	0.14	21,21,21,21	0
5	SO4	D	1001	5/5	0.98	0.14	15,15,15,15	0
5	SO4	B	1003	5/5	0.98	0.16	18,18,18,19	0
5	SO4	D	1005	5/5	0.98	0.12	27,27,27,27	0
5	SO4	O	1010	5/5	0.98	0.17	28,28,29,31	0
5	SO4	H	1007	5/5	0.98	0.11	19,19,19,20	0
5	SO4	H	1008	5/5	0.98	0.17	10,10,10,10	0
5	SO4	H	1009	5/5	0.98	0.15	11,11,11,12	0
5	SO4	B	1004	5/5	0.98	0.11	20,20,20,20	0
3	ZN	N	1002	1/1	0.98	0.11	40,40,40,40	0
5	SO4	K	1025	5/5	0.98	0.13	35,35,36,36	0
5	SO4	D	1009	5/5	0.98	0.11	15,15,15,15	0
5	SO4	A	1007	5/5	0.99	0.15	11,11,11,11	0
5	SO4	C	1009	5/5	0.99	0.15	11,11,11,11	5
5	SO4	E	1008	5/5	0.99	0.14	12,12,12,12	0
3	ZN	B	1001	1/1	0.99	0.16	7,7,7,7	0
3	ZN	J	1001	1/1	0.99	0.13	23,23,23,23	0
3	ZN	O	1001	1/1	0.99	0.14	34,34,34,34	0
3	ZN	D	1002	1/1	0.99	0.14	8,8,8,8	0
5	SO4	D	1008	5/5	0.99	0.18	15,15,15,15	0
3	ZN	Q	1001	1/1	0.99	0.10	46,46,46,46	0

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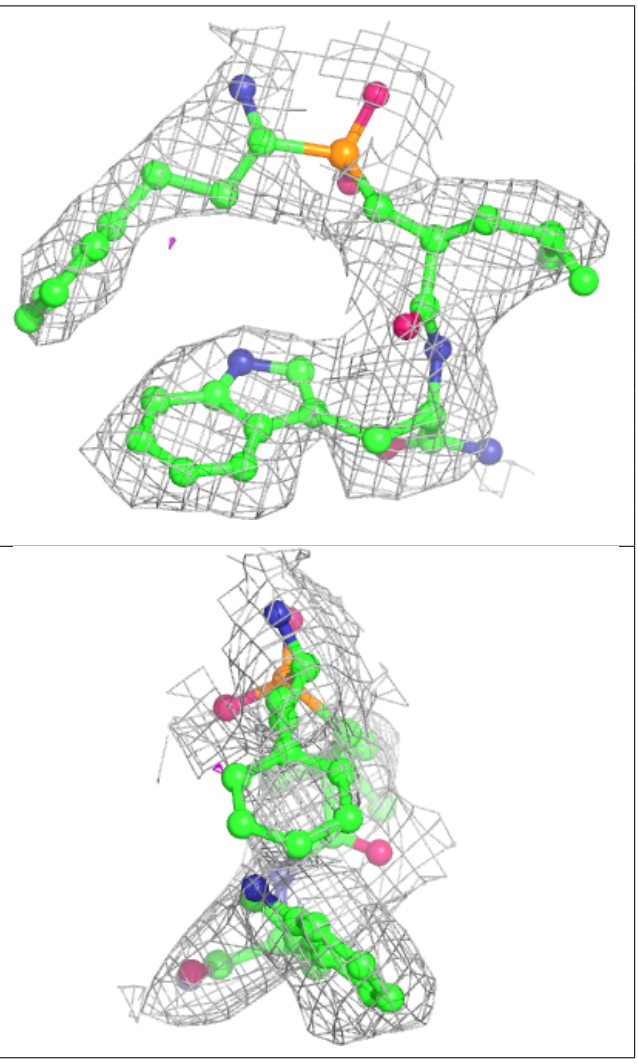
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	G	1007	5/5	0.99	0.17	22,23,23,23	0
3	ZN	H	1002	1/1	0.99	0.18	15,15,15,15	0
3	ZN	F	1002	1/1	1.00	0.15	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

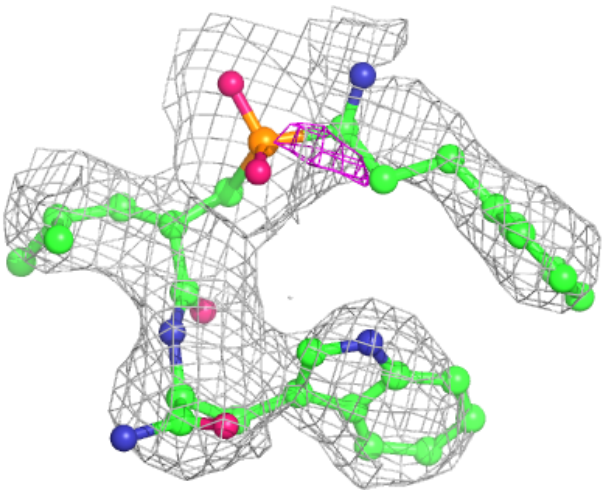
Electron density around P52 V 1002:

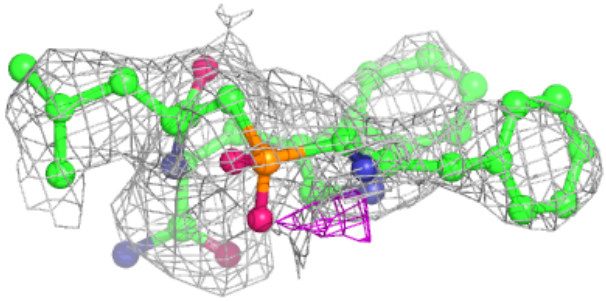
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

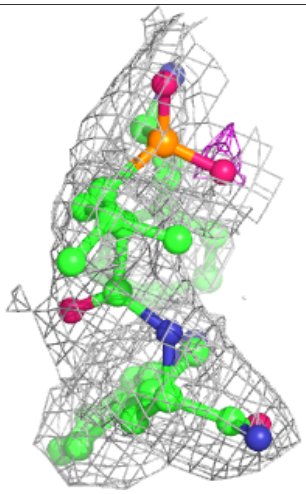


Electron density around P52 U 1003:

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

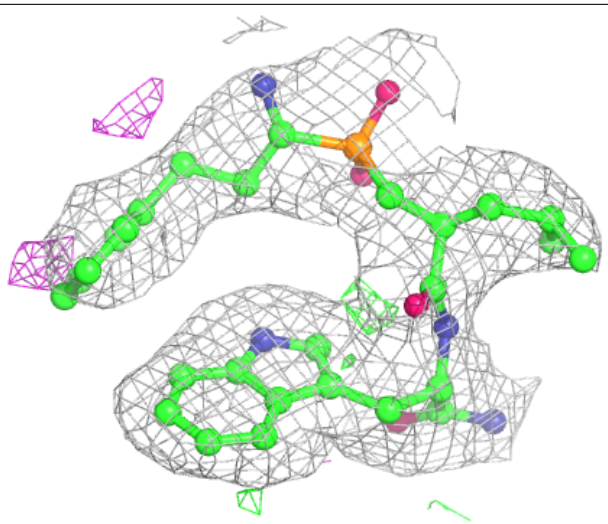


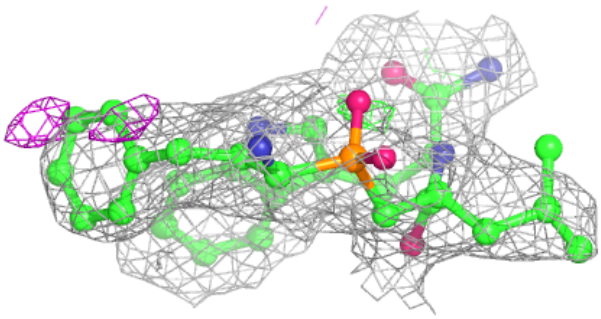


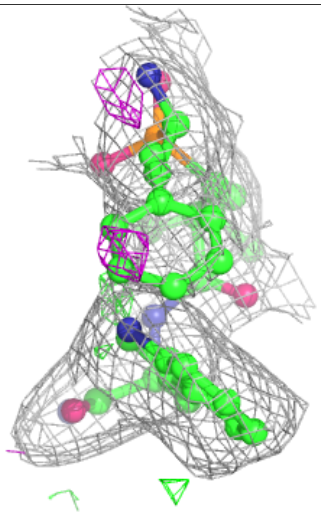


Electron density around P52 R 1002:

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

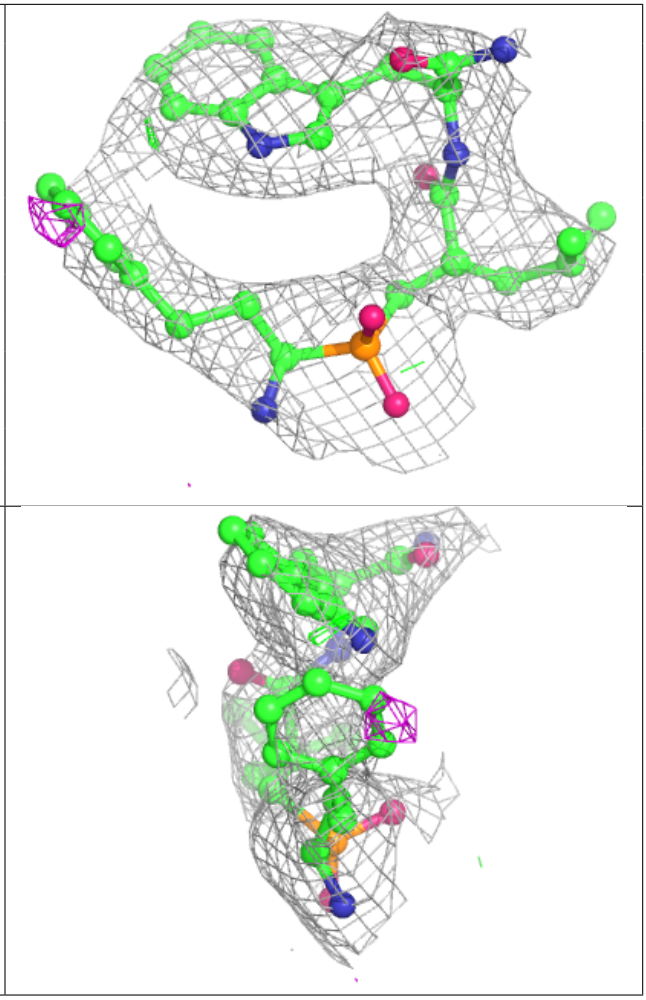






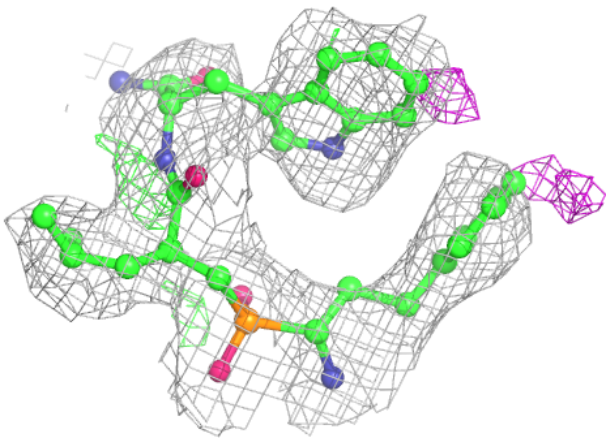
Electron density around P52 T 1003:

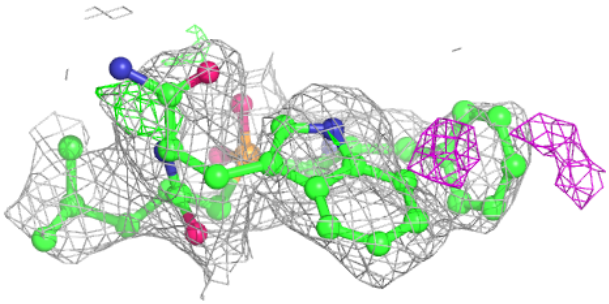
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

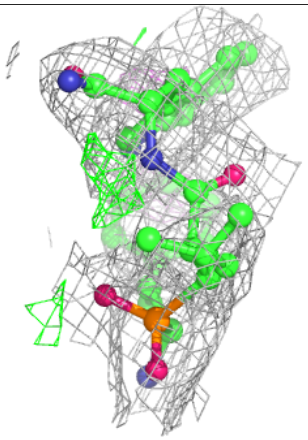


Electron density around P52 M 1003:

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

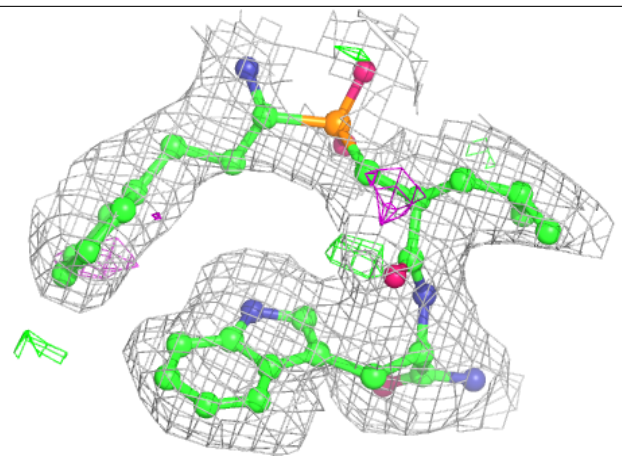


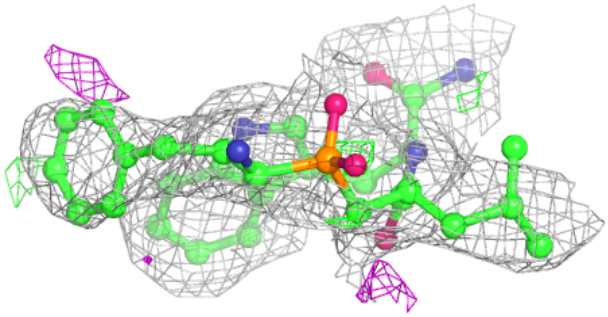


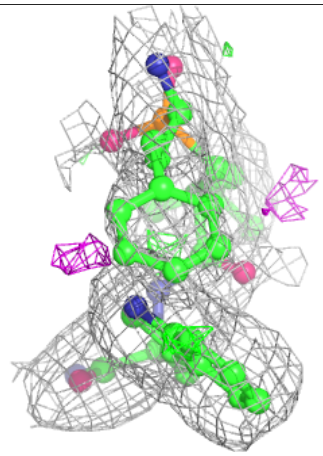


Electron density around P52 J 1002:

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

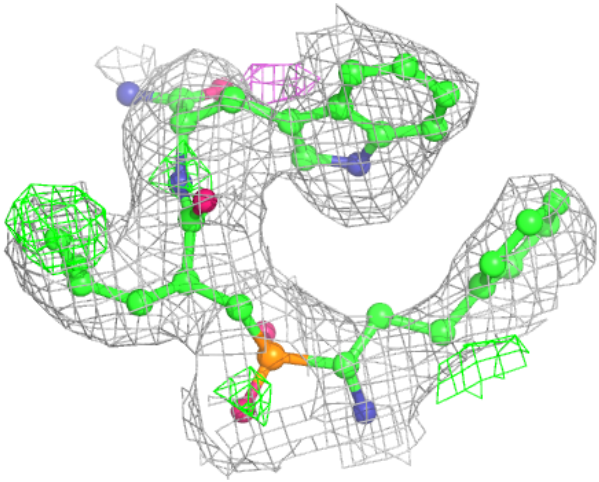


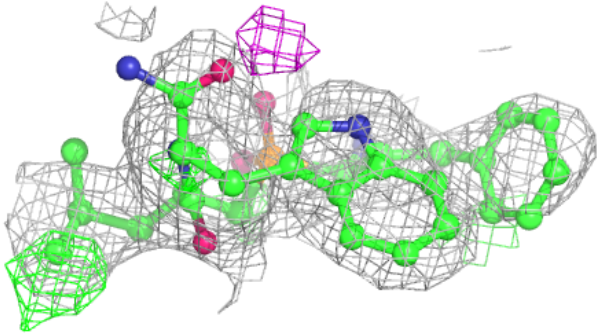


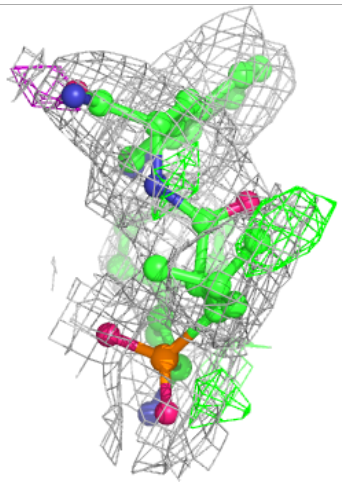


Electron density around P52 L 1003:

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

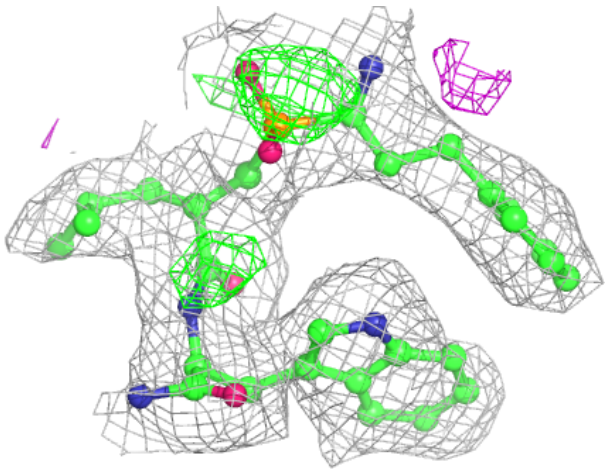


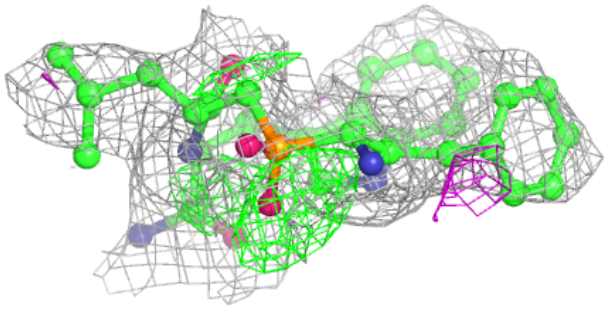


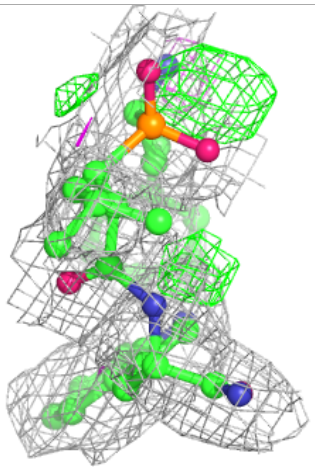


Electron density around P52 H 1003:

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

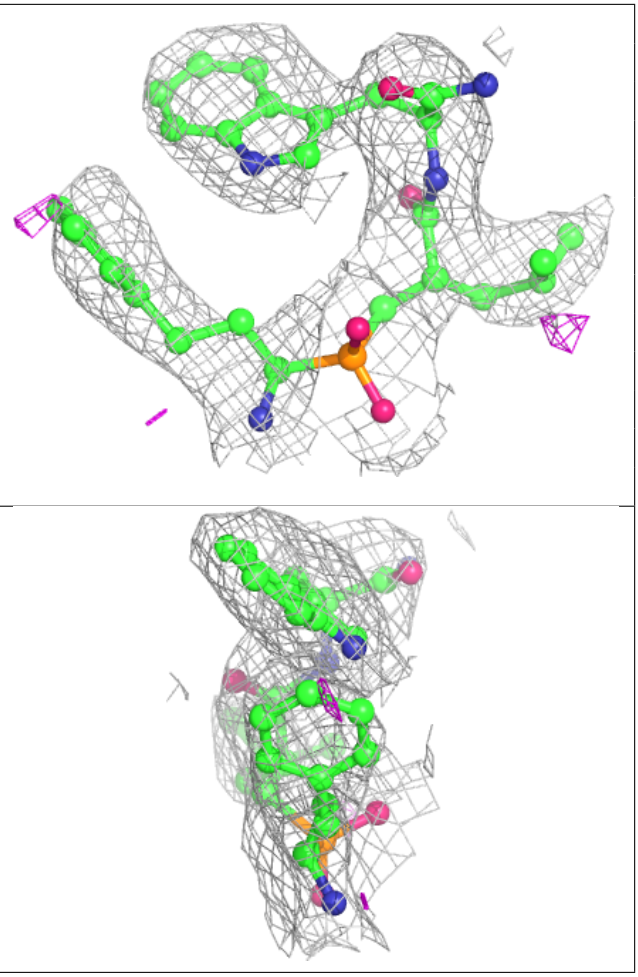






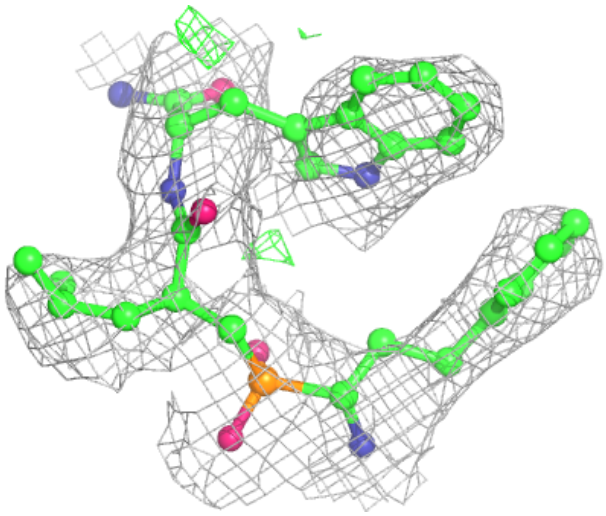
Electron density around P52 N 1003:

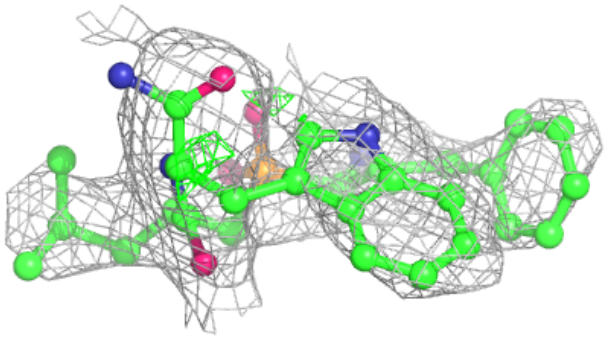
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

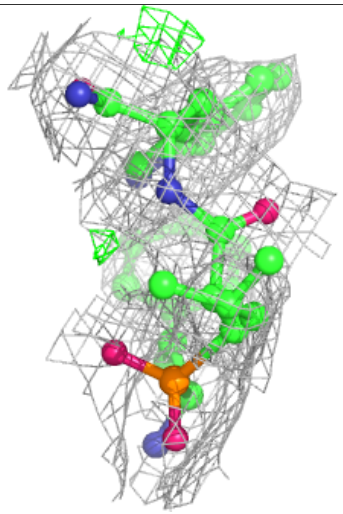


Electron density around P52 P 1002:

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

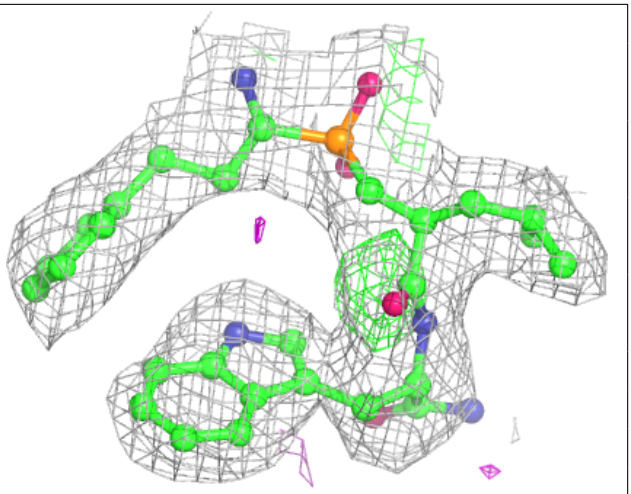


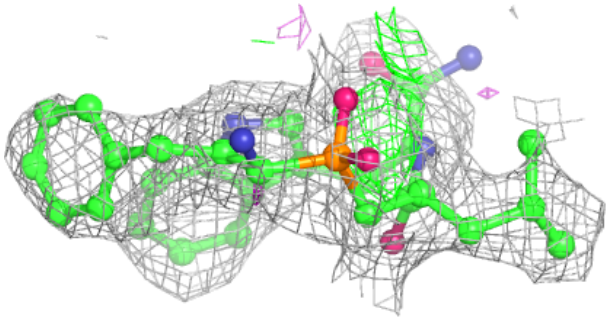


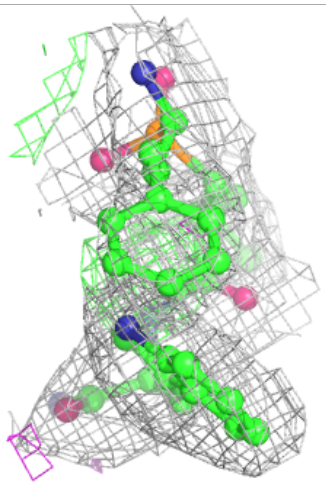


Electron density around P52 I 1003:

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

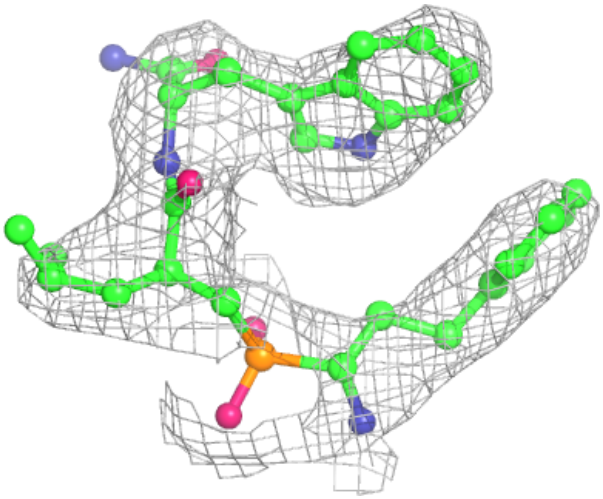


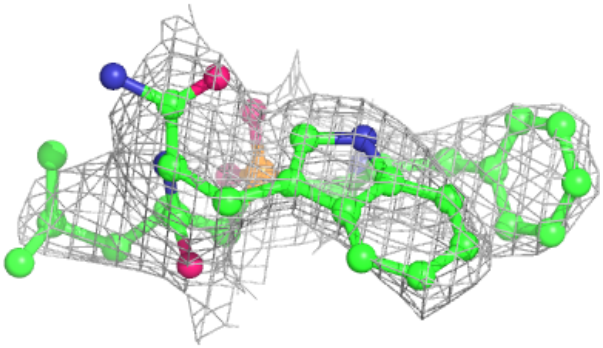


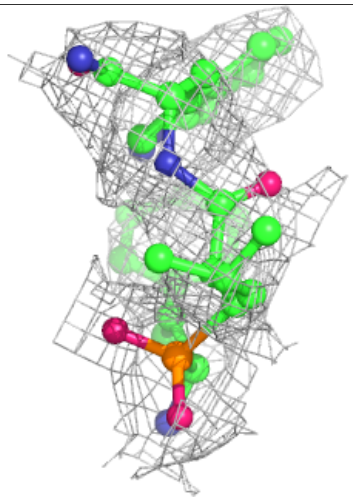


Electron density around P52 S 1003:

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

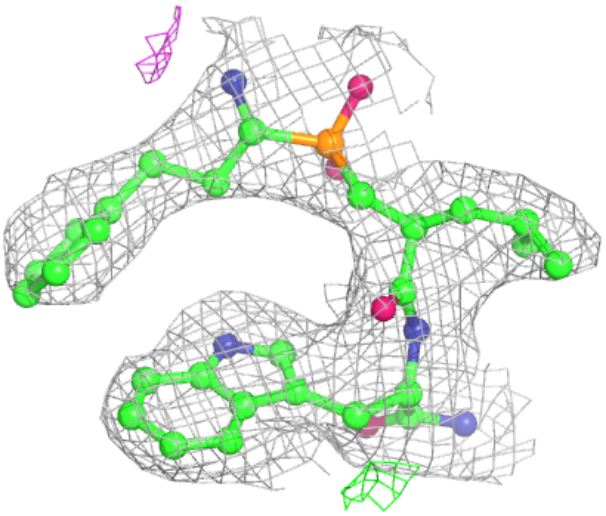


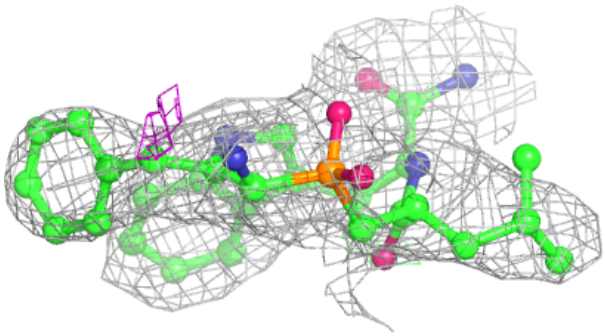


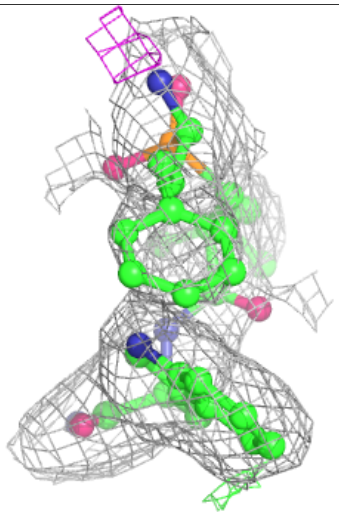


Electron density around P52 Q 1002:

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

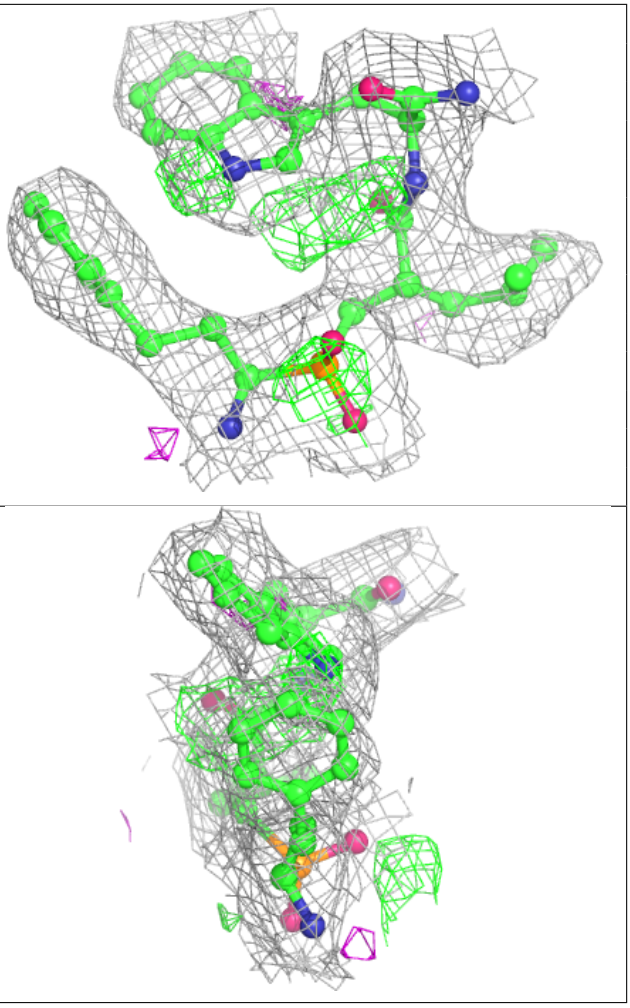






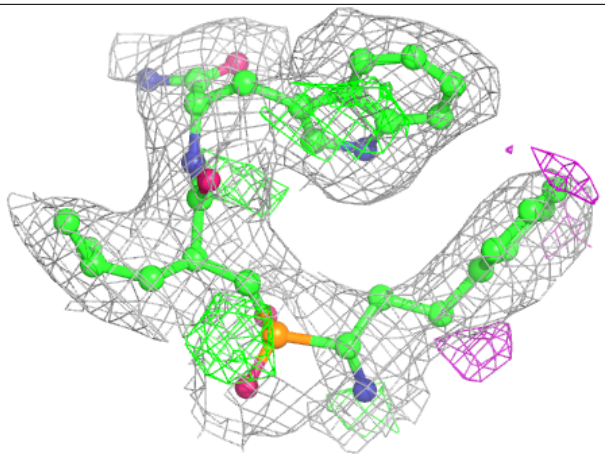
Electron density around P52 B 1002:

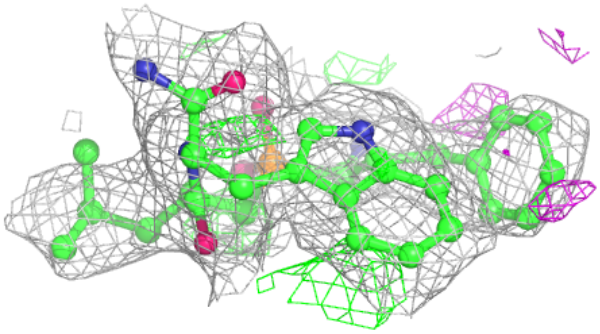
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

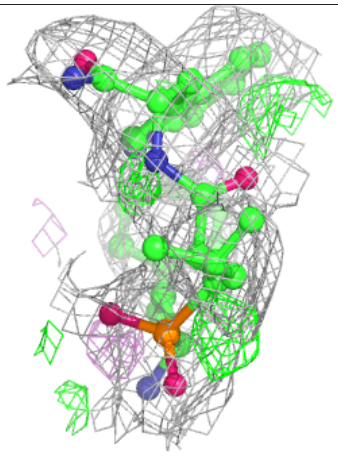


Electron density around P52 E 1003:

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

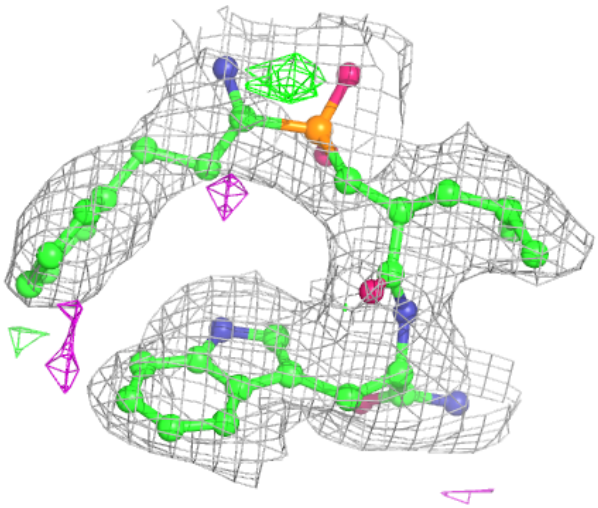


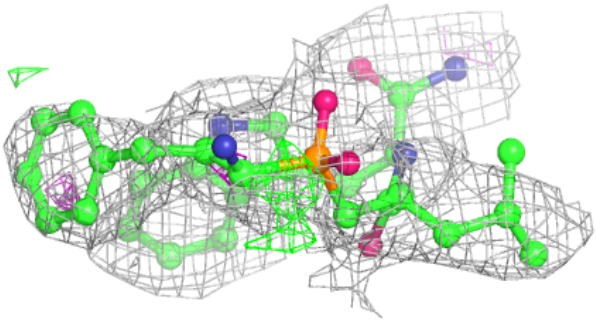


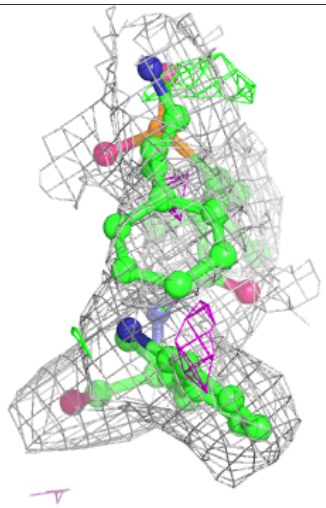


Electron density around P52 K 1002:

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

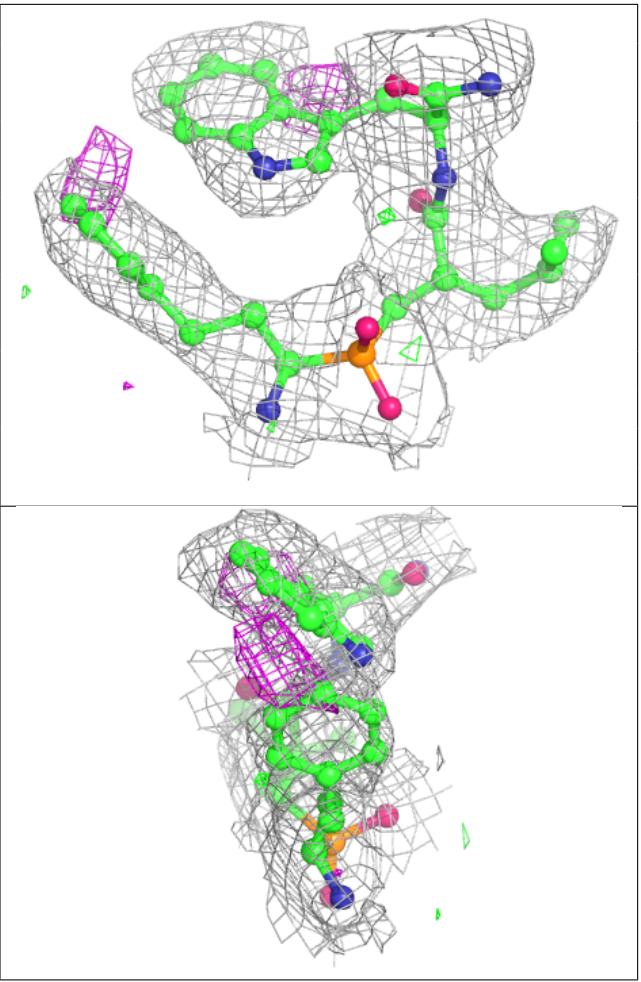






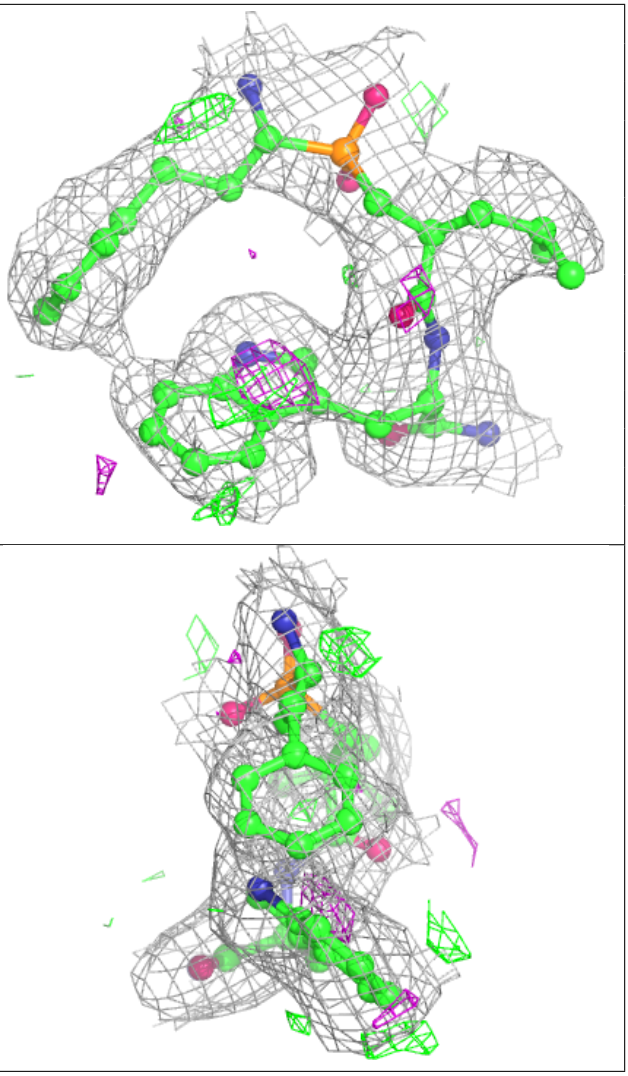
Electron density around P52 A 1002:

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



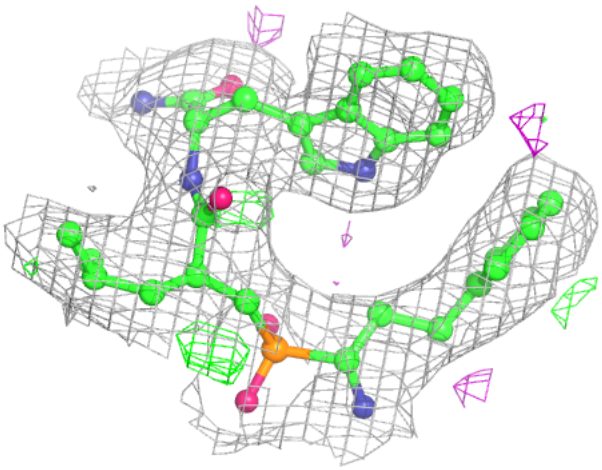
Electron density around P52 C 1002:

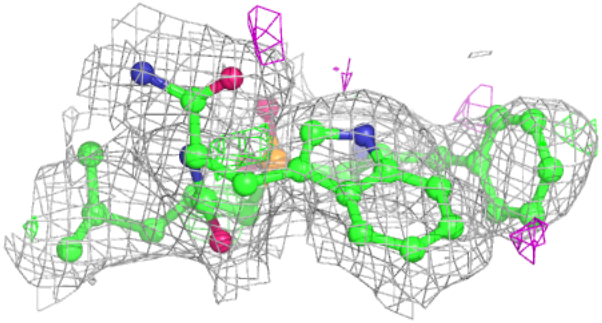
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

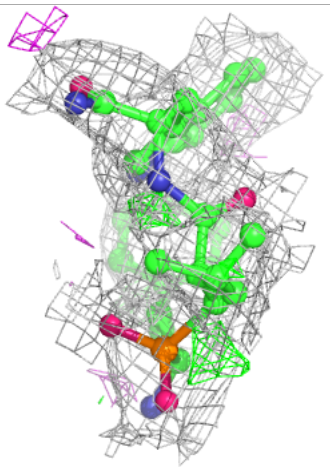


Electron density around P52 D 1003:

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

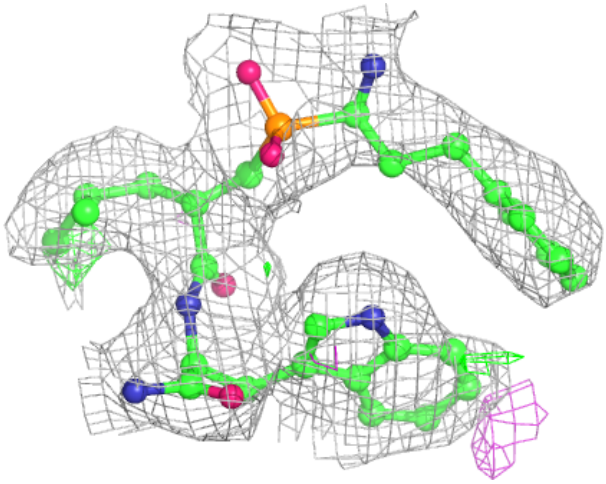


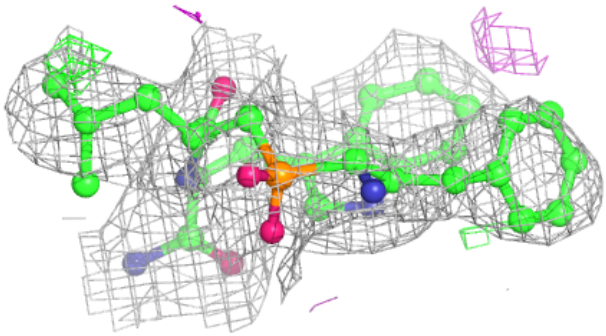


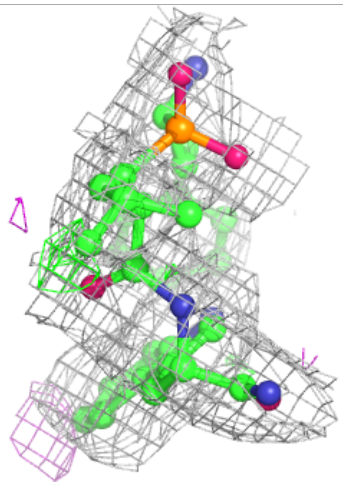


Electron density around P52 F 1003:

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

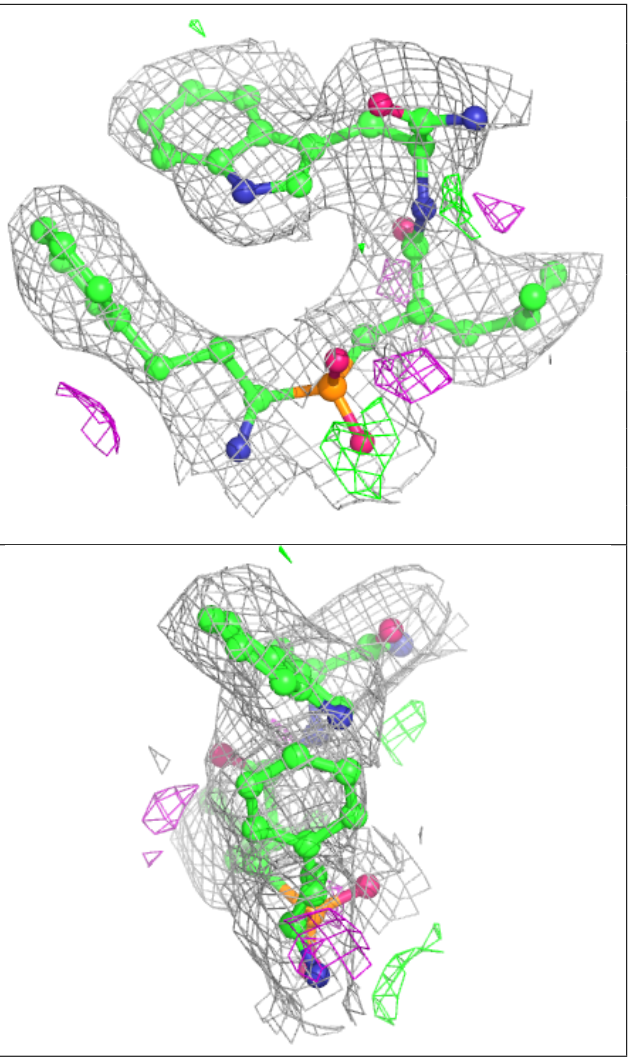






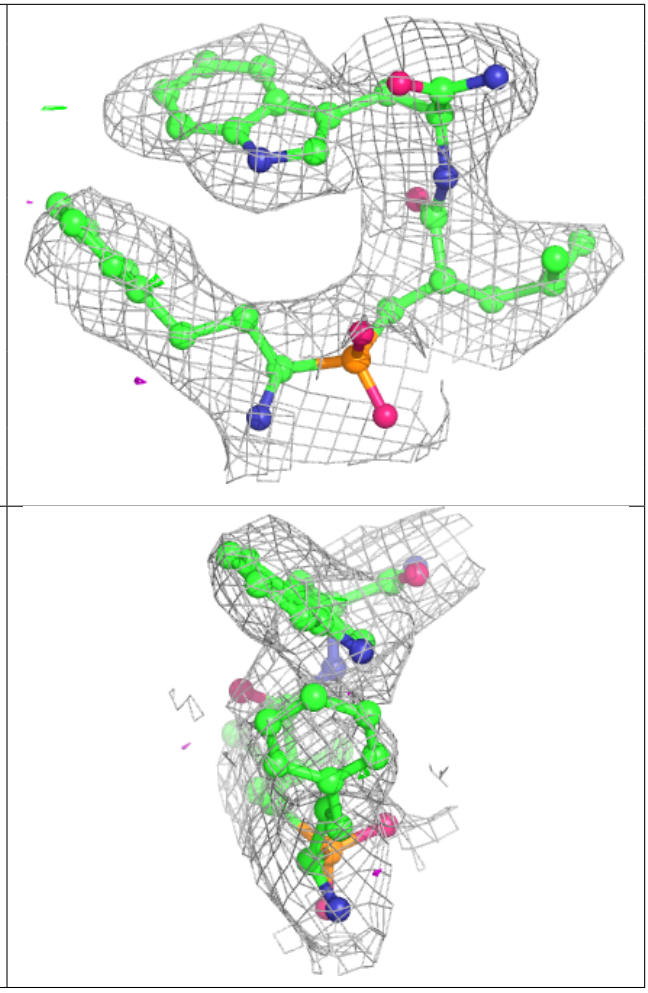
Electron density around P52 G 1002:

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



Electron density around P52 O 1002:

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



6.5 Other polymers (i)

There are no such residues in this entry.