



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:29 PM UTC

PDB ID : 6M8P / pdb_00006m8p
Title : Human ERAP1 bound to phosphinic pseudotriptide 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

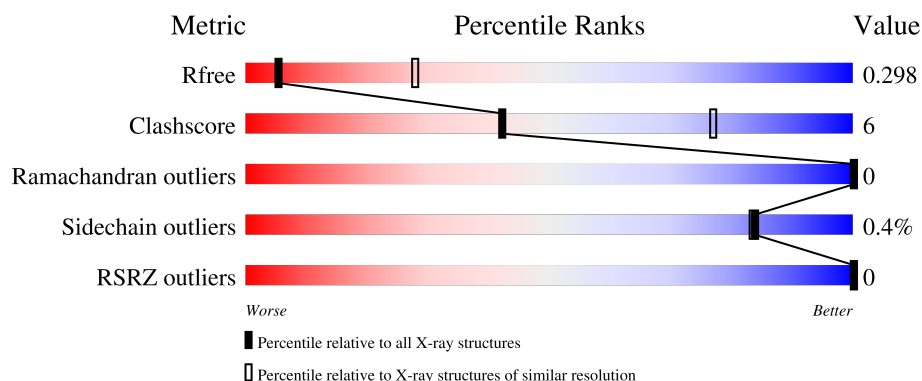
1 Overall quality at a glance

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.



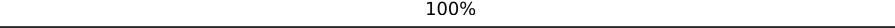
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	899	
1	B	899	
1	C	899	
1	D	899	
1	E	899	

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Mol	Chain	Length	Quality of chain
1	F	899	 82% 14% .
1	G	899	 83% 13% .
1	H	899	 82% 14% .
1	I	899	 83% 13% .
1	J	899	 83% 13% .
1	K	899	 83% 12% .
1	L	899	 81% 15% .
1	M	899	 82% 13% .
1	N	899	 84% 12% .
1	O	899	 82% 13% .
1	P	899	 83% 12% .
1	Q	899	 84% 12% .
1	R	899	 81% 15% .
1	S	899	 84% 12% .
1	T	899	 83% 12% .
1	U	899	 83% 13% .
1	V	899	 83% 12% .
2	0	3	 67% 33%
2	1	3	 33% 67%
2	2	3	 100%
2	3	3	 33% 67%
2	4	3	 67% 33%
2	5	3	 33% 67%
2	6	3	 67% 33%
2	7	3	 33% 67%

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Mol	Chain	Length	Quality of chain
2	8	3	
2	9	3	
2	AA	3	
2	BA	3	
2	CA	3	
2	DA	3	
2	W	3	
2	X	3	
2	Y	3	
2	Z	3	
2	a	3	
2	b	3	
2	c	3	
2	d	3	
2	e	3	
2	f	3	
2	g	3	
2	h	3	
2	i	3	
2	j	3	
2	k	3	
2	l	3	
2	m	3	
2	n	3	
2	o	3	

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Mol	Chain	Length	Quality of chain
2	p	3	
2	q	3	
2	r	3	
2	s	3	
2	t	3	
2	u	3	
2	v	3	
2	w	3	
2	x	3	
2	y	3	
2	z	3	

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	1	-	-	X	-
2	NAG	3	1	-	-	X	-
2	NAG	5	1	-	-	X	-
2	NAG	7	1	-	-	X	-
2	NAG	9	1	-	-	X	-
2	NAG	BA	1	-	-	X	-
2	NAG	DA	1	-	-	X	-
2	NAG	Z	1	-	-	X	-
2	NAG	b	1	-	-	X	-
2	NAG	d	1	-	-	X	-
2	NAG	j	1	-	-	X	-
2	NAG	l	1	-	-	X	-
2	NAG	t	1	-	-	X	-
2	NAG	x	1	-	-	X	-
2	NAG	z	1	-	-	X	-
5	SO4	A	1006	-	-	X	-
5	SO4	B	1006	-	-	X	-
5	SO4	C	1006	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	C	1009	-	-	X	-
5	SO4	D	1007	-	-	X	-
5	SO4	E	1001	-	-	X	-
5	SO4	E	1007	-	-	X	-
5	SO4	E	1010	-	-	X	-
5	SO4	F	1007	-	-	X	-
5	SO4	F	1010	-	-	X	-
5	SO4	G	1006	-	-	X	-
5	SO4	H	1007	-	-	X	-
5	SO4	I	1007	-	-	X	-
5	SO4	I	1010	-	-	X	-
5	SO4	I	1011	-	-	X	-
5	SO4	J	1006	-	-	X	-
5	SO4	K	1006	-	-	X	-
5	SO4	K	1009	-	-	X	-
5	SO4	K	1010	-	-	X	-
5	SO4	K	1024	-	-	X	-
5	SO4	L	1001	-	-	X	-
5	SO4	L	1007	-	-	X	-
5	SO4	L	1010	-	-	X	-
5	SO4	M	1007	-	-	X	-
5	SO4	M	1011	-	-	X	-
5	SO4	M	1012	-	-	X	-
5	SO4	N	1007	-	-	X	-
5	SO4	N	1010	-	-	X	-
5	SO4	O	1006	-	-	X	-
5	SO4	O	1010	-	-	X	-
5	SO4	P	1006	-	-	X	-
5	SO4	P	1009	-	-	X	-
5	SO4	Q	1006	-	-	X	-
5	SO4	Q	1022	-	-	X	-
5	SO4	R	1006	-	-	X	-
5	SO4	S	1007	-	-	X	-
5	SO4	S	1010	-	-	X	-
5	SO4	S	1011	-	-	X	-
5	SO4	T	1007	-	-	X	-
5	SO4	U	1007	-	-	X	-
5	SO4	U	1011	-	-	X	-
5	SO4	V	1006	-	-	X	-
5	SO4	V	1009	-	-	X	-
6	NAG	F	1023	-	-	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
1	A	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	B	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	C	861	Total	C	N	O	S	0	4	0
			6890	4449	1138	1269	34			
1	D	861	Total	C	N	O	S	0	4	0
			6891	4449	1137	1271	34			
1	E	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	F	861	Total	C	N	O	S	0	4	0
			6891	4449	1137	1271	34			
1	G	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	H	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	I	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	J	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	K	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	L	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	M	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	N	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	O	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			
1	P	861	Total	C	N	O	S	0	4	0
			6888	4448	1137	1269	34			

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

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	?	-	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	?	-	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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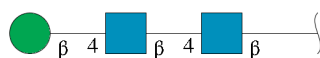
Chain	Residue	Modelled	Actual	Comment	Reference
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	ARG	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	GLN	deletion	UNP Q9NZ08
U	?	-	HIS	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	UNP Q9NZ08
U	?	-	SER	deletion	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
2	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	X	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	Z	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	a	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	b	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	c	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	d	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

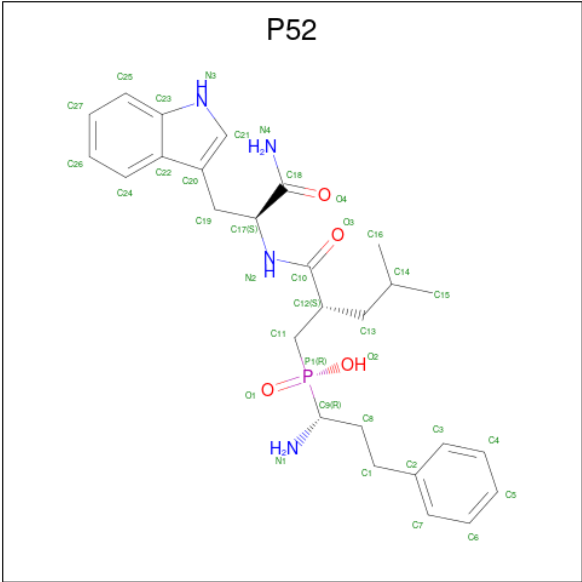
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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

- Molecule 4 is Nalpha-[(2S)-2-{[[(1R)-1-amino-3-phenylpropyl](hydroxy)phosphoryl]methyl}-4-methylpentanoyl]-L-tryptophanamide (CCD ID: P52) (formula: C₂₇H₃₇N₄O₄P).



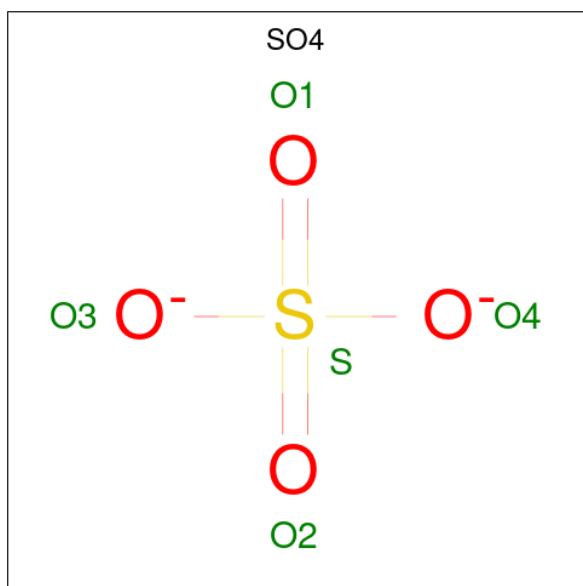
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	B	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	C	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	D	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	E	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	F	1	Total	C	N	O	P	0	0
			36	27	4	4	1		
4	G	1	Total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

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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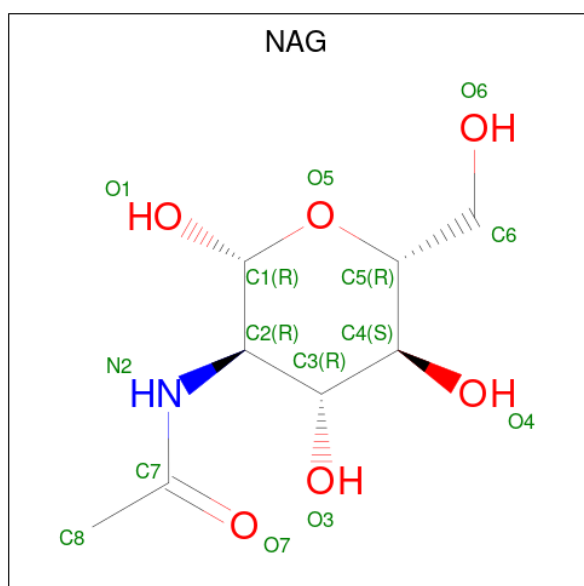
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	T	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		
5	T	1	Total	O	S	0	0
			5	4	1		
5	U	1	Total	O	S	0	0
			5	4	1		
5	U	1	Total	O	S	0	0
			5	4	1		
5	U	1	Total	O	S	0	0
			5	4	1		
5	U	1	Total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

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

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

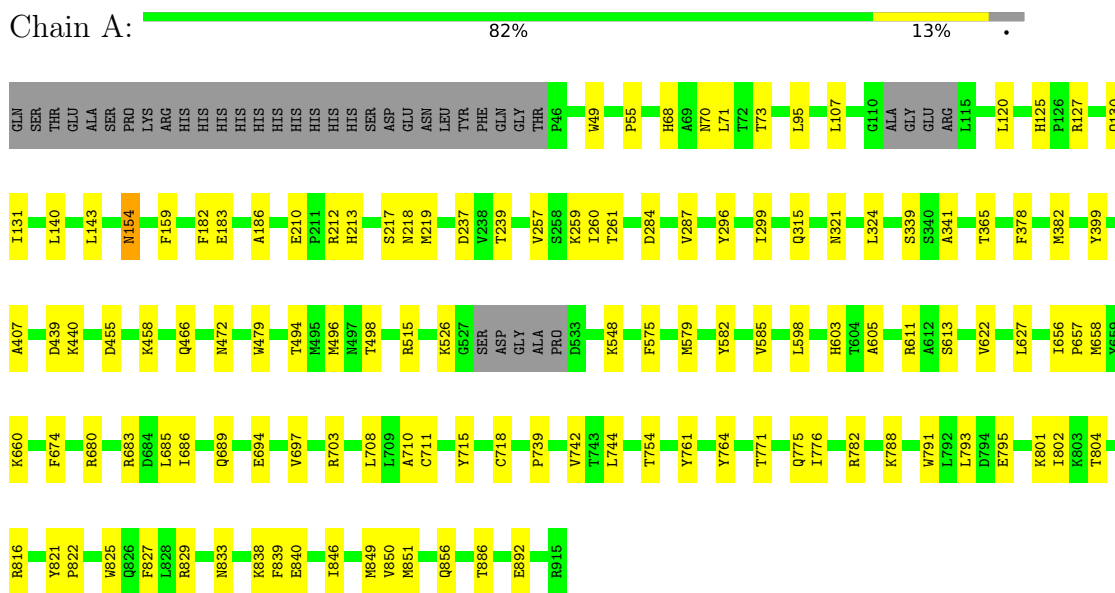


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1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

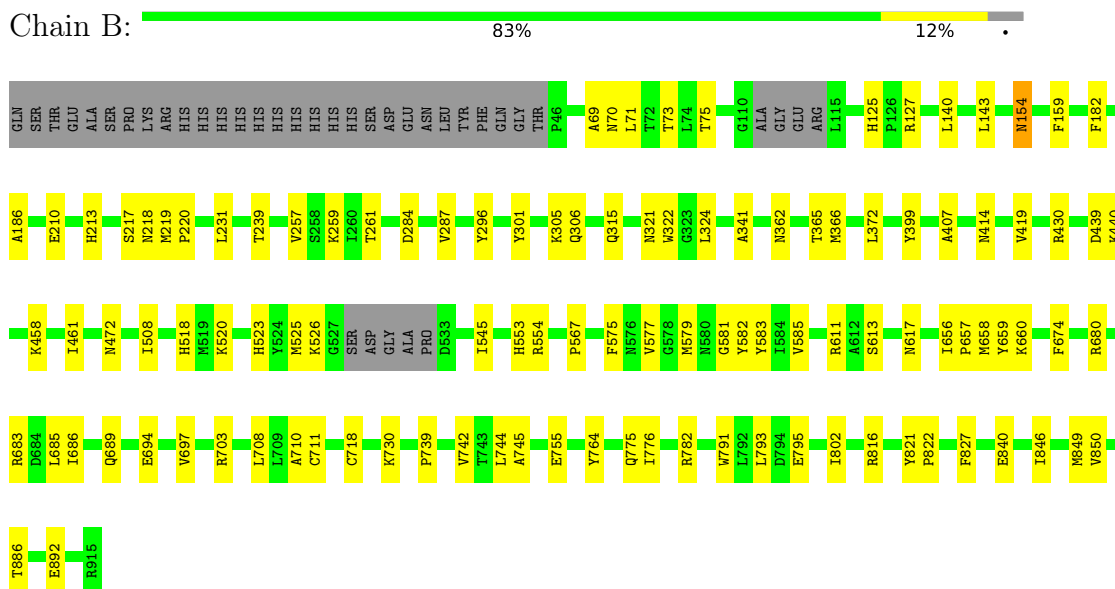
3 Residue-property plots

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

- Molecule 1: Endoplasmic reticulum aminopeptidase 1

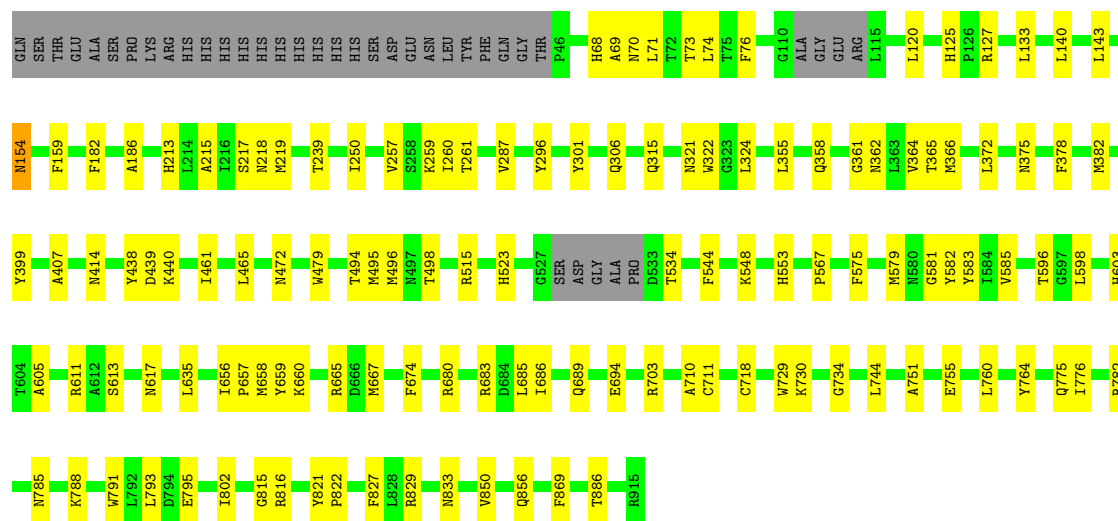


- Molecule 1: Endoplasmic reticulum aminopeptidase 1



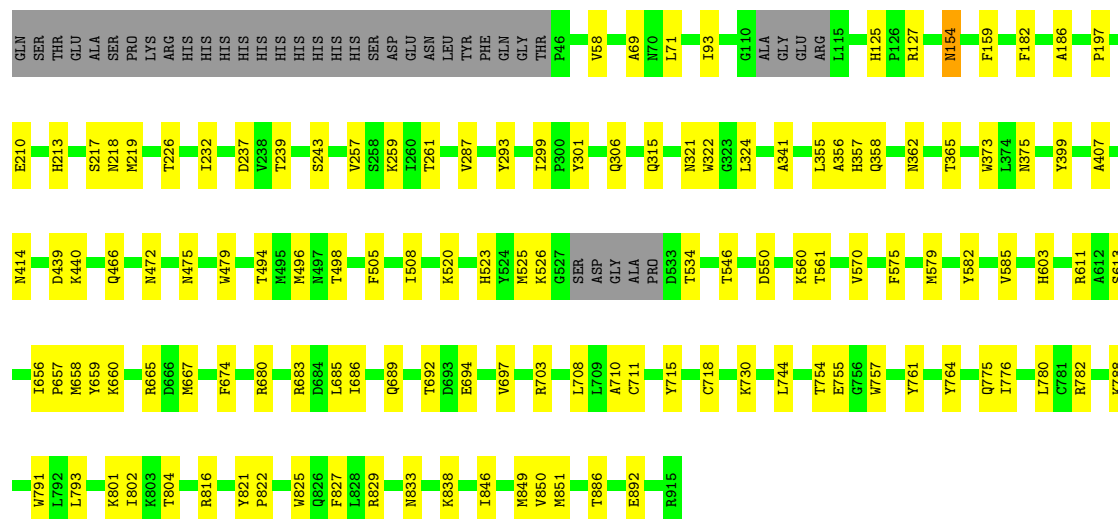
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain C: 82% 14% .



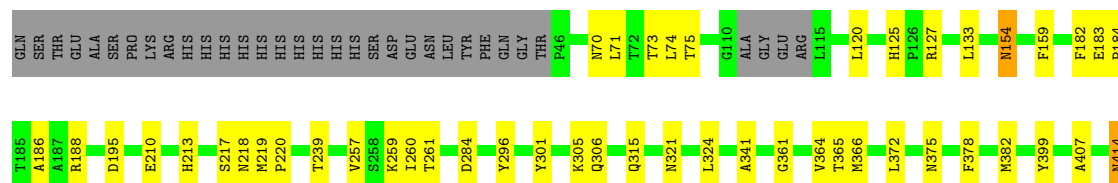
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

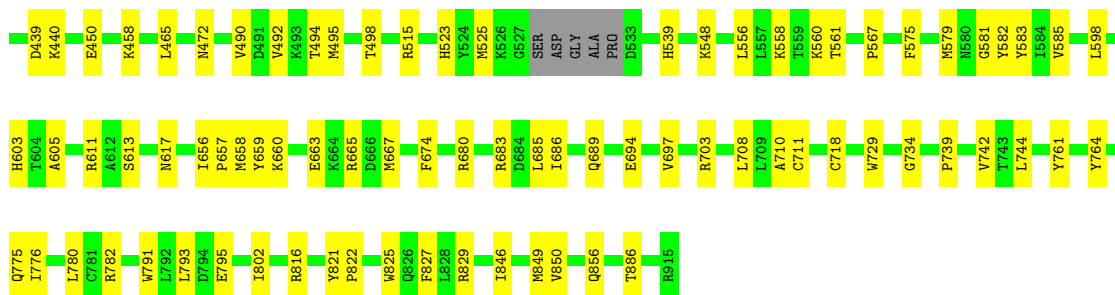
Chain D:  82% 14% .



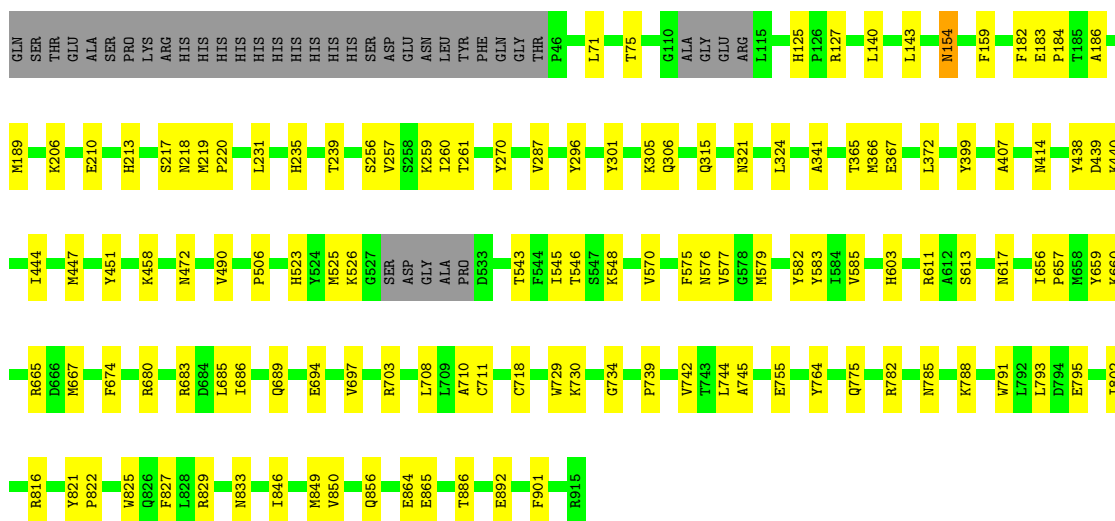
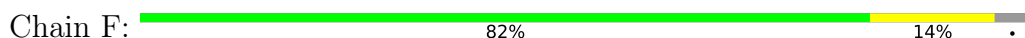
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain E:  82% 14% .

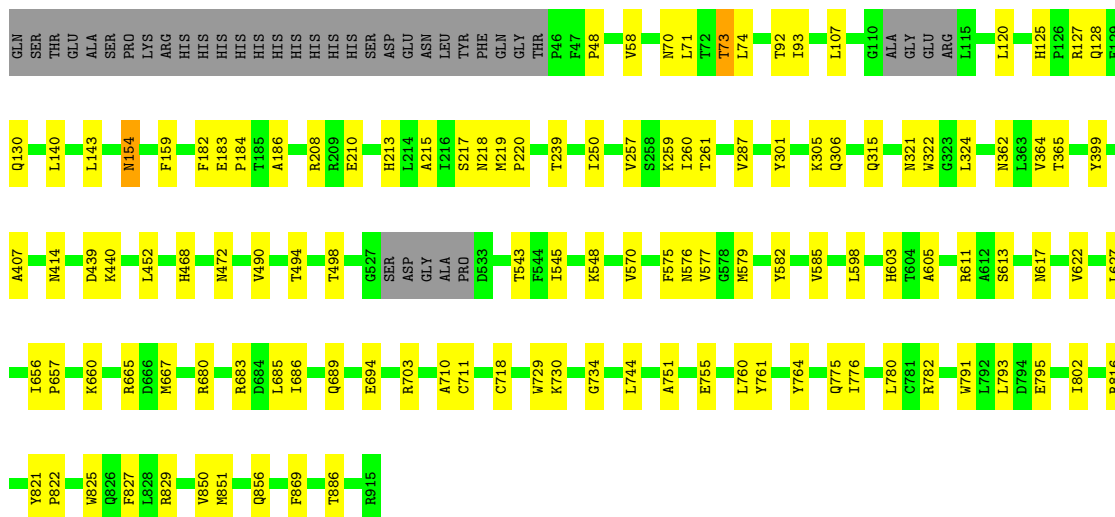
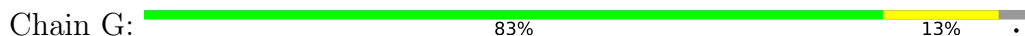




- Molecule 1: Endoplasmic reticulum aminopeptidase 1

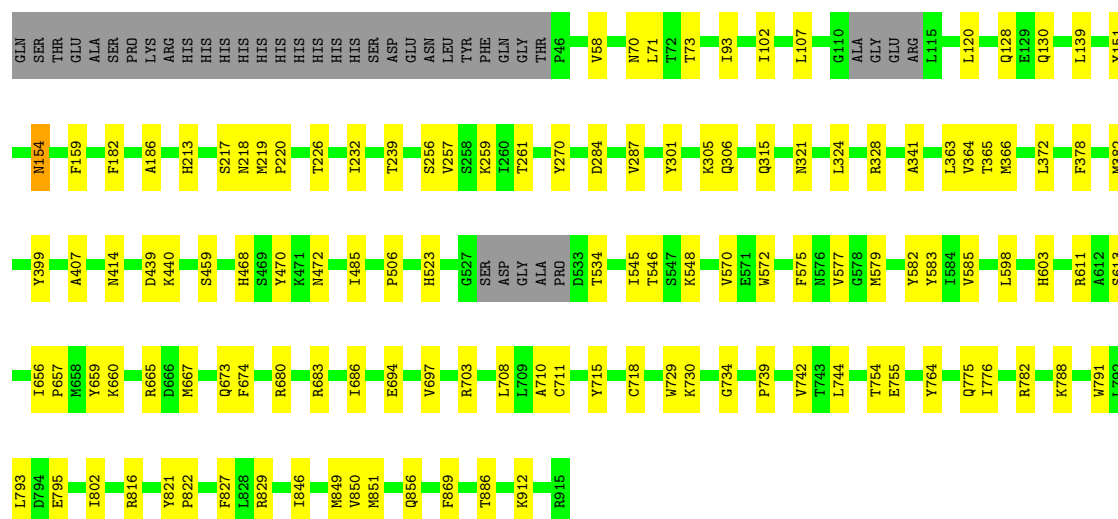


- Molecule 1: Endoplasmic reticulum aminopeptidase 1



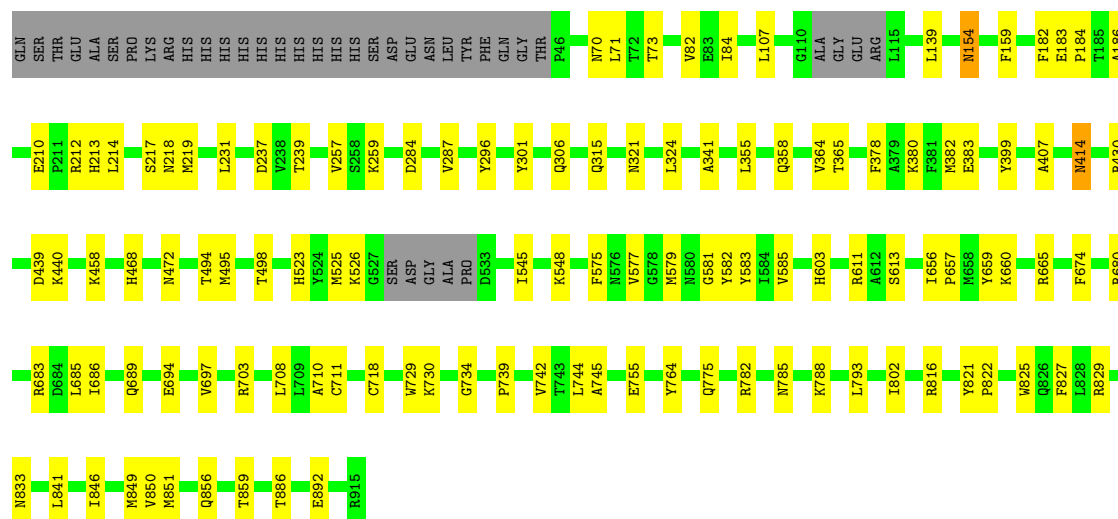
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain H:  82% 14% .



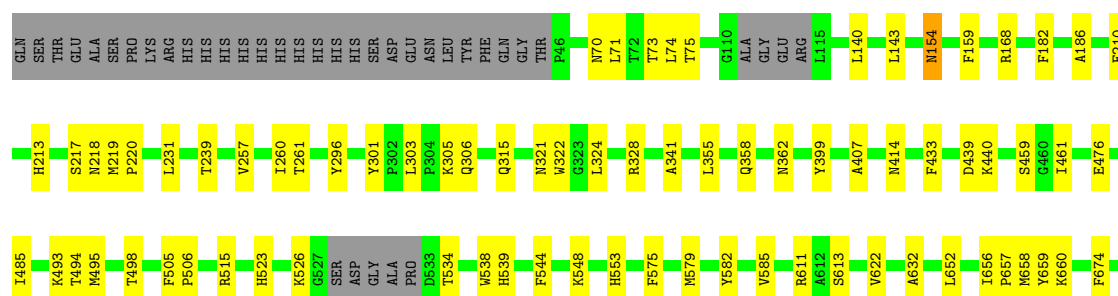
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

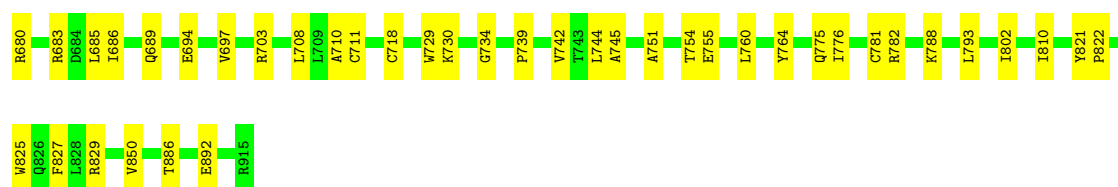
Chain I:  83% 13% .



• Molecule 1: Endoplasmic reticulum aminopeptidase 1

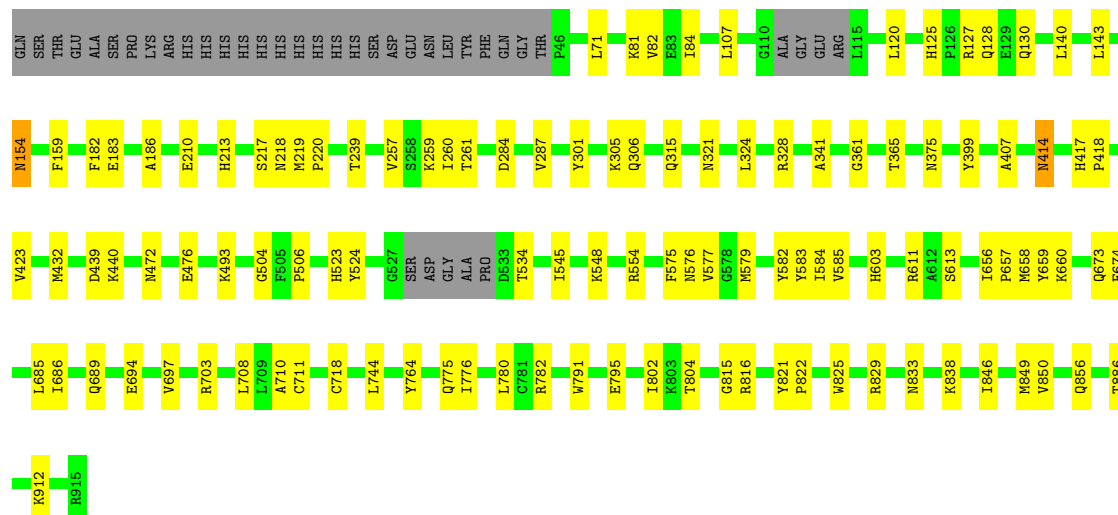
Chain J:  83% 13% .





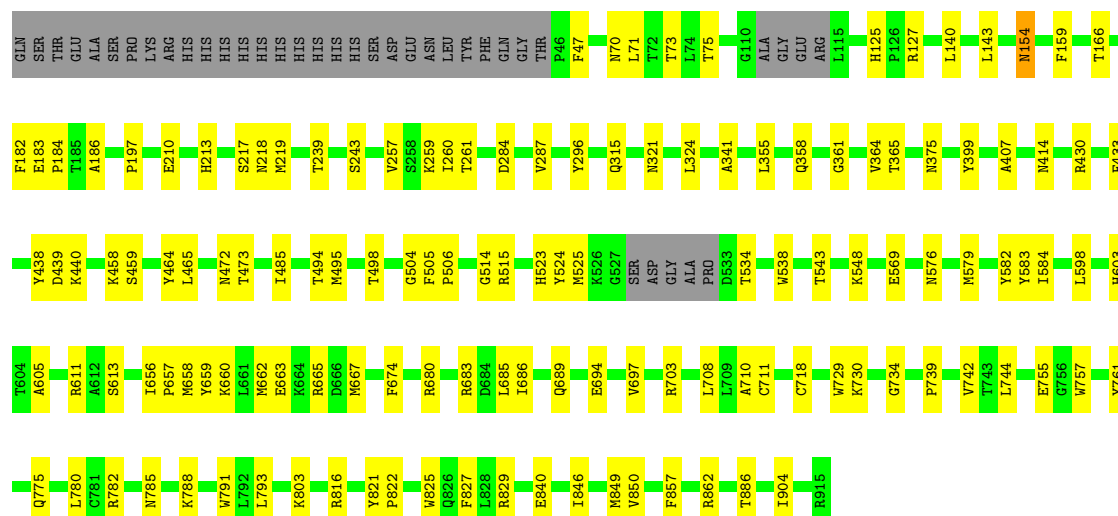
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain K: 83% 12% .



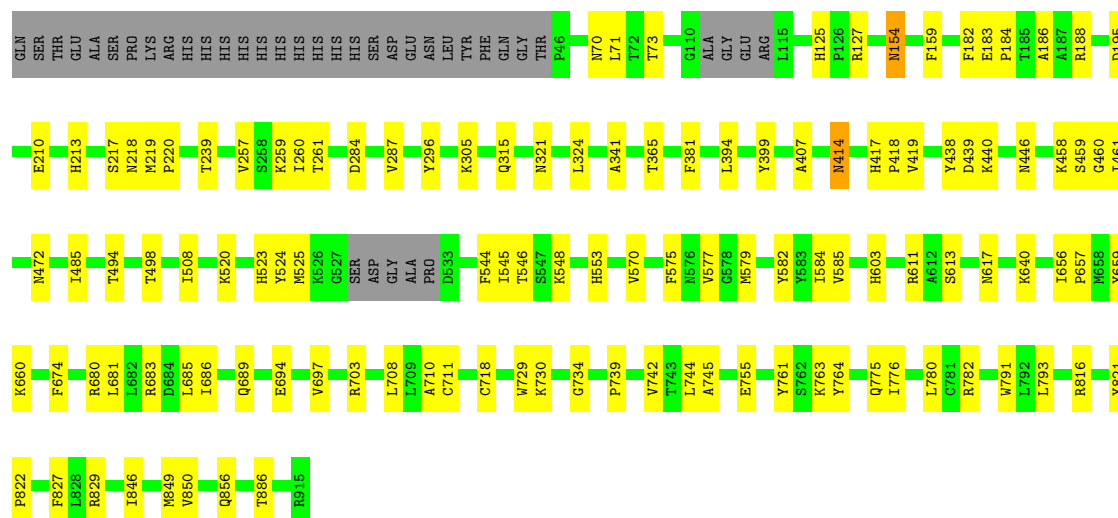
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain L: 81% 15% .



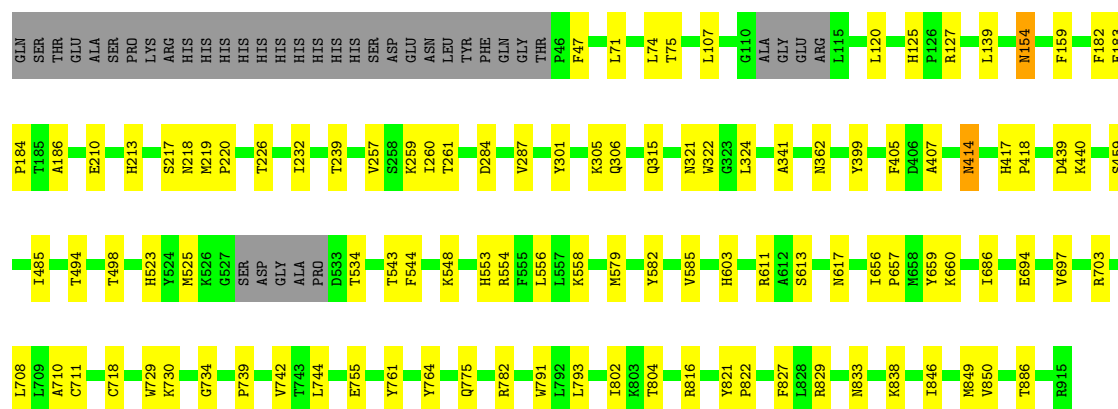
- Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain M: 82% 13% .



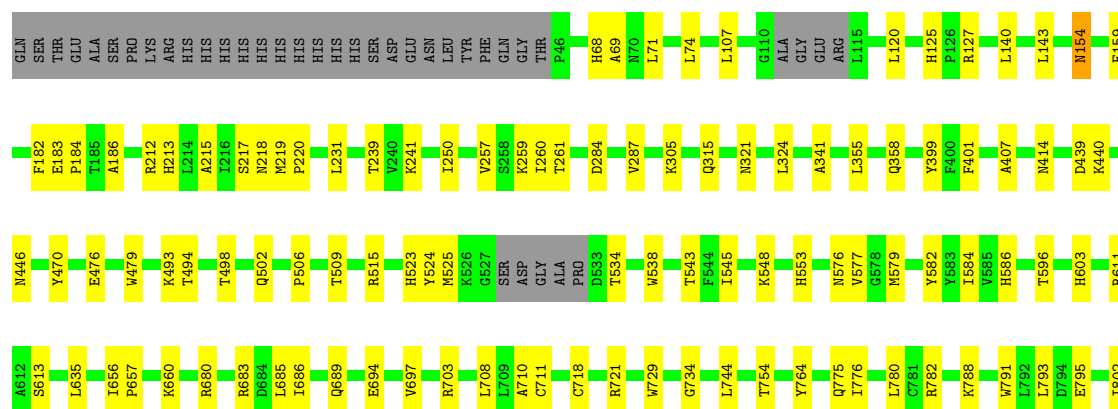
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain N: 84% 12% .

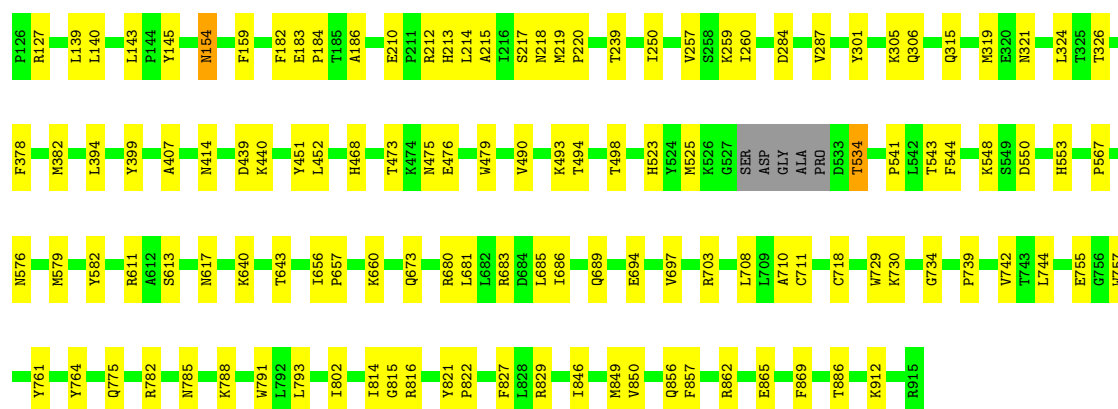


• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain O: 82% 13% .

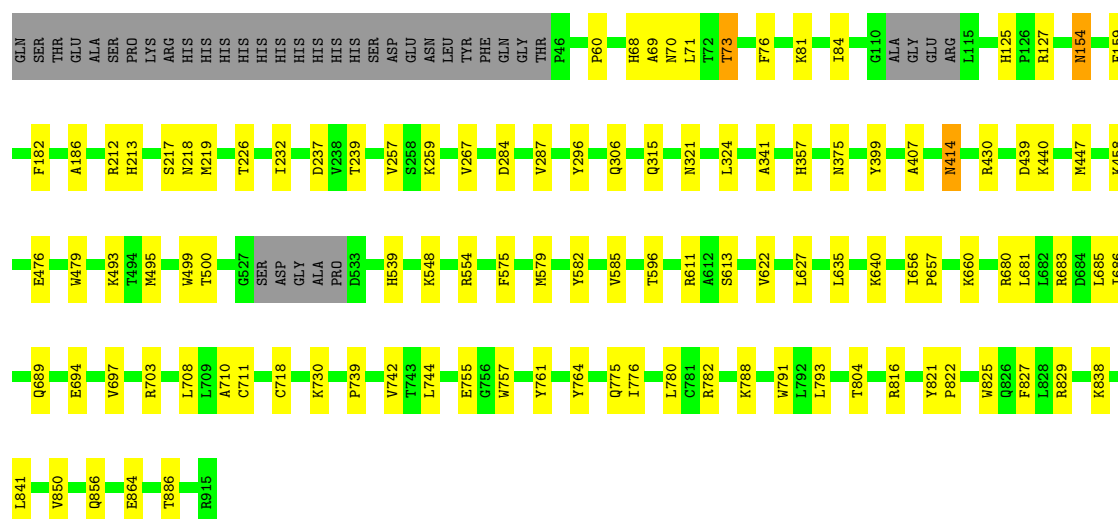






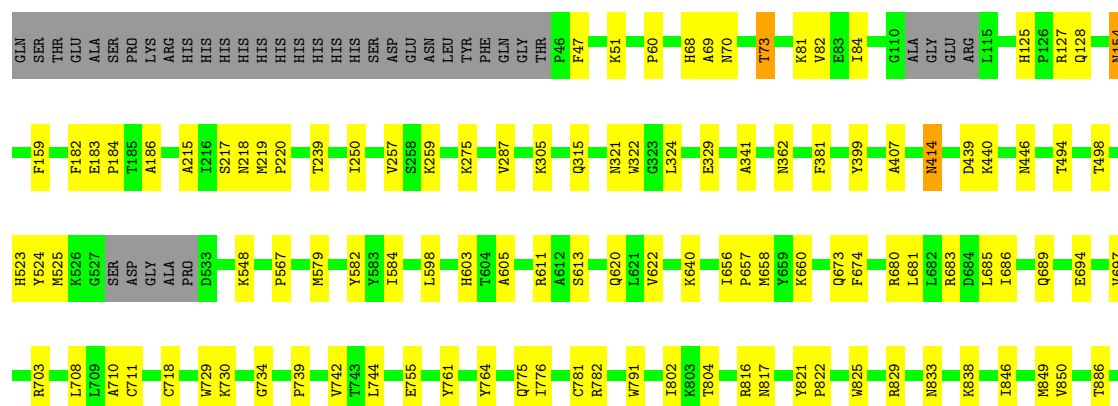
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain S: 84% 12% .



• Molecule 1: Endoplasmic reticulum aminopeptidase 1

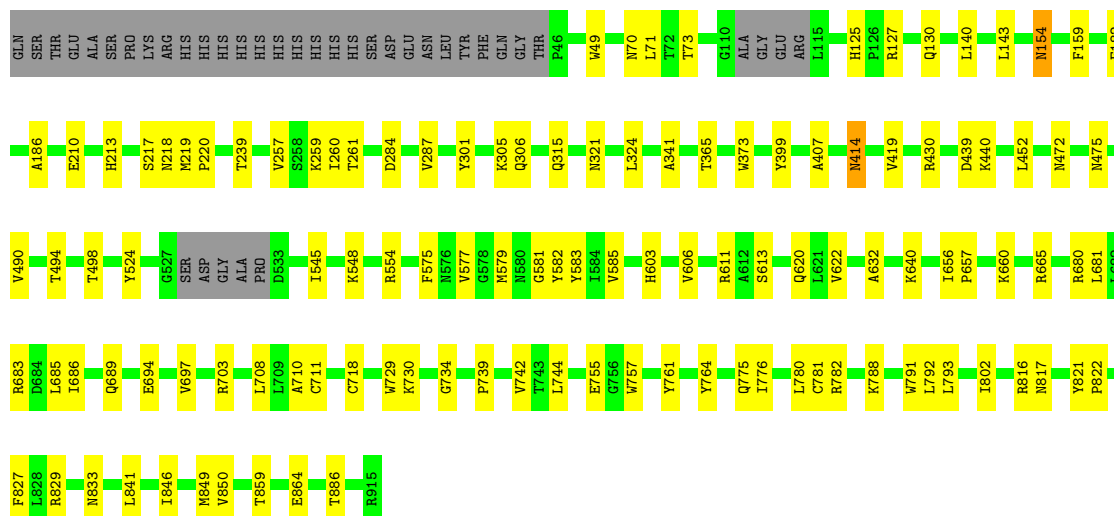
Chain T: 83% 12% .





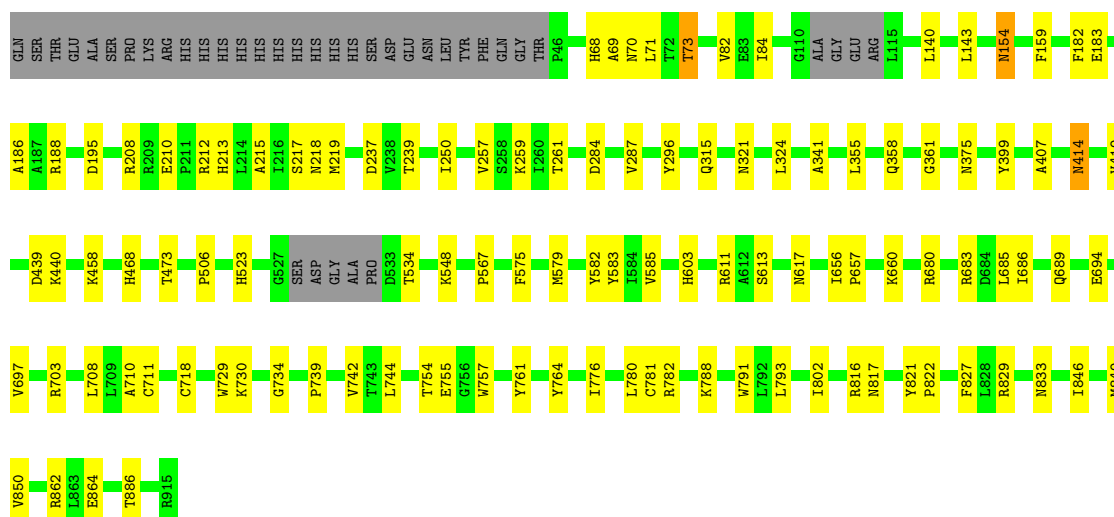
• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain U: 83% 13% .



• Molecule 1: Endoplasmic reticulum aminopeptidase 1

Chain V: 83% 12% .



• 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: 67% 33%



- 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:  67% 33%

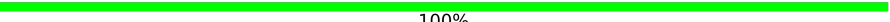


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  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 c:  67% 33%



- 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:  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 e:  67% 33%



- 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:  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 g:  67% 33%



- 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%



- 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:  67% 33%

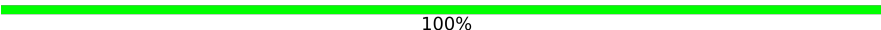


- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  33% 67%



- 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%

MAG1
MAG2
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%

MAG1
MAG2
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:  67% 33%

MAG1
MAG2
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%

MAG1
MAG2
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 o:  67% 33%

MAG1
MAG2
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 p:  33% 67%

MAG1
MAG2
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 q:  67% 33%



- 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:  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 s:  67% 33%



- 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:  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 u:  67% 33%



- 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%



- 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:  67% 33%



- 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%

MAG1
MAG2
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:  67% 33%

MAG1
MAG2
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%

MAG1
MAG2
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:  67% 33%

MAG1
MAG2
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 1:  33% 67%

MAG1
MAG2
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 2:  100%

MAG1
MAG2
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 3:  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



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



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



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



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



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



- 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:  67% 33%



- 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%



- 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:  67% 33%



- 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%



4 Data and refinement statistics

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 41.40 – 3.31	Depositor EDS
% Data completeness (in resolution range)	74.7 (41.40-3.31) 65.5 (41.40-3.31)	Depositor EDS
R_{merge}	1.40	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.285 , 0.295 0.286 , 0.298	Depositor DCC
R_{free} test set	2124 reflections (0.35%)	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 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, NAG, ZN, P52, BMA

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	0.15	0/7075	0.36	0/9602
1	B	0.17	1/7075 (0.0%)	0.36	0/9602
1	C	0.18	1/7077 (0.0%)	0.36	0/9604
1	D	0.16	0/7078	0.37	2/9606 (0.0%)
1	E	0.15	0/7075	0.36	0/9602
1	F	0.14	0/7078	0.36	0/9606
1	G	0.17	1/7075 (0.0%)	0.36	0/9602
1	H	0.15	0/7075	0.37	0/9602
1	I	0.14	0/7075	0.36	0/9602
1	J	0.17	0/7075	0.35	0/9602
1	K	0.15	0/7075	0.36	0/9602
1	L	0.16	0/7075	0.35	0/9602
1	M	0.15	0/7075	0.34	0/9602
1	N	0.16	0/7075	0.35	0/9602
1	O	0.15	0/7075	0.35	3/9602 (0.0%)
1	P	0.16	1/7075 (0.0%)	0.34	0/9602
1	Q	0.14	1/7075 (0.0%)	0.31	0/9602
1	R	0.15	0/7075	0.35	3/9602 (0.0%)
1	S	0.17	2/7075 (0.0%)	0.34	0/9602
1	T	0.15	1/7075 (0.0%)	0.35	2/9602 (0.0%)
1	U	0.14	0/7075	0.34	0/9602
1	V	0.15	1/7075 (0.0%)	0.35	3/9602 (0.0%)
All	All	0.16	9/155658 (0.0%)	0.35	13/211254 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	69	ALA	C-N	-8.11	1.22	1.33
1	B	69	ALA	C-N	-6.07	1.24	1.33
1	S	73	THR	C-N	-5.76	1.25	1.33
1	S	69	ALA	C-N	-5.67	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	73	THR	C-N	-5.56	1.26	1.33
1	V	73	THR	C-N	-5.24	1.26	1.33
1	G	73	THR	C-N	-5.16	1.26	1.33
1	P	69	ALA	C-N	5.16	1.41	1.33
1	T	73	THR	C-N	-5.12	1.26	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	69	ALA	CA-C-N	-5.96	114.37	123.07
1	O	69	ALA	C-N-CA	-5.96	114.37	123.07
1	V	69	ALA	CA-C-N	-5.83	114.56	123.07
1	V	69	ALA	C-N-CA	-5.83	114.56	123.07
1	V	69	ALA	O-C-N	5.38	129.48	123.19
1	O	69	ALA	O-C-N	5.34	129.44	123.19
1	R	69	ALA	O-C-N	5.18	129.25	123.19
1	D	69	ALA	CA-C-N	-5.15	115.56	123.07
1	D	69	ALA	C-N-CA	-5.15	115.56	123.07
1	R	69	ALA	CA-C-N	-5.07	115.66	123.07
1	R	69	ALA	C-N-CA	-5.07	115.66	123.07
1	T	69	ALA	CA-C-N	-5.03	115.73	123.07
1	T	69	ALA	C-N-CA	-5.03	115.73	123.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6888	0	6747	75	0
1	B	6888	0	6749	77	0
1	C	6890	0	6756	91	0
1	D	6891	0	6751	85	0
1	E	6888	0	6749	87	0
1	F	6891	0	6751	92	0
1	G	6888	0	6749	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	6888	0	6749	84	0
1	I	6888	0	6749	87	0
1	J	6888	0	6749	85	0
1	K	6888	0	6749	84	0
1	L	6888	0	6749	97	0
1	M	6888	0	6749	90	0
1	N	6888	0	6749	79	0
1	O	6888	0	6749	88	0
1	P	6888	0	6749	82	0
1	Q	6888	0	6749	79	0
1	R	6888	0	6749	95	0
1	S	6888	0	6749	78	0
1	T	6888	0	6749	77	0
1	U	6888	0	6749	83	0
1	V	6888	0	6749	82	0
2	0	39	0	34	1	0
2	1	39	0	34	8	0
2	2	39	0	34	0	0
2	3	39	0	34	9	0
2	4	39	0	34	2	0
2	5	39	0	34	9	0
2	6	39	0	34	1	0
2	7	39	0	34	9	0
2	8	39	0	34	1	0
2	9	39	0	34	9	0
2	AA	39	0	34	1	0
2	BA	39	0	34	8	0
2	CA	39	0	34	2	0
2	DA	39	0	34	8	0
2	W	39	0	34	2	0
2	X	39	0	34	4	0
2	Y	39	0	34	2	0
2	Z	39	0	34	8	0
2	a	39	0	34	0	0
2	b	39	0	34	8	0
2	c	39	0	34	1	0
2	d	39	0	34	9	0
2	e	39	0	34	1	0
2	f	39	0	34	8	0
2	g	39	0	34	2	0
2	h	39	0	34	8	0
2	i	39	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	j	39	0	34	9	0
2	k	39	0	34	0	0
2	l	39	0	34	8	0
2	m	39	0	34	2	0
2	n	39	0	34	8	0
2	o	39	0	34	2	0
2	p	39	0	34	8	0
2	q	39	0	34	1	0
2	r	39	0	34	8	0
2	s	39	0	34	1	0
2	t	39	0	34	9	0
2	u	39	0	34	1	0
2	v	39	0	34	8	0
2	w	39	0	34	1	0
2	x	39	0	34	9	0
2	y	39	0	34	2	0
2	z	39	0	34	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
3	U	1	0	0	0	0
3	V	1	0	0	0	0
4	A	36	0	37	1	0
4	B	36	0	36	1	0
4	C	36	0	37	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	36	0	37	1	0
4	E	36	0	36	1	0
4	F	36	0	37	1	0
4	G	36	0	37	0	0
4	H	36	0	37	0	0
4	I	36	0	37	1	0
4	J	36	0	37	1	0
4	K	36	0	36	1	0
4	L	36	0	36	3	0
4	M	36	0	37	2	0
4	N	36	0	37	0	0
4	O	36	0	37	0	0
4	P	36	0	36	1	0
4	Q	36	0	37	2	0
4	R	36	0	37	0	0
4	S	36	0	37	0	0
4	T	36	0	36	1	0
4	U	36	0	37	0	0
4	V	36	0	37	1	0
5	A	65	0	0	6	0
5	B	70	0	0	5	0
5	C	70	0	0	9	0
5	D	70	0	0	7	0
5	E	70	0	0	7	0
5	F	70	0	0	9	0
5	G	75	0	0	7	0
5	H	70	0	0	5	0
5	I	70	0	0	10	0
5	J	65	0	0	7	0
5	K	80	0	0	11	0
5	L	70	0	0	9	0
5	M	75	0	0	10	0
5	N	70	0	0	9	0
5	O	70	0	0	10	0
5	P	65	0	0	7	0
5	Q	65	0	0	8	0
5	R	75	0	0	8	0
5	S	70	0	0	12	0
5	T	70	0	0	6	0
5	U	75	0	0	12	0
5	V	65	0	0	11	0
6	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	13	6	0
6	C	14	0	13	5	0
6	D	14	0	13	5	0
6	E	14	0	13	6	0
6	F	14	0	13	7	0
6	G	14	0	13	5	0
6	H	14	0	13	5	0
6	I	14	0	13	6	0
6	J	14	0	13	6	0
6	K	14	0	13	6	0
6	L	14	0	13	6	0
6	M	14	0	13	5	0
6	N	14	0	13	5	0
6	O	14	0	13	5	0
6	P	14	0	13	5	0
6	Q	14	0	13	6	0
6	R	14	0	13	6	0
6	S	14	0	13	5	0
6	T	14	0	13	5	0
6	U	14	0	13	5	0
6	V	14	0	13	6	0
All	All	155927	0	151077	1938	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1938) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:414:ASN:HD21	6:G:1023:NAG:C1	1.18	1.56
1:F:414:ASN:HD21	6:F:1023:NAG:C1	1.14	1.55
1:O:414:ASN:HD21	6:O:1023:NAG:C1	1.18	1.54
1:E:414:ASN:HD21	6:E:1023:NAG:C1	1.22	1.52
1:H:414:ASN:HD21	6:H:1023:NAG:C1	1.23	1.49
1:L:414:ASN:HD21	6:L:1023:NAG:C1	1.23	1.47
1:Q:414:ASN:HD21	6:Q:1021:NAG:C1	1.25	1.47
1:B:414:ASN:HD21	6:B:1022:NAG:C1	1.24	1.46
1:D:414:ASN:HD21	6:D:1023:NAG:C1	1.26	1.46
1:K:414:ASN:HD21	6:K:1023:NAG:C1	1.26	1.46
1:V:414:ASN:HD21	6:V:1022:NAG:C1	1.27	1.45
1:R:414:ASN:HD21	6:R:1023:NAG:C1	1.25	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:414:ASN:HD21	6:I:1023:NAG:C1	1.29	1.45
1:J:414:ASN:HD21	6:J:1022:NAG:C1	1.30	1.45
1:P:414:ASN:HD21	6:P:1022:NAG:C1	1.31	1.43
1:S:414:ASN:HD21	6:S:1023:NAG:C1	1.27	1.43
1:T:414:ASN:HD21	6:T:1023:NAG:C1	1.30	1.42
1:C:414:ASN:HD21	6:C:1022:NAG:C1	1.33	1.42
1:N:414:ASN:HD21	6:N:1023:NAG:C1	1.30	1.41
1:U:414:ASN:HD21	6:U:1024:NAG:C1	1.33	1.39
1:M:414:ASN:HD21	6:M:1024:NAG:C1	1.33	1.39
1:F:414:ASN:ND2	6:F:1023:NAG:C1	1.91	1.31
1:O:414:ASN:ND2	6:O:1023:NAG:C1	1.93	1.30
1:G:414:ASN:ND2	6:G:1023:NAG:C1	1.94	1.29
1:L:414:ASN:ND2	6:L:1023:NAG:C1	1.96	1.27
1:Q:414:ASN:ND2	6:Q:1021:NAG:C1	1.99	1.26
1:E:414:ASN:ND2	6:E:1023:NAG:C1	1.98	1.25
1:H:414:ASN:ND2	6:H:1023:NAG:C1	1.96	1.25
1:B:414:ASN:ND2	6:B:1022:NAG:C1	2.00	1.24
1:K:414:ASN:ND2	6:K:1023:NAG:C1	2.00	1.24
1:S:414:ASN:ND2	6:S:1023:NAG:C1	2.00	1.23
1:N:414:ASN:ND2	6:N:1023:NAG:C1	2.01	1.22
1:D:414:ASN:ND2	6:D:1023:NAG:C1	2.01	1.22
1:R:414:ASN:ND2	6:R:1023:NAG:C1	1.99	1.22
1:I:414:ASN:ND2	6:I:1023:NAG:C1	2.03	1.21
1:T:414:ASN:ND2	6:T:1023:NAG:C1	2.01	1.21
1:V:414:ASN:ND2	6:V:1022:NAG:C1	2.02	1.20
1:J:414:ASN:ND2	6:J:1022:NAG:C1	2.04	1.19
1:M:414:ASN:ND2	6:M:1024:NAG:C1	2.03	1.19
1:P:414:ASN:ND2	6:P:1022:NAG:C1	2.03	1.18
1:C:414:ASN:ND2	6:C:1022:NAG:C1	2.05	1.18
1:U:414:ASN:ND2	6:U:1024:NAG:C1	2.05	1.17
1:T:154:ASN:OD1	2:9:1:NAG:C1	2.03	1.06
1:I:154:ASN:OD1	2:n:1:NAG:C1	2.04	1.06
1:S:154:ASN:OD1	2:7:1:NAG:C1	2.04	1.05
1:B:154:ASN:OD1	2:Z:1:NAG:C1	2.04	1.04
1:F:154:ASN:OD1	2:h:1:NAG:C1	2.06	1.04
1:K:154:ASN:OD1	2:r:1:NAG:C1	2.06	1.03
1:V:154:ASN:OD1	2:DA:1:NAG:C1	2.06	1.03
1:C:154:ASN:OD1	2:b:1:NAG:C1	2.06	1.03
1:U:154:ASN:OD1	2:BA:1:NAG:C1	2.07	1.02
1:L:154:ASN:OD1	2:t:1:NAG:C1	2.07	1.02
1:M:154:ASN:OD1	2:v:1:NAG:C1	2.07	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:154:ASN:OD1	2:x:1:NAG:C1	2.08	1.02
1:D:154:ASN:OD1	2:d:1:NAG:C1	2.09	1.01
1:Q:154:ASN:OD1	2:3:1:NAG:C1	2.09	1.00
1:H:154:ASN:OD1	2:l:1:NAG:C1	2.10	0.99
1:R:154:ASN:OD1	2:5:1:NAG:C1	2.10	0.98
1:P:154:ASN:OD1	2:1:1:NAG:C1	2.11	0.98
1:J:154:ASN:OD1	2:p:1:NAG:C1	2.12	0.98
1:O:154:ASN:OD1	2:z:1:NAG:C1	2.13	0.97
1:E:154:ASN:OD1	2:f:1:NAG:C1	2.12	0.96
1:G:154:ASN:OD1	2:j:1:NAG:C1	2.15	0.94
1:H:414:ASN:CG	6:H:1023:NAG:C1	2.47	0.88
1:L:414:ASN:CG	6:L:1023:NAG:C1	2.48	0.87
1:M:414:ASN:CG	6:M:1024:NAG:C1	2.48	0.86
1:N:414:ASN:CG	6:N:1023:NAG:C1	2.47	0.86
1:O:414:ASN:CG	6:O:1023:NAG:C1	2.48	0.85
1:R:414:ASN:CG	6:R:1023:NAG:C1	2.49	0.84
1:G:414:ASN:CG	6:G:1023:NAG:C1	2.51	0.84
1:S:414:ASN:CG	6:S:1023:NAG:C1	2.51	0.83
1:U:414:ASN:CG	6:U:1024:NAG:C1	2.52	0.83
1:P:414:ASN:CG	6:P:1022:NAG:C1	2.51	0.83
1:C:414:ASN:CG	6:C:1022:NAG:C1	2.53	0.82
1:Q:414:ASN:CG	6:Q:1021:NAG:C1	2.52	0.82
1:F:414:ASN:CG	6:F:1023:NAG:C1	2.52	0.81
1:E:414:ASN:CG	6:E:1023:NAG:C1	2.54	0.80
1:T:414:ASN:CG	6:T:1023:NAG:C1	2.53	0.80
1:K:414:ASN:CG	6:K:1023:NAG:C1	2.54	0.80
1:D:414:ASN:CG	6:D:1023:NAG:C1	2.55	0.79
1:I:414:ASN:CG	6:I:1023:NAG:C1	2.54	0.79
1:B:154:ASN:CG	2:Z:1:NAG:C1	2.55	0.79
1:J:414:ASN:CG	6:J:1022:NAG:C1	2.56	0.77
1:B:414:ASN:HD21	6:B:1022:NAG:C2	1.98	0.77
1:N:414:ASN:OD1	6:N:1023:NAG:C1	2.32	0.77
1:V:414:ASN:CG	6:V:1022:NAG:C1	2.57	0.77
1:M:414:ASN:OD1	6:M:1024:NAG:C1	2.33	0.76
1:B:414:ASN:CG	6:B:1022:NAG:C1	2.59	0.75
2:X:1:NAG:O3	2:X:1:NAG:O7	2.05	0.75
2:b:1:NAG:O3	2:b:1:NAG:O7	2.05	0.75
1:H:680:ARG:HG3	1:H:683:ARG:HH21	1.52	0.75
2:7:1:NAG:O7	2:7:1:NAG:O3	2.05	0.75
2:9:1:NAG:O3	2:9:1:NAG:O7	2.05	0.75
2:z:1:NAG:O7	2:z:1:NAG:O3	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:1:NAG:O3	2:1:1:NAG:O7	2.05	0.75
2:1:2:NAG:O3	2:1:2:NAG:O7	2.05	0.74
2:x:2:NAG:O7	2:x:2:NAG:O3	2.05	0.74
2:z:2:NAG:O3	2:z:2:NAG:O7	2.05	0.74
2:BA:2:NAG:O3	2:BA:2:NAG:O7	2.05	0.74
1:F:365:THR:O	1:F:472:ASN:HA	1.88	0.74
2:h:1:NAG:O3	2:h:1:NAG:O7	2.05	0.74
2:7:2:NAG:O3	2:7:2:NAG:O7	2.05	0.74
2:f:2:NAG:O3	2:f:2:NAG:O7	2.05	0.74
2:X:2:NAG:O3	2:X:2:NAG:O7	2.05	0.74
2:p:1:NAG:O3	2:p:1:NAG:O7	2.05	0.74
2:l:1:NAG:O3	2:l:1:NAG:O7	2.05	0.74
2:r:1:NAG:O3	2:r:1:NAG:O7	2.05	0.74
2:v:2:NAG:O3	2:v:2:NAG:O7	2.05	0.74
1:V:850:VAL:HG12	1:V:886:THR:HG21	1.70	0.74
2:d:2:NAG:O3	2:d:2:NAG:O7	2.05	0.74
2:n:2:NAG:O3	2:n:2:NAG:O7	2.05	0.74
2:5:2:NAG:O3	2:5:2:NAG:O7	2.05	0.74
2:9:2:NAG:O7	2:9:2:NAG:O3	2.05	0.74
2:j:1:NAG:O3	2:j:1:NAG:O7	2.05	0.74
2:p:2:NAG:O7	2:p:2:NAG:O3	2.05	0.74
2:x:1:NAG:O7	2:x:1:NAG:O3	2.05	0.73
2:b:2:NAG:O3	2:b:2:NAG:O7	2.05	0.73
2:3:1:NAG:O3	2:3:1:NAG:O7	2.05	0.73
2:v:1:NAG:O3	2:v:1:NAG:O7	2.05	0.73
1:G:257:VAL:HG12	1:H:257:VAL:HG12	1.70	0.73
1:O:686:ILE:HD13	1:O:710:ALA:HB2	1.71	0.73
1:S:154:ASN:CG	2:7:1:NAG:C1	2.60	0.73
2:BA:1:NAG:O3	2:BA:1:NAG:O7	2.05	0.73
2:DA:1:NAG:O3	2:DA:1:NAG:O7	2.05	0.73
1:U:414:ASN:OD1	6:U:1024:NAG:C1	2.36	0.73
2:t:1:NAG:O3	2:t:1:NAG:O7	2.05	0.73
1:C:154:ASN:CG	2:b:1:NAG:C1	2.61	0.73
1:D:154:ASN:CG	2:d:1:NAG:C1	2.62	0.73
1:S:694:GLU:O	1:S:703:ARG:NH2	2.22	0.73
2:f:1:NAG:O3	2:f:1:NAG:O7	2.05	0.73
2:h:2:NAG:O3	2:h:2:NAG:O7	2.05	0.73
2:n:1:NAG:O3	2:n:1:NAG:O7	2.05	0.73
2:3:2:NAG:O3	2:3:2:NAG:O7	2.05	0.73
2:DA:2:NAG:O3	2:DA:2:NAG:O7	2.05	0.73
1:N:686:ILE:HD13	1:N:710:ALA:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:j:2:NAG:O3	2:j:2:NAG:O7	2.05	0.73
1:M:694:GLU:O	1:M:703:ARG:NH2	2.22	0.73
2:d:1:NAG:O3	2:d:1:NAG:O7	2.05	0.72
1:F:154:ASN:CG	2:h:1:NAG:C1	2.62	0.72
1:L:782:ARG:NH2	5:L:1007:SO4:S	2.62	0.72
1:S:782:ARG:NH2	5:S:1007:SO4:S	2.62	0.72
2:Z:2:NAG:O3	2:Z:2:NAG:O7	2.05	0.72
1:E:154:ASN:CG	2:f:1:NAG:C1	2.62	0.72
2:t:2:NAG:O7	2:t:2:NAG:O3	2.05	0.72
2:1:2:NAG:O3	2:1:2:NAG:O7	2.05	0.72
1:E:816:ARG:HG2	1:E:856:GLN:HE22	1.55	0.72
1:I:154:ASN:CG	2:n:1:NAG:C1	2.62	0.72
1:A:694:GLU:O	1:A:703:ARG:NH2	2.23	0.72
1:E:694:GLU:O	1:E:703:ARG:NH2	2.23	0.72
1:L:414:ASN:OD1	6:L:1023:NAG:C1	2.38	0.72
2:Z:1:NAG:HO3	2:Z:1:NAG:C7	2.03	0.72
1:G:548:LYS:NZ	5:G:1024:SO4:O1	2.23	0.71
1:K:154:ASN:CG	2:r:1:NAG:C1	2.62	0.71
1:D:694:GLU:O	1:D:703:ARG:NH2	2.23	0.71
1:V:154:ASN:CG	2:DA:1:NAG:C1	2.64	0.71
1:H:414:ASN:OD1	6:H:1023:NAG:C1	2.38	0.71
1:P:414:ASN:OD1	6:P:1022:NAG:C1	2.38	0.71
1:U:154:ASN:CG	2:BA:1:NAG:C1	2.63	0.71
1:F:611:ARG:NH2	5:F:1011:SO4:O3	2.24	0.71
1:R:414:ASN:OD1	6:R:1023:NAG:C1	2.38	0.71
1:Q:694:GLU:O	1:Q:703:ARG:NH2	2.24	0.71
1:T:154:ASN:CG	2:9:1:NAG:C1	2.64	0.71
1:E:154:ASN:HD21	2:f:1:NAG:C1	2.02	0.71
1:M:154:ASN:CG	2:v:1:NAG:C1	2.63	0.71
1:H:694:GLU:O	1:H:703:ARG:NH2	2.24	0.71
1:B:154:ASN:ND2	2:Z:1:NAG:C1	2.53	0.71
1:C:414:ASN:OD1	6:C:1022:NAG:C1	2.38	0.71
1:G:694:GLU:O	1:G:703:ARG:NH2	2.24	0.71
1:Q:154:ASN:CG	2:3:1:NAG:C1	2.64	0.71
1:I:829:ARG:NH2	5:I:1010:SO4:O1	2.24	0.71
1:C:548:LYS:NZ	5:C:1023:SO4:O1	2.24	0.70
2:r:2:NAG:O7	2:r:2:NAG:O3	2.05	0.70
1:P:829:ARG:NH2	5:P:1009:SO4:S	2.64	0.70
1:L:154:ASN:CG	2:t:1:NAG:C1	2.63	0.70
1:S:414:ASN:OD1	6:S:1023:NAG:C1	2.40	0.70
2:Z:1:NAG:O7	2:Z:1:NAG:O3	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:257:VAL:HG12	1:U:257:VAL:HG12	1.72	0.70
2:5:1:NAG:O7	2:5:1:NAG:O3	2.05	0.70
1:P:257:VAL:HG12	1:R:257:VAL:HG12	1.72	0.70
1:P:816:ARG:HG2	1:P:856:GLN:HE22	1.57	0.70
1:P:694:GLU:O	1:P:703:ARG:NH2	2.25	0.70
1:E:154:ASN:ND2	2:f:1:NAG:C1	2.55	0.70
1:G:680:ARG:HG3	1:G:683:ARG:HH21	1.56	0.70
1:D:611:ARG:NH2	5:D:1011:SO4:O3	2.23	0.70
1:L:365:THR:O	1:L:472:ASN:HA	1.92	0.69
1:F:829:ARG:NH2	5:F:1010:SO4:O1	2.25	0.69
1:H:611:ARG:NH2	5:H:1011:SO4:O3	2.24	0.69
1:G:365:THR:O	1:G:472:ASN:HA	1.92	0.69
1:I:686:ILE:HD13	1:I:710:ALA:HB2	1.74	0.69
1:N:694:GLU:O	1:N:703:ARG:NH2	2.26	0.69
1:I:611:ARG:NH2	5:I:1011:SO4:O3	2.25	0.69
1:Q:686:ILE:HD13	1:Q:710:ALA:HB2	1.73	0.69
1:R:694:GLU:O	1:R:703:ARG:NH2	2.26	0.69
1:R:154:ASN:CG	2:5:1:NAG:C1	2.66	0.69
1:B:154:ASN:HD21	2:Z:1:NAG:C1	2.05	0.69
1:T:694:GLU:O	1:T:703:ARG:NH2	2.26	0.69
1:F:782:ARG:NH2	5:F:1007:SO4:S	2.66	0.68
1:D:257:VAL:HG12	1:F:257:VAL:HG12	1.75	0.68
1:J:782:ARG:NH2	5:J:1006:SO4:S	2.67	0.68
1:N:154:ASN:CG	2:x:1:NAG:C1	2.66	0.68
1:C:744:LEU:HG	1:C:775:GLN:HG2	1.76	0.68
1:K:365:THR:O	1:K:472:ASN:HA	1.92	0.68
1:R:782:ARG:NH2	5:R:1006:SO4:S	2.66	0.68
1:N:611:ARG:NH2	5:N:1011:SO4:O3	2.25	0.68
1:J:341:ALA:HB1	1:J:697:VAL:HG13	1.76	0.68
1:A:365:THR:O	1:A:472:ASN:HA	1.94	0.68
1:A:611:ARG:NH2	5:A:1010:SO4:O3	2.27	0.68
1:N:548:LYS:NZ	5:N:1001:SO4:O3	2.27	0.67
1:D:154:ASN:HD21	2:d:1:NAG:C1	2.07	0.67
1:F:694:GLU:O	1:F:703:ARG:NH2	2.27	0.67
1:I:414:ASN:OD1	6:I:1023:NAG:C1	2.42	0.67
1:T:68:HIS:NE2	2:8:1:NAG:O7	2.20	0.67
1:U:829:ARG:NH2	5:U:1011:SO4:S	2.67	0.67
1:E:611:ARG:NH2	5:E:1011:SO4:O3	2.27	0.67
1:J:154:ASN:CG	2:p:1:NAG:C1	2.67	0.67
1:P:154:ASN:CG	2:1:1:NAG:C1	2.67	0.67
1:U:816:ARG:NH1	5:U:1007:SO4:O1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:414:ASN:HD21	6:J:1022:NAG:C2	2.05	0.67
1:E:686:ILE:HD13	1:E:710:ALA:HB2	1.77	0.67
1:A:764:TYR:HE2	1:A:802:ILE:HG12	1.57	0.67
1:Q:782:ARG:NH2	5:Q:1006:SO4:S	2.68	0.67
1:L:829:ARG:NH2	5:L:1010:SO4:O4	2.27	0.67
1:J:686:ILE:HD13	1:J:710:ALA:HB2	1.77	0.67
1:O:154:ASN:CG	2:z:1:NAG:C1	2.68	0.67
1:E:782:ARG:NH2	5:E:1007:SO4:O3	2.28	0.67
1:G:154:ASN:HD21	2:j:1:NAG:C1	2.08	0.67
1:L:579:MET:HG2	1:L:613:SER:HB3	1.77	0.67
1:M:381:PHE:HE1	1:M:446:ASN:HD22	1.41	0.67
1:J:782:ARG:NH2	5:J:1006:SO4:O1	2.27	0.67
1:M:159:PHE:HB3	1:M:315:GLN:HB2	1.78	0.66
1:C:694:GLU:O	1:C:703:ARG:NH2	2.28	0.66
1:O:414:ASN:OD1	6:O:1023:NAG:C1	2.42	0.66
1:B:764:TYR:HE2	1:B:802:ILE:HG12	1.59	0.66
1:D:154:ASN:ND2	2:d:1:NAG:C1	2.58	0.66
1:I:694:GLU:O	1:I:703:ARG:NH2	2.28	0.66
1:M:438:TYR:HH	4:M:1003:P52:H1	1.43	0.66
1:U:694:GLU:O	1:U:703:ARG:NH2	2.29	0.66
1:E:579:MET:HG2	1:E:613:SER:HB3	1.78	0.66
1:G:154:ASN:CG	2:j:1:NAG:C1	2.68	0.66
1:N:782:ARG:NH2	5:N:1007:SO4:S	2.69	0.66
1:Q:414:ASN:OD1	6:Q:1021:NAG:C1	2.42	0.66
1:B:341:ALA:HB1	1:B:697:VAL:HG13	1.78	0.66
1:H:154:ASN:CG	2:l:1:NAG:C1	2.69	0.66
1:M:257:VAL:HG12	1:O:257:VAL:HG12	1.78	0.66
1:A:579:MET:HG2	1:A:613:SER:HB3	1.78	0.66
1:S:782:ARG:NH2	5:S:1007:SO4:O2	2.29	0.66
1:G:829:ARG:NH2	5:G:1010:SO4:O1	2.29	0.66
1:L:850:VAL:HG12	1:L:886:THR:HG21	1.78	0.66
1:N:579:MET:HG2	1:N:613:SER:HB3	1.78	0.66
1:S:850:VAL:HG12	1:S:886:THR:HG21	1.77	0.66
1:O:694:GLU:O	1:O:703:ARG:NH2	2.28	0.66
1:P:579:MET:HG2	1:P:613:SER:HB3	1.78	0.66
1:C:71:LEU:HD22	1:C:213:HIS:NE2	2.11	0.65
1:C:365:THR:O	1:C:472:ASN:HA	1.95	0.65
1:K:694:GLU:O	1:K:703:ARG:NH2	2.28	0.65
1:K:548:LYS:NZ	5:K:1024:SO4:O1	2.29	0.65
1:S:154:ASN:HD21	2:7:1:NAG:C1	2.09	0.65
1:J:154:ASN:HD21	2:p:1:NAG:C1	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:816:ARG:NH1	5:I:1007:SO4:O1	2.28	0.65
1:O:764:TYR:HE2	1:O:802:ILE:HG12	1.61	0.65
1:S:154:ASN:ND2	2:7:1:NAG:C1	2.59	0.65
1:D:603:HIS:HB2	1:D:611:ARG:HD3	1.77	0.65
1:J:159:PHE:HB3	1:J:315:GLN:HB2	1.78	0.65
1:V:782:ARG:NH2	5:V:1006:SO4:S	2.70	0.65
1:M:782:ARG:NH2	5:M:1007:SO4:S	2.70	0.65
1:T:414:ASN:OD1	6:T:1023:NAG:C1	2.45	0.65
1:M:686:ILE:HD13	1:M:710:ALA:HB2	1.79	0.64
1:Q:782:ARG:NH2	5:Q:1006:SO4:O1	2.28	0.64
1:J:414:ASN:OD1	6:J:1022:NAG:C1	2.45	0.64
1:J:694:GLU:O	1:J:703:ARG:NH2	2.29	0.64
1:G:660:LYS:NZ	1:G:816:ARG:O	2.29	0.64
1:H:816:ARG:HG2	1:H:856:GLN:HE22	1.61	0.64
1:D:414:ASN:OD1	6:D:1023:NAG:C1	2.46	0.64
1:I:764:TYR:HE2	1:I:802:ILE:HG12	1.60	0.64
1:K:414:ASN:OD1	6:K:1023:NAG:C1	2.45	0.64
1:S:579:MET:HG2	1:S:613:SER:HB3	1.78	0.64
1:D:159:PHE:HB3	1:D:315:GLN:HB2	1.80	0.64
1:E:829:ARG:NH2	5:E:1010:SO4:O4	2.31	0.64
1:R:686:ILE:HD13	1:R:710:ALA:HB2	1.79	0.64
1:V:579:MET:HG2	1:V:613:SER:HB3	1.79	0.64
1:C:850:VAL:HG12	1:C:886:THR:HG21	1.78	0.64
1:G:611:ARG:NH2	5:G:1011:SO4:O3	2.31	0.64
1:Q:548:LYS:NZ	5:Q:1022:SO4:S	2.70	0.64
1:J:611:ARG:NH2	5:J:1010:SO4:O1	2.27	0.64
1:F:686:ILE:HD13	1:F:710:ALA:HB2	1.80	0.64
1:H:71:LEU:HD22	1:H:213:HIS:NE2	2.13	0.64
1:P:341:ALA:HB1	1:P:697:VAL:HG13	1.80	0.64
1:G:414:ASN:OD1	6:G:1023:NAG:C1	2.46	0.63
1:M:154:ASN:HD21	2:v:1:NAG:C1	2.11	0.63
1:R:680:ARG:HG3	1:R:683:ARG:HH21	1.63	0.63
1:V:159:PHE:HB3	1:V:315:GLN:HB2	1.80	0.63
1:F:414:ASN:HD21	6:F:1023:NAG:C2	2.04	0.63
1:G:154:ASN:ND2	2:j:1:NAG:C1	2.62	0.63
1:D:686:ILE:HD13	1:D:710:ALA:HB2	1.79	0.63
1:J:764:TYR:HE2	1:J:802:ILE:HG12	1.61	0.63
1:M:548:LYS:NZ	5:M:1001:SO4:O3	2.31	0.63
1:S:816:ARG:NH1	5:S:1007:SO4:O3	2.30	0.63
1:V:414:ASN:OD1	6:V:1022:NAG:C1	2.47	0.63
1:E:414:ASN:OD1	6:E:1023:NAG:C1	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:364:VAL:HG21	1:Q:465:LEU:HA	1.81	0.63
1:C:154:ASN:ND2	2:b:1:NAG:C1	2.62	0.63
1:C:579:MET:HG2	1:C:613:SER:HB3	1.79	0.63
1:G:782:ARG:NH2	5:G:1006:SO4:O3	2.28	0.63
1:M:154:ASN:ND2	2:v:1:NAG:C1	2.62	0.63
1:Q:548:LYS:NZ	5:Q:1022:SO4:O3	2.32	0.63
1:G:182:PHE:HA	1:G:186:ALA:HB3	1.81	0.63
1:R:708:LEU:HD22	1:R:744:LEU:HD13	1.81	0.63
1:R:782:ARG:NH2	5:R:1006:SO4:O1	2.31	0.63
1:M:579:MET:HG2	1:M:613:SER:HB3	1.81	0.62
1:V:694:GLU:O	1:V:703:ARG:NH2	2.32	0.62
1:F:154:ASN:ND2	2:h:1:NAG:C1	2.62	0.62
1:F:154:ASN:HD21	2:h:1:NAG:C1	2.13	0.62
1:R:764:TYR:HE2	1:R:802:ILE:HG12	1.63	0.62
1:P:686:ILE:HD13	1:P:710:ALA:HB2	1.81	0.62
1:P:708:LEU:HD22	1:P:744:LEU:HD13	1.81	0.62
1:T:782:ARG:NH2	5:T:1007:SO4:S	2.72	0.62
2:x:1:NAG:HO3	2:x:1:NAG:C7	2.11	0.62
1:A:782:ARG:NH2	5:A:1006:SO4:S	2.73	0.62
1:K:154:ASN:ND2	2:r:1:NAG:C1	2.62	0.62
1:K:782:ARG:NH2	5:K:1006:SO4:S	2.72	0.62
5:U:1010:SO4:O3	1:V:548:LYS:NZ	2.28	0.62
1:F:816:ARG:NH1	5:F:1007:SO4:O3	2.32	0.62
1:K:341:ALA:HB1	1:K:697:VAL:HG13	1.82	0.62
1:K:673:GLN:HE22	1:K:912:LYS:HD2	1.64	0.62
1:G:686:ILE:HD13	1:G:710:ALA:HB2	1.81	0.62
1:I:829:ARG:NH2	5:I:1010:SO4:S	2.73	0.62
1:J:154:ASN:ND2	2:p:1:NAG:C1	2.63	0.62
1:Q:816:ARG:NH1	5:Q:1006:SO4:O3	2.33	0.62
1:V:680:ARG:HG3	1:V:683:ARG:HH21	1.65	0.62
1:J:548:LYS:NZ	5:O:1009:SO4:O1	2.32	0.62
1:C:782:ARG:NH2	5:C:1006:SO4:S	2.73	0.62
1:U:680:ARG:HG3	1:U:683:ARG:HH21	1.65	0.62
1:K:476:GLU:OE2	1:K:493:LYS:NZ	2.33	0.61
1:R:611:ARG:NH2	5:R:1011:SO4:O1	2.33	0.61
1:U:686:ILE:HD13	1:U:710:ALA:HB2	1.81	0.61
1:H:548:LYS:NZ	5:H:1001:SO4:O3	2.32	0.61
1:I:154:ASN:ND2	2:n:1:NAG:C1	2.63	0.61
1:O:212:ARG:NH2	5:O:1004:SO4:O4	2.33	0.61
1:U:159:PHE:HB3	1:U:315:GLN:HB2	1.81	0.61
1:V:154:ASN:ND2	2:DA:1:NAG:C1	2.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:154:ASN:HD21	2:z:1:NAG:C1	2.13	0.61
1:S:829:ARG:NH2	5:S:1010:SO4:O3	2.34	0.61
1:B:686:ILE:HD13	1:B:710:ALA:HB2	1.81	0.61
1:K:154:ASN:HD21	2:r:1:NAG:C1	2.13	0.61
1:O:816:ARG:HG2	1:O:856:GLN:HE22	1.65	0.61
1:R:579:MET:HG2	1:R:613:SER:HB3	1.82	0.61
1:R:850:VAL:HG12	1:R:886:THR:HG21	1.81	0.61
1:L:680:ARG:HG3	1:L:683:ARG:HH21	1.64	0.61
1:O:680:ARG:HG3	1:O:683:ARG:HH21	1.66	0.61
1:Q:154:ASN:ND2	2:3:1:NAG:C1	2.63	0.61
1:S:159:PHE:HB3	1:S:315:GLN:HB2	1.82	0.61
1:U:708:LEU:HD22	1:U:744:LEU:HD13	1.82	0.61
1:A:159:PHE:HB3	1:A:315:GLN:HB2	1.82	0.61
1:N:159:PHE:HB3	1:N:315:GLN:HB2	1.82	0.61
1:L:611:ARG:NH2	5:L:1011:SO4:O3	2.33	0.61
1:M:611:ARG:NH2	5:M:1012:SO4:O1	2.25	0.61
1:R:154:ASN:ND2	2:5:1:NAG:C1	2.64	0.61
1:J:257:VAL:HG12	1:L:257:VAL:HG12	1.81	0.61
1:N:257:VAL:HG12	1:Q:257:VAL:HG12	1.82	0.61
1:I:711[B]:CYS:SG	1:I:718[B]:CYS:HB3	2.40	0.61
1:O:515:ARG:NH1	5:O:1007:SO4:O3	2.34	0.61
1:O:850:VAL:HG12	1:O:886:THR:HG21	1.82	0.61
1:T:708:LEU:HD22	1:T:744:LEU:HD13	1.83	0.61
1:T:764:TYR:HE2	1:T:802:ILE:HG12	1.66	0.61
1:V:154:ASN:HD21	2:DA:1:NAG:C1	2.14	0.61
1:C:829:ARG:NH2	5:C:1009:SO4:S	2.73	0.60
1:L:154:ASN:ND2	2:t:1:NAG:C1	2.64	0.60
1:P:829:ARG:NH2	5:P:1009:SO4:O3	2.34	0.60
1:S:476:GLU:OE2	1:S:493:LYS:NZ	2.29	0.60
1:H:259:LYS:NZ	1:H:284[B]:ASP:OD1	2.34	0.60
1:P:850:VAL:HG12	1:P:886:THR:HG21	1.83	0.60
1:C:154:ASN:HD21	2:b:1:NAG:C1	2.14	0.60
1:Q:833:ASN:ND2	5:Q:1012:SO4:O1	2.32	0.60
1:R:154:ASN:HD21	2:5:1:NAG:C1	2.13	0.60
1:U:782:ARG:NH2	5:U:1007:SO4:S	2.75	0.60
1:V:686:ILE:HD13	1:V:710:ALA:HB2	1.83	0.60
1:E:829:ARG:NH2	5:E:1010:SO4:S	2.74	0.60
1:R:829:ARG:NH2	5:R:1010:SO4:O3	2.35	0.60
1:U:154:ASN:ND2	2:BA:1:NAG:C1	2.64	0.60
1:I:414:ASN:HD21	6:I:1023:NAG:C2	2.11	0.60
1:K:523:HIS:HD2	1:K:534:THR:HG21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:816:ARG:NH1	5:O:1006:SO4:O3	2.34	0.60
1:A:154:ASN:N	1:A:154:ASN:OD1	2.35	0.60
1:D:365:THR:O	1:D:472:ASN:HA	2.01	0.60
1:H:764:TYR:HE2	1:H:802:ILE:HG12	1.67	0.60
1:K:182:PHE:HA	1:K:186:ALA:HB3	1.83	0.60
1:T:548:LYS:NZ	5:T:1001:SO4:O1	2.33	0.60
1:B:711[B]:CYS:SG	1:B:718[B]:CYS:HB3	2.41	0.60
1:I:154:ASN:HD21	2:n:1:NAG:C1	2.15	0.60
1:S:341:ALA:HB1	1:S:697:VAL:HG13	1.83	0.60
2:5:1:NAG:HO3	2:5:1:NAG:C7	2.08	0.60
1:D:782:ARG:NH2	5:D:1007:SO4:S	2.75	0.59
1:J:850:VAL:HG12	1:J:886:THR:HG21	1.83	0.59
1:S:611:ARG:NH2	5:S:1011:SO4:O3	2.35	0.59
1:U:373:TRP:HE1	1:U:475:ASN:ND2	1.99	0.59
1:U:579:MET:HG2	1:U:613:SER:HB3	1.82	0.59
2:r:2:NAG:HO3	2:r:2:NAG:C7	2.12	0.59
1:J:579:MET:HG2	1:J:613:SER:HB3	1.83	0.59
1:L:821:TYR:CD1	1:L:822:PRO:HD3	2.37	0.59
1:Q:154:ASN:HD21	2:3:1:NAG:C1	2.14	0.59
1:R:476:GLU:OE2	1:R:493:LYS:NZ	2.35	0.59
1:V:829:ARG:NH2	5:V:1009:SO4:O3	2.31	0.59
1:F:414:ASN:OD1	6:F:1023:NAG:C1	2.49	0.59
1:N:260:ILE:HG13	1:Q:214:LEU:HB2	1.85	0.59
1:O:154:ASN:ND2	2:z:1:NAG:C1	2.65	0.59
1:A:829:ARG:NH2	5:D:1001:SO4:O1	2.36	0.59
1:B:694:GLU:O	1:B:703:ARG:NH2	2.35	0.59
1:C:686:ILE:HD13	1:C:710:ALA:HB2	1.84	0.59
1:J:526:LYS:HD3	1:J:892:GLU:HG2	1.85	0.59
1:Q:579:MET:HG2	1:Q:613:SER:HB3	1.84	0.59
1:D:730:LYS:HE3	1:D:755:GLU:HG2	1.83	0.59
1:E:159:PHE:HB3	1:E:315:GLN:HB2	1.84	0.59
1:F:526:LYS:HD3	1:F:892:GLU:HG2	1.84	0.59
1:C:257:VAL:HG12	1:E:257:VAL:HG12	1.84	0.59
1:G:821:TYR:CD1	1:G:822:PRO:HD3	2.36	0.59
1:L:686:ILE:HD13	1:L:710:ALA:HB2	1.83	0.59
1:O:829:ARG:NH2	5:O:1010:SO4:O3	2.35	0.59
1:S:611:ARG:NH2	5:S:1011:SO4:O1	2.32	0.59
1:V:341:ALA:HB1	1:V:697:VAL:HG13	1.83	0.59
1:B:553:HIS:HE1	1:F:865:GLU:HG2	1.68	0.59
1:I:579:MET:HG2	1:I:613:SER:HB3	1.84	0.59
1:L:159:PHE:HB3	1:L:315:GLN:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:821:TYR:CD1	1:P:822:PRO:HD3	2.38	0.59
1:U:829:ARG:NH2	5:U:1011:SO4:O4	2.35	0.59
1:C:764:TYR:HE2	1:C:802:ILE:HG12	1.67	0.59
1:Q:575:PHE:HB2	1:Q:585:VAL:HG11	1.85	0.59
1:Q:821:TYR:CD1	1:Q:822:PRO:HD3	2.38	0.59
1:T:159:PHE:HB3	1:T:315:GLN:HB2	1.85	0.59
1:U:821:TYR:CD1	1:U:822:PRO:HD3	2.38	0.59
1:E:821:TYR:CD1	1:E:822:PRO:HD3	2.37	0.59
1:Q:373:TRP:HE1	1:Q:475:ASN:ND2	2.00	0.59
1:Q:159:PHE:HB3	1:Q:315:GLN:HB2	1.85	0.58
1:L:782:ARG:NH2	5:L:1007:SO4:O4	2.35	0.58
1:F:744:LEU:HG	1:F:775:GLN:HG2	1.85	0.58
1:M:816:ARG:NH1	5:M:1007:SO4:O4	2.35	0.58
1:P:154:ASN:ND2	2:1:1:NAG:C1	2.66	0.58
1:N:816:ARG:NH1	5:N:1007:SO4:S	2.76	0.58
1:G:603:HIS:HB2	1:G:611:ARG:HD3	1.85	0.58
1:R:821:TYR:CD1	1:R:822:PRO:HD3	2.39	0.58
1:A:257:VAL:HG12	1:B:257:VAL:HG12	1.86	0.58
1:C:603:HIS:HB2	1:C:611:ARG:HD3	1.85	0.58
1:M:708:LEU:HD22	1:M:744:LEU:HD13	1.84	0.58
1:M:821:TYR:CD1	1:M:822:PRO:HD3	2.38	0.58
1:O:182:PHE:HA	1:O:186:ALA:HB3	1.84	0.58
1:P:711[B]:CYS:SG	1:P:718[B]:CYS:HB3	2.44	0.58
1:P:803:LYS:NZ	5:P:1005:SO4:O1	2.36	0.58
1:E:744:LEU:HG	1:E:775:GLN:HG2	1.85	0.58
1:U:154:ASN:HD21	2:BA:1:NAG:C1	2.16	0.58
1:D:821:TYR:CD1	1:D:822:PRO:HD3	2.39	0.58
1:J:711[B]:CYS:SG	1:J:718[B]:CYS:HB3	2.43	0.58
1:K:71:LEU:HD22	1:K:213:HIS:NE2	2.19	0.58
1:T:154:ASN:ND2	2:9:1:NAG:C1	2.66	0.58
1:B:159:PHE:HB3	1:B:315:GLN:HB2	1.84	0.58
1:P:154:ASN:HD21	2:1:1:NAG:C1	2.16	0.58
1:E:414:ASN:HD21	6:E:1023:NAG:C2	2.11	0.57
1:I:257:VAL:HG12	1:K:257:VAL:HG12	1.85	0.57
1:V:414:ASN:HD21	6:V:1022:NAG:C2	2.11	0.57
1:V:708:LEU:HD22	1:V:744:LEU:HD13	1.86	0.57
1:U:365:THR:O	1:U:472:ASN:HA	2.04	0.57
1:A:259:LYS:NZ	1:A:284[B]:ASP:OD1	2.38	0.57
1:G:730:LYS:HE3	1:G:755:GLU:HG2	1.86	0.57
1:N:154:ASN:ND2	2:x:1:NAG:C1	2.67	0.57
1:O:782:ARG:NH2	5:O:1006:SO4:S	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:PHE:HA	1:I:186:ALA:HB3	1.85	0.57
1:A:341:ALA:HB1	1:A:697:VAL:HG13	1.86	0.57
1:I:821:TYR:CD1	1:I:822:PRO:HD3	2.38	0.57
1:L:154:ASN:HD21	2:t:1:NAG:C1	2.17	0.57
1:N:154:ASN:HD21	2:x:1:NAG:C1	2.18	0.57
1:T:220:PRO:HG3	1:T:305:LYS:HG2	1.87	0.57
1:D:526:LYS:HD3	1:D:892:GLU:HG2	1.85	0.57
1:H:341:ALA:HB1	1:H:697:VAL:HG13	1.85	0.57
1:H:711[B]:CYS:SG	1:H:718[B]:CYS:HB3	2.44	0.57
1:K:708:LEU:HD22	1:K:744:LEU:HD13	1.86	0.57
1:K:816:ARG:NH1	5:K:1006:SO4:O3	2.33	0.57
1:L:603:HIS:HB2	1:L:611:ARG:HD3	1.85	0.57
1:R:182:PHE:HA	1:R:186:ALA:HB3	1.86	0.57
1:B:365:THR:O	1:B:472:ASN:HA	2.05	0.57
1:O:579:MET:HG2	1:O:613:SER:HB3	1.87	0.57
1:Q:440:LYS:HG3	1:Q:582:TYR:CZ	2.39	0.57
1:H:154:ASN:HD21	2:l:1:NAG:C1	2.18	0.57
1:H:182:PHE:HA	1:H:186:ALA:HB3	1.86	0.57
1:L:744:LEU:HG	1:L:775:GLN:HG2	1.86	0.57
1:T:686:ILE:HD13	1:T:710:ALA:HB2	1.87	0.57
1:V:821:TYR:CD1	1:V:822:PRO:HD3	2.40	0.57
1:A:744:LEU:HG	1:A:775:GLN:HG2	1.87	0.57
1:L:694:GLU:O	1:L:703:ARG:NH2	2.37	0.57
1:N:829:ARG:NH2	5:N:1010:SO4:S	2.78	0.57
1:Q:708:LEU:HD22	1:Q:744:LEU:HD13	1.87	0.57
1:P:159:PHE:HB3	1:P:315:GLN:HB2	1.87	0.57
1:P:611:ARG:NH2	5:P:1010:SO4:O1	2.37	0.57
1:U:220:PRO:HG3	1:U:305:LYS:HG2	1.85	0.57
1:E:850:VAL:HG12	1:E:886:THR:HG21	1.85	0.56
1:N:816:ARG:NH1	5:N:1007:SO4:O4	2.37	0.56
1:B:567:PRO:HB3	1:F:864:GLU:HG3	1.87	0.56
1:G:579:MET:HG2	1:G:613:SER:HB3	1.86	0.56
1:H:154:ASN:ND2	2:l:1:NAG:C1	2.68	0.56
1:H:579:MET:HG2	1:H:613:SER:HB3	1.86	0.56
1:I:548:LYS:NZ	5:I:1001:SO4:O3	2.34	0.56
1:M:711[B]:CYS:SG	1:M:718[B]:CYS:HB3	2.44	0.56
1:R:816:ARG:NH1	5:R:1006:SO4:O3	2.36	0.56
1:D:579:MET:HG2	1:D:613:SER:HB3	1.88	0.56
1:F:579:MET:HG2	1:F:613:SER:HB3	1.87	0.56
1:I:708:LEU:HD22	1:I:744:LEU:HD13	1.86	0.56
1:O:711[B]:CYS:SG	1:O:718[B]:CYS:HB3	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:821:TYR:CD1	1:O:822:PRO:HD3	2.40	0.56
1:T:154:ASN:HD21	2:9:1:NAG:C1	2.17	0.56
1:N:846:ILE:HA	1:N:849:MET:HE3	1.87	0.56
1:S:757:TRP:CD2	1:S:788:LYS:HD3	2.41	0.56
1:T:579:MET:HG2	1:T:613:SER:HB3	1.87	0.56
1:T:660:LYS:NZ	1:T:816:ARG:O	2.38	0.56
1:U:850:VAL:HG12	1:U:886:THR:HG21	1.86	0.56
1:V:711[B]:CYS:SG	1:V:718[B]:CYS:HB3	2.45	0.56
1:G:816:ARG:HG2	1:G:856:GLN:HE22	1.69	0.56
1:R:57:TYR:CE1	1:R:90:THR:HG21	2.41	0.56
1:R:475:ASN:OD1	1:R:479:TRP:NE1	2.39	0.56
1:T:850:VAL:HG12	1:T:886:THR:HG21	1.88	0.56
1:B:154:ASN:OD1	2:Z:1:NAG:O5	2.24	0.56
1:C:829:ARG:NH2	5:C:1009:SO4:O1	2.38	0.56
1:D:711[B]:CYS:SG	1:D:718[B]:CYS:HB3	2.46	0.56
1:G:711[B]:CYS:SG	1:G:718[B]:CYS:HB3	2.46	0.56
1:I:523:HIS:CE1	1:I:525:MET:HE2	2.41	0.56
1:K:183:GLU:OE1	4:K:1002:P52:N1	2.39	0.56
1:S:686:ILE:HD13	1:S:710:ALA:HB2	1.88	0.56
1:S:708:LEU:HD22	1:S:744:LEU:HD13	1.88	0.56
2:x:2:NAG:HO3	2:x:2:NAG:C7	2.15	0.56
1:K:764:TYR:HE2	1:K:802:ILE:HG12	1.71	0.56
1:M:545:ILE:HG23	1:M:577:VAL:HG21	1.87	0.56
1:N:821:TYR:CD1	1:N:822:PRO:HD3	2.41	0.56
1:B:764:TYR:HB2	1:B:776:ILE:HG21	1.87	0.56
1:H:220:PRO:HG3	1:H:305:LYS:HG2	1.86	0.56
1:J:220:PRO:HG3	1:J:305:LYS:HG2	1.87	0.56
1:A:711[B]:CYS:SG	1:A:718[B]:CYS:HB3	2.46	0.56
1:B:296:TYR:CE1	1:B:458:LYS:HE2	2.41	0.56
1:D:680:ARG:HG3	1:D:683:ARG:HH21	1.71	0.56
1:S:829:ARG:NH2	5:S:1010:SO4:S	2.79	0.56
1:F:711[B]:CYS:SG	1:F:718[B]:CYS:HB3	2.46	0.55
1:F:821:TYR:CD1	1:F:822:PRO:HD3	2.41	0.55
1:J:821:TYR:CD1	1:J:822:PRO:HD3	2.41	0.55
1:U:782:ARG:NH2	5:U:1007:SO4:O2	2.39	0.55
1:G:440:LYS:HG3	1:G:582:TYR:CZ	2.41	0.55
1:Q:548:LYS:NZ	5:Q:1022:SO4:O1	2.38	0.55
1:S:711[B]:CYS:SG	1:S:718[B]:CYS:HB3	2.46	0.55
1:G:208:ARG:NH2	5:G:1015:SO4:O4	2.38	0.55
1:L:711[B]:CYS:SG	1:L:718[B]:CYS:HB3	2.47	0.55
1:B:579:MET:HG2	1:B:613:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:THR:O	1:E:472:ASN:HA	2.07	0.55
1:K:611:ARG:NH2	5:K:1010:SO4:O1	2.40	0.55
1:T:829:ARG:NH2	5:T:1010:SO4:O1	2.39	0.55
1:B:414:ASN:OD1	6:B:1022:NAG:C1	2.54	0.55
1:Q:680:ARG:HG3	1:Q:683:ARG:HH21	1.71	0.55
1:U:575:PHE:HB2	1:U:585:VAL:HG11	1.88	0.55
1:D:373:TRP:HE1	1:D:475:ASN:ND2	2.04	0.55
1:E:711[B]:CYS:SG	1:E:718[B]:CYS:HB3	2.46	0.55
1:I:159:PHE:HB3	1:I:315:GLN:HB2	1.88	0.55
1:K:804:THR:HG21	1:K:838:LYS:HE2	1.86	0.55
1:K:821:TYR:CD1	1:K:822:PRO:HD3	2.42	0.55
1:R:220:PRO:HG3	1:R:305:LYS:HG2	1.89	0.55
1:R:711[B]:CYS:SG	1:R:718[B]:CYS:HB3	2.47	0.55
1:C:821:TYR:CD1	1:C:822:PRO:HD3	2.41	0.55
1:U:548:LYS:NZ	5:U:1001:SO4:O3	2.40	0.55
1:V:764:TYR:HE2	1:V:802:ILE:HG12	1.71	0.55
1:D:219:MET:HG2	1:D:239:THR:HG22	1.89	0.55
1:D:341:ALA:HB1	1:D:697:VAL:HG13	1.89	0.55
1:G:159:PHE:HB3	1:G:315:GLN:HB2	1.88	0.55
1:K:219:MET:HG2	1:K:239:THR:HG22	1.89	0.55
1:L:166:THR:O	1:L:803:LYS:NZ	2.35	0.55
1:N:301:TYR:OH	1:N:306:GLN:NE2	2.40	0.55
1:P:782:ARG:NH2	5:P:1006:SO4:S	2.79	0.55
1:S:864:GLU:HG3	1:T:567:PRO:HB3	1.88	0.55
1:V:70:ASN:OD1	1:V:73:THR:OG1	2.22	0.55
1:V:764:TYR:HB2	1:V:776:ILE:HG21	1.89	0.55
1:D:829:ARG:NH2	5:D:1010:SO4:O1	2.40	0.55
1:H:365:THR:O	1:H:472:ASN:HA	2.07	0.55
1:H:660:LYS:NZ	1:H:816:ARG:O	2.40	0.55
1:O:159:PHE:HB3	1:O:315:GLN:HB2	1.89	0.55
1:S:730:LYS:HE3	1:S:755:GLU:HG2	1.88	0.55
1:I:611:ARG:NH2	5:I:1011:SO4:O1	2.40	0.54
1:F:548:LYS:NZ	5:F:1001:SO4:O1	2.38	0.54
1:F:680:ARG:HG3	1:F:683:ARG:HH21	1.72	0.54
1:D:665:ARG:HH11	1:D:667:MET:HE1	1.72	0.54
1:G:71:LEU:HD22	1:G:213:HIS:NE2	2.23	0.54
1:J:182:PHE:HA	1:J:186:ALA:HB3	1.89	0.54
1:J:708:LEU:HD22	1:J:744:LEU:HD13	1.88	0.54
1:J:829:ARG:NH2	5:J:1009:SO4:O3	2.41	0.54
1:L:816:ARG:NH1	5:L:1007:SO4:O1	2.40	0.54
1:L:829:ARG:NH2	5:L:1010:SO4:S	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:219:MET:HG2	1:P:239:THR:HG22	1.89	0.54
1:Q:764:TYR:HE2	1:Q:802:ILE:HG12	1.72	0.54
1:I:301:TYR:OH	1:I:306:GLN:NE2	2.41	0.54
1:U:70:ASN:OD1	1:U:73:THR:OG1	2.22	0.54
2:9:2:NAG:HO3	2:9:2:NAG:C7	2.15	0.54
1:A:850:VAL:HG12	1:A:886:THR:HG21	1.88	0.54
1:J:407:ALA:HB2	1:J:439:ASP:HB2	1.88	0.54
1:P:182:PHE:HA	1:P:186:ALA:HB3	1.88	0.54
1:G:48:PRO:HG2	1:G:92:THR:HG21	1.88	0.54
1:J:70:ASN:OD1	1:J:73:THR:OG1	2.22	0.54
1:M:744:LEU:HG	1:M:775:GLN:HG2	1.90	0.54
1:R:159:PHE:HB3	1:R:315:GLN:HB2	1.89	0.54
1:I:611:ARG:NH2	5:I:1011:SO4:S	2.80	0.54
1:K:159:PHE:HB3	1:K:315:GLN:HB2	1.90	0.54
1:T:603:HIS:HB2	1:T:611:ARG:HD3	1.90	0.54
1:A:680:ARG:HG3	1:A:683:ARG:HH21	1.73	0.54
1:I:365:THR:O	1:I:472:ASN:HA	2.08	0.54
1:S:71:LEU:HD22	1:S:213:HIS:NE2	2.23	0.54
1:C:154:ASN:OD1	2:b:1:NAG:O5	2.25	0.54
1:E:364:VAL:HG21	1:E:465:LEU:HA	1.90	0.54
1:F:850:VAL:HG12	1:F:886:THR:HG21	1.89	0.54
6:F:1023:NAG:O7	6:F:1023:NAG:O3	2.25	0.54
1:K:315:GLN:O	1:K:328:ARG:NH1	2.41	0.54
1:M:829:ARG:NH2	5:M:1011:SO4:S	2.80	0.54
1:D:182:PHE:HA	1:D:186:ALA:HB3	1.90	0.54
1:E:846:ILE:HA	1:E:849:MET:HE3	1.90	0.54
1:F:523:HIS:CE1	1:F:525:MET:HE2	2.43	0.54
1:H:850:VAL:HG12	1:H:886:THR:HG21	1.89	0.54
1:I:850:VAL:HG12	1:I:886:THR:HG21	1.89	0.54
1:K:154:ASN:OD1	2:r:1:NAG:O5	2.25	0.54
1:K:711[B]:CYS:SG	1:K:718[B]:CYS:HB3	2.48	0.54
1:L:154:ASN:OD1	2:t:1:NAG:O5	2.25	0.54
1:N:523:HIS:CE1	1:N:525:MET:HE2	2.43	0.54
1:P:259:LYS:HD3	1:P:287:VAL:HG21	1.89	0.54
1:C:680:ARG:HG3	1:C:683:ARG:HH21	1.73	0.53
1:I:833:ASN:ND2	5:I:1014:SO4:O1	2.40	0.53
1:K:686:ILE:HD13	1:K:710:ALA:HB2	1.90	0.53
1:O:220:PRO:HG3	1:O:305:LYS:HG2	1.88	0.53
1:P:259:LYS:NZ	1:P:284[B]:ASP:OD1	2.40	0.53
1:Q:219:MET:HG2	1:Q:239:THR:HG22	1.90	0.53
1:Q:259:LYS:NZ	1:Q:284[B]:ASP:OD1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:373:TRP:HE1	1:Q:475:ASN:HD21	1.56	0.53
1:U:182:PHE:HA	1:U:186:ALA:HB3	1.90	0.53
1:C:440:LYS:HG3	1:C:582:TYR:CZ	2.43	0.53
1:D:154:ASN:OD1	2:d:1:NAG:O5	2.25	0.53
1:E:548:LYS:NZ	5:E:1001:SO4:S	2.81	0.53
1:E:764:TYR:HE2	1:E:802:ILE:HG12	1.73	0.53
1:F:71:LEU:HD22	1:F:213:HIS:NE2	2.22	0.53
1:R:452:LEU:HD21	1:R:490:VAL:HG11	1.89	0.53
1:S:154:ASN:OD1	2:7:1:NAG:O5	2.26	0.53
1:C:575:PHE:HB2	1:C:585:VAL:HG11	1.90	0.53
1:E:154:ASN:OD1	2:f:1:NAG:O5	2.26	0.53
1:G:545:ILE:HG23	1:G:577:VAL:HG21	1.90	0.53
1:N:711[B]:CYS:SG	1:N:718[B]:CYS:HB3	2.48	0.53
1:Q:711[B]:CYS:SG	1:Q:718[B]:CYS:HB3	2.48	0.53
2:l:1:NAG:HO3	2:l:1:NAG:C7	2.13	0.53
1:E:182:PHE:HA	1:E:186:ALA:HB3	1.90	0.53
1:E:575:PHE:HB2	1:E:585:VAL:HG11	1.90	0.53
1:F:665:ARG:HH11	1:F:667:MET:HE1	1.73	0.53
1:G:210:GLU:HG2	2:i:1:NAG:H82	1.91	0.53
1:H:782:ARG:NH2	5:H:1007:SO4:O4	2.41	0.53
6:I:1023:NAG:O7	6:I:1023:NAG:O3	2.25	0.53
1:L:440:LYS:HG3	1:L:582:TYR:CZ	2.43	0.53
1:M:680:ARG:HG3	1:M:683:ARG:HH21	1.73	0.53
6:O:1023:NAG:O7	6:O:1023:NAG:O3	2.25	0.53
1:U:440:LYS:HG3	1:U:582:TYR:CZ	2.44	0.53
6:C:1022:NAG:O3	6:C:1022:NAG:O7	2.25	0.53
1:E:598:LEU:HD11	1:E:605:ALA:HB3	1.90	0.53
1:J:71:LEU:HD22	1:J:213:HIS:NE2	2.24	0.53
1:N:660:LYS:NZ	1:N:816:ARG:O	2.42	0.53
1:O:71:LEU:HD22	1:O:213:HIS:NE2	2.24	0.53
1:T:711[B]:CYS:SG	1:T:718[B]:CYS:HB3	2.48	0.53
1:U:622:VAL:HG21	1:U:632:ALA:HB2	1.91	0.53
2:t:2:NAG:HO3	2:t:2:NAG:C7	2.16	0.53
1:A:754:THR:HG23	1:A:788:LYS:HE3	1.89	0.53
1:G:220:PRO:HG3	1:G:305:LYS:HG2	1.90	0.53
1:M:575:PHE:HB2	1:M:585:VAL:HG11	1.91	0.53
1:C:438:TYR:HH	4:C:1002:P52:H1	1.55	0.53
1:E:219:MET:HG2	1:E:239:THR:HG22	1.91	0.53
1:F:782:ARG:NH2	5:F:1007:SO4:O2	2.42	0.53
1:K:576:ASN:ND2	1:K:579:MET:SD	2.82	0.53
1:M:603:HIS:HB2	1:M:611:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:603:HIS:HB2	1:N:611:ARG:HD3	1.89	0.53
1:U:71:LEU:HD22	1:U:213:HIS:NE2	2.24	0.53
1:B:730:LYS:HE3	1:B:755:GLU:HG2	1.91	0.53
1:B:793:LEU:HB3	1:B:827:PHE:CE2	2.44	0.53
1:C:816:ARG:HG2	1:C:856:GLN:HE22	1.74	0.53
1:D:575:PHE:HB2	1:D:585:VAL:HG11	1.89	0.53
1:M:154:ASN:OD1	2:v:1:NAG:O5	2.27	0.53
1:O:603:HIS:HB2	1:O:611:ARG:HD3	1.91	0.53
1:V:182:PHE:HA	1:V:186:ALA:HB3	1.90	0.53
1:B:850:VAL:HG12	1:B:886:THR:HG21	1.91	0.52
1:L:71:LEU:HD22	1:L:213:HIS:NE2	2.24	0.52
1:M:850:VAL:HG12	1:M:886:THR:HG21	1.90	0.52
1:N:182:PHE:HA	1:N:186:ALA:HB3	1.91	0.52
6:Q:1021:NAG:O7	6:Q:1021:NAG:O3	2.25	0.52
1:U:711[B]:CYS:SG	1:U:718[B]:CYS:HB3	2.48	0.52
1:F:301:TYR:OH	1:F:306:GLN:NE2	2.42	0.52
1:G:744:LEU:HG	1:G:775:GLN:HG2	1.91	0.52
1:K:833:ASN:ND2	5:K:1013:SO4:O1	2.42	0.52
1:M:219:MET:HG2	1:M:239:THR:HG22	1.90	0.52
1:Q:495:MET:HG3	1:Q:539:HIS:HB2	1.91	0.52
1:R:673:GLN:HE22	1:R:912:LYS:HD2	1.74	0.52
2:BA:1:NAG:HO3	2:BA:1:NAG:C7	2.17	0.52
1:A:182:PHE:HA	1:A:186:ALA:HB3	1.90	0.52
1:A:821:TYR:CG	1:A:822:PRO:HD3	2.45	0.52
1:E:71:LEU:HD22	1:E:213:HIS:NE2	2.24	0.52
1:K:603:HIS:HB2	1:K:611:ARG:HD3	1.92	0.52
1:N:829:ARG:NH2	5:N:1010:SO4:O4	2.43	0.52
1:S:68:HIS:NE2	2:6:1:NAG:O7	2.30	0.52
1:V:782:ARG:NH2	5:V:1006:SO4:O2	2.42	0.52
1:B:259:LYS:NZ	1:B:284[B]:ASP:OD1	2.42	0.52
1:B:523:HIS:CE1	1:B:525:MET:HE2	2.44	0.52
1:N:708:LEU:HD22	1:N:744:LEU:HD13	1.91	0.52
1:S:611:ARG:NH2	5:S:1011:SO4:S	2.83	0.52
6:U:1024:NAG:O7	6:U:1024:NAG:O3	2.25	0.52
6:E:1023:NAG:O7	6:E:1023:NAG:O3	2.25	0.52
1:F:159:PHE:HB3	1:F:315:GLN:HB2	1.91	0.52
1:L:821:TYR:CG	1:L:822:PRO:HD3	2.44	0.52
1:Q:524:TYR:OH	1:Q:620:GLN:O	2.22	0.52
1:R:140:LEU:HB2	1:R:143:LEU:HD22	1.92	0.52
1:D:821:TYR:CG	1:D:822:PRO:HD3	2.44	0.52
1:D:833:ASN:ND2	5:D:1014:SO4:O1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:TYR:OH	1:E:306:GLN:NE2	2.42	0.52
1:H:821:TYR:CD1	1:H:822:PRO:HD3	2.44	0.52
1:L:761:TYR:CZ	1:L:791:TRP:HH2	2.28	0.52
1:N:730:LYS:HE3	1:N:755:GLU:HG2	1.91	0.52
1:O:764:TYR:HB2	1:O:776:ILE:HG21	1.92	0.52
1:R:259:LYS:NZ	1:R:284[B]:ASP:OD1	2.43	0.52
6:A:1022:NAG:O7	6:A:1022:NAG:O3	2.25	0.52
1:D:58:VAL:HG11	1:D:93:ILE:HG23	1.91	0.52
1:F:603:HIS:HB2	1:F:611:ARG:HD3	1.92	0.52
1:H:321:ASN:HB2	1:H:324:LEU:O	2.10	0.52
1:H:744:LEU:HG	1:H:775:GLN:HG2	1.92	0.52
1:M:829:ARG:NH2	5:M:1011:SO4:O3	2.43	0.52
1:P:260:ILE:HG13	1:R:214:LEU:HB2	1.92	0.52
1:S:829:ARG:NH2	5:S:1010:SO4:O4	2.43	0.52
1:V:575:PHE:HB2	1:V:585:VAL:HG11	1.90	0.52
1:B:708:LEU:HD22	1:B:744:LEU:HD13	1.91	0.52
1:E:680:ARG:HG3	1:E:683:ARG:HH21	1.73	0.52
1:E:708:LEU:HD22	1:E:744:LEU:HD13	1.92	0.52
1:H:729:TRP:CE2	1:H:734:GLY:HA2	2.44	0.52
1:O:407:ALA:HB2	1:O:439:ASP:HB2	1.91	0.52
1:Q:526:LYS:HD3	1:Q:892:GLU:HG2	1.92	0.52
1:U:554:ARG:N	5:U:1017:SO4:O3	2.37	0.52
1:B:140:LEU:HB2	1:B:143:LEU:HD22	1.92	0.52
1:C:159:PHE:HB3	1:C:315:GLN:HB2	1.92	0.52
1:J:495:MET:HG3	1:J:539:HIS:HB2	1.92	0.52
1:M:259:LYS:HD3	1:M:287:VAL:HG21	1.90	0.52
1:S:685:LEU:O	1:S:689:GLN:HG2	2.10	0.52
1:T:523:HIS:CE1	1:T:525:MET:HE2	2.45	0.52
1:A:49:TRP:HD1	1:A:130:GLN:HE22	1.56	0.52
1:A:259:LYS:HD3	1:A:287:VAL:HG21	1.92	0.52
1:B:70:ASN:OD1	1:B:73:THR:OG1	2.22	0.52
1:F:140:LEU:HB2	1:F:143:LEU:HD22	1.92	0.52
1:H:816:ARG:NH1	5:H:1007:SO4:O1	2.43	0.52
1:I:821:TYR:CG	1:I:822:PRO:HD3	2.45	0.52
1:J:440:LYS:HG3	1:J:582:TYR:CZ	2.45	0.52
1:N:744:LEU:HG	1:N:775:GLN:HG2	1.91	0.52
1:Q:182:PHE:HA	1:Q:186:ALA:HB3	1.92	0.52
1:S:764:TYR:HB2	1:S:776:ILE:HG21	1.92	0.52
1:B:71:LEU:HD22	1:B:213:HIS:NE2	2.26	0.51
1:J:821:TYR:CG	1:J:822:PRO:HD3	2.45	0.51
1:Q:70:ASN:OD1	1:Q:73:THR:OG1	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:546:THR:HB	1:Q:570:VAL:HG11	1.91	0.51
1:S:219:MET:HG2	1:S:239:THR:HG22	1.91	0.51
1:U:739:PRO:HB2	1:U:742:VAL:HG22	1.92	0.51
1:C:321:ASN:HB2	1:C:324:LEU:O	2.11	0.51
1:I:154:ASN:OD1	2:n:1:NAG:O5	2.27	0.51
6:J:1022:NAG:O7	6:J:1022:NAG:O3	2.25	0.51
1:P:816:ARG:NH1	5:P:1006:SO4:O3	2.42	0.51
1:R:68:HIS:NE2	2:4:1:NAG:O7	2.32	0.51
1:F:764:TYR:HE2	1:F:802:ILE:HG12	1.74	0.51
1:G:782:ARG:NH2	5:G:1006:SO4:S	2.83	0.51
1:K:744:LEU:HG	1:K:775:GLN:HG2	1.92	0.51
1:M:611:ARG:NH2	5:M:1012:SO4:S	2.83	0.51
1:U:764:TYR:HB2	1:U:776:ILE:HG21	1.92	0.51
1:U:864:GLU:HG3	1:V:567:PRO:HB3	1.92	0.51
1:A:816:ARG:HG2	1:A:856:GLN:HE22	1.74	0.51
1:B:545:ILE:HG23	1:B:577:VAL:HG21	1.92	0.51
1:C:182:PHE:HA	1:C:186:ALA:HB3	1.91	0.51
1:F:182:PHE:HA	1:F:186:ALA:HB3	1.92	0.51
6:M:1024:NAG:O7	6:M:1024:NAG:O3	2.25	0.51
1:N:850:VAL:HG12	1:N:886:THR:HG21	1.91	0.51
1:P:680:ARG:HG3	1:P:683:ARG:HH21	1.75	0.51
1:T:680:ARG:HG3	1:T:683:ARG:HH21	1.75	0.51
1:U:764:TYR:HE2	1:U:802:ILE:HG12	1.74	0.51
1:B:219:MET:HG2	1:B:239:THR:HG22	1.93	0.51
1:F:708:LEU:HD22	1:F:744:LEU:HD13	1.92	0.51
6:G:1023:NAG:O7	6:G:1023:NAG:O3	2.25	0.51
1:L:70:ASN:OD1	1:L:73:THR:OG1	2.22	0.51
1:Q:154:ASN:OD1	2:3:1:NAG:O5	2.28	0.51
1:T:833:ASN:ND2	5:T:1014:SO4:O1	2.40	0.51
1:A:296:TYR:CE1	1:A:458:LYS:HE2	2.45	0.51
1:C:829:ARG:NH2	5:C:1009:SO4:O3	2.43	0.51
1:C:833:ASN:ND2	5:C:1013:SO4:O1	2.43	0.51
6:H:1023:NAG:O7	6:H:1023:NAG:O3	2.25	0.51
1:N:259:LYS:HD3	1:N:287:VAL:HG21	1.93	0.51
1:R:523:HIS:CE1	1:R:525:MET:HE2	2.45	0.51
1:S:680:ARG:HG3	1:S:683:ARG:HH21	1.76	0.51
1:C:821:TYR:CG	1:C:822:PRO:HD3	2.45	0.51
1:F:816:ARG:HG2	1:F:856:GLN:HE22	1.76	0.51
1:H:219:MET:HG2	1:H:239:THR:HG22	1.92	0.51
1:I:782:ARG:NH2	5:I:1007:SO4:S	2.84	0.51
1:F:220:PRO:HG3	1:F:305:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:PHE:HB3	1:H:315:GLN:HB2	1.93	0.51
1:Q:665:ARG:HE	1:Q:859:THR:HG22	1.76	0.51
1:D:782:ARG:NH2	5:D:1007:SO4:O4	2.43	0.51
1:I:210:GLU:HG2	2:m:1:NAG:H82	1.92	0.51
1:N:154:ASN:OD1	2:x:1:NAG:O5	2.29	0.51
1:N:341:ALA:HB1	1:N:697:VAL:HG13	1.93	0.51
1:E:548:LYS:NZ	5:E:1001:SO4:O3	2.44	0.50
1:G:301:TYR:OH	1:G:306:GLN:NE2	2.45	0.50
1:N:764:TYR:HE2	1:N:802:ILE:HG12	1.76	0.50
1:O:611:ARG:NH2	5:O:1011:SO4:O1	2.44	0.50
1:Q:793:LEU:HB3	1:Q:827:PHE:CE2	2.46	0.50
1:Q:821:TYR:CG	1:Q:822:PRO:HD3	2.46	0.50
1:V:407:ALA:HB2	1:V:439:ASP:HB2	1.92	0.50
1:D:744:LEU:HG	1:D:775:GLN:HG2	1.93	0.50
1:E:821:TYR:CG	1:E:822:PRO:HD3	2.47	0.50
1:J:219:MET:HG2	1:J:239:THR:HG22	1.93	0.50
1:L:459:SER:HB2	1:L:485:ILE:HG21	1.93	0.50
6:L:1023:NAG:O7	6:L:1023:NAG:O3	2.25	0.50
1:N:440:LYS:HG3	1:N:582:TYR:CZ	2.46	0.50
1:N:821:TYR:CG	1:N:822:PRO:HD3	2.46	0.50
1:O:219:MET:HG2	1:O:239:THR:HG22	1.92	0.50
1:O:543:THR:O	1:O:576:ASN:N	2.44	0.50
1:P:526:LYS:HD3	1:P:892:GLU:HG2	1.94	0.50
1:Q:816:ARG:HG2	1:Q:856:GLN:HE22	1.76	0.50
1:R:154:ASN:OD1	2:5:1:NAG:O5	2.30	0.50
1:S:259:LYS:NZ	1:S:284[B]:ASP:OD1	2.44	0.50
1:T:70:ASN:OD1	1:T:73:THR:OG1	2.22	0.50
1:V:821:TYR:CG	1:V:822:PRO:HD3	2.46	0.50
1:D:659:TYR:HB3	1:D:674:PHE:CD2	2.46	0.50
1:G:850:VAL:HG12	1:G:886:THR:HG21	1.93	0.50
1:J:321:ASN:HB2	1:J:324:LEU:O	2.12	0.50
1:M:182:PHE:HA	1:M:186:ALA:HB3	1.93	0.50
1:P:440:LYS:HG3	1:P:582:TYR:CZ	2.45	0.50
1:R:259:LYS:HD3	1:R:287:VAL:HG21	1.94	0.50
6:R:1023:NAG:O7	6:R:1023:NAG:O3	2.25	0.50
1:S:660:LYS:NZ	1:S:816:ARG:O	2.44	0.50
1:T:821:TYR:CG	1:T:822:PRO:HD3	2.47	0.50
1:V:816:ARG:NH1	5:V:1006:SO4:S	2.84	0.50
1:B:220:PRO:HG3	1:B:305:LYS:HG2	1.93	0.50
1:D:321:ASN:HB2	1:D:324:LEU:O	2.11	0.50
1:D:523:HIS:CE1	1:D:525:MET:HE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:575:PHE:HB2	1:J:585:VAL:HG11	1.93	0.50
1:J:730:LYS:HE3	1:J:755:GLU:HG2	1.92	0.50
1:N:219:MET:HG2	1:N:239:THR:HG22	1.94	0.50
1:N:259:LYS:NZ	1:N:284[B]:ASP:OD1	2.44	0.50
1:P:764:TYR:HE2	1:P:802:ILE:HG12	1.75	0.50
1:Q:71:LEU:HD22	1:Q:213:HIS:NE2	2.27	0.50
1:U:154:ASN:OD1	2:BA:1:NAG:O5	2.28	0.50
1:D:764:TYR:HB2	1:D:776:ILE:HG21	1.93	0.50
1:D:804:THR:HG21	1:D:838:LYS:HE2	1.94	0.50
1:J:476:GLU:OE2	1:J:493:LYS:NZ	2.33	0.50
1:S:821:TYR:CD1	1:S:822:PRO:HD3	2.47	0.50
1:A:219:MET:HG2	1:A:239:THR:HG22	1.93	0.50
1:A:833:ASN:ND2	5:A:1013:SO4:O1	2.45	0.50
1:C:658:MET:HB2	1:C:674:PHE:HE2	1.76	0.50
6:D:1023:NAG:O7	6:D:1023:NAG:O3	2.25	0.50
1:F:829:ARG:NH2	5:F:1010:SO4:S	2.82	0.50
1:F:846:ILE:HA	1:F:849:MET:HE3	1.94	0.50
1:K:829:ARG:NH2	5:K:1009:SO4:O1	2.44	0.50
1:O:744:LEU:HG	1:O:775:GLN:HG2	1.93	0.50
1:R:846:ILE:HA	1:R:849:MET:HE3	1.93	0.50
1:D:764:TYR:HE2	1:D:802:ILE:HG12	1.75	0.50
1:O:68:HIS:NE2	2:y:1:NAG:O7	2.33	0.50
1:R:761:TYR:CZ	1:R:791:TRP:HH2	2.30	0.50
1:G:140:LEU:HB2	1:G:143:LEU:HD22	1.93	0.50
1:G:321:ASN:HB2	1:G:324:LEU:O	2.11	0.50
1:I:212:ARG:NH2	5:I:1005:SO4:O2	2.44	0.50
1:L:730:LYS:HE3	1:L:755:GLU:HG2	1.94	0.50
1:N:210:GLU:HG2	2:w:1:NAG:H82	1.94	0.50
1:O:729:TRP:CE2	1:O:734:GLY:HA2	2.46	0.50
1:P:495:MET:O	1:P:498:THR:OG1	2.26	0.50
1:S:821:TYR:CG	1:S:822:PRO:HD3	2.47	0.50
1:V:440:LYS:HG3	1:V:582:TYR:CZ	2.47	0.50
2:v:2:NAG:HO3	2:v:2:NAG:C7	2.19	0.50
1:A:782:ARG:NH2	5:A:1006:SO4:O2	2.44	0.50
1:E:729:TRP:CE2	1:E:734:GLY:HA2	2.47	0.50
1:K:850:VAL:HG12	1:K:886:THR:HG21	1.94	0.50
1:L:438:TYR:OH	4:L:1003:P52:O2	2.24	0.50
1:N:761:TYR:CZ	1:N:791:TRP:HH2	2.30	0.50
1:R:793:LEU:HG	1:R:814:ILE:HD12	1.94	0.50
1:U:140:LEU:HB2	1:U:143:LEU:HD22	1.93	0.50
1:V:259:LYS:HD3	1:V:287:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ARG:NH2	5:C:1010:SO4:O3	2.45	0.49
1:G:74:LEU:O	1:G:154:ASN:HB3	2.12	0.49
1:G:793:LEU:HB3	1:G:827:PHE:CD2	2.47	0.49
1:I:341:ALA:HB1	1:I:697:VAL:HG13	1.94	0.49
1:I:659:TYR:HB3	1:I:674:PHE:CD2	2.47	0.49
6:K:1023:NAG:O7	6:K:1023:NAG:O3	2.25	0.49
1:L:729:TRP:CE2	1:L:734:GLY:HA2	2.46	0.49
1:M:341:ALA:HB1	1:M:697:VAL:HG13	1.94	0.49
1:O:821:TYR:CG	1:O:822:PRO:HD3	2.47	0.49
1:U:757:TRP:CD2	1:U:788:LYS:HD3	2.47	0.49
2:z:1:NAG:HO3	2:z:1:NAG:C7	2.12	0.49
1:B:793:LEU:HB3	1:B:827:PHE:CD2	2.47	0.49
1:G:543:THR:O	1:G:576:ASN:N	2.44	0.49
1:I:70:ASN:OD1	1:I:73:THR:OG1	2.22	0.49
1:I:680:ARG:HG3	1:I:683:ARG:HH21	1.77	0.49
1:J:495:MET:O	1:J:498:THR:OG1	2.27	0.49
1:K:259:LYS:NZ	1:K:284[B]:ASP:OD1	2.45	0.49
1:M:659:TYR:HB3	1:M:674:PHE:CD2	2.46	0.49
1:T:182:PHE:HA	1:T:186:ALA:HB3	1.94	0.49
1:T:761:TYR:CZ	1:T:791:TRP:HH2	2.30	0.49
1:O:708:LEU:HD22	1:O:744:LEU:HD13	1.94	0.49
1:P:846:ILE:HA	1:P:849:MET:HE3	1.95	0.49
1:T:407:ALA:HB2	1:T:439:ASP:HB2	1.94	0.49
1:U:321:ASN:HB2	1:U:324:LEU:O	2.13	0.49
1:V:729:TRP:CE2	1:V:734:GLY:HA2	2.47	0.49
6:V:1022:NAG:O7	6:V:1022:NAG:O3	2.25	0.49
1:C:407:ALA:HB2	1:C:439:ASP:HB2	1.94	0.49
1:C:711[B]:CYS:SG	1:C:718[B]:CYS:HB3	2.52	0.49
1:D:850:VAL:HG12	1:D:886:THR:HG21	1.94	0.49
1:F:154:ASN:OD1	2:h:1:NAG:O5	2.29	0.49
1:J:515:ARG:NH1	5:J:1007:SO4:O3	2.44	0.49
1:M:296:TYR:CE1	1:M:458:LYS:HE2	2.48	0.49
1:O:140:LEU:HB2	1:O:143:LEU:HD22	1.95	0.49
1:P:519:MET:HE1	1:P:555:PHE:HE2	1.78	0.49
1:P:622:VAL:HG21	1:P:632:ALA:HB2	1.93	0.49
1:B:259:LYS:HD3	1:B:287:VAL:HG21	1.94	0.49
1:C:261:THR:HG22	1:C:287:VAL:HG13	1.93	0.49
1:D:708:LEU:HD22	1:D:744:LEU:HD13	1.95	0.49
1:D:793:LEU:HB3	1:D:827:PHE:CE2	2.48	0.49
1:F:321:ASN:HB2	1:F:324:LEU:O	2.12	0.49
1:M:321:ASN:HB2	1:M:324:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:739:PRO:HB2	1:S:742:VAL:HG22	1.94	0.49
1:I:665:ARG:HH21	1:I:859:THR:HG22	1.77	0.49
1:N:220:PRO:HG3	1:N:305:LYS:HG2	1.95	0.49
1:F:545:ILE:HG23	1:F:577:VAL:HG21	1.95	0.49
1:I:846:ILE:HA	1:I:849:MET:HE3	1.95	0.49
1:K:548:LYS:NZ	5:K:1024:SO4:S	2.85	0.49
1:M:761:TYR:CZ	1:M:791:TRP:HH2	2.31	0.49
1:O:523:HIS:ND1	1:O:534:THR:HG21	2.27	0.49
1:P:154:ASN:OD1	2:1:1:NAG:O5	2.30	0.49
1:R:523:HIS:ND1	1:R:534:THR:HG21	2.27	0.49
1:T:341:ALA:HB1	1:T:697:VAL:HG13	1.94	0.49
1:V:154:ASN:OD1	2:DA:1:NAG:O5	2.30	0.49
1:C:596:THR:HG23	1:C:635:LEU:HA	1.95	0.49
1:E:603:HIS:HB2	1:E:611:ARG:HD3	1.94	0.49
1:K:575:PHE:HB2	1:K:585:VAL:HG11	1.94	0.49
1:L:217:SER:OG	1:L:218:ASN:N	2.46	0.49
1:O:660:LYS:NZ	1:O:816:ARG:O	2.46	0.49
1:T:259:LYS:HD3	1:T:287:VAL:HG21	1.95	0.49
1:T:622:VAL:HG12	1:T:896:TRP:HE1	1.78	0.49
1:V:71:LEU:HD22	1:V:213:HIS:NE2	2.28	0.49
1:V:217:SER:OG	1:V:218:ASN:N	2.45	0.49
1:A:708:LEU:HD22	1:A:744:LEU:HD13	1.94	0.49
1:B:821:TYR:CG	1:B:822:PRO:HD3	2.48	0.49
1:C:729:TRP:CE2	1:C:734:GLY:HA2	2.48	0.49
1:E:321:ASN:HB2	1:E:324:LEU:O	2.12	0.49
1:N:321:ASN:HB2	1:N:324:LEU:O	2.13	0.49
1:P:49:TRP:HD1	1:P:130:GLN:HE22	1.60	0.49
1:S:575:PHE:HB2	1:S:585:VAL:HG11	1.95	0.49
1:T:744:LEU:HG	1:T:775:GLN:HG2	1.94	0.49
2:d:2:NAG:HO3	2:d:2:NAG:C7	2.20	0.49
6:B:1022:NAG:O7	6:B:1022:NAG:O3	2.25	0.49
1:C:785:ASN:HB3	1:C:788:LYS:HB2	1.95	0.49
1:H:440:LYS:HG3	1:H:582:TYR:CZ	2.47	0.49
1:H:708:LEU:HD22	1:H:744:LEU:HD13	1.93	0.49
1:P:506:PRO:HG2	1:P:583:TYR:HB3	1.94	0.49
1:S:259:LYS:HD3	1:S:287:VAL:HG21	1.93	0.49
1:S:407:ALA:HB2	1:S:439:ASP:HB2	1.94	0.49
6:S:1023:NAG:O7	6:S:1023:NAG:O3	2.25	0.49
1:K:657:PRO:HA	1:K:660:LYS:HB2	1.95	0.48
1:T:781:CYS:O	1:T:817:ASN:ND2	2.39	0.48
1:V:140:LEU:HB2	1:V:143:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ILE:HD13	1:A:710:ALA:HB2	1.95	0.48
1:H:546:THR:HB	1:H:570:VAL:HG11	1.95	0.48
1:J:825:TRP:CE2	1:J:829:ARG:HD2	2.48	0.48
1:M:611:ARG:NH2	5:M:1012:SO4:O3	2.46	0.48
1:P:125:HIS:CE1	1:P:127:ARG:HB2	2.48	0.48
1:B:261:THR:HG22	1:B:287:VAL:HG13	1.94	0.48
1:F:217:SER:OG	1:F:218:ASN:N	2.46	0.48
1:H:603:HIS:HB2	1:H:611:ARG:HD3	1.93	0.48
6:N:1023:NAG:O7	6:N:1023:NAG:O3	2.25	0.48
1:P:140:LEU:HB2	1:P:143:LEU:HD22	1.96	0.48
1:P:782:ARG:NH2	5:P:1006:SO4:O1	2.36	0.48
1:T:685:LEU:O	1:T:689:GLN:HG2	2.13	0.48
1:V:781:CYS:O	1:V:817:ASN:ND2	2.36	0.48
1:B:322:TRP:CD2	1:B:362:ASN:HB3	2.49	0.48
1:F:210:GLU:HG2	2:g:1:NAG:H82	1.95	0.48
1:K:321:ASN:HB2	1:K:324:LEU:O	2.13	0.48
1:L:182:PHE:HA	1:L:186:ALA:HB3	1.95	0.48
1:O:825:TRP:CE2	1:O:829:ARG:HD2	2.48	0.48
1:S:793:LEU:HB3	1:S:827:PHE:CE2	2.48	0.48
1:C:70:ASN:OD1	1:C:73:THR:OG1	2.22	0.48
1:C:361:GLY:HA2	1:C:375:ASN:ND2	2.27	0.48
1:L:846:ILE:HA	1:L:849:MET:HE3	1.95	0.48
1:N:556:LEU:HG	1:N:558:LYS:HG3	1.94	0.48
1:S:125:HIS:CE1	1:S:127:ARG:HB2	2.48	0.48
1:U:757:TRP:CE2	1:U:780:LEU:HD22	2.48	0.48
1:G:70:ASN:OD1	1:G:73:THR:OG1	2.22	0.48
1:I:685:LEU:O	1:I:689:GLN:HG2	2.13	0.48
1:O:846:ILE:HA	1:O:849:MET:HE3	1.94	0.48
1:U:259:LYS:NZ	1:U:284[B]:ASP:OD1	2.46	0.48
1:V:816:ARG:NH1	5:V:1006:SO4:O3	2.46	0.48
1:I:526:LYS:HD3	1:I:892:GLU:HG2	1.96	0.48
1:R:68:HIS:O	1:R:76:PHE:HA	2.13	0.48
1:V:321:ASN:HB2	1:V:324:LEU:O	2.12	0.48
2:d:1:NAG:HO3	2:d:1:NAG:C7	2.21	0.48
1:H:821:TYR:CG	1:H:822:PRO:HD3	2.48	0.48
1:K:579:MET:HG2	1:K:613:SER:HB3	1.95	0.48
1:L:259:LYS:NZ	1:L:284[B]:ASP:OD1	2.46	0.48
1:M:782:ARG:NH2	5:M:1007:SO4:O2	2.47	0.48
1:O:596:THR:HG23	1:O:635:LEU:HA	1.95	0.48
1:S:744:LEU:HG	1:S:775:GLN:HG2	1.96	0.48
1:V:208:ARG:NH2	5:V:1014:SO4:O1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PHE:HA	1:B:186:ALA:HB3	1.94	0.48
1:F:575:PHE:HB2	1:F:585:VAL:HG11	1.96	0.48
1:F:793:LEU:HB3	1:F:827:PHE:CE2	2.49	0.48
1:I:825:TRP:CE2	1:I:829:ARG:HD2	2.48	0.48
1:L:140:LEU:HB2	1:L:143:LEU:HD22	1.96	0.48
1:O:241:LYS:HB2	1:O:470:TYR:HD2	1.77	0.48
1:T:729:TRP:CE2	1:T:734:GLY:HA2	2.49	0.48
2:f:2:NAG:HO3	2:f:2:NAG:C7	2.21	0.48
1:B:658:MET:HB2	1:B:674:PHE:HE2	1.78	0.48
1:E:407:ALA:HB2	1:E:439:ASP:HB2	1.96	0.48
1:F:296:TYR:CE1	1:F:458:LYS:HE2	2.49	0.48
1:F:793:LEU:HB3	1:F:827:PHE:CD2	2.49	0.48
1:H:70:ASN:OD1	1:H:73:THR:OG1	2.22	0.48
1:I:259:LYS:HD3	1:I:287:VAL:HG21	1.96	0.48
1:J:793:LEU:HB3	1:J:827:PHE:CE2	2.49	0.48
1:M:417:HIS:ND1	1:M:418:PRO:O	2.40	0.48
1:C:217:SER:OG	1:C:218:ASN:N	2.45	0.47
1:C:685:LEU:O	1:C:689:GLN:HG2	2.13	0.47
1:E:296:TYR:CE1	1:E:458:LYS:HE2	2.49	0.47
1:E:825:TRP:CE2	1:E:829:ARG:HD2	2.49	0.47
1:I:603:HIS:HB2	1:I:611:ARG:HD3	1.95	0.47
1:L:657:PRO:HA	1:L:660:LYS:HB2	1.95	0.47
1:N:217:SER:OG	1:N:218:ASN:N	2.48	0.47
1:U:744:LEU:HG	1:U:775:GLN:HG2	1.96	0.47
1:B:430:ARG:NH1	1:B:840:GLU:HB3	2.28	0.47
1:E:220:PRO:HG3	1:E:305:LYS:HG2	1.96	0.47
1:H:829:ARG:NH2	5:H:1010:SO4:O1	2.47	0.47
1:K:407:ALA:HB2	1:K:439:ASP:HB2	1.95	0.47
1:K:440:LYS:HG3	1:K:582:TYR:CZ	2.49	0.47
1:L:125:HIS:CE1	1:L:127:ARG:HB2	2.50	0.47
1:L:665:ARG:HH11	1:L:667:MET:HE1	1.79	0.47
6:P:1022:NAG:O7	6:P:1022:NAG:O3	2.25	0.47
1:B:611:ARG:NH2	5:B:1010:SO4:O3	2.33	0.47
1:G:261:THR:HG22	1:G:287:VAL:HG13	1.96	0.47
1:I:744:LEU:HG	1:I:775:GLN:HG2	1.96	0.47
1:J:656:ILE:N	1:J:657:PRO:HD2	2.30	0.47
1:R:212:ARG:NH2	5:R:1004:SO4:O4	2.47	0.47
1:R:321:ASN:HB2	1:R:324:LEU:O	2.14	0.47
1:S:596:THR:HG23	1:S:635:LEU:HA	1.96	0.47
1:B:366:MET:HE2	1:B:372:LEU:HA	1.97	0.47
1:B:685:LEU:O	1:B:689:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:MET:HG2	1:G:239:THR:HG22	1.95	0.47
1:I:219:MET:HG2	1:I:239:THR:HG22	1.95	0.47
1:U:685:LEU:O	1:U:689:GLN:HG2	2.14	0.47
1:E:378:PHE:O	1:E:382:MET:HG2	2.14	0.47
1:L:708:LEU:HD22	1:L:744:LEU:HD13	1.96	0.47
1:R:821:TYR:CG	1:R:822:PRO:HD3	2.49	0.47
1:S:182:PHE:HA	1:S:186:ALA:HB3	1.96	0.47
1:T:804:THR:HG21	1:T:838:LYS:HE2	1.96	0.47
1:T:821:TYR:CD1	1:T:822:PRO:HD3	2.50	0.47
1:T:846:ILE:HA	1:T:849:MET:HE3	1.96	0.47
1:U:407:ALA:HB2	1:U:439:ASP:HB2	1.97	0.47
1:B:711[B]:CYS:SG	1:B:745:ALA:HB1	2.55	0.47
1:F:729:TRP:CE2	1:F:734:GLY:HA2	2.50	0.47
1:F:821:TYR:CG	1:F:822:PRO:HD3	2.50	0.47
1:G:825:TRP:CE2	1:G:829:ARG:HD2	2.50	0.47
1:R:785:ASN:HB3	1:R:788:LYS:HB2	1.96	0.47
1:U:217:SER:OG	1:U:218:ASN:N	2.47	0.47
2:t:1:NAG:HO3	2:t:1:NAG:C7	2.22	0.47
1:B:210:GLU:HG2	2:Y:1:NAG:H82	1.97	0.47
1:D:407:ALA:HB2	1:D:439:ASP:HB2	1.96	0.47
1:F:440:LYS:HG3	1:F:582:TYR:CZ	2.50	0.47
1:H:659:TYR:HB3	1:H:674:PHE:CD2	2.50	0.47
1:I:440:LYS:HG3	1:I:582:TYR:CZ	2.49	0.47
1:K:660:LYS:HD3	1:K:660:LYS:HA	1.72	0.47
1:L:515:ARG:NH1	5:L:1008:SO4:O1	2.48	0.47
1:M:407:ALA:HB2	1:M:439:ASP:HB2	1.97	0.47
1:M:764:TYR:HB2	1:M:776:ILE:HG21	1.96	0.47
1:R:301:TYR:OH	1:R:306:GLN:NE2	2.48	0.47
1:R:739:PRO:HB2	1:R:742:VAL:HG22	1.96	0.47
1:S:257:VAL:HG12	1:V:257:VAL:HG12	1.96	0.47
1:U:341:ALA:HB1	1:U:697:VAL:HG13	1.97	0.47
1:U:729:TRP:CE2	1:U:734:GLY:HA2	2.49	0.47
2:h:2:NAG:HO3	2:h:2:NAG:C7	2.21	0.47
1:A:70:ASN:OD1	1:A:73:THR:OG1	2.22	0.47
1:D:658:MET:HB2	1:D:674:PHE:HE2	1.80	0.47
1:M:70:ASN:OD1	1:M:73:THR:OG1	2.22	0.47
1:U:665:ARG:HH21	1:U:859:THR:HG22	1.79	0.47
1:A:685:LEU:O	1:A:689:GLN:HG2	2.15	0.47
1:C:581:GLY:HA3	1:C:583:TYR:CE1	2.50	0.47
1:C:658:MET:HB2	1:C:674:PHE:CE2	2.50	0.47
1:F:711[B]:CYS:SG	1:F:745:ALA:HB1	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:LYS:HE3	1:F:755:GLU:HG2	1.97	0.47
1:G:259:LYS:HD3	1:G:287:VAL:HG21	1.96	0.47
1:J:659:TYR:HB3	1:J:674:PHE:CD2	2.50	0.47
6:T:1023:NAG:O7	6:T:1023:NAG:O3	2.25	0.47
1:V:215:ALA:HA	1:V:250:ILE:O	2.14	0.47
2:7:1:NAG:HO3	2:7:1:NAG:C7	2.12	0.47
1:D:71:LEU:HD22	1:D:213:HIS:NE2	2.30	0.47
1:H:58:VAL:HG11	1:H:93:ILE:HG23	1.97	0.47
1:H:829:ARG:HA	1:H:869:PHE:CZ	2.50	0.47
1:M:685:LEU:O	1:M:689:GLN:HG2	2.15	0.47
1:O:231:LEU:HD22	2:y:1:NAG:H81	1.97	0.47
1:R:217:SER:OG	1:R:218:ASN:N	2.48	0.47
1:R:219:MET:HG2	1:R:239:THR:HG22	1.96	0.47
1:T:524:TYR:OH	1:T:620:GLN:O	2.21	0.47
1:V:219:MET:HG2	1:V:239:THR:HG22	1.97	0.47
1:B:526:LYS:HD3	1:B:892:GLU:HG2	1.96	0.46
1:F:341:ALA:HB1	1:F:697:VAL:HG13	1.95	0.46
1:F:825:TRP:CE2	1:F:829:ARG:HD2	2.50	0.46
1:G:685:LEU:O	1:G:689:GLN:HG2	2.16	0.46
1:K:791:TRP:CZ2	1:K:795:GLU:HG3	2.51	0.46
1:K:821:TYR:CG	1:K:822:PRO:HD3	2.50	0.46
1:M:659:TYR:HB3	1:M:674:PHE:HD2	1.81	0.46
1:S:548:LYS:NZ	5:S:1001:SO4:O1	2.34	0.46
1:V:657:PRO:HA	1:V:660:LYS:HB2	1.97	0.46
1:V:761:TYR:CZ	1:V:791:TRP:HH2	2.33	0.46
1:B:440:LYS:HG3	1:B:582:TYR:CZ	2.50	0.46
1:C:657:PRO:HA	1:C:660:LYS:HB2	1.97	0.46
1:C:659:TYR:HB3	1:C:674:PHE:CD2	2.50	0.46
1:D:217:SER:OG	1:D:218:ASN:N	2.48	0.46
1:E:739:PRO:HB2	1:E:742:VAL:HG22	1.96	0.46
1:I:729:TRP:CE2	1:I:734:GLY:HA2	2.49	0.46
1:K:815:GLY:HA2	1:K:821:TYR:HA	1.96	0.46
1:L:658:MET:HB2	1:L:674:PHE:HE2	1.81	0.46
1:M:657:PRO:HA	1:M:660:LYS:HB2	1.96	0.46
1:U:761:TYR:CZ	1:U:791:TRP:HH2	2.33	0.46
1:V:523:HIS:ND1	1:V:534:THR:HG21	2.30	0.46
1:B:791:TRP:CE2	1:B:795:GLU:HG3	2.50	0.46
1:F:367:GLU:HA	1:F:472:ASN:HB3	1.98	0.46
1:H:545:ILE:HG23	1:H:577:VAL:HG21	1.98	0.46
1:L:523:HIS:CE1	1:L:525:MET:HE2	2.50	0.46
1:M:188:ARG:HH21	1:M:195:ASP:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:793:LEU:HB3	1:M:827:PHE:CD2	2.50	0.46
1:M:821:TYR:CG	1:M:822:PRO:HD3	2.50	0.46
1:P:217:SER:OG	1:P:218:ASN:N	2.48	0.46
1:A:217:SER:OG	1:A:218:ASN:N	2.46	0.46
1:A:598:LEU:HD11	1:A:605:ALA:HB3	1.96	0.46
1:C:793:LEU:HB3	1:C:827:PHE:CD2	2.51	0.46
1:D:658:MET:HB2	1:D:674:PHE:CE2	2.50	0.46
1:E:685:LEU:O	1:E:689:GLN:HG2	2.15	0.46
1:F:219:MET:HG2	1:F:239:THR:HG22	1.97	0.46
1:I:296:TYR:CE1	1:I:458:LYS:HE2	2.49	0.46
1:I:495:MET:O	1:I:498:THR:OG1	2.32	0.46
1:K:659:TYR:HB3	1:K:674:PHE:CD2	2.51	0.46
1:L:219:MET:HG2	1:L:239:THR:HG22	1.97	0.46
1:N:107:LEU:HD21	1:N:139:LEU:HD21	1.97	0.46
1:O:71:LEU:HD22	1:O:213:HIS:CE1	2.51	0.46
1:Q:217:SER:OG	1:Q:218:ASN:N	2.47	0.46
1:R:729:TRP:CE2	1:R:734:GLY:HA2	2.49	0.46
1:R:744:LEU:HG	1:R:775:GLN:HG2	1.96	0.46
1:U:793:LEU:HB3	1:U:827:PHE:CE2	2.51	0.46
1:U:833:ASN:ND2	5:U:1015:SO4:O4	2.49	0.46
1:U:846:ILE:HA	1:U:849:MET:HE3	1.97	0.46
1:C:495:MET:O	1:C:498:THR:OG1	2.32	0.46
1:E:776:ILE:O	1:E:780:LEU:HG	2.16	0.46
1:H:217:SER:OG	1:H:218:ASN:N	2.48	0.46
1:H:261:THR:HG22	1:H:287:VAL:HG13	1.97	0.46
1:K:301:TYR:OH	1:K:306:GLN:NE2	2.48	0.46
1:T:657:PRO:HA	1:T:660:LYS:HB2	1.98	0.46
1:V:259:LYS:NZ	1:V:284[B]:ASP:OD1	2.48	0.46
2:z:2:NAG:HO3	2:z:2:NAG:C7	2.15	0.46
1:B:125:HIS:HE1	1:B:127:ARG:HH11	1.64	0.46
1:F:438:TYR:OH	4:F:1003:P52:O2	2.28	0.46
1:F:444:ILE:HA	1:F:447:MET:HE2	1.97	0.46
1:H:846:ILE:HA	1:H:849:MET:HE3	1.98	0.46
1:J:680:ARG:HG3	1:J:683:ARG:HH21	1.79	0.46
1:L:341:ALA:HB1	1:L:697:VAL:HG13	1.98	0.46
1:L:407:ALA:HB2	1:L:439:ASP:HB2	1.97	0.46
1:M:125:HIS:CE1	1:M:127:ARG:HB2	2.50	0.46
1:P:321:ASN:HB2	1:P:324:LEU:O	2.16	0.46
1:P:685:LEU:O	1:P:689:GLN:HG2	2.16	0.46
1:P:754:THR:HG23	1:P:788:LYS:HE3	1.98	0.46
1:V:816:ARG:NH1	5:V:1006:SO4:O1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:2:NAG:HO3	2:p:2:NAG:C7	2.21	0.46
1:B:657:PRO:HA	1:B:660:LYS:HB2	1.97	0.46
1:F:657:PRO:HA	1:F:660:LYS:HB2	1.98	0.46
1:M:365:THR:O	1:M:472:ASN:HA	2.16	0.46
1:O:791:TRP:CZ2	1:O:795:GLU:HG3	2.51	0.46
1:R:548:LYS:NZ	5:R:1024:SO4:O1	2.32	0.46
1:S:70:ASN:OD1	1:S:73:THR:OG1	2.22	0.46
1:B:680:ARG:HG3	1:B:683:ARG:HH21	1.80	0.46
1:C:479:TRP:CZ2	1:C:496:MET:HB3	2.51	0.46
1:E:188:ARG:HH21	1:E:195:ASP:HB3	1.80	0.46
1:I:659:TYR:HB3	1:I:674:PHE:HD2	1.80	0.46
1:M:440:LYS:HG3	1:M:582:TYR:CZ	2.51	0.46
1:O:321:ASN:HB2	1:O:324:LEU:O	2.15	0.46
1:O:545:ILE:HG23	1:O:577:VAL:HG21	1.97	0.46
1:P:739:PRO:HB2	1:P:742:VAL:HG22	1.98	0.46
1:R:567:PRO:HB3	1:V:864:GLU:HG3	1.97	0.46
1:S:440:LYS:HG3	1:S:582:TYR:CZ	2.51	0.46
1:S:622:VAL:HA	1:S:627:LEU:O	2.15	0.46
1:T:825:TRP:CE2	1:T:829:ARG:HD2	2.51	0.46
1:V:68:HIS:NE2	2:CA:1:NAG:O7	2.34	0.46
1:B:321:ASN:HB2	1:B:324:LEU:O	2.16	0.46
1:B:782:ARG:NH2	5:B:1006:SO4:S	2.88	0.46
1:D:685:LEU:O	1:D:689:GLN:HG2	2.15	0.46
1:G:793:LEU:HB3	1:G:827:PHE:CE2	2.51	0.46
1:I:71:LEU:HD22	1:I:213:HIS:NE2	2.31	0.46
1:I:217:SER:OG	1:I:218:ASN:N	2.49	0.46
1:I:816:ARG:HG2	1:I:856:GLN:HE22	1.81	0.46
1:L:433:PHE:CZ	4:L:1003:P52:H11	2.51	0.46
1:P:107:LEU:HB2	1:P:120:LEU:HD11	1.98	0.46
1:P:660:LYS:HA	1:P:660:LYS:HD3	1.76	0.46
1:S:212:ARG:NH2	5:S:1005:SO4:O4	2.46	0.46
1:D:440:LYS:HG3	1:D:582:TYR:CZ	2.51	0.46
1:H:791:TRP:CZ2	1:H:795:GLU:HG3	2.50	0.46
1:I:407:ALA:HB2	1:I:439:ASP:HB2	1.98	0.46
1:J:231:LEU:HD22	2:o:1:NAG:H81	1.97	0.46
1:J:523:HIS:ND1	1:J:534:THR:HG21	2.31	0.46
1:J:685:LEU:O	1:J:689:GLN:HG2	2.15	0.46
1:M:217:SER:OG	1:M:218:ASN:N	2.47	0.46
1:M:656:ILE:N	1:M:657:PRO:HD2	2.31	0.46
1:P:407:ALA:HB2	1:P:439:ASP:HB2	1.98	0.46
1:P:730:LYS:HE3	1:P:755:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:430:ARG:HD2	1:Q:841:LEU:O	2.16	0.46
1:Q:793:LEU:HB3	1:Q:827:PHE:CD2	2.51	0.46
1:R:757:TRP:CD2	1:R:788:LYS:HD3	2.50	0.46
1:A:764:TYR:HB2	1:A:776:ILE:HG21	1.98	0.45
1:D:761:TYR:OH	1:D:801:LYS:HB3	2.16	0.45
1:E:660:LYS:HA	1:E:660:LYS:HD3	1.76	0.45
1:F:407:ALA:HB2	1:F:439:ASP:HB2	1.97	0.45
1:F:543:THR:O	1:F:576:ASN:N	2.47	0.45
1:F:685:LEU:O	1:F:689:GLN:HG2	2.16	0.45
1:F:833:ASN:ND2	5:F:1014:SO4:O1	2.49	0.45
1:G:821:TYR:CG	1:G:822:PRO:HD3	2.51	0.45
1:H:154:ASN:OD1	2:I:1:NAG:O5	2.34	0.45
1:H:259:LYS:HD3	1:H:287:VAL:HG21	1.98	0.45
1:J:296:TYR:HE2	1:J:461:ILE:HD11	1.81	0.45
1:O:217:SER:OG	1:O:218:ASN:N	2.47	0.45
1:Q:846:ILE:HA	1:Q:849:MET:HE3	1.97	0.45
1:S:219:MET:HB3	1:S:237:ASP:HB3	1.98	0.45
1:T:381:PHE:HE1	1:T:446:ASN:HD22	1.64	0.45
1:A:575:PHE:HB2	1:A:585:VAL:HG11	1.97	0.45
1:C:140:LEU:HB2	1:C:143:LEU:HD22	1.98	0.45
1:H:739:PRO:HB2	1:H:742:VAL:HG22	1.99	0.45
1:H:754:THR:HG23	1:H:788:LYS:HE3	1.97	0.45
1:L:548:LYS:NZ	5:L:1001:SO4:O4	2.44	0.45
1:O:782:ARG:NH2	5:O:1006:SO4:O1	2.49	0.45
1:S:554:ARG:N	5:S:1016:SO4:O1	2.36	0.45
1:V:833:ASN:ND2	5:V:1013:SO4:O3	2.49	0.45
1:A:804:THR:HG21	1:A:838:LYS:HE2	1.97	0.45
1:C:125:HIS:CE1	1:C:127:ARG:HB2	2.50	0.45
1:E:782:ARG:NH2	5:E:1007:SO4:S	2.88	0.45
1:P:656:ILE:N	1:P:657:PRO:HD2	2.32	0.45
1:R:71:LEU:HD22	1:R:213:HIS:NE2	2.32	0.45
1:S:640:LYS:HA	1:S:681:LEU:O	2.16	0.45
1:T:154:ASN:OD1	2:9:1:NAG:O5	2.32	0.45
2:b:1:NAG:HO3	2:b:1:NAG:C7	2.19	0.45
1:A:851:MET:HE3	1:A:886:THR:HG22	1.98	0.45
1:B:217:SER:OG	1:B:218:ASN:N	2.48	0.45
1:G:452:LEU:HD21	1:G:490:VAL:HG11	1.99	0.45
1:G:729:TRP:CE2	1:G:734:GLY:HA2	2.51	0.45
1:I:231:LEU:HD22	2:m:1:NAG:H81	1.97	0.45
1:I:660:LYS:HA	1:I:660:LYS:HD3	1.70	0.45
1:J:506:PRO:HB3	1:J:538:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:PRO:HG3	1:K:305:LYS:HG2	1.98	0.45
1:L:659:TYR:HB3	1:L:674:PHE:CD2	2.51	0.45
1:O:476:GLU:HG3	1:O:493:LYS:HE3	1.98	0.45
1:Q:431:GLU:OE2	1:Q:881:ARG:N	2.44	0.45
1:Q:659:TYR:HB3	1:Q:674:PHE:CD2	2.52	0.45
1:Q:744:LEU:HG	1:Q:775:GLN:HG2	1.98	0.45
1:T:321:ASN:HB2	1:T:324:LEU:O	2.17	0.45
1:V:685:LEU:O	1:V:689:GLN:HG2	2.16	0.45
1:D:816:ARG:NH1	5:D:1007:SO4:O1	2.44	0.45
2:1:1:NAG:HO3	2:1:1:NAG:C7	2.22	0.45
1:B:125:HIS:CE1	1:B:127:ARG:HB2	2.52	0.45
1:C:523:HIS:ND1	1:C:534:THR:HG21	2.32	0.45
1:K:829:ARG:NH2	5:K:1009:SO4:S	2.89	0.45
1:M:782:ARG:NH2	5:M:1007:SO4:O3	2.40	0.45
1:P:494:THR:O	1:P:498:THR:HG23	2.17	0.45
1:Q:120:LEU:HD13	1:Q:133:LEU:HB3	1.97	0.45
1:U:816:ARG:NH1	5:U:1007:SO4:S	2.90	0.45
1:C:751:ALA:HB2	1:C:760:LEU:HD12	1.98	0.45
1:D:560:LYS:HG2	1:D:561:THR:HG23	1.98	0.45
1:F:659:TYR:HB3	1:F:674:PHE:CD2	2.51	0.45
1:G:107:LEU:HB2	1:G:120:LEU:HD11	1.99	0.45
1:J:322:TRP:CD2	1:J:362:ASN:HB3	2.51	0.45
1:J:782:ARG:NH2	5:J:1006:SO4:O2	2.50	0.45
1:P:821:TYR:CG	1:P:822:PRO:HD3	2.52	0.45
1:Q:761:TYR:CZ	1:Q:791:TRP:HH2	2.34	0.45
1:R:494:THR:O	1:R:498:THR:HG23	2.16	0.45
1:T:764:TYR:HB2	1:T:776:ILE:HG21	1.98	0.45
1:V:506:PRO:HG2	1:V:583:TYR:HB3	1.99	0.45
1:V:739:PRO:HB2	1:V:742:VAL:HG22	1.98	0.45
1:C:815:GLY:HA2	1:C:821:TYR:HA	1.99	0.45
1:D:355:LEU:HA	1:D:358:GLN:HG2	1.98	0.45
1:D:692:THR:O	1:D:703:ARG:NE	2.50	0.45
1:E:764:TYR:HB2	1:E:776:ILE:HG21	1.98	0.45
1:I:851:MET:HE3	1:I:886:THR:HG22	1.99	0.45
1:K:506:PRO:HG2	1:K:583:TYR:HB3	1.99	0.45
1:L:210:GLU:HG2	2:s:1:NAG:H82	1.98	0.45
1:M:660:LYS:HD3	1:M:660:LYS:HA	1.72	0.45
1:P:659:TYR:HB3	1:P:674:PHE:CD2	2.52	0.45
1:Q:407:ALA:HB2	1:Q:439:ASP:HB2	1.99	0.45
1:S:479:TRP:HZ2	1:S:500:THR:HG21	1.82	0.45
1:S:761:TYR:CZ	1:S:791:TRP:HH2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:782:ARG:NH2	5:T:1007:SO4:O2	2.50	0.45
2:5:2:NAG:HO3	2:5:2:NAG:C7	2.22	0.45
1:A:793:LEU:HB3	1:A:827:PHE:CD2	2.52	0.45
1:D:226:THR:HG22	1:D:232:ILE:HD12	1.99	0.45
1:D:683:ARG:HD3	1:D:715:TYR:HE1	1.82	0.45
1:E:217:SER:OG	1:E:218:ASN:N	2.48	0.45
1:E:494:THR:O	1:E:498:THR:HG23	2.16	0.45
1:E:581:GLY:HA3	1:E:583:TYR:CE1	2.52	0.45
1:E:657:PRO:HA	1:E:660:LYS:HB2	1.99	0.45
1:H:660:LYS:HD3	1:H:660:LYS:HA	1.76	0.45
1:H:665:ARG:HH11	1:H:667:MET:HE1	1.82	0.45
1:H:686:ILE:HD13	1:H:710:ALA:HB2	1.99	0.45
1:I:785:ASN:HB3	1:I:788:LYS:HB2	1.99	0.45
1:J:459:SER:HB2	1:J:485:ILE:HG21	1.99	0.45
1:L:197:PRO:HA	1:L:243:SER:HB3	1.98	0.45
1:O:685:LEU:O	1:O:689:GLN:HG2	2.17	0.45
1:P:660:LYS:HE3	1:P:816:ARG:NH1	2.32	0.45
1:Q:140:LEU:HB2	1:Q:143:LEU:HD22	1.97	0.45
1:Q:523:HIS:CE1	1:Q:525:MET:HE2	2.52	0.45
1:Q:599:LEU:HB3	1:Q:638:TYR:CG	2.51	0.45
1:R:57:TYR:HE1	1:R:90:THR:HG21	1.81	0.45
1:S:217:SER:OG	1:S:218:ASN:N	2.48	0.45
1:T:219:MET:HG2	1:T:239:THR:HG22	1.99	0.45
1:A:210:GLU:HG2	2:W:1:NAG:H82	1.99	0.45
1:B:656:ILE:N	1:B:657:PRO:HD2	2.32	0.45
1:C:730:LYS:HE3	1:C:755:GLU:HG2	1.99	0.45
1:G:217:SER:OG	1:G:218:ASN:N	2.49	0.45
1:J:217:SER:OG	1:J:218:ASN:N	2.47	0.45
1:L:857:PHE:CD2	1:L:862:ARG:HB3	2.52	0.45
1:N:657:PRO:HA	1:N:660:LYS:HB2	1.98	0.45
1:P:506:PRO:HB3	1:P:538:TRP:CE3	2.52	0.45
1:T:217:SER:OG	1:T:218:ASN:N	2.46	0.45
1:U:545:ILE:HG23	1:U:577:VAL:HG21	1.98	0.45
1:V:829:ARG:NH2	5:V:1009:SO4:S	2.83	0.45
1:H:673:GLN:HE22	1:H:912:LYS:HD2	1.82	0.44
1:M:159:PHE:CB	1:M:315:GLN:HB2	2.47	0.44
1:P:519:MET:HE1	1:P:555:PHE:CE2	2.52	0.44
1:V:757:TRP:CE2	1:V:780:LEU:HD22	2.52	0.44
1:C:68:HIS:O	1:C:76:PHE:HA	2.17	0.44
1:D:825:TRP:CE2	1:D:829:ARG:HD2	2.51	0.44
1:I:656:ILE:N	1:I:657:PRO:HD2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:LEU:HD22	1:N:213:HIS:NE2	2.32	0.44
1:R:407:ALA:HB2	1:R:439:ASP:HB2	1.98	0.44
1:T:494:THR:O	1:T:498:THR:HG23	2.17	0.44
1:T:739:PRO:HB2	1:T:742:VAL:HG22	1.98	0.44
1:A:739:PRO:HB2	1:A:742:VAL:HG22	2.00	0.44
1:F:729:TRP:NE1	1:F:734:GLY:HA2	2.32	0.44
1:H:659:TYR:HB3	1:H:674:PHE:HD2	1.83	0.44
1:L:414:ASN:HD21	6:L:1023:NAG:C2	2.16	0.44
1:P:524:TYR:OH	1:P:620:GLN:O	2.30	0.44
1:R:414:ASN:HD21	6:R:1023:NAG:C2	2.15	0.44
1:T:275:LYS:NZ	1:T:329:GLU:OE1	2.42	0.44
1:U:219:MET:HG2	1:U:239:THR:HG22	2.00	0.44
1:G:494:THR:O	1:G:498:THR:HG23	2.17	0.44
1:L:793:LEU:HB3	1:L:827:PHE:CE2	2.52	0.44
1:M:508:ILE:HA	1:M:520:LYS:O	2.16	0.44
1:U:125:HIS:CE1	1:U:127:ARG:HB2	2.53	0.44
1:U:259:LYS:HD3	1:U:287:VAL:HG21	2.00	0.44
1:V:660:LYS:NZ	1:V:816:ARG:O	2.49	0.44
1:C:656:ILE:N	1:C:657:PRO:HD2	2.33	0.44
1:C:782:ARG:NH2	5:C:1006:SO4:O2	2.50	0.44
1:D:494:THR:O	1:D:498:THR:HG23	2.18	0.44
1:E:495:MET:HG3	1:E:539:HIS:HB2	1.99	0.44
1:E:560:LYS:HG2	1:E:561:THR:HG23	1.99	0.44
1:F:125:HIS:CE1	1:F:127:ARG:HB2	2.52	0.44
1:M:438:TYR:OH	4:M:1003:P52:O2	2.23	0.44
1:N:656:ILE:HG12	1:N:659:TYR:HE2	1.82	0.44
1:N:782:ARG:NH2	5:N:1007:SO4:O4	2.50	0.44
1:B:231:LEU:HD22	2:Y:1:NAG:H81	1.99	0.44
1:B:407:ALA:HB2	1:B:439:ASP:HB2	2.00	0.44
1:B:656:ILE:HG12	1:B:659:TYR:HE2	1.82	0.44
1:E:70:ASN:OD1	1:E:73:THR:OG1	2.22	0.44
1:E:515:ARG:NH2	1:E:567:PRO:O	2.50	0.44
1:K:846:ILE:HA	1:K:849:MET:HE3	2.00	0.44
1:L:659:TYR:HB3	1:L:674:PHE:HD2	1.83	0.44
1:N:107:LEU:HB2	1:N:120:LEU:HD11	1.99	0.44
1:N:544:PHE:CE1	1:N:553:HIS:HB2	2.53	0.44
1:O:259:LYS:HD3	1:O:287:VAL:HG21	2.00	0.44
1:U:780:LEU:HB3	1:U:792:LEU:HD11	1.98	0.44
1:U:821:TYR:CG	1:U:822:PRO:HD3	2.53	0.44
1:A:660:LYS:NZ	1:A:816:ARG:O	2.49	0.44
1:B:554:ARG:N	5:B:1015:SO4:O3	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:GLU:HA	1:E:184:PRO:HA	1.78	0.44
1:H:793:LEU:HB3	1:H:827:PHE:CE2	2.53	0.44
1:J:159:PHE:CB	1:J:315:GLN:HB2	2.47	0.44
1:L:785:ASN:HB3	1:L:788:LYS:HB2	1.99	0.44
1:M:846:ILE:HA	1:M:849:MET:HE3	2.00	0.44
1:N:804:THR:HG21	1:N:838:LYS:HE2	2.00	0.44
1:O:440:LYS:HG3	1:O:582:TYR:CZ	2.52	0.44
1:V:846:ILE:HA	1:V:849:MET:HE3	2.00	0.44
2:X:1:NAG:HO3	2:X:1:NAG:C7	2.27	0.44
1:D:197:PRO:HA	1:D:243:SER:HB3	2.00	0.44
1:D:757:TRP:CE2	1:D:780:LEU:HD22	2.53	0.44
1:H:315:GLN:O	1:H:328:ARG:NH1	2.51	0.44
1:I:107:LEU:HD21	1:I:139:LEU:HD21	2.00	0.44
1:I:575:PHE:HB2	1:I:585:VAL:HG11	2.00	0.44
1:J:74:LEU:O	1:J:154:ASN:HB3	2.17	0.44
1:L:495:MET:O	1:L:498:THR:OG1	2.36	0.44
1:O:729:TRP:NE1	1:O:734:GLY:HA2	2.32	0.44
1:R:394:LEU:HD23	1:R:697:VAL:HG21	2.00	0.44
1:T:82:VAL:HG22	1:T:84:ILE:HG23	2.00	0.44
1:T:183:GLU:HA	1:T:184:PRO:HA	1.79	0.44
1:U:660:LYS:HA	1:U:660:LYS:HD3	1.78	0.44
1:C:660:LYS:HD3	1:C:660:LYS:HA	1.76	0.44
1:D:505:PHE:HB3	1:D:582:TYR:CE2	2.53	0.44
1:D:793:LEU:HB3	1:D:827:PHE:CD2	2.52	0.44
1:K:504:GLY:HA3	1:K:523:HIS:CE1	2.53	0.44
1:L:825:TRP:CE2	1:L:829:ARG:HD2	2.53	0.44
1:N:494:THR:O	1:N:498:THR:HG23	2.18	0.44
1:O:125:HIS:CE1	1:O:127:ARG:HB2	2.53	0.44
1:O:341:ALA:HB1	1:O:697:VAL:HG13	2.00	0.44
1:O:524:TYR:CD1	1:O:584:ILE:HD11	2.52	0.44
1:P:47:PHE:CE1	1:P:125:HIS:HB2	2.53	0.44
1:P:71:LEU:HD22	1:P:213:HIS:NE2	2.33	0.44
1:P:125:HIS:HE1	1:P:127:ARG:HH11	1.66	0.44
1:R:656:ILE:N	1:R:657:PRO:HD2	2.33	0.44
1:R:793:LEU:HB3	1:R:827:PHE:CD2	2.53	0.44
1:U:640:LYS:HA	1:U:681:LEU:O	2.18	0.44
1:V:219:MET:HB3	1:V:237:ASP:HB3	2.00	0.44
1:A:71:LEU:HD22	1:A:213:HIS:NE2	2.33	0.43
1:D:259:LYS:HD3	1:D:287:VAL:HG21	1.99	0.43
1:F:256:SER:HB3	1:F:270:TYR:CD2	2.53	0.43
1:I:321:ASN:HB2	1:I:324:LEU:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:414:ASN:HD21	6:K:1023:NAG:C2	2.16	0.43
1:N:125:HIS:CE1	1:N:127:ARG:HB2	2.53	0.43
1:N:793:LEU:HB3	1:N:827:PHE:CE2	2.53	0.43
1:O:829:ARG:NH2	5:O:1010:SO4:S	2.91	0.43
1:T:640:LYS:HA	1:T:681:LEU:O	2.18	0.43
1:U:524:TYR:OH	1:U:620:GLN:O	2.27	0.43
1:A:548:LYS:NZ	5:G:1009:SO4:O3	2.50	0.43
1:D:159:PHE:CB	1:D:315:GLN:HB2	2.46	0.43
1:G:761:TYR:CZ	1:G:791:TRP:HH2	2.36	0.43
1:J:754:THR:HG23	1:J:788:LYS:HE3	1.99	0.43
1:K:524:TYR:CD1	1:K:584:ILE:HD11	2.53	0.43
1:L:183:GLU:HA	1:L:184:PRO:HA	1.76	0.43
1:L:321:ASN:HB2	1:L:324:LEU:O	2.18	0.43
1:L:464:TYR:HE1	1:L:473:THR:HG21	1.82	0.43
1:P:210:GLU:HG2	2:O:1:NAG:H82	1.99	0.43
1:P:657:PRO:HA	1:P:660:LYS:HB2	2.00	0.43
1:S:321:ASN:HB2	1:S:324:LEU:O	2.18	0.43
1:A:68:HIS:NE2	2:W:1:NAG:O7	2.31	0.43
1:A:440:LYS:HG3	1:A:582:TYR:CZ	2.53	0.43
1:A:515:ARG:HD2	5:A:1007:SO4:O1	2.18	0.43
1:A:622:VAL:HA	1:A:627:LEU:O	2.18	0.43
1:A:821:TYR:CD1	1:A:822:PRO:HD3	2.53	0.43
1:B:816:ARG:NH1	5:B:1006:SO4:O1	2.45	0.43
1:E:120:LEU:HD13	1:E:133:LEU:HB3	2.00	0.43
1:F:259:LYS:HD3	1:F:287:VAL:HG21	2.01	0.43
1:F:739:PRO:HB2	1:F:742:VAL:HG22	1.99	0.43
1:G:660:LYS:HA	1:G:660:LYS:HD3	1.77	0.43
1:J:301:TYR:OH	1:J:306:GLN:NE2	2.51	0.43
1:Q:259:LYS:HD3	1:Q:287:VAL:HG21	2.00	0.43
1:T:730:LYS:HE3	1:T:755:GLU:HG2	2.00	0.43
1:V:188:ARG:HH21	1:V:195:ASP:HB3	1.83	0.43
1:V:212:ARG:NH2	5:V:1004:SO4:O2	2.48	0.43
1:A:825:TRP:CE2	1:A:829:ARG:HD2	2.53	0.43
1:B:301:TYR:OH	1:B:306:GLN:NE2	2.52	0.43
1:F:183:GLU:HA	1:F:184:PRO:HA	1.80	0.43
1:I:364:VAL:HG22	1:I:468:HIS:O	2.18	0.43
1:J:140:LEU:HB2	1:J:143:LEU:HD22	2.00	0.43
1:J:315:GLN:O	1:J:328:ARG:NH1	2.51	0.43
1:L:543:THR:O	1:L:576:ASN:N	2.50	0.43
1:M:296:TYR:HE2	1:M:461:ILE:HD11	1.83	0.43
1:U:603:HIS:HB2	1:U:611:ARG:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:611:ARG:NH2	5:U:1012:SO4:O3	2.36	0.43
2:3:2:NAG:HO3	2:3:2:NAG:C7	2.24	0.43
1:A:479:TRP:CH2	1:A:496:MET:HB3	2.54	0.43
1:A:494:THR:O	1:A:498:THR:HG23	2.19	0.43
1:D:846:ILE:HA	1:D:849:MET:HE3	2.00	0.43
1:H:93:ILE:HD11	1:H:139:LEU:HD11	2.01	0.43
1:L:656:ILE:N	1:L:657:PRO:HD2	2.33	0.43
1:M:220:PRO:HG3	1:M:305:LYS:HG2	2.01	0.43
1:M:656:ILE:HA	1:M:659:TYR:CE2	2.54	0.43
1:N:47:PHE:CE1	1:N:125:HIS:HB2	2.52	0.43
1:N:74:LEU:O	1:N:154:ASN:HB3	2.18	0.43
1:N:660:LYS:HD3	1:N:660:LYS:HA	1.82	0.43
1:O:479:TRP:HB3	1:O:493:LYS:HA	2.01	0.43
1:P:260:ILE:HG22	1:P:261:THR:O	2.19	0.43
1:Q:220:PRO:HG3	1:Q:305:LYS:HG2	2.00	0.43
1:R:183:GLU:HA	1:R:184:PRO:HA	1.77	0.43
1:R:543:THR:O	1:R:576:ASN:N	2.51	0.43
1:T:47:PHE:CE1	1:T:125:HIS:HB2	2.53	0.43
1:U:419:VAL:HG22	1:U:440:LYS:HD3	1.99	0.43
1:U:656:ILE:N	1:U:657:PRO:HD2	2.33	0.43
1:V:296:TYR:CE1	1:V:458:LYS:HE2	2.54	0.43
1:V:603:HIS:HB2	1:V:611:ARG:HD3	2.00	0.43
1:A:219:MET:HB3	1:A:237:ASP:HB3	2.00	0.43
1:C:515:ARG:NH2	1:C:567:PRO:O	2.52	0.43
1:D:219:MET:HB3	1:D:237:ASP:HB3	2.00	0.43
1:D:546:THR:HB	1:D:570:VAL:HG11	2.00	0.43
1:E:658:MET:HB2	1:E:674:PHE:HE2	1.83	0.43
1:M:183:GLU:HA	1:M:184:PRO:HA	1.78	0.43
1:O:776:ILE:O	1:O:780:LEU:HG	2.18	0.43
1:R:70:ASN:OD1	1:R:73:THR:OG1	2.22	0.43
1:R:657:PRO:HA	1:R:660:LYS:HB2	2.01	0.43
1:V:729:TRP:NE1	1:V:734:GLY:HA2	2.34	0.43
1:A:656:ILE:N	1:A:657:PRO:HD2	2.33	0.43
1:A:846:ILE:HA	1:A:849:MET:HE3	2.00	0.43
1:D:508:ILE:HA	1:D:520:LYS:O	2.18	0.43
1:D:754:THR:HG23	1:D:788:LYS:HE3	1.99	0.43
1:H:656:ILE:N	1:H:657:PRO:HD2	2.33	0.43
1:I:494:THR:O	1:I:498:THR:HG23	2.19	0.43
1:I:545:ILE:HG23	1:I:577:VAL:HG21	2.00	0.43
1:I:711[B]:CYS:SG	1:I:745:ALA:HB1	2.59	0.43
1:J:751:ALA:HB2	1:J:760:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:523:HIS:CE1	1:M:525:MET:HE2	2.53	0.43
1:P:793:LEU:HG	1:P:814:ILE:HD12	2.01	0.43
1:R:793:LEU:HB3	1:R:827:PHE:CE2	2.54	0.43
1:S:816:ARG:HG2	1:S:856:GLN:HE22	1.83	0.43
1:A:378:PHE:O	1:A:382:MET:HG2	2.19	0.43
1:D:322:TRP:CD2	1:D:362:ASN:HB3	2.54	0.43
1:E:125:HIS:HE1	1:E:127:ARG:HH11	1.66	0.43
1:F:260:ILE:HG22	1:F:261:THR:O	2.18	0.43
1:F:659:TYR:HB3	1:F:674:PHE:HD2	1.83	0.43
1:H:107:LEU:HB2	1:H:120:LEU:HD11	2.01	0.43
1:R:640:LYS:HA	1:R:681:LEU:O	2.19	0.43
1:T:656:ILE:N	1:T:657:PRO:HD2	2.34	0.43
1:A:603:HIS:HB2	1:A:611:ARG:HD3	2.00	0.43
1:A:791:TRP:HZ2	1:A:801:LYS:HD3	1.84	0.43
1:B:658:MET:HB2	1:B:674:PHE:CE2	2.53	0.43
1:C:659:TYR:HB3	1:C:674:PHE:HD2	1.83	0.43
1:C:764:TYR:HB2	1:C:776:ILE:HG21	2.00	0.43
1:D:656:ILE:N	1:D:657:PRO:HD2	2.34	0.43
1:E:791:TRP:CE2	1:E:795:GLU:HG3	2.54	0.43
1:G:407:ALA:HB2	1:G:439:ASP:HB2	2.00	0.43
1:G:851:MET:HE3	1:G:886:THR:HG22	2.00	0.43
1:I:219:MET:HB3	1:I:237:ASP:HB3	2.01	0.43
1:J:660:LYS:HD3	1:J:660:LYS:HA	1.74	0.43
1:J:739:PRO:HB2	1:J:742:VAL:HG22	2.01	0.43
1:K:545:ILE:HG23	1:K:577:VAL:HG21	2.01	0.43
1:M:816:ARG:HG2	1:M:856:GLN:HE22	1.83	0.43
1:S:226:THR:HG22	1:S:232:ILE:HD12	2.00	0.43
1:A:212:ARG:NH2	5:A:1004:SO4:O2	2.49	0.43
1:C:301:TYR:OH	1:C:306:GLN:NE2	2.51	0.43
1:H:364:VAL:HG22	1:H:468:HIS:O	2.18	0.43
1:H:575:PHE:HB2	1:H:585:VAL:HG11	2.01	0.43
1:I:657:PRO:HA	1:I:660:LYS:HB2	2.01	0.43
1:J:744:LEU:HG	1:J:775:GLN:HG2	2.01	0.43
1:N:793:LEU:HB3	1:N:827:PHE:CD2	2.54	0.43
1:Q:739:PRO:HB2	1:Q:742:VAL:HG22	2.01	0.43
1:R:685:LEU:O	1:R:689:GLN:HG2	2.18	0.43
1:A:407:ALA:HB2	1:A:439:ASP:HB2	2.00	0.42
1:A:791:TRP:CE2	1:A:795:GLU:HG3	2.54	0.42
1:C:322:TRP:CD2	1:C:362:ASN:HB3	2.54	0.42
1:C:665:ARG:HH11	1:C:667:MET:HE1	1.84	0.42
1:H:729:TRP:NE1	1:H:734:GLY:HA2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:355:LEU:HA	1:I:358:GLN:HG2	1.99	0.42
1:I:764:TYR:CE2	1:I:802:ILE:HG12	2.49	0.42
1:J:154:ASN:OD1	2:p:1:NAG:O5	2.36	0.42
1:J:658:MET:HB2	1:J:674:PHE:CE2	2.54	0.42
1:K:816:ARG:HG2	1:K:856:GLN:HE22	1.83	0.42
1:N:322:TRP:CD2	1:N:362:ASN:HB3	2.54	0.42
1:N:459:SER:HB2	1:N:485:ILE:HG21	2.01	0.42
1:O:154:ASN:OD1	2:z:1:NAG:O5	2.35	0.42
1:O:215:ALA:HA	1:O:250:ILE:O	2.19	0.42
1:S:757:TRP:CE2	1:S:780:LEU:HD22	2.54	0.42
2:X:2:NAG:HO3	2:X:2:NAG:C7	2.19	0.42
1:A:299:ILE:HD11	1:A:466:GLN:HG3	2.00	0.42
1:C:71:LEU:HD22	1:C:213:HIS:HE2	1.83	0.42
1:F:414:ASN:ND2	6:F:1023:NAG:C2	2.74	0.42
1:F:617:ASN:N	1:F:617:ASN:HD22	2.16	0.42
1:H:572:TRP:CE2	1:H:598:LEU:HD22	2.54	0.42
1:K:140:LEU:HB2	1:K:143:LEU:HD22	2.01	0.42
1:K:660:LYS:NZ	1:K:816:ARG:O	2.48	0.42
1:O:506:PRO:HB3	1:O:538:TRP:CE3	2.54	0.42
1:Q:301:TYR:CE2	1:Q:303:LEU:HB2	2.54	0.42
1:Q:414:ASN:HD21	6:Q:1021:NAG:C2	2.13	0.42
1:Q:576:ASN:HB2	1:Q:583:TYR:CE2	2.53	0.42
1:S:657:PRO:HA	1:S:660:LYS:HB2	2.01	0.42
1:A:125:HIS:CE1	1:A:127:ARG:HB2	2.55	0.42
1:B:419:VAL:HG22	1:B:440:LYS:HD3	2.02	0.42
1:B:575:PHE:HB2	1:B:585:VAL:HG11	2.00	0.42
1:C:120:LEU:HD13	1:C:133:LEU:HB3	2.01	0.42
1:D:125:HIS:HE1	1:D:127:ARG:HH11	1.67	0.42
1:K:125:HIS:CE1	1:K:127:ARG:HB2	2.54	0.42
1:K:685:LEU:O	1:K:689:GLN:HG2	2.18	0.42
1:M:210:GLU:HG2	2:u:1:NAG:H82	2.01	0.42
1:M:460:GLY:HA2	1:M:485:ILE:HG13	2.00	0.42
1:M:544:PHE:CE1	1:M:553:HIS:HB2	2.55	0.42
1:M:739:PRO:HB2	1:M:742:VAL:HG22	2.00	0.42
1:N:585:VAL:H	1:N:617:ASN:ND2	2.18	0.42
1:R:468:HIS:CD2	1:R:473:THR:HG22	2.54	0.42
1:R:815:GLY:HA2	1:R:821:TYR:HA	2.02	0.42
1:V:261:THR:HG22	1:V:287:VAL:HG13	2.00	0.42
1:V:419:VAL:HG22	1:V:440:LYS:HD3	2.01	0.42
1:V:730:LYS:HE3	1:V:755:GLU:HG2	2.01	0.42
2:3:1:NAG:HO3	2:3:1:NAG:C7	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:LYS:HD3	1:A:892:GLU:HG2	2.02	0.42
1:D:210:GLU:HG2	2:c:1:NAG:H82	2.00	0.42
1:J:793:LEU:HB3	1:J:827:PHE:CD2	2.54	0.42
1:K:656:ILE:N	1:K:657:PRO:HD2	2.34	0.42
1:L:506:PRO:HB3	1:L:538:TRP:CE3	2.55	0.42
1:M:640:LYS:HA	1:M:681:LEU:O	2.20	0.42
1:P:785:ASN:HB3	1:P:788:LYS:HB2	2.00	0.42
1:R:57:TYR:O	1:R:86:ALA:HA	2.19	0.42
1:C:219:MET:HG2	1:C:239:THR:HG22	2.00	0.42
1:C:544:PHE:CE1	1:C:553:HIS:HB2	2.54	0.42
1:C:598:LEU:HD11	1:C:605:ALA:HB3	2.01	0.42
1:D:301:TYR:OH	1:D:306:GLN:NE2	2.53	0.42
1:E:440:LYS:HG3	1:E:582:TYR:CZ	2.53	0.42
1:E:656:ILE:N	1:E:657:PRO:HD2	2.34	0.42
1:E:665:ARG:HH11	1:E:667:MET:HE1	1.83	0.42
1:F:656:ILE:N	1:F:657:PRO:HD2	2.34	0.42
1:F:785:ASN:HB3	1:F:788:LYS:HB2	2.01	0.42
1:G:622:VAL:HA	1:G:627:LEU:O	2.19	0.42
1:G:657:PRO:HA	1:G:660:LYS:HB2	2.01	0.42
1:K:417:HIS:ND1	1:K:418:PRO:O	2.46	0.42
1:L:504:GLY:HA3	1:L:523:HIS:HE2	1.84	0.42
1:M:71:LEU:HD22	1:M:213:HIS:NE2	2.34	0.42
1:N:656:ILE:N	1:N:657:PRO:HD2	2.35	0.42
1:P:220:PRO:HG3	1:P:305:LYS:HG2	2.00	0.42
1:R:544:PHE:CE1	1:R:553:HIS:HB2	2.54	0.42
1:T:729:TRP:NE1	1:T:734:GLY:HA2	2.35	0.42
1:A:107:LEU:HB2	1:A:120:LEU:HD11	2.01	0.42
1:B:508:ILE:HA	1:B:520:LYS:O	2.19	0.42
1:C:494:THR:O	1:C:498:THR:HG23	2.18	0.42
1:E:617:ASN:N	1:E:617:ASN:HD22	2.18	0.42
1:E:793:LEU:HB3	1:E:827:PHE:CE2	2.54	0.42
1:H:407:ALA:HB2	1:H:439:ASP:HB2	2.01	0.42
1:J:494:THR:O	1:J:498:THR:HG23	2.20	0.42
1:K:361:GLY:HA2	1:K:375:ASN:ND2	2.35	0.42
1:M:394:LEU:HD23	1:M:697:VAL:HG21	2.02	0.42
1:M:524:TYR:CD1	1:M:584:ILE:HD11	2.54	0.42
1:N:183:GLU:HA	1:N:184:PRO:HA	1.80	0.42
1:O:523:HIS:CE1	1:O:525:MET:HE2	2.55	0.42
1:Q:219:MET:HB3	1:Q:237:ASP:HB3	2.01	0.42
1:R:829:ARG:HA	1:R:869:PHE:CZ	2.55	0.42
1:A:183:GLU:OE1	4:A:1002:P52:N1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:744:LEU:HG	1:B:775:GLN:HG2	2.02	0.42
4:D:1003:P52:H34	4:D:1003:P52:C5	2.50	0.42
1:E:523:HIS:CE1	1:E:525:MET:HE2	2.54	0.42
1:I:730:LYS:HE3	1:I:755:GLU:HG2	2.02	0.42
1:J:729:TRP:CE2	1:J:734:GLY:HA2	2.54	0.42
1:L:729:TRP:NE1	1:L:734:GLY:HA2	2.35	0.42
1:M:546:THR:HB	1:M:570:VAL:HG11	2.01	0.42
1:N:159:PHE:CB	1:N:315:GLN:HB2	2.49	0.42
1:O:260:ILE:HG22	1:O:261:THR:O	2.20	0.42
1:O:548:LYS:NZ	5:R:1009:SO4:O1	2.48	0.42
1:P:744:LEU:HG	1:P:775:GLN:HG2	2.02	0.42
1:Q:74:LEU:O	1:Q:154:ASN:HB3	2.19	0.42
1:R:107:LEU:HD11	1:R:145:TYR:HB3	2.02	0.42
1:R:215:ALA:HA	1:R:250:ILE:O	2.20	0.42
1:R:319:MET:HB3	1:R:326:THR:OG1	2.20	0.42
1:R:643:THR:HG22	1:R:685:LEU:HD13	2.01	0.42
1:T:673:GLN:OE1	1:T:912:LYS:HD2	2.20	0.42
1:V:656:ILE:N	1:V:657:PRO:HD2	2.34	0.42
1:A:683:ARG:HD3	1:A:715:TYR:HE1	1.84	0.42
1:B:581:GLY:HA3	1:B:583:TYR:CE1	2.55	0.42
1:B:617:ASN:HD22	1:B:617:ASN:N	2.17	0.42
1:D:660:LYS:HA	1:D:660:LYS:HD3	1.81	0.42
1:G:364:VAL:HG22	1:G:468:HIS:O	2.20	0.42
1:G:776:ILE:O	1:G:780:LEU:HG	2.19	0.42
1:I:739:PRO:HB2	1:I:742:VAL:HG22	2.02	0.42
1:J:301:TYR:CE2	1:J:303:LEU:HB2	2.54	0.42
1:N:543:THR:HG22	1:N:554:ARG:HG2	2.02	0.42
1:O:74:LEU:O	1:O:154:ASN:HB3	2.20	0.42
1:S:495:MET:HG3	1:S:539:HIS:HB2	2.02	0.42
1:U:606:VAL:HG23	1:U:611:ARG:HG3	2.01	0.42
1:U:730:LYS:HE3	1:U:755:GLU:HG2	2.01	0.42
1:A:95:LEU:HD11	1:A:131:ILE:HD11	2.01	0.42
1:C:159:PHE:CB	1:C:315:GLN:HB2	2.50	0.42
1:F:451:TYR:HE2	1:F:490:VAL:HG13	1.85	0.42
1:F:667:MET:HE2	1:F:901:PHE:CE2	2.55	0.42
1:G:58:VAL:HG11	1:G:93:ILE:HG23	2.02	0.42
1:G:764:TYR:HB2	1:G:776:ILE:HG21	2.00	0.42
1:H:378:PHE:O	1:H:382:MET:HG2	2.20	0.42
1:H:730:LYS:HE3	1:H:755:GLU:HG2	2.01	0.42
1:J:658:MET:HB2	1:J:674:PHE:HE2	1.84	0.42
1:K:825:TRP:CE2	1:K:829:ARG:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:355:LEU:HA	1:L:358:GLN:HG2	2.02	0.42
1:L:464:TYR:CE1	1:L:473:THR:HG21	2.55	0.42
1:L:685:LEU:O	1:L:689:GLN:HG2	2.20	0.42
1:L:757:TRP:CE2	1:L:780:LEU:HD22	2.55	0.42
1:N:125:HIS:HE1	1:N:127:ARG:HH11	1.68	0.42
1:P:214:LEU:HB2	1:R:260:ILE:HG13	2.02	0.42
1:P:355:LEU:HA	1:P:358:GLN:HG2	2.01	0.42
1:S:357:HIS:HE1	1:S:375:ASN:HB3	1.85	0.42
1:S:430:ARG:HD2	1:S:841:LEU:O	2.19	0.42
1:V:82:VAL:HG22	1:V:84:ILE:HG23	2.02	0.42
1:A:321:ASN:HB2	1:A:324:LEU:O	2.20	0.42
1:A:658:MET:HB2	1:A:674:PHE:HE2	1.84	0.42
1:E:366:MET:HE2	1:E:372:LEU:HA	2.02	0.42
1:F:656:ILE:HA	1:F:659:TYR:CE2	2.55	0.42
1:G:183:GLU:HA	1:G:184:PRO:HA	1.83	0.42
1:G:665:ARG:HH11	1:G:667:MET:HE1	1.85	0.42
1:H:226:THR:HG22	1:H:232:ILE:HD12	2.02	0.42
1:J:168:ARG:N	5:J:1005:SO4:O4	2.41	0.42
1:J:433:PHE:CE1	4:J:1002:P52:H11	2.55	0.42
1:J:781:CYS:SG	1:J:810:ILE:HG23	2.60	0.42
1:L:430:ARG:NH1	1:L:840:GLU:HB3	2.35	0.42
1:O:553:HIS:HE1	1:R:865:GLU:HG2	1.84	0.42
1:O:793:LEU:HB3	1:O:827:PHE:CE2	2.55	0.42
1:O:829:ARG:HA	1:O:869:PHE:CZ	2.55	0.42
1:T:60:PRO:HA	1:T:84:ILE:HG22	2.02	0.42
1:U:430:ARG:HD2	1:U:841:LEU:O	2.20	0.42
1:U:781:CYS:O	1:U:817:ASN:ND2	2.50	0.42
1:V:210:GLU:HG2	2:CA:1:NAG:H82	2.01	0.42
1:A:49:TRP:CZ3	1:A:55:PRO:HG3	2.55	0.41
1:D:261:THR:HG22	1:D:287:VAL:HG13	2.02	0.41
1:E:159:PHE:CB	1:E:315:GLN:HB2	2.50	0.41
1:G:154:ASN:OD1	2:j:1:NAG:O5	2.35	0.41
1:H:793:LEU:HB3	1:H:827:PHE:CD2	2.55	0.41
1:H:851:MET:HE3	1:H:886:THR:HG22	2.02	0.41
1:K:210:GLU:HG2	2:q:1:NAG:H82	2.02	0.41
5:K:1025:SO4:O1	1:Q:829:ARG:NH2	2.53	0.41
1:L:598:LEU:HD11	1:L:605:ALA:HB3	2.01	0.41
1:M:729:TRP:NE1	1:M:734:GLY:HA2	2.35	0.41
1:R:210:GLU:HG2	2:4:1:NAG:H82	2.02	0.41
1:R:730:LYS:HE3	1:R:755:GLU:HG2	2.02	0.41
2:n:2:NAG:HO3	2:n:2:NAG:C7	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:LYS:HD3	1:C:287:VAL:HG21	2.03	0.41
1:C:515:ARG:HD2	5:C:1007:SO4:O1	2.21	0.41
1:D:357:HIS:HE1	1:D:375:ASN:HB3	1.85	0.41
1:E:260:ILE:HG22	1:E:261:THR:O	2.20	0.41
1:E:659:TYR:O	1:E:663:GLU:HG3	2.20	0.41
1:G:322:TRP:CD2	1:G:362:ASN:HB3	2.54	0.41
1:H:256:SER:HB3	1:H:270:TYR:CD2	2.55	0.41
1:J:544:PHE:CE1	1:J:553:HIS:HB2	2.55	0.41
1:L:361:GLY:HA2	1:L:375:ASN:ND2	2.35	0.41
1:L:433:PHE:CE1	4:L:1003:P52:H11	2.55	0.41
1:L:506:PRO:HG2	1:L:583:TYR:HB3	2.01	0.41
1:M:259:LYS:NZ	1:M:284[B]:ASP:OD1	2.53	0.41
1:N:729:TRP:CE2	1:N:734:GLY:HA2	2.55	0.41
1:O:509:THR:HG23	1:O:586:HIS:HD2	1.85	0.41
1:P:70:ASN:OD1	1:P:73:THR:OG1	2.22	0.41
1:R:107:LEU:HB2	1:R:120:LEU:HD11	2.02	0.41
1:R:451:TYR:CD1	1:R:541:PRO:HB3	2.55	0.41
1:U:729:TRP:NE1	1:U:734:GLY:HA2	2.36	0.41
1:V:468:HIS:CD2	1:V:473:THR:HG22	2.56	0.41
1:V:754:THR:HG23	1:V:788:LYS:HE3	2.01	0.41
1:A:140:LEU:HB2	1:A:143:LEU:HD22	2.03	0.41
1:A:658:MET:HB2	1:A:674:PHE:CE2	2.55	0.41
1:C:378:PHE:O	1:C:382:MET:HG2	2.20	0.41
1:C:617:ASN:N	1:C:617:ASN:HD22	2.16	0.41
1:E:74:LEU:O	1:E:154:ASN:HB3	2.19	0.41
1:E:210:GLU:HG2	2:e:1:NAG:H82	2.03	0.41
1:F:189:MET:HE2	1:F:189:MET:HB3	1.95	0.41
1:F:206:LYS:HD3	1:F:235:HIS:CE1	2.55	0.41
1:G:125:HIS:CE1	1:G:127:ARG:HB2	2.56	0.41
1:G:575:PHE:HB2	1:G:585:VAL:HG11	2.02	0.41
1:G:656:ILE:N	1:G:657:PRO:HD2	2.34	0.41
1:H:657:PRO:HA	1:H:660:LYS:HB2	2.02	0.41
1:H:764:TYR:HB2	1:H:776:ILE:HG21	2.01	0.41
1:I:183:GLU:OE1	4:I:1003:P52:N1	2.53	0.41
1:I:214:LEU:HB2	1:K:260:ILE:HG13	2.02	0.41
1:J:210:GLU:HG2	2:o:1:NAG:H82	2.02	0.41
1:J:260:ILE:HG22	1:J:261:THR:O	2.20	0.41
1:L:548:LYS:NZ	5:L:1001:SO4:O3	2.50	0.41
1:M:729:TRP:CE2	1:M:734:GLY:HA2	2.56	0.41
1:O:721:ARG:NH2	5:O:1003:SO4:O1	2.41	0.41
1:P:417:HIS:NE2	1:P:434:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:159:PHE:CB	1:Q:315:GLN:HB2	2.50	0.41
1:A:761:TYR:CE1	1:A:791:TRP:HH2	2.38	0.41
1:B:739:PRO:HB2	1:B:742:VAL:HG22	2.01	0.41
1:E:761:TYR:CZ	1:E:791:TRP:HH2	2.38	0.41
1:F:366:MET:HE2	1:F:372:LEU:HA	2.02	0.41
1:H:366:MET:HE2	1:H:372:LEU:HA	2.03	0.41
1:I:793:LEU:HB3	1:I:827:PHE:CE2	2.55	0.41
1:N:226:THR:HG22	1:N:232:ILE:HD12	2.01	0.41
1:N:833:ASN:ND2	5:N:1014:SO4:O1	2.53	0.41
1:O:502:GLN:HE21	1:O:538:TRP:CD1	2.37	0.41
1:R:816:ARG:HG2	1:R:856:GLN:HE22	1.85	0.41
1:T:215:ALA:HA	1:T:250:ILE:O	2.21	0.41
4:T:1003:P52:H34	4:T:1003:P52:C5	2.50	0.41
1:U:210:GLU:HG2	2:AA:1:NAG:H82	2.02	0.41
1:U:452:LEU:HD21	1:U:490:VAL:HG11	2.02	0.41
1:A:260:ILE:HG22	1:A:261:THR:O	2.20	0.41
1:C:125:HIS:HE1	1:C:127:ARG:HH11	1.68	0.41
1:D:299:ILE:HD11	1:D:466:GLN:HG3	2.03	0.41
1:D:761:TYR:CZ	1:D:791:TRP:HH2	2.38	0.41
1:F:231:LEU:HD22	2:g:1:NAG:H81	2.01	0.41
1:F:546:THR:HB	1:F:570:VAL:HG11	2.01	0.41
1:H:363:LEU:O	1:H:470:TYR:N	2.53	0.41
1:K:658:MET:HB2	1:K:674:PHE:HE2	1.84	0.41
1:L:659:TYR:O	1:L:663:GLU:HG3	2.21	0.41
1:R:125:HIS:CE1	1:R:127:ARG:HB2	2.55	0.41
1:V:355:LEU:HA	1:V:358:GLN:HG2	2.02	0.41
1:C:829:ARG:HA	1:C:869:PHE:CZ	2.56	0.41
1:I:430:ARG:HD2	1:I:841:LEU:O	2.21	0.41
1:K:261:THR:HG22	1:K:287:VAL:HG13	2.03	0.41
1:N:405:PHE:CZ	1:N:613:SER:HA	2.55	0.41
1:N:739:PRO:HB2	1:N:742:VAL:HG22	2.02	0.41
1:O:656:ILE:N	1:O:657:PRO:HD2	2.35	0.41
1:R:617:ASN:HD22	1:R:617:ASN:N	2.19	0.41
1:V:829:ARG:NH2	5:V:1009:SO4:O4	2.53	0.41
1:D:293:TYR:CZ	1:D:356:ALA:HB2	2.55	0.41
1:E:341:ALA:HB1	1:E:697:VAL:HG13	2.03	0.41
1:H:683:ARG:HD3	1:H:715:TYR:HE1	1.84	0.41
1:J:622:VAL:HG21	1:J:632:ALA:HB2	2.02	0.41
1:J:729:TRP:NE1	1:J:734:GLY:HA2	2.35	0.41
1:K:128:GLN:O	1:K:130:GLN:HG3	2.21	0.41
1:K:659:TYR:HB3	1:K:674:PHE:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:PHE:CE1	1:L:125:HIS:HB2	2.55	0.41
1:L:125:HIS:HE1	1:L:127:ARG:HH11	1.69	0.41
1:L:660:LYS:HD3	1:L:660:LYS:HA	1.72	0.41
1:N:417:HIS:ND1	1:N:418:PRO:O	2.54	0.41
1:O:754:THR:HG23	1:O:788:LYS:HE3	2.02	0.41
1:P:659:TYR:HB3	1:P:674:PHE:HD2	1.86	0.41
1:Q:316:SER:OG	4:Q:1002:P52:H4	2.21	0.41
1:Q:433:PHE:CE1	4:Q:1002:P52:H11	2.56	0.41
1:S:296:TYR:CE1	1:S:458:LYS:HE2	2.56	0.41
1:S:656:ILE:N	1:S:657:PRO:HD2	2.35	0.41
1:S:825:TRP:CE2	1:S:829:ARG:HD2	2.56	0.41
1:T:598:LEU:HD11	1:T:605:ALA:HB3	2.02	0.41
1:T:660:LYS:HD3	1:T:660:LYS:HA	1.78	0.41
1:U:782:ARG:NH2	5:U:1007:SO4:O3	2.53	0.41
1:B:846:ILE:HA	1:B:849:MET:HE3	2.03	0.41
1:E:556:LEU:HG	1:E:558:LYS:HG3	2.02	0.41
1:H:506:PRO:HG2	1:H:583:TYR:HB3	2.03	0.41
1:J:652:LEU:HD23	1:J:652:LEU:HA	1.90	0.41
1:L:261:THR:HG22	1:L:287:VAL:HG13	2.03	0.41
1:L:505:PHE:HB3	1:L:582:TYR:CE2	2.56	0.41
1:M:617:ASN:N	1:M:617:ASN:HD22	2.19	0.41
1:Q:260:ILE:HG22	1:Q:261:THR:O	2.20	0.41
1:T:658:MET:HB2	1:T:674:PHE:HE2	1.85	0.41
1:B:296:TYR:HE2	1:B:461:ILE:HD11	1.86	0.41
1:C:260:ILE:HG22	1:C:261:THR:O	2.20	0.41
1:G:260:ILE:HG22	1:G:261:THR:O	2.21	0.41
1:G:829:ARG:HA	1:G:869:PHE:CZ	2.56	0.41
1:H:523:HIS:ND1	1:H:534:THR:HG21	2.36	0.41
1:I:183:GLU:HA	1:I:184:PRO:HA	1.78	0.41
1:I:581:GLY:HA3	1:I:583:TYR:CE1	2.55	0.41
1:I:793:LEU:HD23	1:I:793:LEU:HA	1.91	0.41
1:J:764:TYR:HB2	1:J:776:ILE:HG21	2.02	0.41
1:K:82:VAL:HG22	1:K:84:ILE:HG23	2.02	0.41
1:K:217:SER:OG	1:K:218:ASN:N	2.47	0.41
1:K:776:ILE:O	1:K:780:LEU:HG	2.20	0.41
1:L:662:MET:HE1	1:L:904:ILE:HG21	2.03	0.41
1:M:260:ILE:HG22	1:M:261:THR:O	2.20	0.41
1:M:459:SER:HB2	1:M:485:ILE:HG21	2.02	0.41
1:N:407:ALA:HB2	1:N:439:ASP:HB2	2.01	0.41
1:O:183:GLU:HA	1:O:184:PRO:HA	1.77	0.41
1:O:259:LYS:NZ	1:O:284[B]:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:401:PHE:HE1	1:O:446:ASN:ND2	2.19	0.41
1:O:494:THR:O	1:O:498:THR:HG23	2.21	0.41
1:O:880:LEU:HB3	1:O:882:CYS:SG	2.61	0.41
1:P:523:HIS:ND1	1:P:534:THR:HG21	2.36	0.41
1:Q:656:ILE:HA	1:Q:659:TYR:CE2	2.56	0.41
1:R:107:LEU:HD21	1:R:139:LEU:HD21	2.03	0.41
1:R:440:LYS:HG3	1:R:582:TYR:CZ	2.55	0.41
1:R:550:ASP:H	1:V:862:ARG:HH22	1.67	0.41
1:T:125:HIS:CE1	1:T:127:ARG:HB2	2.56	0.41
1:T:524:TYR:CD2	1:T:584:ILE:HD11	2.55	0.41
1:U:581:GLY:HA3	1:U:583:TYR:CE1	2.55	0.41
2:9:1:NAG:HO3	2:9:1:NAG:C7	2.26	0.41
2:DA:1:NAG:HO3	2:DA:1:NAG:C7	2.21	0.41
1:A:339:SER:HA	1:A:771:THR:HB	2.02	0.41
1:B:518:HIS:NE2	5:B:1008:SO4:O3	2.51	0.41
1:C:74:LEU:O	1:C:154:ASN:HB3	2.21	0.41
1:E:361:GLY:HA2	1:E:375:ASN:ND2	2.36	0.41
1:E:490:VAL:HG12	1:E:492:VAL:HG22	2.03	0.41
1:F:829:ARG:NH2	5:F:1010:SO4:O3	2.54	0.41
1:I:259:LYS:NZ	1:I:284[B]:ASP:OD1	2.54	0.41
1:I:378:PHE:O	1:I:382:MET:HG2	2.20	0.41
1:K:107:LEU:HB2	1:K:120:LEU:HD11	2.02	0.41
1:K:611:ARG:NH2	5:K:1010:SO4:S	2.93	0.41
1:L:260:ILE:HG22	1:L:261:THR:O	2.21	0.41
1:L:524:TYR:CD2	1:L:584:ILE:HD11	2.56	0.41
1:M:711[B]:CYS:SG	1:M:745:ALA:HB1	2.61	0.41
1:M:776:ILE:O	1:M:780:LEU:HG	2.21	0.41
1:N:260:ILE:HG22	1:N:261:THR:O	2.21	0.41
1:O:509:THR:HG23	1:O:586:HIS:CD2	2.56	0.41
1:P:364:VAL:HG22	1:P:468:HIS:O	2.21	0.41
1:P:622:VAL:HA	1:P:627:LEU:O	2.21	0.41
1:Q:208:ARG:NH2	5:Q:1013:SO4:O4	2.54	0.41
1:Q:665:ARG:HH11	1:Q:667:MET:HE1	1.86	0.41
1:Q:730:LYS:HE3	1:Q:755:GLU:HG2	2.03	0.41
1:S:81:LYS:HB2	1:S:81:LYS:HE3	1.87	0.41
1:S:267:VAL:HA	1:S:306:GLN:O	2.21	0.41
1:T:81:LYS:HB2	1:T:81:LYS:HE3	1.88	0.41
1:T:322:TRP:CD2	1:T:362:ASN:HB3	2.56	0.41
1:T:816:ARG:NH1	5:T:1007:SO4:O4	2.54	0.41
2:7:2:NAG:HO3	2:7:2:NAG:C7	2.25	0.41
1:C:355:LEU:HA	1:C:358:GLN:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:660:LYS:HA	1:F:660:LYS:HD3	1.77	0.40
1:G:128:GLN:O	1:G:130:GLN:HG3	2.21	0.40
1:G:751:ALA:HB2	1:G:760:LEU:HD12	2.03	0.40
1:G:791:TRP:CZ2	1:G:795:GLU:HG3	2.56	0.40
1:H:102:ILE:HD13	1:H:151:TYR:HB3	2.04	0.40
1:H:459:SER:HB2	1:H:485:ILE:HG21	2.03	0.40
1:I:82:VAL:HG22	1:I:84:ILE:HG23	2.03	0.40
1:K:81:LYS:HB2	1:K:81:LYS:HE3	1.90	0.40
1:L:494:THR:O	1:L:498:THR:HG23	2.21	0.40
1:L:514:GLY:C	1:L:569:GLU:HG2	2.46	0.40
1:L:523:HIS:ND1	1:L:534:THR:HG21	2.36	0.40
1:M:763:LYS:HA	1:M:763:LYS:HD3	1.87	0.40
1:N:523:HIS:ND1	1:N:534:THR:HG21	2.35	0.40
1:O:657:PRO:HA	1:O:660:LYS:HB2	2.02	0.40
1:P:575:PHE:HB2	1:P:585:VAL:HG11	2.02	0.40
1:Q:478:LEU:HD11	1:Q:482:MET:HE2	2.03	0.40
1:Q:660:LYS:HD3	1:Q:660:LYS:HA	1.77	0.40
1:U:49:TRP:HD1	1:U:130:GLN:HE22	1.69	0.40
1:U:494:THR:O	1:U:498:THR:HG23	2.21	0.40
1:C:296:TYR:HE2	1:C:461:ILE:HD11	1.86	0.40
1:E:183:GLU:OE1	4:E:1003:P52:N1	2.53	0.40
1:F:791:TRP:CZ2	1:F:795:GLU:HG3	2.56	0.40
1:J:355:LEU:HA	1:J:358:GLN:HG2	2.03	0.40
1:K:554:ARG:N	5:K:1015:SO4:O2	2.38	0.40
1:L:739:PRO:HB2	1:L:742:VAL:HG22	2.03	0.40
1:O:107:LEU:HB2	1:O:120:LEU:HD11	2.03	0.40
1:R:378:PHE:O	1:R:382:MET:HG2	2.21	0.40
1:R:857:PHE:CD2	1:R:862:ARG:HB3	2.57	0.40
1:S:447:MET:HE1	1:S:499:TRP:CE2	2.55	0.40
1:V:361:GLY:HA2	1:V:375:ASN:ND2	2.36	0.40
1:B:660:LYS:HA	1:B:660:LYS:HD3	1.76	0.40
4:B:1002:P52:C5	4:B:1002:P52:H34	2.52	0.40
1:D:479:TRP:CH2	1:D:496:MET:HB3	2.56	0.40
1:E:125:HIS:CE1	1:E:127:ARG:HB2	2.57	0.40
1:G:548:LYS:HG2	1:G:570:VAL:HG12	2.03	0.40
1:G:598:LEU:HD11	1:G:605:ALA:HB3	2.03	0.40
1:G:764:TYR:HE2	1:G:802:ILE:HG12	1.87	0.40
1:H:128:GLN:O	1:H:130:GLN:HG3	2.21	0.40
1:H:301:TYR:OH	1:H:306:GLN:NE2	2.53	0.40
1:M:494:THR:O	1:M:498:THR:HG23	2.21	0.40
1:M:730:LYS:HE3	1:M:755:GLU:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:355:LEU:HA	1:O:358:GLN:HG2	2.03	0.40
1:Q:656:ILE:N	1:Q:657:PRO:HD2	2.36	0.40
1:R:140:LEU:HD23	1:R:140:LEU:HA	1.94	0.40
1:S:60:PRO:HA	1:S:84:ILE:HG22	2.04	0.40
1:S:68:HIS:O	1:S:76:PHE:HA	2.21	0.40
1:S:804:THR:HG21	1:S:838:LYS:HD3	2.04	0.40
1:U:260:ILE:HG22	1:U:261:THR:O	2.21	0.40
1:V:183:GLU:OE1	4:V:1002:P52:N1	2.53	0.40
1:V:585:VAL:H	1:V:617:ASN:ND2	2.18	0.40
1:A:839:PHE:O	1:A:840:GLU:HB2	2.20	0.40
1:C:215:ALA:HA	1:C:250:ILE:O	2.21	0.40
1:C:364:VAL:HG21	1:C:465:LEU:HA	2.01	0.40
1:D:776:ILE:O	1:D:780:LEU:HG	2.22	0.40
1:G:215:ALA:HA	1:G:250:ILE:O	2.21	0.40
1:G:617:ASN:N	1:G:617:ASN:HD22	2.19	0.40
1:J:505:PHE:HB3	1:J:582:TYR:CE2	2.57	0.40
1:J:711[B]:CYS:SG	1:J:745:ALA:HB1	2.62	0.40
1:L:296:TYR:CE1	1:L:458:LYS:HE2	2.56	0.40
1:L:364:VAL:HG21	1:L:465:LEU:HA	2.02	0.40
1:M:419:VAL:HG22	1:M:440:LYS:HD3	2.02	0.40
1:O:660:LYS:HA	1:O:660:LYS:HD3	1.77	0.40
1:P:301:TYR:CE2	1:P:303:LEU:HB2	2.57	0.40
1:Q:556:LEU:HG	1:Q:558:LYS:HG3	2.03	0.40
1:T:51:LYS:O	1:T:128:GLN:NE2	2.55	0.40
1:T:125:HIS:HE1	1:T:127:ARG:HH11	1.68	0.40
1:V:793:LEU:HB3	1:V:827:PHE:CE2	2.56	0.40
2:j:1:NAG:HO3	2:j:1:NAG:C7	2.26	0.40
2:j:2:NAG:HO3	2:j:2:NAG:C7	2.22	0.40
1:C:366:MET:HE2	1:C:372:LEU:HA	2.02	0.40
1:C:791:TRP:CE2	1:C:795:GLU:HG3	2.57	0.40
1:D:851:MET:HE3	1:D:886:THR:HG22	2.04	0.40
1:E:259:LYS:NZ	1:E:284[B]:ASP:OD1	2.55	0.40
1:F:506:PRO:HG2	1:F:583:TYR:HB3	2.04	0.40
1:I:380:LYS:O	1:I:383:GLU:HB2	2.20	0.40
1:K:260:ILE:HG22	1:K:261:THR:O	2.21	0.40
1:K:423:VAL:HG11	1:K:432:MET:HG2	2.03	0.40
1:P:183:GLU:OE1	4:P:1002:P52:N1	2.55	0.40
1:T:440:LYS:HG3	1:T:582:TYR:CZ	2.56	0.40
1:U:301:TYR:OH	1:U:306:GLN:NE2	2.54	0.40
1:U:657:PRO:HA	1:U:660:LYS:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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
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 ⓘ

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%)	741 (100%)	3 (0%)	84	83
1	B	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	C	745/799 (93%)	743 (100%)	2 (0%)	86	85
1	D	745/799 (93%)	741 (100%)	4 (0%)	81	82
1	E	744/799 (93%)	739 (99%)	5 (1%)	76	79
1	F	745/799 (93%)	742 (100%)	3 (0%)	84	83
1	G	744/799 (93%)	742 (100%)	2 (0%)	86	85
1	H	744/799 (93%)	742 (100%)	2 (0%)	86	85
1	I	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	J	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	K	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	L	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	M	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	N	744/799 (93%)	740 (100%)	4 (0%)	81	82
1	O	744/799 (93%)	742 (100%)	2 (0%)	86	85
1	P	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	Q	744/799 (93%)	739 (99%)	5 (1%)	76	79
1	R	744/799 (93%)	739 (99%)	5 (1%)	76	79
1	S	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	T	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	U	744/799 (93%)	741 (100%)	3 (0%)	84	83
1	V	744/799 (93%)	741 (100%)	3 (0%)	84	83
All	All	16371/17578 (93%)	16301 (100%)	70 (0%)	84	83

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	399	TYR
1	A	455	ASP
1	B	75	THR
1	B	154	ASN
1	B	399	TYR
1	C	154	ASN
1	C	399	TYR
1	D	154	ASN
1	D	399	TYR
1	D	534	THR
1	D	550	ASP
1	E	75	THR
1	E	154	ASN
1	E	399	TYR
1	E	414	ASN
1	E	450	GLU
1	F	75	THR
1	F	154	ASN
1	F	399	TYR
1	G	154	ASN
1	G	399	TYR
1	H	154	ASN
1	H	399	TYR
1	I	154	ASN
1	I	399	TYR
1	I	414	ASN
1	J	75	THR
1	J	154	ASN
1	J	399	TYR
1	K	154	ASN
1	K	399	TYR
1	K	414	ASN
1	L	75	THR
1	L	154	ASN
1	L	399	TYR
1	M	154	ASN
1	M	399	TYR
1	M	414	ASN
1	N	75	THR
1	N	154	ASN
1	N	399	TYR
1	N	414	ASN

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Mol	Chain	Res	Type
1	O	154	ASN
1	O	399	TYR
1	P	154	ASN
1	P	399	TYR
1	P	414	ASN
1	Q	154	ASN
1	Q	399	TYR
1	Q	414	ASN
1	Q	711[A]	CYS
1	Q	711[B]	CYS
1	R	87	SER
1	R	88	GLN
1	R	154	ASN
1	R	399	TYR
1	R	534	THR
1	S	154	ASN
1	S	399	TYR
1	S	414	ASN
1	T	154	ASN
1	T	399	TYR
1	T	414	ASN
1	U	154	ASN
1	U	399	TYR
1	U	414	ASN
1	V	154	ASN
1	V	399	TYR
1	V	414	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (236) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	130	GLN
1	A	306	GLN
1	A	358	GLN
1	A	468	HIS
1	A	765	GLN
1	A	775	GLN
1	A	784	GLN
1	A	826	GLN
1	A	856	GLN
1	A	879	GLN

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Mol	Chain	Res	Type
1	A	909	GLN
1	B	125	HIS
1	B	130	GLN
1	B	306	GLN
1	B	414	ASN
1	B	553	HIS
1	B	616	ASN
1	B	617	ASN
1	B	620	GLN
1	B	765	GLN
1	B	775	GLN
1	B	784	GLN
1	B	826	GLN
1	B	879	GLN
1	C	125	HIS
1	C	130	GLN
1	C	306	GLN
1	C	414	ASN
1	C	463	GLN
1	C	580	ASN
1	C	616	ASN
1	C	617	ASN
1	C	620	GLN
1	C	765	GLN
1	C	826	GLN
1	C	856	GLN
1	D	125	HIS
1	D	358	GLN
1	D	414	ASN
1	D	475	ASN
1	D	518	HIS
1	D	620	GLN
1	D	765	GLN
1	D	826	GLN
1	D	856	GLN
1	D	879	GLN
1	E	306	GLN
1	E	358	GLN
1	E	414	ASN
1	E	603	HIS
1	E	616	ASN
1	E	617	ASN

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Mol	Chain	Res	Type
1	E	620	GLN
1	E	765	GLN
1	E	826	GLN
1	E	856	GLN
1	E	879	GLN
1	F	99	HIS
1	F	306	GLN
1	F	414	ASN
1	F	616	ASN
1	F	617	ASN
1	F	620	GLN
1	F	765	GLN
1	F	775	GLN
1	F	826	GLN
1	F	879	GLN
1	G	306	GLN
1	G	358	GLN
1	G	414	ASN
1	G	616	ASN
1	G	617	ASN
1	G	620	GLN
1	G	733	ASN
1	G	765	GLN
1	G	826	GLN
1	G	879	GLN
1	H	306	GLN
1	H	414	ASN
1	H	446	ASN
1	H	580	ASN
1	H	616	ASN
1	H	617	ASN
1	H	620	GLN
1	H	673	GLN
1	H	765	GLN
1	H	826	GLN
1	H	856	GLN
1	H	879	GLN
1	I	125	HIS
1	I	358	GLN
1	I	414	ASN
1	I	603	HIS
1	I	616	ASN

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Mol	Chain	Res	Type
1	I	620	GLN
1	I	765	GLN
1	I	775	GLN
1	I	790	GLN
1	I	826	GLN
1	I	879	GLN
1	I	900	ASN
1	J	306	GLN
1	J	414	ASN
1	J	472	ASN
1	J	620	GLN
1	J	765	GLN
1	J	826	GLN
1	J	856	GLN
1	K	130	GLN
1	K	306	GLN
1	K	414	ASN
1	K	425	ASN
1	K	518	HIS
1	K	523	HIS
1	K	553	HIS
1	K	673	GLN
1	K	765	GLN
1	K	826	GLN
1	K	879	GLN
1	K	909	GLN
1	L	125	HIS
1	L	306	GLN
1	L	358	GLN
1	L	414	ASN
1	L	425	ASN
1	L	463	GLN
1	L	468	HIS
1	L	475	ASN
1	L	765	GLN
1	L	826	GLN
1	L	879	GLN
1	M	306	GLN
1	M	414	ASN
1	M	446	ASN
1	M	468	HIS
1	M	603	HIS

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Mol	Chain	Res	Type
1	M	616	ASN
1	M	617	ASN
1	M	620	GLN
1	M	765	GLN
1	M	826	GLN
1	M	879	GLN
1	M	893	ASN
1	N	125	HIS
1	N	306	GLN
1	N	414	ASN
1	N	468	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	N	879	GLN
1	O	358	GLN
1	O	414	ASN
1	O	518	HIS
1	O	553	HIS
1	O	580	ASN
1	O	765	GLN
1	O	809	GLN
1	O	826	GLN
1	O	856	GLN
1	O	879	GLN
1	O	909	GLN
1	P	125	HIS
1	P	130	GLN
1	P	306	GLN
1	P	358	GLN
1	P	414	ASN
1	P	553	HIS
1	P	580	ASN
1	P	616	ASN
1	P	620	GLN
1	P	765	GLN
1	P	826	GLN
1	P	879	GLN

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Mol	Chain	Res	Type
1	Q	99	HIS
1	Q	414	ASN
1	Q	616	ASN
1	Q	650	GLN
1	Q	765	GLN
1	Q	826	GLN
1	Q	879	GLN
1	R	88	GLN
1	R	306	GLN
1	R	414	ASN
1	R	468	HIS
1	R	553	HIS
1	R	616	ASN
1	R	617	ASN
1	R	620	GLN
1	R	673	GLN
1	R	765	GLN
1	R	826	GLN
1	R	856	GLN
1	R	879	GLN
1	S	99	HIS
1	S	358	GLN
1	S	414	ASN
1	S	616	ASN
1	S	620	GLN
1	S	765	GLN
1	S	826	GLN
1	S	831	ASN
1	S	856	GLN
1	S	879	GLN
1	S	909	GLN
1	T	125	HIS
1	T	306	GLN
1	T	414	ASN
1	T	446	ASN
1	T	518	HIS
1	T	765	GLN
1	T	826	GLN
1	T	879	GLN
1	T	900	ASN
1	U	358	GLN
1	U	414	ASN

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Mol	Chain	Res	Type
1	U	475	ASN
1	U	617	ASN
1	U	765	GLN
1	U	790	GLN
1	U	826	GLN
1	U	879	GLN
1	V	414	ASN
1	V	468	HIS
1	V	603	HIS
1	V	616	ASN
1	V	620	GLN
1	V	673	GLN
1	V	765	GLN
1	V	826	GLN
1	V	879	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	0.73	0
2	NAG	0	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	0	3	2	11,11,12	0.22	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.98	1 (5%)
2	BMA	1	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	2	1	1,2	14,14,15	0.31	0	17,19,21	0.72	0
2	NAG	2	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	2	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	3	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	4	1	1,2	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	4	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	4	3	2	11,11,12	0.23	0	15,15,17	0.84	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	0.97	1 (5%)
2	BMA	5	3	2	11,11,12	0.27	0	15,15,17	0.79	0
2	NAG	6	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	6	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	6	3	2	11,11,12	0.21	0	15,15,17	0.85	0
2	NAG	7	1	2	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
2	NAG	7	2	2	14,14,15	0.29	0	17,19,21	0.98	1 (5%)
2	BMA	7	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	8	1	1,2	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	8	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	8	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.99	1 (5%)
2	BMA	9	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	AA	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	AA	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	AA	3	2	11,11,12	0.21	0	15,15,17	0.84	0
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	0.30	0	17,19,21	0.98	1 (5%)
2	BMA	BA	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	CA	1	1,2	14,14,15	0.32	0	17,19,21	0.74	0
2	NAG	CA	2	2	14,14,15	0.36	0	17,19,21	0.78	0
2	BMA	CA	3	2	11,11,12	0.21	0	15,15,17	0.84	0
2	NAG	DA	1	2	14,14,15	0.33	0	17,19,21	1.03	1 (5%)
2	NAG	DA	2	2	14,14,15	0.27	0	17,19,21	0.98	1 (5%)
2	BMA	DA	3	2	11,11,12	0.25	0	15,15,17	0.79	0
2	NAG	W	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	W	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	BMA	W	3	2	11,11,12	0.22	0	15,15,17	0.84	0
2	NAG	X	1	1,2	14,14,15	0.33	0	17,19,21	1.03	1 (5%)
2	NAG	X	2	2	14,14,15	0.28	0	17,19,21	0.99	1 (5%)
2	BMA	X	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	Y	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	Y	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	BMA	Y	3	2	11,11,12	0.23	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	Z	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	a	1	1,2	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	a	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	a	3	2	11,11,12	0.21	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	b	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	c	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	c	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	BMA	c	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	d	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	e	1	1,2	14,14,15	0.33	0	17,19,21	0.72	0
2	NAG	e	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	e	3	2	11,11,12	0.21	0	15,15,17	0.84	0
2	NAG	f	1	2	14,14,15	0.32	0	17,19,21	1.02	1 (5%)
2	NAG	f	2	2	14,14,15	0.28	0	17,19,21	0.97	1 (5%)
2	BMA	f	3	2	11,11,12	0.25	0	15,15,17	0.79	0
2	NAG	g	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	g	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	BMA	g	3	2	11,11,12	0.22	0	15,15,17	0.84	0
2	NAG	h	1	2	14,14,15	0.33	0	17,19,21	1.02	1 (5%)
2	NAG	h	2	2	14,14,15	0.28	0	17,19,21	0.98	1 (5%)
2	BMA	h	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	i	1	1,2	14,14,15	0.31	0	17,19,21	0.73	0
2	NAG	i	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	BMA	i	3	2	11,11,12	0.21	0	15,15,17	0.84	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	0.98	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	j	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	k	1	1,2	14,14,15	0.32	0	17,19,21	0.72	0
2	NAG	k	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	BMA	k	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	l	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	m	1	1,2	14,14,15	0.31	0	17,19,21	0.73	0
2	NAG	m	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	m	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.29	0	17,19,21	0.98	1 (5%)
2	BMA	n	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	o	1	1,2	14,14,15	0.31	0	17,19,21	0.73	0
2	NAG	o	2	2	14,14,15	0.34	0	17,19,21	0.79	0
2	BMA	o	3	2	11,11,12	0.22	0	15,15,17	0.84	0
2	NAG	p	1	2	14,14,15	0.32	0	17,19,21	1.03	1 (5%)
2	NAG	p	2	2	14,14,15	0.28	0	17,19,21	0.98	1 (5%)
2	BMA	p	3	2	11,11,12	0.26	0	15,15,17	0.77	0
2	NAG	q	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	q	2	2	14,14,15	0.35	0	17,19,21	0.78	0
2	BMA	q	3	2	11,11,12	0.21	0	15,15,17	0.84	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	0.97	1 (5%)
2	BMA	r	3	2	11,11,12	0.25	0	15,15,17	0.78	0
2	NAG	s	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	s	2	2	14,14,15	0.33	0	17,19,21	0.78	0
2	BMA	s	3	2	11,11,12	0.21	0	15,15,17	0.83	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	0.98	1 (5%)
2	BMA	t	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	u	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	u	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	u	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.98	1 (5%)
2	BMA	v	3	2	11,11,12	0.26	0	15,15,17	0.78	0
2	NAG	w	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	w	2	2	14,14,15	0.34	0	17,19,21	0.78	0
2	BMA	w	3	2	11,11,12	0.22	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	0.98	1 (5%)
2	BMA	x	3	2	11,11,12	0.24	0	15,15,17	0.78	0
2	NAG	y	1	1,2	14,14,15	0.32	0	17,19,21	0.73	0
2	NAG	y	2	2	14,14,15	0.35	0	17,19,21	0.79	0
2	BMA	y	3	2	11,11,12	0.22	0	15,15,17	0.84	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	0.29	0	17,19,21	0.99	1 (5%)
2	BMA	z	3	2	11,11,12	0.25	0	15,15,17	0.78	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	-	1/6/23/26	0/1/1/1
2	NAG	1	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	3	2	2	-	1/6/23/26	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
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	-	1/6/23/26	0/1/1/1
2	NAG	5	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	7	2	2	-	1/6/23/26	0/1/1/1
2	BMA	7	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/23/26	0/1/1/1
2	NAG	9	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	BA	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	DA	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	X	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	Z	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	b	2	2	-	1/6/23/26	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	d	1	2	-	1/6/23/26	0/1/1/1
2	NAG	d	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	f	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	h	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	j	2	2	-	1/6/23/26	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
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	-	1/6/23/26	0/1/1/1
2	NAG	l	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	n	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	p	2	2	-	1/6/23/26	0/1/1/1
2	BMA	p	3	2	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	1/6/23/26	0/1/1/1
2	NAG	r	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	t	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	v	2	2	-	1/6/23/26	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
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	-	1/6/23/26	0/1/1/1
2	NAG	x	2	2	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	z	2	2	-	1/6/23/26	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(°)	Ideal(°)
2	z	2	NAG	C1-O5-C5	2.28	115.24	112.19
2	X	2	NAG	C1-O5-C5	2.26	115.21	112.19
2	DA	2	NAG	C1-O5-C5	2.25	115.20	112.19
2	t	2	NAG	C1-O5-C5	2.24	115.19	112.19
2	Z	2	NAG	C1-O5-C5	2.23	115.18	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	x	2	NAG	C1-O5-C5	2.23	115.17	112.19
2	n	2	NAG	C1-O5-C5	2.23	115.17	112.19
2	9	2	NAG	C1-O5-C5	2.23	115.17	112.19
2	r	2	NAG	C1-O5-C5	2.22	115.17	112.19
2	7	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	d	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	p	2	NAG	C1-O5-C5	2.22	115.16	112.19
2	h	2	NAG	C1-O5-C5	2.21	115.14	112.19
2	b	2	NAG	C1-O5-C5	2.20	115.14	112.19
2	BA	2	NAG	C1-O5-C5	2.20	115.14	112.19
2	v	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	f	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	1	2	NAG	C1-O5-C5	2.20	115.13	112.19
2	3	2	NAG	C1-O5-C5	2.19	115.13	112.19
2	j	2	NAG	C1-O5-C5	2.19	115.12	112.19
2	l	2	NAG	C1-O5-C5	2.17	115.10	112.19
2	5	2	NAG	C1-O5-C5	2.17	115.10	112.19
2	X	1	NAG	C1-O5-C5	2.17	115.09	112.19
2	7	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	b	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	t	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	DA	1	NAG	C1-O5-C5	2.15	115.07	112.19
2	1	1	NAG	C1-O5-C5	2.15	115.07	112.19
2	p	1	NAG	C1-O5-C5	2.15	115.07	112.19
2	3	1	NAG	C1-O5-C5	2.15	115.07	112.19
2	5	1	NAG	C1-O5-C5	2.15	115.07	112.19
2	j	1	NAG	C1-O5-C5	2.14	115.06	112.19
2	f	1	NAG	C1-O5-C5	2.14	115.06	112.19
2	d	1	NAG	C1-O5-C5	2.14	115.05	112.19
2	x	1	NAG	C1-O5-C5	2.13	115.05	112.19
2	h	1	NAG	C1-O5-C5	2.13	115.04	112.19
2	BA	1	NAG	C1-O5-C5	2.13	115.04	112.19
2	l	1	NAG	C1-O5-C5	2.13	115.03	112.19
2	n	1	NAG	C1-O5-C5	2.12	115.03	112.19
2	z	1	NAG	C1-O5-C5	2.12	115.02	112.19
2	v	1	NAG	C1-O5-C5	2.11	115.01	112.19
2	r	1	NAG	C1-O5-C5	2.11	115.01	112.19
2	9	1	NAG	C1-O5-C5	2.11	115.01	112.19
2	Z	1	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (220) 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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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	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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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

There are no ring outliers.

63 monomers are involved in 208 short contacts:

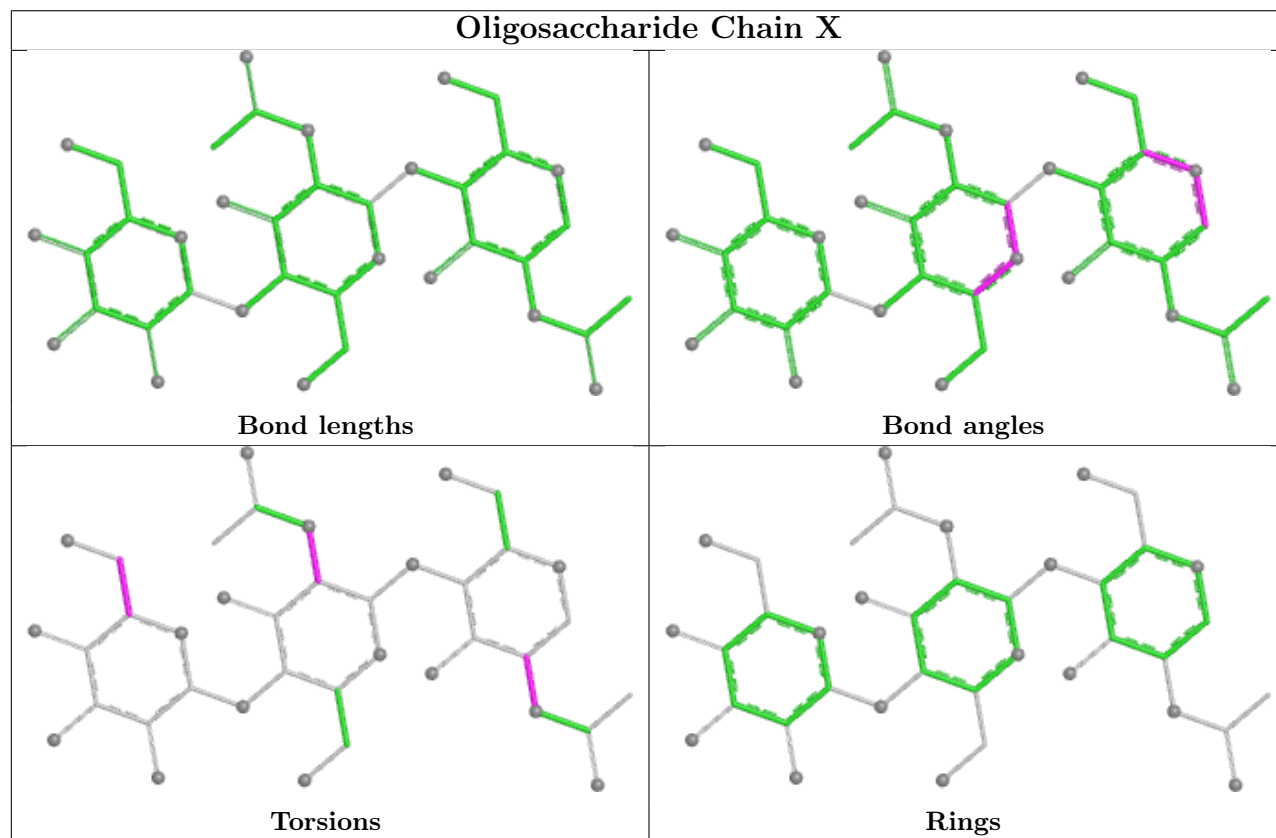
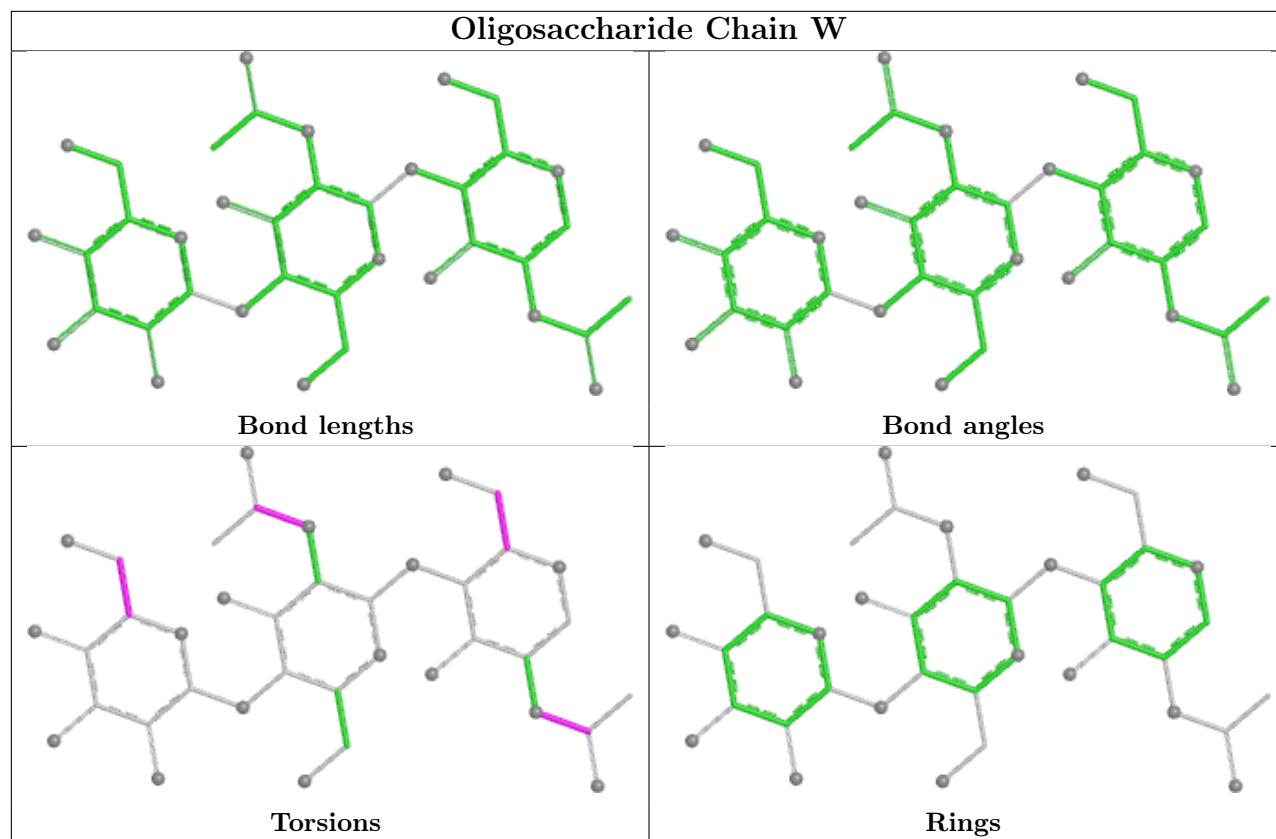
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	v	1	NAG	6	0
2	7	2	NAG	2	0
2	BA	1	NAG	7	0
2	n	1	NAG	6	0
2	6	1	NAG	1	0
2	W	1	NAG	2	0
2	l	2	NAG	1	0
2	X	1	NAG	2	0
2	j	2	NAG	2	0
2	Z	1	NAG	7	0
2	x	2	NAG	2	0
2	u	1	NAG	1	0
2	d	1	NAG	7	0
2	7	1	NAG	7	0
2	n	2	NAG	2	0
2	z	2	NAG	2	0
2	AA	1	NAG	1	0
2	p	1	NAG	6	0
2	i	1	NAG	1	0
2	d	2	NAG	2	0
2	Y	1	NAG	2	0
2	0	1	NAG	1	0
2	Z	2	NAG	1	0
2	DA	1	NAG	7	0
2	h	2	NAG	2	0
2	o	1	NAG	2	0
2	t	1	NAG	7	0
2	b	1	NAG	7	0

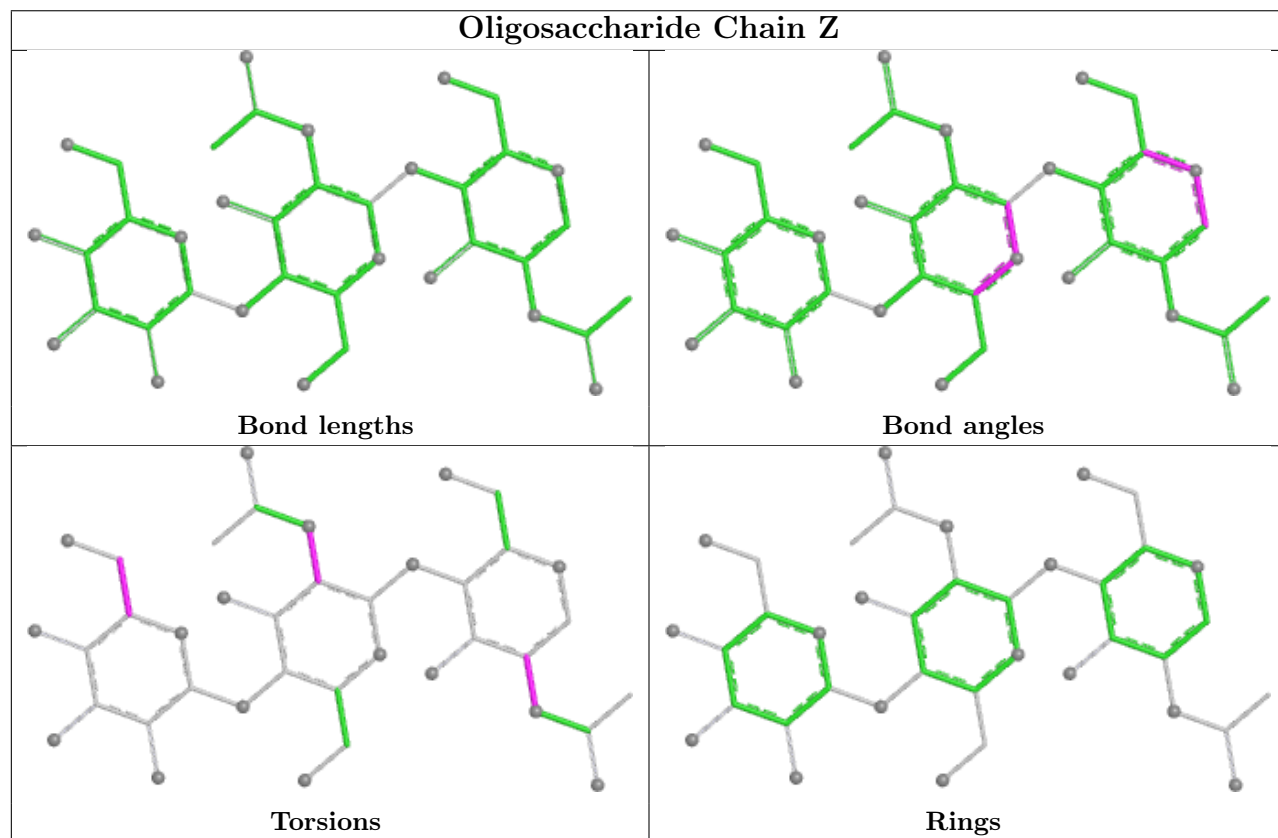
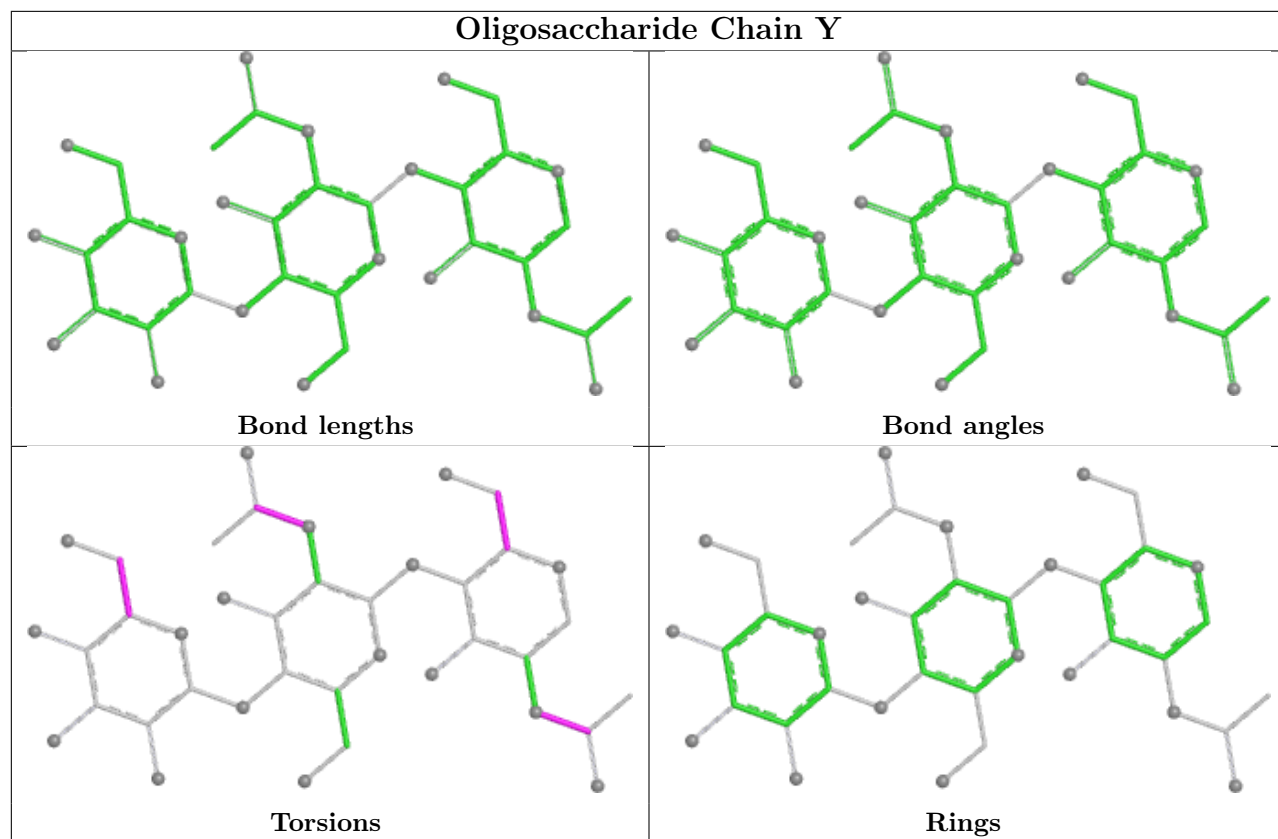
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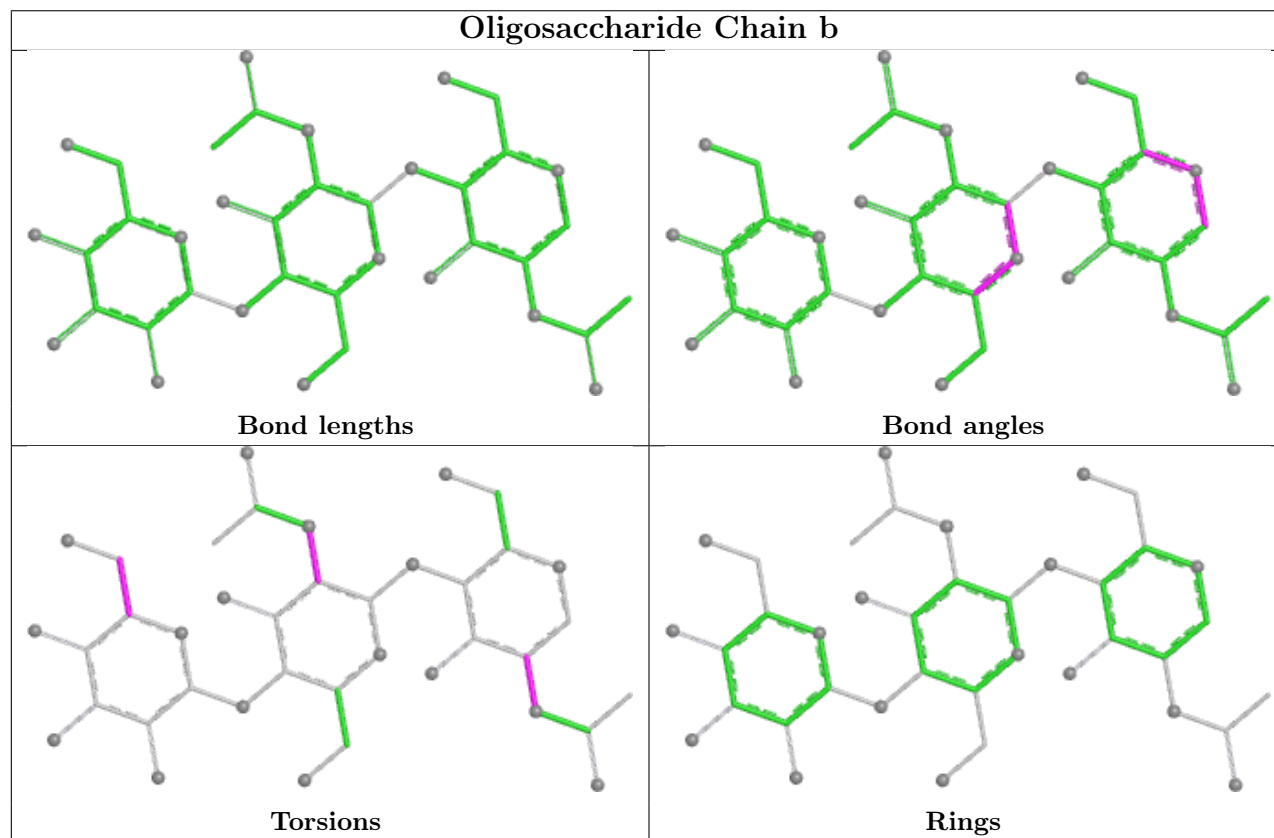
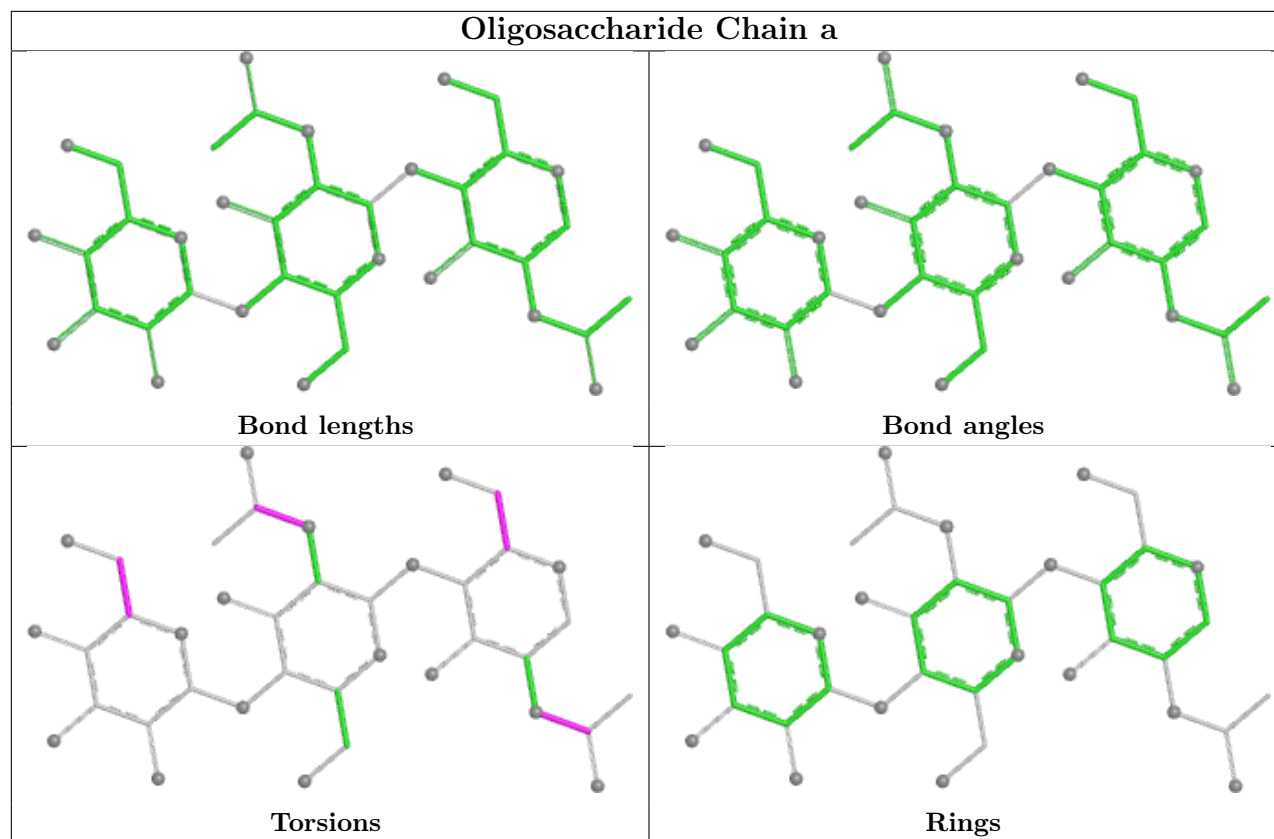
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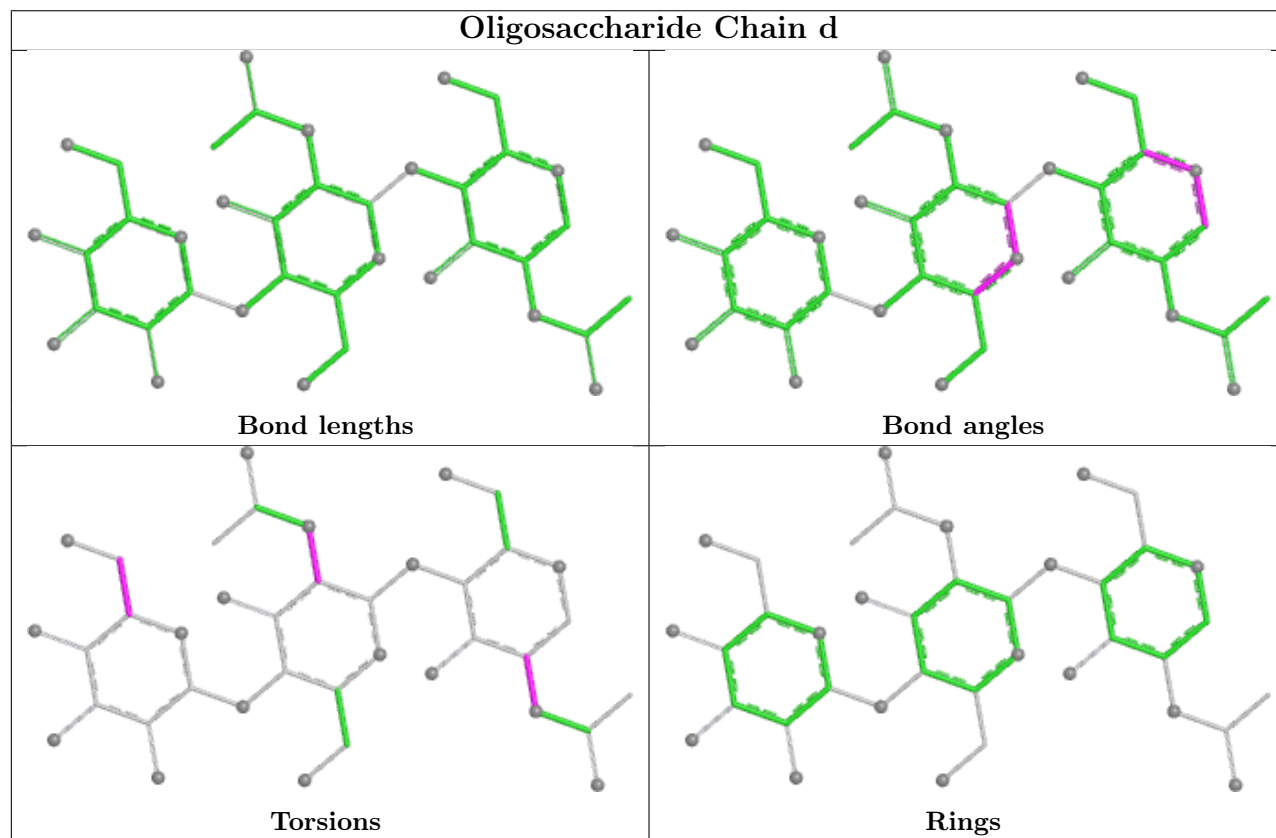
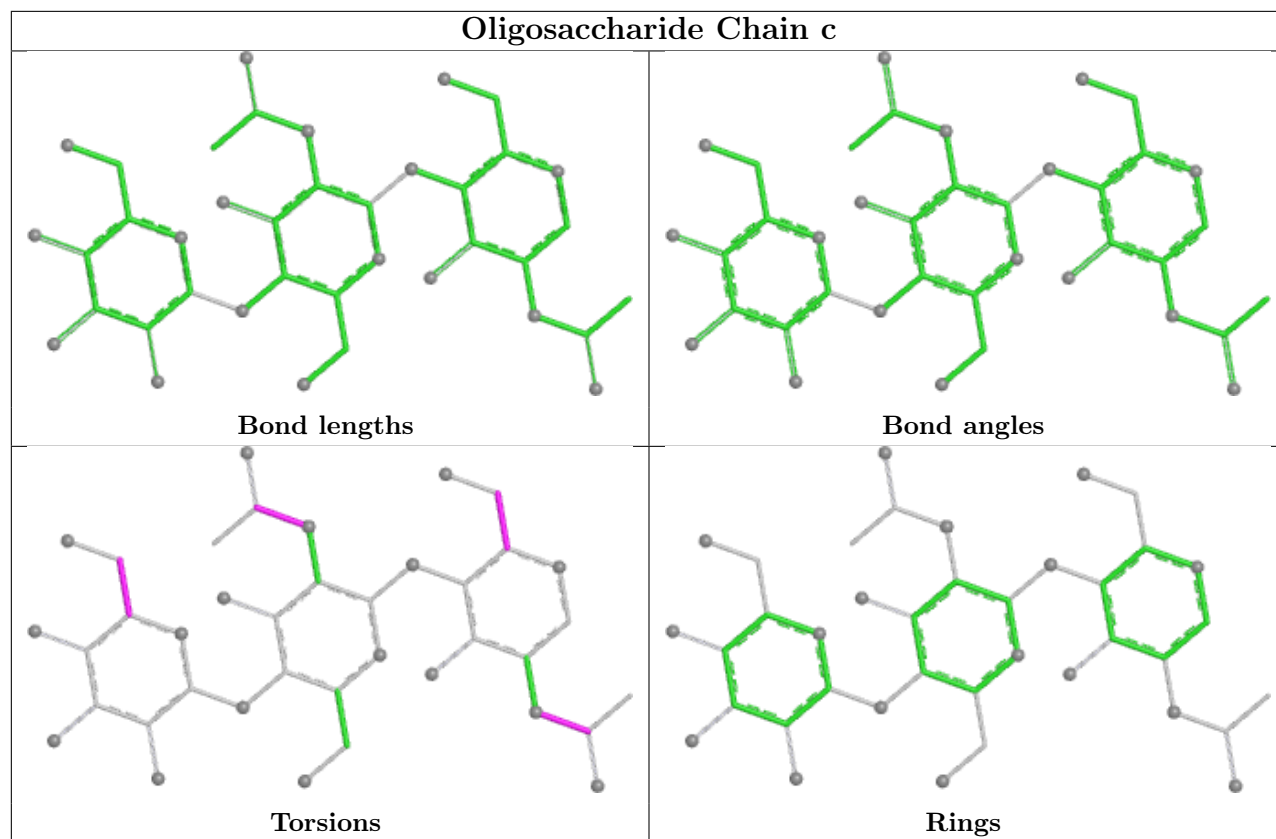
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	v	2	NAG	2	0
2	p	2	NAG	2	0
2	1	2	NAG	1	0
2	BA	2	NAG	1	0
2	w	1	NAG	1	0
2	4	1	NAG	2	0
2	1	1	NAG	7	0
2	8	1	NAG	1	0
2	DA	2	NAG	1	0
2	X	2	NAG	2	0
2	z	1	NAG	7	0
2	9	2	NAG	2	0
2	f	1	NAG	6	0
2	t	2	NAG	2	0
2	5	1	NAG	7	0
2	s	1	NAG	1	0
2	CA	1	NAG	2	0
2	r	2	NAG	2	0
2	f	2	NAG	2	0
2	3	1	NAG	7	0
2	3	2	NAG	2	0
2	r	1	NAG	6	0
2	9	1	NAG	7	0
2	m	1	NAG	2	0
2	q	1	NAG	1	0
2	e	1	NAG	1	0
2	l	1	NAG	7	0
2	j	1	NAG	7	0
2	h	1	NAG	6	0
2	x	1	NAG	7	0
2	5	2	NAG	2	0
2	g	1	NAG	2	0
2	c	1	NAG	1	0
2	y	1	NAG	2	0
2	b	2	NAG	1	0

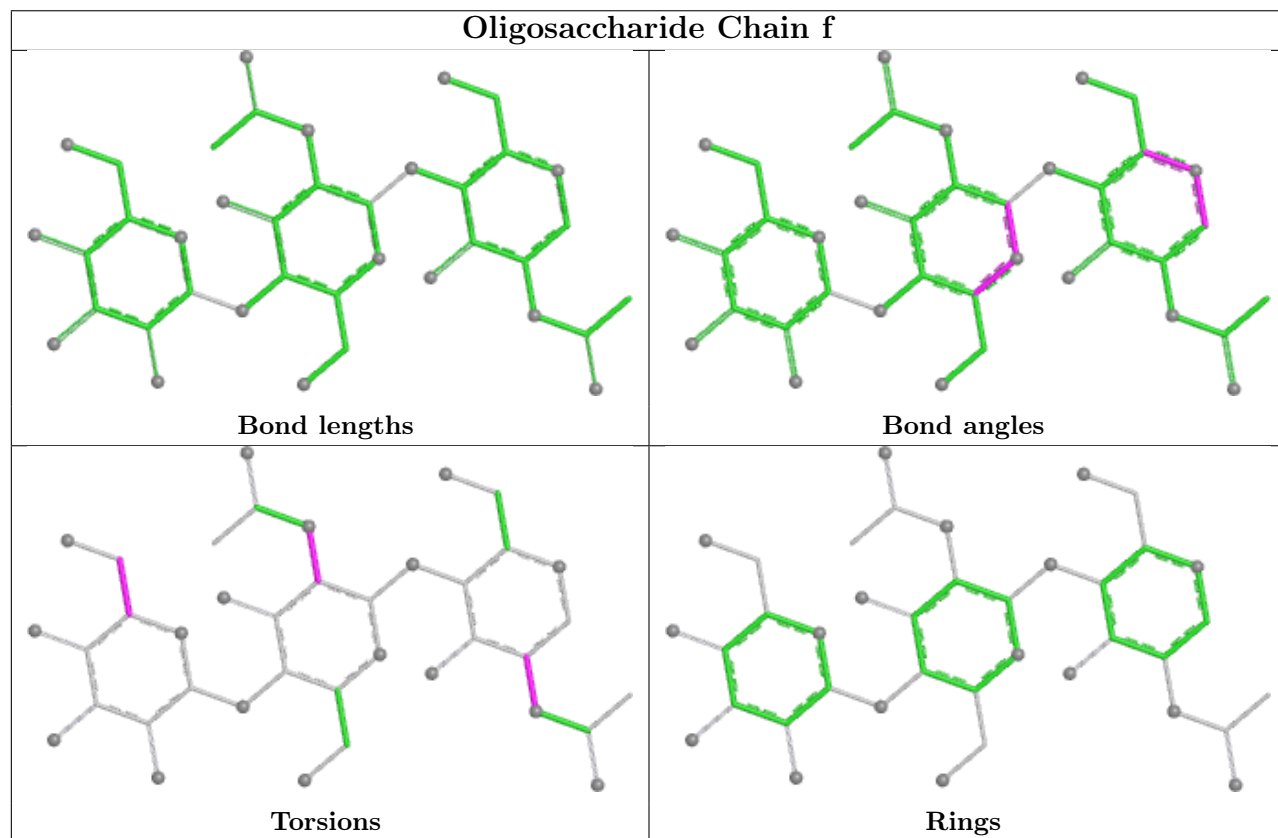
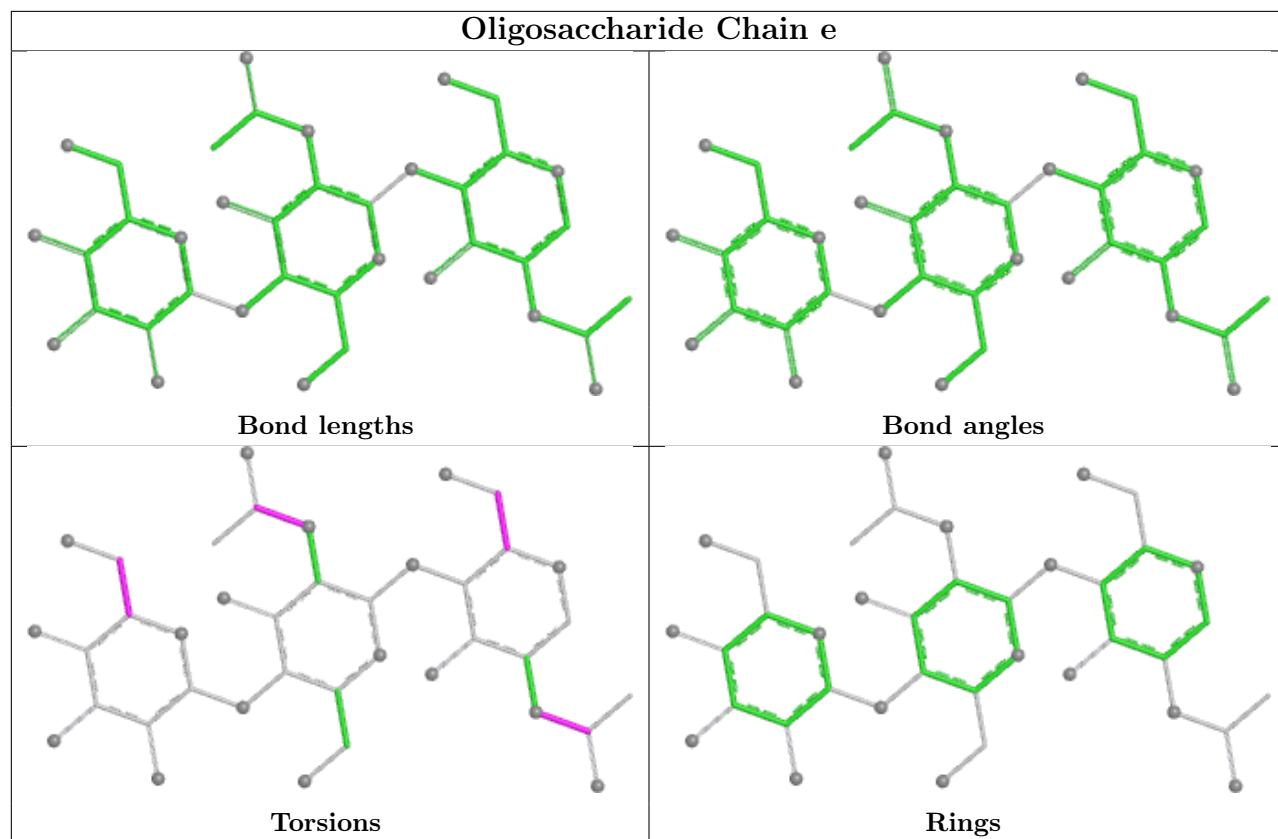
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

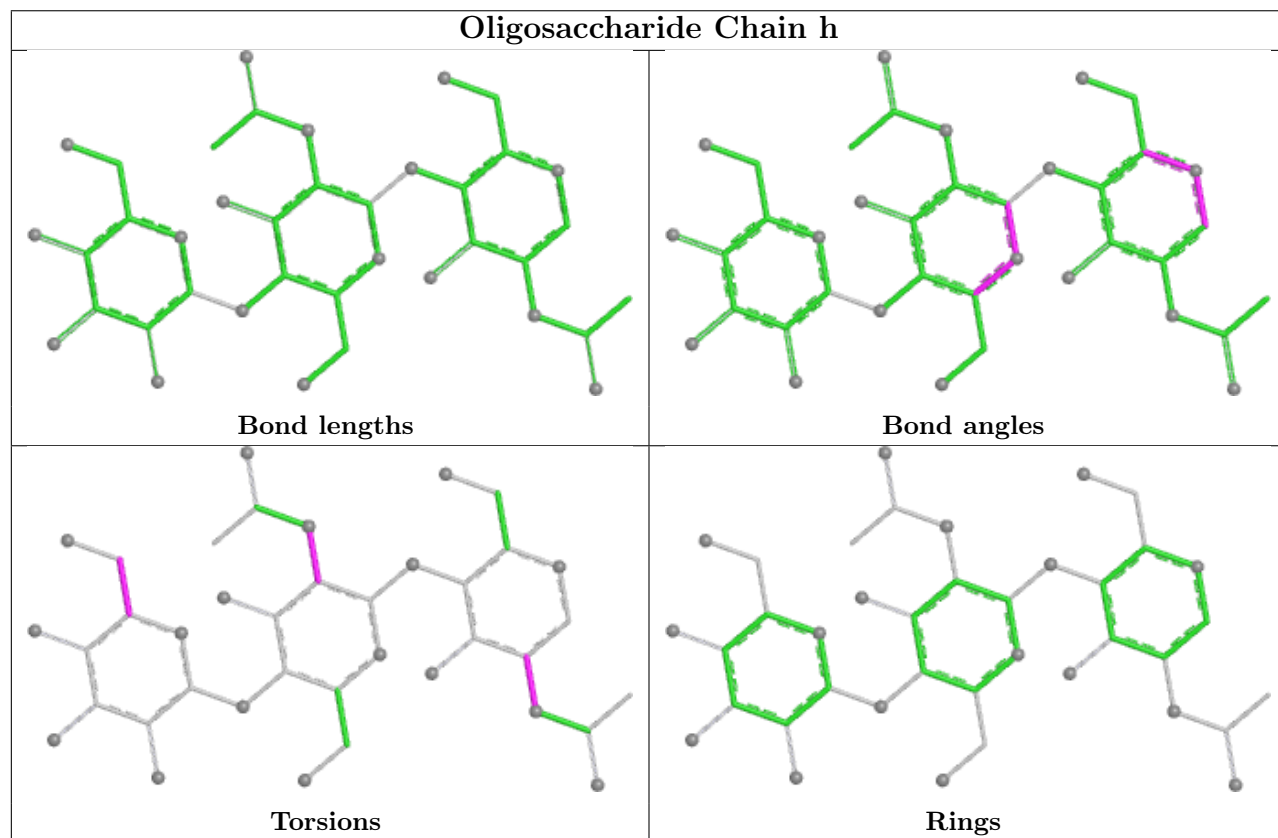
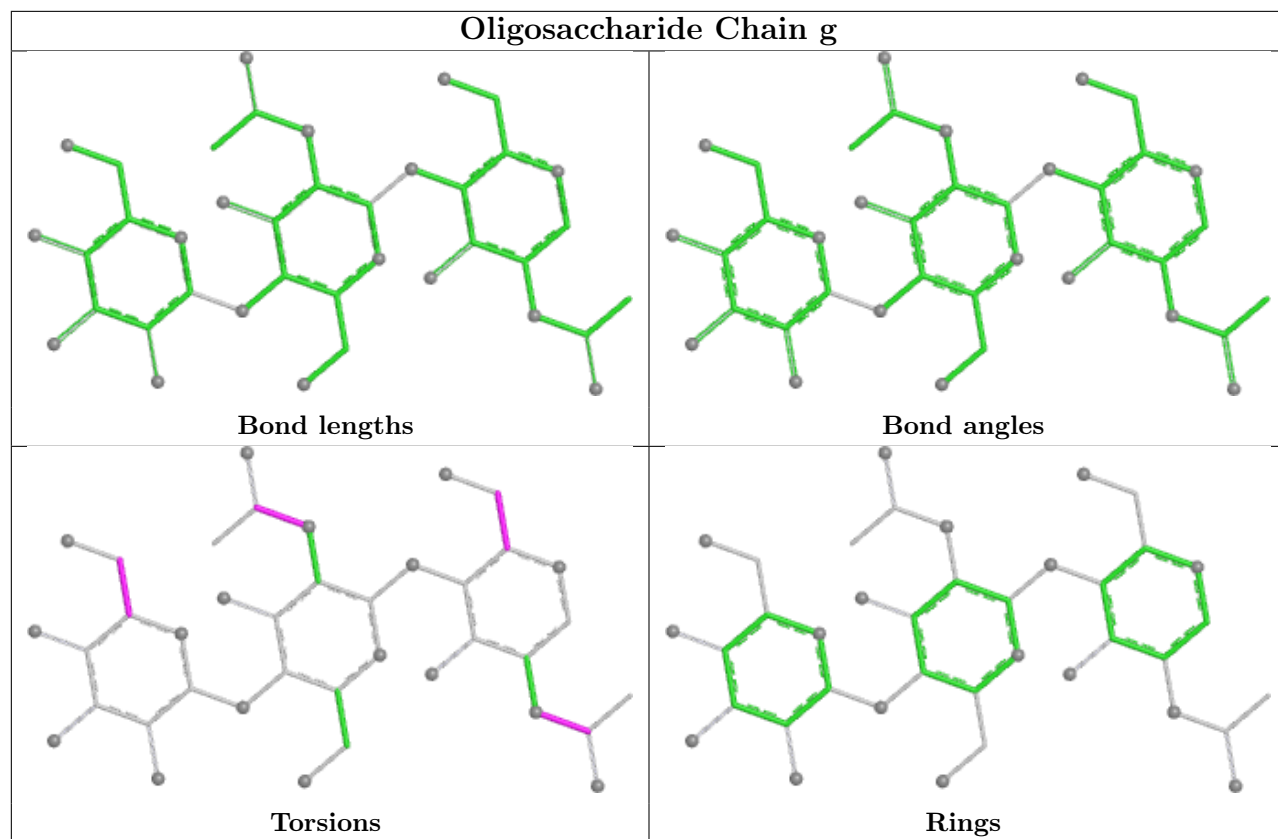


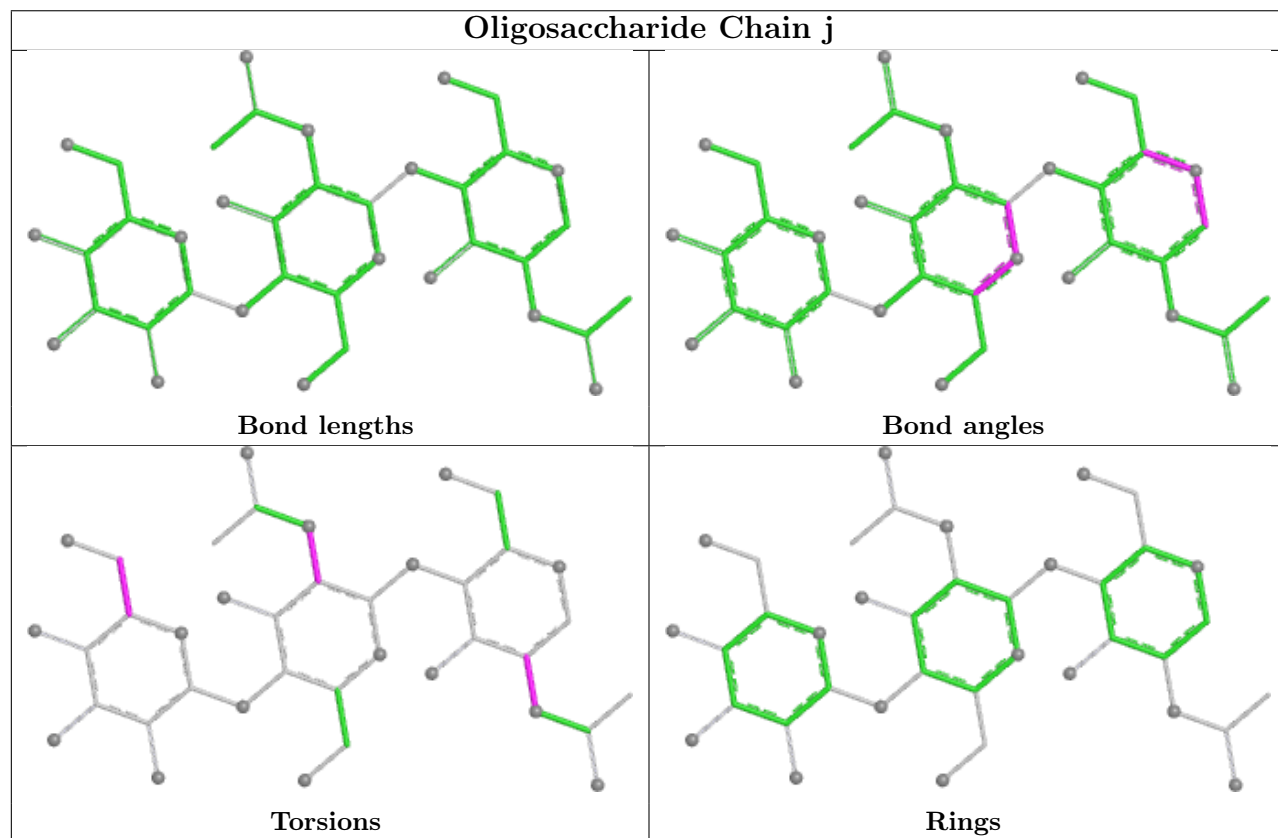
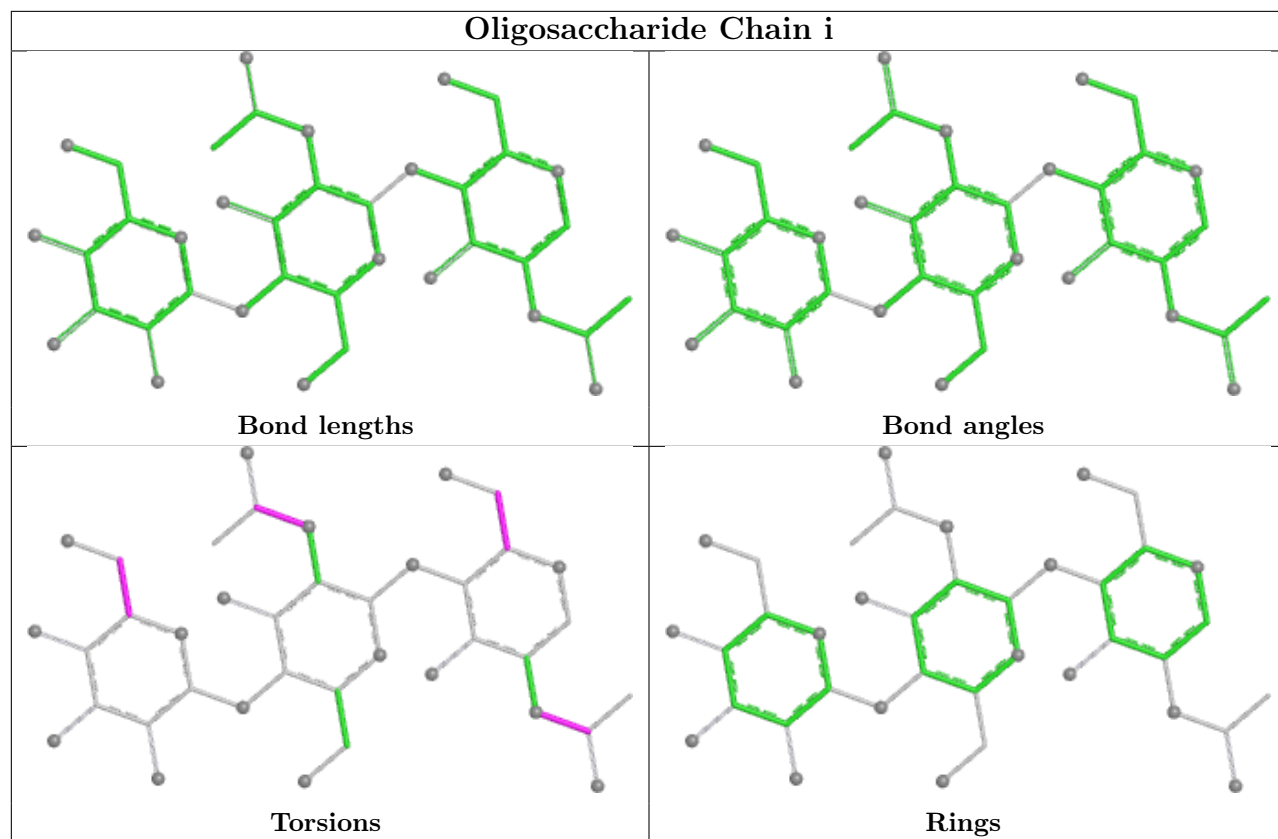


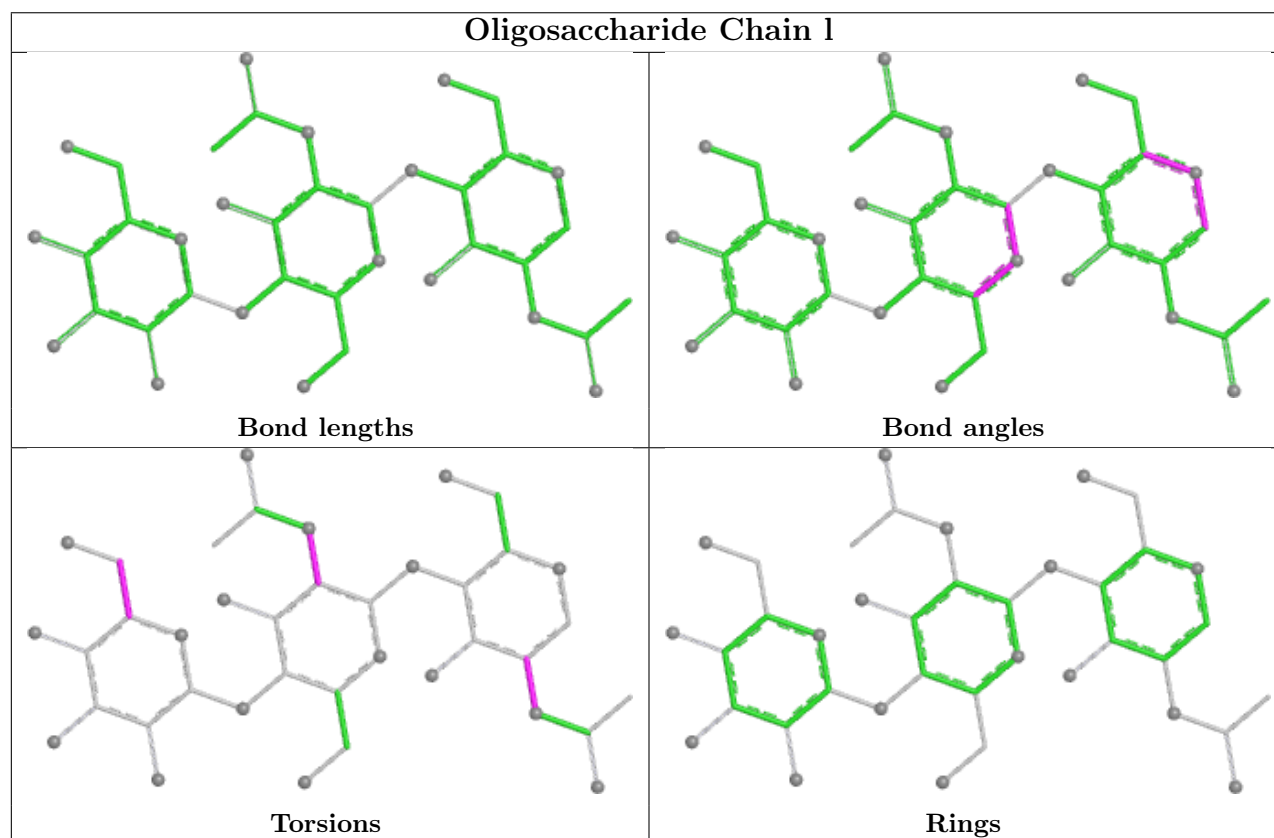
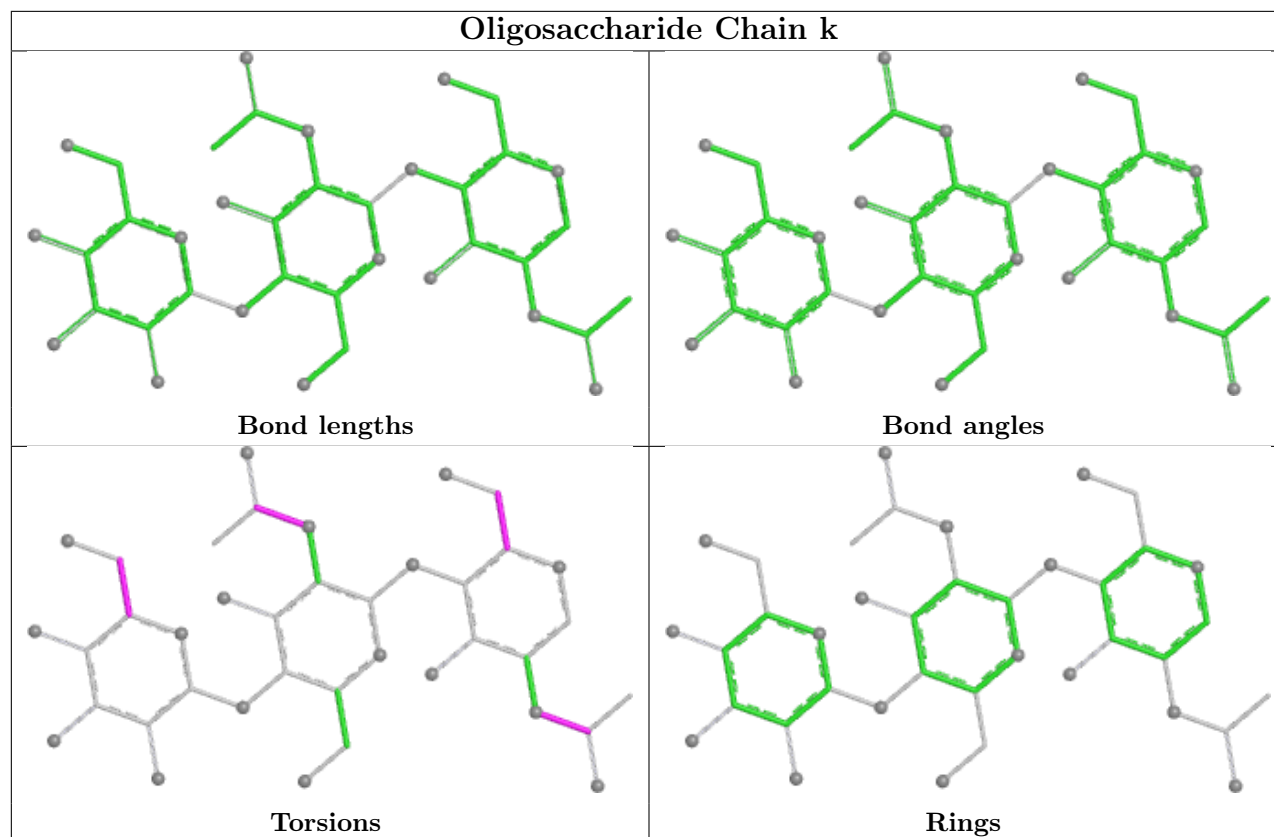


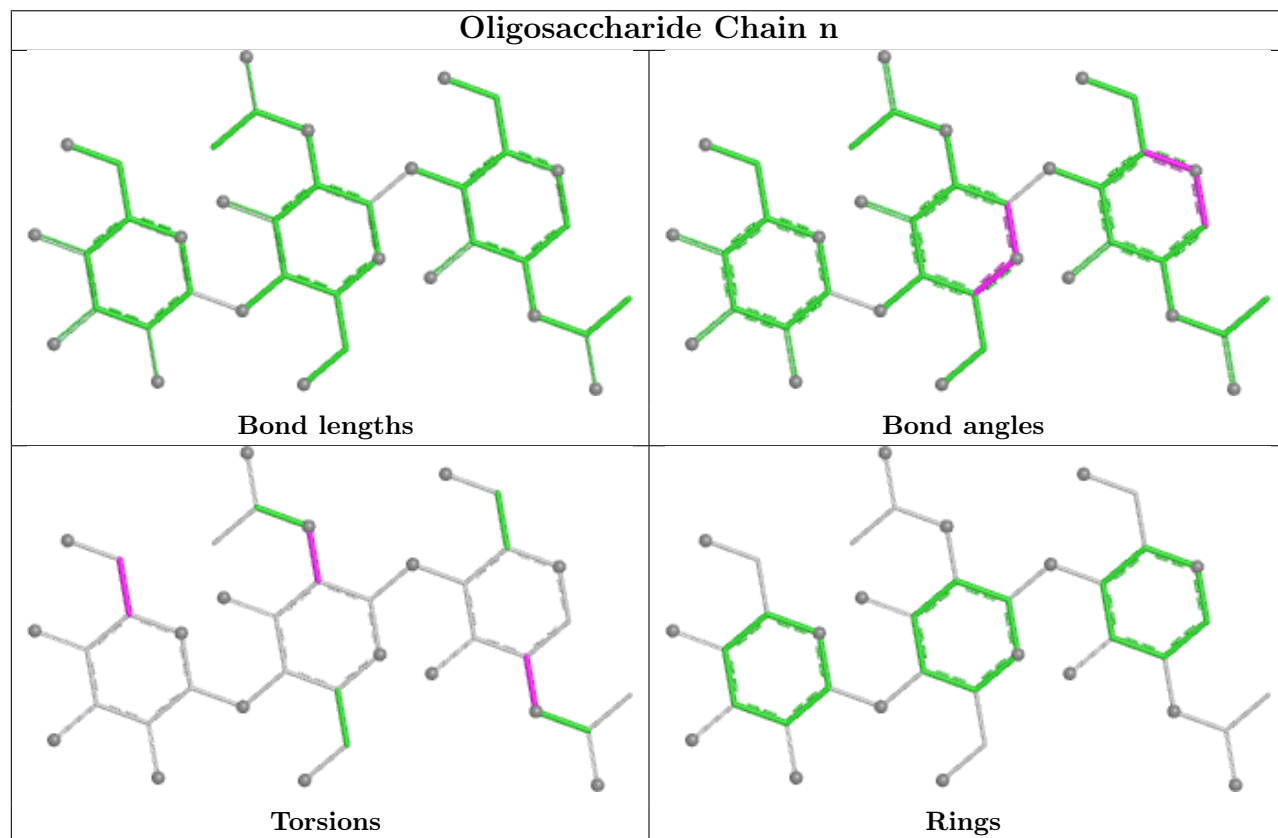
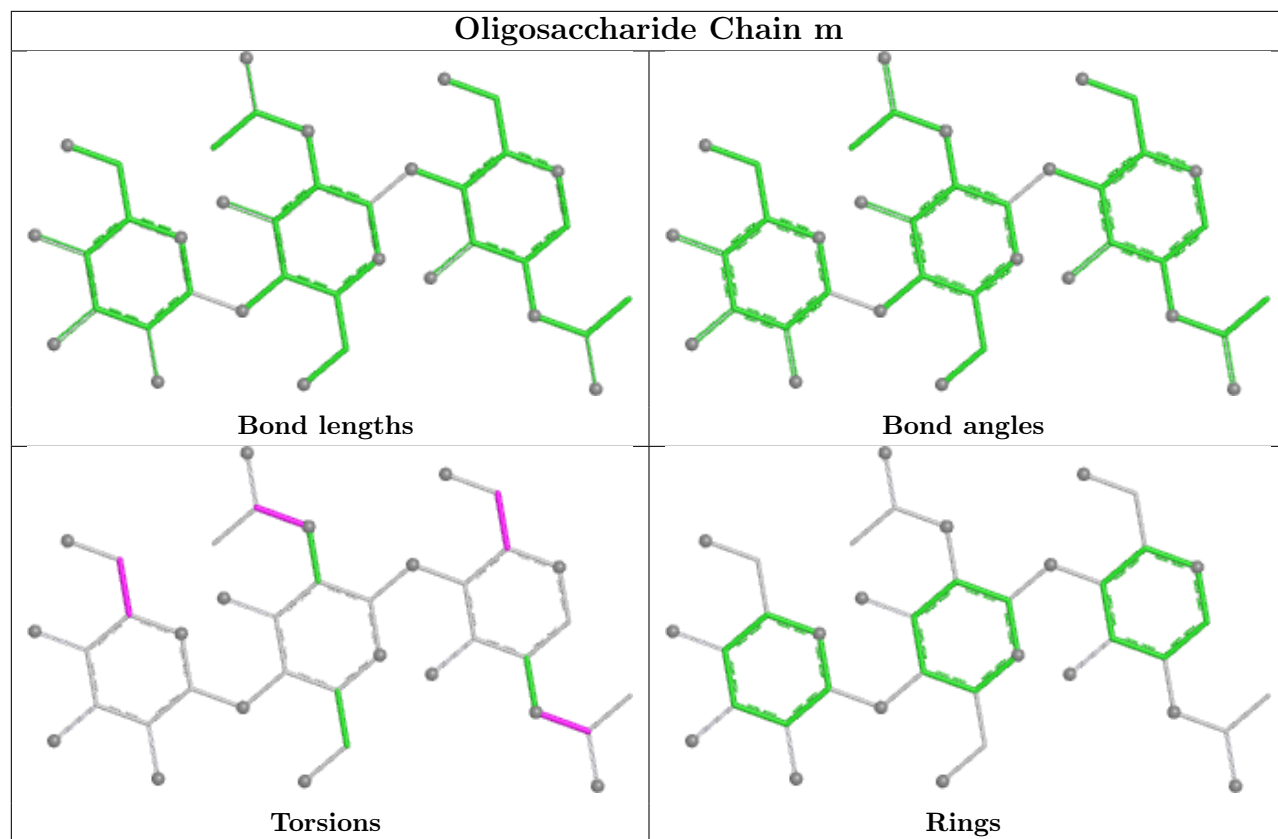


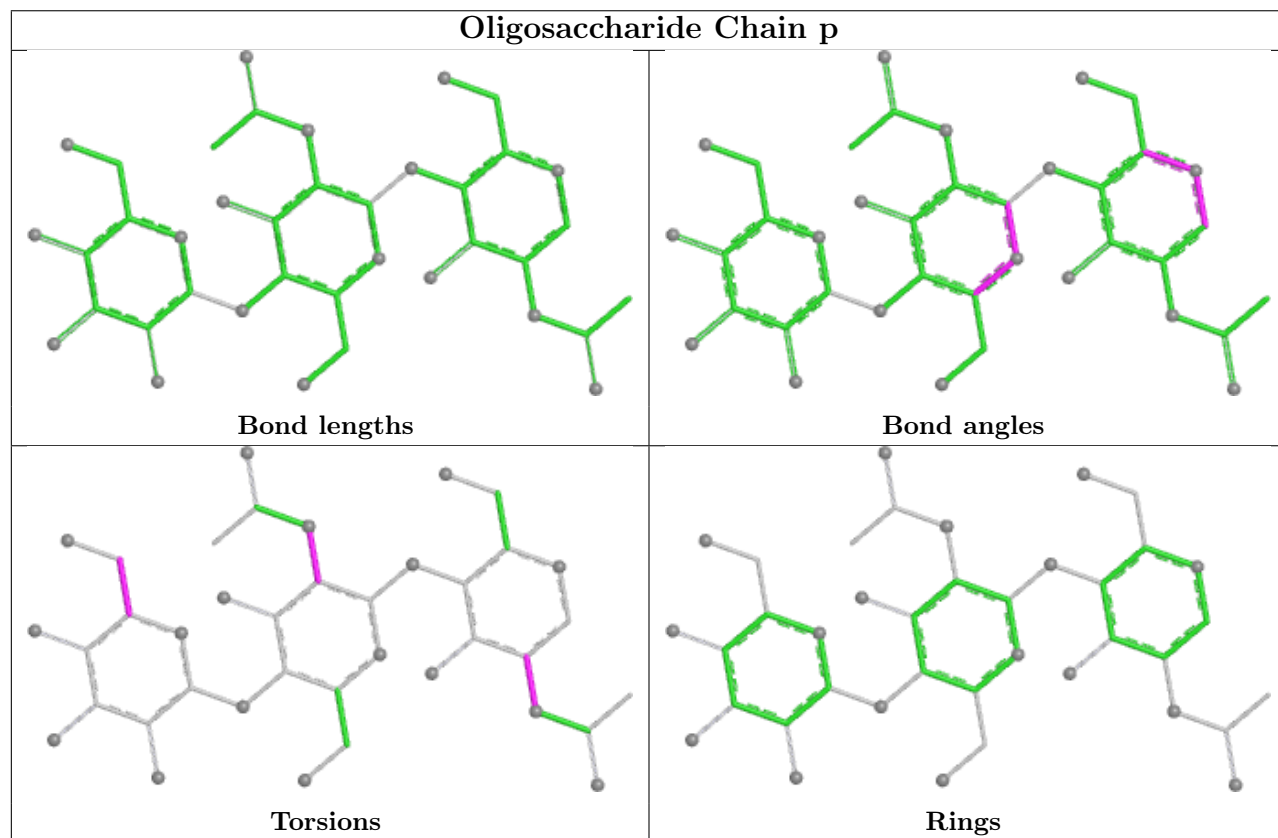
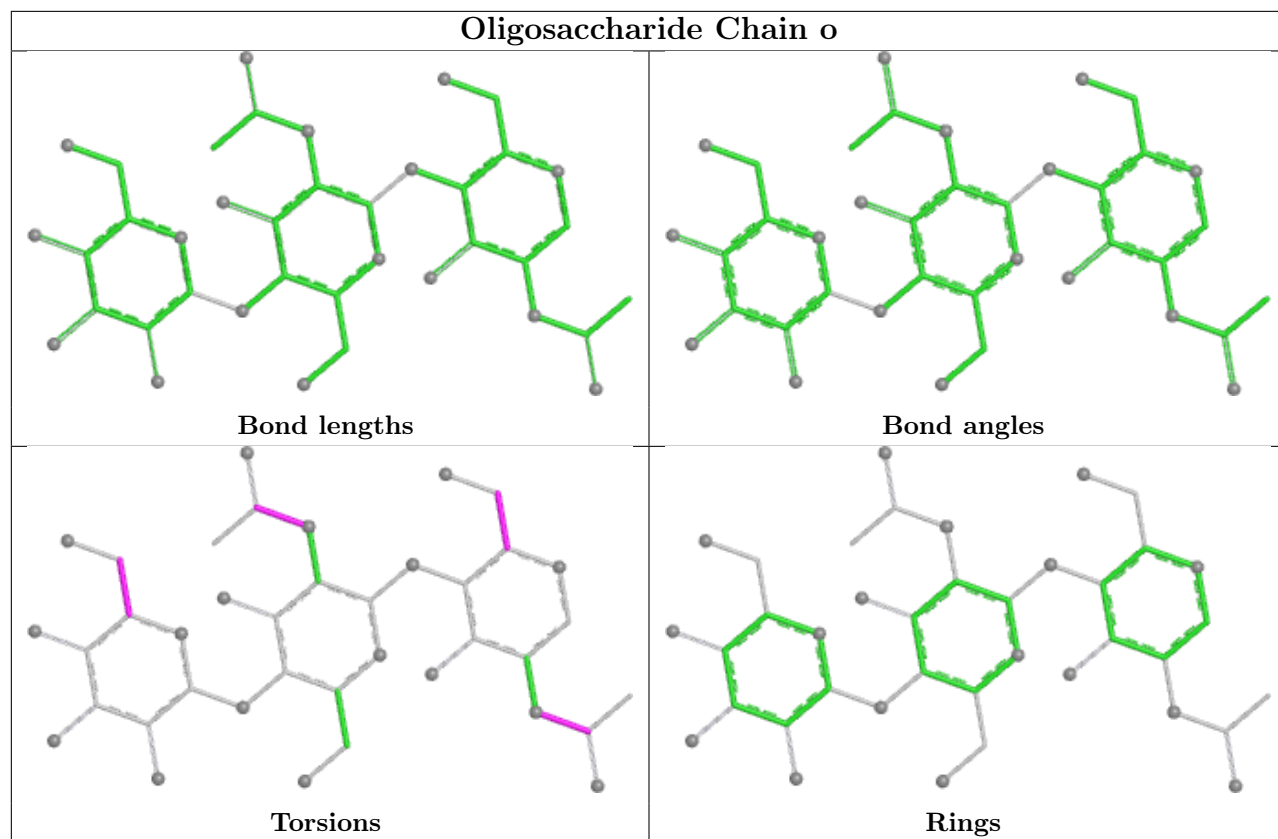


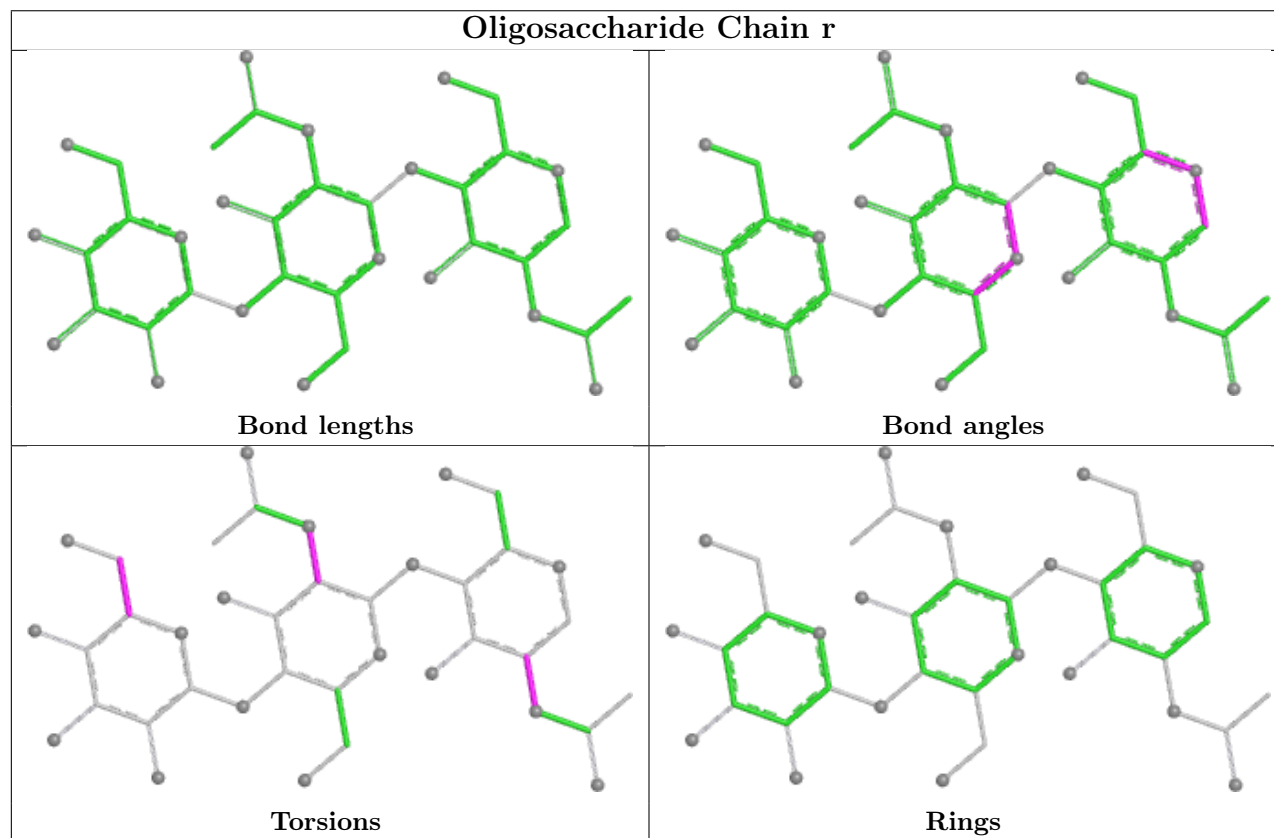
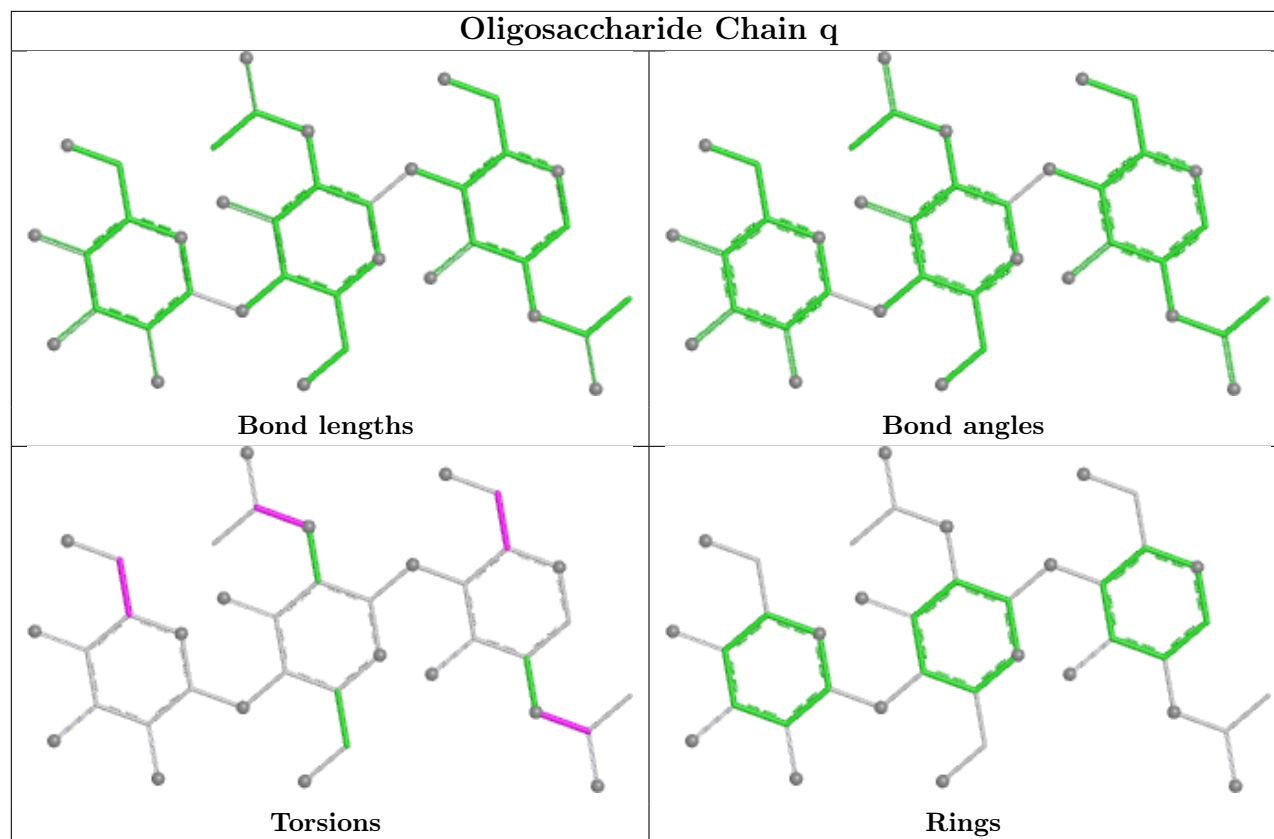


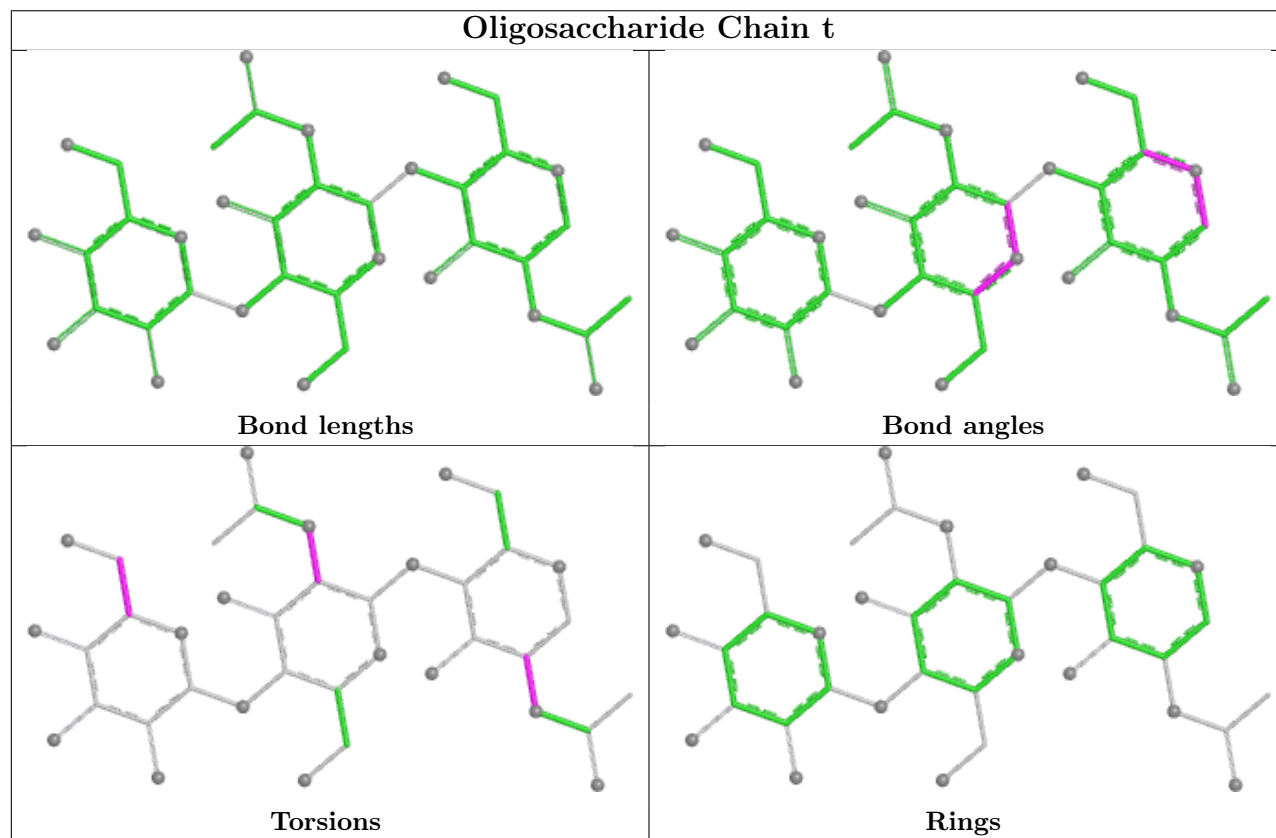
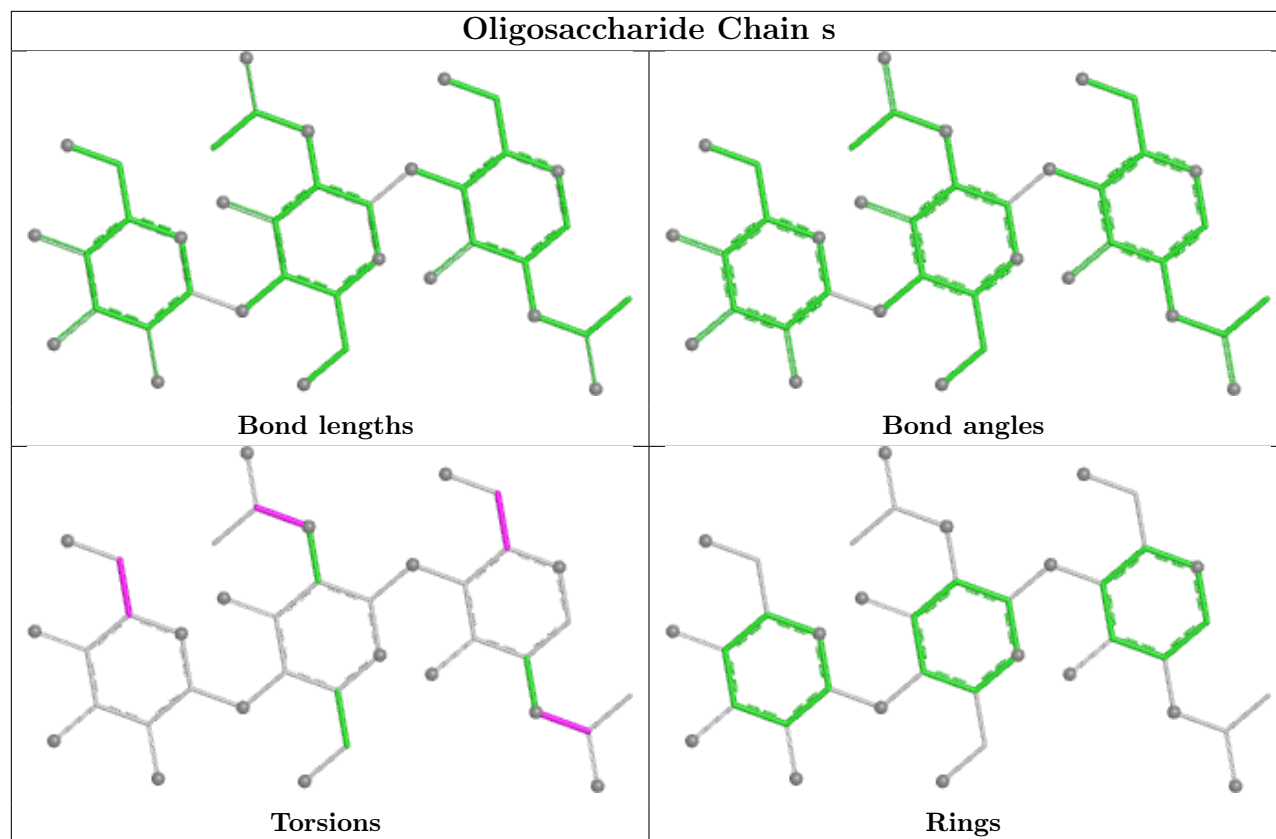


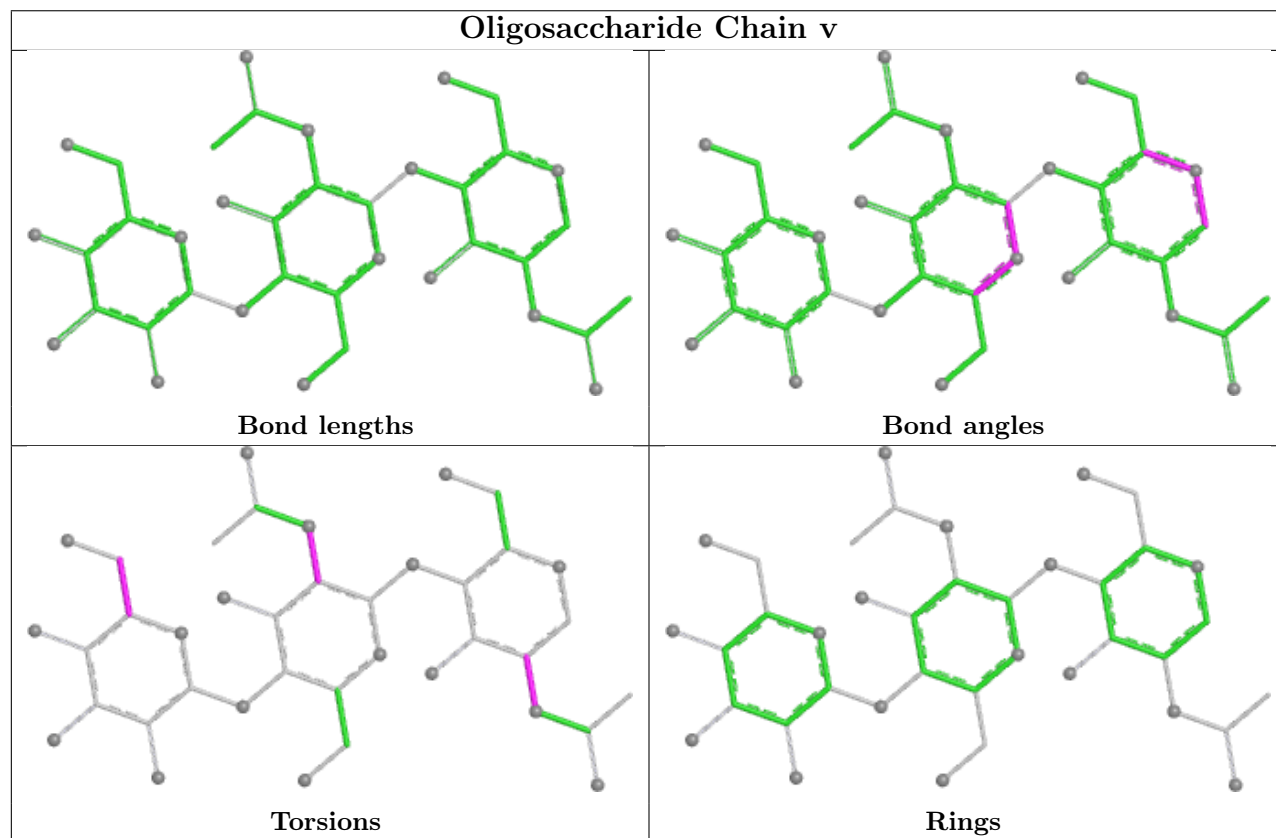
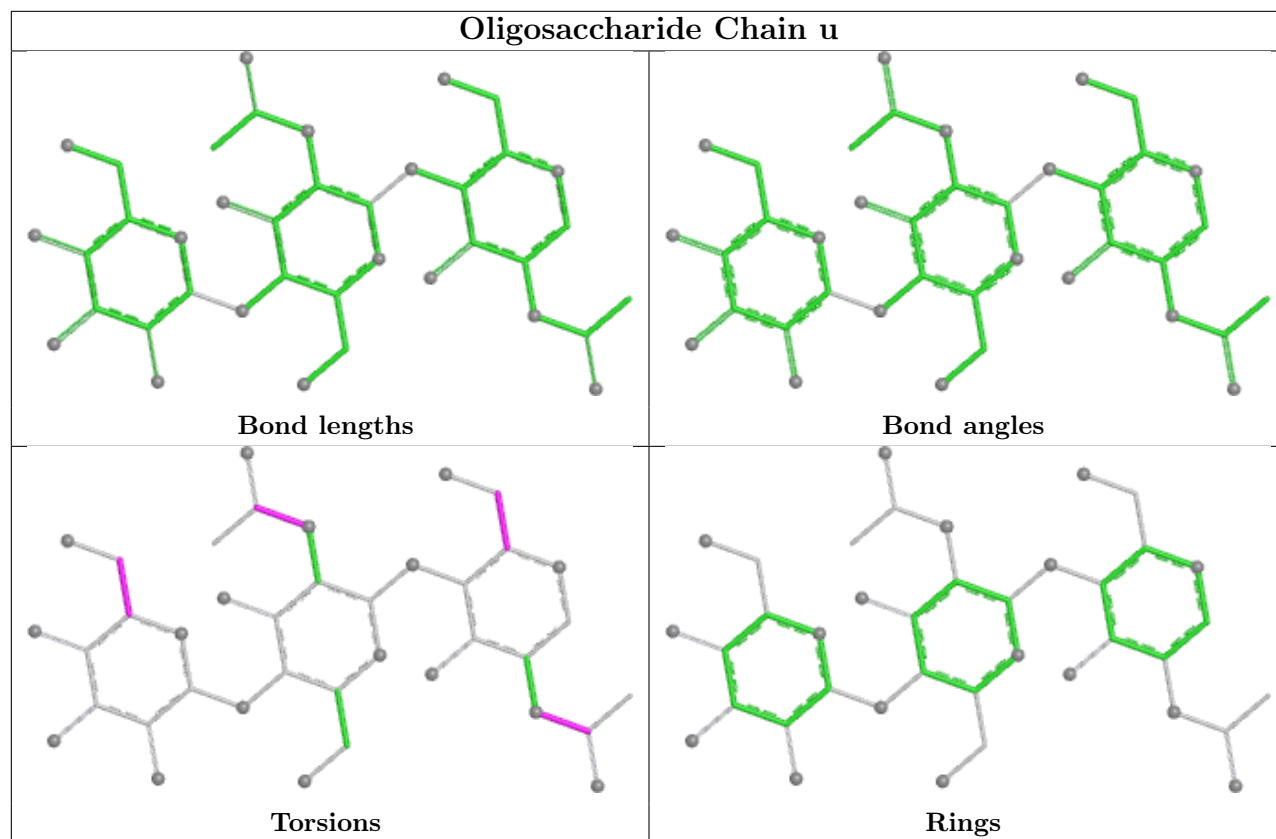


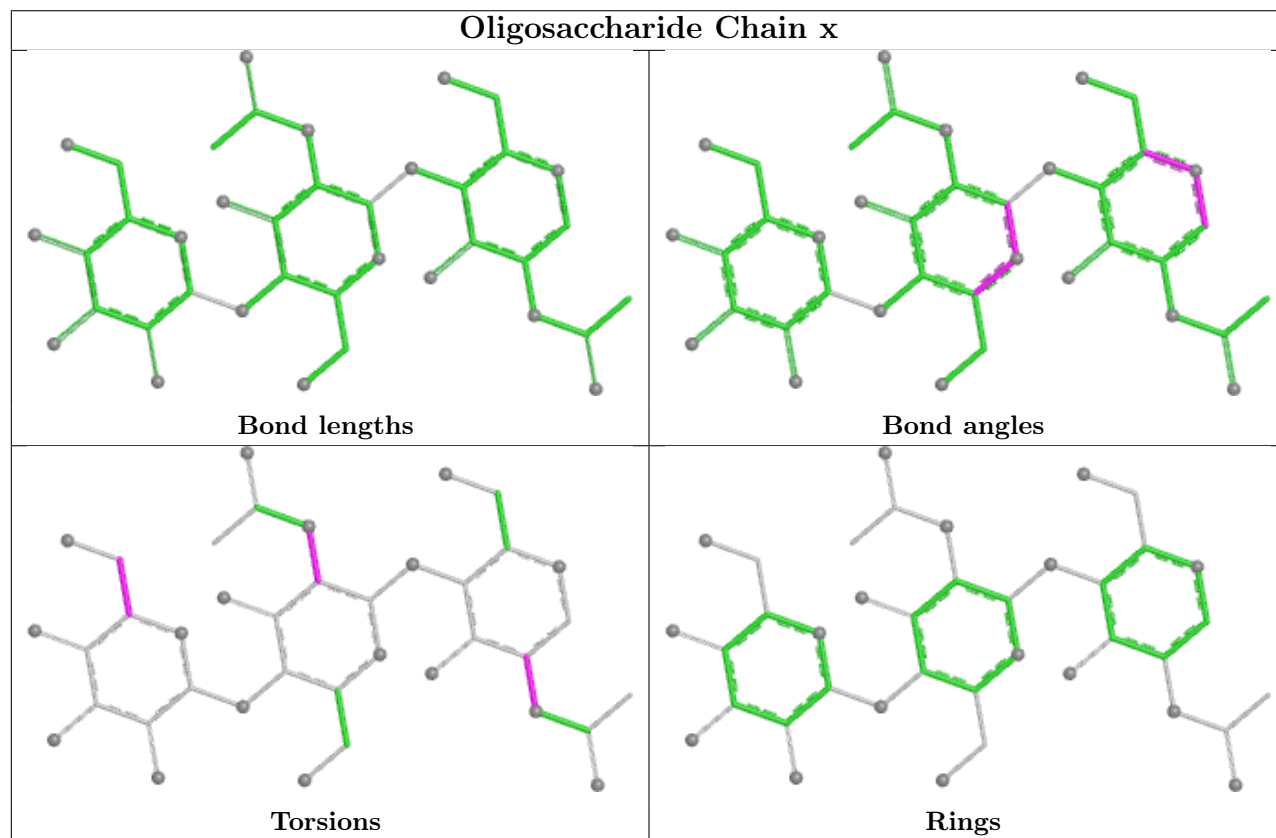
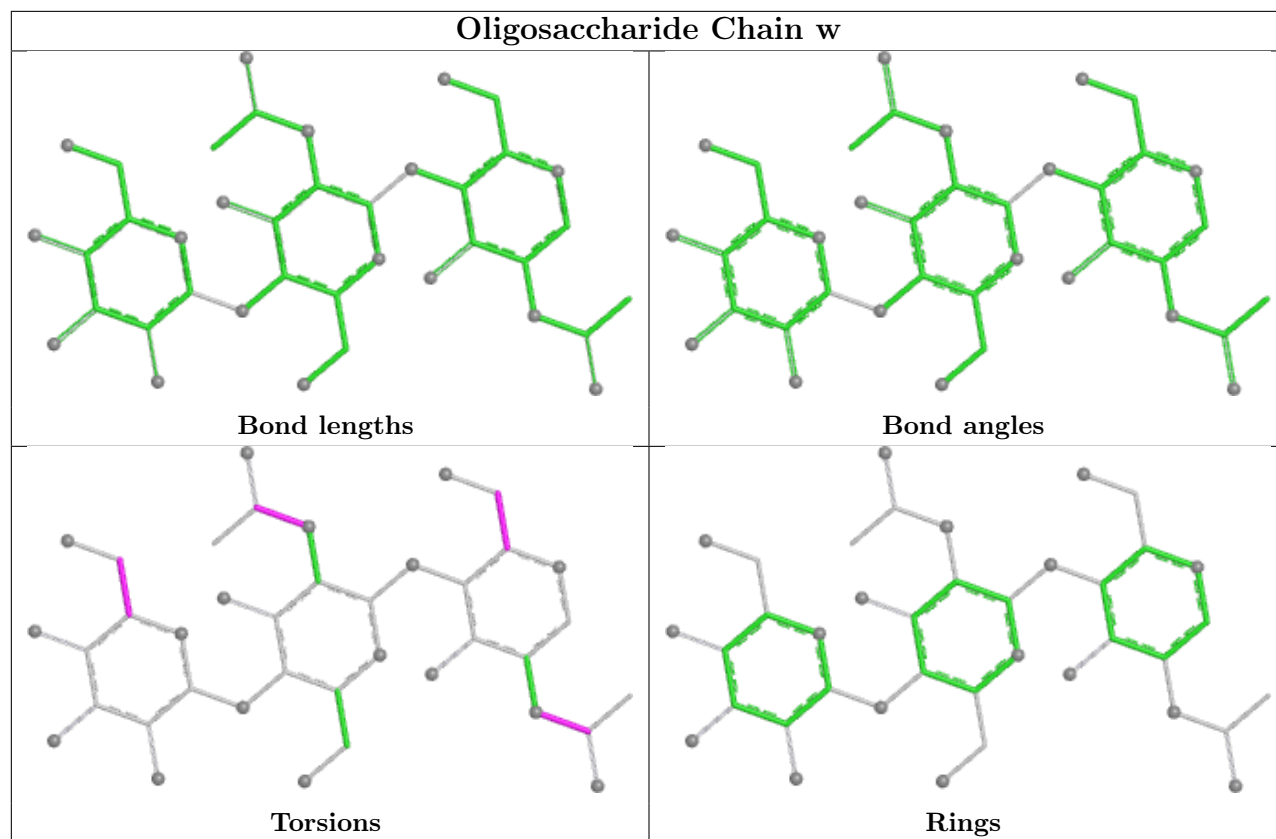


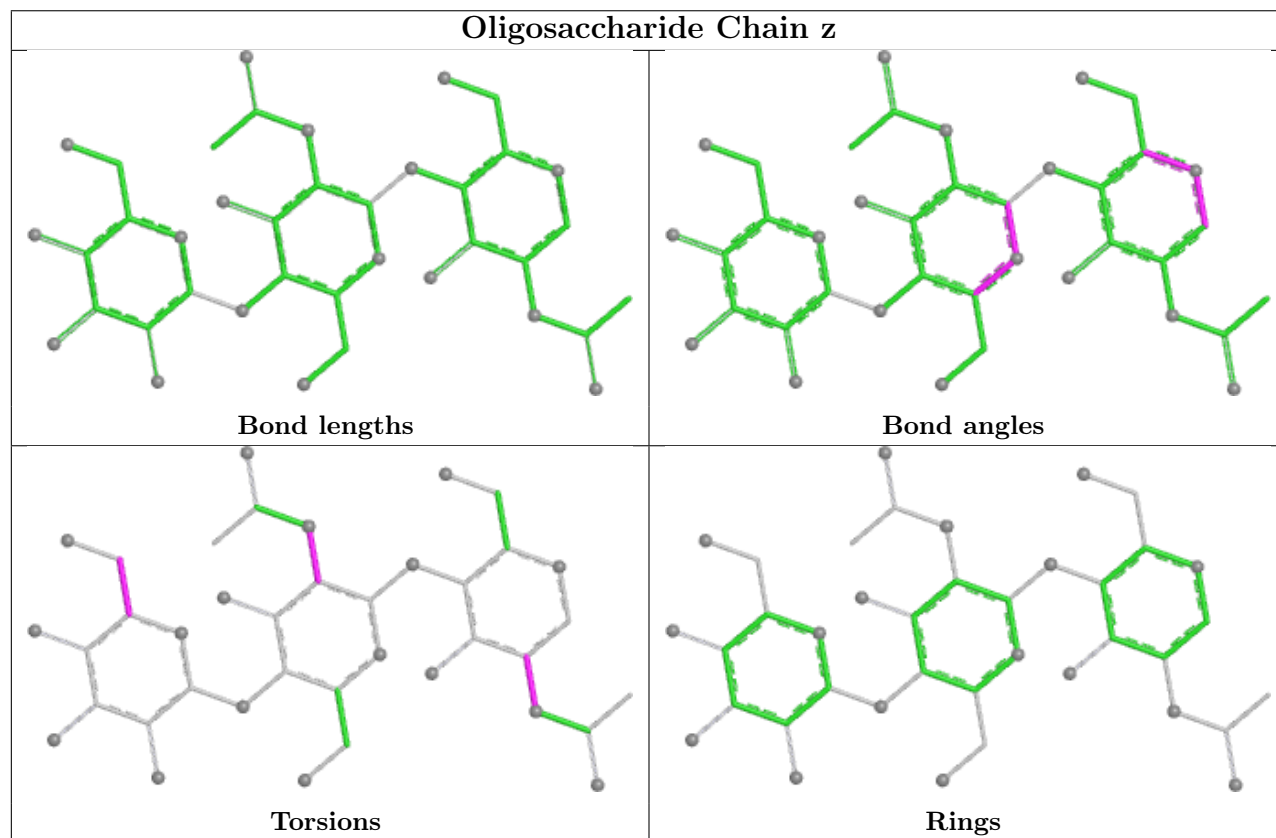
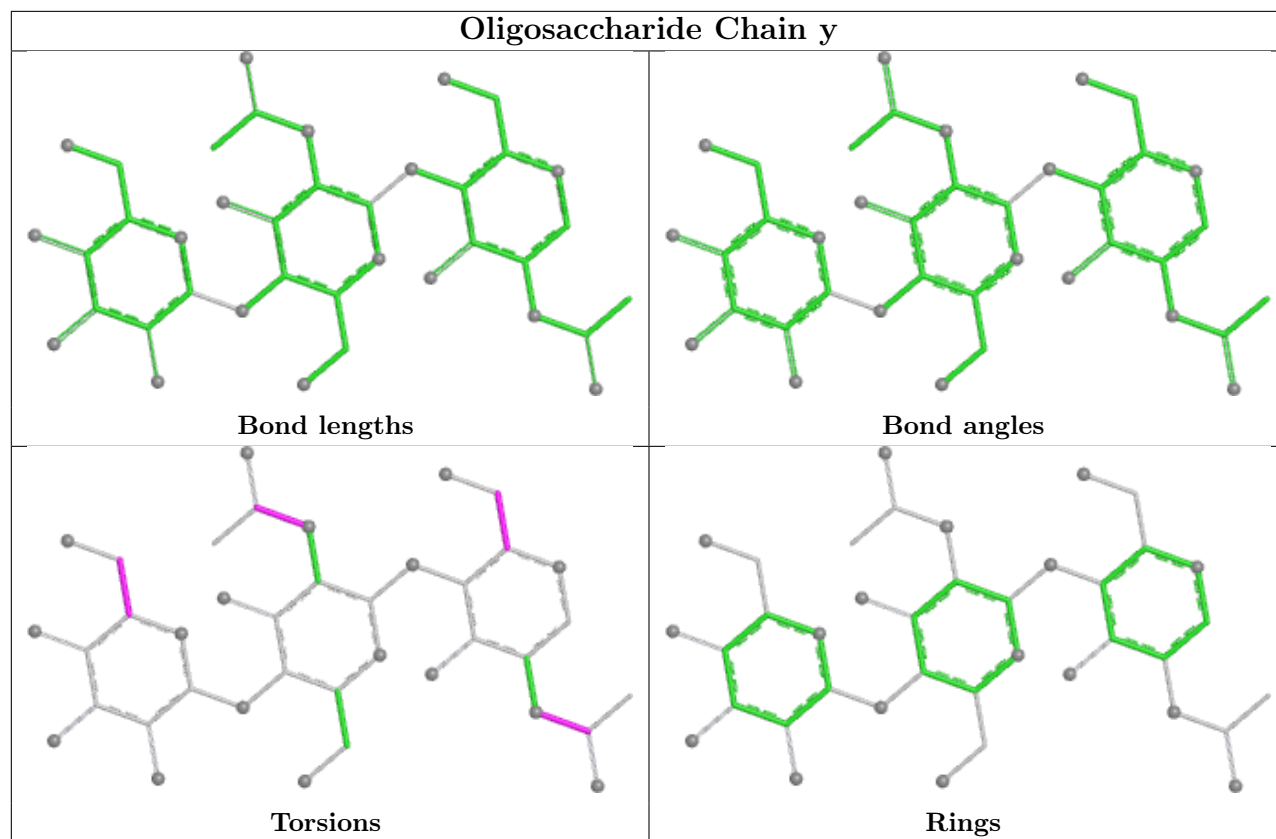


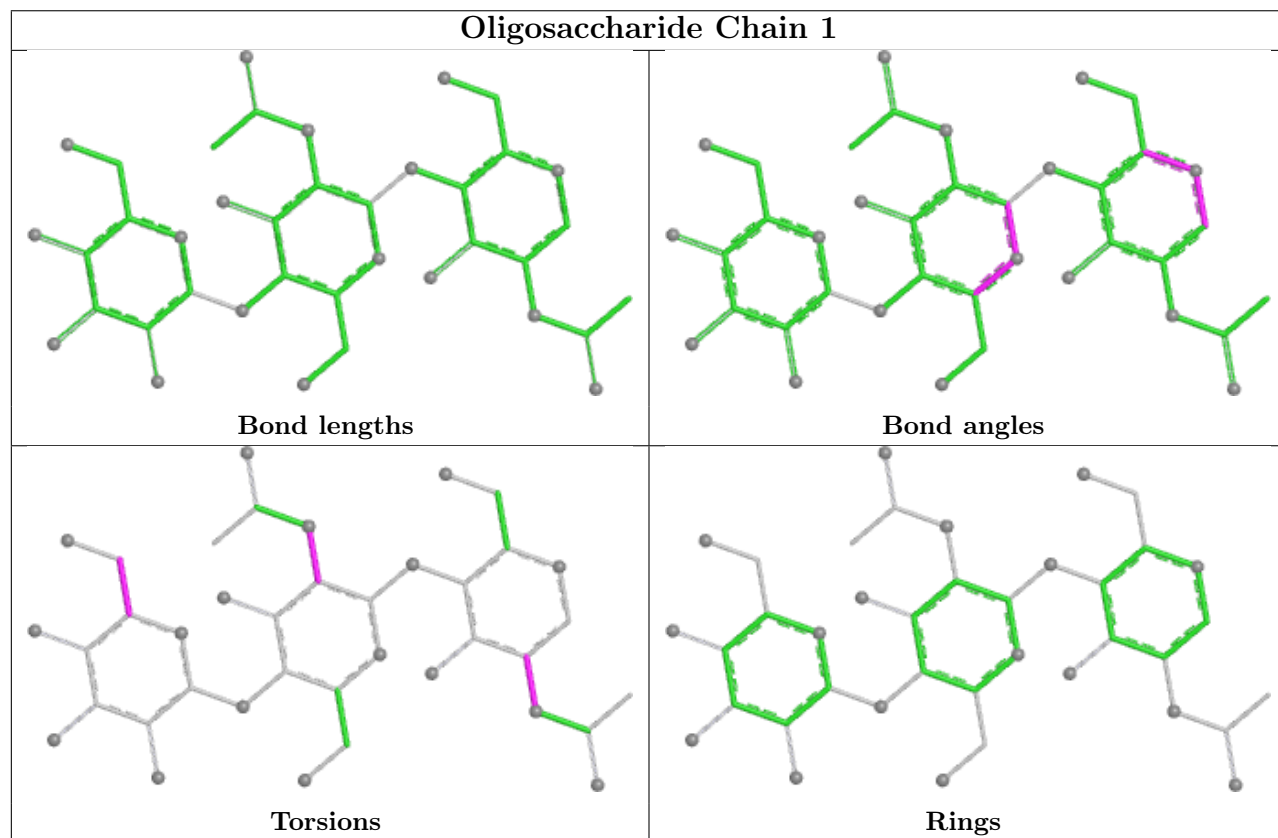
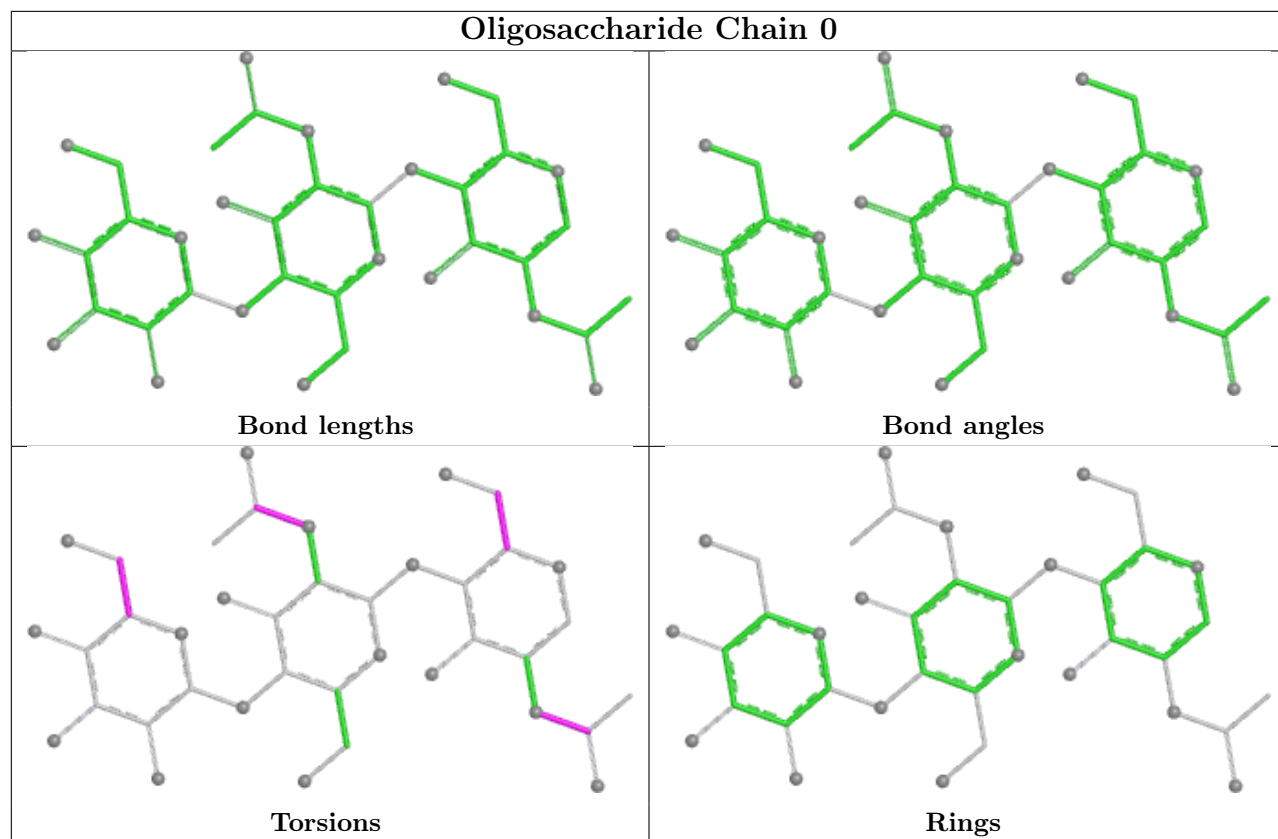




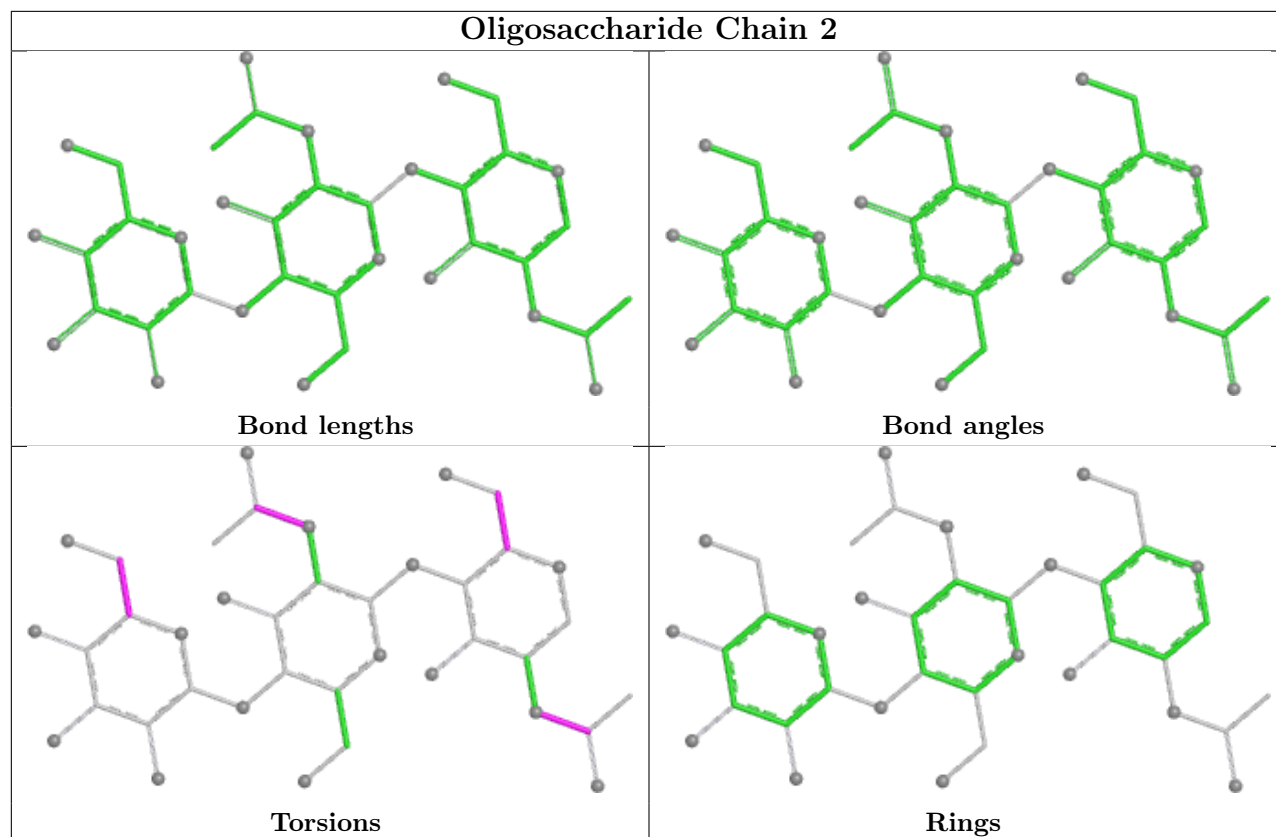




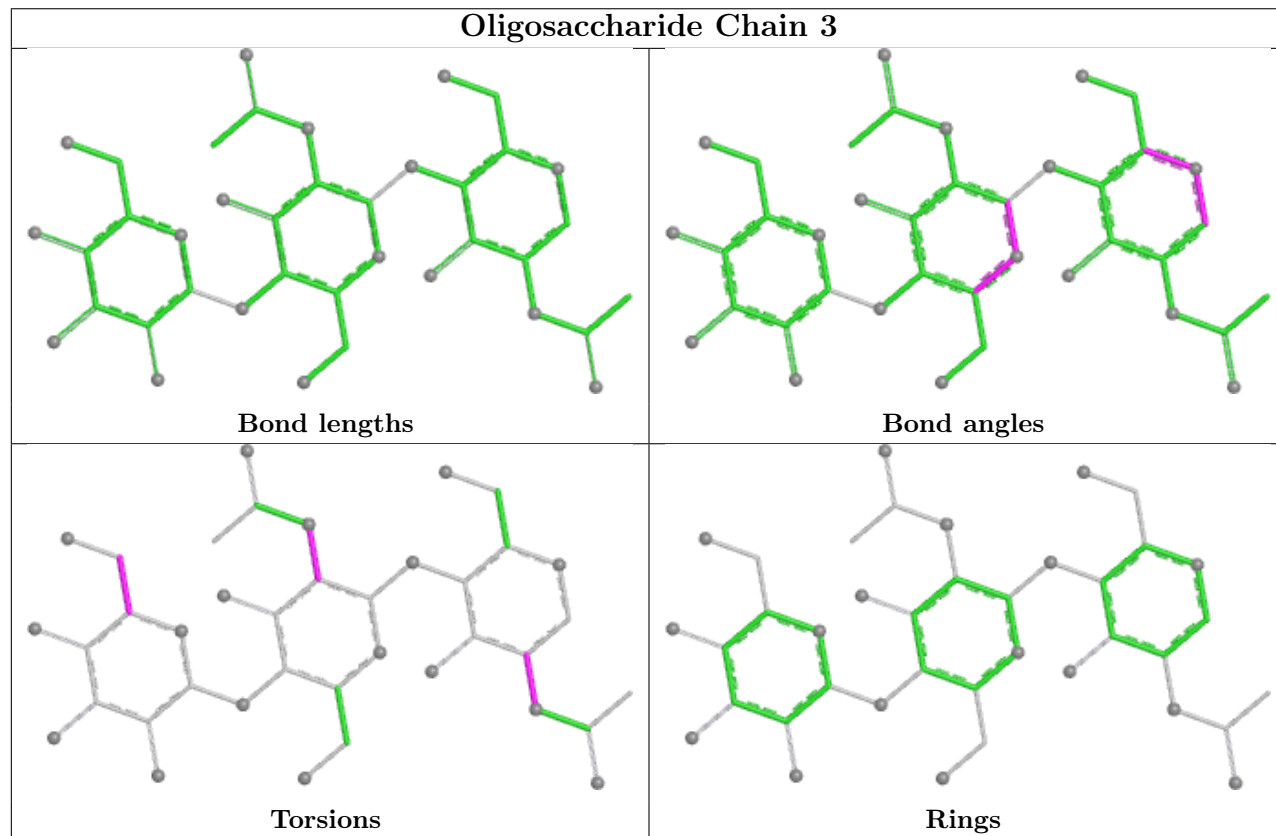




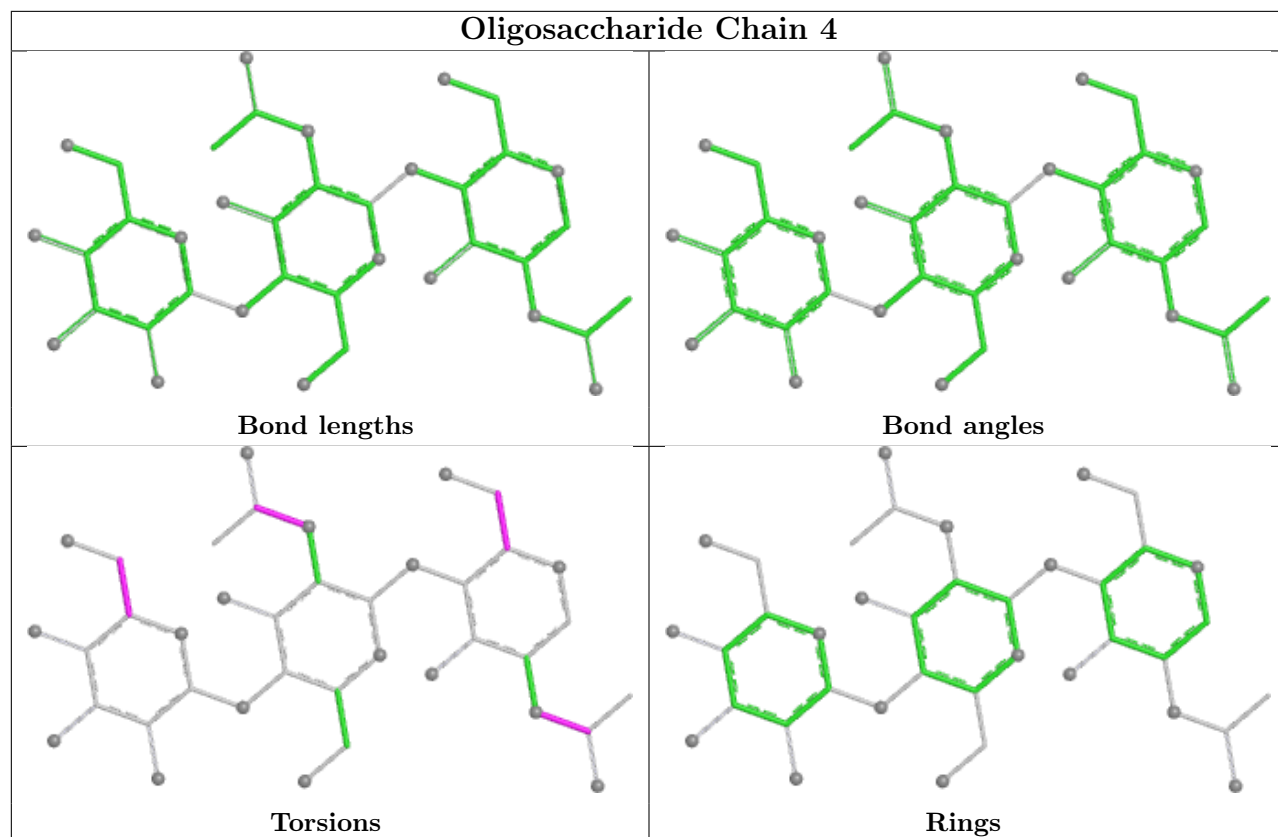
Oligosaccharide Chain 2



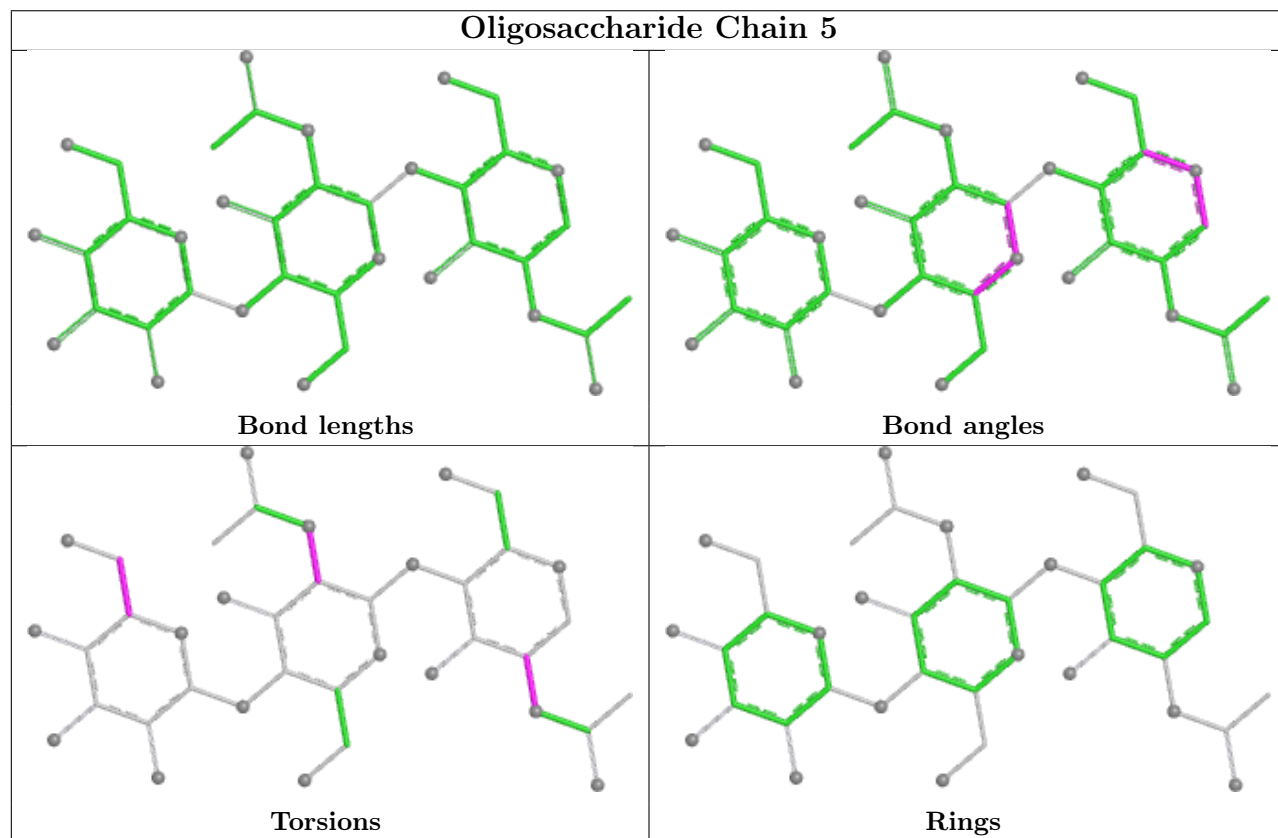
Oligosaccharide Chain 3



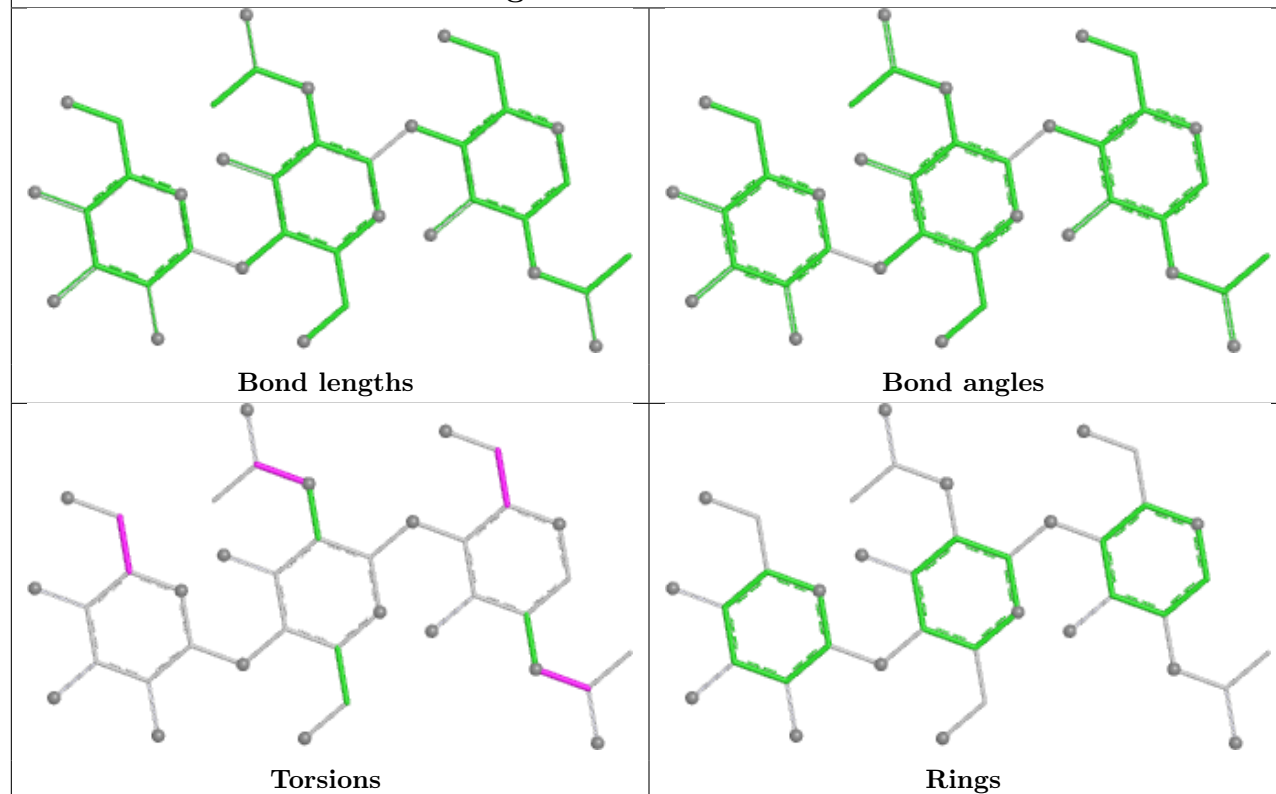
Oligosaccharide Chain 4



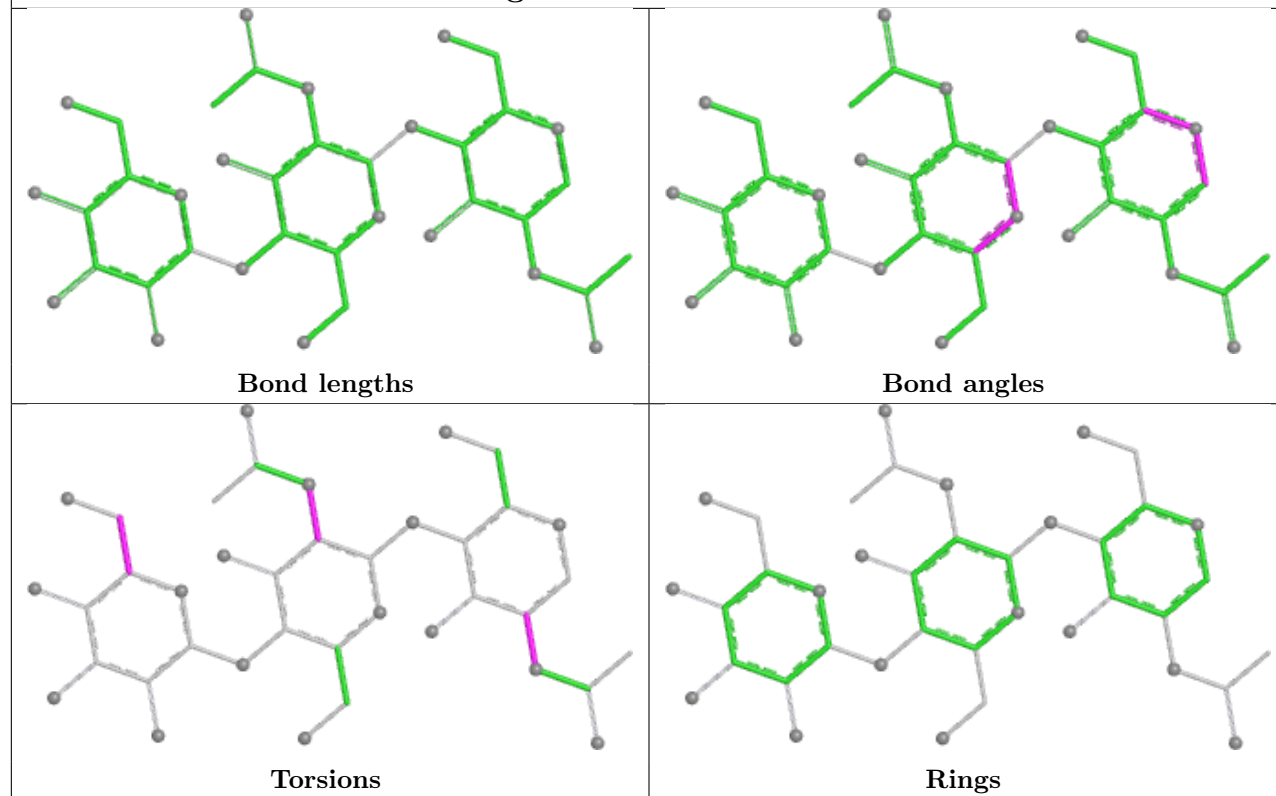
Oligosaccharide Chain 5



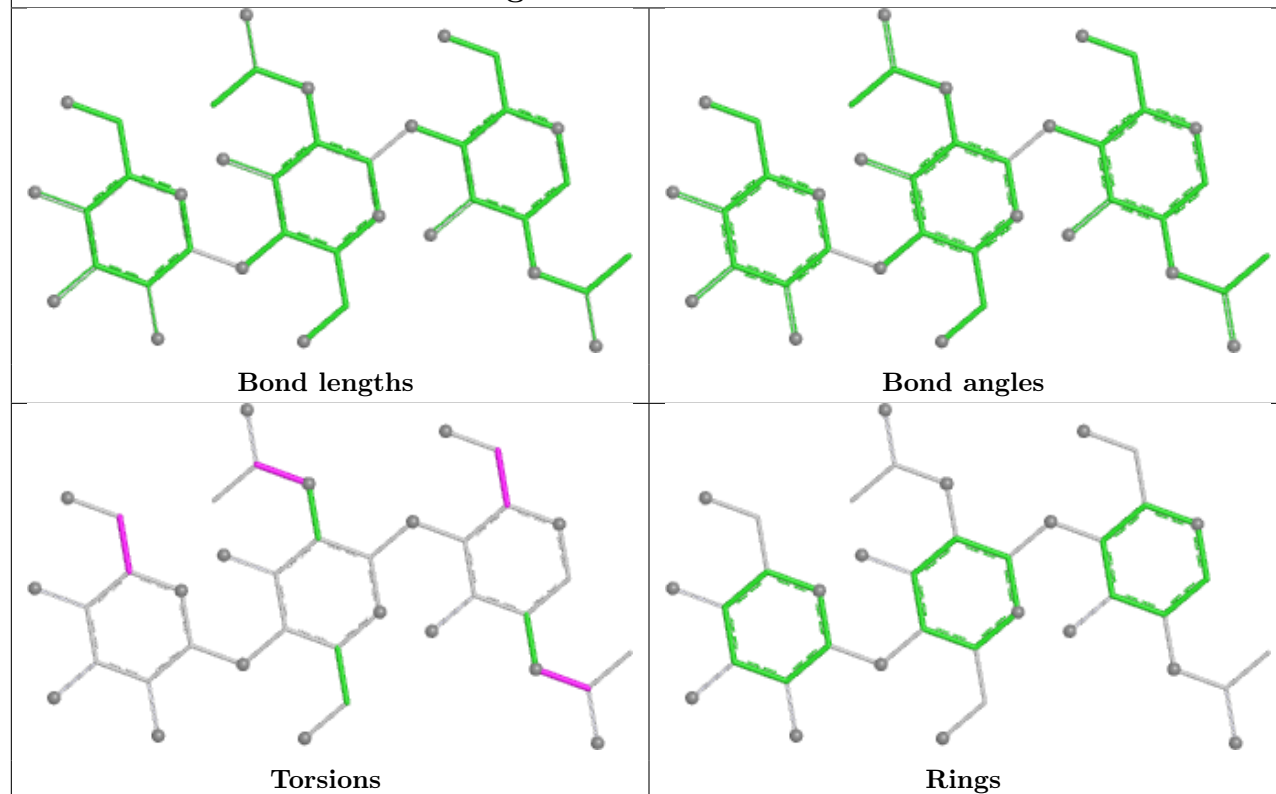
Oligosaccharide Chain 6



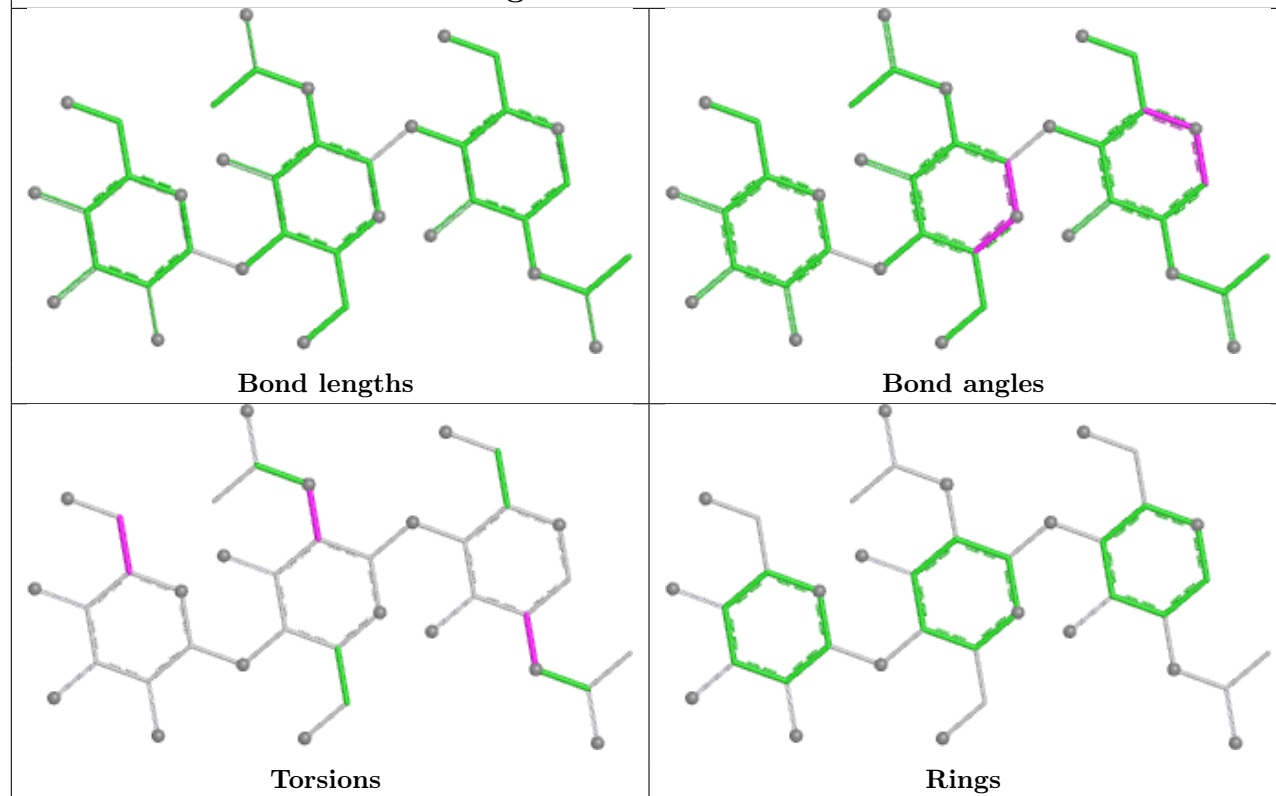
Oligosaccharide Chain 7



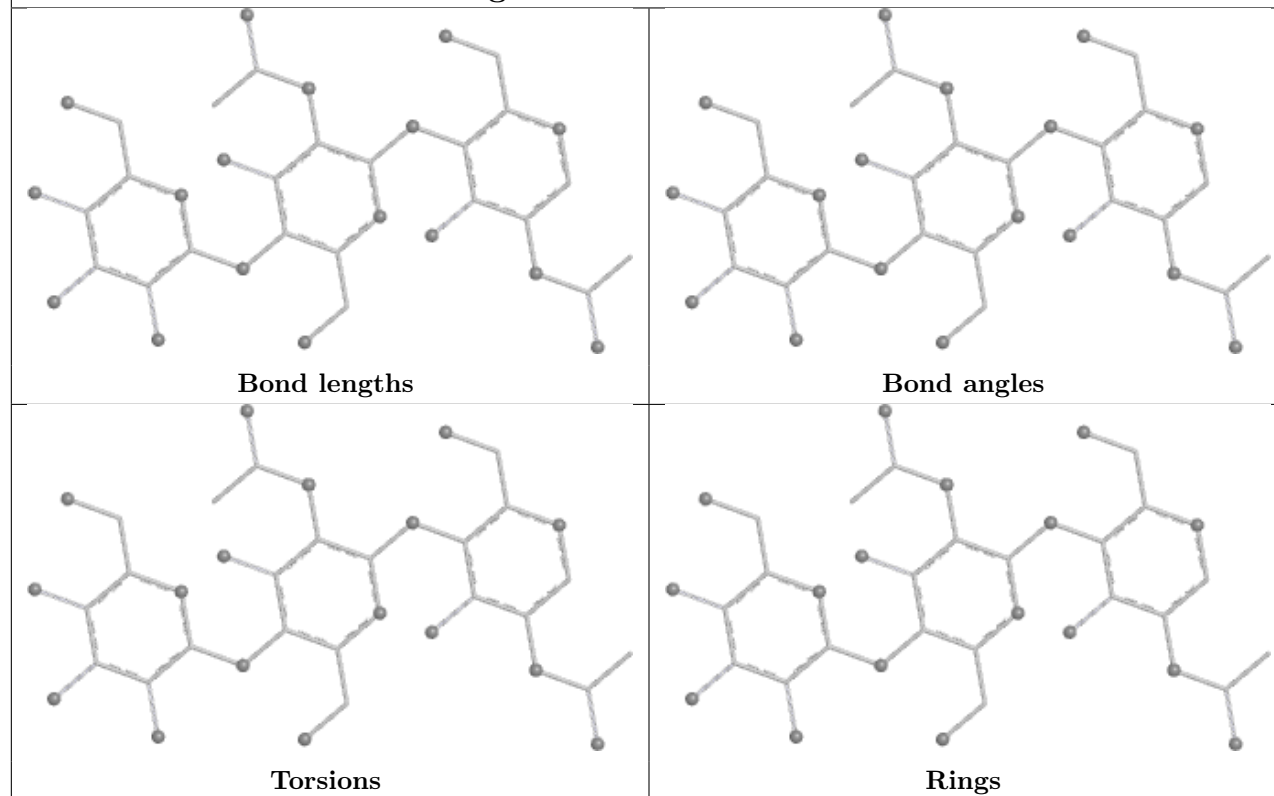
Oligosaccharide Chain 8



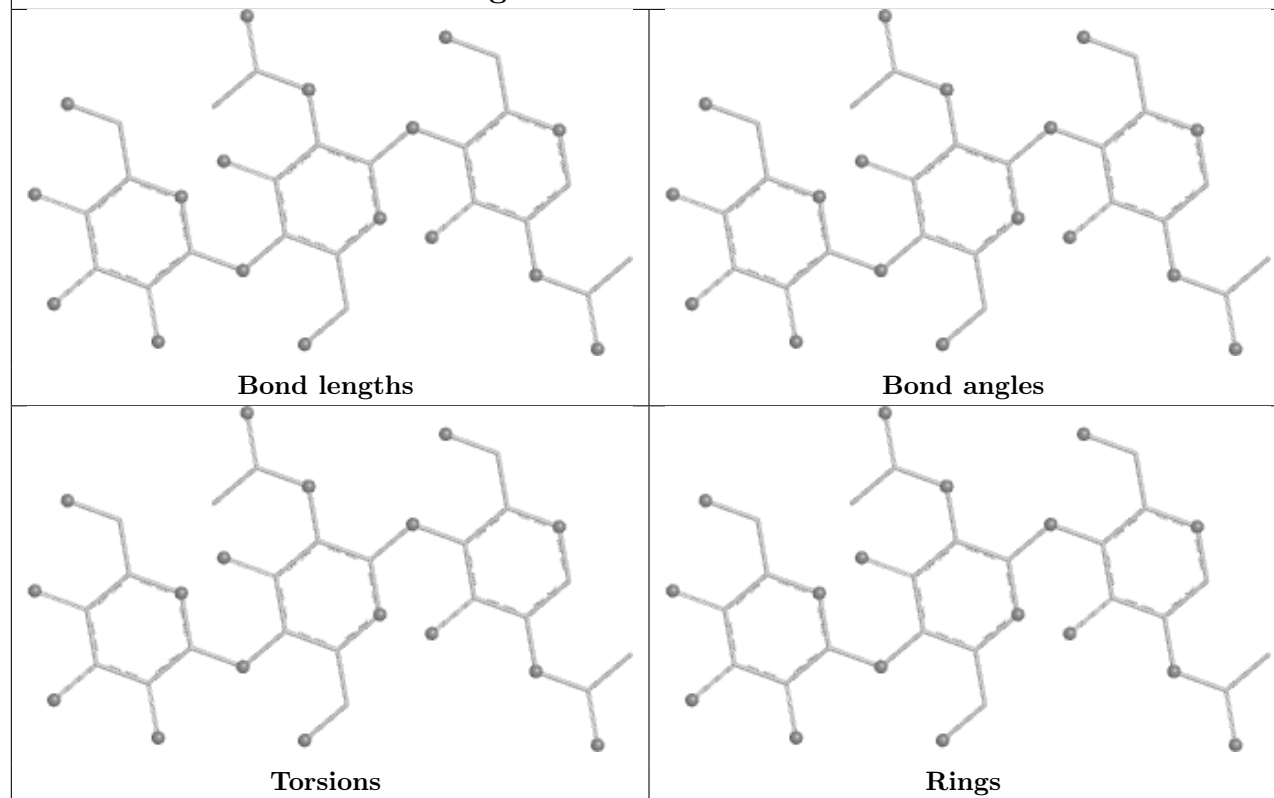
Oligosaccharide Chain 9



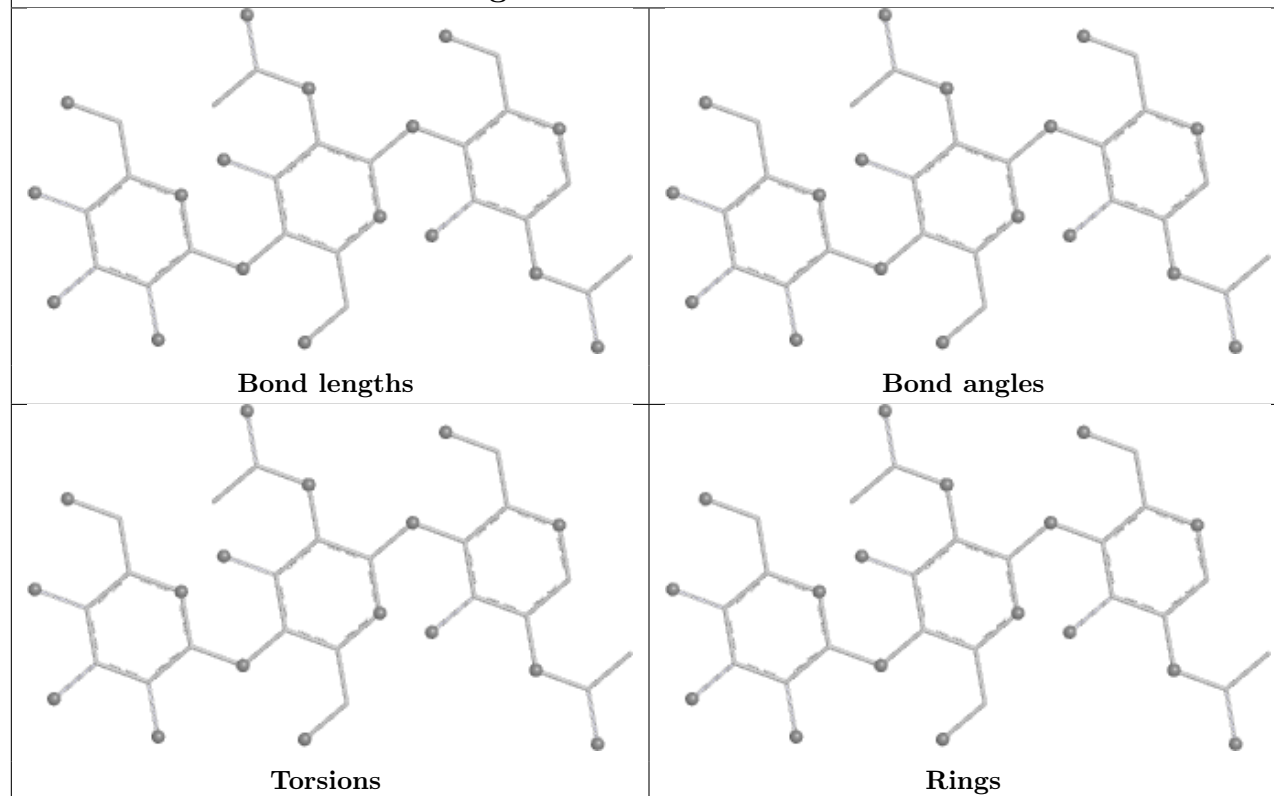
Oligosaccharide Chain AA



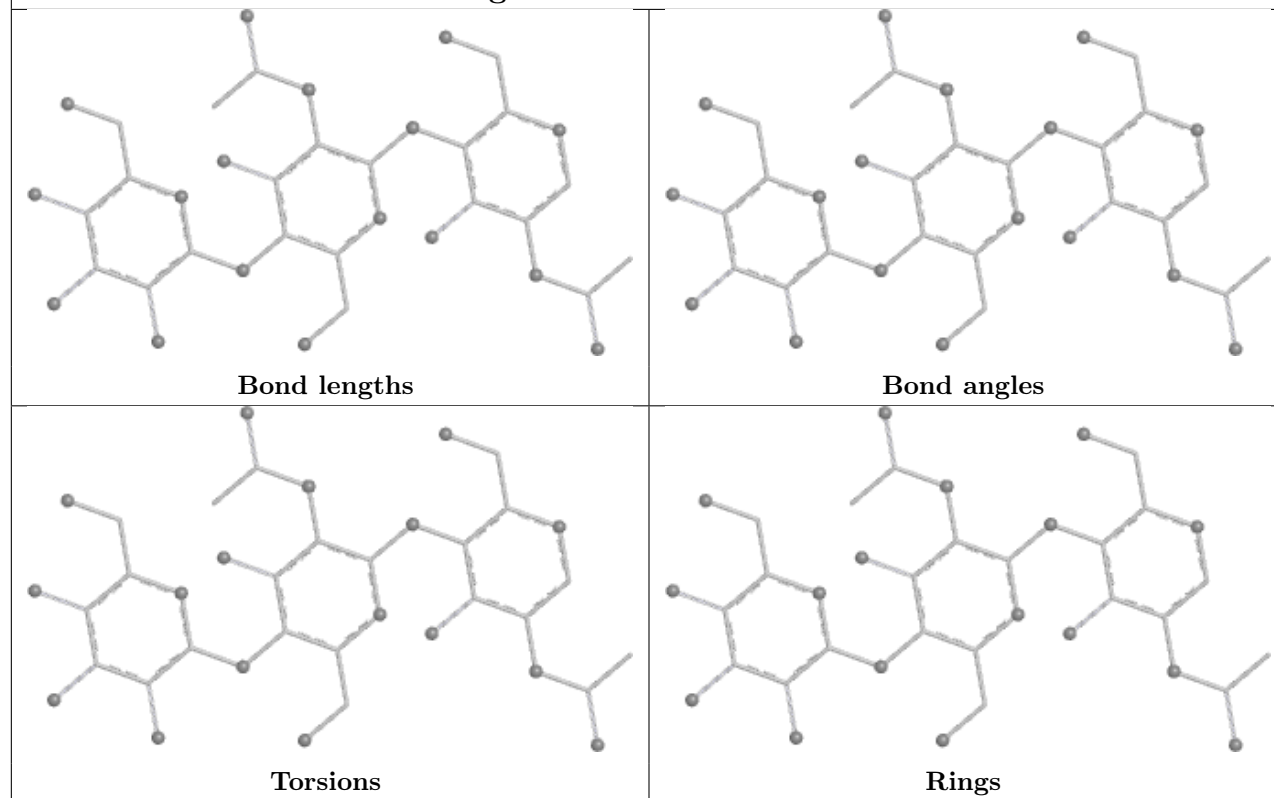
Oligosaccharide Chain BA



Oligosaccharide Chain CA



Oligosaccharide Chain DA



5.6 Ligand geometry

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	I	1011	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	T	1016	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	R	1006	-	4,4,4	0.24	0	6,6,6	0.05	0
4	P52	V	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.14	5 (11%)
6	NAG	T	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	V	1004	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	E	1010	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	N	1005	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	N	1009	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	E	1004	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	S	1015	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	U	1001	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	A	1006	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	P	1011	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	U	1014	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	M	1017	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	P	1004	-	4,4,4	0.24	0	6,6,6	0.08	0
6	NAG	D	1023	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	A	1013	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	L	1007	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	A	1015	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	L	1011	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	L	1009	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	A	1010	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	G	1024	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	S	1011	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	A	1008	-	4,4,4	0.24	0	6,6,6	0.13	0
4	P52	P	1002	3	34,38,38	3.63	8 (23%)	42,53,53	1.12	4 (9%)
5	SO4	T	1009	-	4,4,4	0.23	0	6,6,6	0.07	0
6	NAG	U	1024	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	K	1003	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	U	1013	-	4,4,4	0.23	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	T	1014	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	J	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	F	1007	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	U	1015	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	R	1011	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	V	1012	-	4,4,4	0.24	0	6,6,6	0.08	0
6	NAG	H	1023	-	14,14,15	0.22	0	17,19,21	0.76	0
5	SO4	J	1008	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	D	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	K	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	I	1015	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	O	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	D	1015	-	4,4,4	0.24	0	6,6,6	0.10	0
4	P52	M	1003	3	34,38,38	3.61	8 (23%)	42,53,53	1.13	5 (11%)
5	SO4	K	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	P	1005	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	O	1014	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	S	1004	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	R	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	F	1012	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	O	1016	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	T	1015	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	F	1006	-	4,4,4	0.23	0	6,6,6	0.14	0
6	NAG	I	1023	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	S	1012	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	K	1004	-	4,4,4	0.24	0	6,6,6	0.06	0
6	NAG	K	1023	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	C	1013	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	T	1004	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	1005	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	M	1012	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	K	1012	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	N	1006	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	S	1001	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	A	1005	-	4,4,4	0.22	0	6,6,6	0.14	0
5	SO4	T	1012	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	Q	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
6	NAG	Q	1021	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	F	1009	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	E	1014	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	B	1008	-	4,4,4	0.23	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	P52	J	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.15	5 (11%)
4	P52	R	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.15	6 (14%)
5	SO4	T	1010	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	G	1010	-	4,4,4	0.24	0	6,6,6	0.12	0
6	NAG	N	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	S	1008	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	1013	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	H	1014	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	H	1005	-	4,4,4	0.23	0	6,6,6	0.17	0
5	SO4	P	1014	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	E	1007	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	F	1010	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	R	1013	-	4,4,4	0.23	0	6,6,6	0.08	0
4	P52	K	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.14	3 (7%)
5	SO4	D	1012	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	K	1014	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	L	1010	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	U	1017	-	4,4,4	0.23	0	6,6,6	0.08	0
4	P52	A	1002	3	34,38,38	3.60	8 (23%)	42,53,53	1.16	5 (11%)
5	SO4	G	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	L	1016	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	P	1006	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	A	1014	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	H	1007	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	Q	1014	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	Q	1005	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	P	1010	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	K	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	H	1011	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	V	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	M	1011	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	C	1009	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	B	1006	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	K	1015	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	H	1012	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	H	1004	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	B	1023	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	K	1008	-	4,4,4	0.24	0	6,6,6	0.06	0
6	NAG	O	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	M	1006	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	H	1016	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	Q	1013	-	4,4,4	0.24	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	T	1011	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	N	1016	-	4,4,4	0.24	0	6,6,6	0.06	0
4	P52	G	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.12	4 (9%)
5	SO4	C	1011	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	F	1001	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	D	1010	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	M	1010	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	B	1012	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	M	1007	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	D	1011	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	L	1001	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	I	1004	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	I	1008	-	4,4,4	0.25	0	6,6,6	0.13	0
5	SO4	Q	1012	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	L	1014	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	N	1015	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	M	1004	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	N	1001	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	R	1015	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	F	1016	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	N	1014	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	E	1013	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	V	1014	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	V	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	J	1015	-	4,4,4	0.23	0	6,6,6	0.12	0
6	NAG	R	1023	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	J	1010	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	U	1011	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	F	1014	-	4,4,4	0.24	0	6,6,6	0.06	0
4	P52	I	1003	3	34,38,38	3.59	8 (23%)	42,53,53	1.11	3 (7%)
4	P52	B	1002	3	34,38,38	3.61	8 (23%)	42,53,53	1.15	3 (7%)
5	SO4	P	1007	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	N	1008	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	F	1008	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	L	1004	-	4,4,4	0.23	0	6,6,6	0.10	0
6	NAG	G	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
4	P52	T	1003	3	34,38,38	3.62	8 (23%)	42,53,53	1.14	5 (11%)
5	SO4	N	1004	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	M	1014	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	M	1005	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	S	1016	-	4,4,4	0.22	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	O	1007	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	B	1011	-	4,4,4	0.24	0	6,6,6	0.07	0
6	NAG	C	1022	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	R	1008	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	N	1012	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	H	1006	-	4,4,4	0.23	0	6,6,6	0.08	0
4	P52	D	1003	3	34,38,38	3.61	7 (20%)	42,53,53	1.21	5 (11%)
5	SO4	S	1006	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	S	1005	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	O	1012	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	S	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
6	NAG	S	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	I	1010	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	J	1014	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	J	1005	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	K	1010	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	D	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	Q	1010	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	E	1001	-	4,4,4	0.24	0	6,6,6	0.08	0
4	P52	E	1003	3	34,38,38	3.60	8 (23%)	42,53,53	1.14	3 (7%)
5	SO4	O	1004	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	R	1007	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	M	1016	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	P	1012	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	A	1003	-	4,4,4	0.23	0	6,6,6	0.08	0
4	P52	H	1003	3	34,38,38	3.62	8 (23%)	42,53,53	1.24	6 (14%)
5	SO4	G	1005	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	U	1012	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	N	1010	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	E	1009	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	J	1012	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	R	1012	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	J	1006	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	G	1008	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	H	1009	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	L	1006	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	I	1005	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	S	1014	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	E	1011	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	G	1007	-	4,4,4	0.25	0	6,6,6	0.12	0
6	NAG	J	1022	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	V	1010	-	4,4,4	0.24	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	V	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
6	NAG	B	1022	-	14,14,15	0.22	0	17,19,21	0.77	0
5	SO4	M	1001	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	G	1012	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	H	1010	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	V	1013	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	H	1013	-	4,4,4	0.24	0	6,6,6	0.07	0
6	NAG	P	1022	-	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	B	1005	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	H	1015	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	I	1009	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	C	1005	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	T	1007	-	4,4,4	0.23	0	6,6,6	0.05	0
4	P52	Q	1002	3	34,38,38	3.60	8 (23%)	42,53,53	1.17	4 (9%)
5	SO4	A	1007	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	A	1009	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	I	1014	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	D	1005	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	B	1004	-	4,4,4	0.24	0	6,6,6	0.06	0
4	P52	S	1003	3	34,38,38	3.61	8 (23%)	42,53,53	1.09	4 (9%)
5	SO4	C	1023	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	U	1007	-	4,4,4	0.24	0	6,6,6	0.04	0
5	SO4	D	1016	-	4,4,4	0.24	0	6,6,6	0.07	0
4	P52	L	1003	3	34,38,38	3.64	8 (23%)	42,53,53	1.10	3 (7%)
5	SO4	M	1013	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	1006	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	N	1007	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	U	1004	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	I	1007	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	D	1007	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	N	1011	-	4,4,4	0.24	0	6,6,6	0.06	0
6	NAG	L	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	M	1008	-	4,4,4	0.21	0	6,6,6	0.12	0
5	SO4	C	1012	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	T	1001	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	H	1001	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	R	1010	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	E	1008	-	4,4,4	0.24	0	6,6,6	0.15	0
5	SO4	V	1009	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	F	1013	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	O	1003	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	V	1007	-	4,4,4	0.23	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	F	1015	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	F	1011	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	V	1011	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	S	1010	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	1013	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	J	1011	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	L	1015	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	I	1001	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	J	1009	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	1001	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	N	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	L	1008	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	D	1014	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	R	1024	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	K	1024	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	Q	1006	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	C	1006	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	U	1005	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	T	1013	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	P	1009	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	O	1011	-	4,4,4	0.23	0	6,6,6	0.10	0
6	NAG	A	1022	1	14,14,15	0.24	0	17,19,21	0.76	0
5	SO4	S	1009	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	E	1006	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1015	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	K	1009	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	O	1015	-	4,4,4	0.23	0	6,6,6	0.05	0
5	SO4	T	1008	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	C	1015	-	4,4,4	0.23	0	6,6,6	0.07	0
4	P52	U	1003	3	34,38,38	3.60	8 (23%)	42,53,53	1.14	6 (14%)
5	SO4	L	1012	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	J	1007	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	C	1007	-	4,4,4	0.23	0	6,6,6	0.14	0
5	SO4	C	1008	-	4,4,4	0.24	0	6,6,6	0.14	0
6	NAG	E	1023	-	14,14,15	0.24	0	17,19,21	0.75	0
4	P52	O	1002	3	34,38,38	3.60	8 (23%)	42,53,53	1.15	5 (11%)
5	SO4	R	1003	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	J	1004	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	R	1014	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	R	1005	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	O	1005	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	B	1014	-	4,4,4	0.24	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	S	1007	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	U	1008	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	I	1013	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	D	1004	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	B	1013	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	O	1013	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	D	1008	-	4,4,4	0.25	0	6,6,6	0.12	0
5	SO4	K	1007	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	G	1015	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	B	1007	-	4,4,4	0.24	0	6,6,6	0.12	0
5	SO4	C	1010	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	O	1008	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	K	1011	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	E	1015	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	M	1009	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	I	1016	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	G	1011	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	R	1004	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	I	1006	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	G	1016	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	H	1008	-	4,4,4	0.25	0	6,6,6	0.15	0
6	NAG	V	1022	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	P	1003	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	R	1016	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	E	1005	-	4,4,4	0.23	0	6,6,6	0.11	0
5	SO4	C	1003	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	E	1016	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	K	1025	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	A	1011	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	G	1004	-	4,4,4	0.24	0	6,6,6	0.11	0
6	NAG	F	1023	-	14,14,15	0.23	0	17,19,21	0.76	0
5	SO4	G	1014	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	Q	1007	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	Q	1008	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	F	1004	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	Q	1011	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	Q	1009	-	4,4,4	0.23	0	6,6,6	0.08	0
4	P52	N	1003	3	34,38,38	3.61	8 (23%)	42,53,53	1.09	3 (7%)
4	P52	C	1002	3	34,38,38	3.61	7 (20%)	42,53,53	1.17	5 (11%)
5	SO4	B	1009	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	P	1015	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	O	1006	-	4,4,4	0.23	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	U	1009	-	4,4,4	0.24	0	6,6,6	0.06	0
5	SO4	P	1008	-	4,4,4	0.23	0	6,6,6	0.12	0
5	SO4	U	1006	-	4,4,4	0.23	0	6,6,6	0.06	0
5	SO4	I	1012	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	B	1010	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	A	1004	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	O	1010	-	4,4,4	0.24	0	6,6,6	0.13	0
5	SO4	D	1006	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	U	1010	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	Q	1022	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	A	1012	-	4,4,4	0.24	0	6,6,6	0.05	0
4	P52	F	1003	3	34,38,38	3.58	8 (23%)	42,53,53	1.13	3 (7%)
5	SO4	U	1016	-	4,4,4	0.24	0	6,6,6	0.05	0
5	SO4	T	1006	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	P	1013	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	M	1015	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	T	1005	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	Q	1004	-	4,4,4	0.24	0	6,6,6	0.11	0
5	SO4	C	1004	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	J	1003	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	1014	-	4,4,4	0.24	0	6,6,6	0.10	0
5	SO4	V	1015	-	4,4,4	0.24	0	6,6,6	0.05	0
6	NAG	M	1024	-	14,14,15	0.24	0	17,19,21	0.77	0
5	SO4	K	1016	-	4,4,4	0.24	0	6,6,6	0.09	0
5	SO4	E	1012	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	V	1008	-	4,4,4	0.24	0	6,6,6	0.08	0
5	SO4	F	1005	-	4,4,4	0.23	0	6,6,6	0.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P52	J	1002	3	-	11/30/36/36	0/3/3/3
4	P52	R	1002	3	-	11/30/36/36	0/3/3/3
4	P52	V	1002	3	-	11/30/36/36	0/3/3/3
6	NAG	J	1022	-	-	5/6/23/26	0/1/1/1
4	P52	H	1003	3	-	8/30/36/36	0/3/3/3
4	P52	S	1003	3	-	12/30/36/36	0/3/3/3
6	NAG	T	1023	-	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P52	U	1003	3	-	11/30/36/36	0/3/3/3
4	P52	I	1003	3	-	11/30/36/36	0/3/3/3
4	P52	B	1002	3	-	8/30/36/36	0/3/3/3
6	NAG	B	1022	-	-	5/6/23/26	0/1/1/1
6	NAG	I	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	N	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	E	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	S	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	F	1023	-	-	5/6/23/26	0/1/1/1
4	P52	L	1003	3	-	10/30/36/36	0/3/3/3
4	P52	O	1002	3	-	11/30/36/36	0/3/3/3
4	P52	P	1002	3	-	10/30/36/36	0/3/3/3
6	NAG	K	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	U	1024	-	-	5/6/23/26	0/1/1/1
4	P52	F	1003	3	-	9/30/36/36	0/3/3/3
6	NAG	P	1022	-	-	5/6/23/26	0/1/1/1
6	NAG	G	1023	-	-	5/6/23/26	0/1/1/1
4	P52	K	1002	3	-	10/30/36/36	0/3/3/3
4	P52	T	1003	3	-	11/30/36/36	0/3/3/3
6	NAG	O	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	L	1023	-	-	5/6/23/26	0/1/1/1
4	P52	Q	1002	3	-	12/30/36/36	0/3/3/3
6	NAG	H	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	V	1022	-	-	5/6/23/26	0/1/1/1
4	P52	N	1003	3	-	10/30/36/36	0/3/3/3
4	P52	C	1002	3	-	9/30/36/36	0/3/3/3
6	NAG	Q	1021	-	-	5/6/23/26	0/1/1/1
4	P52	E	1003	3	-	12/30/36/36	0/3/3/3
4	P52	A	1002	3	-	11/30/36/36	0/3/3/3
6	NAG	M	1024	-	-	5/6/23/26	0/1/1/1
6	NAG	R	1023	-	-	5/6/23/26	0/1/1/1
6	NAG	C	1022	-	-	5/6/23/26	0/1/1/1
4	P52	G	1002	3	-	13/30/36/36	0/3/3/3
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
4	P52	M	1003	3	-	9/30/36/36	0/3/3/3
4	P52	D	1003	3	-	12/30/36/36	0/3/3/3
6	NAG	D	1023	-	-	5/6/23/26	0/1/1/1

All (174) 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	8.43	1.52	1.34
4	R	1002	P52	C10-N2	8.38	1.52	1.34
4	B	1002	P52	C10-N2	8.36	1.52	1.34
4	P	1002	P52	C10-N2	8.34	1.51	1.34
4	G	1002	P52	C10-N2	8.34	1.51	1.34
4	V	1002	P52	C10-N2	8.34	1.51	1.34
4	C	1002	P52	C10-N2	8.32	1.51	1.34
4	J	1002	P52	C10-N2	8.32	1.51	1.34
4	A	1002	P52	C10-N2	8.32	1.51	1.34
4	E	1003	P52	C10-N2	8.31	1.51	1.34
4	O	1002	P52	C10-N2	8.30	1.51	1.34
4	D	1003	P52	C10-N2	8.29	1.51	1.34
4	Q	1002	P52	C10-N2	8.29	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1003	P52	C10-N2	8.29	1.51	1.34
4	U	1003	P52	C10-N2	8.28	1.51	1.34
4	T	1003	P52	C10-N2	8.28	1.51	1.34
4	L	1003	P52	C10-N2	8.28	1.51	1.34
4	S	1003	P52	C10-N2	8.26	1.51	1.34
4	I	1003	P52	C10-N2	8.23	1.51	1.34
4	K	1002	P52	C10-N2	8.22	1.51	1.34
4	F	1003	P52	C10-N2	8.17	1.51	1.34
4	N	1003	P52	C10-N2	8.15	1.51	1.34
4	G	1002	P52	C18-N4	6.51	1.48	1.32
4	D	1003	P52	C18-N4	6.50	1.48	1.32
4	I	1003	P52	C18-N4	6.46	1.48	1.32
4	J	1002	P52	C18-N4	6.45	1.48	1.32
4	B	1002	P52	C18-N4	6.44	1.48	1.32
4	M	1003	P52	C18-N4	6.44	1.48	1.32
4	C	1002	P52	C18-N4	6.44	1.48	1.32
4	E	1003	P52	C18-N4	6.44	1.48	1.32
4	L	1003	P52	C18-N4	6.44	1.48	1.32
4	K	1002	P52	C18-N4	6.43	1.48	1.32
4	O	1002	P52	C18-N4	6.43	1.48	1.32
4	H	1003	P52	C18-N4	6.42	1.48	1.32
4	N	1003	P52	C18-N4	6.42	1.48	1.32
4	F	1003	P52	C18-N4	6.42	1.48	1.32
4	T	1003	P52	C18-N4	6.41	1.48	1.32
4	S	1003	P52	C18-N4	6.41	1.48	1.32
4	U	1003	P52	C18-N4	6.40	1.48	1.32
4	V	1002	P52	C18-N4	6.40	1.48	1.32
4	Q	1002	P52	C18-N4	6.40	1.48	1.32
4	A	1002	P52	C18-N4	6.40	1.48	1.32
4	P	1002	P52	C18-N4	6.39	1.48	1.32
4	R	1002	P52	C18-N4	6.39	1.48	1.32
4	D	1003	P52	C19-C20	5.18	1.60	1.50
4	Q	1002	P52	C19-C20	5.17	1.60	1.50
4	H	1003	P52	C19-C20	5.16	1.60	1.50
4	P	1002	P52	C19-C20	5.15	1.60	1.50
4	N	1003	P52	C19-C20	5.14	1.59	1.50
4	L	1003	P52	C19-C20	5.14	1.59	1.50
4	C	1002	P52	C19-C20	5.14	1.59	1.50
4	K	1002	P52	C19-C20	5.13	1.59	1.50
4	J	1002	P52	C19-C20	5.12	1.59	1.50
4	B	1002	P52	C19-C20	5.11	1.59	1.50
4	F	1003	P52	C19-C20	5.11	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1003	P52	C19-C20	5.11	1.59	1.50
4	M	1003	P52	C19-C20	5.11	1.59	1.50
4	O	1002	P52	C19-C20	5.09	1.59	1.50
4	V	1002	P52	C19-C20	5.08	1.59	1.50
4	U	1003	P52	C19-C20	5.08	1.59	1.50
4	R	1002	P52	C19-C20	5.07	1.59	1.50
4	T	1003	P52	C19-C20	5.07	1.59	1.50
4	S	1003	P52	C19-C20	5.06	1.59	1.50
4	G	1002	P52	C19-C20	5.06	1.59	1.50
4	A	1002	P52	C19-C20	5.04	1.59	1.50
4	E	1003	P52	C19-C20	5.03	1.59	1.50
4	A	1002	P52	C22-C23	-3.21	1.37	1.41
4	H	1003	P52	C22-C23	-3.17	1.37	1.41
4	T	1003	P52	C22-C23	-3.15	1.37	1.41
4	F	1003	P52	C22-C23	-3.14	1.37	1.41
4	D	1003	P52	C22-C23	-3.14	1.37	1.41
4	E	1003	P52	C22-C23	-3.13	1.37	1.41
4	G	1002	P52	C22-C23	-3.12	1.37	1.41
4	O	1002	P52	C22-C23	-3.12	1.37	1.41
4	U	1003	P52	C22-C23	-3.11	1.37	1.41
4	V	1002	P52	C22-C23	-3.11	1.37	1.41
4	N	1003	P52	C22-C23	-3.10	1.37	1.41
4	P	1002	P52	C22-C23	-3.10	1.37	1.41
4	I	1003	P52	C22-C23	-3.10	1.37	1.41
4	S	1003	P52	C22-C23	-3.09	1.37	1.41
4	B	1002	P52	C22-C23	-3.08	1.37	1.41
4	R	1002	P52	C22-C23	-3.08	1.37	1.41
4	J	1002	P52	C22-C23	-3.07	1.37	1.41
4	K	1002	P52	C22-C23	-3.06	1.37	1.41
4	Q	1002	P52	C22-C23	-3.06	1.37	1.41
4	M	1003	P52	C22-C23	-3.05	1.37	1.41
4	L	1003	P52	C22-C23	-3.03	1.37	1.41
4	C	1002	P52	C22-C23	-2.94	1.37	1.41
4	S	1003	P52	C12-C10	2.65	1.56	1.51
4	N	1003	P52	C12-C10	2.64	1.56	1.51
4	A	1002	P52	C12-C10	2.62	1.56	1.51
4	P	1002	P52	C12-C10	2.62	1.56	1.51
4	R	1002	P52	C12-C10	2.58	1.56	1.51
4	H	1003	P52	C17-N2	2.57	1.51	1.45
4	F	1003	P52	C12-C10	2.56	1.56	1.51
4	B	1002	P52	C17-N2	2.56	1.51	1.45
4	L	1003	P52	C12-C10	2.55	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1002	P52	C12-C10	2.55	1.56	1.51
4	T	1003	P52	C12-C10	2.55	1.56	1.51
4	M	1003	P52	C12-C10	2.53	1.56	1.51
4	J	1002	P52	C12-C10	2.53	1.56	1.51
4	I	1003	P52	C12-C10	2.52	1.56	1.51
4	R	1002	P52	C17-N2	2.51	1.51	1.45
4	P	1002	P52	C17-N2	2.51	1.51	1.45
4	V	1002	P52	C12-C10	2.49	1.55	1.51
4	Q	1002	P52	C17-N2	2.49	1.51	1.45
4	G	1002	P52	C17-N2	2.49	1.51	1.45
4	U	1003	P52	C17-N2	2.49	1.51	1.45
4	H	1003	P52	C12-C10	2.49	1.55	1.51
4	U	1003	P52	C12-C10	2.49	1.55	1.51
4	V	1002	P52	C17-N2	2.48	1.51	1.45
4	C	1002	P52	C17-N2	2.48	1.51	1.45
4	Q	1002	P52	C12-C10	2.48	1.55	1.51
4	B	1002	P52	C12-C10	2.47	1.55	1.51
4	O	1002	P52	C12-C10	2.47	1.55	1.51
4	D	1003	P52	C17-N2	2.46	1.51	1.45
4	D	1003	P52	C12-C10	2.46	1.55	1.51
4	I	1003	P52	C17-N2	2.46	1.51	1.45
4	J	1002	P52	C17-N2	2.46	1.51	1.45
4	K	1002	P52	C12-C10	2.46	1.55	1.51
4	O	1002	P52	C17-N2	2.45	1.51	1.45
4	G	1002	P52	C12-C10	2.45	1.55	1.51
4	K	1002	P52	C17-N2	2.45	1.51	1.45
4	L	1003	P52	C17-N2	2.45	1.51	1.45
4	T	1003	P52	C17-N2	2.44	1.51	1.45
4	M	1003	P52	C17-N2	2.44	1.51	1.45
4	E	1003	P52	C12-C10	2.44	1.55	1.51
4	E	1003	P52	C17-N2	2.43	1.50	1.45
4	F	1003	P52	C17-N2	2.42	1.50	1.45
4	S	1003	P52	C17-N2	2.39	1.50	1.45
4	N	1003	P52	C17-N2	2.37	1.50	1.45
4	A	1002	P52	C17-N2	2.37	1.50	1.45
4	O	1002	P52	C21-N3	-2.13	1.33	1.37
4	T	1003	P52	C21-N3	-2.08	1.33	1.37
4	N	1003	P52	C21-N3	-2.07	1.33	1.37
4	P	1002	P52	C21-N3	-2.07	1.33	1.37
4	U	1003	P52	C21-N3	-2.07	1.33	1.37
4	S	1003	P52	C21-N3	-2.07	1.33	1.37
4	G	1002	P52	C21-N3	-2.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1002	P52	C21-N3	-2.06	1.33	1.37
4	K	1002	P52	C21-N3	-2.06	1.33	1.37
4	H	1003	P52	C21-N3	-2.05	1.33	1.37
4	Q	1002	P52	C21-N3	-2.05	1.33	1.37
4	R	1002	P52	C21-N3	-2.05	1.33	1.37
4	A	1002	P52	C21-N3	-2.05	1.33	1.37
4	J	1002	P52	C21-N3	-2.04	1.33	1.37
4	M	1003	P52	C21-N3	-2.04	1.33	1.37
4	E	1003	P52	C21-N3	-2.02	1.33	1.37
4	I	1003	P52	C21-N3	-2.02	1.33	1.37
4	F	1003	P52	C21-N3	-2.02	1.33	1.37
4	B	1002	P52	C21-N3	-2.00	1.34	1.37
4	L	1003	P52	C21-N3	-2.00	1.34	1.37

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1003	P52	C17-C19-C20	2.83	118.80	113.44
4	H	1003	P52	C19-C17-N2	2.78	115.95	110.64
4	F	1003	P52	C19-C17-N2	2.74	115.86	110.64
4	D	1003	P52	C17-C19-C20	2.72	118.60	113.44
4	Q	1002	P52	C19-C17-N2	2.67	115.74	110.64
4	E	1003	P52	C12-C10-N2	2.65	120.75	116.19
4	N	1003	P52	C17-C19-C20	2.65	118.46	113.44
4	K	1002	P52	C19-C17-N2	2.64	115.67	110.64
4	K	1002	P52	C17-C19-C20	2.63	118.42	113.44
4	D	1003	P52	C25-C23-C22	-2.62	119.65	122.19
4	M	1003	P52	C25-C23-C22	-2.62	119.65	122.19
4	E	1003	P52	C25-C23-C22	-2.62	119.66	122.19
4	A	1002	P52	C25-C23-C22	-2.61	119.66	122.19
4	C	1002	P52	C25-C23-C22	-2.59	119.68	122.19
4	Q	1002	P52	C17-C19-C20	2.58	118.33	113.44
4	T	1003	P52	C25-C23-C22	-2.58	119.69	122.19
4	N	1003	P52	C19-C17-N2	2.57	115.55	110.64
4	G	1002	P52	C25-C23-C22	-2.57	119.70	122.19
4	L	1003	P52	C25-C23-C22	-2.57	119.70	122.19
4	H	1003	P52	C25-C23-C22	-2.57	119.70	122.19
4	B	1002	P52	C25-C23-C22	-2.57	119.70	122.19
4	J	1002	P52	C25-C23-C22	-2.55	119.72	122.19
4	E	1003	P52	O3-C10-C12	-2.55	118.25	122.19
4	O	1002	P52	C17-C19-C20	2.53	118.25	113.44
4	P	1002	P52	C25-C23-C22	-2.53	119.73	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1003	P52	C17-C19-C20	2.51	118.21	113.44
4	I	1003	P52	C25-C23-C22	-2.51	119.76	122.19
4	S	1003	P52	C25-C23-C22	-2.51	119.76	122.19
4	U	1003	P52	C19-C17-N2	2.49	115.39	110.64
4	R	1002	P52	C25-C23-C22	-2.49	119.78	122.19
4	K	1002	P52	C25-C23-C22	-2.48	119.78	122.19
4	O	1002	P52	C19-C17-N2	2.48	115.37	110.64
4	V	1002	P52	C25-C23-C22	-2.46	119.81	122.19
4	Q	1002	P52	C25-C23-C22	-2.46	119.81	122.19
4	C	1002	P52	C17-C19-C20	2.45	118.09	113.44
4	U	1003	P52	C25-C23-C22	-2.44	119.82	122.19
4	D	1003	P52	C19-C17-N2	2.44	115.30	110.64
4	H	1003	P52	O3-C10-C12	-2.44	118.43	122.19
4	F	1003	P52	C25-C23-C22	-2.43	119.84	122.19
4	C	1002	P52	C19-C17-N2	2.42	115.25	110.64
4	B	1002	P52	C19-C17-N2	2.40	115.22	110.64
4	B	1002	P52	O3-C10-C12	-2.40	118.49	122.19
4	U	1003	P52	C17-C19-C20	2.40	117.99	113.44
4	N	1003	P52	C25-C23-C22	-2.39	119.87	122.19
4	V	1002	P52	C19-C17-N2	2.39	115.19	110.64
4	M	1003	P52	C19-C17-N2	2.38	115.19	110.64
4	A	1002	P52	C17-C19-C20	2.38	117.95	113.44
4	H	1003	P52	C13-C12-C11	-2.37	108.07	111.55
4	I	1003	P52	C19-C17-N2	2.37	115.15	110.64
4	T	1003	P52	C19-C17-N2	2.36	115.15	110.64
4	O	1002	P52	C13-C12-C11	-2.35	108.10	111.55
4	H	1003	P52	C17-N2-C10	2.34	126.67	121.65
4	P	1002	P52	C19-C17-N2	2.33	115.09	110.64
4	R	1002	P52	O3-C10-C12	-2.32	118.60	122.19
4	J	1002	P52	C17-C19-C20	2.32	117.85	113.44
4	J	1002	P52	C19-C17-N2	2.32	115.06	110.64
4	R	1002	P52	C19-C17-N2	2.32	115.06	110.64
4	O	1002	P52	C25-C23-C22	-2.30	119.96	122.19
4	M	1003	P52	C13-C12-C11	-2.30	108.18	111.55
4	G	1002	P52	C13-C12-C11	-2.29	108.19	111.55
4	C	1002	P52	C13-C12-C11	-2.28	108.20	111.55
4	D	1003	P52	O3-C10-C12	-2.27	118.69	122.19
4	Q	1002	P52	O3-C10-C12	-2.26	118.70	122.19
4	A	1002	P52	O3-C10-C12	-2.26	118.70	122.19
4	G	1002	P52	C12-C10-N2	2.25	120.06	116.19
4	T	1003	P52	C17-C19-C20	2.25	117.70	113.44
4	A	1002	P52	C19-C17-N2	2.24	114.92	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	1003	P52	C19-C17-N2	2.24	114.92	110.64
4	P	1002	P52	C17-C19-C20	2.24	117.68	113.44
4	V	1002	P52	C17-C19-C20	2.23	117.67	113.44
4	M	1003	P52	C17-C19-C20	2.22	117.66	113.44
4	G	1002	P52	O3-C10-C12	-2.21	118.78	122.19
4	S	1003	P52	C17-C19-C20	2.21	117.62	113.44
4	I	1003	P52	C17-C19-C20	2.20	117.62	113.44
4	L	1003	P52	C17-C19-C20	2.20	117.61	113.44
4	V	1002	P52	O3-C10-C12	-2.20	118.80	122.19
4	R	1002	P52	C12-C10-N2	2.20	119.97	116.19
4	U	1003	P52	O3-C10-C12	-2.18	118.82	122.19
4	J	1002	P52	C13-C12-C11	-2.18	108.35	111.55
4	C	1002	P52	O3-C10-C12	-2.18	118.83	122.19
4	R	1002	P52	C13-C12-C11	-2.18	108.36	111.55
4	S	1003	P52	C12-C10-N2	2.16	119.91	116.19
4	A	1002	P52	C12-C10-N2	2.15	119.89	116.19
4	T	1003	P52	O3-C10-C12	-2.14	118.89	122.19
4	T	1003	P52	C12-C10-N2	2.13	119.86	116.19
4	O	1002	P52	O3-C10-C12	-2.12	118.92	122.19
4	U	1003	P52	C13-C12-C11	-2.11	108.46	111.55
4	R	1002	P52	C17-C19-C20	2.10	117.42	113.44
4	D	1003	P52	C12-C10-N2	2.10	119.80	116.19
4	J	1002	P52	O3-C10-C12	-2.09	118.96	122.19
4	P	1002	P52	O3-C10-C12	-2.08	118.97	122.19
4	U	1003	P52	C12-C10-N2	2.08	119.77	116.19
4	L	1003	P52	O3-C10-C12	-2.06	119.01	122.19
4	V	1002	P52	C13-C12-C11	-2.02	108.59	111.55
4	M	1003	P52	O3-C10-C12	-2.01	119.08	122.19

There are no chirality outliers.

All (342) 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	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

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Mol	Chain	Res	Type	Atoms
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
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	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

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Mol	Chain	Res	Type	Atoms
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
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

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Mol	Chain	Res	Type	Atoms
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	B	1002	P52	C12-C13-C14-C16
4	I	1003	P52	C12-C13-C14-C16
4	K	1002	P52	C12-C13-C14-C16
4	N	1003	P52	C12-C13-C14-C16
4	S	1003	P52	C12-C13-C14-C16
4	U	1003	P52	C12-C13-C14-C16
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
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	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	J	1002	P52	C12-C13-C14-C16
4	L	1003	P52	C12-C13-C14-C16
4	M	1003	P52	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
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	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	F	1003	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	D	1003	P52	C12-C13-C14-C15
4	G	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
4	A	1002	P52	C12-C13-C14-C16
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

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Mol	Chain	Res	Type	Atoms
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	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
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	A	1002	P52	C12-C13-C14-C15
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	R	1023	NAG	O5-C5-C6-O6
6	O	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

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Mol	Chain	Res	Type	Atoms
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
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	M	1003	P52	C2-C1-C8-C9
4	T	1003	P52	C2-C1-C8-C9
4	E	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	O	1002	P52	C1-C8-C9-N1
4	G	1002	P52	C18-C17-N2-C10
4	S	1003	P52	C18-C17-N2-C10
4	S	1003	P52	C2-C1-C8-C9
4	D	1003	P52	C19-C17-C18-O4
4	E	1003	P52	C19-C17-C18-O4
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

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Mol	Chain	Res	Type	Atoms
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	N	1003	P52	C18-C17-N2-C10
4	C	1002	P52	C17-C19-C20-C22
4	R	1002	P52	C17-C19-C20-C22
4	R	1002	P52	C17-C19-C20-C21
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	L	1003	P52	C18-C17-N2-C10
4	T	1003	P52	C17-C19-C20-C22
4	U	1003	P52	C17-C19-C20-C22
4	C	1002	P52	C17-C19-C20-C21
4	T	1003	P52	C17-C19-C20-C21
4	A	1002	P52	C18-C17-N2-C10
4	O	1002	P52	N2-C17-C18-O4
4	T	1003	P52	N2-C17-C18-O4
4	U	1003	P52	C17-C19-C20-C21
4	O	1002	P52	C18-C17-N2-C10
4	G	1002	P52	C17-C19-C20-C22
4	S	1003	P52	C17-C19-C20-C22
4	V	1002	P52	C17-C19-C20-C22
4	D	1003	P52	C19-C17-C18-N4
4	E	1003	P52	C19-C17-C18-N4
4	G	1002	P52	C17-C19-C20-C21
4	S	1003	P52	C17-C19-C20-C21
4	V	1002	P52	C17-C19-C20-C21
4	I	1003	P52	C17-C19-C20-C22
4	E	1003	P52	C17-C19-C20-C21
4	I	1003	P52	C17-C19-C20-C21
4	L	1003	P52	C17-C19-C20-C21
4	N	1003	P52	C17-C19-C20-C21
4	Q	1002	P52	C17-C19-C20-C21
4	A	1002	P52	C17-C19-C20-C21
4	E	1003	P52	C17-C19-C20-C22
4	L	1003	P52	C17-C19-C20-C22

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Mol	Chain	Res	Type	Atoms
4	N	1003	P52	C17-C19-C20-C22
4	Q	1002	P52	C17-C19-C20-C22
4	D	1003	P52	C17-C19-C20-C21
4	O	1002	P52	C17-C19-C20-C21
4	D	1003	P52	C18-C17-N2-C10
4	P	1002	P52	C18-C17-N2-C10
4	D	1003	P52	C17-C19-C20-C22
4	O	1002	P52	C17-C19-C20-C22
4	M	1003	P52	C17-C19-C20-C21
4	P	1002	P52	C17-C19-C20-C21
4	G	1002	P52	C19-C17-C18-O4
4	T	1003	P52	C18-C17-N2-C10
4	U	1003	P52	C18-C17-N2-C10
4	A	1002	P52	C17-C19-C20-C22
4	J	1002	P52	C17-C19-C20-C21
4	K	1002	P52	C17-C19-C20-C21
4	B	1002	P52	C17-C19-C20-C21
4	H	1003	P52	C17-C19-C20-C21
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	R	1002	P52	C18-C17-N2-C10
4	I	1003	P52	C18-C17-N2-C10
4	F	1003	P52	C17-C19-C20-C21
4	S	1003	P52	N2-C17-C18-N4
4	U	1003	P52	N2-C17-C18-O4
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	K	1002	P52	C18-C17-N2-C10
4	Q	1002	P52	C18-C17-N2-C10
4	G	1002	P52	C19-C17-C18-N4

There are no ring outliers.

151 monomers are involved in 321 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1011	SO4	3	0
5	R	1006	SO4	3	0
4	V	1002	P52	1	0
6	T	1023	NAG	5	0
5	V	1004	SO4	1	0
5	E	1010	SO4	2	0
5	U	1001	SO4	1	0
5	A	1006	SO4	2	0
6	D	1023	NAG	5	0
5	A	1013	SO4	1	0
5	L	1007	SO4	3	0
5	L	1011	SO4	1	0
5	A	1010	SO4	1	0
5	G	1024	SO4	1	0
5	S	1011	SO4	3	0
4	P	1002	P52	1	0
6	U	1024	NAG	5	0
5	T	1014	SO4	1	0
5	F	1007	SO4	3	0
5	U	1015	SO4	1	0
5	R	1011	SO4	1	0
6	H	1023	NAG	5	0
5	K	1006	SO4	2	0
5	O	1009	SO4	1	0
4	M	1003	P52	2	0
5	P	1005	SO4	1	0
5	R	1009	SO4	1	0
6	I	1023	NAG	6	0
6	K	1023	NAG	6	0
5	C	1013	SO4	1	0
5	M	1012	SO4	3	0
5	S	1001	SO4	1	0
6	Q	1021	NAG	6	0
5	B	1008	SO4	1	0
4	J	1002	P52	1	0
5	T	1010	SO4	1	0
5	G	1010	SO4	1	0
6	N	1023	NAG	5	0
5	E	1007	SO4	2	0
5	F	1010	SO4	3	0
4	K	1002	P52	1	0
5	L	1010	SO4	2	0
5	U	1017	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	P52	1	0
5	G	1009	SO4	1	0
5	P	1006	SO4	3	0
5	H	1007	SO4	2	0
5	P	1010	SO4	1	0
5	K	1013	SO4	1	0
5	H	1011	SO4	1	0
5	M	1011	SO4	2	0
5	C	1009	SO4	3	0
5	B	1006	SO4	2	0
5	K	1015	SO4	1	0
6	O	1023	NAG	5	0
5	Q	1013	SO4	1	0
5	F	1001	SO4	1	0
5	D	1010	SO4	1	0
5	M	1007	SO4	4	0
5	D	1011	SO4	1	0
5	L	1001	SO4	2	0
5	Q	1012	SO4	1	0
5	N	1001	SO4	1	0
5	N	1014	SO4	1	0
5	V	1014	SO4	1	0
6	R	1023	NAG	6	0
5	J	1010	SO4	1	0
5	U	1011	SO4	2	0
5	F	1014	SO4	1	0
4	I	1003	P52	1	0
4	B	1002	P52	1	0
6	G	1023	NAG	5	0
4	T	1003	P52	1	0
5	S	1016	SO4	1	0
5	O	1007	SO4	1	0
6	C	1022	NAG	5	0
4	D	1003	P52	1	0
5	S	1005	SO4	1	0
6	S	1023	NAG	5	0
5	I	1010	SO4	2	0
5	J	1005	SO4	1	0
5	K	1010	SO4	2	0
5	E	1001	SO4	2	0
4	E	1003	P52	1	0
5	O	1004	SO4	1	0

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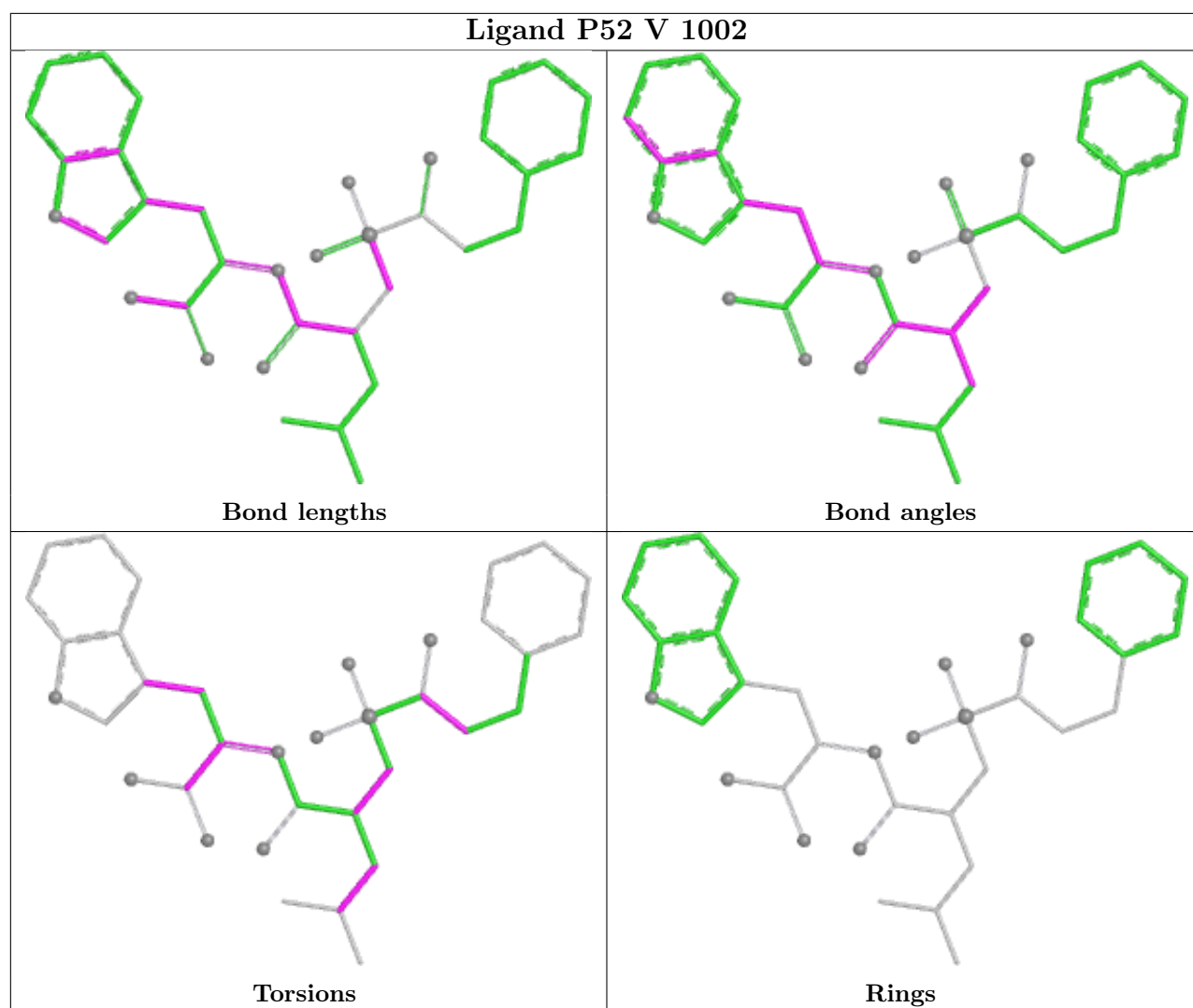
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	1012	SO4	1	0
5	N	1010	SO4	2	0
5	J	1006	SO4	3	0
5	I	1005	SO4	1	0
5	E	1011	SO4	1	0
6	J	1022	NAG	6	0
5	V	1006	SO4	5	0
6	B	1022	NAG	6	0
5	M	1001	SO4	1	0
5	H	1010	SO4	1	0
5	V	1013	SO4	1	0
6	P	1022	NAG	5	0
5	T	1007	SO4	3	0
4	Q	1002	P52	2	0
5	A	1007	SO4	1	0
5	I	1014	SO4	1	0
5	C	1023	SO4	1	0
5	U	1007	SO4	5	0
4	L	1003	P52	3	0
5	G	1006	SO4	2	0
5	N	1007	SO4	4	0
5	I	1007	SO4	2	0
5	D	1007	SO4	3	0
5	N	1011	SO4	1	0
6	L	1023	NAG	6	0
5	T	1001	SO4	1	0
5	H	1001	SO4	1	0
5	R	1010	SO4	1	0
5	V	1009	SO4	3	0
5	O	1003	SO4	1	0
5	F	1011	SO4	1	0
5	S	1010	SO4	3	0
5	I	1001	SO4	1	0
5	J	1009	SO4	1	0
5	D	1001	SO4	1	0
5	L	1008	SO4	1	0
5	D	1014	SO4	1	0
5	R	1024	SO4	1	0
5	K	1024	SO4	2	0
5	Q	1006	SO4	3	0
5	C	1006	SO4	2	0
5	P	1009	SO4	2	0

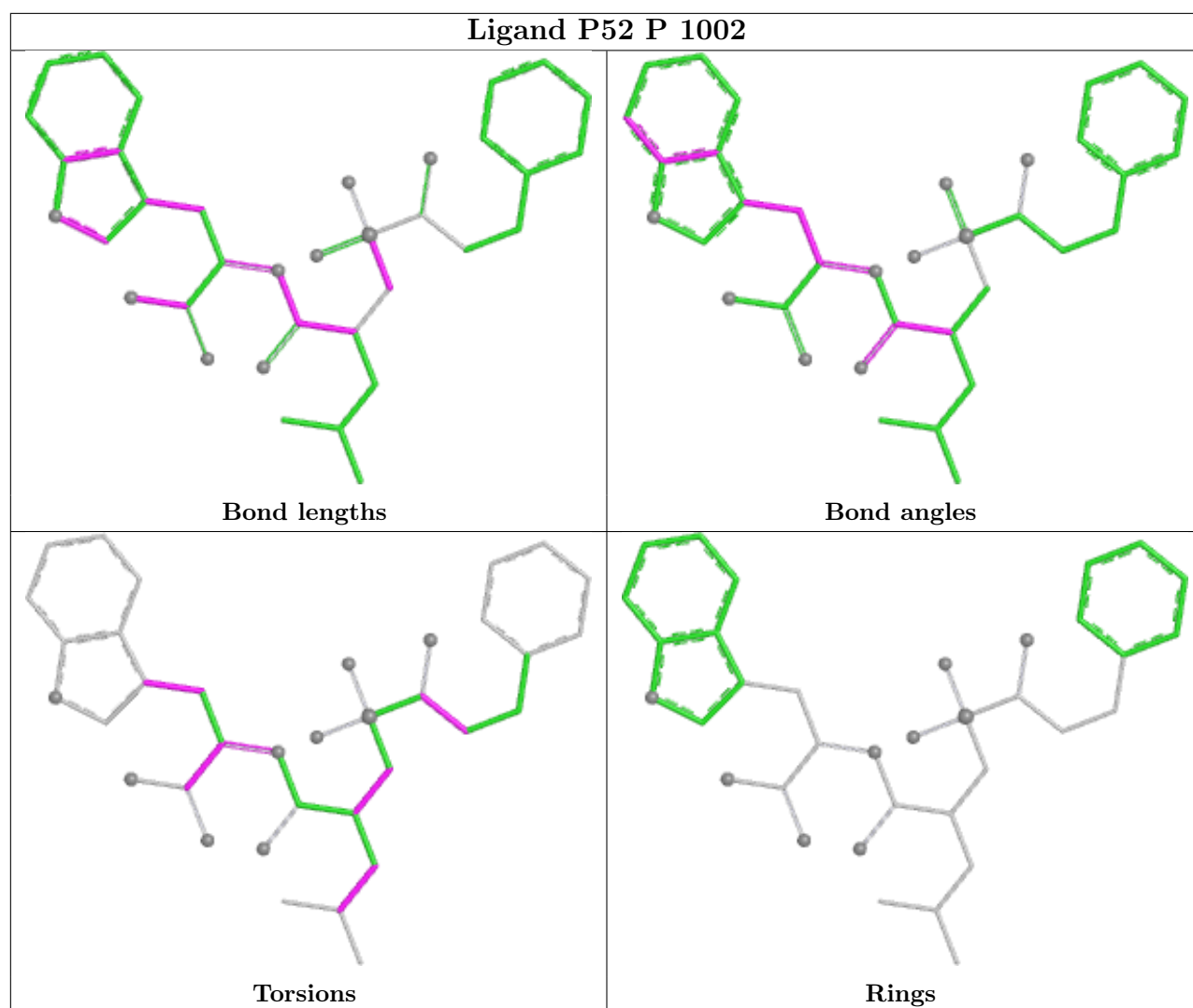
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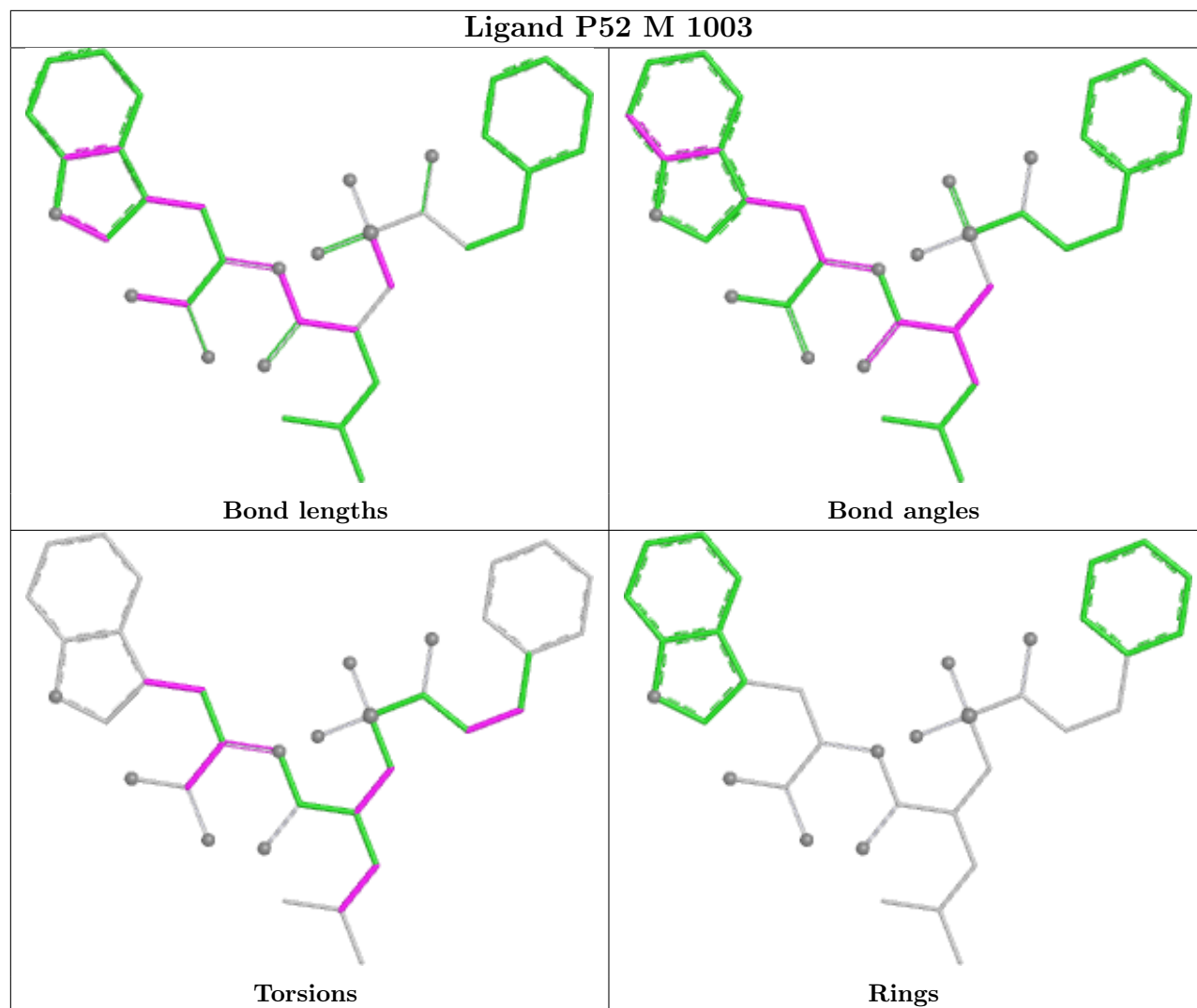
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1011	SO4	1	0
6	A	1022	NAG	1	0
5	B	1015	SO4	1	0
5	K	1009	SO4	2	0
5	J	1007	SO4	1	0
5	C	1007	SO4	1	0
6	E	1023	NAG	6	0
5	S	1007	SO4	3	0
5	G	1015	SO4	1	0
5	C	1010	SO4	1	0
5	G	1011	SO4	1	0
5	R	1004	SO4	1	0
6	V	1022	NAG	6	0
5	K	1025	SO4	1	0
6	F	1023	NAG	7	0
4	C	1002	P52	1	0
5	O	1006	SO4	3	0
5	B	1010	SO4	1	0
5	A	1004	SO4	1	0
5	O	1010	SO4	2	0
5	U	1010	SO4	1	0
5	Q	1022	SO4	3	0
4	F	1003	P52	1	0
6	M	1024	NAG	5	0

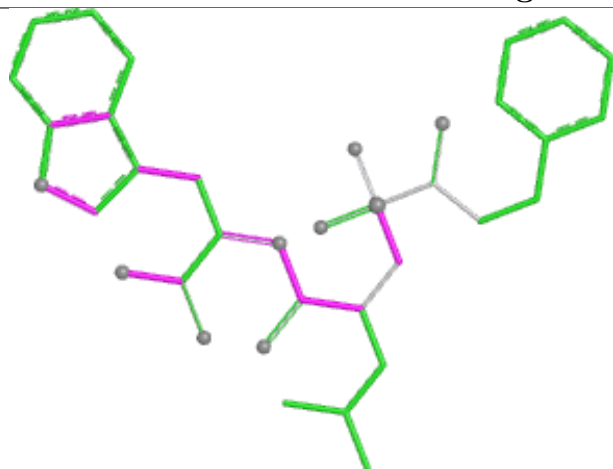
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.



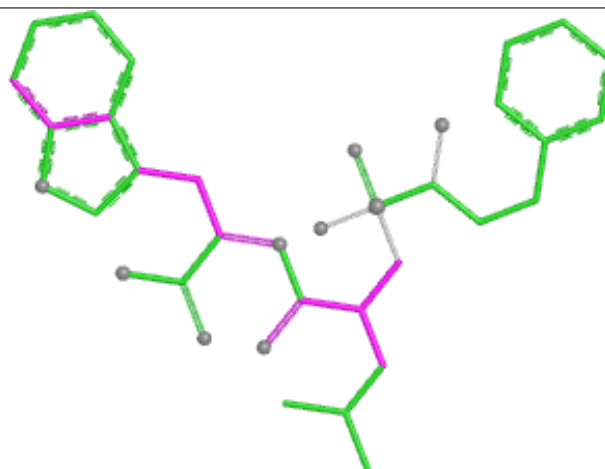




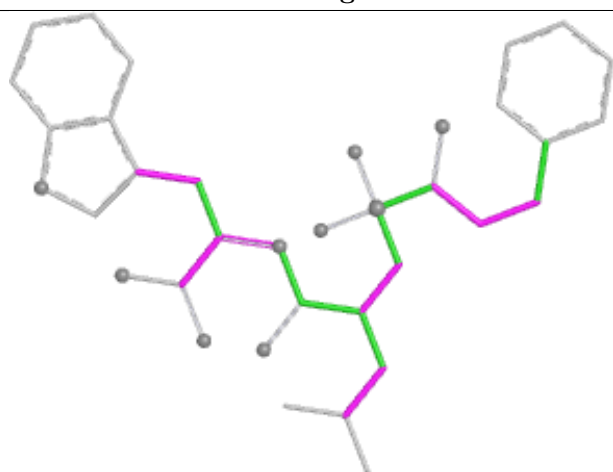
Ligand P52 J 1002



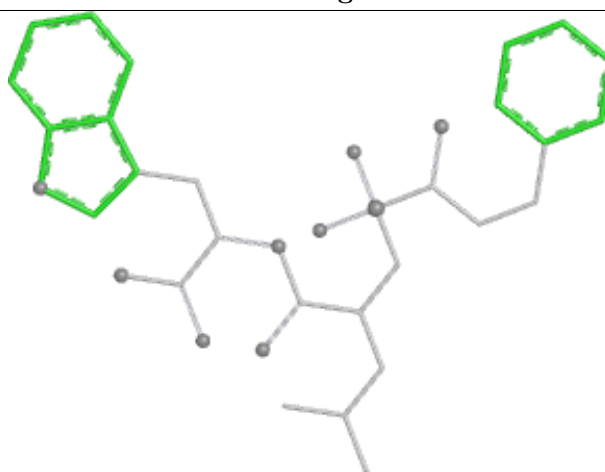
Bond lengths



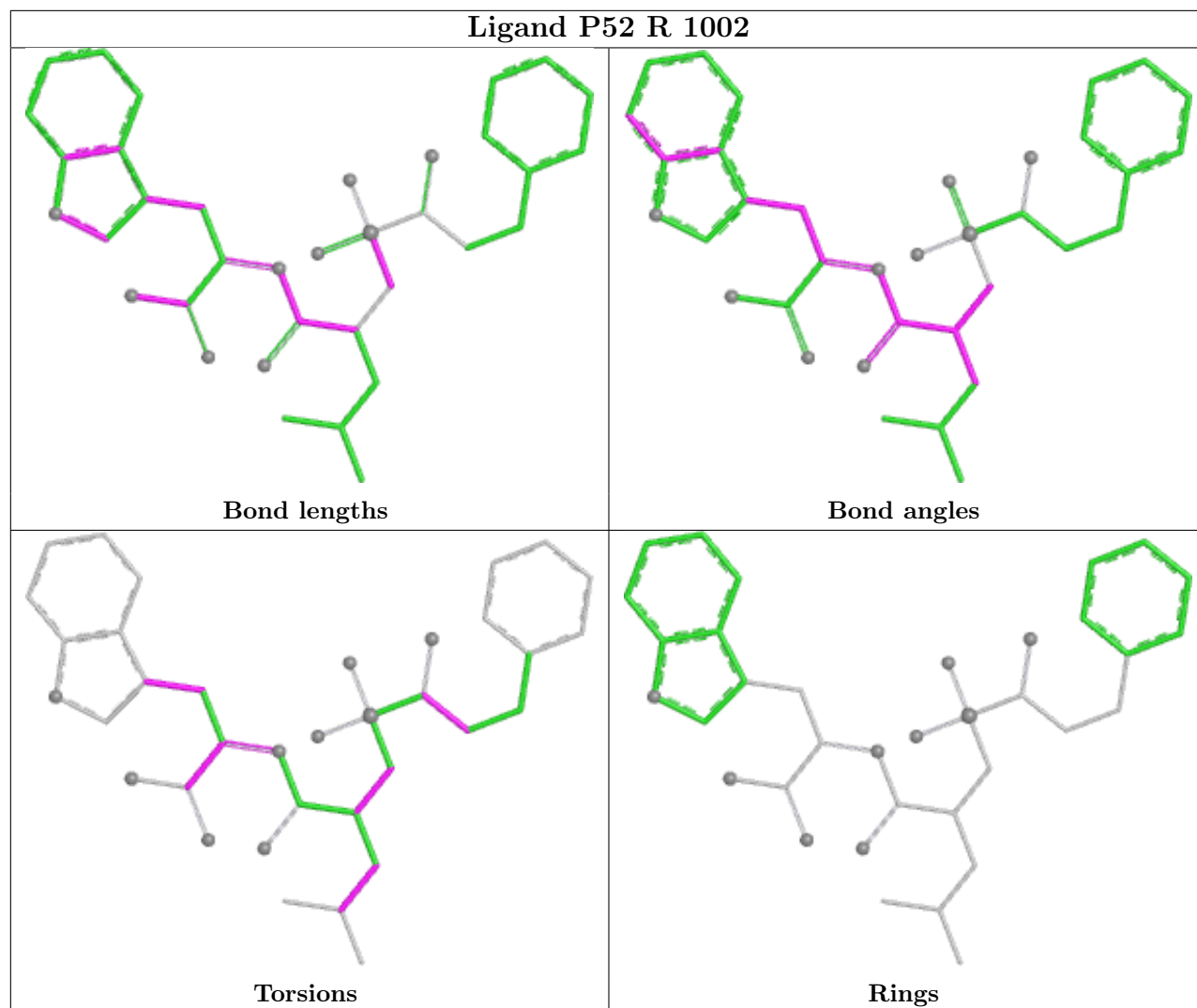
Bond angles

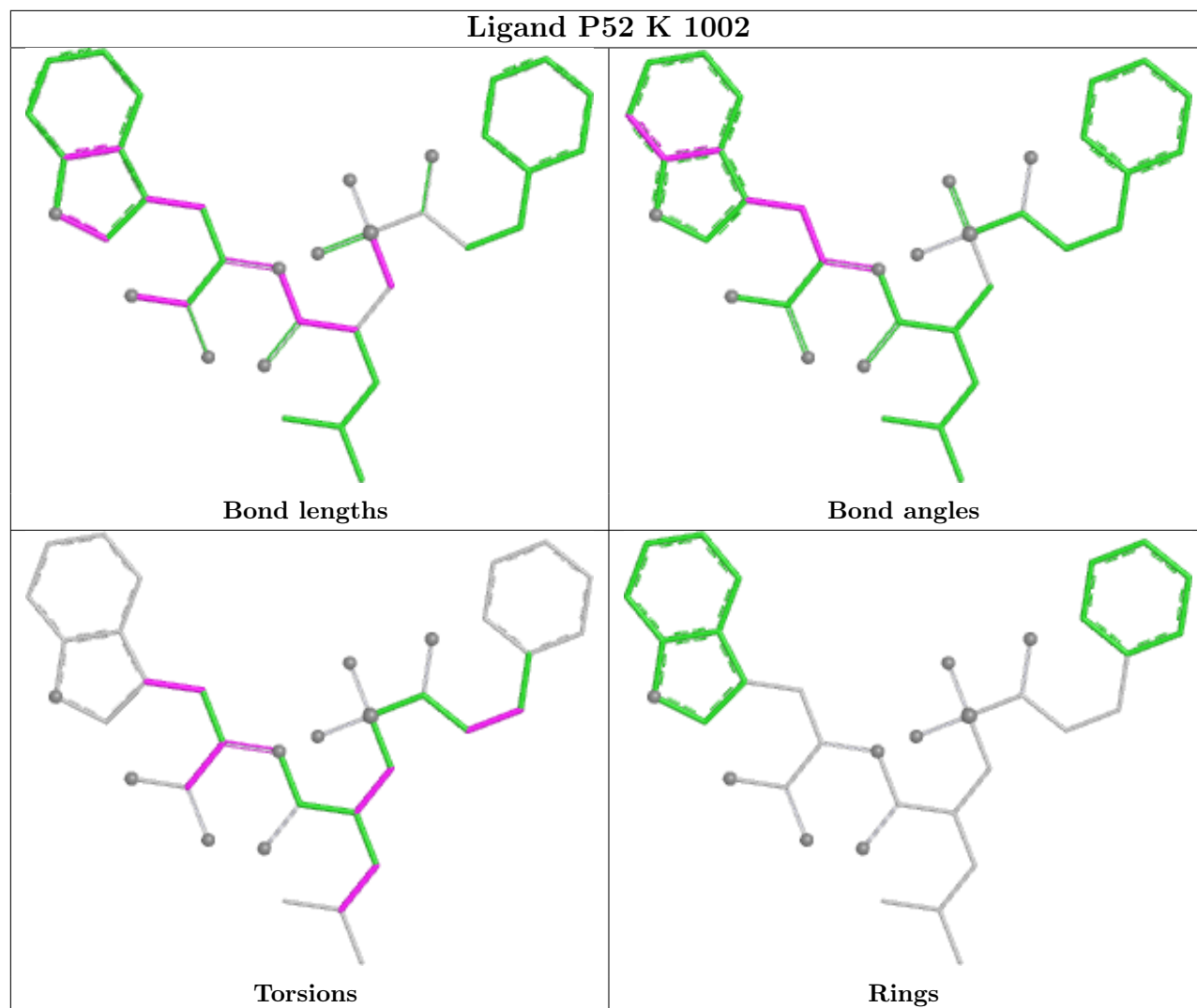


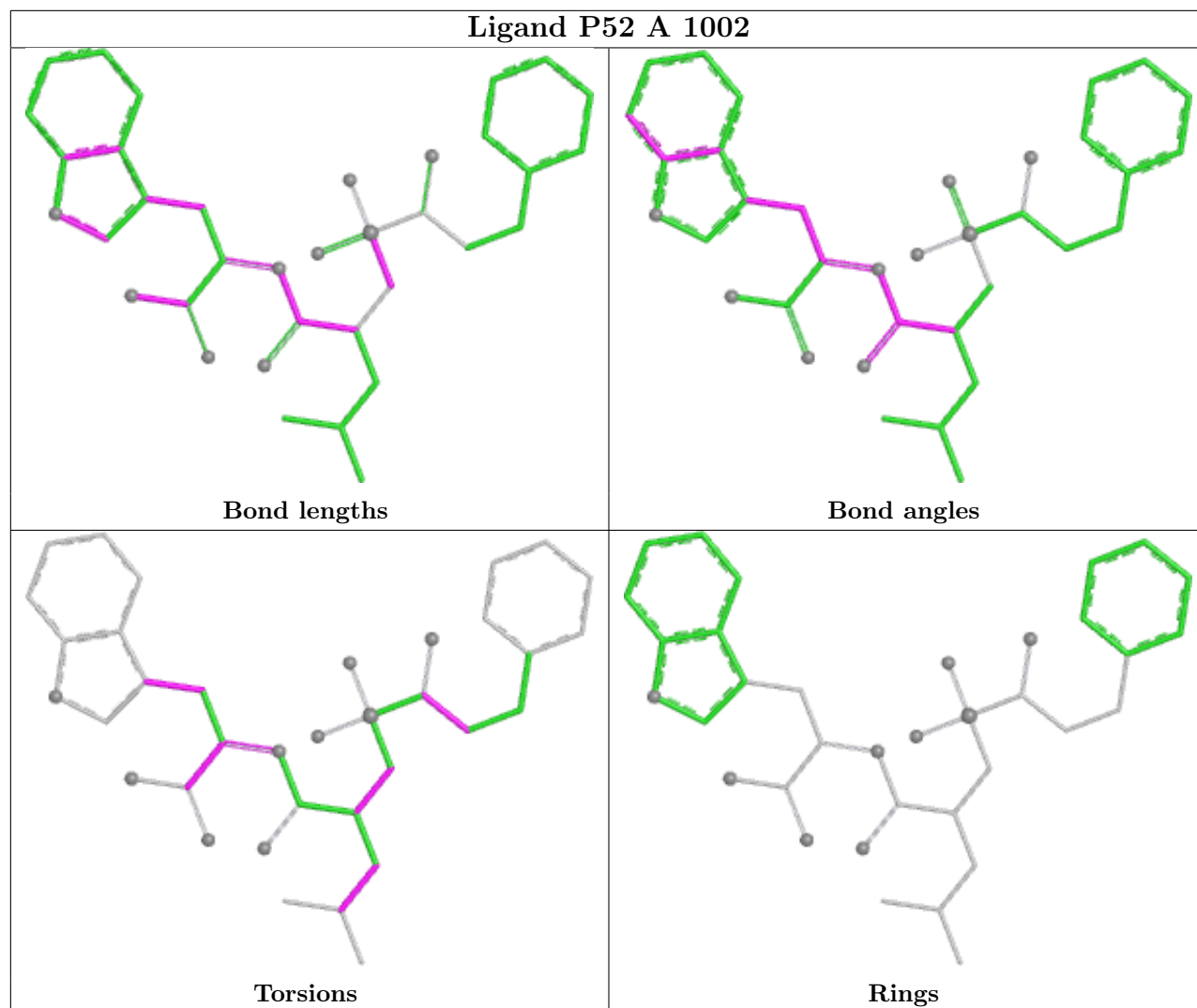
Torsions

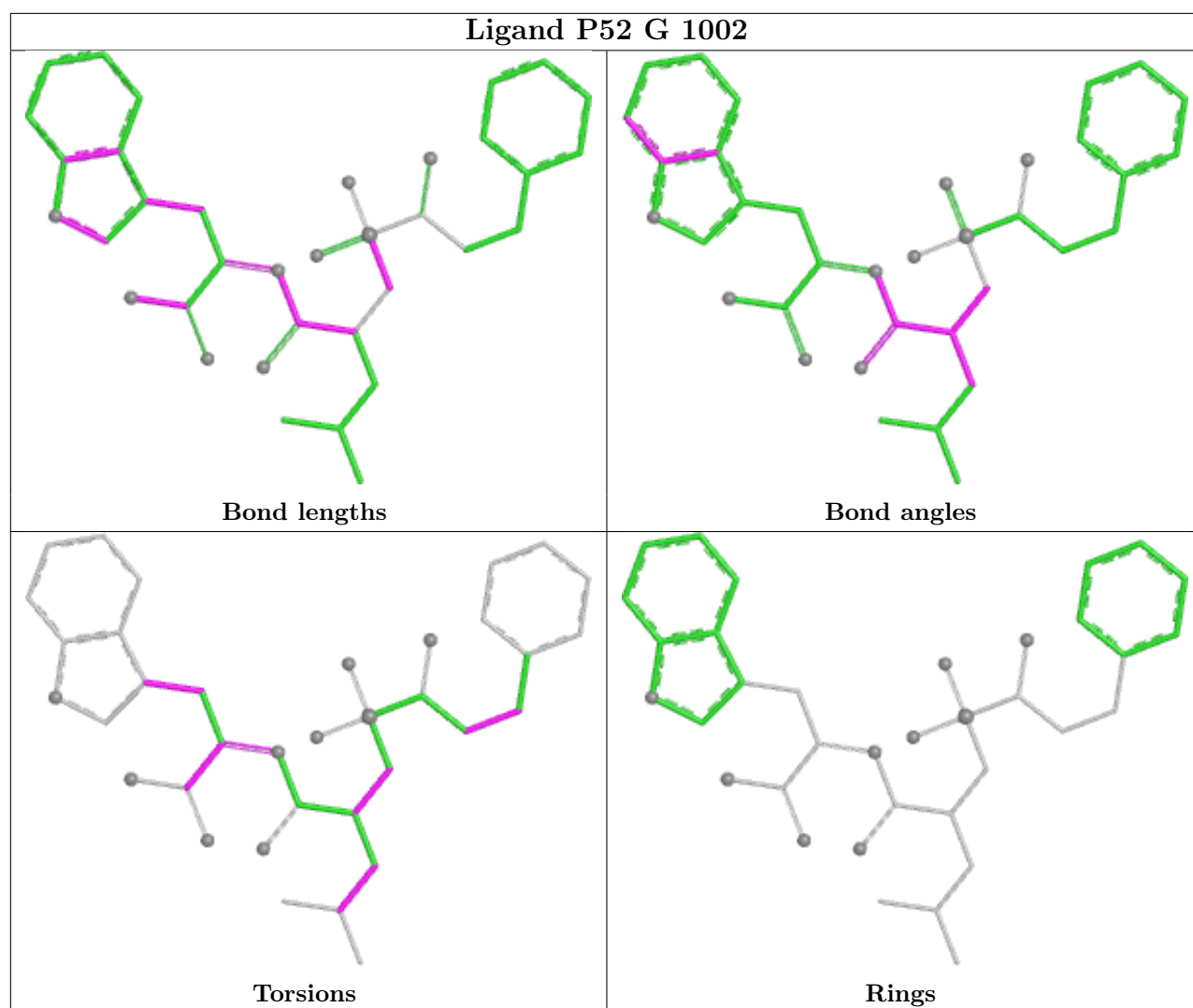


Rings

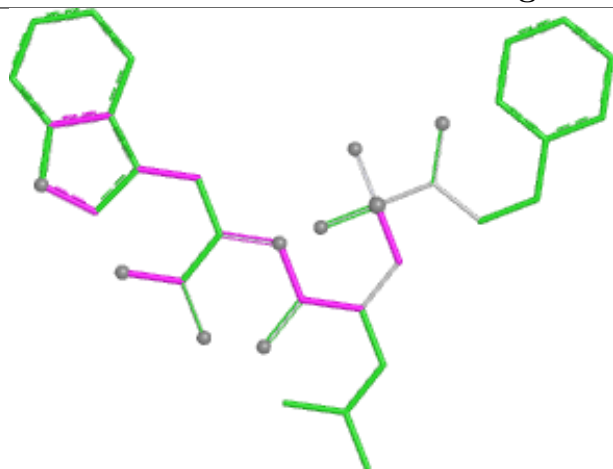




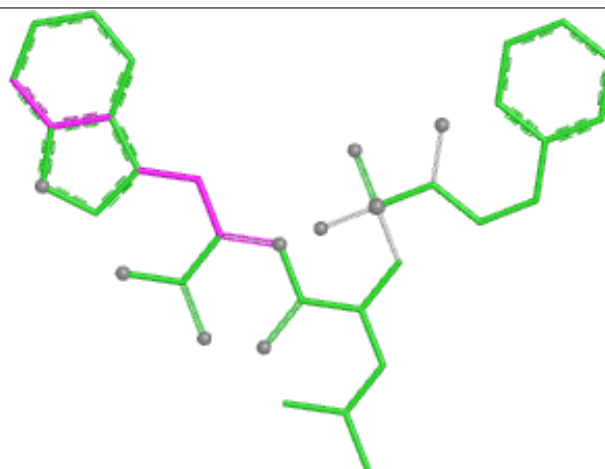




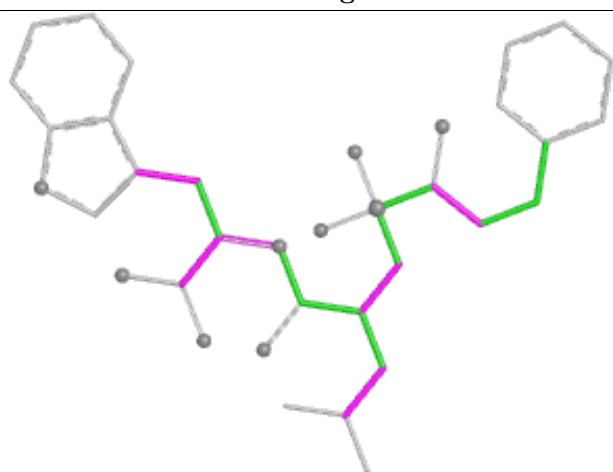
Ligand P52 I 1003



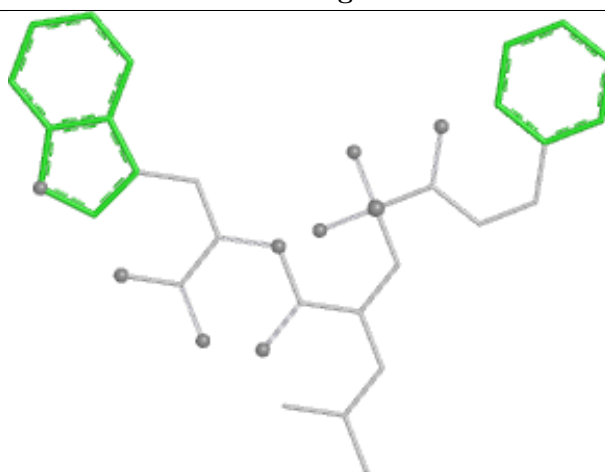
Bond lengths



Bond angles

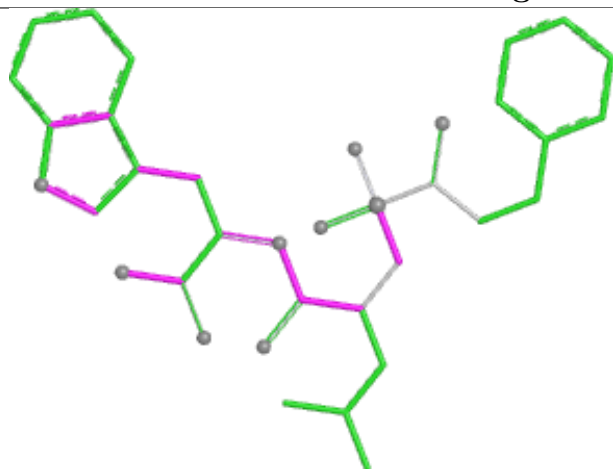


Torsions

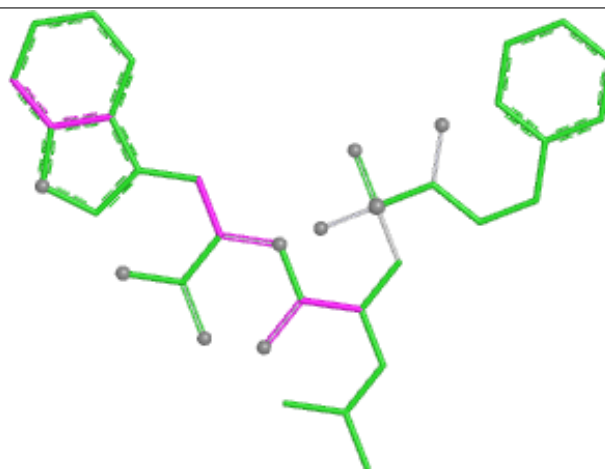


Rings

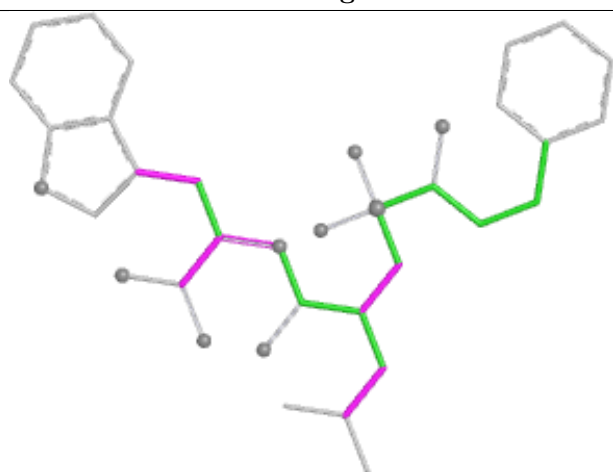
Ligand P52 B 1002



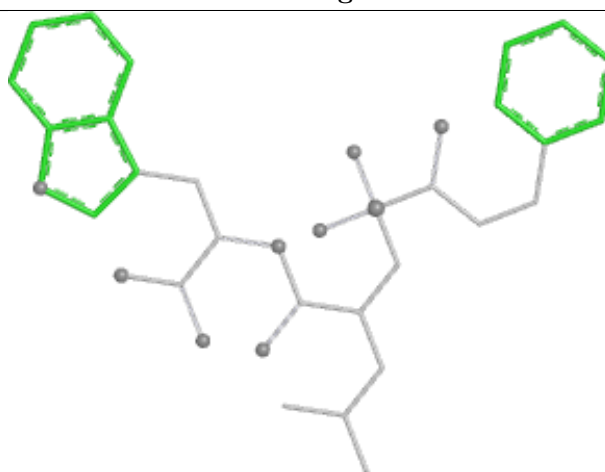
Bond lengths



Bond angles

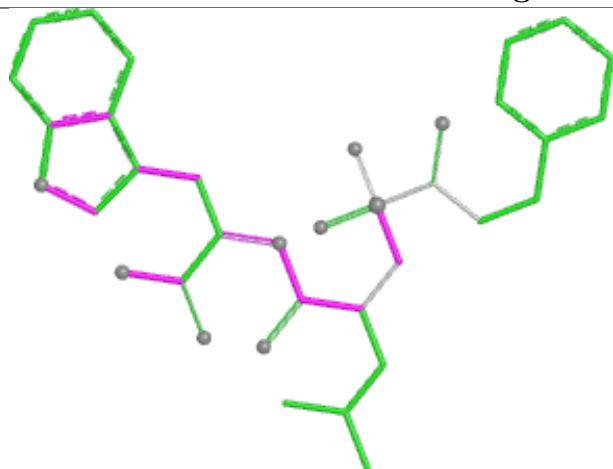


Torsions

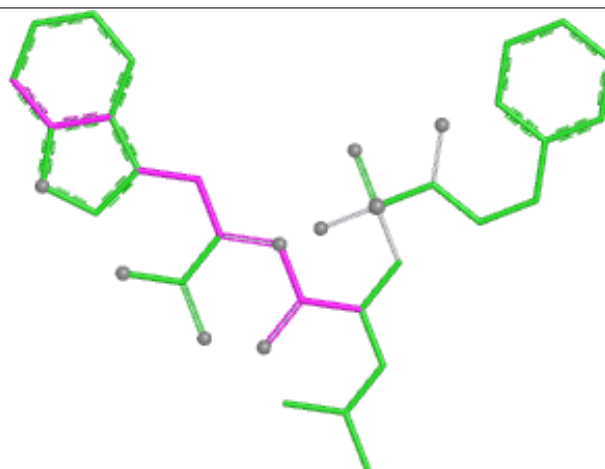


Rings

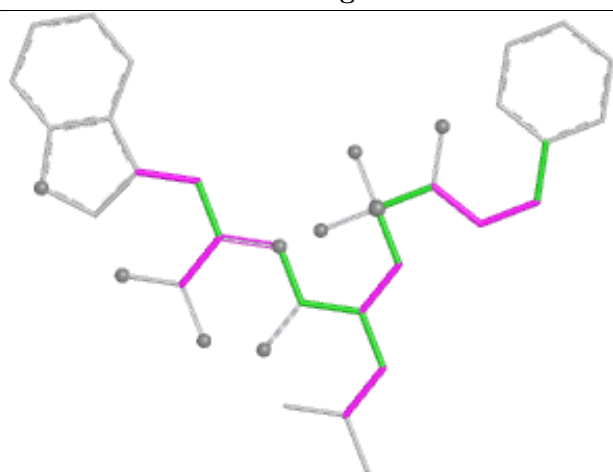
Ligand P52 T 1003



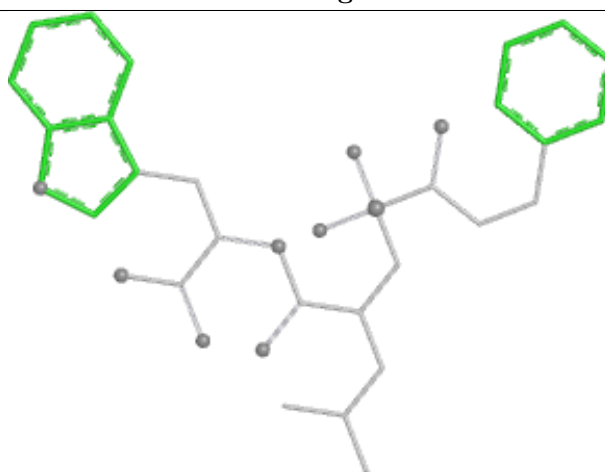
Bond lengths



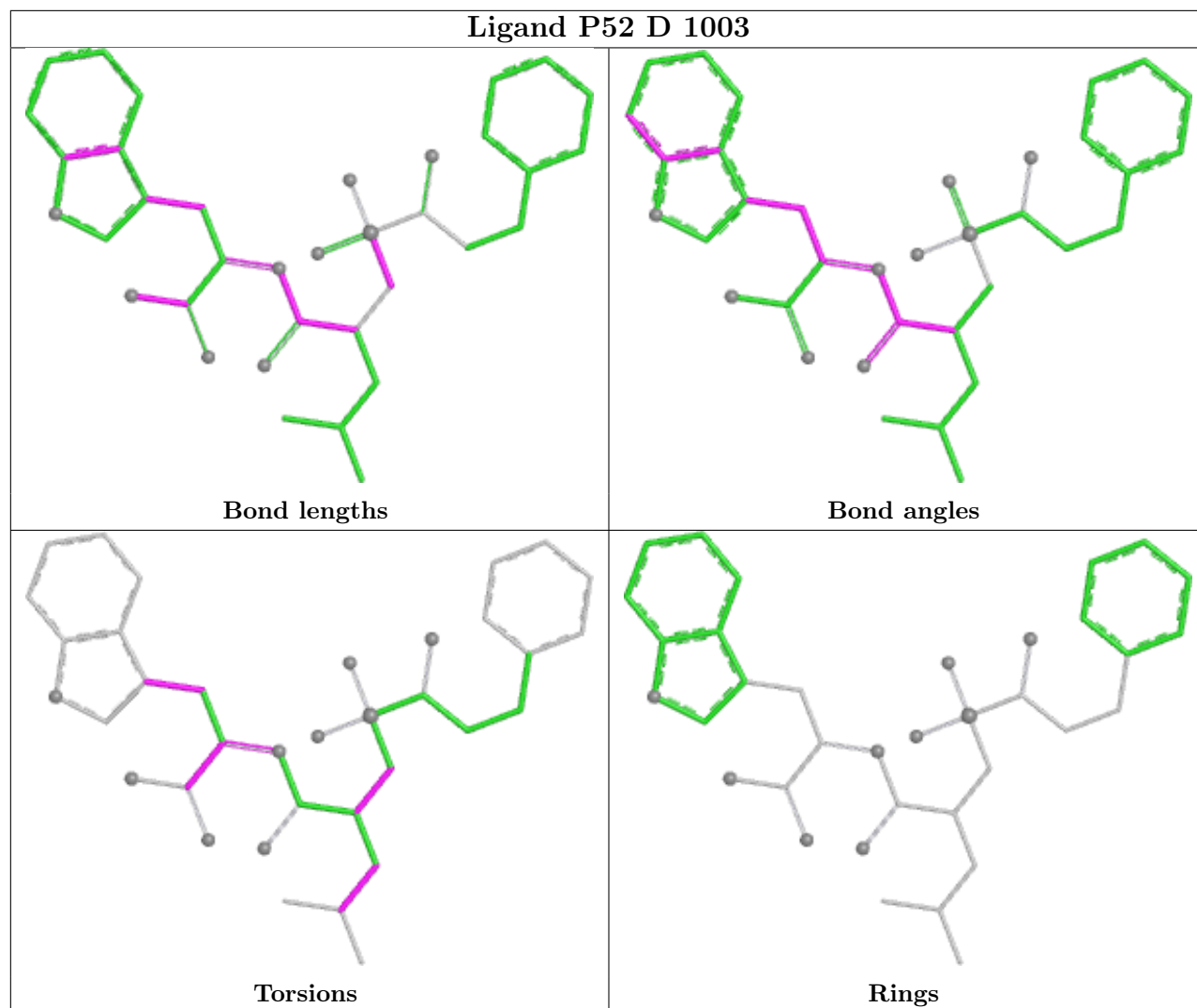
Bond angles



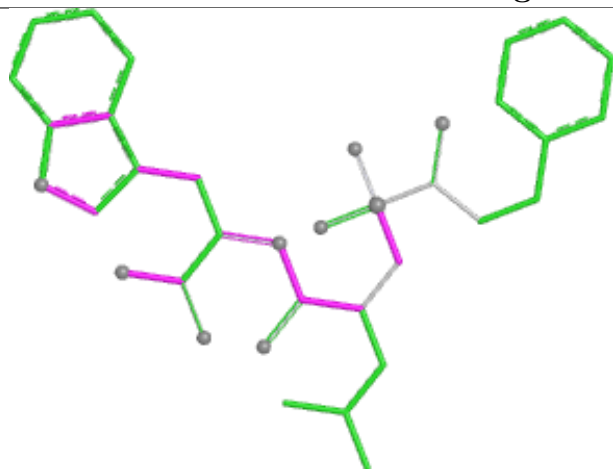
Torsions



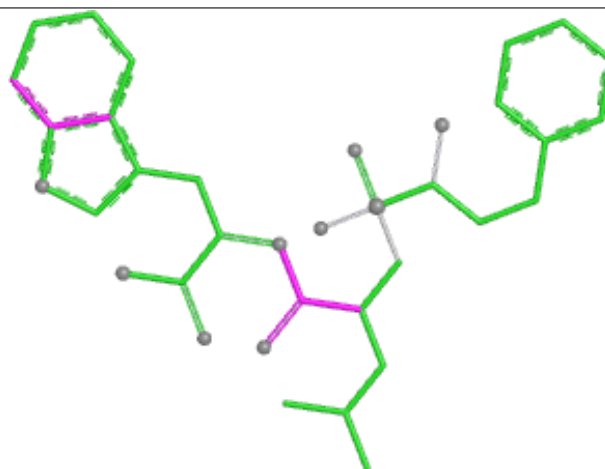
Rings



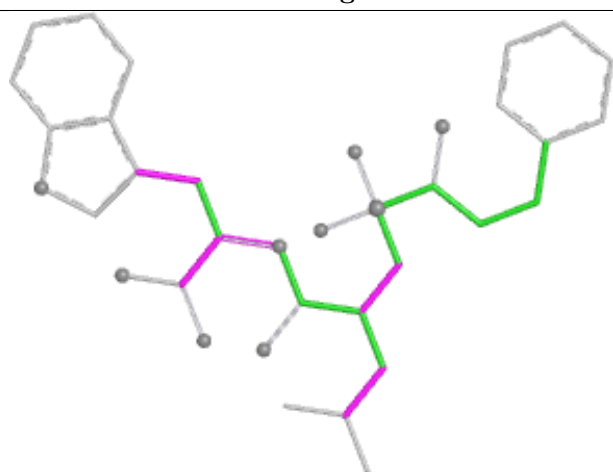
Ligand P52 E 1003



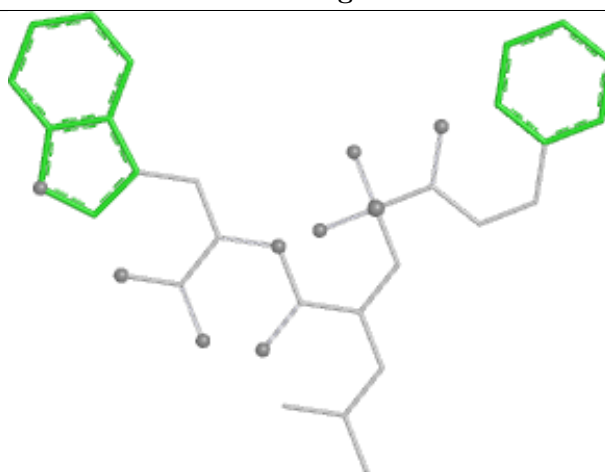
Bond lengths



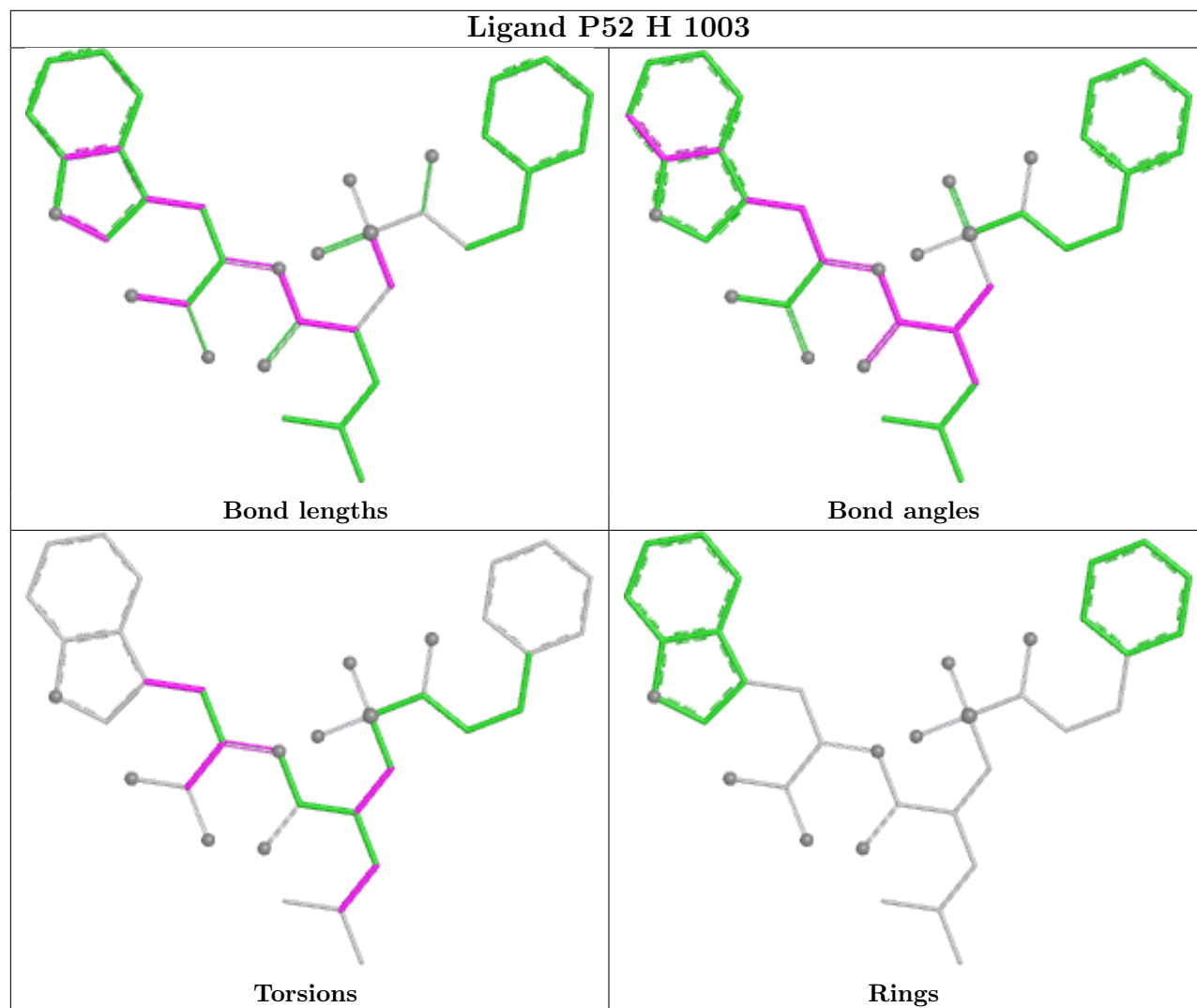
Bond angles

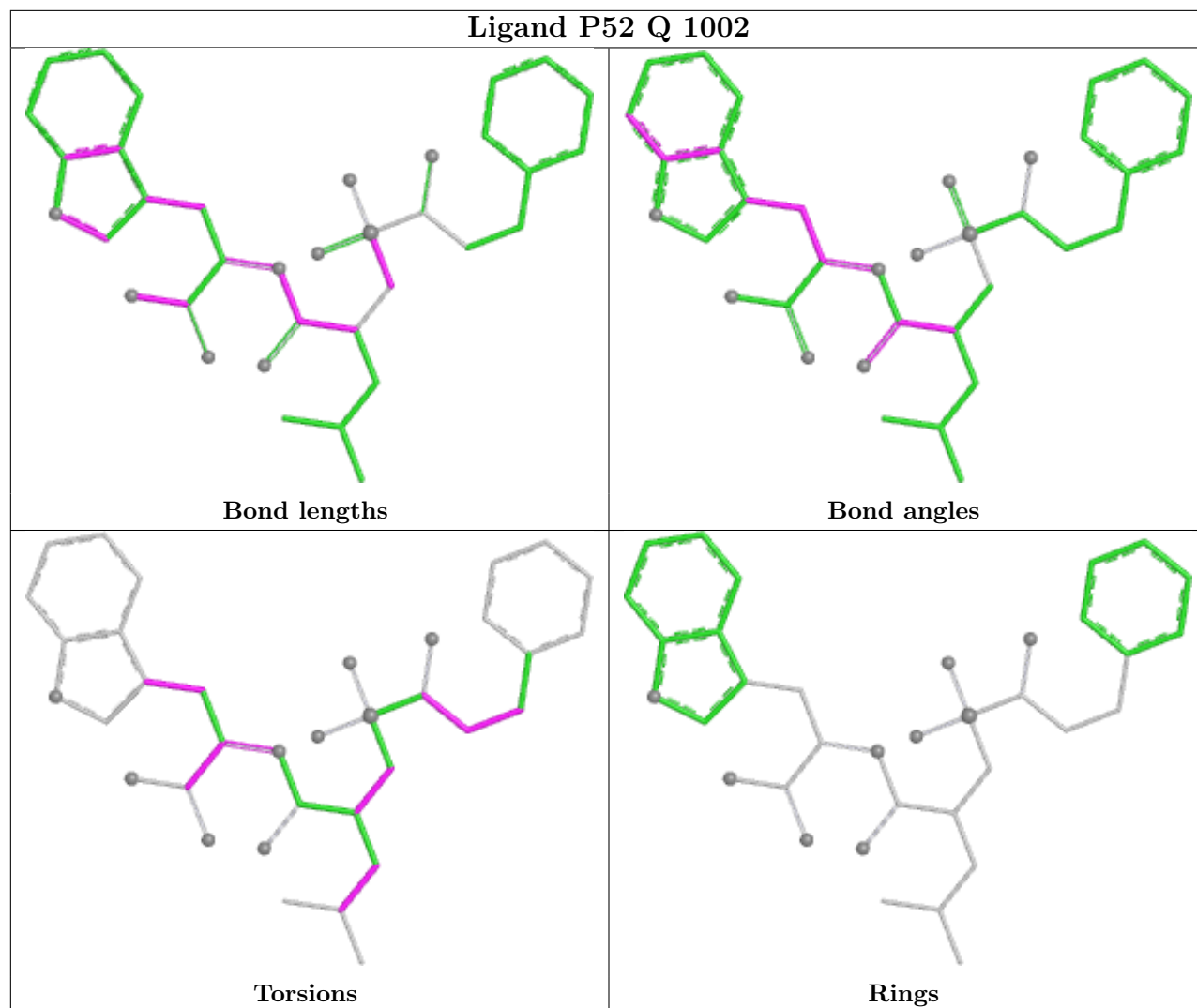


Torsions

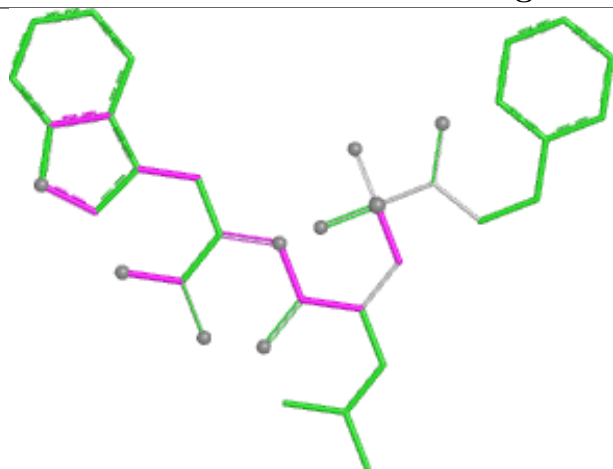


Rings

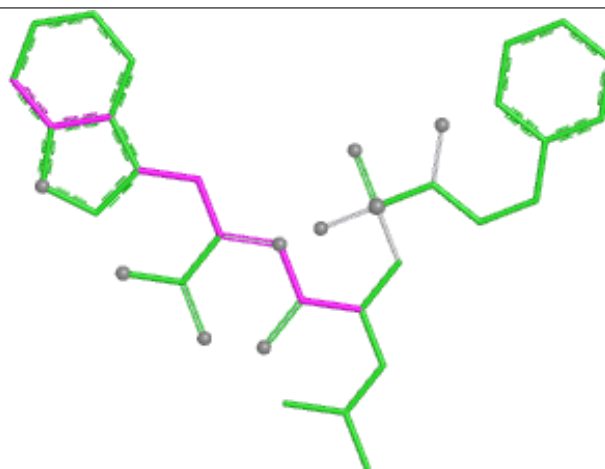




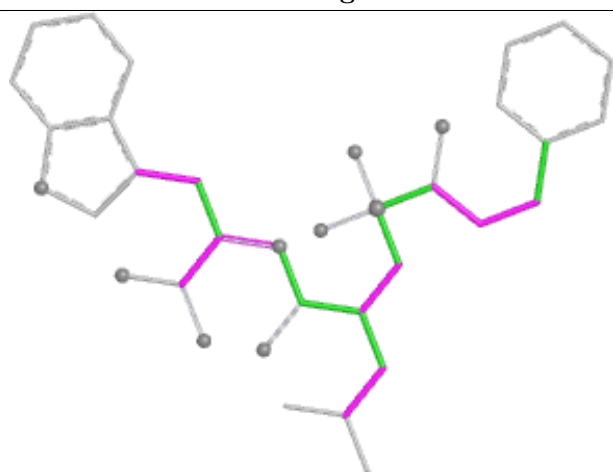
Ligand P52 S 1003



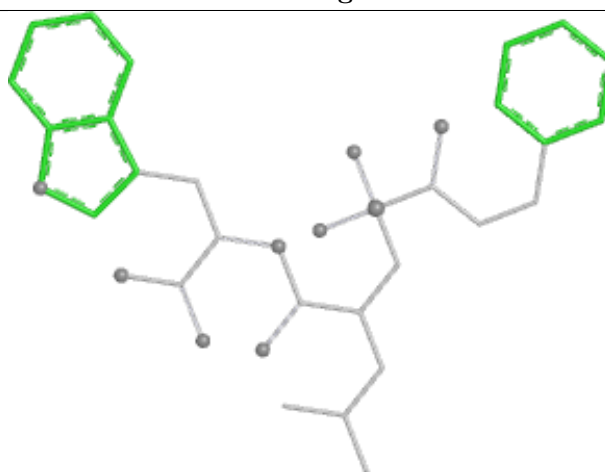
Bond lengths



Bond angles

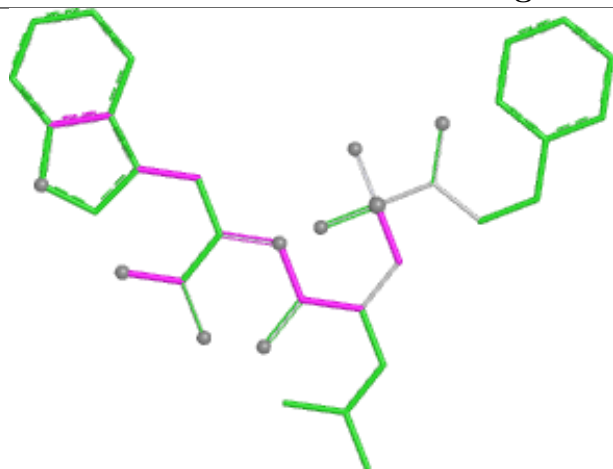


Torsions

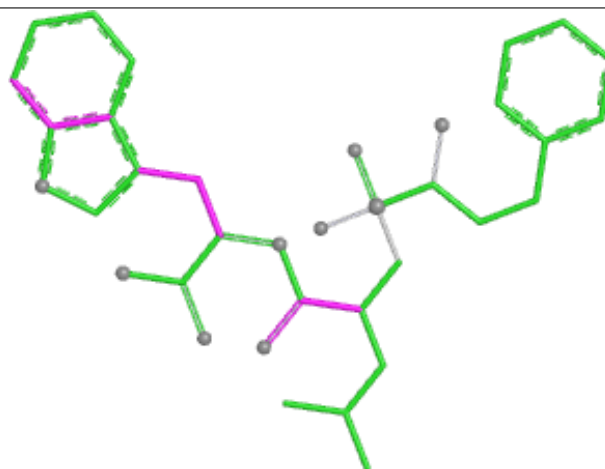


Rings

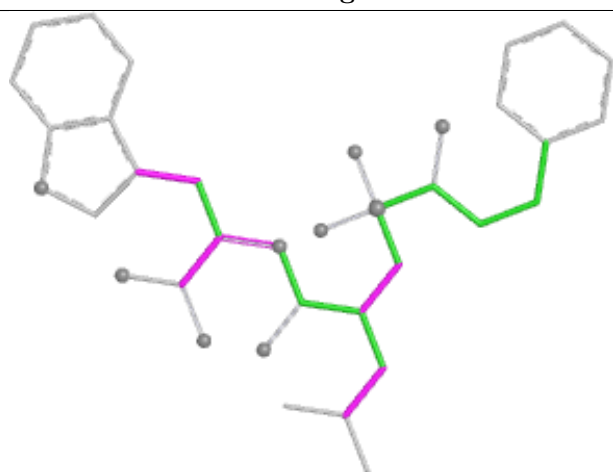
Ligand P52 L 1003



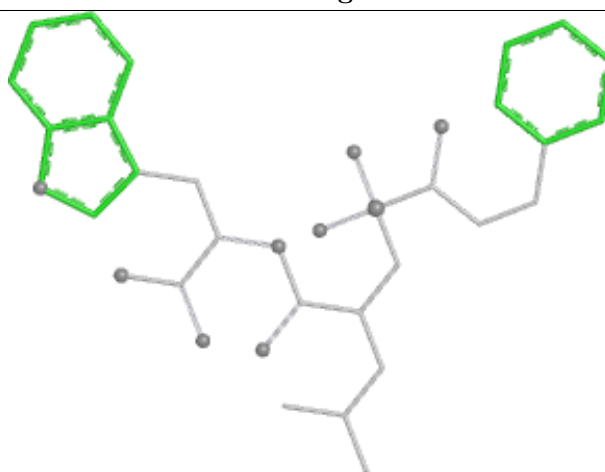
Bond lengths



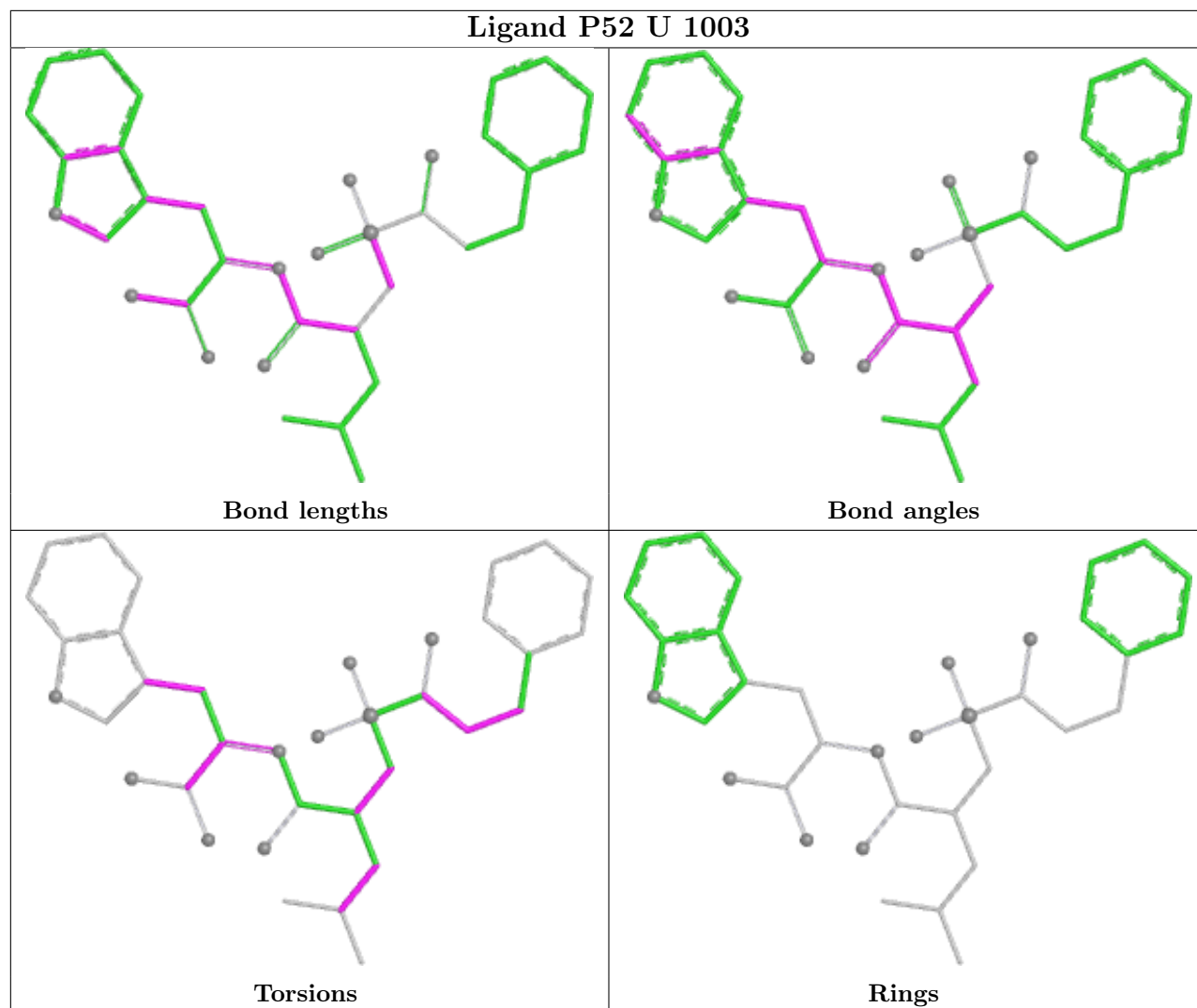
Bond angles

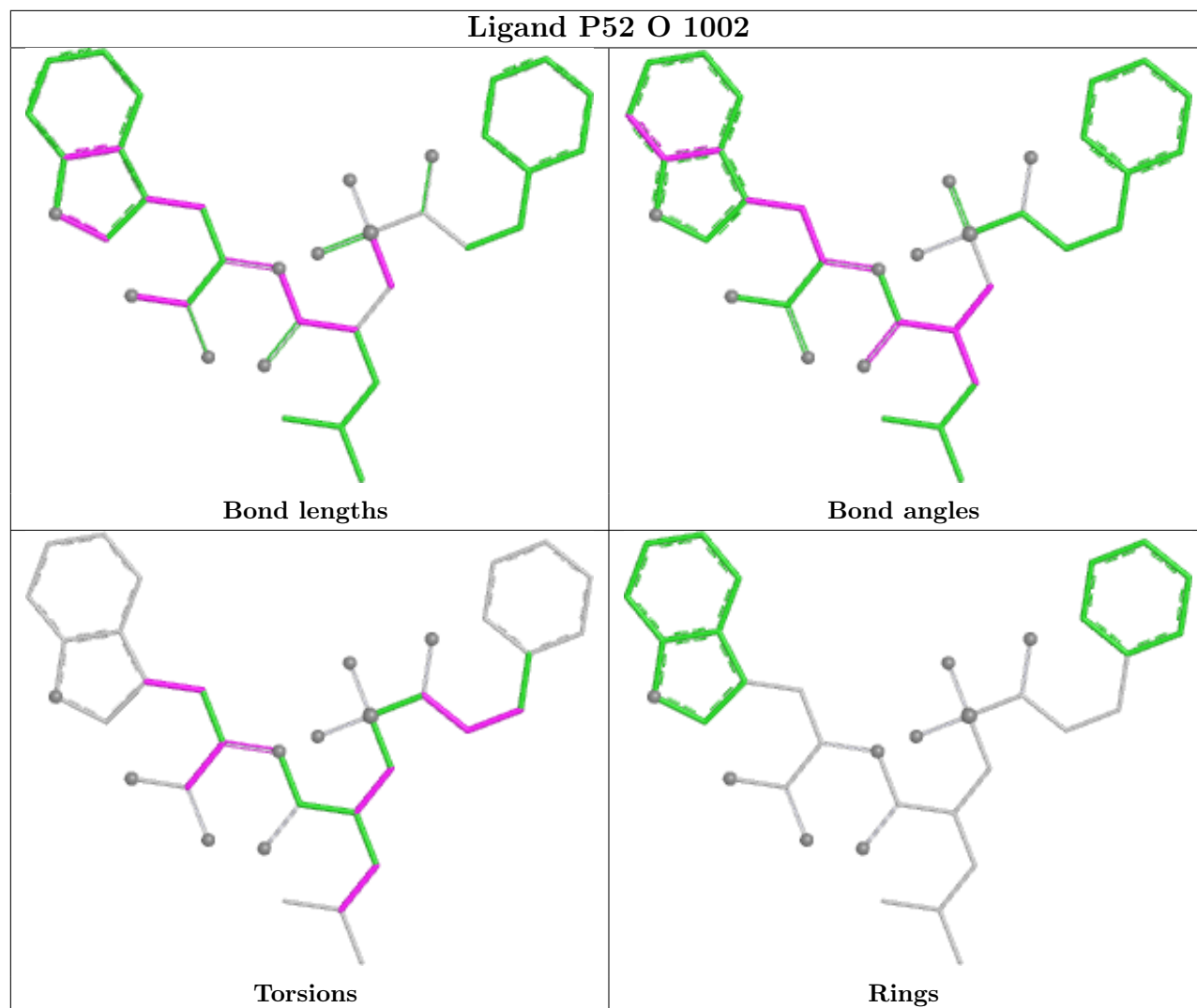


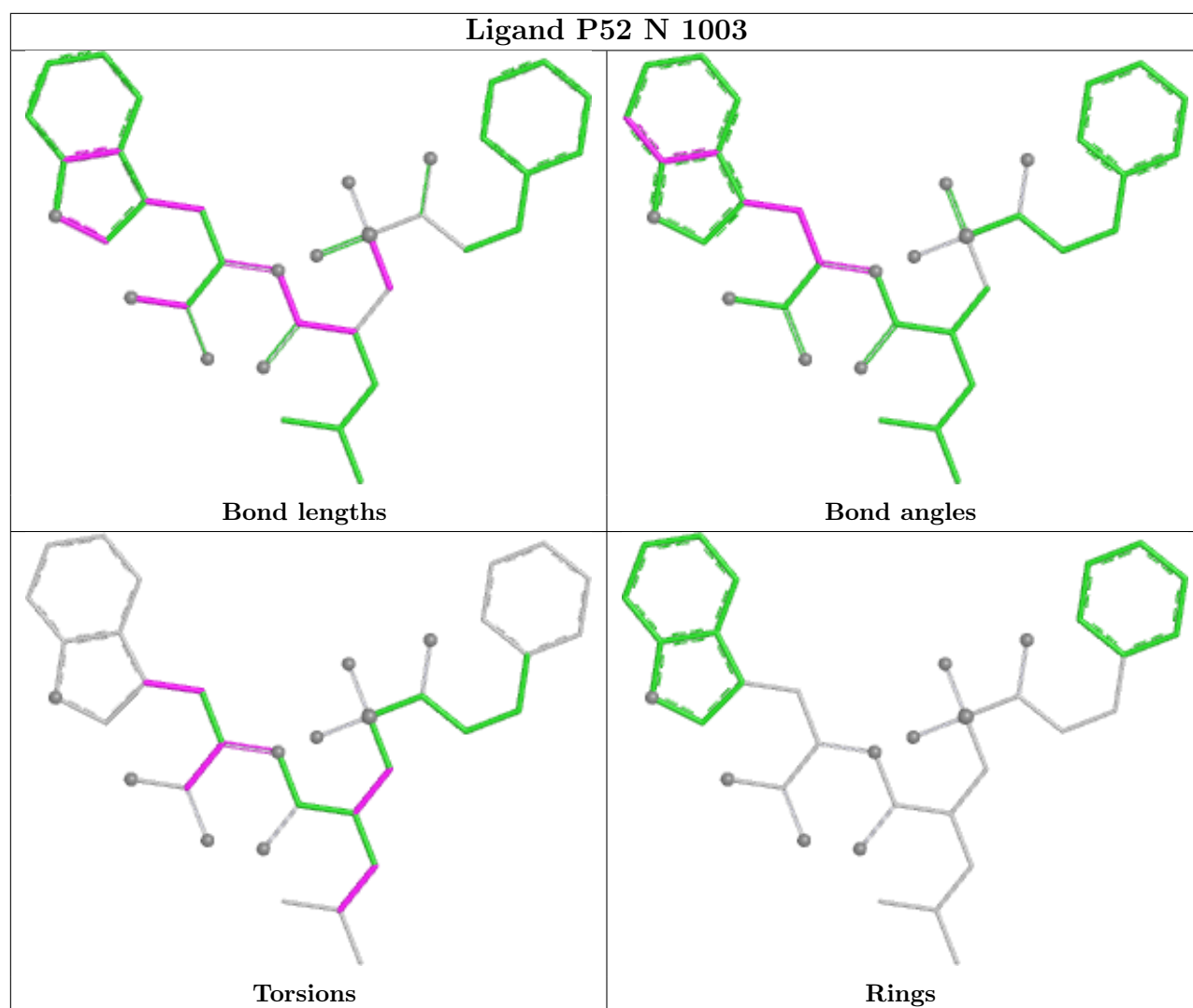
Torsions

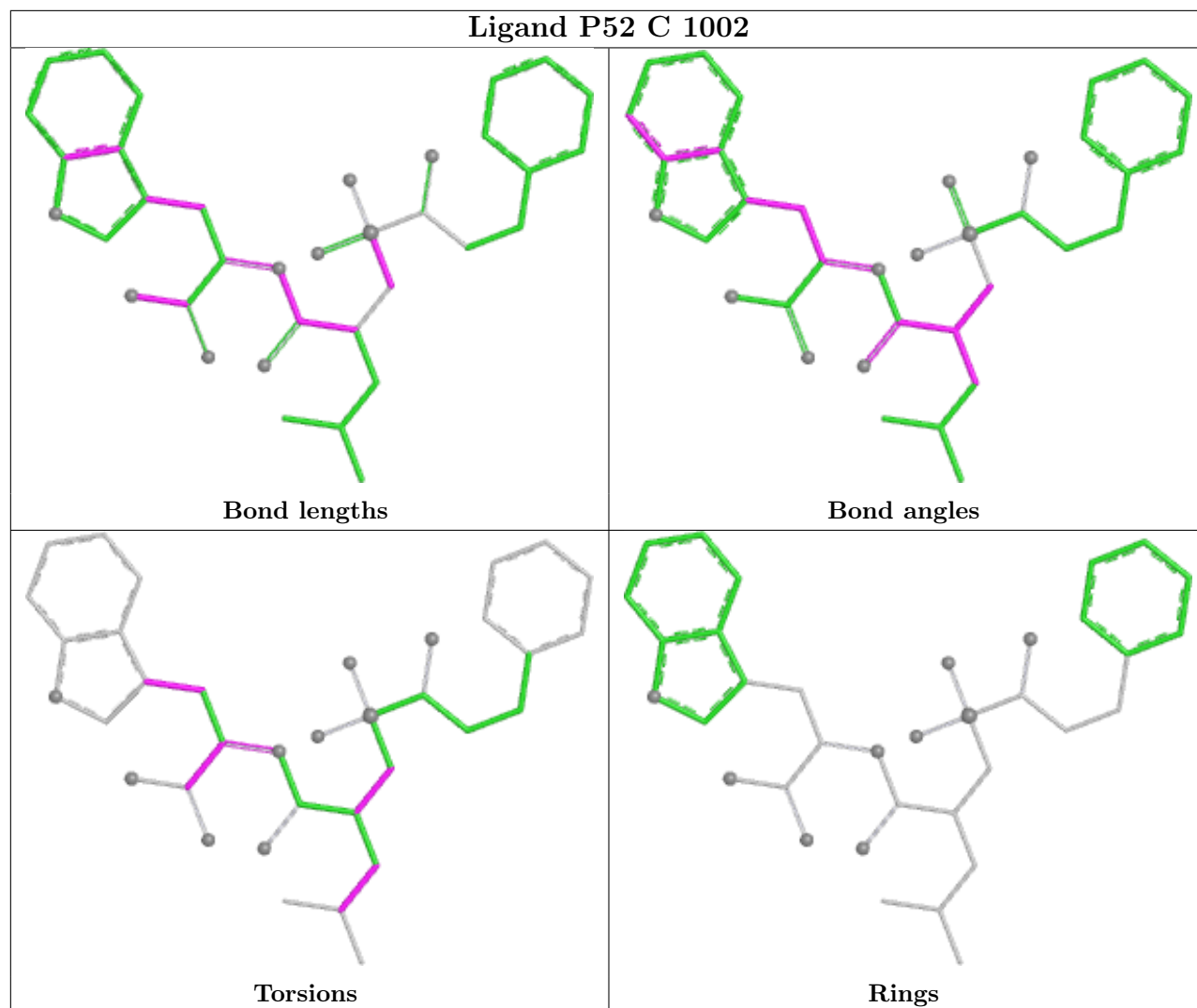


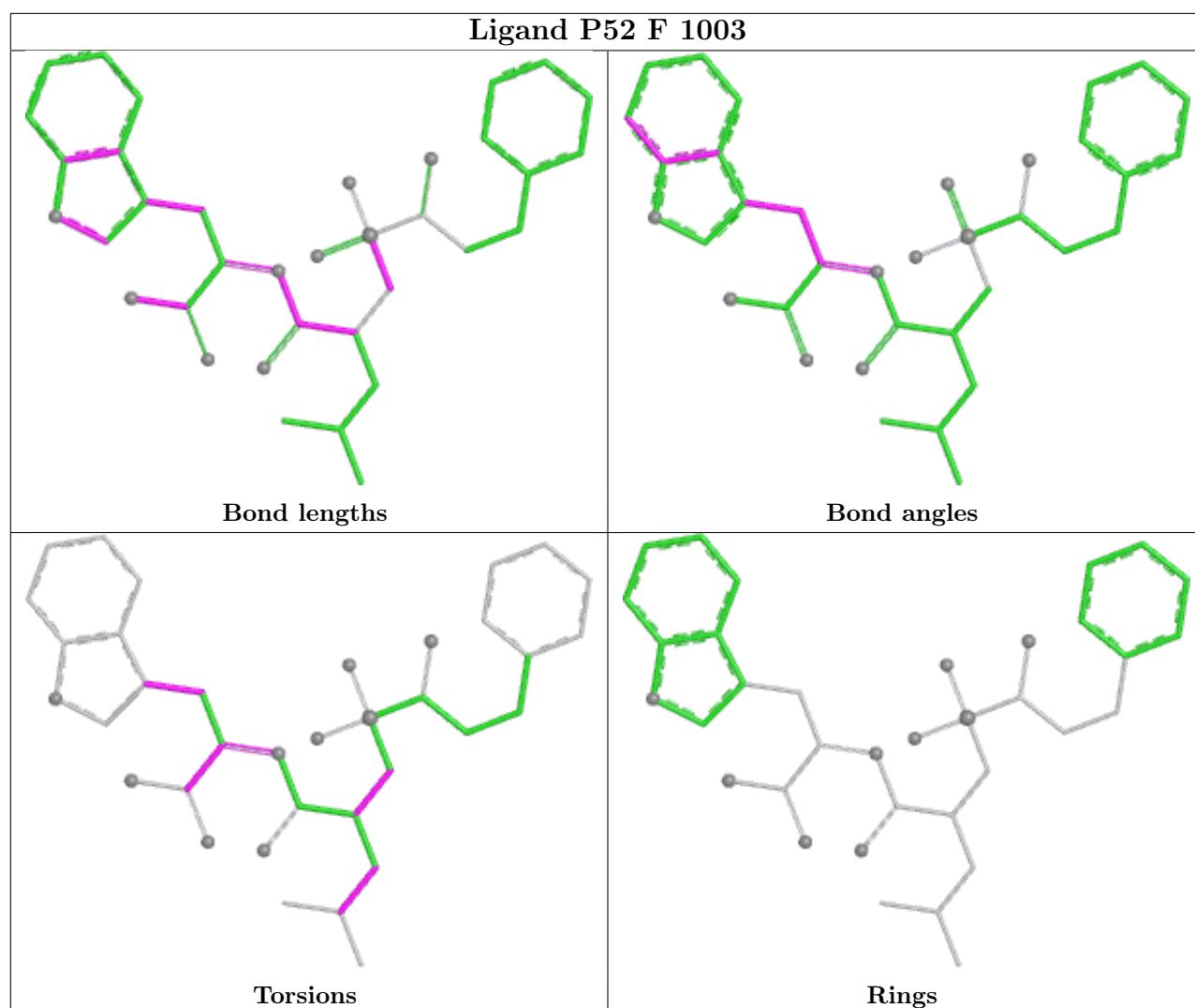
Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-1.62	0 100 100	7, 14, 27, 59	4 (0%)
1	B	861/899 (95%)	-1.62	0 100 100	8, 14, 29, 53	4 (0%)
1	C	861/899 (95%)	-1.62	0 100 100	8, 16, 29, 54	4 (0%)
1	D	861/899 (95%)	-1.62	0 100 100	8, 15, 32, 56	4 (0%)
1	E	861/899 (95%)	-1.63	0 100 100	8, 16, 33, 58	4 (0%)
1	F	861/899 (95%)	-1.61	0 100 100	7, 15, 34, 57	4 (0%)
1	G	861/899 (95%)	-1.63	0 100 100	11, 18, 39, 60	4 (0%)
1	H	861/899 (95%)	-1.62	0 100 100	10, 19, 38, 55	4 (0%)
1	I	861/899 (95%)	-1.60	0 100 100	19, 31, 40, 68	4 (0%)
1	J	861/899 (95%)	-1.56	0 100 100	18, 29, 51, 82	4 (0%)
1	K	861/899 (95%)	-1.56	0 100 100	20, 31, 53, 81	4 (0%)
1	L	861/899 (95%)	-1.55	0 100 100	16, 28, 50, 68	4 (0%)
1	M	861/899 (95%)	-1.46	0 100 100	22, 37, 51, 59	4 (0%)
1	N	861/899 (95%)	-1.31	0 100 100	28, 50, 73, 88	4 (0%)
1	O	861/899 (95%)	-1.39	0 100 100	26, 41, 67, 89	4 (0%)
1	P	861/899 (95%)	-1.21	0 100 100	30, 55, 69, 78	4 (0%)
1	Q	861/899 (95%)	-1.25	0 100 100	25, 51, 73, 95	4 (0%)
1	R	861/899 (95%)	-1.18	0 100 100	25, 53, 79, 101	4 (0%)
1	S	861/899 (95%)	-0.90	0 100 100	42, 74, 85, 94	4 (0%)
1	T	861/899 (95%)	-0.96	0 100 100	41, 73, 84, 95	4 (0%)
1	U	861/899 (95%)	-1.00	0 100 100	37, 71, 82, 96	4 (0%)
1	V	861/899 (95%)	-0.92	0 100 100	45, 79, 89, 100	4 (0%)
All	All	18942/19778 (95%)	-1.40	0 100 100	7, 34, 79, 101	88 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

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	DA	3	11/12	0.96	0.08	135,135,135,135	0
2	NAG	DA	2	14/15	0.97	0.10	127,128,128,128	0
2	NAG	BA	2	14/15	0.98	0.07	124,124,125,125	0
2	NAG	Z	2	14/15	0.98	0.08	93,93,94,94	0
2	BMA	Z	3	11/12	0.98	0.06	105,106,106,106	0
2	NAG	Y	1	14/15	0.99	0.04	20,21,21,21	0
2	NAG	Y	2	14/15	0.99	0.03	31,31,31,31	0
2	BMA	Y	3	11/12	0.99	0.04	38,38,38,38	11
2	NAG	Z	1	14/15	0.99	0.04	63,63,64,64	0
2	NAG	W	2	14/15	0.99	0.03	31,31,31,31	0
2	BMA	W	3	11/12	0.99	0.04	36,36,36,36	11
2	NAG	AA	1	14/15	0.99	0.04	72,73,73,73	0
2	NAG	a	1	14/15	-	-	22,22,23,23	0
2	NAG	a	2	14/15	-	-	32,32,33,33	0
2	BMA	a	3	11/12	-	-	36,36,36,36	11
2	NAG	b	1	14/15	-	-	64,64,64,65	0
2	NAG	b	2	14/15	-	-	89,89,89,89	0
2	BMA	b	3	11/12	-	-	94,95,95,95	0
2	NAG	c	1	14/15	-	-	32,32,33,33	0
2	NAG	c	2	14/15	-	-	43,43,43,43	0
2	BMA	c	3	11/12	-	-	49,49,49,49	11
2	NAG	d	1	14/15	-	-	68,68,69,69	0
2	NAG	d	2	14/15	-	-	103,103,103,103	0
2	BMA	d	3	11/12	-	-	115,115,115,115	0
2	NAG	e	1	14/15	-	-	28,28,29,29	0
2	NAG	e	2	14/15	-	-	44,45,45,45	0
2	BMA	e	3	11/12	-	-	49,49,50,50	11
2	NAG	f	1	14/15	-	-	71,71,72,72	0
2	NAG	f	2	14/15	-	-	97,97,97,97	0
2	BMA	f	3	11/12	-	-	105,105,106,106	0
2	NAG	g	1	14/15	-	-	24,24,24,24	0
2	NAG	g	2	14/15	-	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	g	3	11/12	-	-	45,45,45,45	11
2	NAG	h	1	14/15	-	-	70,70,70,70	0
2	NAG	h	2	14/15	-	-	94,94,94,94	0
2	BMA	h	3	11/12	-	-	106,106,106,106	0
2	NAG	i	1	14/15	-	-	27,27,28,28	0
2	NAG	i	2	14/15	-	-	39,39,40,40	0
2	BMA	i	3	11/12	-	-	45,45,46,46	11
2	NAG	j	1	14/15	-	-	66,66,66,67	0
2	NAG	j	2	14/15	-	-	89,90,90,90	0
2	BMA	j	3	11/12	-	-	97,97,97,97	0
2	NAG	k	1	14/15	-	-	38,39,39,39	0
2	NAG	k	2	14/15	-	-	47,47,48,48	0
2	BMA	k	3	11/12	-	-	54,54,54,54	11
2	NAG	l	1	14/15	-	-	76,76,77,77	0
2	NAG	l	2	14/15	-	-	106,107,107,107	0
2	BMA	l	3	11/12	-	-	116,117,117,117	0
2	NAG	m	1	14/15	-	-	38,38,39,39	0
2	NAG	m	2	14/15	-	-	50,50,51,51	0
2	BMA	m	3	11/12	-	-	52,52,53,53	11
2	NAG	n	1	14/15	-	-	82,83,83,83	0
2	NAG	n	2	14/15	-	-	110,110,110,110	0
2	BMA	n	3	11/12	-	-	117,117,117,117	0
2	NAG	o	1	14/15	-	-	43,43,44,44	0
2	NAG	o	2	14/15	-	-	54,55,55,55	0
2	BMA	o	3	11/12	-	-	65,65,65,65	11
2	NAG	p	1	14/15	-	-	77,77,78,78	0
2	NAG	p	2	14/15	-	-	97,97,98,98	0
2	BMA	p	3	11/12	-	-	106,107,107,107	0
2	NAG	q	1	14/15	-	-	39,39,40,40	0
2	NAG	q	2	14/15	-	-	50,51,51,51	0
2	BMA	q	3	11/12	-	-	62,62,62,62	11
2	NAG	r	1	14/15	-	-	78,78,78,79	0
2	NAG	r	2	14/15	-	-	113,113,114,114	0
2	BMA	r	3	11/12	-	-	124,124,124,125	0
2	NAG	s	1	14/15	-	-	41,41,42,42	0
2	NAG	s	2	14/15	-	-	59,60,60,60	0
2	BMA	s	3	11/12	-	-	64,64,64,64	11
2	NAG	t	1	14/15	-	-	84,84,84,84	0
2	NAG	t	2	14/15	-	-	115,115,116,116	0
2	BMA	t	3	11/12	-	-	134,134,134,134	0
2	NAG	u	1	14/15	-	-	42,42,43,43	0
2	NAG	u	2	14/15	-	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	u	3	11/12	-	-	61,61,61,61	11
2	NAG	v	1	14/15	-	-	73,73,74,74	0
2	NAG	v	2	14/15	-	-	102,103,103,103	0
2	BMA	v	3	11/12	-	-	113,113,113,113	0
2	NAG	w	1	14/15	-	-	60,60,61,61	0
2	NAG	w	2	14/15	-	-	68,68,68,68	0
2	BMA	w	3	11/12	-	-	67,67,67,67	11
2	NAG	x	1	14/15	-	-	89,89,89,89	0
2	NAG	x	2	14/15	-	-	114,114,114,114	0
2	BMA	x	3	11/12	-	-	122,122,123,123	0
2	NAG	y	1	14/15	-	-	44,45,45,46	0
2	NAG	y	2	14/15	-	-	54,55,56,56	0
2	BMA	y	3	11/12	-	-	61,61,61,61	11
2	NAG	z	1	14/15	-	-	89,90,90,90	0
2	NAG	z	2	14/15	-	-	113,114,114,114	0
2	BMA	z	3	11/12	-	-	121,121,121,121	0
2	NAG	0	1	14/15	-	-	62,62,62,62	0
2	NAG	0	2	14/15	-	-	71,71,72,72	0
2	BMA	0	3	11/12	-	-	74,74,74,74	11
2	NAG	1	1	14/15	-	-	96,96,96,96	0
2	NAG	1	2	14/15	-	-	117,117,117,117	0
2	BMA	1	3	11/12	-	-	120,120,120,120	0
2	NAG	2	1	14/15	-	-	48,48,49,49	0
2	NAG	2	2	14/15	-	-	57,57,58,58	0
2	BMA	2	3	11/12	-	-	64,64,64,64	11
2	NAG	3	1	14/15	-	-	93,93,94,94	0
2	NAG	3	2	14/15	-	-	114,115,115,115	0
2	BMA	3	3	11/12	-	-	120,120,120,121	0
2	NAG	4	1	14/15	-	-	50,51,51,51	0
2	NAG	4	2	14/15	-	-	59,59,60,60	0
2	BMA	4	3	11/12	-	-	66,66,66,66	11
2	NAG	5	1	14/15	-	-	91,91,91,92	0
2	NAG	5	2	14/15	-	-	104,104,104,104	0
2	BMA	5	3	11/12	-	-	109,109,109,109	0
2	NAG	6	1	14/15	-	-	81,81,81,81	0
2	NAG	6	2	14/15	-	-	96,96,97,97	0
2	BMA	6	3	11/12	-	-	93,93,93,93	11
2	NAG	7	1	14/15	-	-	108,109,109,109	0
2	NAG	7	2	14/15	-	-	132,133,133,133	0
2	BMA	7	3	11/12	-	-	139,140,140,140	0
2	NAG	8	1	14/15	-	-	77,77,77,77	0
2	NAG	8	2	14/15	-	-	85,85,85,85	0

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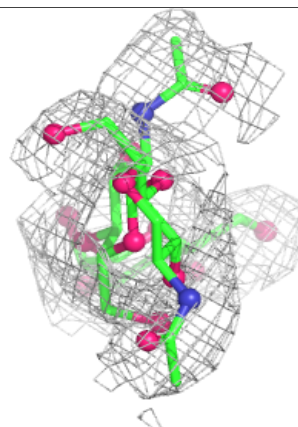
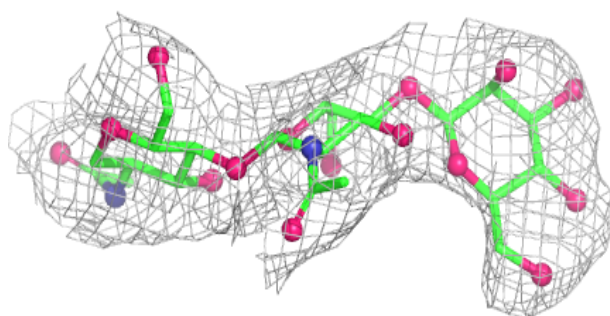
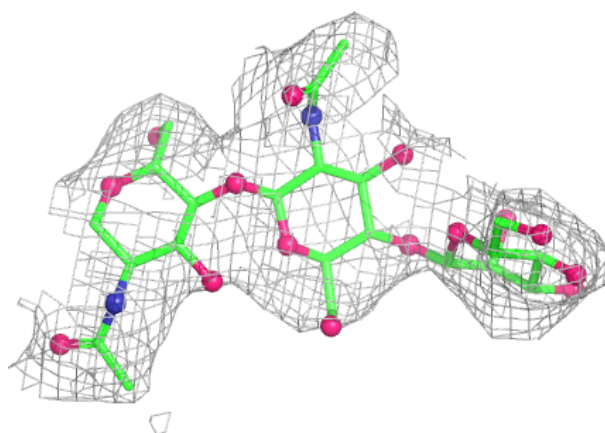
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BMA	8	3	11/12	-	-	85,85,85,85	11
2	NAG	9	1	14/15	-	-	100,100,100,100	0
2	NAG	9	2	14/15	-	-	113,113,113,113	0
2	BMA	9	3	11/12	-	-	119,119,119,119	0
2	NAG	AA	2	14/15	0.99	0.04	81,81,81,81	0
2	BMA	AA	3	11/12	0.99	0.05	79,79,80,80	11
2	NAG	BA	1	14/15	0.99	0.04	104,104,105,105	0
2	NAG	X	1	14/15	0.99	0.04	39,39,39,39	0
2	BMA	BA	3	11/12	0.99	0.04	127,128,128,128	0
2	NAG	CA	2	14/15	0.99	0.04	88,89,89,89	0
2	BMA	CA	3	11/12	0.99	0.05	86,86,86,86	11
2	NAG	DA	1	14/15	0.99	0.04	115,115,115,115	0
2	NAG	X	2	14/15	0.99	0.04	52,52,52,52	0
2	BMA	X	3	11/12	0.99	0.03	56,56,56,56	0
2	NAG	CA	1	14/15	1.00	0.03	82,82,82,82	0
2	NAG	W	1	14/15	1.00	0.02	20,20,20,20	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.

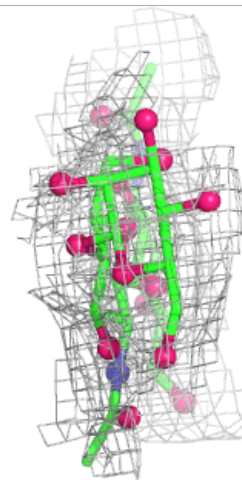
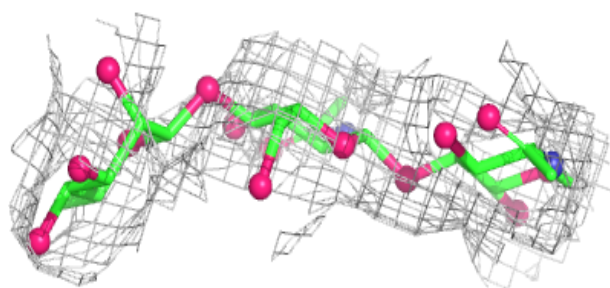
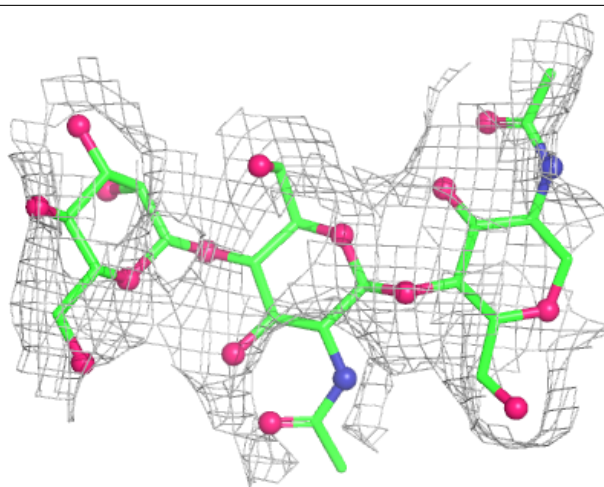
Electron density around Chain W:

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



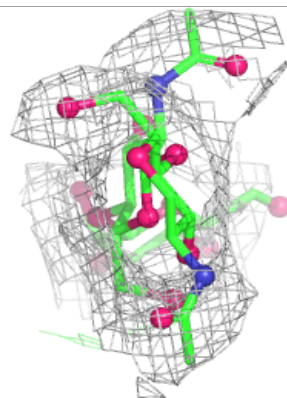
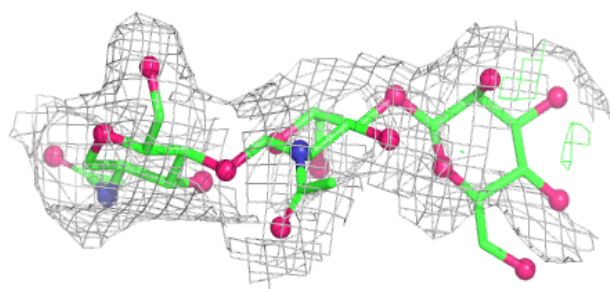
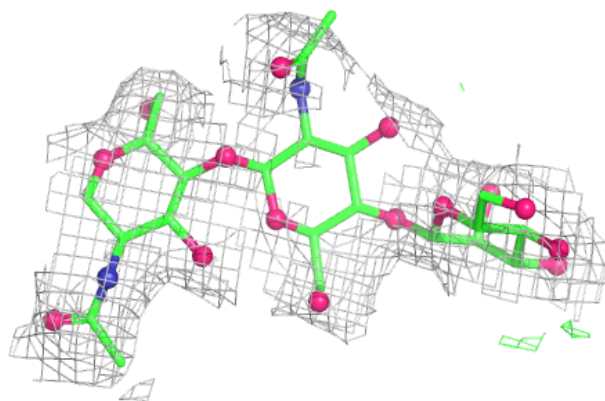
Electron density around Chain X:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



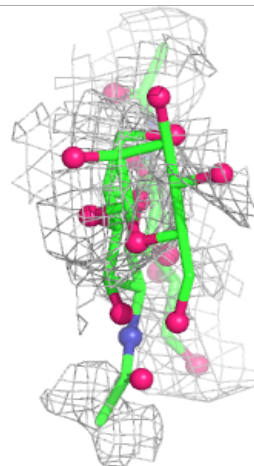
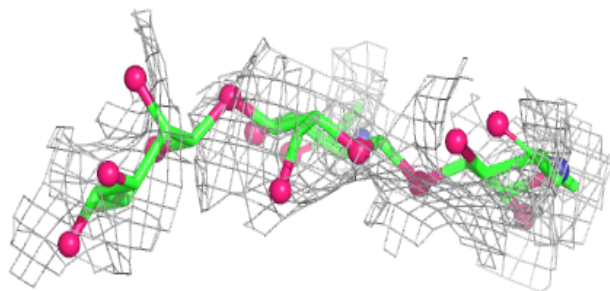
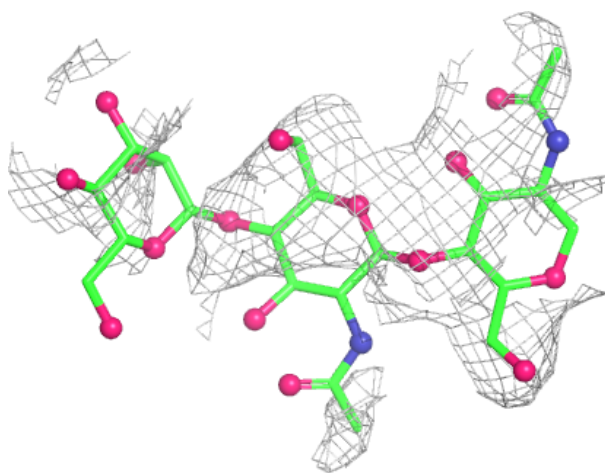
Electron density around Chain Y:

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



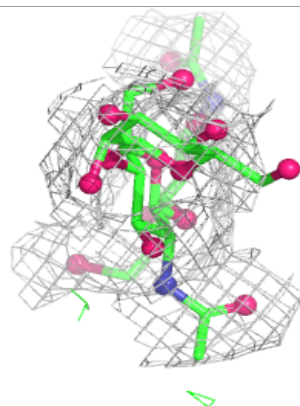
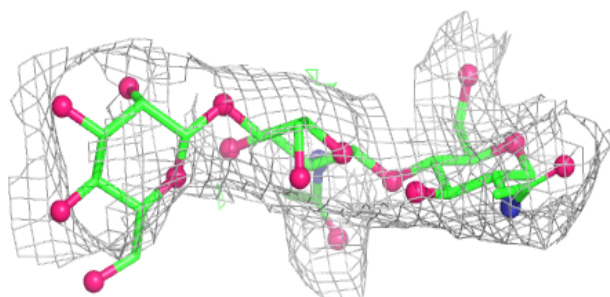
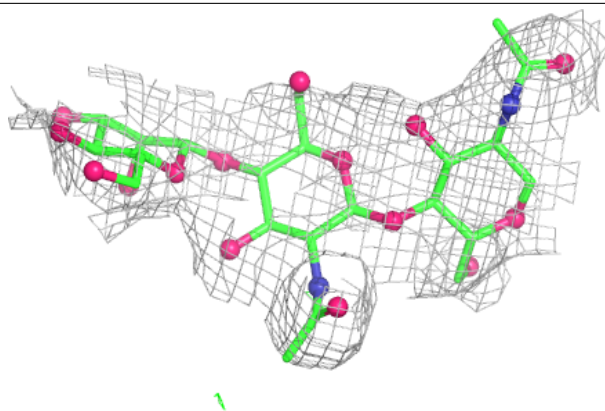
Electron density around Chain Z:

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



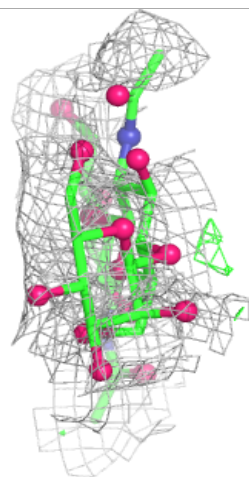
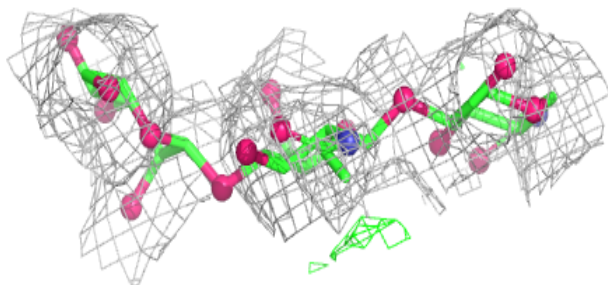
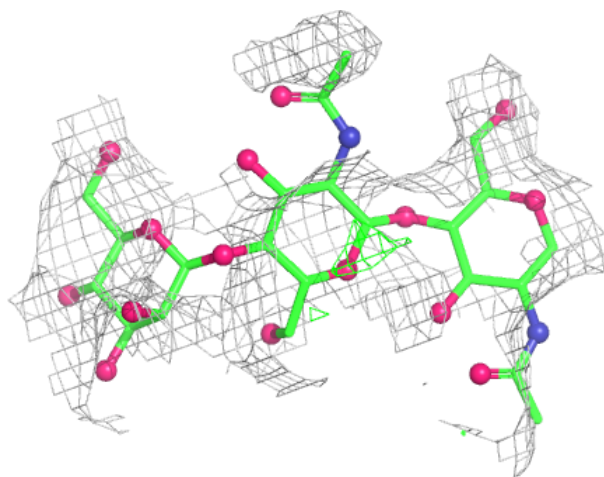
Electron density around Chain a:

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



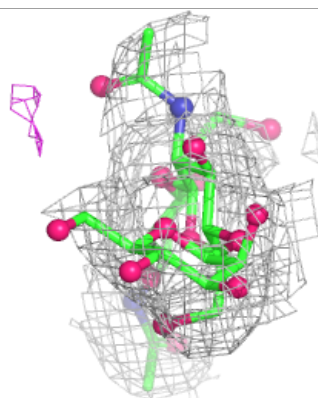
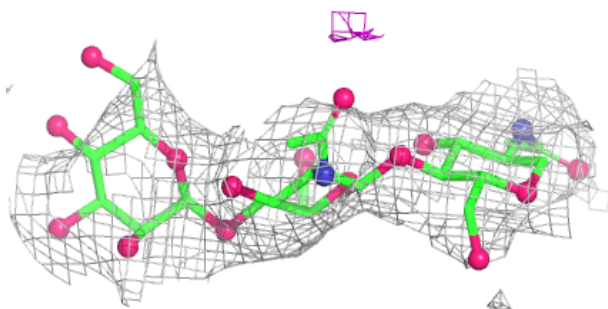
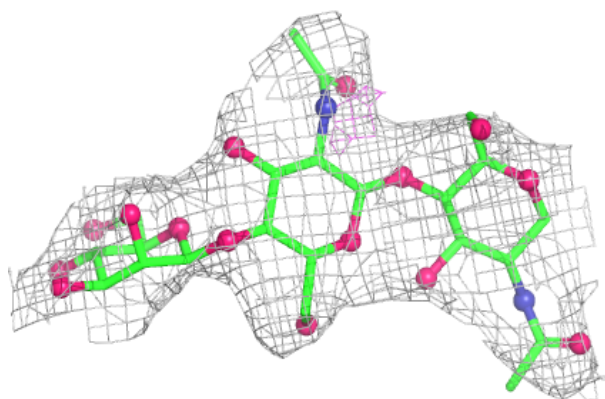
Electron density around Chain b:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

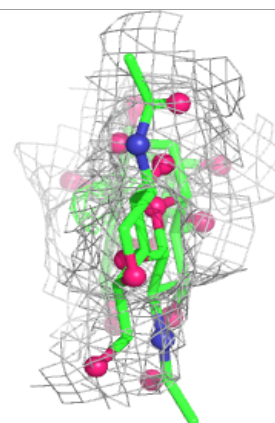
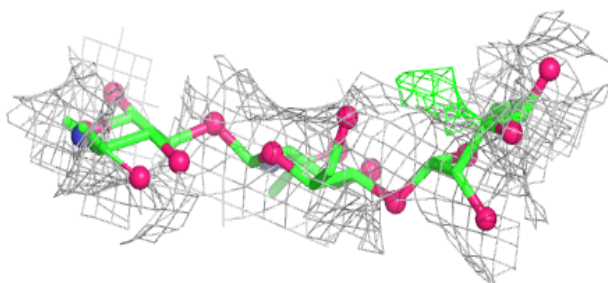
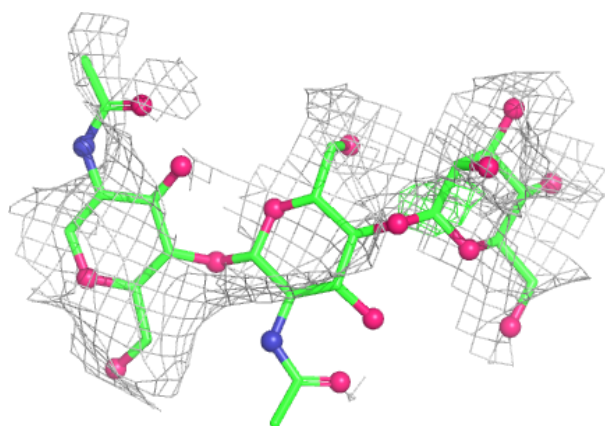


Electron density around Chain c:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

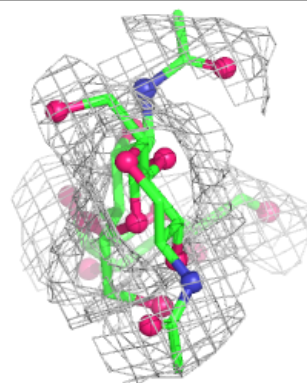
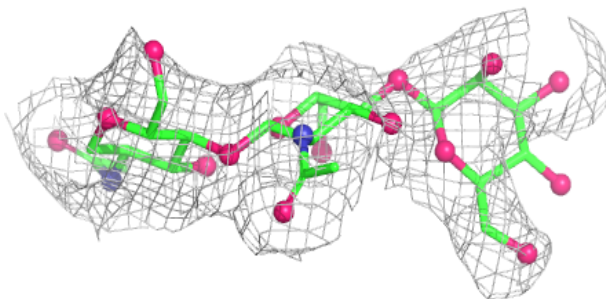
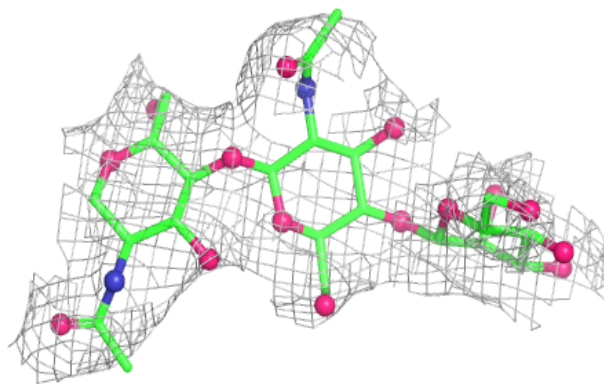
**Electron density around Chain d:**

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



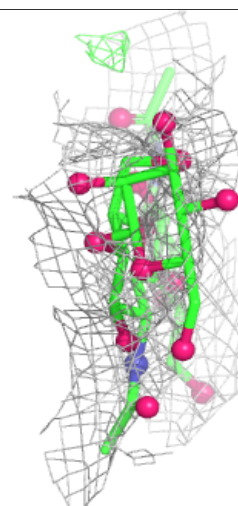
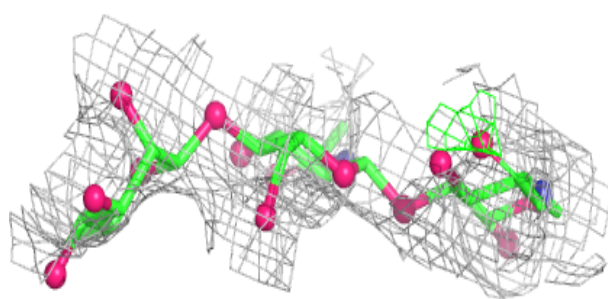
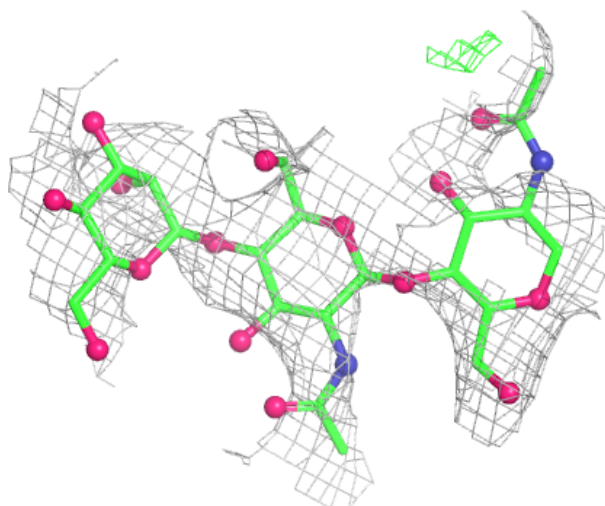
Electron density around Chain e:

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



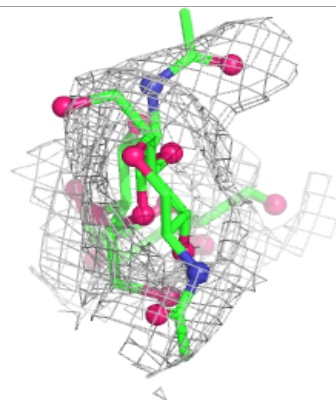
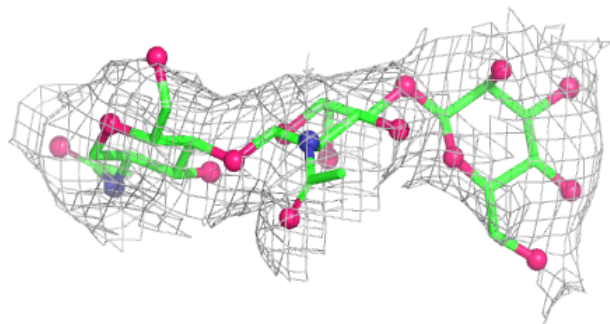
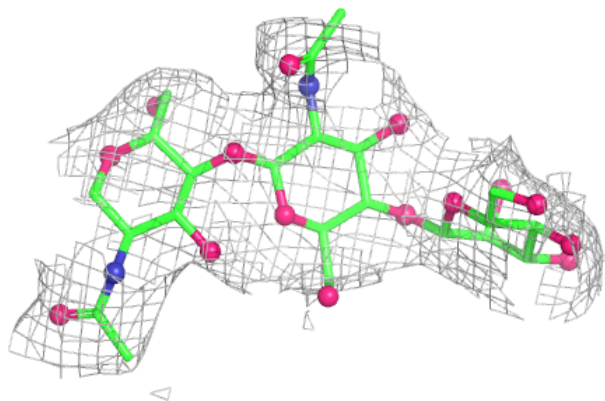
Electron density around Chain f:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



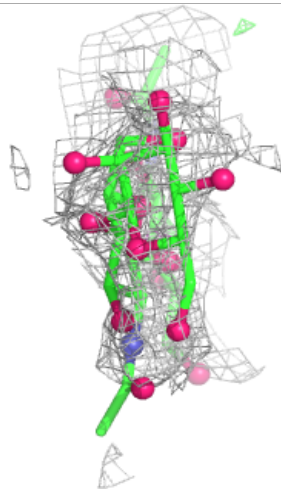
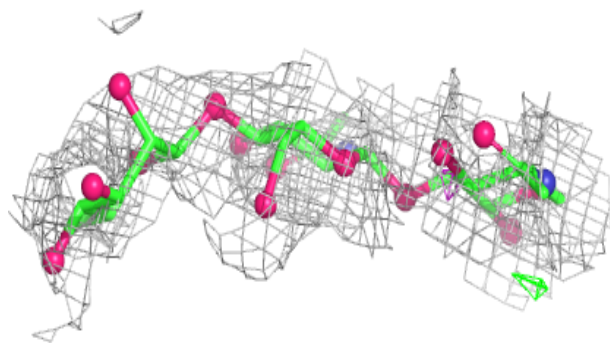
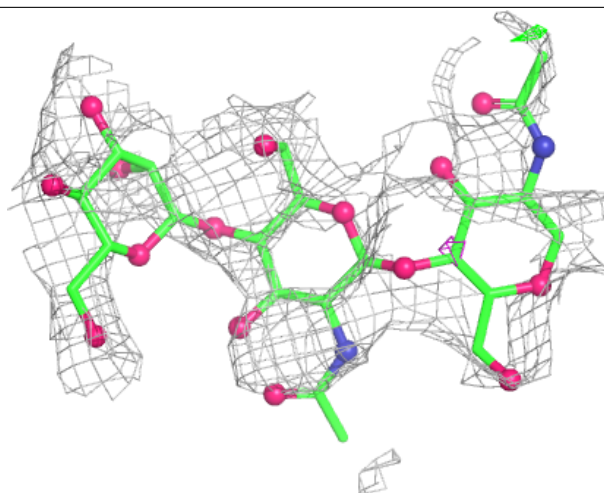
Electron density around Chain g:

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



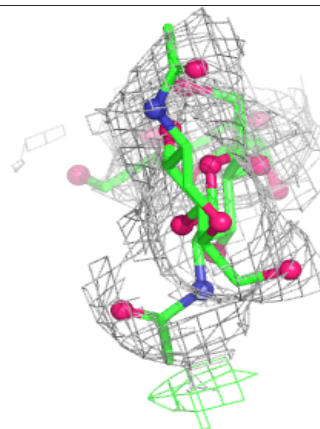
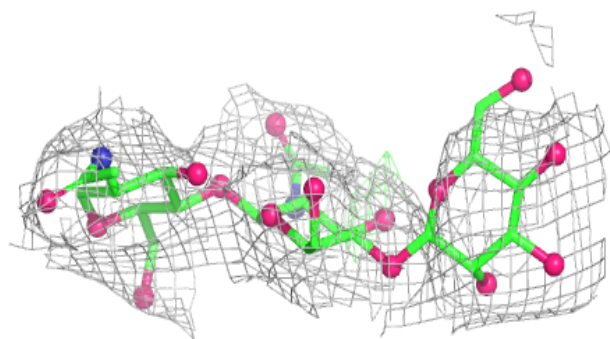
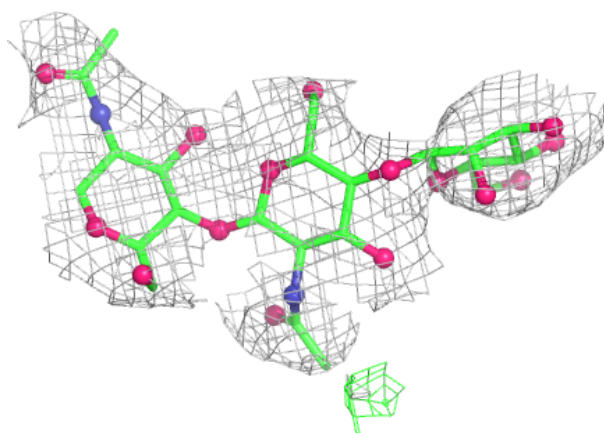
Electron density around Chain h:

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



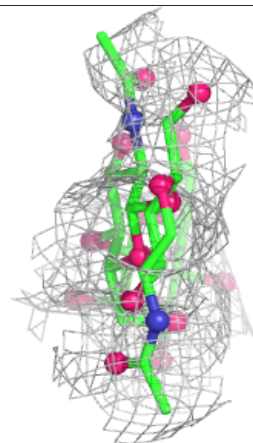
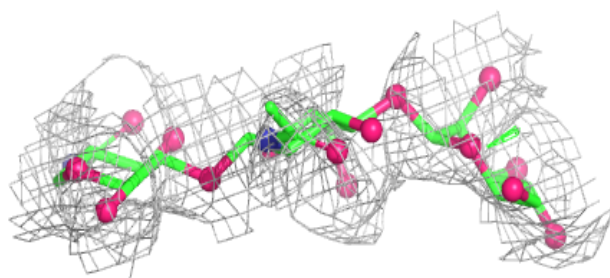
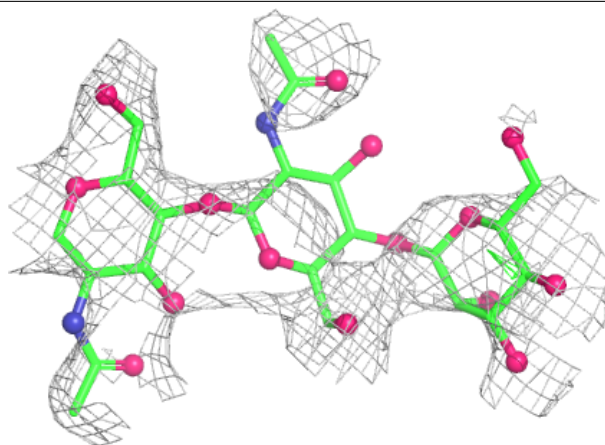
Electron density around Chain i:

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

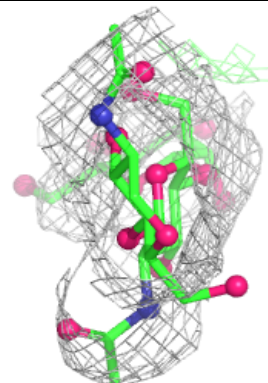
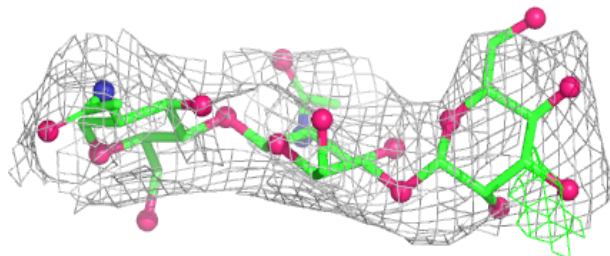
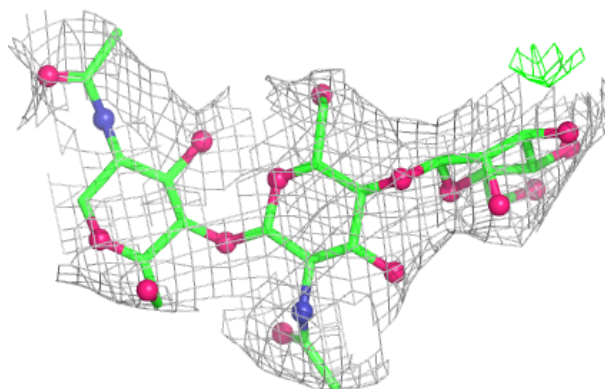


Electron density around Chain j:

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

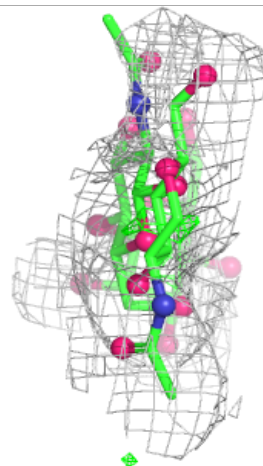
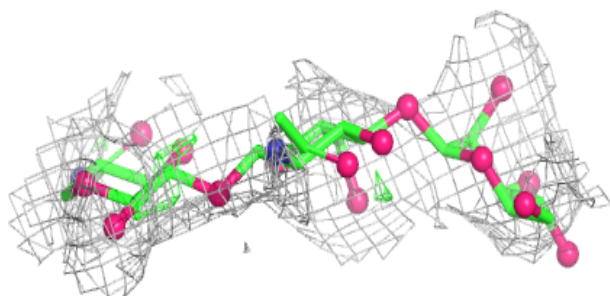
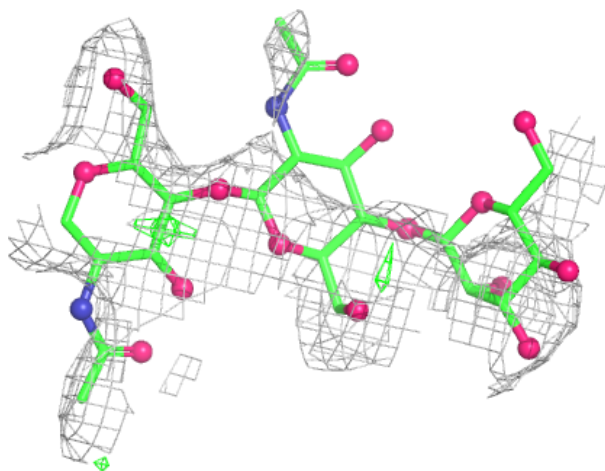
**Electron density around Chain k:**

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



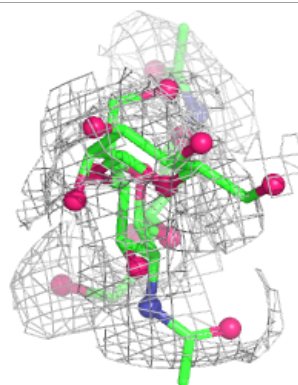
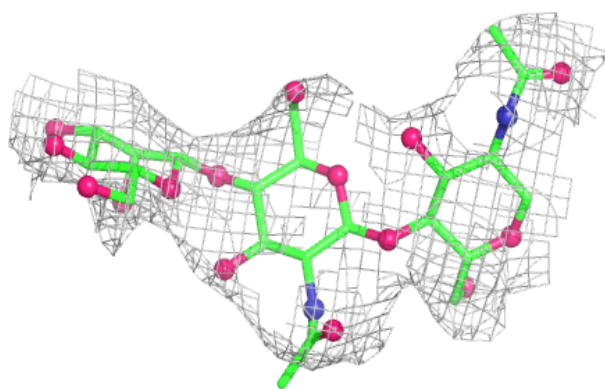
Electron density around Chain 1:

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



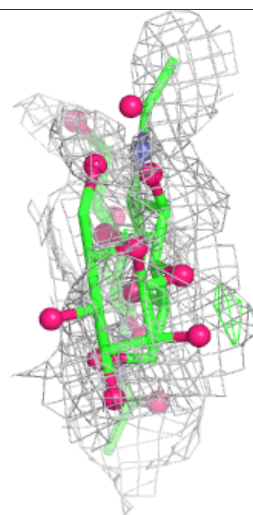
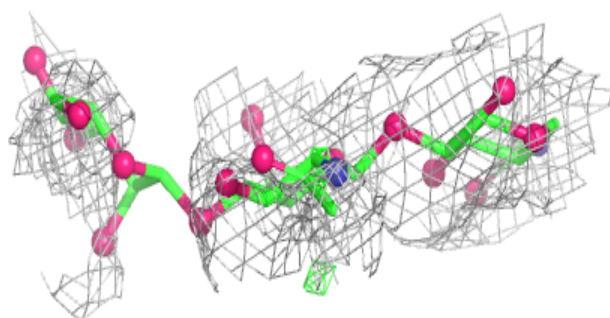
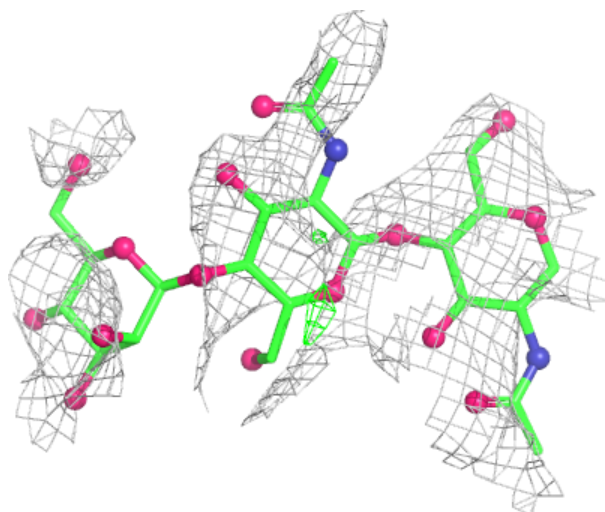
Electron density around Chain m:

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



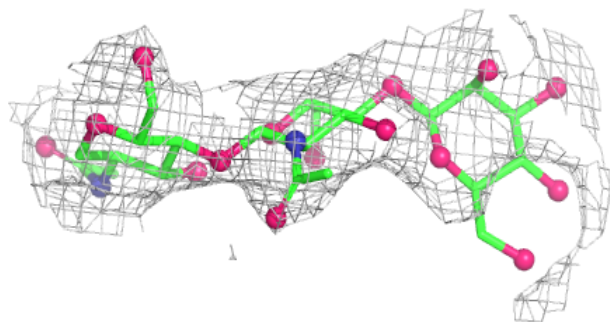
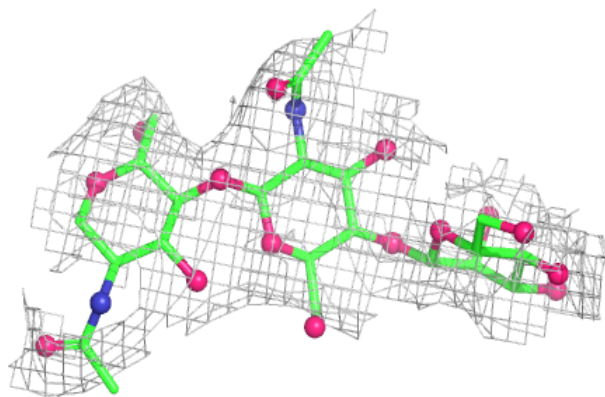
Electron density around Chain n:

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



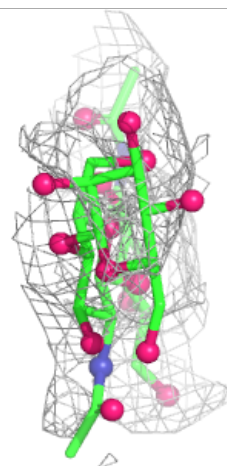
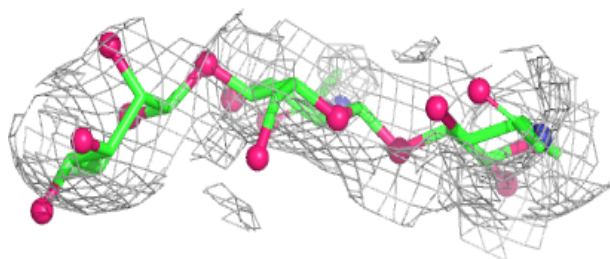
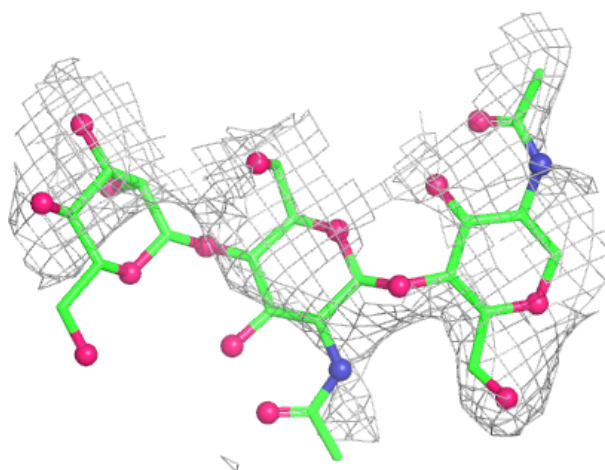
Electron density around Chain o:

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



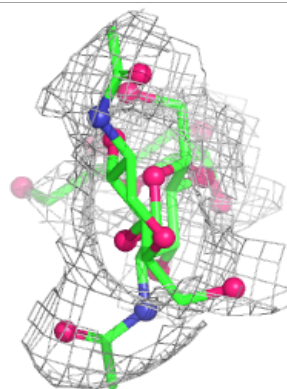
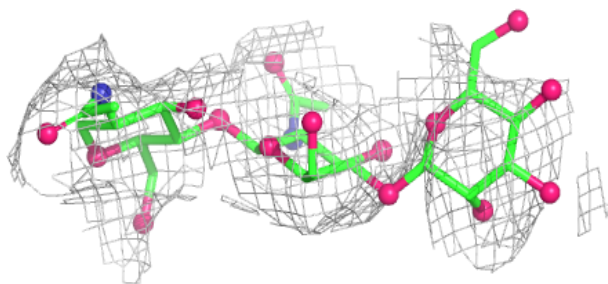
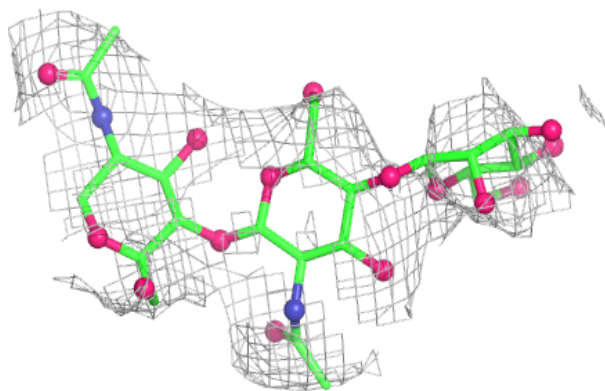
Electron density around Chain p:

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



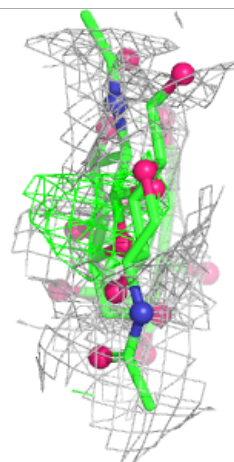
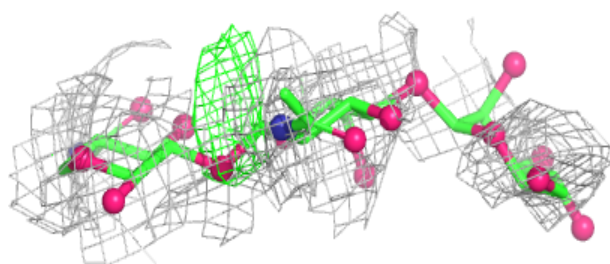
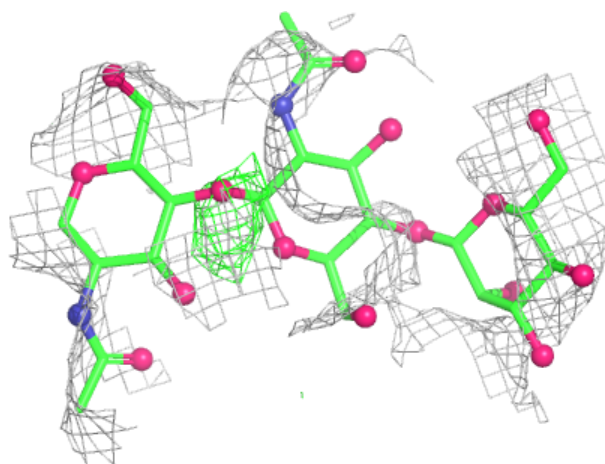
Electron density around Chain q:

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



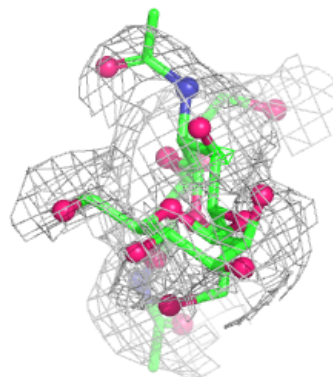
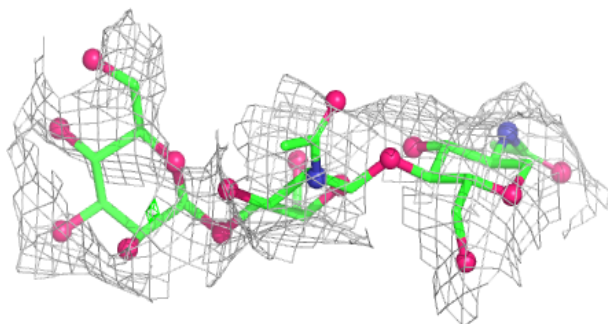
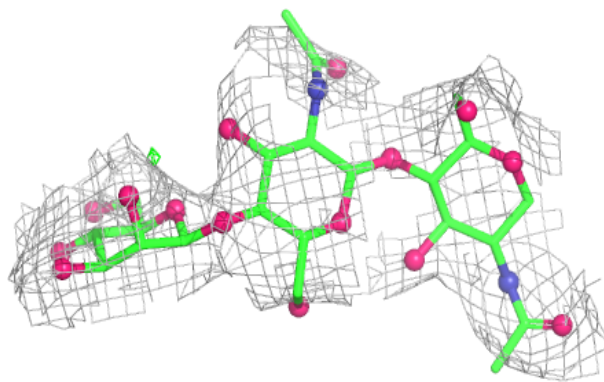
Electron density around Chain r:

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



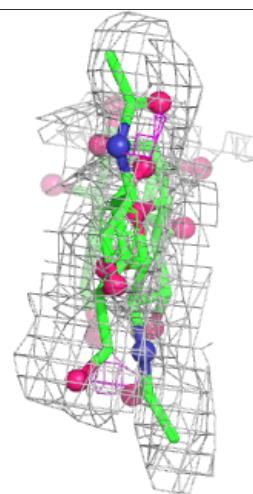
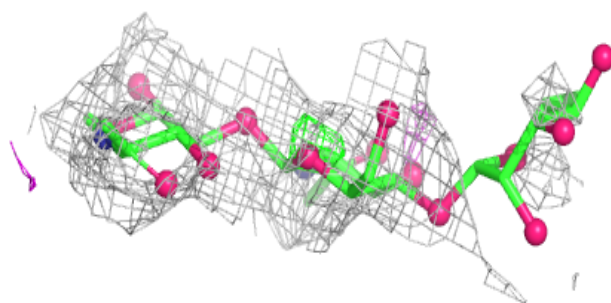
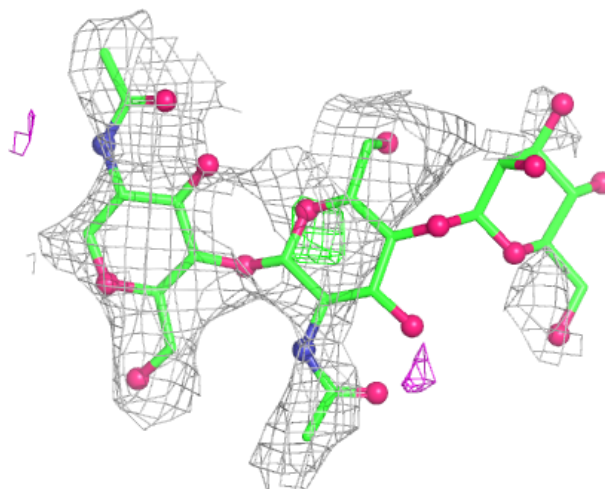
Electron density around Chain s:

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



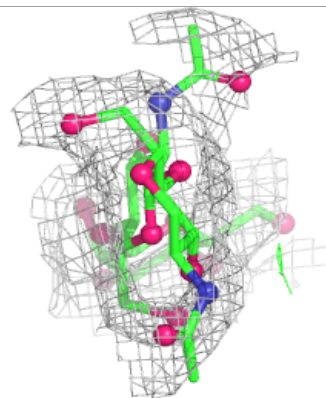
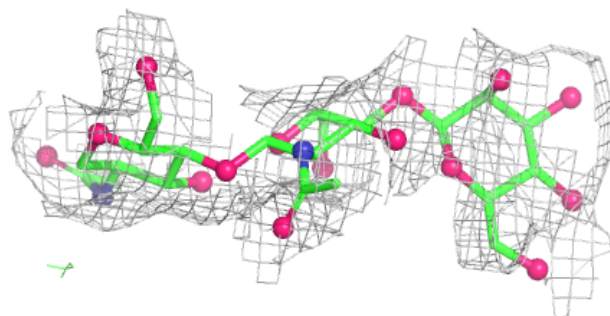
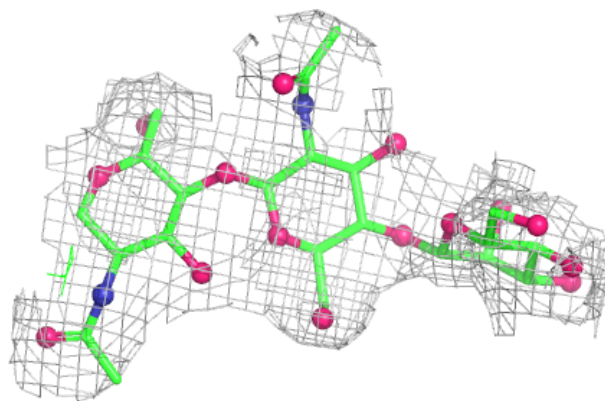
Electron density around Chain t:

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



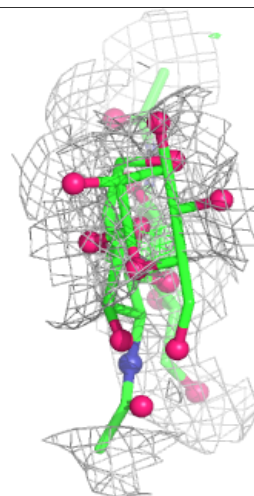
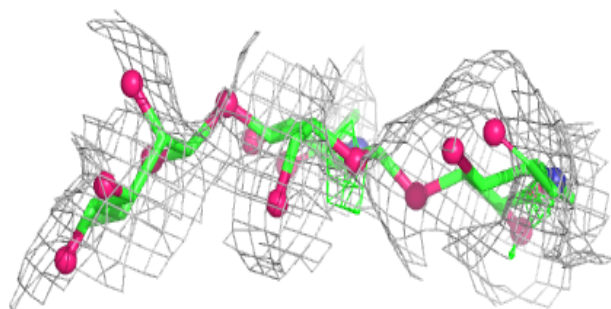
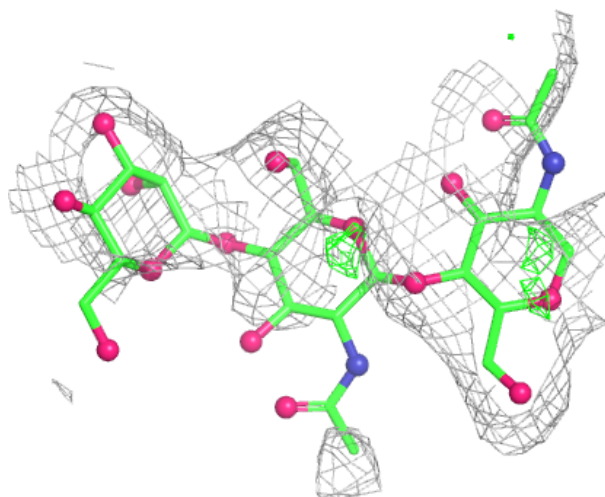
Electron density around Chain u:

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



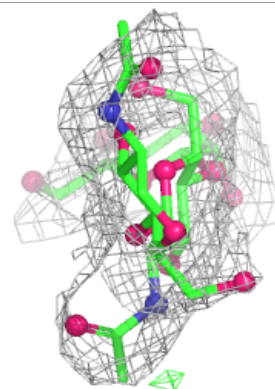
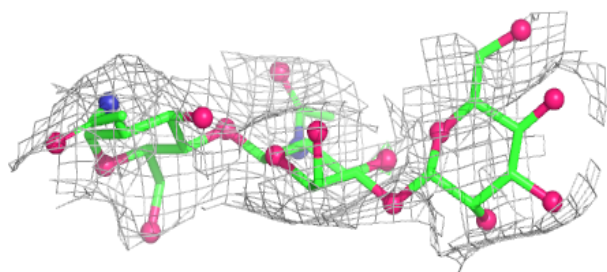
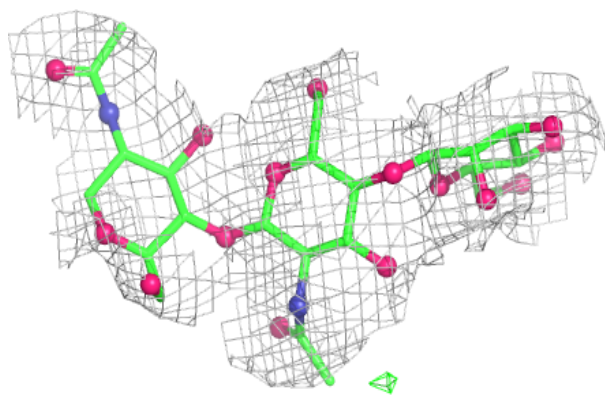
Electron density around Chain v:

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



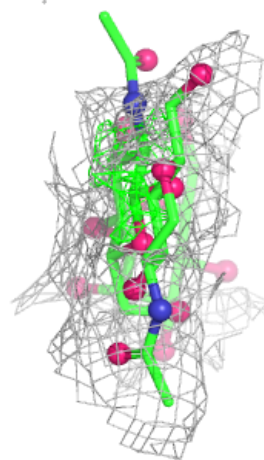
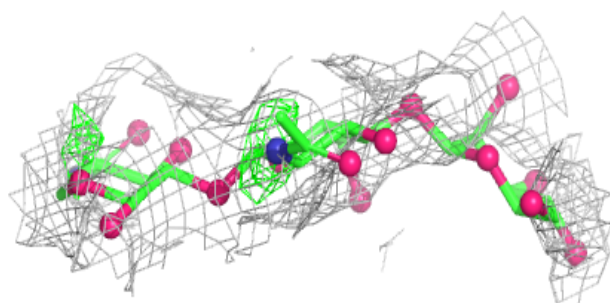
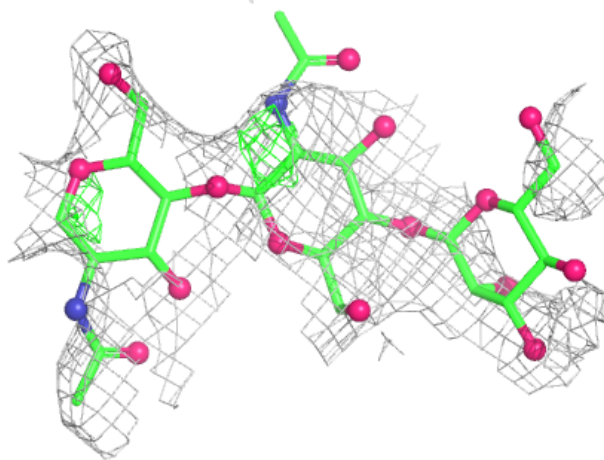
Electron density around Chain w:

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



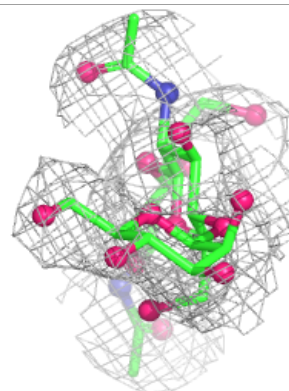
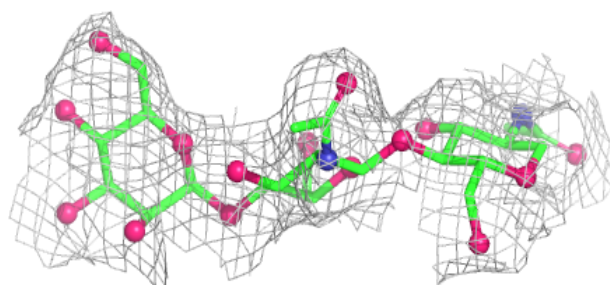
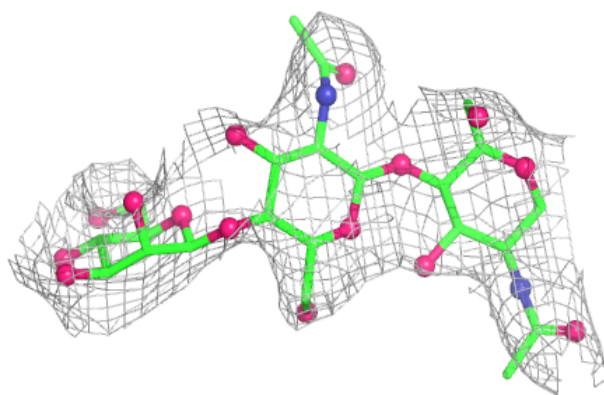
Electron density around Chain x:

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

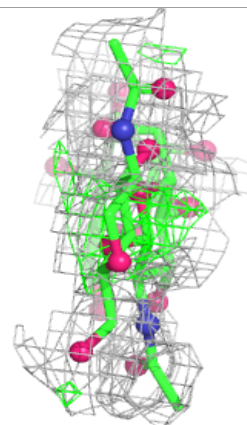
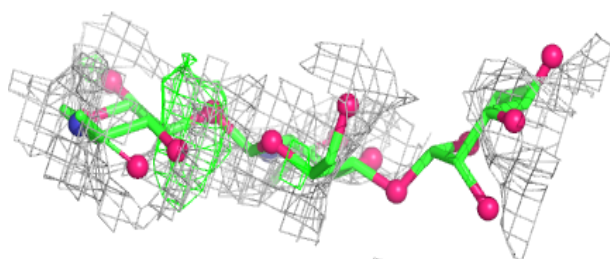
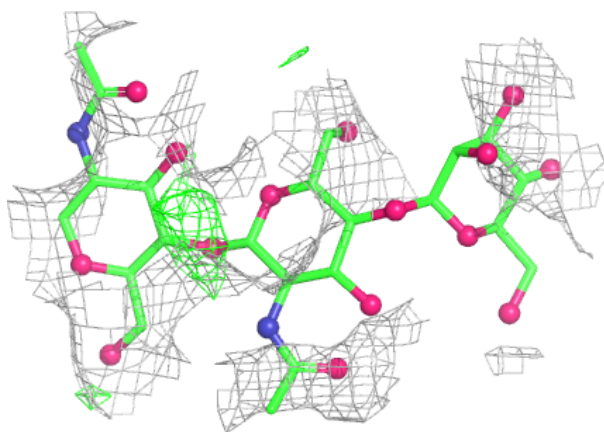


Electron density around Chain y:

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

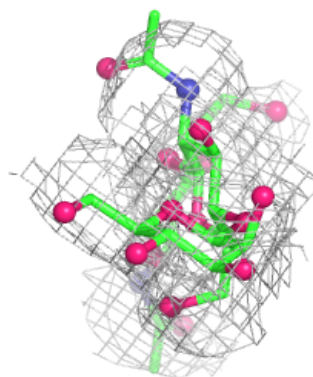
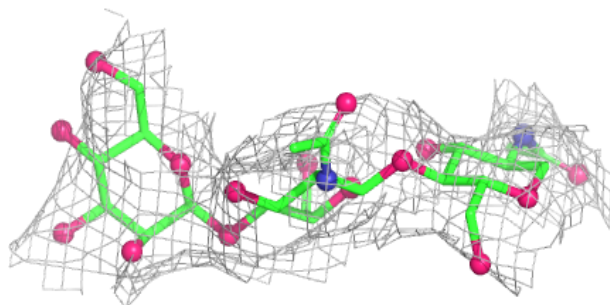
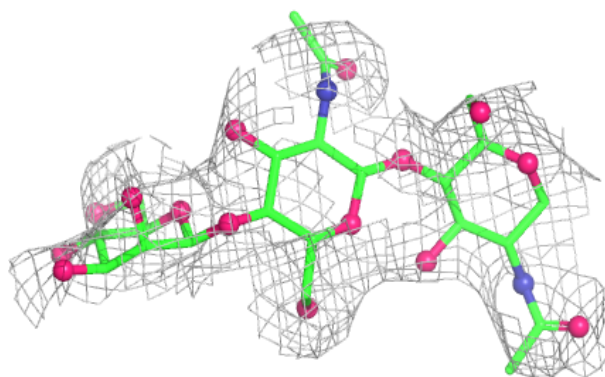
**Electron density around Chain z:**

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

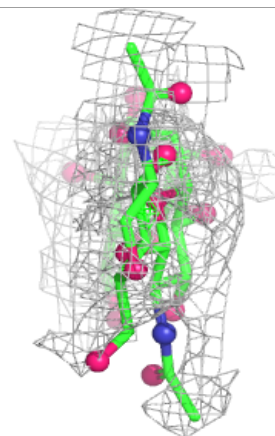
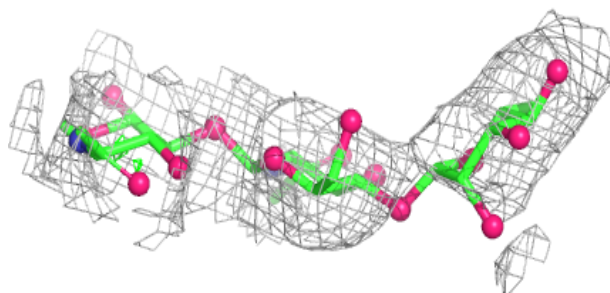
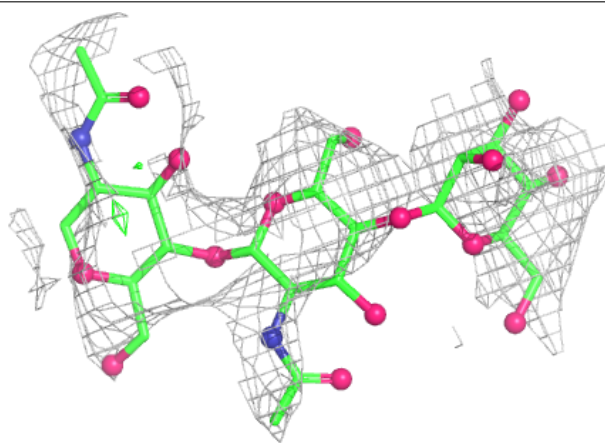


Electron density around Chain 0:

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

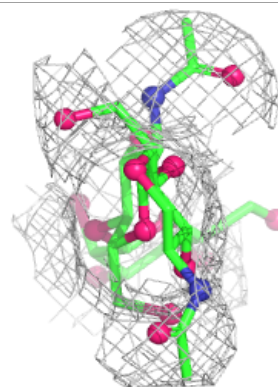
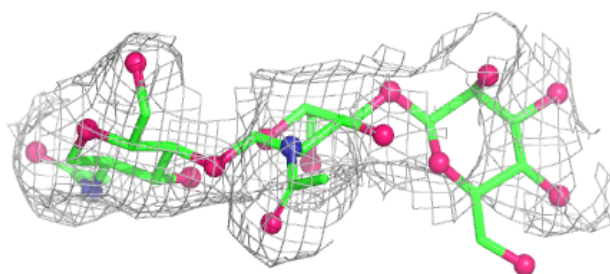
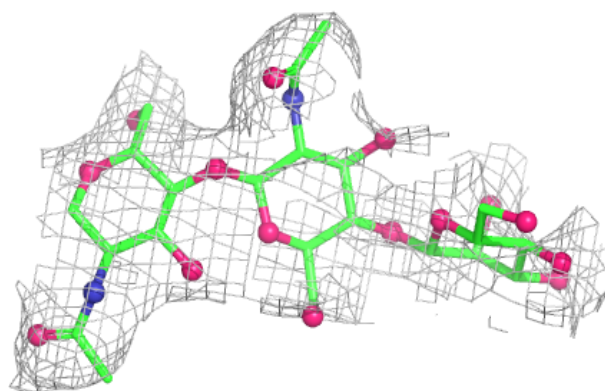
**Electron density around Chain 1:**

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

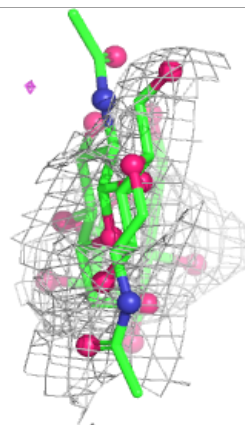
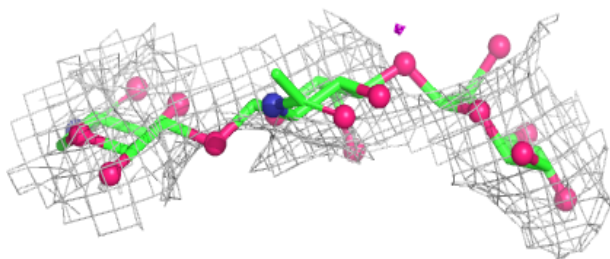
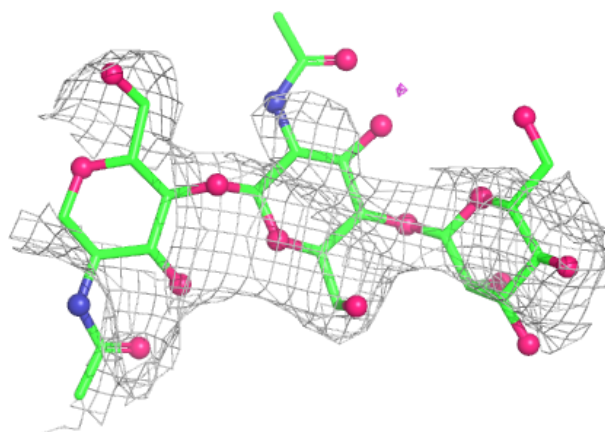


Electron density around Chain 2:

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

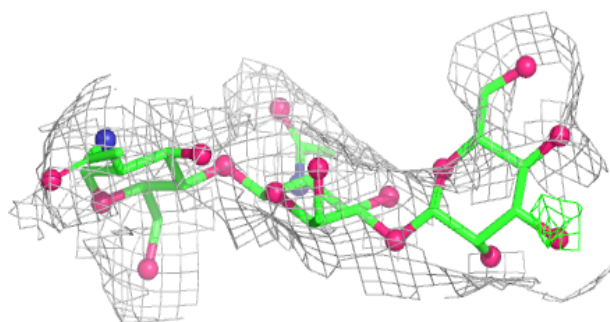
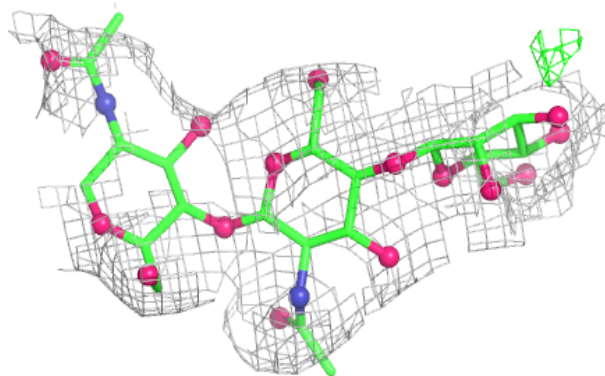
**Electron density around Chain 3:**

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

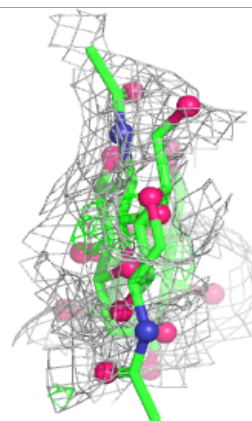
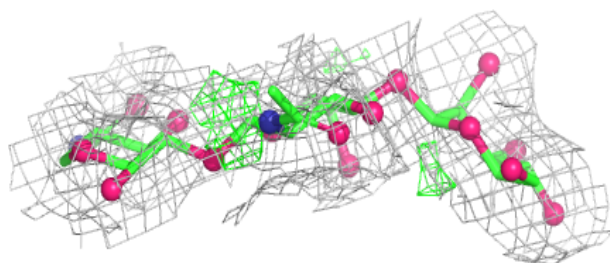
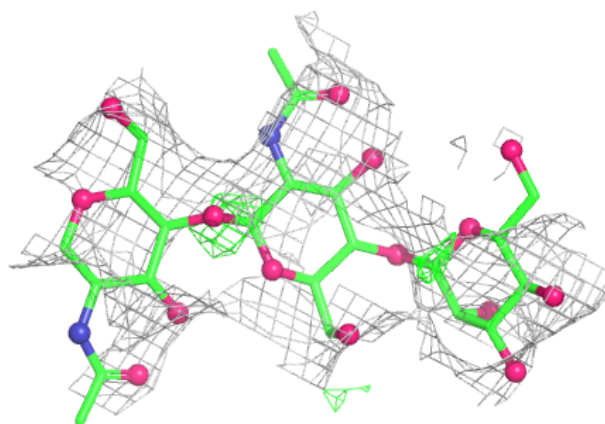


Electron density around Chain 4:

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

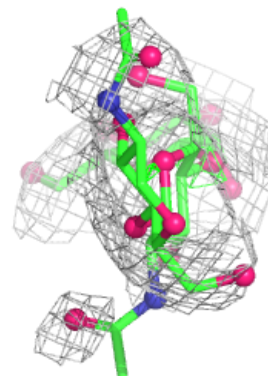
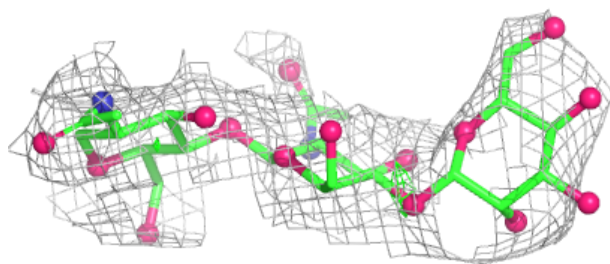
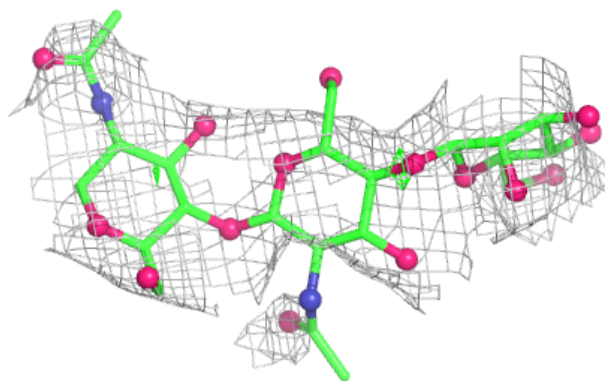
**Electron density around Chain 5:**

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



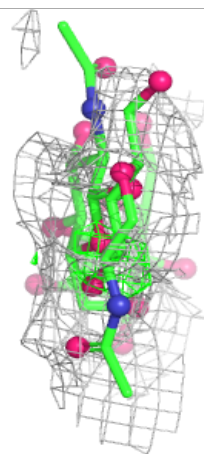
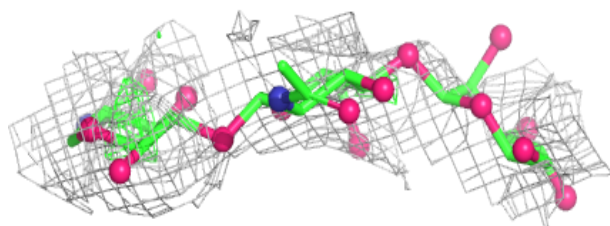
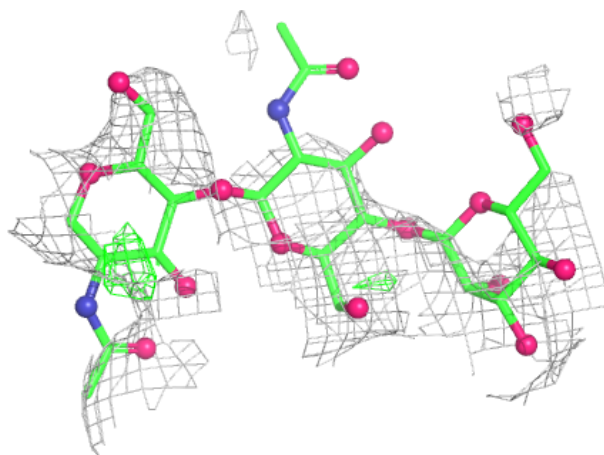
Electron density around Chain 6:

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



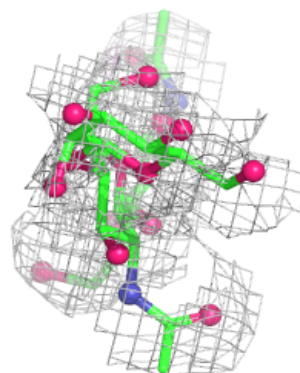
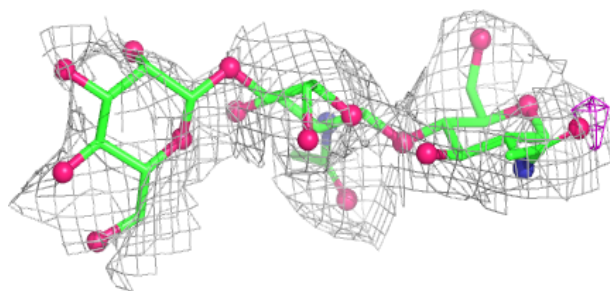
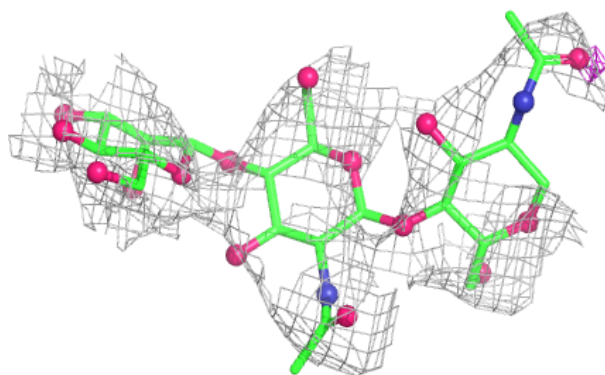
Electron density around Chain 7:

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

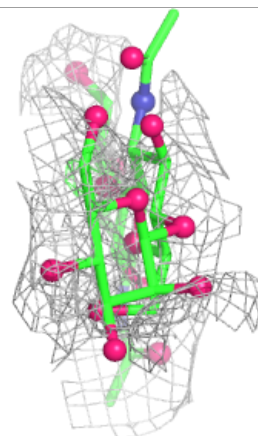
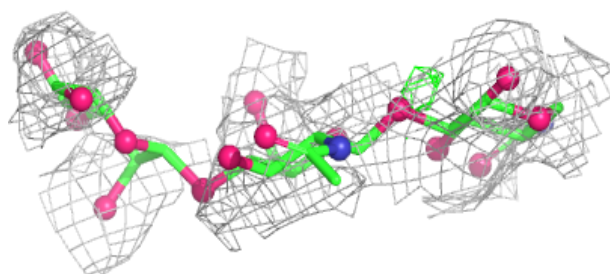
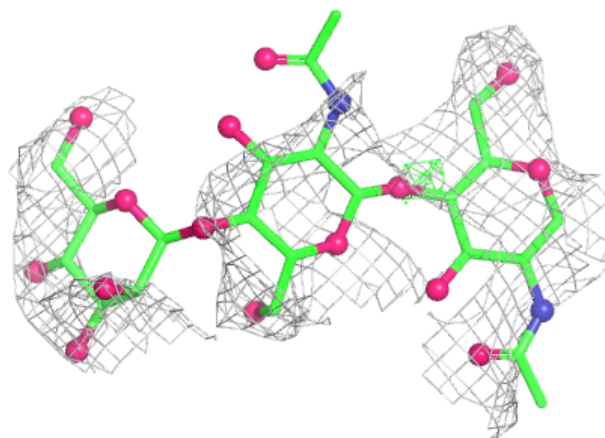


Electron density around Chain 8:

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

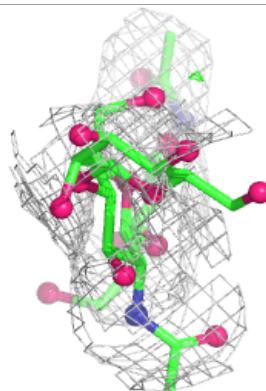
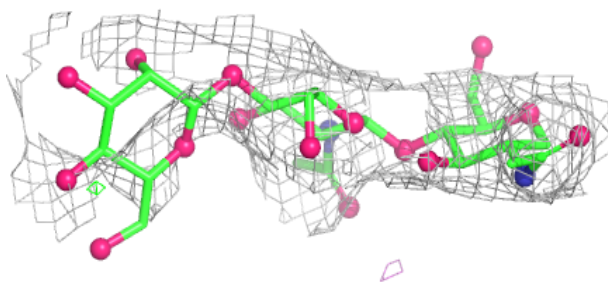
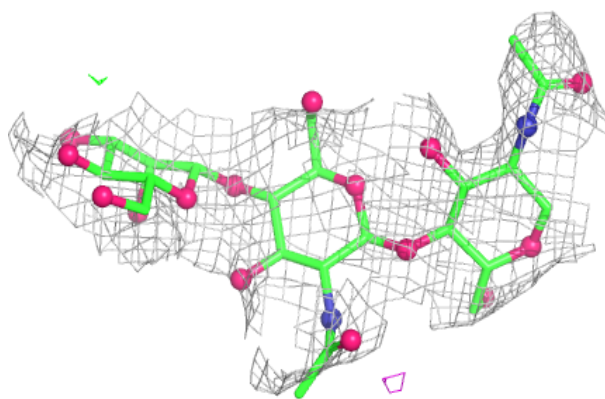
**Electron density around Chain 9:**

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

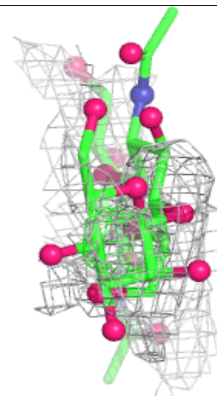
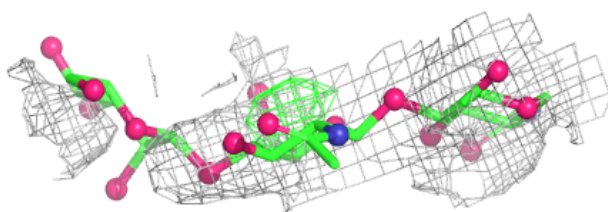
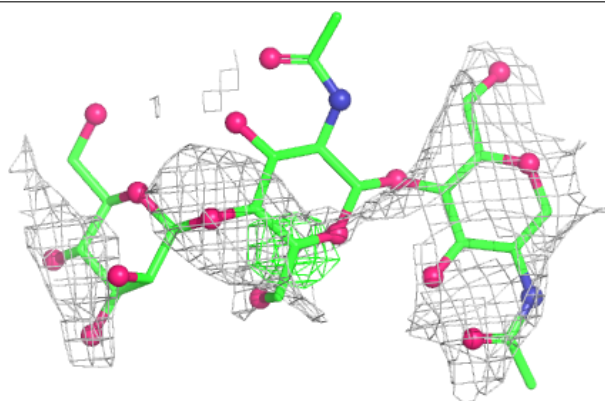


Electron density around Chain AA:

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

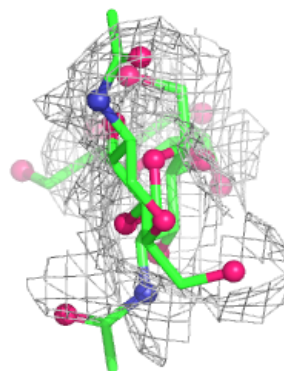
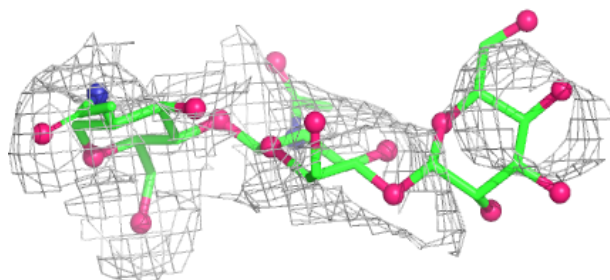
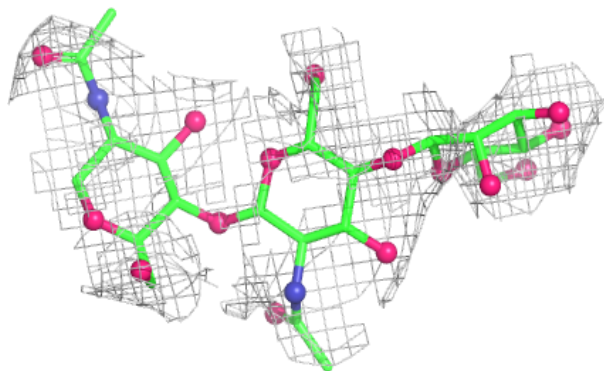
**Electron density around Chain BA:**

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

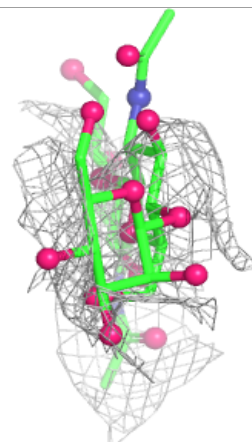
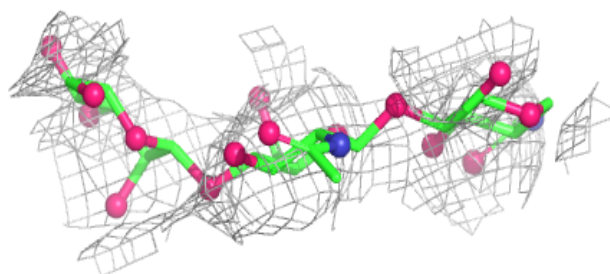
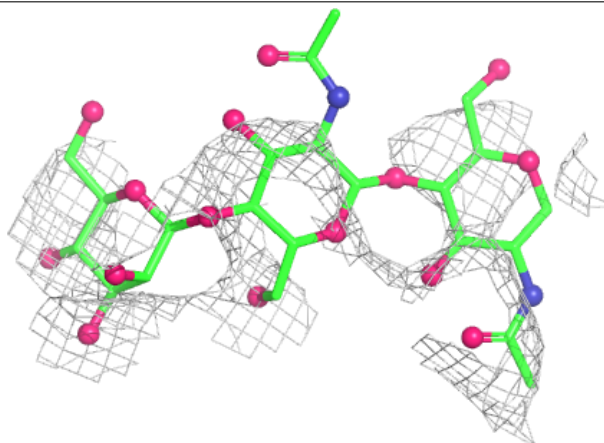


Electron density around Chain CA:

$2mF_o-DF_c$ (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

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	T	1016	5/5	0.94	0.06	89,89,89,90	5
5	SO4	S	1016	5/5	0.96	0.05	93,93,94,94	5
6	NAG	P	1022	14/15	0.96	0.07	70,70,70,70	0
6	NAG	R	1023	14/15	0.96	0.08	71,71,71,71	0
5	SO4	R	1016	5/5	0.97	0.06	78,79,81,81	5
5	SO4	Q	1007	5/5	0.97	0.11	88,88,89,89	5
5	SO4	Q	1013	5/5	0.97	0.04	66,67,67,67	5
5	SO4	U	1017	5/5	0.97	0.07	68,68,68,69	5
5	SO4	V	1010	5/5	0.97	0.05	90,90,90,90	0
6	NAG	D	1023	14/15	0.97	0.06	38,38,38,38	0
6	NAG	J	1022	14/15	0.97	0.07	51,52,52,52	0
6	NAG	M	1024	14/15	0.97	0.06	51,51,52,52	0
6	NAG	N	1023	14/15	0.97	0.07	65,66,66,66	0
5	SO4	R	1007	5/5	0.97	0.10	91,91,92,92	5
5	SO4	R	1008	5/5	0.97	0.07	84,85,85,85	5
6	NAG	S	1023	14/15	0.97	0.07	79,80,80,80	0
6	NAG	T	1023	14/15	0.97	0.06	80,80,81,81	0
6	NAG	V	1022	14/15	0.97	0.09	88,88,88,88	0
5	SO4	Q	1008	5/5	0.98	0.07	88,88,88,91	5
5	SO4	T	1006	5/5	0.98	0.07	82,82,82,82	5
5	SO4	T	1008	5/5	0.98	0.06	77,78,78,78	5
5	SO4	T	1009	5/5	0.98	0.05	68,69,69,69	5
5	SO4	T	1011	5/5	0.98	0.04	94,94,94,94	0
5	SO4	T	1014	5/5	0.98	0.06	81,81,82,82	5
5	SO4	M	1015	5/5	0.98	0.05	47,47,47,47	5
5	SO4	U	1004	5/5	0.98	0.04	85,86,86,86	0
5	SO4	U	1008	5/5	0.98	0.05	81,81,81,81	0
5	SO4	U	1009	5/5	0.98	0.06	75,75,75,75	5
5	SO4	U	1012	5/5	0.98	0.06	83,83,83,84	0
5	SO4	U	1014	5/5	0.98	0.04	81,82,83,84	5
5	SO4	U	1015	5/5	0.98	0.05	84,84,85,85	5
5	SO4	Q	1022	5/5	0.98	0.04	81,81,82,82	5
5	SO4	V	1007	5/5	0.98	0.06	75,76,76,76	5
5	SO4	O	1015	5/5	0.98	0.06	61,61,62,62	5
5	SO4	V	1011	5/5	0.98	0.09	83,84,84,84	5
6	NAG	A	1022	14/15	0.98	0.07	32,33,33,33	0
6	NAG	B	1022	14/15	0.98	0.06	30,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	P	1013	5/5	0.98	0.06	83,83,84,84	5
6	NAG	E	1023	14/15	0.98	0.06	39,39,40,40	0
6	NAG	F	1023	14/15	0.98	0.04	30,30,30,30	0
5	SO4	R	1014	5/5	0.98	0.04	55,55,55,55	5
5	SO4	J	1012	5/5	0.98	0.04	68,69,69,69	5
5	SO4	S	1007	5/5	0.98	0.07	81,81,81,82	0
6	NAG	O	1023	14/15	0.98	0.06	50,50,51,51	0
5	SO4	S	1008	5/5	0.98	0.07	90,90,91,91	5
6	NAG	Q	1021	14/15	0.98	0.05	66,67,67,67	0
5	SO4	S	1009	5/5	0.98	0.08	97,97,98,98	5
5	SO4	S	1011	5/5	0.98	0.05	86,86,86,86	5
5	SO4	S	1014	5/5	0.98	0.04	69,69,70,70	5
6	NAG	U	1024	14/15	0.98	0.06	77,77,78,78	0
5	SO4	S	1015	5/5	0.98	0.05	76,76,77,78	5
3	ZN	P	1001	1/1	0.99	0.02	44,44,44,44	0
5	SO4	J	1013	5/5	0.99	0.04	28,28,29,29	5
5	SO4	J	1014	5/5	0.99	0.03	49,49,50,50	5
5	SO4	K	1007	5/5	0.99	0.03	40,41,41,44	0
5	SO4	K	1010	5/5	0.99	0.05	36,36,36,38	5
5	SO4	K	1011	5/5	0.99	0.06	30,30,31,31	5
5	SO4	K	1013	5/5	0.99	0.04	36,36,37,37	5
5	SO4	K	1014	5/5	0.99	0.03	47,48,48,48	5
5	SO4	K	1015	5/5	0.99	0.06	35,36,36,39	5
5	SO4	K	1016	5/5	0.99	0.05	31,31,31,31	5
5	SO4	K	1024	5/5	0.99	0.03	50,51,54,54	0
5	SO4	L	1006	5/5	0.99	0.05	40,40,41,43	5
5	SO4	L	1011	5/5	0.99	0.03	30,31,31,31	5
5	SO4	L	1012	5/5	0.99	0.04	31,31,32,34	5
5	SO4	L	1013	5/5	0.99	0.04	48,48,50,50	5
5	SO4	L	1014	5/5	0.99	0.05	33,33,34,36	5
5	SO4	L	1015	5/5	0.99	0.03	42,43,43,45	5
5	SO4	M	1007	5/5	0.99	0.04	39,39,39,40	0
5	SO4	M	1012	5/5	0.99	0.05	37,38,38,38	5
5	SO4	M	1014	5/5	0.99	0.06	55,55,55,56	5
3	ZN	U	1002	1/1	0.99	0.02	66,66,66,66	0
5	SO4	M	1016	5/5	0.99	0.07	41,41,41,41	5
5	SO4	M	1017	5/5	0.99	0.04	31,31,32,32	5
5	SO4	N	1006	5/5	0.99	0.05	60,60,60,61	5
5	SO4	N	1007	5/5	0.99	0.03	56,56,56,57	0
5	SO4	N	1010	5/5	0.99	0.04	57,57,57,57	5
5	SO4	N	1011	5/5	0.99	0.05	51,52,52,52	5
5	SO4	N	1012	5/5	0.99	0.10	72,72,72,73	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	N	1013	5/5	0.99	0.04	75,75,75,75	5
5	SO4	N	1014	5/5	0.99	0.05	64,64,64,65	5
5	SO4	N	1015	5/5	0.99	0.04	61,61,61,61	5
5	SO4	N	1016	5/5	0.99	0.03	43,44,47,47	5
5	SO4	O	1005	5/5	0.99	0.04	44,44,46,46	5
5	SO4	O	1008	5/5	0.99	0.04	63,63,63,67	0
5	SO4	O	1010	5/5	0.99	0.03	28,28,29,31	0
5	SO4	O	1011	5/5	0.99	0.07	57,57,57,61	5
5	SO4	O	1012	5/5	0.99	0.06	42,43,43,43	5
5	SO4	O	1013	5/5	0.99	0.05	76,76,76,76	5
5	SO4	O	1014	5/5	0.99	0.03	36,36,36,39	5
4	P52	E	1003	36/36	0.99	0.05	12,12,14,14	0
5	SO4	O	1016	5/5	0.99	0.06	54,54,54,55	5
5	SO4	P	1003	5/5	0.99	0.03	51,52,52,53	0
5	SO4	P	1004	5/5	0.99	0.04	67,67,67,67	0
5	SO4	P	1005	5/5	0.99	0.05	66,67,67,67	0
5	SO4	P	1009	5/5	0.99	0.04	68,68,68,68	0
5	SO4	P	1010	5/5	0.99	0.05	66,67,67,67	5
5	SO4	P	1011	5/5	0.99	0.04	66,66,66,66	5
5	SO4	P	1012	5/5	0.99	0.03	63,63,63,63	5
4	P52	M	1003	36/36	0.99	0.06	34,35,36,36	0
5	SO4	P	1015	5/5	0.99	0.03	60,60,60,60	5
5	SO4	Q	1003	5/5	0.99	0.03	62,62,63,63	0
5	SO4	Q	1004	5/5	0.99	0.03	46,46,46,47	0
5	SO4	Q	1005	5/5	0.99	0.05	41,42,42,42	5
4	P52	N	1003	36/36	0.99	0.06	44,45,46,49	0
4	P52	P	1002	36/36	0.99	0.06	46,47,49,49	0
5	SO4	Q	1009	5/5	0.99	0.04	65,65,65,66	5
5	SO4	Q	1010	5/5	0.99	0.06	50,51,51,51	5
5	SO4	Q	1011	5/5	0.99	0.03	72,72,72,73	5
4	P52	Q	1002	36/36	0.99	0.05	43,44,45,45	0
5	SO4	Q	1014	5/5	0.99	0.05	74,74,74,74	5
4	P52	R	1002	36/36	0.99	0.05	45,45,46,47	0
5	SO4	R	1003	5/5	0.99	0.02	65,65,66,66	0
5	SO4	R	1005	5/5	0.99	0.07	49,49,49,49	5
4	P52	S	1003	36/36	0.99	0.07	66,68,69,69	0
4	P52	T	1003	36/36	0.99	0.08	67,69,71,71	0
5	SO4	R	1011	5/5	0.99	0.03	78,78,78,79	5
5	SO4	R	1012	5/5	0.99	0.06	57,57,58,58	0
5	SO4	R	1013	5/5	0.99	0.04	83,83,83,83	5
4	P52	U	1003	36/36	0.99	0.07	66,67,67,68	0
4	P52	V	1002	36/36	0.99	0.07	70,72,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	R	1024	5/5	0.99	0.04	83,83,84,84	0
5	SO4	S	1001	5/5	0.99	0.04	80,80,81,81	0
5	SO4	S	1004	5/5	0.99	0.04	84,84,84,84	0
5	SO4	S	1005	5/5	0.99	0.03	67,67,67,68	0
5	SO4	S	1006	5/5	0.99	0.07	76,76,76,77	0
5	SO4	A	1012	5/5	0.99	0.03	39,40,40,40	5
5	SO4	A	1013	5/5	0.99	0.03	25,25,25,25	5
5	SO4	A	1014	5/5	0.99	0.05	26,26,26,26	5
5	SO4	S	1010	5/5	0.99	0.04	69,69,69,69	5
5	SO4	B	1012	5/5	0.99	0.02	27,27,27,27	5
5	SO4	S	1012	5/5	0.99	0.05	81,81,81,82	0
5	SO4	S	1013	5/5	0.99	0.04	90,90,91,91	0
5	SO4	B	1013	5/5	0.99	0.04	18,18,18,18	5
5	SO4	C	1005	5/5	0.99	0.03	23,23,23,24	5
5	SO4	C	1010	5/5	0.99	0.04	24,24,25,25	5
5	SO4	T	1001	5/5	0.99	0.03	75,76,76,76	0
5	SO4	T	1004	5/5	0.99	0.03	82,82,82,83	5
5	SO4	T	1005	5/5	0.99	0.03	79,79,79,79	0
5	SO4	C	1012	5/5	0.99	0.03	38,38,38,39	5
5	SO4	T	1007	5/5	0.99	0.04	80,81,81,81	0
5	SO4	C	1013	5/5	0.99	0.03	19,19,19,19	5
5	SO4	C	1015	5/5	0.99	0.03	19,20,20,20	5
5	SO4	T	1010	5/5	0.99	0.04	68,68,68,68	5
5	SO4	D	1011	5/5	0.99	0.03	24,24,24,24	5
5	SO4	T	1012	5/5	0.99	0.07	73,73,73,74	5
5	SO4	T	1013	5/5	0.99	0.03	98,99,99,99	0
5	SO4	D	1013	5/5	0.99	0.02	40,40,40,40	5
5	SO4	T	1015	5/5	0.99	0.04	67,67,67,68	5
5	SO4	D	1014	5/5	0.99	0.02	18,18,18,19	5
5	SO4	U	1001	5/5	0.99	0.04	65,65,65,66	5
5	SO4	E	1005	5/5	0.99	0.03	32,33,33,33	0
5	SO4	U	1005	5/5	0.99	0.04	74,74,74,74	0
5	SO4	U	1006	5/5	0.99	0.06	73,73,73,74	5
5	SO4	U	1007	5/5	0.99	0.04	83,83,83,83	0
5	SO4	E	1006	5/5	0.99	0.05	22,23,24,24	5
5	SO4	E	1012	5/5	0.99	0.06	17,17,20,21	5
5	SO4	U	1011	5/5	0.99	0.05	75,75,75,75	5
5	SO4	E	1013	5/5	0.99	0.03	43,43,43,43	5
5	SO4	U	1013	5/5	0.99	0.06	78,78,78,78	5
5	SO4	E	1014	5/5	0.99	0.04	17,17,18,18	5
5	SO4	E	1015	5/5	0.99	0.03	42,42,43,43	5
5	SO4	U	1016	5/5	0.99	0.04	67,67,68,68	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	F	1011	5/5	0.99	0.04	25,25,25,25	5
5	SO4	V	1003	5/5	0.99	0.04	81,82,82,82	0
5	SO4	V	1004	5/5	0.99	0.03	78,78,78,78	0
5	SO4	V	1005	5/5	0.99	0.06	84,84,84,84	5
5	SO4	V	1006	5/5	0.99	0.05	86,86,87,87	0
5	SO4	F	1012	5/5	0.99	0.06	15,15,15,15	5
5	SO4	V	1008	5/5	0.99	0.04	75,75,75,75	5
5	SO4	V	1009	5/5	0.99	0.04	81,81,81,81	0
5	SO4	F	1014	5/5	0.99	0.04	16,16,16,17	5
5	SO4	F	1015	5/5	0.99	0.04	36,36,36,36	5
5	SO4	V	1012	5/5	0.99	0.04	93,94,94,94	0
5	SO4	V	1013	5/5	0.99	0.05	88,88,88,88	5
5	SO4	V	1014	5/5	0.99	0.03	75,75,75,78	5
5	SO4	V	1015	5/5	0.99	0.02	78,79,79,79	5
5	SO4	G	1005	5/5	0.99	0.03	26,26,27,27	5
5	SO4	G	1013	5/5	0.99	0.04	49,49,50,50	5
6	NAG	C	1022	14/15	0.99	0.06	31,31,32,32	0
5	SO4	G	1015	5/5	0.99	0.05	34,34,34,34	5
5	SO4	H	1006	5/5	0.99	0.04	33,34,35,35	5
5	SO4	H	1011	5/5	0.99	0.04	16,17,19,20	5
6	NAG	G	1023	14/15	0.99	0.06	32,33,33,34	0
6	NAG	H	1023	14/15	0.99	0.06	41,41,41,41	0
6	NAG	I	1023	14/15	0.99	0.05	40,41,41,41	0
5	SO4	H	1013	5/5	0.99	0.03	43,43,43,44	5
6	NAG	K	1023	14/15	0.99	0.06	42,42,43,43	0
6	NAG	L	1023	14/15	0.99	0.06	41,41,41,41	0
5	SO4	H	1014	5/5	0.99	0.04	27,28,28,28	5
5	SO4	H	1015	5/5	0.99	0.03	43,43,44,46	5
5	SO4	I	1010	5/5	0.99	0.04	36,36,37,40	5
5	SO4	I	1011	5/5	0.99	0.04	25,26,26,28	5
5	SO4	I	1012	5/5	0.99	0.04	36,37,37,40	0
5	SO4	I	1013	5/5	0.99	0.03	45,45,45,48	5
5	SO4	I	1014	5/5	0.99	0.03	35,35,35,35	5
5	SO4	I	1015	5/5	0.99	0.03	42,42,42,47	5
5	SO4	J	1005	5/5	0.99	0.04	31,32,32,32	5
5	SO4	J	1010	5/5	0.99	0.04	43,44,44,46	0
5	SO4	L	1001	5/5	1.00	0.02	17,17,18,19	0
5	SO4	L	1004	5/5	1.00	0.02	32,32,34,35	0
5	SO4	L	1005	5/5	1.00	0.03	45,45,45,45	0
5	SO4	B	1008	5/5	1.00	0.02	13,13,13,13	0
5	SO4	L	1007	5/5	1.00	0.02	24,24,25,26	0
5	SO4	L	1008	5/5	1.00	0.02	14,14,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	L	1009	5/5	1.00	0.02	18,18,19,19	0
5	SO4	L	1010	5/5	1.00	0.02	28,28,29,29	5
5	SO4	B	1009	5/5	1.00	0.02	11,11,11,11	0
5	SO4	B	1010	5/5	1.00	0.04	18,18,18,18	5
5	SO4	B	1011	5/5	1.00	0.06	12,12,13,13	5
3	ZN	A	1001	1/1	1.00	0.02	8,8,8,8	0
3	ZN	Q	1001	1/1	1.00	0.02	46,46,46,46	0
5	SO4	L	1016	5/5	1.00	0.02	23,24,24,24	5
5	SO4	M	1001	5/5	1.00	0.02	26,28,29,30	0
5	SO4	M	1004	5/5	1.00	0.02	41,42,42,43	5
5	SO4	M	1005	5/5	1.00	0.03	42,42,42,42	0
5	SO4	M	1006	5/5	1.00	0.02	45,45,45,46	5
5	SO4	B	1014	5/5	1.00	0.03	25,25,26,26	5
5	SO4	M	1008	5/5	1.00	0.02	27,28,28,31	0
5	SO4	M	1009	5/5	1.00	0.02	28,28,28,29	0
5	SO4	M	1010	5/5	1.00	0.02	44,44,44,45	0
5	SO4	M	1011	5/5	1.00	0.03	45,46,46,46	0
5	SO4	B	1015	5/5	1.00	0.03	18,18,18,18	5
5	SO4	M	1013	5/5	1.00	0.03	43,43,43,44	5
5	SO4	B	1023	5/5	1.00	0.02	16,16,16,16	0
5	SO4	C	1003	5/5	1.00	0.02	21,21,22,22	0
5	SO4	C	1004	5/5	1.00	0.02	20,20,20,20	0
3	ZN	R	1001	1/1	1.00	0.01	43,43,43,43	0
5	SO4	N	1001	5/5	1.00	0.01	34,34,37,38	0
5	SO4	N	1004	5/5	1.00	0.03	45,46,46,46	0
5	SO4	N	1005	5/5	1.00	0.02	58,58,58,58	0
5	SO4	C	1006	5/5	1.00	0.02	13,13,13,13	0
5	SO4	C	1007	5/5	1.00	0.02	19,19,20,20	0
5	SO4	N	1008	5/5	1.00	0.03	35,35,35,36	0
5	SO4	N	1009	5/5	1.00	0.02	41,41,45,45	0
5	SO4	C	1008	5/5	1.00	0.02	18,18,18,18	0
5	SO4	C	1009	5/5	1.00	0.02	11,11,11,11	5
3	ZN	S	1002	1/1	1.00	0.02	59,59,59,59	0
5	SO4	C	1011	5/5	1.00	0.02	16,16,17,17	5
3	ZN	T	1002	1/1	1.00	0.01	57,57,57,57	0
3	ZN	B	1001	1/1	1.00	0.02	7,7,7,7	0
5	SO4	C	1014	5/5	1.00	0.03	29,29,30,30	5
5	SO4	O	1003	5/5	1.00	0.02	42,43,43,43	0
5	SO4	O	1004	5/5	1.00	0.02	39,39,39,39	0
3	ZN	V	1001	1/1	1.00	0.01	67,67,67,67	0
5	SO4	O	1006	5/5	1.00	0.03	36,36,36,37	0
5	SO4	O	1007	5/5	1.00	0.03	55,56,56,59	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	1023	5/5	1.00	0.02	20,21,23,24	0
5	SO4	O	1009	5/5	1.00	0.02	34,35,35,37	0
5	SO4	D	1001	5/5	1.00	0.02	15,15,15,15	0
5	SO4	D	1004	5/5	1.00	0.02	21,21,21,21	0
5	SO4	D	1005	5/5	1.00	0.02	27,27,27,27	0
5	SO4	D	1006	5/5	1.00	0.04	24,24,24,24	5
5	SO4	D	1007	5/5	1.00	0.02	15,15,15,15	0
5	SO4	D	1008	5/5	1.00	0.02	15,15,15,15	0
5	SO4	D	1009	5/5	1.00	0.01	15,15,15,15	0
5	SO4	D	1010	5/5	1.00	0.03	11,11,11,12	5
4	P52	A	1002	36/36	1.00	0.04	9,10,10,10	0
5	SO4	D	1012	5/5	1.00	0.03	20,20,20,20	5
5	SO4	P	1006	5/5	1.00	0.02	55,55,55,56	0
5	SO4	P	1007	5/5	1.00	0.03	49,49,49,52	0
5	SO4	P	1008	5/5	1.00	0.02	54,55,55,55	0
4	P52	B	1002	36/36	1.00	0.04	10,11,12,12	36
4	P52	C	1002	36/36	1.00	0.04	12,13,14,14	0
5	SO4	D	1015	5/5	1.00	0.02	43,43,43,43	5
5	SO4	D	1016	5/5	1.00	0.04	20,20,20,20	5
5	SO4	E	1001	5/5	1.00	0.02	16,16,16,16	0
5	SO4	P	1014	5/5	1.00	0.04	57,57,58,58	5
5	SO4	E	1004	5/5	1.00	0.02	19,20,21,21	0
4	P52	D	1003	36/36	1.00	0.04	17,17,17,17	0
3	ZN	C	1001	1/1	1.00	0.01	20,20,20,20	0
5	SO4	E	1007	5/5	1.00	0.03	17,18,18,18	0
5	SO4	Q	1006	5/5	1.00	0.03	45,45,46,46	0
5	SO4	E	1008	5/5	1.00	0.02	12,12,12,12	0
5	SO4	E	1009	5/5	1.00	0.02	11,11,12,12	0
5	SO4	E	1010	5/5	1.00	0.03	17,18,18,18	5
5	SO4	E	1011	5/5	1.00	0.04	19,19,20,20	5
4	P52	F	1003	36/36	1.00	0.04	12,12,12,12	0
5	SO4	Q	1012	5/5	1.00	0.02	38,39,39,39	5
4	P52	G	1002	36/36	1.00	0.03	14,15,15,15	0
4	P52	H	1003	36/36	1.00	0.05	15,16,17,17	0
4	P52	I	1003	36/36	1.00	0.05	28,29,31,31	0
5	SO4	E	1016	5/5	1.00	0.03	12,12,13,13	5
5	SO4	R	1004	5/5	1.00	0.02	56,56,56,56	0
5	SO4	F	1001	5/5	1.00	0.02	17,17,18,18	0
5	SO4	R	1006	5/5	1.00	0.03	54,55,55,55	5
5	SO4	F	1004	5/5	1.00	0.02	23,23,24,24	0
5	SO4	F	1005	5/5	1.00	0.02	22,22,22,22	0
5	SO4	R	1009	5/5	1.00	0.02	53,54,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	R	1010	5/5	1.00	0.02	45,45,45,45	0
5	SO4	F	1006	5/5	1.00	0.04	22,22,22,22	5
5	SO4	F	1007	5/5	1.00	0.01	16,16,16,16	0
5	SO4	F	1008	5/5	1.00	0.02	12,12,13,13	0
5	SO4	F	1009	5/5	1.00	0.02	11,11,11,12	0
5	SO4	R	1015	5/5	1.00	0.03	53,53,53,53	5
5	SO4	F	1010	5/5	1.00	0.02	14,14,14,14	0
4	P52	J	1002	36/36	1.00	0.04	22,24,33,35	0
4	P52	K	1002	36/36	1.00	0.04	27,28,29,29	0
5	SO4	F	1013	5/5	1.00	0.02	37,37,37,38	5
4	P52	L	1003	36/36	1.00	0.04	22,24,28,29	36
3	ZN	D	1002	1/1	1.00	0.01	8,8,8,8	0
5	SO4	F	1016	5/5	1.00	0.02	18,18,19,19	5
5	SO4	G	1003	5/5	1.00	0.02	18,18,19,19	0
5	SO4	G	1004	5/5	1.00	0.02	25,25,25,25	0
3	ZN	E	1002	1/1	1.00	0.01	12,12,12,12	0
5	SO4	G	1006	5/5	1.00	0.02	13,14,14,14	0
5	SO4	G	1007	5/5	1.00	0.02	22,23,23,23	0
5	SO4	G	1008	5/5	1.00	0.03	20,20,20,21	0
5	SO4	G	1009	5/5	1.00	0.02	11,11,11,12	0
5	SO4	G	1010	5/5	1.00	0.02	10,10,10,10	5
5	SO4	G	1011	5/5	1.00	0.02	22,22,22,23	5
5	SO4	G	1012	5/5	1.00	0.03	17,18,18,20	5
4	P52	O	1002	36/36	1.00	0.04	32,33,35,35	0
5	SO4	G	1014	5/5	1.00	0.03	11,11,11,12	5
3	ZN	F	1002	1/1	1.00	0.02	8,8,8,8	0
5	SO4	G	1016	5/5	1.00	0.02	21,21,22,22	5
5	SO4	G	1024	5/5	1.00	0.02	22,22,22,23	0
5	SO4	H	1001	5/5	1.00	0.01	10,10,10,10	0
5	SO4	H	1004	5/5	1.00	0.02	23,23,24,24	0
5	SO4	H	1005	5/5	1.00	0.03	40,40,40,40	0
3	ZN	G	1001	1/1	1.00	0.02	16,16,16,16	0
5	SO4	H	1007	5/5	1.00	0.03	19,19,19,20	0
5	SO4	H	1008	5/5	1.00	0.03	10,10,10,10	0
5	SO4	H	1009	5/5	1.00	0.02	11,11,11,12	0
5	SO4	H	1010	5/5	1.00	0.02	22,24,24,25	0
3	ZN	H	1002	1/1	1.00	0.01	15,15,15,15	0
5	SO4	H	1012	5/5	1.00	0.04	24,24,24,25	5
3	ZN	I	1002	1/1	1.00	0.01	29,29,29,29	0
3	ZN	J	1001	1/1	1.00	0.01	23,23,23,23	0
3	ZN	K	1001	1/1	1.00	0.02	29,29,29,29	0
5	SO4	H	1016	5/5	1.00	0.02	13,14,14,14	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	I	1001	5/5	1.00	0.02	19,20,20,20	0
5	SO4	U	1010	5/5	1.00	0.03	71,72,72,72	0
5	SO4	I	1004	5/5	1.00	0.02	29,29,30,33	0
5	SO4	I	1005	5/5	1.00	0.02	36,36,36,36	0
5	SO4	I	1006	5/5	1.00	0.03	36,36,40,42	5
5	SO4	I	1007	5/5	1.00	0.03	29,30,30,31	5
5	SO4	I	1008	5/5	1.00	0.02	19,20,20,20	0
5	SO4	I	1009	5/5	1.00	0.02	22,22,22,22	0
3	ZN	L	1002	1/1	1.00	0.01	26,26,26,26	0
5	SO4	A	1003	5/5	1.00	0.02	20,20,20,21	0
5	SO4	A	1004	5/5	1.00	0.01	18,18,18,19	0
5	SO4	A	1005	5/5	1.00	0.03	23,23,23,23	5
5	SO4	A	1006	5/5	1.00	0.02	16,16,16,16	0
5	SO4	A	1007	5/5	1.00	0.02	11,11,11,11	0
5	SO4	I	1016	5/5	1.00	0.03	30,30,30,31	5
5	SO4	J	1003	5/5	1.00	0.02	31,31,31,32	5
5	SO4	J	1004	5/5	1.00	0.02	37,37,37,37	0
5	SO4	A	1008	5/5	1.00	0.02	9,9,10,10	0
5	SO4	J	1006	5/5	1.00	0.01	25,25,26,26	0
5	SO4	J	1007	5/5	1.00	0.02	29,29,30,32	0
5	SO4	J	1008	5/5	1.00	0.02	28,30,31,31	0
5	SO4	J	1009	5/5	1.00	0.02	19,19,19,20	0
5	SO4	A	1009	5/5	1.00	0.02	17,17,17,17	0
5	SO4	J	1011	5/5	1.00	0.07	32,32,32,34	5
5	SO4	A	1010	5/5	1.00	0.03	21,21,22,22	5
5	SO4	A	1011	5/5	1.00	0.04	14,14,14,14	5
3	ZN	M	1002	1/1	1.00	0.01	35,35,35,35	0
5	SO4	J	1015	5/5	1.00	0.03	38,39,42,42	5
5	SO4	K	1003	5/5	1.00	0.01	37,37,37,38	0
5	SO4	K	1004	5/5	1.00	0.02	30,30,30,31	0
5	SO4	K	1005	5/5	1.00	0.06	36,36,37,37	0
5	SO4	K	1006	5/5	1.00	0.02	25,25,26,28	0
3	ZN	N	1002	1/1	1.00	0.01	40,40,40,40	0
5	SO4	K	1008	5/5	1.00	0.02	42,43,43,43	0
5	SO4	K	1009	5/5	1.00	0.01	21,21,21,21	0
3	ZN	O	1001	1/1	1.00	0.02	34,34,34,34	0
5	SO4	A	1015	5/5	1.00	0.04	16,16,16,17	5
5	SO4	K	1012	5/5	1.00	0.02	59,59,60,60	0
5	SO4	B	1003	5/5	1.00	0.01	18,18,18,19	0
5	SO4	B	1004	5/5	1.00	0.02	20,20,20,20	0
5	SO4	B	1005	5/5	1.00	0.02	25,25,25,25	5
5	SO4	B	1006	5/5	1.00	0.01	12,12,12,12	0

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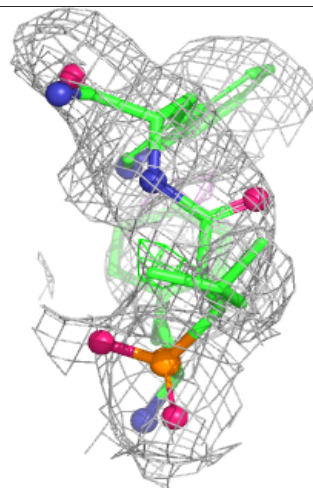
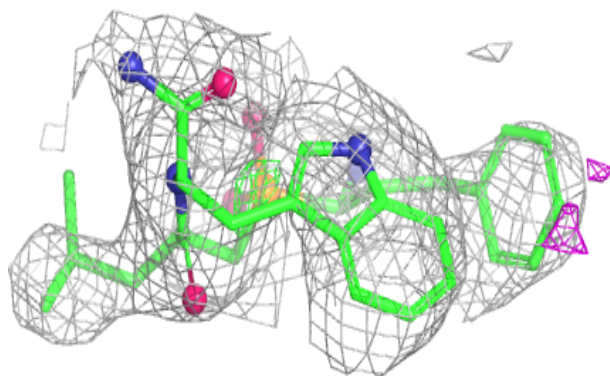
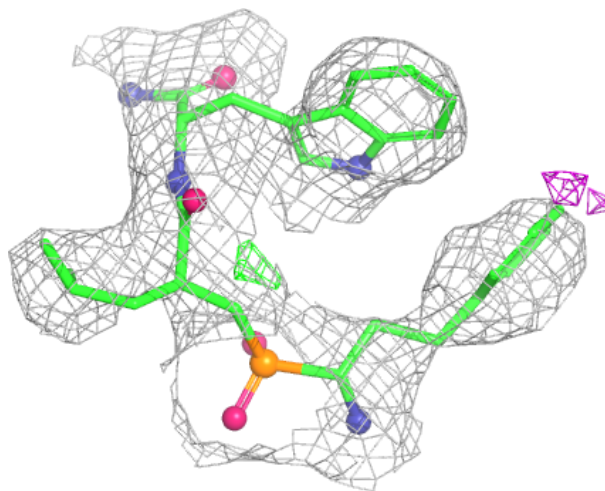
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	1007	5/5	1.00	0.02	15,15,15,15	0
5	SO4	K	1025	5/5	1.00	0.02	35,35,36,36	0

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.

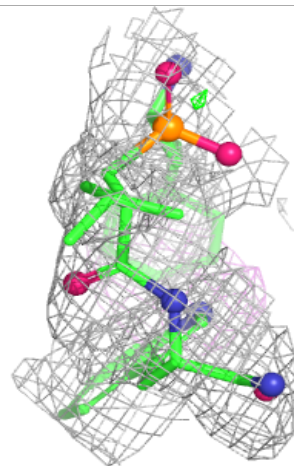
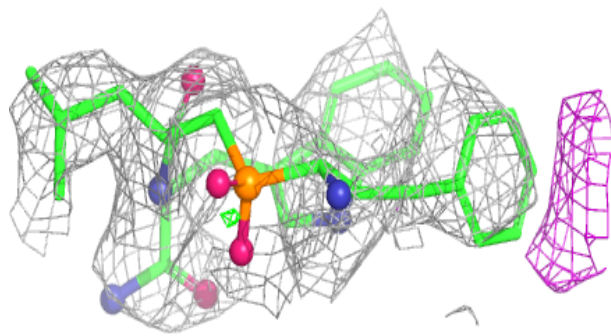
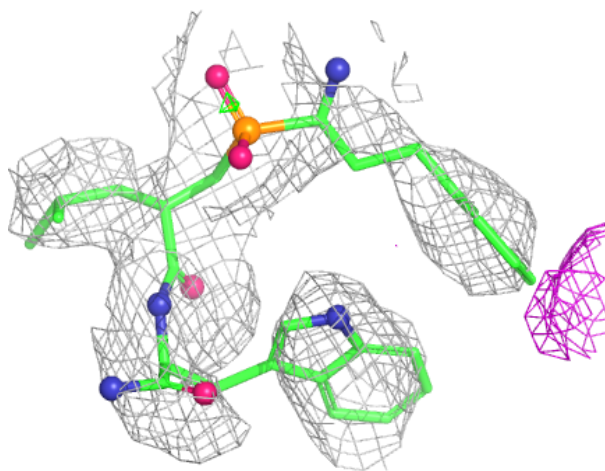
Electron density around P52 E 1003:

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



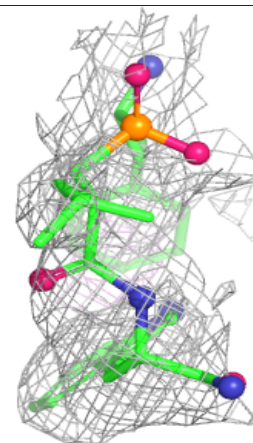
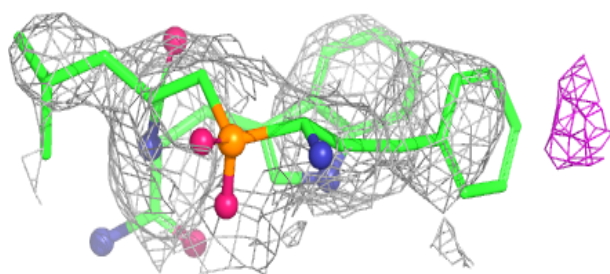
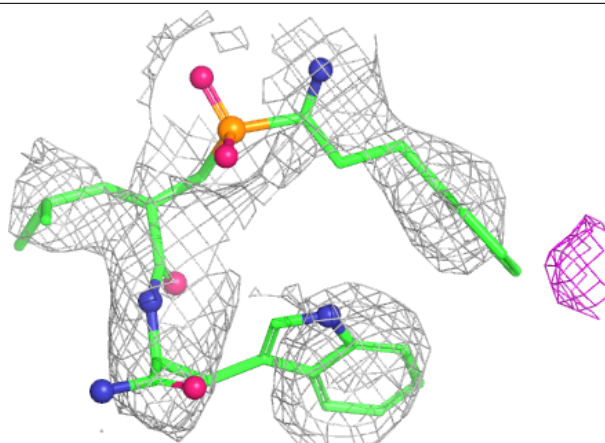
Electron density around P52 M 1003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



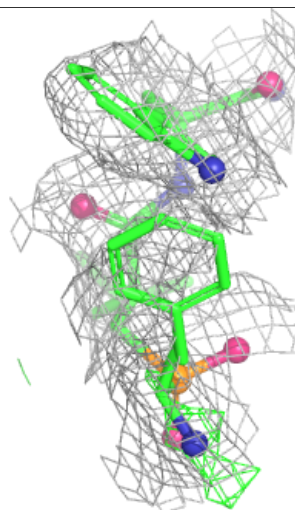
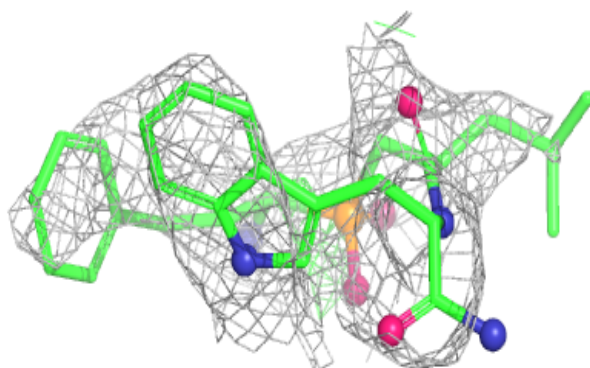
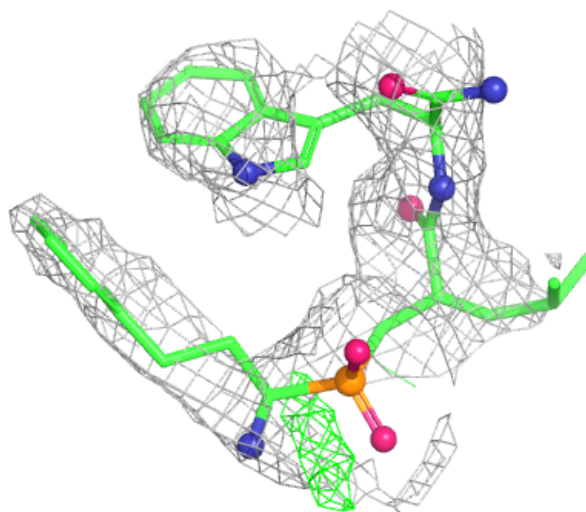
Electron density around P52 N 1003:

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and green (positive)



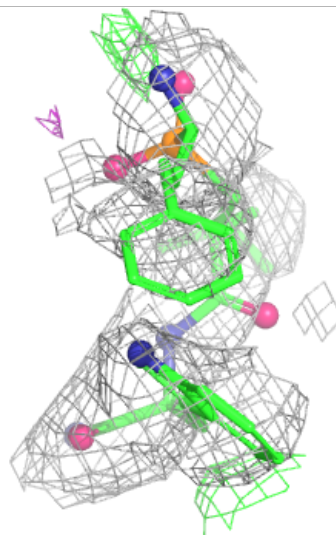
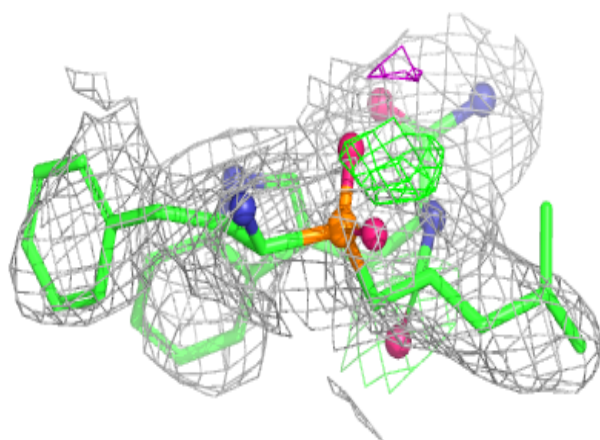
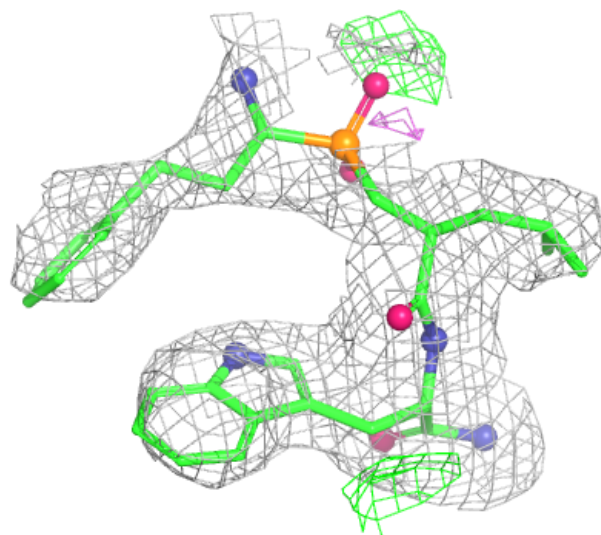
Electron density around P52 P 1002:

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



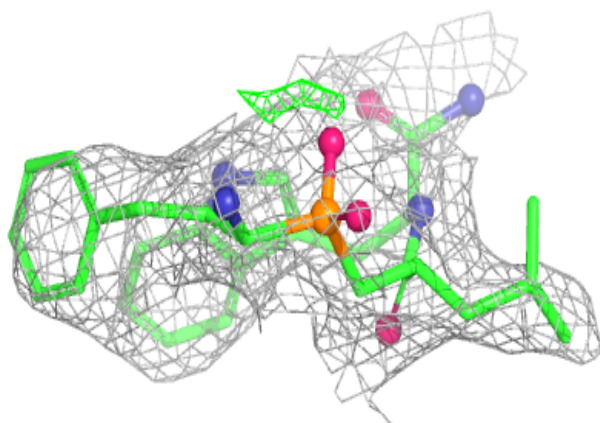
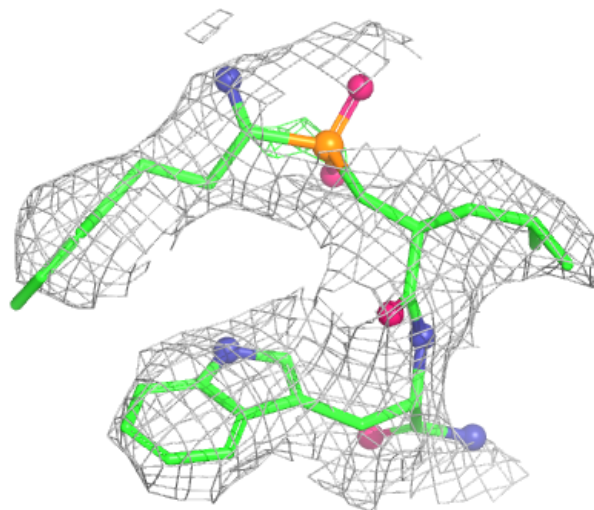
Electron density around P52 Q 1002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



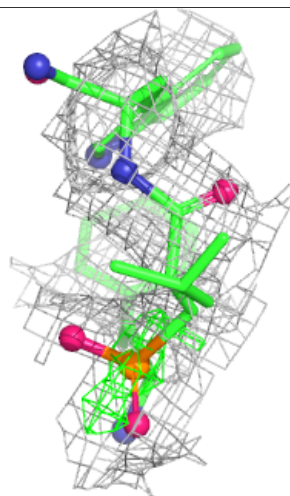
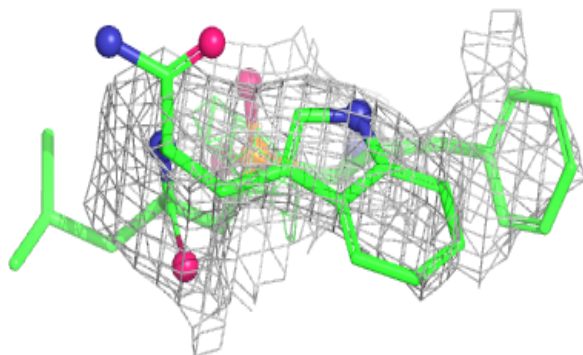
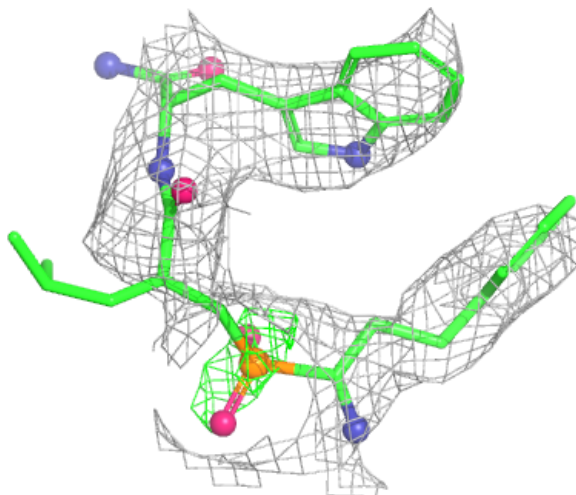
Electron density around P52 R 1002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



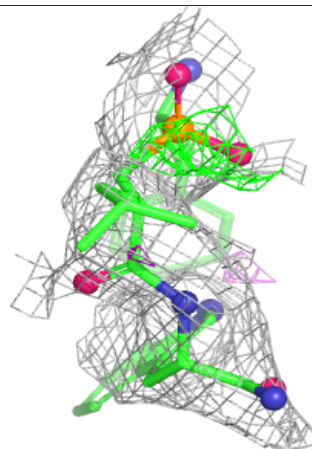
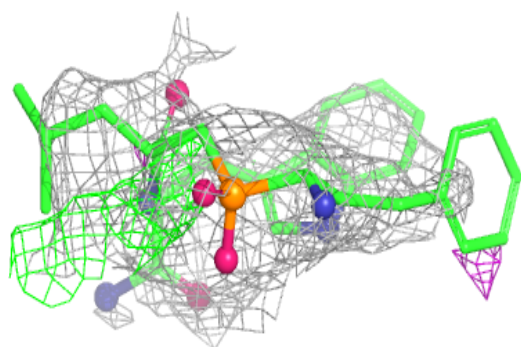
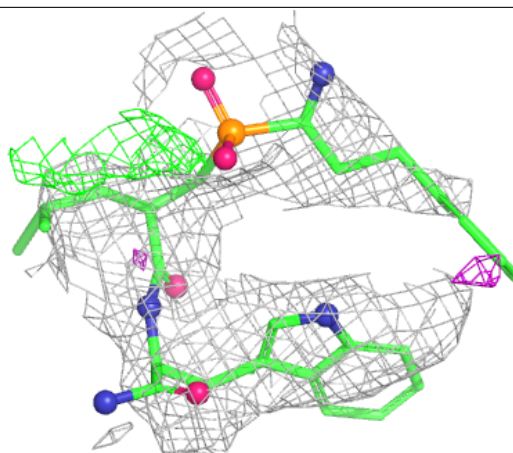
Electron density around P52 S 1003:

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



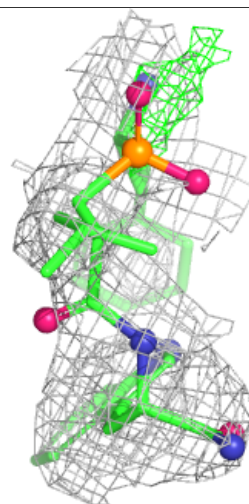
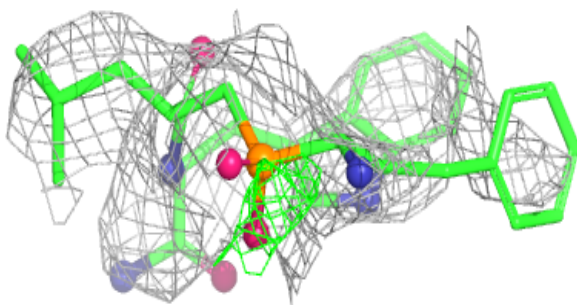
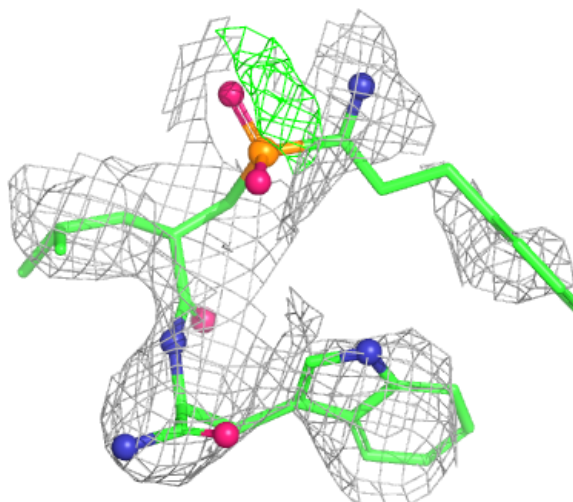
Electron density around P52 T 1003:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



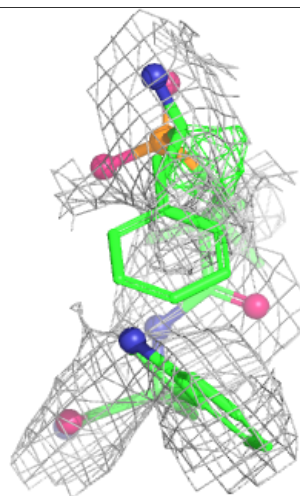
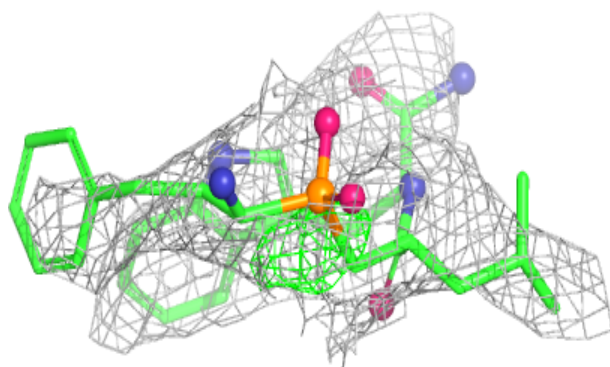
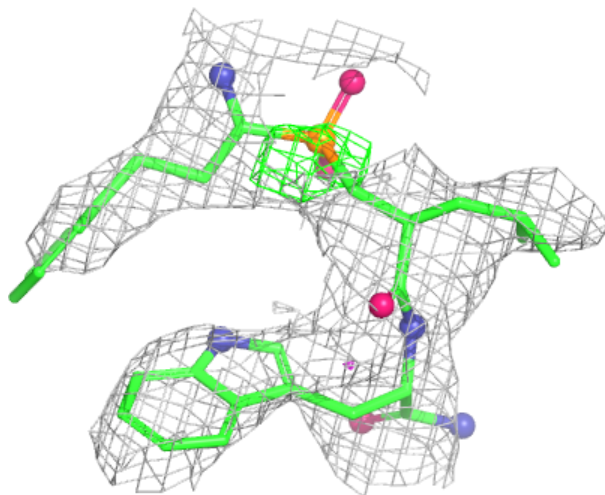
Electron density around P52 U 1003:

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



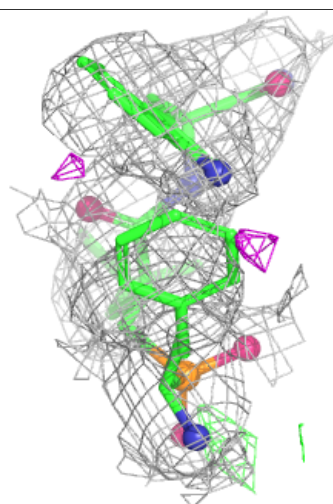
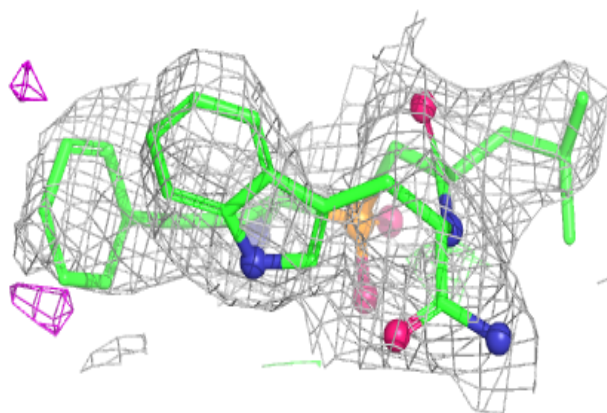
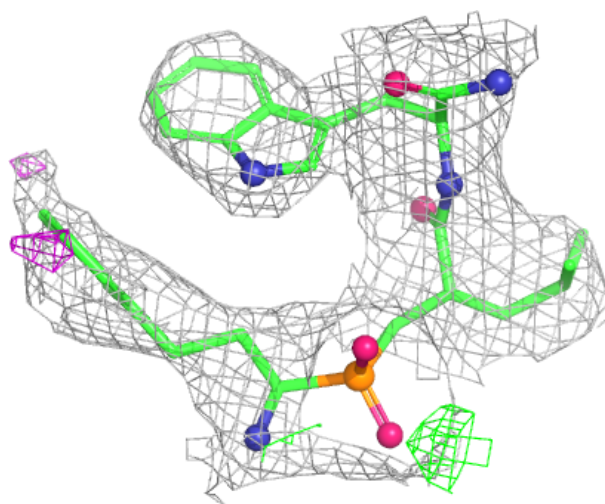
Electron density around P52 V 1002:

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



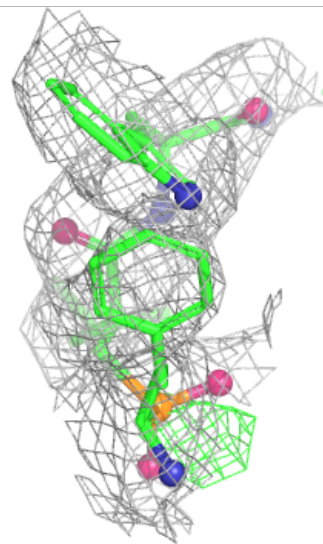
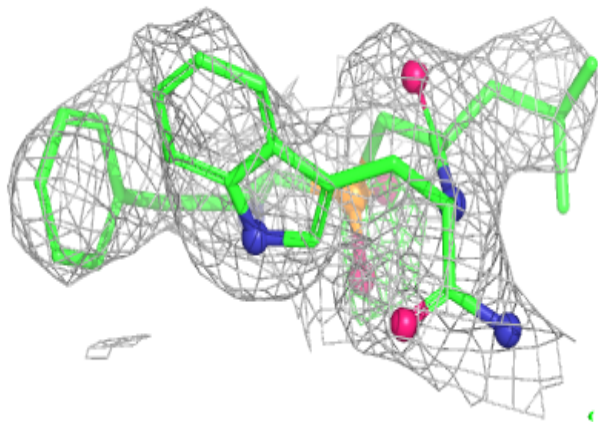
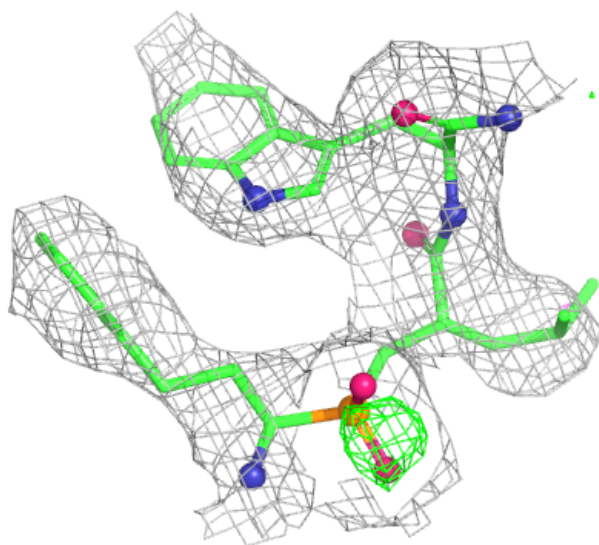
Electron density around P52 A 1002:

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



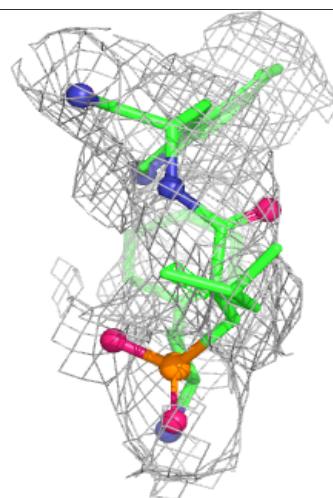
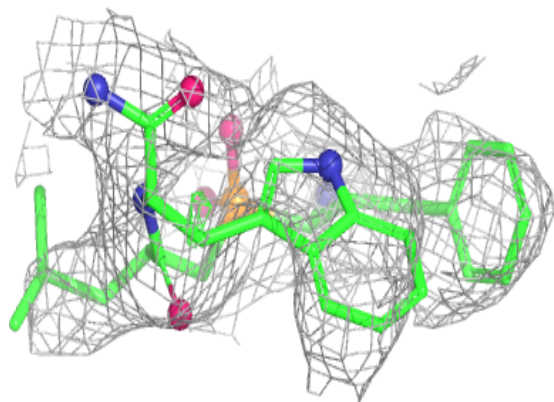
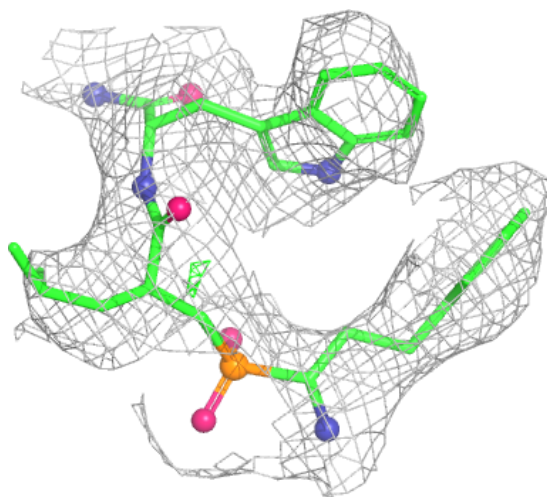
Electron density around P52 B 1002:

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



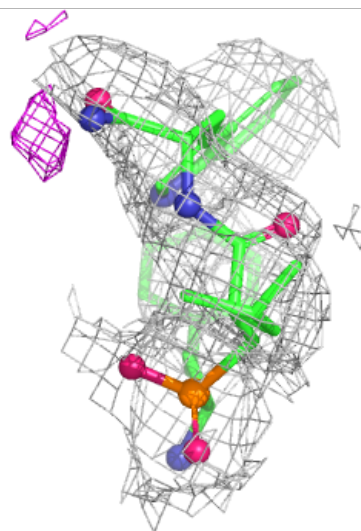
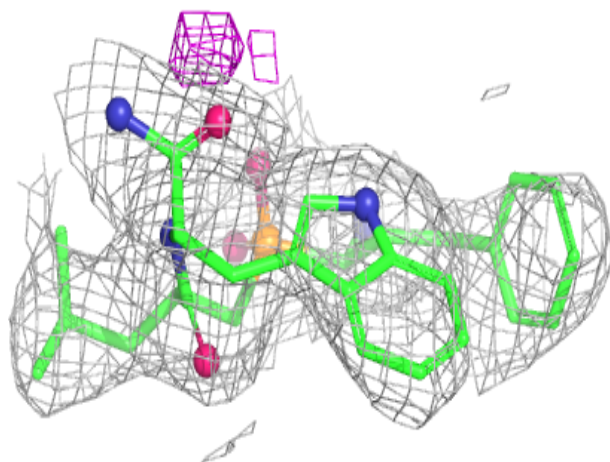
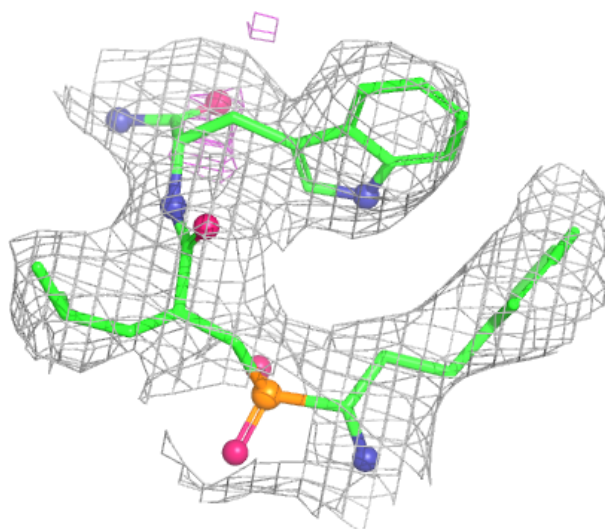
Electron density around P52 C 1002:

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



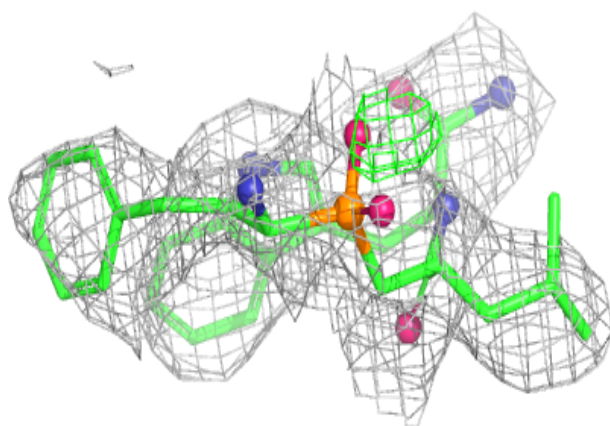
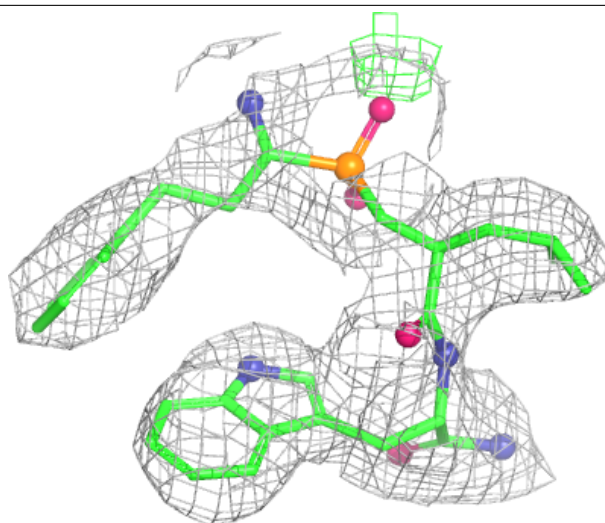
Electron density around P52 D 1003:

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



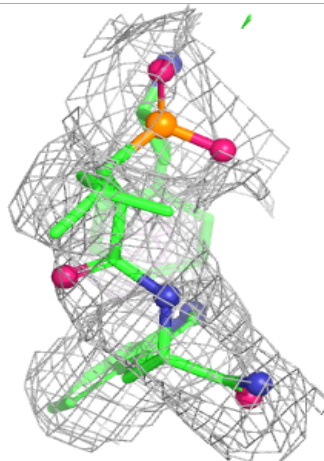
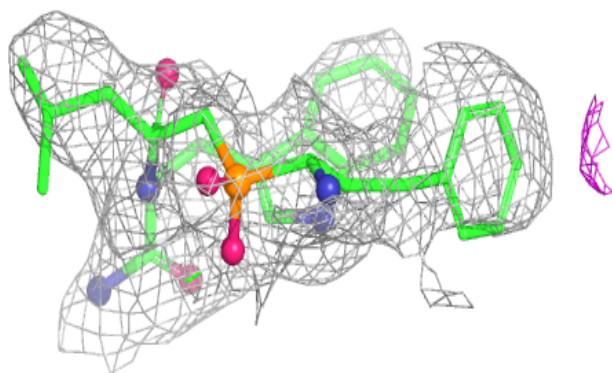
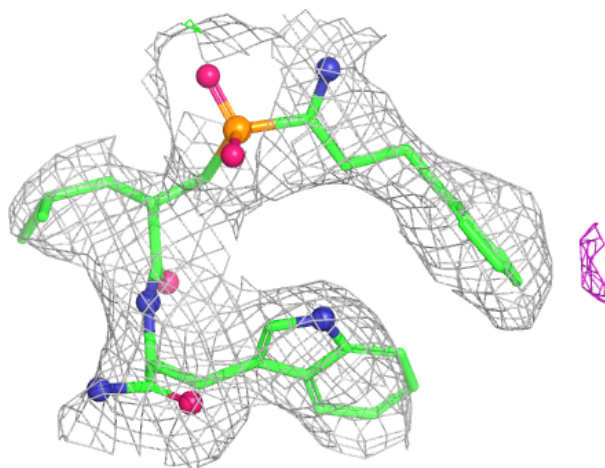
Electron density around P52 F 1003:

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



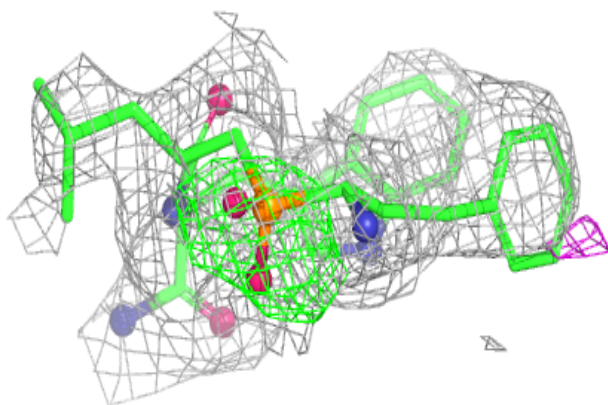
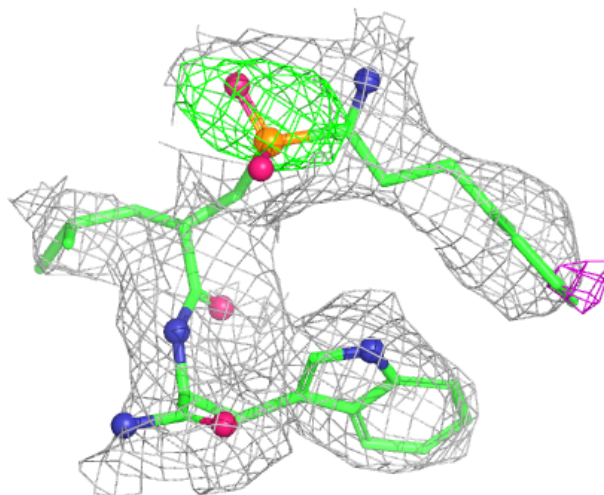
Electron density around P52 G 1002:

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



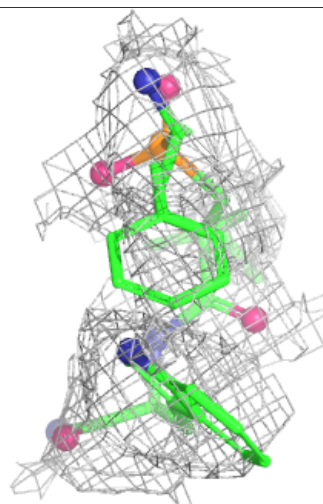
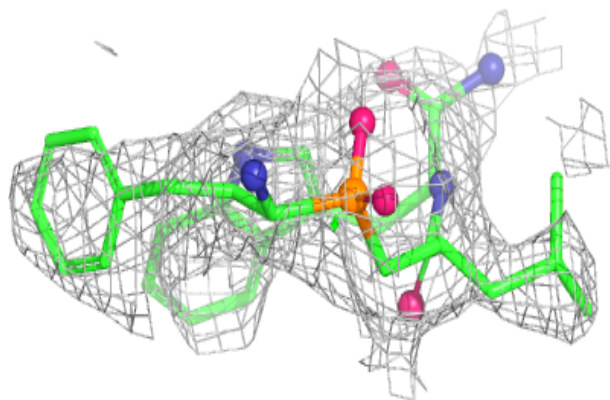
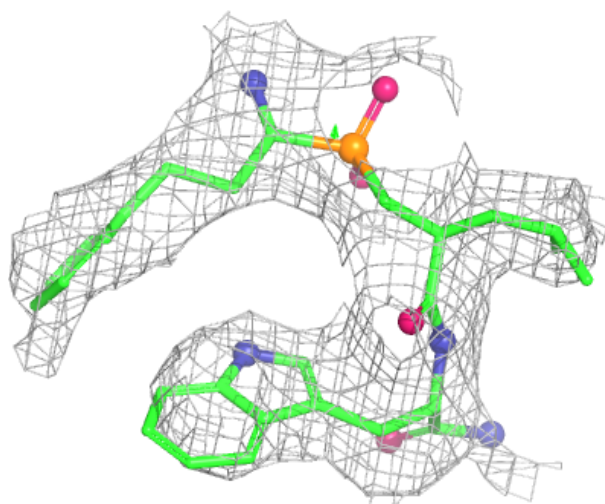
Electron density around P52 H 1003:

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



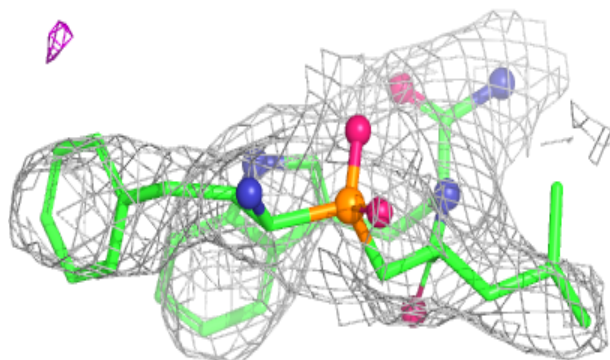
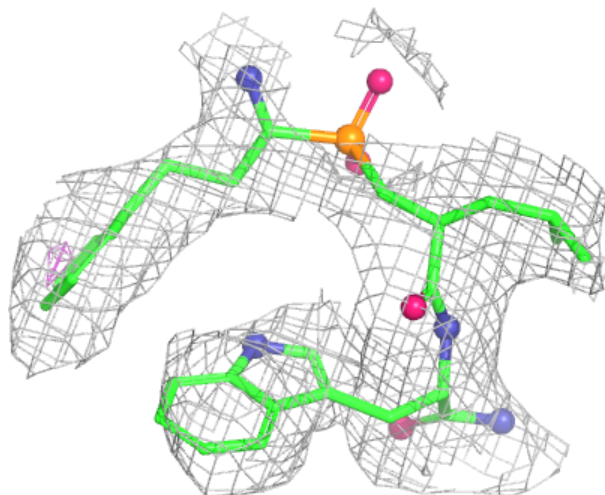
Electron density around P52 I 1003:

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



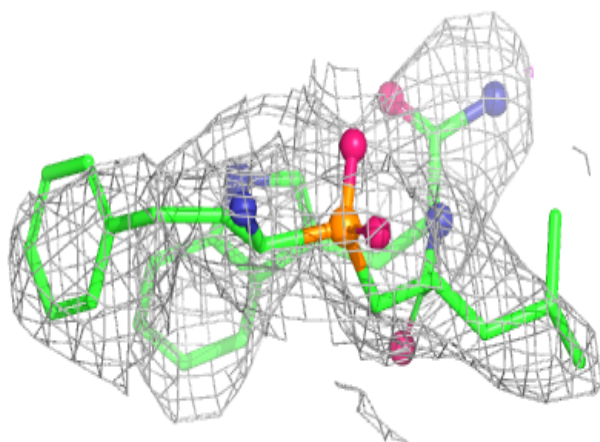
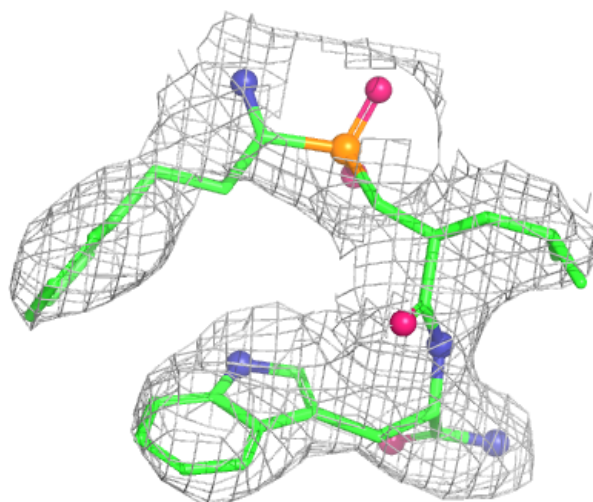
Electron density around P52 J 1002:

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



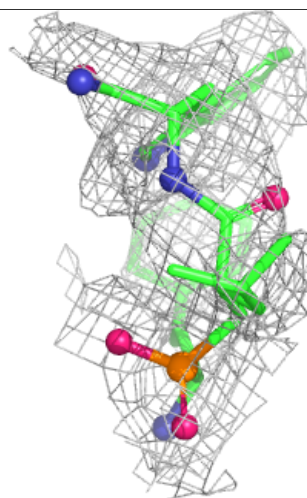
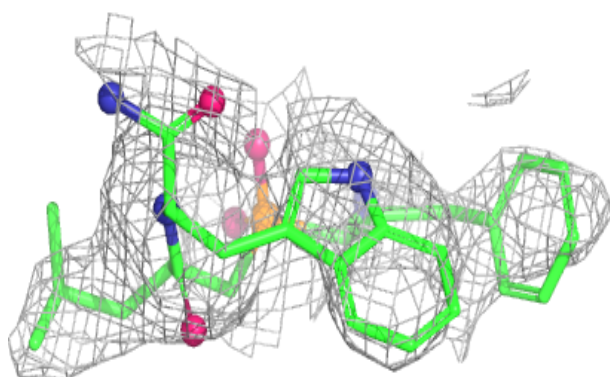
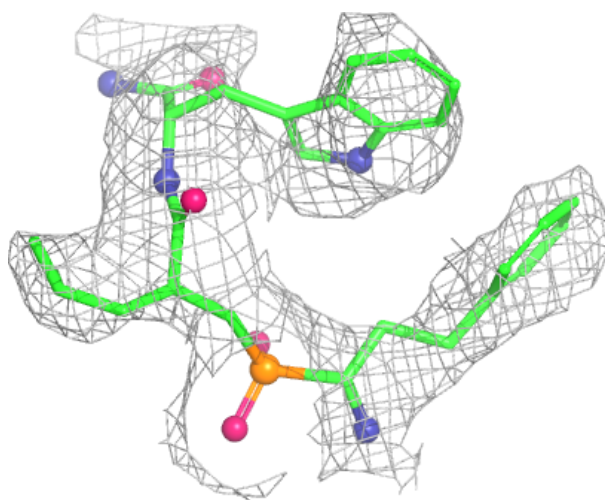
Electron density around P52 K 1002:

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



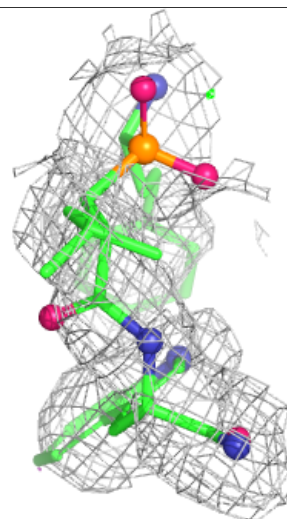
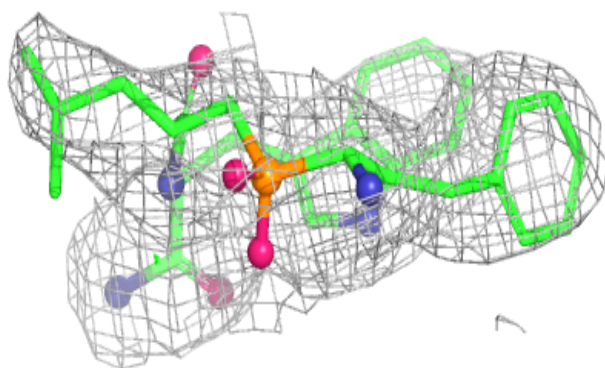
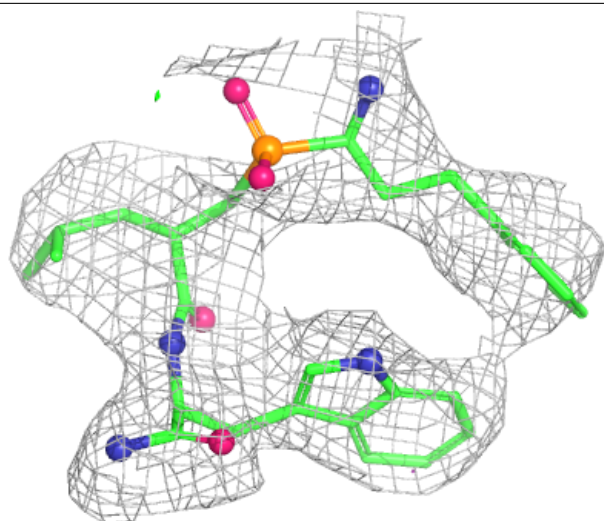
Electron density around P52 L 1003:

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



Electron density around P52 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.