Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 02:34 PM JST

PDB ID	:	8WHU
EMDB ID	:	EMD-37548
Title	:	Spike Trimer of BA.2.86 in complex with two hACE2s
Authors	:	Yue, C.; Liu, P.
Deposited on	:	2023-09-23
Resolution	:	3.30 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

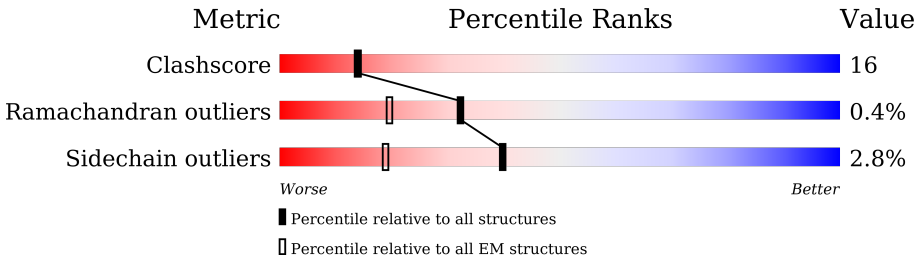
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1206	61% 26% • 12%
1	B	1206	61% 26% • 12%
1	C	1206	57% 29% • 12%
2	D	597	69% 30% •
2	E	597	68% 30% •
3	F	2	50% 50%
3	G	2	100%
3	H	2	50% 50%
3	I	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	J	2	100%
3	K	2	50% 50%
3	L	2	100%
3	M	2	50% 50%
3	N	2	100%
3	O	2	100%
3	P	2	100%
3	Q	2	100%
3	R	2	50% 50%
3	S	2	100%
3	T	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35548 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		
1	B	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		
1	C	1059	Total	C	N	O	S	0	0
			8285	5302	1376	1569	38		

There are 273 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	0	MET	-	expression tag	UNP P0DTC2
A	1	PHE	-	expression tag	UNP P0DTC2
A	2	VAL	-	expression tag	UNP P0DTC2
A	3	PHE	-	expression tag	UNP P0DTC2
A	4	LEU	-	expression tag	UNP P0DTC2
A	5	VAL	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	LEU	-	expression tag	UNP P0DTC2
A	8	PRO	-	expression tag	UNP P0DTC2
A	9	LEU	-	expression tag	UNP P0DTC2
A	10	VAL	-	expression tag	UNP P0DTC2
A	11	SER	-	expression tag	UNP P0DTC2
A	12	SER	-	expression tag	UNP P0DTC2
A	13	GLN	-	expression tag	UNP P0DTC2
A	14	CYS	-	expression tag	UNP P0DTC2
A	15	VAL	-	expression tag	UNP P0DTC2
A	16	MET	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	PHE	-	expression tag	UNP P0DTC2
A	20	ASN	-	expression tag	UNP P0DTC2
A	21	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	-	expression tag	UNP P0DTC2
A	23	THR	-	expression tag	UNP P0DTC2
A	24	THR	-	expression tag	UNP P0DTC2
A	25	THR	-	expression tag	UNP P0DTC2
A	26	GLN	-	expression tag	UNP P0DTC2
A	27	SER	-	expression tag	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	variant	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	0	MET	-	expression tag	UNP P0DTC2
B	1	PHE	-	expression tag	UNP P0DTC2
B	2	VAL	-	expression tag	UNP P0DTC2
B	3	PHE	-	expression tag	UNP P0DTC2
B	4	LEU	-	expression tag	UNP P0DTC2
B	5	VAL	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	LEU	-	expression tag	UNP P0DTC2
B	8	PRO	-	expression tag	UNP P0DTC2
B	9	LEU	-	expression tag	UNP P0DTC2
B	10	VAL	-	expression tag	UNP P0DTC2
B	11	SER	-	expression tag	UNP P0DTC2
B	12	SER	-	expression tag	UNP P0DTC2
B	13	GLN	-	expression tag	UNP P0DTC2
B	14	CYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	VAL	-	expression tag	UNP P0DTC2
B	16	MET	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	PHE	-	expression tag	UNP P0DTC2
B	20	ASN	-	expression tag	UNP P0DTC2
B	21	LEU	-	expression tag	UNP P0DTC2
B	22	ILE	-	expression tag	UNP P0DTC2
B	23	THR	-	expression tag	UNP P0DTC2
B	24	THR	-	expression tag	UNP P0DTC2
B	25	THR	-	expression tag	UNP P0DTC2
B	26	GLN	-	expression tag	UNP P0DTC2
B	27	SER	-	expression tag	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	variant	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	0	MET	-	expression tag	UNP P0DTC2
C	1	PHE	-	expression tag	UNP P0DTC2
C	2	VAL	-	expression tag	UNP P0DTC2
C	3	PHE	-	expression tag	UNP P0DTC2
C	4	LEU	-	expression tag	UNP P0DTC2
C	5	VAL	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	PRO	-	expression tag	UNP P0DTC2
C	9	LEU	-	expression tag	UNP P0DTC2
C	10	VAL	-	expression tag	UNP P0DTC2
C	11	SER	-	expression tag	UNP P0DTC2
C	12	SER	-	expression tag	UNP P0DTC2
C	13	GLN	-	expression tag	UNP P0DTC2
C	14	CYS	-	expression tag	UNP P0DTC2
C	15	VAL	-	expression tag	UNP P0DTC2
C	16	MET	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	PHE	-	expression tag	UNP P0DTC2
C	20	ASN	-	expression tag	UNP P0DTC2
C	21	LEU	-	expression tag	UNP P0DTC2
C	22	ILE	-	expression tag	UNP P0DTC2
C	23	THR	-	expression tag	UNP P0DTC2
C	24	THR	-	expression tag	UNP P0DTC2
C	25	THR	-	expression tag	UNP P0DTC2
C	26	GLN	-	expression tag	UNP P0DTC2
C	27	SER	-	expression tag	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	variant	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

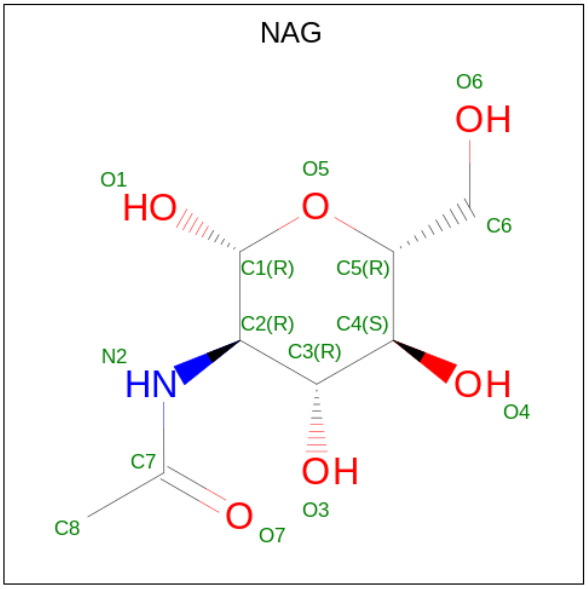
- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	E	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			25	14	1	10		
3	G	2	Total	C	N	O	0	0
			25	14	1	10		
3	H	2	Total	C	N	O	0	0
			25	14	1	10		
3	I	2	Total	C	N	O	0	0
			25	14	1	10		
3	J	2	Total	C	N	O	0	0
			25	14	1	10		
3	K	2	Total	C	N	O	0	0
			25	14	1	10		
3	L	2	Total	C	N	O	0	0
			25	14	1	10		
3	M	2	Total	C	N	O	0	0
			25	14	1	10		
3	N	2	Total	C	N	O	0	0
			25	14	1	10		
3	O	2	Total	C	N	O	0	0
			25	14	1	10		
3	P	2	Total	C	N	O	0	0
			25	14	1	10		
3	Q	2	Total	C	N	O	0	0
			25	14	1	10		
3	R	2	Total	C	N	O	0	0
			25	14	1	10		
3	S	2	Total	C	N	O	0	0
			25	14	1	10		
3	T	2	Total	C	N	O	0	0
			25	14	1	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0

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Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	D	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0
4	E	1	Total C N O 14 8 1 5	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	D	1	Total Zn 1 1	0
5	E	1	Total Zn 1 1	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

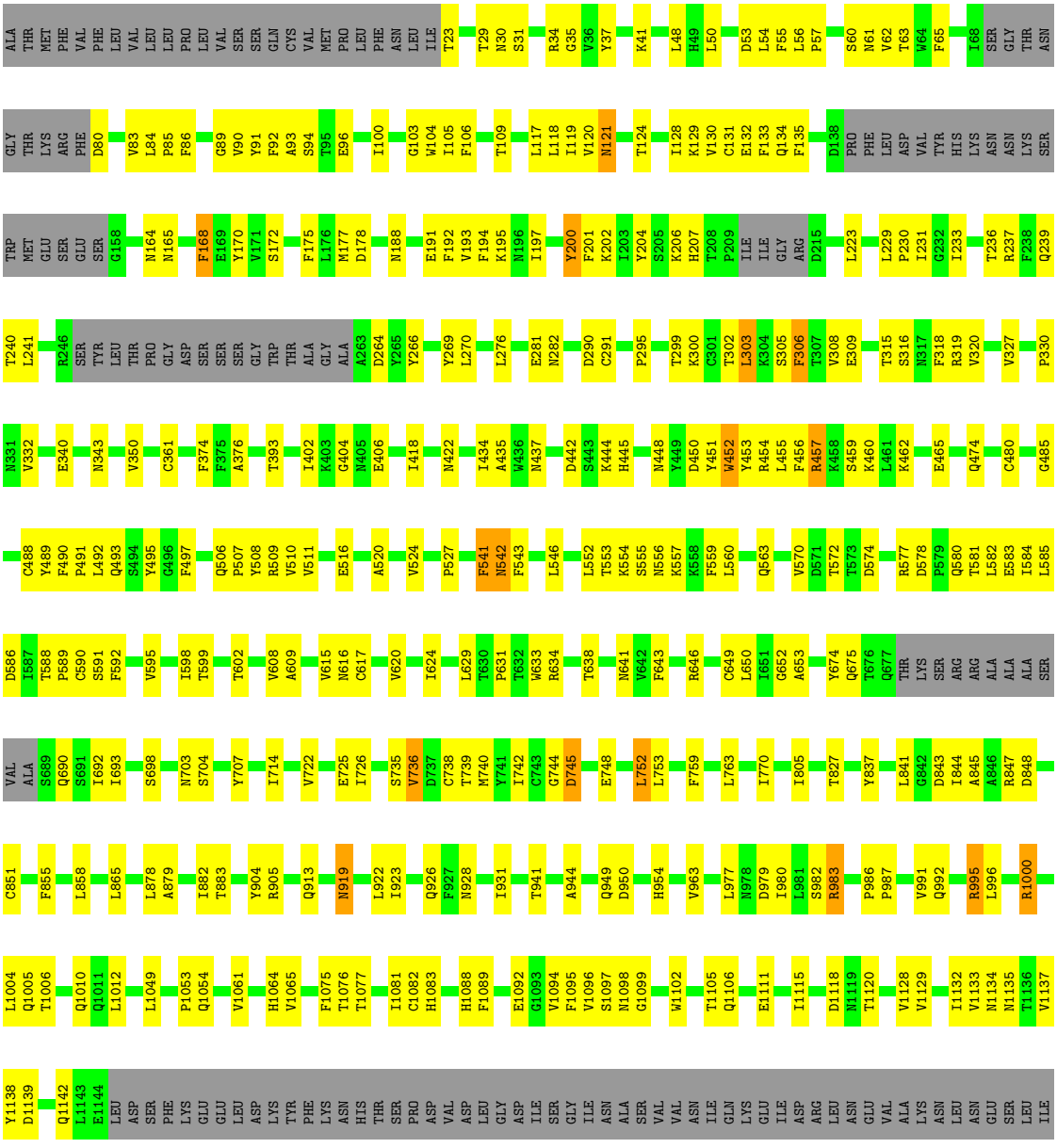
Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total Cl 1 1	0
6	E	1	Total Cl 1 1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

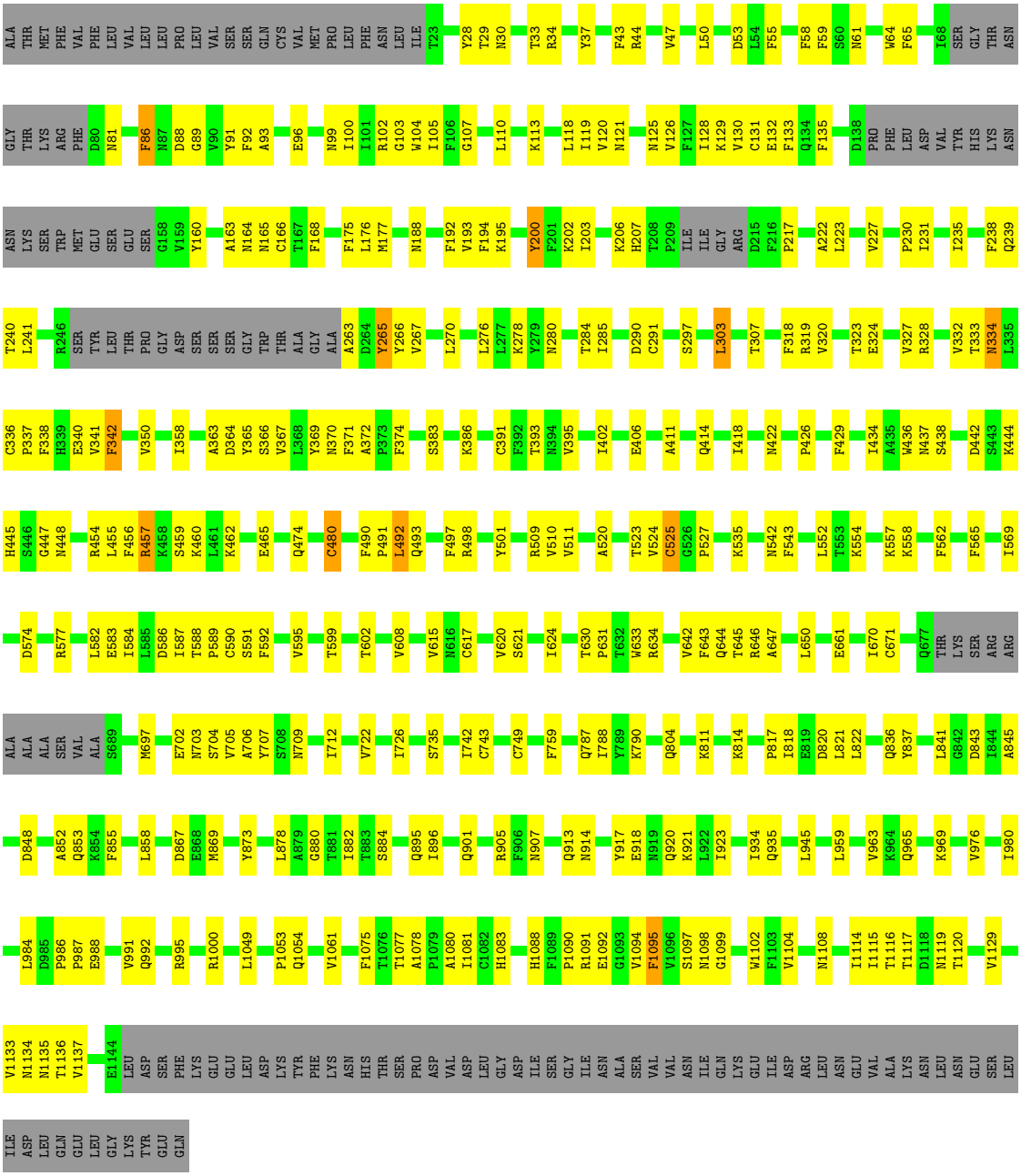
- Molecule 1: Spike glycoprotein

Chain A:



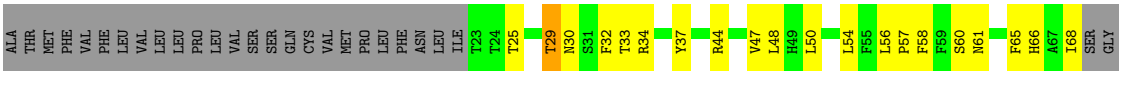
• Molecule 1: Spike glycoprotein

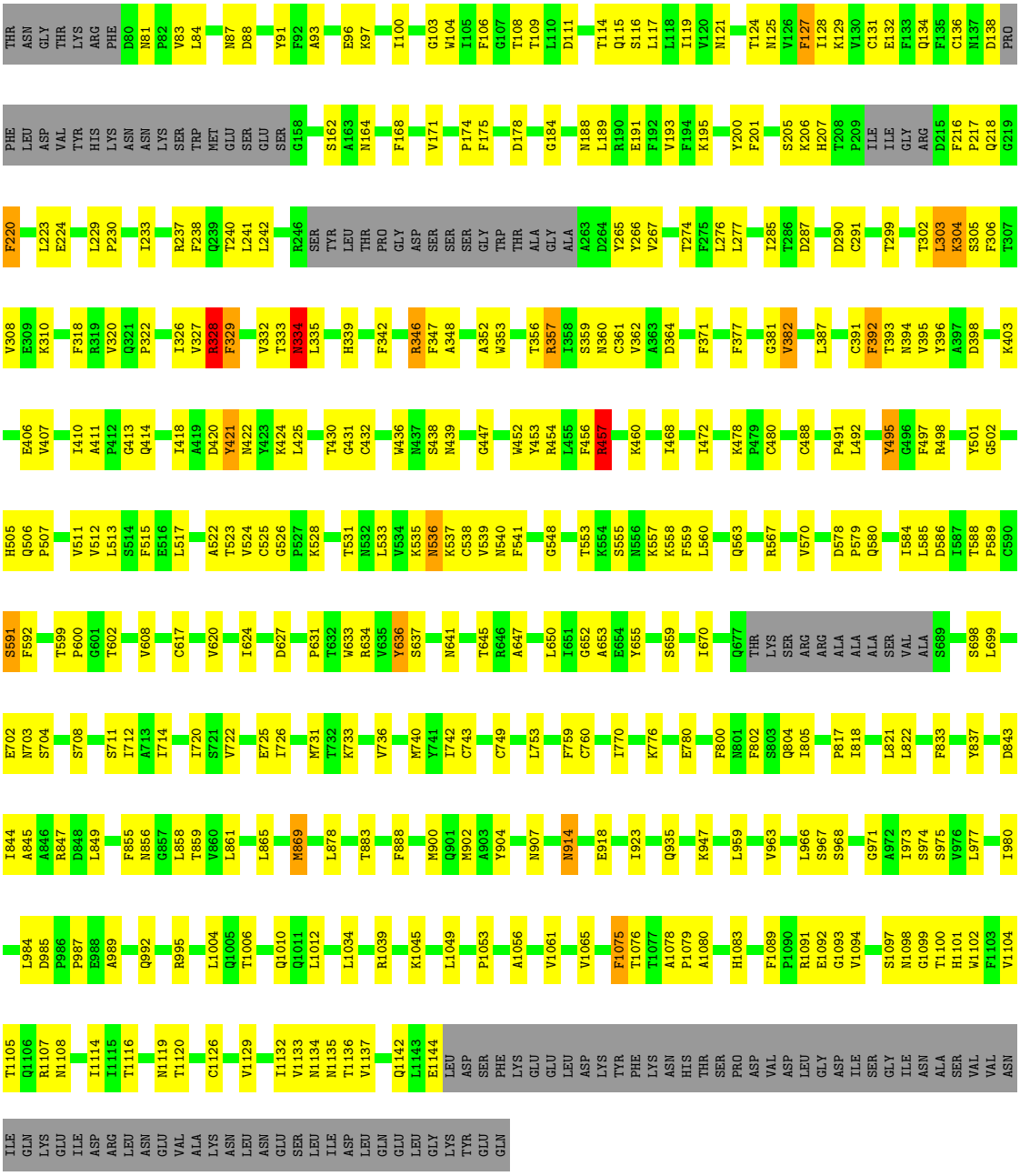
Chain B:



• Molecule 1: Spike glycoprotein

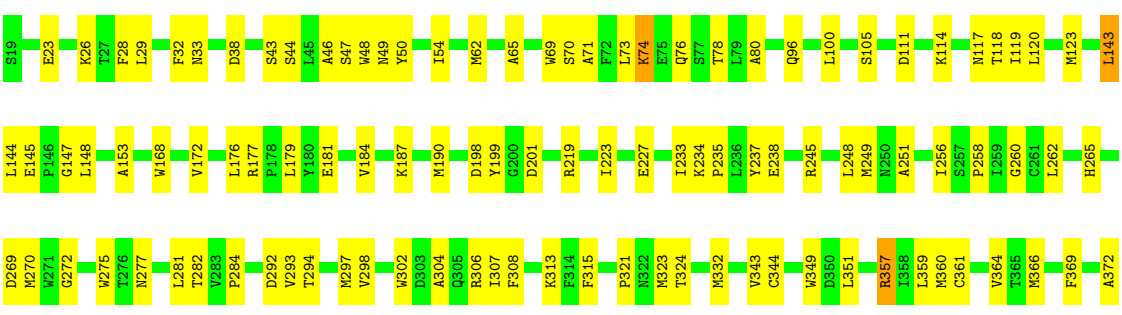
Chain C:

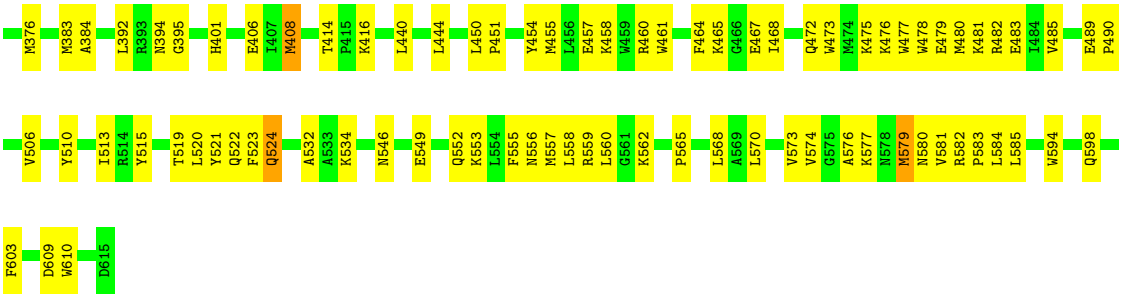




• Molecule 2: Processed angiotensin-converting enzyme 2

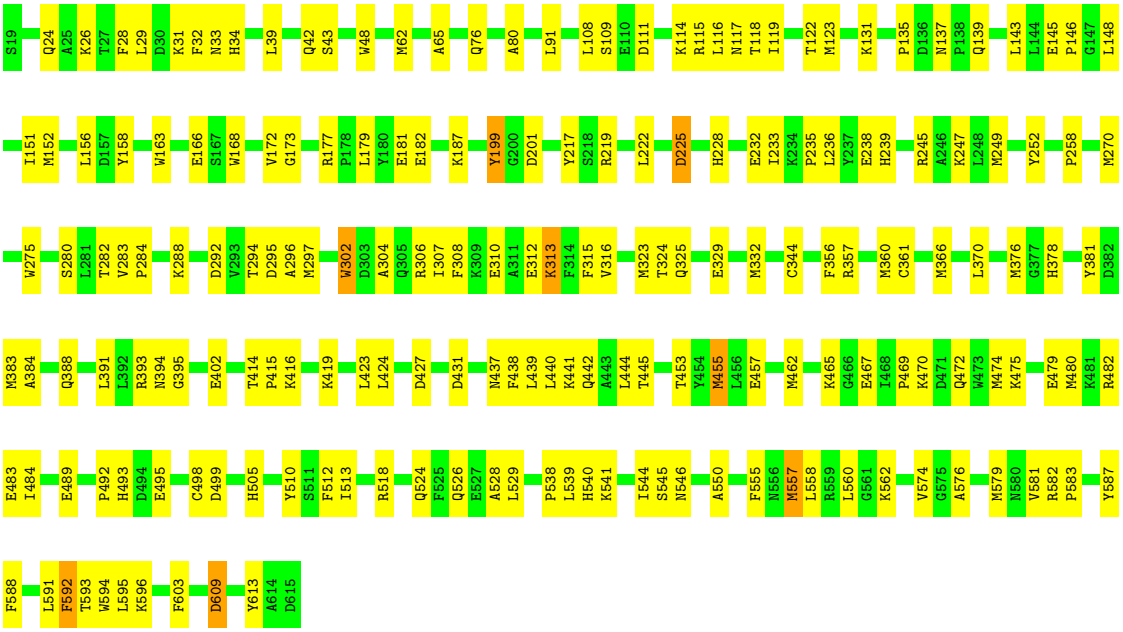
Chain D:





• Molecule 2: Processed angiotensin-converting enzyme 2

Chain E:

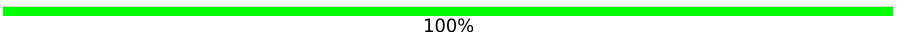


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

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

Chain G:



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

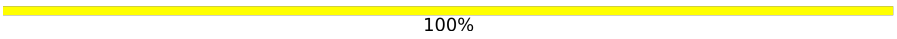
Chain H:

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

Chain I:

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

Chain J:

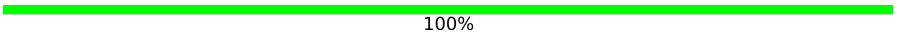


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

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

Chain L:

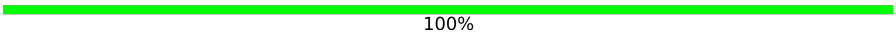


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

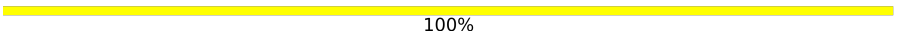
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain O:

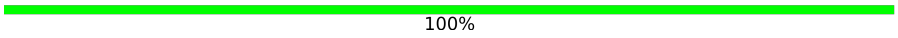


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain Q:

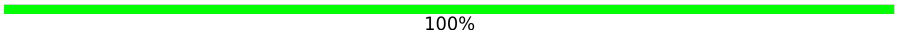


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

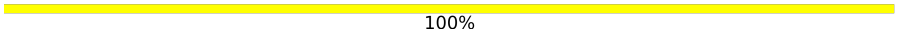
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	284921	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	1/8484 (0.0%)	0.53	0/11547
1	B	0.36	0/8484	0.52	0/11547
1	C	0.39	0/8484	0.55	0/11547
2	D	0.31	0/5007	0.47	0/6803
2	E	0.32	0/5007	0.48	0/6803
All	All	0.36	1/35466 (0.0%)	0.52	0/48247

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	4
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	736	VAL	CB-CG2	-5.10	1.42	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	995	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	328	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	357	ARG	Sidechain
1	C	457	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8285	0	8061	269	0
1	B	8285	0	8063	238	0
1	C	8285	0	8064	300	0
2	D	4870	0	4639	171	0
2	E	4870	0	4639	146	0
3	F	25	0	22	1	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	1	0
3	J	25	0	22	0	0
3	K	25	0	22	0	0
3	L	25	0	22	0	0
3	M	25	0	22	0	0
3	N	25	0	22	0	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
3	R	25	0	22	1	0
3	S	25	0	22	0	0
3	T	25	0	22	0	0
4	A	154	0	143	6	0
4	B	154	0	143	4	0
4	C	154	0	143	3	0
4	D	56	0	52	0	0
4	E	56	0	52	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	D	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	1	0
All	All	35548	0	34329	1083	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 16.

All (1083) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:476:LYS:HE3	2:D:480:MET:CE	1.72	1.19
1:B:586:ASP:O	1:B:587:ILE:HD13	1.43	1.16
2:E:302:TRP:CD1	2:E:306:ARG:HD3	1.86	1.09
1:C:726:ILE:HD12	1:C:1061:VAL:HG22	1.36	1.07
1:A:763:LEU:HD11	1:A:1005:GLN:HE22	0.99	1.07
2:D:476:LYS:HE3	2:D:480:MET:HE2	1.37	1.01
1:B:1135:ASN:OD1	1:B:1136:THR:N	1.95	0.99
1:C:127:PHE:CE1	1:C:129:LYS:HD2	2.00	0.95
1:C:34:ARG:HH22	1:C:189:LEU:HD22	1.30	0.94
2:D:476:LYS:HE3	2:D:480:MET:HE1	1.46	0.94
1:C:452:TRP:HB3	1:C:492:LEU:HD11	1.49	0.94
1:A:763:LEU:HD11	1:A:1005:GLN:NE2	1.82	0.93
2:D:521:TYR:CE1	2:D:579:MET:SD	2.61	0.93
2:E:455:MET:SD	6:E:902:CL:CL	2.64	0.93
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.54	0.89
2:D:148:LEU:HB3	2:D:270:MET:HE1	1.54	0.89
1:A:104:TRP:CH2	1:A:194:PHE:CZ	2.61	0.89
1:A:982:SER:O	1:A:983:ARG:HG3	1.71	0.89
1:B:118:LEU:HD21	1:B:120:VAL:HG12	1.52	0.89
1:A:541:PHE:HZ	1:A:546:LEU:CD2	1.87	0.88
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.54	0.88
2:D:47:SER:HA	2:D:62:MET:CE	2.02	0.88
1:C:352:ALA:HB2	1:C:468:ILE:HD11	1.56	0.87
1:A:609:ALA:HB2	1:A:692:ILE:HD11	1.55	0.87
1:B:586:ASP:C	1:B:587:ILE:HD13	1.96	0.86
1:C:973:ILE:HD12	1:C:992:GLN:HG3	1.57	0.86
2:E:582:ARG:HG2	2:E:583:PRO:HD3	1.57	0.86
1:C:533:LEU:HD23	1:C:535:LYS:HZ1	1.39	0.86
1:A:104:TRP:CZ3	1:A:194:PHE:CZ	2.63	0.85
2:D:119:ILE:O	2:D:123:MET:SD	2.33	0.85
1:C:326:ILE:HA	1:C:531:THR:OG1	1.75	0.85
1:B:1081:ILE:HD11	1:B:1135:ASN:HB3	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:HD23	1:C:535:LYS:NZ	1.92	0.83
1:C:726:ILE:CD1	1:C:1061:VAL:HG22	2.07	0.83
1:A:93:ALA:HB3	1:A:266:TYR:HB2	1.61	0.83
1:B:131:CYS:SG	1:B:132:GLU:N	2.52	0.82
1:A:759:PHE:HE1	1:B:965:GLN:HE21	1.27	0.82
1:B:105:ILE:HD11	1:B:110:LEU:HD21	1.60	0.82
1:C:533:LEU:CD2	1:C:578:ASP:OD2	2.28	0.82
1:A:759:PHE:CE1	1:B:965:GLN:NE2	2.48	0.82
1:C:636:TYR:HD1	1:C:637:SER:H	1.27	0.81
1:A:541:PHE:HZ	1:A:546:LEU:HD23	1.46	0.81
1:C:456:PHE:HB2	1:C:491:PRO:HA	1.61	0.81
1:C:328:ARG:HG3	1:C:580:GLN:HG2	1.61	0.81
1:C:537:LYS:O	1:C:539:VAL:HG23	1.79	0.81
1:A:131:CYS:SG	1:A:132:GLU:N	2.52	0.81
1:A:1133:VAL:HG22	1:A:1134:ASN:H	1.44	0.81
1:B:119:ILE:HD11	1:B:175:PHE:CE2	2.16	0.81
2:E:152:MET:SD	2:E:270:MET:SD	2.78	0.81
1:B:991:VAL:O	1:B:995:ARG:HG2	1.79	0.80
1:A:1081:ILE:HD11	1:A:1135:ASN:HB3	1.64	0.80
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.64	0.79
2:E:152:MET:SD	2:E:270:MET:HA	2.21	0.79
1:A:541:PHE:CE1	1:A:543:PHE:HB2	2.18	0.79
1:C:636:TYR:HD1	1:C:637:SER:N	1.81	0.79
1:B:1135:ASN:OD1	1:B:1136:THR:O	2.00	0.79
1:C:242:LEU:HD23	1:C:242:LEU:H	1.48	0.79
1:B:557:LYS:HB2	1:B:584:ILE:HG21	1.66	0.78
2:D:321:PRO:HG2	2:D:383:MET:CE	2.14	0.78
1:A:982:SER:O	1:A:983:ARG:CG	2.32	0.77
2:D:50:TYR:HB3	2:D:62:MET:HE2	1.67	0.77
2:E:526:GLN:HE22	2:E:544:ILE:HD11	1.48	0.77
1:A:650:LEU:HD21	1:A:653:ALA:HB3	1.65	0.77
1:C:636:TYR:CD1	1:C:637:SER:N	2.54	0.76
2:E:152:MET:SD	2:E:270:MET:HG3	2.24	0.76
1:A:759:PHE:HE1	1:B:965:GLN:NE2	1.84	0.76
1:B:119:ILE:HD11	1:B:175:PHE:HE2	1.48	0.76
2:D:520:LEU:HB3	2:D:579:MET:HE2	1.67	0.76
1:A:200:TYR:HA	1:A:230:PRO:HA	1.65	0.75
1:C:34:ARG:NH2	1:C:189:LEU:HD22	2.02	0.75
1:C:360:ASN:H	1:C:523:THR:HB	1.51	0.75
1:C:645:THR:HG23	1:C:670:ILE:HD12	1.69	0.75
1:C:84:LEU:HD22	1:C:267:VAL:HG11	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:CE3	1:B:119:ILE:HG21	2.22	0.74
1:C:328:ARG:HG3	1:C:580:GLN:CG	2.16	0.74
2:D:468:ILE:HG23	2:D:472:GLN:HE21	1.52	0.74
2:D:532:ALA:O	2:D:534:LYS:HE2	1.86	0.74
2:D:47:SER:HA	2:D:62:MET:HE2	1.70	0.74
1:C:131:CYS:SG	1:C:132:GLU:N	2.56	0.74
2:D:321:PRO:HG2	2:D:383:MET:HE2	1.70	0.73
2:E:152:MET:SD	2:E:270:MET:CG	2.76	0.73
1:C:560:LEU:HB2	1:C:563:GLN:HG3	1.70	0.73
1:C:61:ASN:HB2	4:C:1302:NAG:N2	2.02	0.73
1:C:1091:ARG:HB3	1:C:1092:GLU:OE1	1.88	0.73
1:B:455:LEU:HD12	1:B:493:GLN:HG3	1.70	0.73
2:E:302:TRP:NE1	2:E:306:ARG:HD3	2.04	0.72
1:C:659:SER:HB3	1:C:698:SER:HB2	1.70	0.72
1:A:641:ASN:HB2	1:A:652:GLY:H	1.53	0.72
1:C:589:PRO:HB3	1:C:592:PHE:CE1	2.25	0.72
2:D:574:VAL:HG23	2:D:576:ALA:H	1.55	0.72
2:E:378:HIS:HE1	2:E:402:GLU:HA	1.53	0.72
1:C:726:ILE:HD12	1:C:1061:VAL:CG2	2.19	0.72
1:B:569:ILE:HD12	1:B:569:ILE:H	1.55	0.72
1:C:804:GLN:HG2	3:R:1:NAG:H61	1.72	0.72
1:B:105:ILE:CD1	1:B:110:LEU:HD21	2.20	0.71
1:B:358:ILE:HB	1:B:395:VAL:HB	1.72	0.71
1:C:535:LYS:O	1:C:536:ASN:HB2	1.89	0.71
2:D:521:TYR:CD1	2:D:579:MET:SD	2.83	0.71
1:A:1128:VAL:HG21	1:C:918:GLU:OE1	1.92	0.70
1:A:541:PHE:HE1	1:A:543:PHE:HB2	1.53	0.70
1:C:115:GLN:HE21	1:C:233:ILE:HB	1.55	0.70
2:D:47:SER:HA	2:D:62:MET:SD	2.31	0.70
1:A:541:PHE:CZ	1:A:546:LEU:HD23	2.27	0.70
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.73	0.70
1:C:127:PHE:HE1	1:C:129:LYS:HD2	1.56	0.69
1:C:326:ILE:HG23	1:C:539:VAL:HG11	1.73	0.69
1:A:422:ASN:HD21	1:A:454:ARG:H	1.39	0.69
1:A:759:PHE:HD1	1:B:965:GLN:HE22	1.39	0.69
1:C:328:ARG:CZ	1:C:579:PRO:HB2	2.23	0.69
1:A:560:LEU:HD13	1:A:563:GLN:HE21	1.57	0.69
1:C:984:LEU:HB3	1:C:989:ALA:HB2	1.74	0.69
2:D:594:TRP:O	2:D:598:GLN:NE2	2.26	0.69
2:D:524:GLN:NE2	2:D:579:MET:HE1	2.08	0.69
1:A:442:ASP:HB2	1:A:509:ARG:HH21	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:557:MET:HE3	2:D:573:VAL:HG21	1.75	0.68
2:E:465:LYS:HB3	2:E:467:GLU:HG3	1.73	0.68
1:C:392:PHE:HD1	1:C:524:VAL:HG23	1.58	0.68
1:C:971:GLY:O	1:C:995:ARG:NH1	2.24	0.68
1:A:595:VAL:HG11	1:A:633:TRP:HZ2	1.58	0.68
1:C:914:ASN:O	1:C:918:GLU:HG2	1.94	0.68
2:E:474:MET:HE1	2:E:499:ASP:H	1.58	0.68
1:C:776:LYS:O	1:C:780:GLU:HG2	1.94	0.68
1:B:535:LYS:HG2	1:B:552:LEU:HD11	1.75	0.68
1:B:914:ASN:O	1:B:918:GLU:HG2	1.94	0.67
1:C:570:VAL:O	1:C:570:VAL:HG23	1.94	0.67
2:E:529:LEU:HD12	2:E:550:ALA:HB1	1.77	0.67
1:A:448:ASN:HB3	1:A:497:PHE:HB2	1.77	0.67
1:A:1133:VAL:CG2	1:A:1134:ASN:H	2.08	0.67
1:C:339:HIS:HA	1:C:371:PHE:HE2	1.60	0.67
1:C:50:LEU:HD21	1:C:274:THR:CG2	2.25	0.67
2:D:476:LYS:CE	2:D:480:MET:HE2	2.19	0.67
2:E:474:MET:CE	2:E:499:ASP:H	2.07	0.67
2:D:451:PRO:HB2	2:D:485:VAL:HG23	1.77	0.66
1:C:206:LYS:HB3	1:C:223:LEU:HD13	1.78	0.66
2:E:457:GLU:HG2	2:E:513:ILE:HB	1.78	0.66
1:C:96:GLU:OE1	1:C:100:ILE:N	2.28	0.66
2:D:477:TRP:NE1	6:D:902:CL:CL	2.65	0.65
2:E:479:GLU:OE2	2:E:482:ARG:NH1	2.29	0.65
1:A:541:PHE:HZ	1:A:546:LEU:HD22	1.60	0.65
1:A:1105:THR:CG2	1:A:1111:GLU:H	2.10	0.65
1:B:118:LEU:CD2	1:B:120:VAL:HG12	2.25	0.65
1:B:643:PHE:HB3	1:B:650:LEU:HB3	1.78	0.65
1:B:853:GLN:HG2	1:B:963:VAL:HG21	1.79	0.65
2:D:308:PHE:HE2	2:D:376:MET:HE1	1.61	0.65
1:C:533:LEU:CD2	1:C:535:LYS:NZ	2.60	0.65
1:C:431:GLY:HA2	1:C:515:PHE:CD2	2.31	0.65
1:A:577:ARG:HD3	1:A:582:LEU:HD13	1.77	0.65
1:C:334:ASN:ND2	1:C:361:CYS:HA	2.12	0.65
2:E:187:LYS:HD2	2:E:199:TYR:CZ	2.32	0.65
1:C:736:VAL:HG22	1:C:858:LEU:HD22	1.78	0.65
2:D:457:GLU:HG2	2:D:513:ILE:HB	1.79	0.65
2:D:48:TRP:HZ3	2:D:359:LEU:HB2	1.62	0.64
1:B:457:ARG:HD3	1:B:459:SER:H	1.62	0.64
1:C:533:LEU:HD22	1:C:578:ASP:OD2	1.97	0.64
1:C:736:VAL:HG22	1:C:858:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ARG:HD3	1:A:459:SER:H	1.63	0.64
1:B:96:GLU:OE1	1:B:100:ILE:N	2.30	0.64
1:A:309:GLU:OE2	1:A:309:GLU:N	2.30	0.64
1:B:200:TYR:HA	1:B:230:PRO:HA	1.80	0.64
2:E:114:LYS:O	2:E:118:THR:HG23	1.97	0.64
1:A:609:ALA:HB2	1:A:692:ILE:CD1	2.27	0.64
2:E:574:VAL:HG23	2:E:576:ALA:H	1.62	0.64
1:C:557:LYS:HB2	1:C:584:ILE:HD13	1.80	0.63
2:D:364:VAL:HG12	2:D:364:VAL:O	1.97	0.63
1:A:350:VAL:HG11	1:A:418:ILE:HD11	1.80	0.63
1:B:448:ASN:HB3	1:B:497:PHE:HB2	1.81	0.63
2:D:565:PRO:HD2	2:D:568:LEU:HD21	1.79	0.63
1:A:1133:VAL:HG22	1:A:1134:ASN:N	2.12	0.62
2:D:521:TYR:HD1	2:D:579:MET:HE1	1.63	0.62
1:B:350:VAL:HG11	1:B:418:ILE:HD11	1.80	0.62
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.80	0.62
2:D:50:TYR:HB3	2:D:62:MET:CE	2.29	0.62
2:E:111:ASP:HA	2:E:114:LYS:HE3	1.82	0.62
1:A:121:ASN:N	1:A:121:ASN:HD22	1.97	0.62
1:A:320:VAL:O	1:A:590:CYS:SG	2.58	0.62
1:A:879:ALA:O	1:A:883:THR:HG22	1.98	0.62
1:C:736:VAL:HG11	1:C:1004:LEU:HD11	1.81	0.62
1:B:43:PHE:N	1:C:563:GLN:OE1	2.33	0.62
2:E:505:HIS:HA	2:E:510:TYR:HD2	1.65	0.62
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.80	0.62
2:D:524:GLN:HG2	2:D:574:VAL:HG11	1.82	0.62
2:E:284:PRO:HD2	2:E:437:ASN:HD22	1.65	0.62
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.80	0.62
2:D:556:ASN:HD22	2:D:559:ARG:HH22	1.48	0.62
1:A:117:LEU:HD21	1:A:119:ILE:HD11	1.82	0.62
1:B:535:LYS:HG2	1:B:552:LEU:CD1	2.30	0.62
1:C:108:THR:HG22	1:C:109:THR:HG23	1.82	0.62
1:C:200:TYR:HA	1:C:230:PRO:HA	1.81	0.62
1:B:1083:HIS:ND1	1:B:1137:VAL:HG22	2.15	0.61
2:D:148:LEU:HB3	2:D:270:MET:CE	2.29	0.61
1:A:759:PHE:CD1	1:B:965:GLN:NE2	2.64	0.61
1:A:599:THR:HB	1:A:608:VAL:HG12	1.82	0.61
2:E:116:LEU:HD11	2:E:187:LYS:HE2	1.83	0.61
2:D:120:LEU:HA	2:D:123:MET:CE	2.31	0.61
1:B:290:ASP:OD1	1:B:291:CYS:N	2.34	0.61
1:A:1094:VAL:HG22	1:C:904:TYR:OH	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:OD1	1:A:291:CYS:N	2.33	0.60
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.64	0.60
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.82	0.60
1:C:108:THR:HB	1:C:114:THR:HG21	1.83	0.60
2:D:383:MET:SD	2:D:383:MET:C	2.79	0.60
2:D:395:GLY:H	2:D:401:HIS:HE2	1.49	0.60
1:B:586:ASP:O	1:B:587:ILE:CD1	2.36	0.60
2:D:515:TYR:O	2:D:519:THR:HG23	2.02	0.60
1:B:337:PRO:HB2	1:B:340:GLU:HB2	1.83	0.60
1:C:277:LEU:HD22	1:C:285:ILE:HD13	1.84	0.60
1:C:878:LEU:HD13	1:C:1053:PRO:HD2	1.82	0.60
2:D:119:ILE:HG22	2:D:123:MET:SD	2.41	0.60
1:A:177:MET:H	1:A:207:HIS:CE1	2.19	0.60
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.60
1:C:328:ARG:HD3	1:C:328:ARG:C	2.22	0.60
2:E:233:ILE:HD11	2:E:581:VAL:HB	1.82	0.60
2:D:48:TRP:HH2	2:D:332:MET:HG3	1.67	0.60
2:E:332:MET:O	2:E:332:MET:HG2	2.00	0.60
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.84	0.60
1:B:620:VAL:HG12	1:B:624:ILE:HD11	1.84	0.60
1:A:56:LEU:HD13	1:A:91:TYR:HB3	1.84	0.59
1:C:627:ASP:HA	1:C:634:ARG:HH22	1.67	0.59
2:D:521:TYR:CD1	2:D:579:MET:HE1	2.37	0.59
1:C:328:ARG:HD2	1:C:579:PRO:HG2	1.84	0.59
2:D:23:GLU:HA	2:D:26:LYS:HG3	1.85	0.59
2:D:29:LEU:O	2:D:33:ASN:ND2	2.35	0.59
1:A:474:GLN:NE2	1:A:480:CYS:SG	2.75	0.59
2:E:118:THR:O	2:E:122:THR:HG23	2.03	0.59
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.85	0.59
2:E:143:LEU:HB3	2:E:146:PRO:HG2	1.84	0.59
1:B:422:ASN:HD21	1:B:454:ARG:H	1.50	0.59
1:B:1117:THR:HA	1:B:1120:THR:HG22	1.85	0.59
2:E:228:HIS:O	2:E:232:GLU:HG3	2.03	0.59
2:E:469:PRO:HD2	2:E:472:GLN:NE2	2.16	0.59
1:A:195:LYS:HD2	1:A:197:ILE:HG22	1.83	0.59
1:B:30:ASN:HD21	1:B:59:PHE:HD1	1.49	0.59
1:C:406:GLU:OE1	1:C:406:GLU:N	2.36	0.59
2:D:284:PRO:HD3	2:D:440:LEU:HD22	1.85	0.59
2:D:321:PRO:HG2	2:D:383:MET:HE1	1.84	0.59
2:D:520:LEU:C	2:D:579:MET:HE2	2.23	0.59
1:C:536:ASN:O	1:C:537:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:SER:HB3	1:C:584:ILE:HG22	1.85	0.58
1:C:539:VAL:O	1:C:540:ASN:C	2.39	0.58
1:C:977:LEU:HA	1:C:980:ILE:HG22	1.84	0.58
1:A:104:TRP:CZ3	1:A:194:PHE:CE2	2.91	0.58
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.84	0.58
1:A:1075:PHE:O	1:A:1076:THR:OG1	2.19	0.58
1:C:393:THR:HA	1:C:522:ALA:HA	1.85	0.58
2:D:235:PRO:HA	2:D:238:GLU:OE2	2.03	0.58
2:E:297:MET:HG2	2:E:302:TRP:CE3	2.39	0.58
1:A:124:THR:OG1	4:A:1301:NAG:O7	2.21	0.58
1:A:574:ASP:OD2	1:C:847:ARG:N	2.26	0.58
2:D:332:MET:SD	2:D:359:LEU:HD12	2.43	0.58
2:D:120:LEU:HD23	2:D:123:MET:CE	2.33	0.58
2:E:378:HIS:CE1	2:E:402:GLU:HA	2.38	0.58
1:A:41:LYS:HD2	1:B:562:PHE:O	2.02	0.58
1:A:50:LEU:HD12	1:A:276:LEU:HD12	1.84	0.58
1:A:61:ASN:HB3	4:A:1302:NAG:HN2	1.69	0.58
1:B:366:SER:HA	1:B:369:TYR:CZ	2.39	0.58
1:C:178:ASP:N	1:C:178:ASP:OD1	2.35	0.58
2:E:315:PHE:CE2	2:E:376:MET:HB3	2.38	0.58
1:A:653:ALA:HB2	1:A:692:ILE:CD1	2.34	0.58
2:D:43:SER:HA	2:D:65:ALA:HB1	1.86	0.58
1:C:66:HIS:HE1	1:C:68:ILE:HB	1.69	0.58
1:C:497:PHE:HA	1:C:501:TYR:HE2	1.68	0.58
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.68	0.58
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.86	0.58
1:C:357:ARG:HG3	1:C:396:TYR:HE1	1.69	0.58
1:C:357:ARG:HG3	1:C:396:TYR:CE1	2.39	0.57
2:D:120:LEU:HD23	2:D:123:MET:HE1	1.86	0.57
2:D:235:PRO:HA	2:D:238:GLU:CD	2.24	0.57
2:D:406:GLU:HB3	2:D:522:GLN:OE1	2.05	0.57
1:B:363:ALA:HB1	1:B:365:TYR:CE1	2.39	0.57
2:E:62:MET:HE3	2:E:62:MET:O	2.04	0.57
1:C:1116:THR:OG1	1:C:1119:ASN:ND2	2.36	0.57
1:C:81:ASN:ND2	1:C:240:THR:O	2.30	0.57
1:C:865:LEU:CD2	1:C:869:MET:HE3	2.35	0.57
2:D:372:ALA:O	2:D:376:MET:HG2	2.03	0.57
1:A:206:LYS:HB3	1:A:223:LEU:HD23	1.87	0.57
2:E:482:ARG:NH2	2:E:489:GLU:OE1	2.37	0.57
1:B:1135:ASN:CG	1:B:1136:THR:H	2.09	0.57
1:C:326:ILE:HG23	1:C:539:VAL:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.34	0.57
1:C:974:SER:HB3	1:C:980:ILE:HD13	1.87	0.57
1:C:57:PRO:HB2	1:C:60:SER:HB3	1.86	0.57
1:C:303:LEU:HD11	1:C:308:VAL:HG12	1.85	0.57
1:A:118:LEU:HD21	1:A:120:VAL:HG12	1.86	0.56
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.86	0.56
1:A:979:ASP:OD1	1:A:983:ARG:NH2	2.32	0.56
1:C:472:ILE:HG21	1:C:488:CYS:HB2	1.86	0.56
1:C:1133:VAL:HG12	1:C:1134:ASN:H	1.70	0.56
2:D:251:ALA:HB2	2:D:281:LEU:HD11	1.86	0.56
2:D:609:ASP:OD1	2:D:610:TRP:N	2.38	0.56
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.88	0.56
1:B:363:ALA:HB1	1:B:365:TYR:HE1	1.70	0.56
1:C:856:ASN:HD22	1:C:966:LEU:HD12	1.71	0.56
2:D:233:ILE:HD11	2:D:581:VAL:HB	1.87	0.56
2:D:237:TYR:OH	2:D:485:VAL:O	2.23	0.56
2:E:152:MET:SD	2:E:270:MET:CA	2.94	0.56
2:E:440:LEU:HD21	2:E:594:TRP:HZ3	1.70	0.56
1:A:1092:GLU:N	1:A:1092:GLU:OE1	2.39	0.56
1:B:474:GLN:NE2	1:B:480:CYS:SG	2.77	0.56
1:B:712:ILE:HG12	1:B:1077:THR:HB	1.86	0.56
2:D:143:LEU:HD23	2:D:144:LEU:H	1.70	0.56
1:A:437:ASN:HD21	1:A:506:GLN:HG2	1.71	0.56
2:E:593:THR:HA	2:E:596:LYS:HG2	1.87	0.56
1:A:742:ILE:HG22	1:A:1000:ARG:HB3	1.86	0.56
1:B:195:LYS:HE3	1:B:202:LYS:HD3	1.87	0.56
2:D:227:GLU:OE1	2:D:454:TYR:OH	2.22	0.56
1:C:822:LEU:HD23	1:C:1056:ALA:HB2	1.88	0.56
2:D:472:GLN:HE22	2:D:476:LYS:HB2	1.70	0.56
2:D:472:GLN:NE2	2:D:476:LYS:HB2	2.21	0.56
2:E:245:ARG:O	2:E:249:MET:HG3	2.05	0.56
1:A:318:PHE:CZ	1:A:615:VAL:HG11	2.41	0.56
1:C:712:ILE:O	1:C:1075:PHE:N	2.39	0.56
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.87	0.55
1:A:692:ILE:HG13	1:A:692:ILE:O	2.06	0.55
2:D:48:TRP:CH2	2:D:332:MET:HG3	2.41	0.55
2:D:476:LYS:CE	2:D:480:MET:CE	2.67	0.55
2:E:29:LEU:O	2:E:33:ASN:ND2	2.39	0.55
2:E:474:MET:HE1	2:E:499:ASP:N	2.20	0.55
2:E:555:PHE:HA	2:E:558:LEU:HB2	1.88	0.55
1:A:48:LEU:HD12	1:A:276:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASP:HB2	1:B:509:ARG:HH21	1.72	0.55
1:B:1135:ASN:CG	1:B:1136:THR:N	2.58	0.55
1:A:451:TYR:C	1:A:452:TRP:CE3	2.80	0.55
1:C:725:GLU:O	1:C:726:ILE:HD13	2.06	0.55
1:A:55:PHE:HA	1:A:270:LEU:HD23	1.89	0.55
1:A:541:PHE:CZ	1:A:546:LEU:O	2.60	0.55
1:B:787:GLN:OE1	1:C:703:ASN:ND2	2.39	0.55
1:C:391:CYS:HG	1:C:525:CYS:HG	1.55	0.55
1:B:1133:VAL:HG22	1:B:1134:ASN:H	1.71	0.55
2:D:184:VAL:HG22	2:D:464:PHE:HE1	1.71	0.55
2:D:260:GLY:HA3	2:D:610:TRP:CE3	2.42	0.55
1:A:675:GLN:HG2	1:A:693:ILE:HD13	1.88	0.55
1:B:125:ASN:HB2	4:B:1301:NAG:H62	1.89	0.55
1:A:406:GLU:N	1:A:406:GLU:OE1	2.40	0.55
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.89	0.55
1:C:328:ARG:NE	1:C:579:PRO:HB2	2.22	0.55
1:C:398:ASP:HB2	1:C:512:VAL:HG12	1.89	0.55
2:D:524:GLN:NE2	2:D:579:MET:CE	2.69	0.55
1:A:319:ARG:NH2	1:C:740:MET:SD	2.79	0.55
1:A:847:ARG:HD2	1:A:851:CYS:HB3	1.89	0.55
1:B:456:PHE:HB2	1:B:491:PRO:HB3	1.89	0.55
1:B:558:LYS:HE2	3:F:1:NAG:H62	1.89	0.55
1:C:856:ASN:ND2	1:C:966:LEU:HD12	2.22	0.55
1:A:281:GLU:OE2	1:A:281:GLU:N	2.32	0.54
1:B:855:PHE:HA	1:C:589:PRO:HG3	1.89	0.54
1:C:191:GLU:HB2	1:C:223:LEU:HD11	1.90	0.54
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.87	0.54
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.89	0.54
2:E:119:ILE:O	2:E:123:MET:HG2	2.08	0.54
1:A:130:VAL:HG21	1:A:231:ILE:HD12	1.90	0.54
1:B:705:VAL:HG12	1:B:706:ALA:N	2.23	0.54
1:C:91:TYR:HD1	1:C:193:VAL:HG22	1.73	0.54
2:E:441:LYS:O	2:E:445:THR:HG23	2.07	0.54
1:A:735:SER:O	1:A:735:SER:OG	2.24	0.54
1:B:206:LYS:NZ	1:B:222:ALA:H	2.05	0.54
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.37	0.54
2:D:223:ILE:HG23	2:D:458:LYS:HE2	1.88	0.54
1:B:133:PHE:HB3	1:B:160:TYR:HB2	1.89	0.54
1:B:599:THR:HB	1:B:608:VAL:HG12	1.90	0.54
2:D:521:TYR:CD1	2:D:579:MET:CE	2.90	0.54
2:E:302:TRP:NE1	2:E:306:ARG:CD	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:O	1:A:60:SER:OG	2.26	0.54
1:B:132:GLU:N	1:B:166:CYS:SG	2.72	0.54
1:B:574:ASP:C	1:B:574:ASP:OD2	2.46	0.54
1:A:86:PHE:HE2	1:A:90:VAL:HG12	1.73	0.54
1:A:589:PRO:HG3	1:C:855:PHE:HA	1.89	0.54
2:D:524:GLN:HA	2:D:583:PRO:HG2	1.90	0.54
1:C:361:CYS:O	1:C:524:VAL:HA	2.09	0.54
1:C:382:VAL:HG11	1:C:387:LEU:HD13	1.90	0.54
1:C:109:THR:OG1	1:C:111:ASP:OD1	2.23	0.53
2:D:523:PHE:CD2	2:D:584:LEU:HD13	2.42	0.53
2:D:524:GLN:HE21	2:D:579:MET:CE	2.21	0.53
2:E:148:LEU:O	2:E:152:MET:HE2	2.08	0.53
1:B:917:TYR:HD1	1:C:1089:PHE:HE2	1.55	0.53
2:D:482:ARG:NH2	2:D:489:GLU:OE1	2.41	0.53
1:C:106:PHE:CE1	1:C:119:ILE:CD1	2.91	0.53
1:A:195:LYS:HE2	1:A:202:LYS:HD3	1.90	0.53
1:B:1104:VAL:HG13	1:B:1115:ILE:HG12	1.90	0.53
2:D:332:MET:SD	2:D:359:LEU:HA	2.48	0.53
1:B:118:LEU:HD21	1:B:120:VAL:CG1	2.31	0.53
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.89	0.53
1:A:646:ARG:HE	1:C:833:PHE:HB2	1.73	0.53
1:A:979:ASP:CG	1:A:983:ARG:HH22	2.11	0.53
1:C:134:GLN:HG2	1:C:162:SER:HB2	1.91	0.53
2:E:492:PRO:HD3	2:E:613:TYR:CG	2.44	0.53
1:A:29:THR:HG22	1:A:30:ASN:H	1.72	0.53
1:B:30:ASN:ND2	1:B:59:PHE:HD1	2.07	0.53
1:B:307:THR:HA	1:B:602:THR:HG21	1.91	0.53
1:B:976:VAL:O	1:B:980:ILE:HG23	2.09	0.53
2:D:117:ASN:OD1	2:D:118:THR:N	2.42	0.53
2:D:321:PRO:CG	2:D:383:MET:CE	2.86	0.53
1:B:104:TRP:HD1	1:B:240:THR:HG23	1.73	0.53
1:A:1105:THR:HG22	1:A:1106:GLN:H	1.73	0.53
1:B:858:LEU:HD22	1:B:963:VAL:HG22	1.90	0.53
2:E:48:TRP:CH2	2:E:357:ARG:HB3	2.44	0.53
1:A:202:LYS:HB3	1:A:204:TYR:CE2	2.44	0.52
1:A:1129:VAL:HB	1:A:1132:ILE:HB	1.92	0.52
1:B:742:ILE:O	1:B:1000:ARG:NH1	2.42	0.52
1:C:303:LEU:O	1:C:304:LYS:C	2.47	0.52
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.09	0.52
2:D:476:LYS:CE	2:D:480:MET:HE1	2.31	0.52
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:HA	2:D:123:MET:HE2	1.90	0.52
2:E:366:MET:HE3	2:E:370:LEU:CD2	2.39	0.52
1:A:991:VAL:HG12	1:A:995:ARG:HH12	1.73	0.52
1:B:621:SER:HA	1:B:624:ILE:HD12	1.92	0.52
1:B:342:PHE:CE1	1:B:511:VAL:HG11	2.44	0.52
1:C:617:CYS:HA	1:C:620:VAL:HG22	1.91	0.52
2:E:137:ASN:HD21	2:E:139:GLN:HE21	1.58	0.52
1:A:65:PHE:HE1	1:A:84:LEU:HD21	1.74	0.52
1:A:451:TYR:O	1:A:452:TRP:HE3	1.92	0.52
1:C:1126:CYS:O	1:C:1126:CYS:SG	2.68	0.52
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.92	0.52
1:B:44:ARG:HG2	1:B:47:VAL:HG21	1.92	0.52
1:C:865:LEU:CD2	1:C:869:MET:CE	2.87	0.52
1:C:888:PHE:CZ	1:C:1034:LEU:HD22	2.45	0.52
1:C:631:PRO:HA	1:C:633:TRP:CH2	2.44	0.52
1:A:201:PHE:N	1:A:229:LEU:O	2.43	0.52
1:B:709:ASN:HB3	4:B:1308:NAG:N2	2.25	0.52
2:D:187:LYS:HA	2:D:190:MET:HG3	1.92	0.52
2:D:582:ARG:HH12	2:D:585:LEU:HD12	1.74	0.52
1:A:178:ASP:N	1:A:178:ASP:OD1	2.42	0.51
1:C:290:ASP:OD1	1:C:291:CYS:N	2.38	0.51
2:D:555:PHE:HA	2:D:558:LEU:HB2	1.92	0.51
1:B:206:LYS:HD2	1:B:222:ALA:O	2.10	0.51
1:B:374:PHE:HA	1:B:436:TRP:HD1	1.75	0.51
1:C:128:ILE:HD11	1:C:175:PHE:HZ	1.74	0.51
1:C:392:PHE:CD1	1:C:524:VAL:HG23	2.42	0.51
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.92	0.51
1:C:650:LEU:HD21	1:C:653:ALA:HB3	1.92	0.51
1:A:318:PHE:HZ	1:A:615:VAL:HG11	1.73	0.51
1:A:343:ASN:OD1	4:A:1305:NAG:N2	2.44	0.51
1:B:841:LEU:HB3	1:C:588:THR:HG21	1.91	0.51
1:B:105:ILE:O	1:B:105:ILE:HG13	2.11	0.51
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.92	0.51
2:D:414:THR:HG22	2:D:416:LYS:H	1.75	0.51
1:B:843:ASP:O	1:B:845:ALA:N	2.43	0.51
1:A:638:THR:HG22	1:A:641:ASN:ND2	2.26	0.51
1:A:1081:ILE:HG23	1:A:1088:HIS:HB2	1.93	0.51
2:E:156:LEU:O	2:E:252:TYR:OH	2.26	0.51
1:A:31:SER:HB3	1:A:62:VAL:HG13	1.93	0.51
1:C:103:GLY:H	1:C:241:LEU:HB3	1.76	0.51
1:B:92:PHE:HB3	1:B:192:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:PHE:CE1	1:C:119:ILE:HD12	2.46	0.51
1:A:418:ILE:HD12	1:A:422:ASN:HD22	1.76	0.50
1:C:56:LEU:HD22	1:C:91:TYR:CD2	2.46	0.50
2:E:114:LYS:HA	2:E:117:ASN:ND2	2.26	0.50
2:E:414:THR:HG22	2:E:416:LYS:H	1.75	0.50
2:E:538:PRO:HG2	2:E:541:LYS:HB3	1.93	0.50
1:A:456:PHE:HB2	1:A:491:PRO:HB3	1.93	0.50
1:A:580:GLN:HA	4:A:1307:NAG:H82	1.93	0.50
1:A:177:MET:H	1:A:207:HIS:HE1	1.58	0.50
1:B:164:ASN:OD1	1:B:165:ASN:N	2.42	0.50
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.10	0.50
1:C:364:ASP:OD1	1:C:364:ASP:N	2.44	0.50
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.92	0.50
2:D:304:ALA:O	2:D:308:PHE:HD1	1.94	0.50
1:A:738:CYS:SG	1:A:739:THR:N	2.84	0.50
1:B:705:VAL:CG1	1:B:706:ALA:N	2.75	0.50
1:C:50:LEU:HD21	1:C:274:THR:HG21	1.93	0.50
2:D:465:LYS:HD2	2:D:467:GLU:HG3	1.93	0.50
2:D:245:ARG:O	2:D:249:MET:HE2	2.11	0.50
2:E:344:CYS:HB2	2:E:360:MET:HA	1.94	0.50
2:E:557:MET:HA	2:E:560:LEU:HD12	1.92	0.50
1:B:959:LEU:O	1:B:963:VAL:HG23	2.10	0.50
1:C:54:LEU:HD22	1:C:88:ASP:HB3	1.94	0.50
1:C:436:TRP:NE1	1:C:438:SER:OG	2.45	0.50
1:C:1092:GLU:OE1	1:C:1092:GLU:N	2.45	0.50
1:B:104:TRP:HE3	1:B:119:ILE:HG21	1.73	0.50
1:C:865:LEU:HD23	1:C:869:MET:CE	2.42	0.50
2:D:248:LEU:HD12	2:D:262:LEU:HD22	1.94	0.49
1:A:361:CYS:H	1:A:524:VAL:HG12	1.77	0.49
1:A:1133:VAL:CG2	1:A:1134:ASN:N	2.74	0.49
1:C:37:TYR:CE2	1:C:193:VAL:HG11	2.46	0.49
2:E:32:PHE:CE1	2:E:76:GLN:HG3	2.47	0.49
2:E:235:PRO:O	2:E:238:GLU:HG3	2.12	0.49
1:B:712:ILE:HG23	1:B:1077:THR:HG21	1.93	0.49
1:C:624:ILE:HA	1:C:634:ARG:HH21	1.77	0.49
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.45	0.49
1:A:616:ASN:HB2	4:A:1308:NAG:H62	1.95	0.49
1:B:645:THR:C	1:B:647:ALA:H	2.16	0.49
2:D:176:LEU:HD23	2:D:179:LEU:HD12	1.94	0.49
2:E:475:LYS:O	2:E:479:GLU:HG2	2.12	0.49
1:A:201:PHE:HB2	1:A:231:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ASP:HB3	1:A:581:THR:HB	1.94	0.49
1:B:735:SER:O	1:B:735:SER:OG	2.23	0.49
1:C:30:ASN:HB2	1:C:32:PHE:CE2	2.48	0.49
1:C:888:PHE:CZ	1:C:1034:LEU:CD2	2.95	0.49
2:E:270:MET:SD	2:E:270:MET:N	2.85	0.49
2:E:325:GLN:O	2:E:329:GLU:HG2	2.12	0.49
2:E:545:SER:O	2:E:546:ASN:HB3	2.12	0.49
1:B:29:THR:CA	4:B:1302:NAG:H82	2.43	0.49
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.47	0.49
1:C:34:ARG:NH1	1:C:217:PRO:O	2.46	0.49
1:C:393:THR:O	1:C:523:THR:OG1	2.25	0.49
2:D:282:THR:HG21	2:D:444:LEU:HD11	1.95	0.49
2:D:307:ILE:HD12	2:D:369:PHE:HD1	1.77	0.49
1:A:332:VAL:HG11	1:A:527:PRO:HB3	1.94	0.49
1:B:86:PHE:HE2	1:B:89:GLY:H	1.60	0.49
1:A:131:CYS:HB3	1:A:133:PHE:CZ	2.47	0.49
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.95	0.49
1:C:327:VAL:O	1:C:328:ARG:C	2.51	0.49
1:A:282:ASN:OD1	1:A:282:ASN:O	2.31	0.49
1:A:552:LEU:HG	1:A:585:LEU:HB3	1.95	0.49
1:A:1094:VAL:HG12	1:A:1095:PHE:N	2.28	0.49
1:C:714:ILE:HD11	1:C:1094:VAL:HG21	1.95	0.49
1:C:1079:PRO:HD2	1:C:1080:ALA:H	1.77	0.49
2:E:524:GLN:HA	2:E:583:PRO:HG2	1.95	0.49
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.48	0.48
1:B:459:SER:OG	1:B:460:LYS:N	2.46	0.48
1:C:1114:ILE:O	1:C:1116:THR:HG23	2.13	0.48
2:D:349:TRP:HB2	2:D:357:ARG:HG3	1.95	0.48
2:E:297:MET:HG2	2:E:302:TRP:HE3	1.77	0.48
2:E:439:LEU:HD23	2:E:591:LEU:HB2	1.95	0.48
1:A:841:LEU:HB3	1:B:588:THR:OG1	2.13	0.48
2:D:294:THR:O	2:D:298:VAL:HG23	2.13	0.48
2:E:528:ALA:HB2	2:E:574:VAL:HG12	1.96	0.48
1:B:333:THR:OG1	1:B:334:ASN:N	2.45	0.48
1:B:406:GLU:N	1:B:406:GLU:OE1	2.43	0.48
1:B:788:ILE:O	1:B:788:ILE:HG13	2.13	0.48
1:C:800:PHE:HB3	1:C:802:PHE:HE2	1.79	0.48
2:D:54:ILE:HD11	2:D:343:VAL:HG23	1.96	0.48
2:E:384:ALA:HB1	2:E:558:LEU:HB3	1.95	0.48
2:E:540:HIS:HB3	2:E:587:TYR:HE1	1.77	0.48
1:A:490:PHE:CE2	1:A:492:LEU:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.95	0.48
2:E:115:ARG:O	2:E:119:ILE:HG23	2.14	0.48
1:A:104:TRP:CH2	1:A:194:PHE:HZ	2.23	0.48
1:C:533:LEU:HD21	1:C:578:ASP:OD2	2.09	0.48
2:D:521:TYR:HA	2:D:579:MET:HE1	1.95	0.48
2:E:388:GLN:O	2:E:393:ARG:NH2	2.37	0.48
1:B:37:TYR:CE2	1:B:193:VAL:HG11	2.49	0.48
1:B:661:GLU:OE1	1:B:661:GLU:N	2.43	0.48
1:C:502:GLY:O	1:C:506:GLN:HG2	2.14	0.48
1:C:1107:ARG:C	1:C:1108:ASN:HD22	2.17	0.48
2:D:308:PHE:HE2	2:D:376:MET:CE	2.24	0.48
1:A:541:PHE:CD1	1:A:543:PHE:HB2	2.49	0.48
1:B:81:ASN:HB2	1:B:239:GLN:HE21	1.78	0.48
2:E:480:MET:HA	2:E:483:GLU:HG2	1.95	0.48
1:C:326:ILE:HA	1:C:531:THR:HG1	1.76	0.48
1:A:444:LYS:NZ	1:A:445:HIS:O	2.36	0.48
1:B:99:ASN:OD1	1:B:102:ARG:NH1	2.47	0.48
1:B:160:TYR:HE2	1:B:163:ALA:HB2	1.79	0.48
1:B:438:SER:OG	1:B:509:ARG:NH2	2.47	0.48
2:D:237:TYR:CE1	2:D:451:PRO:HG2	2.49	0.48
2:D:384:ALA:HB1	2:D:558:LEU:HB3	1.95	0.48
2:E:217:TYR:OH	2:E:225:ASP:OD2	2.32	0.48
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.96	0.47
1:B:722:VAL:O	1:B:934:ILE:HD11	2.14	0.47
1:C:555:SER:CB	1:C:586:ASP:OD2	2.62	0.47
1:C:918:GLU:OE1	1:C:918:GLU:HA	2.14	0.47
1:C:1107:ARG:HB3	1:C:1108:ASN:ND2	2.29	0.47
2:D:468:ILE:HG22	2:D:473:TRP:HD1	1.79	0.47
2:D:553:LYS:HD2	2:D:573:VAL:HA	1.96	0.47
2:E:177:ARG:NH1	2:E:495:GLU:O	2.46	0.47
1:A:29:THR:HG22	1:A:30:ASN:N	2.28	0.47
1:A:1083:HIS:HB2	1:A:1137:VAL:HG13	1.96	0.47
1:B:119:ILE:O	1:B:119:ILE:CG1	2.62	0.47
1:B:418:ILE:HD12	1:B:422:ASN:HD22	1.78	0.47
1:C:420:ASP:HB3	1:C:460:LYS:HD2	1.95	0.47
2:D:394:ASN:HB3	2:D:562:LYS:HD3	1.96	0.47
1:A:843:ASP:O	1:A:845:ALA:N	2.46	0.47
1:A:103:GLY:C	1:A:104:TRP:HD1	2.17	0.47
1:C:91:TYR:HE1	1:C:191:GLU:HB3	1.78	0.47
1:C:703:ASN:OD1	1:C:704:SER:N	2.47	0.47
2:D:457:GLU:OE2	2:D:461:TRP:NE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ILE:HG22	1:A:233:ILE:HG23	1.96	0.47
1:B:338:PHE:HE1	1:B:358:ILE:HD13	1.79	0.47
1:C:188:ASN:ND2	1:C:207:HIS:HB3	2.30	0.47
2:D:460:ARG:NH2	2:D:510:TYR:O	2.45	0.47
2:E:236:LEU:HD21	2:E:588:PHE:HD2	1.80	0.47
2:E:402:GLU:HB3	2:E:518:ARG:HD3	1.97	0.47
1:A:168:PHE:CE1	1:A:229:LEU:HD22	2.49	0.47
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.36	0.47
2:D:292:ASP:N	2:D:292:ASP:OD1	2.47	0.47
2:E:288:LYS:NZ	2:E:431:ASP:OD2	2.38	0.47
2:E:366:MET:HE3	2:E:370:LEU:HD21	1.97	0.47
1:A:742:ILE:HD11	1:A:753:LEU:HD22	1.96	0.47
1:B:332:VAL:HG11	1:B:527:PRO:HB3	1.96	0.47
1:B:595:VAL:HG21	1:B:633:TRP:HZ2	1.80	0.47
1:B:818:ILE:O	1:B:822:LEU:HG	2.15	0.47
1:C:326:ILE:CG2	1:C:539:VAL:HG11	2.43	0.47
2:D:111:ASP:O	2:D:114:LYS:HG2	2.15	0.47
2:E:438:PHE:O	2:E:442:GLN:HG2	2.15	0.47
1:A:922:LEU:HD11	3:I:1:NAG:H3	1.96	0.47
1:B:104:TRP:CD1	1:B:240:THR:HG23	2.50	0.47
1:B:176:LEU:O	1:B:176:LEU:HD12	2.14	0.47
1:B:444:LYS:NZ	1:B:447:GLY:O	2.39	0.47
1:B:814:LYS:HA	1:B:814:LYS:HD3	1.64	0.47
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.97	0.47
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.33	0.47
2:E:115:ARG:NH2	2:E:118:THR:HG21	2.30	0.47
2:E:469:PRO:HB2	2:E:472:GLN:OE1	2.15	0.47
2:E:541:LYS:HB2	2:E:541:LYS:HE2	1.65	0.47
1:A:119:ILE:HG22	1:A:175:PHE:HE2	1.80	0.47
1:B:203:ILE:HB	1:B:227:VAL:HG22	1.96	0.47
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.80	0.47
2:E:323:MET:HG2	2:E:324:THR:H	1.80	0.47
1:A:164:ASN:OD1	1:A:165:ASN:N	2.45	0.47
1:C:125:ASN:HD22	1:C:171:VAL:HG12	1.80	0.47
1:C:164:ASN:OD1	1:C:164:ASN:N	2.46	0.47
1:C:1116:THR:O	1:C:1120:THR:HG22	2.14	0.47
2:D:148:LEU:CB	2:D:270:MET:HE1	2.36	0.47
2:E:166:GLU:OE1	2:E:493:HIS:NE2	2.36	0.47
1:B:569:ILE:HD12	1:B:569:ILE:N	2.27	0.46
1:C:555:SER:HB2	1:C:586:ASP:OD2	2.14	0.46
2:D:111:ASP:HA	2:D:114:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:N	1:A:270:LEU:HD23	2.31	0.46
1:B:880:GLY:O	1:B:884:SER:OG	2.29	0.46
1:C:104:TRP:CD1	1:C:240:THR:HG23	2.50	0.46
1:C:124:THR:OG1	4:C:1301:NAG:O7	2.32	0.46
1:C:334:ASN:HD21	1:C:361:CYS:HA	1.78	0.46
1:C:432:CYS:O	1:C:513:LEU:N	2.31	0.46
2:E:201:ASP:OD1	2:E:219:ARG:HD2	2.14	0.46
1:A:48:LEU:HD11	1:A:306:PHE:CD1	2.51	0.46
1:B:370:ASN:OD1	1:B:371:PHE:N	2.48	0.46
1:C:359:SER:OG	1:C:394:ASN:OD1	2.23	0.46
1:A:1105:THR:HG23	1:A:1111:GLU:O	2.16	0.46
1:B:88:ASP:O	1:B:270:LEU:HB2	2.14	0.46
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.16	0.46
2:D:298:VAL:HG22	2:D:364:VAL:HG11	1.97	0.46
2:D:557:MET:HE3	2:D:573:VAL:CG2	2.43	0.46
1:A:327:VAL:HG12	1:A:542:ASN:HB2	1.97	0.46
1:B:444:LYS:NZ	1:B:445:HIS:O	2.39	0.46
1:B:498:ARG:HB2	1:B:501:TYR:CZ	2.51	0.46
1:B:917:TYR:HD1	1:C:1089:PHE:CE2	2.34	0.46
1:B:1114:ILE:HG23	1:B:1116:THR:HG23	1.96	0.46
1:C:985:ASP:HB3	1:C:987:PRO:HD2	1.97	0.46
2:E:117:ASN:OD1	2:E:118:THR:N	2.48	0.46
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.97	0.46
1:A:552:LEU:HD11	1:A:585:LEU:HD13	1.98	0.46
1:A:570:VAL:HG23	1:A:572:THR:HG23	1.97	0.46
1:A:1105:THR:HG23	1:A:1111:GLU:C	2.35	0.46
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.51	0.46
1:B:645:THR:O	1:B:647:ALA:N	2.49	0.46
1:B:963:VAL:HG11	1:C:570:VAL:HG21	1.98	0.46
1:B:1092:GLU:HG2	1:B:1092:GLU:O	2.16	0.46
1:B:1102:TRP:CZ2	1:B:1133:VAL:HG21	2.50	0.46
2:E:295:ASP:OD1	2:E:296:ALA:N	2.49	0.46
2:E:539:LEU:HD12	2:E:539:LEU:H	1.81	0.46
1:A:206:LYS:HD2	1:A:207:HIS:H	1.80	0.46
1:A:459:SER:OG	1:A:460:LYS:N	2.47	0.46
1:A:858:LEU:CD1	1:A:963:VAL:HG23	2.46	0.46
1:C:195:LYS:HB2	1:C:195:LYS:HE2	1.79	0.46
2:D:450:LEU:HB2	2:D:451:PRO:HD3	1.98	0.46
2:E:181:GLU:OE1	2:E:470:LYS:HD3	2.16	0.46
1:A:239:GLN:HE22	1:A:241:LEU:HD23	1.81	0.46
1:A:624:ILE:HG23	1:A:634:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:ASP:OD1	1:A:954:HIS:NE2	2.49	0.46
1:A:1094:VAL:HG13	1:C:900:MET:CE	2.46	0.46
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.48	0.46
1:C:320:VAL:HB	1:C:591:SER:HB2	1.97	0.46
1:C:395:VAL:O	1:C:396:TYR:HD1	1.99	0.46
1:C:1083:HIS:CD2	1:C:1137:VAL:H	2.32	0.46
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.49	0.46
1:B:319:ARG:O	1:B:630:THR:OG1	2.29	0.46
1:C:712:ILE:HD11	1:C:1094:VAL:HG11	1.98	0.46
1:C:843:ASP:O	1:C:845:ALA:N	2.49	0.46
2:D:344:CYS:HB2	2:D:360:MET:HA	1.97	0.46
2:D:360:MET:SD	2:D:361:CYS:O	2.73	0.46
2:D:549:GLU:O	2:D:552:GLN:NE2	2.49	0.46
2:E:108:LEU:HD12	2:E:109:SER:H	1.81	0.46
2:E:168:TRP:O	2:E:172:VAL:HG22	2.16	0.46
1:A:129:LYS:HA	1:A:168:PHE:O	2.16	0.46
1:A:592:PHE:CE2	1:C:859:THR:HB	2.51	0.46
1:A:855:PHE:HD1	1:B:589:PRO:HG3	1.80	0.46
1:B:280:ASN:N	1:B:284:THR:O	2.38	0.46
1:B:630:THR:HB	1:B:631:PRO:HD3	1.98	0.46
1:C:136:CYS:SG	1:C:138:ASP:HB2	2.56	0.46
1:A:541:PHE:CZ	1:A:546:LEU:HD22	2.47	0.45
1:A:837:TYR:OH	1:B:589:PRO:O	2.30	0.45
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.49	0.45
1:B:645:THR:C	1:B:647:ALA:N	2.68	0.45
1:C:339:HIS:HA	1:C:371:PHE:CE2	2.46	0.45
1:C:418:ILE:H	1:C:418:ILE:HD12	1.81	0.45
2:D:144:LEU:HB2	2:D:168:TRP:CZ2	2.51	0.45
2:E:135:PRO:HD3	2:E:163:TRP:HE1	1.81	0.45
2:E:356:PHE:CE1	2:E:383:MET:HG3	2.51	0.45
1:A:858:LEU:HD12	1:A:963:VAL:CG2	2.46	0.45
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.38	0.45
1:B:33:THR:HG22	1:B:58:PHE:CD2	2.51	0.45
1:C:407:VAL:HA	1:C:410:ILE:HG22	1.97	0.45
1:C:865:LEU:HD23	1:C:869:MET:HE3	1.96	0.45
2:E:31:LYS:HA	2:E:34:HIS:CD2	2.51	0.45
1:A:23:THR:N	1:A:80:ASP:OD1	2.50	0.45
1:B:383:SER:HB3	1:B:386:LYS:HB2	1.98	0.45
1:C:553:THR:O	1:C:585:LEU:HA	2.17	0.45
2:D:114:LYS:HA	2:D:117:ASN:ND2	2.31	0.45
1:A:714:ILE:HD12	1:A:1096:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLU:HG3	1:A:1064:HIS:CD2	2.51	0.45
1:A:1006:THR:O	1:A:1010:GLN:HG2	2.17	0.45
1:C:48:LEU:HD13	1:C:305:SER:HA	1.98	0.45
1:C:106:PHE:CD1	1:C:106:PHE:N	2.85	0.45
2:D:198:ASP:OD1	2:D:201:ASP:N	2.45	0.45
2:E:28:PHE:CE2	2:E:80:ALA:HB2	2.51	0.45
2:E:302:TRP:CH2	2:E:423:LEU:HD11	2.51	0.45
1:A:592:PHE:HE2	1:C:859:THR:HB	1.81	0.45
1:A:609:ALA:CB	1:A:692:ILE:HD11	2.38	0.45
1:A:703:ASN:OD1	1:A:704:SER:N	2.49	0.45
1:B:119:ILE:CD1	1:B:175:PHE:HE2	2.24	0.45
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.84	0.45
1:C:822:LEU:HD21	1:C:1061:VAL:HG21	1.98	0.45
2:D:46:ALA:HA	2:D:49:ASN:ND2	2.32	0.45
2:E:115:ARG:HA	2:E:115:ARG:NE	2.32	0.45
1:A:595:VAL:HG11	1:A:633:TRP:CZ2	2.46	0.45
1:C:406:GLU:HG3	1:C:418:ILE:HD13	1.97	0.45
1:C:599:THR:HB	1:C:608:VAL:HG12	1.97	0.45
2:E:222:LEU:HA	2:E:225:ASP:OD2	2.17	0.45
2:E:555:PHE:HA	2:E:558:LEU:HD12	1.99	0.45
1:A:86:PHE:N	1:A:236:THR:O	2.45	0.45
1:B:43:PHE:HE2	1:C:558:LYS:HB2	1.81	0.45
1:C:431:GLY:HA3	1:C:513:LEU:O	2.16	0.45
2:E:131:LYS:HE3	2:E:131:LYS:HB3	1.83	0.45
2:E:440:LEU:HD11	2:E:594:TRP:CH2	2.52	0.45
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.99	0.45
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.32	0.45
1:B:1081:ILE:HG23	1:B:1088:HIS:HB2	1.99	0.45
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.98	0.45
1:A:118:LEU:HB2	1:A:133:PHE:CE2	2.52	0.45
1:A:489:TYR:OH	2:E:24:GLN:OE1	2.35	0.45
1:B:64:TRP:HE1	1:B:263:ALA:N	2.15	0.45
1:B:643:PHE:HE1	1:B:670:ILE:HG21	1.82	0.45
1:B:1115:ILE:HG21	1:B:1137:VAL:HG12	1.99	0.45
1:B:1116:THR:OG1	1:B:1119:ASN:OD1	2.34	0.45
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.52	0.45
1:C:641:ASN:HB2	1:C:652:GLY:H	1.81	0.45
2:E:388:GLN:HE22	2:E:562:LYS:H	1.64	0.45
1:A:63:THR:O	1:A:63:THR:OG1	2.35	0.44
1:A:65:PHE:CE1	1:A:84:LEU:HD21	2.52	0.44
1:B:462:LYS:HB2	1:B:465:GLU:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:O	1:C:97:LYS:NZ	2.45	0.44
2:E:579:MET:SD	2:E:579:MET:N	2.90	0.44
1:A:299:THR:O	1:A:302:THR:HG22	2.17	0.44
1:C:116:SER:N	1:C:131:CYS:O	2.26	0.44
2:D:187:LYS:HD2	2:D:199:TYR:CZ	2.52	0.44
2:D:323:MET:SD	2:D:324:THR:O	2.75	0.44
2:D:580:ASN:OD1	2:D:582:ARG:HG2	2.16	0.44
1:A:393:THR:OG1	1:A:516:GLU:OE2	2.34	0.44
1:A:707:TYR:HB2	1:C:883:THR:HB	2.00	0.44
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.00	0.44
1:C:536:ASN:O	1:C:537:LYS:CG	2.65	0.44
1:C:818:ILE:O	1:C:822:LEU:HD13	2.18	0.44
2:D:71:ALA:O	2:D:74:LYS:HG3	2.17	0.44
2:D:223:ILE:HG12	2:D:461:TRP:CZ3	2.52	0.44
2:E:310:GLU:O	2:E:313:LYS:HG3	2.17	0.44
2:E:394:ASN:HB3	2:E:562:LYS:HD3	1.98	0.44
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.83	0.44
1:B:320:VAL:H	1:B:591:SER:HB2	1.82	0.44
1:B:589:PRO:HB3	1:B:592:PHE:CE1	2.52	0.44
1:B:963:VAL:CG1	1:C:570:VAL:HG21	2.47	0.44
1:A:318:PHE:HD2	1:A:629:LEU:HD22	1.81	0.44
1:C:299:THR:O	1:C:302:THR:HG22	2.16	0.44
1:C:645:THR:HG22	1:C:647:ALA:H	1.83	0.44
1:C:947:LYS:HB2	1:C:947:LYS:HE3	1.81	0.44
2:D:520:LEU:HB3	2:D:579:MET:CE	2.40	0.44
1:A:192:PHE:HB3	1:A:194:PHE:CZ	2.52	0.44
1:A:617:CYS:HB3	1:A:649:CYS:HB3	1.67	0.44
1:A:1076:THR:HG22	1:A:1077:THR:N	2.33	0.44
1:B:340:GLU:OE1	1:B:340:GLU:N	2.50	0.44
1:C:119:ILE:HG23	1:C:128:ILE:HG12	2.00	0.44
1:A:556:ASN:HB3	1:C:844:ILE:HG23	2.00	0.44
1:A:748:GLU:OE1	1:A:748:GLU:N	2.34	0.44
1:B:624:ILE:CG2	1:B:634:ARG:HD2	2.47	0.44
1:C:570:VAL:O	1:C:570:VAL:CG2	2.64	0.44
2:D:32:PHE:CE1	2:D:76:GLN:HG3	2.52	0.44
2:E:145:GLU:HB2	2:E:146:PRO:HD3	1.99	0.44
1:A:555:SER:HB2	1:A:586:ASP:OD1	2.17	0.44
1:A:557:LYS:HG2	1:C:844:ILE:O	2.18	0.44
1:B:338:PHE:HA	1:B:341:VAL:HG12	2.00	0.44
1:C:33:THR:HG22	1:C:220:PHE:CD1	2.53	0.44
1:C:205:SER:OG	1:C:206:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:SER:O	1:C:360:ASN:ND2	2.51	0.44
1:C:902:MET:CE	1:C:1049:LEU:HD13	2.47	0.44
1:C:974:SER:OG	1:C:975:SER:N	2.50	0.44
2:D:577:LYS:HE2	2:D:577:LYS:HB3	1.91	0.44
2:E:39:LEU:O	2:E:42:GLN:HG2	2.17	0.44
1:A:904:TYR:OH	1:B:1094:VAL:HG12	2.17	0.44
1:B:364:ASP:OD1	1:B:364:ASP:N	2.50	0.44
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.53	0.44
1:B:901:GLN:HE21	1:B:905:ARG:HH21	1.65	0.44
1:C:631:PRO:HA	1:C:633:TRP:CZ3	2.53	0.44
2:E:297:MET:HG2	2:E:302:TRP:CB	2.48	0.44
1:B:34:ARG:NH2	1:B:217:PRO:O	2.51	0.43
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.99	0.43
1:C:362:VAL:HG13	1:C:526:GLY:HA2	2.00	0.43
2:E:239:HIS:HB3	2:E:595:LEU:HG	1.99	0.43
1:A:53:ASP:OD1	1:A:54:LEU:N	2.52	0.43
1:A:752:LEU:HD13	1:A:752:LEU:HA	1.84	0.43
1:B:402:ILE:HD11	1:B:510:VAL:HG21	1.99	0.43
2:D:153:ALA:O	2:D:277:ASN:ND2	2.51	0.43
2:D:302:TRP:CG	2:D:306:ARG:HD3	2.52	0.43
2:D:570:LEU:O	2:D:574:VAL:HG22	2.18	0.43
1:A:86:PHE:CE2	1:A:90:VAL:HG12	2.51	0.43
1:A:541:PHE:CZ	1:A:546:LEU:CD2	2.79	0.43
1:A:837:TYR:OH	1:B:590:CYS:O	2.36	0.43
1:A:913:GLN:H	1:A:913:GLN:HG2	1.63	0.43
1:B:372:ALA:HB1	1:B:436:TRP:CE2	2.53	0.43
1:B:878:LEU:O	1:B:882:ILE:HG23	2.18	0.43
2:D:475:LYS:HD2	2:D:475:LYS:HA	1.86	0.43
2:E:26:LYS:O	2:E:29:LEU:HG	2.18	0.43
2:E:366:MET:CE	2:E:370:LEU:HD21	2.48	0.43
1:A:376:ALA:HB3	1:A:435:ALA:HB3	2.01	0.43
1:A:736:VAL:HG13	1:A:858:LEU:HD23	2.00	0.43
1:B:367:VAL:HA	1:B:370:ASN:OD1	2.18	0.43
1:B:374:PHE:HA	1:B:436:TRP:CD1	2.53	0.43
1:B:703:ASN:OD1	1:B:704:SER:N	2.51	0.43
1:C:34:ARG:NH1	1:C:217:PRO:HD2	2.33	0.43
1:C:403:LYS:N	1:C:495:TYR:OH	2.51	0.43
1:C:1100:THR:HG22	1:C:1101:HIS:CE1	2.54	0.43
2:D:557:MET:O	2:D:557:MET:HG2	2.19	0.43
2:E:116:LEU:HA	2:E:119:ILE:HG12	2.00	0.43
2:E:312:GLU:O	2:E:316:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:GLU:OE1	1:A:340:GLU:N	2.52	0.43
1:A:588:THR:HG23	1:A:589:PRO:HD2	1.99	0.43
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.54	0.43
1:C:91:TYR:CE1	1:C:191:GLU:HB3	2.53	0.43
1:C:631:PRO:HB3	1:C:633:TRP:CE2	2.54	0.43
1:A:300:LYS:HE3	1:A:306:PHE:HA	2.01	0.43
1:B:498:ARG:NH1	2:D:38:ASP:OD1	2.51	0.43
1:C:447:GLY:HA2	1:C:498:ARG:HG2	2.01	0.43
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.18	0.43
2:D:234:LYS:HG2	2:D:235:PRO:HD3	2.00	0.43
2:D:293:VAL:HG22	2:D:366:MET:SD	2.59	0.43
2:E:48:TRP:CE2	2:E:357:ARG:HD3	2.53	0.43
2:E:245:ARG:NH2	2:E:603:PHE:O	2.51	0.43
1:A:168:PHE:HE1	1:A:229:LEU:HD22	1.84	0.43
1:B:113:LYS:HE2	1:B:113:LYS:HB3	1.74	0.43
1:B:434:ILE:HB	1:B:511:VAL:HG13	2.00	0.43
1:B:790:LYS:NZ	1:C:702:GLU:OE2	2.47	0.43
2:D:245:ARG:NH2	2:D:603:PHE:O	2.51	0.43
1:B:554:LYS:NZ	1:B:583:GLU:HB3	2.34	0.43
1:B:969:LYS:HE2	1:B:969:LYS:HB2	1.77	0.43
1:C:65:PHE:HB2	1:C:265:TYR:CB	2.48	0.43
1:C:108:THR:O	1:C:109:THR:OG1	2.37	0.43
1:C:1108:ASN:ND2	1:C:1108:ASN:N	2.66	0.43
2:D:520:LEU:HD11	2:D:581:VAL:HG12	2.00	0.43
2:E:111:ASP:O	2:E:115:ARG:HG2	2.19	0.43
2:E:143:LEU:HD23	2:E:146:PRO:HD2	1.99	0.43
1:A:83:VAL:HG12	1:A:237:ARG:HB3	2.01	0.43
1:A:206:LYS:HB2	1:A:223:LEU:HA	2.01	0.43
1:A:455:LEU:HD12	1:A:493:GLN:HG3	2.01	0.43
1:B:624:ILE:HG23	1:B:634:ARG:HD2	2.00	0.43
2:D:332:MET:SD	2:D:332:MET:O	2.77	0.43
2:D:384:ALA:CB	2:D:558:LEU:HB3	2.48	0.43
2:E:280:SER:O	2:E:283:VAL:HG12	2.19	0.43
2:E:609:ASP:OD1	2:E:609:ASP:N	2.52	0.43
1:A:485:GLY:H	1:A:488:CYS:HB2	1.84	0.43
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.01	0.43
1:C:1083:HIS:HD2	1:C:1136:THR:HA	1.84	0.43
2:D:460:ARG:NH1	2:D:506:VAL:HA	2.33	0.43
2:E:415:PRO:HD2	2:E:541:LYS:HZ3	1.84	0.43
1:A:96:GLU:OE1	1:A:100:ILE:N	2.52	0.42
1:A:827:THR:OG1	1:A:949:GLN:NE2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.42
1:A:1139:ASP:OD1	1:A:1142:GLN:N	2.33	0.42
1:B:920:GLN:HA	1:B:923:ILE:HG22	2.00	0.42
1:C:533:LEU:CD2	1:C:535:LYS:HZ1	2.19	0.42
2:D:44:SER:HB3	2:D:351:LEU:HG	2.00	0.42
2:D:557:MET:HA	2:D:560:LEU:HG	2.01	0.42
1:B:105:ILE:HG23	1:B:241:LEU:HD21	2.01	0.42
1:C:361:CYS:SG	1:C:524:VAL:HG12	2.59	0.42
2:E:440:LEU:HD11	2:E:594:TRP:CZ3	2.54	0.42
1:A:170:TYR:CE1	1:A:172:SER:HB3	2.55	0.42
1:A:315:THR:OG1	1:A:316:SER:N	2.53	0.42
1:C:303:LEU:H	1:C:303:LEU:HG	1.65	0.42
1:C:342:PHE:HE2	1:C:511:VAL:HB	1.84	0.42
1:C:421:TYR:HB3	1:C:457:ARG:HB2	2.02	0.42
1:C:422:ASN:ND2	1:C:454:ARG:O	2.33	0.42
1:C:720:ILE:HD12	1:C:923:ILE:HG13	2.01	0.42
1:C:725:GLU:C	1:C:726:ILE:HD13	2.40	0.42
2:D:321:PRO:CG	2:D:383:MET:HE1	2.46	0.42
2:D:468:ILE:HG23	2:D:472:GLN:NE2	2.28	0.42
2:E:148:LEU:O	2:E:152:MET:CE	2.68	0.42
1:A:119:ILE:HG23	1:A:128:ILE:HG12	2.02	0.42
1:A:191:GLU:HB2	1:A:223:LEU:HD21	2.01	0.42
1:A:451:TYR:O	1:A:452:TRP:CE3	2.72	0.42
1:C:634:ARG:HA	1:C:634:ARG:HD2	1.88	0.42
1:C:736:VAL:HG22	1:C:858:LEU:HD23	2.00	0.42
1:C:742:ILE:HD13	1:C:753:LEU:HD13	2.00	0.42
2:E:43:SER:HA	2:E:65:ALA:HB1	2.01	0.42
2:E:236:LEU:HD13	2:E:592:PHE:HB2	2.01	0.42
2:E:444:LEU:HD23	2:E:444:LEU:HA	1.86	0.42
1:A:34:ARG:HG3	1:A:35:GLY:N	2.34	0.42
1:A:85:PRO:O	1:A:269:TYR:OH	2.28	0.42
1:B:869:MET:SD	1:C:699:LEU:HD21	2.60	0.42
1:B:907:ASN:HB2	1:B:913:GLN:HG3	2.02	0.42
1:B:921:LYS:HD2	1:B:921:LYS:HA	1.93	0.42
1:B:995:ARG:HG2	1:B:995:ARG:H	1.59	0.42
1:C:878:LEU:HD12	1:C:878:LEU:HA	1.87	0.42
2:D:74:LYS:O	2:D:78:THR:HG22	2.20	0.42
2:D:119:ILE:HD13	2:D:119:ILE:HA	1.92	0.42
2:D:265:HIS:ND1	2:D:490:PRO:HG3	2.34	0.42
1:A:94:SER:HB2	1:A:264:ASP:HB2	2.01	0.42
1:A:631:PRO:HB3	1:A:633:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASP:HB3	1:B:55:PHE:CZ	2.54	0.42
1:A:86:PHE:CZ	1:A:89:GLY:HA2	2.55	0.42
1:A:206:LYS:HD2	1:A:207:HIS:N	2.35	0.42
1:A:878:LEU:O	1:A:882:ILE:HG23	2.20	0.42
1:B:1080:ALA:HB3	1:B:1129:VAL:HG11	2.02	0.42
1:C:106:PHE:CE1	1:C:119:ILE:HD11	2.54	0.42
1:C:218:GLN:OE1	1:C:218:GLN:N	2.49	0.42
1:C:497:PHE:CD1	1:C:507:PRO:HG3	2.53	0.42
1:C:959:LEU:O	1:C:963:VAL:HG23	2.19	0.42
2:D:275:TRP:HB3	2:D:444:LEU:HD22	2.00	0.42
2:D:455:MET:CE	2:D:477:TRP:HD1	2.32	0.42
1:A:48:LEU:HD11	1:A:306:PHE:HD1	1.85	0.42
1:A:103:GLY:C	1:A:104:TRP:CD1	2.93	0.42
1:A:404:GLY:HA2	1:A:508:TYR:HD2	1.84	0.42
1:A:450:ASP:C	1:A:452:TRP:CZ3	2.93	0.42
1:A:560:LEU:HD13	1:A:563:GLN:NE2	2.31	0.42
1:A:883:THR:OG1	1:B:707:TYR:HB2	2.20	0.42
1:B:50:LEU:HB2	1:B:276:LEU:HD12	2.02	0.42
1:B:444:LYS:HE2	1:B:444:LYS:HB2	1.83	0.42
1:C:44:ARG:HB3	1:C:47:VAL:HG11	2.02	0.42
1:C:127:PHE:CD1	1:C:127:PHE:O	2.73	0.42
1:C:478:LYS:HE3	1:C:478:LYS:HB2	1.86	0.42
1:C:1091:ARG:N	1:C:1119:ASN:O	2.40	0.42
1:A:118:LEU:HB3	1:A:129:LYS:HG3	2.01	0.42
1:A:553:THR:OG1	1:A:554:LYS:N	2.53	0.42
1:A:559:PHE:HB3	1:A:577:ARG:NH2	2.34	0.42
1:B:126:VAL:HG11	1:B:175:PHE:CE2	2.54	0.42
1:B:671:CYS:SG	1:B:697:MET:HG2	2.60	0.42
1:C:411:ALA:C	1:C:425:LEU:HD12	2.40	0.42
2:D:479:GLU:HG3	2:D:483:GLU:OE2	2.20	0.42
2:E:173:GLY:HA3	2:E:498:CYS:H	1.85	0.42
1:B:91:TYR:HD1	1:B:193:VAL:HG22	1.85	0.42
1:B:177:MET:H	1:B:207:HIS:CE1	2.37	0.42
1:B:817:PRO:O	1:B:821:LEU:HG	2.20	0.42
1:B:984:LEU:HB3	1:B:988:GLU:HB2	2.00	0.42
1:B:992:GLN:H	1:B:992:GLN:HG2	1.65	0.42
1:C:206:LYS:HD3	1:C:224:GLU:OE1	2.20	0.42
1:C:655:TYR:CD2	4:C:1306:NAG:H61	2.54	0.42
1:A:848:ASP:N	1:A:848:ASP:OD1	2.42	0.41
1:B:278:LYS:O	1:B:285:ILE:HA	2.20	0.41
1:B:702:GLU:OE1	1:B:703:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:GLN:O	1:B:837:TYR:C	2.58	0.41
1:C:48:LEU:HD22	1:C:276:LEU:HD21	2.01	0.41
1:C:334:ASN:N	1:C:334:ASN:HD22	2.18	0.41
1:C:381:GLY:HA3	1:C:430:THR:HA	2.02	0.41
1:C:1129:VAL:HB	1:C:1132:ILE:HB	2.01	0.41
2:D:248:LEU:HB3	2:D:256:ILE:HD13	2.01	0.41
2:D:476:LYS:HG3	2:D:480:MET:CE	2.50	0.41
1:A:109:THR:H	1:A:237:ARG:CZ	2.33	0.41
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.20	0.41
1:B:86:PHE:HE1	1:B:235:ILE:HB	1.86	0.41
1:B:852:ALA:HB1	1:C:570:VAL:HG22	2.01	0.41
1:C:308:VAL:HG22	1:C:602:THR:HB	2.02	0.41
1:C:322:PRO:HA	1:C:538:CYS:HB2	2.02	0.41
1:A:744:GLY:O	1:A:745:ASP:C	2.59	0.41
1:C:849:LEU:HD12	1:C:849:LEU:H	1.85	0.41
1:C:1108:ASN:HD22	1:C:1108:ASN:N	2.17	0.41
2:D:177:ARG:O	2:D:181:GLU:HG3	2.20	0.41
2:D:392:LEU:HD12	2:D:562:LYS:HG3	2.02	0.41
2:D:524:GLN:HE21	2:D:579:MET:HE3	1.84	0.41
1:A:350:VAL:HG22	1:A:422:ASN:HB3	2.03	0.41
1:C:33:THR:HG23	1:C:58:PHE:CZ	2.56	0.41
1:C:34:ARG:HH22	1:C:189:LEU:CD2	2.16	0.41
1:C:708:SER:HB3	1:C:711:SER:HB2	2.02	0.41
2:D:168:TRP:O	2:D:172:VAL:HG22	2.20	0.41
2:D:249:MET:SD	2:D:258:PRO:HA	2.60	0.41
2:E:247:LYS:HG3	2:E:282:THR:HG22	2.02	0.41
2:E:284:PRO:HD3	2:E:440:LEU:HD13	2.01	0.41
2:E:297:MET:SD	2:E:307:ILE:HD11	2.59	0.41
2:E:540:HIS:HB3	2:E:587:TYR:CE1	2.55	0.41
1:A:91:TYR:OH	1:A:93:ALA:HB2	2.21	0.41
1:A:164:ASN:HB2	4:A:1304:NAG:O7	2.20	0.41
1:A:308:VAL:HG22	1:A:602:THR:HB	2.02	0.41
1:A:462:LYS:HB2	1:A:465:GLU:HG3	2.02	0.41
1:A:922:LEU:O	1:A:926:GLN:HG3	2.21	0.41
1:B:290:ASP:O	1:B:297:SER:HB3	2.21	0.41
1:B:1081:ILE:CG2	1:B:1088:HIS:HB2	2.51	0.41
1:B:1097:SER:C	1:B:1099:GLY:N	2.72	0.41
2:D:29:LEU:HD12	2:D:96:GLN:HE21	1.85	0.41
2:D:269:ASP:OD1	2:D:272:GLY:N	2.54	0.41
2:E:148:LEU:HD23	2:E:151:ILE:HD12	2.02	0.41
2:E:344:CYS:HB2	2:E:361:CYS:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ASN:OD1	1:A:188:ASN:N	2.51	0.41
1:A:239:GLN:NE2	1:A:240:THR:O	2.54	0.41
1:A:738:CYS:HA	1:A:1004:LEU:HD21	2.03	0.41
1:A:941:THR:HG21	1:A:944:ALA:HB2	2.03	0.41
1:B:895:GLN:O	1:B:896:ILE:HG12	2.20	0.41
1:C:329:PHE:HB3	1:C:528:LYS:HD2	2.01	0.41
2:D:80:ALA:HB3	2:D:100:LEU:HD22	2.02	0.41
2:E:384:ALA:CB	2:E:558:LEU:HB3	2.50	0.41
1:A:303:LEU:HD13	1:A:305:SER:HB3	2.03	0.41
1:A:495:TYR:HB3	1:A:497:PHE:CZ	2.56	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CE3	2.56	0.41
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG21	2.56	0.41
1:B:848:ASP:OD1	1:B:848:ASP:N	2.45	0.41
1:C:29:THR:HG22	1:C:30:ASN:H	1.84	0.41
1:C:87:ASN:N	1:C:87:ASN:OD1	2.54	0.41
1:C:242:LEU:H	1:C:242:LEU:CD2	2.25	0.41
1:C:984:LEU:HD12	1:C:984:LEU:HA	1.92	0.41
2:D:455:MET:HE2	2:D:477:TRP:CD1	2.56	0.41
2:E:304:ALA:O	2:E:308:PHE:HD1	2.02	0.41
1:A:444:LYS:HE2	1:A:444:LYS:HB2	1.85	0.41
1:A:506:GLN:HA	1:A:507:PRO:HD3	1.93	0.41
1:A:977:LEU:O	1:A:980:ILE:HG12	2.21	0.41
1:A:1089:PHE:O	1:A:1120:THR:HA	2.20	0.41
1:B:129:LYS:HE2	1:B:129:LYS:HB3	1.90	0.41
1:B:303:LEU:H	1:B:303:LEU:HG	1.70	0.41
1:C:346:ARG:HD3	1:C:346:ARG:HA	1.94	0.41
1:C:480:CYS:HB3	1:C:488:CYS:HB3	1.89	0.41
2:D:315:PHE:HE1	2:D:408:MET:CE	2.33	0.41
2:D:534:LYS:HA	2:D:534:LYS:HD3	1.94	0.41
2:E:179:LEU:HD23	2:E:182:GLU:CD	2.41	0.41
1:A:295:PRO:HG3	1:A:633:TRP:CD1	2.55	0.41
1:A:374:PHE:CZ	1:A:434:ILE:HG23	2.56	0.41
1:A:589:PRO:O	1:C:837:TYR:HE2	2.04	0.41
1:A:674:TYR:CZ	1:A:690:GLN:HB3	2.56	0.41
1:A:919:ASN:O	1:A:923:ILE:HG22	2.21	0.41
1:A:931:ILE:HD12	1:A:931:ILE:HA	1.94	0.41
1:B:28:TYR:HB3	1:B:61:ASN:HD21	1.86	0.41
1:B:1102:TRP:CH2	1:B:1133:VAL:HG11	2.56	0.41
1:C:25:THR:HG23	1:C:66:HIS:HB3	2.02	0.41
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.56	0.41
2:D:69:TRP:NE1	2:D:73:LEU:HD11	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:ASP:OD1	2:D:219:ARG:HD2	2.21	0.41
2:D:293:VAL:O	2:D:297:MET:N	2.48	0.41
2:D:555:PHE:HA	2:D:558:LEU:HD12	2.03	0.41
2:E:483:GLU:HG3	2:E:484:ILE:N	2.36	0.41
1:A:104:TRP:CD1	1:A:104:TRP:N	2.88	0.41
1:A:453:TYR:HB3	1:A:495:TYR:CE2	2.56	0.41
1:C:588:THR:HB	1:C:589:PRO:HD2	2.03	0.41
1:A:434:ILE:HB	1:A:511:VAL:HG13	2.02	0.40
1:A:577:ARG:HA	1:A:583:GLU:O	2.21	0.40
1:A:865:LEU:HD23	1:A:865:LEU:HA	1.92	0.40
1:B:107:GLY:N	1:B:235:ILE:HG23	2.36	0.40
1:B:323:THR:OG1	1:B:324:GLU:N	2.54	0.40
1:C:342:PHE:CE2	1:C:511:VAL:HB	2.56	0.40
1:C:733:LYS:HD2	1:C:861:LEU:HB2	2.03	0.40
2:D:308:PHE:CE2	2:D:376:MET:CE	3.04	0.40
2:E:32:PHE:CE2	2:E:391:LEU:HD21	2.57	0.40
2:E:32:PHE:CD2	2:E:391:LEU:HD21	2.56	0.40
2:E:419:LYS:HG3	2:E:424:LEU:HD23	2.03	0.40
1:A:105:ILE:CG2	1:A:239:GLN:HB3	2.52	0.40
1:B:265:TYR:O	1:B:267:VAL:HG23	2.21	0.40
1:B:582:LEU:HD23	4:B:1306:NAG:H81	2.02	0.40
1:C:83:VAL:HG11	1:C:237:ARG:HE	1.86	0.40
1:C:1144:GLU:OE1	1:C:1144:GLU:N	2.52	0.40
2:D:50:TYR:CD2	2:D:62:MET:CE	3.04	0.40
2:D:70:SER:HA	2:D:73:LEU:HD12	2.04	0.40
2:D:308:PHE:CE2	2:D:376:MET:HE1	2.47	0.40
2:D:478:TRP:HB3	2:D:482:ARG:NH2	2.37	0.40
2:E:275:TRP:HB3	2:E:444:LEU:HD22	2.02	0.40
1:A:598:ILE:O	1:A:598:ILE:HG13	2.22	0.40
1:A:653:ALA:HB2	1:A:692:ILE:HD12	2.01	0.40
1:A:805:ILE:HB	1:A:878:LEU:HD11	2.03	0.40
1:A:986:PRO:HB2	1:A:987:PRO:HD3	2.02	0.40
1:A:996:LEU:HA	1:A:996:LEU:HD23	1.83	0.40
1:A:1115:ILE:O	1:A:1138:TYR:HB2	2.21	0.40
1:C:124:THR:O	1:C:174:PRO:HD3	2.21	0.40
1:C:201:PHE:N	1:C:229:LEU:O	2.54	0.40
1:C:555:SER:HB2	1:C:586:ASP:CG	2.42	0.40
1:C:1039:ARG:H	1:C:1039:ARG:HG2	1.67	0.40
1:C:1078:ALA:HB2	1:C:1102:TRP:CZ3	2.56	0.40
2:E:292:ASP:OD2	2:E:294:THR:HG23	2.22	0.40
2:E:557:MET:SD	2:E:557:MET:C	3.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.02	0.40
1:A:589:PRO:HG3	1:C:855:PHE:CA	2.51	0.40
1:A:844:ILE:O	1:B:557:LYS:HG2	2.20	0.40
1:B:1091:ARG:HG2	1:B:1119:ASN:C	2.41	0.40
1:C:97:LYS:HE2	1:C:184:GLY:HA3	2.03	0.40
1:C:413:GLY:HA2	1:C:424:LYS:NZ	2.36	0.40
1:C:541:PHE:N	1:C:548:GLY:O	2.46	0.40
1:C:1098:ASN:OD1	1:C:1099:GLY:N	2.55	0.40
2:D:47:SER:CA	2:D:62:MET:SD	3.07	0.40
2:D:245:ARG:HA	2:D:262:LEU:HD21	2.04	0.40
2:D:478:TRP:HA	2:D:481:LYS:HE3	2.03	0.40
2:E:297:MET:CG	2:E:302:TRP:HE3	2.34	0.40
1:A:928:ASN:O	1:A:931:ILE:HG22	2.22	0.40
1:A:992:GLN:HA	1:A:995:ARG:HH11	1.85	0.40
1:B:37:TYR:HA	1:B:223:LEU:HB2	2.03	0.40
1:B:121:ASN:HD21	1:B:175:PHE:HB2	1.87	0.40
1:B:631:PRO:HB3	1:B:633:TRP:CE2	2.57	0.40
1:B:705:VAL:CG1	1:B:706:ALA:H	2.35	0.40
1:C:731:MET:HB3	1:C:731:MET:HE2	1.87	0.40
1:C:817:PRO:O	1:C:821:LEU:HG	2.22	0.40
1:C:865:LEU:HD22	1:C:869:MET:CE	2.51	0.40
2:D:28:PHE:CE2	2:D:80:ALA:HB2	2.57	0.40
2:E:249:MET:SD	2:E:258:PRO:HA	2.62	0.40
2:E:297:MET:CG	2:E:302:TRP:CE3	3.04	0.40
2:E:395:GLY:O	2:E:562:LYS:HB3	2.21	0.40
2:E:453:THR:HA	2:E:512:PHE:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1047/1206 (87%)	960 (92%)	83 (8%)	4 (0%)	30	61
1	B	1047/1206 (87%)	952 (91%)	91 (9%)	4 (0%)	30	61
1	C	1047/1206 (87%)	949 (91%)	90 (9%)	8 (1%)	16	46
2	D	595/597 (100%)	576 (97%)	18 (3%)	1 (0%)	44	71
2	E	595/597 (100%)	573 (96%)	22 (4%)	0	100	100
All	All	4331/4812 (90%)	4010 (93%)	304 (7%)	17 (0%)	32	61

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	591	SER
1	A	983	ARG
1	C	348	ALA
1	C	536	ASN
1	C	591	SER
1	C	1135	ASN
1	A	745	ASP
1	C	335	LEU
1	C	347	PHE
2	D	147	GLY
1	C	304	LYS
1	C	334	ASN
1	B	646	ARG
1	B	1098	ASN
1	B	334	ASN
1	A	330	PRO
1	B	642	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	922/1054 (88%)	902 (98%)	20 (2%)	47	69
1	B	922/1054 (88%)	894 (97%)	28 (3%)	36	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	922/1054 (88%)	885 (96%)	37 (4%)	27 55
2	D	527/527 (100%)	517 (98%)	10 (2%)	52 72
2	E	527/527 (100%)	514 (98%)	13 (2%)	42 67
All	All	3820/4216 (91%)	3712 (97%)	108 (3%)	40 64

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	134	GLN
1	A	135	PHE
1	A	168	PHE
1	A	200	TYR
1	A	303	LEU
1	A	306	PHE
1	A	452	TRP
1	A	457	ARG
1	A	541	PHE
1	A	542	ASN
1	A	620	VAL
1	A	643	PHE
1	A	698	SER
1	A	740	MET
1	A	752	LEU
1	A	919	ASN
1	A	1000	ARG
1	A	1082	CYS
1	A	1118	ASP
1	B	86	PHE
1	B	135	PHE
1	B	168	PHE
1	B	188	ASN
1	B	194	PHE
1	B	200	TYR
1	B	238	PHE
1	B	265	TYR
1	B	303	LEU
1	B	336	CYS
1	B	342	PHE
1	B	437	ASN
1	B	457	ARG

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Mol	Chain	Res	Type
1	B	480	CYS
1	B	492	LEU
1	B	523	THR
1	B	524	VAL
1	B	525	CYS
1	B	543	PHE
1	B	565	PHE
1	B	617	CYS
1	B	644	GLN
1	B	759	PHE
1	B	867	ASP
1	B	873	TYR
1	B	1075	PHE
1	B	1095	PHE
1	B	1108	ASN
1	C	29	THR
1	C	121	ASN
1	C	127	PHE
1	C	168	PHE
1	C	216	PHE
1	C	220	PHE
1	C	238	PHE
1	C	287	ASP
1	C	303	LEU
1	C	306	PHE
1	C	318	PHE
1	C	328	ARG
1	C	329	PHE
1	C	332	VAL
1	C	333	THR
1	C	334	ASN
1	C	353	TRP
1	C	356	THR
1	C	377	PHE
1	C	382	VAL
1	C	392	PHE
1	C	421	TYR
1	C	457	ARG
1	C	495	TYR
1	C	559	PHE
1	C	567	ARG
1	C	636	TYR

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Mol	Chain	Res	Type
1	C	759	PHE
1	C	760	CYS
1	C	869	MET
1	C	907	ASN
1	C	914	ASN
1	C	967	SER
1	C	968	SER
1	C	1045	LYS
1	C	1075	PHE
1	C	1104	VAL
2	D	74	LYS
2	D	105	SER
2	D	143	LEU
2	D	145	GLU
2	D	313	LYS
2	D	357	ARG
2	D	408	MET
2	D	524	GLN
2	D	546	ASN
2	D	579	MET
2	E	91	LEU
2	E	158	TYR
2	E	199	TYR
2	E	225	ASP
2	E	302	TRP
2	E	313	LYS
2	E	381	TYR
2	E	427	ASP
2	E	455	MET
2	E	462	MET
2	E	557	MET
2	E	592	PHE
2	E	609	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	207	HIS
1	A	422	ASN
1	A	506	GLN
1	A	913	GLN

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Mol	Chain	Res	Type
1	A	978	ASN
1	A	1005	GLN
1	B	30	ASN
1	B	49	HIS
1	B	207	HIS
1	B	422	ASN
1	B	644	GLN
1	B	965	GLN
1	C	321	GLN
1	C	334	ASN
1	C	360	ASN
1	C	1083	HIS
1	C	1108	ASN
1	C	1119	ASN
2	D	472	GLN
2	D	556	ASN
2	D	598	GLN
2	E	139	GLN
2	E	401	HIS
2	E	437	ASN
2	E	526	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

30 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	$\#\|Z\|>2$
3	NAG	F	1	3,1	14,14,15	0.49	0	17,19,21	0.97	1 (5%)
3	BMA	F	2	3	11,11,12	0.85	1 (9%)	15,15,17	0.84	0
3	NAG	G	1	3,1	14,14,15	0.20	0	17,19,21	0.40	0
3	BMA	G	2	3	11,11,12	0.66	0	15,15,17	0.71	0
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.96	2 (11%)
3	BMA	H	2	3	11,11,12	0.61	0	15,15,17	0.74	0
3	NAG	I	1	3,1	14,14,15	0.25	0	17,19,21	0.43	0
3	BMA	I	2	3	11,11,12	0.59	0	15,15,17	0.77	0
3	NAG	J	1	3,1	14,14,15	1.53	1 (7%)	17,19,21	1.31	1 (5%)
3	BMA	J	2	3	11,11,12	0.80	0	15,15,17	1.41	3 (20%)
3	NAG	K	1	3,1	14,14,15	0.21	0	17,19,21	0.38	0
3	BMA	K	2	3	11,11,12	0.83	1 (9%)	15,15,17	0.78	0
3	NAG	L	1	3,1	14,14,15	0.33	0	17,19,21	0.42	0
3	BMA	L	2	3	11,11,12	0.50	0	15,15,17	0.76	0
3	NAG	M	1	3,1	14,14,15	0.39	0	17,19,21	0.90	2 (11%)
3	BMA	M	2	3	11,11,12	0.72	0	15,15,17	0.70	0
3	NAG	N	1	3,1	14,14,15	0.24	0	17,19,21	0.43	0
3	BMA	N	2	3	11,11,12	0.66	0	15,15,17	0.74	0
3	NAG	O	1	3,1	14,14,15	1.51	1 (7%)	17,19,21	1.30	1 (5%)
3	BMA	O	2	3	11,11,12	1.00	2 (18%)	15,15,17	1.39	2 (13%)
3	NAG	P	1	3,1	14,14,15	0.32	0	17,19,21	0.37	0
3	BMA	P	2	3	11,11,12	0.90	0	15,15,17	0.91	0
3	NAG	Q	1	3,1	14,14,15	0.27	0	17,19,21	0.52	0
3	BMA	Q	2	3	11,11,12	0.63	0	15,15,17	0.72	0
3	NAG	R	1	3,1	14,14,15	0.39	0	17,19,21	0.87	2 (11%)
3	BMA	R	2	3	11,11,12	0.83	0	15,15,17	0.64	0
3	NAG	S	1	3,1	14,14,15	0.29	0	17,19,21	0.47	0
3	BMA	S	2	3	11,11,12	0.66	0	15,15,17	0.76	0
3	NAG	T	1	3,1	14,14,15	1.58	1 (7%)	17,19,21	1.36	1 (5%)
3	BMA	T	2	3	11,11,12	0.91	1 (9%)	15,15,17	1.09	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	H	2	3	-	2/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	J	2	3	-	2/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	BMA	K	2	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	L	2	3	-	0/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	M	2	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	1/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	4/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	Q	2	3	-	0/2/19/22	0/1/1/1
3	NAG	R	1	3,1	-	5/6/23/26	0/1/1/1
3	BMA	R	2	3	-	1/2/19/22	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	S	2	3	-	0/2/19/22	0/1/1/1
3	NAG	T	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	T	2	3	-	1/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	1	NAG	O5-C1	-5.53	1.34	1.43
3	J	1	NAG	O5-C1	-5.32	1.35	1.43
3	O	1	NAG	O5-C1	-5.18	1.35	1.43
3	O	2	BMA	O5-C1	-2.37	1.39	1.43
3	K	2	BMA	C1-C2	2.13	1.57	1.52
3	F	2	BMA	C1-C2	2.13	1.57	1.52
3	T	2	BMA	C2-C3	2.12	1.55	1.52
3	O	2	BMA	C2-C3	2.05	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	T	1	NAG	C3-C4-C5	4.55	118.36	110.24
3	O	1	NAG	C3-C4-C5	4.15	117.65	110.24
3	J	1	NAG	C3-C4-C5	4.06	117.49	110.24
3	F	1	NAG	C1-O5-C5	3.37	116.76	112.19
3	J	2	BMA	C1-O5-C5	2.93	116.16	112.19
3	O	2	BMA	C1-C2-C3	2.76	113.06	109.67
3	O	2	BMA	C1-O5-C5	2.58	115.69	112.19
3	J	2	BMA	C1-C2-C3	2.55	112.80	109.67
3	J	2	BMA	O5-C1-C2	2.45	114.55	110.77
3	R	1	NAG	C1-C2-N2	2.44	114.66	110.49
3	M	1	NAG	C1-C2-N2	2.30	114.41	110.49
3	H	1	NAG	C1-C2-N2	2.25	114.33	110.49
3	T	2	BMA	C1-C2-C3	2.22	112.39	109.67
3	H	1	NAG	C2-N2-C7	2.21	126.05	122.90
3	M	1	NAG	C2-N2-C7	2.16	125.98	122.90
3	R	1	NAG	C2-N2-C7	2.04	125.80	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1	NAG	C3-C2-N2-C7
3	M	1	NAG	C3-C2-N2-C7
3	R	1	NAG	C3-C2-N2-C7
3	S	1	NAG	O5-C5-C6-O6
3	O	2	BMA	O5-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	O	2	BMA	C4-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	K	1	NAG	C8-C7-N2-C2
3	K	1	NAG	O7-C7-N2-C2
3	P	1	NAG	C8-C7-N2-C2
3	P	1	NAG	O7-C7-N2-C2
3	J	2	BMA	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	J	2	BMA	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	M	2	BMA	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	H	2	BMA	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	R	2	BMA	O5-C5-C6-O6
3	M	2	BMA	C4-C5-C6-O6
3	M	1	NAG	C8-C7-N2-C2
3	R	1	NAG	C8-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
3	M	1	NAG	C1-C2-N2-C7
3	R	1	NAG	C1-C2-N2-C7
3	T	2	BMA	O5-C5-C6-O6
3	R	1	NAG	O7-C7-N2-C2
3	M	1	NAG	O7-C7-N2-C2
3	N	1	NAG	O5-C5-C6-O6
3	H	2	BMA	C4-C5-C6-O6
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2

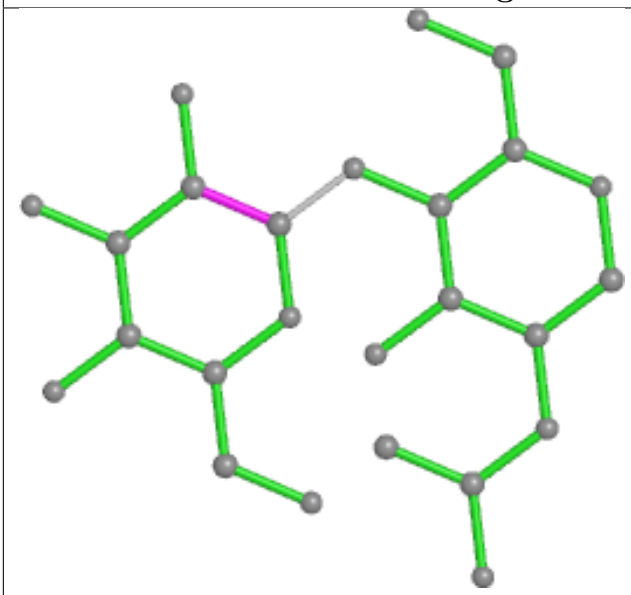
There are no ring outliers.

3 monomers are involved in 3 short contacts:

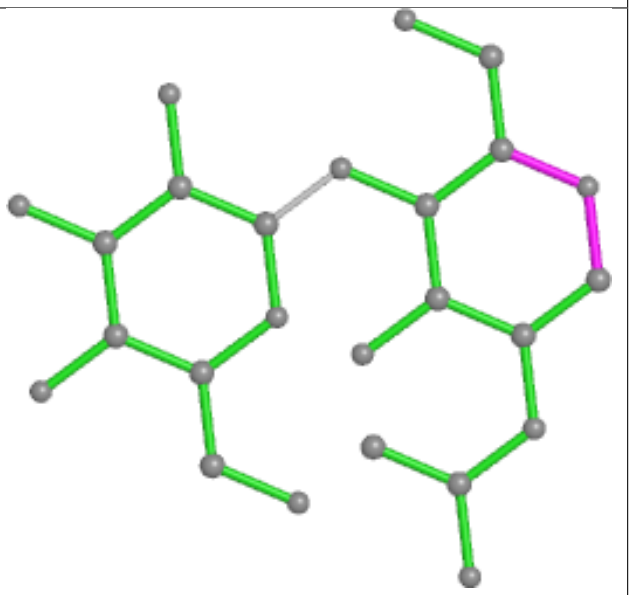
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	1	NAG	1	0
3	I	1	NAG	1	0
3	F	1	NAG	1	0

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

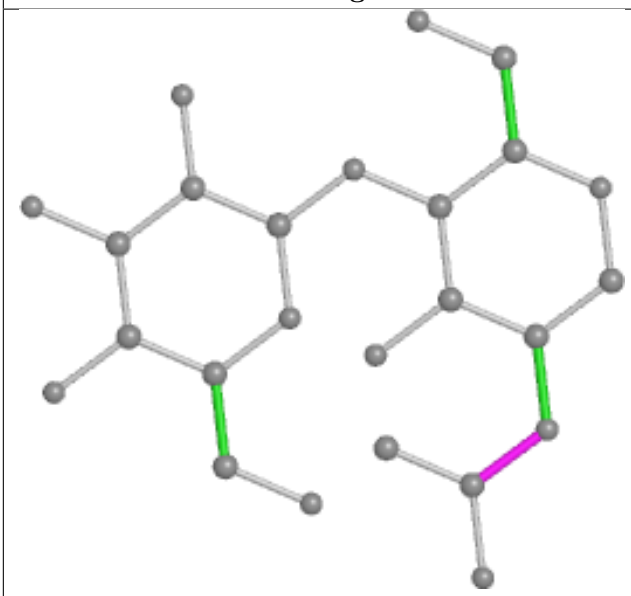
Oligosaccharide Chain F



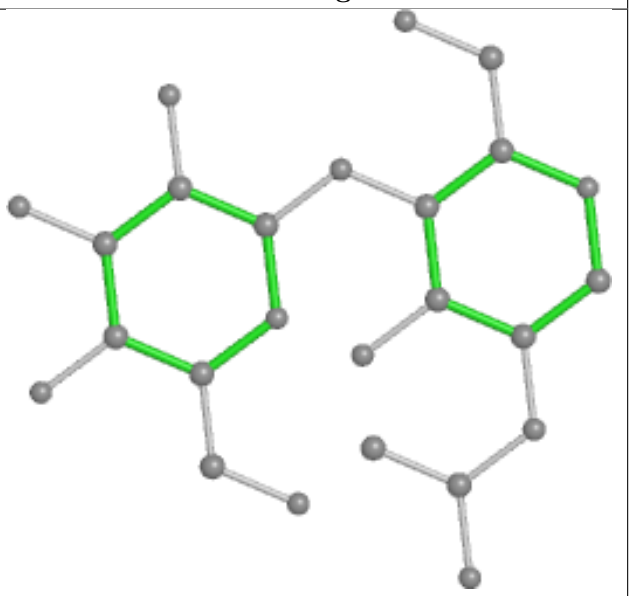
Bond lengths



Bond angles

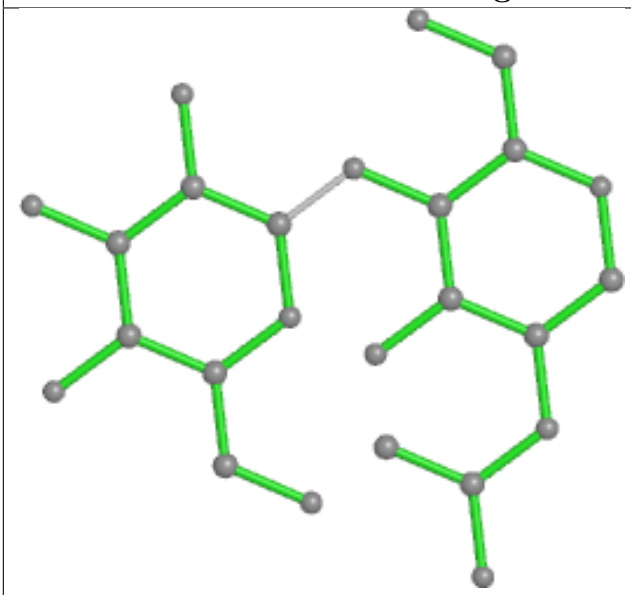


Torsions

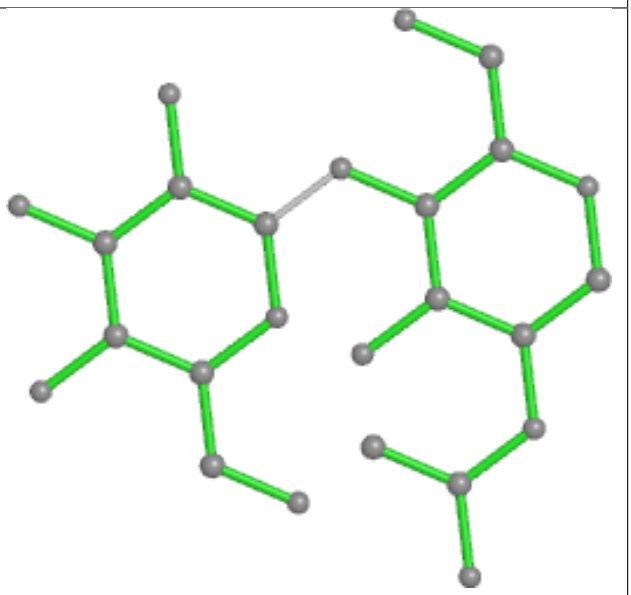


Rings

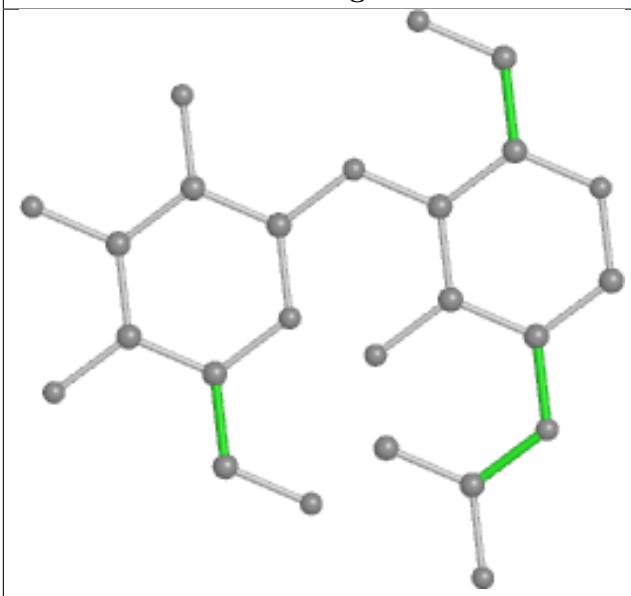
Oligosaccharide Chain G



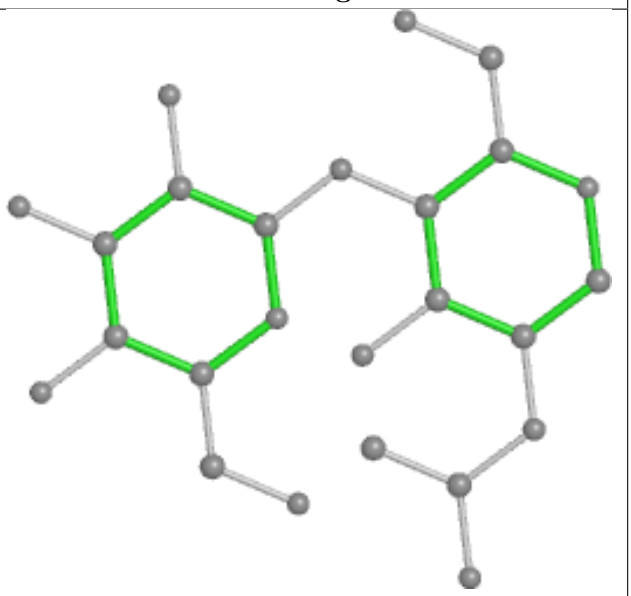
Bond lengths



Bond angles

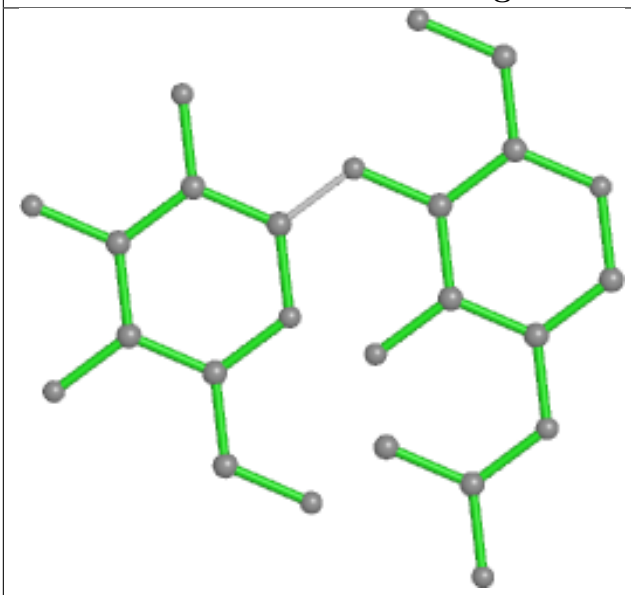


Torsions



Rings

Oligosaccharide Chain H



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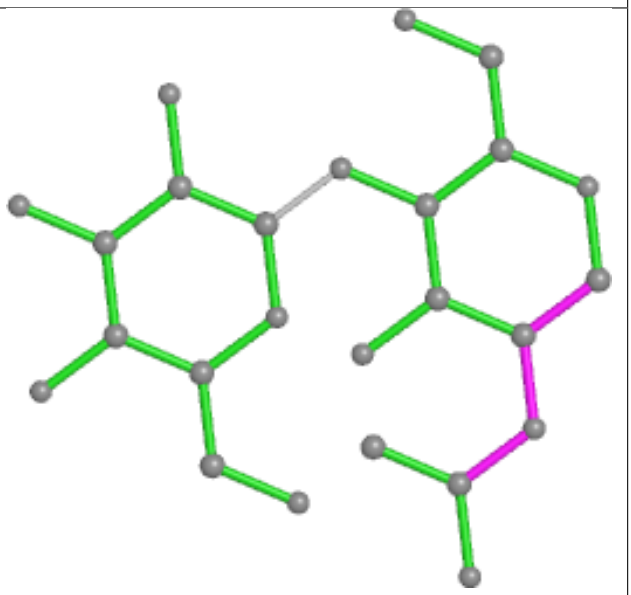
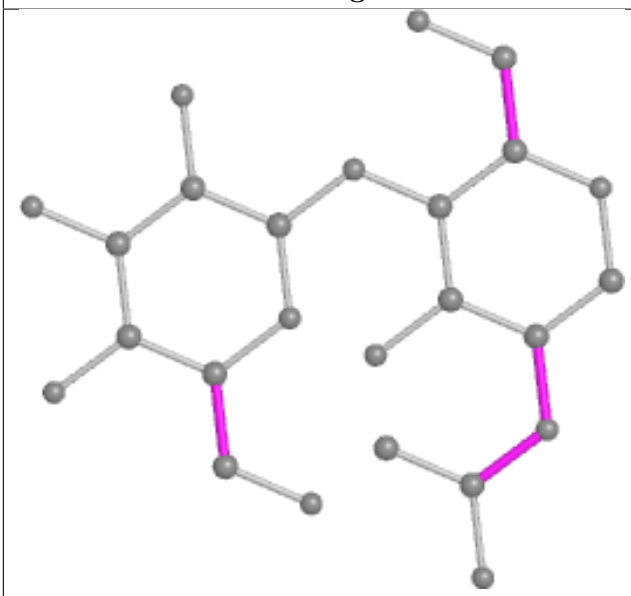


Bond angles



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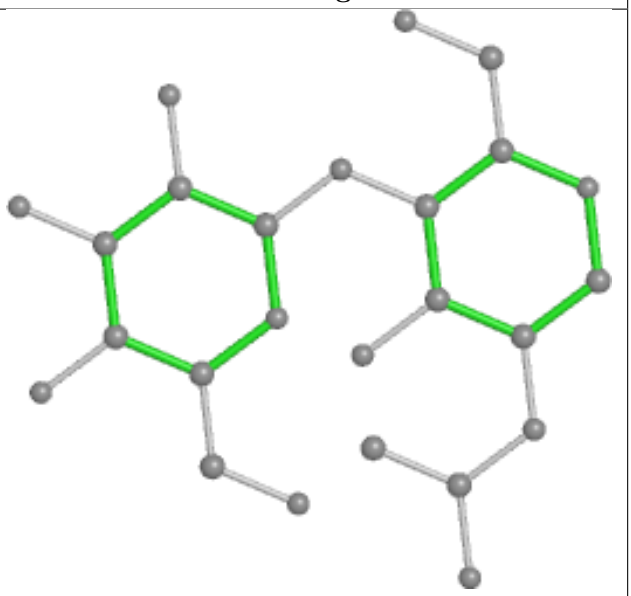
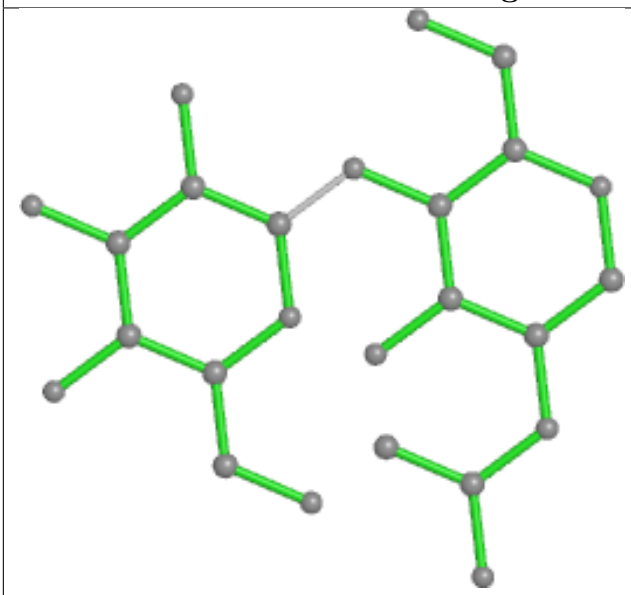


Rings

Oligosaccharide Chain I



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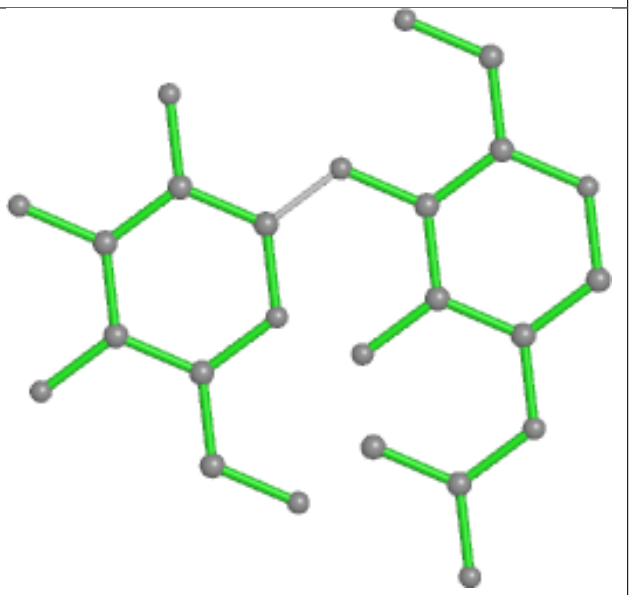
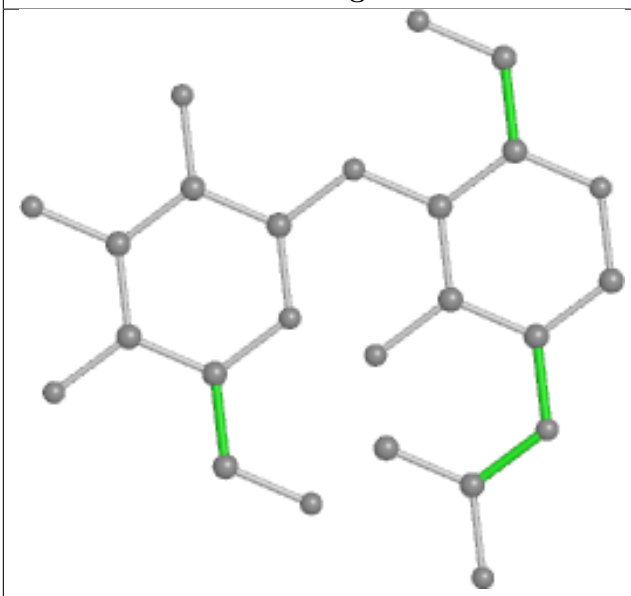


Bond angles



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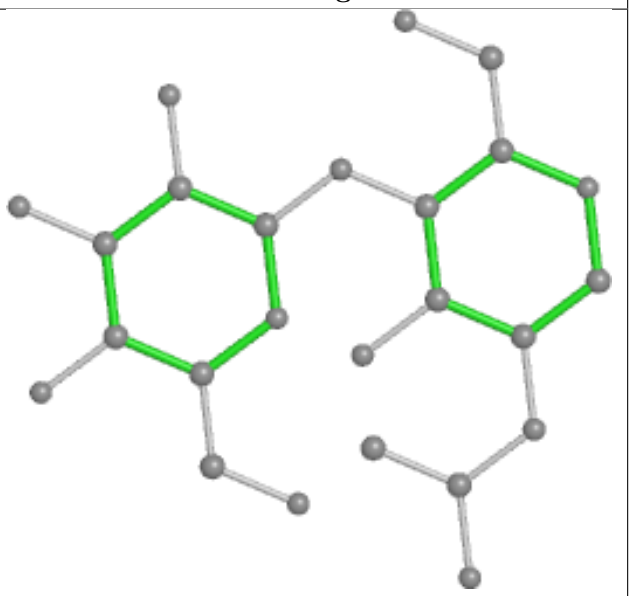
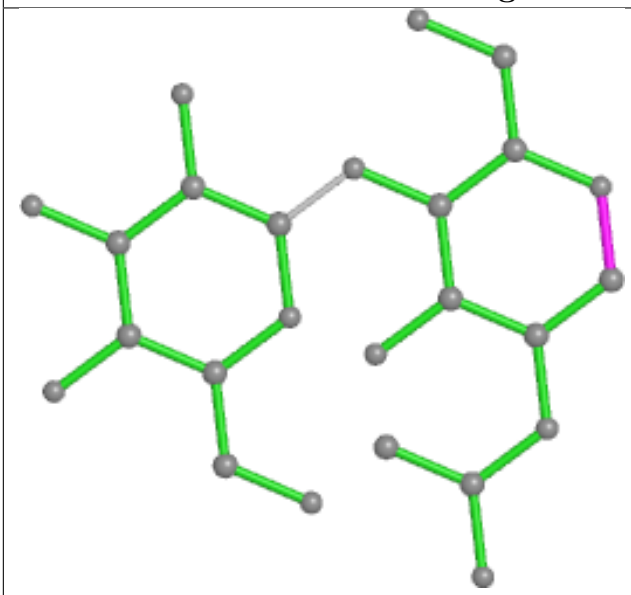
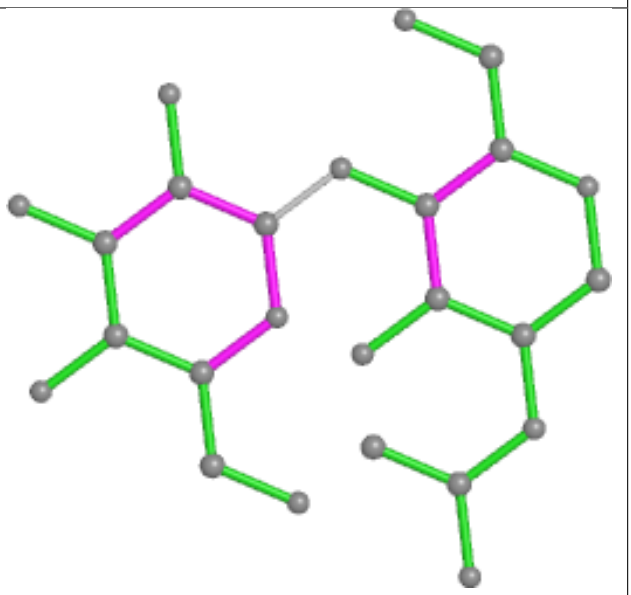


Rings

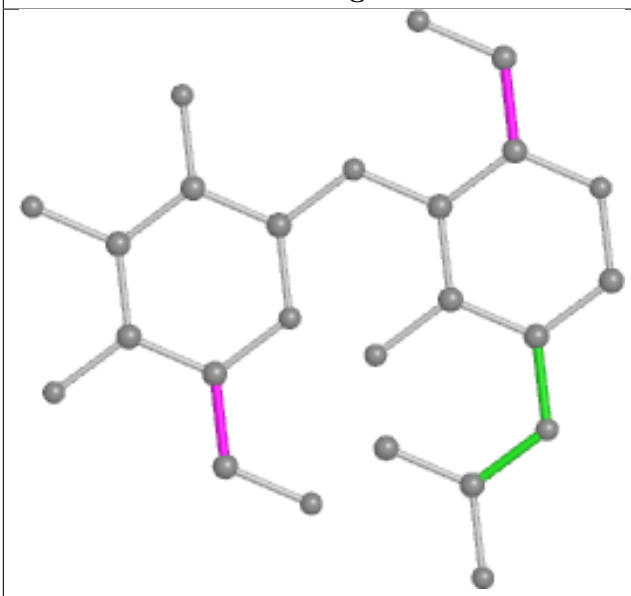
Oligosaccharide Chain J



Bond lengths



Bond angles



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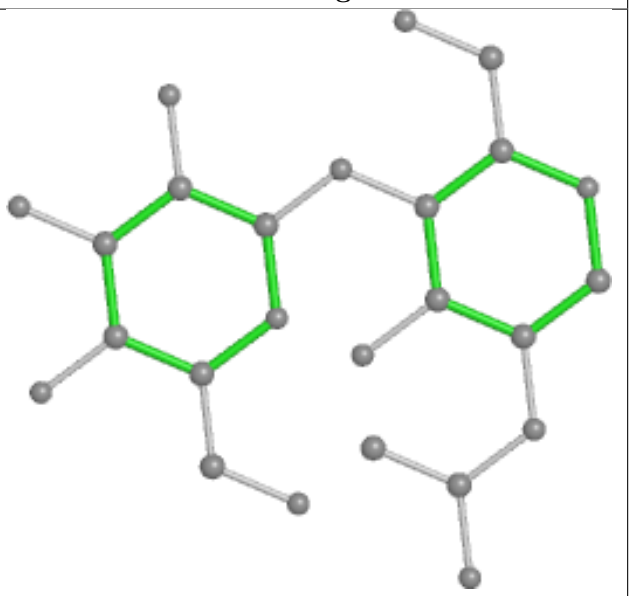
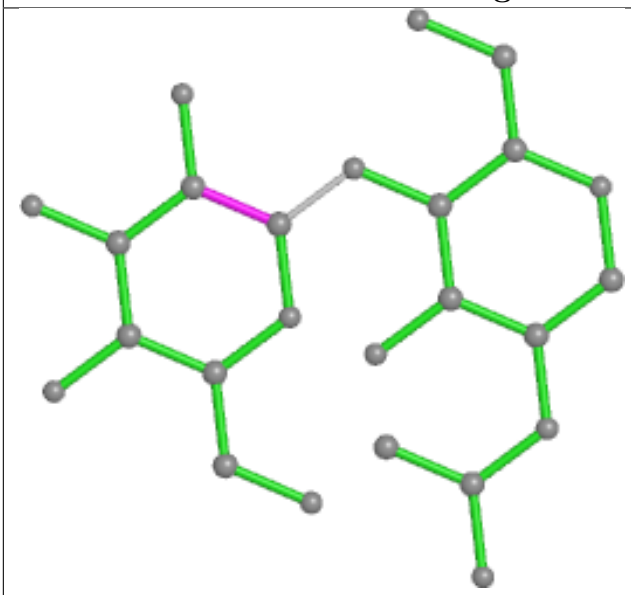


Rings

Oligosaccharide Chain K



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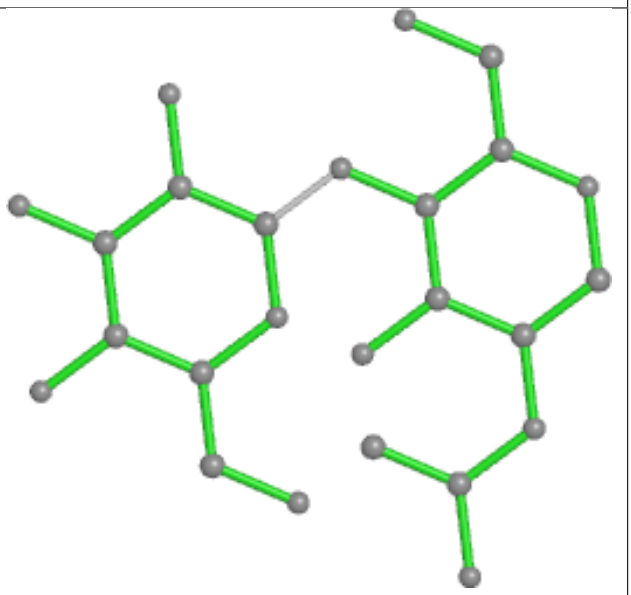
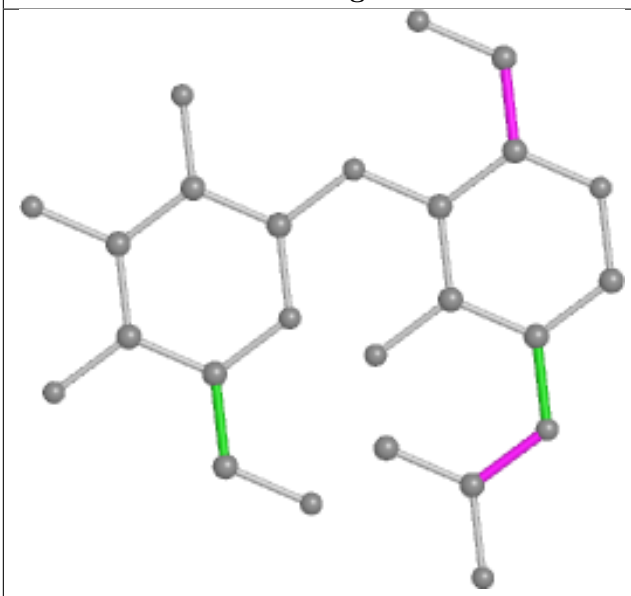


Bond angles



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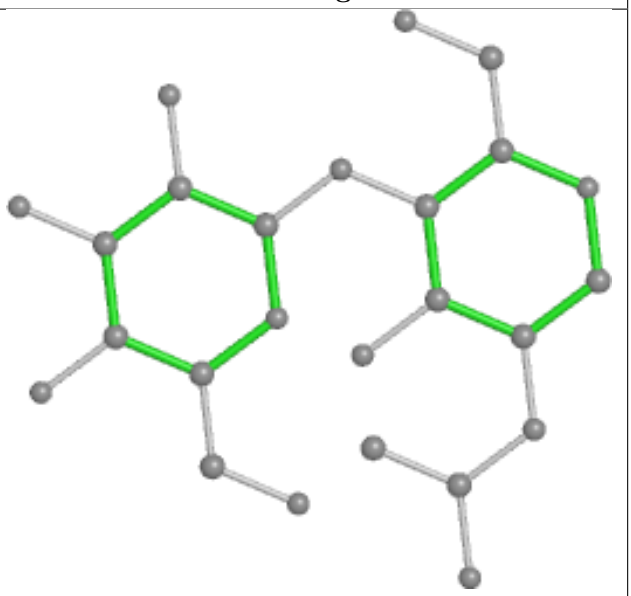
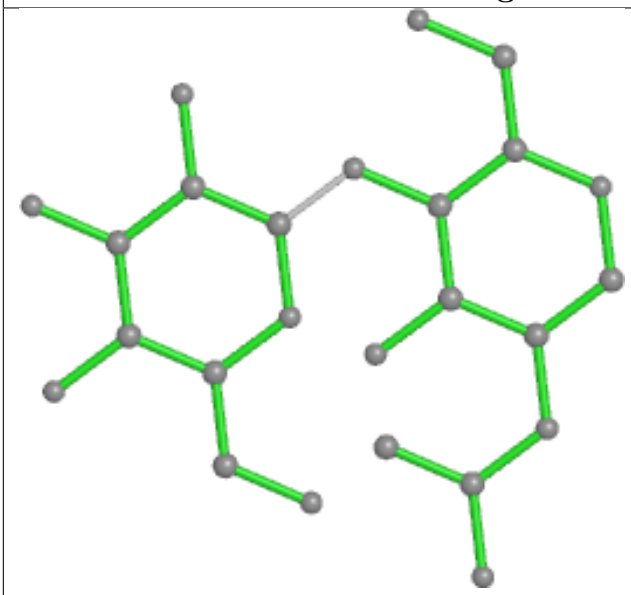
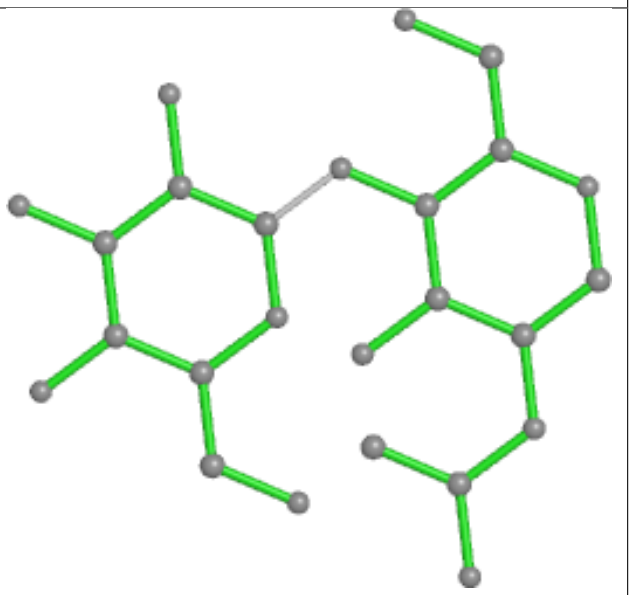


Rings

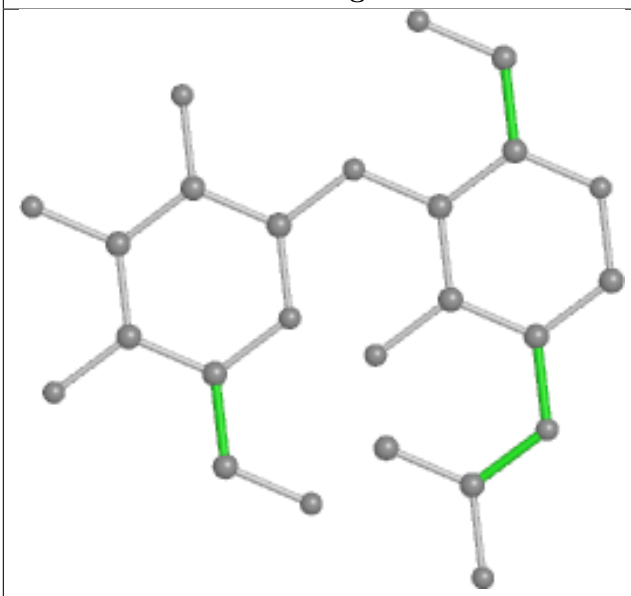
Oligosaccharide Chain L



Bond lengths



Bond angles



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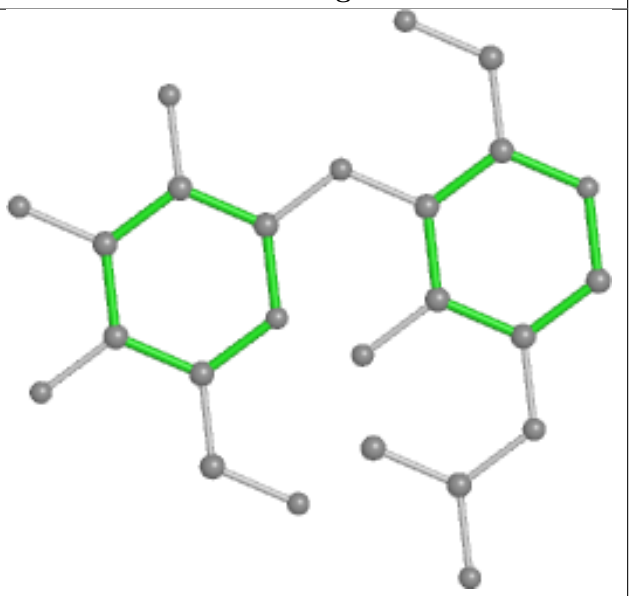
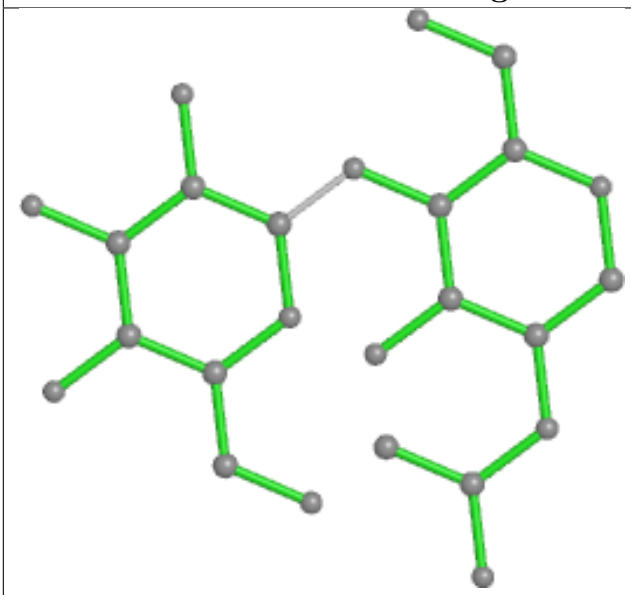
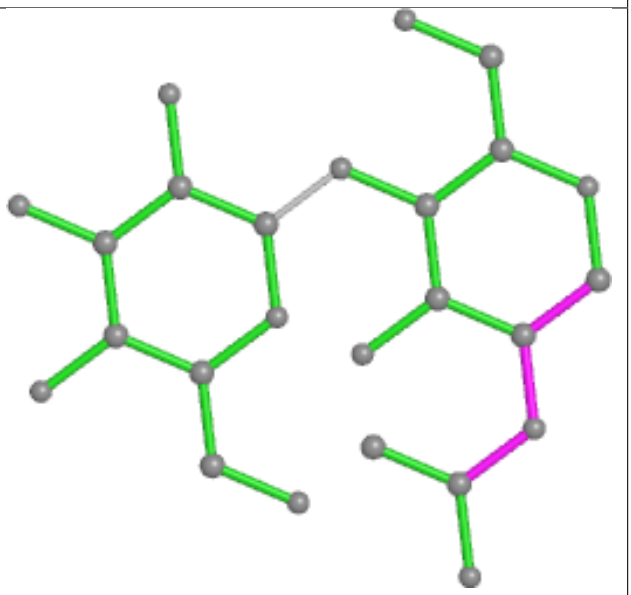


Rings

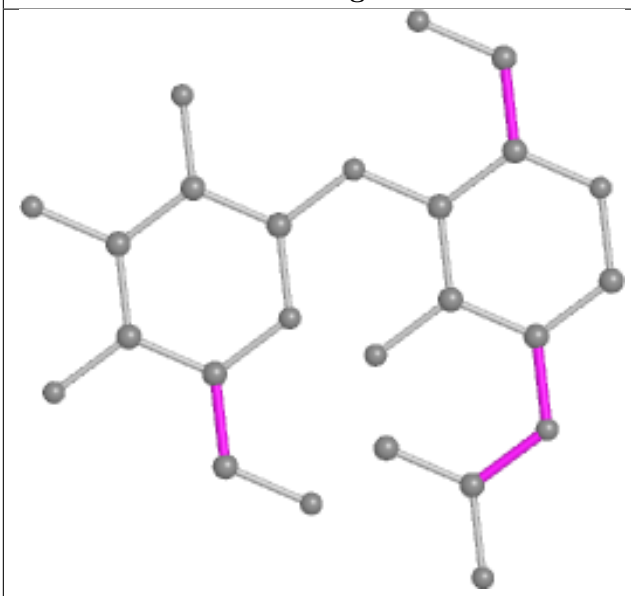
Oligosaccharide Chain M



Bond lengths



Bond angles



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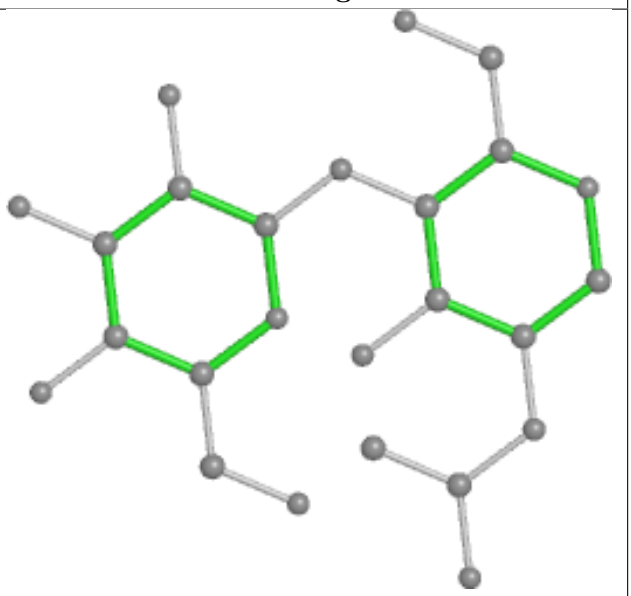
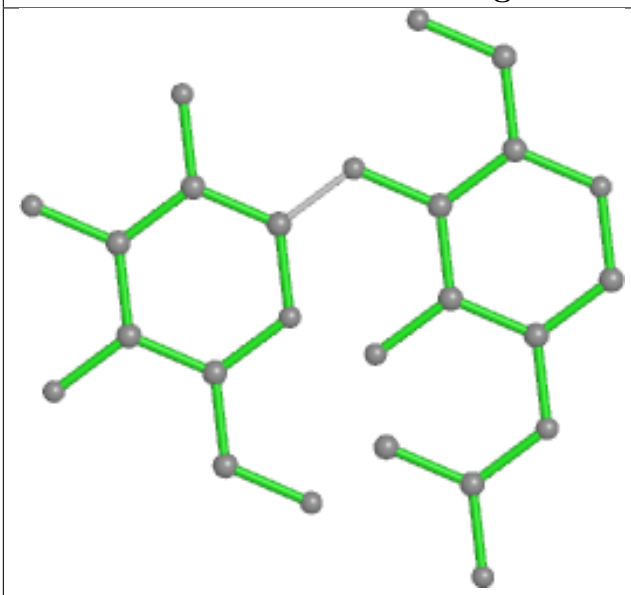


Rings

Oligosaccharide Chain N



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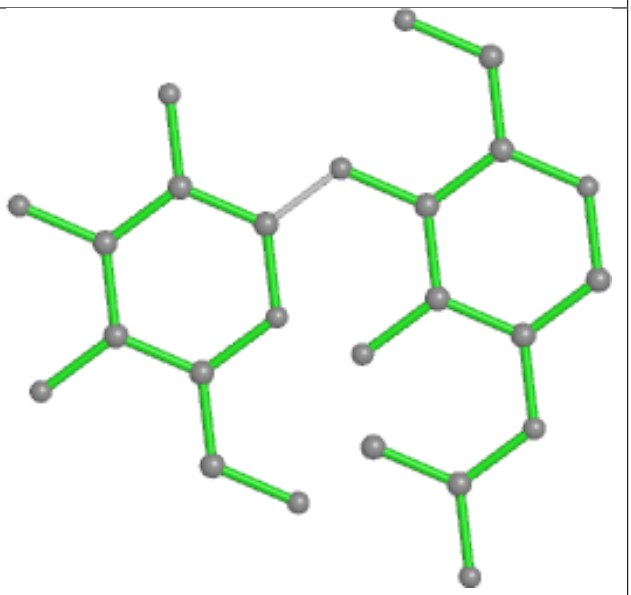
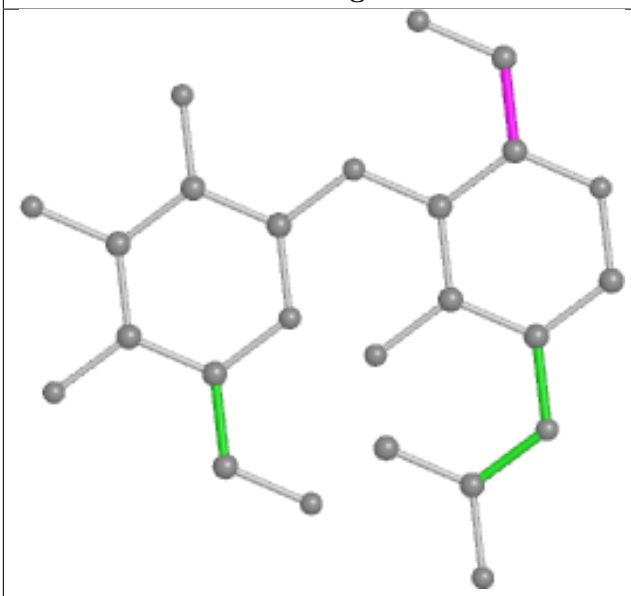


Bond angles



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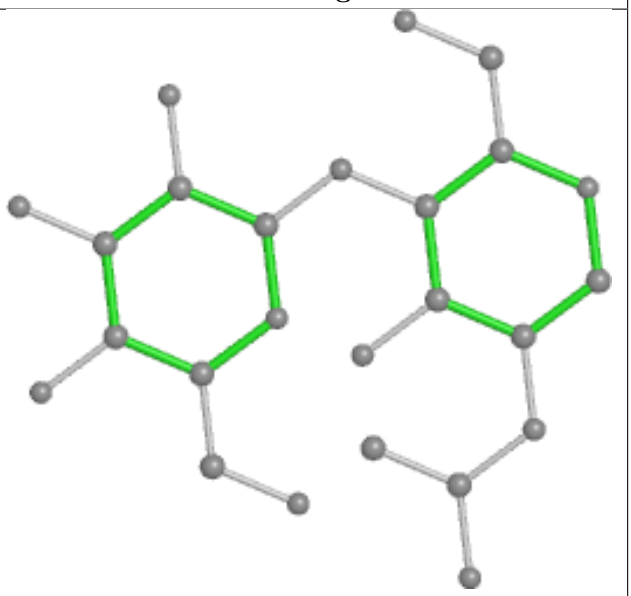
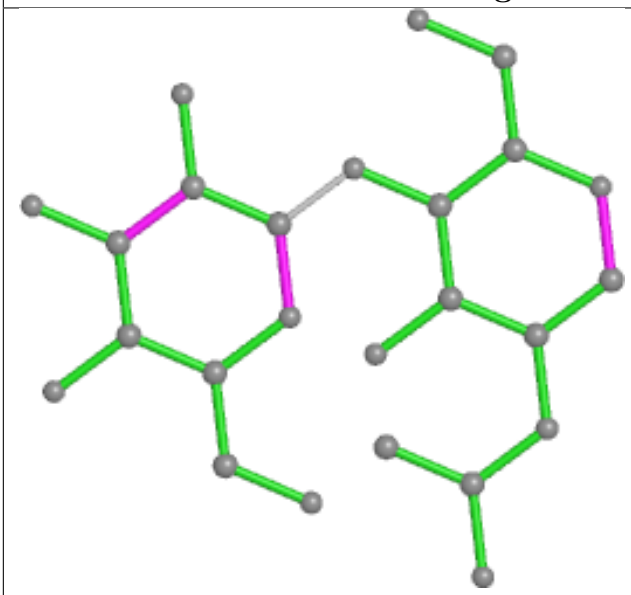
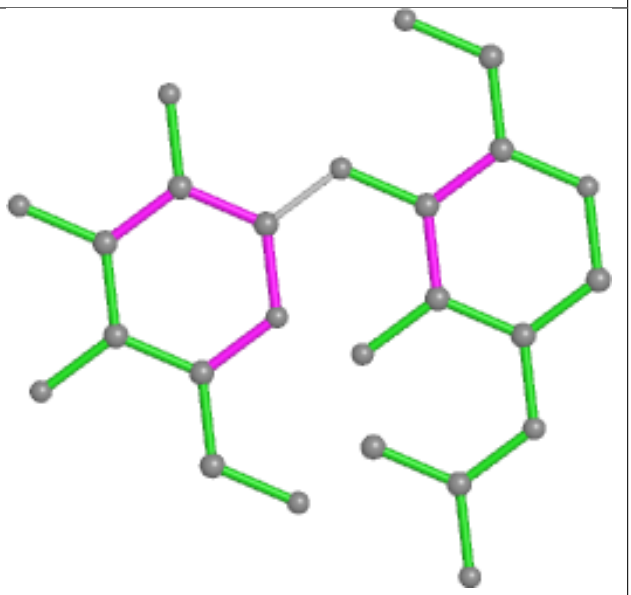


Rings

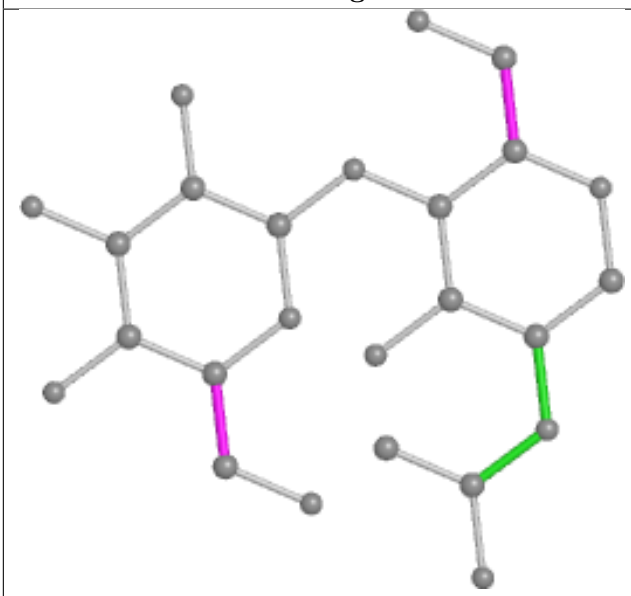
Oligosaccharide Chain O



Bond lengths



Bond angles



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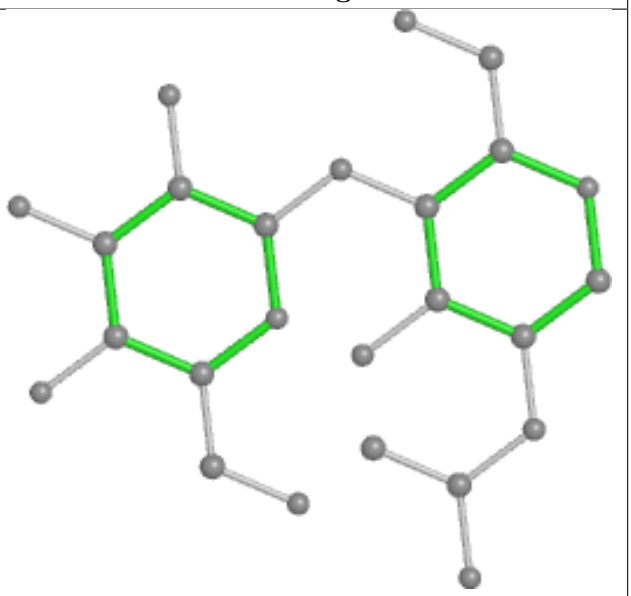
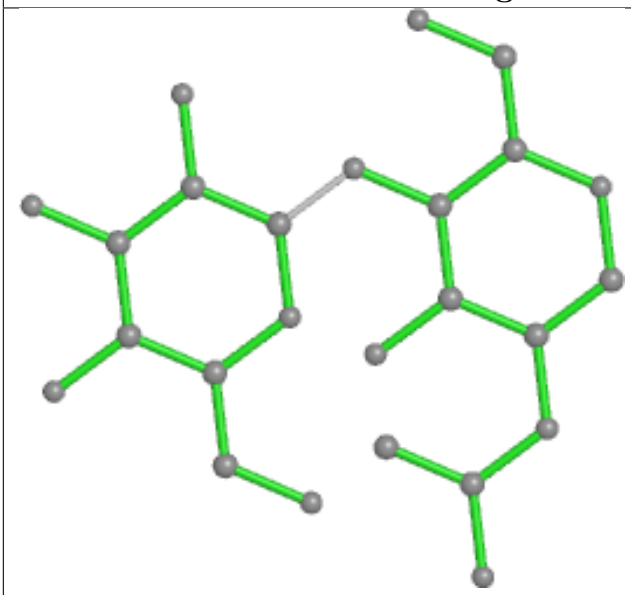
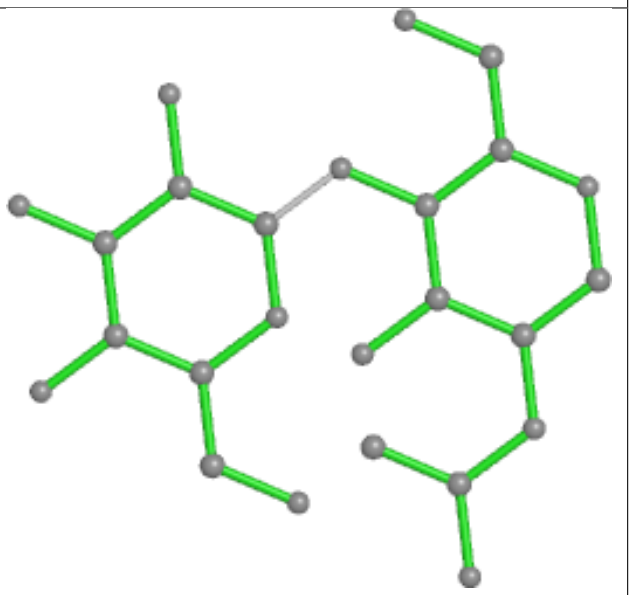


Rings

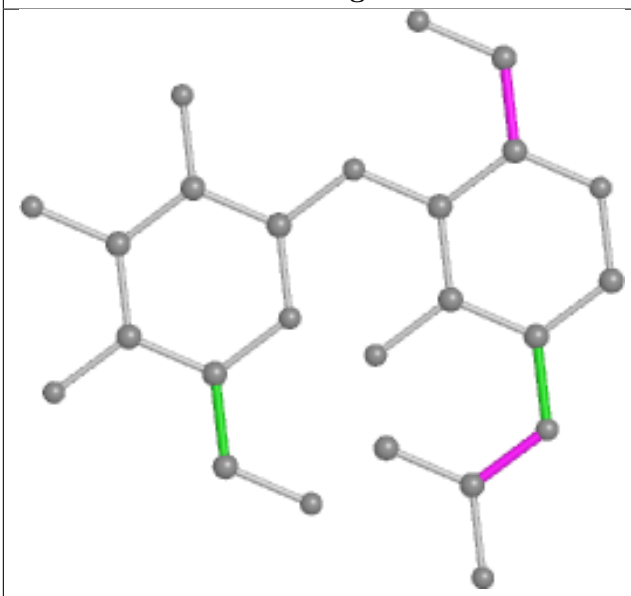
Oligosaccharide Chain P



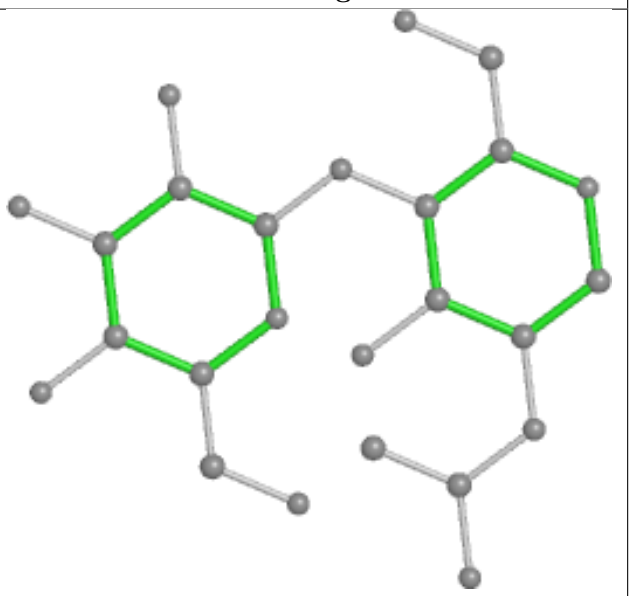
Bond lengths



Bond angles

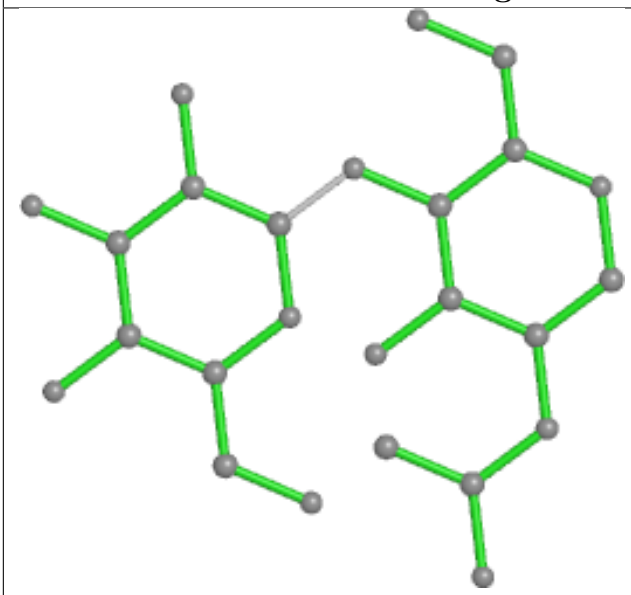


Torsions

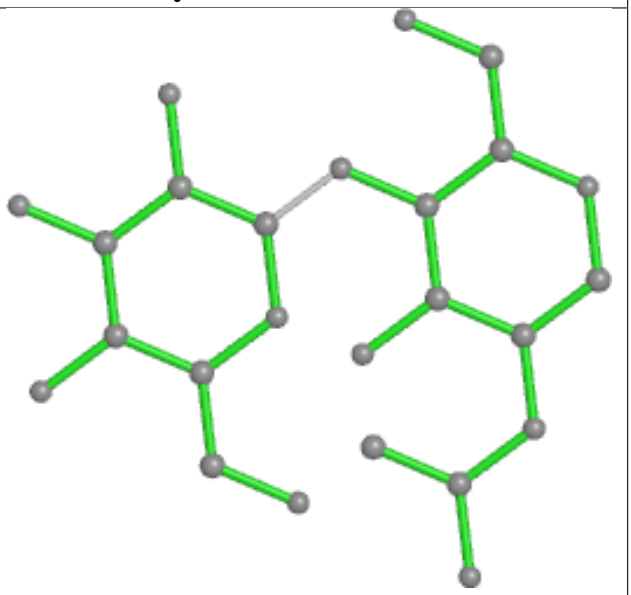


Rings

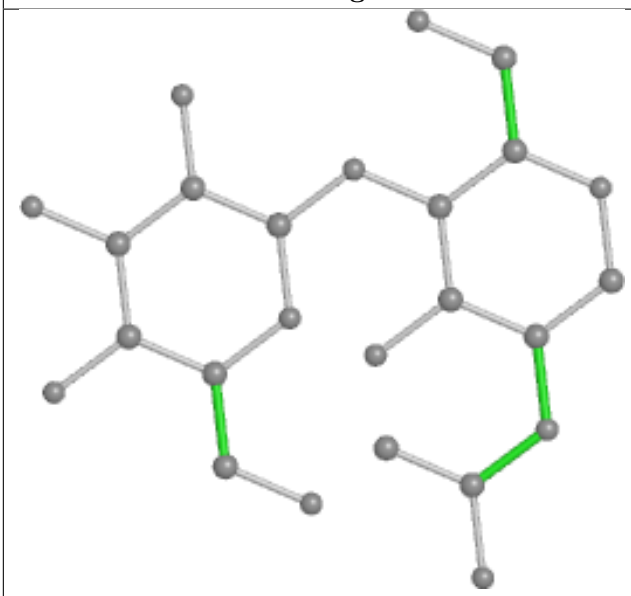
Oligosaccharide Chain Q



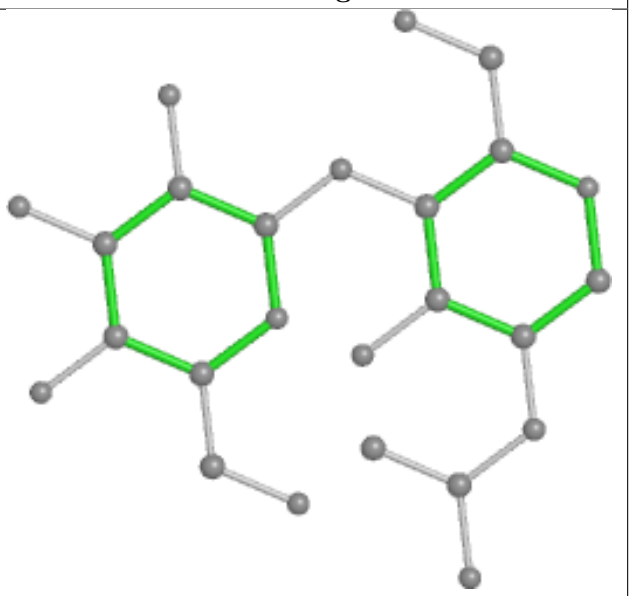
Bond lengths



Bond angles

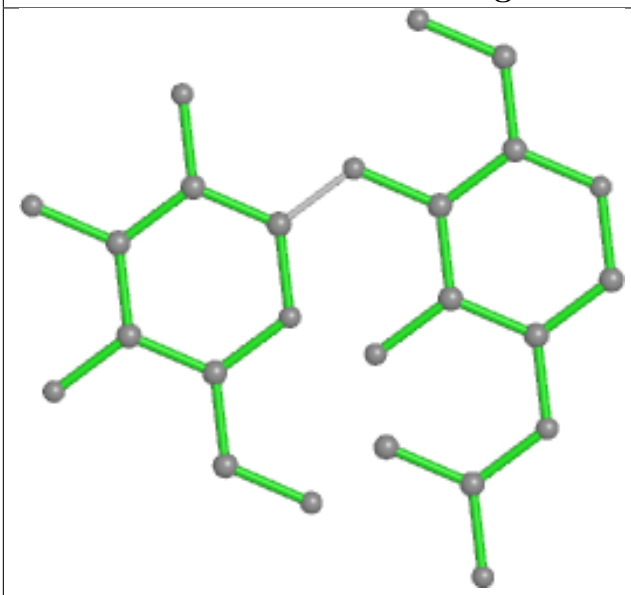


Torsions

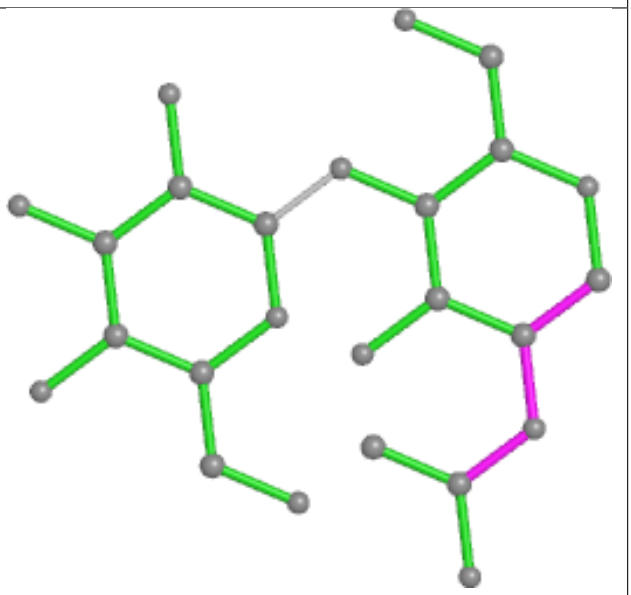


Rings

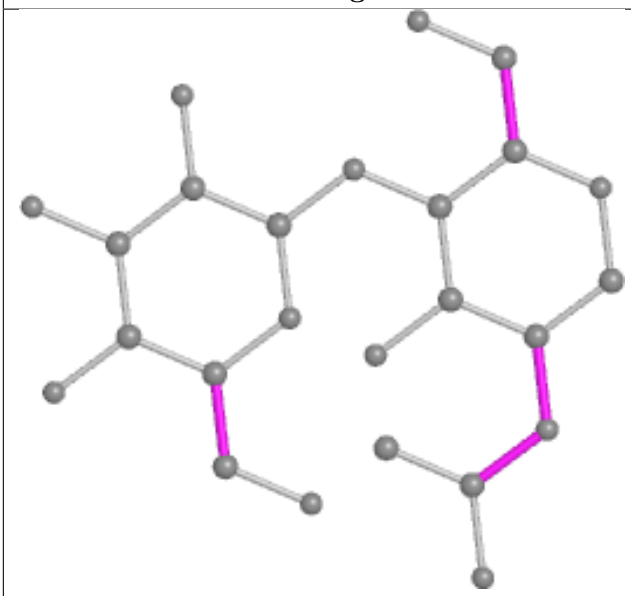
Oligosaccharide Chain R



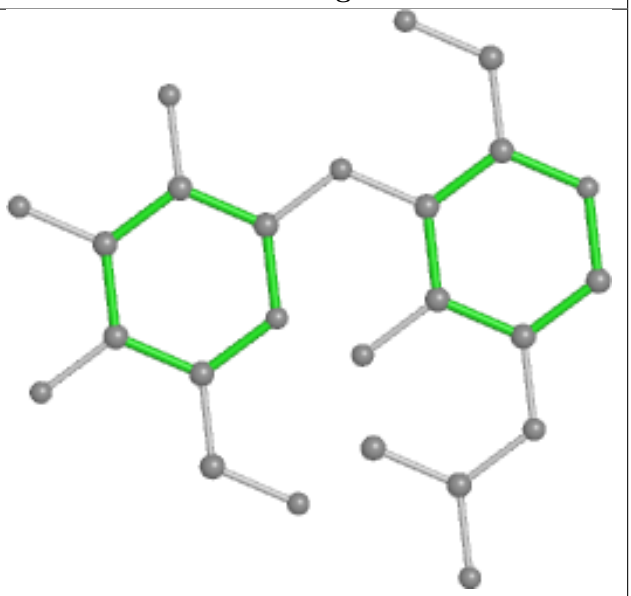
Bond lengths



Bond angles

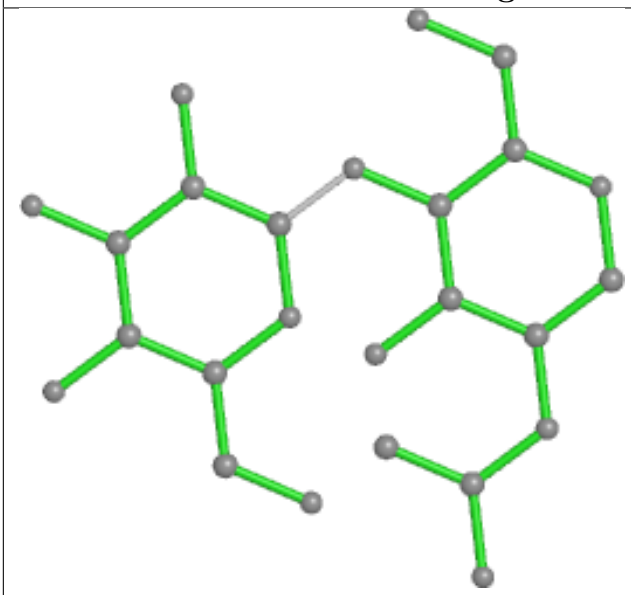


Torsions

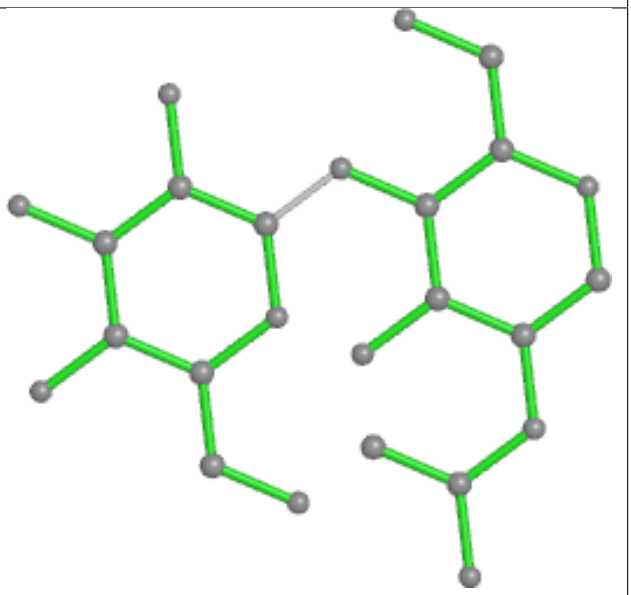


Rings

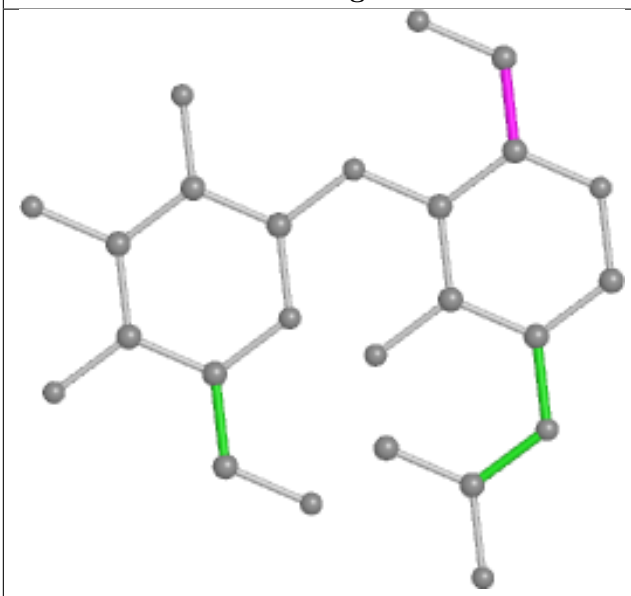
Oligosaccharide Chain S



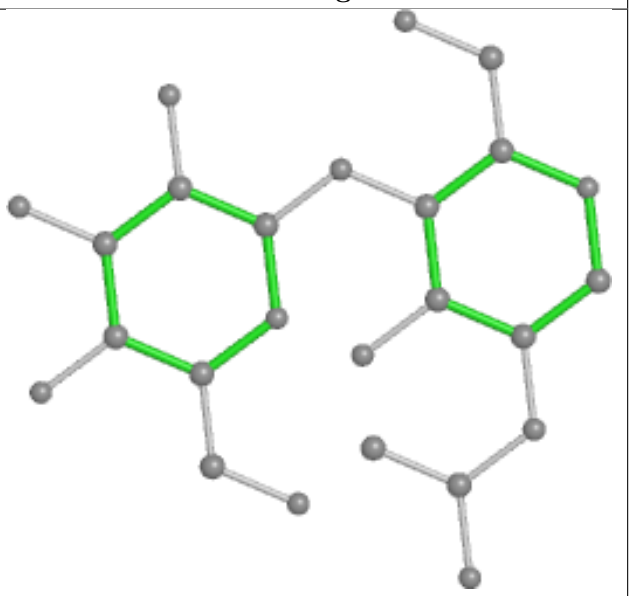
Bond lengths



Bond angles

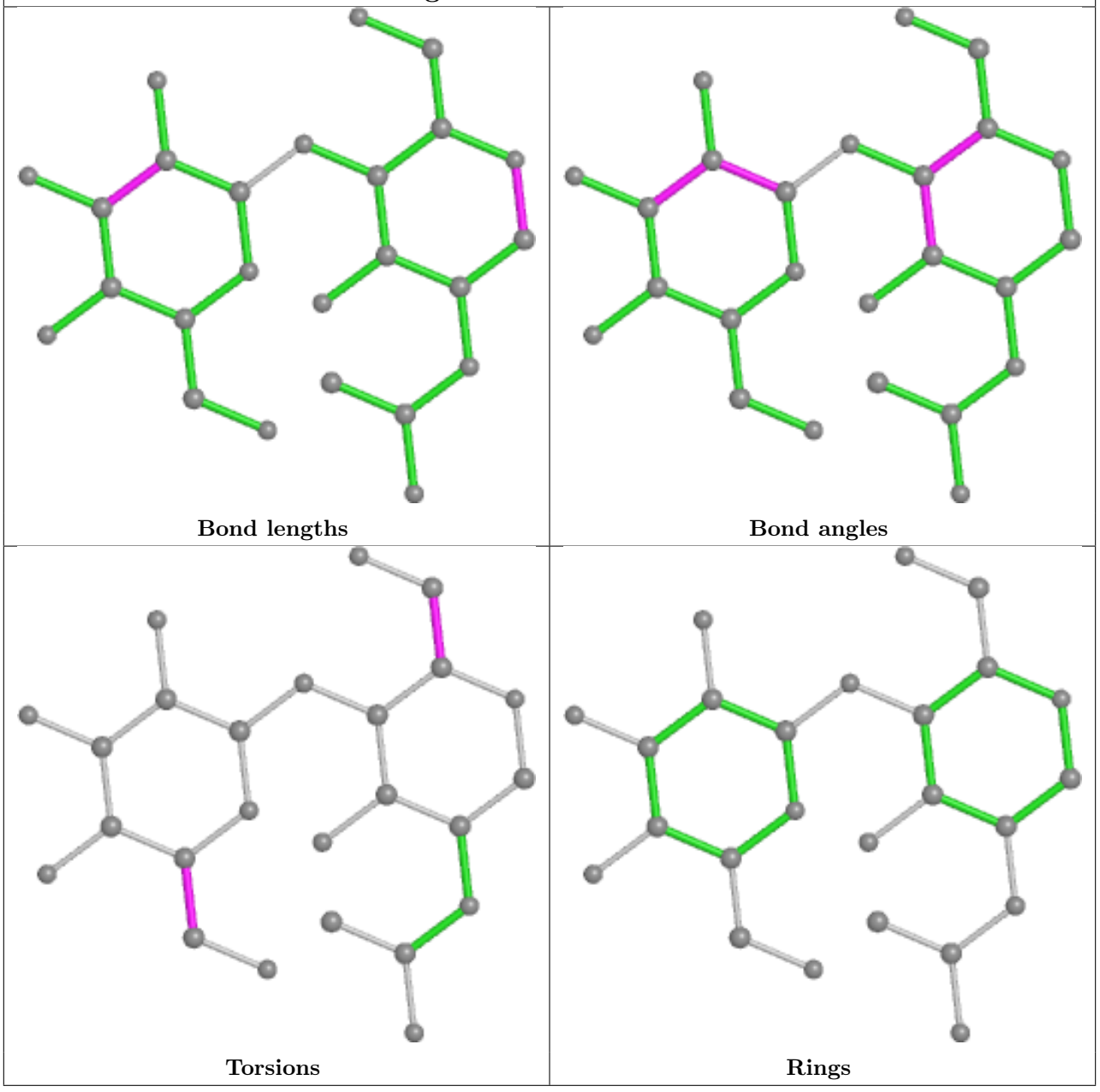


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 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	$\#\|Z\|>2$
4	NAG	A	1304	1	14,14,15	0.42	0	17,19,21	0.53	0
4	NAG	B	1309	1	14,14,15	0.41	0	17,19,21	0.65	1 (5%)
4	NAG	B	1307	1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	C	1302	1	14,14,15	0.71	1 (7%)	17,19,21	0.65	1 (5%)
4	NAG	C	1307	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.55	0
4	NAG	C	1309	1	14,14,15	0.40	0	17,19,21	0.53	0
4	NAG	B	1306	1	14,14,15	0.67	1 (7%)	17,19,21	0.69	0
4	NAG	E	903	2	14,14,15	0.79	1 (7%)	17,19,21	1.58	2 (11%)
4	NAG	A	1306	1	14,14,15	0.19	0	17,19,21	0.45	0
4	NAG	A	1305	1	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	B	1305	1	14,14,15	0.30	0	17,19,21	0.46	0
4	NAG	E	906	2	14,14,15	0.40	0	17,19,21	0.81	0
4	NAG	A	1309	1	14,14,15	0.36	0	17,19,21	0.40	0
4	NAG	C	1311	1	14,14,15	0.38	0	17,19,21	0.56	0
4	NAG	E	904	2	14,14,15	0.62	1 (7%)	17,19,21	0.52	0
4	NAG	B	1304	1	14,14,15	0.41	0	17,19,21	0.83	1 (5%)
4	NAG	B	1302	1	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.46	0
4	NAG	B	1301	1	14,14,15	0.38	0	17,19,21	0.77	1 (5%)
4	NAG	E	905	2	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	D	905	2	14,14,15	0.57	0	17,19,21	0.53	0
4	NAG	A	1307	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	D	903	2	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	C	1304	1	14,14,15	0.20	0	17,19,21	0.52	0
4	NAG	C	1306	1	14,14,15	0.28	0	17,19,21	0.31	0
4	NAG	C	1308	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
4	NAG	D	906	2	14,14,15	0.28	0	17,19,21	0.37	0
4	NAG	A	1310	1	14,14,15	0.36	0	17,19,21	0.61	1 (5%)
4	NAG	B	1303	1	14,14,15	0.27	0	17,19,21	0.45	0
4	NAG	D	904	2	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
4	NAG	C	1303	1	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	A	1311	1	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.54	0
4	NAG	A	1301	1	14,14,15	0.22	0	17,19,21	0.58	0
4	NAG	A	1308	1	14,14,15	0.57	0	17,19,21	1.52	3 (17%)
4	NAG	C	1310	1	14,14,15	0.40	0	17,19,21	0.59	1 (5%)
4	NAG	C	1305	1	14,14,15	0.43	0	17,19,21	1.26	2 (11%)
4	NAG	A	1303	1	14,14,15	0.36	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1308	1	14,14,15	0.58	1 (7%)	17,19,21	0.64	1 (5%)

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	NAG	A	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	E	903	2	-	1/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	E	906	2	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	E	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
4	NAG	E	905	2	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	D	903	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	D	906	2	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	904	2	-	1/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	903	NAG	O5-C1	-2.84	1.39	1.43
4	C	1302	NAG	C1-C2	2.34	1.55	1.52
4	B	1306	NAG	C1-C2	2.30	1.55	1.52
4	E	904	NAG	O5-C1	-2.09	1.40	1.43
4	B	1308	NAG	C1-C2	2.01	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	903	NAG	C1-O5-C5	5.11	119.12	112.19
4	A	1308	NAG	C1-O5-C5	4.46	118.24	112.19
4	A	1308	NAG	C3-C4-C5	3.24	116.01	110.24
4	C	1305	NAG	O5-C1-C2	3.04	116.08	111.29
4	C	1305	NAG	C1-O5-C5	2.98	116.23	112.19
4	C	1308	NAG	C1-O5-C5	2.86	116.06	112.19
4	E	903	NAG	C3-C4-C5	2.71	115.07	110.24
4	B	1304	NAG	C1-C2-N2	2.46	114.69	110.49
4	B	1301	NAG	C2-N2-C7	2.42	126.35	122.90
4	B	1309	NAG	C1-O5-C5	2.27	115.26	112.19
4	D	904	NAG	C1-O5-C5	2.18	115.14	112.19
4	C	1302	NAG	C1-O5-C5	2.17	115.13	112.19
4	C	1310	NAG	C1-O5-C5	2.13	115.08	112.19
4	A	1310	NAG	C1-O5-C5	2.10	115.03	112.19
4	A	1308	NAG	O5-C5-C4	2.06	115.84	110.83
4	B	1308	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1311	NAG	C8-C7-N2-C2
4	B	1311	NAG	O7-C7-N2-C2
4	B	1306	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	D	906	NAG	C4-C5-C6-O6
4	E	905	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	D	905	NAG	O5-C5-C6-O6
4	E	905	NAG	O5-C5-C6-O6
4	A	1305	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	A	1303	NAG	C8-C7-N2-C2
4	A	1303	NAG	O7-C7-N2-C2
4	A	1304	NAG	C8-C7-N2-C2
4	A	1304	NAG	O7-C7-N2-C2
4	A	1311	NAG	C8-C7-N2-C2
4	A	1311	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	C	1303	NAG	C8-C7-N2-C2
4	C	1303	NAG	O7-C7-N2-C2
4	C	1308	NAG	C8-C7-N2-C2
4	C	1308	NAG	O7-C7-N2-C2
4	D	906	NAG	C8-C7-N2-C2
4	D	906	NAG	O7-C7-N2-C2
4	E	905	NAG	C8-C7-N2-C2
4	E	905	NAG	O7-C7-N2-C2
4	D	906	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	D	905	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1306	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	D	903	NAG	O5-C5-C6-O6
4	E	903	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1301	NAG	C4-C5-C6-O6
4	B	1302	NAG	C1-C2-N2-C7
4	B	1303	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1304	NAG	O5-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	C	1307	NAG	C1-C2-N2-C7
4	B	1309	NAG	C4-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	C	1302	NAG	C1-C2-N2-C7
4	A	1303	NAG	O5-C5-C6-O6
4	B	1311	NAG	C1-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	B	1308	NAG	C1-C2-N2-C7
4	A	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	C3-C2-N2-C7
4	B	1302	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C1-C2-N2-C7
4	D	904	NAG	C1-C2-N2-C7
4	C	1301	NAG	C1-C2-N2-C7

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1304	NAG	1	0
4	C	1302	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1301	NAG	1	0
4	B	1306	NAG	1	0
4	A	1305	NAG	1	0
4	B	1302	NAG	1	0
4	B	1301	NAG	1	0
4	A	1307	NAG	1	0
4	C	1306	NAG	1	0
4	A	1302	NAG	1	0
4	A	1301	NAG	1	0
4	A	1308	NAG	1	0
4	B	1308	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.