Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 05:07 PM EST

PDB ID	:	6EDU
EMDB ID	:	EMD-9038
Title	:	B41 SOSIP.664 in complex with soluble CD4 (D1-D2), the co-receptor mimicking antibody 21c and the broadly neutralizing antibody 8ANC195
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2018-08-11
Resolution	:	4.06 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:

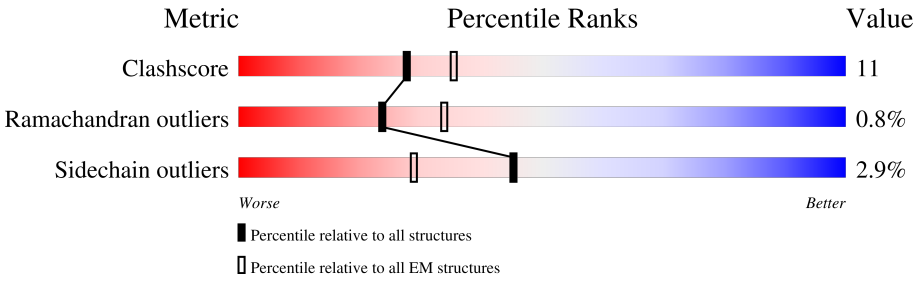
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.06 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	12% 62% 12% •• 24%
1	B	153	13% 65% 10% • 24%
1	C	153	12% 68% 7% • 24%
2	D	516	17% 58% 17% • • 22%
2	E	516	16% 59% 16% • 22%
2	F	516	15% 56% 18% • • 22%
3	G	185	7% 43% 10% 48%
3	H	185	9% 42% 10% 48%

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Mol	Chain	Length	Quality of chain
3	I	185	9% 44% 8% 48%
4	J	231	27% 39% 14% 46%
4	L	231	27% 39% 13% 46%
4	N	231	24% 41% 12% 46%
5	K	217	29% 39% 11% 49%
5	M	217	29% 39% 11% 49%
5	O	217	28% 38% 12% 49%
6	P	244	7% 39% 14% 46%
6	R	244	7% 40% 14% 46%
6	T	244	7% 39% 15% 46%
7	Q	215	10% 40% 10% 50%
7	S	215	11% 40% 10% 50%
7	U	215	10% 40% 9% 50%
8	V	2	50% 50% 50%
8	W	2	50% 50% 50%
8	X	2	50% 50% 50%
8	Y	2	50% 100%
8	c	2	50% 50% 50%
8	d	2	50% 50% 50%
8	e	2	50% 50%
8	f	2	50% 100%
8	j	2	50% 50% 50%
8	k	2	50% 50% 50%
8	l	2	50% 50%
8	m	2	50% 100%

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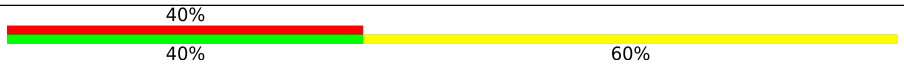
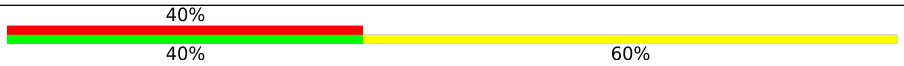
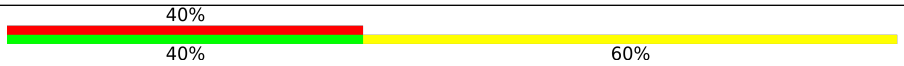
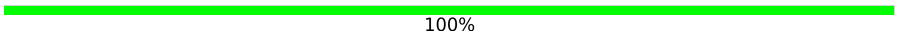
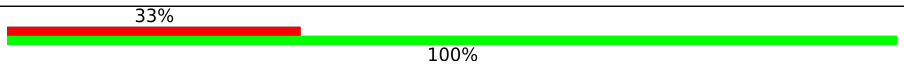
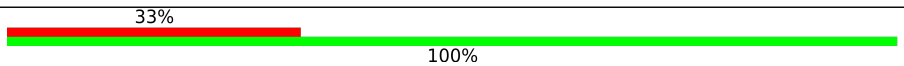
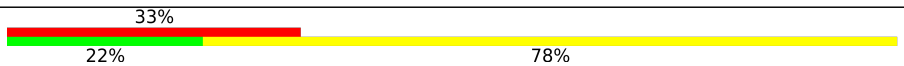
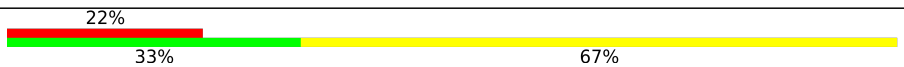
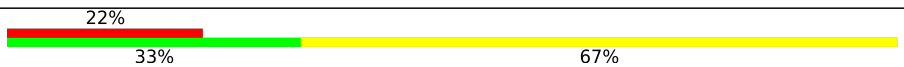
Mol	Chain	Length	Quality of chain
8	q	2	
8	r	2	
8	s	2	
9	Z	5	
9	g	5	
9	n	5	
10	a	5	
10	h	5	
10	o	5	
11	b	3	
11	i	3	
11	p	3	
12	t	9	
12	u	9	
12	v	9	

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 26271 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	116	Total	C	N	O	S	0	0
			884	564	152	161	7		
1	B	116	Total	C	N	O	S	0	0
			884	564	152	161	7		
1	C	116	Total	C	N	O	S	0	0
			884	564	152	161	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP B3UEZ6
A	605	CYS	THR	conflict	UNP B3UEZ6
B	559	PRO	ILE	conflict	UNP B3UEZ6
B	605	CYS	THR	conflict	UNP B3UEZ6
C	559	PRO	ILE	conflict	UNP B3UEZ6
C	605	CYS	THR	conflict	UNP B3UEZ6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	401	Total	C	N	O	S	0	0
			2989	1874	531	559	25		
2	E	401	Total	C	N	O	S	0	0
			2989	1874	531	559	25		
2	F	401	Total	C	N	O	S	0	0
			2989	1874	531	559	25		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	MET	-	initiating methionine	UNP B3UES2
D	-3	ASP	-	expression tag	UNP B3UES2
D	-2	ALA	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	MET	-	expression tag	UNP B3UES2
D	0	LYS	-	expression tag	UNP B3UES2
D	1	ARG	-	expression tag	UNP B3UES2
D	2	GLY	-	expression tag	UNP B3UES2
D	3	LEU	-	expression tag	UNP B3UES2
D	4	CYS	-	expression tag	UNP B3UES2
D	5	CYS	-	expression tag	UNP B3UES2
D	6	VAL	-	expression tag	UNP B3UES2
D	7	LEU	-	expression tag	UNP B3UES2
D	8	LEU	-	expression tag	UNP B3UES2
D	9	LEU	-	expression tag	UNP B3UES2
D	10	CYS	-	expression tag	UNP B3UES2
D	11	GLY	-	expression tag	UNP B3UES2
D	12	ALA	-	expression tag	UNP B3UES2
D	13	VAL	-	expression tag	UNP B3UES2
D	14	PHE	-	expression tag	UNP B3UES2
D	15	VAL	-	expression tag	UNP B3UES2
D	16	SER	-	expression tag	UNP B3UES2
D	17	PRO	-	expression tag	UNP B3UES2
D	18	SER	-	expression tag	UNP B3UES2
D	19	GLN	-	expression tag	UNP B3UES2
D	20	GLU	-	expression tag	UNP B3UES2
D	21	ILE	-	expression tag	UNP B3UES2
D	22	HIS	-	expression tag	UNP B3UES2
D	23	ALA	-	expression tag	UNP B3UES2
D	24	ARG	-	expression tag	UNP B3UES2
D	25	PHE	-	expression tag	UNP B3UES2
D	26	ARG	-	expression tag	UNP B3UES2
D	27	ARG	-	expression tag	UNP B3UES2
D	28	GLY	-	expression tag	UNP B3UES2
D	29	ALA	-	expression tag	UNP B3UES2
D	30	ARG	-	expression tag	UNP B3UES2
D	501	CYS	ALA	conflict	UNP B3UES2
E	-4	MET	-	initiating methionine	UNP B3UES2
E	-3	ASP	-	expression tag	UNP B3UES2
E	-2	ALA	-	expression tag	UNP B3UES2
E	-1	MET	-	expression tag	UNP B3UES2
E	0	LYS	-	expression tag	UNP B3UES2
E	1	ARG	-	expression tag	UNP B3UES2
E	2	GLY	-	expression tag	UNP B3UES2
E	3	LEU	-	expression tag	UNP B3UES2
E	4	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	5	CYS	-	expression tag	UNP B3UES2
E	6	VAL	-	expression tag	UNP B3UES2
E	7	LEU	-	expression tag	UNP B3UES2
E	8	LEU	-	expression tag	UNP B3UES2
E	9	LEU	-	expression tag	UNP B3UES2
E	10	CYS	-	expression tag	UNP B3UES2
E	11	GLY	-	expression tag	UNP B3UES2
E	12	ALA	-	expression tag	UNP B3UES2
E	13	VAL	-	expression tag	UNP B3UES2
E	14	PHE	-	expression tag	UNP B3UES2
E	15	VAL	-	expression tag	UNP B3UES2
E	16	SER	-	expression tag	UNP B3UES2
E	17	PRO	-	expression tag	UNP B3UES2
E	18	SER	-	expression tag	UNP B3UES2
E	19	GLN	-	expression tag	UNP B3UES2
E	20	GLU	-	expression tag	UNP B3UES2
E	21	ILE	-	expression tag	UNP B3UES2
E	22	HIS	-	expression tag	UNP B3UES2
E	23	ALA	-	expression tag	UNP B3UES2
E	24	ARG	-	expression tag	UNP B3UES2
E	25	PHE	-	expression tag	UNP B3UES2
E	26	ARG	-	expression tag	UNP B3UES2
E	27	ARG	-	expression tag	UNP B3UES2
E	28	GLY	-	expression tag	UNP B3UES2
E	29	ALA	-	expression tag	UNP B3UES2
E	30	ARG	-	expression tag	UNP B3UES2
E	501	CYS	ALA	conflict	UNP B3UES2
F	-4	MET	-	initiating methionine	UNP B3UES2
F	-3	ASP	-	expression tag	UNP B3UES2
F	-2	ALA	-	expression tag	UNP B3UES2
F	-1	MET	-	expression tag	UNP B3UES2
F	0	LYS	-	expression tag	UNP B3UES2
F	1	ARG	-	expression tag	UNP B3UES2
F	2	GLY	-	expression tag	UNP B3UES2
F	3	LEU	-	expression tag	UNP B3UES2
F	4	CYS	-	expression tag	UNP B3UES2
F	5	CYS	-	expression tag	UNP B3UES2
F	6	VAL	-	expression tag	UNP B3UES2
F	7	LEU	-	expression tag	UNP B3UES2
F	8	LEU	-	expression tag	UNP B3UES2
F	9	LEU	-	expression tag	UNP B3UES2
F	10	CYS	-	expression tag	UNP B3UES2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	11	GLY	-	expression tag	UNP B3UES2
F	12	ALA	-	expression tag	UNP B3UES2
F	13	VAL	-	expression tag	UNP B3UES2
F	14	PHE	-	expression tag	UNP B3UES2
F	15	VAL	-	expression tag	UNP B3UES2
F	16	SER	-	expression tag	UNP B3UES2
F	17	PRO	-	expression tag	UNP B3UES2
F	18	SER	-	expression tag	UNP B3UES2
F	19	GLN	-	expression tag	UNP B3UES2
F	20	GLU	-	expression tag	UNP B3UES2
F	21	ILE	-	expression tag	UNP B3UES2
F	22	HIS	-	expression tag	UNP B3UES2
F	23	ALA	-	expression tag	UNP B3UES2
F	24	ARG	-	expression tag	UNP B3UES2
F	25	PHE	-	expression tag	UNP B3UES2
F	26	ARG	-	expression tag	UNP B3UES2
F	27	ARG	-	expression tag	UNP B3UES2
F	28	GLY	-	expression tag	UNP B3UES2
F	29	ALA	-	expression tag	UNP B3UES2
F	30	ARG	-	expression tag	UNP B3UES2
F	501	CYS	ALA	conflict	UNP B3UES2

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	97	Total	C	N	O	S	0	0
			775	487	136	150	2		
3	H	97	Total	C	N	O	S	0	0
			775	487	136	150	2		
3	I	97	Total	C	N	O	S	0	0
			775	487	136	150	2		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	184	ASN	-	expression tag	UNP P01730
G	185	THR	-	expression tag	UNP P01730
H	184	ASN	-	expression tag	UNP P01730
H	185	THR	-	expression tag	UNP P01730
I	184	ASN	-	expression tag	UNP P01730
I	185	THR	-	expression tag	UNP P01730

- Molecule 4 is a protein called 21c Fab VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	124	Total	C	N	O	S	0	0
			958	609	158	186	5		
4	L	124	Total	C	N	O	S	0	0
			958	609	158	186	5		
4	N	124	Total	C	N	O	S	0	0
			958	609	158	186	5		

- Molecule 5 is a protein called 21c Fab VL domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	111	Total	C	N	O	S	0	0
			802	501	133	166	2		
5	M	111	Total	C	N	O	S	0	0
			802	501	133	166	2		
5	O	111	Total	C	N	O	S	0	0
			802	501	133	166	2		

- Molecule 6 is a protein called 8ANC195 G52K5 Fab VH domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		
6	R	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		
6	T	131	Total	C	N	O	S	0	0
			1007	639	173	192	3		

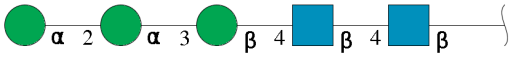
- Molecule 7 is a protein called 8ANC195 G52K5 Fab VL domain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Q	107	Total	C	N	O	S	0	0
			810	509	140	158	3		
7	S	107	Total	C	N	O	S	0	0
			810	509	140	158	3		
7	U	107	Total	C	N	O	S	0	0
			810	509	140	158	3		

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

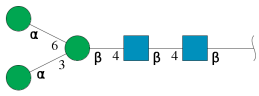
Mol	Chain	Residues	Atoms	AltConf	Trace
8	V	2	Total C N O 28 16 2 10	0	0
8	W	2	Total C N O 28 16 2 10	0	0
8	X	2	Total C N O 28 16 2 10	0	0
8	Y	2	Total C N O 28 16 2 10	0	0
8	c	2	Total C N O 28 16 2 10	0	0
8	d	2	Total C N O 28 16 2 10	0	0
8	e	2	Total C N O 28 16 2 10	0	0
8	f	2	Total C N O 28 16 2 10	0	0
8	j	2	Total C N O 28 16 2 10	0	0
8	k	2	Total C N O 28 16 2 10	0	0
8	l	2	Total C N O 28 16 2 10	0	0
8	m	2	Total C N O 28 16 2 10	0	0
8	q	2	Total C N O 28 16 2 10	0	0
8	r	2	Total C N O 28 16 2 10	0	0
8	s	2	Total C N O 28 16 2 10	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



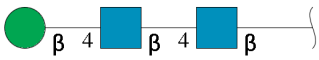
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Z	5	Total	C	N	O	0	0
			61	34	2	25		
9	g	5	Total	C	N	O	0	0
			61	34	2	25		
9	n	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



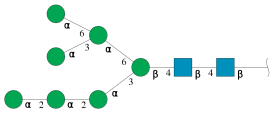
Mol	Chain	Residues	Atoms				AltConf	Trace
10	a	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		
10	o	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



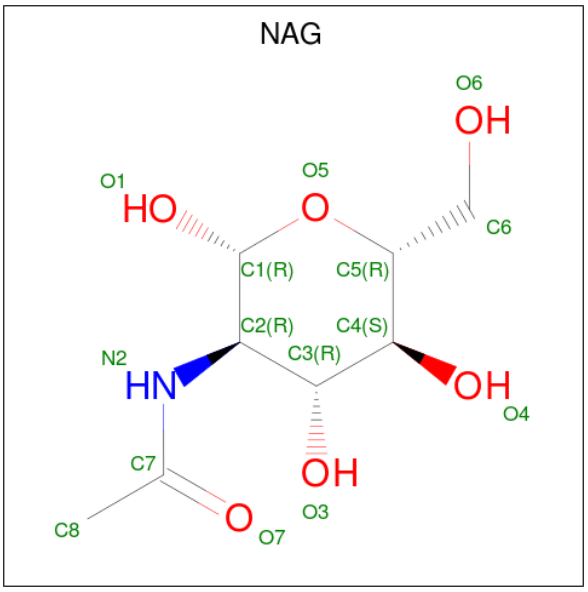
Mol	Chain	Residues	Atoms				AltConf	Trace
11	b	3	Total	C	N	O	0	0
			39	22	2	15		
11	i	3	Total	C	N	O	0	0
			39	22	2	15		
11	p	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	AltConf	Trace
12	t	9	Total C N O 105 58 2 45	0	0
12	u	9	Total C N O 105 58 2 45	0	0
12	v	9	Total C N O 105 58 2 45	0	0

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C N O 14 8 1 5	0
13	B	1	Total C N O 14 8 1 5	0
13	C	1	Total C N O 14 8 1 5	0
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0

Continued on next page...

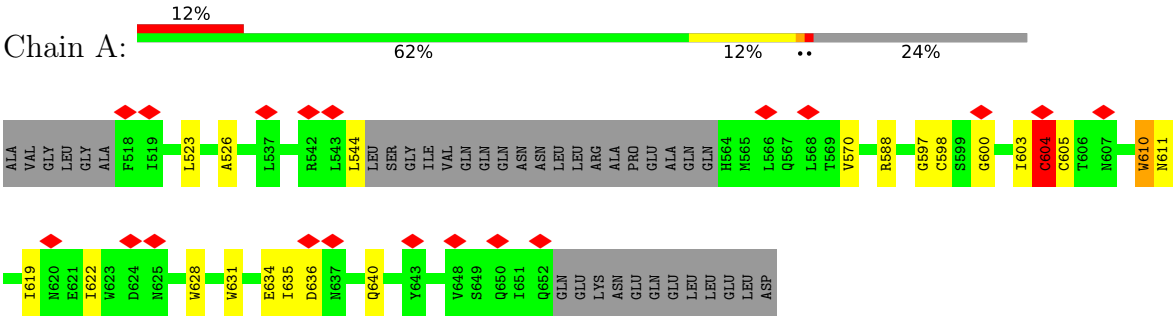
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0
13	D	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	E	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0
13	F	1	Total C N O 112 64 8 40	0

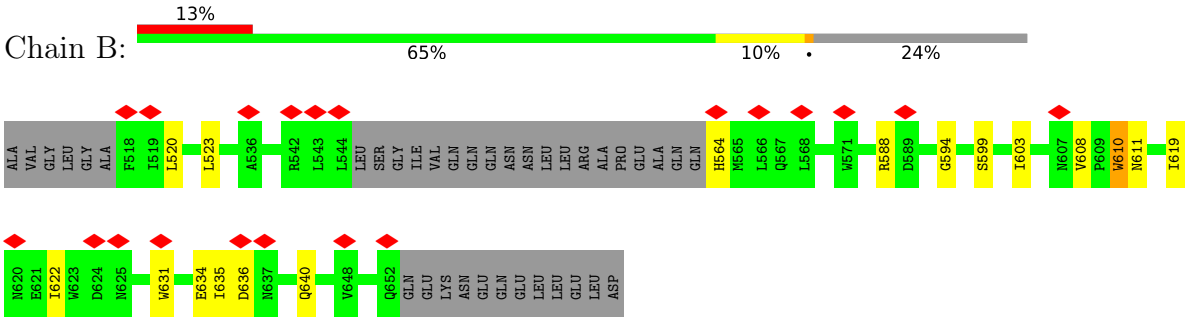
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

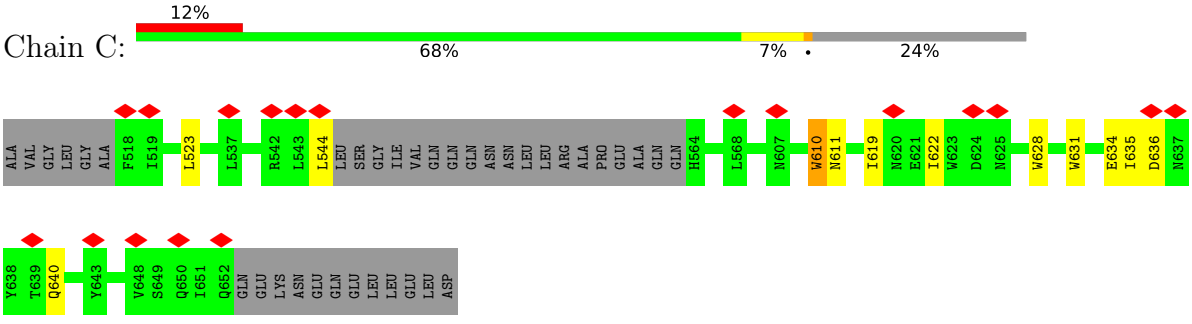
• Molecule 1: Envelope glycoprotein gp160



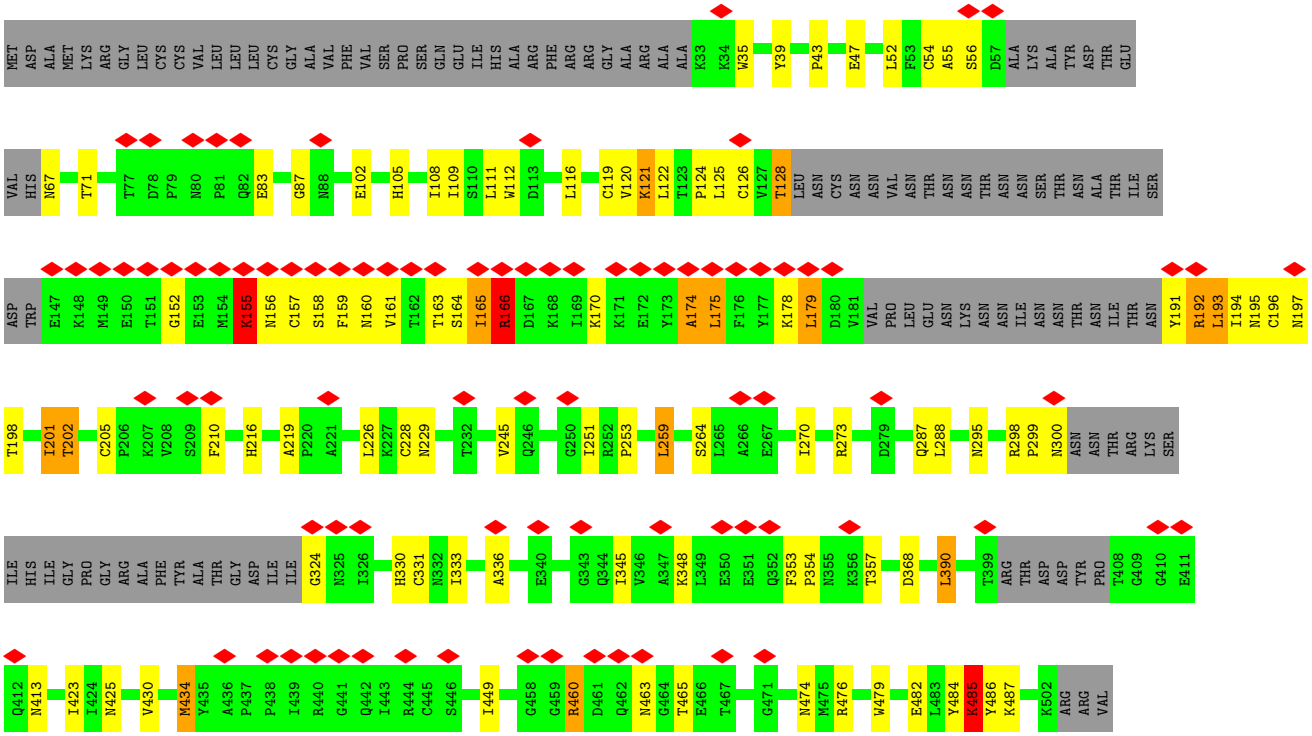
• Molecule 1: Envelope glycoprotein gp160



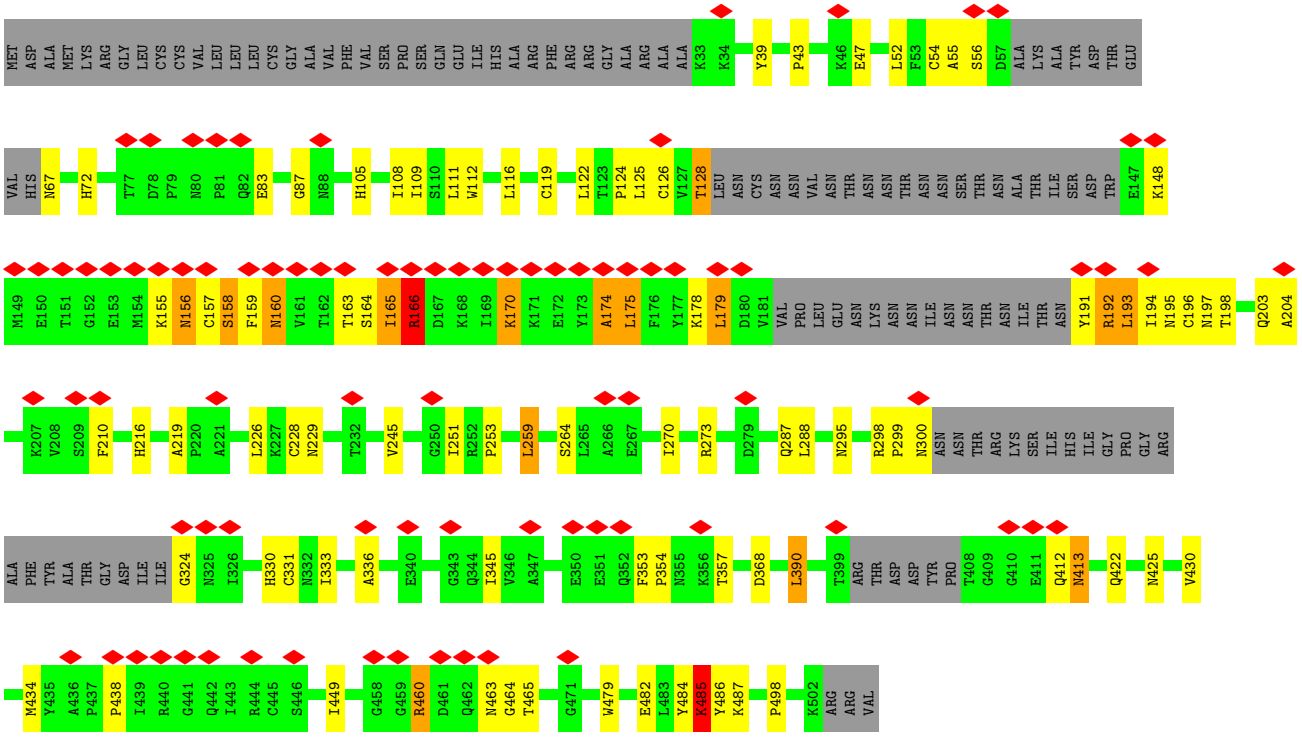
• Molecule 1: Envelope glycoprotein gp160



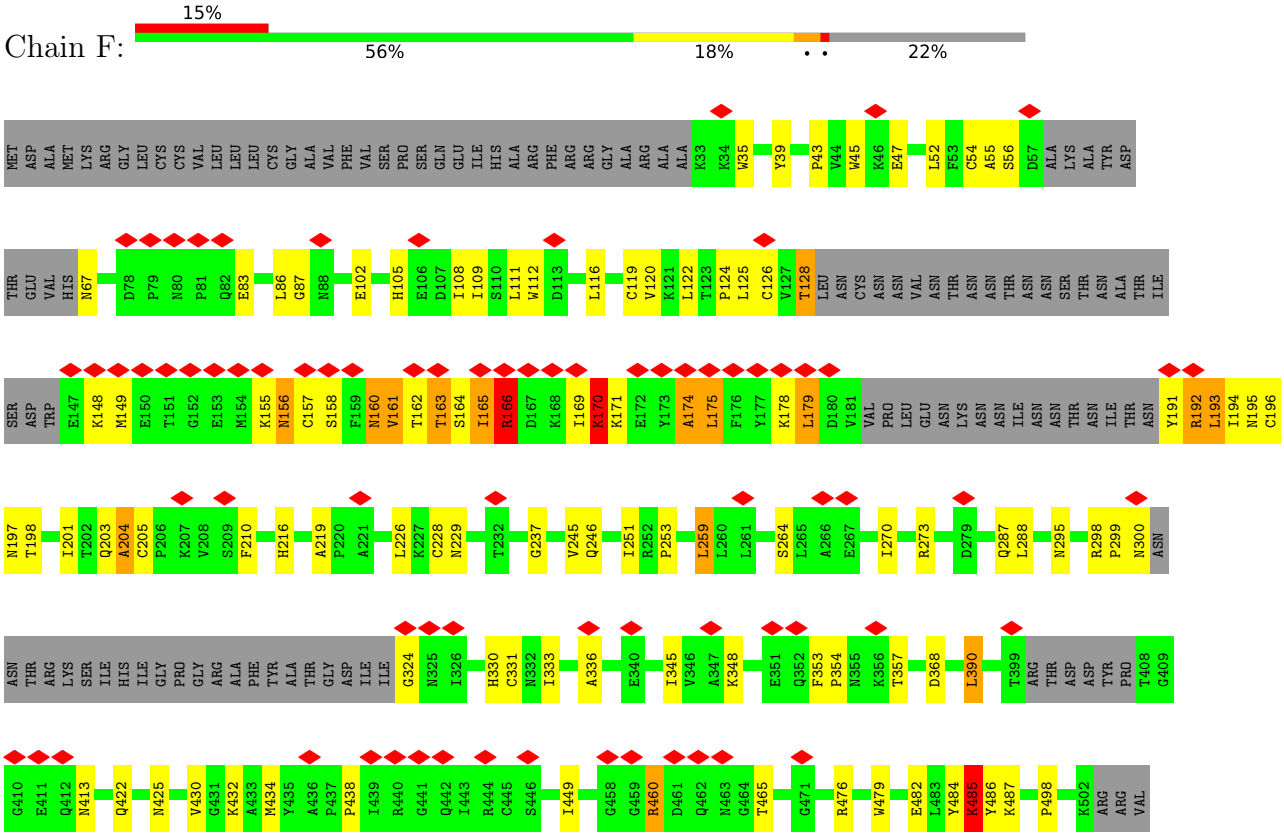
• Molecule 2: Envelope glycoprotein gp160



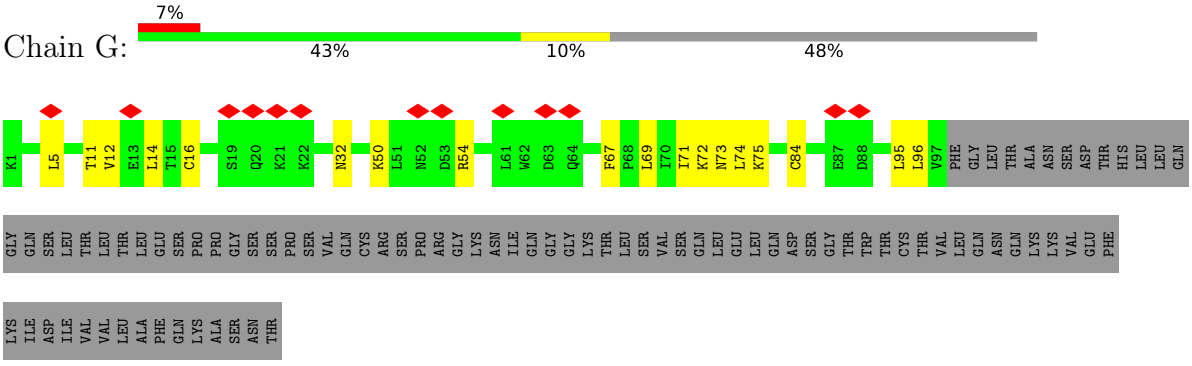
• Molecule 2: Envelope glycoprotein gp160



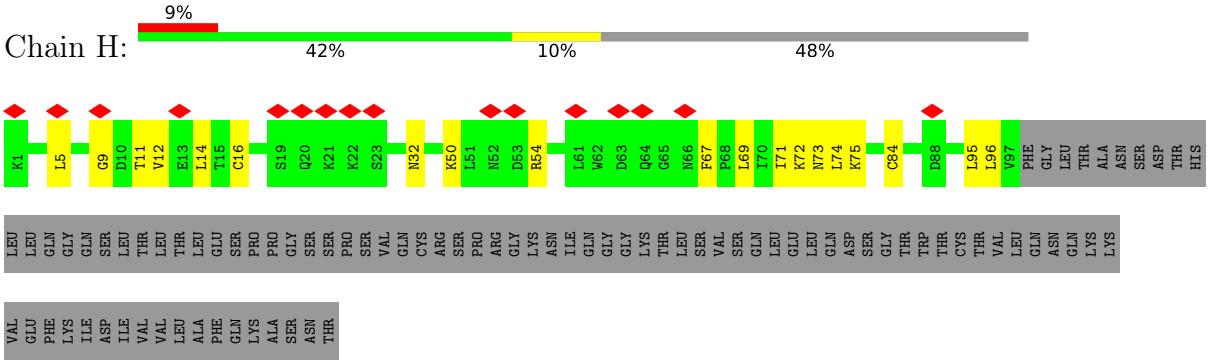
• Molecule 2: Envelope glycoprotein gp160



• Molecule 3: T-cell surface glycoprotein CD4

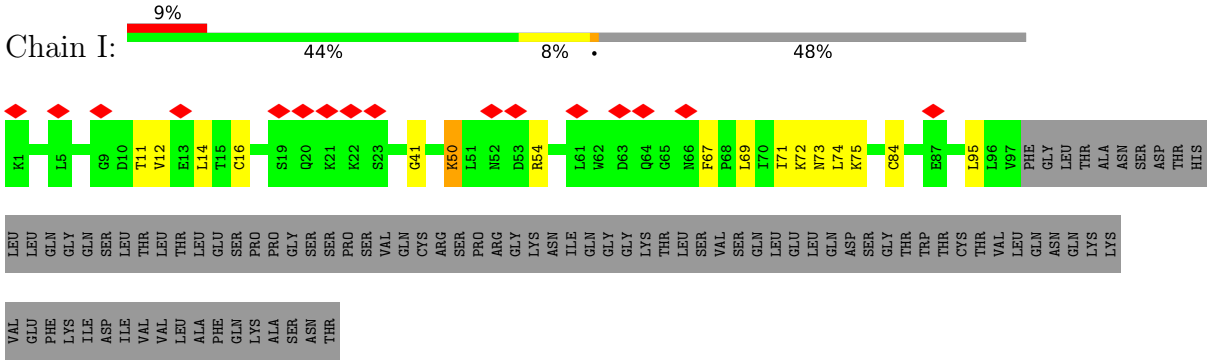


• Molecule 3: T-cell surface glycoprotein CD4



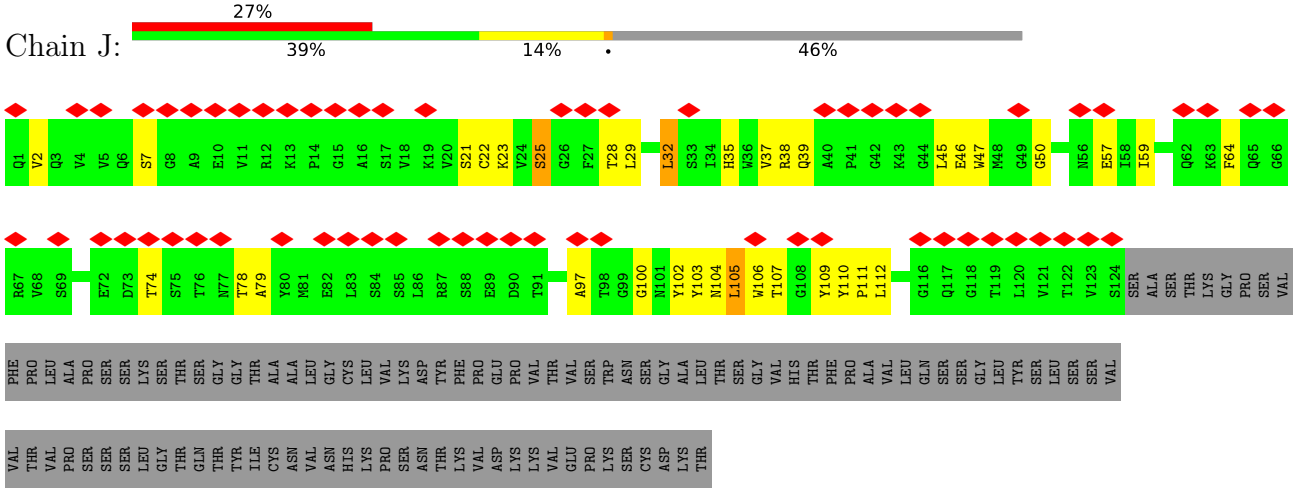
• Molecule 3: T-cell surface glycoprotein CD4

Chain I:



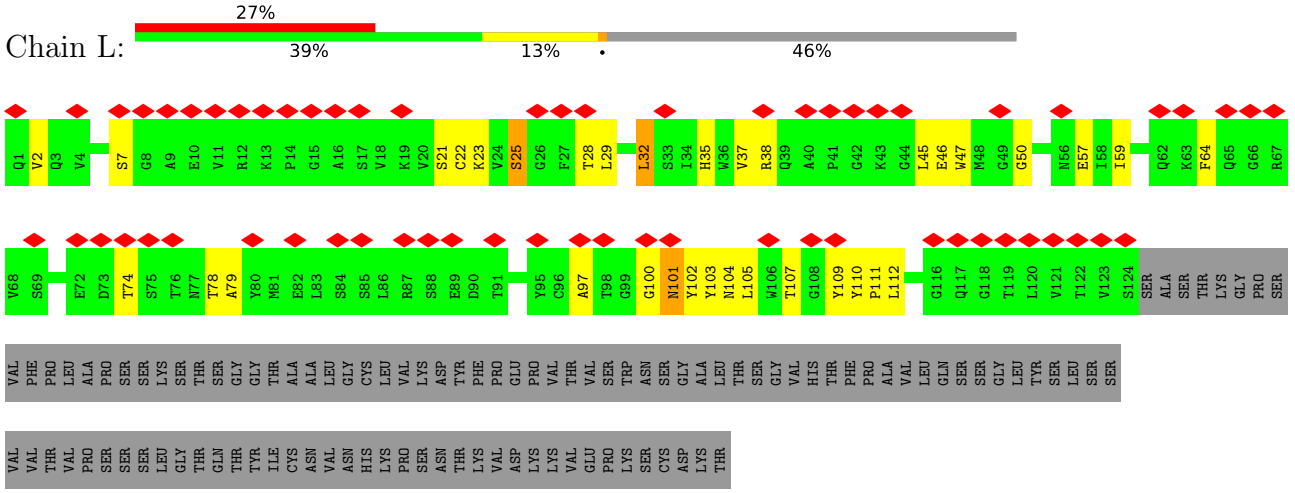
• Molecule 4: 21c Fab VH domain

Chain J:



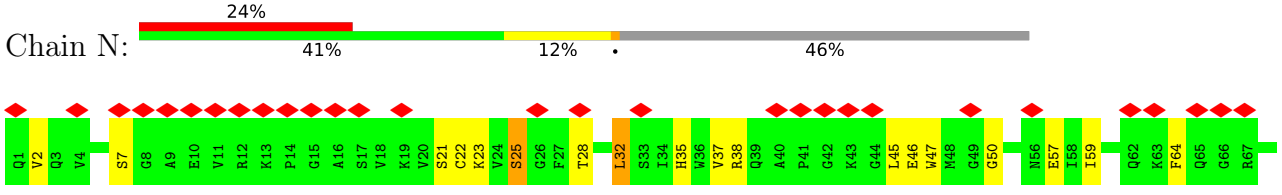
• Molecule 4: 21c Fab VH domain

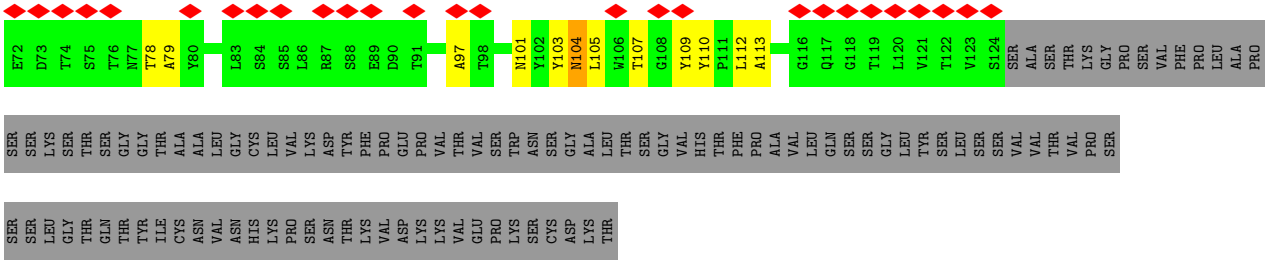
Chain L:



• Molecule 4: 21c Fab VH domain

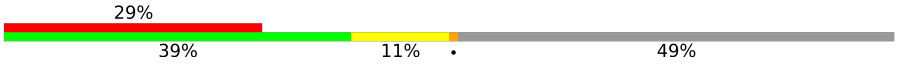
Chain N:

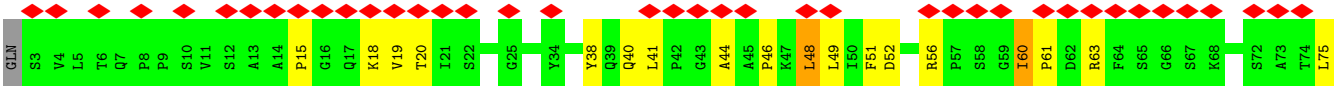




• Molecule 5: 21c Fab VL domain

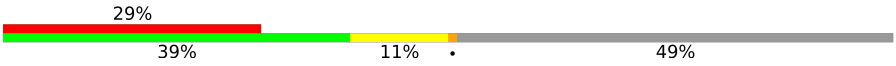
Chain K:

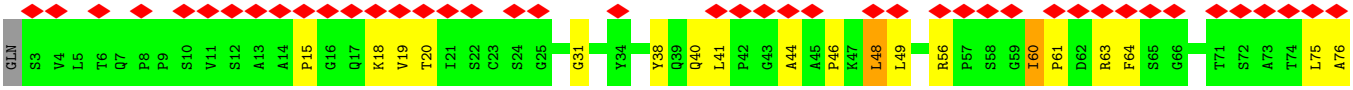




• Molecule 5: 21c Fab VL domain

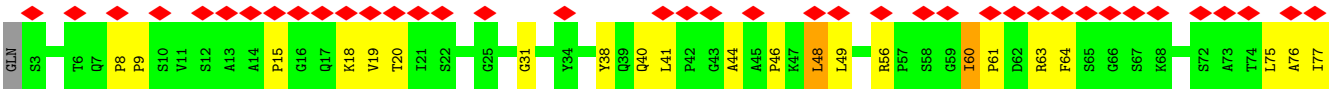
Chain M:

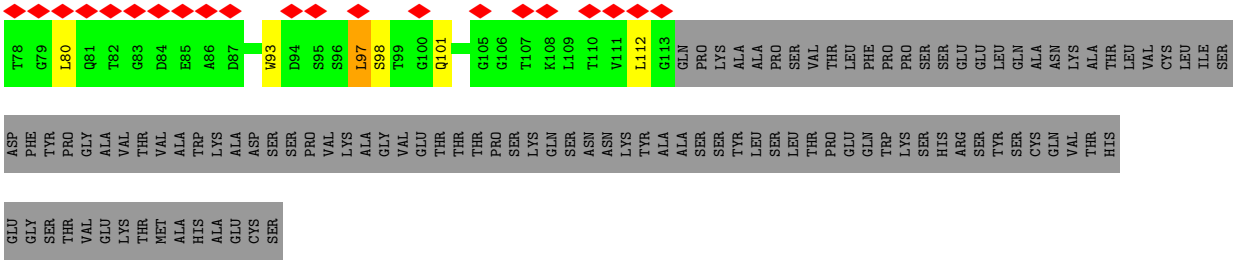




• Molecule 5: 21c Fab VL domain

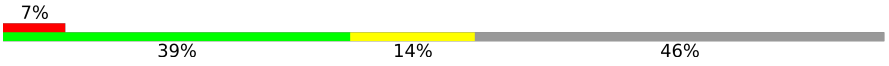
Chain O:

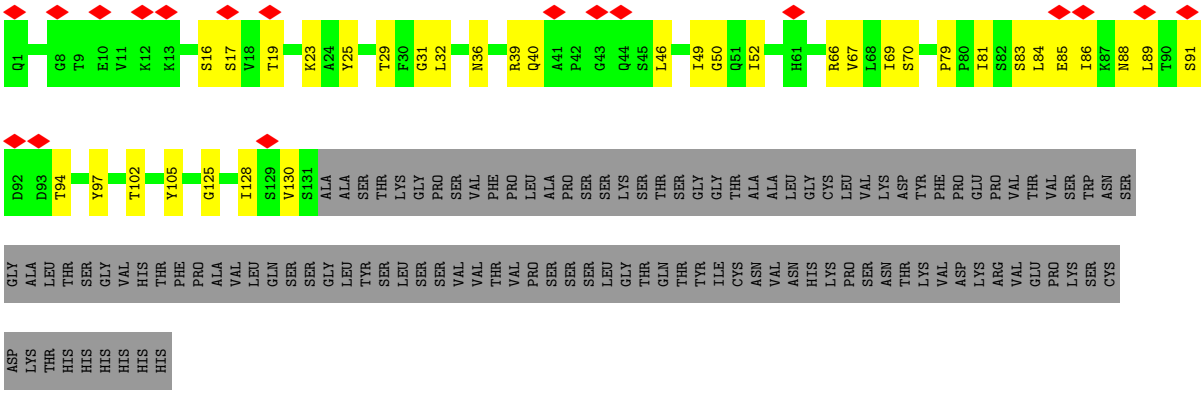




• Molecule 6: 8ANC195 G52K5 Fab VH domain

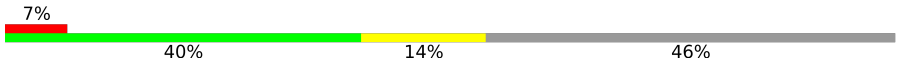
Chain P:

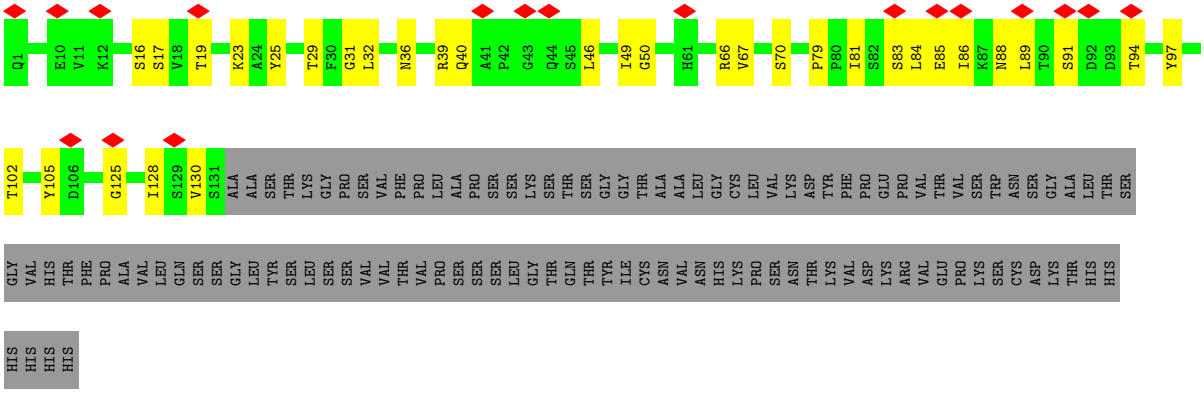




• Molecule 6: 8ANC195 G52K5 Fab VH domain

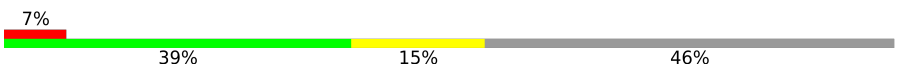
Chain R:

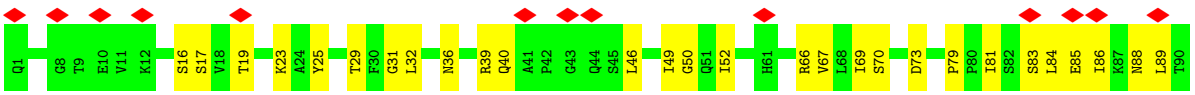


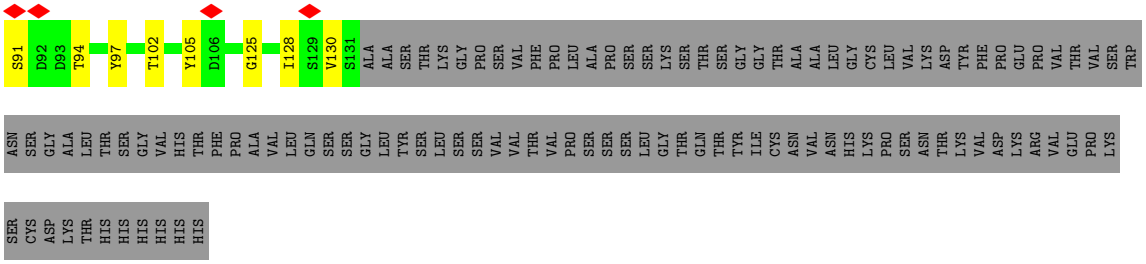


• Molecule 6: 8ANC195 G52K5 Fab VH domain

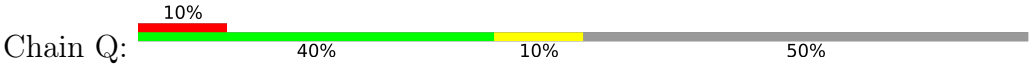
Chain T:

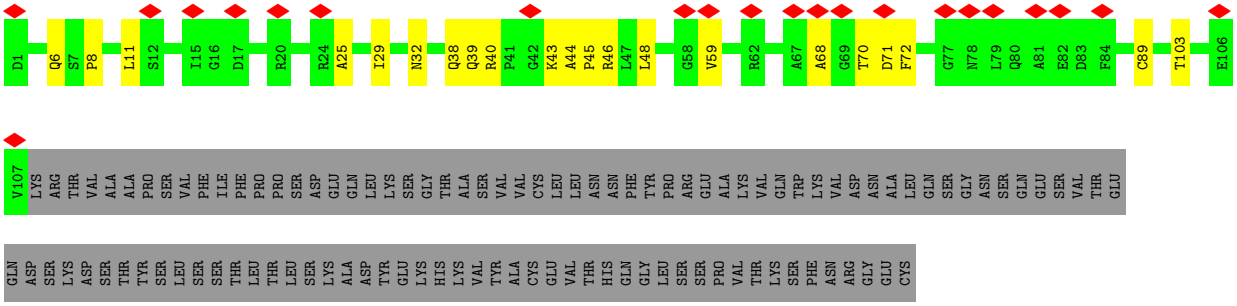




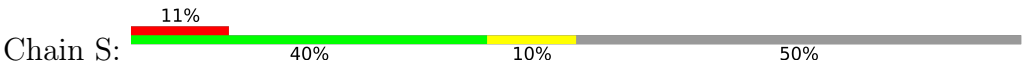


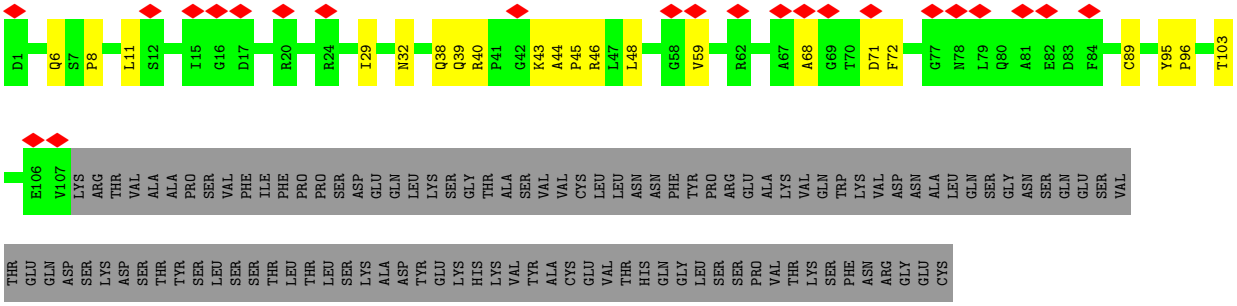
• Molecule 7: 8ANC195 G52K5 Fab VL domain



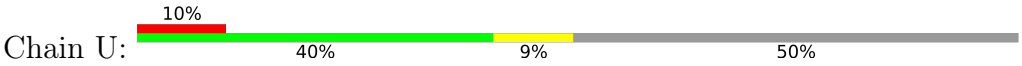


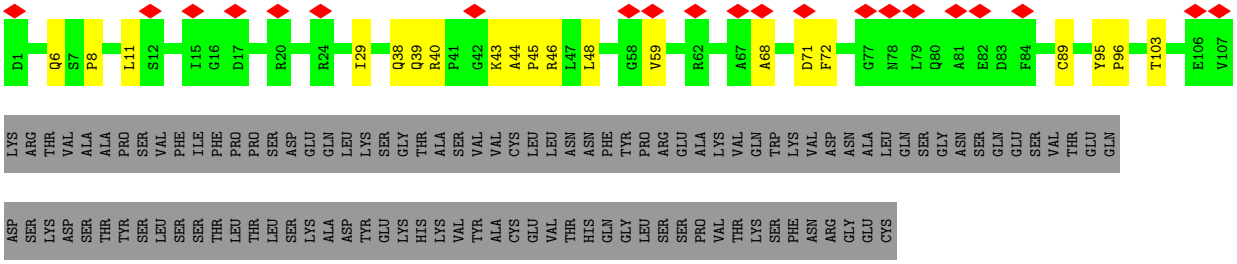
• Molecule 7: 8ANC195 G52K5 Fab VL domain





• Molecule 7: 8ANC195 G52K5 Fab VL domain





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

Chain V:

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

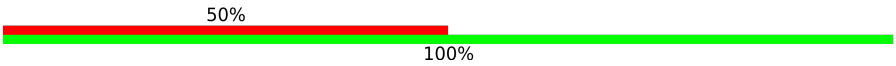
Chain W:

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

Chain X:

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

Chain Y:



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

Chain c:

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

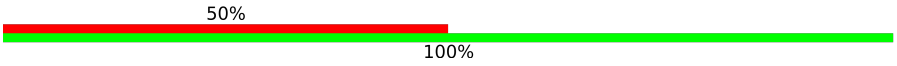
Chain d:

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

Chain e:

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

Chain f:



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

Chain j:

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

Chain k:

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

Chain l:

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

Chain m:

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

Chain q:

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

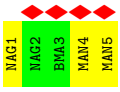
Chain r:

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

Chain s:

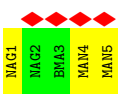
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



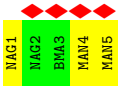
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

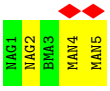


• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

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

Chain h:

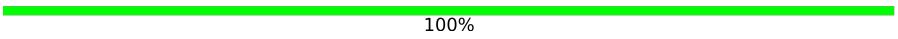


• Molecule 10: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:

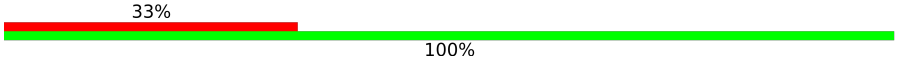
• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



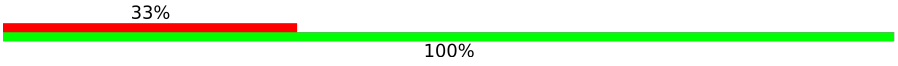
• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

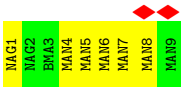


• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

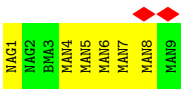
• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u:



• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	305469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.102	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.041	Depositor
Map size (Å)	377.27997, 377.27997, 377.27997	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.38	0/901	0.79	4/1228 (0.3%)
1	B	0.32	0/901	0.61	0/1228
1	C	0.32	0/901	0.61	0/1228
2	D	0.42	0/3049	0.74	3/4156 (0.1%)
2	E	0.44	1/3049 (0.0%)	0.86	8/4156 (0.2%)
2	F	0.41	0/3049	0.91	9/4156 (0.2%)
3	G	0.32	0/785	0.64	0/1053
3	H	0.32	0/785	0.64	0/1053
3	I	0.32	0/785	0.64	0/1053
4	J	0.36	0/982	0.62	0/1335
4	L	0.36	0/982	0.64	0/1335
4	N	0.36	0/982	0.62	0/1335
5	K	0.30	0/819	0.66	1/1115 (0.1%)
5	M	0.30	0/819	0.66	1/1115 (0.1%)
5	O	0.32	0/819	0.63	0/1115
6	P	0.31	0/1034	0.59	0/1408
6	R	0.31	0/1034	0.59	0/1408
6	T	0.31	0/1034	0.59	0/1408
7	Q	0.28	0/828	0.57	0/1125
7	S	0.28	0/828	0.57	0/1125
7	U	0.28	0/828	0.57	0/1125
All	All	0.36	1/25194 (0.0%)	0.71	26/34260 (0.1%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	6
2	E	0	6
2	F	0	6
3	G	0	1
3	H	0	1
3	I	0	1
5	K	0	3
5	M	0	3
5	O	0	3
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	204	ALA	C-N	8.88	1.54	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	204	ALA	O-C-N	21.88	157.71	122.70
2	E	204	ALA	O-C-N	18.86	152.88	122.70
2	F	204	ALA	CA-C-N	-17.25	79.26	117.20
2	E	204	ALA	CA-C-N	-14.45	85.42	117.20
2	F	204	ALA	C-N-CA	-12.29	90.97	121.70
2	E	204	ALA	C-N-CA	-9.92	96.91	121.70
1	A	597	GLY	C-N-CA	-9.16	98.79	121.70
1	A	604	CYS	CB-CA-C	-9.12	92.15	110.40
2	D	164	SER	N-CA-CB	7.78	122.17	110.50
2	E	164	SER	N-CA-CB	7.78	122.17	110.50
2	F	164	SER	N-CA-CB	7.78	122.16	110.50
1	A	604	CYS	CA-CB-SG	-6.28	102.70	114.00
5	K	48	LEU	CA-CB-CG	6.16	129.47	115.30
5	M	48	LEU	CA-CB-CG	6.15	129.44	115.30
2	D	354	PRO	C-N-CA	6.12	137.00	121.70
2	F	354	PRO	C-N-CA	6.12	136.99	121.70
2	E	354	PRO	C-N-CA	6.11	136.98	121.70
2	F	155	LYS	CB-CA-C	-6.05	98.31	110.40
2	E	155	LYS	CB-CA-C	-6.04	98.31	110.40
2	F	149	MET	C-N-CA	5.36	135.10	121.70
2	F	156	ASN	N-CA-CB	5.21	119.98	110.60
2	E	156	ASN	N-CA-CB	5.19	119.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	598	CYS	CA-CB-SG	-5.09	104.83	114.00
2	E	259	LEU	CA-CB-CG	5.09	127.00	115.30
2	F	259	LEU	CA-CB-CG	5.09	127.01	115.30
2	D	259	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	TRP	Peptide
1	B	610	TRP	Peptide
1	C	610	TRP	Peptide
2	D	166	ARG	Sidechain
2	D	192	ARG	Sidechain
2	D	336	ALA	Peptide
2	D	353	PHE	Peptide
2	D	460	ARG	Peptide
2	D	485	LYS	Peptide
2	E	166	ARG	Sidechain
2	E	192	ARG	Sidechain
2	E	336	ALA	Peptide
2	E	353	PHE	Peptide
2	E	460	ARG	Peptide
2	E	485	LYS	Peptide
2	F	166	ARG	Sidechain
2	F	192	ARG	Sidechain
2	F	336	ALA	Peptide
2	F	353	PHE	Peptide
2	F	460	ARG	Peptide
2	F	485	LYS	Peptide
3	G	84	CYS	Peptide
3	H	84	CYS	Peptide
3	I	84	CYS	Peptide
5	K	60	ILE	Peptide
5	K	97	LEU	Peptide
5	K	98	SER	Peptide
5	M	60	ILE	Peptide
5	M	97	LEU	Peptide
5	M	98	SER	Peptide
5	O	60	ILE	Peptide
5	O	97	LEU	Peptide
5	O	98	SER	Peptide

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	884	0	843	23	0
1	B	884	0	841	21	0
1	C	884	0	841	8	0
2	D	2989	0	2792	97	0
2	E	2989	0	2792	80	0
2	F	2989	0	2792	88	0
3	G	775	0	795	7	0
3	H	775	0	795	9	0
3	I	775	0	795	8	0
4	J	958	0	919	37	0
4	L	958	0	919	35	0
4	N	958	0	919	40	0
5	K	802	0	780	21	0
5	M	802	0	780	17	0
5	O	802	0	780	19	0
6	P	1007	0	979	20	0
6	R	1007	0	979	18	0
6	T	1007	0	979	19	0
7	Q	810	0	783	11	0
7	S	810	0	783	11	0
7	U	810	0	783	10	0
8	V	28	0	25	1	0
8	W	28	0	25	1	0
8	X	28	0	25	0	0
8	Y	28	0	25	0	0
8	c	28	0	25	0	0
8	d	28	0	25	0	0
8	e	28	0	25	0	0
8	f	28	0	25	0	0
8	j	28	0	25	0	0
8	k	28	0	25	0	0
8	l	28	0	25	0	0
8	m	28	0	25	0	0
8	q	28	0	25	0	0
8	r	28	0	25	0	0
8	s	28	0	25	0	0
9	Z	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	g	61	0	52	0	0
9	n	61	0	52	0	0
10	a	61	0	52	0	0
10	h	61	0	52	0	0
10	o	61	0	52	0	0
11	b	39	0	34	0	0
11	i	39	0	34	0	0
11	p	39	0	34	0	0
12	t	105	0	87	0	0
12	u	105	0	87	0	0
12	v	105	0	87	0	0
13	A	14	0	13	0	0
13	B	14	0	13	0	0
13	C	14	0	13	0	0
13	D	112	0	104	1	0
13	E	112	0	104	1	0
13	F	112	0	104	1	0
All	All	26271	0	25070	530	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 11.

All (530) 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)
4:N:97:ALA:CB	4:N:112:LEU:HD13	1.40	1.50
2:E:198:THR:CG2	4:N:103:TYR:HA	1.50	1.39
4:L:102:TYR:OH	4:L:111:PRO:HD2	1.44	1.18
2:F:198:THR:HG21	4:J:104:ASN:O	1.40	1.18
4:N:97:ALA:HB1	4:N:112:LEU:HD13	1.17	1.14
4:L:102:TYR:HD1	4:L:103:TYR:CE2	1.65	1.13
2:D:423:ILE:HG23	2:D:434:MET:SD	1.88	1.12
4:N:97:ALA:HB3	4:N:112:LEU:HD13	1.14	1.05
4:N:97:ALA:CB	4:N:112:LEU:CD1	2.33	1.05
1:A:604:CYS:O	1:A:605:CYS:SG	2.14	1.05
2:E:198:THR:CG2	4:N:103:TYR:CA	2.37	1.02
2:E:198:THR:HG23	4:N:103:TYR:CA	1.89	1.02
2:E:198:THR:HG23	4:N:103:TYR:HA	1.05	1.01
2:D:198:THR:HG21	4:L:104:ASN:O	1.60	1.00
4:J:103:TYR:OH	5:K:52:ASP:OD2	1.78	0.99
4:N:97:ALA:HB3	4:N:112:LEU:CD1	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:18:LYS:HA	5:O:77:ILE:O	1.65	0.96
5:M:18:LYS:HA	5:M:77:ILE:O	1.65	0.96
2:F:198:THR:CG2	4:J:104:ASN:O	2.13	0.95
4:L:102:TYR:CD1	4:L:103:TYR:CE2	2.54	0.95
5:K:18:LYS:HA	5:K:77:ILE:O	1.65	0.94
4:N:97:ALA:HB1	4:N:112:LEU:CD1	1.98	0.93
4:L:102:TYR:HH	4:L:111:PRO:HD2	1.27	0.93
1:A:604:CYS:SG	1:A:605:CYS:N	2.35	0.92
2:F:160:ASN:ND2	2:F:160:ASN:H	1.65	0.92
2:E:198:THR:HG21	4:N:103:TYR:HA	1.50	0.92
6:T:97:TYR:O	6:T:125:GLY:HA2	1.72	0.89
6:P:97:TYR:O	6:P:125:GLY:HA2	1.72	0.88
6:R:97:TYR:O	6:R:125:GLY:HA2	1.72	0.87
2:F:122:LEU:CD2	4:J:105:LEU:HA	2.03	0.87
2:E:122:LEU:CD2	4:N:105:LEU:HA	2.05	0.86
2:D:152:GLY:O	2:D:159:PHE:CE2	2.30	0.85
2:E:178:LYS:HA	2:E:191:TYR:CB	2.07	0.85
2:D:122:LEU:CD2	4:L:105:LEU:HA	2.07	0.84
2:F:178:LYS:HA	2:F:191:TYR:CB	2.07	0.83
2:D:152:GLY:O	2:D:159:PHE:HE2	1.60	0.83
2:D:178:LYS:HA	2:D:191:TYR:CB	2.07	0.83
2:E:122:LEU:HD21	4:N:105:LEU:HA	1.61	0.82
1:A:600:GLY:HA3	1:B:599:SER:CB	2.11	0.81
2:F:160:ASN:H	2:F:160:ASN:HD22	1.28	0.79
4:N:113:ALA:HA	5:O:48:LEU:HD23	1.63	0.79
2:E:160:ASN:N	2:E:160:ASN:OD1	2.15	0.78
2:D:122:LEU:HD21	4:L:105:LEU:HA	1.66	0.78
1:A:600:GLY:HA3	1:B:599:SER:HB3	1.67	0.77
2:E:198:THR:HG21	4:N:103:TYR:CA	2.08	0.77
2:D:423:ILE:CG2	2:D:434:MET:SD	2.71	0.76
1:A:603:ILE:HD12	1:A:603:ILE:O	1.85	0.75
2:E:124:PRO:HG2	2:E:430:VAL:HG13	1.66	0.75
2:F:193:LEU:HD13	2:F:193:LEU:O	1.89	0.72
2:E:193:LEU:HD13	2:E:193:LEU:O	1.89	0.72
2:D:124:PRO:HG2	2:D:430:VAL:HG13	1.72	0.71
2:D:193:LEU:HD13	2:D:193:LEU:O	1.89	0.71
2:F:170:LYS:O	2:F:170:LYS:HG3	1.91	0.71
2:E:178:LYS:C	2:E:191:TYR:CB	2.59	0.70
2:F:119:CYS:O	2:F:203:GLN:N	2.21	0.70
2:F:160:ASN:ND2	2:F:160:ASN:N	2.39	0.70
2:D:178:LYS:C	2:D:191:TYR:CB	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:THR:HG21	4:N:103:TYR:C	2.12	0.70
2:D:198:THR:CG2	4:L:104:ASN:O	2.37	0.70
2:F:158:SER:O	2:F:158:SER:OG	1.98	0.70
2:F:178:LYS:C	2:F:191:TYR:CB	2.59	0.70
2:D:119:CYS:HA	2:D:205:CYS:SG	2.32	0.70
1:B:523:LEU:HA	2:F:43:PRO:HB3	1.75	0.68
2:F:259:LEU:HD11	2:F:449:ILE:HG12	1.76	0.68
2:E:170:LYS:HG2	2:E:170:LYS:O	1.94	0.68
2:E:259:LEU:HD11	2:E:449:ILE:HG12	1.76	0.68
4:J:103:TYR:HD2	4:J:103:TYR:O	1.77	0.68
2:D:160:ASN:HB3	2:D:170:LYS:H	1.57	0.67
3:I:73:ASN:ND2	5:M:31:GLY:O	2.27	0.67
2:D:170:LYS:HG3	2:D:170:LYS:O	1.92	0.67
2:F:193:LEU:HD22	2:F:193:LEU:C	2.15	0.67
2:D:121:LYS:HG2	2:D:201:ILE:HB	1.77	0.67
4:J:103:TYR:O	4:J:103:TYR:CD2	2.46	0.67
2:E:56:SER:HB3	2:E:216:HIS:HD2	1.60	0.67
2:E:178:LYS:CA	2:E:191:TYR:CB	2.73	0.67
2:E:193:LEU:C	2:E:193:LEU:HD22	2.15	0.67
2:D:193:LEU:C	2:D:193:LEU:HD22	2.15	0.66
2:D:259:LEU:HD11	2:D:449:ILE:HG12	1.76	0.66
2:F:178:LYS:CA	2:F:191:TYR:CB	2.73	0.66
2:D:56:SER:HB3	2:D:216:HIS:HD2	1.60	0.66
2:F:56:SER:HB3	2:F:216:HIS:HD2	1.60	0.66
2:D:178:LYS:CA	2:D:191:TYR:CB	2.73	0.66
5:O:48:LEU:C	5:O:48:LEU:HD12	2.16	0.65
2:D:191:TYR:O	2:D:192:ARG:HG2	1.97	0.65
1:A:600:GLY:O	1:B:594:GLY:O	2.14	0.65
2:E:174:ALA:O	2:E:175:LEU:CB	2.44	0.65
2:F:122:LEU:HD21	4:J:105:LEU:HA	1.76	0.65
5:O:63:ARG:HD2	5:O:80:LEU:HD11	1.79	0.65
2:D:174:ALA:O	2:D:175:LEU:CB	2.44	0.65
2:F:191:TYR:O	2:F:192:ARG:HG2	1.97	0.65
5:K:63:ARG:HD2	5:K:80:LEU:HD11	1.79	0.64
2:E:191:TYR:O	2:E:192:ARG:HG2	1.97	0.64
2:F:174:ALA:O	2:F:175:LEU:CB	2.44	0.64
1:A:603:ILE:HG22	2:D:39:TYR:CD1	2.32	0.64
2:E:124:PRO:HG2	2:E:430:VAL:CG1	2.28	0.64
5:M:63:ARG:HD2	5:M:80:LEU:HD11	1.79	0.64
1:A:600:GLY:CA	1:B:599:SER:CB	2.77	0.63
2:F:178:LYS:O	2:F:179:LEU:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:102:TYR:OH	4:L:111:PRO:CD	2.36	0.63
2:E:178:LYS:O	2:E:179:LEU:CB	2.46	0.62
2:E:198:THR:HG23	4:N:103:TYR:CB	2.29	0.62
4:L:35:HIS:HD2	4:L:47:TRP:HE1	1.47	0.62
6:T:94:THR:HA	6:T:128:ILE:O	1.99	0.62
2:D:178:LYS:O	2:D:179:LEU:CB	2.46	0.62
4:N:35:HIS:HB2	4:N:112:LEU:HD21	1.81	0.62
4:N:107:THR:HA	4:N:110:TYR:CD1	2.35	0.62
2:F:128:THR:O	2:F:128:THR:OG1	2.16	0.62
6:P:94:THR:HA	6:P:128:ILE:O	1.99	0.62
6:R:94:THR:HA	6:R:128:ILE:O	1.99	0.62
6:T:29:THR:HG23	6:T:31:GLY:H	1.65	0.61
4:N:35:HIS:HE1	4:N:110:TYR:CZ	2.18	0.61
2:E:124:PRO:CG	2:E:430:VAL:HG13	2.31	0.61
4:J:35:HIS:HD2	4:J:47:TRP:HE1	1.47	0.61
4:N:35:HIS:HD2	4:N:47:TRP:HE1	1.47	0.61
4:J:103:TYR:HE2	4:J:106:TRP:HZ2	1.49	0.60
4:N:109:TYR:CD1	5:O:93:TRP:HB3	2.37	0.60
2:E:368:ASP:OD2	2:E:425:ASN:ND2	2.35	0.60
2:D:124:PRO:CG	2:D:430:VAL:HG13	2.32	0.60
3:H:11:THR:HG22	3:H:72:LYS:HG2	1.84	0.60
6:P:29:THR:HG23	6:P:31:GLY:H	1.65	0.60
6:R:29:THR:HG23	6:R:31:GLY:H	1.65	0.60
2:D:87:GLY:HA3	13:D:601:NAG:H82	1.84	0.60
2:E:87:GLY:HA3	13:E:601:NAG:H82	1.84	0.60
4:J:103:TYR:CZ	5:K:52:ASP:OD2	2.54	0.60
1:A:600:GLY:O	1:B:594:GLY:CA	2.49	0.60
2:D:124:PRO:HG2	2:D:430:VAL:CG1	2.32	0.60
2:F:368:ASP:OD2	2:F:425:ASN:ND2	2.35	0.60
3:I:11:THR:HG22	3:I:72:LYS:HG2	1.84	0.60
2:F:87:GLY:HA3	13:F:601:NAG:H82	1.84	0.60
2:D:368:ASP:OD2	2:D:425:ASN:ND2	2.35	0.59
5:M:38:TYR:HA	5:M:48:LEU:HA	1.83	0.59
2:D:120:VAL:HG13	2:D:120:VAL:O	2.03	0.59
2:D:423:ILE:HG12	2:D:434:MET:SD	2.43	0.59
2:F:264:SER:O	2:F:287:GLN:NE2	2.36	0.59
5:K:38:TYR:HA	5:K:48:LEU:HA	1.83	0.59
2:D:264:SER:O	2:D:287:GLN:NE2	2.36	0.59
3:G:11:THR:HG22	3:G:72:LYS:HG2	1.84	0.59
1:A:603:ILE:HD12	1:A:603:ILE:C	2.24	0.58
4:L:102:TYR:CD1	4:L:103:TYR:CZ	2.90	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:104:ASN:OD1	4:N:104:ASN:N	2.33	0.58
2:E:264:SER:O	2:E:287:GLN:NE2	2.36	0.58
5:K:49:LEU:HD12	5:K:60:ILE:HG12	1.86	0.58
5:M:49:LEU:HD12	5:M:60:ILE:HG12	1.86	0.58
2:D:198:THR:HG23	4:L:103:TYR:HA	1.86	0.58
2:F:198:THR:HG21	4:J:104:ASN:C	2.22	0.57
2:E:157:CYS:HB2	2:E:174:ALA:H	1.70	0.57
1:B:564:HIS:HB3	2:E:72:HIS:HB2	1.86	0.57
2:F:157:CYS:HB2	2:F:174:ALA:H	1.70	0.57
5:O:49:LEU:HD12	5:O:60:ILE:HG12	1.86	0.57
7:S:43:LYS:NZ	7:S:44:ALA:O	2.38	0.57
2:E:119:CYS:O	2:E:203:GLN:N	2.36	0.57
7:Q:68:ALA:HB3	7:Q:71:ASP:HB2	1.87	0.57
7:S:68:ALA:HB3	7:S:71:ASP:HB2	1.87	0.57
7:Q:43:LYS:NZ	7:Q:44:ALA:O	2.38	0.56
2:F:163:THR:HG22	2:F:169:ILE:O	2.04	0.56
4:J:32:LEU:HD13	4:J:107:THR:HG21	1.87	0.56
7:U:43:LYS:NZ	7:U:44:ALA:O	2.38	0.56
7:U:68:ALA:HB3	7:U:71:ASP:HB2	1.87	0.56
2:D:198:THR:HG21	4:L:104:ASN:C	2.26	0.56
4:N:32:LEU:HD13	4:N:107:THR:HG21	1.87	0.56
2:D:121:LYS:NZ	2:D:121:LYS:HB3	2.21	0.55
4:L:32:LEU:HD13	4:L:107:THR:HG21	1.87	0.55
5:O:38:TYR:HA	5:O:48:LEU:HA	1.87	0.55
4:N:23:LYS:HA	4:N:78:THR:HG22	1.89	0.55
3:G:16:CYS:HB2	3:G:67:PHE:HB2	1.89	0.55
6:T:67:VAL:HA	6:T:85:GLU:O	2.07	0.55
2:E:128:THR:O	2:E:128:THR:OG1	2.16	0.55
1:A:628:TRP:HH2	2:D:39:TYR:HD2	1.54	0.55
6:R:67:VAL:HA	6:R:85:GLU:O	2.07	0.55
2:D:128:THR:O	2:D:128:THR:OG1	2.16	0.55
2:F:124:PRO:HG2	2:F:430:VAL:HG13	1.89	0.55
4:L:23:LYS:HA	4:L:78:THR:HG22	1.89	0.55
2:D:121:LYS:HB3	2:D:121:LYS:HZ3	1.71	0.55
3:H:16:CYS:HB2	3:H:67:PHE:HB2	1.89	0.55
5:K:56:ARG:NH1	5:K:61:PRO:O	2.41	0.55
2:E:119:CYS:N	2:E:434:MET:O	2.41	0.54
6:P:67:VAL:HA	6:P:85:GLU:O	2.07	0.54
1:A:588:ARG:NH1	1:C:544:LEU:O	2.40	0.54
2:E:193:LEU:H	2:E:193:LEU:CD1	2.21	0.54
5:M:56:ARG:NH1	5:M:61:PRO:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:273:ARG:NH2	2:F:484:TYR:OH	2.41	0.54
5:O:56:ARG:NH1	5:O:61:PRO:O	2.41	0.54
3:I:16:CYS:HB2	3:I:67:PHE:HB2	1.89	0.54
4:J:23:LYS:HA	4:J:78:THR:HG22	1.89	0.54
2:D:119:CYS:CB	2:D:205:CYS:SG	2.96	0.53
2:E:273:ARG:NH2	2:E:484:TYR:OH	2.41	0.53
2:F:193:LEU:CD1	2:F:193:LEU:H	2.21	0.53
2:D:193:LEU:H	2:D:193:LEU:CD1	2.21	0.53
2:D:273:ARG:NH2	2:D:484:TYR:OH	2.41	0.53
4:L:32:LEU:O	4:L:110:TYR:OH	2.27	0.53
5:O:20:THR:HA	5:O:75:LEU:O	2.09	0.53
1:A:600:GLY:CA	1:B:599:SER:HB2	2.39	0.53
2:F:119:CYS:HA	2:F:203:GLN:O	2.08	0.53
4:N:103:TYR:HD2	4:N:103:TYR:O	1.92	0.53
6:R:66:ARG:NH2	6:R:88:ASN:O	2.41	0.53
6:R:19:THR:HA	6:R:84:LEU:O	2.09	0.53
6:T:19:THR:HA	6:T:84:LEU:O	2.09	0.53
2:E:54:CYS:HB2	2:E:55:ALA:HB2	1.91	0.53
5:K:20:THR:HA	5:K:75:LEU:O	2.09	0.53
2:E:193:LEU:O	2:E:193:LEU:HD22	2.10	0.52
4:J:32:LEU:O	4:J:110:TYR:OH	2.27	0.52
6:P:19:THR:HA	6:P:84:LEU:O	2.09	0.52
2:D:54:CYS:HB2	2:D:55:ALA:HB2	1.91	0.52
5:M:20:THR:HA	5:M:75:LEU:O	2.09	0.52
2:D:202:THR:O	2:D:202:THR:HG22	2.08	0.52
2:D:193:LEU:O	2:D:193:LEU:HD22	2.10	0.52
2:D:434:MET:HE2	2:D:434:MET:N	2.25	0.52
2:E:165:ILE:HG12	2:E:166:ARG:HG2	1.92	0.52
2:F:165:ILE:HG12	2:F:166:ARG:HG2	1.92	0.52
4:J:39:GLN:OE1	5:K:40:GLN:NE2	2.38	0.52
6:R:16:SER:HB3	6:R:89:LEU:HD12	1.92	0.52
2:D:165:ILE:HG12	2:D:166:ARG:HG2	1.92	0.52
5:O:19:VAL:O	5:O:76:ALA:HA	2.10	0.52
2:D:121:LYS:NZ	2:D:121:LYS:CB	2.73	0.52
2:E:165:ILE:HG23	2:E:166:ARG:H	1.75	0.52
4:J:102:TYR:O	4:J:102:TYR:CD1	2.62	0.52
6:R:67:VAL:HG22	6:R:86:ILE:HA	1.92	0.52
2:F:157:CYS:SG	2:F:158:SER:N	2.83	0.51
6:P:67:VAL:HG22	6:P:86:ILE:HA	1.92	0.51
2:F:54:CYS:HB2	2:F:55:ALA:HB2	1.91	0.51
2:F:165:ILE:HG23	2:F:166:ARG:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:LEU:O	2:F:197:ASN:HB2	2.11	0.51
5:K:19:VAL:O	5:K:76:ALA:HA	2.10	0.51
6:P:16:SER:HB3	6:P:89:LEU:HD12	1.91	0.51
2:F:193:LEU:O	2:F:193:LEU:HD22	2.10	0.51
2:D:157:CYS:SG	2:D:158:SER:N	2.84	0.51
2:D:108:ILE:HD13	2:D:111:LEU:HD12	1.92	0.51
6:T:66:ARG:NH2	6:T:88:ASN:O	2.41	0.51
2:D:165:ILE:HG23	2:D:166:ARG:H	1.75	0.51
2:F:460:ARG:NH1	3:G:32:ASN:O	2.44	0.51
1:A:523:LEU:HA	2:D:43:PRO:HB3	1.92	0.50
2:E:108:ILE:HD13	2:E:111:LEU:HD12	1.93	0.50
2:F:108:ILE:HD13	2:F:111:LEU:HD12	1.93	0.50
2:D:119:CYS:CA	2:D:205:CYS:SG	2.99	0.50
5:M:41:LEU:HB2	5:M:44:ALA:HB3	1.93	0.50
5:O:20:THR:HG22	5:O:76:ALA:HB2	1.93	0.50
5:M:19:VAL:O	5:M:76:ALA:HA	2.10	0.50
5:M:20:THR:HG22	5:M:76:ALA:HB2	1.93	0.50
6:T:16:SER:HB3	6:T:89:LEU:HD12	1.91	0.50
6:T:67:VAL:HG22	6:T:86:ILE:HA	1.92	0.50
2:E:125:LEU:O	2:E:197:ASN:HB2	2.11	0.50
5:K:20:THR:HG22	5:K:76:ALA:HB2	1.93	0.50
6:R:91:SER:HA	6:R:130:VAL:HG21	1.94	0.50
2:D:198:THR:HG21	4:L:104:ASN:N	2.26	0.50
2:D:333:ILE:HD12	2:D:390:LEU:HD11	1.94	0.50
2:F:126:CYS:HA	2:F:196:CYS:HA	1.93	0.50
2:F:198:THR:HG21	4:J:104:ASN:N	2.26	0.50
2:F:333:ILE:HD12	2:F:390:LEU:HD11	1.94	0.50
2:D:126:CYS:HA	2:D:196:CYS:HA	1.93	0.49
6:P:40:GLN:HB2	6:P:46:LEU:HD23	1.94	0.49
2:E:198:THR:CB	4:N:103:TYR:HA	2.32	0.49
2:E:333:ILE:HD12	2:E:390:LEU:HD11	1.94	0.49
5:O:41:LEU:HB2	5:O:44:ALA:HB3	1.93	0.49
6:T:40:GLN:HB2	6:T:46:LEU:HD23	1.94	0.49
6:T:91:SER:HA	6:T:130:VAL:HG21	1.94	0.49
2:F:119:CYS:N	2:F:434:MET:O	2.45	0.49
4:J:47:TRP:CD2	5:K:101:GLN:HB3	2.47	0.49
5:K:41:LEU:HB2	5:K:44:ALA:HB3	1.93	0.49
6:R:40:GLN:HB2	6:R:46:LEU:HD23	1.94	0.49
4:L:109:TYR:CD1	5:M:93:TRP:HB3	2.47	0.49
6:P:70:SER:OG	6:P:83:SER:OG	2.31	0.49
2:D:165:ILE:HG12	2:D:166:ARG:CG	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:CYS:HA	2:E:196:CYS:HA	1.93	0.49
2:F:165:ILE:HG12	2:F:166:ARG:CG	2.43	0.49
6:P:91:SER:HA	6:P:130:VAL:HG21	1.94	0.49
2:F:160:ASN:HD22	2:F:160:ASN:N	2.05	0.49
4:J:111:PRO:HG3	5:K:51:PHE:HB2	1.95	0.49
4:J:37:VAL:HG11	4:J:45:LEU:HD23	1.95	0.48
4:N:104:ASN:O	4:N:107:THR:HG23	2.13	0.48
1:A:544:LEU:O	1:B:588:ARG:NH1	2.46	0.48
4:J:103:TYR:CE2	4:J:106:TRP:HZ2	2.31	0.48
4:N:35:HIS:HE1	4:N:110:TYR:CE2	2.31	0.48
6:T:70:SER:OG	6:T:83:SER:OG	2.31	0.48
2:D:125:LEU:O	2:D:197:ASN:HB2	2.12	0.48
2:E:165:ILE:HG12	2:E:166:ARG:CG	2.43	0.48
2:E:193:LEU:CD1	2:E:193:LEU:N	2.76	0.48
2:E:460:ARG:NH1	3:H:32:ASN:O	2.46	0.48
6:R:70:SER:OG	6:R:83:SER:OG	2.31	0.48
2:D:193:LEU:H	2:D:193:LEU:HD12	1.79	0.48
5:K:93:TRP:HA	5:K:101:GLN:HA	1.95	0.48
4:L:37:VAL:HG11	4:L:45:LEU:HD23	1.95	0.48
4:N:37:VAL:HG11	4:N:45:LEU:HD23	1.95	0.48
1:C:628:TRP:HH2	2:E:39:TYR:HD2	1.62	0.48
5:M:93:TRP:HA	5:M:101:GLN:HA	1.95	0.48
7:Q:40:ARG:HB2	7:Q:43:LYS:HD3	1.95	0.48
2:F:193:LEU:H	2:F:193:LEU:HD12	1.79	0.48
2:F:237:GLY:HA2	6:P:31:GLY:HA3	1.95	0.48
2:F:193:LEU:CD1	2:F:193:LEU:N	2.76	0.48
1:B:610:TRP:HE1	2:F:498:PRO:HB3	1.79	0.47
2:D:193:LEU:CD1	2:D:193:LEU:N	2.76	0.47
2:E:193:LEU:H	2:E:193:LEU:HD12	1.78	0.47
4:L:102:TYR:CD1	4:L:102:TYR:O	2.67	0.47
1:C:523:LEU:HA	2:E:43:PRO:HB3	1.96	0.47
7:Q:32:ASN:ND2	8:W:1:NAG:O7	2.48	0.47
7:U:40:ARG:HB2	7:U:43:LYS:HD3	1.95	0.47
2:D:288:LEU:HD21	2:D:345:ILE:HD11	1.97	0.47
4:L:102:TYR:HD1	4:L:103:TYR:CD2	2.25	0.47
5:O:93:TRP:HA	5:O:101:GLN:HA	1.95	0.47
2:F:288:LEU:HD21	2:F:345:ILE:HD11	1.97	0.47
1:B:603:ILE:HG23	2:F:39:TYR:HE1	1.79	0.46
6:P:66:ARG:NH2	6:P:88:ASN:O	2.41	0.46
4:J:97:ALA:HB1	4:J:112:LEU:HB3	1.97	0.46
4:L:97:ALA:HB1	4:L:112:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:40:ARG:HB2	7:S:43:LYS:HD3	1.95	0.46
2:E:295:ASN:O	2:E:331:CYS:HA	2.16	0.46
4:N:107:THR:HA	4:N:110:TYR:HD1	1.76	0.46
2:D:47:GLU:HG2	2:D:487:LYS:HE2	1.98	0.46
3:I:12:VAL:HB	3:I:74:LEU:HD11	1.98	0.46
4:L:22:CYS:HB3	4:L:79:ALA:HB3	1.98	0.46
1:B:608:VAL:O	2:F:35:TRP:HB2	2.15	0.46
2:F:295:ASN:O	2:F:331:CYS:HA	2.15	0.46
4:J:100:GLY:H	4:J:102:TYR:HE2	1.64	0.46
6:R:17:SER:HA	6:R:86:ILE:O	2.15	0.46
6:R:39:ARG:HB3	6:R:49:ILE:HD11	1.98	0.46
1:A:619:ILE:HD13	1:A:622:ILE:HD12	1.98	0.46
6:T:39:ARG:HB3	6:T:49:ILE:HD11	1.98	0.46
1:B:619:ILE:HD13	1:B:622:ILE:HD12	1.98	0.46
4:N:22:CYS:HB3	4:N:79:ALA:HB3	1.98	0.46
4:J:22:CYS:HB3	4:J:79:ALA:HB3	1.98	0.46
6:T:17:SER:HA	6:T:86:ILE:O	2.15	0.46
6:T:32:LEU:HD12	6:T:105:TYR:HA	1.98	0.45
1:C:634:GLU:HG2	1:C:635:ILE:HG23	1.99	0.45
2:D:423:ILE:HG12	2:D:434:MET:CG	2.46	0.45
2:E:47:GLU:HG2	2:E:487:LYS:HE2	1.98	0.45
5:K:15:PRO:HD3	5:K:112:LEU:H	1.82	0.45
2:E:288:LEU:HD21	2:E:345:ILE:HD11	1.97	0.45
2:F:47:GLU:HG2	2:F:487:LYS:HE2	1.98	0.45
3:G:12:VAL:HB	3:G:74:LEU:HD11	1.98	0.45
4:N:35:HIS:CD2	4:N:50:GLY:HA3	2.52	0.45
6:P:17:SER:HA	6:P:86:ILE:O	2.15	0.45
7:S:48:LEU:HA	7:S:59:VAL:HG21	1.98	0.45
2:D:295:ASN:O	2:D:331:CYS:HA	2.16	0.45
2:E:124:PRO:HD3	2:E:430:VAL:O	2.16	0.45
6:P:32:LEU:HD12	6:P:105:TYR:HA	1.98	0.45
1:B:634:GLU:HG2	1:B:635:ILE:HG23	1.99	0.45
4:J:35:HIS:CD2	4:J:50:GLY:HA3	2.52	0.45
7:Q:48:LEU:HA	7:Q:59:VAL:HG21	1.99	0.45
1:A:526:ALA:HB2	2:D:43:PRO:HB2	1.99	0.45
4:J:2:VAL:HA	4:J:25:SER:O	2.17	0.45
7:S:38:GLN:HB2	7:S:48:LEU:HD11	1.99	0.45
4:J:102:TYR:OH	4:J:111:PRO:HD2	2.15	0.45
4:L:2:VAL:HA	4:L:25:SER:O	2.17	0.45
2:E:300:ASN:HB2	2:E:324:GLY:HA2	1.99	0.45
4:L:35:HIS:CD2	4:L:50:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:32:LEU:HD12	6:R:105:TYR:HA	1.98	0.45
7:U:95:TYR:HA	7:U:96:PRO:HA	1.77	0.45
2:E:157:CYS:SG	2:E:158:SER:N	2.90	0.44
4:L:103:TYR:O	4:L:103:TYR:CD1	2.70	0.44
7:Q:38:GLN:HB2	7:Q:48:LEU:HD11	1.99	0.44
6:R:32:LEU:HD13	6:R:32:LEU:HA	1.86	0.44
3:H:12:VAL:HB	3:H:74:LEU:HD11	1.98	0.44
4:N:35:HIS:ND1	4:N:112:LEU:HD21	2.32	0.44
1:A:634:GLU:HG2	1:A:635:ILE:HG23	1.99	0.44
2:D:300:ASN:HB2	2:D:324:GLY:HA2	1.99	0.44
2:E:228:CYS:H	2:E:485:LYS:HB3	1.82	0.44
4:N:38:ARG:O	4:N:46:GLU:N	2.49	0.44
7:U:38:GLN:HB2	7:U:48:LEU:HD11	1.99	0.44
2:D:191:TYR:C	2:D:192:ARG:HG2	2.38	0.44
2:E:270:ILE:HG12	2:E:288:LEU:HA	1.99	0.44
2:F:191:TYR:C	2:F:192:ARG:HG2	2.38	0.44
4:L:102:TYR:CE1	4:L:103:TYR:CZ	3.05	0.44
5:M:15:PRO:HD3	5:M:112:LEU:H	1.82	0.44
7:U:48:LEU:HA	7:U:59:VAL:HG21	1.98	0.44
1:C:619:ILE:HD13	1:C:622:ILE:HD12	1.98	0.44
2:D:460:ARG:O	2:D:463:ASN:N	2.44	0.44
2:F:204:ALA:C	2:F:205:CYS:SG	2.96	0.44
2:F:270:ILE:HG12	2:F:288:LEU:HA	1.99	0.44
6:T:23:LYS:HG2	6:T:81:ILE:HG12	2.00	0.44
6:P:32:LEU:HD13	6:P:32:LEU:HA	1.86	0.44
2:D:191:TYR:O	2:D:192:ARG:CG	2.65	0.44
2:E:124:PRO:CD	2:E:430:VAL:HG13	2.48	0.44
1:B:523:LEU:HD12	2:F:86:LEU:HD21	2.00	0.44
1:C:622:ILE:HG12	1:C:631:TRP:HH2	1.83	0.44
2:D:122:LEU:HD21	4:L:104:ASN:O	2.17	0.44
2:D:423:ILE:HG12	2:D:434:MET:HG3	1.99	0.44
2:F:228:CYS:H	2:F:485:LYS:HB3	1.82	0.44
3:I:54:ARG:HD2	3:I:73:ASN:HB2	2.00	0.44
4:N:2:VAL:HA	4:N:25:SER:O	2.17	0.44
2:D:270:ILE:HG12	2:D:288:LEU:HA	1.99	0.44
2:E:463:ASN:HA	2:E:464:GLY:HA3	1.76	0.44
5:O:15:PRO:HD3	5:O:112:LEU:H	1.82	0.44
2:D:155:LYS:HA	2:D:155:LYS:HD2	1.61	0.43
3:H:73:ASN:ND2	5:O:31:GLY:O	2.51	0.43
6:P:23:LYS:HG2	6:P:81:ILE:HG12	1.99	0.43
6:P:39:ARG:HB3	6:P:49:ILE:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:23:LYS:HG2	6:R:81:ILE:HG12	1.99	0.43
2:F:52:LEU:HG	2:F:219:ALA:HA	2.00	0.43
1:A:622:ILE:HG12	1:A:631:TRP:HH2	1.83	0.43
2:D:116:LEU:HD21	2:D:210:PHE:HB2	2.00	0.43
2:E:116:LEU:HD21	2:E:210:PHE:HB2	2.00	0.43
2:F:300:ASN:HB2	2:F:324:GLY:HA2	1.99	0.43
3:H:54:ARG:HD2	3:H:73:ASN:HB2	2.00	0.43
5:M:56:ARG:NH2	5:M:64:PHE:O	2.51	0.43
7:S:32:ASN:ND2	8:V:1:NAG:O7	2.51	0.43
2:F:102:GLU:OE2	2:F:476:ARG:NH1	2.44	0.43
2:F:119:CYS:N	2:F:205:CYS:SG	2.91	0.43
3:I:50:LYS:HE2	3:I:50:LYS:HB3	1.83	0.43
4:L:100:GLY:O	4:L:102:TYR:CD2	2.72	0.43
2:E:251:ILE:HD12	2:E:482:GLU:HB3	2.00	0.43
2:F:116:LEU:HD21	2:F:210:PHE:HB2	2.00	0.43
3:H:9:GLY:N	3:H:74:LEU:O	2.46	0.43
6:T:29:THR:OG1	6:T:73:ASP:OD1	2.29	0.43
2:E:191:TYR:C	2:E:192:ARG:HG2	2.38	0.43
1:A:570:VAL:HG11	2:D:71:THR:HG23	2.00	0.43
2:D:423:ILE:CG1	2:D:434:MET:SD	3.07	0.43
6:R:25:TYR:HE1	6:R:79:PRO:HG3	1.84	0.43
7:S:29:ILE:HD12	7:S:72:PHE:HE2	1.84	0.43
2:F:251:ILE:HD12	2:F:482:GLU:HB3	2.00	0.43
2:F:348:LYS:HB3	2:F:348:LYS:HE3	1.85	0.43
1:B:622:ILE:HG12	1:B:631:TRP:HH2	1.83	0.42
4:L:7:SER:HB3	4:L:21:SER:H	1.84	0.42
5:O:40:GLN:HB2	5:O:46:PRO:HB3	2.01	0.42
5:O:56:ARG:NH2	5:O:64:PHE:O	2.51	0.42
2:D:52:LEU:HG	2:D:219:ALA:HA	2.00	0.42
2:D:251:ILE:HD12	2:D:482:GLU:HB3	2.00	0.42
2:E:228:CYS:SG	2:E:229:ASN:N	2.92	0.42
2:F:126:CYS:HB3	2:F:194:ILE:HG21	2.00	0.42
2:F:228:CYS:SG	2:F:229:ASN:N	2.92	0.42
4:J:7:SER:HB3	4:J:21:SER:H	1.84	0.42
4:J:57:GLU:HG2	4:J:59:ILE:HA	2.01	0.42
5:M:40:GLN:HB2	5:M:46:PRO:HB3	2.01	0.42
4:N:103:TYR:O	4:N:103:TYR:CD2	2.70	0.42
7:Q:29:ILE:HD12	7:Q:72:PHE:HE2	1.84	0.42
7:U:29:ILE:HD12	7:U:72:PHE:HE2	1.84	0.42
2:D:126:CYS:HB3	2:D:194:ILE:HG21	2.00	0.42
4:N:7:SER:HB3	4:N:21:SER:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:228:CYS:H	2:D:485:LYS:HB3	1.83	0.42
2:E:126:CYS:HB3	2:E:194:ILE:HG21	2.00	0.42
4:J:29:LEU:O	4:J:74:THR:OG1	2.31	0.42
6:T:25:TYR:HE1	6:T:79:PRO:HG3	1.84	0.42
2:F:226:LEU:O	2:F:486:TYR:HA	2.19	0.42
6:P:25:TYR:HE1	6:P:79:PRO:HG3	1.84	0.42
2:D:348:LYS:HE3	2:D:348:LYS:HB3	1.85	0.42
2:F:163:THR:CG2	2:F:169:ILE:O	2.66	0.42
5:K:56:ARG:HG2	5:K:61:PRO:HA	2.01	0.42
5:M:56:ARG:HG2	5:M:61:PRO:HA	2.01	0.42
5:O:56:ARG:HG2	5:O:61:PRO:HA	2.01	0.42
2:D:226:LEU:O	2:D:486:TYR:HA	2.19	0.42
2:F:432:LYS:NZ	4:J:106:TRP:O	2.46	0.42
4:J:38:ARG:O	4:J:46:GLU:N	2.49	0.42
6:P:36:ASN:HA	6:P:50:GLY:O	2.20	0.42
6:T:36:ASN:HA	6:T:50:GLY:O	2.20	0.42
2:E:299:PRO:HG2	2:E:330:HIS:HE1	1.85	0.42
4:L:38:ARG:O	4:L:46:GLU:N	2.49	0.42
4:N:38:ARG:HH12	4:N:64:PHE:HZ	1.68	0.42
6:R:36:ASN:HA	6:R:50:GLY:O	2.20	0.42
2:D:102:GLU:OE2	2:D:476:ARG:NH1	2.44	0.42
3:G:14:LEU:HD12	3:G:69:LEU:HD23	2.02	0.42
3:G:54:ARG:HD2	3:G:73:ASN:HB2	2.00	0.42
4:J:38:ARG:HH12	4:J:64:PHE:HZ	1.68	0.42
5:M:18:LYS:HZ2	5:M:78:THR:HG22	1.84	0.42
2:D:228:CYS:SG	2:D:229:ASN:N	2.92	0.42
2:F:191:TYR:O	2:F:192:ARG:CG	2.65	0.42
3:G:5:LEU:HG	3:G:96:LEU:HB2	2.02	0.42
2:D:474:ASN:OD1	3:I:41:GLY:N	2.53	0.41
2:E:357:THR:HB	2:E:465:THR:HG22	2.02	0.41
3:H:5:LEU:HG	3:H:96:LEU:HB2	2.02	0.41
3:H:14:LEU:HD12	3:H:69:LEU:HD23	2.02	0.41
3:I:14:LEU:HD12	3:I:69:LEU:HD23	2.02	0.41
4:L:57:GLU:HG2	4:L:59:ILE:HA	2.02	0.41
2:D:357:THR:HB	2:D:465:THR:HG22	2.02	0.41
1:A:600:GLY:O	1:B:594:GLY:C	2.58	0.41
2:D:124:PRO:HD3	2:D:430:VAL:O	2.20	0.41
2:E:52:LEU:HG	2:E:219:ALA:HA	2.00	0.41
2:E:226:LEU:O	2:E:486:TYR:HA	2.19	0.41
2:F:120:VAL:HA	2:F:201:ILE:O	2.21	0.41
2:F:160:ASN:HB2	2:F:161:VAL:H	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:8:PRO:HA	5:O:9:PRO:HD3	1.95	0.41
7:Q:6:GLN:NE2	7:Q:103:THR:OG1	2.54	0.41
4:J:47:TRP:CG	5:K:101:GLN:HB3	2.55	0.41
7:Q:8:PRO:HG2	7:Q:11:LEU:HD23	2.02	0.41
2:D:161:VAL:HG12	2:D:161:VAL:O	2.21	0.41
2:F:83:GLU:HG3	2:F:245:VAL:HG12	2.02	0.41
2:F:111:LEU:HB3	2:F:112:TRP:CD1	2.56	0.41
2:F:160:ASN:HA	2:F:171:LYS:HA	2.01	0.41
2:F:299:PRO:HG2	2:F:330:HIS:HE1	1.85	0.41
6:T:52:ILE:HD11	6:T:69:ILE:HB	2.03	0.41
7:U:6:GLN:NE2	7:U:103:THR:OG1	2.54	0.41
1:A:636:ASP:O	1:A:640:GLN:NE2	2.54	0.41
2:D:253:PRO:HA	2:D:479:TRP:HH2	1.85	0.41
2:E:191:TYR:O	2:E:192:ARG:CG	2.65	0.41
5:K:40:GLN:HB2	5:K:46:PRO:HB3	2.01	0.41
4:L:38:ARG:HH12	4:L:64:PHE:HZ	1.68	0.41
7:U:39:GLN:HB2	7:U:45:PRO:HB3	2.03	0.41
2:F:253:PRO:HA	2:F:479:TRP:HH2	1.85	0.41
2:F:357:THR:HB	2:F:465:THR:HG22	2.02	0.41
7:Q:39:GLN:HB2	7:Q:45:PRO:HB3	2.03	0.41
7:S:8:PRO:HG2	7:S:11:LEU:HD23	2.02	0.41
1:C:636:ASP:O	1:C:640:GLN:NE2	2.54	0.41
4:J:109:TYR:CD1	5:K:93:TRP:HB3	2.56	0.41
7:S:6:GLN:NE2	7:S:103:THR:OG1	2.54	0.41
7:S:95:TYR:HA	7:S:96:PRO:HA	1.77	0.41
2:D:119:CYS:N	2:D:434:MET:O	2.54	0.41
2:D:299:PRO:HG2	2:D:330:HIS:HE1	1.85	0.41
2:D:357:THR:HB	2:D:465:THR:HA	2.03	0.41
2:E:83:GLU:HG3	2:E:245:VAL:HG12	2.02	0.41
2:E:105:HIS:O	2:E:109:ILE:HG12	2.21	0.41
2:E:357:THR:HB	2:E:465:THR:HA	2.03	0.41
2:F:56:SER:HB3	2:F:216:HIS:CD2	2.49	0.41
2:F:105:HIS:O	2:F:109:ILE:HG12	2.21	0.41
2:F:422:GLN:HE22	2:F:438:PRO:HA	1.86	0.41
2:E:111:LEU:HB3	2:E:112:TRP:CD1	2.56	0.41
1:C:610:TRP:HE1	2:E:498:PRO:HB3	1.86	0.40
2:D:111:LEU:HB3	2:D:112:TRP:CD1	2.56	0.40
2:E:412:GLN:HG2	2:E:413:ASN:HB2	2.03	0.40
2:E:460:ARG:O	2:E:463:ASN:N	2.44	0.40
2:D:105:HIS:O	2:D:109:ILE:HG12	2.21	0.40
2:D:124:PRO:CD	2:D:430:VAL:HG13	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:THR:HB	2:F:465:THR:HA	2.03	0.40
4:N:57:GLU:HG2	4:N:59:ILE:HA	2.01	0.40
7:Q:25:ALA:N	7:Q:70:THR:O	2.55	0.40
7:S:39:GLN:HB2	7:S:45:PRO:HB3	2.03	0.40
1:B:636:ASP:O	1:B:640:GLN:NE2	2.54	0.40
2:D:155:LYS:HB3	2:D:156:ASN:H	1.58	0.40
2:D:193:LEU:C	2:D:193:LEU:CD2	2.85	0.40
2:E:413:ASN:HD22	2:E:413:ASN:HA	1.72	0.40
4:J:35:HIS:CD2	4:J:47:TRP:HE1	2.34	0.40
5:K:18:LYS:HZ2	5:K:78:THR:HG22	1.86	0.40
6:P:52:ILE:HD11	6:P:69:ILE:HB	2.03	0.40
1:B:523:LEU:HD22	2:F:45:TRP:HE1	1.85	0.40
2:D:83:GLU:HG3	2:D:245:VAL:HG12	2.02	0.40
2:E:422:GLN:HE22	2:E:438:PRO:HA	1.86	0.40
4:J:112:LEU:HA	4:J:112:LEU:HD23	1.91	0.40
7:U:8:PRO:HG2	7:U:11:LEU:HD23	2.02	0.40
1:A:610:TRP:CD1	2:D:35:TRP:HA	2.56	0.40
1:B:520:LEU:HD21	2:F:246:GLN:HB2	2.03	0.40
1:B:523:LEU:HD22	2:F:45:TRP:NE1	2.36	0.40
2:E:253:PRO:HA	2:E:479:TRP:HH2	1.85	0.40
4:L:29:LEU:O	4:L:74:THR:OG1	2.31	0.40
4:L:101:ASN:C	4:L:101:ASN:HD22	2.25	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	112/153 (73%)	106 (95%)	5 (4%)	1 (1%)	17	55
1	B	112/153 (73%)	107 (96%)	5 (4%)	0	100	100
1	C	112/153 (73%)	107 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	389/516 (75%)	324 (83%)	59 (15%)	6 (2%)	10 45
2	E	389/516 (75%)	326 (84%)	55 (14%)	8 (2%)	7 39
2	F	389/516 (75%)	326 (84%)	53 (14%)	10 (3%)	5 34
3	G	95/185 (51%)	79 (83%)	16 (17%)	0	100 100
3	H	95/185 (51%)	78 (82%)	17 (18%)	0	100 100
3	I	95/185 (51%)	78 (82%)	17 (18%)	0	100 100
4	J	122/231 (53%)	109 (89%)	12 (10%)	1 (1%)	19 58
4	L	122/231 (53%)	109 (89%)	13 (11%)	0	100 100
4	N	122/231 (53%)	110 (90%)	12 (10%)	0	100 100
5	K	109/217 (50%)	93 (85%)	16 (15%)	0	100 100
5	M	109/217 (50%)	93 (85%)	16 (15%)	0	100 100
5	O	109/217 (50%)	93 (85%)	16 (15%)	0	100 100
6	P	129/244 (53%)	115 (89%)	14 (11%)	0	100 100
6	R	129/244 (53%)	115 (89%)	14 (11%)	0	100 100
6	T	129/244 (53%)	115 (89%)	14 (11%)	0	100 100
7	Q	105/215 (49%)	96 (91%)	9 (9%)	0	100 100
7	S	105/215 (49%)	96 (91%)	9 (9%)	0	100 100
7	U	105/215 (49%)	96 (91%)	9 (9%)	0	100 100
All	All	3183/5283 (60%)	2771 (87%)	386 (12%)	26 (1%)	24 58

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	163	THR
2	D	179	LEU
2	E	156	ASN
2	E	163	THR
2	E	179	LEU
2	F	156	ASN
2	F	163	THR
2	F	179	LEU
1	A	604	CYS
2	D	165	ILE
2	D	175	LEU
2	E	148	LYS
2	E	165	ILE

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Mol	Chain	Res	Type
2	E	175	LEU
2	F	161	VAL
2	F	165	ILE
2	F	175	LEU
2	D	155	LYS
2	E	159	PHE
2	F	162	THR
2	D	174	ALA
2	E	174	ALA
2	F	148	LYS
2	F	170	LYS
2	F	174	ALA
4	J	105	LEU

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	89/130 (68%)	88 (99%)	1 (1%)	73	85
1	B	89/130 (68%)	88 (99%)	1 (1%)	73	85
1	C	89/130 (68%)	88 (99%)	1 (1%)	73	85
2	D	314/453 (69%)	300 (96%)	14 (4%)	27	54
2	E	314/453 (69%)	302 (96%)	12 (4%)	33	59
2	F	314/453 (69%)	303 (96%)	11 (4%)	36	61
3	G	89/167 (53%)	85 (96%)	4 (4%)	27	54
3	H	89/167 (53%)	85 (96%)	4 (4%)	27	54
3	I	89/167 (53%)	85 (96%)	4 (4%)	27	54
4	J	101/194 (52%)	98 (97%)	3 (3%)	41	64
4	L	101/194 (52%)	97 (96%)	4 (4%)	31	57
4	N	101/194 (52%)	96 (95%)	5 (5%)	24	52
5	K	89/180 (49%)	88 (99%)	1 (1%)	73	85
5	M	89/180 (49%)	88 (99%)	1 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	O	89/180 (49%)	87 (98%)	2 (2%)	52 71
6	P	112/210 (53%)	111 (99%)	1 (1%)	78 88
6	R	112/210 (53%)	111 (99%)	1 (1%)	78 88
6	T	112/210 (53%)	111 (99%)	1 (1%)	78 88
7	Q	85/182 (47%)	83 (98%)	2 (2%)	49 69
7	S	85/182 (47%)	83 (98%)	2 (2%)	49 69
7	U	85/182 (47%)	83 (98%)	2 (2%)	49 69
All	All	2637/4548 (58%)	2560 (97%)	77 (3%)	45 64

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	611	ASN
1	B	611	ASN
1	C	611	ASN
2	D	67	ASN
2	D	121	LYS
2	D	128	THR
2	D	155	LYS
2	D	166	ARG
2	D	193	LEU
2	D	195	ASN
2	D	201	ILE
2	D	202	THR
2	D	298	ARG
2	D	390	LEU
2	D	413	ASN
2	D	434	MET
2	D	485	LYS
2	E	67	ASN
2	E	128	THR
2	E	158	SER
2	E	160	ASN
2	E	166	ARG
2	E	170	LYS
2	E	193	LEU
2	E	195	ASN
2	E	298	ARG
2	E	390	LEU
2	E	413	ASN

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Mol	Chain	Res	Type
2	E	485	LYS
2	F	67	ASN
2	F	128	THR
2	F	160	ASN
2	F	166	ARG
2	F	170	LYS
2	F	193	LEU
2	F	195	ASN
2	F	298	ARG
2	F	390	LEU
2	F	413	ASN
2	F	485	LYS
3	G	50	LYS
3	G	71	ILE
3	G	75	LYS
3	G	95	LEU
3	H	50	LYS
3	H	71	ILE
3	H	75	LYS
3	H	95	LEU
3	I	50	LYS
3	I	71	ILE
3	I	75	LYS
3	I	95	LEU
4	J	25	SER
4	J	28	THR
4	J	32	LEU
5	K	97	LEU
4	L	25	SER
4	L	28	THR
4	L	32	LEU
4	L	101	ASN
5	M	97	LEU
4	N	25	SER
4	N	28	THR
4	N	32	LEU
4	N	101	ASN
4	N	104	ASN
5	O	48	LEU
5	O	97	LEU
6	P	102	THR
7	Q	46	ARG

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Mol	Chain	Res	Type
7	Q	89	CYS
6	R	102	THR
7	S	46	ARG
7	S	89	CYS
6	T	102	THR
7	U	46	ARG
7	U	89	CYS

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	611	ASN
1	A	630	GLN
1	A	640	GLN
1	B	611	ASN
1	B	630	GLN
1	B	640	GLN
1	C	611	ASN
1	C	630	GLN
1	C	640	GLN
2	D	67	ASN
2	D	195	ASN
2	D	229	ASN
2	E	67	ASN
2	E	195	ASN
2	E	229	ASN
2	F	67	ASN
2	F	160	ASN
2	F	229	ASN
3	H	66	ASN
3	I	66	ASN
4	J	35	HIS
4	J	39	GLN
5	K	40	GLN
4	L	35	HIS
4	L	101	ASN
4	N	35	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

96 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	$\#\|Z\| > 2$
8	NAG	V	1	8,1	14,14,15	1.25	1 (7%)	17,19,21	1.14	3 (17%)
8	NAG	V	2	8	14,14,15	0.60	0	17,19,21	0.32	0
8	NAG	W	1	8,1	14,14,15	1.26	1 (7%)	17,19,21	1.13	3 (17%)
8	NAG	W	2	8	14,14,15	0.61	0	17,19,21	0.32	0
8	NAG	X	1	8,1	14,14,15	1.25	1 (7%)	17,19,21	1.14	3 (17%)
8	NAG	X	2	8	14,14,15	0.61	0	17,19,21	0.32	0
8	NAG	Y	1	2,8	14,14,15	0.28	0	17,19,21	0.48	0
8	NAG	Y	2	8	14,14,15	0.32	0	17,19,21	0.46	0
9	NAG	Z	1	9,2	14,14,15	0.21	0	17,19,21	0.61	1 (5%)
9	NAG	Z	2	9	14,14,15	0.27	0	17,19,21	0.53	0
9	BMA	Z	3	9	11,11,12	0.68	0	15,15,17	0.82	0
9	MAN	Z	4	9	11,11,12	0.70	0	15,15,17	1.35	2 (13%)
9	MAN	Z	5	9	11,11,12	0.84	0	15,15,17	1.17	2 (13%)
10	NAG	a	1	10,2	14,14,15	0.25	0	17,19,21	0.61	0
10	NAG	a	2	10	14,14,15	0.40	0	17,19,21	0.79	1 (5%)
10	BMA	a	3	10	11,11,12	0.69	0	15,15,17	0.94	0
10	MAN	a	4	10	11,11,12	0.73	0	15,15,17	1.07	2 (13%)
10	MAN	a	5	10	11,11,12	0.81	0	15,15,17	1.11	2 (13%)
11	NAG	b	1	2,11	14,14,15	0.33	0	17,19,21	0.47	0
11	NAG	b	2	11	14,14,15	0.22	0	17,19,21	0.61	0
11	BMA	b	3	11	11,11,12	0.91	0	15,15,17	0.80	0
8	NAG	c	1	2,8	14,14,15	0.40	0	17,19,21	0.79	0
8	NAG	c	2	8	14,14,15	0.82	1 (7%)	17,19,21	0.92	1 (5%)
8	NAG	d	1	2,8	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
8	NAG	d	2	8	14,14,15	0.43	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	e	1	2,8	14,14,15	0.58	0	17,19,21	1.75	4 (23%)
8	NAG	e	2	8	14,14,15	0.27	0	17,19,21	0.63	0
8	NAG	f	1	2,8	14,14,15	0.29	0	17,19,21	0.48	0
8	NAG	f	2	8	14,14,15	0.30	0	17,19,21	0.47	0
9	NAG	g	1	9,2	14,14,15	0.21	0	17,19,21	0.61	1 (5%)
9	NAG	g	2	9	14,14,15	0.27	0	17,19,21	0.53	0
9	BMA	g	3	9	11,11,12	0.68	0	15,15,17	0.83	0
9	MAN	g	4	9	11,11,12	0.69	0	15,15,17	1.34	2 (13%)
9	MAN	g	5	9	11,11,12	0.82	0	15,15,17	1.17	2 (13%)
10	NAG	h	1	10,2	14,14,15	0.25	0	17,19,21	0.62	0
10	NAG	h	2	10	14,14,15	0.41	0	17,19,21	0.79	1 (5%)
10	BMA	h	3	10	11,11,12	0.70	0	15,15,17	0.94	0
10	MAN	h	4	10	11,11,12	0.73	0	15,15,17	1.07	2 (13%)
10	MAN	h	5	10	11,11,12	0.80	0	15,15,17	1.12	2 (13%)
11	NAG	i	1	2,11	14,14,15	0.32	0	17,19,21	0.47	0
11	NAG	i	2	11	14,14,15	0.22	0	17,19,21	0.61	0
11	BMA	i	3	11	11,11,12	0.90	0	15,15,17	0.81	0
8	NAG	j	1	2,8	14,14,15	0.40	0	17,19,21	0.80	0
8	NAG	j	2	8	14,14,15	0.82	1 (7%)	17,19,21	0.92	1 (5%)
8	NAG	k	1	2,8	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
8	NAG	k	2	8	14,14,15	0.42	0	17,19,21	0.43	0
8	NAG	l	1	2,8	14,14,15	0.50	0	17,19,21	1.53	4 (23%)
8	NAG	l	2	8	14,14,15	0.28	0	17,19,21	0.63	0
8	NAG	m	1	2,8	14,14,15	0.28	0	17,19,21	0.48	0
8	NAG	m	2	8	14,14,15	0.32	0	17,19,21	0.46	0
9	NAG	n	1	9,2	14,14,15	0.22	0	17,19,21	0.62	1 (5%)
9	NAG	n	2	9	14,14,15	0.28	0	17,19,21	0.53	0
9	BMA	n	3	9	11,11,12	0.67	0	15,15,17	0.83	0
9	MAN	n	4	9	11,11,12	0.69	0	15,15,17	1.34	2 (13%)
9	MAN	n	5	9	11,11,12	0.83	0	15,15,17	1.17	2 (13%)
10	NAG	o	1	10,2	14,14,15	0.25	0	17,19,21	0.61	0
10	NAG	o	2	10	14,14,15	0.41	0	17,19,21	0.79	1 (5%)
10	BMA	o	3	10	11,11,12	0.69	0	15,15,17	0.94	0
10	MAN	o	4	10	11,11,12	0.74	0	15,15,17	1.08	2 (13%)
10	MAN	o	5	10	11,11,12	0.80	0	15,15,17	1.11	2 (13%)
11	NAG	p	1	2,11	14,14,15	0.32	0	17,19,21	0.47	0
11	NAG	p	2	11	14,14,15	0.22	0	17,19,21	0.61	0
11	BMA	p	3	11	11,11,12	0.91	0	15,15,17	0.81	0
8	NAG	q	1	2,8	14,14,15	0.40	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	q	2	8	14,14,15	0.83	1 (7%)	17,19,21	0.92	1 (5%)
8	NAG	r	1	2,8	14,14,15	0.43	0	17,19,21	0.96	1 (5%)
8	NAG	r	2	8	14,14,15	0.42	0	17,19,21	0.43	0
8	NAG	s	1	2,8	14,14,15	0.36	0	17,19,21	1.09	2 (11%)
8	NAG	s	2	8	14,14,15	0.30	0	17,19,21	0.77	0
12	NAG	t	1	2,12	14,14,15	0.60	0	17,19,21	0.92	1 (5%)
12	NAG	t	2	12	14,14,15	0.34	0	17,19,21	0.64	1 (5%)
12	BMA	t	3	12	11,11,12	0.73	0	15,15,17	0.82	0
12	MAN	t	4	12	11,11,12	0.68	0	15,15,17	1.33	2 (13%)
12	MAN	t	5	6,12	11,11,12	0.90	1 (9%)	15,15,17	1.25	1 (6%)
12	MAN	t	6	12	11,11,12	0.91	1 (9%)	15,15,17	0.91	1 (6%)
12	MAN	t	7	12	11,11,12	0.79	0	15,15,17	1.42	2 (13%)
12	MAN	t	8	12	11,11,12	0.92	1 (9%)	15,15,17	1.38	2 (13%)
12	MAN	t	9	12	11,11,12	0.24	0	15,15,17	0.84	0
12	NAG	u	1	2,12	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
12	NAG	u	2	12	14,14,15	0.33	0	17,19,21	0.63	0
12	BMA	u	3	12	11,11,12	0.73	0	15,15,17	0.82	0
12	MAN	u	4	12	11,11,12	0.68	0	15,15,17	1.33	2 (13%)
12	MAN	u	5	6,12	11,11,12	0.89	1 (9%)	15,15,17	1.25	1 (6%)
12	MAN	u	6	12	11,11,12	0.91	1 (9%)	15,15,17	0.91	1 (6%)
12	MAN	u	7	12	11,11,12	0.80	0	15,15,17	1.42	2 (13%)
12	MAN	u	8	12	11,11,12	0.92	1 (9%)	15,15,17	1.38	2 (13%)
12	MAN	u	9	12	11,11,12	0.25	0	15,15,17	0.85	0
12	NAG	v	1	2,12	14,14,15	0.61	0	17,19,21	0.92	1 (5%)
12	NAG	v	2	12	14,14,15	0.33	0	17,19,21	0.63	0
12	BMA	v	3	12	11,11,12	0.72	0	15,15,17	0.83	0
12	MAN	v	4	12	11,11,12	0.67	0	15,15,17	1.32	2 (13%)
12	MAN	v	5	6,12	11,11,12	0.90	1 (9%)	15,15,17	1.25	1 (6%)
12	MAN	v	6	12	11,11,12	0.92	1 (9%)	15,15,17	0.91	1 (6%)
12	MAN	v	7	12	11,11,12	0.79	0	15,15,17	1.42	2 (13%)
12	MAN	v	8	12	11,11,12	0.91	1 (9%)	15,15,17	1.38	2 (13%)
12	MAN	v	9	12	11,11,12	0.25	0	15,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	V	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	NAG	Y	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
9	NAG	Z	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	Z	2	9	-	2/6/23/26	0/1/1/1
9	BMA	Z	3	9	-	2/2/19/22	0/1/1/1
9	MAN	Z	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Z	5	9	-	2/2/19/22	0/1/1/1
10	NAG	a	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	a	2	10	-	2/6/23/26	0/1/1/1
10	BMA	a	3	10	-	0/2/19/22	0/1/1/1
10	MAN	a	4	10	-	0/2/19/22	0/1/1/1
10	MAN	a	5	10	-	2/2/19/22	0/1/1/1
11	NAG	b	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	b	2	11	-	0/6/23/26	0/1/1/1
11	BMA	b	3	11	-	1/2/19/22	0/1/1/1
8	NAG	c	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	c	2	8	-	2/6/23/26	0/1/1/1
8	NAG	d	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	d	2	8	-	1/6/23/26	0/1/1/1
8	NAG	e	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	e	2	8	-	3/6/23/26	0/1/1/1
8	NAG	f	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
9	NAG	g	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
9	BMA	g	3	9	-	2/2/19/22	0/1/1/1
9	MAN	g	4	9	-	0/2/19/22	0/1/1/1
9	MAN	g	5	9	-	2/2/19/22	0/1/1/1
10	NAG	h	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	h	2	10	-	2/6/23/26	0/1/1/1
10	BMA	h	3	10	-	0/2/19/22	0/1/1/1
10	MAN	h	4	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	h	5	10	-	2/2/19/22	0/1/1/1
11	NAG	i	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	i	2	11	-	0/6/23/26	0/1/1/1
11	BMA	i	3	11	-	1/2/19/22	0/1/1/1
8	NAG	j	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1
8	NAG	k	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	k	2	8	-	1/6/23/26	0/1/1/1
8	NAG	l	1	2,8	-	3/6/23/26	0/1/1/1
8	NAG	l	2	8	-	3/6/23/26	0/1/1/1
8	NAG	m	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	m	2	8	-	2/6/23/26	0/1/1/1
9	NAG	n	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	n	2	9	-	2/6/23/26	0/1/1/1
9	BMA	n	3	9	-	2/2/19/22	0/1/1/1
9	MAN	n	4	9	-	0/2/19/22	0/1/1/1
9	MAN	n	5	9	-	2/2/19/22	0/1/1/1
10	NAG	o	1	10,2	-	1/6/23/26	0/1/1/1
10	NAG	o	2	10	-	2/6/23/26	0/1/1/1
10	BMA	o	3	10	-	0/2/19/22	0/1/1/1
10	MAN	o	4	10	-	0/2/19/22	0/1/1/1
10	MAN	o	5	10	-	2/2/19/22	0/1/1/1
11	NAG	p	1	2,11	-	0/6/23/26	0/1/1/1
11	NAG	p	2	11	-	0/6/23/26	0/1/1/1
11	BMA	p	3	11	-	1/2/19/22	0/1/1/1
8	NAG	q	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	q	2	8	-	2/6/23/26	0/1/1/1
8	NAG	r	1	2,8	-	0/6/23/26	0/1/1/1
8	NAG	r	2	8	-	1/6/23/26	0/1/1/1
8	NAG	s	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	s	2	8	-	5/6/23/26	0/1/1/1
12	NAG	t	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	t	2	12	-	2/6/23/26	0/1/1/1
12	BMA	t	3	12	-	2/2/19/22	0/1/1/1
12	MAN	t	4	12	-	2/2/19/22	0/1/1/1
12	MAN	t	5	6,12	-	1/2/19/22	0/1/1/1
12	MAN	t	6	12	-	0/2/19/22	0/1/1/1
12	MAN	t	7	12	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MAN	t	8	12	-	0/2/19/22	0/1/1/1
12	MAN	t	9	12	-	0/2/19/22	0/1/1/1
12	NAG	u	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	u	2	12	-	2/6/23/26	0/1/1/1
12	BMA	u	3	12	-	2/2/19/22	0/1/1/1
12	MAN	u	4	12	-	2/2/19/22	0/1/1/1
12	MAN	u	5	6,12	-	1/2/19/22	0/1/1/1
12	MAN	u	6	12	-	0/2/19/22	0/1/1/1
12	MAN	u	7	12	-	0/2/19/22	0/1/1/1
12	MAN	u	8	12	-	0/2/19/22	0/1/1/1
12	MAN	u	9	12	-	0/2/19/22	0/1/1/1
12	NAG	v	1	2,12	-	2/6/23/26	0/1/1/1
12	NAG	v	2	12	-	2/6/23/26	0/1/1/1
12	BMA	v	3	12	-	2/2/19/22	0/1/1/1
12	MAN	v	4	12	-	2/2/19/22	0/1/1/1
12	MAN	v	5	6,12	-	1/2/19/22	0/1/1/1
12	MAN	v	6	12	-	0/2/19/22	0/1/1/1
12	MAN	v	7	12	-	0/2/19/22	0/1/1/1
12	MAN	v	8	12	-	0/2/19/22	0/1/1/1
12	MAN	v	9	12	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	1	NAG	O5-C1	-4.50	1.36	1.43
8	V	1	NAG	O5-C1	-4.47	1.36	1.43
8	X	1	NAG	O5-C1	-4.47	1.36	1.43
12	t	8	MAN	C1-C2	2.59	1.58	1.52
12	v	8	MAN	C1-C2	2.55	1.58	1.52
12	u	8	MAN	C1-C2	2.53	1.58	1.52
8	q	2	NAG	C1-C2	2.40	1.55	1.52
8	j	2	NAG	C1-C2	2.38	1.55	1.52
8	c	2	NAG	C1-C2	2.36	1.55	1.52
12	v	5	MAN	C1-C2	2.22	1.57	1.52
12	u	5	MAN	C1-C2	2.22	1.57	1.52
12	t	5	MAN	C1-C2	2.21	1.57	1.52
12	t	6	MAN	O5-C1	-2.03	1.40	1.43
12	v	6	MAN	O5-C1	-2.03	1.40	1.43
12	u	6	MAN	O5-C1	-2.03	1.40	1.43

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	e	1	NAG	O5-C1-C2	-4.66	103.93	111.29
9	Z	4	MAN	C1-O5-C5	4.11	117.76	112.19
9	g	4	MAN	C1-O5-C5	4.07	117.71	112.19
9	n	4	MAN	C1-O5-C5	4.06	117.69	112.19
8	l	1	NAG	O5-C1-C2	-3.94	105.07	111.29
12	u	7	MAN	C1-O5-C5	3.78	117.32	112.19
12	t	7	MAN	C1-O5-C5	3.77	117.30	112.19
12	v	7	MAN	C1-O5-C5	3.76	117.29	112.19
12	u	4	MAN	C1-O5-C5	3.71	117.22	112.19
12	t	4	MAN	C1-O5-C5	3.69	117.19	112.19
12	v	4	MAN	C1-O5-C5	3.69	117.19	112.19
12	t	8	MAN	C1-O5-C5	3.45	116.86	112.19
12	v	8	MAN	C1-O5-C5	3.45	116.86	112.19
12	u	8	MAN	C1-O5-C5	3.42	116.82	112.19
8	e	1	NAG	C1-O5-C5	3.39	116.79	112.19
9	Z	5	MAN	C1-O5-C5	3.33	116.71	112.19
9	n	5	MAN	C1-O5-C5	3.33	116.70	112.19
9	g	5	MAN	C1-O5-C5	3.32	116.69	112.19
8	e	1	NAG	C3-C4-C5	-3.27	104.40	110.24
8	r	1	NAG	C1-O5-C5	3.26	116.60	112.19
8	d	1	NAG	C1-O5-C5	3.24	116.59	112.19
8	k	1	NAG	C1-O5-C5	3.23	116.56	112.19
12	v	1	NAG	C1-O5-C5	3.20	116.52	112.19
12	t	1	NAG	C1-O5-C5	3.17	116.49	112.19
12	u	1	NAG	C1-O5-C5	3.17	116.49	112.19
12	t	4	MAN	O2-C2-C3	-3.15	103.84	110.14
12	v	4	MAN	O2-C2-C3	-3.13	103.87	110.14
12	u	4	MAN	O2-C2-C3	-3.12	103.89	110.14
12	u	5	MAN	O2-C2-C3	-3.09	103.95	110.14
12	t	5	MAN	O2-C2-C3	-3.09	103.96	110.14
12	v	5	MAN	O2-C2-C3	-3.08	103.98	110.14
8	j	2	NAG	C2-N2-C7	3.04	127.23	122.90
8	q	2	NAG	C2-N2-C7	3.00	127.18	122.90
8	c	2	NAG	C2-N2-C7	2.98	127.14	122.90
8	l	1	NAG	C1-O5-C5	2.79	115.98	112.19
10	o	4	MAN	C1-O5-C5	2.73	115.89	112.19
10	h	4	MAN	C1-O5-C5	2.70	115.85	112.19
10	a	4	MAN	C1-O5-C5	2.70	115.84	112.19
10	h	5	MAN	C1-O5-C5	2.63	115.75	112.19
8	l	1	NAG	O4-C4-C5	2.62	115.81	109.30
10	o	5	MAN	C1-O5-C5	2.60	115.72	112.19
9	n	4	MAN	O2-C2-C3	-2.60	104.92	110.14
9	g	4	MAN	O2-C2-C3	-2.60	104.93	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Z	4	MAN	O2-C2-C3	-2.59	104.94	110.14
10	a	5	MAN	C1-O5-C5	2.59	115.70	112.19
10	o	2	NAG	C1-O5-C5	2.55	115.65	112.19
10	h	2	NAG	C1-O5-C5	2.55	115.65	112.19
10	a	2	NAG	C1-O5-C5	2.55	115.64	112.19
8	l	1	NAG	C3-C4-C5	-2.53	105.73	110.24
12	v	7	MAN	O2-C2-C3	-2.32	105.49	110.14
12	t	7	MAN	O2-C2-C3	-2.32	105.50	110.14
12	u	7	MAN	O2-C2-C3	-2.31	105.51	110.14
8	V	1	NAG	C3-C4-C5	2.28	114.30	110.24
8	W	1	NAG	C3-C4-C5	2.26	114.28	110.24
8	X	1	NAG	C3-C4-C5	2.26	114.27	110.24
8	e	1	NAG	O4-C4-C5	2.23	114.84	109.30
10	h	5	MAN	O2-C2-C3	-2.22	105.69	110.14
10	o	5	MAN	O2-C2-C3	-2.21	105.71	110.14
8	s	1	NAG	O4-C4-C5	2.21	114.78	109.30
12	t	6	MAN	O2-C2-C3	-2.20	105.72	110.14
12	v	6	MAN	O2-C2-C3	-2.20	105.73	110.14
12	u	6	MAN	O2-C2-C3	-2.20	105.73	110.14
10	a	5	MAN	O2-C2-C3	-2.19	105.75	110.14
12	u	8	MAN	O2-C2-C3	-2.19	105.76	110.14
8	X	1	NAG	C4-C3-C2	2.18	114.21	111.02
12	v	8	MAN	O2-C2-C3	-2.17	105.80	110.14
8	V	1	NAG	C4-C3-C2	2.16	114.19	111.02
12	t	8	MAN	O2-C2-C3	-2.16	105.81	110.14
8	W	1	NAG	C4-C3-C2	2.15	114.17	111.02
10	o	4	MAN	O2-C2-C3	-2.12	105.90	110.14
10	a	4	MAN	O2-C2-C3	-2.11	105.92	110.14
10	h	4	MAN	O2-C2-C3	-2.10	105.93	110.14
9	g	5	MAN	O2-C2-C3	-2.09	105.94	110.14
9	n	5	MAN	O2-C2-C3	-2.09	105.96	110.14
9	Z	5	MAN	O2-C2-C3	-2.08	105.97	110.14
9	n	1	NAG	C1-O5-C5	2.06	114.98	112.19
8	W	1	NAG	O4-C4-C3	-2.06	105.60	110.35
8	V	1	NAG	O4-C4-C3	-2.04	105.63	110.35
8	s	1	NAG	O4-C4-C3	-2.04	105.64	110.35
8	X	1	NAG	O4-C4-C3	-2.04	105.64	110.35
12	t	2	NAG	C1-O5-C5	2.03	114.94	112.19
9	Z	1	NAG	C1-O5-C5	2.01	114.92	112.19
9	g	1	NAG	C1-O5-C5	2.00	114.91	112.19

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	e	1	NAG	C8-C7-N2-C2
8	l	1	NAG	C8-C7-N2-C2
8	l	1	NAG	O7-C7-N2-C2
8	l	2	NAG	C3-C2-N2-C7
8	l	2	NAG	C8-C7-N2-C2
8	l	2	NAG	O7-C7-N2-C2
8	s	2	NAG	C3-C2-N2-C7
8	e	1	NAG	O7-C7-N2-C2
8	V	1	NAG	O5-C5-C6-O6
8	W	1	NAG	O5-C5-C6-O6
8	X	1	NAG	O5-C5-C6-O6
8	Y	2	NAG	O5-C5-C6-O6
8	f	2	NAG	O5-C5-C6-O6
8	m	2	NAG	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	a	5	MAN	O5-C5-C6-O6
10	h	2	NAG	O5-C5-C6-O6
10	h	5	MAN	O5-C5-C6-O6
10	o	2	NAG	O5-C5-C6-O6
10	o	5	MAN	O5-C5-C6-O6
8	V	2	NAG	C4-C5-C6-O6
8	s	1	NAG	C8-C7-N2-C2
8	V	2	NAG	O5-C5-C6-O6
8	W	2	NAG	O5-C5-C6-O6
8	X	2	NAG	O5-C5-C6-O6
8	W	2	NAG	C4-C5-C6-O6
8	X	2	NAG	C4-C5-C6-O6
12	t	4	MAN	O5-C5-C6-O6
12	t	7	MAN	O5-C5-C6-O6
12	u	4	MAN	O5-C5-C6-O6
12	v	4	MAN	O5-C5-C6-O6
9	Z	5	MAN	O5-C5-C6-O6
9	g	5	MAN	O5-C5-C6-O6
9	n	5	MAN	O5-C5-C6-O6
12	t	2	NAG	O5-C5-C6-O6
12	u	2	NAG	O5-C5-C6-O6
12	v	2	NAG	O5-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
8	j	1	NAG	C4-C5-C6-O6
8	q	1	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
10	h	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
10	o	2	NAG	C4-C5-C6-O6
12	t	1	NAG	O5-C5-C6-O6
12	u	1	NAG	O5-C5-C6-O6
12	v	1	NAG	O5-C5-C6-O6
8	s	1	NAG	O7-C7-N2-C2
9	Z	2	NAG	O5-C5-C6-O6
9	g	2	NAG	O5-C5-C6-O6
9	n	2	NAG	O5-C5-C6-O6
8	V	1	NAG	C4-C5-C6-O6
8	W	1	NAG	C4-C5-C6-O6
8	X	1	NAG	C4-C5-C6-O6
12	t	1	NAG	C4-C5-C6-O6
12	u	1	NAG	C4-C5-C6-O6
12	v	1	NAG	C4-C5-C6-O6
8	f	2	NAG	C4-C5-C6-O6
8	m	2	NAG	C4-C5-C6-O6
9	Z	2	NAG	C4-C5-C6-O6
9	g	2	NAG	C4-C5-C6-O6
9	n	2	NAG	C4-C5-C6-O6
12	t	2	NAG	C4-C5-C6-O6
12	u	2	NAG	C4-C5-C6-O6
12	v	2	NAG	C4-C5-C6-O6
10	a	5	MAN	C4-C5-C6-O6
10	h	5	MAN	C4-C5-C6-O6
10	o	5	MAN	C4-C5-C6-O6
12	t	4	MAN	C4-C5-C6-O6
12	u	4	MAN	C4-C5-C6-O6
12	v	4	MAN	C4-C5-C6-O6
8	V	1	NAG	C8-C7-N2-C2
8	V	1	NAG	O7-C7-N2-C2
8	W	1	NAG	C8-C7-N2-C2
8	W	1	NAG	O7-C7-N2-C2
8	X	1	NAG	C8-C7-N2-C2
8	X	1	NAG	O7-C7-N2-C2
8	Y	2	NAG	C4-C5-C6-O6
8	d	2	NAG	O5-C5-C6-O6
8	k	2	NAG	O5-C5-C6-O6
8	r	2	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
8	j	1	NAG	O5-C5-C6-O6
8	q	1	NAG	O5-C5-C6-O6
12	t	7	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
12	t	5	MAN	O5-C5-C6-O6
12	u	5	MAN	O5-C5-C6-O6
12	v	5	MAN	O5-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
11	b	3	BMA	O5-C5-C6-O6
11	i	3	BMA	O5-C5-C6-O6
11	p	3	BMA	O5-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
10	h	1	NAG	O5-C5-C6-O6
10	o	1	NAG	O5-C5-C6-O6
8	l	1	NAG	O5-C5-C6-O6
8	s	2	NAG	O5-C5-C6-O6
8	e	2	NAG	C3-C2-N2-C7
8	e	2	NAG	C1-C2-N2-C7
12	t	3	BMA	C4-C5-C6-O6
12	u	3	BMA	C4-C5-C6-O6
12	v	3	BMA	C4-C5-C6-O6
9	Z	5	MAN	C4-C5-C6-O6
9	g	5	MAN	C4-C5-C6-O6
8	s	2	NAG	C8-C7-N2-C2
9	n	5	MAN	C4-C5-C6-O6
8	s	2	NAG	O7-C7-N2-C2
12	t	3	BMA	O5-C5-C6-O6
12	u	3	BMA	O5-C5-C6-O6
12	v	3	BMA	O5-C5-C6-O6
9	n	3	BMA	O5-C5-C6-O6
9	Z	3	BMA	O5-C5-C6-O6
9	g	3	BMA	O5-C5-C6-O6
9	n	3	BMA	C4-C5-C6-O6
9	Z	3	BMA	C4-C5-C6-O6
9	g	3	BMA	C4-C5-C6-O6
8	c	2	NAG	C3-C2-N2-C7
8	j	2	NAG	C3-C2-N2-C7
8	q	2	NAG	C3-C2-N2-C7
8	s	2	NAG	C1-C2-N2-C7
8	c	2	NAG	C4-C5-C6-O6
8	j	2	NAG	C4-C5-C6-O6
8	q	2	NAG	C4-C5-C6-O6

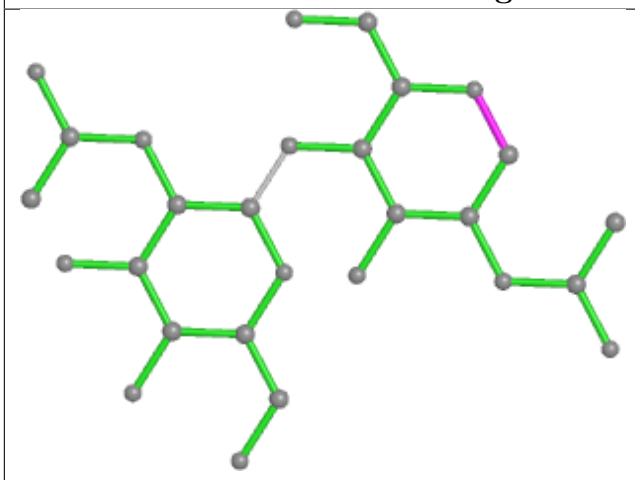
There are no ring outliers.

2 monomers are involved in 2 short contacts:

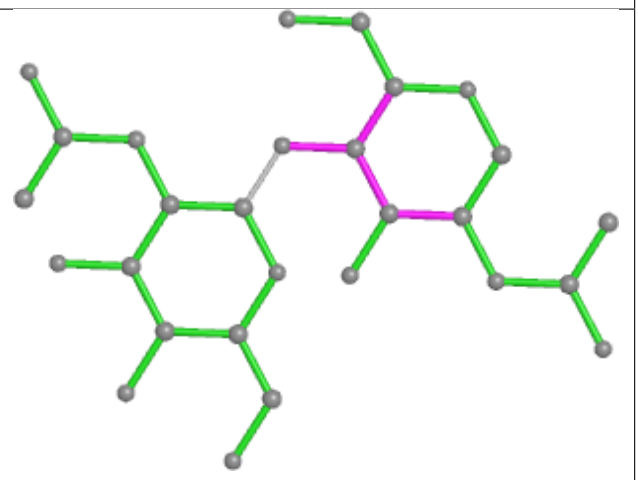
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	1	NAG	1	0
8	V	1	NAG	1	0

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

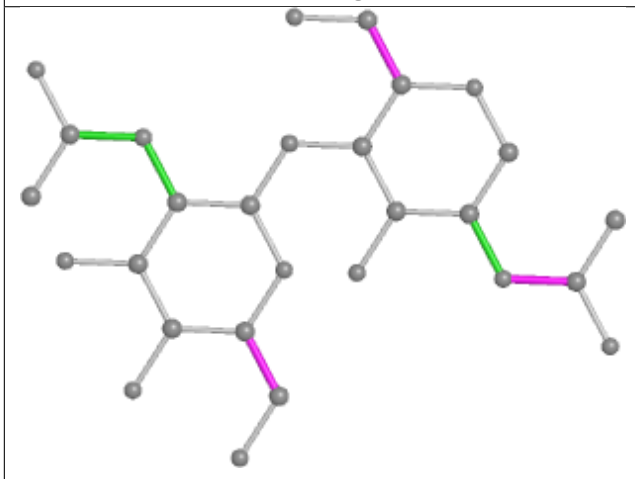
Oligosaccharide Chain V



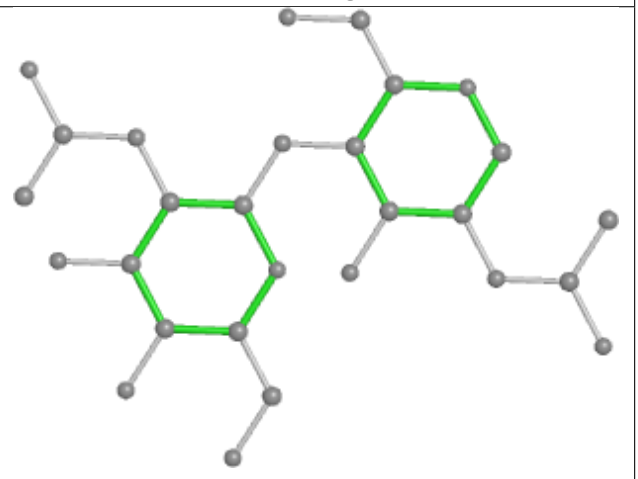
Bond lengths



Bond angles

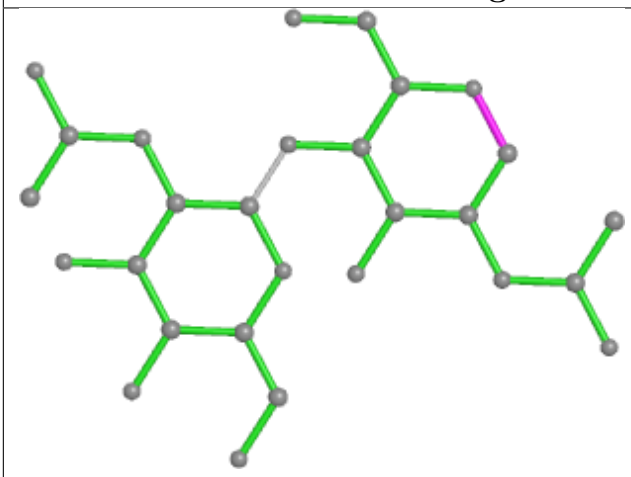


Torsions

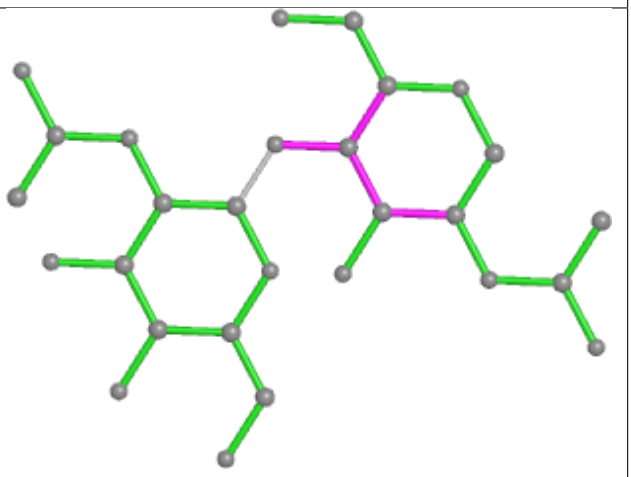


Rings

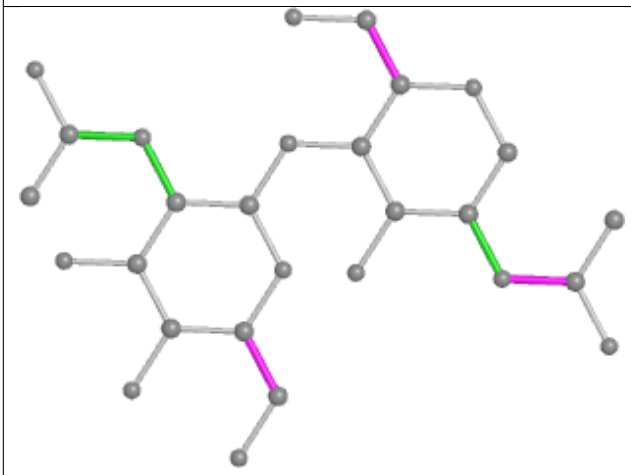
Oligosaccharide Chain W



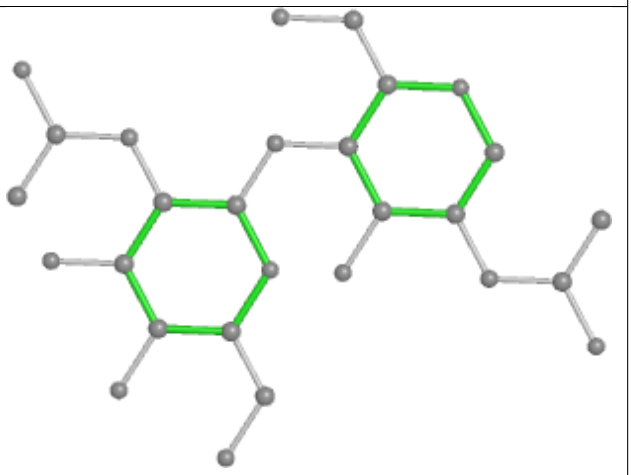
Bond lengths



Bond angles

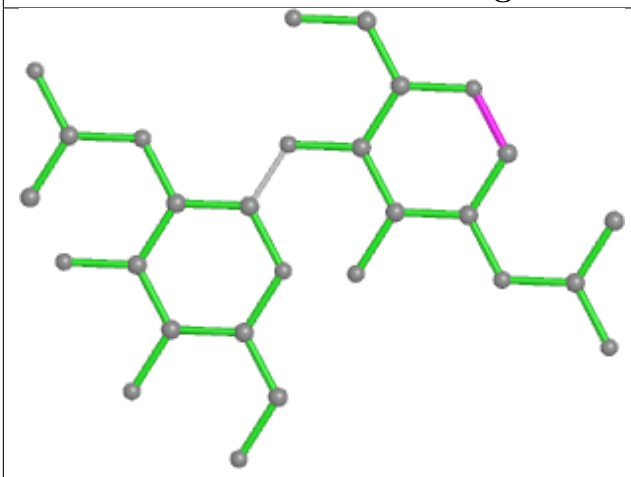


Torsions

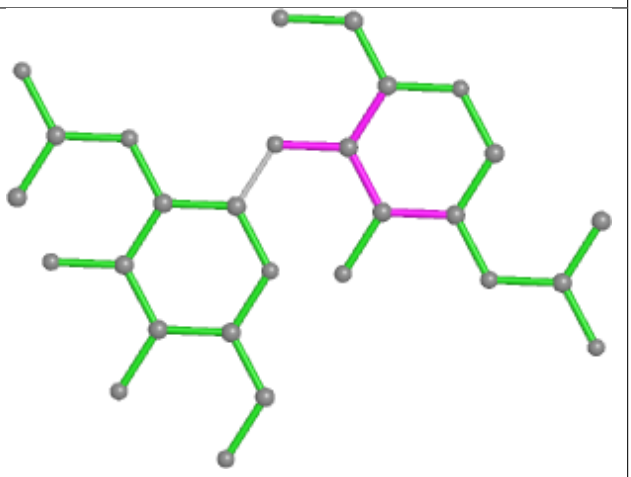


Rings

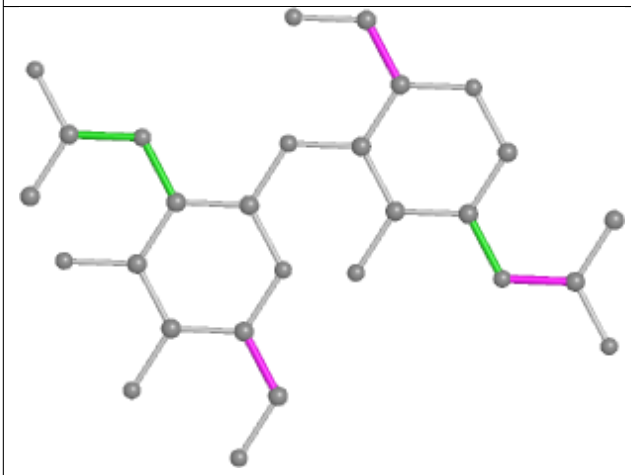
Oligosaccharide Chain X



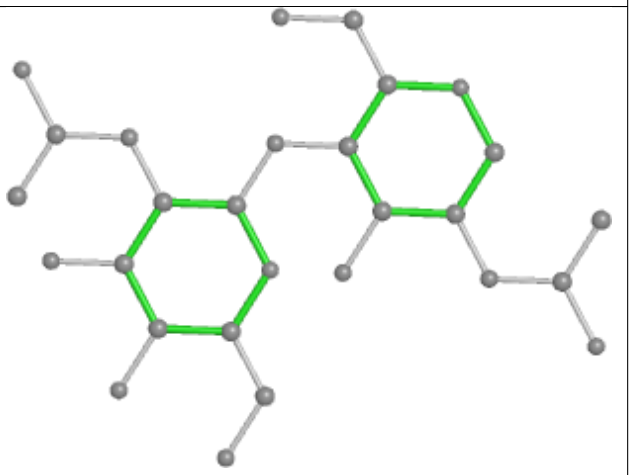
Bond lengths



Bond angles

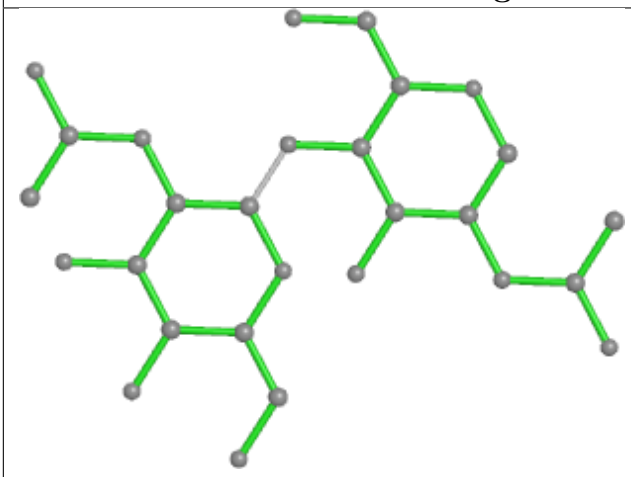


Torsions

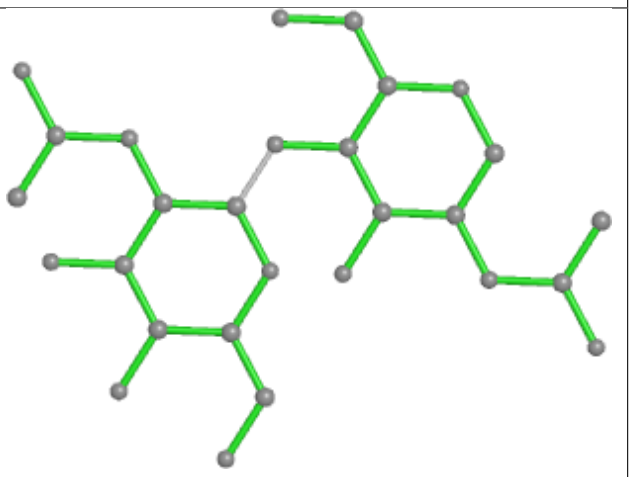


Rings

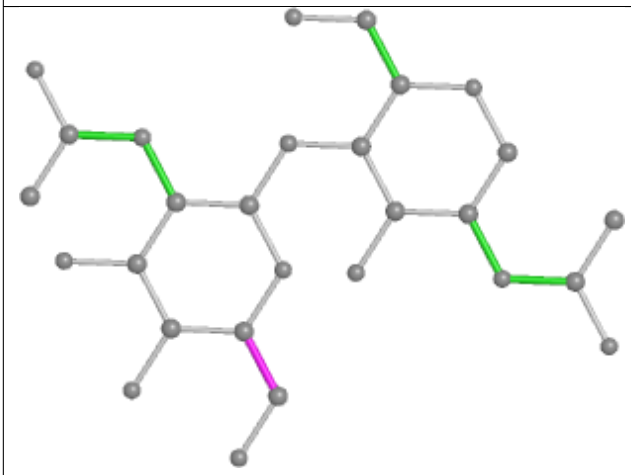
Oligosaccharide Chain Y



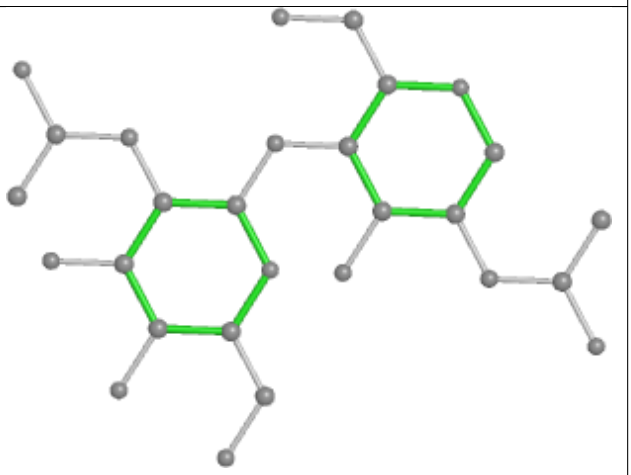
Bond lengths



Bond angles

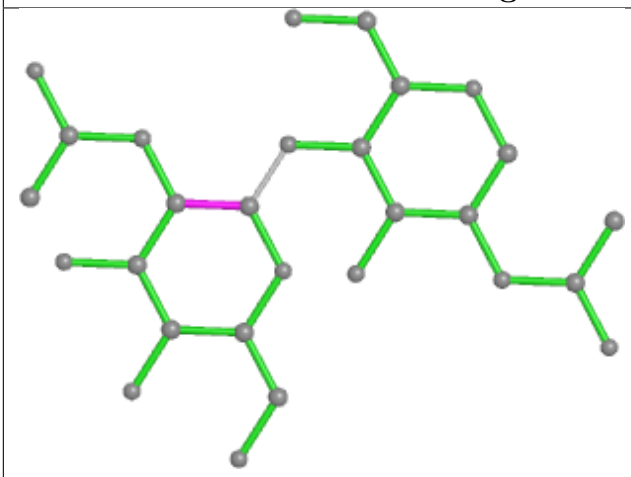


Torsions

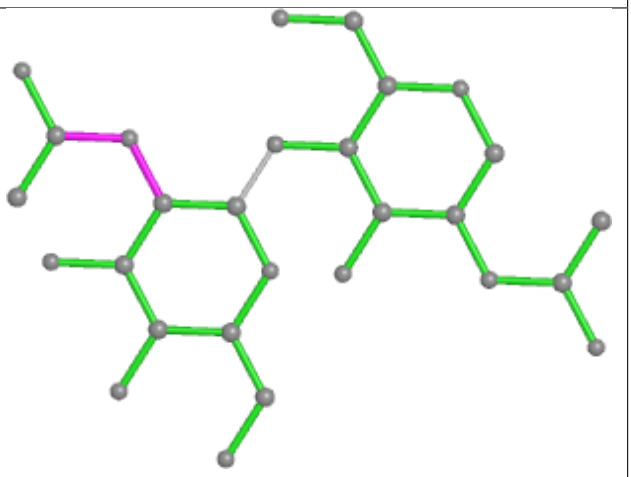


Rings

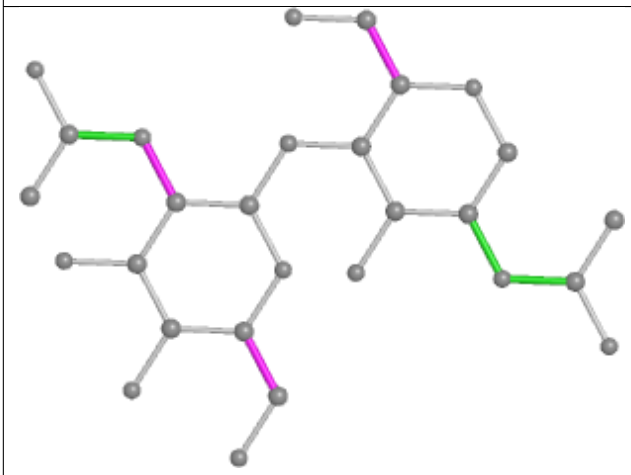
Oligosaccharide Chain c



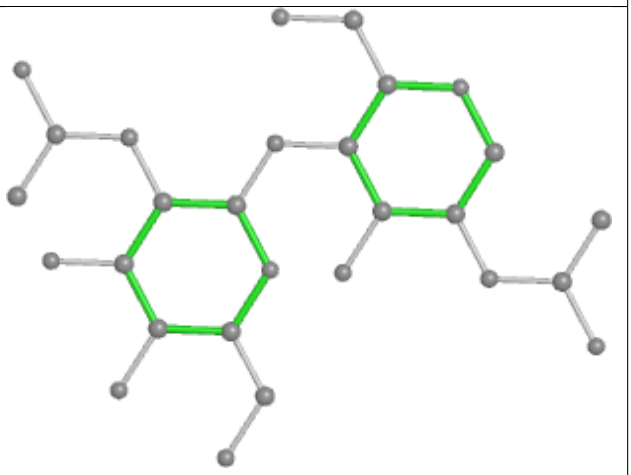
Bond lengths



Bond angles

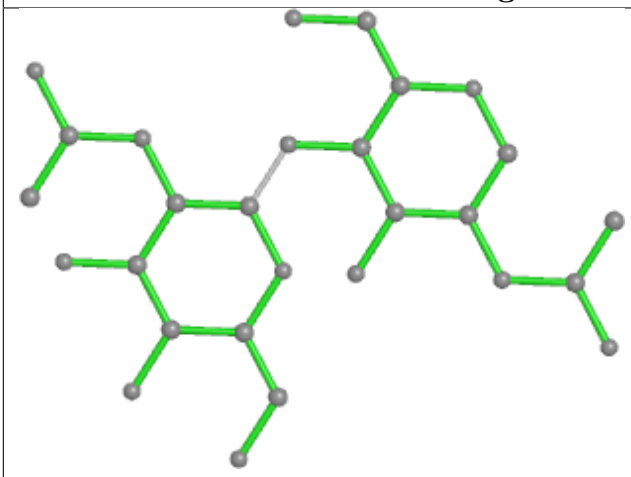


Torsions

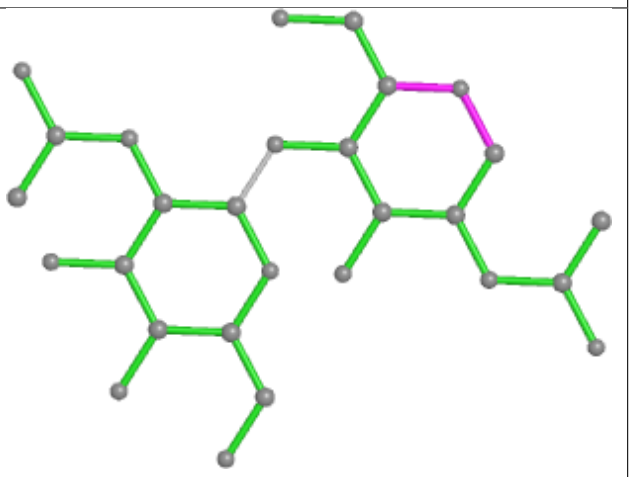


Rings

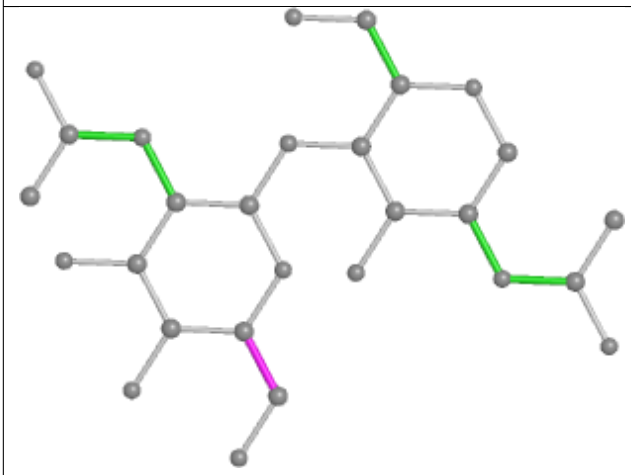
Oligosaccharide Chain d



Bond lengths



Bond angles



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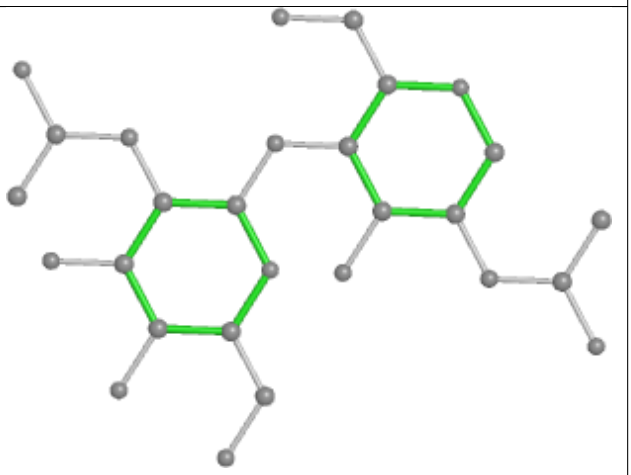
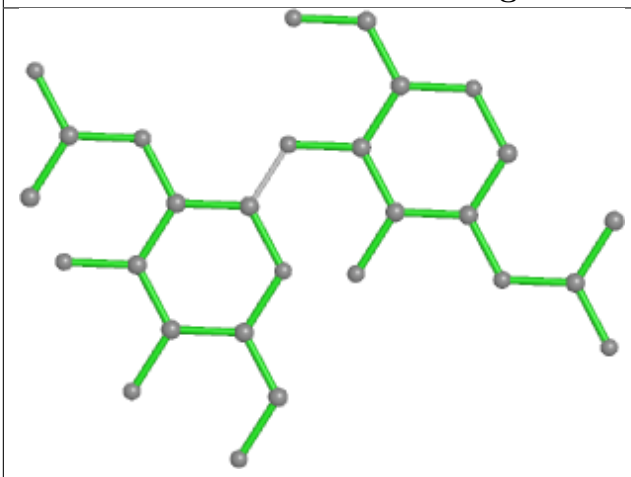


Rings

Oligosaccharide Chain e



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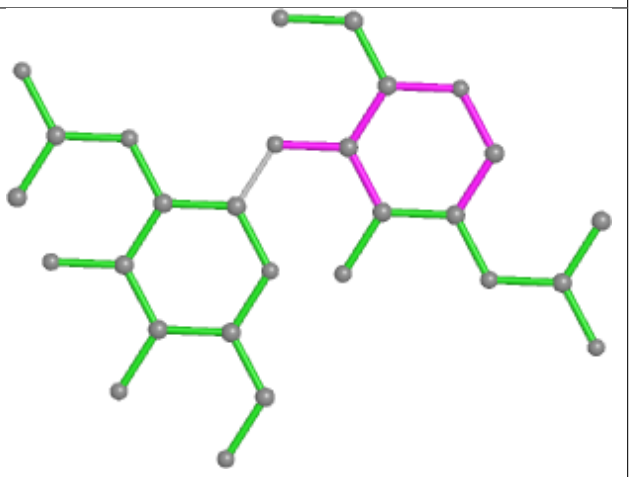

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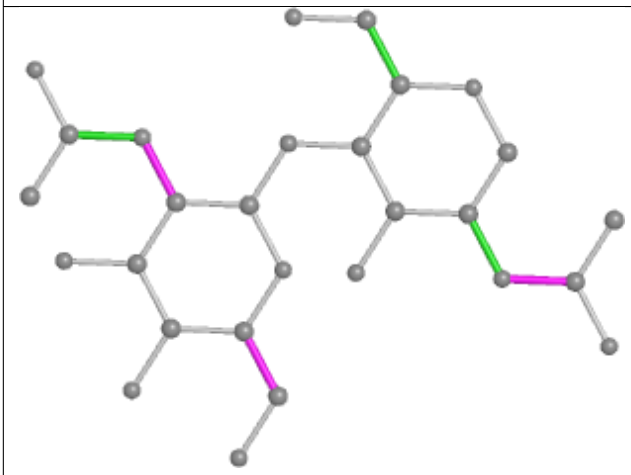

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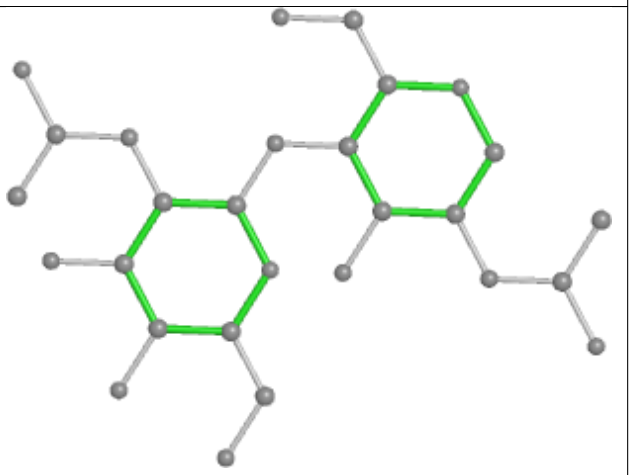
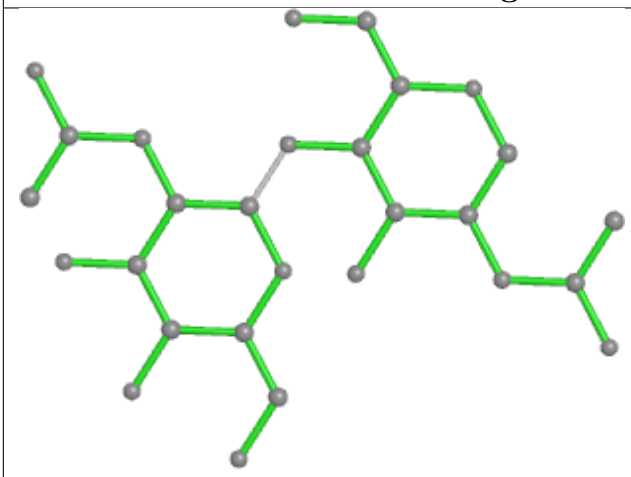


Rings

Oligosaccharide Chain f



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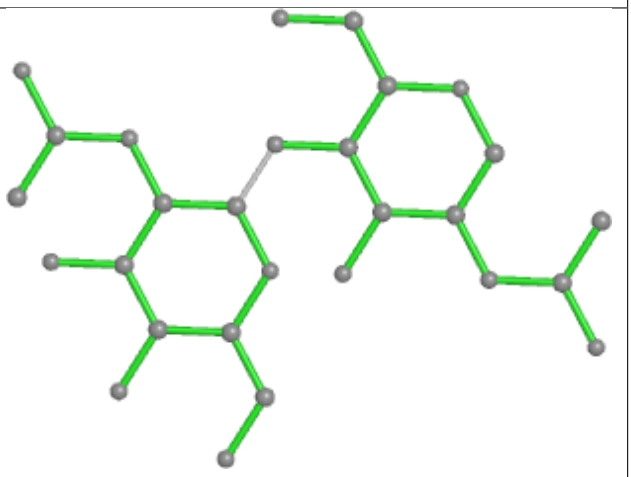

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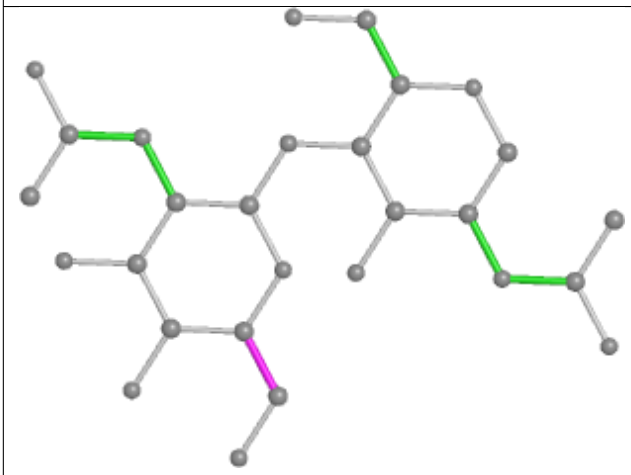

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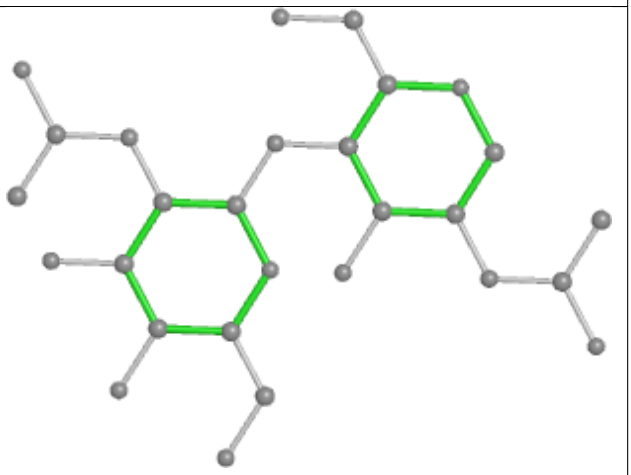
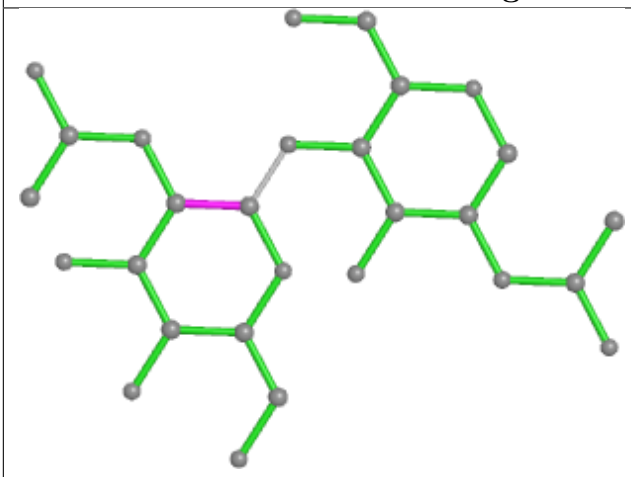


Rings

Oligosaccharide Chain j



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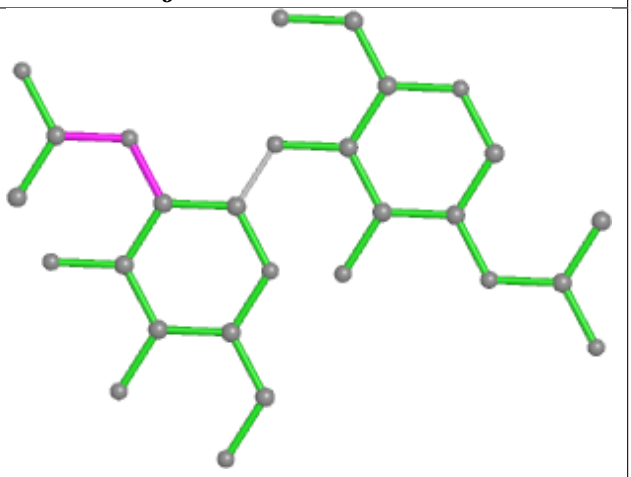

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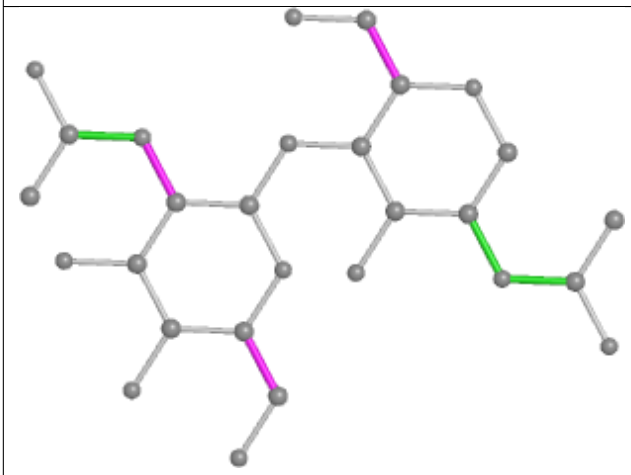

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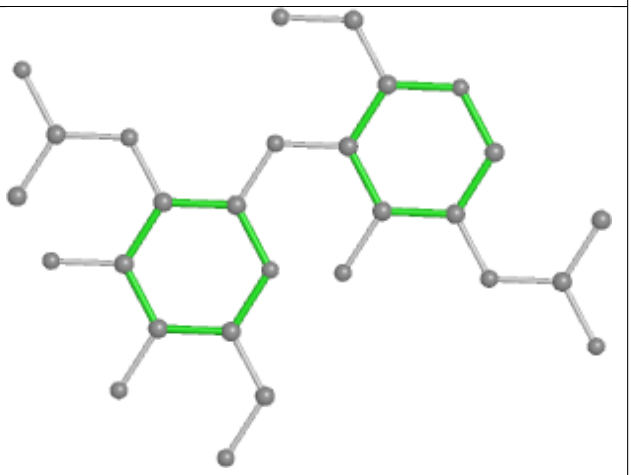
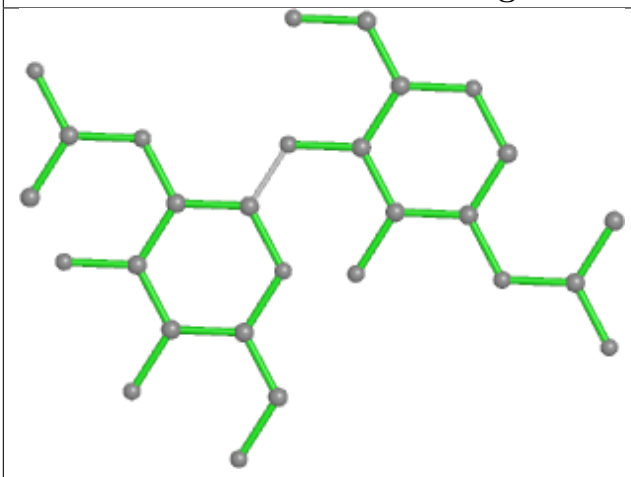


Rings

Oligosaccharide Chain k



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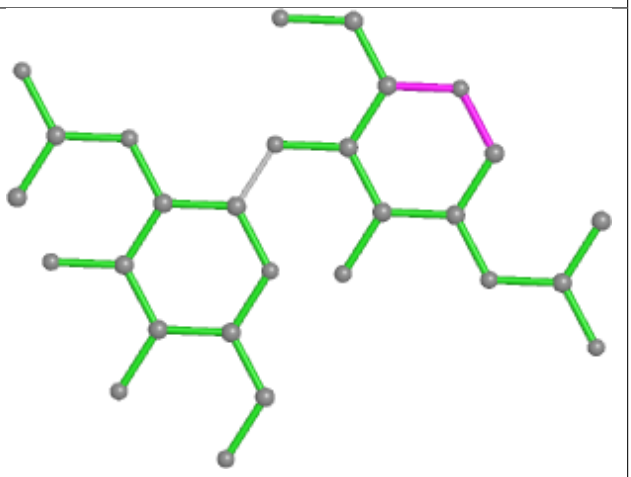

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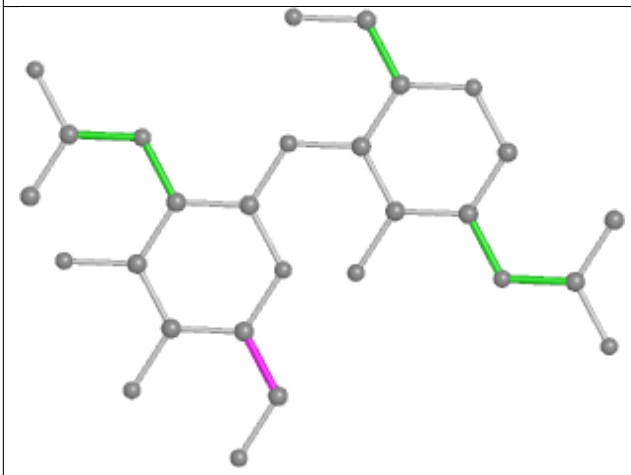

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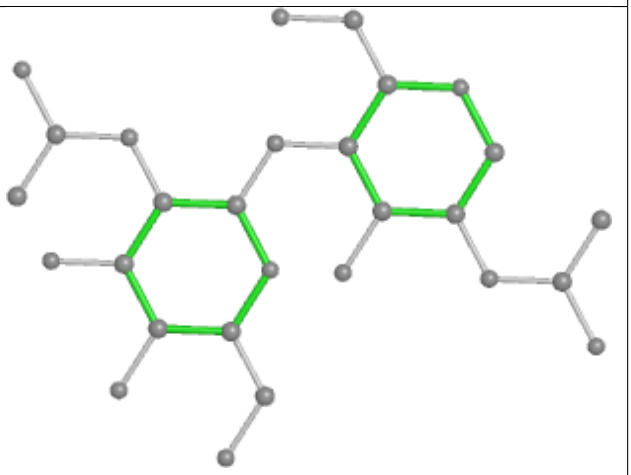
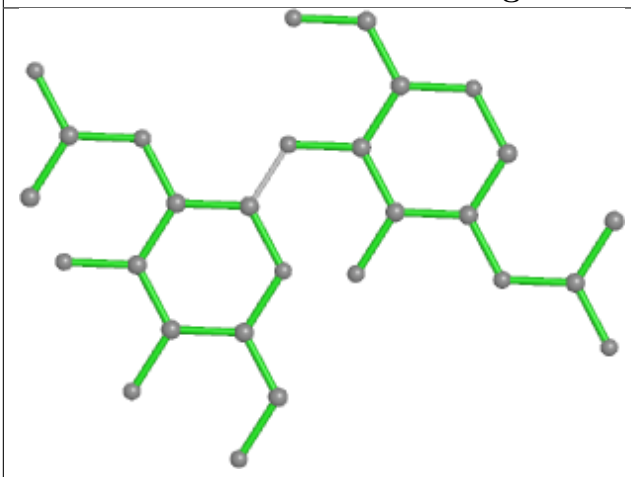


Rings

Oligosaccharide Chain l



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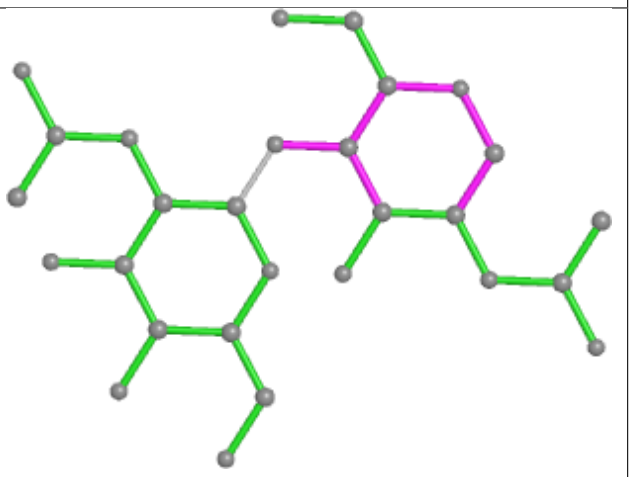

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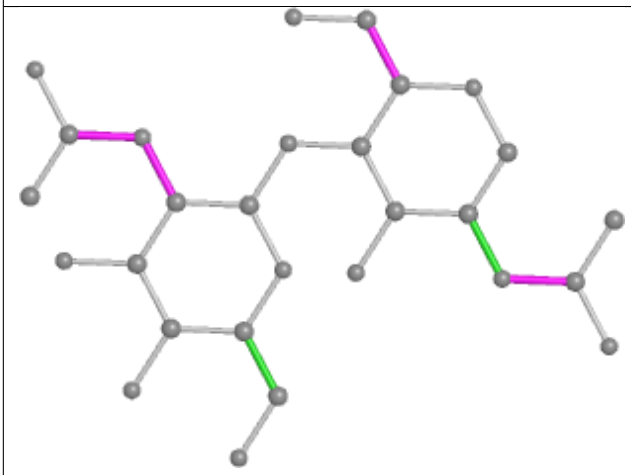

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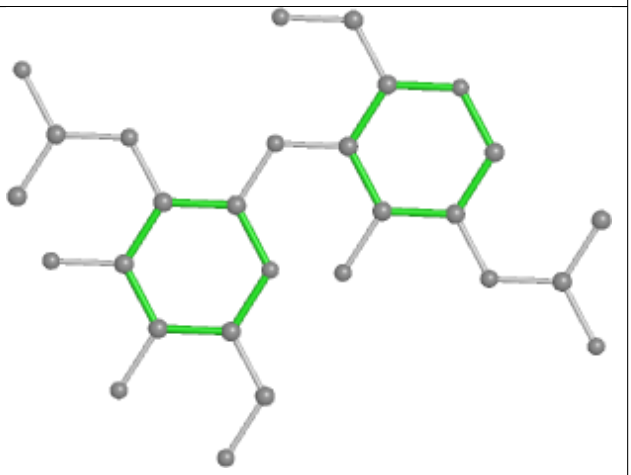
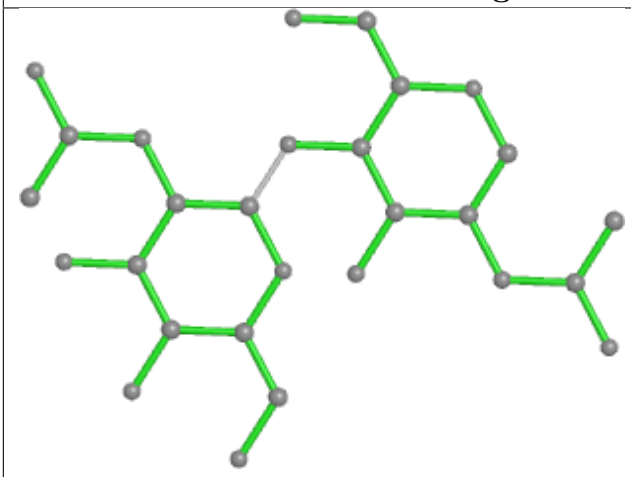


Rings

Oligosaccharide Chain m



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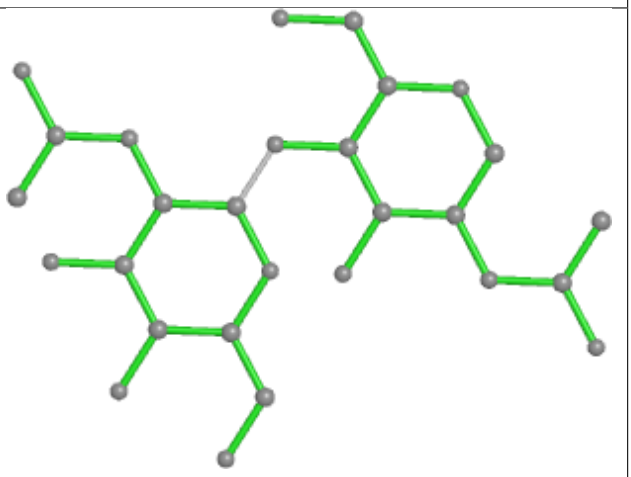

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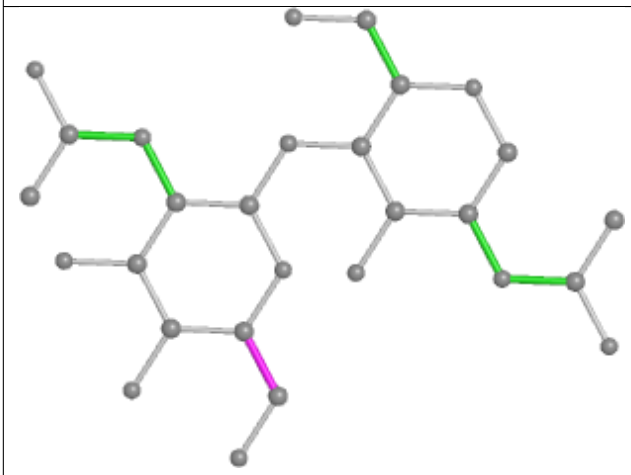

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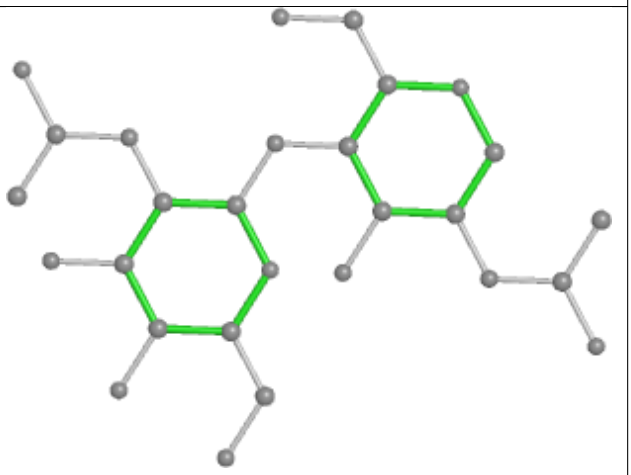
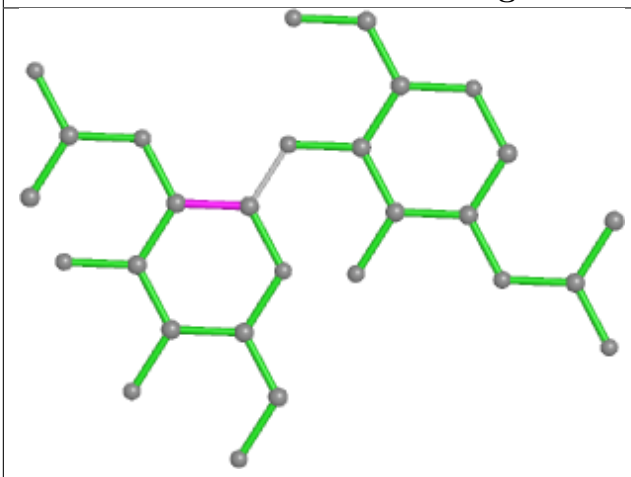


Rings

Oligosaccharide Chain q



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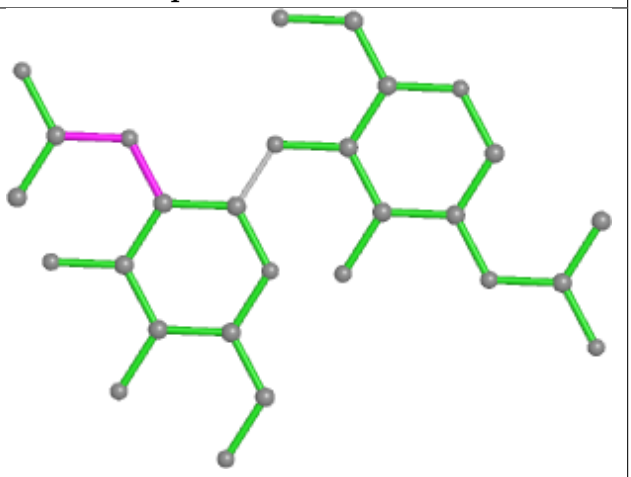
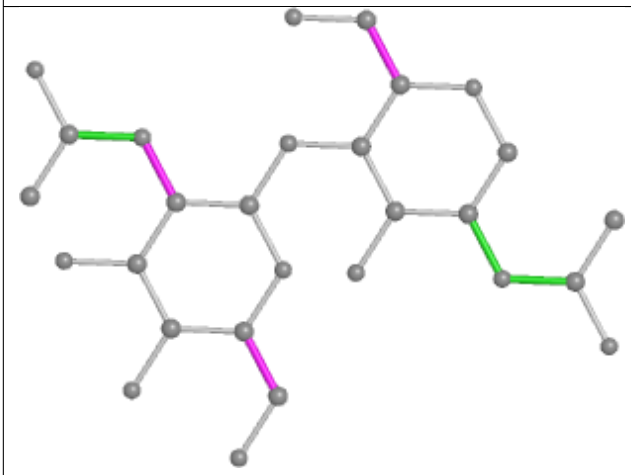


Bond angles



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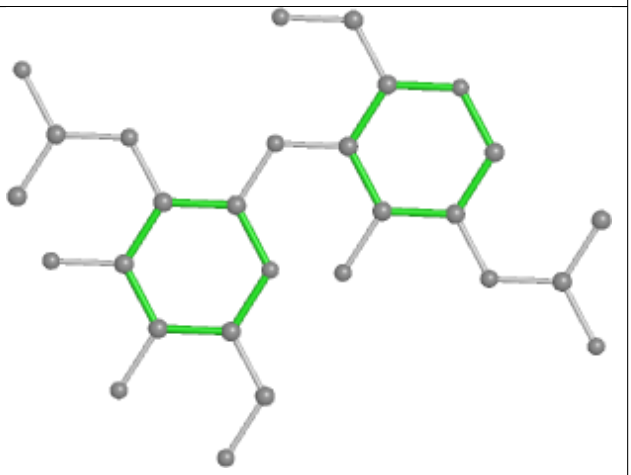
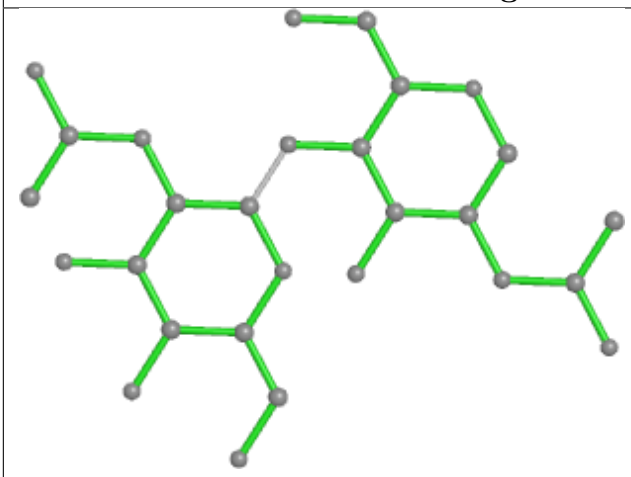


Rings

Oligosaccharide Chain r



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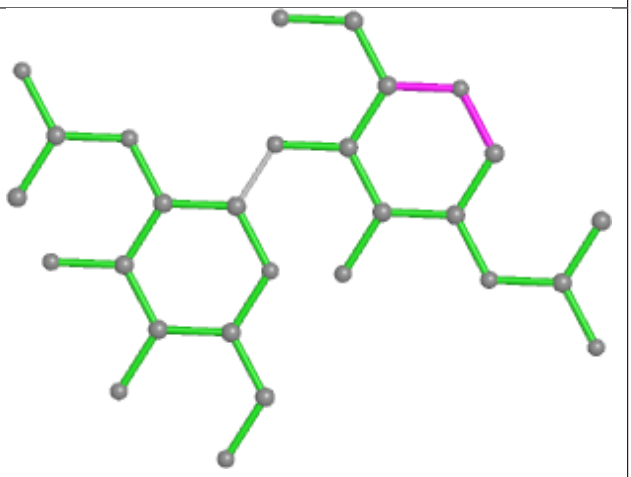

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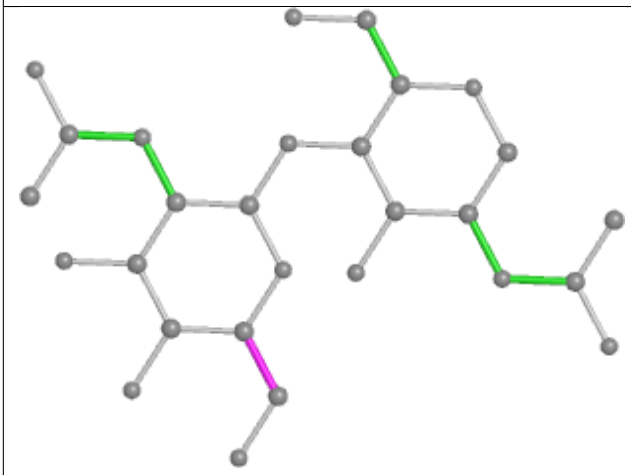

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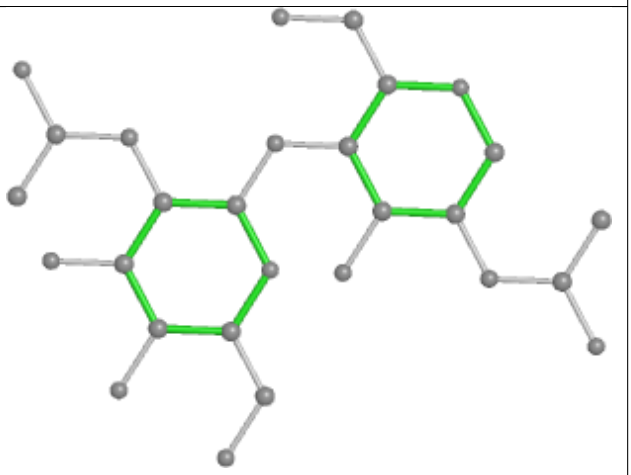
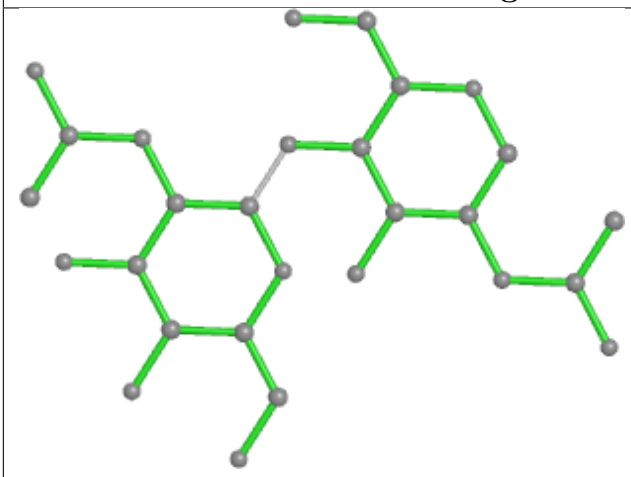
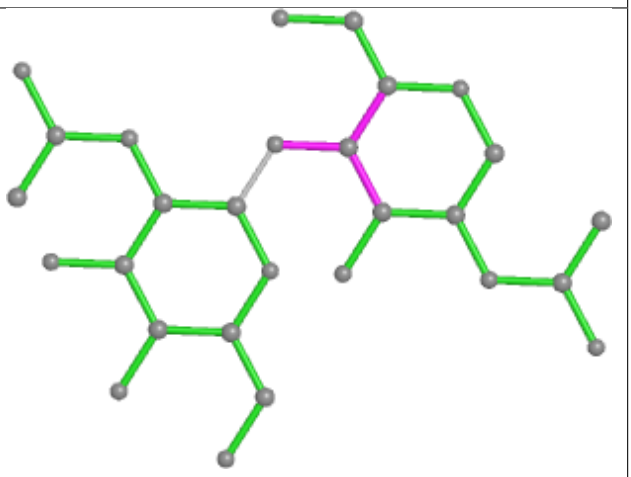
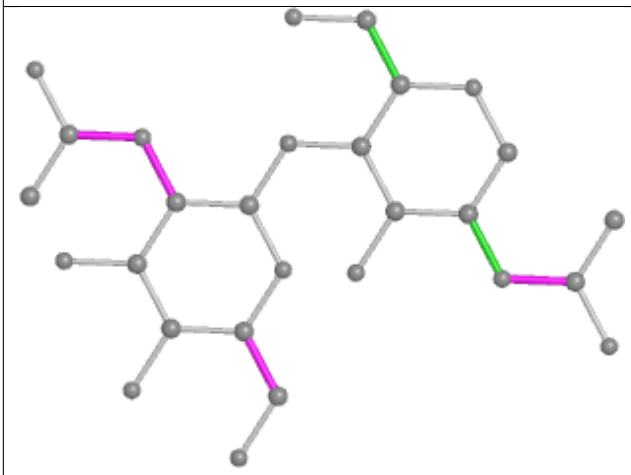
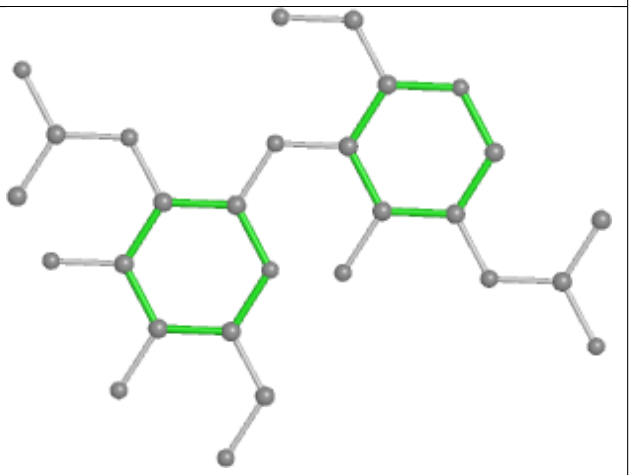
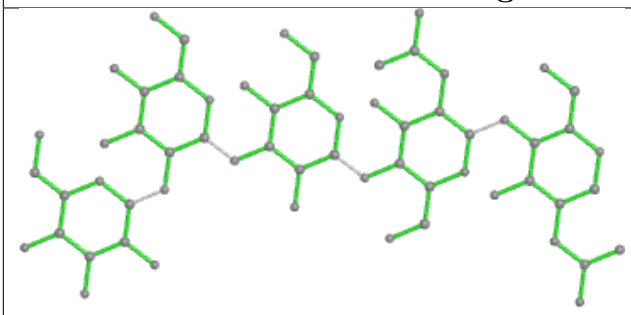


Rings

Oligosaccharide Chain s	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain Z



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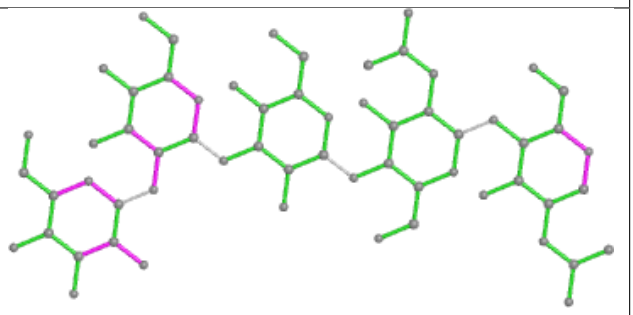
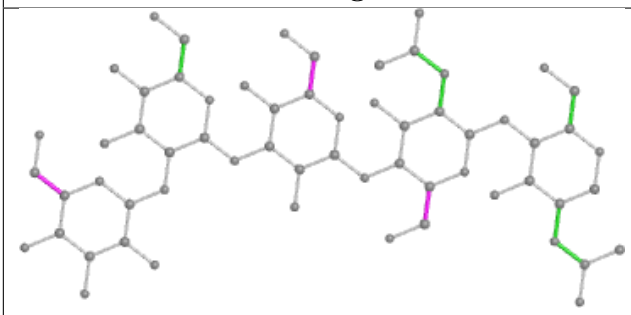
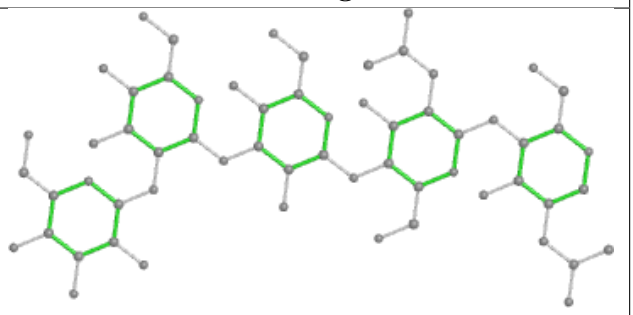


Bond angles

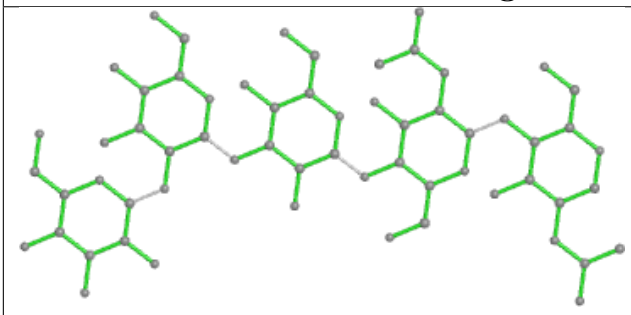


Torsions



Rings

Oligosaccharide Chain g



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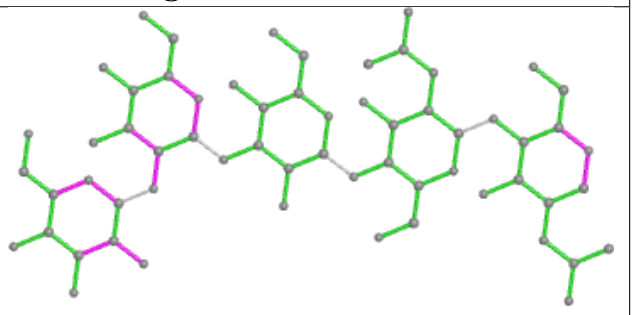
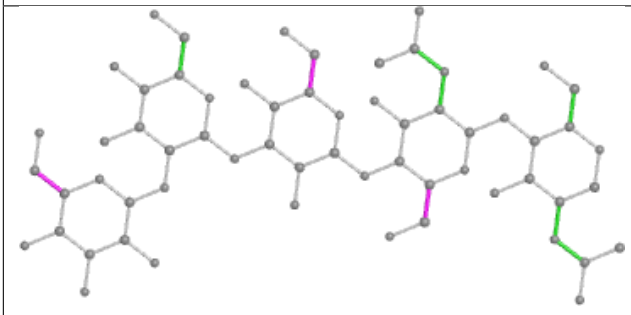


Bond angles



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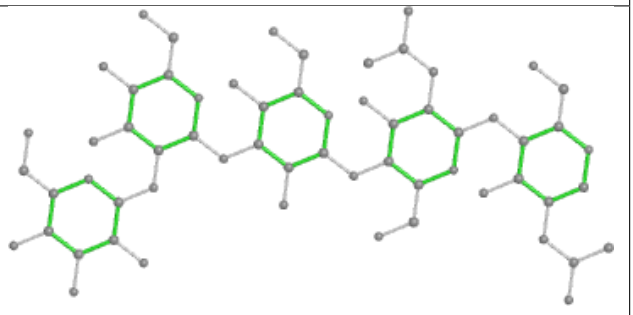
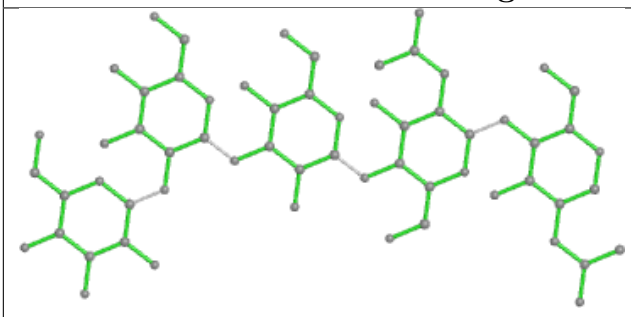


Rings

Oligosaccharide Chain n



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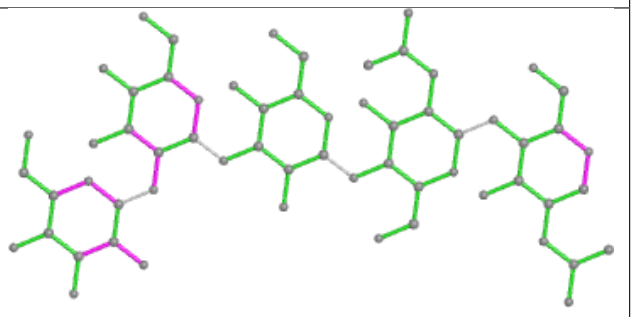
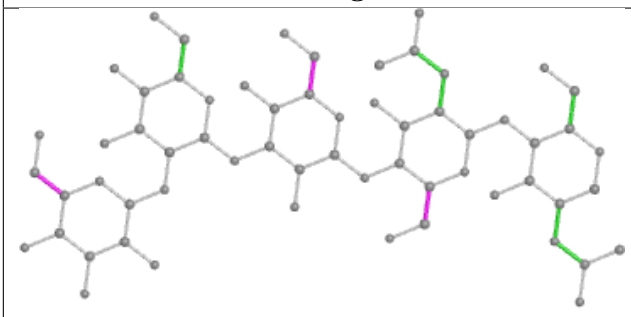


Bond angles



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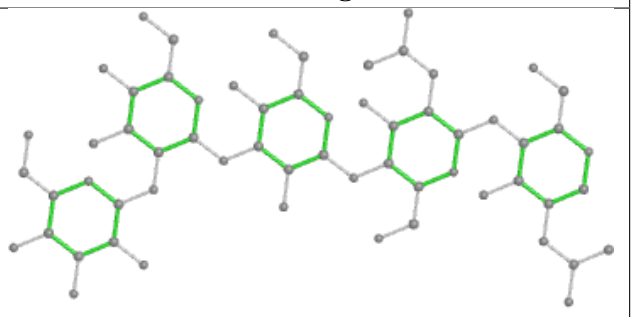
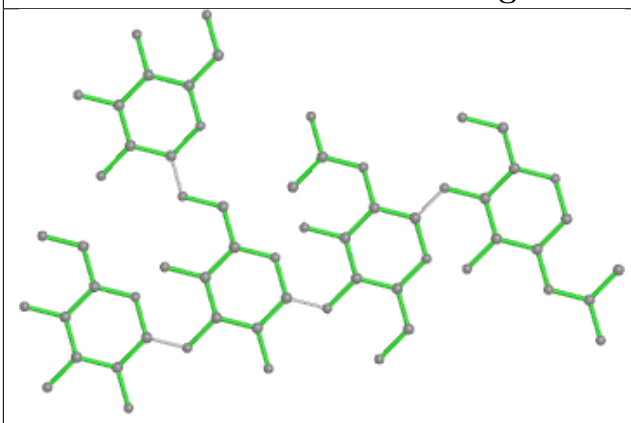
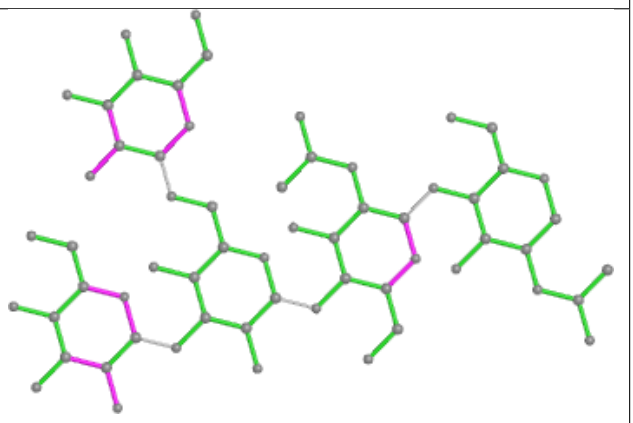


Rings

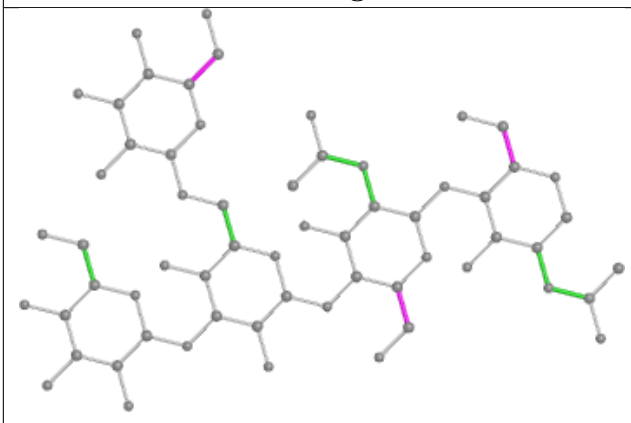
Oligosaccharide Chain a



Bond lengths



Bond angles



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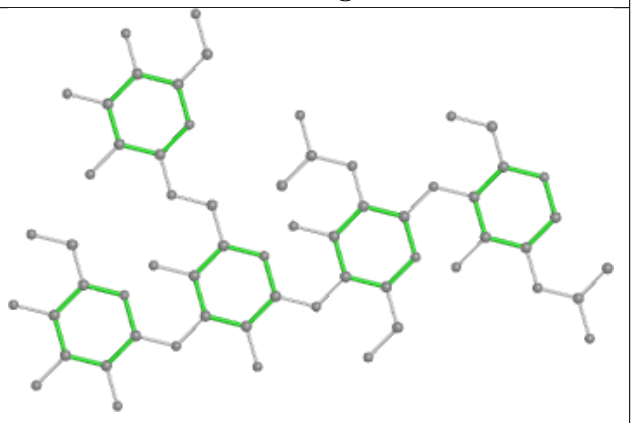
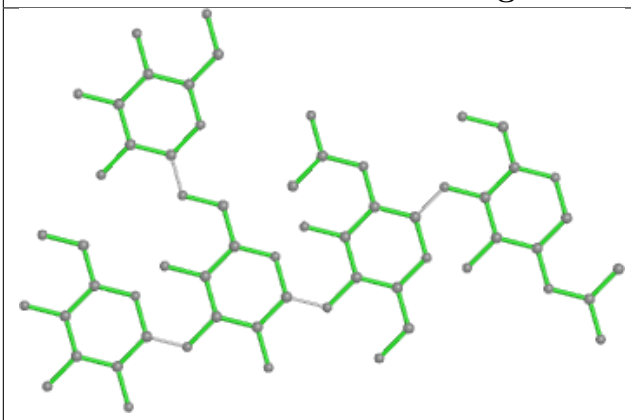
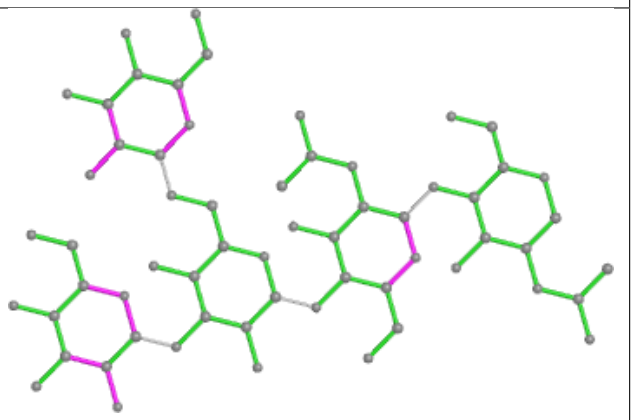


Rings

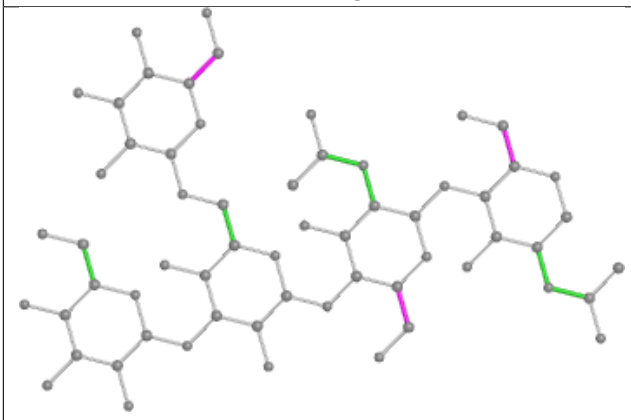
Oligosaccharide Chain h



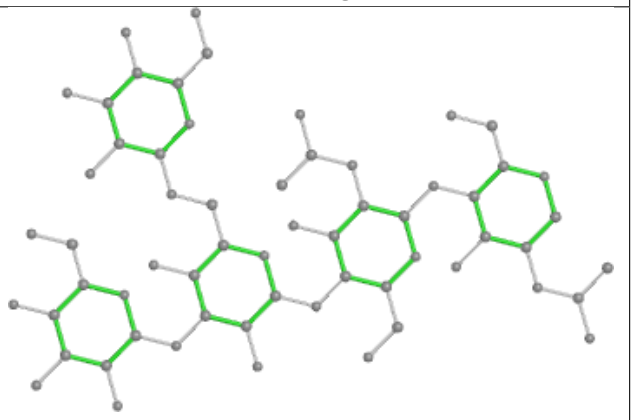
Bond lengths



Bond angles

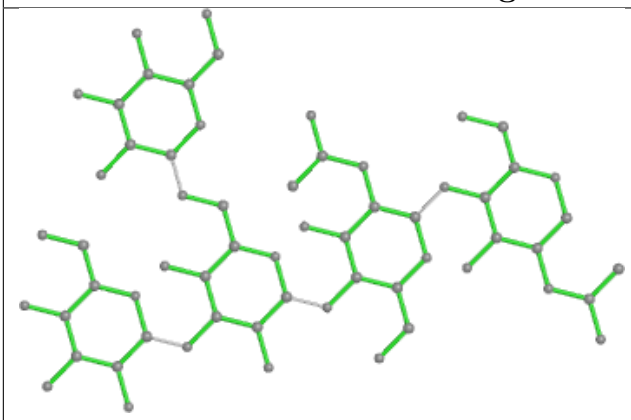


Torsions

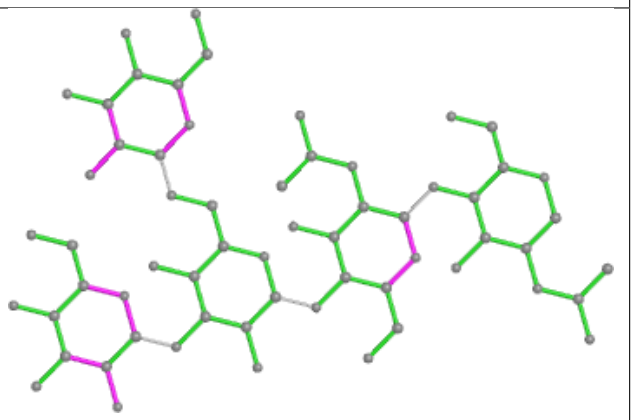


Rings

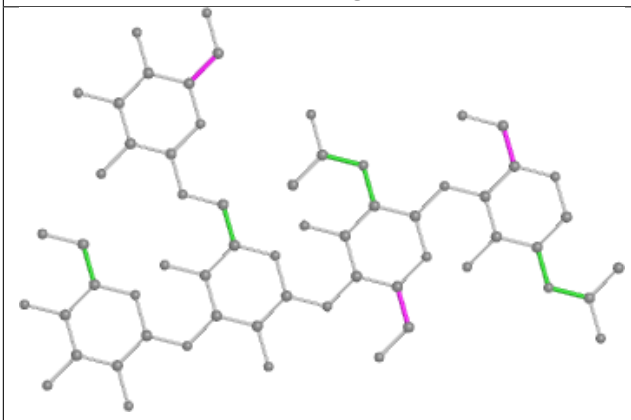
Oligosaccharide Chain o



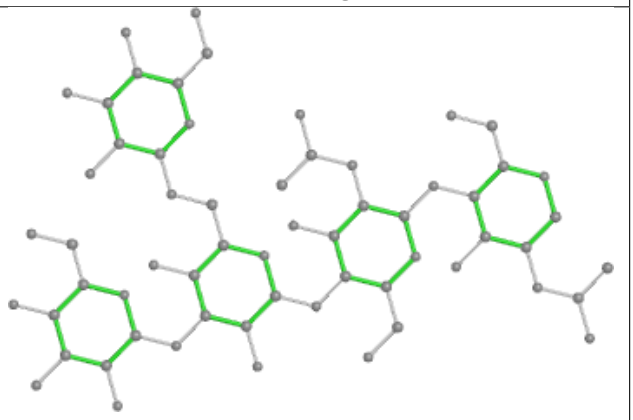
Bond lengths



Bond angles

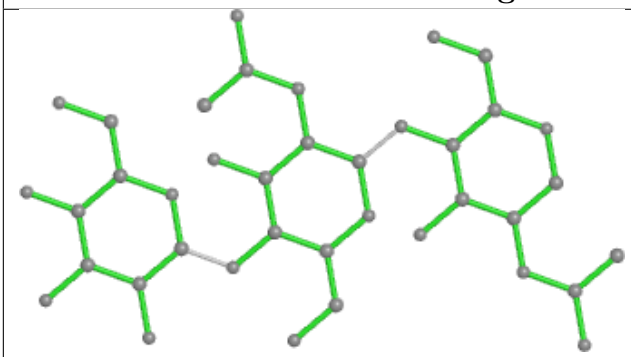


Torsions

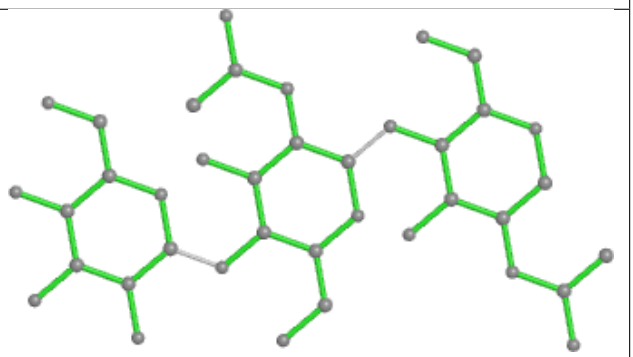


Rings

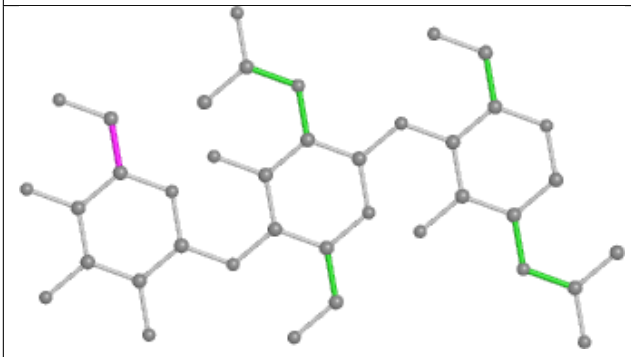
Oligosaccharide Chain b



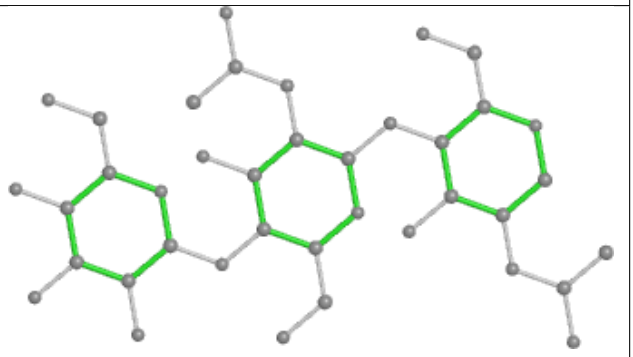
Bond lengths



Bond angles

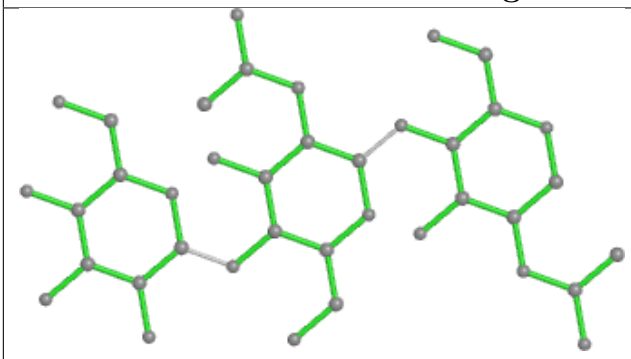


Torsions

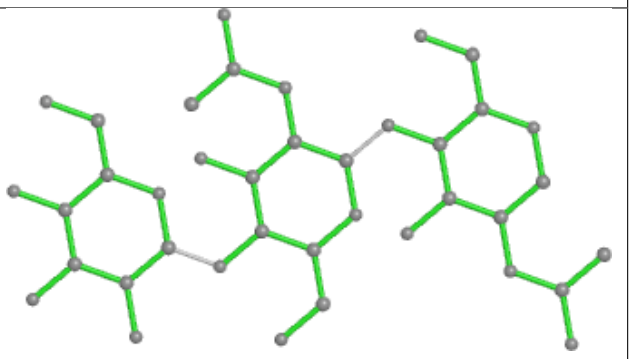


Rings

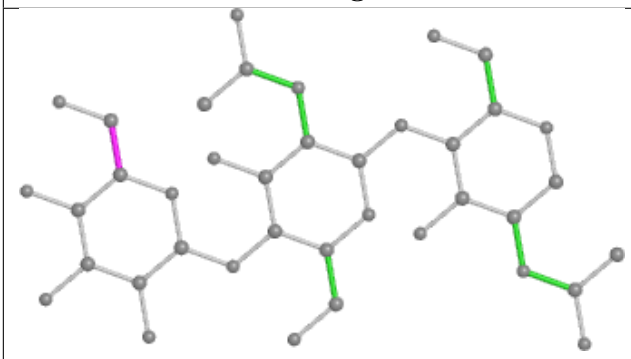
Oligosaccharide Chain i



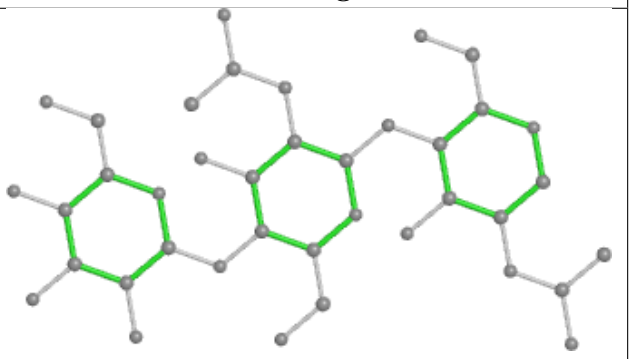
Bond lengths



Bond angles

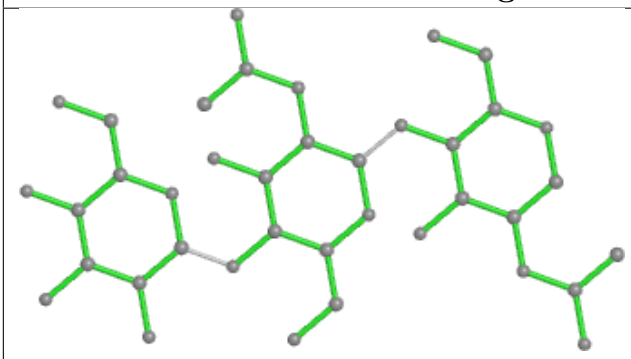


Torsions

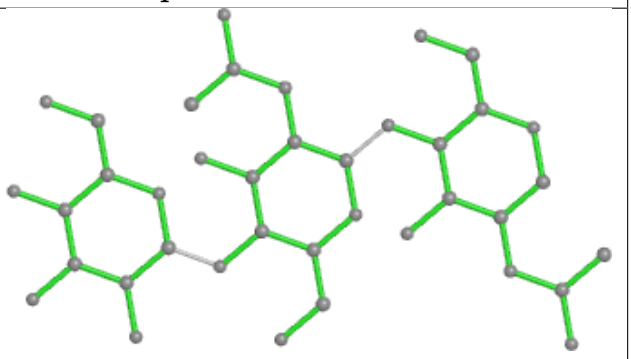


Rings

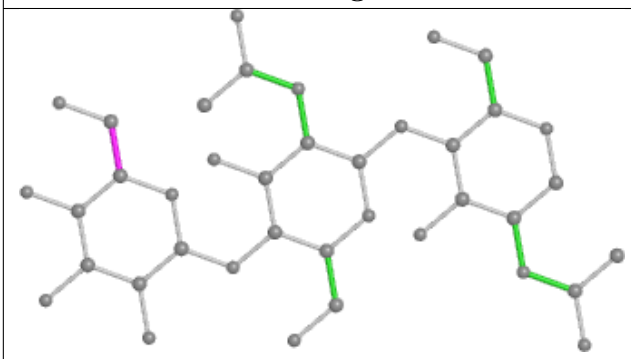
Oligosaccharide Chain p



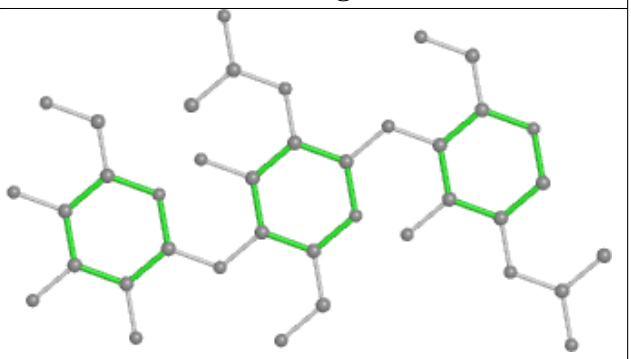
Bond lengths



Bond angles

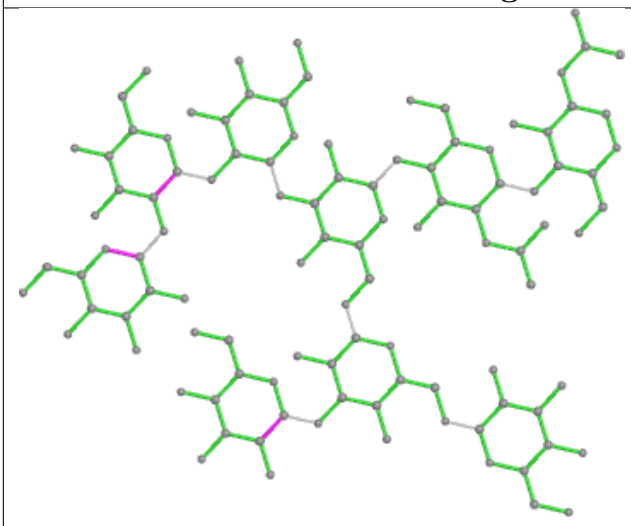


Torsions

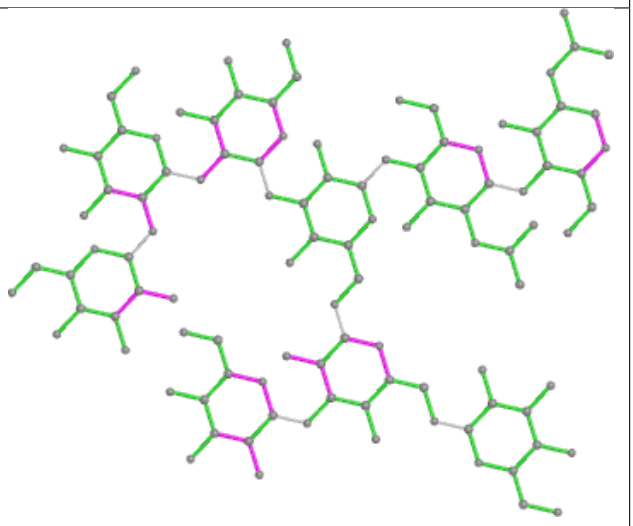


Rings

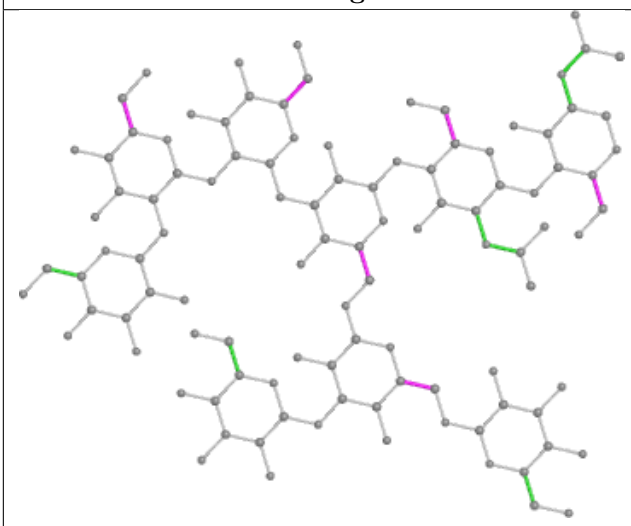
Oligosaccharide Chain t



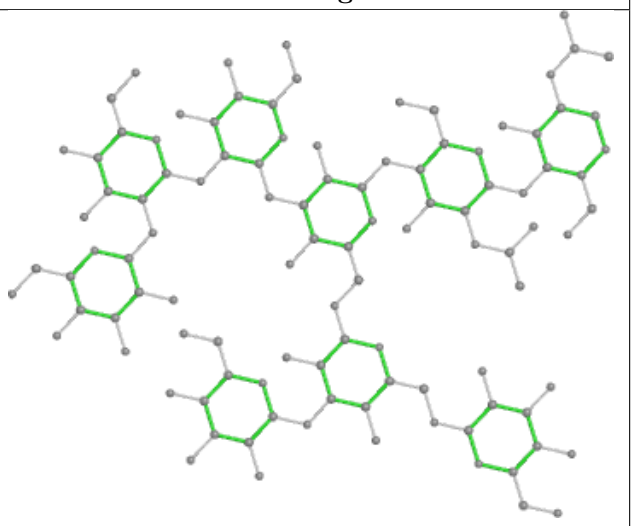
Bond lengths



Bond angles

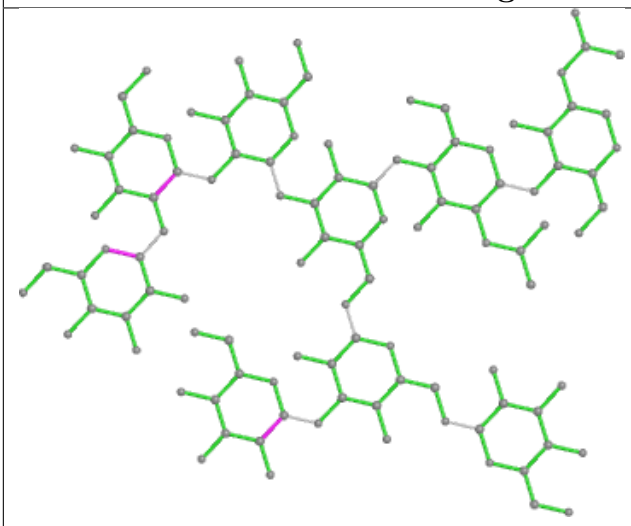


Torsions

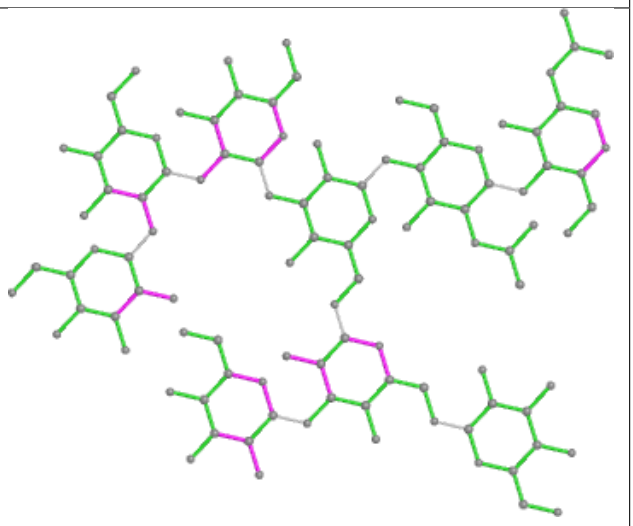


Rings

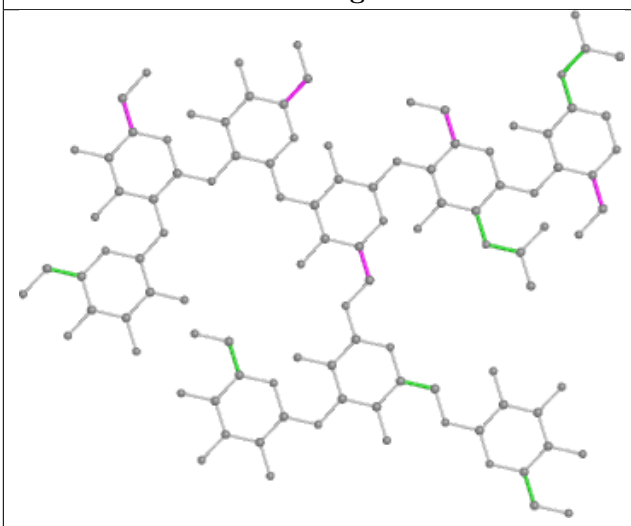
Oligosaccharide Chain u



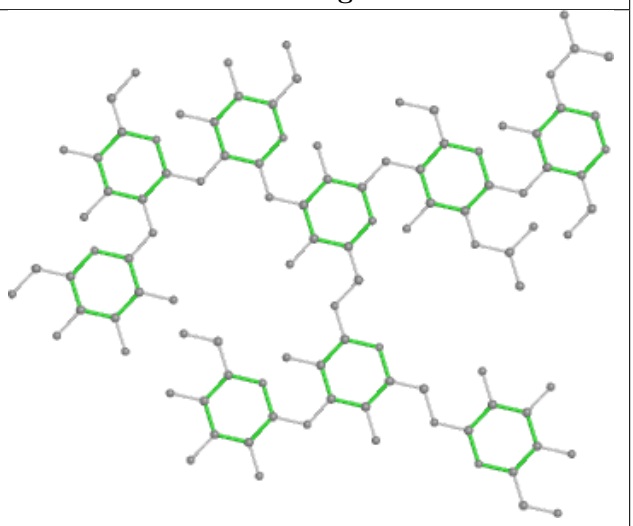
Bond lengths



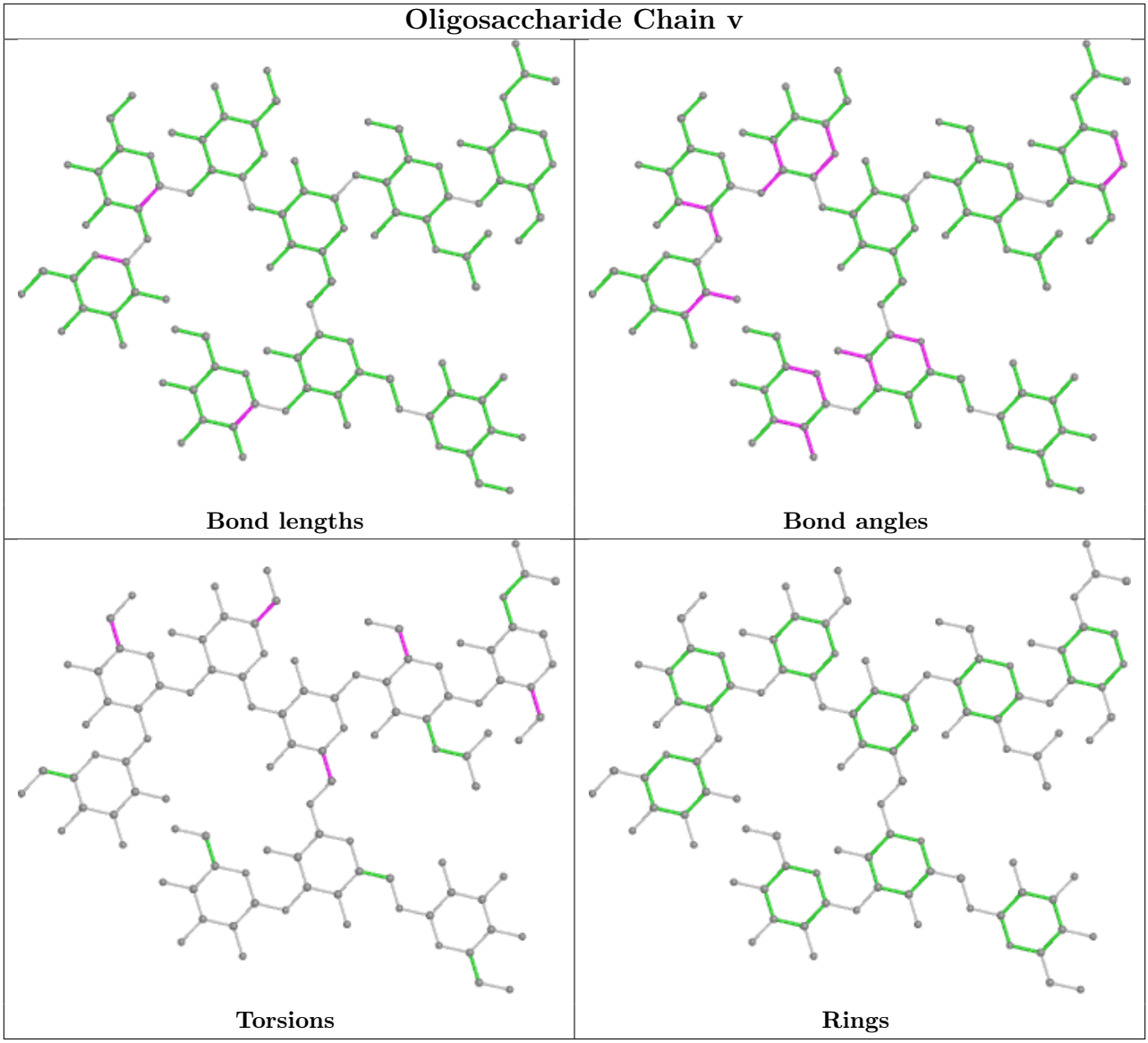
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	E	627	2	14,14,15	0.31	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	E	617	2	14,14,15	0.42	0	17,19,21	0.56	0
13	NAG	D	623	2	14,14,15	0.51	0	17,19,21	0.40	0
13	NAG	F	624	2	14,14,15	0.29	0	17,19,21	0.57	0
13	NAG	E	601	2	14,14,15	0.26	0	17,19,21	0.44	0
13	NAG	F	615	2	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
13	NAG	B	701	1	14,14,15	0.51	0	17,19,21	0.43	0
13	NAG	D	617	2	14,14,15	0.43	0	17,19,21	0.56	0
13	NAG	E	614	2	14,14,15	0.38	0	17,19,21	0.50	0
13	NAG	F	623	2	14,14,15	0.50	0	17,19,21	0.40	0
13	NAG	F	616	2	14,14,15	0.44	0	17,19,21	0.51	0
13	NAG	F	617	2	14,14,15	0.44	0	17,19,21	0.56	0
13	NAG	E	616	2	14,14,15	0.44	0	17,19,21	0.51	0
13	NAG	F	614	2	14,14,15	0.37	0	17,19,21	0.49	0
13	NAG	D	601	2	14,14,15	0.25	0	17,19,21	0.44	0
13	NAG	D	624	2	14,14,15	0.28	0	17,19,21	0.57	0
13	NAG	F	627	2	14,14,15	0.31	0	17,19,21	0.61	0
13	NAG	C	701	1	14,14,15	0.51	0	17,19,21	0.43	0
13	NAG	E	623	2	14,14,15	0.51	0	17,19,21	0.40	0
13	NAG	D	615	2	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
13	NAG	D	616	2	14,14,15	0.45	0	17,19,21	0.51	0
13	NAG	D	627	2	14,14,15	0.32	0	17,19,21	0.61	0
13	NAG	D	614	2	14,14,15	0.38	0	17,19,21	0.49	0
13	NAG	E	624	2	14,14,15	0.29	0	17,19,21	0.57	0
13	NAG	A	703	1	14,14,15	0.26	0	17,19,21	0.64	0
13	NAG	F	601	2	14,14,15	0.25	0	17,19,21	0.44	0
13	NAG	E	615	2	14,14,15	0.31	0	17,19,21	0.65	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
13	NAG	E	627	2	-	4/6/23/26	0/1/1/1
13	NAG	E	617	2	-	2/6/23/26	0/1/1/1
13	NAG	D	623	2	-	2/6/23/26	0/1/1/1
13	NAG	F	624	2	-	0/6/23/26	0/1/1/1
13	NAG	E	601	2	-	2/6/23/26	0/1/1/1
13	NAG	F	615	2	-	0/6/23/26	0/1/1/1
13	NAG	B	701	1	-	2/6/23/26	0/1/1/1
13	NAG	D	617	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	NAG	E	614	2	-	2/6/23/26	0/1/1/1
13	NAG	F	623	2	-	2/6/23/26	0/1/1/1
13	NAG	F	616	2	-	1/6/23/26	0/1/1/1
13	NAG	F	617	2	-	2/6/23/26	0/1/1/1
13	NAG	E	616	2	-	1/6/23/26	0/1/1/1
13	NAG	F	614	2	-	2/6/23/26	0/1/1/1
13	NAG	D	601	2	-	2/6/23/26	0/1/1/1
13	NAG	D	624	2	-	0/6/23/26	0/1/1/1
13	NAG	F	627	2	-	4/6/23/26	0/1/1/1
13	NAG	C	701	1	-	2/6/23/26	0/1/1/1
13	NAG	E	623	2	-	2/6/23/26	0/1/1/1
13	NAG	D	615	2	-	0/6/23/26	0/1/1/1
13	NAG	D	616	2	-	1/6/23/26	0/1/1/1
13	NAG	D	627	2	-	4/6/23/26	0/1/1/1
13	NAG	D	614	2	-	2/6/23/26	0/1/1/1
13	NAG	E	624	2	-	0/6/23/26	0/1/1/1
13	NAG	A	703	1	-	2/6/23/26	0/1/1/1
13	NAG	F	601	2	-	2/6/23/26	0/1/1/1
13	NAG	E	615	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	615	NAG	C1-O5-C5	2.09	115.02	112.19
13	F	615	NAG	C1-O5-C5	2.09	115.02	112.19
13	D	615	NAG	C1-O5-C5	2.09	115.02	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	614	NAG	C4-C5-C6-O6
13	D	627	NAG	C4-C5-C6-O6
13	E	614	NAG	C4-C5-C6-O6
13	E	627	NAG	C4-C5-C6-O6
13	F	614	NAG	C4-C5-C6-O6
13	F	627	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
13	B	701	NAG	O5-C5-C6-O6
13	C	701	NAG	O5-C5-C6-O6
13	D	601	NAG	O5-C5-C6-O6
13	E	601	NAG	O5-C5-C6-O6
13	F	601	NAG	O5-C5-C6-O6
13	B	701	NAG	C4-C5-C6-O6
13	C	701	NAG	C4-C5-C6-O6
13	D	614	NAG	O5-C5-C6-O6
13	D	627	NAG	O5-C5-C6-O6
13	E	614	NAG	O5-C5-C6-O6
13	E	627	NAG	O5-C5-C6-O6
13	F	614	NAG	O5-C5-C6-O6
13	F	627	NAG	O5-C5-C6-O6
13	D	601	NAG	C4-C5-C6-O6
13	E	601	NAG	C4-C5-C6-O6
13	F	601	NAG	C4-C5-C6-O6
13	D	627	NAG	C8-C7-N2-C2
13	D	627	NAG	O7-C7-N2-C2
13	E	627	NAG	C8-C7-N2-C2
13	E	627	NAG	O7-C7-N2-C2
13	F	627	NAG	C8-C7-N2-C2
13	F	627	NAG	O7-C7-N2-C2
13	D	617	NAG	O5-C5-C6-O6
13	E	617	NAG	O5-C5-C6-O6
13	F	617	NAG	O5-C5-C6-O6
13	D	617	NAG	C4-C5-C6-O6
13	E	617	NAG	C4-C5-C6-O6
13	F	617	NAG	C4-C5-C6-O6
13	D	623	NAG	C4-C5-C6-O6
13	E	623	NAG	C4-C5-C6-O6
13	F	623	NAG	C4-C5-C6-O6
13	A	703	NAG	C1-C2-N2-C7
13	D	623	NAG	O5-C5-C6-O6
13	E	623	NAG	O5-C5-C6-O6
13	F	623	NAG	O5-C5-C6-O6
13	D	616	NAG	C4-C5-C6-O6
13	E	616	NAG	C4-C5-C6-O6
13	F	616	NAG	C4-C5-C6-O6
13	A	703	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	601	NAG	1	0
13	D	601	NAG	1	0
13	F	601	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

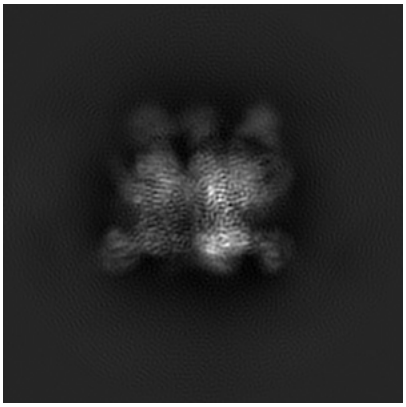
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9038. These allow visual inspection of the internal detail of the map and identification of artifacts.

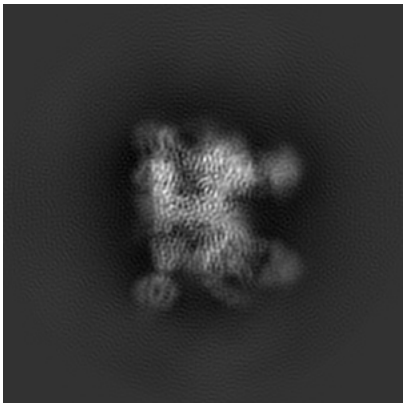
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

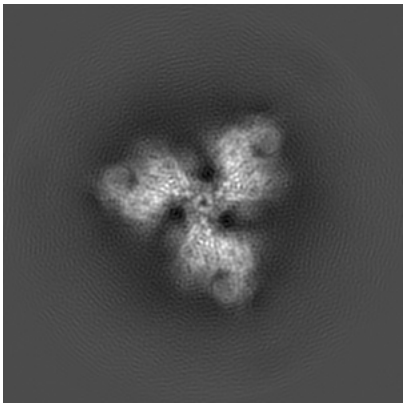
6.1.1 Primary map



X



Y

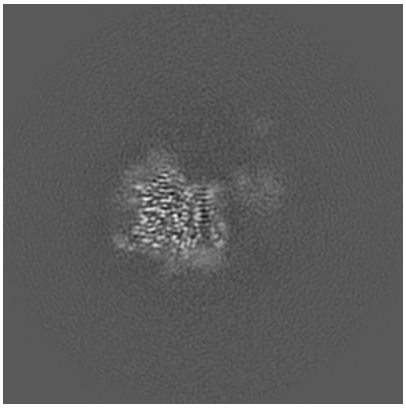


Z

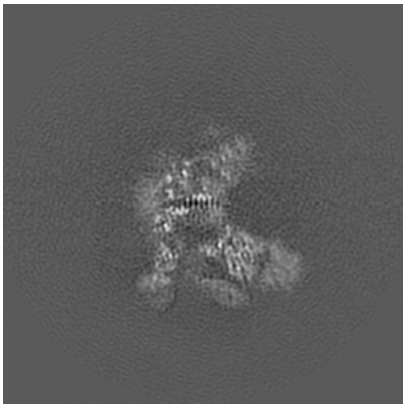
The images above show the map projected in three orthogonal directions.

6.2 Central slices

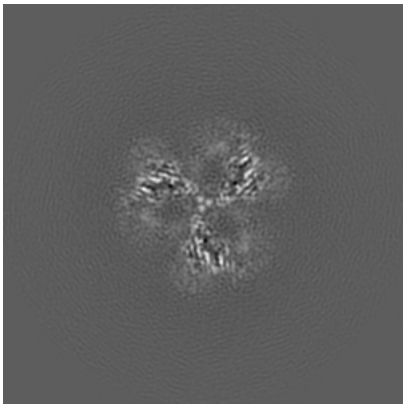
6.2.1 Primary map



X Index: 144



Y Index: 144

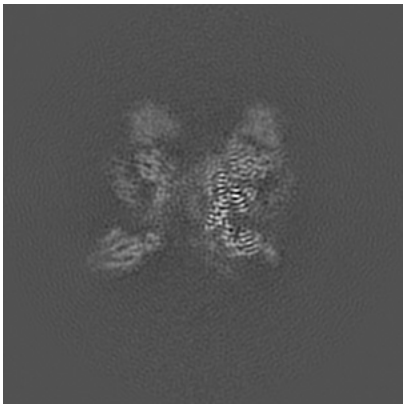


Z Index: 144

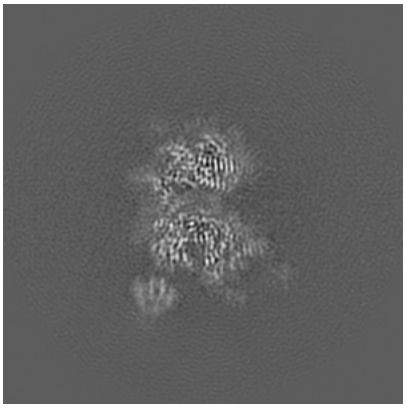
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

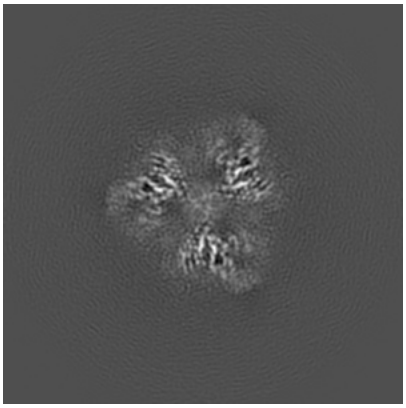
6.3.1 Primary map



X Index: 169



Y Index: 157



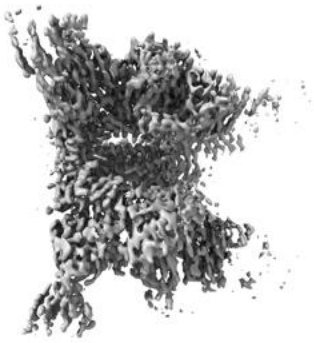
Z Index: 153

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.041. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

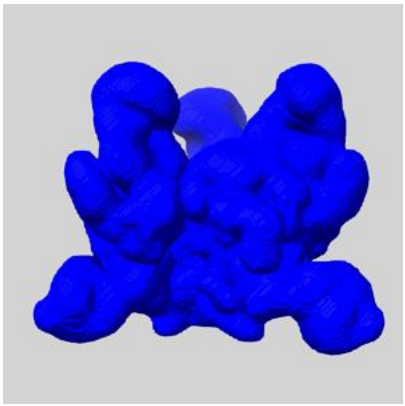
6.5 Mask visualisation

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

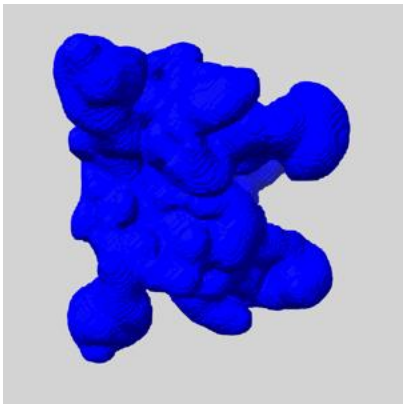
A mask typically either:

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

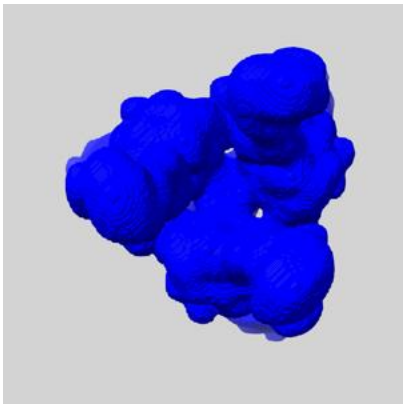
6.5.1 emd_9038_msk_1.map



X

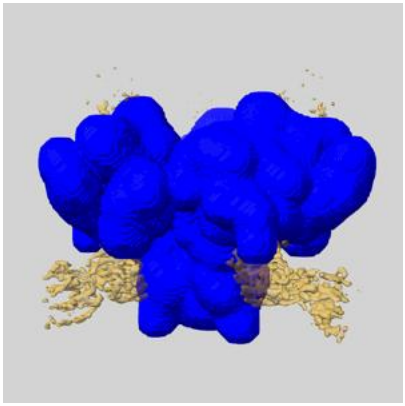


Y

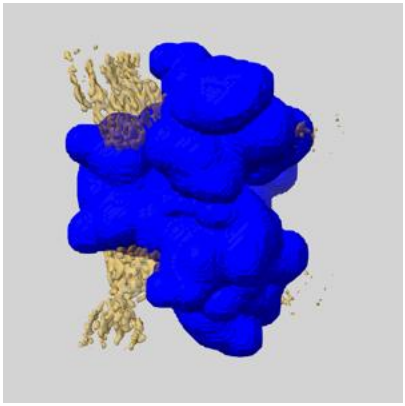


Z

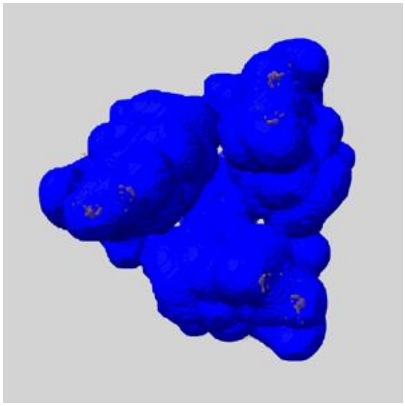
6.5.2 emd_9038_msk_2.map



X



Y

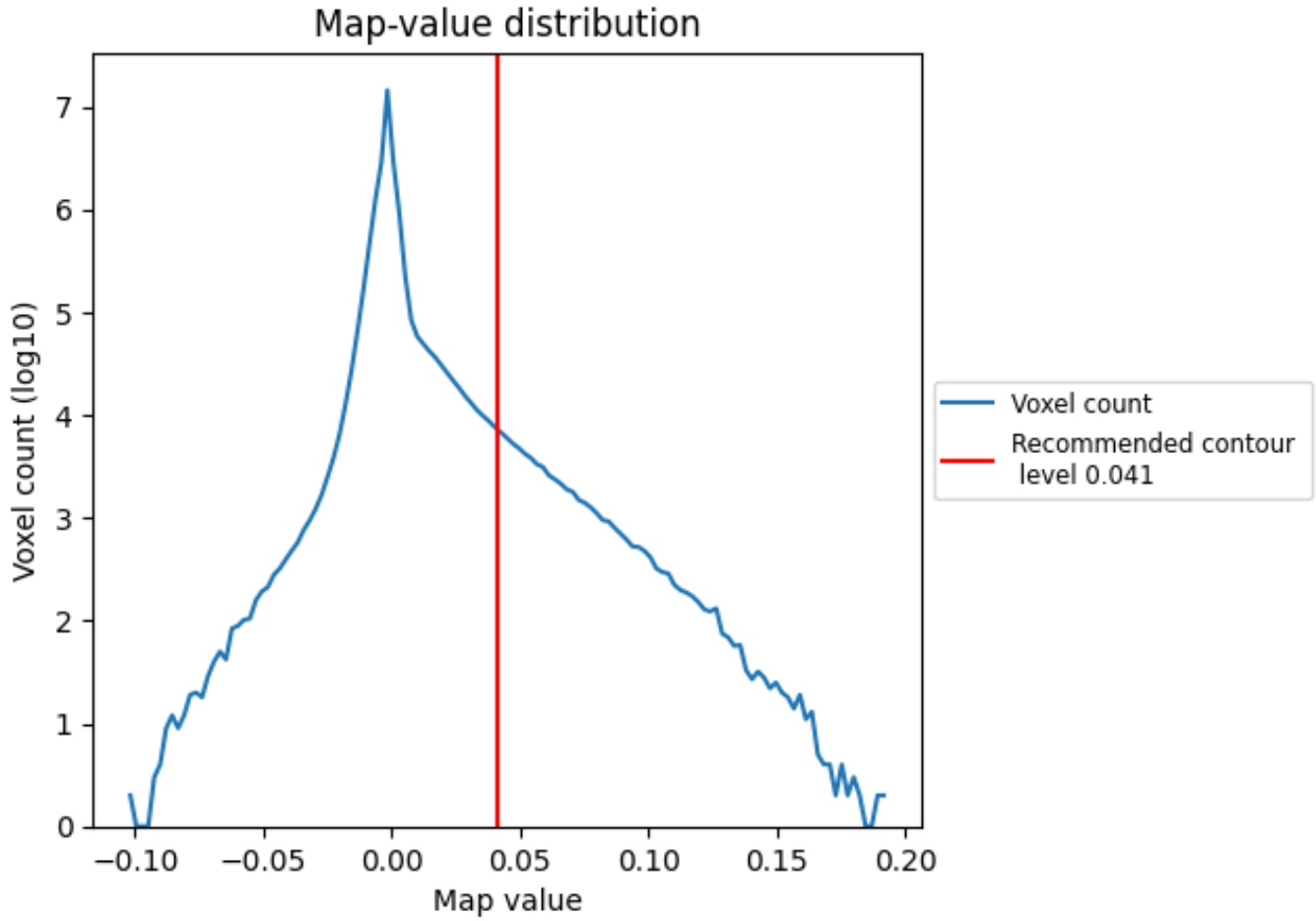


Z

7 Map analysis

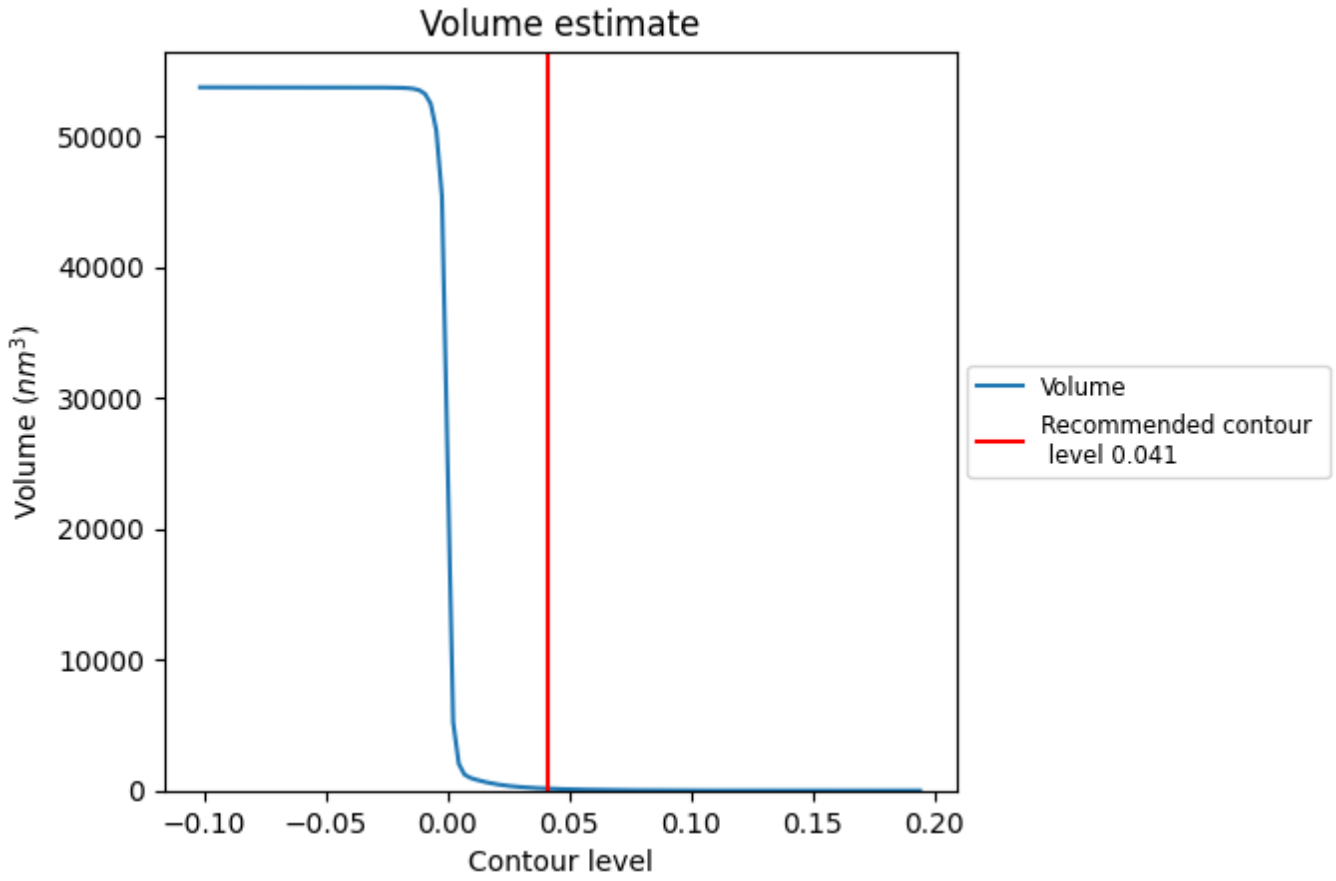
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

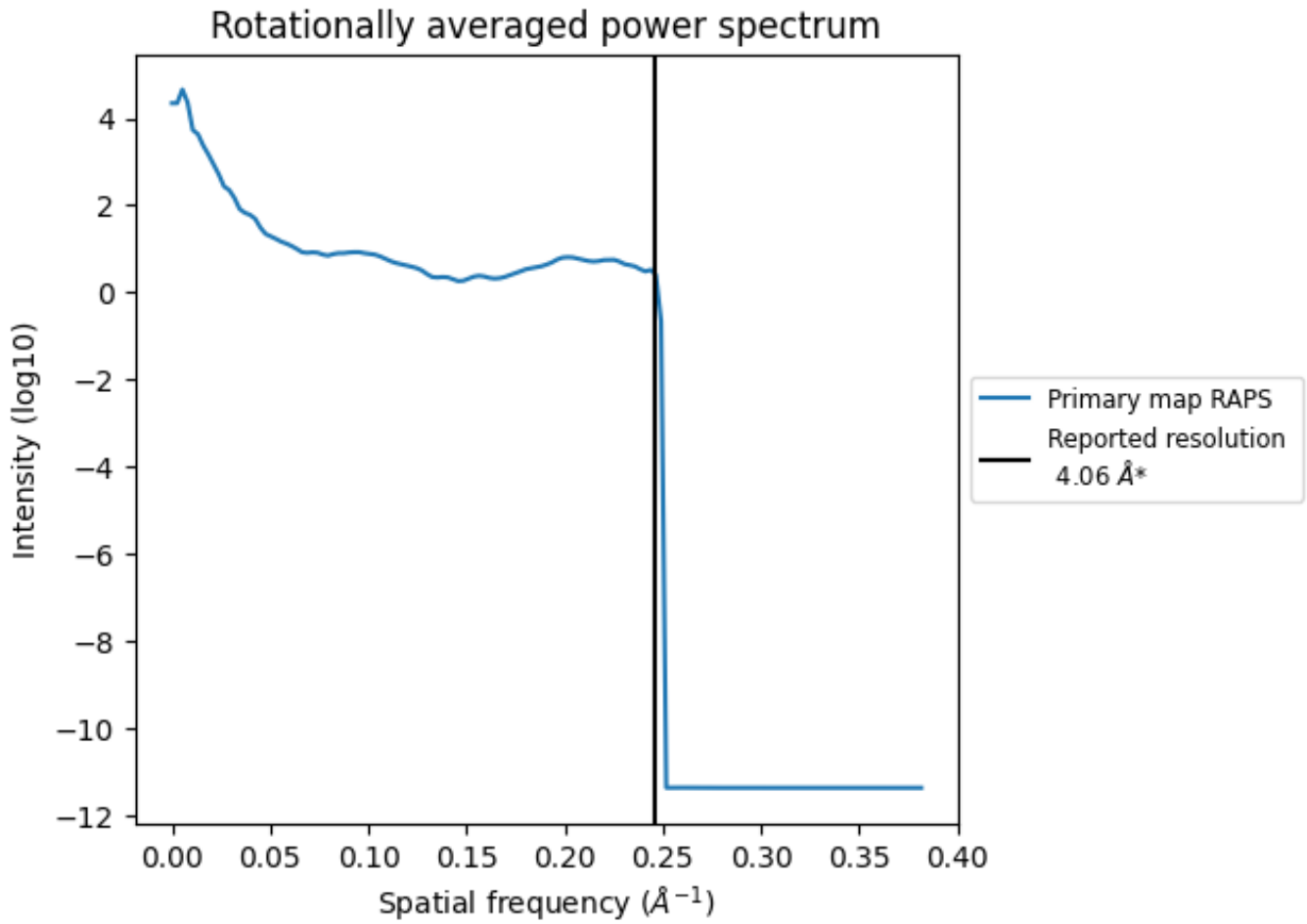
7.2 Volume estimate



The volume at the recommended contour level is 152 nm^3; this corresponds to an approximate mass of 138 kDa.

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

7.3 Rotationally averaged power spectrum (i)

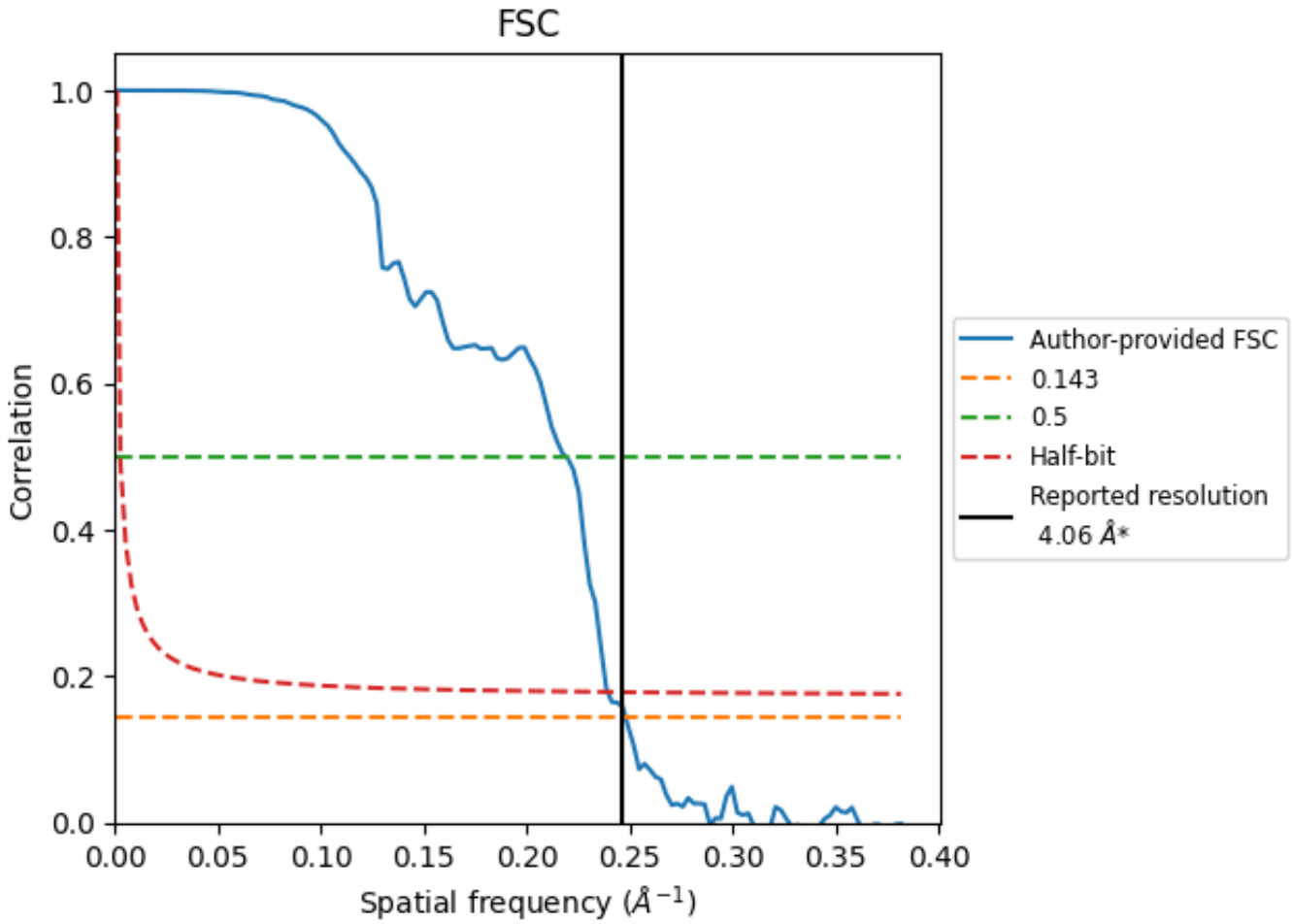


*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.246 Å^{-1}

8.2 Resolution estimates (i)

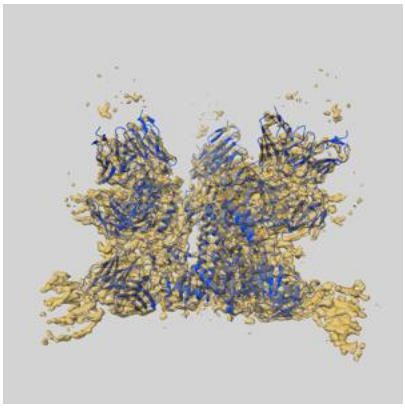
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.06	-	-
Author-provided FSC curve	4.03	4.57	4.18
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

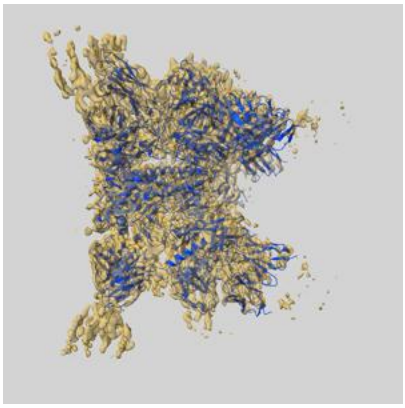
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9038 and PDB model 6EDU. Per-residue inclusion information can be found in section 3 on page 14.

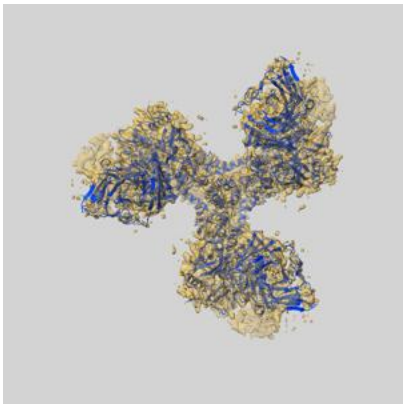
9.1 Map-model overlay



X



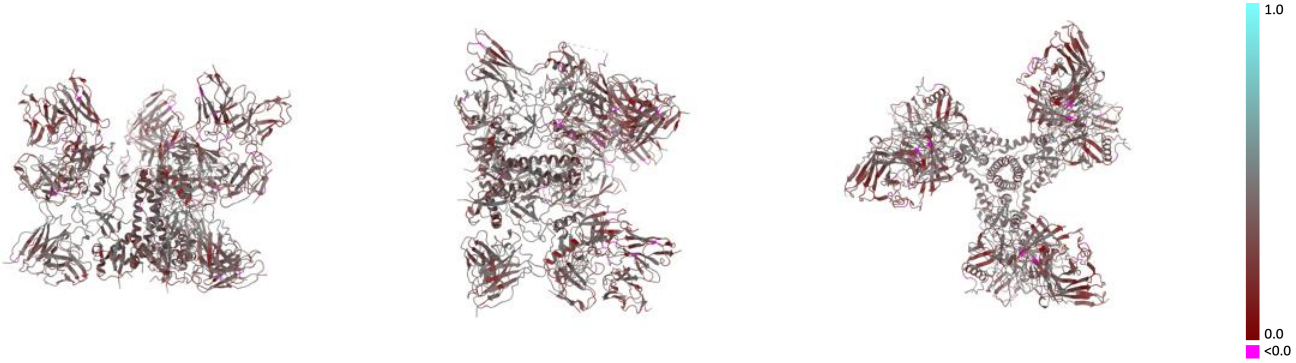
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.041 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

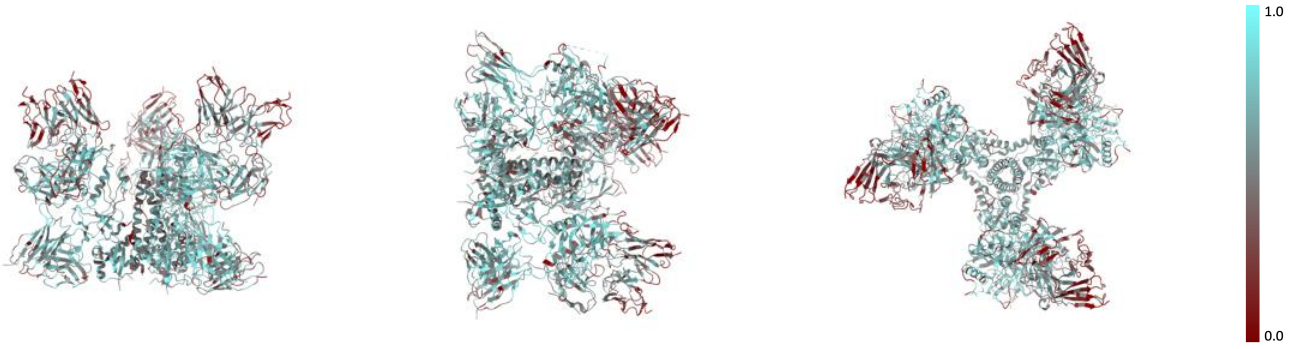
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

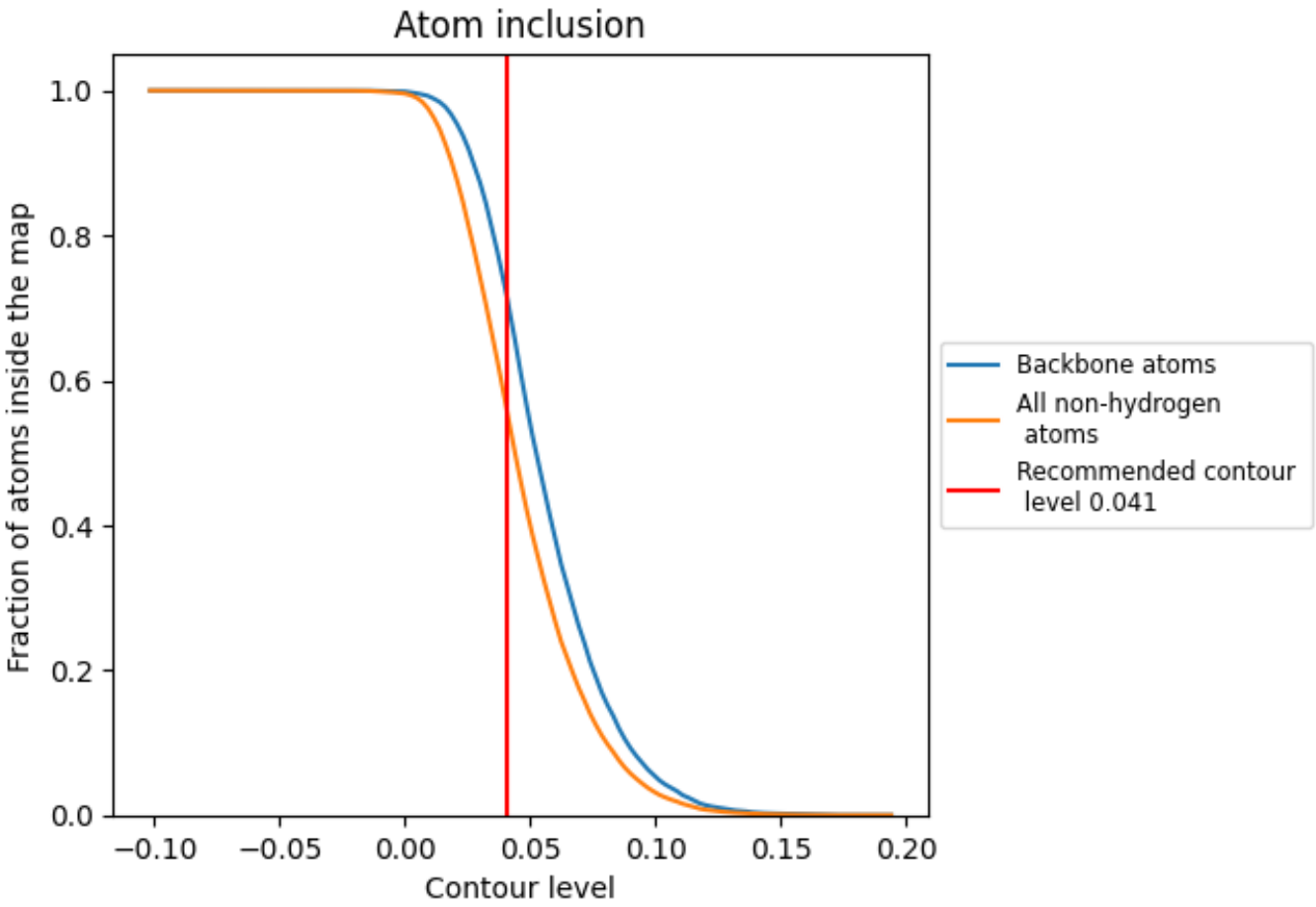
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.041).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.041) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5530	0.3600
A	0.5991	0.3560
B	0.5832	0.3420
C	0.5946	0.3550
D	0.5927	0.3650
E	0.5960	0.3650
F	0.5950	0.3620
G	0.6018	0.4000
H	0.6123	0.4030
I	0.6149	0.4040
J	0.4055	0.3030
K	0.3586	0.3190
L	0.4045	0.3000
M	0.3826	0.3230
N	0.4162	0.3060
O	0.3674	0.3160
P	0.6289	0.3790
Q	0.5967	0.3890
R	0.6229	0.3870
S	0.5967	0.3900
T	0.6279	0.3890
U	0.5841	0.3830
V	0.4286	0.3140
W	0.4286	0.3080
X	0.4286	0.3270
Y	0.2500	0.3640
Z	0.3115	0.3200
a	0.5246	0.4100
b	0.5641	0.3790
c	0.5357	0.3710
d	0.2857	0.2420
e	0.5714	0.3120
f	0.2500	0.3960
g	0.2459	0.3030
h	0.5410	0.4170

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Chain	Atom inclusion	Q-score
i	0.5385	0.3850
j	0.5357	0.3640
k	0.2857	0.2060
l	0.6429	0.3020
m	0.2500	0.3740
n	0.2623	0.3090
o	0.5902	0.3970
p	0.5128	0.4020
q	0.5357	0.3660
r	0.2500	0.1720
s	0.6429	0.2760
t	0.5810	0.4290
u	0.6476	0.4360
v	0.6286	0.4310