Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 06:27 pm GMT

PDB ID	:	8AS0
Title	:	PD-1 extracellular domain in complex with Fab fragment from D12 antibody
Authors	:	Ongaro, T.; Scietti, L.; Pluss, L.; Peissert, F.; Villa, A.; Puca, E.; De Luca, R.; Neri, D.; Forneris, F.
Deposited on	:	2022-08-17
Resolution	:	3.50 Å(reported)

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

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

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

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

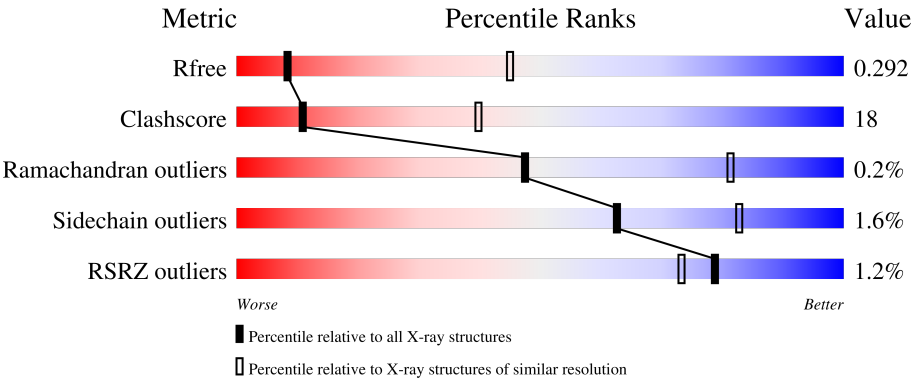
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	C	214	71% 26% .
1	D	214	69% 29% .
1	G	214	73% 25% .
1	J	214	73% 25% .
1	M	214	73% 25% .

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Mol	Chain	Length	Quality of chain
1	P	214	2% 72% 27%
1	S	214	73% 25%
1	V	214	4% 73% 26%
2	B	225	67% 27% 5%
2	E	225	65% 28% 5%
2	H	225	67% 24% 7%
2	K	225	64% 28% 6%
2	N	225	66% 25% 7%
2	Q	225	3% 69% 22% 7%
2	T	225	3% 62% 30% 6%
2	W	225	2% 64% 25% 8%
3	A	168	% 36% 29% 34%
3	F	168	% 43% 26% 30%
3	I	168	% 42% 25% 33%
3	L	168	% 40% 26% 33%
3	O	168	2% 43% 27% 30%
3	R	168	% 40% 24% 35%
3	X	168	2% 36% 32% 30%
3	Y	168	5% 44% 26% 30%
4	U	4	100%
5	Z	4	50% 50%
5	g	4	100%
5	h	4	75% 25%
5	k	4	75% 25%
6	a	3	100%

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Mol	Chain	Length	Quality of chain
6	e	3	100%
6	j	3	100%
7	b	2	100%
8	c	4	100%
9	d	2	50% 50%
9	i	2	50% 50%
10	f	6	83% 17%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MAN	f	4	-	-	-	X
11	NAG	F	207	-	-	-	X
11	NAG	Y	206	-	-	-	X
4	NAG	U	2	-	-	-	X
9	FUC	d	2	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 33524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called D12 antibody light chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	D	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	G	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	J	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	M	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	P	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	V	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			
1	S	213	Total	C	N	O	S	0	0	0
			1634	1023	272	334	5			

- Molecule 2 is a protein called D12 antibody heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1593	1007	265	314	7			
2	E	214	Total	C	N	O	S	0	0	0
			1593	1007	265	314	7			
2	H	210	Total	C	N	O	S	0	0	0
			1562	988	260	307	7			
2	K	212	Total	C	N	O	S	0	0	0
			1578	998	262	311	7			
2	N	209	Total	C	N	O	S	0	0	0
			1555	983	259	306	7			
2	Q	210	Total	C	N	O	S	0	0	0
			1562	988	260	307	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	206	Total	C	N	O	S	0	0	0
			1540	975	256	302	7			
2	T	212	Total	C	N	O	S	0	0	0
			1578	998	262	311	7			

- Molecule 3 is a protein called Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	111	Total	C	N	O	S	0	0	0
			879	549	159	166	5			
3	F	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	I	113	Total	C	N	O	S	0	0	0
			891	555	161	170	5			
3	L	112	Total	C	N	O	S	0	0	0
			887	553	160	169	5			
3	O	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	R	110	Total	C	N	O	S	0	0	0
			870	544	157	164	5			
3	X	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			
3	Y	117	Total	C	N	O	S	0	0	0
			924	574	169	176	5			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q15116
A	172	LEU	-	expression tag	UNP Q15116
A	173	ASN	-	expression tag	UNP Q15116
A	174	ASP	-	expression tag	UNP Q15116
A	175	ILE	-	expression tag	UNP Q15116
A	176	PHE	-	expression tag	UNP Q15116
A	177	GLU	-	expression tag	UNP Q15116
A	178	ALA	-	expression tag	UNP Q15116
A	179	GLN	-	expression tag	UNP Q15116
A	180	LYS	-	expression tag	UNP Q15116
A	181	ILE	-	expression tag	UNP Q15116
A	182	GLU	-	expression tag	UNP Q15116
A	183	TRP	-	expression tag	UNP Q15116
A	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
A	185	GLU	-	expression tag	UNP Q15116
A	186	HIS	-	expression tag	UNP Q15116
A	187	HIS	-	expression tag	UNP Q15116
A	188	HIS	-	expression tag	UNP Q15116
A	189	HIS	-	expression tag	UNP Q15116
A	190	HIS	-	expression tag	UNP Q15116
A	191	HIS	-	expression tag	UNP Q15116
F	171	GLY	-	expression tag	UNP Q15116
F	172	LEU	-	expression tag	UNP Q15116
F	173	ASN	-	expression tag	UNP Q15116
F	174	ASP	-	expression tag	UNP Q15116
F	175	ILE	-	expression tag	UNP Q15116
F	176	PHE	-	expression tag	UNP Q15116
F	177	GLU	-	expression tag	UNP Q15116
F	178	ALA	-	expression tag	UNP Q15116
F	179	GLN	-	expression tag	UNP Q15116
F	180	LYS	-	expression tag	UNP Q15116
F	181	ILE	-	expression tag	UNP Q15116
F	182	GLU	-	expression tag	UNP Q15116
F	183	TRP	-	expression tag	UNP Q15116
F	184	HIS	-	expression tag	UNP Q15116
F	185	GLU	-	expression tag	UNP Q15116
F	186	HIS	-	expression tag	UNP Q15116
F	187	HIS	-	expression tag	UNP Q15116
F	188	HIS	-	expression tag	UNP Q15116
F	189	HIS	-	expression tag	UNP Q15116
F	190	HIS	-	expression tag	UNP Q15116
F	191	HIS	-	expression tag	UNP Q15116
I	171	GLY	-	expression tag	UNP Q15116
I	172	LEU	-	expression tag	UNP Q15116
I	173	ASN	-	expression tag	UNP Q15116
I	174	ASP	-	expression tag	UNP Q15116
I	175	ILE	-	expression tag	UNP Q15116
I	176	PHE	-	expression tag	UNP Q15116
I	177	GLU	-	expression tag	UNP Q15116
I	178	ALA	-	expression tag	UNP Q15116
I	179	GLN	-	expression tag	UNP Q15116
I	180	LYS	-	expression tag	UNP Q15116
I	181	ILE	-	expression tag	UNP Q15116
I	182	GLU	-	expression tag	UNP Q15116
I	183	TRP	-	expression tag	UNP Q15116
I	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
I	185	GLU	-	expression tag	UNP Q15116
I	186	HIS	-	expression tag	UNP Q15116
I	187	HIS	-	expression tag	UNP Q15116
I	188	HIS	-	expression tag	UNP Q15116
I	189	HIS	-	expression tag	UNP Q15116
I	190	HIS	-	expression tag	UNP Q15116
I	191	HIS	-	expression tag	UNP Q15116
L	171	GLY	-	expression tag	UNP Q15116
L	172	LEU	-	expression tag	UNP Q15116
L	173	ASN	-	expression tag	UNP Q15116
L	174	ASP	-	expression tag	UNP Q15116
L	175	ILE	-	expression tag	UNP Q15116
L	176	PHE	-	expression tag	UNP Q15116
L	177	GLU	-	expression tag	UNP Q15116
L	178	ALA	-	expression tag	UNP Q15116
L	179	GLN	-	expression tag	UNP Q15116
L	180	LYS	-	expression tag	UNP Q15116
L	181	ILE	-	expression tag	UNP Q15116
L	182	GLU	-	expression tag	UNP Q15116
L	183	TRP	-	expression tag	UNP Q15116
L	184	HIS	-	expression tag	UNP Q15116
L	185	GLU	-	expression tag	UNP Q15116
L	186	HIS	-	expression tag	UNP Q15116
L	187	HIS	-	expression tag	UNP Q15116
L	188	HIS	-	expression tag	UNP Q15116
L	189	HIS	-	expression tag	UNP Q15116
L	190	HIS	-	expression tag	UNP Q15116
L	191	HIS	-	expression tag	UNP Q15116
O	171	GLY	-	expression tag	UNP Q15116
O	172	LEU	-	expression tag	UNP Q15116
O	173	ASN	-	expression tag	UNP Q15116
O	174	ASP	-	expression tag	UNP Q15116
O	175	ILE	-	expression tag	UNP Q15116
O	176	PHE	-	expression tag	UNP Q15116
O	177	GLU	-	expression tag	UNP Q15116
O	178	ALA	-	expression tag	UNP Q15116
O	179	GLN	-	expression tag	UNP Q15116
O	180	LYS	-	expression tag	UNP Q15116
O	181	ILE	-	expression tag	UNP Q15116
O	182	GLU	-	expression tag	UNP Q15116
O	183	TRP	-	expression tag	UNP Q15116
O	184	HIS	-	expression tag	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
O	185	GLU	-	expression tag	UNP Q15116
O	186	HIS	-	expression tag	UNP Q15116
O	187	HIS	-	expression tag	UNP Q15116
O	188	HIS	-	expression tag	UNP Q15116
O	189	HIS	-	expression tag	UNP Q15116
O	190	HIS	-	expression tag	UNP Q15116
O	191	HIS	-	expression tag	UNP Q15116
R	171	GLY	-	expression tag	UNP Q15116
R	172	LEU	-	expression tag	UNP Q15116
R	173	ASN	-	expression tag	UNP Q15116
R	174	ASP	-	expression tag	UNP Q15116
R	175	ILE	-	expression tag	UNP Q15116
R	176	PHE	-	expression tag	UNP Q15116
R	177	GLU	-	expression tag	UNP Q15116
R	178	ALA	-	expression tag	UNP Q15116
R	179	GLN	-	expression tag	UNP Q15116
R	180	LYS	-	expression tag	UNP Q15116
R	181	ILE	-	expression tag	UNP Q15116
R	182	GLU	-	expression tag	UNP Q15116
R	183	TRP	-	expression tag	UNP Q15116
R	184	HIS	-	expression tag	UNP Q15116
R	185	GLU	-	expression tag	UNP Q15116
R	186	HIS	-	expression tag	UNP Q15116
R	187	HIS	-	expression tag	UNP Q15116
R	188	HIS	-	expression tag	UNP Q15116
R	189	HIS	-	expression tag	UNP Q15116
R	190	HIS	-	expression tag	UNP Q15116
R	191	HIS	-	expression tag	UNP Q15116
X	171	GLY	-	expression tag	UNP Q15116
X	172	LEU	-	expression tag	UNP Q15116
X	173	ASN	-	expression tag	UNP Q15116
X	174	ASP	-	expression tag	UNP Q15116
X	175	ILE	-	expression tag	UNP Q15116
X	176	PHE	-	expression tag	UNP Q15116
X	177	GLU	-	expression tag	UNP Q15116
X	178	ALA	-	expression tag	UNP Q15116
X	179	GLN	-	expression tag	UNP Q15116
X	180	LYS	-	expression tag	UNP Q15116
X	181	ILE	-	expression tag	UNP Q15116
X	182	GLU	-	expression tag	UNP Q15116
X	183	TRP	-	expression tag	UNP Q15116
X	184	HIS	-	expression tag	UNP Q15116

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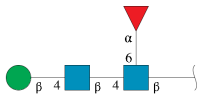
Chain	Residue	Modelled	Actual	Comment	Reference
X	185	GLU	-	expression tag	UNP Q15116
X	186	HIS	-	expression tag	UNP Q15116
X	187	HIS	-	expression tag	UNP Q15116
X	188	HIS	-	expression tag	UNP Q15116
X	189	HIS	-	expression tag	UNP Q15116
X	190	HIS	-	expression tag	UNP Q15116
X	191	HIS	-	expression tag	UNP Q15116
Y	171	GLY	-	expression tag	UNP Q15116
Y	172	LEU	-	expression tag	UNP Q15116
Y	173	ASN	-	expression tag	UNP Q15116
Y	174	ASP	-	expression tag	UNP Q15116
Y	175	ILE	-	expression tag	UNP Q15116
Y	176	PHE	-	expression tag	UNP Q15116
Y	177	GLU	-	expression tag	UNP Q15116
Y	178	ALA	-	expression tag	UNP Q15116
Y	179	GLN	-	expression tag	UNP Q15116
Y	180	LYS	-	expression tag	UNP Q15116
Y	181	ILE	-	expression tag	UNP Q15116
Y	182	GLU	-	expression tag	UNP Q15116
Y	183	TRP	-	expression tag	UNP Q15116
Y	184	HIS	-	expression tag	UNP Q15116
Y	185	GLU	-	expression tag	UNP Q15116
Y	186	HIS	-	expression tag	UNP Q15116
Y	187	HIS	-	expression tag	UNP Q15116
Y	188	HIS	-	expression tag	UNP Q15116
Y	189	HIS	-	expression tag	UNP Q15116
Y	190	HIS	-	expression tag	UNP Q15116
Y	191	HIS	-	expression tag	UNP Q15116

- Molecule 4 is an oligosaccharide called 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				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	U	4	50	28	2	20	0	0	0

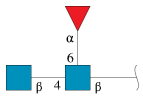
- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Z	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	g	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	h	4	Total	C	N	O	0	0	0
			49	28	2	19			
5	k	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



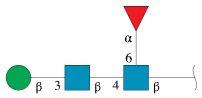
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	e	3	Total	C	N	O	0	0	0
			38	22	2	14			
6	j	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	b	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopy ranose.

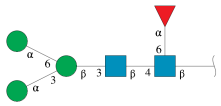


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	c	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 9 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-bet a-D-glucopyranose.

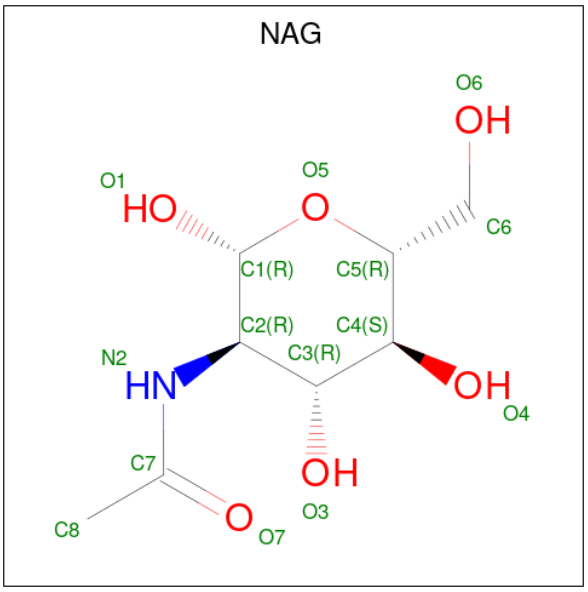
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	d	2	Total	C	N	O	0	0	0
			24	14	1	9			
9	i	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	f	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



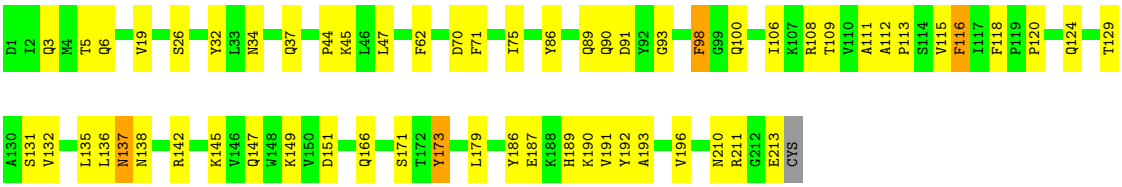
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total C N O 14 8 1 5	0	0
11	I	1	Total C N O 14 8 1 5	0	0
11	L	1	Total C N O 14 8 1 5	0	0
11	L	1	Total C N O 14 8 1 5	0	0
11	O	1	Total C N O 14 8 1 5	0	0
11	R	1	Total C N O 14 8 1 5	0	0
11	Y	1	Total C N O 14 8 1 5	0	0
11	Y	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

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

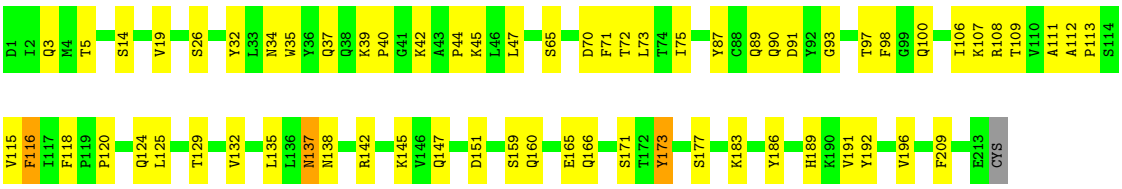
• Molecule 1: D12 antibody light chain, Fab fragment

Chain C:



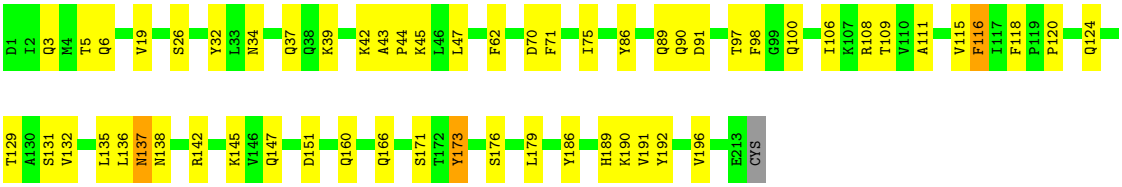
• Molecule 1: D12 antibody light chain, Fab fragment

Chain D:



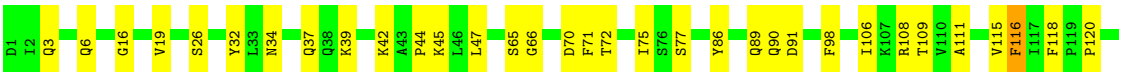
• Molecule 1: D12 antibody light chain, Fab fragment

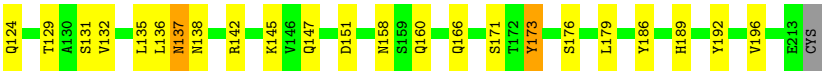
Chain G:



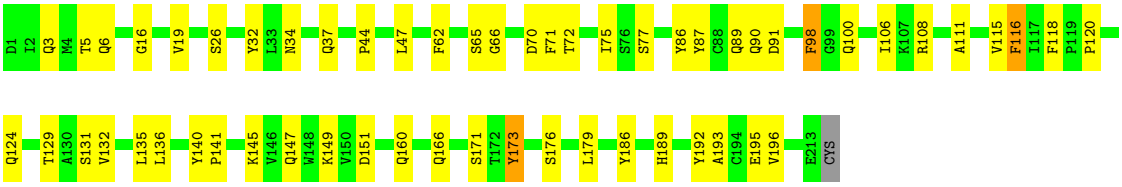
• Molecule 1: D12 antibody light chain, Fab fragment

Chain J:

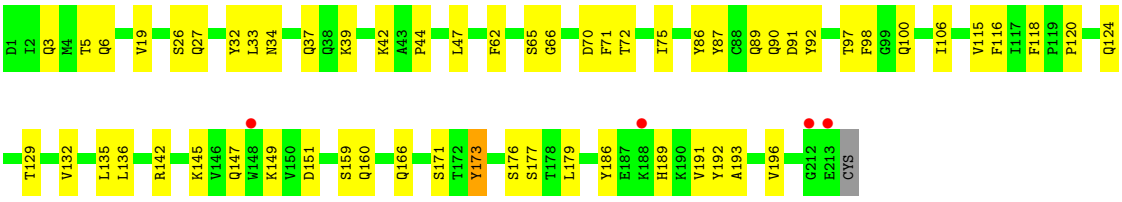




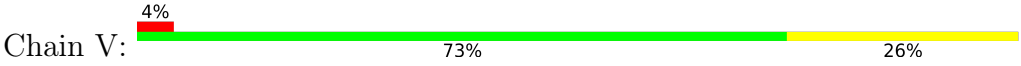
• Molecule 1: D12 antibody light chain, Fab fragment

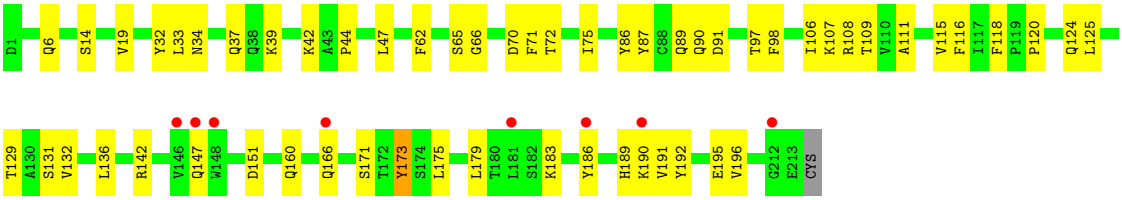


• Molecule 1: D12 antibody light chain, Fab fragment

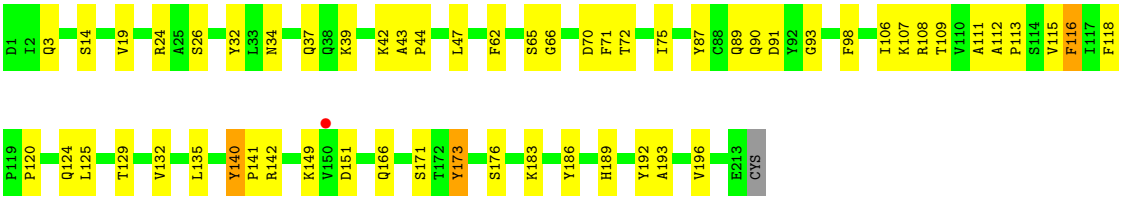


• Molecule 1: D12 antibody light chain, Fab fragment

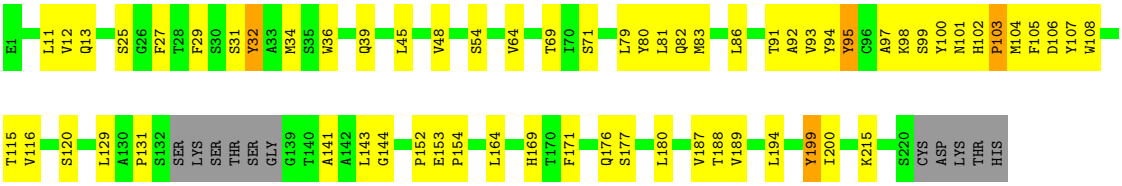




• Molecule 1: D12 antibody light chain, Fab fragment

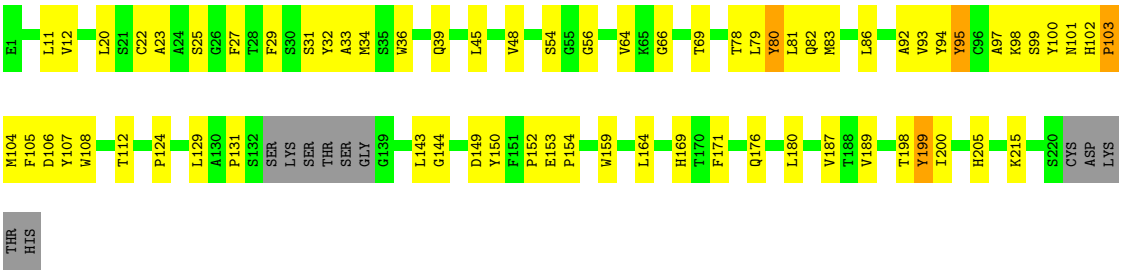


• Molecule 2: D12 antibody heavy chain, Fab fragment



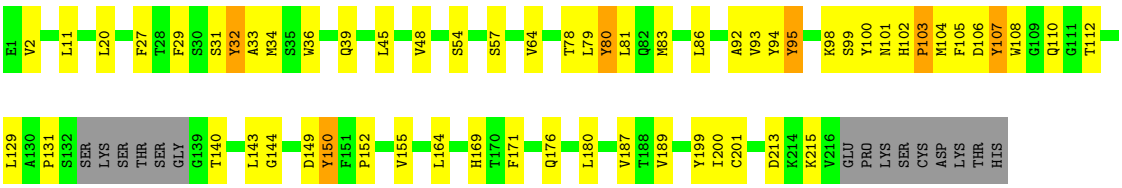
• Molecule 2: D12 antibody heavy chain, Fab fragment

Chain E:



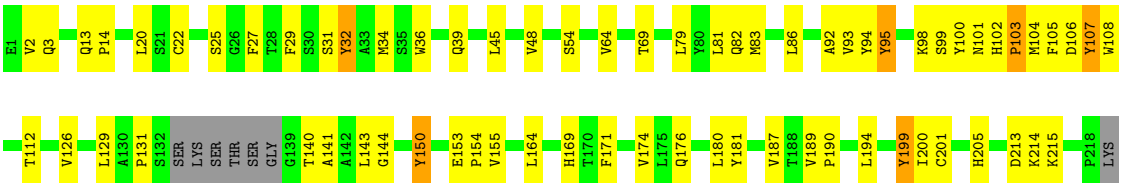
• Molecule 2: D12 antibody heavy chain, Fab fragment

Chain H:



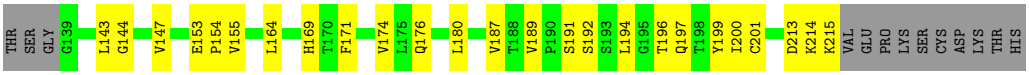
• Molecule 2: D12 antibody heavy chain, Fab fragment

Chain K:

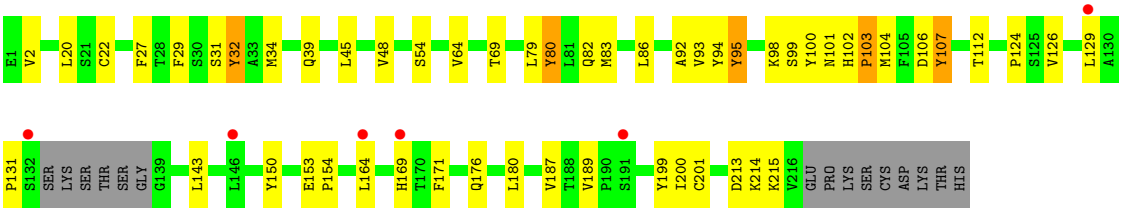


• Molecule 2: D12 antibody heavy chain, Fab fragment

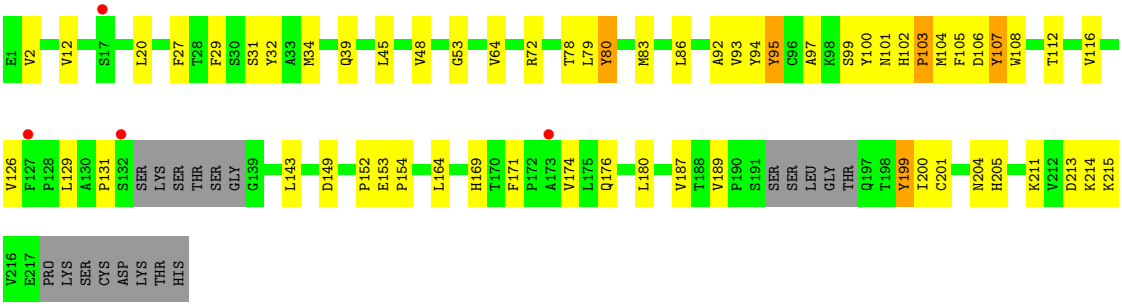
Chain N:



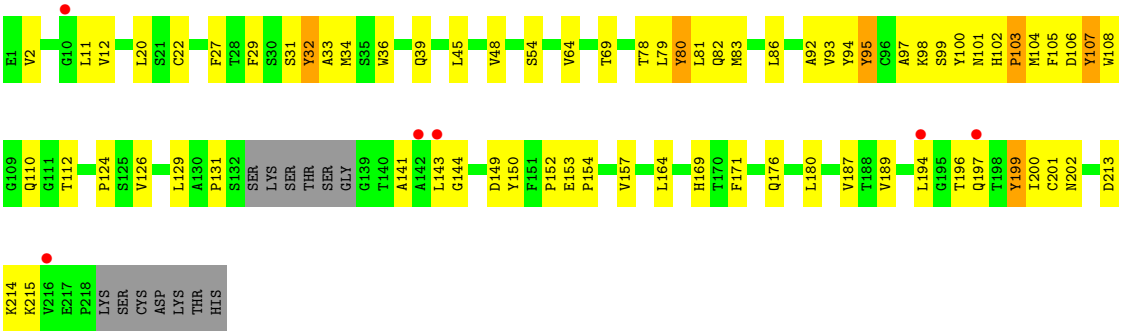
• Molecule 2: D12 antibody heavy chain, Fab fragment



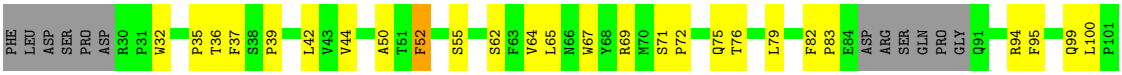
• Molecule 2: D12 antibody heavy chain, Fab fragment

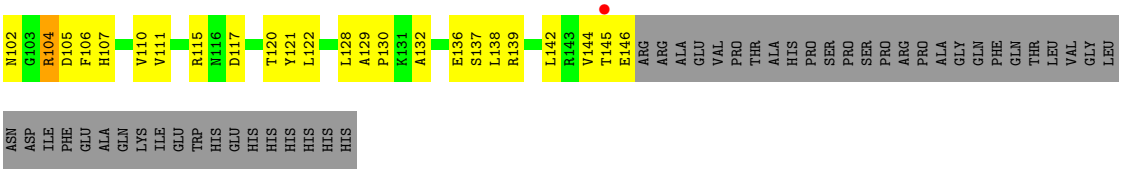


• Molecule 2: D12 antibody heavy chain, Fab fragment



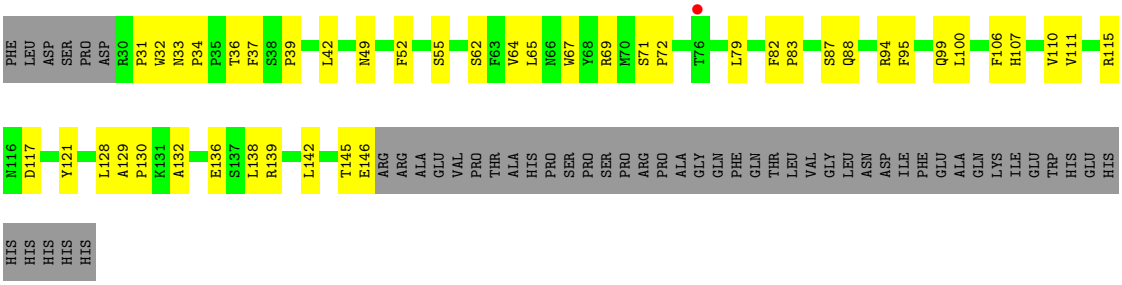
• Molecule 3: Programmed cell death protein 1





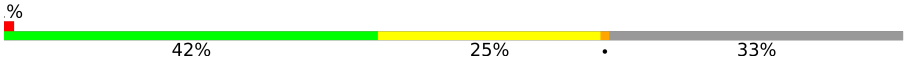
• Molecule 3: Programmed cell death protein 1

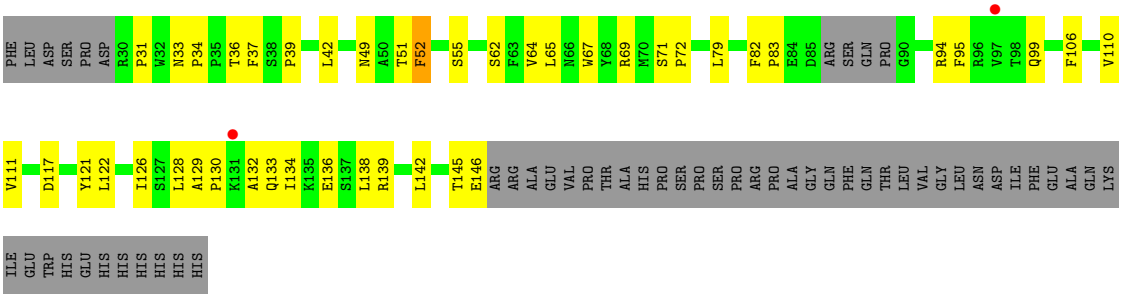
Chain F:



• Molecule 3: Programmed cell death protein 1

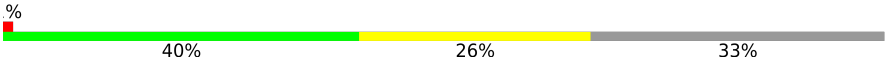
Chain I:

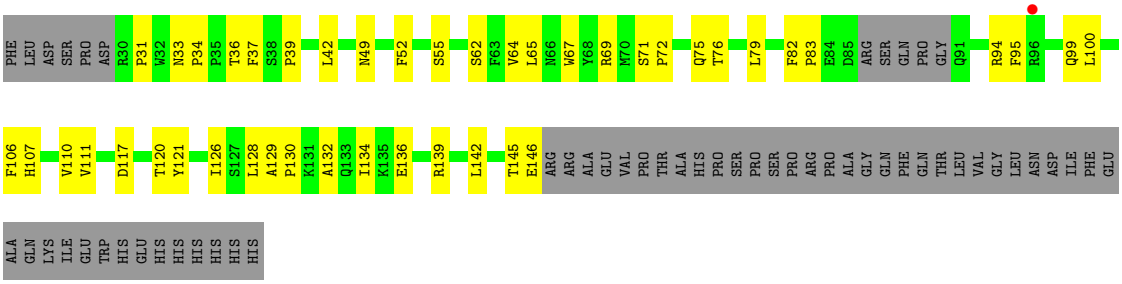




• Molecule 3: Programmed cell death protein 1

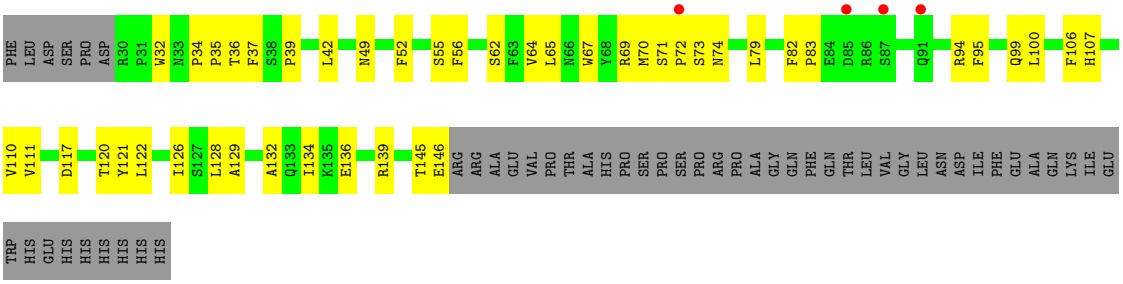
Chain L:





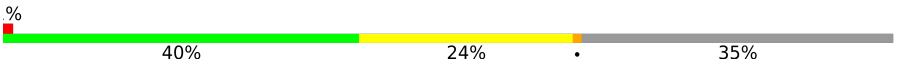
• Molecule 3: Programmed cell death protein 1

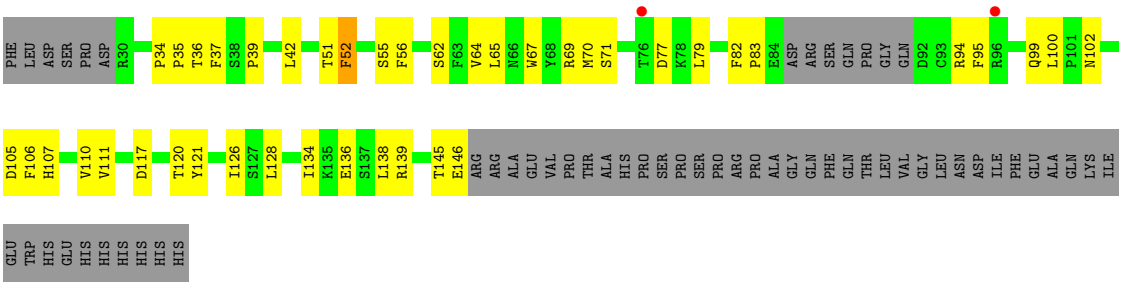
Chain O:



• Molecule 3: Programmed cell death protein 1

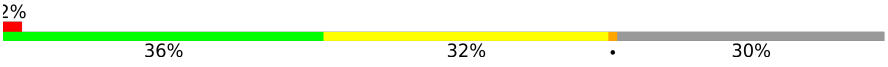
Chain R:

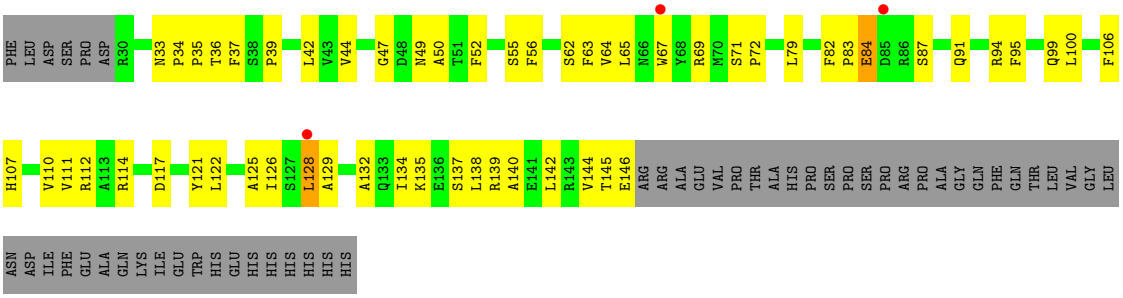




• Molecule 3: Programmed cell death protein 1

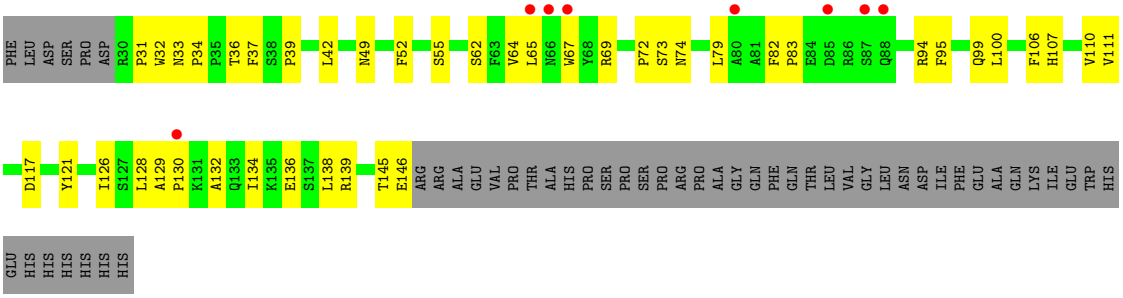
Chain X:





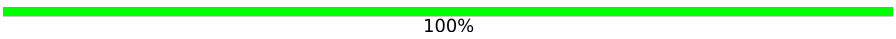
• Molecule 3: Programmed cell death protein 1

Chain Y:



• Molecule 4: 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 U:



• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

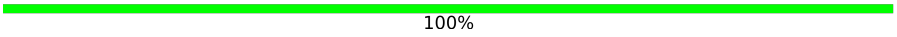
Chain h:

• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

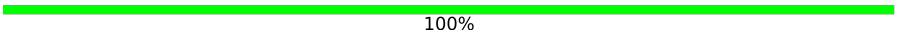
Chain e:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

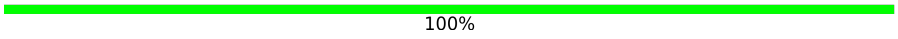
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 8: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 9: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

• Molecule 9: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

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

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.19Å 187.09Å 190.84Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	95.42 – 3.50 95.42 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (95.42-3.50) 94.6 (95.42-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.243 , 0.293 0.246 , 0.292	Depositor DCC
R_{free} test set	3527 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.661	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.053 for -h,l,k 0.049 for -h,-l,-k 0.176 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	33524	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	C	0.29	0/1669	0.54	0/2265
1	D	0.27	0/1669	0.53	0/2265
1	G	0.26	0/1669	0.53	0/2265
1	J	0.26	0/1669	0.52	0/2265
1	M	0.26	0/1669	0.53	0/2265
1	P	0.27	0/1669	0.52	0/2265
1	S	0.28	0/1669	0.55	0/2265
1	V	0.27	0/1669	0.53	0/2265
2	B	0.28	0/1632	0.54	0/2221
2	E	0.27	0/1632	0.53	0/2221
2	H	0.29	0/1600	0.55	0/2178
2	K	0.29	0/1617	0.55	0/2202
2	N	0.28	0/1593	0.55	0/2168
2	Q	0.28	0/1600	0.55	0/2178
2	T	0.28	0/1617	0.56	0/2202
2	W	0.28	0/1577	0.54	0/2145
3	A	0.29	0/899	0.62	0/1220
3	F	0.28	0/946	0.62	0/1285
3	I	0.27	0/911	0.61	0/1236
3	L	0.27	0/907	0.60	0/1231
3	O	0.28	0/946	0.61	0/1285
3	R	0.30	0/890	0.61	0/1208
3	X	0.28	0/946	0.60	0/1285
3	Y	0.27	0/946	0.60	0/1285
All	All	0.28	0/33611	0.55	0/45670

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	C	1634	0	1586	51	0
1	D	1634	0	1586	50	0
1	G	1634	0	1586	49	0
1	J	1634	0	1586	49	0
1	M	1634	0	1586	51	0
1	P	1634	0	1586	53	0
1	S	1634	0	1586	53	0
1	V	1634	0	1586	51	0
2	B	1593	0	1556	57	0
2	E	1593	0	1556	61	0
2	H	1562	0	1525	57	0
2	K	1578	0	1538	65	0
2	N	1555	0	1516	63	0
2	Q	1562	0	1525	53	0
2	T	1578	0	1538	70	0
2	W	1540	0	1499	63	0
3	A	879	0	849	60	0
3	F	924	0	889	47	0
3	I	891	0	854	46	0
3	L	887	0	852	46	0
3	O	924	0	890	50	0
3	R	870	0	841	46	0
3	X	924	0	889	65	0
3	Y	924	0	889	49	0
4	U	50	0	43	0	0
5	Z	49	0	43	3	0
5	g	49	0	43	0	0
5	h	49	0	43	0	0
5	k	49	0	43	0	0
6	a	38	0	34	0	0
6	e	38	0	34	0	0
6	j	38	0	34	0	0
7	b	28	0	25	0	0
8	c	49	0	43	0	0
9	d	24	0	22	0	0
9	i	24	0	22	0	0
10	f	71	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	14	0	13	0	0
11	I	14	0	13	0	0
11	L	28	0	26	0	0
11	O	14	0	13	0	0
11	R	14	0	13	0	0
11	Y	28	0	26	0	0
All	All	33524	0	32488	1164	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 18.

All (1164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:140:TYR:HD1	1:S:141:PRO:HA	1.23	1.01
1:P:115:VAL:HG21	1:P:196:VAL:HG11	1.55	0.88
1:S:140:TYR:CD1	1:S:141:PRO:HA	2.09	0.86
3:A:82:PHE:HE2	3:A:99:GLN:HB2	1.39	0.85
1:M:115:VAL:HG21	1:M:196:VAL:HG11	1.59	0.85
1:V:115:VAL:HG21	1:V:196:VAL:HG11	1.58	0.85
1:S:115:VAL:HG21	1:S:196:VAL:HG11	1.59	0.84
1:G:115:VAL:HG21	1:G:196:VAL:HG11	1.61	0.83
1:D:151:ASP:OD2	1:D:189:HIS:ND1	2.13	0.82
1:D:115:VAL:HG21	1:D:196:VAL:HG11	1.61	0.82
3:X:129:ALA:HB3	3:X:132:ALA:HB2	1.62	0.80
1:J:115:VAL:HG21	1:J:196:VAL:HG11	1.63	0.80
2:W:83:MET:HB3	2:W:86:LEU:HD21	1.63	0.80
1:C:151:ASP:OD2	1:C:189:HIS:ND1	2.13	0.80
1:D:118:PHE:HD2	2:E:129:LEU:HB3	1.47	0.80
1:G:151:ASP:OD2	1:G:189:HIS:ND1	2.16	0.78
1:V:89:GLN:NE2	1:V:90:GLN:O	2.17	0.78
3:A:79:LEU:HB3	3:A:95:PHE:HD2	1.48	0.78
3:I:79:LEU:HB3	3:I:95:PHE:HD2	1.49	0.77
2:Q:101:ASN:HD22	3:R:138:LEU:HD12	1.49	0.77
2:E:31:SER:HA	3:F:139:ARG:HE	1.48	0.77
1:G:118:PHE:HD2	2:H:129:LEU:HB3	1.49	0.77
5:Z:1:NAG:H61	5:Z:4:FUC:H3	1.67	0.77
1:G:89:GLN:NE2	1:G:90:GLN:O	2.18	0.77
1:P:89:GLN:NE2	1:P:90:GLN:O	2.16	0.77
1:J:151:ASP:OD2	1:J:189:HIS:ND1	2.18	0.77
1:S:140:TYR:HD1	1:S:141:PRO:CA	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:118:PHE:HD2	2:K:129:LEU:HB3	1.50	0.76
2:T:31:SER:HA	3:Y:139:ARG:HE	1.50	0.76
3:F:79:LEU:HB3	3:F:95:PHE:HD2	1.51	0.76
3:R:82:PHE:HE2	3:R:99:GLN:HB2	1.51	0.75
2:N:197:GLN:OE1	3:Y:74:ASN:ND2	2.19	0.75
1:C:115:VAL:HG21	1:C:196:VAL:HG11	1.69	0.74
3:X:62:SER:HB3	3:X:128:LEU:HB2	1.70	0.74
1:C:89:GLN:NE2	1:C:90:GLN:O	2.20	0.74
1:M:89:GLN:NE2	1:M:90:GLN:O	2.21	0.73
3:A:82:PHE:CE2	3:A:99:GLN:HB2	2.23	0.73
2:N:99:SER:OG	2:N:104:MET:SD	2.42	0.73
3:X:82:PHE:CE2	3:X:99:GLN:HB2	2.23	0.73
2:Q:100:TYR:HB3	2:Q:103:PRO:HG2	1.71	0.73
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.71	0.73
1:J:89:GLN:NE2	1:J:90:GLN:O	2.21	0.73
1:D:89:GLN:NE2	1:D:90:GLN:O	2.21	0.72
3:O:82:PHE:HE2	3:O:99:GLN:HB2	1.53	0.72
1:C:118:PHE:HD2	2:B:129:LEU:HB3	1.54	0.72
1:M:118:PHE:HD2	2:N:129:LEU:HB3	1.54	0.72
1:S:89:GLN:NE2	1:S:90:GLN:O	2.23	0.72
3:X:82:PHE:HD1	3:X:83:PRO:HA	1.55	0.72
3:A:115:ARG:NH1	3:A:144:VAL:O	2.23	0.71
1:G:32:TYR:HB3	1:G:91:ASP:HB2	1.72	0.71
2:K:31:SER:HA	3:L:139:ARG:HE	1.54	0.71
3:Y:79:LEU:HB3	3:Y:95:PHE:HD2	1.55	0.71
2:H:31:SER:HA	3:I:139:ARG:HE	1.54	0.71
2:K:200:ILE:HD12	2:K:215:LYS:HG2	1.72	0.71
3:L:117:ASP:O	3:L:121:TYR:OH	2.08	0.71
3:L:62:SER:HB3	3:L:128:LEU:HB2	1.74	0.70
2:N:196:THR:HG21	3:Y:73:SER:HA	1.73	0.70
3:O:79:LEU:HB3	3:O:95:PHE:HD2	1.54	0.70
2:B:101:ASN:HD22	3:A:138:LEU:HD12	1.56	0.70
2:N:169:HIS:HB3	2:N:171:PHE:HE1	1.56	0.70
3:F:69:ARG:HB2	3:F:79:LEU:HD11	1.73	0.70
2:N:83:MET:HB3	2:N:86:LEU:HD21	1.73	0.70
2:N:31:SER:HA	3:O:139:ARG:HE	1.57	0.69
1:P:32:TYR:HB3	1:P:91:ASP:HB2	1.73	0.69
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.73	0.69
3:R:94:ARG:HA	3:R:111:VAL:HG22	1.74	0.69
3:Y:145:THR:HG22	3:Y:146:GLU:H	1.58	0.69
2:H:131:PRO:HD3	2:H:143:LEU:HG	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:145:THR:HG22	3:R:146:GLU:H	1.57	0.69
3:O:36:THR:OG1	3:O:55:SER:OG	2.10	0.69
3:O:117:ASP:O	3:O:121:TYR:OH	2.09	0.69
3:R:36:THR:OG1	3:R:55:SER:OG	2.11	0.69
3:A:62:SER:HB3	3:A:128:LEU:HB2	1.74	0.69
3:I:145:THR:HG22	3:I:146:GLU:H	1.58	0.69
3:O:145:THR:HG22	3:O:146:GLU:H	1.58	0.69
3:L:82:PHE:HE2	3:L:99:GLN:HB2	1.57	0.68
3:L:145:THR:HG22	3:L:146:GLU:H	1.58	0.68
3:F:145:THR:HG22	3:F:146:GLU:H	1.59	0.68
3:R:64:VAL:HG12	3:R:83:PRO:HD2	1.74	0.68
2:K:34:MET:HB3	2:K:79:LEU:HD22	1.75	0.68
3:R:69:ARG:HB2	3:R:79:LEU:HD11	1.76	0.68
3:F:36:THR:OG1	3:F:55:SER:OG	2.11	0.68
1:C:44:PRO:HD3	2:B:95:TYR:HE2	1.59	0.68
3:A:145:THR:HG22	3:A:146:GLU:H	1.58	0.68
2:B:34:MET:HB3	2:B:79:LEU:HD22	1.76	0.68
3:I:129:ALA:HB3	3:I:132:ALA:HB2	1.76	0.68
2:B:11:LEU:HD12	2:B:152:PRO:HD3	1.74	0.68
3:F:115:ARG:HH22	3:F:146:GLU:HA	1.58	0.68
1:V:32:TYR:HB3	1:V:91:ASP:HB2	1.76	0.67
3:X:69:ARG:HB2	3:X:79:LEU:HD11	1.77	0.67
2:H:83:MET:HB3	2:H:86:LEU:HD21	1.74	0.67
1:C:32:TYR:HB3	1:C:91:ASP:HB2	1.76	0.67
3:Y:62:SER:HB3	3:Y:128:LEU:HB2	1.76	0.67
3:A:36:THR:OG1	3:A:55:SER:OG	2.12	0.67
3:L:79:LEU:HB3	3:L:95:PHE:HD2	1.58	0.67
3:X:36:THR:OG1	3:X:55:SER:OG	2.12	0.67
3:R:62:SER:HB3	3:R:128:LEU:HB2	1.76	0.67
3:I:69:ARG:HB2	3:I:79:LEU:HD11	1.75	0.67
3:Y:69:ARG:HB2	3:Y:79:LEU:HD11	1.76	0.67
3:A:117:ASP:O	3:A:121:TYR:OH	2.09	0.66
2:B:83:MET:HB3	2:B:86:LEU:HD21	1.76	0.66
3:F:117:ASP:O	3:F:121:TYR:OH	2.11	0.66
1:J:145:LYS:HE3	1:J:147:GLN:HE21	1.60	0.66
3:X:64:VAL:HG12	3:X:83:PRO:HG2	1.77	0.66
2:T:83:MET:HB3	2:T:86:LEU:HD21	1.76	0.66
2:W:149:ASP:OD1	2:W:176:GLN:NE2	2.28	0.66
1:S:118:PHE:HD2	2:T:129:LEU:HB3	1.61	0.66
3:Y:117:ASP:O	3:Y:121:TYR:OH	2.10	0.66
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:36:THR:OG1	3:I:55:SER:OG	2.10	0.66
2:T:34:MET:HB3	2:T:79:LEU:HD22	1.76	0.66
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.77	0.66
1:J:118:PHE:CD2	2:K:129:LEU:HB3	2.31	0.66
2:Q:169:HIS:HB3	2:Q:171:PHE:HE1	1.59	0.66
3:R:82:PHE:CE2	3:R:99:GLN:HB2	2.31	0.66
3:O:69:ARG:HB2	3:O:79:LEU:HD11	1.77	0.65
1:P:44:PRO:HD3	2:Q:95:TYR:HE2	1.61	0.65
2:B:31:SER:HA	3:A:139:ARG:HE	1.60	0.65
2:K:169:HIS:HB3	2:K:171:PHE:HE1	1.60	0.65
3:R:64:VAL:HG13	3:R:128:LEU:HD11	1.77	0.65
1:V:37:GLN:HB2	1:V:47:LEU:HD11	1.78	0.65
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.79	0.65
3:L:69:ARG:HB2	3:L:79:LEU:HD11	1.78	0.65
2:B:169:HIS:HB3	2:B:171:PHE:HE1	1.61	0.65
2:H:169:HIS:HB3	2:H:171:PHE:HE1	1.61	0.65
1:M:37:GLN:HB2	1:M:47:LEU:HD11	1.79	0.65
2:W:99:SER:OG	2:W:104:MET:HG2	1.96	0.64
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.79	0.64
1:D:189:HIS:HB2	1:D:192:TYR:HE1	1.61	0.64
1:P:37:GLN:HB2	1:P:47:LEU:HD11	1.79	0.64
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.78	0.64
1:V:118:PHE:HD2	2:W:129:LEU:HB3	1.63	0.64
3:Y:36:THR:OG1	3:Y:55:SER:OG	2.15	0.64
3:I:39:PRO:HB3	1:V:70:ASP:OD2	1.98	0.64
2:W:34:MET:HB3	2:W:79:LEU:HD22	1.78	0.64
2:T:126:VAL:O	2:T:214:LYS:NZ	2.27	0.64
3:A:69:ARG:HB2	3:A:79:LEU:HD11	1.79	0.64
3:L:36:THR:OG1	3:L:55:SER:OG	2.15	0.64
1:G:118:PHE:CD2	2:H:129:LEU:HB3	2.31	0.64
3:Y:94:ARG:HA	3:Y:111:VAL:HG22	1.80	0.64
1:C:118:PHE:CD2	2:B:129:LEU:HB3	2.33	0.63
1:M:44:PRO:HD3	2:N:95:TYR:HE2	1.63	0.63
2:T:200:ILE:HD12	2:T:215:LYS:HG2	1.79	0.63
3:X:138:LEU:HD12	3:X:138:LEU:H	1.63	0.63
2:H:102:HIS:O	2:H:104:MET:N	2.32	0.63
3:X:79:LEU:HB3	3:X:95:PHE:HD2	1.61	0.63
3:A:39:PRO:HB3	1:P:70:ASP:OD2	1.99	0.63
2:K:99:SER:OG	2:K:104:MET:HG2	1.99	0.63
1:S:44:PRO:HD3	2:T:95:TYR:CE2	2.34	0.63
2:Q:31:SER:HA	3:R:139:ARG:HE	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:145:LYS:HE3	1:G:147:GLN:HE21	1.64	0.62
3:O:94:ARG:HA	3:O:111:VAL:HG22	1.80	0.62
1:V:44:PRO:HD3	2:W:95:TYR:CE2	2.34	0.62
3:A:102:ASN:HD21	3:A:105:ASP:HB2	1.64	0.62
1:J:44:PRO:HD3	2:K:95:TYR:CE2	2.34	0.62
3:L:82:PHE:CE2	3:L:99:GLN:HB2	2.34	0.62
3:X:82:PHE:HE2	3:X:99:GLN:HB2	1.62	0.62
1:C:89:GLN:HG3	1:C:98:PHE:CE1	2.35	0.62
2:B:102:HIS:O	2:B:104:MET:N	2.33	0.62
3:F:129:ALA:HB3	3:F:132:ALA:HB2	1.82	0.62
1:G:44:PRO:HD3	2:H:95:TYR:CE2	2.34	0.62
3:I:117:ASP:O	3:I:121:TYR:OH	2.09	0.62
1:M:145:LYS:HE3	1:M:147:GLN:HE21	1.64	0.62
3:R:117:ASP:O	3:R:121:TYR:OH	2.09	0.62
2:W:189:VAL:HG21	2:W:199:TYR:HE2	1.65	0.62
2:N:101:ASN:HD21	3:O:34:PRO:HB2	1.63	0.62
1:C:187:GLU:HA	1:C:211:ARG:HH12	1.64	0.62
1:D:118:PHE:CD2	2:E:129:LEU:HB3	2.33	0.62
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.81	0.62
3:O:82:PHE:CE2	3:O:99:GLN:HB2	2.34	0.62
1:D:44:PRO:HD3	2:E:95:TYR:HE2	1.63	0.62
1:V:160:GLN:HE21	2:W:174:VAL:HG22	1.64	0.62
2:E:25:SER:HB2	2:K:140:THR:HG22	1.80	0.62
2:E:99:SER:OG	2:E:104:MET:HG2	2.00	0.62
1:J:44:PRO:HD3	2:K:95:TYR:HE2	1.65	0.62
2:N:131:PRO:HD3	2:N:143:LEU:HG	1.80	0.62
3:O:64:VAL:HG13	3:O:128:LEU:HD11	1.81	0.61
2:W:93:VAL:HG13	2:W:95:TYR:HE1	1.64	0.61
1:G:44:PRO:HD3	2:H:95:TYR:HE2	1.64	0.61
1:V:151:ASP:OD2	1:V:189:HIS:ND1	2.29	0.61
3:X:94:ARG:HA	3:X:111:VAL:HG22	1.82	0.61
2:T:101:ASN:ND2	3:Y:138:LEU:HD12	2.15	0.61
1:J:37:GLN:HB2	1:J:47:LEU:HD11	1.83	0.61
2:W:100:TYR:HB3	2:W:103:PRO:HG2	1.82	0.61
2:Q:34:MET:HB3	2:Q:79:LEU:HD22	1.81	0.61
2:Q:102:HIS:O	2:Q:104:MET:N	2.34	0.61
2:E:169:HIS:HB3	2:E:171:PHE:HE1	1.64	0.61
3:L:129:ALA:HB3	3:L:132:ALA:HB2	1.83	0.61
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.82	0.61
1:M:118:PHE:CD2	2:N:129:LEU:HB3	2.35	0.61
3:F:82:PHE:HE2	3:F:99:GLN:HB2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:TYR:HB3	1:J:91:ASP:HB2	1.83	0.61
1:V:189:HIS:HB2	1:V:192:TYR:HE1	1.65	0.61
1:S:37:GLN:HB2	1:S:47:LEU:HD11	1.82	0.61
3:A:67:TRP:CD1	3:A:79:LEU:HB2	2.35	0.61
3:F:62:SER:O	3:F:128:LEU:N	2.28	0.61
2:N:189:VAL:HG21	2:N:199:TYR:HE2	1.64	0.61
2:Q:99:SER:OG	2:Q:104:MET:SD	2.48	0.61
2:T:93:VAL:HG13	2:T:95:TYR:HE1	1.65	0.61
2:W:189:VAL:HG21	2:W:199:TYR:CE2	2.36	0.60
2:H:99:SER:OG	2:H:104:MET:HG2	2.01	0.60
1:J:89:GLN:HG3	1:J:98:PHE:CE1	2.35	0.60
2:Q:83:MET:HB3	2:Q:86:LEU:HD21	1.82	0.60
3:F:39:PRO:HB3	1:M:70:ASP:OD2	2.02	0.60
3:I:82:PHE:HE2	3:I:99:GLN:HB2	1.65	0.60
2:T:102:HIS:O	2:T:104:MET:N	2.35	0.60
1:S:151:ASP:OD2	1:S:189:HIS:ND1	2.31	0.60
2:T:169:HIS:HB3	2:T:171:PHE:HE1	1.66	0.60
1:M:44:PRO:HD3	2:N:95:TYR:CE2	2.36	0.60
2:N:34:MET:HB3	2:N:79:LEU:HD22	1.81	0.60
1:S:32:TYR:HB3	1:S:91:ASP:HB2	1.83	0.60
2:H:2:VAL:HB	2:H:107:TYR:CD2	2.37	0.60
3:O:71:SER:HB3	3:O:72:PRO:HD2	1.83	0.60
3:Y:129:ALA:HB3	3:Y:132:ALA:HB2	1.83	0.60
1:P:166:GLN:HE21	1:P:171:SER:HB3	1.66	0.60
1:P:44:PRO:HD3	2:Q:95:TYR:CE2	2.36	0.60
3:F:62:SER:HB3	3:F:128:LEU:HB2	1.83	0.59
3:I:62:SER:HB3	3:I:128:LEU:HB2	1.83	0.59
2:N:189:VAL:HG21	2:N:199:TYR:CE2	2.36	0.59
3:R:67:TRP:CD1	3:R:79:LEU:HB2	2.36	0.59
2:H:93:VAL:HG13	2:H:95:TYR:HE1	1.66	0.59
3:I:62:SER:O	3:I:128:LEU:N	2.30	0.59
2:B:54:SER:OG	3:A:136:GLU:OE2	2.16	0.59
2:E:102:HIS:O	2:E:104:MET:N	2.35	0.59
3:L:67:TRP:CD1	3:L:79:LEU:HB2	2.38	0.59
1:P:118:PHE:HD2	2:Q:129:LEU:HB3	1.67	0.59
1:D:145:LYS:HE3	1:D:147:GLN:HE21	1.67	0.59
3:R:82:PHE:HD1	3:R:83:PRO:HA	1.67	0.59
3:X:64:VAL:HA	3:X:83:PRO:HD2	1.83	0.59
2:N:93:VAL:HG13	2:N:95:TYR:HE1	1.68	0.59
2:K:102:HIS:O	2:K:104:MET:N	2.36	0.59
1:S:118:PHE:CD2	2:T:129:LEU:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:126:VAL:O	2:N:214:LYS:NZ	2.30	0.58
3:O:64:VAL:HG12	3:O:83:PRO:HD2	1.85	0.58
3:O:73:SER:C	2:T:196:THR:HG21	2.24	0.58
2:Q:39:GLN:HB2	2:Q:45:LEU:HD23	1.85	0.58
2:W:169:HIS:HB3	2:W:171:PHE:HE1	1.68	0.58
1:G:39:LYS:HB2	1:G:42:LYS:HD2	1.84	0.58
1:C:44:PRO:HD3	2:B:95:TYR:CE2	2.38	0.58
3:L:37:PHE:CZ	3:L:52:PHE:HD2	2.22	0.58
3:X:84:GLU:HG2	3:X:87:SER:HB3	1.84	0.58
2:T:99:SER:OG	2:T:104:MET:HG2	2.04	0.58
3:A:37:PHE:CZ	3:A:67:TRP:HZ3	2.21	0.58
3:R:99:GLN:HG3	3:R:106:PHE:CE1	2.38	0.58
2:T:39:GLN:HB2	2:T:45:LEU:HD23	1.84	0.58
2:B:143:LEU:HD22	2:B:199:TYR:CD2	2.39	0.58
3:A:67:TRP:O	3:A:79:LEU:N	2.32	0.58
2:E:100:TYR:HB3	2:E:103:PRO:HG2	1.86	0.58
2:E:176:GLN:HG2	2:E:180:LEU:O	2.04	0.58
3:F:82:PHE:CE2	3:F:99:GLN:HB2	2.39	0.58
1:G:160:GLN:HE22	2:H:176:GLN:HA	1.68	0.58
1:V:44:PRO:HD3	2:W:95:TYR:HE2	1.66	0.58
3:A:37:PHE:CZ	3:A:52:PHE:HD2	2.21	0.58
1:D:89:GLN:HG3	1:D:98:PHE:CE1	2.38	0.58
2:H:101:ASN:HB2	3:I:138:LEU:HD11	1.84	0.58
2:K:39:GLN:HB2	2:K:45:LEU:HD23	1.86	0.58
3:X:82:PHE:CD1	3:X:83:PRO:HA	2.37	0.58
3:I:82:PHE:CE2	3:I:99:GLN:HB2	2.39	0.57
1:M:160:GLN:HE22	2:N:176:GLN:HA	1.68	0.57
1:S:89:GLN:HG3	1:S:98:PHE:CE1	2.38	0.57
3:A:82:PHE:HD1	3:A:83:PRO:HA	1.69	0.57
2:K:150:TYR:HE2	2:K:155:VAL:HB	1.70	0.57
2:N:102:HIS:O	2:N:104:MET:N	2.38	0.57
2:N:92:ALA:HB3	2:N:94:TYR:HE1	1.69	0.57
2:B:101:ASN:ND2	3:A:138:LEU:HD12	2.18	0.57
3:I:64:VAL:HG13	3:I:128:LEU:HD11	1.86	0.57
2:K:93:VAL:HG13	2:K:95:TYR:HE1	1.69	0.57
1:M:34:ASN:ND2	1:M:91:ASP:OD2	2.37	0.57
3:I:64:VAL:HG12	3:I:83:PRO:HD2	1.86	0.57
3:R:37:PHE:CZ	3:R:52:PHE:HD2	2.22	0.57
1:J:115:VAL:C	1:J:116:PHE:HD1	2.08	0.57
2:Q:126:VAL:O	2:Q:214:LYS:NZ	2.27	0.57
3:R:37:PHE:CZ	3:R:67:TRP:HZ3	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:82:PHE:CD1	3:R:83:PRO:HA	2.40	0.57
3:X:145:THR:O	3:X:146:GLU:C	2.41	0.57
1:S:108:ARG:HB3	1:S:140:TYR:CD2	2.39	0.57
3:X:63:PHE:HA	3:X:128:LEU:HD13	1.85	0.57
2:E:54:SER:OG	3:F:136:GLU:OE2	2.18	0.57
3:F:67:TRP:CD1	3:F:79:LEU:HB2	2.40	0.57
2:T:2:VAL:HB	2:T:107:TYR:CD2	2.39	0.57
3:Y:99:GLN:HG3	3:Y:106:PHE:CE1	2.40	0.57
2:E:101:ASN:ND2	3:F:138:LEU:HD12	2.19	0.56
3:R:70:MET:SD	3:R:139:ARG:NH1	2.78	0.56
1:D:3:GLN:HB2	1:D:26:SER:HB2	1.87	0.56
1:D:37:GLN:HB2	1:D:47:LEU:HD11	1.87	0.56
3:I:94:ARG:HA	3:I:111:VAL:HG22	1.86	0.56
1:D:44:PRO:HD3	2:E:95:TYR:CE2	2.40	0.56
2:H:11:LEU:HB2	2:H:152:PRO:HG3	1.87	0.56
3:I:37:PHE:CZ	3:I:67:TRP:HZ3	2.23	0.56
2:K:150:TYR:CE1	2:K:181:TYR:HB2	2.39	0.56
2:E:143:LEU:HD22	2:E:199:TYR:CD2	2.40	0.56
3:I:67:TRP:CD1	3:I:79:LEU:HB2	2.40	0.56
2:Q:93:VAL:HG13	2:Q:95:TYR:HE1	1.70	0.56
3:L:94:ARG:HA	3:L:111:VAL:HG22	1.87	0.56
1:D:39:LYS:HB2	1:D:42:LYS:HD2	1.86	0.56
3:X:99:GLN:HG3	3:X:106:PHE:CE1	2.41	0.56
1:D:106:ILE:HB	1:D:166:GLN:NE2	2.19	0.56
2:W:126:VAL:O	2:W:214:LYS:NZ	2.28	0.56
3:Y:62:SER:O	3:Y:128:LEU:N	2.32	0.56
1:M:151:ASP:OD2	1:M:189:HIS:ND1	2.31	0.56
1:D:5:THR:HA	1:D:100:GLN:HE22	1.70	0.56
1:J:160:GLN:HE21	2:K:174:VAL:HG22	1.70	0.56
2:T:31:SER:HA	3:Y:139:ARG:NE	2.18	0.56
3:I:99:GLN:HG3	3:I:106:PHE:CE1	2.41	0.55
1:P:149:LYS:HB2	1:P:193:ALA:HB3	1.88	0.55
3:R:100:LEU:HD11	3:R:107:HIS:CG	2.41	0.55
2:W:2:VAL:HB	2:W:107:TYR:CD2	2.41	0.55
3:X:37:PHE:CZ	3:X:52:PHE:HD2	2.24	0.55
1:S:44:PRO:HD3	2:T:95:TYR:HE2	1.69	0.55
2:E:33:ALA:HB3	2:E:99:SER:HB3	1.88	0.55
2:H:189:VAL:HG21	2:H:199:TYR:CE2	2.42	0.55
3:L:99:GLN:HG3	3:L:106:PHE:CE1	2.42	0.55
1:P:65:SER:O	1:P:72:THR:N	2.39	0.55
1:V:189:HIS:HB2	1:V:192:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:189:HIS:HB2	1:S:192:TYR:HE1	1.71	0.55
3:Y:82:PHE:CE2	3:Y:99:GLN:HB2	2.40	0.55
3:A:99:GLN:HG3	3:A:106:PHE:CE1	2.41	0.55
1:D:115:VAL:C	1:D:116:PHE:HD1	2.09	0.55
1:G:115:VAL:C	1:G:116:PHE:HD1	2.09	0.55
1:M:106:ILE:HB	1:M:166:GLN:NE2	2.21	0.55
2:Q:189:VAL:HG21	2:Q:199:TYR:CE2	2.42	0.55
1:C:166:GLN:HE21	1:C:171:SER:HB3	1.71	0.55
1:M:89:GLN:HG3	1:M:98:PHE:CE1	2.41	0.55
1:S:93:GLY:HA2	3:Y:32:TRP:H	1.71	0.55
2:W:31:SER:HA	3:X:139:ARG:HE	1.72	0.55
3:X:67:TRP:CD1	3:X:79:LEU:HB2	2.41	0.55
2:E:69:THR:OG1	2:E:82:GLN:HB3	2.07	0.55
3:F:64:VAL:HG12	3:F:83:PRO:HD2	1.87	0.55
2:H:31:SER:HA	3:I:139:ARG:NE	2.22	0.55
2:H:189:VAL:HG21	2:H:199:TYR:HE2	1.71	0.55
2:K:31:SER:HA	3:L:139:ARG:NE	2.22	0.55
3:O:37:PHE:CZ	3:O:52:PHE:HD2	2.25	0.55
3:O:74:ASN:HD21	2:T:197:GLN:CD	2.09	0.55
2:B:189:VAL:HG21	2:B:199:TYR:CE2	2.42	0.55
2:E:189:VAL:HG21	2:E:199:TYR:CE2	2.42	0.55
2:Q:106:ASP:OD1	2:Q:107:TYR:N	2.40	0.55
2:Q:189:VAL:HG21	2:Q:199:TYR:HE2	1.72	0.55
2:H:200:ILE:HD12	2:H:215:LYS:HG2	1.89	0.55
2:K:189:VAL:HG21	2:K:199:TYR:CE2	2.42	0.55
3:R:102:ASN:HD21	3:R:105:ASP:HB2	1.72	0.55
2:K:126:VAL:O	2:K:214:LYS:NZ	2.29	0.54
2:Q:131:PRO:HD3	2:Q:143:LEU:HG	1.89	0.54
2:T:143:LEU:HD22	2:T:199:TYR:CD2	2.42	0.54
3:Y:37:PHE:CZ	3:Y:52:PHE:HD2	2.25	0.54
3:A:64:VAL:HG12	3:A:83:PRO:HG2	1.89	0.54
1:V:115:VAL:HG22	1:V:136:LEU:HG	1.89	0.54
2:B:92:ALA:HB3	2:B:94:TYR:HE1	1.73	0.54
1:D:160:GLN:HE22	2:E:176:GLN:HA	1.72	0.54
1:G:166:GLN:HE21	1:G:171:SER:HB3	1.72	0.54
1:V:118:PHE:CD2	2:W:129:LEU:HB3	2.41	0.54
1:C:115:VAL:C	1:C:116:PHE:HD1	2.10	0.54
1:C:187:GLU:HA	1:C:211:ARG:NH1	2.22	0.54
2:H:92:ALA:HB3	2:H:94:TYR:HE1	1.73	0.54
2:Q:200:ILE:HD12	2:Q:215:LYS:HG2	1.89	0.54
2:W:102:HIS:O	2:W:104:MET:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:65:LEU:HD22	3:X:106:PHE:CD2	2.43	0.54
2:H:54:SER:OG	3:I:136:GLU:OE2	2.20	0.54
2:K:92:ALA:HB3	2:K:94:TYR:HE1	1.72	0.54
2:T:131:PRO:HD3	2:T:143:LEU:HG	1.90	0.54
2:Q:92:ALA:HB3	2:Q:94:TYR:HE1	1.73	0.54
1:C:189:HIS:HB2	1:C:192:TYR:HE1	1.71	0.54
2:B:131:PRO:HD3	2:B:143:LEU:HG	1.90	0.54
1:M:19:VAL:HG22	1:M:75:ILE:HB	1.89	0.54
1:P:151:ASP:OD2	1:P:189:HIS:ND1	2.38	0.54
2:W:92:ALA:HB3	2:W:94:TYR:HE1	1.73	0.54
1:C:145:LYS:HE3	1:C:147:GLN:HE21	1.73	0.53
2:E:149:ASP:OD1	2:E:176:GLN:NE2	2.41	0.53
3:O:62:SER:O	3:O:128:LEU:N	2.32	0.53
2:B:189:VAL:HG21	2:B:199:TYR:HE2	1.73	0.53
1:D:32:TYR:HB3	1:D:91:ASP:HB2	1.89	0.53
1:D:189:HIS:HB2	1:D:192:TYR:CE1	2.41	0.53
2:K:54:SER:OG	3:L:136:GLU:OE2	2.18	0.53
2:K:143:LEU:HD22	2:K:199:TYR:CD2	2.42	0.53
2:W:39:GLN:HB2	2:W:45:LEU:HD23	1.89	0.53
2:T:100:TYR:HB3	2:T:103:PRO:HG2	1.90	0.53
1:G:6:GLN:NE2	1:G:86:TYR:O	2.41	0.53
1:J:160:GLN:HE22	2:K:176:GLN:HA	1.74	0.53
2:K:176:GLN:HG2	2:K:180:LEU:O	2.07	0.53
2:W:176:GLN:HG2	2:W:180:LEU:O	2.09	0.53
1:S:106:ILE:HB	1:S:166:GLN:NE2	2.23	0.53
1:P:176:SER:HG	2:Q:171:PHE:HD2	1.55	0.53
3:X:42:LEU:HD22	3:X:52:PHE:CE1	2.43	0.53
1:S:115:VAL:C	1:S:116:PHE:HD1	2.12	0.53
3:Y:82:PHE:HE2	3:Y:99:GLN:HB2	1.74	0.53
3:F:37:PHE:CZ	3:F:52:PHE:HD2	2.26	0.53
3:I:79:LEU:HD22	3:I:95:PHE:HE2	1.74	0.53
2:T:176:GLN:HG2	2:T:180:LEU:O	2.09	0.53
3:A:100:LEU:HD11	3:A:107:HIS:CG	2.43	0.53
2:K:22:CYS:HB3	2:K:79:LEU:HB3	1.91	0.53
1:P:6:GLN:NE2	1:P:86:TYR:O	2.39	0.53
2:Q:106:ASP:C	2:Q:107:TYR:HD1	2.12	0.53
2:E:31:SER:HA	3:F:139:ARG:NE	2.21	0.53
1:M:115:VAL:C	1:M:116:PHE:HD1	2.11	0.53
1:P:145:LYS:HE3	1:P:147:GLN:HE21	1.73	0.53
2:H:176:GLN:HG2	2:H:180:LEU:O	2.08	0.53
3:I:69:ARG:HB3	3:I:79:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:ILE:HB	1:J:166:GLN:NE2	2.24	0.53
2:N:54:SER:OG	3:O:136:GLU:OE2	2.21	0.53
3:O:99:GLN:HG3	3:O:106:PHE:CE1	2.44	0.53
3:Y:65:LEU:HD22	3:Y:106:PHE:CD2	2.44	0.53
1:C:34:ASN:ND2	1:C:91:ASP:OD2	2.42	0.53
2:B:99:SER:OG	2:B:104:MET:SD	2.51	0.53
3:I:37:PHE:CZ	3:I:52:PHE:HD2	2.26	0.53
3:I:49:ASN:OD1	3:I:111:VAL:HA	2.09	0.53
1:J:120:PRO:HB3	1:J:131:SER:H	1.73	0.53
1:P:39:LYS:HB2	1:P:42:LYS:HD2	1.91	0.53
3:R:42:LEU:HD22	3:R:52:PHE:CE1	2.43	0.53
3:X:126:ILE:HG12	3:X:134:ILE:HG23	1.89	0.53
3:F:99:GLN:HG3	3:F:106:PHE:CE1	2.43	0.52
3:O:74:ASN:HD22	2:T:196:THR:HB	1.74	0.52
2:W:200:ILE:HD12	2:W:215:LYS:HG2	1.90	0.52
2:B:93:VAL:HG13	2:B:95:TYR:HE1	1.74	0.52
2:B:200:ILE:HD12	2:B:215:LYS:HG2	1.90	0.52
3:A:42:LEU:HD22	3:A:52:PHE:CE1	2.44	0.52
2:H:150:TYR:HE2	2:H:155:VAL:HB	1.74	0.52
3:L:65:LEU:HD22	3:L:106:PHE:CD2	2.44	0.52
3:Y:42:LEU:HD22	3:Y:52:PHE:CE1	2.45	0.52
3:A:82:PHE:HE2	3:A:99:GLN:CB	2.17	0.52
2:E:189:VAL:HG21	2:E:199:TYR:HE2	1.74	0.52
2:N:106:ASP:C	2:N:107:TYR:HD1	2.12	0.52
3:F:65:LEU:HD22	3:F:106:PHE:CD2	2.45	0.52
1:J:34:ASN:ND2	1:J:91:ASP:OD2	2.41	0.52
2:T:189:VAL:HG21	2:T:199:TYR:CE2	2.44	0.52
1:C:93:GLY:HA2	3:A:32:TRP:H	1.74	0.52
3:I:67:TRP:O	3:I:79:LEU:N	2.38	0.52
1:M:115:VAL:HG22	1:M:136:LEU:HG	1.89	0.52
2:N:31:SER:HA	3:O:139:ARG:NE	2.22	0.52
3:O:65:LEU:HD22	3:O:106:PHE:CD2	2.45	0.52
1:C:3:GLN:HB2	1:C:26:SER:HB2	1.92	0.52
3:A:65:LEU:HD22	3:A:106:PHE:CD2	2.44	0.52
1:G:145:LYS:HE3	1:G:147:GLN:NE2	2.24	0.52
3:L:49:ASN:OD1	3:L:111:VAL:HA	2.09	0.52
2:W:31:SER:HA	3:X:139:ARG:CD	2.39	0.52
2:K:101:ASN:HD21	3:L:34:PRO:HB2	1.73	0.52
2:W:101:ASN:HD21	3:X:34:PRO:HB2	1.74	0.52
1:S:65:SER:O	1:S:72:THR:N	2.42	0.52
1:G:106:ILE:HB	1:G:166:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:122:LEU:HD23	3:I:139:ARG:HG2	1.92	0.52
1:P:34:ASN:ND2	1:P:91:ASP:OD2	2.42	0.52
2:W:31:SER:HA	3:X:139:ARG:NE	2.25	0.52
1:S:189:HIS:HB2	1:S:192:TYR:CE1	2.44	0.52
3:O:70:MET:SD	3:O:139:ARG:NH1	2.83	0.52
1:S:34:ASN:ND2	1:S:91:ASP:OD2	2.42	0.52
2:T:102:HIS:CE1	3:Y:34:PRO:HD2	2.45	0.52
3:F:37:PHE:CZ	3:F:67:TRP:HZ3	2.28	0.52
2:K:100:TYR:HD2	2:K:103:PRO:HG2	1.75	0.52
2:Q:164:LEU:HD21	2:Q:187:VAL:HG21	1.91	0.52
2:K:189:VAL:HG21	2:K:199:TYR:HE2	1.75	0.51
2:T:164:LEU:HD21	2:T:187:VAL:HG21	1.91	0.51
3:A:82:PHE:CD1	3:A:83:PRO:HA	2.45	0.51
1:D:166:GLN:HE21	1:D:171:SER:HB3	1.75	0.51
1:G:186:TYR:HA	1:G:192:TYR:OH	2.11	0.51
1:M:145:LYS:HE3	1:M:147:GLN:NE2	2.26	0.51
3:O:95:PHE:CE1	3:O:110:VAL:HG13	2.45	0.51
1:V:166:GLN:HE21	1:V:171:SER:HB3	1.76	0.51
1:S:89:GLN:NE2	1:S:91:ASP:OD1	2.42	0.51
2:B:31:SER:HA	3:A:139:ARG:NE	2.24	0.51
1:G:62:PHE:CD1	1:G:75:ILE:HG12	2.45	0.51
3:A:129:ALA:HB3	3:A:132:ALA:HB2	1.91	0.51
2:H:57:SER:OG	3:I:133:GLN:OE1	2.22	0.51
2:Q:176:GLN:HG2	2:Q:180:LEU:O	2.10	0.51
2:H:164:LEU:HD21	2:H:187:VAL:HG21	1.92	0.51
1:J:166:GLN:HE21	1:J:171:SER:HB3	1.76	0.51
2:K:2:VAL:HB	2:K:107:TYR:CD2	2.46	0.51
2:N:153:GLU:HB2	2:N:154:PRO:HA	1.91	0.51
2:W:131:PRO:HD3	2:W:143:LEU:HG	1.92	0.51
3:Y:49:ASN:OD1	3:Y:111:VAL:HA	2.10	0.51
3:I:65:LEU:HD22	3:I:106:PHE:CD2	2.46	0.51
1:J:19:VAL:HG22	1:J:75:ILE:HB	1.93	0.51
3:O:62:SER:HB3	3:O:128:LEU:HB2	1.93	0.51
1:V:62:PHE:CD1	1:V:75:ILE:HG12	2.46	0.51
2:W:106:ASP:C	2:W:107:TYR:HD1	2.14	0.51
2:T:92:ALA:HB3	2:T:94:TYR:HE1	1.76	0.51
2:K:131:PRO:HD3	2:K:143:LEU:HG	1.91	0.51
3:L:64:VAL:HG12	3:L:83:PRO:HD2	1.93	0.51
5:Z:1:NAG:H61	5:Z:4:FUC:C3	2.33	0.51
1:C:210:ASN:HB3	1:C:213:GLU:OE1	2.11	0.51
1:M:62:PHE:CD1	1:M:75:ILE:HG12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:106:ASP:OD1	2:N:107:TYR:N	2.44	0.51
1:P:70:ASP:C	1:P:71:PHE:HD1	2.14	0.51
2:Q:153:GLU:HB2	2:Q:154:PRO:HA	1.92	0.51
1:V:70:ASP:C	1:V:71:PHE:HD1	2.14	0.51
2:W:106:ASP:OD1	2:W:107:TYR:N	2.43	0.51
1:D:145:LYS:HE3	1:D:147:GLN:NE2	2.26	0.51
1:G:34:ASN:ND2	1:G:91:ASP:OD2	2.43	0.51
3:I:42:LEU:HD22	3:I:52:PHE:CE1	2.46	0.51
1:M:5:THR:HA	1:M:100:GLN:HE22	1.76	0.51
2:N:39:GLN:HB2	2:N:45:LEU:HD23	1.91	0.51
2:Q:54:SER:OG	3:R:136:GLU:OE2	2.24	0.51
2:Q:143:LEU:HD22	2:Q:199:TYR:CD2	2.46	0.51
1:V:6:GLN:NE2	1:V:86:TYR:O	2.41	0.51
3:X:67:TRP:O	3:X:79:LEU:N	2.39	0.51
1:G:136:LEU:HD21	1:G:196:VAL:HG21	1.93	0.51
1:P:98:PHE:CD2	2:Q:45:LEU:HB2	2.46	0.51
3:R:67:TRP:O	3:R:79:LEU:N	2.32	0.51
1:S:43:ALA:HB2	2:T:110:GLN:HA	1.92	0.51
3:A:69:ARG:HB3	3:A:79:LEU:HD21	1.92	0.50
2:E:23:ALA:HB1	2:K:190:PRO:HB2	1.93	0.50
2:K:20:LEU:HD22	2:K:112:THR:HG21	1.94	0.50
2:T:106:ASP:C	2:T:107:TYR:HD1	2.15	0.50
1:C:145:LYS:HE3	1:C:147:GLN:NE2	2.26	0.50
3:A:75:GLN:NE2	3:A:76:THR:O	2.43	0.50
1:D:34:ASN:ND2	1:D:91:ASP:OD2	2.43	0.50
2:N:196:THR:OG1	3:Y:74:ASN:ND2	2.44	0.50
2:W:143:LEU:HD22	2:W:199:TYR:CD2	2.46	0.50
1:M:166:GLN:HE21	1:M:171:SER:HB3	1.75	0.50
3:O:49:ASN:OD1	3:O:111:VAL:HA	2.12	0.50
2:B:106:ASP:OD1	2:B:107:TYR:N	2.44	0.50
3:L:37:PHE:CZ	3:L:67:TRP:HZ3	2.30	0.50
2:N:2:VAL:HB	2:N:107:TYR:CD2	2.47	0.50
3:R:65:LEU:HD22	3:R:106:PHE:CD2	2.47	0.50
3:A:104:ARG:HH21	1:P:27:GLN:HB3	1.77	0.50
3:O:129:ALA:HB3	3:O:132:ALA:HB2	1.93	0.50
1:S:120:PRO:HD3	1:S:132:VAL:HG12	1.94	0.50
2:B:120:SER:H	2:E:56:GLY:HA2	1.76	0.50
2:K:106:ASP:C	2:K:107:TYR:HD1	2.14	0.50
3:R:126:ILE:HG12	3:R:134:ILE:HG12	1.93	0.50
2:T:54:SER:OG	3:Y:136:GLU:OE2	2.21	0.50
3:Y:79:LEU:HD22	3:Y:95:PHE:HE2	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:PHE:CD2	2:N:45:LEU:HB2	2.47	0.50
1:P:118:PHE:CD2	2:Q:129:LEU:HB3	2.46	0.50
3:Y:67:TRP:CD1	3:Y:79:LEU:HB2	2.46	0.50
2:H:106:ASP:C	2:H:107:TYR:HD1	2.15	0.50
1:J:98:PHE:CD2	2:K:45:LEU:HB2	2.46	0.50
2:K:164:LEU:HD21	2:K:187:VAL:HG21	1.93	0.50
3:O:79:LEU:HD22	3:O:95:PHE:HE2	1.77	0.50
1:C:62:PHE:CD1	1:C:75:ILE:HG12	2.47	0.50
1:C:106:ILE:HB	1:C:166:GLN:NE2	2.27	0.50
1:C:136:LEU:HD21	1:C:196:VAL:HG21	1.93	0.50
1:J:3:GLN:HB2	1:J:26:SER:HB2	1.93	0.50
1:S:62:PHE:CD1	1:S:75:ILE:HG12	2.47	0.50
2:H:48:VAL:HG23	2:H:64:VAL:HG11	1.94	0.49
3:L:42:LEU:HD22	3:L:52:PHE:CE1	2.47	0.49
2:W:95:TYR:N	2:W:95:TYR:HD1	2.10	0.49
3:X:82:PHE:HA	3:X:83:PRO:C	2.32	0.49
2:B:25:SER:HB2	2:H:140:THR:HG22	1.94	0.49
2:E:131:PRO:HD3	2:E:143:LEU:HG	1.94	0.49
3:F:69:ARG:HB3	3:F:79:LEU:HD21	1.94	0.49
2:W:164:LEU:HD21	2:W:187:VAL:HG21	1.92	0.49
1:D:137:ASN:HD22	1:D:138:ASN:N	2.10	0.49
1:G:120:PRO:HB3	1:G:131:SER:H	1.77	0.49
2:N:191:SER:O	2:N:194:LEU:HD13	2.12	0.49
1:S:19:VAL:HG22	1:S:75:ILE:HB	1.94	0.49
1:C:137:ASN:HD22	1:C:138:ASN:N	2.10	0.49
2:E:92:ALA:HB3	2:E:94:TYR:HE1	1.77	0.49
2:K:129:LEU:HB2	2:K:144:GLY:C	2.31	0.49
3:L:79:LEU:HB3	3:L:95:PHE:CD2	2.45	0.49
3:O:100:LEU:HD11	3:O:107:HIS:CD2	2.47	0.49
1:V:39:LYS:HB2	1:V:42:LYS:HD2	1.94	0.49
2:W:101:ASN:ND2	3:X:34:PRO:HB2	2.27	0.49
2:W:189:VAL:HG11	2:W:199:TYR:CE2	2.47	0.49
2:B:100:TYR:O	2:B:103:PRO:HD2	2.12	0.49
3:L:79:LEU:HD22	3:L:95:PHE:HE2	1.77	0.49
1:M:70:ASP:C	1:M:71:PHE:HD1	2.16	0.49
1:M:149:LYS:HB2	1:M:193:ALA:HB3	1.95	0.49
2:N:102:HIS:CE1	3:O:34:PRO:HD2	2.46	0.49
1:P:106:ILE:HB	1:P:166:GLN:NE2	2.26	0.49
2:W:102:HIS:NE2	3:X:34:PRO:HD2	2.28	0.49
3:X:44:VAL:O	3:X:144:VAL:HA	2.12	0.49
1:S:70:ASP:C	1:S:71:PHE:HD1	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:SER:OG	1:D:177:SER:OG	2.30	0.49
3:L:126:ILE:HG12	3:L:134:ILE:HG12	1.94	0.49
3:O:37:PHE:CZ	3:O:67:TRP:HZ3	2.31	0.49
3:O:42:LEU:HD22	3:O:52:PHE:CE1	2.47	0.49
1:P:5:THR:HA	1:P:100:GLN:HE22	1.78	0.49
1:P:19:VAL:HG22	1:P:75:ILE:HB	1.94	0.49
3:R:71:SER:OG	3:R:77:ASP:HB2	2.12	0.49
2:W:95:TYR:N	2:W:95:TYR:CD1	2.80	0.49
3:X:100:LEU:HD11	3:X:107:HIS:CG	2.47	0.49
1:D:70:ASP:OD2	3:O:39:PRO:HB3	2.13	0.49
1:D:98:PHE:CD2	2:E:45:LEU:HB2	2.47	0.49
2:E:152:PRO:O	2:E:205:HIS:NE2	2.45	0.49
2:W:152:PRO:O	2:W:205:HIS:NE2	2.46	0.49
2:E:93:VAL:HG13	2:E:95:TYR:HE1	1.77	0.49
1:G:189:HIS:HB2	1:G:192:TYR:HE1	1.76	0.49
2:N:176:GLN:HG2	2:N:180:LEU:O	2.13	0.49
1:P:115:VAL:C	1:P:116:PHE:HD1	2.16	0.49
1:V:132:VAL:HG23	1:V:179:LEU:HB3	1.94	0.49
3:Y:126:ILE:HG12	3:Y:134:ILE:HG12	1.94	0.49
2:N:164:LEU:HD21	2:N:187:VAL:HG21	1.94	0.49
2:W:31:SER:HA	3:X:139:ARG:HD2	1.95	0.49
3:X:71:SER:HB3	3:X:72:PRO:HD2	1.94	0.49
2:T:95:TYR:N	2:T:95:TYR:HD1	2.11	0.49
3:I:95:PHE:CE1	3:I:110:VAL:HG13	2.48	0.49
2:K:27:PHE:CZ	2:K:98:LYS:HD3	2.48	0.49
1:M:65:SER:O	1:M:72:THR:N	2.43	0.49
3:X:64:VAL:HG13	3:X:128:LEU:HD11	1.95	0.49
2:E:105:PHE:HB3	2:E:108:TRP:CZ2	2.48	0.48
2:E:164:LEU:HD21	2:E:187:VAL:HG21	1.93	0.48
2:H:95:TYR:N	2:H:95:TYR:HD1	2.10	0.48
1:J:136:LEU:HD21	1:J:196:VAL:HG21	1.95	0.48
2:T:95:TYR:N	2:T:95:TYR:CD1	2.81	0.48
1:D:186:TYR:HA	1:D:192:TYR:OH	2.14	0.48
1:J:186:TYR:HA	1:J:192:TYR:OH	2.13	0.48
3:O:74:ASN:ND2	2:T:196:THR:HB	2.29	0.48
3:O:100:LEU:HD11	3:O:107:HIS:CG	2.48	0.48
1:P:145:LYS:HE3	1:P:147:GLN:NE2	2.28	0.48
3:X:47:GLY:HA2	3:X:114:ARG:HH12	1.78	0.48
1:C:6:GLN:NE2	1:C:86:TYR:O	2.46	0.48
2:H:102:HIS:HB2	2:H:103:PRO:HD3	1.94	0.48
2:N:48:VAL:HG23	2:N:64:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:67:TRP:CD1	3:O:79:LEU:HB2	2.48	0.48
1:V:120:PRO:HD3	1:V:132:VAL:HG12	1.95	0.48
3:F:49:ASN:OD1	3:F:111:VAL:HA	2.13	0.48
1:M:189:HIS:HB2	1:M:192:TYR:HE1	1.78	0.48
1:S:166:GLN:HE21	1:S:171:SER:HB3	1.78	0.48
3:F:95:PHE:CE1	3:F:110:VAL:HG13	2.48	0.48
1:J:120:PRO:HD3	1:J:132:VAL:HG12	1.94	0.48
1:J:137:ASN:HD22	1:J:138:ASN:N	2.11	0.48
3:F:100:LEU:HD11	3:F:107:HIS:CG	2.49	0.48
2:N:100:TYR:HB3	2:N:103:PRO:HG2	1.95	0.48
3:O:82:PHE:CD1	3:O:83:PRO:HA	2.48	0.48
1:V:19:VAL:HG22	1:V:75:ILE:HB	1.96	0.48
2:W:48:VAL:HG23	2:W:64:VAL:HG11	1.94	0.48
3:Y:95:PHE:CE1	3:Y:110:VAL:HG13	2.48	0.48
1:G:137:ASN:HD22	1:G:138:ASN:N	2.11	0.48
2:H:95:TYR:N	2:H:95:TYR:CD1	2.81	0.48
1:M:32:TYR:HB3	1:M:91:ASP:HB2	1.95	0.48
1:M:108:ARG:NH1	1:M:111:ALA:HB2	2.28	0.48
2:T:97:ALA:HB1	2:T:105:PHE:HA	1.96	0.48
1:D:14:SER:HA	1:D:107:LYS:HB3	1.96	0.48
3:F:42:LEU:HD22	3:F:52:PHE:CE1	2.49	0.48
3:F:67:TRP:O	3:F:79:LEU:N	2.41	0.48
1:G:120:PRO:HD3	1:G:132:VAL:HG12	1.96	0.48
2:H:100:TYR:O	2:H:103:PRO:HD2	2.14	0.48
1:S:107:LYS:HA	1:S:140:TYR:OH	2.14	0.48
1:C:70:ASP:C	1:C:71:PHE:HD1	2.18	0.48
1:V:66:GLY:HA3	1:V:71:PHE:HA	1.95	0.48
2:W:78:THR:HB	2:W:80:TYR:HE1	1.79	0.48
2:T:20:LEU:HD22	2:T:112:THR:HG21	1.96	0.48
1:D:65:SER:O	1:D:72:THR:N	2.43	0.47
2:E:97:ALA:HB1	2:E:105:PHE:HA	1.95	0.47
2:N:200:ILE:HG13	2:N:215:LYS:HG2	1.94	0.47
2:Q:31:SER:HA	3:R:139:ARG:NE	2.27	0.47
1:V:106:ILE:HB	1:V:166:GLN:NE2	2.28	0.47
1:V:115:VAL:C	1:V:116:PHE:HD1	2.16	0.47
2:E:27:PHE:CE2	2:E:29:PHE:HA	2.49	0.47
1:J:132:VAL:HG11	1:J:192:TYR:HD2	1.79	0.47
2:N:101:ASN:ND2	3:O:34:PRO:HB2	2.29	0.47
5:Z:1:NAG:O5	5:Z:4:FUC:H5	2.14	0.47
1:D:70:ASP:C	1:D:71:PHE:HD1	2.18	0.47
2:E:48:VAL:HG23	2:E:64:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:62:PHE:CD1	1:P:75:ILE:HG12	2.50	0.47
3:Y:100:LEU:HD11	3:Y:107:HIS:CG	2.49	0.47
1:C:186:TYR:HA	1:C:192:TYR:OH	2.13	0.47
2:B:12:VAL:O	2:B:116:VAL:HA	2.14	0.47
2:H:129:LEU:HB2	2:H:144:GLY:C	2.34	0.47
1:M:189:HIS:HB2	1:M:192:TYR:CE1	2.48	0.47
2:Q:31:SER:C	2:Q:32:TYR:HD1	2.18	0.47
3:X:69:ARG:HB3	3:X:79:LEU:HD21	1.96	0.47
2:W:97:ALA:HB1	2:W:105:PHE:HA	1.96	0.47
3:A:79:LEU:HB3	3:A:95:PHE:CD2	2.39	0.47
2:K:95:TYR:N	2:K:95:TYR:CD1	2.83	0.47
2:N:31:SER:C	2:N:32:TYR:HD1	2.18	0.47
3:O:122:LEU:HD23	3:O:139:ARG:HG2	1.96	0.47
3:X:79:LEU:HD22	3:X:95:PHE:HE2	1.79	0.47
1:C:132:VAL:HG23	1:C:179:LEU:HB3	1.96	0.47
2:E:27:PHE:CZ	2:E:98:LYS:HD3	2.50	0.47
3:F:37:PHE:HZ	3:F:67:TRP:HZ3	1.63	0.47
1:G:5:THR:HA	1:G:100:GLN:HE22	1.79	0.47
1:G:70:ASP:OD2	3:X:39:PRO:HB3	2.15	0.47
1:J:70:ASP:OD2	3:Y:39:PRO:HB3	2.14	0.47
3:L:75:GLN:NE2	3:L:76:THR:O	2.47	0.47
2:N:95:TYR:CD1	2:N:95:TYR:N	2.82	0.47
1:V:136:LEU:HB2	1:V:175:LEU:HB3	1.96	0.47
2:W:200:ILE:CD1	2:W:215:LYS:HG2	2.45	0.47
2:B:153:GLU:HB2	2:B:154:PRO:HA	1.97	0.47
3:L:95:PHE:CE1	3:L:110:VAL:HG13	2.50	0.47
2:W:153:GLU:HB2	2:W:154:PRO:HA	1.96	0.47
3:X:95:PHE:CE1	3:X:110:VAL:HG13	2.50	0.47
1:S:14:SER:HA	1:S:107:LYS:HB3	1.96	0.47
2:T:105:PHE:HB3	2:T:108:TRP:CZ2	2.50	0.47
2:T:200:ILE:CD1	2:T:215:LYS:HG2	2.44	0.47
2:T:201:CYS:O	2:T:213:ASP:HA	2.15	0.47
2:H:149:ASP:OD1	2:H:176:GLN:NE2	2.48	0.47
1:J:37:GLN:O	1:J:45:LYS:N	2.46	0.47
1:V:186:TYR:HA	1:V:192:TYR:OH	2.14	0.47
1:S:108:ARG:HG2	1:S:109:THR:N	2.29	0.47
2:T:101:ASN:HD22	3:Y:138:LEU:HD12	1.78	0.47
3:L:39:PRO:HB3	1:S:70:ASP:OD2	2.15	0.47
1:P:189:HIS:HB2	1:P:192:TYR:CE1	2.49	0.47
3:A:39:PRO:HG2	3:A:42:LEU:HG	1.97	0.46
2:E:124:PRO:HB3	2:E:150:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:LEU:HD22	3:F:95:PHE:HE2	1.80	0.46
1:G:98:PHE:CD2	2:H:45:LEU:HB2	2.50	0.46
1:J:39:LYS:HB2	1:J:42:LYS:HD2	1.97	0.46
1:J:145:LYS:HE3	1:J:147:GLN:NE2	2.29	0.46
2:K:95:TYR:N	2:K:95:TYR:HD1	2.13	0.46
2:N:27:PHE:CE2	2:N:29:PHE:HA	2.50	0.46
1:P:124:GLN:HG2	1:P:129:THR:O	2.15	0.46
3:R:95:PHE:CD2	3:R:110:VAL:HG22	2.50	0.46
3:X:37:PHE:CE2	3:X:140:ALA:HB3	2.50	0.46
1:S:108:ARG:N	1:S:140:TYR:CE2	2.84	0.46
2:T:141:ALA:HB3	2:T:194:LEU:HD11	1.96	0.46
1:G:115:VAL:HA	1:G:135:LEU:O	2.16	0.46
2:H:143:LEU:HD22	2:H:199:TYR:CD2	2.50	0.46
1:D:19:VAL:HG22	1:D:75:ILE:HB	1.98	0.46
1:M:120:PRO:HB3	1:M:131:SER:H	1.80	0.46
1:M:149:LYS:HE2	1:M:195:GLU:HB2	1.98	0.46
2:W:105:PHE:HB3	2:W:108:TRP:CZ2	2.51	0.46
3:A:94:ARG:HA	3:A:111:VAL:HG22	1.97	0.46
2:E:200:ILE:HG13	2:E:215:LYS:HG2	1.97	0.46
3:F:94:ARG:HA	3:F:111:VAL:HG22	1.96	0.46
1:G:116:PHE:N	1:G:116:PHE:CD1	2.83	0.46
1:V:160:GLN:HE22	2:W:176:GLN:HA	1.80	0.46
1:S:108:ARG:HB3	1:S:140:TYR:CE2	2.50	0.46
2:T:199:TYR:CD1	2:T:199:TYR:N	2.84	0.46
2:B:13:GLN:N	2:B:13:GLN:OE1	2.48	0.46
2:B:105:PHE:HB3	2:B:108:TRP:CZ2	2.50	0.46
1:J:108:ARG:NH1	1:J:111:ALA:HB2	2.31	0.46
2:K:3:GLN:HB2	2:K:25:SER:OG	2.14	0.46
3:R:100:LEU:HD11	3:R:107:HIS:CD2	2.51	0.46
1:S:24:ARG:HG3	1:S:70:ASP:OD1	2.16	0.46
2:E:20:LEU:HD22	2:E:112:THR:HG21	1.98	0.46
2:K:102:HIS:NE2	3:L:34:PRO:HD2	2.31	0.46
1:V:120:PRO:HB3	1:V:131:SER:H	1.80	0.46
1:D:142:ARG:HD2	1:D:173:TYR:HE2	1.81	0.46
2:K:199:TYR:CD1	2:K:199:TYR:N	2.84	0.46
3:O:126:ILE:HG12	3:O:134:ILE:HG12	1.98	0.46
1:V:98:PHE:CD2	2:W:45:LEU:HB2	2.51	0.46
1:S:115:VAL:HA	1:S:135:LEU:O	2.16	0.46
1:S:186:TYR:HA	1:S:192:TYR:OH	2.15	0.46
2:T:33:ALA:HB3	2:T:99:SER:HB3	1.98	0.46
1:C:108:ARG:HG2	1:C:109:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:TYR:CD1	2:B:199:TYR:N	2.84	0.46
1:D:124:GLN:HG2	1:D:129:THR:O	2.15	0.46
3:F:64:VAL:HG13	3:F:128:LEU:HD11	1.97	0.46
1:G:19:VAL:HG22	1:G:75:ILE:HB	1.98	0.46
3:L:67:TRP:O	3:L:79:LEU:N	2.40	0.46
2:W:199:TYR:N	2:W:199:TYR:CD1	2.84	0.46
2:B:12:VAL:HG11	2:B:86:LEU:HD13	1.97	0.46
2:B:31:SER:C	2:B:32:TYR:HD1	2.19	0.46
2:B:69:THR:OG1	2:B:82:GLN:HB3	2.16	0.46
2:K:200:ILE:CD1	2:K:215:LYS:HG2	2.44	0.46
2:Q:95:TYR:CD1	2:Q:95:TYR:N	2.82	0.46
3:X:82:PHE:HE2	3:X:99:GLN:CB	2.28	0.46
3:F:94:ARG:HG3	3:F:111:VAL:HG22	1.97	0.46
2:H:199:TYR:N	2:H:199:TYR:CD1	2.84	0.46
2:H:200:ILE:CD1	2:H:215:LYS:HG2	2.46	0.46
2:K:48:VAL:HG23	2:K:64:VAL:HG11	1.98	0.46
2:K:106:ASP:OD1	2:K:107:TYR:N	2.49	0.46
3:O:79:LEU:HD22	3:O:95:PHE:CE2	2.50	0.46
2:W:27:PHE:CE2	2:W:29:PHE:HA	2.51	0.46
1:S:98:PHE:CD2	2:T:45:LEU:HB2	2.51	0.46
2:B:176:GLN:HG2	2:B:180:LEU:O	2.15	0.45
1:G:70:ASP:C	1:G:71:PHE:HD1	2.20	0.45
2:Q:27:PHE:CE2	2:Q:29:PHE:HA	2.51	0.45
1:C:120:PRO:HB3	1:C:131:SER:H	1.81	0.45
2:E:199:TYR:N	2:E:199:TYR:CD1	2.84	0.45
3:F:71:SER:HB3	3:F:72:PRO:HD2	1.98	0.45
1:P:191:VAL:C	1:P:192:TYR:HD1	2.19	0.45
2:Q:48:VAL:HG23	2:Q:64:VAL:HG21	1.97	0.45
3:R:82:PHE:HA	3:R:83:PRO:C	2.36	0.45
1:C:120:PRO:HD3	1:C:132:VAL:HG12	1.98	0.45
1:D:120:PRO:HD3	1:D:132:VAL:HG12	1.99	0.45
2:N:48:VAL:HG23	2:N:64:VAL:HG21	1.98	0.45
3:O:69:ARG:HB3	3:O:79:LEU:HD21	1.97	0.45
1:S:124:GLN:HG2	1:S:129:THR:O	2.16	0.45
3:A:64:VAL:HA	3:A:83:PRO:HD2	1.99	0.45
3:F:82:PHE:HA	3:F:83:PRO:C	2.37	0.45
1:G:132:VAL:HG23	1:G:179:LEU:HB3	1.98	0.45
1:J:108:ARG:HG2	1:J:109:THR:N	2.31	0.45
2:K:31:SER:C	2:K:32:TYR:HD1	2.20	0.45
2:K:150:TYR:HE1	2:K:181:TYR:HB2	1.81	0.45
2:B:95:TYR:N	2:B:95:TYR:CD1	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:HIS:HB2	2:B:103:PRO:HD3	1.99	0.45
3:A:67:TRP:CZ2	3:A:121:TYR:HD2	2.35	0.45
1:D:116:PHE:N	1:D:116:PHE:CD1	2.84	0.45
3:F:79:LEU:HD22	3:F:95:PHE:CE2	2.52	0.45
3:F:129:ALA:HB1	3:F:130:PRO:HD2	1.99	0.45
3:I:79:LEU:HD22	3:I:95:PHE:CE2	2.50	0.45
1:J:6:GLN:NE2	1:J:86:TYR:O	2.50	0.45
1:J:132:VAL:HG23	1:J:179:LEU:HB3	1.99	0.45
3:X:121:TYR:CE1	3:X:142:LEU:HB3	2.50	0.45
2:T:27:PHE:CE2	2:T:29:PHE:HA	2.51	0.45
1:G:108:ARG:HG2	1:G:109:THR:N	2.31	0.45
3:I:52:PHE:N	3:I:52:PHE:CD1	2.85	0.45
2:K:98:LYS:HE3	2:K:106:ASP:OD2	2.17	0.45
2:N:98:LYS:HE3	2:N:106:ASP:OD2	2.17	0.45
2:Q:200:ILE:CD1	2:Q:215:LYS:HG2	2.46	0.45
3:Y:64:VAL:HG12	3:Y:83:PRO:HD2	1.98	0.45
1:D:37:GLN:O	1:D:45:LYS:N	2.47	0.45
1:J:116:PHE:CD1	1:J:116:PHE:N	2.85	0.45
2:N:95:TYR:N	2:N:95:TYR:HD1	2.13	0.45
2:T:69:THR:OG1	2:T:82:GLN:HB3	2.17	0.45
1:C:98:PHE:CD2	2:B:45:LEU:HB2	2.51	0.45
2:N:129:LEU:HB2	2:N:144:GLY:C	2.37	0.45
3:O:94:ARG:HH12	3:O:117:ASP:CG	2.20	0.45
1:P:120:PRO:HD3	1:P:132:VAL:HG12	1.99	0.45
2:Q:48:VAL:HG23	2:Q:64:VAL:HG11	1.99	0.45
2:W:201:CYS:O	2:W:213:ASP:HA	2.17	0.45
2:T:12:VAL:HG11	2:T:86:LEU:HD13	1.99	0.45
2:E:106:ASP:OD1	2:E:107:TYR:N	2.49	0.45
1:M:3:GLN:HB2	1:M:26:SER:HB2	1.98	0.45
2:Q:69:THR:OG1	2:Q:82:GLN:HB3	2.17	0.45
2:Q:102:HIS:CE1	3:R:34:PRO:HD2	2.52	0.45
3:R:52:PHE:CD1	3:R:52:PHE:N	2.85	0.45
3:X:52:PHE:HZ	3:X:142:LEU:HB2	1.82	0.45
1:C:19:VAL:HG22	1:C:75:ILE:HB	2.00	0.44
3:A:129:ALA:HB1	3:A:130:PRO:HD2	2.00	0.44
2:E:12:VAL:HG11	2:E:86:LEU:HD13	1.99	0.44
2:E:69:THR:HG1	2:E:82:GLN:HB3	1.82	0.44
1:G:189:HIS:HB2	1:G:192:TYR:CE1	2.52	0.44
3:I:37:PHE:HZ	3:I:67:TRP:HZ3	1.65	0.44
3:O:82:PHE:HA	3:O:83:PRO:C	2.37	0.44
1:V:132:VAL:HG11	1:V:192:TYR:HD2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:79:LEU:HD22	3:X:95:PHE:CE2	2.52	0.44
1:C:149:LYS:HB2	1:C:193:ALA:HB3	1.98	0.44
2:B:200:ILE:CD1	2:B:215:LYS:HG2	2.46	0.44
2:E:95:TYR:CD1	2:E:95:TYR:N	2.85	0.44
1:G:89:GLN:HG3	1:G:98:PHE:CE1	2.52	0.44
2:H:27:PHE:CZ	2:H:98:LYS:HD3	2.52	0.44
2:H:98:LYS:HE3	2:H:106:ASP:OD2	2.18	0.44
3:I:79:LEU:HB3	3:I:95:PHE:CD2	2.41	0.44
1:J:66:GLY:HA3	1:J:71:PHE:HA	1.98	0.44
2:N:199:TYR:N	2:N:199:TYR:CD1	2.85	0.44
3:O:67:TRP:O	3:O:79:LEU:N	2.44	0.44
2:Q:95:TYR:N	2:Q:95:TYR:HD1	2.14	0.44
1:P:66:GLY:HA3	1:P:71:PHE:HA	1.98	0.44
2:W:20:LEU:HD22	2:W:112:THR:HG21	1.98	0.44
3:X:64:VAL:HG12	3:X:83:PRO:CG	2.47	0.44
3:A:82:PHE:HA	3:A:83:PRO:C	2.38	0.44
2:H:31:SER:C	2:H:32:TYR:HD1	2.21	0.44
3:L:71:SER:HB3	3:L:72:PRO:HD2	2.00	0.44
2:Q:101:ASN:ND2	3:R:138:LEU:HD12	2.24	0.44
1:C:37:GLN:O	1:C:45:LYS:N	2.47	0.44
3:A:62:SER:O	3:A:128:LEU:N	2.35	0.44
1:J:70:ASP:C	1:J:71:PHE:HD1	2.21	0.44
1:V:33:LEU:HA	1:V:89:GLN:O	2.18	0.44
1:V:108:ARG:NH1	1:V:111:ALA:HB2	2.32	0.44
3:X:87:SER:O	3:X:91:GLN:HB2	2.18	0.44
2:T:189:VAL:HG21	2:T:199:TYR:HE2	1.79	0.44
2:B:27:PHE:CE2	2:B:29:PHE:HA	2.52	0.44
3:A:44:VAL:HG21	3:A:50:ALA:HB2	2.00	0.44
3:A:52:PHE:CD1	3:A:52:PHE:N	2.86	0.44
1:D:125:LEU:O	1:D:183:LYS:HD2	2.17	0.44
2:H:27:PHE:CE2	2:H:29:PHE:HA	2.53	0.44
3:L:79:LEU:HD22	3:L:95:PHE:CE2	2.53	0.44
2:T:11:LEU:HB2	2:T:152:PRO:HG3	1.99	0.44
2:T:31:SER:C	2:T:32:TYR:HD1	2.20	0.44
1:C:142:ARG:HD2	1:C:173:TYR:HE2	1.82	0.44
3:A:35:PRO:HG2	3:A:137:SER:HB3	1.99	0.44
2:N:147:VAL:HG11	2:N:155:VAL:HG11	1.99	0.44
3:X:87:SER:HA	3:X:91:GLN:OE1	2.18	0.44
1:S:39:LYS:HB2	1:S:42:LYS:HD2	2.00	0.44
3:Y:79:LEU:HB3	3:Y:95:PHE:CD2	2.45	0.44
2:B:129:LEU:HB2	2:B:144:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:129:ALA:HB1	3:L:130:PRO:HD2	2.00	0.44
2:W:48:VAL:HG23	2:W:64:VAL:HG21	2.00	0.44
1:C:190:LYS:HG3	1:C:191:VAL:HG13	1.99	0.44
3:A:37:PHE:CZ	3:A:67:TRP:CZ3	3.05	0.44
1:D:115:VAL:HA	1:D:135:LEU:O	2.17	0.44
2:K:141:ALA:HB3	2:K:194:LEU:HD11	2.00	0.44
2:N:92:ALA:HB3	2:N:94:TYR:CE1	2.53	0.44
3:R:94:ARG:HG2	3:R:111:VAL:O	2.17	0.44
1:S:108:ARG:NH1	1:S:111:ALA:HB2	2.33	0.44
2:T:107:TYR:HD1	2:T:107:TYR:N	2.16	0.44
3:Y:37:PHE:CZ	3:Y:67:TRP:HZ3	2.36	0.44
2:B:164:LEU:HD21	2:B:187:VAL:HG21	1.99	0.43
1:D:87:TYR:HE2	2:E:45:LEU:HG	1.83	0.43
1:D:108:ARG:NH1	1:D:111:ALA:HB2	2.33	0.43
2:K:153:GLU:HB2	2:K:154:PRO:HA	1.99	0.43
2:N:192:SER:C	3:Y:72:PRO:HB2	2.38	0.43
2:Q:199:TYR:CD1	2:Q:199:TYR:N	2.85	0.43
1:V:173:TYR:N	1:V:173:TYR:HD1	2.16	0.43
2:T:149:ASP:OD1	2:T:176:GLN:NE2	2.51	0.43
1:G:116:PHE:HD1	1:G:116:PHE:N	2.15	0.43
2:K:105:PHE:HB3	2:K:108:TRP:CZ2	2.53	0.43
1:M:116:PHE:N	1:M:116:PHE:CD1	2.86	0.43
3:Y:69:ARG:HB3	3:Y:79:LEU:HD21	1.99	0.43
3:A:65:LEU:HD13	3:A:106:PHE:CE2	2.53	0.43
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.33	0.43
3:I:71:SER:HB3	3:I:72:PRO:HD2	2.01	0.43
3:R:67:TRP:CH2	3:R:121:TYR:HD2	2.36	0.43
1:V:89:GLN:HG3	1:V:98:PHE:CE1	2.53	0.43
3:X:49:ASN:OD1	3:X:111:VAL:HA	2.18	0.43
2:B:95:TYR:N	2:B:95:TYR:HD1	2.17	0.43
1:D:191:VAL:HA	1:D:209:PHE:O	2.18	0.43
2:E:102:HIS:CE1	3:F:34:PRO:HD2	2.53	0.43
1:G:43:ALA:HB2	2:H:110:GLN:HA	2.00	0.43
3:I:31:PRO:HB2	3:I:33:ASN:OD1	2.18	0.43
1:M:124:GLN:HG2	1:M:129:THR:O	2.19	0.43
1:P:87:TYR:HE2	2:Q:45:LEU:HG	1.84	0.43
3:R:145:THR:HG22	3:R:146:GLU:N	2.31	0.43
2:W:12:VAL:O	2:W:116:VAL:HA	2.18	0.43
2:W:53:GLY:O	2:W:72:ARG:NH1	2.51	0.43
3:X:37:PHE:CZ	3:X:67:TRP:HZ3	2.36	0.43
1:S:87:TYR:HE2	2:T:45:LEU:HG	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:106:ASP:OD1	2:T:107:TYR:N	2.51	0.43
1:C:124:GLN:HG2	1:C:129:THR:O	2.17	0.43
3:A:52:PHE:HZ	3:A:142:LEU:HB2	1.83	0.43
2:H:20:LEU:HD22	2:H:112:THR:HG21	2.00	0.43
3:L:62:SER:O	3:L:128:LEU:N	2.36	0.43
1:V:124:GLN:HG2	1:V:129:THR:O	2.17	0.43
3:A:69:ARG:HD3	3:A:121:TYR:CE1	2.54	0.43
1:D:116:PHE:HD1	1:D:116:PHE:N	2.16	0.43
2:E:22:CYS:HB3	2:E:79:LEU:HB3	2.00	0.43
2:Q:201:CYS:O	2:Q:213:ASP:HA	2.18	0.43
3:X:84:GLU:OE2	3:X:87:SER:N	2.52	0.43
3:Y:52:PHE:CD1	3:Y:52:PHE:N	2.86	0.43
2:E:159:TRP:HB3	2:E:164:LEU:HD23	2.00	0.43
1:J:116:PHE:HD1	1:J:116:PHE:N	2.16	0.43
2:Q:22:CYS:HB3	2:Q:79:LEU:HB3	2.01	0.43
3:X:52:PHE:CD1	3:X:52:PHE:N	2.86	0.43
3:Y:94:ARG:HH12	3:Y:117:ASP:CG	2.22	0.43
2:B:36:TRP:NE1	2:B:81:LEU:HB2	2.34	0.43
2:E:199:TYR:N	2:E:199:TYR:HD1	2.17	0.43
3:F:52:PHE:CE1	3:F:142:LEU:HD12	2.53	0.43
3:F:52:PHE:CD1	3:F:52:PHE:N	2.87	0.43
1:G:124:GLN:HG2	1:G:129:THR:O	2.19	0.43
1:J:132:VAL:CG2	1:J:179:LEU:HB3	2.49	0.43
1:J:176:SER:HG	2:K:171:PHE:HD2	1.65	0.43
2:K:201:CYS:O	2:K:213:ASP:HA	2.18	0.43
3:L:69:ARG:HB3	3:L:79:LEU:HD21	2.00	0.43
3:L:145:THR:HG22	3:L:146:GLU:N	2.31	0.43
2:Q:2:VAL:HB	2:Q:107:TYR:CD2	2.54	0.43
1:V:173:TYR:N	1:V:173:TYR:CD1	2.87	0.43
2:W:107:TYR:HD1	2:W:107:TYR:N	2.17	0.43
1:S:142:ARG:HD2	1:S:173:TYR:HE2	1.84	0.43
3:Y:129:ALA:HB1	3:Y:130:PRO:HD2	2.01	0.43
3:A:104:ARG:NH1	1:P:92:TYR:OH	2.52	0.43
3:A:145:THR:HG22	3:A:146:GLU:N	2.31	0.43
1:D:108:ARG:HG2	1:D:109:THR:N	2.34	0.43
2:E:36:TRP:NE1	2:E:81:LEU:HB2	2.34	0.43
3:F:100:LEU:HD11	3:F:107:HIS:CD2	2.54	0.43
3:L:31:PRO:HB2	3:L:33:ASN:OD1	2.19	0.43
2:Q:98:LYS:HE3	2:Q:106:ASP:OD2	2.19	0.43
1:V:132:VAL:CG2	1:V:179:LEU:HB3	2.49	0.43
2:T:2:VAL:HB	2:T:107:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:153:GLU:HB2	2:T:154:PRO:HA	2.01	0.43
3:Y:31:PRO:HB2	3:Y:33:ASN:OD1	2.18	0.43
2:H:105:PHE:HB3	2:H:108:TRP:CZ2	2.54	0.43
1:M:120:PRO:HD3	1:M:132:VAL:HG12	2.01	0.43
2:W:79:LEU:C	2:W:80:TYR:HD1	2.22	0.43
3:X:35:PRO:CG	3:X:125:ALA:HB2	2.48	0.43
1:S:149:LYS:HB2	1:S:193:ALA:HB3	2.01	0.43
2:T:98:LYS:HE3	2:T:106:ASP:OD2	2.19	0.43
1:C:98:PHE:CD1	1:C:98:PHE:N	2.86	0.42
2:B:97:ALA:HB1	2:B:105:PHE:HA	2.01	0.42
2:E:129:LEU:HB2	2:E:144:GLY:C	2.40	0.42
1:G:142:ARG:HD2	1:G:173:TYR:HE2	1.83	0.42
1:J:65:SER:O	1:J:72:THR:N	2.48	0.42
1:J:124:GLN:HG2	1:J:129:THR:O	2.18	0.42
1:J:142:ARG:HD2	1:J:173:TYR:HE2	1.84	0.42
2:K:101:ASN:ND2	3:L:34:PRO:HB2	2.33	0.42
3:L:100:LEU:HD11	3:L:107:HIS:CG	2.54	0.42
1:P:160:GLN:HE22	2:Q:176:GLN:HA	1.84	0.42
1:V:14:SER:HA	1:V:107:LYS:HB3	2.00	0.42
1:V:108:ARG:HG2	1:V:109:THR:N	2.34	0.42
1:S:176:SER:HB3	2:T:171:PHE:CE2	2.54	0.42
3:Y:82:PHE:HA	3:Y:83:PRO:C	2.38	0.42
2:E:31:SER:C	2:E:32:TYR:HD1	2.22	0.42
1:G:176:SER:HG	2:H:171:PHE:HD2	1.63	0.42
3:I:145:THR:HG22	3:I:146:GLU:N	2.31	0.42
2:K:48:VAL:HG23	2:K:64:VAL:HG21	2.01	0.42
2:B:141:ALA:HB3	2:B:194:LEU:HD11	2.01	0.42
2:E:153:GLU:HB2	2:E:154:PRO:HA	2.02	0.42
1:M:132:VAL:HG11	1:M:192:TYR:HD2	1.83	0.42
3:O:145:THR:HG22	3:O:146:GLU:N	2.31	0.42
3:Y:79:LEU:HD22	3:Y:95:PHE:CE2	2.52	0.42
2:E:198:THR:C	2:E:199:TYR:HD1	2.23	0.42
3:F:87:SER:OG	3:F:88:GLN:OE1	2.31	0.42
1:J:189:HIS:HB2	1:J:192:TYR:HE1	1.85	0.42
2:K:107:TYR:HD1	2:K:107:TYR:N	2.17	0.42
2:K:199:TYR:N	2:K:199:TYR:HD1	2.17	0.42
1:P:87:TYR:CE2	2:Q:45:LEU:HG	2.54	0.42
3:X:117:ASP:OD1	3:X:117:ASP:N	2.53	0.42
2:T:199:TYR:N	2:T:199:TYR:HD1	2.16	0.42
1:D:40:PRO:HB2	1:D:165:GLU:HG3	2.01	0.42
2:E:189:VAL:HG11	2:E:199:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:52:PHE:N	3:I:52:PHE:HD1	2.18	0.42
3:L:52:PHE:HZ	3:L:142:LEU:HB2	1.84	0.42
3:L:94:ARG:HH12	3:L:117:ASP:CG	2.23	0.42
2:N:196:THR:CG2	3:Y:73:SER:HA	2.47	0.42
3:O:35:PRO:HG3	3:O:56:PHE:CD1	2.54	0.42
3:R:67:TRP:CZ2	3:R:121:TYR:HD2	2.37	0.42
3:A:52:PHE:CE1	3:A:142:LEU:HD12	2.55	0.42
1:G:108:ARG:NH1	1:G:111:ALA:HB2	2.35	0.42
1:M:98:PHE:CD1	1:M:98:PHE:N	2.87	0.42
1:M:132:VAL:HG23	1:M:179:LEU:HB3	2.02	0.42
1:M:176:SER:HG	2:N:171:PHE:HD2	1.66	0.42
1:P:173:TYR:CD1	1:P:173:TYR:N	2.88	0.42
2:Q:124:PRO:HB3	2:Q:150:TYR:HB3	2.02	0.42
2:W:12:VAL:HG11	2:W:86:LEU:HD13	2.00	0.42
2:W:199:TYR:N	2:W:199:TYR:HD1	2.16	0.42
1:S:66:GLY:HA3	1:S:71:PHE:HA	2.02	0.42
1:C:108:ARG:NH1	1:C:111:ALA:HB2	2.34	0.42
2:B:48:VAL:HG23	2:B:64:VAL:HG11	2.01	0.42
2:H:201:CYS:O	2:H:213:ASP:HA	2.18	0.42
1:J:16:GLY:HA2	1:J:77:SER:OG	2.20	0.42
2:K:13:GLN:HG3	2:K:14:PRO:HD2	2.01	0.42
3:L:82:PHE:HA	3:L:83:PRO:C	2.40	0.42
2:N:100:TYR:HD2	2:N:103:PRO:HG2	1.84	0.42
2:Q:101:ASN:HB2	3:R:138:LEU:HD11	2.02	0.42
3:R:120:THR:C	3:R:121:TYR:HD1	2.23	0.42
2:W:32:TYR:HB3	2:W:99:SER:O	2.20	0.42
2:T:107:TYR:N	2:T:107:TYR:CD1	2.87	0.42
2:E:11:LEU:HB2	2:E:152:PRO:HG3	2.02	0.42
3:I:126:ILE:HG12	3:I:134:ILE:HG12	2.02	0.42
1:P:97:THR:C	1:P:98:PHE:HD1	2.22	0.42
2:T:124:PRO:HB3	2:T:150:TYR:HB3	2.02	0.42
1:C:115:VAL:HA	1:C:135:LEU:O	2.19	0.42
2:H:199:TYR:N	2:H:199:TYR:HD1	2.18	0.42
2:K:27:PHE:CE2	2:K:29:PHE:HA	2.55	0.42
3:L:65:LEU:HD13	3:L:106:PHE:CE2	2.55	0.42
1:P:71:PHE:CD1	1:P:71:PHE:N	2.88	0.42
1:P:142:ARG:HD2	1:P:173:TYR:HE2	1.85	0.42
1:V:34:ASN:ND2	1:V:91:ASP:OD2	2.50	0.42
2:T:36:TRP:NE1	2:T:81:LEU:HB2	2.34	0.42
1:C:116:PHE:CD1	1:C:116:PHE:N	2.88	0.42
3:A:67:TRP:CH2	3:A:121:TYR:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:VAL:HA	1:M:135:LEU:O	2.20	0.42
3:O:120:THR:C	3:O:121:TYR:HD1	2.24	0.42
3:X:37:PHE:CE1	3:X:67:TRP:HZ3	2.37	0.42
1:C:173:TYR:N	1:C:173:TYR:CD1	2.88	0.41
3:A:122:LEU:HD23	3:A:139:ARG:HG2	2.01	0.41
1:J:115:VAL:HA	1:J:135:LEU:O	2.20	0.41
1:M:16:GLY:HA2	1:M:77:SER:OG	2.20	0.41
2:N:189:VAL:HG11	2:N:199:TYR:CE2	2.55	0.41
3:R:37:PHE:CZ	3:R:67:TRP:CZ3	3.06	0.41
3:X:37:PHE:HB2	3:X:137:SER:HB2	2.02	0.41
3:X:122:LEU:HD12	3:X:122:LEU:C	2.40	0.41
1:G:132:VAL:HG11	1:G:192:TYR:HD2	1.84	0.41
2:H:33:ALA:HB3	2:H:99:SER:HB3	2.02	0.41
1:P:159:SER:OG	1:P:177:SER:OG	2.38	0.41
1:V:190:LYS:HG3	1:V:191:VAL:HG13	2.02	0.41
2:W:31:SER:C	2:W:32:TYR:HD1	2.23	0.41
2:T:48:VAL:HG23	2:T:64:VAL:HG11	2.02	0.41
1:C:132:VAL:CG2	1:C:179:LEU:HB3	2.50	0.41
2:B:27:PHE:CZ	2:B:98:LYS:HD3	2.55	0.41
2:B:177:SER:OG	2:E:66:GLY:HA2	2.21	0.41
3:A:105:ASP:C	3:A:106:PHE:HD1	2.22	0.41
3:I:129:ALA:HB1	3:I:130:PRO:HD2	2.01	0.41
2:K:155:VAL:HG23	2:K:205:HIS:HD2	1.85	0.41
1:M:160:GLN:HE21	2:N:174:VAL:HG22	1.84	0.41
3:R:39:PRO:HG2	3:R:42:LEU:HG	2.03	0.41
1:V:87:TYR:CE2	2:W:45:LEU:HG	2.55	0.41
2:W:189:VAL:HG11	2:W:199:TYR:HE2	1.85	0.41
2:T:157:VAL:HA	2:T:202:ASN:O	2.20	0.41
1:C:189:HIS:HB2	1:C:192:TYR:CE1	2.52	0.41
3:F:67:TRP:CH2	3:F:121:TYR:HD2	2.38	0.41
2:H:78:THR:HB	2:H:80:TYR:HE1	1.85	0.41
1:M:6:GLN:NE2	1:M:86:TYR:O	2.51	0.41
1:M:116:PHE:HD1	1:M:116:PHE:N	2.18	0.41
1:P:115:VAL:HA	1:P:135:LEU:O	2.20	0.41
1:P:176:SER:HB3	2:Q:171:PHE:CE2	2.54	0.41
3:A:120:THR:C	3:A:121:TYR:HD1	2.23	0.41
1:D:35:TRP:CG	1:D:73:LEU:HD12	2.56	0.41
2:H:48:VAL:HG23	2:H:64:VAL:HG21	2.02	0.41
3:I:52:PHE:CE1	3:I:142:LEU:HD12	2.56	0.41
1:J:189:HIS:HB2	1:J:192:TYR:CE1	2.55	0.41
3:L:120:THR:C	3:L:121:TYR:HD1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:66:GLY:HA3	1:M:71:PHE:HA	2.02	0.41
1:M:87:TYR:CE2	2:N:45:LEU:HG	2.56	0.41
1:M:186:TYR:HA	1:M:192:TYR:OH	2.20	0.41
1:P:132:VAL:HG23	1:P:179:LEU:HB3	2.02	0.41
2:W:204:ASN:ND2	2:W:211:LYS:HE2	2.35	0.41
1:S:3:GLN:HB2	1:S:26:SER:HB2	2.01	0.41
3:A:79:LEU:HD22	3:A:95:PHE:CE2	2.55	0.41
1:G:190:LYS:HG3	1:G:191:VAL:HG13	2.01	0.41
2:H:102:HIS:NE2	3:I:34:PRO:HD2	2.36	0.41
2:K:36:TRP:NE1	2:K:81:LEU:HB2	2.35	0.41
2:N:69:THR:OG1	2:N:82:GLN:HB3	2.21	0.41
2:N:199:TYR:N	2:N:199:TYR:HD1	2.19	0.41
1:P:98:PHE:N	1:P:98:PHE:CD1	2.88	0.41
1:V:33:LEU:HB3	1:V:71:PHE:CD2	2.56	0.41
1:V:71:PHE:N	1:V:71:PHE:CD1	2.88	0.41
3:Y:100:LEU:HD11	3:Y:107:HIS:CD2	2.55	0.41
1:C:5:THR:HA	1:C:100:GLN:HE22	1.85	0.41
1:C:137:ASN:OD1	2:B:188:THR:OG1	2.29	0.41
1:D:93:GLY:HA2	3:F:32:TRP:H	1.85	0.41
1:G:37:GLN:O	1:G:45:LYS:N	2.52	0.41
1:J:120:PRO:HD3	1:J:132:VAL:CG1	2.51	0.41
3:L:52:PHE:N	3:L:52:PHE:CD1	2.88	0.41
1:M:173:TYR:N	1:M:173:TYR:CD1	2.89	0.41
2:N:192:SER:HB3	3:Y:72:PRO:CG	2.49	0.41
1:V:125:LEU:O	1:V:183:LYS:HD2	2.21	0.41
2:T:105:PHE:HB3	2:T:108:TRP:CE2	2.56	0.41
2:B:11:LEU:HB2	2:B:152:PRO:HG3	2.03	0.41
2:B:91:THR:HG23	2:B:115:THR:HA	2.02	0.41
2:B:177:SER:O	2:E:69:THR:HG22	2.20	0.41
3:A:71:SER:HB3	3:A:72:PRO:HD2	2.02	0.41
3:A:95:PHE:CE1	3:A:110:VAL:HG13	2.56	0.41
1:D:98:PHE:CD1	1:D:98:PHE:N	2.88	0.41
1:D:173:TYR:N	1:D:173:TYR:CD1	2.89	0.41
2:H:2:VAL:HB	2:H:107:TYR:CE2	2.55	0.41
2:H:189:VAL:HG11	2:H:199:TYR:CE2	2.56	0.41
3:I:39:PRO:HG2	3:I:42:LEU:HG	2.03	0.41
2:N:27:PHE:CZ	2:N:98:LYS:HD3	2.56	0.41
3:O:67:TRP:CH2	3:O:121:TYR:HD2	2.39	0.41
3:X:112:ARG:HB3	3:X:114:ARG:NH2	2.35	0.41
2:T:22:CYS:HB3	2:T:79:LEU:HB3	2.03	0.41
2:T:129:LEU:HB2	2:T:144:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:VAL:HG11	2:B:199:TYR:CE2	2.56	0.41
3:A:52:PHE:N	3:A:52:PHE:HD1	2.19	0.41
3:A:104:ARG:HG2	3:A:105:ASP:OD1	2.21	0.41
3:F:31:PRO:HB2	3:F:33:ASN:OD1	2.20	0.41
3:I:51:THR:C	3:I:52:PHE:HD1	2.25	0.41
3:I:82:PHE:HA	3:I:83:PRO:C	2.41	0.41
2:K:107:TYR:N	2:K:107:TYR:CD1	2.88	0.41
1:M:176:SER:HB3	2:N:171:PHE:CE2	2.55	0.41
2:N:105:PHE:HB3	2:N:108:TRP:CZ2	2.56	0.41
2:N:201:CYS:O	2:N:213:ASP:HA	2.21	0.41
1:P:3:GLN:HB2	1:P:26:SER:HB2	2.03	0.41
1:P:173:TYR:N	1:P:173:TYR:HD1	2.18	0.41
3:R:51:THR:C	3:R:52:PHE:HD1	2.25	0.41
1:V:142:ARG:HD2	1:V:173:TYR:CE2	2.55	0.41
2:W:107:TYR:N	2:W:107:TYR:CD1	2.88	0.41
3:X:33:ASN:H	3:X:135:LYS:HE2	1.86	0.41
3:X:44:VAL:HG21	3:X:50:ALA:HB2	2.02	0.41
1:S:87:TYR:CE2	2:T:45:LEU:HG	2.55	0.41
1:S:112:ALA:HA	1:S:113:PRO:HD3	1.97	0.41
3:Y:94:ARG:HG3	3:Y:111:VAL:HG22	2.03	0.41
1:C:173:TYR:N	1:C:173:TYR:HD1	2.19	0.41
2:E:78:THR:HB	2:E:80:TYR:HE1	1.86	0.41
1:G:97:THR:C	1:G:98:PHE:HD1	2.24	0.41
1:G:98:PHE:N	1:G:98:PHE:CD1	2.88	0.41
2:N:196:THR:HG21	3:Y:73:SER:CA	2.46	0.41
2:Q:20:LEU:HD22	2:Q:112:THR:HG21	2.02	0.41
1:V:98:PHE:N	1:V:98:PHE:CD1	2.89	0.41
3:X:62:SER:O	3:X:128:LEU:N	2.46	0.41
1:D:97:THR:C	1:D:98:PHE:HD1	2.25	0.40
1:J:158:ASN:O	1:J:179:LEU:HD12	2.22	0.40
2:K:36:TRP:CE2	2:K:81:LEU:HB2	2.56	0.40
1:P:33:LEU:HB3	1:P:71:PHE:CD2	2.56	0.40
1:V:65:SER:O	1:V:72:THR:N	2.53	0.40
3:X:100:LEU:HD11	3:X:107:HIS:CD2	2.56	0.40
2:T:78:THR:HB	2:T:80:TYR:HE1	1.86	0.40
1:C:112:ALA:HA	1:C:113:PRO:HD3	1.98	0.40
1:G:3:GLN:HB2	1:G:26:SER:HB2	2.03	0.40
3:O:32:TRP:NE1	3:O:34:PRO:HG3	2.37	0.40
1:P:89:GLN:HG3	1:P:98:PHE:CE1	2.56	0.40
1:P:186:TYR:HA	1:P:192:TYR:OH	2.21	0.40
2:W:101:ASN:HB3	2:W:102:HIS:H	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:125:LEU:O	1:S:183:LYS:HD2	2.22	0.40
3:Y:67:TRP:O	3:Y:79:LEU:N	2.47	0.40
2:E:95:TYR:N	2:E:95:TYR:HD1	2.20	0.40
3:F:94:ARG:HH12	3:F:117:ASP:CG	2.25	0.40
3:F:145:THR:HG22	3:F:146:GLU:N	2.31	0.40
1:P:115:VAL:HG22	1:P:136:LEU:HG	2.03	0.40
3:R:52:PHE:N	3:R:52:PHE:HD1	2.19	0.40
1:V:97:THR:C	1:V:98:PHE:HD1	2.25	0.40
1:S:116:PHE:N	1:S:116:PHE:CD1	2.89	0.40
2:T:79:LEU:C	2:T:80:TYR:HD1	2.25	0.40
1:C:70:ASP:OD2	3:R:39:PRO:HB3	2.22	0.40
1:D:112:ALA:HA	1:D:113:PRO:HD3	1.98	0.40
2:K:69:THR:OG1	2:K:82:GLN:HB3	2.21	0.40
3:L:52:PHE:CE1	3:L:142:LEU:HD12	2.56	0.40
1:M:140:TYR:CD1	1:M:141:PRO:HA	2.57	0.40
2:N:12:VAL:HG11	2:N:86:LEU:HD13	2.03	0.40
2:Q:79:LEU:C	2:Q:80:TYR:HD1	2.25	0.40
3:X:35:PRO:HG3	3:X:125:ALA:HB2	2.04	0.40
3:X:35:PRO:HG3	3:X:56:PHE:CD1	2.56	0.40
1:S:71:PHE:N	1:S:71:PHE:CD1	2.89	0.40
1:S:98:PHE:CD1	1:S:98:PHE:N	2.89	0.40
2:B:71:SER:OG	2:B:80:TYR:HB2	2.22	0.40
2:B:171:PHE:N	2:B:171:PHE:CD1	2.89	0.40
1:G:132:VAL:CG2	1:G:179:LEU:HB3	2.52	0.40
1:M:173:TYR:N	1:M:173:TYR:HD1	2.20	0.40
1:P:33:LEU:HA	1:P:89:GLN:O	2.21	0.40
1:P:136:LEU:HD21	1:P:196:VAL:HG21	2.02	0.40
3:R:35:PRO:HG3	3:R:56:PHE:CD1	2.57	0.40
1:V:147:GLN:HG3	1:V:195:GLU:HB3	2.02	0.40
3:X:39:PRO:HG2	3:X:42:LEU:HG	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	D	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	G	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	J	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	M	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	P	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	S	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
1	V	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
2	B	210/225 (93%)	200 (95%)	9 (4%)	1 (0%)	29	68
2	E	210/225 (93%)	201 (96%)	8 (4%)	1 (0%)	29	68
2	H	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	29	68
2	K	208/225 (92%)	200 (96%)	7 (3%)	1 (0%)	29	68
2	N	205/225 (91%)	197 (96%)	7 (3%)	1 (0%)	29	68
2	Q	206/225 (92%)	197 (96%)	8 (4%)	1 (0%)	29	68
2	T	208/225 (92%)	197 (95%)	10 (5%)	1 (0%)	29	68
2	W	200/225 (89%)	193 (96%)	6 (3%)	1 (0%)	29	68
3	A	107/168 (64%)	102 (95%)	5 (5%)	0	100	100
3	F	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
3	I	109/168 (65%)	102 (94%)	7 (6%)	0	100	100
3	L	108/168 (64%)	103 (95%)	5 (5%)	0	100	100
3	O	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
3	R	106/168 (63%)	100 (94%)	6 (6%)	0	100	100
3	X	115/168 (68%)	107 (93%)	7 (6%)	1 (1%)	17	56
3	Y	115/168 (68%)	107 (93%)	8 (7%)	0	100	100
All	All	4231/4856 (87%)	4049 (96%)	173 (4%)	9 (0%)	47	81

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	X	84	GLU
2	B	103	PRO
2	H	103	PRO

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Mol	Chain	Res	Type
2	Q	103	PRO
2	N	103	PRO
2	K	103	PRO
2	W	103	PRO
2	E	103	PRO
2	T	103	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	187/188 (100%)	183 (98%)	4 (2%)	53 79
1	D	187/188 (100%)	184 (98%)	3 (2%)	62 83
1	G	187/188 (100%)	184 (98%)	3 (2%)	62 83
1	J	187/188 (100%)	184 (98%)	3 (2%)	62 83
1	M	187/188 (100%)	184 (98%)	3 (2%)	62 83
1	P	187/188 (100%)	186 (100%)	1 (0%)	88 94
1	S	187/188 (100%)	184 (98%)	3 (2%)	62 83
1	V	187/188 (100%)	186 (100%)	1 (0%)	88 94
2	B	178/188 (95%)	175 (98%)	3 (2%)	60 82
2	E	178/188 (95%)	175 (98%)	3 (2%)	60 82
2	H	174/188 (93%)	169 (97%)	5 (3%)	42 71
2	K	176/188 (94%)	171 (97%)	5 (3%)	43 72
2	N	173/188 (92%)	169 (98%)	4 (2%)	50 77
2	Q	174/188 (93%)	170 (98%)	4 (2%)	50 77
2	T	176/188 (94%)	171 (97%)	5 (3%)	43 72
2	W	171/188 (91%)	167 (98%)	4 (2%)	50 77
3	A	98/148 (66%)	96 (98%)	2 (2%)	55 79
3	F	103/148 (70%)	103 (100%)	0	100 100
3	I	99/148 (67%)	98 (99%)	1 (1%)	76 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	99/148 (67%)	99 (100%)	0	100 100
3	O	103/148 (70%)	103 (100%)	0	100 100
3	R	97/148 (66%)	96 (99%)	1 (1%)	76 88
3	X	103/148 (70%)	102 (99%)	1 (1%)	76 88
3	Y	103/148 (70%)	103 (100%)	0	100 100
All	All	3701/4192 (88%)	3642 (98%)	59 (2%)	62 83

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	98	PHE
1	C	116	PHE
1	C	137	ASN
1	C	173	TYR
2	B	32	TYR
2	B	95	TYR
2	B	199	TYR
3	A	52	PHE
3	A	104	ARG
1	D	116	PHE
1	D	137	ASN
1	D	173	TYR
2	E	80	TYR
2	E	95	TYR
2	E	199	TYR
1	G	116	PHE
1	G	137	ASN
1	G	173	TYR
2	H	32	TYR
2	H	80	TYR
2	H	95	TYR
2	H	107	TYR
2	H	150	TYR
3	I	52	PHE
1	J	116	PHE
1	J	137	ASN
1	J	173	TYR
2	K	32	TYR
2	K	95	TYR
2	K	107	TYR

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Mol	Chain	Res	Type
2	K	150	TYR
2	K	199	TYR
1	M	98	PHE
1	M	116	PHE
1	M	173	TYR
2	N	32	TYR
2	N	80	TYR
2	N	95	TYR
2	N	107	TYR
1	P	173	TYR
2	Q	32	TYR
2	Q	80	TYR
2	Q	95	TYR
2	Q	107	TYR
3	R	52	PHE
1	V	173	TYR
2	W	80	TYR
2	W	95	TYR
2	W	107	TYR
2	W	199	TYR
3	X	128	LEU
1	S	116	PHE
1	S	140	TYR
1	S	173	TYR
2	T	32	TYR
2	T	80	TYR
2	T	95	TYR
2	T	107	TYR
2	T	199	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	147	GLN
2	B	101	ASN
1	D	147	GLN
1	G	147	GLN
1	J	147	GLN
1	J	160	GLN
1	M	147	GLN
1	M	160	GLN
3	O	74	ASN

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Mol	Chain	Res	Type
1	P	147	GLN
1	P	166	GLN
2	Q	101	ASN
1	V	160	GLN
2	T	101	ASN
3	Y	74	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

45 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	$\#\|Z\| > 2$
4	NAG	U	1	4,3	14,14,15	0.30	0	17,19,21	0.59	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.59	0
4	BMA	U	3	4	11,11,12	0.26	0	15,15,17	0.70	0
4	MAN	U	4	4	11,11,12	0.23	0	15,15,17	0.67	0
5	NAG	Z	1	3,5	14,14,15	0.41	0	17,19,21	0.67	0
5	NAG	Z	2	5	14,14,15	0.26	0	17,19,21	0.35	0
5	BMA	Z	3	5	11,11,12	0.64	0	15,15,17	0.73	0
5	FUC	Z	4	5	10,10,11	0.35	0	14,14,16	0.71	0
6	NAG	a	1	6,3	14,14,15	0.42	0	17,19,21	0.79	0
6	NAG	a	2	6	14,14,15	0.23	0	17,19,21	0.48	0
6	FUC	a	3	6	10,10,11	0.24	0	14,14,16	0.66	0
7	NAG	b	1	3,7	14,14,15	0.20	0	17,19,21	0.60	0
7	NAG	b	2	7	14,14,15	0.32	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	c	1	3,8	14,14,15	0.40	0	17,19,21	0.66	0
8	NAG	c	2	8	14,14,15	0.38	0	17,19,21	0.48	0
8	BMA	c	3	8	11,11,12	0.55	0	15,15,17	0.79	0
8	FUC	c	4	8	10,10,11	0.26	0	14,14,16	0.63	0
9	NAG	d	1	9,3	14,14,15	0.29	0	17,19,21	0.62	0
9	FUC	d	2	9	10,10,11	0.25	0	14,14,16	1.06	1 (7%)
6	NAG	e	1	6,3	14,14,15	0.39	0	17,19,21	0.64	0
6	NAG	e	2	6	14,14,15	0.24	0	17,19,21	0.46	0
6	FUC	e	3	6	10,10,11	0.26	0	14,14,16	0.68	0
10	NAG	f	1	10,3	14,14,15	0.42	0	17,19,21	0.55	0
10	NAG	f	2	10	14,14,15	0.31	0	17,19,21	0.85	1 (5%)
10	BMA	f	3	10	11,11,12	0.26	0	15,15,17	0.68	0
10	MAN	f	4	10	11,11,12	0.24	0	15,15,17	0.96	0
10	MAN	f	5	10	11,11,12	0.21	0	15,15,17	0.64	0
10	FUC	f	6	10	10,10,11	0.24	0	14,14,16	0.69	0
5	NAG	g	1	3,5	14,14,15	0.42	0	17,19,21	0.79	0
5	NAG	g	2	5	14,14,15	0.29	0	17,19,21	0.72	0
5	BMA	g	3	5	11,11,12	0.24	0	15,15,17	0.68	0
5	FUC	g	4	5	10,10,11	0.26	0	14,14,16	0.71	0
5	NAG	h	1	3,5	14,14,15	0.43	0	17,19,21	0.87	1 (5%)
5	NAG	h	2	5	14,14,15	0.21	0	17,19,21	0.45	0
5	BMA	h	3	5	11,11,12	0.52	0	15,15,17	0.71	0
5	FUC	h	4	5	10,10,11	0.24	0	14,14,16	0.66	0
9	NAG	i	1	9,3	14,14,15	0.29	0	17,19,21	0.68	1 (5%)
9	FUC	i	2	9	10,10,11	0.26	0	14,14,16	0.56	0
6	NAG	j	1	6,3	14,14,15	0.43	0	17,19,21	0.48	0
6	NAG	j	2	6	14,14,15	0.31	0	17,19,21	0.54	0
6	FUC	j	3	6	10,10,11	0.25	0	14,14,16	0.61	0
5	NAG	k	1	3,5	14,14,15	0.42	0	17,19,21	0.65	0
5	NAG	k	2	5	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
5	BMA	k	3	5	11,11,12	0.56	0	15,15,17	0.71	0
5	FUC	k	4	5	10,10,11	0.25	0	14,14,16	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	U	3	4	-	0/2/19/22	0/1/1/1
4	MAN	U	4	4	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	0/2/19/22	0/1/1/1
5	FUC	Z	4	5	-	-	0/1/1/1
6	NAG	a	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	a	2	6	-	0/6/23/26	0/1/1/1
6	FUC	a	3	6	-	-	0/1/1/1
7	NAG	b	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	b	2	7	-	0/6/23/26	0/1/1/1
8	NAG	c	1	3,8	-	4/6/23/26	0/1/1/1
8	NAG	c	2	8	-	0/6/23/26	0/1/1/1
8	BMA	c	3	8	-	0/2/19/22	0/1/1/1
8	FUC	c	4	8	-	-	0/1/1/1
9	NAG	d	1	9,3	-	0/6/23/26	0/1/1/1
9	FUC	d	2	9	-	-	0/1/1/1
6	NAG	e	1	6,3	-	4/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	FUC	e	3	6	-	-	0/1/1/1
10	NAG	f	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	f	2	10	-	2/6/23/26	0/1/1/1
10	BMA	f	3	10	-	0/2/19/22	0/1/1/1
10	MAN	f	4	10	-	0/2/19/22	0/1/1/1
10	MAN	f	5	10	-	0/2/19/22	0/1/1/1
10	FUC	f	6	10	-	-	0/1/1/1
5	NAG	g	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1
5	BMA	g	3	5	-	0/2/19/22	0/1/1/1
5	FUC	g	4	5	-	-	0/1/1/1
5	NAG	h	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	h	2	5	-	0/6/23/26	0/1/1/1
5	BMA	h	3	5	-	0/2/19/22	0/1/1/1
5	FUC	h	4	5	-	-	0/1/1/1
9	NAG	i	1	9,3	-	4/6/23/26	0/1/1/1
9	FUC	i	2	9	-	-	0/1/1/1
6	NAG	j	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	j	2	6	-	0/6/23/26	0/1/1/1
6	FUC	j	3	6	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	k	1	3,5	-	4/6/23/26	0/1/1/1
5	NAG	k	2	5	-	0/6/23/26	0/1/1/1
5	BMA	k	3	5	-	0/2/19/22	0/1/1/1
5	FUC	k	4	5	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	d	2	FUC	O5-C1-C2	2.73	114.98	110.77
5	k	2	NAG	C4-C3-C2	-2.52	107.32	111.02
5	h	1	NAG	C1-O5-C5	2.33	115.35	112.19
10	f	2	NAG	O3-C3-C2	-2.28	104.74	109.47
9	i	1	NAG	O5-C5-C6	2.23	110.70	107.20

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
9	i	1	NAG	C8-C7-N2-C2
9	i	1	NAG	O7-C7-N2-C2
9	i	1	NAG	O5-C5-C6-O6
5	k	1	NAG	C8-C7-N2-C2
6	j	1	NAG	O5-C5-C6-O6
5	k	1	NAG	O7-C7-N2-C2
6	a	1	NAG	C8-C7-N2-C2
6	e	1	NAG	C8-C7-N2-C2
8	c	1	NAG	C8-C7-N2-C2
10	f	2	NAG	C8-C7-N2-C2
6	j	1	NAG	C4-C5-C6-O6
9	i	1	NAG	C4-C5-C6-O6
6	e	1	NAG	O7-C7-N2-C2
10	f	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
8	c	1	NAG	O5-C5-C6-O6
10	f	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	k	1	NAG	O5-C5-C6-O6
6	a	1	NAG	O7-C7-N2-C2
8	c	1	NAG	O7-C7-N2-C2
10	f	2	NAG	O7-C7-N2-C2
6	e	1	NAG	O5-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
8	c	1	NAG	C4-C5-C6-O6
6	e	1	NAG	C4-C5-C6-O6
5	k	1	NAG	C4-C5-C6-O6
5	g	2	NAG	C8-C7-N2-C2
5	h	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O7-C7-N2-C2
5	h	1	NAG	O7-C7-N2-C2
6	a	1	NAG	O5-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C8-C7-N2-C2
5	h	1	NAG	O5-C5-C6-O6
5	h	1	NAG	C4-C5-C6-O6

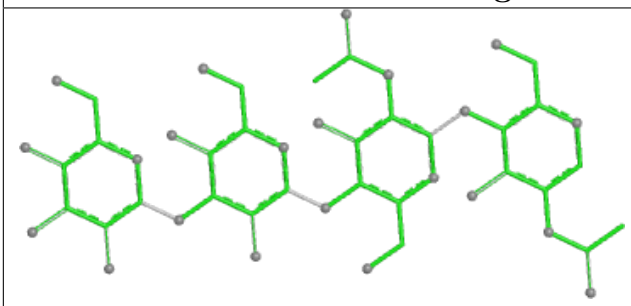
There are no ring outliers.

2 monomers are involved in 3 short contacts:

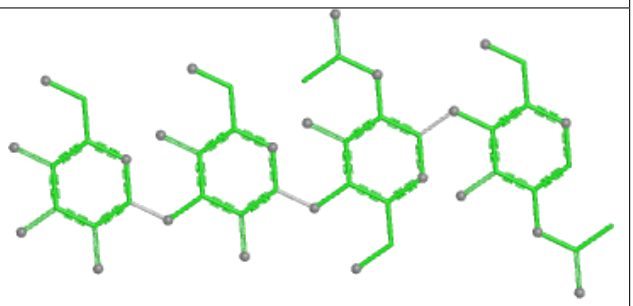
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	4	FUC	3	0
5	Z	1	NAG	3	0

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

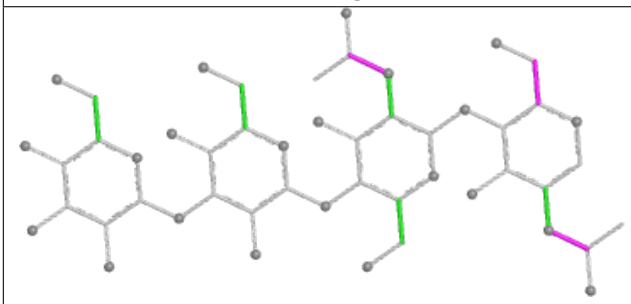
Oligosaccharide Chain U



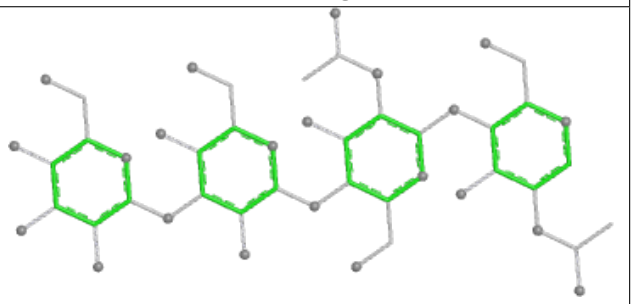
Bond lengths



Bond angles

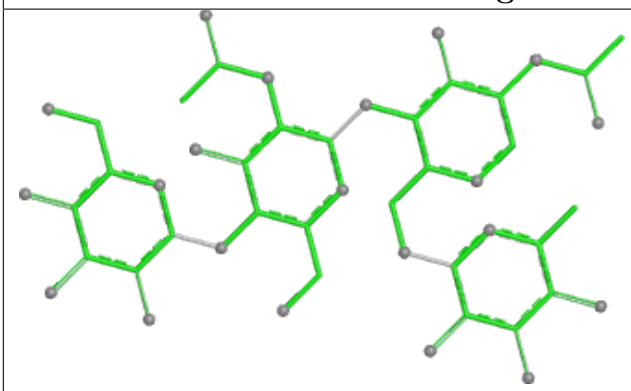


Torsions

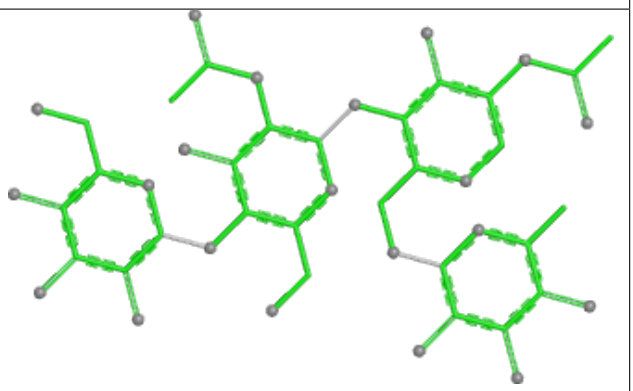


Rings

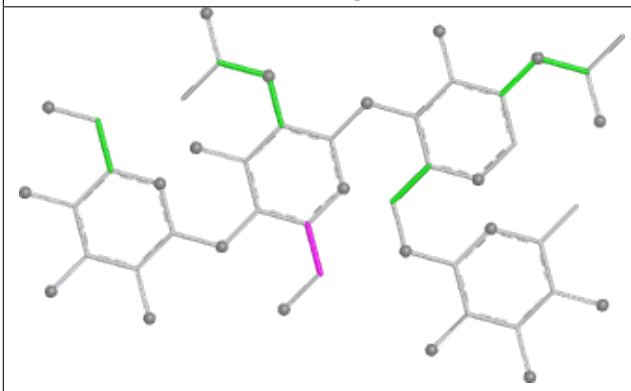
Oligosaccharide Chain Z



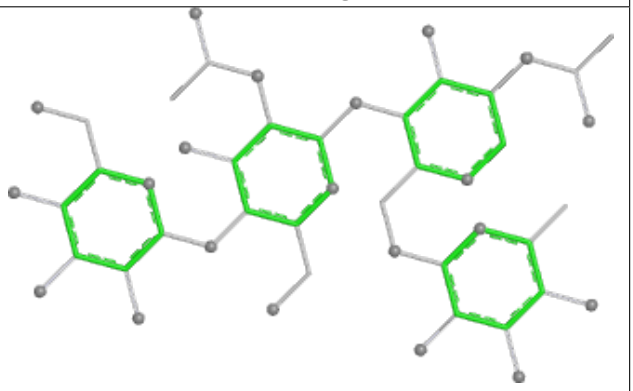
Bond lengths



Bond angles

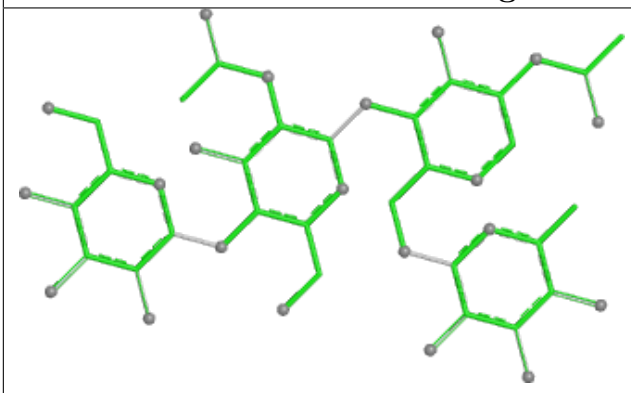


Torsions

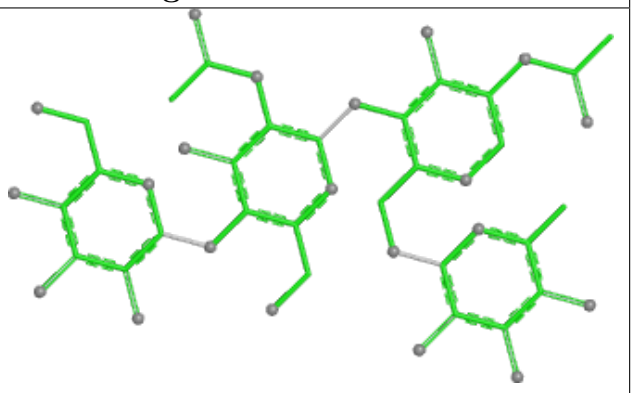


Rings

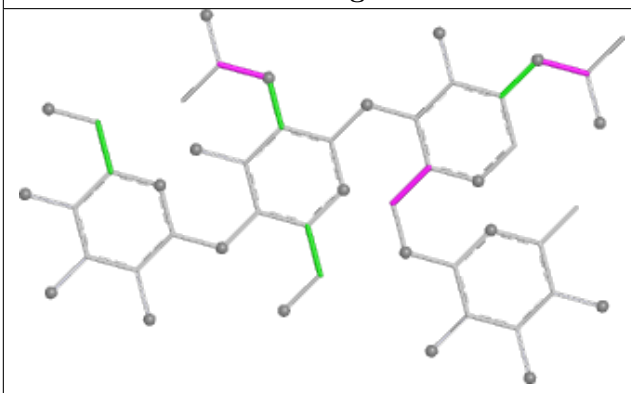
Oligosaccharide Chain g



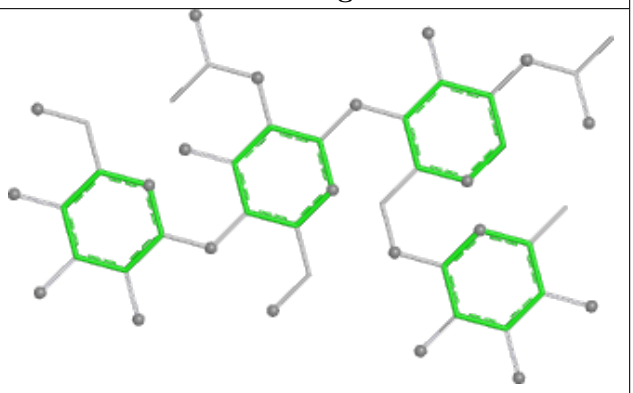
Bond lengths



Bond angles

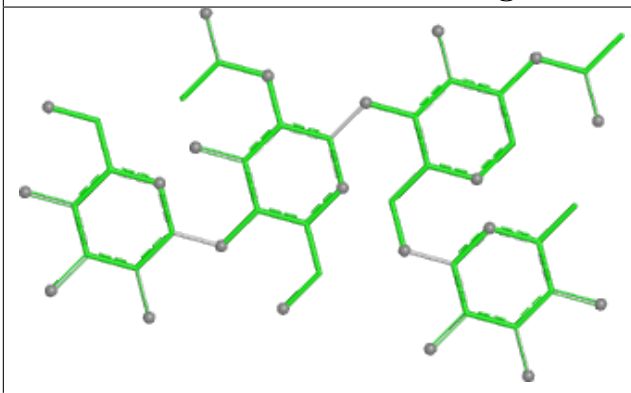


Torsions

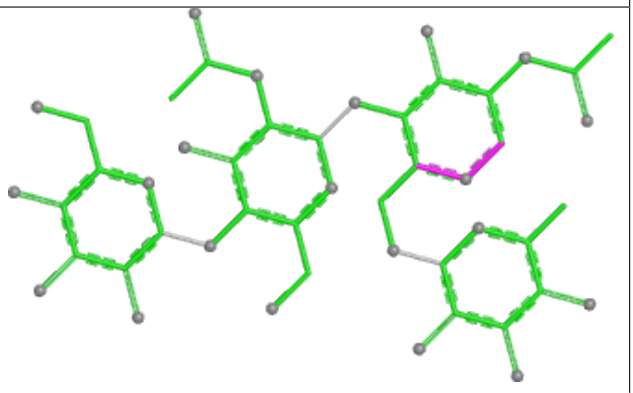


Rings

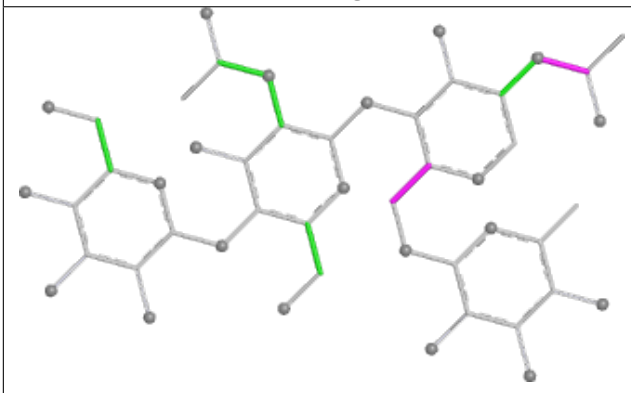
Oligosaccharide Chain h



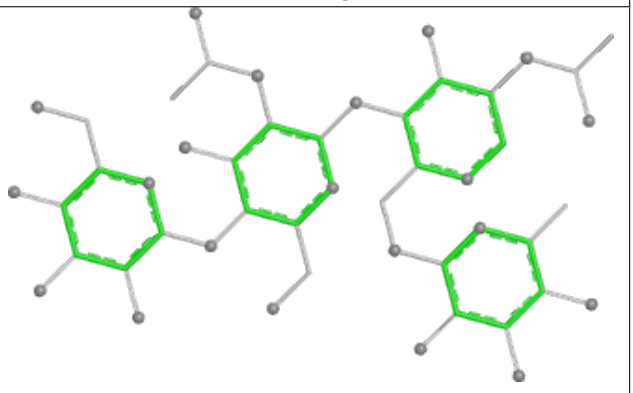
Bond lengths



Bond angles

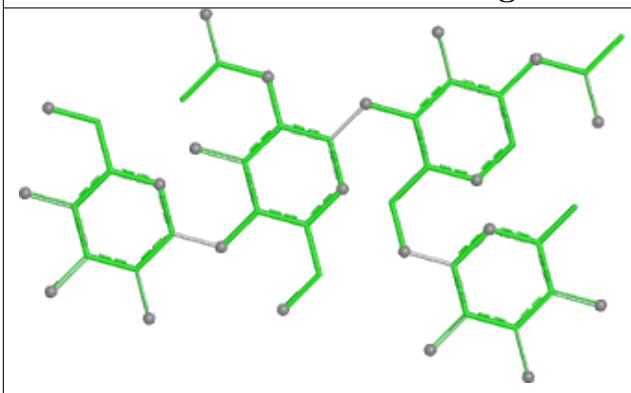


Torsions

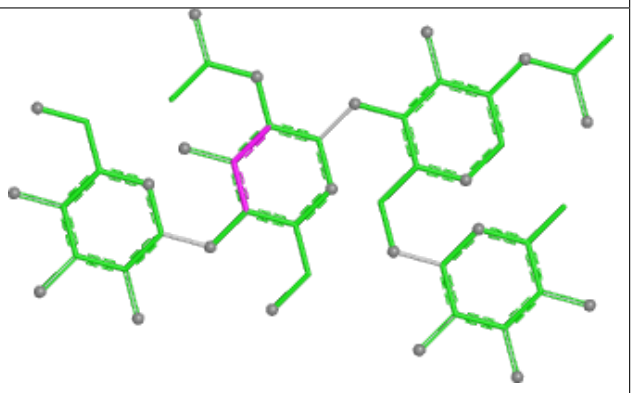


Rings

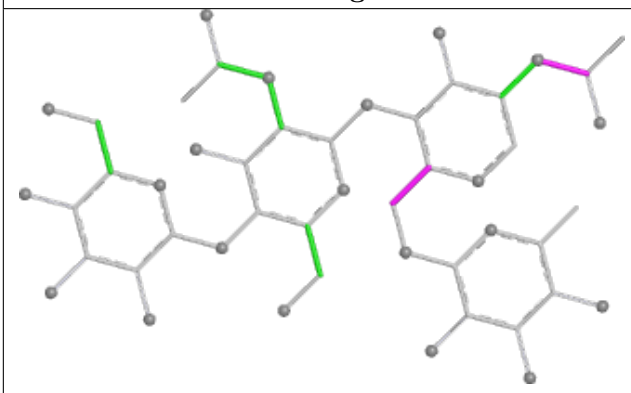
Oligosaccharide Chain k



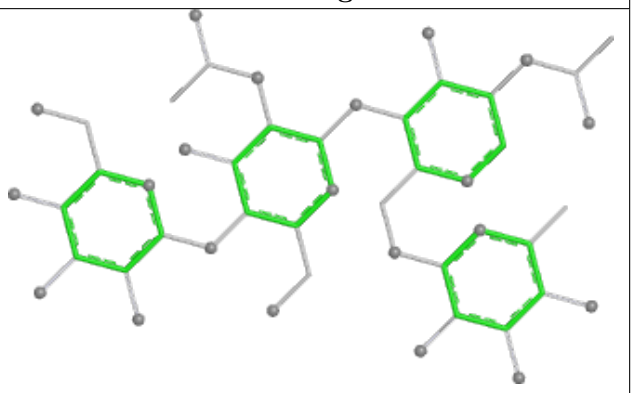
Bond lengths



Bond angles

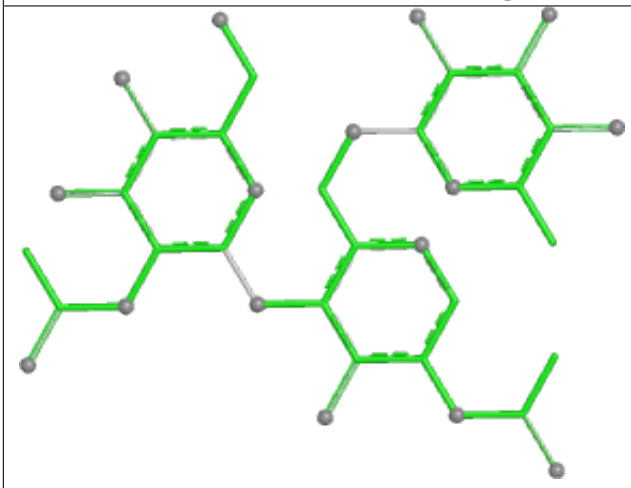


Torsions

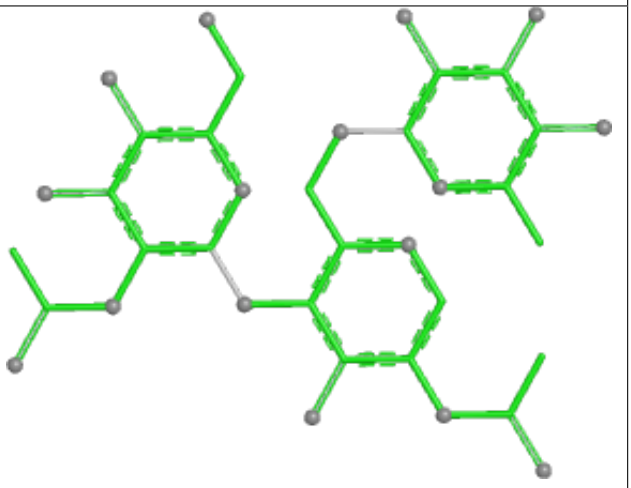


Rings

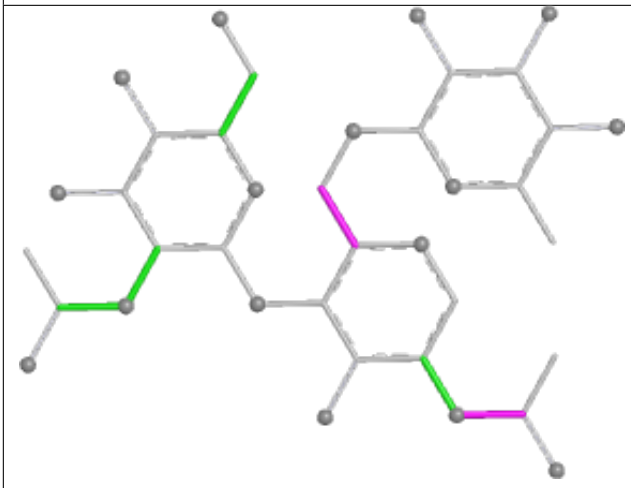
Oligosaccharide Chain a



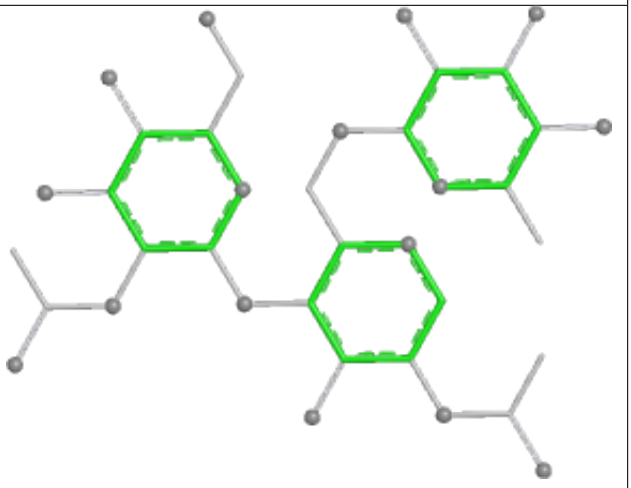
Bond lengths



Bond angles

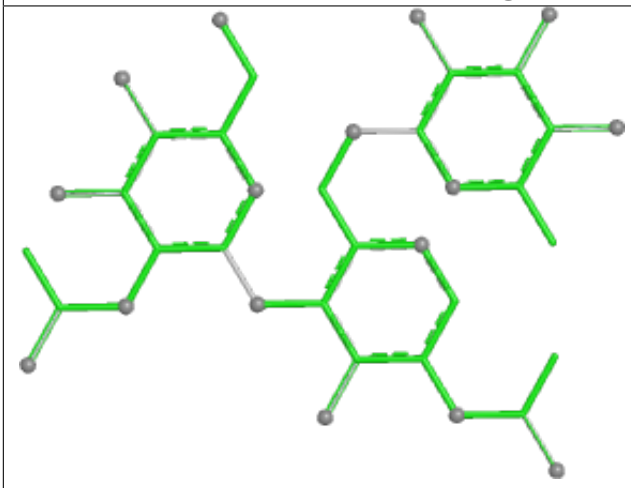


Torsions

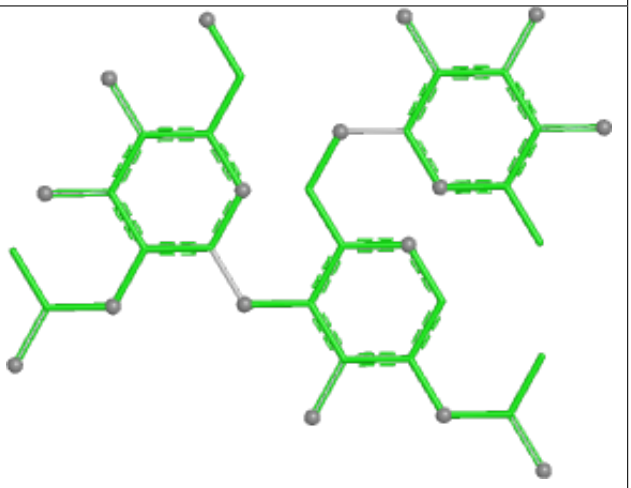


Rings

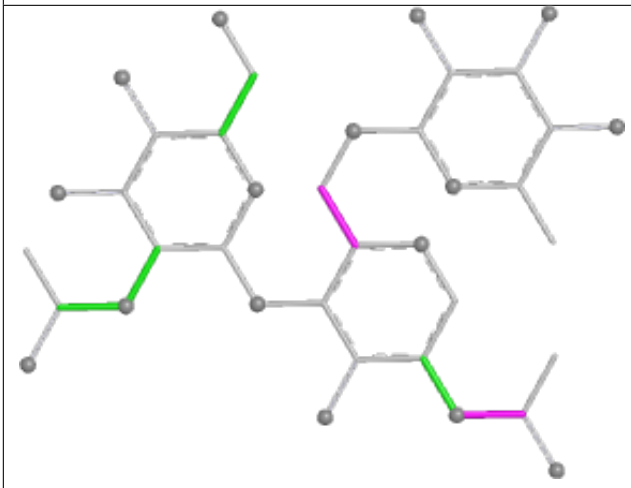
Oligosaccharide Chain e



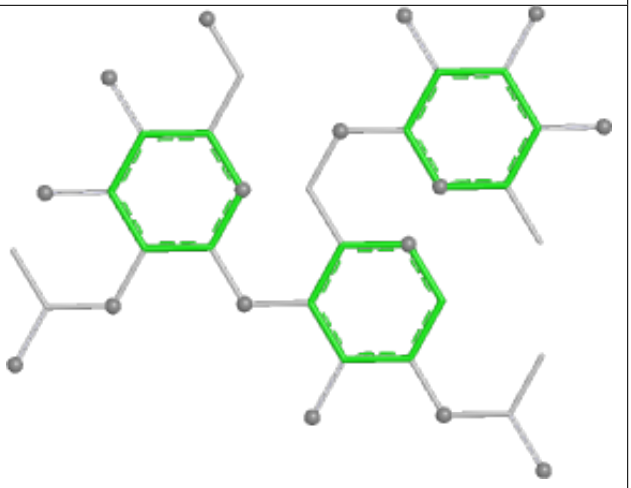
Bond lengths



Bond angles

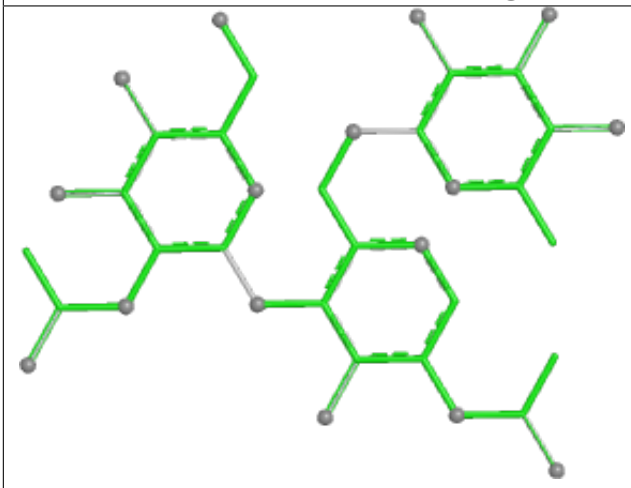


Torsions

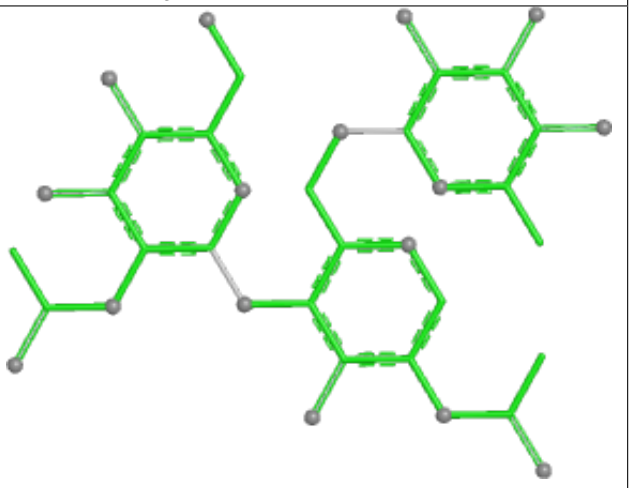


Rings

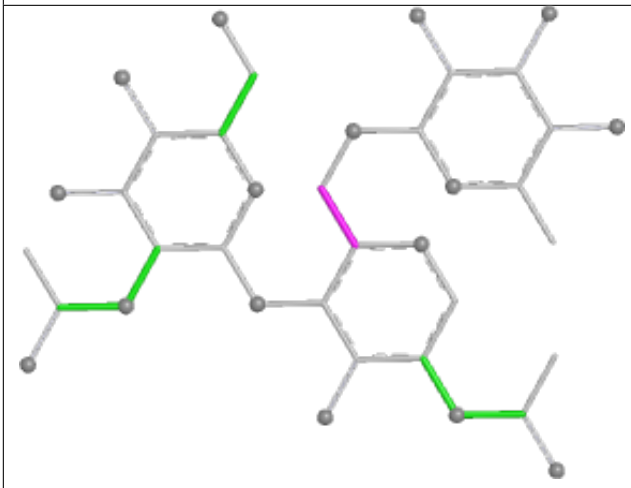
Oligosaccharide Chain j



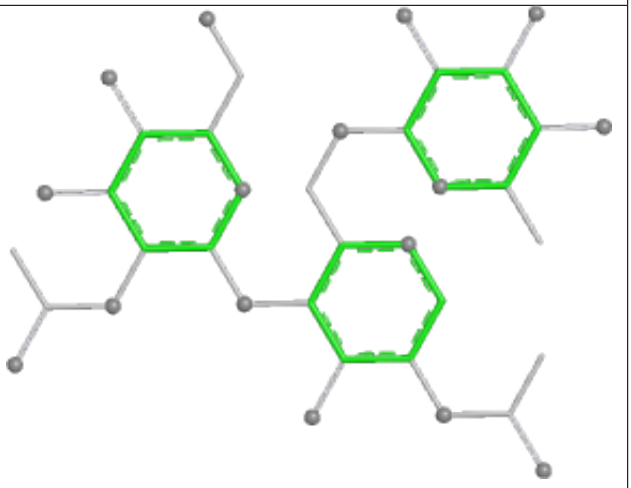
Bond lengths



Bond angles

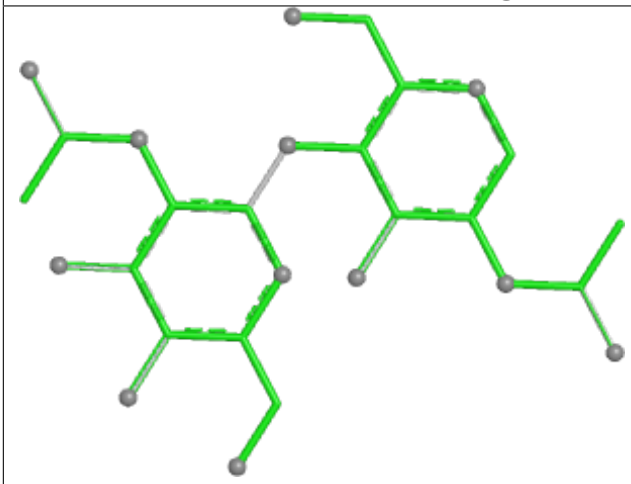


Torsions

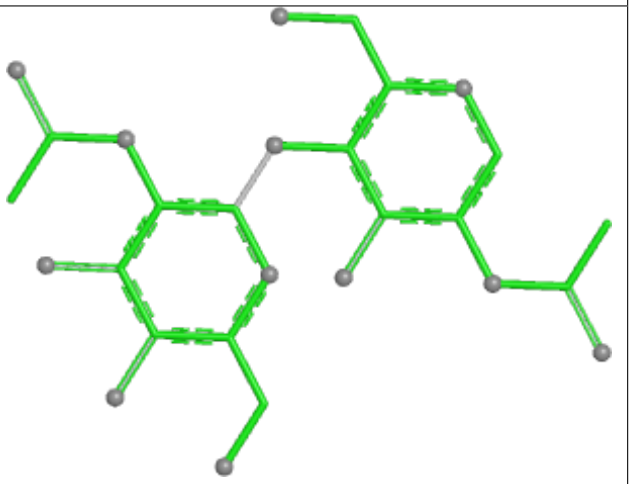


Rings

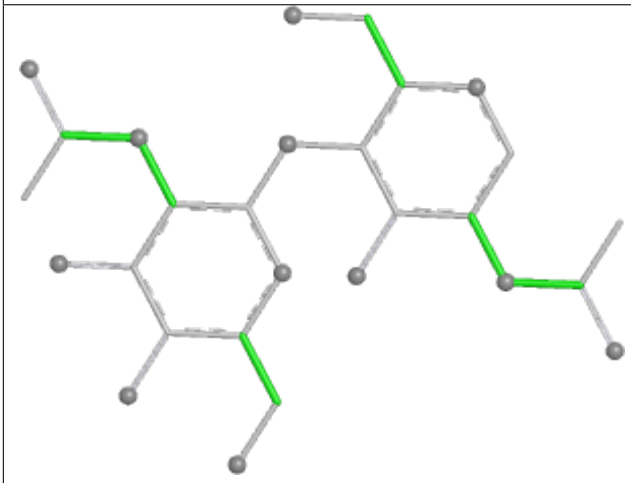
Oligosaccharide Chain b



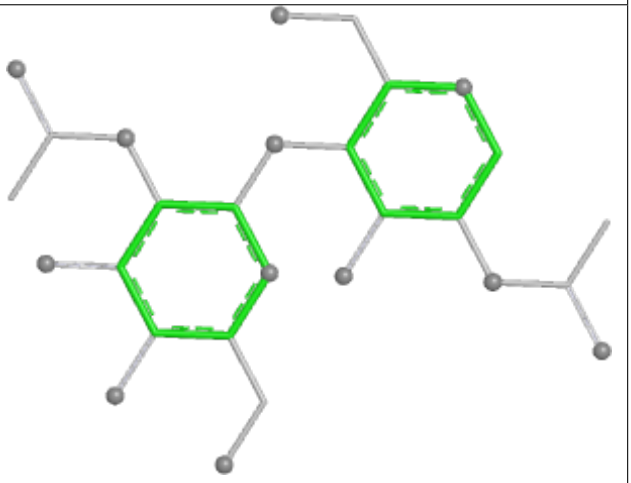
Bond lengths



Bond angles

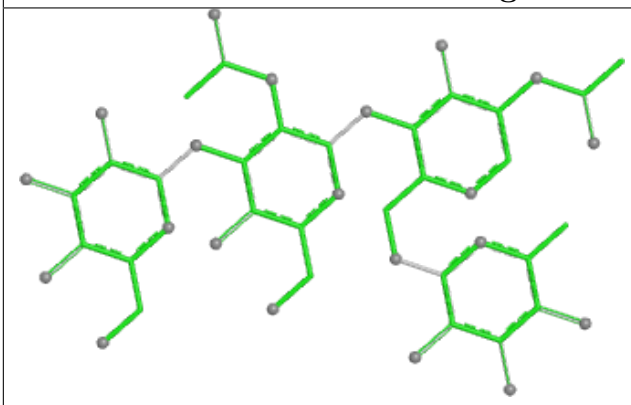


Torsions

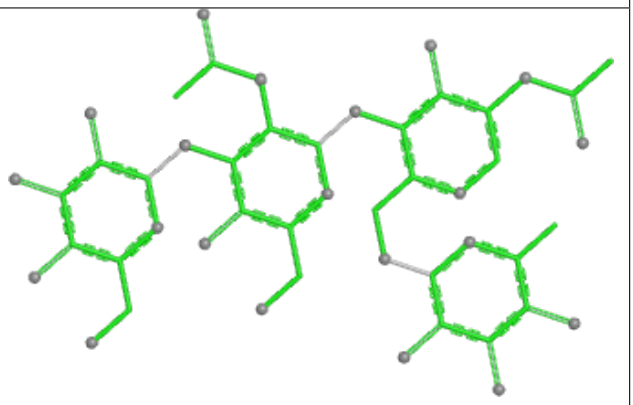


Rings

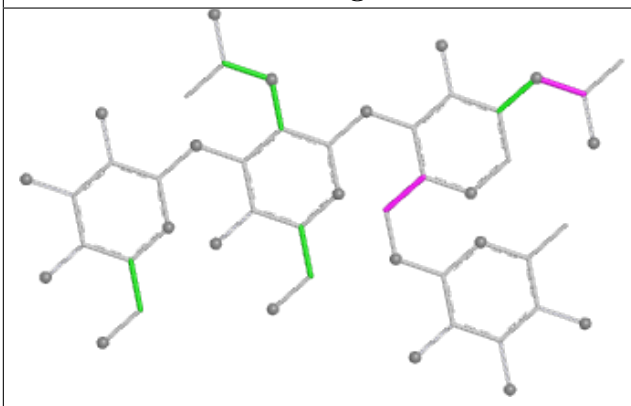
Oligosaccharide Chain c



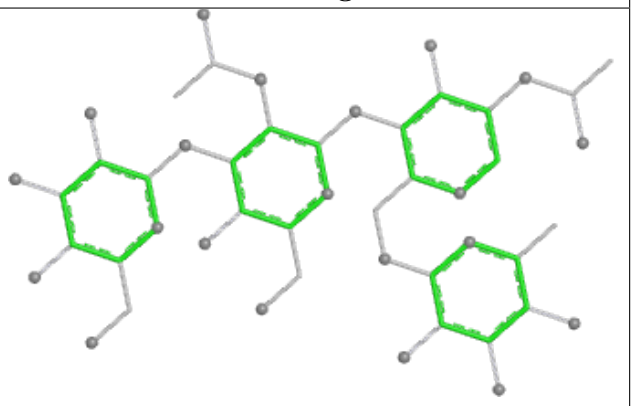
Bond lengths



Bond angles

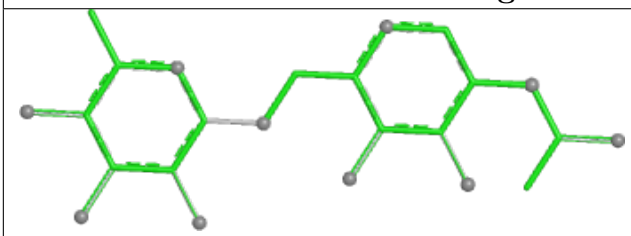


Torsions

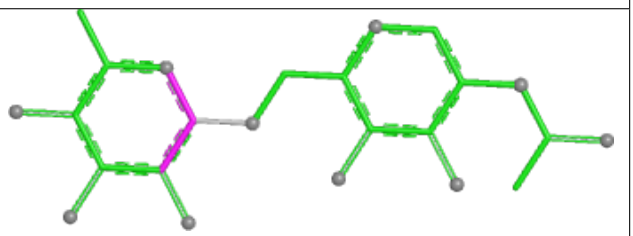


Rings

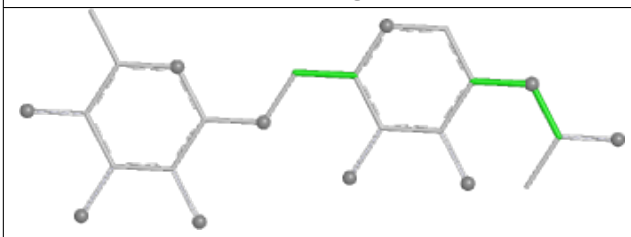
Oligosaccharide Chain d



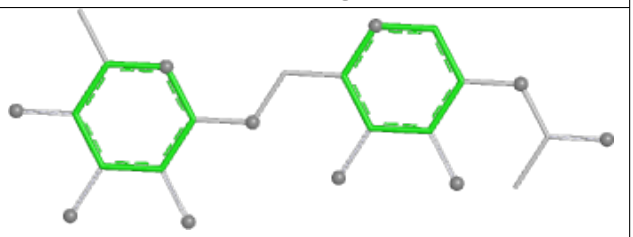
Bond lengths



Bond angles

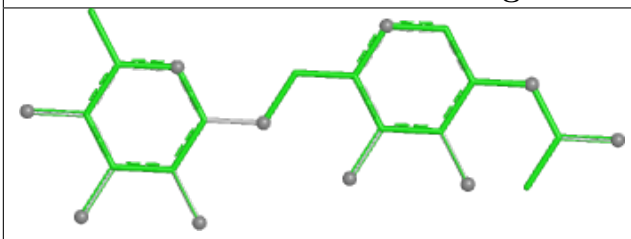


Torsions

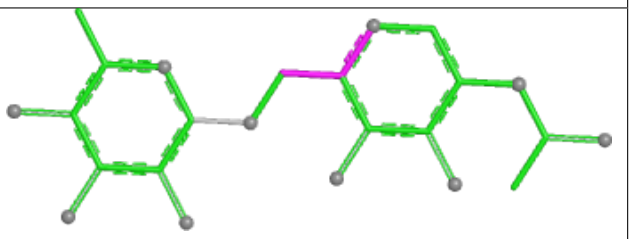


Rings

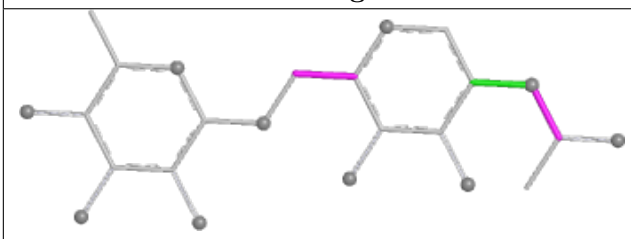
Oligosaccharide Chain i



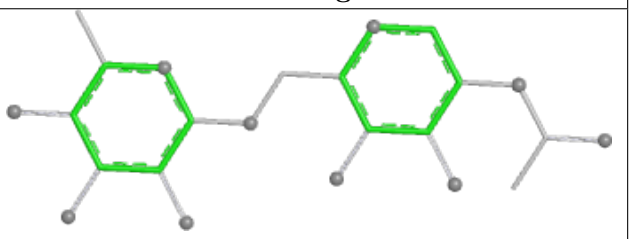
Bond lengths



Bond angles

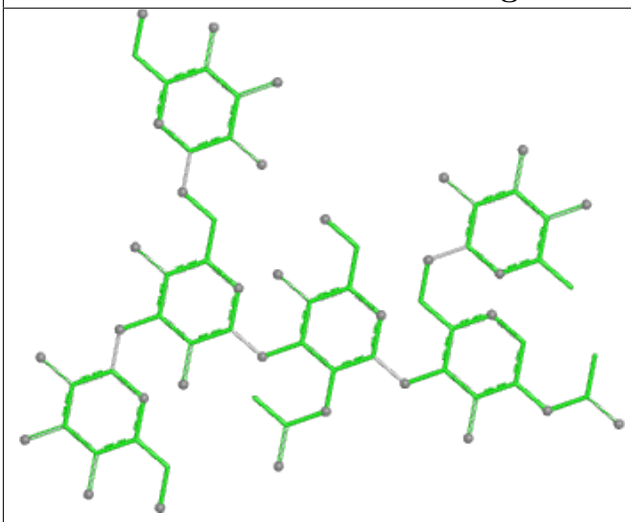


Torsions

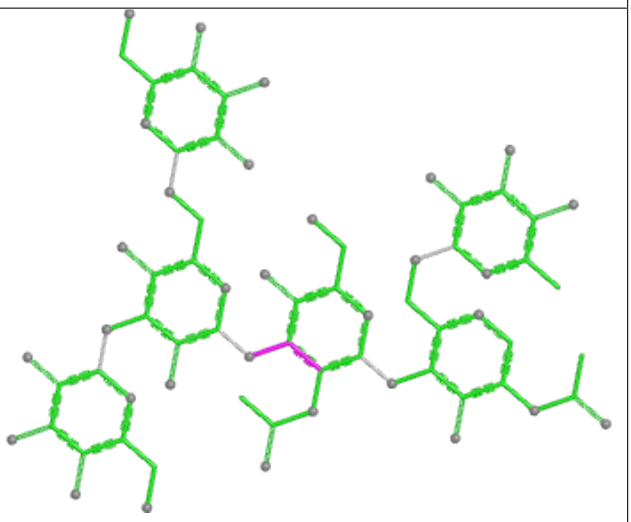


Rings

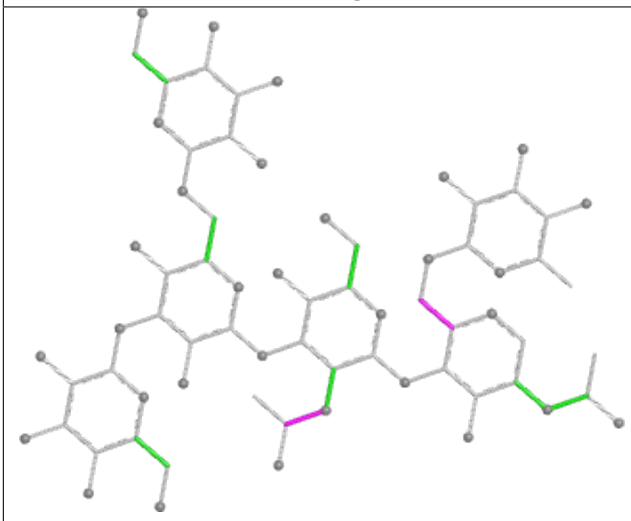
Oligosaccharide Chain f



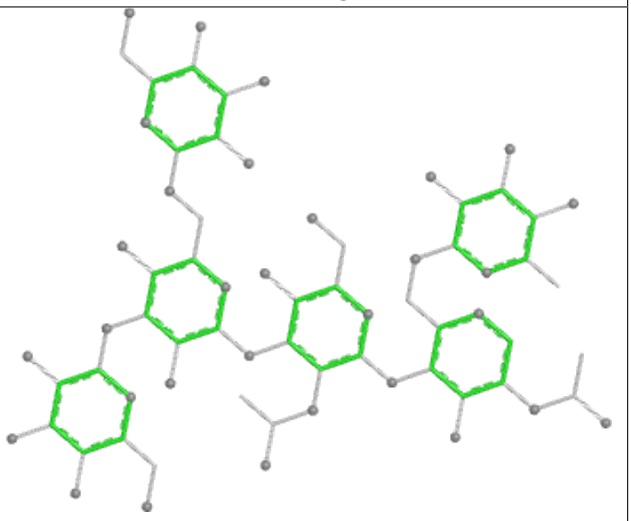
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
11	NAG	I	206	3	14,14,15	0.72	1 (7%)	17,19,21	0.73	0
11	NAG	F	207	3	14,14,15	0.28	0	17,19,21	0.48	0
11	NAG	Y	206	3	14,14,15	0.28	0	17,19,21	0.49	0
11	NAG	L	208	3	14,14,15	0.30	0	17,19,21	0.48	0
11	NAG	R	201	3	14,14,15	0.25	0	17,19,21	0.55	0
11	NAG	O	201	3	14,14,15	0.22	0	17,19,21	0.49	0
11	NAG	Y	201	3	14,14,15	0.23	0	17,19,21	0.48	0
11	NAG	L	201	3	14,14,15	0.22	0	17,19,21	0.48	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
11	NAG	I	206	3	-	2/6/23/26	0/1/1/1
11	NAG	F	207	3	-	2/6/23/26	0/1/1/1
11	NAG	Y	206	3	-	1/6/23/26	0/1/1/1
11	NAG	L	208	3	-	1/6/23/26	0/1/1/1
11	NAG	R	201	3	-	2/6/23/26	0/1/1/1
11	NAG	O	201	3	-	2/6/23/26	0/1/1/1
11	NAG	Y	201	3	-	2/6/23/26	0/1/1/1
11	NAG	L	201	3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	206	NAG	O5-C1	-2.27	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	R	201	NAG	O5-C5-C6-O6
11	I	206	NAG	O5-C5-C6-O6
11	R	201	NAG	C4-C5-C6-O6
11	I	206	NAG	C4-C5-C6-O6
11	F	207	NAG	O5-C5-C6-O6
11	L	208	NAG	O5-C5-C6-O6
11	F	207	NAG	C4-C5-C6-O6
11	Y	206	NAG	O5-C5-C6-O6
11	O	201	NAG	C4-C5-C6-O6
11	Y	201	NAG	C4-C5-C6-O6
11	O	201	NAG	O5-C5-C6-O6
11	Y	201	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	213/214 (99%)	0.02	0	100	100	57, 84, 123, 174	0
1	D	213/214 (99%)	0.03	0	100	100	59, 96, 132, 165	0
1	G	213/214 (99%)	-0.12	0	100	100	64, 90, 118, 152	0
1	J	213/214 (99%)	-0.14	0	100	100	61, 82, 116, 145	0
1	M	213/214 (99%)	0.08	0	100	100	59, 94, 135, 177	0
1	P	213/214 (99%)	0.17	4 (1%)	66	61	59, 93, 146, 174	0
1	S	213/214 (99%)	0.27	1 (0%)	91	88	77, 109, 155, 189	0
1	V	213/214 (99%)	0.22	8 (3%)	40	36	62, 102, 154, 190	0
2	B	214/225 (95%)	-0.03	0	100	100	46, 73, 112, 140	0
2	E	214/225 (95%)	0.10	0	100	100	51, 78, 119, 154	0
2	H	210/225 (93%)	-0.05	0	100	100	57, 79, 111, 137	0
2	K	212/225 (94%)	-0.08	0	100	100	58, 81, 113, 150	0
2	N	209/225 (92%)	-0.06	0	100	100	61, 86, 131, 204	0
2	Q	210/225 (93%)	0.13	6 (2%)	51	45	62, 90, 146, 221	0
2	T	212/225 (94%)	0.11	6 (2%)	53	47	80, 107, 159, 252	0
2	W	206/225 (91%)	0.24	4 (1%)	66	61	87, 115, 151, 209	0
3	A	111/168 (66%)	0.03	1 (0%)	84	79	68, 98, 134, 173	0
3	F	117/168 (69%)	0.08	1 (0%)	84	79	59, 90, 152, 203	0
3	I	113/168 (67%)	0.17	2 (1%)	68	62	69, 112, 164, 190	0
3	L	112/168 (66%)	0.28	1 (0%)	84	79	75, 123, 161, 195	0
3	O	117/168 (69%)	0.28	4 (3%)	45	40	73, 100, 199, 287	0
3	R	110/168 (65%)	0.05	2 (1%)	68	62	69, 102, 147, 200	0
3	X	117/168 (69%)	0.21	3 (2%)	56	49	87, 136, 185, 266	0
3	Y	117/168 (69%)	0.36	8 (6%)	17	16	87, 123, 206, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	4305/4856 (88%)	0.08	51 (1%)	79	73	46, 95, 149, 287	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	132	SER	7.1
3	O	72	PRO	4.7
3	Y	85	ASP	4.6
3	O	85	ASP	4.4
3	O	87	SER	4.3
1	P	213	GLU	4.2
3	X	85	ASP	4.1
2	T	194	LEU	3.9
1	V	181	LEU	3.8
3	Y	66	ASN	3.8
3	X	67	TRP	3.2
1	P	188	LYS	3.2
3	F	76	THR	3.1
3	Y	87	SER	3.1
2	W	17	SER	2.9
3	A	145	THR	2.8
1	V	166	GLN	2.7
3	Y	88	GLN	2.6
3	Y	65	LEU	2.6
2	T	142	ALA	2.5
2	T	10	GLY	2.5
2	Q	169	HIS	2.5
2	T	143	LEU	2.5
1	V	148	TRP	2.5
2	Q	129	LEU	2.4
1	V	146	VAL	2.4
3	I	97	VAL	2.4
1	P	212	GLY	2.4
3	X	128	LEU	2.3
3	Y	67	TRP	2.3
3	R	96	ARG	2.3
2	W	127	PHE	2.3
2	W	173	ALA	2.2
3	L	96	ARG	2.2
2	Q	191	SER	2.2
1	V	186	TYR	2.2
1	V	190	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	148	TRP	2.2
2	T	197	GLN	2.2
2	Q	146	LEU	2.2
2	Q	164	LEU	2.1
1	V	147	GLN	2.1
3	R	76	THR	2.1
1	S	150	VAL	2.1
2	T	216	VAL	2.1
3	I	131	LYS	2.0
3	Y	130	PRO	2.0
1	V	212	GLY	2.0
3	Y	80	ALA	2.0
2	W	132	SER	2.0
3	O	91	GLN	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	d	1	14/15	0.67	0.29	123,130,133,134	0
9	NAG	i	1	14/15	0.68	0.26	113,121,128,130	0
9	FUC	d	2	10/11	0.70	0.45	108,122,124,125	0
4	NAG	U	1	14/15	0.73	0.21	109,131,136,138	0
10	MAN	f	4	11/12	0.73	0.49	97,108,110,110	0
4	NAG	U	2	14/15	0.74	0.60	91,114,123,125	0
6	NAG	e	1	14/15	0.77	0.17	109,118,126,132	0
6	NAG	e	2	14/15	0.77	0.32	105,119,123,123	0
4	BMA	U	3	11/12	0.78	0.29	98,103,108,112	0
4	MAN	U	4	11/12	0.78	0.29	94,102,106,109	0
6	NAG	j	2	14/15	0.81	0.30	102,109,115,115	0
7	NAG	b	1	14/15	0.81	0.19	105,112,114,117	0
5	FUC	Z	4	10/11	0.81	0.30	93,103,106,111	0
6	NAG	a	2	14/15	0.82	0.34	95,103,111,111	0

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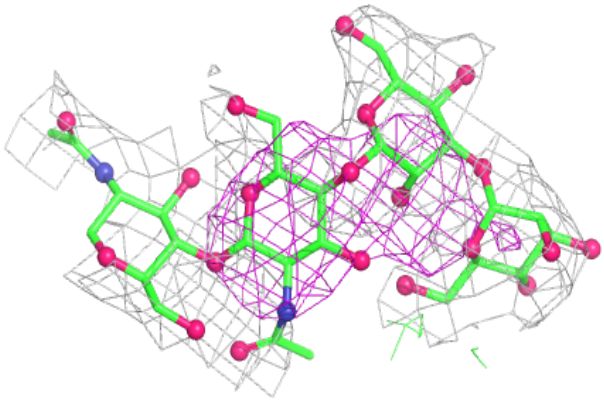
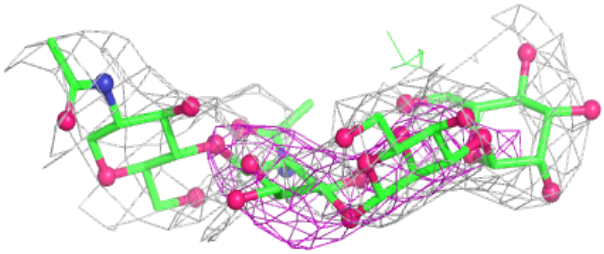
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BMA	Z	3	11/12	0.82	0.20	89,95,102,103	0
10	BMA	f	3	11/12	0.82	0.41	96,111,115,117	0
5	BMA	g	3	11/12	0.82	0.20	92,103,111,113	0
8	BMA	c	3	11/12	0.83	0.21	78,93,97,98	0
5	NAG	k	2	14/15	0.83	0.21	108,116,123,126	0
5	BMA	h	3	11/12	0.83	0.17	92,97,100,101	0
9	FUC	i	2	10/11	0.84	0.29	125,131,135,137	0
5	NAG	g	2	14/15	0.84	0.24	89,101,112,122	0
5	FUC	h	4	10/11	0.84	0.40	93,97,101,101	0
6	FUC	j	3	10/11	0.85	0.36	113,119,123,123	0
5	NAG	k	1	14/15	0.85	0.16	114,122,130,131	0
5	NAG	Z	1	14/15	0.85	0.24	102,110,113,114	0
7	NAG	b	2	14/15	0.86	0.17	100,107,111,112	0
8	FUC	c	4	10/11	0.86	0.23	79,82,83,84	0
5	NAG	Z	2	14/15	0.87	0.24	93,103,106,109	0
10	NAG	f	2	14/15	0.87	0.26	93,108,112,114	0
5	NAG	g	1	14/15	0.87	0.20	75,88,94,98	0
6	NAG	a	1	14/15	0.87	0.16	102,107,116,116	0
5	BMA	k	3	11/12	0.88	0.23	101,106,113,115	0
10	NAG	f	1	14/15	0.88	0.22	110,116,127,136	0
6	FUC	e	3	10/11	0.88	0.24	105,109,113,115	0
6	NAG	j	1	14/15	0.88	0.15	106,120,132,133	0
5	NAG	h	1	14/15	0.88	0.17	75,90,97,99	0
5	FUC	g	4	10/11	0.89	0.33	92,95,100,102	0
5	FUC	k	4	10/11	0.90	0.21	112,121,122,128	0
10	MAN	f	5	11/12	0.90	0.23	88,99,103,105	0
10	FUC	f	6	10/11	0.90	0.32	102,106,110,111	0
5	NAG	h	2	14/15	0.91	0.19	84,91,101,102	0
6	FUC	a	3	10/11	0.91	0.39	90,97,102,105	0
8	NAG	c	1	14/15	0.92	0.18	78,85,91,99	0
8	NAG	c	2	14/15	0.92	0.26	81,90,98,107	0

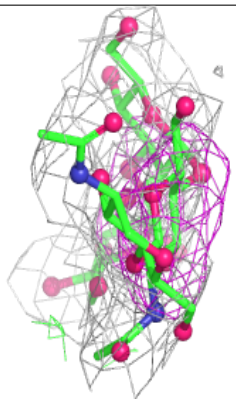
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

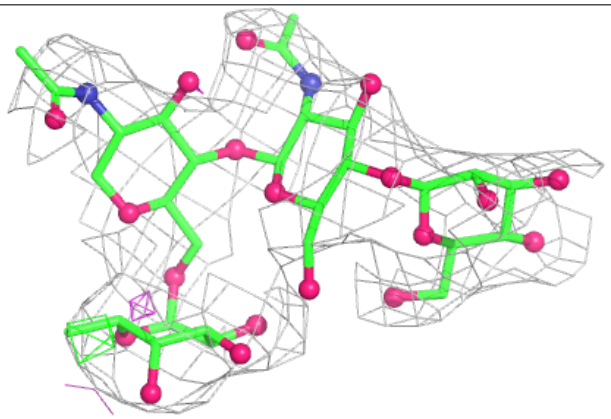


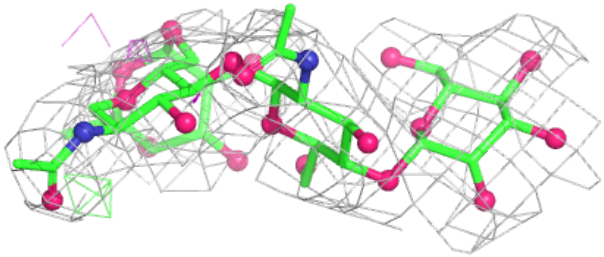


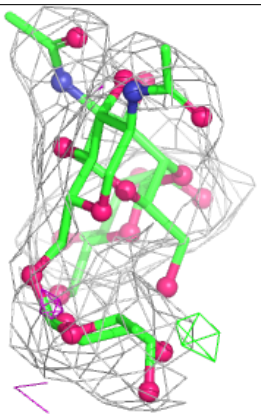


Electron density around Chain Z:

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

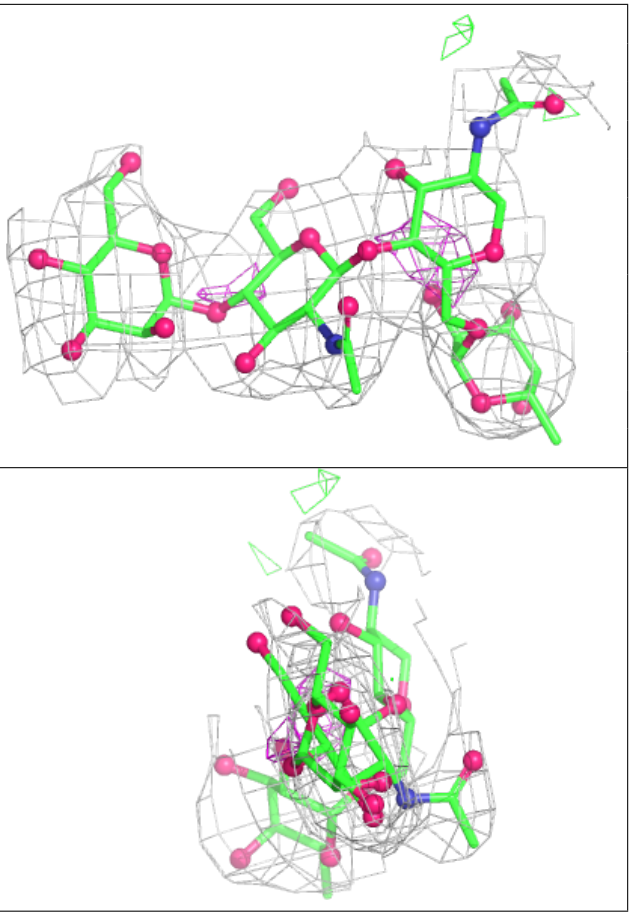






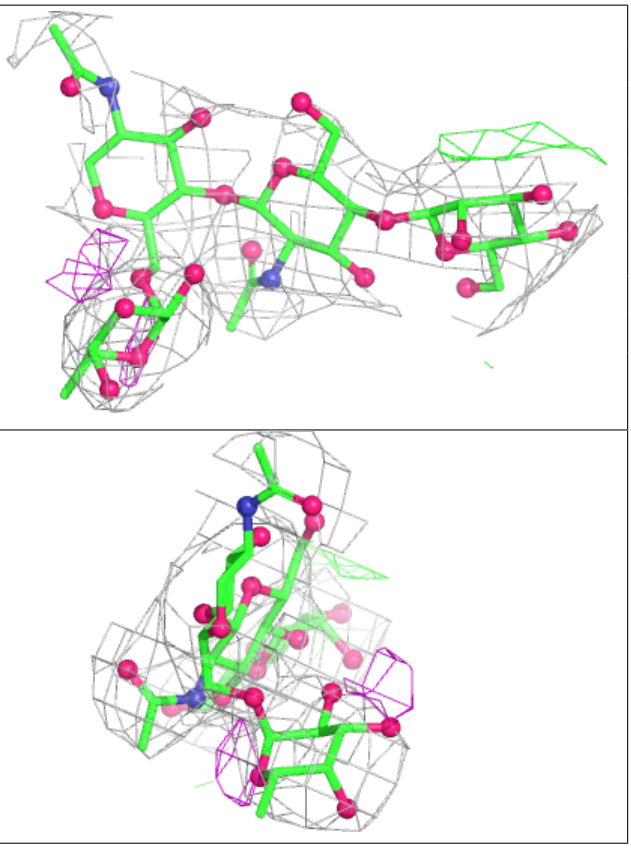
Electron density around Chain g:

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



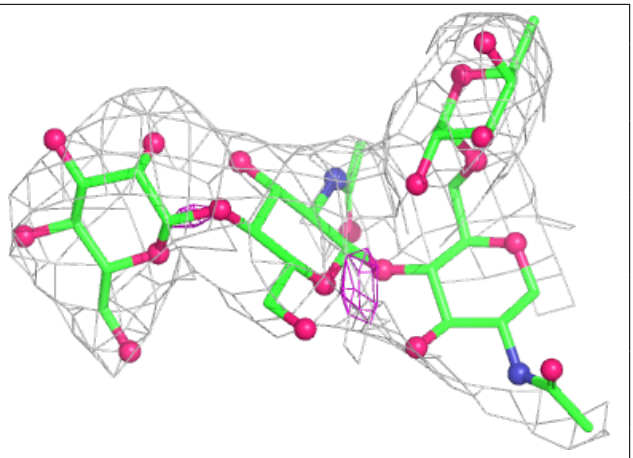
Electron density around Chain h:

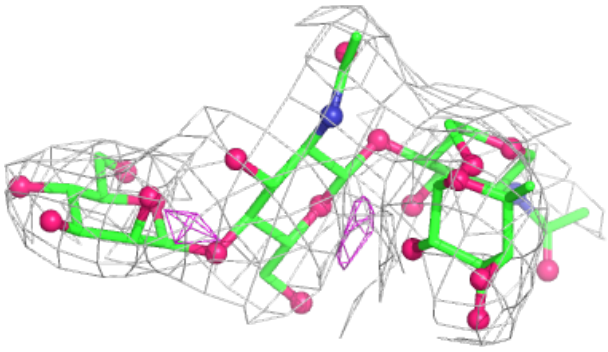
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

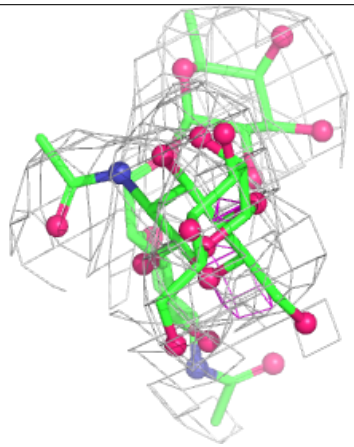


Electron density around Chain k:

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

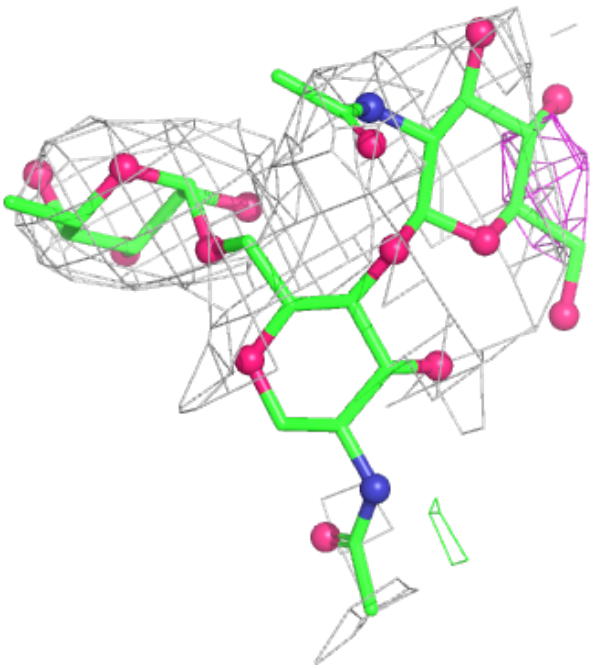


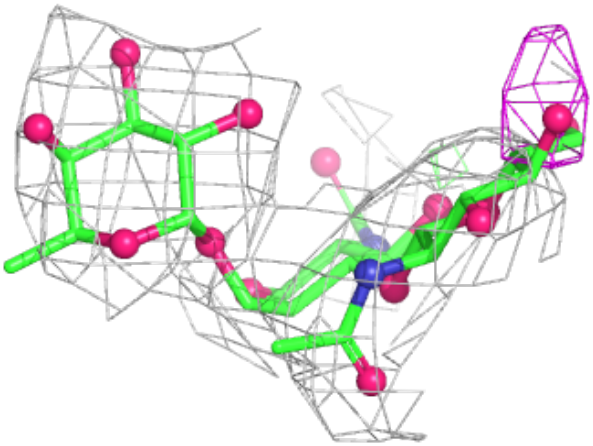


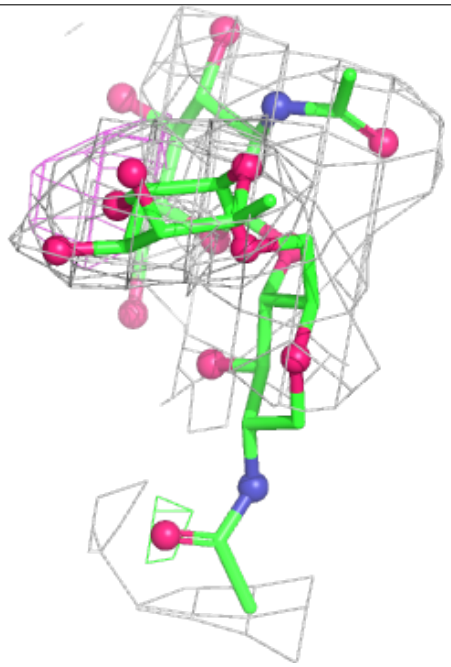


Electron density around Chain a:

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

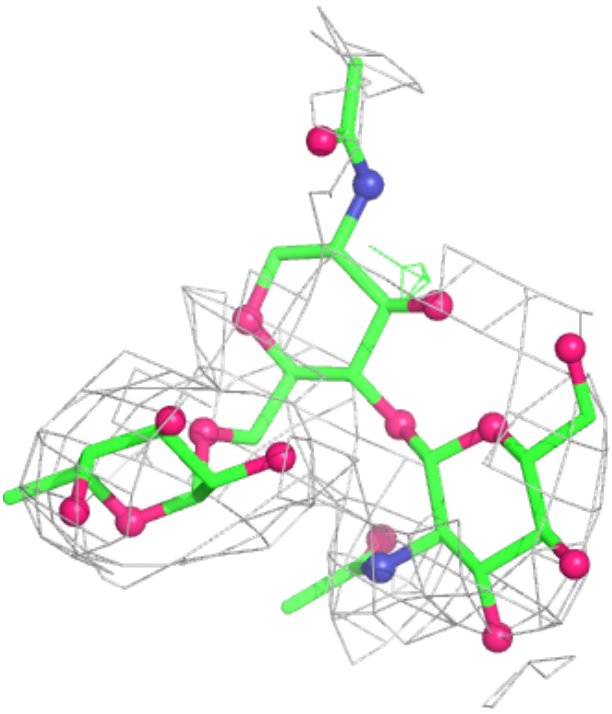


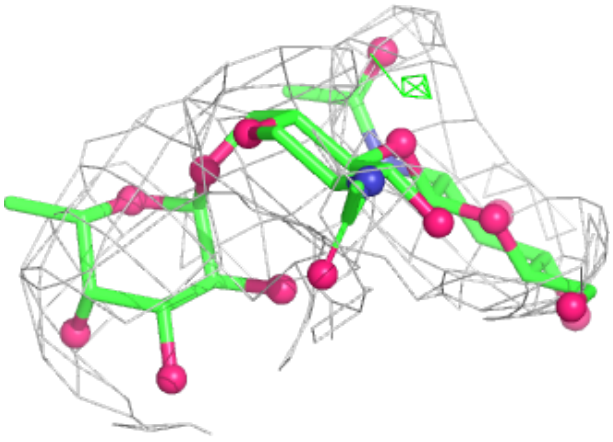


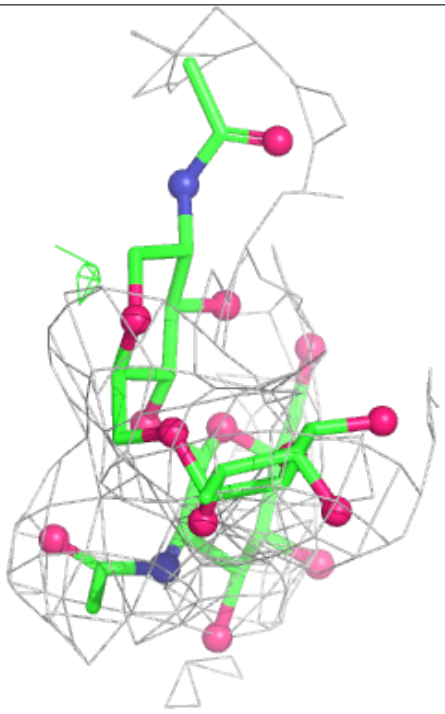


Electron density around Chain e:

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

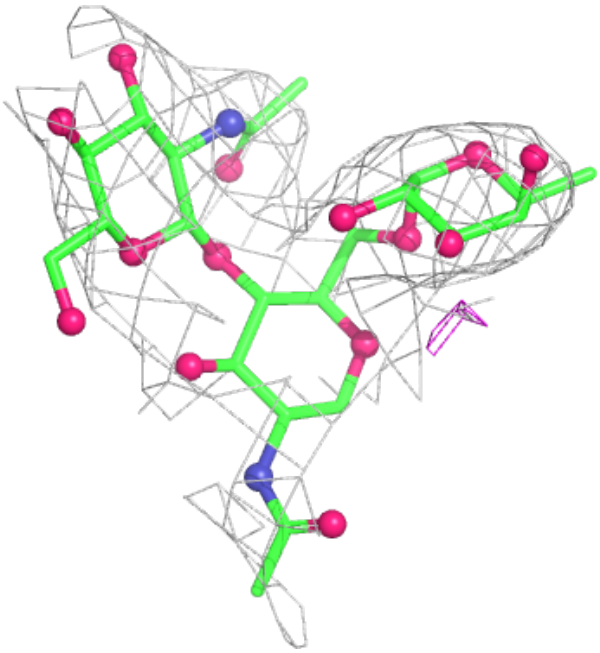


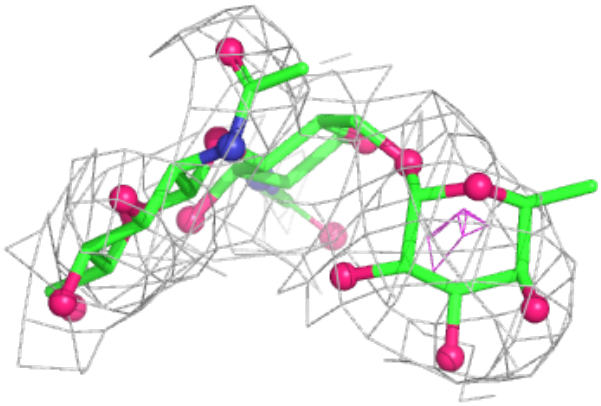


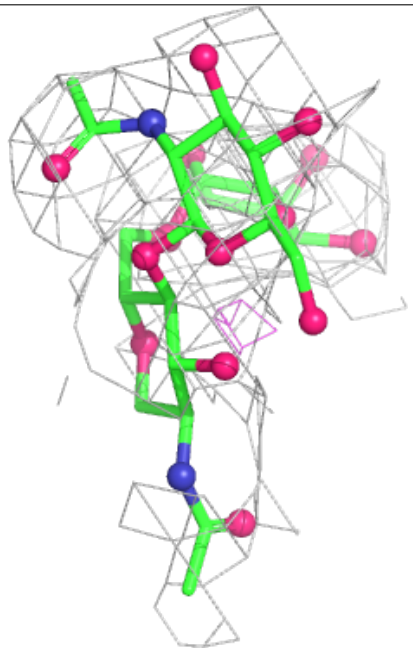


Electron density around Chain j:

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

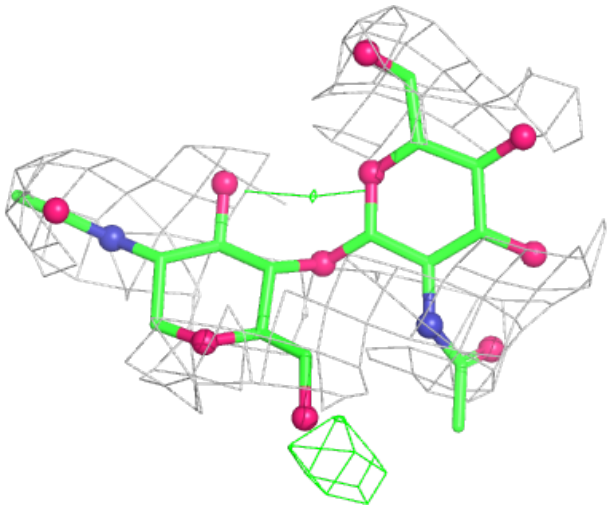


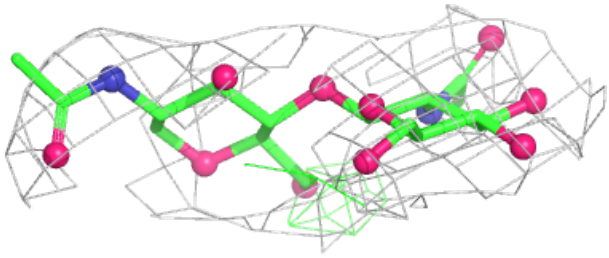


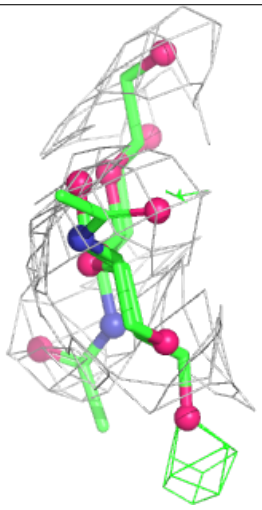


Electron density around Chain b:

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

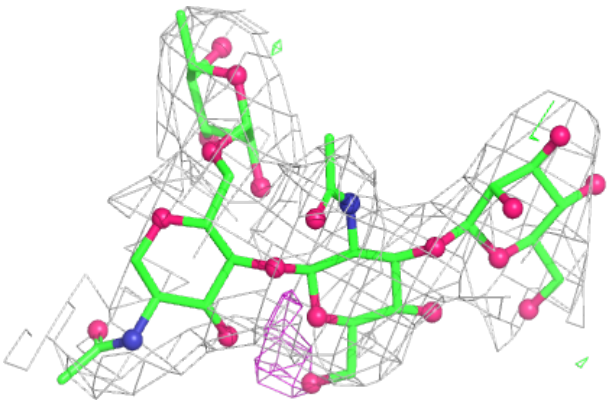


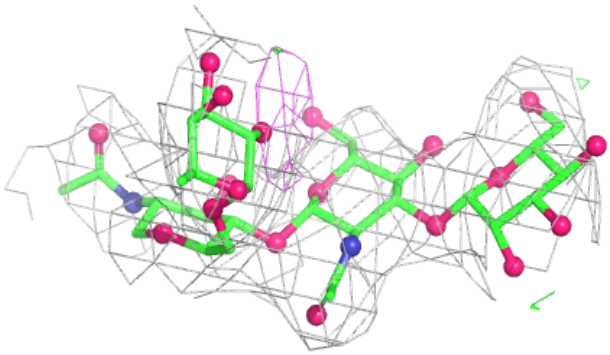


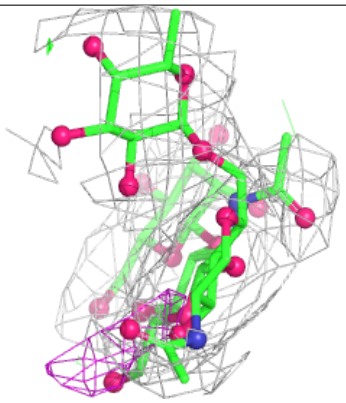


Electron density around Chain c:

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

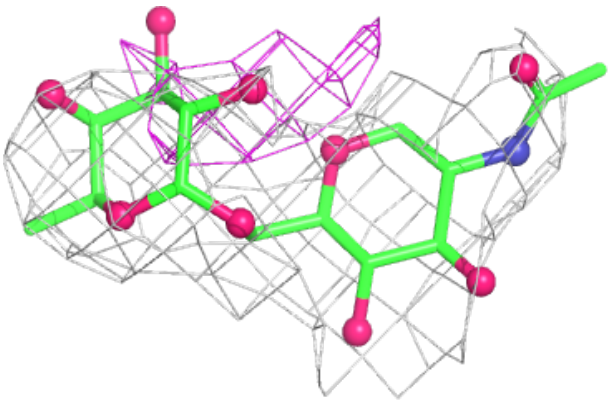


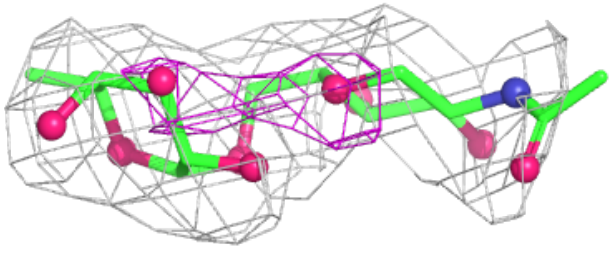


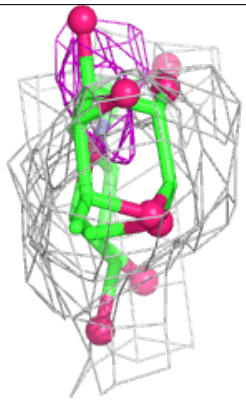


Electron density around Chain d:

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

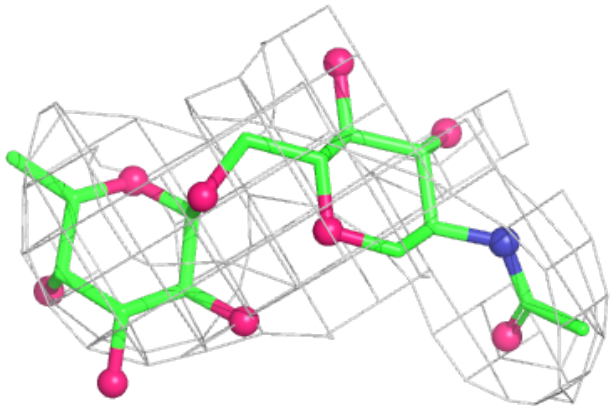


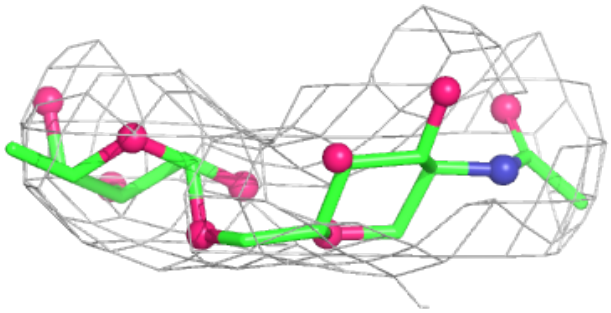


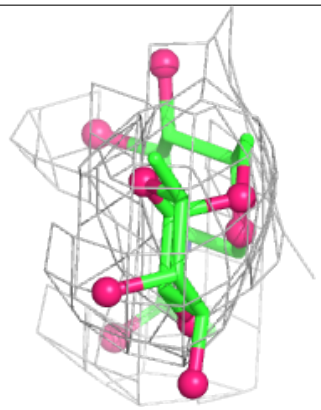


Electron density around Chain i:

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

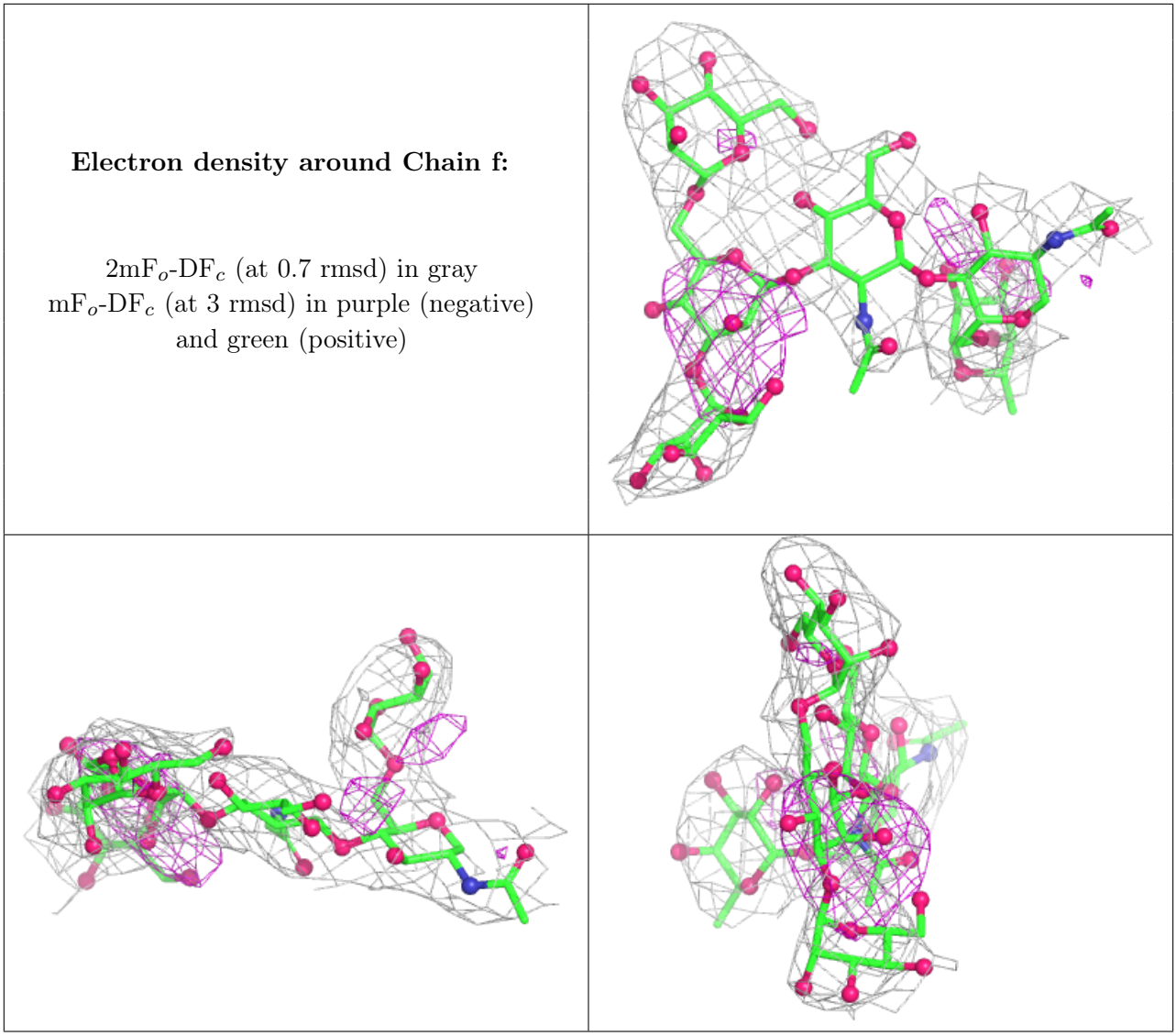






Electron density around Chain f:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	F	207	14/15	0.59	0.42	98,113,121,122	0
11	NAG	Y	206	14/15	0.66	0.45	122,137,141,143	0
11	NAG	L	201	14/15	0.73	0.22	122,138,141,142	0
11	NAG	L	208	14/15	0.75	0.30	115,122,125,127	0
11	NAG	Y	201	14/15	0.77	0.26	106,112,118,118	0
11	NAG	R	201	14/15	0.78	0.25	109,113,120,121	0
11	NAG	O	201	14/15	0.81	0.20	84,93,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	I	206	14/15	0.84	0.29	104,108,111,111	0

6.5 Other polymers (i)

There are no such residues in this entry.