Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 06:11 AM EDT

PDB ID	:	6WEO
Title	:	IL-22 Signaling Complex with IL-22R1 and IL-10Rbeta
Authors	:	Saxton, R.A.; Jude, K.M.; Henneberg, L.T.; Garcia, K.C.
Deposited on	:	2020-04-02
Resolution	:	2.60 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:

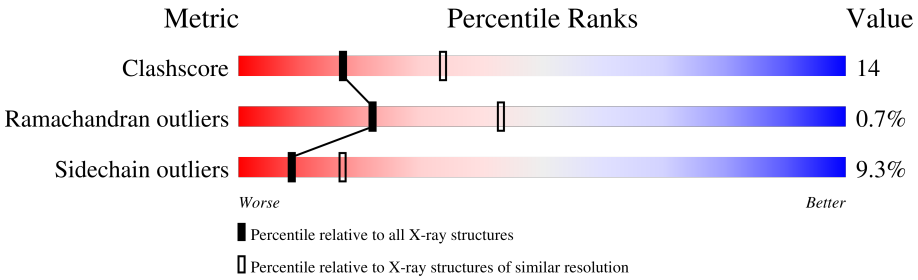
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	0	204	61% 31% • 5%
1	3	204	58% 30% 7% •
1	6	204	58% 33% • •
1	9	204	58% 25% 7% 9%
1	C	204	70% 24% • •
1	E	204	73% 21% • •
1	H	204	65% 27% • •
1	K	204	61% 30% • •

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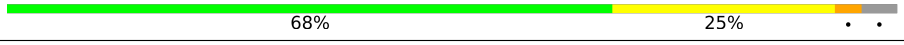
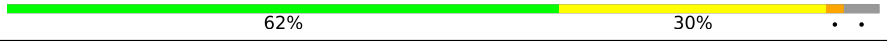
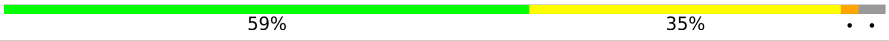
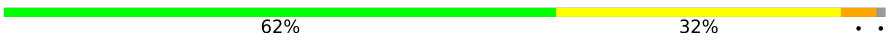
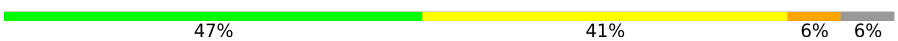
Mol	Chain	Length	Quality of chain
1	O	204	
1	R	204	
1	U	204	
1	X	204	
2	1	204	
2	4	204	
2	7	204	
2	A	204	
2	B	204	
2	F	204	
2	I	204	
2	M	204	
2	P	204	
2	S	204	
2	V	204	
2	Y	204	
3	2	149	
3	5	149	
3	8	149	
3	D	149	
3	G	149	
3	J	149	
3	L	149	
3	N	149	
3	Q	149	

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Mol	Chain	Length	Quality of chain
3	T	149	60% 29% 6% • 5%
3	W	149	60% 32% • 5%
3	Z	149	60% 30% 5% 5%
4	a	4	100%
4	c	4	100%
4	n	4	50% 50%
5	b	3	33% 67%
5	e	3	100%
5	i	3	33% 67%
5	j	3	67% 33%
5	l	3	100%
5	m	3	33% 67%
5	s	3	67% 33%
6	d	2	50% 50%
6	o	2	100%
6	p	2	100%
6	r	2	100%
6	t	2	100%
6	u	2	100%
6	v	2	50% 50%
7	f	2	50% 50%
8	g	3	67% 33%
9	h	5	20% 80%
9	k	5	40% 60%
10	q	2	50% 50%

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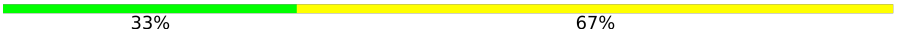
Mol	Chain	Length	Quality of chain
11	w	3	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 53140 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 Interleukin-10 receptor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	193	Total	C	N	O	S	0	0	0
			1579	1007	261	303	8			
1	3	195	Total	C	N	O	S	0	0	0
			1595	1016	263	308	8			
1	6	195	Total	C	N	O	S	0	0	0
			1607	1024	266	309	8			
1	9	186	Total	C	N	O	S	0	0	0
			1532	980	254	290	8			
1	C	195	Total	C	N	O	S	0	0	0
			1614	1026	270	310	8			
1	E	195	Total	C	N	O	S	0	0	0
			1593	1014	263	308	8			
1	H	195	Total	C	N	O	S	0	0	0
			1602	1021	264	309	8			
1	K	195	Total	C	N	O	S	0	0	0
			1605	1022	267	308	8			
1	O	196	Total	C	N	O	S	0	0	0
			1609	1025	268	308	8			
1	R	195	Total	C	N	O	S	0	0	0
			1611	1025	269	309	8			
1	U	195	Total	C	N	O	S	0	0	0
			1603	1020	266	309	8			
1	X	197	Total	C	N	O	S	0	0	0
			1619	1031	269	311	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	49	GLN	ASN	conflict	UNP Q61190
0	102	GLN	ASN	conflict	UNP Q61190
0	161	GLN	ASN	conflict	UNP Q61190
0	199	GLN	ASN	conflict	UNP Q61190
0	221	GLY	-	expression tag	UNP Q61190

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Chain	Residue	Modelled	Actual	Comment	Reference
0	222	GLY	-	expression tag	UNP Q61190
0	223	SER	-	expression tag	UNP Q61190
3	49	GLN	ASN	conflict	UNP Q61190
3	102	GLN	ASN	conflict	UNP Q61190
3	161	GLN	ASN	conflict	UNP Q61190
3	199	GLN	ASN	conflict	UNP Q61190
3	221	GLY	-	expression tag	UNP Q61190
3	222	GLY	-	expression tag	UNP Q61190
3	223	SER	-	expression tag	UNP Q61190
6	49	GLN	ASN	conflict	UNP Q61190
6	102	GLN	ASN	conflict	UNP Q61190
6	161	GLN	ASN	conflict	UNP Q61190
6	199	GLN	ASN	conflict	UNP Q61190
6	221	GLY	-	expression tag	UNP Q61190
6	222	GLY	-	expression tag	UNP Q61190
6	223	SER	-	expression tag	UNP Q61190
9	49	GLN	ASN	conflict	UNP Q61190
9	102	GLN	ASN	conflict	UNP Q61190
9	161	GLN	ASN	conflict	UNP Q61190
9	199	GLN	ASN	conflict	UNP Q61190
9	221	GLY	-	expression tag	UNP Q61190
9	222	GLY	-	expression tag	UNP Q61190
9	223	SER	-	expression tag	UNP Q61190
C	49	GLN	ASN	conflict	UNP Q61190
C	102	GLN	ASN	conflict	UNP Q61190
C	161	GLN	ASN	conflict	UNP Q61190
C	199	GLN	ASN	conflict	UNP Q61190
C	221	GLY	-	expression tag	UNP Q61190
C	222	GLY	-	expression tag	UNP Q61190
C	223	SER	-	expression tag	UNP Q61190
E	49	GLN	ASN	conflict	UNP Q61190
E	102	GLN	ASN	conflict	UNP Q61190
E	161	GLN	ASN	conflict	UNP Q61190
E	199	GLN	ASN	conflict	UNP Q61190
E	221	GLY	-	expression tag	UNP Q61190
E	222	GLY	-	expression tag	UNP Q61190
E	223	SER	-	expression tag	UNP Q61190
H	49	GLN	ASN	conflict	UNP Q61190
H	102	GLN	ASN	conflict	UNP Q61190
H	161	GLN	ASN	conflict	UNP Q61190
H	199	GLN	ASN	conflict	UNP Q61190
H	221	GLY	-	expression tag	UNP Q61190

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Chain	Residue	Modelled	Actual	Comment	Reference
H	222	GLY	-	expression tag	UNP Q61190
H	223	SER	-	expression tag	UNP Q61190
K	49	GLN	ASN	conflict	UNP Q61190
K	102	GLN	ASN	conflict	UNP Q61190
K	161	GLN	ASN	conflict	UNP Q61190
K	199	GLN	ASN	conflict	UNP Q61190
K	221	GLY	-	expression tag	UNP Q61190
K	222	GLY	-	expression tag	UNP Q61190
K	223	SER	-	expression tag	UNP Q61190
O	49	GLN	ASN	conflict	UNP Q61190
O	102	GLN	ASN	conflict	UNP Q61190
O	161	GLN	ASN	conflict	UNP Q61190
O	199	GLN	ASN	conflict	UNP Q61190
O	221	GLY	-	expression tag	UNP Q61190
O	222	GLY	-	expression tag	UNP Q61190
O	223	SER	-	expression tag	UNP Q61190
R	49	GLN	ASN	conflict	UNP Q61190
R	102	GLN	ASN	conflict	UNP Q61190
R	161	GLN	ASN	conflict	UNP Q61190
R	199	GLN	ASN	conflict	UNP Q61190
R	221	GLY	-	expression tag	UNP Q61190
R	222	GLY	-	expression tag	UNP Q61190
R	223	SER	-	expression tag	UNP Q61190
U	49	GLN	ASN	conflict	UNP Q61190
U	102	GLN	ASN	conflict	UNP Q61190
U	161	GLN	ASN	conflict	UNP Q61190
U	199	GLN	ASN	conflict	UNP Q61190
U	221	GLY	-	expression tag	UNP Q61190
U	222	GLY	-	expression tag	UNP Q61190
U	223	SER	-	expression tag	UNP Q61190
X	49	GLN	ASN	conflict	UNP Q61190
X	102	GLN	ASN	conflict	UNP Q61190
X	161	GLN	ASN	conflict	UNP Q61190
X	199	GLN	ASN	conflict	UNP Q61190
X	221	GLY	-	expression tag	UNP Q61190
X	222	GLY	-	expression tag	UNP Q61190
X	223	SER	-	expression tag	UNP Q61190

- Molecule 2 is a protein called Interleukin-22 receptor subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	201	Total	C	N	O	S	0	0	0
			1613	1032	270	303	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	4	201	Total	C	N	O	S	0	0	0
			1610	1030	269	303	8			
2	7	201	Total	C	N	O	S	0	0	0
			1604	1027	266	303	8			
2	A	201	Total	C	N	O	S	0	0	0
			1605	1026	268	303	8			
2	B	201	Total	C	N	O	S	0	0	0
			1609	1029	269	303	8			
2	F	201	Total	C	N	O	S	0	0	0
			1608	1030	267	303	8			
2	I	201	Total	C	N	O	S	0	0	0
			1614	1032	269	305	8			
2	M	201	Total	C	N	O	S	0	0	0
			1605	1029	265	303	8			
2	P	201	Total	C	N	O	S	0	0	0
			1621	1037	271	305	8			
2	S	201	Total	C	N	O	S	0	0	0
			1617	1035	271	303	8			
2	V	201	Total	C	N	O	S	0	0	0
			1611	1032	268	303	8			
2	Y	201	Total	C	N	O	S	0	0	0
			1610	1032	265	305	8			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	80	ASP	ASN	conflict	UNP Q80XZ4
1	87	ASP	ASN	conflict	UNP Q80XZ4
1	89	GLN	THR	conflict	UNP Q80XZ4
1	225	GLY	-	expression tag	UNP Q80XZ4
1	226	GLY	-	expression tag	UNP Q80XZ4
1	227	SER	-	expression tag	UNP Q80XZ4
4	80	ASP	ASN	conflict	UNP Q80XZ4
4	87	ASP	ASN	conflict	UNP Q80XZ4
4	89	GLN	THR	conflict	UNP Q80XZ4
4	225	GLY	-	expression tag	UNP Q80XZ4
4	226	GLY	-	expression tag	UNP Q80XZ4
4	227	SER	-	expression tag	UNP Q80XZ4
7	80	ASP	ASN	conflict	UNP Q80XZ4
7	87	ASP	ASN	conflict	UNP Q80XZ4
7	89	GLN	THR	conflict	UNP Q80XZ4
7	225	GLY	-	expression tag	UNP Q80XZ4
7	226	GLY	-	expression tag	UNP Q80XZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
7	227	SER	-	expression tag	UNP Q80XZ4
A	80	ASP	ASN	conflict	UNP Q80XZ4
A	87	ASP	ASN	conflict	UNP Q80XZ4
A	89	GLN	THR	conflict	UNP Q80XZ4
A	225	GLY	-	expression tag	UNP Q80XZ4
A	226	GLY	-	expression tag	UNP Q80XZ4
A	227	SER	-	expression tag	UNP Q80XZ4
B	80	ASP	ASN	conflict	UNP Q80XZ4
B	87	ASP	ASN	conflict	UNP Q80XZ4
B	89	GLN	THR	conflict	UNP Q80XZ4
B	225	GLY	-	expression tag	UNP Q80XZ4
B	226	GLY	-	expression tag	UNP Q80XZ4
B	227	SER	-	expression tag	UNP Q80XZ4
F	80	ASP	ASN	conflict	UNP Q80XZ4
F	87	ASP	ASN	conflict	UNP Q80XZ4
F	89	GLN	THR	conflict	UNP Q80XZ4
F	225	GLY	-	expression tag	UNP Q80XZ4
F	226	GLY	-	expression tag	UNP Q80XZ4
F	227	SER	-	expression tag	UNP Q80XZ4
I	80	ASP	ASN	conflict	UNP Q80XZ4
I	87	ASP	ASN	conflict	UNP Q80XZ4
I	89	GLN	THR	conflict	UNP Q80XZ4
I	225	GLY	-	expression tag	UNP Q80XZ4
I	226	GLY	-	expression tag	UNP Q80XZ4
I	227	SER	-	expression tag	UNP Q80XZ4
M	80	ASP	ASN	conflict	UNP Q80XZ4
M	87	ASP	ASN	conflict	UNP Q80XZ4
M	89	GLN	THR	conflict	UNP Q80XZ4
M	225	GLY	-	expression tag	UNP Q80XZ4
M	226	GLY	-	expression tag	UNP Q80XZ4
M	227	SER	-	expression tag	UNP Q80XZ4
P	80	ASP	ASN	conflict	UNP Q80XZ4
P	87	ASP	ASN	conflict	UNP Q80XZ4
P	89	GLN	THR	conflict	UNP Q80XZ4
P	225	GLY	-	expression tag	UNP Q80XZ4
P	226	GLY	-	expression tag	UNP Q80XZ4
P	227	SER	-	expression tag	UNP Q80XZ4
S	80	ASP	ASN	conflict	UNP Q80XZ4
S	87	ASP	ASN	conflict	UNP Q80XZ4
S	89	GLN	THR	conflict	UNP Q80XZ4
S	225	GLY	-	expression tag	UNP Q80XZ4
S	226	GLY	-	expression tag	UNP Q80XZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
S	227	SER	-	expression tag	UNP Q80XZ4
V	80	ASP	ASN	conflict	UNP Q80XZ4
V	87	ASP	ASN	conflict	UNP Q80XZ4
V	89	GLN	THR	conflict	UNP Q80XZ4
V	225	GLY	-	expression tag	UNP Q80XZ4
V	226	GLY	-	expression tag	UNP Q80XZ4
V	227	SER	-	expression tag	UNP Q80XZ4
Y	80	ASP	ASN	conflict	UNP Q80XZ4
Y	87	ASP	ASN	conflict	UNP Q80XZ4
Y	89	GLN	THR	conflict	UNP Q80XZ4
Y	225	GLY	-	expression tag	UNP Q80XZ4
Y	226	GLY	-	expression tag	UNP Q80XZ4
Y	227	SER	-	expression tag	UNP Q80XZ4

- Molecule 3 is a protein called Interleukin-22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	140	Total	C	N	O	S	0	0	0
			1096	700	186	202	8			
3	5	141	Total	C	N	O	S	0	0	0
			1126	715	197	206	8			
3	8	140	Total	C	N	O	S	0	0	0
			1107	704	191	204	8			
3	D	141	Total	C	N	O	S	0	0	0
			1131	718	198	207	8			
3	G	141	Total	C	N	O	S	0	0	0
			1123	715	196	204	8			
3	J	140	Total	C	N	O	S	0	0	0
			1117	711	193	205	8			
3	L	141	Total	C	N	O	S	0	0	0
			1125	716	195	206	8			
3	N	140	Total	C	N	O	S	0	0	0
			1093	695	187	203	8			
3	Q	142	Total	C	N	O	S	0	0	0
			1120	713	191	208	8			
3	T	142	Total	C	N	O	S	0	0	0
			1133	720	196	209	8			
3	W	141	Total	C	N	O	S	0	0	0
			1124	714	195	207	8			
3	Z	141	Total	C	N	O	S	0	0	0
			1129	718	197	206	8			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	43	HIS	GLU	conflict	UNP Q9JJY9
2	45	ARG	SER	conflict	UNP Q9JJY9
2	49	SER	GLN	conflict	UNP Q9JJY9
2	68	GLN	ASN	conflict	UNP Q9JJY9
2	97	GLN	ASN	conflict	UNP Q9JJY9
2	116	TRP	GLN	conflict	UNP Q9JJY9
2	128	LYS	GLN	conflict	UNP Q9JJY9
2	180	GLY	-	expression tag	UNP Q9JJY9
2	181	GLY	-	expression tag	UNP Q9JJY9
2	182	SER	-	expression tag	UNP Q9JJY9
5	43	HIS	GLU	conflict	UNP Q9JJY9
5	45	ARG	SER	conflict	UNP Q9JJY9
5	49	SER	GLN	conflict	UNP Q9JJY9
5	68	GLN	ASN	conflict	UNP Q9JJY9
5	97	GLN	ASN	conflict	UNP Q9JJY9
5	116	TRP	GLN	conflict	UNP Q9JJY9
5	128	LYS	GLN	conflict	UNP Q9JJY9
5	180	GLY	-	expression tag	UNP Q9JJY9
5	181	GLY	-	expression tag	UNP Q9JJY9
5	182	SER	-	expression tag	UNP Q9JJY9
8	43	HIS	GLU	conflict	UNP Q9JJY9
8	45	ARG	SER	conflict	UNP Q9JJY9
8	49	SER	GLN	conflict	UNP Q9JJY9
8	68	GLN	ASN	conflict	UNP Q9JJY9
8	97	GLN	ASN	conflict	UNP Q9JJY9
8	116	TRP	GLN	conflict	UNP Q9JJY9
8	128	LYS	GLN	conflict	UNP Q9JJY9
8	180	GLY	-	expression tag	UNP Q9JJY9
8	181	GLY	-	expression tag	UNP Q9JJY9
8	182	SER	-	expression tag	UNP Q9JJY9
D	43	HIS	GLU	conflict	UNP Q9JJY9
D	45	ARG	SER	conflict	UNP Q9JJY9
D	49	SER	GLN	conflict	UNP Q9JJY9
D	68	GLN	ASN	conflict	UNP Q9JJY9
D	97	GLN	ASN	conflict	UNP Q9JJY9
D	116	TRP	GLN	conflict	UNP Q9JJY9
D	128	LYS	GLN	conflict	UNP Q9JJY9
D	180	GLY	-	expression tag	UNP Q9JJY9
D	181	GLY	-	expression tag	UNP Q9JJY9
D	182	SER	-	expression tag	UNP Q9JJY9
G	43	HIS	GLU	conflict	UNP Q9JJY9
G	45	ARG	SER	conflict	UNP Q9JJY9
G	49	SER	GLN	conflict	UNP Q9JJY9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	68	GLN	ASN	conflict	UNP Q9JJY9
G	97	GLN	ASN	conflict	UNP Q9JJY9
G	116	TRP	GLN	conflict	UNP Q9JJY9
G	128	LYS	GLN	conflict	UNP Q9JJY9
G	180	GLY	-	expression tag	UNP Q9JJY9
G	181	GLY	-	expression tag	UNP Q9JJY9
G	182	SER	-	expression tag	UNP Q9JJY9
J	43	HIS	GLU	conflict	UNP Q9JJY9
J	45	ARG	SER	conflict	UNP Q9JJY9
J	49	SER	GLN	conflict	UNP Q9JJY9
J	68	GLN	ASN	conflict	UNP Q9JJY9
J	97	GLN	ASN	conflict	UNP Q9JJY9
J	116	TRP	GLN	conflict	UNP Q9JJY9
J	128	LYS	GLN	conflict	UNP Q9JJY9
J	180	GLY	-	expression tag	UNP Q9JJY9
J	181	GLY	-	expression tag	UNP Q9JJY9
J	182	SER	-	expression tag	UNP Q9JJY9
L	43	HIS	GLU	conflict	UNP Q9JJY9
L	45	ARG	SER	conflict	UNP Q9JJY9
L	49	SER	GLN	conflict	UNP Q9JJY9
L	68	GLN	ASN	conflict	UNP Q9JJY9
L	97	GLN	ASN	conflict	UNP Q9JJY9
L	116	TRP	GLN	conflict	UNP Q9JJY9
L	128	LYS	GLN	conflict	UNP Q9JJY9
L	180	GLY	-	expression tag	UNP Q9JJY9
L	181	GLY	-	expression tag	UNP Q9JJY9
L	182	SER	-	expression tag	UNP Q9JJY9
N	43	HIS	GLU	conflict	UNP Q9JJY9
N	45	ARG	SER	conflict	UNP Q9JJY9
N	49	SER	GLN	conflict	UNP Q9JJY9
N	68	GLN	ASN	conflict	UNP Q9JJY9
N	97	GLN	ASN	conflict	UNP Q9JJY9
N	116	TRP	GLN	conflict	UNP Q9JJY9
N	128	LYS	GLN	conflict	UNP Q9JJY9
N	180	GLY	-	expression tag	UNP Q9JJY9
N	181	GLY	-	expression tag	UNP Q9JJY9
N	182	SER	-	expression tag	UNP Q9JJY9
Q	43	HIS	GLU	conflict	UNP Q9JJY9
Q	45	ARG	SER	conflict	UNP Q9JJY9
Q	49	SER	GLN	conflict	UNP Q9JJY9
Q	68	GLN	ASN	conflict	UNP Q9JJY9
Q	97	GLN	ASN	conflict	UNP Q9JJY9

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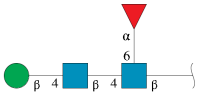
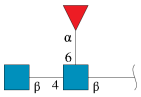
Chain	Residue	Modelled	Actual	Comment	Reference
Q	116	TRP	GLN	conflict	UNP Q9JJY9
Q	128	LYS	GLN	conflict	UNP Q9JJY9
Q	180	GLY	-	expression tag	UNP Q9JJY9
Q	181	GLY	-	expression tag	UNP Q9JJY9
Q	182	SER	-	expression tag	UNP Q9JJY9
T	43	HIS	GLU	conflict	UNP Q9JJY9
T	45	ARG	SER	conflict	UNP Q9JJY9
T	49	SER	GLN	conflict	UNP Q9JJY9
T	68	GLN	ASN	conflict	UNP Q9JJY9
T	97	GLN	ASN	conflict	UNP Q9JJY9
T	116	TRP	GLN	conflict	UNP Q9JJY9
T	128	LYS	GLN	conflict	UNP Q9JJY9
T	180	GLY	-	expression tag	UNP Q9JJY9
T	181	GLY	-	expression tag	UNP Q9JJY9
T	182	SER	-	expression tag	UNP Q9JJY9
W	43	HIS	GLU	conflict	UNP Q9JJY9
W	45	ARG	SER	conflict	UNP Q9JJY9
W	49	SER	GLN	conflict	UNP Q9JJY9
W	68	GLN	ASN	conflict	UNP Q9JJY9
W	97	GLN	ASN	conflict	UNP Q9JJY9
W	116	TRP	GLN	conflict	UNP Q9JJY9
W	128	LYS	GLN	conflict	UNP Q9JJY9
W	180	GLY	-	expression tag	UNP Q9JJY9
W	181	GLY	-	expression tag	UNP Q9JJY9
W	182	SER	-	expression tag	UNP Q9JJY9
Z	43	HIS	GLU	conflict	UNP Q9JJY9
Z	45	ARG	SER	conflict	UNP Q9JJY9
Z	49	SER	GLN	conflict	UNP Q9JJY9
Z	68	GLN	ASN	conflict	UNP Q9JJY9
Z	97	GLN	ASN	conflict	UNP Q9JJY9
Z	116	TRP	GLN	conflict	UNP Q9JJY9
Z	128	LYS	GLN	conflict	UNP Q9JJY9
Z	180	GLY	-	expression tag	UNP Q9JJY9
Z	181	GLY	-	expression tag	UNP Q9JJY9
Z	182	SER	-	expression tag	UNP Q9JJY9

- Molecule 4 is an oligosaccharide called 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.



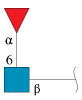
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	a	4	Total C N O 49 28 2 19	0	0	0
4	c	4	Total C N O 49 28 2 19	0	0	0
4	n	4	Total C N O 49 28 2 19	0	0	0

- Molecule 5 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
5	b	3	Total C N O 38 22 2 14	0	0	0
5	e	3	Total C N O 38 22 2 14	0	0	0
5	i	3	Total C N O 38 22 2 14	0	0	0
5	j	3	Total C N O 38 22 2 14	0	0	0
5	l	3	Total C N O 38 22 2 14	0	0	0
5	m	3	Total C N O 38 22 2 14	0	0	0
5	s	3	Total C N O 38 22 2 14	0	0	0

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



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

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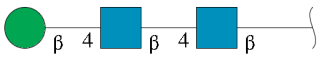
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	p	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	r	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	t	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	u	2	Total	C	N	O	0	0	0
			24	14	1	9			
6	v	2	Total	C	N	O	0	0	0
			24	14	1	9			

- Molecule 7 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

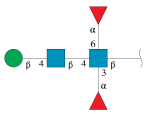
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	f	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	g	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

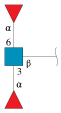


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	h	5	Total C N O 59 34 2 23	0	0	0
9	k	5	Total C N O 59 34 2 23	0	0	0

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

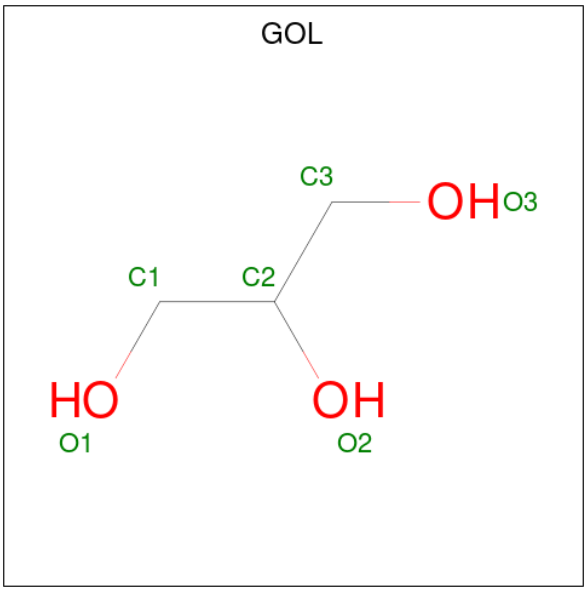
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	q	2	Total C N O 28 16 2 10	0	0	0

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



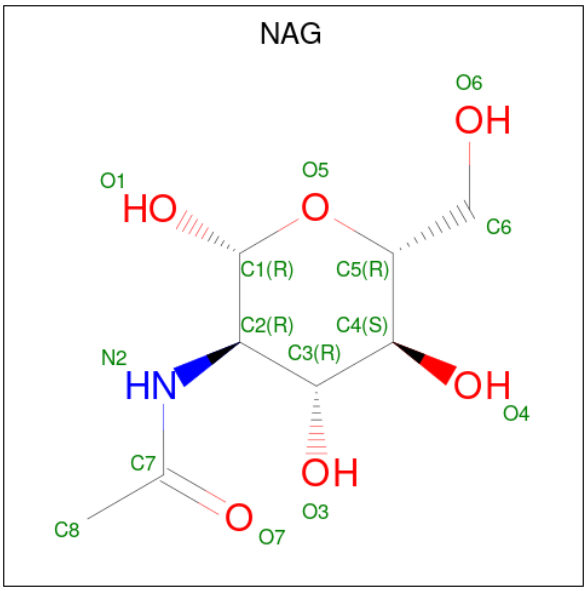
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	w	3	Total C N O 34 20 1 13	0	0	0

- Molecule 12 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 6 3 3	0	0
12	H	1	Total C O 6 3 3	0	0
12	J	1	Total C O 6 3 3	0	0
12	K	1	Total C O 6 3 3	0	0
12	M	1	Total C O 6 3 3	0	0
12	O	1	Total C O 6 3 3	0	0
12	Y	1	Total C O 6 3 3	0	0

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



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

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	1	9	Total O 9 9	0	0
14	2	6	Total O 6 6	0	0
14	3	6	Total O 6 6	0	0
14	4	7	Total O 7 7	0	0
14	5	2	Total O 2 2	0	0
14	6	5	Total O 5 5	0	0
14	7	12	Total O 12 12	0	0
14	8	6	Total O 6 6	0	0
14	9	3	Total O 3 3	0	0
14	A	22	Total O 22 22	0	0
14	B	16	Total O 16 16	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	22	Total O 22 22	0	0
14	D	14	Total O 14 14	0	0
14	E	15	Total O 15 15	0	0
14	F	10	Total O 10 10	0	0
14	G	5	Total O 5 5	0	0
14	H	17	Total O 17 17	0	0
14	I	9	Total O 9 9	0	0
14	J	6	Total O 6 6	0	0
14	K	9	Total O 9 9	0	0
14	L	8	Total O 8 8	0	0
14	M	8	Total O 8 8	0	0
14	N	5	Total O 5 5	0	0
14	O	14	Total O 14 14	0	0
14	P	6	Total O 6 6	0	0
14	Q	7	Total O 7 7	0	0
14	R	9	Total O 9 9	0	0
14	S	13	Total O 13 13	0	0
14	T	6	Total O 6 6	0	0
14	U	14	Total O 14 14	0	0
14	V	12	Total O 12 12	0	0
14	W	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	X	11	Total O 11 11	0	0
14	Y	20	Total O 20 20	0	0
14	Z	5	Total O 5 5	0	0

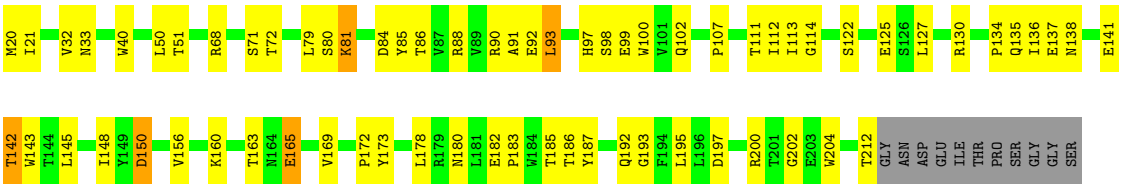
3 Residue-property plots (i)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

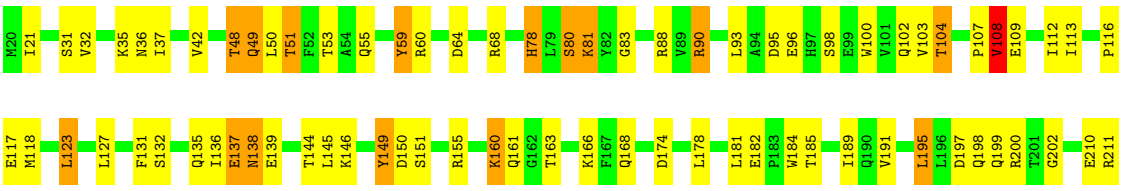
• Molecule 1: Interleukin-10 receptor subunit beta

Chain 0:



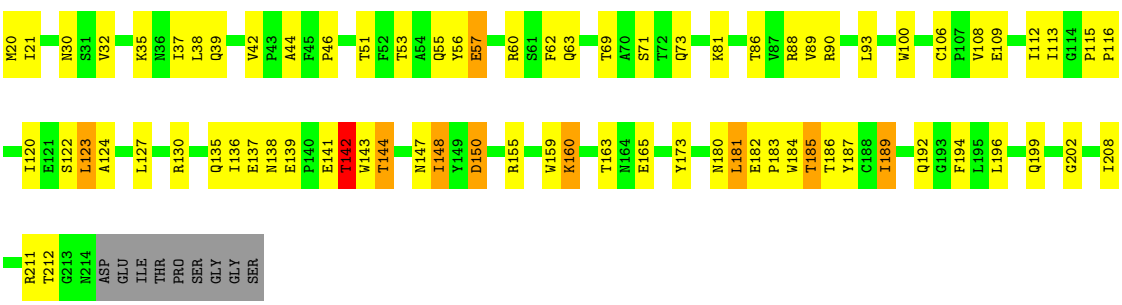
• Molecule 1: Interleukin-10 receptor subunit beta

Chain 3:



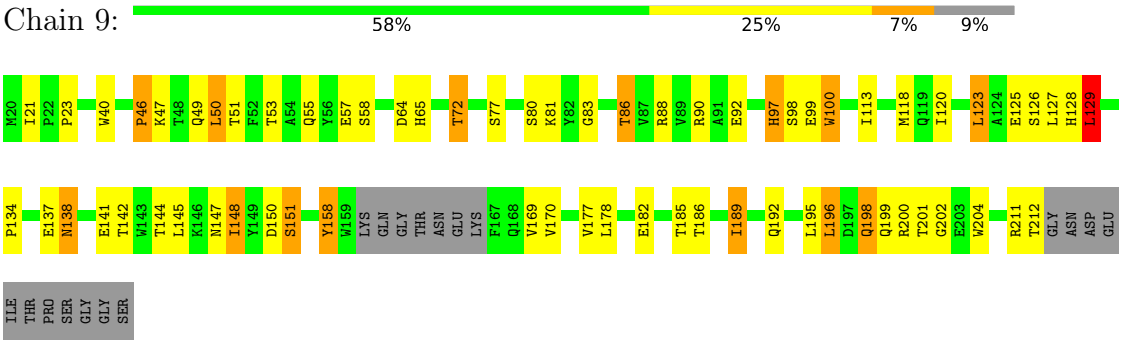
• Molecule 1: Interleukin-10 receptor subunit beta

Chain 6:



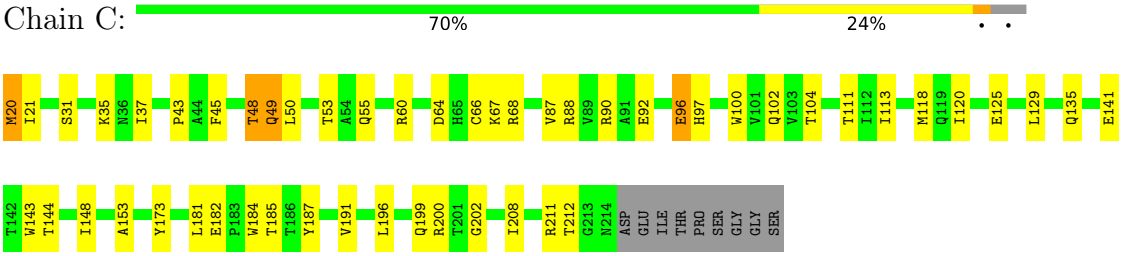
• Molecule 1: Interleukin-10 receptor subunit beta

Chain 9:



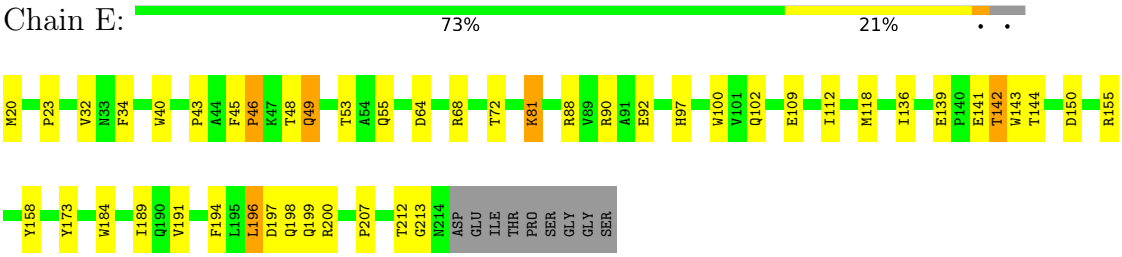
• Molecule 1: Interleukin-10 receptor subunit beta

Chain C:



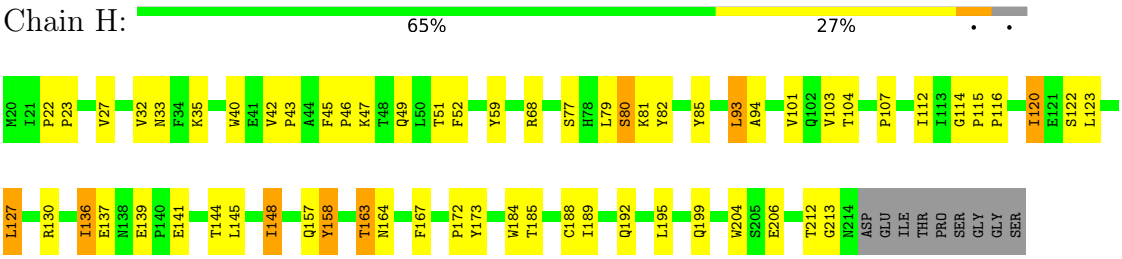
• Molecule 1: Interleukin-10 receptor subunit beta

Chain E:



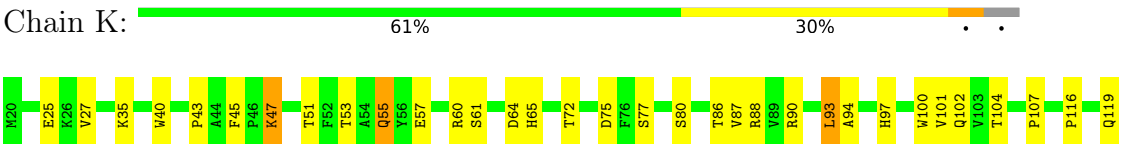
• Molecule 1: Interleukin-10 receptor subunit beta

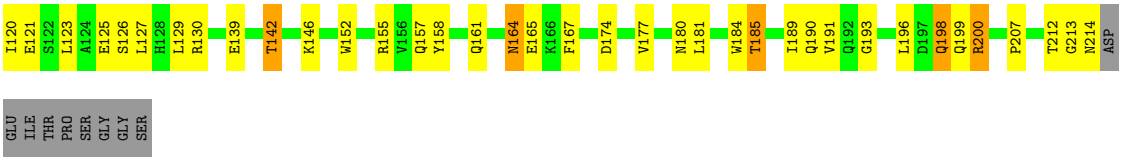
Chain H:



• Molecule 1: Interleukin-10 receptor subunit beta

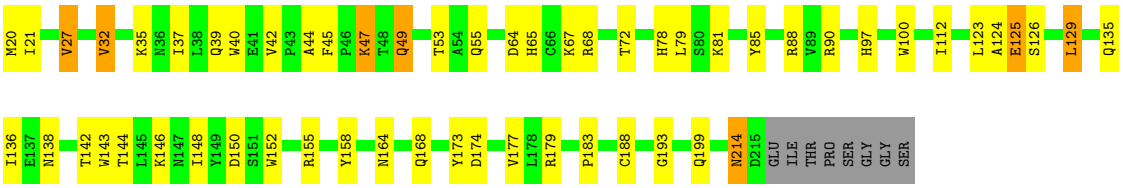
Chain K:





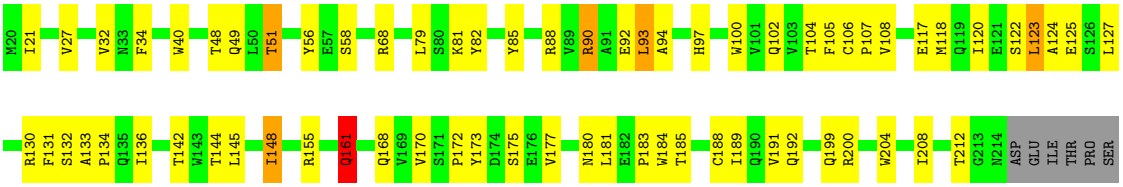
• Molecule 1: Interleukin-10 receptor subunit beta

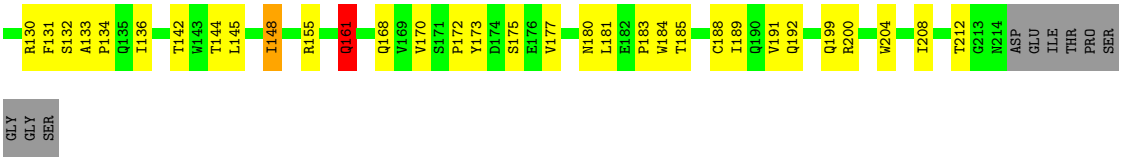
Chain O:



• Molecule 1: Interleukin-10 receptor subunit beta

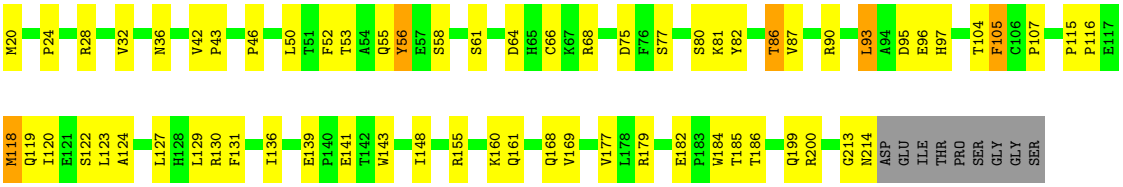
Chain R:





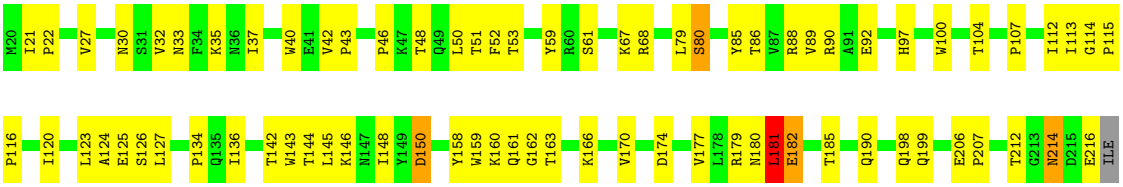
• Molecule 1: Interleukin-10 receptor subunit beta

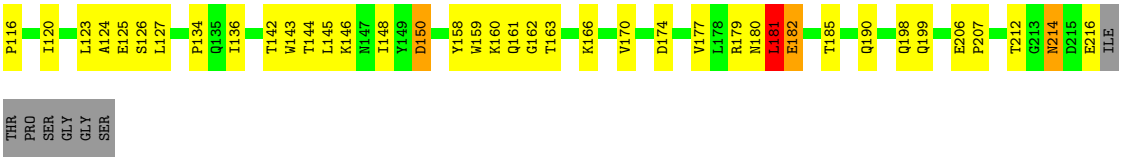
Chain U:



• Molecule 1: Interleukin-10 receptor subunit beta

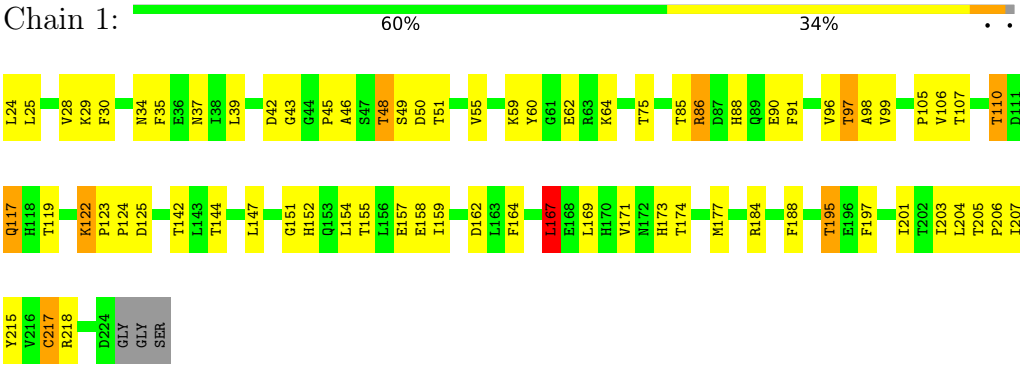
Chain X:





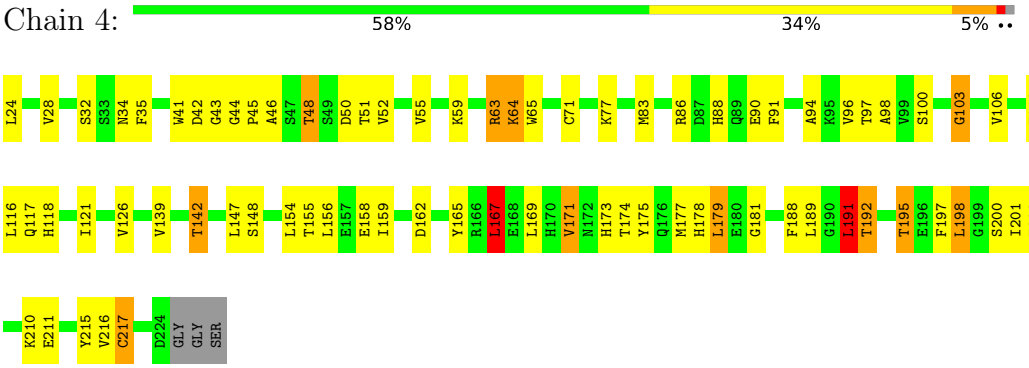
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain 1:



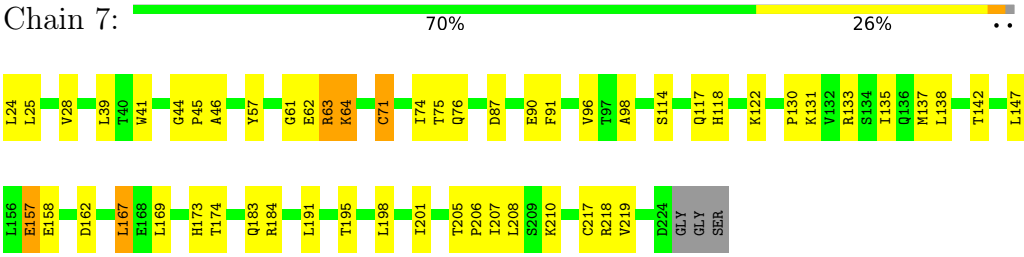
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain 4:



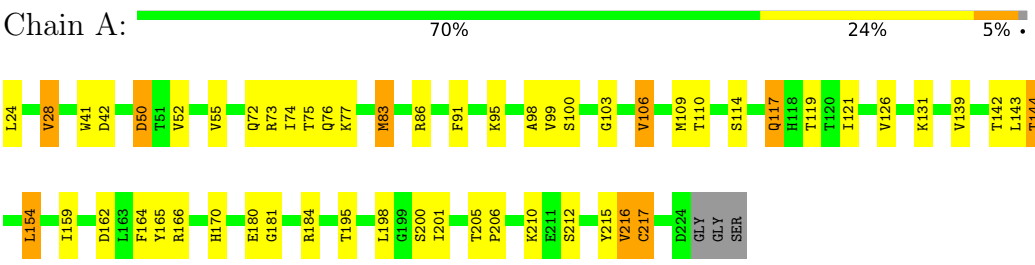
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain 7:



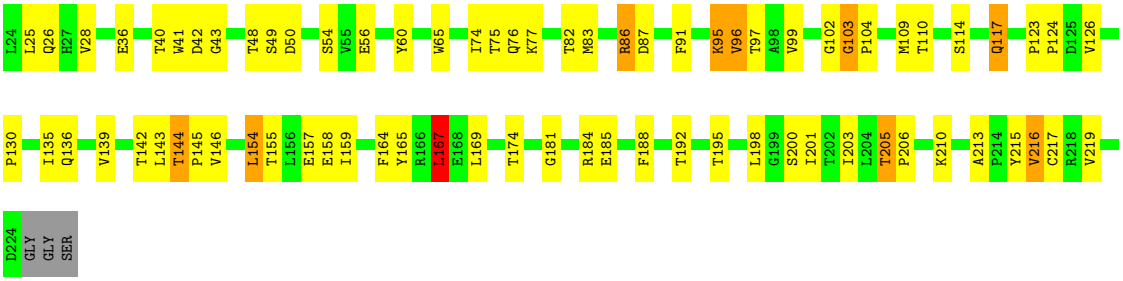
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain A:



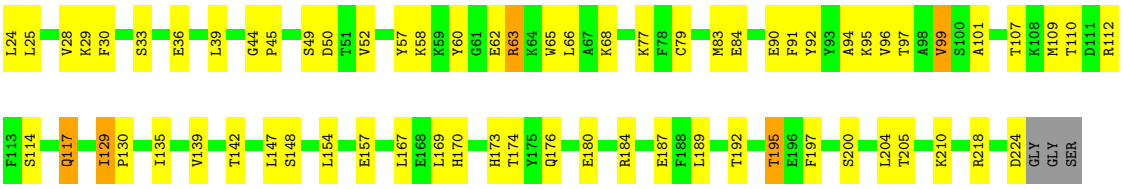
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain B:



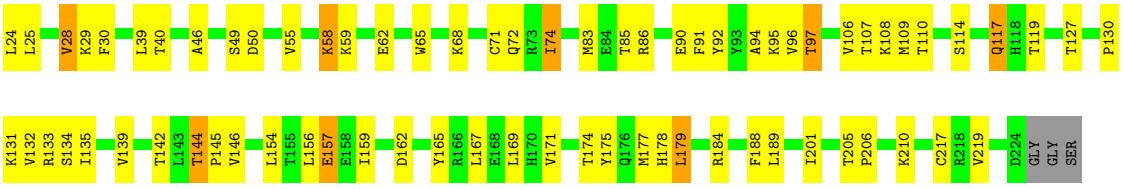
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain F:



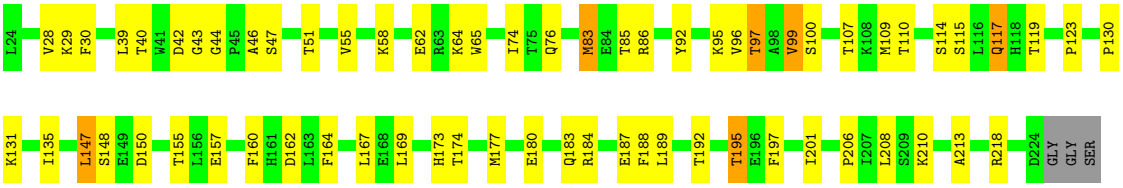
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain I:



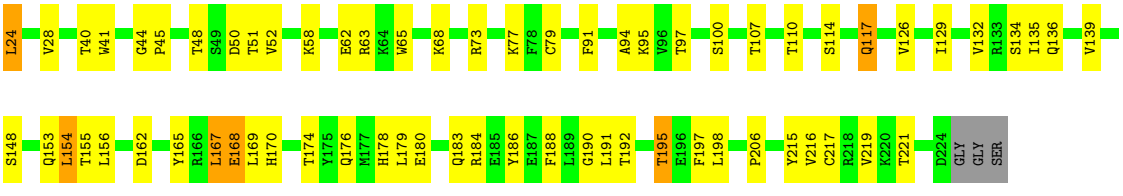
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain M:



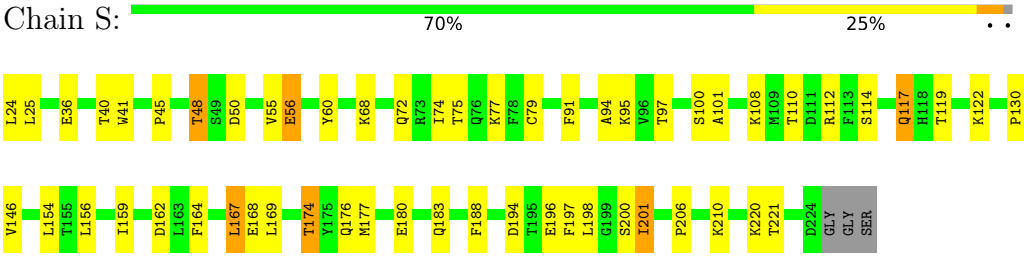
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain P:



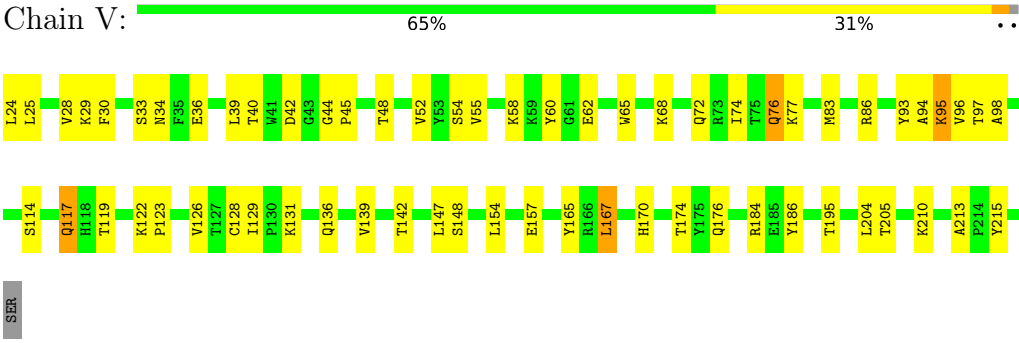
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain S:



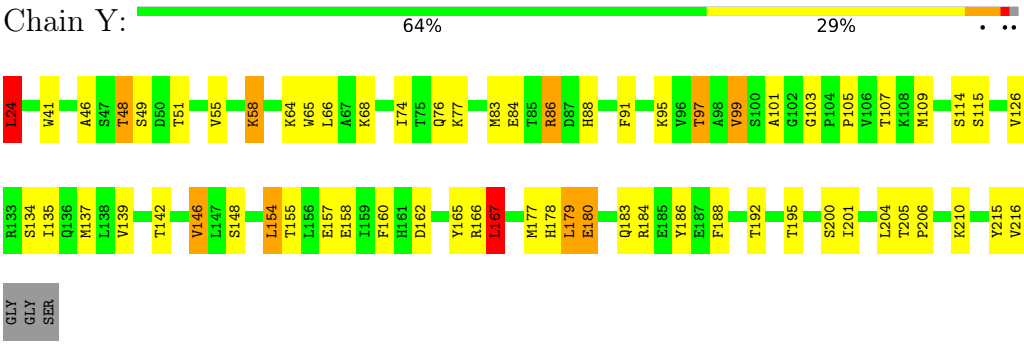
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain V:



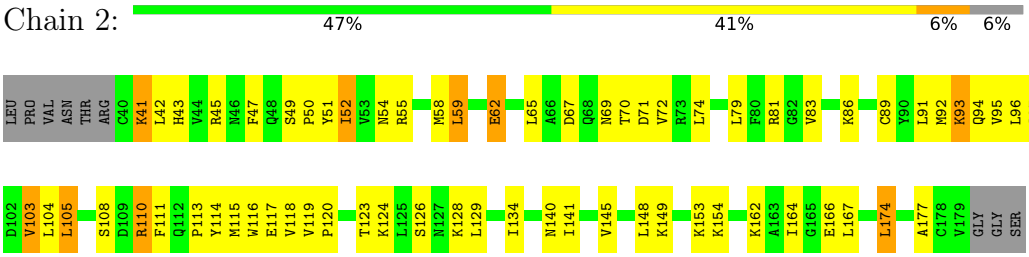
• Molecule 2: Interleukin-22 receptor subunit alpha-1

Chain Y:



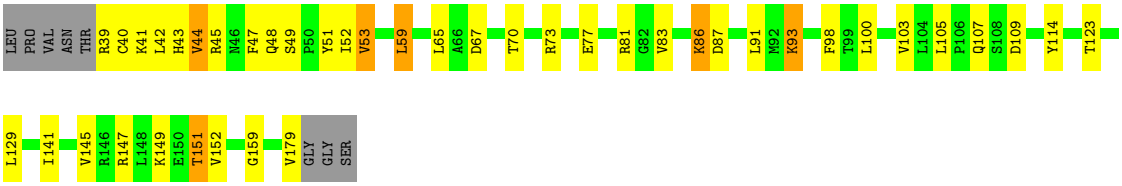
• Molecule 3: Interleukin-22

Chain 2:



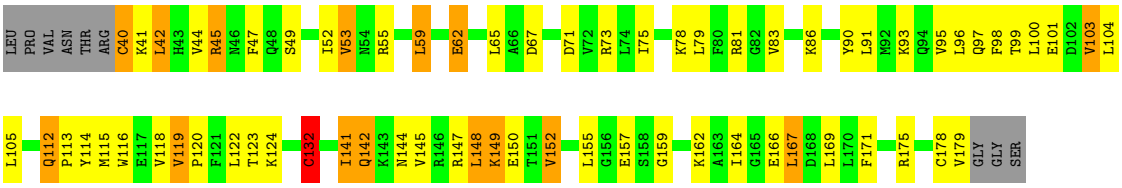
• Molecule 3: Interleukin-22

Chain 5:



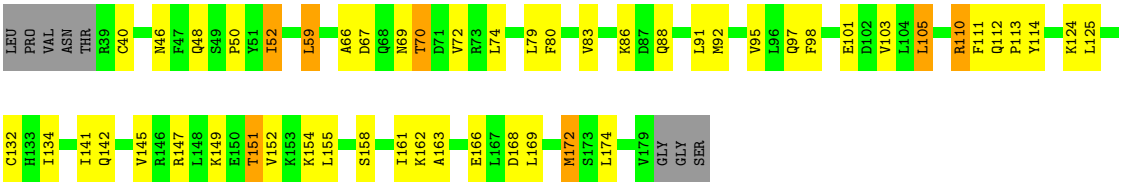
• Molecule 3: Interleukin-22

Chain 8:



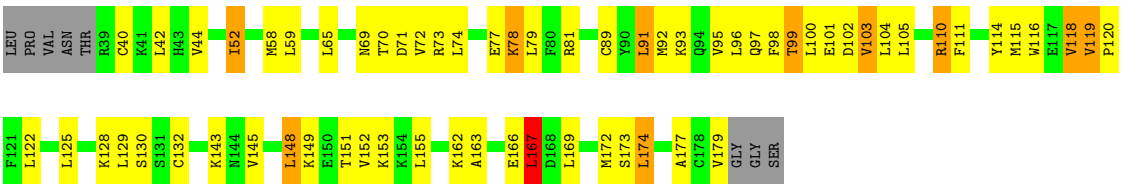
• Molecule 3: Interleukin-22

Chain D:



• Molecule 3: Interleukin-22

Chain G:



• Molecule 3: Interleukin-22

Chain J:

• Molecule 3: Interleukin-22

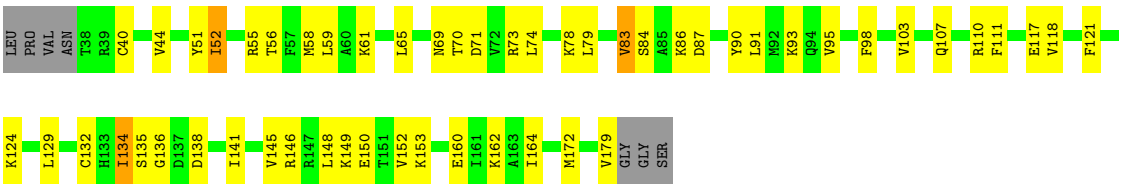
Chain L:

• Molecule 3: Interleukin-22

Chain N:

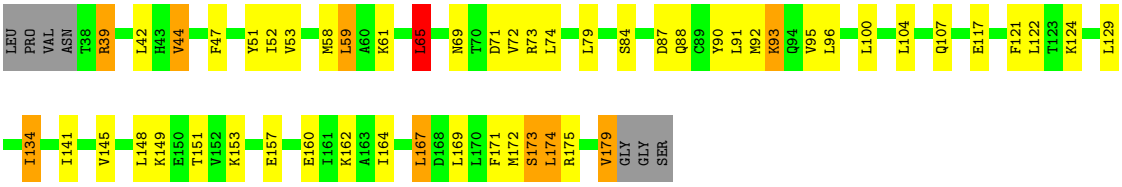
• Molecule 3: Interleukin-22

Chain Q:



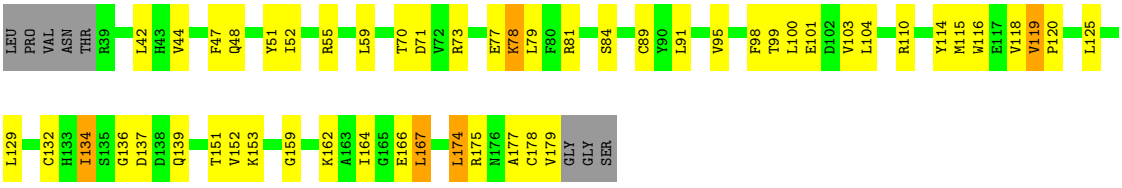
• Molecule 3: Interleukin-22

Chain T:



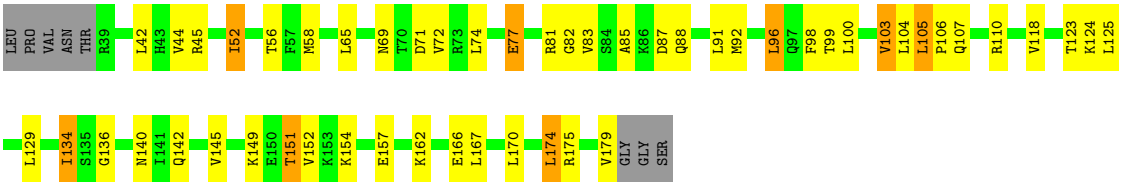
• Molecule 3: Interleukin-22

Chain W:



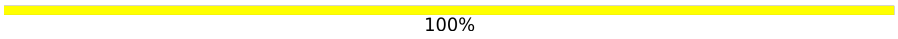
• Molecule 3: Interleukin-22

Chain Z:



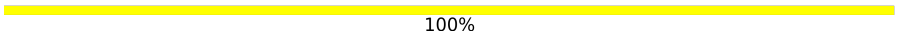
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



• Molecule 4: 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 c:

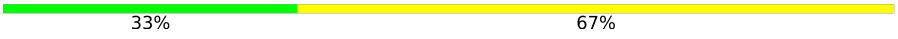


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

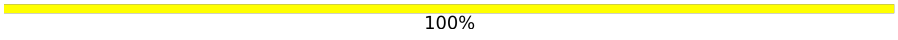
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



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

Chain e:



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

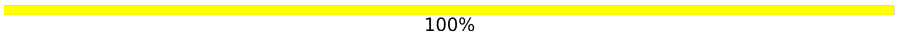
Chain i:

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

Chain j:

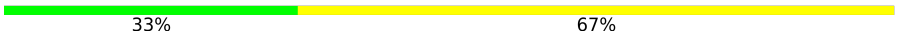
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:



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

Chain m:



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

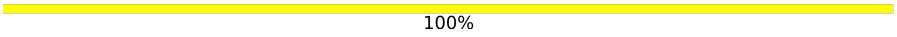
Chain s:

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

Chain d:

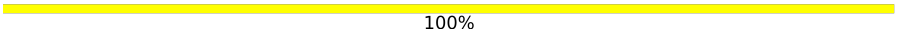
• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:



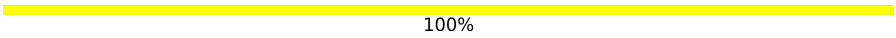
• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



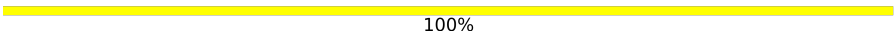
• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



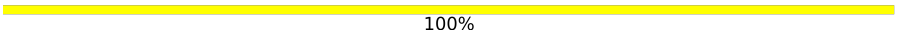
• Molecule 6: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:



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

Chain u:



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

Chain v:

• Molecule 7: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

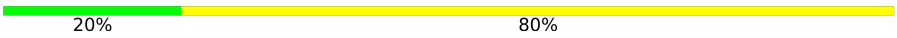
Chain f:

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

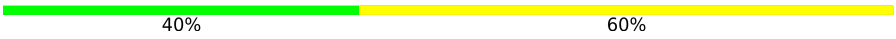
Chain g:

• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



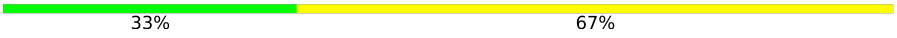
• Molecule 9: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 

• Molecule 10: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q: 

• Molecule 11: alpha-L-fucopyranose-(1-3)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	134.49Å 145.22Å 152.04Å 71.06° 81.84° 62.48°	Depositor
Resolution (Å)	48.09 – 2.60	Depositor
% Data completeness (in resolution range)	97.5 (48.09-2.60)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.236 , 0.296	Depositor
Wilson B-factor (Å^2)	69.1	Xtriage
Anisotropy	0.199	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	53140	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5066e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, FUC, NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.53	0/1627	0.74	1/2223 (0.0%)
1	3	0.45	1/1643 (0.1%)	0.67	0/2244
1	6	0.48	0/1655	0.67	0/2258
1	9	0.46	0/1579	0.72	2/2155 (0.1%)
1	C	0.60	0/1662	0.75	0/2267
1	E	0.57	0/1641	0.72	1/2242 (0.0%)
1	H	0.58	1/1650 (0.1%)	0.74	0/2252
1	K	0.54	0/1653	0.71	0/2256
1	O	0.56	0/1657	0.76	2/2261 (0.1%)
1	R	0.54	0/1659	0.69	0/2263
1	U	0.55	0/1651	0.72	1/2254 (0.0%)
1	X	0.49	0/1667	0.73	1/2274 (0.0%)
2	1	0.53	1/1655 (0.1%)	0.75	1/2250 (0.0%)
2	4	0.57	1/1652 (0.1%)	0.81	4/2247 (0.2%)
2	7	0.52	1/1646 (0.1%)	0.73	1/2240 (0.0%)
2	A	0.60	1/1647 (0.1%)	0.78	1/2242 (0.0%)
2	B	0.56	0/1651	0.78	1/2246 (0.0%)
2	F	0.55	0/1650	0.72	0/2244
2	I	0.53	0/1656	0.74	0/2252
2	M	0.56	0/1647	0.74	0/2240
2	P	0.61	0/1663	0.83	0/2259
2	S	0.59	0/1659	0.77	1/2254 (0.0%)
2	V	0.53	0/1653	0.70	0/2247
2	Y	0.60	0/1652	0.82	3/2246 (0.1%)
3	2	0.59	1/1113 (0.1%)	0.79	1/1500 (0.1%)
3	5	0.45	0/1143	0.65	0/1536
3	8	0.62	2/1124 (0.2%)	0.79	1/1513 (0.1%)
3	D	0.52	0/1148	0.77	2/1543 (0.1%)
3	G	0.48	0/1140	0.77	2/1533 (0.1%)
3	J	0.45	0/1134	0.68	0/1525
3	L	0.54	0/1142	0.72	0/1536
3	N	0.49	0/1110	0.72	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	Q	0.60	0/1137	0.84	2/1532 (0.1%)
3	T	0.54	0/1150	0.77	1/1547 (0.1%)
3	W	0.49	0/1141	0.70	0/1534
3	Z	0.57	0/1146	0.79	0/1540
All	All	0.54	9/53203 (0.0%)	0.74	29/72253 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	1
2	Y	0	1
3	2	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	8	40	CYS	CB-SG	-9.55	1.66	1.82
3	2	62	GLU	CG-CD	9.31	1.66	1.51
3	8	132	CYS	CB-SG	8.11	1.96	1.82
2	7	71	CYS	CB-SG	-7.13	1.70	1.82
2	4	217	CYS	CB-SG	-6.00	1.72	1.82
2	1	217	CYS	CB-SG	-5.84	1.72	1.81
1	H	82	TYR	CD1-CE1	5.63	1.47	1.39
2	A	217	CYS	CB-SG	-5.22	1.73	1.81
1	3	108	VAL	CB-CG1	-5.13	1.42	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	8	148	LEU	CB-CG-CD2	-10.11	93.81	111.00
3	Q	110	ARG	NE-CZ-NH2	9.99	125.29	120.30
2	Y	167	LEU	CA-CB-CG	7.51	132.57	115.30
2	4	167	LEU	CA-CB-CG	6.99	131.37	115.30
2	B	167	LEU	CB-CG-CD1	-6.89	99.28	111.00
3	T	65	LEU	CA-CB-CG	6.59	130.45	115.30
1	0	178	LEU	CB-CG-CD1	-6.57	99.82	111.00
3	D	110	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	9	129	LEU	CA-CB-CG	6.02	129.14	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	73	ARG	NE-CZ-NH2	-6.01	117.29	120.30
2	Y	179	LEU	CA-CB-CG	5.93	128.93	115.30
2	A	154	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	9	150	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	O	129	LEU	CA-CB-CG	5.40	127.73	115.30
3	2	59	LEU	CB-CG-CD2	5.40	120.17	111.00
2	7	167	LEU	CA-CB-CG	5.28	127.44	115.30
1	X	181	LEU	CA-CB-CG	5.26	127.39	115.30
1	U	75	ASP	CB-CG-OD1	5.22	123.00	118.30
1	E	197	ASP	CB-CG-OD1	5.21	122.99	118.30
2	S	112	ARG	NE-CZ-NH1	-5.21	117.70	120.30
3	G	155	LEU	CA-CB-CG	5.17	127.20	115.30
1	O	138	ASN	C-N-CA	-5.12	108.91	121.70
2	4	191	LEU	CA-CB-CG	5.11	127.04	115.30
2	1	167	LEU	CA-CB-CG	5.07	126.96	115.30
2	4	198	LEU	CB-CG-CD2	-5.06	102.40	111.00
3	G	167	LEU	CA-CB-CG	5.04	126.89	115.30
2	4	191	LEU	CB-CG-CD1	5.03	119.55	111.00
3	D	59	LEU	CB-CG-CD1	-5.01	102.48	111.00
2	Y	24	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	58	MET	Mainchain
2	4	103	GLY	Peptide
2	Y	103	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1579	0	1468	51	0
1	3	1595	0	1479	53	0
1	6	1607	0	1505	44	0
1	9	1532	0	1422	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1614	0	1516	31	0
1	E	1593	0	1474	26	0
1	H	1602	0	1499	46	0
1	K	1605	0	1500	41	0
1	O	1609	0	1508	25	0
1	R	1611	0	1512	46	0
1	U	1603	0	1491	41	0
1	X	1619	0	1516	50	0
2	1	1613	0	1583	54	0
2	4	1610	0	1574	58	0
2	7	1604	0	1563	39	0
2	A	1605	0	1561	39	0
2	B	1609	0	1572	59	0
2	F	1608	0	1574	40	0
2	I	1614	0	1578	53	0
2	M	1605	0	1572	43	0
2	P	1621	0	1598	44	0
2	S	1617	0	1594	39	0
2	V	1611	0	1583	42	0
2	Y	1610	0	1578	47	0
3	2	1096	0	1100	58	0
3	5	1126	0	1144	33	0
3	8	1107	0	1114	52	0
3	D	1131	0	1155	44	0
3	G	1123	0	1142	50	0
3	J	1117	0	1138	30	0
3	L	1125	0	1143	21	0
3	N	1093	0	1083	16	0
3	Q	1120	0	1127	33	0
3	T	1133	0	1153	36	0
3	W	1124	0	1139	30	0
3	Z	1129	0	1153	40	0
4	a	49	0	43	0	0
4	c	49	0	43	0	0
4	n	49	0	43	0	0
5	b	38	0	34	0	0
5	e	38	0	34	0	0
5	i	38	0	34	0	0
5	j	38	0	34	0	0
5	l	38	0	34	0	0
5	m	38	0	34	0	0
5	s	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	d	24	0	22	0	0
6	o	24	0	22	0	0
6	p	24	0	22	0	0
6	r	24	0	22	0	0
6	t	24	0	22	0	0
6	u	24	0	22	0	0
6	v	24	0	22	0	0
7	f	24	0	22	0	0
8	g	39	0	34	0	0
9	h	59	0	52	0	0
9	k	59	0	52	0	0
10	q	28	0	25	0	0
11	w	34	0	31	0	0
12	A	6	0	8	0	0
12	H	6	0	8	0	0
12	J	6	0	8	0	0
12	K	6	0	8	0	0
12	M	6	0	8	2	0
12	O	6	0	8	0	0
12	Y	6	0	8	1	0
13	B	14	0	13	0	0
14	1	9	0	0	4	0
14	2	6	0	0	1	0
14	3	6	0	0	4	0
14	4	7	0	0	2	0
14	5	2	0	0	1	0
14	6	5	0	0	4	0
14	7	12	0	0	2	0
14	8	6	0	0	3	0
14	9	3	0	0	1	0
14	A	22	0	0	2	0
14	B	16	0	0	5	0
14	C	22	0	0	0	0
14	D	14	0	0	2	0
14	E	15	0	0	2	0
14	F	10	0	0	0	0
14	G	5	0	0	4	0
14	H	17	0	0	3	0
14	I	9	0	0	2	0
14	J	6	0	0	1	0
14	K	9	0	0	3	0
14	L	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	M	8	0	0	0	0
14	N	5	0	0	0	0
14	O	14	0	0	0	0
14	P	6	0	0	0	0
14	Q	7	0	0	2	0
14	R	9	0	0	5	0
14	S	13	0	0	6	0
14	T	6	0	0	1	0
14	U	14	0	0	1	0
14	V	12	0	0	2	0
14	W	1	0	0	0	0
14	X	11	0	0	0	0
14	Y	20	0	0	2	0
14	Z	5	0	0	0	0
All	All	53140	0	51217	1419	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 14.

All (1419) 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)
1:0:136:ILE:HD13	1:0:148:ILE:HD11	1.43	1.01
3:2:59:LEU:HD22	3:2:118:VAL:HG11	1.39	0.99
2:V:157:GLU:OE1	2:V:184:ARG:NH2	1.97	0.98
2:B:146:VAL:O	14:B:401:HOH:O	1.83	0.96
1:0:32:VAL:HG12	1:0:112:ILE:HB	1.51	0.93
2:B:205:THR:HG23	2:B:210:LYS:HB2	1.52	0.92
3:G:102:ASP:O	14:G:301:HOH:O	1.90	0.90
1:9:123:LEU:HD22	1:9:128:HIS:CE1	2.07	0.89
1:0:111:THR:O	1:0:200:ARG:NH2	2.06	0.89
3:T:92:MET:HB3	3:T:174:LEU:HD12	1.54	0.88
1:6:71:SER:O	14:6:301:HOH:O	1.91	0.88
2:7:205:THR:HB	2:7:210:LYS:HB2	1.55	0.87
2:A:83:MET:SD	2:A:86:ARG:NH1	2.48	0.87
3:2:100:LEU:HD23	3:2:104:LEU:HD21	1.57	0.86
2:P:139:VAL:HG23	2:P:184:ARG:HD2	1.58	0.86
1:U:184:TRP:HD1	1:U:213:GLY:HA2	1.41	0.86
1:3:210:GLU:O	14:3:301:HOH:O	1.93	0.86
2:I:25:LEU:HD21	2:I:96:VAL:HG13	1.59	0.85
1:9:123:LEU:HD22	1:9:128:HIS:HE1	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:184:TRP:CD1	1:U:213:GLY:HA2	2.12	0.84
1:K:88:ARG:HB3	1:K:102:GLN:HG2	1.59	0.84
1:K:161:GLN:O	14:K:401:HOH:O	1.94	0.84
1:R:106:CYS:SG	14:R:301:HOH:O	2.36	0.83
1:3:100:TRP:O	14:3:302:HOH:O	1.95	0.83
2:M:83:MET:SD	2:M:86:ARG:NH1	2.51	0.83
2:V:25:LEU:HD21	2:V:96:VAL:HG23	1.60	0.83
2:Y:216:VAL:H	12:Y:303:GOL:H31	1.45	0.82
3:T:107:GLN:NE2	3:T:157:GLU:OE2	2.10	0.82
2:I:144:THR:HG23	2:I:146:VAL:H	1.45	0.82
3:D:147:ARG:O	3:D:151:THR:OG1	1.98	0.81
3:G:162:LYS:O	14:G:302:HOH:O	1.98	0.81
3:G:77:GLU:OE1	3:G:81:ARG:NH1	2.14	0.81
1:X:120:ILE:HD11	1:X:127:LEU:HD22	1.63	0.81
3:8:83:VAL:HG21	3:8:91:LEU:HD22	1.61	0.80
1:H:136:ILE:HG21	1:H:148:ILE:HD11	1.62	0.80
2:Y:157:GLU:OE1	2:Y:184:ARG:NH2	2.14	0.80
3:5:67:ASP:OD2	14:5:301:HOH:O	2.01	0.79
1:9:55:GLN:NE2	1:9:64:ASP:OD1	2.14	0.79
1:C:182:GLU:O	1:C:212:THR:HG21	1.82	0.79
3:Q:153:LYS:NZ	14:Q:301:HOH:O	2.15	0.78
1:R:123:LEU:HD13	1:R:124:ALA:H	1.47	0.78
2:A:50:ASP:N	2:A:50:ASP:OD1	2.16	0.77
2:Y:24:LEU:HD12	2:Y:46:ALA:HB3	1.66	0.77
3:N:103:VAL:HG11	3:N:163:ALA:HB3	1.66	0.76
3:Z:103:VAL:O	3:Z:107:GLN:HB3	1.85	0.76
2:B:74:ILE:HD12	2:B:76:GLN:HG2	1.67	0.76
3:Z:92:MET:HB3	3:Z:174:LEU:HD12	1.68	0.76
1:3:108:VAL:O	1:3:200:ARG:NH2	2.13	0.76
2:B:87:ASP:OD2	14:B:402:HOH:O	2.04	0.76
2:F:205:THR:HB	2:F:210:LYS:HB2	1.68	0.76
2:I:83:MET:SD	2:I:86:ARG:NH1	2.59	0.76
2:S:220:LYS:O	14:S:401:HOH:O	2.03	0.76
1:9:65:HIS:ND1	14:9:401:HOH:O	2.17	0.75
2:Y:148:SER:HB2	2:Y:154:LEU:HD11	1.67	0.75
2:P:129:ILE:HB	2:P:136:GLN:HB3	1.68	0.75
1:X:185:THR:H	1:X:212:THR:HG22	1.50	0.75
3:5:49:SER:HB3	3:5:52:ILE:HG12	1.68	0.75
1:9:81:LYS:NZ	1:9:138:ASN:OD1	2.19	0.75
2:7:184:ARG:NH2	14:7:401:HOH:O	2.11	0.74
1:C:20:MET:N	1:C:96:GLU:OE2	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:90:ARG:HD2	1:0:97:HIS:HB2	1.68	0.74
1:0:122:SER:HB2	1:0:127:LEU:HD23	1.69	0.74
1:0:84:ASP:OD2	3:Z:124:LYS:HE2	1.87	0.74
2:1:157:GLU:OE1	2:1:184:ARG:NH2	2.20	0.73
2:I:97:THR:HG23	2:I:107:THR:OG1	1.88	0.73
2:B:126:VAL:HG21	2:B:201:ILE:HG21	1.70	0.73
3:5:44:VAL:HG13	3:5:179:VAL:HG21	1.69	0.73
3:G:92:MET:HB3	3:G:174:LEU:HD12	1.71	0.73
3:Q:107:GLN:NE2	3:Q:160:GLU:OE1	2.19	0.73
1:R:81:LYS:O	14:R:301:HOH:O	2.06	0.73
2:I:157:GLU:OE1	2:I:184:ARG:NH2	2.22	0.73
3:2:83:VAL:HG21	3:2:91:LEU:HD22	1.70	0.73
1:6:185:THR:H	1:6:212:THR:HG22	1.53	0.73
1:6:35:LYS:HE2	1:6:37:ILE:HD11	1.69	0.73
2:F:157:GLU:OE1	2:F:184:ARG:NH2	2.20	0.73
3:5:41:LYS:NZ	3:5:86:LYS:HD3	2.04	0.73
3:8:95:VAL:HG13	3:8:148:LEU:HD21	1.70	0.72
1:9:90:ARG:HH11	1:9:97:HIS:HB3	1.54	0.72
3:D:83:VAL:HG11	3:D:91:LEU:HD22	1.71	0.72
3:T:121:PHE:HD2	3:T:122:LEU:HD12	1.54	0.72
1:X:42:VAL:HG12	1:X:52:PHE:HZ	1.51	0.72
2:Y:48:THR:HG23	2:Y:51:THR:HB	1.72	0.72
3:W:98:PHE:HZ	3:W:152:VAL:HG11	1.55	0.72
2:1:86:ARG:HD2	2:1:147:LEU:HD23	1.70	0.72
1:6:32:VAL:HG12	1:6:112:ILE:HB	1.72	0.71
2:Y:97:THR:HG23	2:Y:107:THR:OG1	1.89	0.71
2:A:24:LEU:N	14:A:403:HOH:O	2.23	0.71
1:0:195:LEU:HD13	1:0:200:ARG:HB3	1.71	0.71
2:7:25:LEU:HD11	2:7:96:VAL:HG23	1.73	0.71
3:5:107:GLN:HE21	3:5:109:ASP:HB2	1.54	0.71
2:M:177:MET:HE2	2:M:188:PHE:HD1	1.54	0.71
1:H:120:ILE:HD11	1:H:127:LEU:HG	1.73	0.71
2:4:42:ASP:HA	2:4:77:LYS:HD3	1.72	0.70
2:V:58:LYS:HE3	2:V:65:TRP:CD1	2.26	0.70
2:1:144:THR:OG1	14:1:401:HOH:O	2.09	0.70
3:J:147:ARG:O	3:J:151:THR:HG22	1.92	0.70
1:0:145:LEU:HA	1:0:148:ILE:HD12	1.72	0.70
2:7:74:ILE:HD12	2:7:76:GLN:HG2	1.73	0.70
2:F:58:LYS:HD3	2:F:65:TRP:CD1	2.27	0.70
3:2:62:GLU:N	3:2:62:GLU:OE1	2.25	0.70
1:6:39:GLN:NE2	14:6:302:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:123:LEU:HD23	1:9:126:SER:H	1.56	0.69
1:R:177:VAL:O	14:R:302:HOH:O	2.10	0.69
1:U:86:THR:HG23	1:U:104:THR:HG22	1.74	0.69
1:3:35:LYS:HE2	1:3:37:ILE:HD11	1.75	0.69
2:A:52:VAL:HG21	2:A:73:ARG:HG3	1.75	0.69
1:C:185:THR:H	1:C:212:THR:HG22	1.56	0.69
3:T:96:LEU:HD22	3:T:174:LEU:HD21	1.74	0.69
2:A:162:ASP:OD2	14:A:401:HOH:O	2.10	0.69
3:J:114:TYR:O	3:J:118:VAL:HG23	1.93	0.69
3:W:59:LEU:HD13	3:W:114:TYR:HB2	1.75	0.69
3:5:93:LYS:HB2	3:5:129:LEU:HD13	1.74	0.69
2:I:58:LYS:NZ	3:J:70:THR:OG1	2.23	0.69
2:A:74:ILE:HD12	2:A:76:GLN:HG2	1.75	0.68
3:T:87:ASP:HB3	3:T:141:ILE:HD11	1.73	0.68
2:1:97:THR:HG23	2:1:107:THR:OG1	1.94	0.68
1:E:88:ARG:HB3	1:E:102:GLN:HG2	1.76	0.68
2:1:167:LEU:HB3	2:1:201:ILE:HG13	1.75	0.68
2:A:144:THR:HG23	2:A:146:VAL:H	1.58	0.68
2:B:165:TYR:HB3	2:B:201:ILE:HD11	1.74	0.68
1:O:214:ASN:OD1	1:O:214:ASN:N	2.27	0.68
1:O:35:LYS:HE2	1:O:37:ILE:HD11	1.76	0.68
2:S:97:THR:O	14:S:402:HOH:O	2.12	0.68
2:4:83:MET:SD	2:4:86:ARG:NH1	2.67	0.67
2:F:58:LYS:NZ	2:F:62:GLU:O	2.27	0.67
1:R:51:THR:OG1	1:R:92:GLU:OE2	2.12	0.67
2:1:218:ARG:NH2	1:C:50:LEU:O	2.27	0.67
1:0:156:VAL:HB	1:0:169:VAL:HG12	1.77	0.67
1:6:135:GLN:HA	1:6:144:THR:HA	1.76	0.67
3:D:110:ARG:NH2	3:D:161:ILE:HG22	2.08	0.67
2:V:58:LYS:NZ	2:V:62:GLU:O	2.28	0.67
2:B:126:VAL:HB	2:B:215:TYR:CD2	2.30	0.67
3:Z:85:ALA:HA	3:Z:88:GLN:HG3	1.76	0.67
1:0:163:THR:HG22	1:0:165:GLU:H	1.60	0.66
2:V:58:LYS:HG2	2:V:95:LYS:HZ1	1.60	0.66
3:D:151:THR:HG22	3:D:154:LYS:HE2	1.76	0.66
2:F:192:THR:HG23	2:F:195:THR:OG1	1.95	0.66
2:4:173:HIS:HB2	1:E:68:ARG:HB2	1.78	0.66
2:7:71:CYS:HB3	2:7:74:ILE:HD13	1.77	0.66
3:D:97:GLN:NE2	14:D:301:HOH:O	2.27	0.66
2:S:144:THR:HG23	2:S:146:VAL:H	1.59	0.66
1:K:86:THR:HG22	1:K:104:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:120:ILE:HD12	1:9:129:LEU:HD12	1.78	0.66
2:A:126:VAL:HG22	2:A:139:VAL:HG22	1.76	0.66
3:G:42:LEU:HG	3:G:129:LEU:HD21	1.78	0.66
3:2:120:PRO:HB3	1:3:83:GLY:HA2	1.78	0.66
2:I:130:PRO:HA	2:I:135:ILE:HD13	1.78	0.66
3:L:151:THR:HA	3:L:154:LYS:HE2	1.78	0.66
2:4:48:THR:HG23	2:4:50:ASP:H	1.61	0.65
1:K:155:ARG:NH1	14:K:402:HOH:O	2.28	0.65
1:K:196:LEU:O	1:K:198:GLN:NE2	2.29	0.65
3:T:74:LEU:HB3	3:T:148:LEU:HD11	1.78	0.65
2:4:178:HIS:CD2	1:6:130:ARG:HD2	2.32	0.65
2:B:65:TRP:CG	2:B:95:LYS:HE3	2.31	0.65
2:F:33:SER:O	2:F:36:GLU:HG2	1.95	0.65
1:K:57:GLU:OE1	2:M:64:LYS:NZ	2.23	0.65
2:A:144:THR:HG23	2:A:146:VAL:HG13	1.77	0.65
2:M:97:THR:HG22	2:M:107:THR:HG23	1.77	0.65
3:Q:146:ARG:NH1	3:Q:150:GLU:OE2	2.29	0.65
1:9:90:ARG:NH1	1:9:97:HIS:HB3	2.11	0.65
3:N:93:LYS:NZ	3:N:132:CYS:O	2.25	0.65
3:G:115:MET:O	3:G:119:VAL:HG13	1.96	0.65
2:M:58:LYS:HE3	2:M:65:TRP:CE2	2.32	0.65
2:Y:205:THR:HB	2:Y:210:LYS:HB2	1.77	0.65
2:1:177:MET:HE2	2:1:188:PHE:CD1	2.31	0.65
3:2:116:TRP:HD1	1:3:80:SER:OG	1.79	0.65
3:2:99:THR:HA	3:2:103:VAL:HG23	1.78	0.65
3:N:97:GLN:NE2	3:N:101:GLU:OE2	2.30	0.65
2:P:63:ARG:NH1	3:Q:71:ASP:OD2	2.28	0.65
2:F:58:LYS:HD3	2:F:65:TRP:HD1	1.61	0.65
2:7:62:GLU:HB3	2:7:64:LYS:HD2	1.78	0.65
2:I:95:LYS:HA	2:I:109:MET:HA	1.78	0.65
3:5:98:PHE:HZ	3:5:152:VAL:HG11	1.61	0.64
3:G:166:GLU:HG3	14:G:302:HOH:O	1.96	0.64
2:4:63:ARG:HB3	2:4:63:ARG:HH11	1.62	0.64
3:Z:107:GLN:HE21	3:Z:110:ARG:HG2	1.60	0.64
3:2:96:LEU:HD13	3:2:126:SER:HB3	1.80	0.64
3:8:67:ASP:CG	3:8:162:LYS:HE2	2.18	0.64
3:G:116:TRP:O	1:H:80:SER:OG	2.15	0.64
1:O:90:ARG:HD2	1:O:97:HIS:HB2	1.80	0.64
3:G:110:ARG:HD3	3:G:111:PHE:H	1.63	0.64
3:L:103:VAL:HG11	3:L:163:ALA:HB3	1.80	0.64
1:9:123:LEU:HG	1:9:125:GLU:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:188:CYS:C	1:H:189:ILE:HD13	2.18	0.64
1:R:161:GLN:HG2	1:R:188:CYS:SG	2.38	0.64
3:8:59:LEU:HD12	3:8:118:VAL:HG11	1.77	0.63
3:G:59:LEU:HD13	3:G:114:TYR:HB2	1.80	0.63
2:Y:48:THR:HG21	2:Y:101:ALA:H	1.62	0.63
1:R:120:ILE:HD13	1:R:189:ILE:HD12	1.80	0.63
1:3:146:LYS:NZ	1:3:174:ASP:OD1	2.31	0.63
2:4:167:LEU:HB3	2:4:201:ILE:HG13	1.81	0.63
2:M:157:GLU:OE1	2:M:184:ARG:NH2	2.31	0.63
3:8:164:ILE:HA	3:8:167:LEU:HD13	1.80	0.63
1:3:116:PRO:HG2	1:3:191:VAL:HG13	1.81	0.63
2:S:24:LEU:HD22	2:S:45:PRO:HD2	1.80	0.63
1:3:104:THR:O	14:3:303:HOH:O	2.16	0.63
2:M:148:SER:OG	2:M:150:ASP:OD1	2.11	0.63
2:S:176:GLN:HE21	1:U:130:ARG:HH12	1.46	0.63
1:H:32:VAL:HG22	1:H:112:ILE:HB	1.80	0.63
3:Z:145:VAL:O	3:Z:149:LYS:HG3	1.99	0.63
3:2:98:PHE:CD1	3:2:149:LYS:HE2	2.34	0.62
3:D:151:THR:HA	3:D:154:LYS:HG2	1.80	0.62
3:Z:107:GLN:NE2	3:Z:110:ARG:HG2	2.14	0.62
2:1:25:LEU:HD12	2:1:98:ALA:HB2	1.82	0.62
2:B:103:GLY:H	2:B:104:PRO:HD2	1.64	0.62
1:H:195:LEU:O	14:H:401:HOH:O	2.15	0.62
2:P:168:GLU:HG3	2:P:170:HIS:NE2	2.13	0.62
3:T:121:PHE:CD2	3:T:122:LEU:HD12	2.34	0.62
3:W:98:PHE:CZ	3:W:152:VAL:HG11	2.34	0.62
3:Z:110:ARG:NH2	3:Z:157:GLU:OE2	2.32	0.62
1:9:77:SER:O	1:9:138:ASN:ND2	2.26	0.62
2:B:157:GLU:OE1	2:B:184:ARG:NH2	2.33	0.62
1:3:160:LYS:NZ	1:3:182:GLU:OE1	2.25	0.62
2:P:52:VAL:HG21	2:P:73:ARG:HG3	1.81	0.62
2:P:126:VAL:HB	2:P:215:TYR:CD2	2.34	0.62
2:A:131:LYS:HE2	2:Y:41:TRP:O	2.00	0.62
1:0:134:PRO:HB2	1:0:145:LEU:HD13	1.80	0.62
3:J:142:GLN:HA	3:J:145:VAL:HG22	1.81	0.62
1:X:42:VAL:HG12	1:X:52:PHE:CZ	2.34	0.62
3:2:98:PHE:HA	3:2:101:GLU:HG2	1.82	0.62
3:L:98:PHE:HZ	3:L:152:VAL:HG11	1.64	0.62
2:V:94:ALA:O	2:V:110:THR:HG23	1.99	0.62
3:W:79:LEU:HD21	3:W:95:VAL:HG21	1.82	0.62
1:0:130:ARG:HD2	2:Y:178:HIS:CD2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:24:LEU:HB2	2:7:46:ALA:HB3	1.82	0.62
1:9:123:LEU:HD21	1:9:125:GLU:HB2	1.81	0.62
3:D:172:MET:HA	3:D:172:MET:CE	2.30	0.62
2:M:160:PHE:HD1	12:M:305:GOL:H12	1.65	0.62
2:P:24:LEU:HB3	2:P:44:GLY:HA3	1.81	0.62
3:5:49:SER:O	3:5:53:VAL:HG13	2.00	0.61
2:P:165:TYR:OH	2:P:184:ARG:NH1	2.33	0.61
1:3:48:THR:O	1:3:50:LEU:N	2.33	0.61
3:G:73:ARG:HB3	3:G:78:LYS:HZ2	1.65	0.61
2:M:95:LYS:HA	2:M:109:MET:HA	1.82	0.61
2:I:139:VAL:O	2:I:184:ARG:HD3	2.00	0.61
2:V:28:VAL:HG22	2:V:110:THR:HG22	1.83	0.61
3:Z:77:GLU:HB2	3:Z:81:ARG:HH12	1.65	0.61
1:0:79:LEU:HB3	1:0:85:TYR:CE2	2.34	0.61
1:3:88:ARG:HB3	1:3:102:GLN:HG2	1.82	0.61
2:1:91:PHE:CE2	2:1:114:SER:HB2	2.35	0.61
3:2:96:LEU:HD12	3:2:97:GLN:N	2.16	0.61
1:6:160:LYS:HE3	1:6:165:GLU:HB2	1.81	0.61
1:9:88:ARG:HD3	1:9:100:TRP:CG	2.36	0.61
2:4:204:LEU:HG	2:4:211:GLU:HG3	1.82	0.61
2:P:48:THR:OG1	2:P:50:ASP:OD1	2.12	0.61
2:4:91:PHE:CE2	2:4:114:SER:HB2	2.35	0.61
2:A:98:ALA:HB3	2:A:106:VAL:HG23	1.82	0.61
2:4:155:THR:HG23	2:4:158:GLU:H	1.66	0.60
2:P:195:THR:O	2:P:221:THR:HG22	2.01	0.60
3:Z:72:VAL:HG13	3:Z:162:LYS:HE3	1.83	0.60
3:Z:170:LEU:HD23	3:Z:174:LEU:HD22	1.83	0.60
2:B:91:PHE:CE2	2:B:114:SER:HB2	2.36	0.60
1:U:55:GLN:NE2	1:U:64:ASP:OD1	2.30	0.60
1:0:51:THR:O	1:0:92:GLU:N	2.32	0.60
3:2:96:LEU:HD21	3:2:129:LEU:HD12	1.83	0.60
3:2:141:ILE:O	3:2:145:VAL:HG23	2.02	0.60
2:M:167:LEU:HG	2:M:201:ILE:HG23	1.84	0.60
1:H:80:SER:O	1:H:107:PRO:HG2	2.02	0.60
2:I:144:THR:HG21	2:I:159:ILE:HD11	1.83	0.60
3:Z:100:LEU:HD23	3:Z:104:LEU:HD12	1.84	0.60
3:8:49:SER:OG	1:9:148:ILE:O	2.11	0.60
3:W:115:MET:O	3:W:119:VAL:HG13	2.01	0.60
2:S:114:SER:HB3	2:S:117:GLN:HG3	1.83	0.60
3:W:42:LEU:N	3:W:178:CYS:O	2.32	0.60
3:Z:92:MET:HB3	3:Z:174:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:LEU:HB3	2:F:44:GLY:HA3	1.83	0.59
3:Z:103:VAL:O	3:Z:107:GLN:CB	2.50	0.59
3:Z:98:PHE:HZ	3:Z:152:VAL:HG11	1.66	0.59
2:S:194:ASP:HA	2:S:221:THR:O	2.02	0.59
3:L:98:PHE:CZ	3:L:152:VAL:HG11	2.36	0.59
1:U:119:GLN:OE1	14:U:301:HOH:O	2.17	0.59
2:V:170:HIS:ND1	2:V:176:GLN:HG2	2.18	0.59
1:H:35:LYS:HD3	1:H:137:GLU:HG3	1.83	0.59
2:1:154:LEU:O	14:1:401:HOH:O	2.17	0.59
1:K:116:PRO:HG2	1:K:191:VAL:HG22	1.84	0.59
2:M:58:LYS:NZ	2:M:62:GLU:O	2.24	0.59
2:S:25:LEU:O	2:S:108:LYS:NZ	2.28	0.59
2:4:51:THR:HA	2:4:100:SER:HB3	1.85	0.59
2:A:148:SER:HB3	2:A:154:LEU:HD21	1.84	0.59
2:P:94:ALA:H	2:P:110:THR:HG22	1.66	0.59
1:C:120:ILE:HD12	1:C:208:ILE:HG22	1.84	0.59
3:T:117:GLU:HG3	14:T:301:HOH:O	2.02	0.59
3:8:119:VAL:HG22	3:8:120:PRO:HD3	1.85	0.59
3:G:149:LYS:O	3:G:153:LYS:HG2	2.03	0.59
2:V:131:LYS:NZ	14:V:402:HOH:O	2.34	0.59
1:X:32:VAL:HG22	1:X:112:ILE:HB	1.84	0.59
2:7:130:PRO:HA	2:7:135:ILE:HD13	1.85	0.59
1:R:79:LEU:HB3	1:R:85:TYR:CE2	2.38	0.59
2:V:33:SER:O	2:V:36:GLU:HG2	2.02	0.59
2:V:148:SER:HB3	2:V:154:LEU:HD21	1.84	0.59
1:X:179:ARG:O	1:X:181:LEU:HD13	2.03	0.59
2:7:133:ARG:HG3	2:7:191:LEU:O	2.02	0.58
2:1:123:PRO:HG3	2:1:213:ALA:HB3	1.85	0.58
1:R:21:ILE:HG12	1:R:93:LEU:HD23	1.85	0.58
2:4:126:VAL:HG22	2:4:139:VAL:HG22	1.84	0.58
1:9:127:LEU:HD21	1:9:212:THR:HG22	1.85	0.58
1:E:136:ILE:HD12	1:E:143:TRP:HB3	1.85	0.58
1:H:145:LEU:HA	1:H:148:ILE:HD12	1.85	0.58
3:W:137:ASP:OD1	3:W:139:GLN:HG2	2.04	0.58
1:E:142:THR:O	1:E:142:THR:OG1	2.21	0.58
1:X:146:LYS:NZ	1:X:174:ASP:OD1	2.32	0.58
2:7:155:THR:HG23	2:7:158:GLU:H	1.67	0.58
1:R:145:LEU:HA	1:R:148:ILE:HD12	1.86	0.58
1:R:183:PRO:HB2	1:R:184:TRP:CE3	2.38	0.58
1:X:136:ILE:CD1	1:X:148:ILE:HD11	2.34	0.58
1:6:142:THR:O	1:6:142:THR:OG1	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:HD12	2:B:217:CYS:O	2.04	0.58
1:0:125:GLU:HG2	1:0:183:PRO:HB3	1.86	0.58
3:G:58:MET:HG2	3:G:114:TYR:CZ	2.39	0.58
3:5:41:LYS:HZ1	3:5:86:LYS:HD3	1.69	0.57
1:6:81:LYS:O	1:6:108:VAL:HG13	2.05	0.57
1:X:136:ILE:HG23	1:X:145:LEU:HD12	1.86	0.57
3:N:99:THR:HA	3:N:103:VAL:HG23	1.85	0.57
2:V:24:LEU:HD22	2:V:45:PRO:HD2	1.86	0.57
2:1:34:ASN:HB2	2:1:122:LYS:HD2	1.85	0.57
3:8:45:ARG:NH2	1:9:151:SER:OG	2.37	0.57
1:R:108:VAL:HG12	14:R:301:HOH:O	2.04	0.57
1:H:22:PRO:HG2	1:H:43:PRO:HB2	1.86	0.57
2:P:195:THR:H	2:P:221:THR:HG23	1.70	0.57
3:W:175:ARG:O	3:W:179:VAL:HG12	2.04	0.57
2:4:216:VAL:HG11	1:E:48:THR:HG23	1.85	0.57
1:6:183:PRO:HB2	1:6:184:TRP:CE3	2.39	0.57
1:9:195:LEU:HD13	1:9:200:ARG:HD2	1.87	0.57
1:K:35:LYS:HD2	1:K:77:SER:OG	2.04	0.57
1:6:123:LEU:HD13	1:6:124:ALA:H	1.69	0.57
3:T:169:LEU:O	3:T:173:SER:OG	2.23	0.57
3:N:91:LEU:O	3:N:95:VAL:HG23	2.05	0.57
3:W:100:LEU:HD23	3:W:104:LEU:HD12	1.86	0.57
1:X:136:ILE:HD11	1:X:143:TRP:HB2	1.86	0.57
2:7:218:ARG:NH2	1:X:50:LEU:O	2.35	0.57
2:B:144:THR:HG22	14:B:401:HOH:O	2.05	0.57
2:F:114:SER:HB3	2:F:117:GLN:HG3	1.87	0.57
1:H:136:ILE:HG22	1:H:145:LEU:HD12	1.87	0.57
3:8:120:PRO:HB3	1:9:83:GLY:HA2	1.87	0.57
3:L:79:LEU:HD21	3:L:148:LEU:HB2	1.87	0.57
2:4:177:MET:HE2	2:4:188:PHE:CD1	2.40	0.56
1:X:30:ASN:N	1:X:37:ILE:O	2.36	0.56
2:4:64:LYS:HD3	2:4:65:TRP:N	2.20	0.56
2:B:48:THR:C	2:B:50:ASP:H	2.09	0.56
2:I:58:LYS:HZ2	2:I:65:TRP:HE1	1.53	0.56
3:J:83:VAL:HG13	3:J:141:ILE:HG12	1.87	0.56
2:P:169:LEU:HD11	2:P:197:PHE:HB3	1.87	0.56
3:W:120:PRO:HG2	1:X:80:SER:OG	2.05	0.56
1:X:48:THR:HG22	1:X:48:THR:O	2.04	0.56
2:1:173:HIS:HB2	1:C:68:ARG:HB2	1.87	0.56
1:3:109:GLU:N	1:3:109:GLU:OE1	2.36	0.56
2:4:192:THR:HG23	2:4:195:THR:OG1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:186:THR:OG1	1:9:212:THR:HG23	2.05	0.56
2:B:65:TRP:CD2	2:B:95:LYS:HE3	2.41	0.56
2:A:181:GLY:HA2	1:C:173:TYR:CZ	2.41	0.56
1:X:214:ASN:ND2	1:X:216:GLU:O	2.38	0.56
1:3:21:ILE:HG13	1:3:98:SER:HB2	1.87	0.56
3:8:55:ARG:NH2	1:9:141:GLU:OE1	2.39	0.56
1:9:134:PRO:HB2	1:9:145:LEU:HD13	1.87	0.56
3:D:103:VAL:HG11	3:D:163:ALA:HB3	1.88	0.56
3:G:93:LYS:HZ1	3:G:130:SER:HA	1.70	0.56
3:J:49:SER:O	3:J:53:VAL:HG13	2.05	0.56
2:M:173:HIS:HB2	1:U:68:ARG:HB2	1.88	0.56
3:W:99:THR:O	3:W:103:VAL:HG22	2.06	0.56
3:8:98:PHE:HZ	3:8:152:VAL:HG21	1.71	0.56
1:9:123:LEU:CD2	1:9:125:GLU:HB2	2.35	0.56
1:9:158:TYR:HB3	1:9:189:ILE:HG22	1.86	0.56
2:V:65:TRP:CZ2	2:V:95:LYS:HD2	2.41	0.56
3:2:99:THR:HA	3:2:103:VAL:CG2	2.36	0.56
1:3:31:SER:OG	1:3:36:ASN:OD1	2.20	0.56
2:4:91:PHE:CD2	2:4:114:SER:HB2	2.41	0.56
3:8:67:ASP:OD2	3:8:162:LYS:HE2	2.05	0.56
3:D:59:LEU:HD13	3:D:114:TYR:HB2	1.87	0.56
2:I:59:LYS:O	2:I:62:GLU:HG2	2.06	0.56
3:J:99:THR:HA	3:J:103:VAL:HG13	1.87	0.56
3:L:107:GLN:NE2	3:L:160:GLU:OE1	2.39	0.56
2:M:218:ARG:NH2	1:U:50:LEU:O	2.39	0.56
2:1:88:HIS:HA	2:1:115:SER:OG	2.06	0.55
2:P:126:VAL:HG22	2:P:139:VAL:HG12	1.87	0.55
1:R:180:ASN:O	1:R:181:LEU:HD23	2.06	0.55
1:U:160:LYS:NZ	1:U:182:GLU:OE1	2.32	0.55
2:1:91:PHE:HD2	2:1:112:ARG:HG2	1.71	0.55
1:3:127:LEU:HB2	1:3:178:LEU:HD12	1.88	0.55
3:L:107:GLN:NE2	3:L:157:GLU:OE2	2.39	0.55
2:M:162:ASP:HB2	2:M:206:PRO:HD2	1.88	0.55
1:E:194:PHE:CE2	1:E:196:LEU:HD12	2.42	0.55
2:V:34:ASN:CG	2:V:122:LYS:HG2	2.27	0.55
3:W:42:LEU:HD13	3:W:125:LEU:HD22	1.89	0.55
2:4:178:HIS:O	2:4:179:LEU:HD22	2.06	0.55
2:4:191:LEU:HD23	2:4:197:PHE:CE1	2.41	0.55
1:O:32:VAL:HG12	1:O:112:ILE:HB	1.88	0.55
3:2:124:LYS:HE3	1:3:109:GLU:OE2	2.07	0.55
1:9:21:ILE:HG13	1:9:98:SER:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:126:SER:HB3	1:9:178:LEU:O	2.05	0.55
3:J:143:LYS:O	3:J:146:ARG:HG2	2.07	0.55
1:K:120:ILE:HD13	1:K:189:ILE:HD13	1.89	0.55
2:S:146:VAL:HG23	2:S:154:LEU:HD12	1.88	0.55
2:V:65:TRP:CH2	2:V:95:LYS:HD2	2.42	0.55
2:7:61:GLY:HA3	3:8:73:ARG:HB2	1.89	0.55
2:B:167:LEU:HD23	2:B:167:LEU:N	2.22	0.55
3:Q:51:TYR:HD2	3:Q:52:ILE:HD13	1.72	0.55
3:T:145:VAL:O	3:T:149:LYS:HG3	2.06	0.55
1:X:35:LYS:HE2	1:X:37:ILE:HD11	1.87	0.55
1:0:136:ILE:HG21	1:0:148:ILE:HD11	1.89	0.54
1:0:172:PRO:HG2	1:0:173:TYR:CE2	2.41	0.54
2:1:35:PHE:CE2	2:1:159:ILE:HD13	2.43	0.54
1:K:40:TRP:O	1:K:72:THR:OG1	2.25	0.54
2:M:164:PHE:HE1	2:M:206:PRO:HG3	1.72	0.54
1:0:113:ILE:HD12	1:0:145:LEU:HD23	1.89	0.54
2:1:119:THR:O	2:1:210:LYS:HE3	2.07	0.54
1:E:23:PRO:O	1:E:43:PRO:HB3	2.08	0.54
1:H:122:SER:OG	1:H:212:THR:O	2.25	0.54
3:J:146:ARG:O	3:J:150:GLU:HG2	2.07	0.54
2:S:144:THR:HG21	2:S:159:ILE:HD11	1.88	0.54
1:X:160:LYS:NZ	1:X:185:THR:HG21	2.21	0.54
1:9:55:GLN:HG2	1:9:64:ASP:HA	1.87	0.54
2:A:139:VAL:HG11	2:A:165:TYR:CZ	2.42	0.54
2:F:200:SER:OG	1:U:46:PRO:HG2	2.07	0.54
1:X:159:TRP:HZ3	1:X:162:GLY:H	1.54	0.54
2:1:24:LEU:HB2	2:1:46:ALA:HB3	1.89	0.54
2:7:207:ILE:HG22	2:7:208:LEU:HD12	1.90	0.54
1:K:142:THR:O	1:K:142:THR:OG1	2.25	0.54
2:V:83:MET:HE3	2:V:86:ARG:HD2	1.89	0.54
1:0:40:TRP:NE1	1:0:72:THR:HA	2.22	0.54
1:0:197:ASP:OD2	3:Z:45:ARG:HD3	2.07	0.54
1:H:45:PHE:CD1	1:H:46:PRO:HD2	2.43	0.54
2:1:147:LEU:HD12	2:1:151:GLY:O	2.07	0.54
1:3:135:GLN:NE2	14:3:304:HOH:O	2.40	0.54
1:E:53:THR:N	14:E:303:HOH:O	2.39	0.54
3:G:77:GLU:CD	3:G:81:ARG:NH1	2.60	0.54
2:V:126:VAL:HB	2:V:215:TYR:CD2	2.43	0.54
1:6:159:TRP:HZ3	1:6:163:THR:H	1.56	0.54
1:U:155:ARG:NH1	1:U:168:GLN:OE1	2.37	0.54
3:W:47:PHE:HE2	3:W:174:LEU:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:151:THR:HG22	3:Z:154:LYS:HE2	1.90	0.54
3:8:100:LEU:O	3:8:105:LEU:HD13	2.08	0.54
3:D:88:GLN:O	3:D:92:MET:HG2	2.07	0.54
3:J:93:LYS:NZ	3:J:132:CYS:O	2.37	0.54
3:L:91:LEU:O	3:L:95:VAL:HG13	2.08	0.54
2:S:60:TYR:CE2	3:T:73:ARG:HG3	2.43	0.54
3:8:75:ILE:HG22	3:8:166:GLU:OE1	2.08	0.54
2:M:29:LYS:HA	2:M:110:THR:HG22	1.90	0.54
1:O:67:LYS:HE3	1:O:68:ARG:NH2	2.23	0.54
1:R:117:GLU:HB2	1:R:132:SER:HB2	1.89	0.54
3:2:108:SER:HA	3:2:115:MET:HE1	1.90	0.54
2:4:156:LEU:N	14:4:401:HOH:O	2.41	0.54
3:D:67:ASP:OD1	3:D:162:LYS:NZ	2.39	0.54
3:G:44:VAL:HG13	3:G:179:VAL:HG21	1.90	0.54
3:J:75:ILE:HD11	3:J:173:SER:HB2	1.90	0.54
2:V:24:LEU:CD2	2:V:45:PRO:HD2	2.38	0.54
2:V:74:ILE:HD13	2:V:76:GLN:HG2	1.90	0.54
2:A:42:ASP:OD2	2:Y:132:VAL:HG22	2.08	0.53
3:D:147:ARG:HH22	3:D:154:LYS:HD3	1.73	0.53
1:H:188:CYS:O	1:H:189:ILE:HD13	2.07	0.53
1:U:141:GLU:HB2	1:U:143:TRP:CD1	2.43	0.53
1:U:184:TRP:HD1	1:U:213:GLY:CA	2.18	0.53
3:8:115:MET:O	3:8:119:VAL:HG13	2.07	0.53
1:9:192:GLN:HG2	1:9:204:TRP:CZ3	2.44	0.53
1:C:181:LEU:HB3	1:C:187:TYR:CZ	2.43	0.53
3:D:48:GLN:O	3:D:50:PRO:HD3	2.07	0.53
1:K:164:ASN:OD1	1:K:164:ASN:N	2.41	0.53
2:Y:130:PRO:HA	2:Y:135:ILE:HD13	1.89	0.53
2:4:86:ARG:HH21	2:4:147:LEU:HD11	1.73	0.53
3:T:79:LEU:HD21	3:T:95:VAL:HG21	1.90	0.53
1:9:51:THR:O	1:9:92:GLU:N	2.41	0.53
2:A:144:THR:CG2	2:A:146:VAL:HG13	2.38	0.53
2:F:94:ALA:O	2:F:110:THR:HG23	2.07	0.53
1:H:158:TYR:CB	1:H:189:ILE:HD12	2.38	0.53
1:H:184:TRP:CD2	1:H:213:GLY:HA2	2.44	0.53
2:M:123:PRO:HG3	2:M:213:ALA:HB3	1.91	0.53
1:0:135:GLN:HG3	1:0:143:TRP:O	2.08	0.53
1:3:55:GLN:HG2	1:3:64:ASP:HA	1.90	0.53
2:7:173:HIS:HB2	1:X:68:ARG:HB2	1.90	0.53
3:8:116:TRP:N	14:8:302:HOH:O	2.41	0.53
3:N:57:PHE:HZ	3:N:172:MET:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:131:PHE:CE1	1:R:191:VAL:HG11	2.44	0.53
2:7:24:LEU:HD13	2:7:45:PRO:HD2	1.91	0.53
2:7:173:HIS:HA	1:X:68:ARG:HH21	1.74	0.53
2:M:58:LYS:HE3	2:M:65:TRP:CZ2	2.44	0.53
1:R:68:ARG:HA	1:R:92:GLU:OE2	2.09	0.53
2:S:162:ASP:HB2	2:S:206:PRO:HD2	1.90	0.53
3:2:51:TYR:OH	1:3:139:GLU:OE2	2.20	0.53
2:4:177:MET:HE2	2:4:188:PHE:HD1	1.73	0.53
3:8:67:ASP:OD1	3:8:162:LYS:HE2	2.09	0.53
2:B:86:ARG:HD3	2:B:145:PRO:O	2.09	0.53
2:F:29:LYS:O	2:F:39:LEU:HD12	2.09	0.53
1:C:48:THR:O	1:C:50:LEU:N	2.37	0.53
1:C:184:TRP:HD1	1:C:211:ARG:HH21	1.56	0.53
2:I:83:MET:O	2:I:86:ARG:HG3	2.08	0.53
2:V:58:LYS:HE3	2:V:65:TRP:NE1	2.23	0.53
2:1:110:THR:HB	14:1:407:HOH:O	2.10	0.53
3:8:78:LYS:HD2	3:8:78:LYS:N	2.24	0.53
3:8:120:PRO:HG2	1:9:80:SER:OG	2.09	0.53
1:9:57:GLU:HB3	1:9:86:THR:HG23	1.90	0.53
3:J:134:ILE:HD13	3:J:136:GLY:N	2.24	0.53
3:W:164:ILE:HA	3:W:167:LEU:HD13	1.90	0.53
1:X:124:ALA:O	1:X:126:SER:N	2.42	0.53
2:Y:115:SER:HA	14:Y:406:HOH:O	2.09	0.53
3:5:147:ARG:O	3:5:151:THR:OG1	2.27	0.52
2:M:195:THR:HB	2:M:197:PHE:CE1	2.44	0.52
2:V:114:SER:HB3	2:V:117:GLN:HG3	1.91	0.52
2:4:142:THR:O	14:4:401:HOH:O	2.19	0.52
1:9:51:THR:HG23	1:9:92:GLU:HB2	1.90	0.52
1:6:57:GLU:HA	1:6:62:PHE:HA	1.92	0.52
1:6:143:TRP:O	1:6:147:ASN:ND2	2.43	0.52
3:J:143:LYS:HA	3:J:146:ARG:HG2	1.89	0.52
1:O:124:ALA:O	1:O:126:SER:N	2.42	0.52
1:U:139:GLU:HG2	1:U:143:TRP:CD1	2.44	0.52
2:Y:74:ILE:HD12	2:Y:76:GLN:HG2	1.90	0.52
2:1:155:THR:HG23	2:1:158:GLU:H	1.75	0.52
1:3:151:SER:HB3	1:3:195:LEU:HD12	1.91	0.52
1:X:190:GLN:HE21	1:X:207:PRO:N	2.08	0.52
2:Y:146:VAL:HG22	2:Y:154:LEU:HD23	1.92	0.52
3:2:116:TRP:O	1:3:80:SER:OG	2.28	0.52
2:P:155:THR:OG1	2:P:156:LEU:N	2.43	0.52
2:7:25:LEU:HD21	2:7:28:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ILE:HG23	2:B:215:TYR:HB3	1.91	0.52
1:C:55:GLN:HG2	1:C:64:ASP:HA	1.92	0.52
1:O:143:TRP:HB3	1:O:148:ILE:HD11	1.91	0.52
1:X:33:ASN:HD21	1:X:114:GLY:HA3	1.75	0.52
3:G:44:VAL:HG12	3:G:179:VAL:HG11	1.91	0.52
1:O:125:GLU:HG2	1:O:183:PRO:HB3	1.91	0.52
1:O:177:VAL:HG11	1:O:179:ARG:NH2	2.24	0.52
3:Q:69:ASN:O	3:Q:162:LYS:NZ	2.38	0.52
1:R:68:ARG:HG2	1:R:92:GLU:OE2	2.10	0.52
2:S:156:LEU:HA	14:S:410:HOH:O	2.09	0.52
2:V:58:LYS:HG2	2:V:95:LYS:NZ	2.25	0.52
3:8:49:SER:O	3:8:53:VAL:HG12	2.09	0.52
3:G:163:ALA:O	3:G:167:LEU:HD13	2.09	0.52
3:Q:145:VAL:O	3:Q:149:LYS:HG3	2.10	0.52
2:7:162:ASP:HB2	2:7:206:PRO:HD2	1.92	0.52
1:C:35:LYS:HE2	1:C:37:ILE:HD11	1.91	0.52
1:C:111:THR:O	1:C:200:ARG:NH2	2.43	0.52
3:N:41:LYS:HG3	3:N:178:CYS:O	2.10	0.52
3:Q:103:VAL:O	3:Q:107:GLN:HB2	2.10	0.52
2:B:123:PRO:O	14:B:403:HOH:O	2.19	0.52
2:I:90:GLU:OE2	3:J:73:ARG:NH2	2.29	0.52
3:2:92:MET:HA	3:2:95:VAL:HG22	1.92	0.51
2:7:25:LEU:HD12	2:7:98:ALA:HB2	1.92	0.51
1:9:51:THR:CG2	1:9:92:GLU:HB2	2.40	0.51
1:9:151:SER:HB3	1:9:196:LEU:HB3	1.92	0.51
2:P:180:GLU:OE1	1:R:173:TYR:HB3	2.10	0.51
2:P:195:THR:H	2:P:221:THR:CG2	2.22	0.51
3:T:47:PHE:CD2	3:T:175:ARG:HB2	2.44	0.51
1:X:159:TRP:CZ3	1:X:161:GLN:HA	2.45	0.51
2:Y:155:THR:HG23	2:Y:158:GLU:H	1.75	0.51
3:Z:69:ASN:OD1	3:Z:72:VAL:HG12	2.10	0.51
3:Z:99:THR:HA	3:Z:103:VAL:HG13	1.92	0.51
1:H:33:ASN:HD21	1:H:114:GLY:HA3	1.75	0.51
1:3:149:TYR:N	1:3:149:TYR:HD1	2.08	0.51
1:6:184:TRP:HB3	1:6:211:ARG:NH2	2.25	0.51
3:G:99:THR:HA	3:G:103:VAL:HG23	1.93	0.51
3:J:75:ILE:HD11	3:J:173:SER:CB	2.40	0.51
1:O:40:TRP:O	1:O:72:THR:OG1	2.28	0.51
1:O:177:VAL:HG11	1:O:179:ARG:HH21	1.76	0.51
2:P:195:THR:HB	2:P:197:PHE:CE1	2.45	0.51
1:0:21:ILE:HD11	1:0:91:ALA:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:PHE:CD2	1:E:136:ILE:HG23	2.46	0.51
1:H:172:PRO:HG2	1:H:173:TYR:CE2	2.44	0.51
2:B:144:THR:HG23	2:B:146:VAL:HG13	1.93	0.51
1:E:184:TRP:H	1:E:213:GLY:H	1.57	0.51
1:H:27:VAL:HG22	1:H:40:TRP:HB3	1.92	0.51
2:P:168:GLU:HA	2:P:178:HIS:HB3	1.91	0.51
1:U:55:GLN:HG2	1:U:64:ASP:HA	1.92	0.51
1:3:149:TYR:N	1:3:149:TYR:CD1	2.79	0.51
2:4:41:TRP:CE2	2:4:77:LYS:HA	2.46	0.51
1:H:185:THR:O	1:H:212:THR:HG23	2.10	0.51
1:U:118:MET:HE3	1:U:131:PHE:HE1	1.76	0.51
3:2:110:ARG:NE	3:2:111:PHE:H	2.08	0.51
3:D:98:PHE:HZ	3:D:152:VAL:HG11	1.76	0.51
3:G:105:LEU:O	1:H:59:TYR:OH	2.19	0.51
3:T:53:VAL:HG22	3:T:171:PHE:CZ	2.45	0.51
1:0:33:ASN:HD21	1:0:114:GLY:HA3	1.75	0.51
1:3:160:LYS:O	1:3:163:THR:HG22	2.10	0.51
3:5:49:SER:HB3	3:5:52:ILE:CG1	2.38	0.51
3:Q:74:LEU:HB3	3:Q:148:LEU:HD11	1.93	0.51
2:V:60:TYR:CD1	2:V:93:TYR:HE1	2.29	0.51
2:4:117:GLN:HG3	2:4:118:HIS:CE1	2.46	0.51
1:C:48:THR:OG1	1:C:49:GLN:N	2.41	0.51
1:E:155:ARG:O	1:E:191:VAL:HA	2.11	0.51
1:H:52:PHE:HE2	2:Y:218:ARG:NH2	2.08	0.51
1:H:206:GLU:N	1:H:206:GLU:OE1	2.44	0.50
3:T:44:VAL:HG13	3:T:179:VAL:HG21	1.92	0.50
1:U:123:LEU:HG	1:U:124:ALA:H	1.75	0.50
2:F:28:VAL:HG12	2:F:110:THR:HG22	1.93	0.50
3:G:125:LEU:HD23	3:G:174:LEU:HD23	1.93	0.50
1:H:136:ILE:HD11	1:H:139:GLU:HG3	1.92	0.50
2:P:179:LEU:HD11	2:P:186:TYR:HD1	1.76	0.50
2:V:98:ALA:HB3	2:V:106:VAL:HG23	1.93	0.50
1:X:136:ILE:HD11	1:X:143:TRP:CB	2.40	0.50
2:1:164:PHE:HE1	2:1:206:PRO:HG3	1.76	0.50
1:6:194:PHE:CE2	1:6:196:LEU:HG	2.47	0.50
2:7:114:SER:H	2:7:118:HIS:CD2	2.29	0.50
2:B:26:GLN:NE2	2:B:43:GLY:O	2.43	0.50
1:E:92:GLU:HG3	14:E:303:HOH:O	2.11	0.50
2:I:94:ALA:O	2:I:110:THR:HG23	2.10	0.50
3:Z:175:ARG:O	3:Z:179:VAL:HG12	2.12	0.50
2:A:126:VAL:HB	2:A:215:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ARG:HD2	1:E:97:HIS:HB2	1.94	0.50
2:A:91:PHE:CE2	2:A:114:SER:HB2	2.47	0.50
3:D:79:LEU:HD21	3:D:95:VAL:HG21	1.93	0.50
2:F:24:LEU:HG	2:F:45:PRO:HG2	1.94	0.50
3:G:73:ARG:HB3	3:G:78:LYS:NZ	2.26	0.50
3:G:95:VAL:HG13	3:G:148:LEU:HD11	1.93	0.50
1:H:136:ILE:CG2	1:H:148:ILE:HD11	2.38	0.50
3:T:72:VAL:CG2	3:T:162:LYS:HE3	2.42	0.50
1:U:105:PHE:CE2	1:U:107:PRO:HG3	2.47	0.50
2:1:29:LYS:HA	2:1:110:THR:HG23	1.92	0.50
3:D:59:LEU:HD11	3:D:111:PHE:HB3	1.93	0.50
2:F:167:LEU:HD12	2:F:167:LEU:N	2.27	0.50
3:J:61:LYS:O	3:J:65:LEU:HD12	2.10	0.50
3:L:92:MET:HB3	3:L:174:LEU:HD13	1.93	0.50
2:B:201:ILE:CG2	2:B:215:TYR:HB3	2.41	0.50
1:C:88:ARG:HB3	1:C:102:GLN:HG2	1.93	0.50
3:T:100:LEU:HD23	3:T:104:LEU:HD12	1.93	0.50
2:7:28:VAL:HG22	2:7:41:TRP:HB3	1.93	0.50
3:8:78:LYS:HB2	14:8:301:HOH:O	2.11	0.50
2:I:144:THR:HG22	2:I:154:LEU:O	2.12	0.50
3:W:79:LEU:HG	3:W:91:LEU:HD11	1.92	0.50
2:1:25:LEU:HD21	2:1:28:VAL:HG23	1.93	0.50
2:S:144:THR:CG2	2:S:146:VAL:H	2.25	0.50
2:V:29:LYS:O	2:V:39:LEU:HD12	2.12	0.50
1:0:21:ILE:HG13	1:0:98:SER:HB2	1.94	0.49
2:1:205:THR:OG1	2:1:210:LYS:HB2	2.11	0.49
2:4:41:TRP:O	2:4:77:LYS:HB3	2.12	0.49
2:A:119:THR:O	2:A:210:LYS:HE3	2.12	0.49
2:F:97:THR:HG23	2:F:107:THR:OG1	2.12	0.49
3:N:74:LEU:HB3	3:N:148:LEU:HD11	1.93	0.49
3:W:116:TRP:O	1:X:80:SER:OG	2.29	0.49
3:2:96:LEU:HD23	3:2:174:LEU:HD21	1.94	0.49
3:2:98:PHE:HD1	3:2:149:LYS:HE2	1.77	0.49
1:9:118:MET:HE2	1:9:120:ILE:HD11	1.94	0.49
2:F:139:VAL:O	2:F:184:ARG:HD3	2.12	0.49
3:G:110:ARG:HD3	3:G:111:PHE:N	2.27	0.49
1:U:177:VAL:HB	1:U:179:ARG:NH2	2.26	0.49
1:X:160:LYS:HZ3	1:X:185:THR:HG21	1.77	0.49
1:3:81:LYS:O	1:3:108:VAL:HG12	2.12	0.49
1:3:88:ARG:CB	1:3:102:GLN:HG2	2.42	0.49
2:B:123:PRO:HG3	2:B:213:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:MET:HE2	1:C:191:VAL:HG12	1.93	0.49
2:P:162:ASP:HB2	2:P:206:PRO:HD2	1.94	0.49
2:P:178:HIS:NE2	1:R:130:ARG:CZ	2.75	0.49
1:X:214:ASN:OD1	1:X:214:ASN:N	2.38	0.49
3:5:48:GLN:NE2	1:6:150:ASP:OD2	2.44	0.49
2:P:97:THR:HG23	2:P:107:THR:OG1	2.12	0.49
1:R:27:VAL:HG22	1:R:40:TRP:HB3	1.94	0.49
1:3:48:THR:C	1:3:50:LEU:H	2.16	0.49
3:5:145:VAL:O	3:5:149:LYS:HG2	2.13	0.49
2:F:169:LEU:HD11	2:F:197:PHE:HB3	1.94	0.49
3:Z:77:GLU:HB2	3:Z:81:ARG:NH1	2.28	0.49
2:F:170:HIS:ND1	2:F:176:GLN:HG2	2.27	0.49
1:K:185:THR:O	1:K:212:THR:HG23	2.13	0.49
3:L:115:MET:O	3:L:119:VAL:HG13	2.12	0.49
1:U:36:ASN:N	1:U:77:SER:OG	2.42	0.49
3:W:119:VAL:HG22	3:W:120:PRO:HD3	1.94	0.49
3:2:45:ARG:NE	1:3:197:ASP:OD2	2.45	0.49
1:H:79:LEU:HB3	1:H:85:TYR:CE2	2.48	0.49
2:I:58:LYS:HG2	2:I:65:TRP:CD1	2.48	0.49
2:Y:126:VAL:HG11	2:Y:201:ILE:HD13	1.94	0.49
3:2:42:LEU:HD11	3:2:47:PHE:HE1	1.77	0.49
3:5:141:ILE:O	3:5:145:VAL:HG13	2.13	0.49
1:6:184:TRP:HB3	1:6:211:ARG:HH21	1.78	0.49
3:8:99:THR:HA	3:8:103:VAL:HG13	1.94	0.49
2:B:144:THR:HG21	2:B:159:ILE:HD11	1.94	0.49
2:B:200:SER:HA	2:B:215:TYR:O	2.12	0.49
3:D:91:LEU:HD13	3:D:141:ILE:HG23	1.95	0.49
2:F:173:HIS:HD1	1:U:20:MET:N	2.10	0.49
2:I:167:LEU:HG	2:I:201:ILE:HG23	1.95	0.49
3:Q:83:VAL:HG11	3:Q:91:LEU:HD22	1.95	0.49
2:V:139:VAL:HG11	2:V:165:TYR:CE1	2.48	0.49
2:Y:95:LYS:HA	2:Y:109:MET:HA	1.94	0.49
3:Z:82:GLY:O	3:Z:140:ASN:ND2	2.34	0.49
3:Z:83:VAL:HG21	3:Z:91:LEU:HD22	1.94	0.49
1:3:88:ARG:HD2	1:3:100:TRP:CG	2.48	0.49
2:7:137:MET:SD	2:7:201:ILE:HD11	2.53	0.49
3:8:79:LEU:HD21	3:8:91:LEU:HD11	1.95	0.49
1:9:88:ARG:HD3	1:9:100:TRP:CD2	2.47	0.49
2:B:155:THR:HG23	2:B:158:GLU:H	1.78	0.49
2:F:173:HIS:CD2	2:F:174:THR:HG23	2.47	0.49
2:V:54:SER:HA	14:V:401:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:49:SER:CB	3:5:52:ILE:HG12	2.40	0.49
1:9:90:ARG:NH1	1:9:92:GLU:HG2	2.28	0.49
2:B:136:GLN:NE2	2:B:185:GLU:OE2	2.45	0.49
3:D:162:LYS:HB2	3:D:162:LYS:HZ2	1.77	0.49
2:M:85:THR:HA	2:M:92:TYR:CZ	2.48	0.49
3:D:158:SER:O	3:D:161:ILE:HG12	2.13	0.48
3:D:172:MET:HA	3:D:172:MET:HE3	1.95	0.48
1:E:118:MET:HE2	1:E:191:VAL:HG12	1.95	0.48
1:H:42:VAL:HG12	1:H:52:PHE:CZ	2.48	0.48
1:R:88:ARG:HB3	1:R:102:GLN:HG2	1.95	0.48
1:R:192:GLN:NE2	1:R:204:TRP:CE2	2.81	0.48
2:V:205:THR:HB	2:V:210:LYS:HB2	1.94	0.48
3:2:79:LEU:HD23	3:2:148:LEU:HG	1.95	0.48
3:2:116:TRP:CD1	1:3:80:SER:OG	2.65	0.48
3:5:49:SER:HB3	3:5:52:ILE:CD1	2.43	0.48
1:6:35:LYS:HB2	1:6:137:GLU:HG3	1.95	0.48
2:7:91:PHE:CE2	2:7:114:SER:HB2	2.48	0.48
3:8:62:GLU:N	3:8:62:GLU:OE1	2.45	0.48
1:C:53:THR:HA	1:C:66:CYS:O	2.12	0.48
2:M:74:ILE:HD12	2:M:76:GLN:HB2	1.93	0.48
2:S:159:ILE:HD12	14:S:410:HOH:O	2.12	0.48
1:0:137:GLU:HG3	1:0:137:GLU:O	2.13	0.48
2:1:55:VAL:HG22	2:1:96:VAL:HG22	1.94	0.48
2:1:117:GLN:O	2:1:117:GLN:HG2	2.13	0.48
1:6:181:LEU:HB3	1:6:187:TYR:HE2	1.78	0.48
2:7:157:GLU:OE1	2:7:184:ARG:NH2	2.43	0.48
3:8:73:ARG:HH21	3:8:169:LEU:HD21	1.78	0.48
2:A:205:THR:OG1	2:A:210:LYS:HB2	2.13	0.48
2:Y:200:SER:HA	2:Y:215:TYR:O	2.13	0.48
1:0:122:SER:HB2	1:0:127:LEU:CD2	2.42	0.48
1:0:192:GLN:HG2	1:0:204:TRP:CZ3	2.49	0.48
1:C:90:ARG:HH11	1:C:97:HIS:CB	2.27	0.48
3:G:72:VAL:HG23	3:G:162:LYS:NZ	2.28	0.48
1:3:155:ARG:HD3	1:3:168:GLN:OE1	2.13	0.48
2:7:74:ILE:HB	2:7:76:GLN:CD	2.33	0.48
2:A:198:LEU:HD12	2:A:217:CYS:O	2.14	0.48
2:B:124:PRO:HB3	2:B:203:ILE:HD11	1.95	0.48
2:P:24:LEU:HD22	2:P:45:PRO:HD2	1.94	0.48
3:T:39:ARG:HA	3:T:39:ARG:HD3	1.53	0.48
1:3:184:TRP:HE3	1:3:211:ARG:HH21	1.60	0.48
3:8:141:ILE:HG13	3:8:142:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ILE:HG13	1:C:96:GLU:HG2	1.95	0.48
3:D:124:LYS:NZ	1:E:109:GLU:OE2	2.39	0.48
3:Q:160:GLU:O	3:Q:164:ILE:HG13	2.13	0.48
3:5:100:LEU:O	3:5:105:LEU:HB2	2.13	0.48
3:8:164:ILE:HG23	3:8:167:LEU:HD22	1.95	0.48
2:B:103:GLY:H	2:B:104:PRO:CD	2.25	0.48
3:D:69:ASN:OD1	3:D:72:VAL:HG22	2.14	0.48
1:U:86:THR:CG2	1:U:104:THR:HG22	2.42	0.48
3:W:91:LEU:O	3:W:95:VAL:HG23	2.12	0.48
2:Y:58:LYS:HE3	2:Y:65:TRP:CE2	2.49	0.48
2:1:59:LYS:HB3	2:1:62:GLU:OE2	2.14	0.48
2:1:195:THR:HB	2:1:197:PHE:CE1	2.49	0.48
3:5:42:LEU:HD11	3:5:47:PHE:HE1	1.79	0.48
1:6:120:ILE:HD13	1:6:208:ILE:HG21	1.94	0.48
3:8:47:PHE:HD1	3:8:171:PHE:CE1	2.32	0.48
1:H:127:LEU:HD11	1:H:212:THR:HG22	1.96	0.48
2:S:174:THR:O	2:S:174:THR:OG1	2.31	0.48
3:T:124:LYS:HD2	1:U:82:TYR:HD2	1.77	0.48
1:X:134:PRO:HB2	1:X:145:LEU:HD13	1.96	0.48
3:Z:96:LEU:HD23	3:Z:170:LEU:HD21	1.96	0.48
1:0:160:LYS:HG3	1:0:187:TYR:CE2	2.49	0.48
2:A:143:LEU:HD13	2:A:143:LEU:HA	1.74	0.48
2:I:29:LYS:O	2:I:39:LEU:HD12	2.14	0.48
1:K:80:SER:O	1:K:107:PRO:HG2	2.13	0.48
1:K:139:GLU:N	1:K:139:GLU:OE1	2.47	0.48
3:L:154:LYS:HG3	3:L:155:LEU:HD22	1.96	0.48
2:S:169:LEU:HD11	2:S:197:PHE:HB3	1.95	0.48
3:T:93:LYS:HB2	3:T:129:LEU:HD13	1.94	0.48
2:Y:167:LEU:HD11	2:Y:186:TYR:HB2	1.96	0.48
1:0:88:ARG:HD2	1:0:100:TRP:CG	2.49	0.48
2:B:42:ASP:OD1	2:B:43:GLY:N	2.47	0.48
2:S:91:PHE:CE2	2:S:114:SER:HB2	2.48	0.48
1:U:53:THR:HA	1:U:66:CYS:O	2.13	0.48
1:U:122:SER:HA	1:U:127:LEU:HD23	1.96	0.48
2:Y:167:LEU:HD11	2:Y:186:TYR:CB	2.44	0.48
3:5:83:VAL:HG11	3:5:91:LEU:HD22	1.96	0.47
1:6:30:ASN:HB3	14:6:302:HOH:O	2.14	0.47
2:7:131:LYS:HE2	2:B:41:TRP:O	2.14	0.47
2:I:28:VAL:HG11	2:I:108:LYS:HB3	1.95	0.47
2:I:177:MET:HE2	2:I:188:PHE:CD1	2.49	0.47
3:Q:56:THR:HA	3:Q:118:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:ILE:HD11	1:X:97:HIS:HA	1.96	0.47
2:4:162:ASP:OD2	2:4:206:PRO:HD2	2.15	0.47
1:6:122:SER:HA	1:6:127:LEU:HD23	1.96	0.47
2:A:114:SER:HB3	2:A:117:GLN:HG3	1.97	0.47
1:K:184:TRP:HD1	1:K:213:GLY:HA2	1.78	0.47
1:R:134:PRO:HB2	1:R:145:LEU:HD13	1.95	0.47
2:V:24:LEU:HB3	2:V:44:GLY:HA3	1.97	0.47
2:1:125:ASP:OD1	14:1:402:HOH:O	2.20	0.47
3:8:147:ARG:HA	3:8:150:GLU:HG2	1.96	0.47
2:I:177:MET:HE2	2:I:188:PHE:HD1	1.79	0.47
1:K:27:VAL:HG22	1:K:40:TRP:HB3	1.96	0.47
3:T:164:ILE:O	3:T:167:LEU:HD22	2.14	0.47
3:W:89:CYS:HB2	3:W:177:ALA:O	2.14	0.47
2:1:24:LEU:HD23	2:1:45:PRO:HD2	1.96	0.47
1:3:81:LYS:O	1:3:107:PRO:HD2	2.14	0.47
2:7:87:ASP:OD2	2:7:90:GLU:HG2	2.15	0.47
3:8:162:LYS:HE3	3:8:162:LYS:HB2	1.67	0.47
2:A:28:VAL:HG22	2:A:110:THR:HG22	1.95	0.47
3:Q:44:VAL:HG12	3:Q:179:VAL:HG11	1.95	0.47
1:6:44:ALA:O	1:6:46:PRO:HD3	2.14	0.47
3:8:78:LYS:HD2	3:8:78:LYS:H	1.79	0.47
3:8:97:GLN:NE2	3:8:101:GLU:OE2	2.44	0.47
3:G:73:ARG:NH1	3:G:169:LEU:HD21	2.29	0.47
1:K:152:TRP:CH2	1:K:193:GLY:HA3	2.50	0.47
1:0:92:GLU:CD	1:0:97:HIS:HB3	2.35	0.47
3:8:40:CYS:HA	3:8:132:CYS:HB2	1.94	0.47
3:Z:134:ILE:HG22	3:Z:136:GLY:H	1.80	0.47
2:1:174:THR:O	2:1:174:THR:OG1	2.32	0.47
2:4:205:THR:OG1	2:4:210:LYS:HB2	2.14	0.47
3:8:45:ARG:HH22	1:9:196:LEU:HD23	1.79	0.47
2:A:216:VAL:HG13	1:H:46:PRO:HB2	1.96	0.47
2:B:41:TRP:O	2:B:77:LYS:HB3	2.14	0.47
3:D:40:CYS:HB2	3:D:132:CYS:HB2	1.72	0.47
1:H:192:GLN:HG2	1:H:204:TRP:CZ3	2.50	0.47
2:I:91:PHE:CE2	2:I:114:SER:HB2	2.49	0.47
2:I:167:LEU:HB2	2:I:179:LEU:HD12	1.96	0.47
3:Q:52:ILE:HG12	1:R:82:TYR:CE1	2.50	0.47
2:V:97:THR:HG23	2:V:107:THR:OG1	2.15	0.47
2:Y:88:HIS:HA	2:Y:115:SER:OG	2.14	0.47
1:0:93:LEU:HD23	1:0:93:LEU:HA	1.77	0.47
3:2:93:LYS:HD3	3:2:94:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:24:LEU:HD13	2:4:45:PRO:HD2	1.97	0.47
2:B:181:GLY:HA2	1:E:173:TYR:CZ	2.50	0.47
3:J:96:LEU:HB2	3:J:174:LEU:HD11	1.96	0.47
2:Y:215:TYR:HE1	2:Y:217:CYS:SG	2.38	0.47
2:1:173:HIS:ND1	1:C:68:ARG:HD3	2.30	0.47
3:2:50:PRO:O	3:2:54:ASN:N	2.35	0.47
2:4:94:ALA:O	2:4:110:THR:HG23	2.15	0.47
2:F:63:ARG:NH1	3:G:71:ASP:HB3	2.29	0.47
1:H:35:LYS:HD2	1:H:77:SER:OG	2.13	0.47
1:O:79:LEU:HB3	1:O:85:TYR:CE2	2.50	0.47
2:P:135:ILE:HG21	2:P:169:LEU:HD22	1.97	0.47
3:T:72:VAL:HG23	3:T:162:LYS:HE3	1.96	0.47
2:Y:48:THR:O	2:Y:51:THR:HG22	2.14	0.47
3:2:117:GLU:O	14:2:301:HOH:O	2.21	0.47
1:3:48:THR:C	1:3:50:LEU:N	2.68	0.47
3:5:45:ARG:HG2	1:6:150:ASP:OD1	2.15	0.47
1:K:190:GLN:HE21	1:K:207:PRO:HG3	1.80	0.47
2:P:51:THR:HA	2:P:100:SER:HA	1.96	0.47
3:Q:61:LYS:O	3:Q:65:LEU:HD13	2.15	0.47
1:0:86:THR:OG1	1:0:102:GLN:NE2	2.47	0.46
3:2:164:ILE:HA	3:2:167:LEU:HD13	1.95	0.46
2:4:97:THR:HA	2:4:106:VAL:O	2.15	0.46
3:D:147:ARG:HA	3:D:147:ARG:HD2	1.64	0.46
1:K:123:LEU:HB3	1:K:126:SER:OG	2.15	0.46
2:M:177:MET:HE2	2:M:188:PHE:CD1	2.43	0.46
3:T:69:ASN:O	3:T:162:LYS:NZ	2.43	0.46
2:P:148:SER:HB2	2:P:154:LEU:HD11	1.96	0.46
1:R:34:PHE:HE2	1:R:148:ILE:HD13	1.80	0.46
3:Z:44:VAL:HB	3:Z:179:VAL:HG21	1.96	0.46
1:0:40:TRP:CE2	1:0:72:THR:HA	2.51	0.46
3:2:89:CYS:HB2	3:2:177:ALA:O	2.15	0.46
1:3:48:THR:HG22	1:3:49:GLN:H	1.79	0.46
1:3:117:GLU:HB2	1:3:132:SER:HB2	1.97	0.46
2:P:114:SER:HB3	2:P:117:GLN:HG3	1.96	0.46
2:S:24:LEU:CD2	2:S:45:PRO:HD2	2.45	0.46
1:U:115:PRO:HA	1:U:116:PRO:HD3	1.85	0.46
1:X:136:ILE:HD13	1:X:148:ILE:HD11	1.95	0.46
1:6:69:THR:HG23	14:6:301:HOH:O	2.14	0.46
1:E:32:VAL:HG12	1:E:112:ILE:HB	1.98	0.46
1:E:88:ARG:HD2	1:E:100:TRP:CG	2.50	0.46
2:I:24:LEU:HB2	2:I:46:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:217:CYS:HB3	2:P:219:VAL:HG13	1.97	0.46
2:Y:177:MET:HE2	2:Y:188:PHE:HB3	1.98	0.46
1:0:51:THR:OG1	1:0:68:ARG:HA	2.15	0.46
2:4:24:LEU:HB3	2:4:44:GLY:HA3	1.96	0.46
3:N:175:ARG:O	3:N:179:VAL:HB	2.15	0.46
2:S:159:ILE:HB	14:S:410:HOH:O	2.15	0.46
3:W:42:LEU:HG	3:W:129:LEU:HD21	1.97	0.46
1:X:182:GLU:O	1:X:212:THR:HG21	2.15	0.46
3:2:42:LEU:CD1	3:2:47:PHE:HE1	2.28	0.46
2:4:24:LEU:HD23	2:4:24:LEU:HA	1.56	0.46
2:A:41:TRP:O	2:A:77:LYS:HB3	2.16	0.46
1:H:158:TYR:HB3	1:H:189:ILE:HD12	1.97	0.46
1:R:155:ARG:HD3	1:R:168:GLN:NE2	2.30	0.46
2:1:29:LYS:HA	2:1:110:THR:CG2	2.46	0.46
2:B:114:SER:HB3	2:B:117:GLN:HG3	1.96	0.46
3:G:119:VAL:HG22	3:G:120:PRO:HD3	1.97	0.46
3:G:120:PRO:HG2	1:H:80:SER:OG	2.16	0.46
3:N:83:VAL:HG13	3:N:141:ILE:HG12	1.98	0.46
3:T:61:LYS:O	3:T:65:LEU:HD12	2.15	0.46
3:W:119:VAL:HG21	1:X:59:TYR:OH	2.14	0.46
1:X:90:ARG:HD2	1:X:97:HIS:HB2	1.97	0.46
2:Y:99:VAL:CG1	2:Y:105:PRO:HB3	2.45	0.46
2:1:124:PRO:HB3	2:1:203:ILE:HD11	1.98	0.46
3:2:140:ASN:OD1	3:2:141:ILE:N	2.49	0.46
2:B:144:THR:HG23	2:B:146:VAL:H	1.80	0.46
2:B:167:LEU:HD22	2:B:201:ILE:CD1	2.46	0.46
2:M:114:SER:HB3	2:M:117:GLN:HG3	1.98	0.46
2:B:60:TYR:OH	3:D:166:GLU:OE2	2.14	0.46
2:S:194:ASP:N	2:S:221:THR:OG1	2.49	0.46
2:1:59:LYS:HD2	2:1:90:GLU:HG3	1.97	0.46
2:1:147:LEU:HD13	2:1:152:HIS:C	2.36	0.46
1:3:90:ARG:HB2	1:3:100:TRP:CZ3	2.51	0.46
1:6:38:LEU:O	1:6:73:GLN:HA	2.16	0.46
1:9:118:MET:CE	1:9:120:ILE:HD11	2.46	0.46
2:F:77:LYS:HB2	2:M:131:LYS:HE3	1.97	0.46
3:G:77:GLU:O	3:G:81:ARG:NH1	2.49	0.46
3:L:92:MET:HA	3:L:95:VAL:HG22	1.98	0.46
1:O:88:ARG:HD3	1:O:100:TRP:CD2	2.51	0.46
3:Z:170:LEU:CD2	3:Z:174:LEU:HD22	2.46	0.46
3:D:98:PHE:CZ	3:D:152:VAL:HG11	2.52	0.45
2:I:72:GLN:H	2:I:74:ILE:HD11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:114:SER:HB3	2:I:117:GLN:HG3	1.98	0.45
1:R:122:SER:HA	1:R:127:LEU:HD23	1.97	0.45
2:4:32:SER:HB2	2:4:113:PHE:HZ	1.81	0.45
3:D:110:ARG:HG2	3:D:111:PHE:N	2.31	0.45
2:F:52:VAL:HG23	2:F:99:VAL:HG13	1.99	0.45
2:I:55:VAL:HG13	2:I:68:LYS:HB3	1.99	0.45
2:P:129:ILE:HD12	2:P:136:GLN:HG2	1.98	0.45
3:Q:98:PHE:CD1	3:Q:149:LYS:HE3	2.51	0.45
3:Q:152:VAL:HG12	3:Q:153:LYS:HD2	1.99	0.45
3:Z:77:GLU:HB2	3:Z:81:ARG:HH22	1.82	0.45
2:1:48:THR:C	2:1:50:ASP:H	2.20	0.45
2:1:177:MET:HE2	2:1:188:PHE:HD1	1.80	0.45
2:B:25:LEU:HD21	2:B:96:VAL:HG22	1.98	0.45
3:D:147:ARG:NH2	3:D:154:LYS:HD3	2.31	0.45
2:F:57:TYR:CE2	2:F:84:GLU:HB3	2.52	0.45
2:F:96:VAL:O	2:F:107:THR:HA	2.17	0.45
3:G:97:GLN:O	3:G:101:GLU:HG2	2.16	0.45
2:S:48:THR:HG23	2:S:100:SER:OG	2.17	0.45
3:Z:87:ASP:HA	3:Z:134:ILE:HD11	1.99	0.45
1:0:142:THR:O	1:0:142:THR:OG1	2.23	0.45
3:8:98:PHE:CD1	3:8:149:LYS:HE2	2.51	0.45
1:9:113:ILE:HB	1:9:202:GLY:CA	2.46	0.45
2:B:36:GLU:HG3	2:B:82:THR:OG1	2.16	0.45
3:D:52:ILE:HD12	3:D:52:ILE:HA	1.82	0.45
1:H:35:LYS:HB2	1:H:137:GLU:HG3	1.97	0.45
3:J:57:PHE:HZ	3:J:172:MET:HE3	1.81	0.45
3:T:52:ILE:HD12	3:T:121:PHE:CE1	2.51	0.45
1:0:113:ILE:CD1	1:0:145:LEU:HD23	2.46	0.45
3:2:45:ARG:HG2	1:3:150:ASP:OD2	2.16	0.45
2:4:116:LEU:O	2:4:116:LEU:HD22	2.17	0.45
2:4:179:LEU:HD13	2:4:179:LEU:HA	1.65	0.45
3:8:42:LEU:HD12	3:8:42:LEU:HA	1.76	0.45
3:D:125:LEU:HD23	3:D:125:LEU:HA	1.84	0.45
1:E:189:ILE:O	1:E:207:PRO:HA	2.16	0.45
2:F:95:LYS:HA	2:F:109:MET:HA	1.98	0.45
3:G:52:ILE:HD12	3:G:52:ILE:HA	1.83	0.45
3:G:145:VAL:O	3:G:149:LYS:HG2	2.15	0.45
2:P:65:TRP:CD2	2:P:95:LYS:HE2	2.52	0.45
2:S:55:VAL:O	2:S:72:GLN:NE2	2.49	0.45
1:X:88:ARG:HG3	1:X:100:TRP:CE3	2.52	0.45
2:4:59:LYS:NZ	2:4:90:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:9:169:VAL:HG21	1:9:178:LEU:HD21	1.97	0.45
2:I:175:TYR:HE1	1:K:121:GLU:OE2	2.00	0.45
1:X:27:VAL:HG22	1:X:40:TRP:HB3	1.98	0.45
2:4:167:LEU:HA	2:4:200:SER:O	2.15	0.45
2:7:41:TRP:CE3	2:7:96:VAL:HG11	2.51	0.45
3:L:119:VAL:HG22	3:L:120:PRO:HD3	1.99	0.45
3:Q:93:LYS:HB2	3:Q:129:LEU:HD13	1.99	0.45
1:R:192:GLN:HB3	1:R:204:TRP:HA	1.98	0.45
1:U:118:MET:HE1	1:U:129:LEU:HD22	1.99	0.45
1:X:53:THR:O	1:X:89:VAL:HA	2.17	0.45
2:1:42:ASP:OD1	2:1:43:GLY:N	2.50	0.45
1:E:81:LYS:HE2	1:E:139:GLU:OE2	2.16	0.45
2:F:224:ASP:OD1	2:F:224:ASP:N	2.48	0.45
1:H:27:VAL:HG22	1:H:40:TRP:CB	2.47	0.45
2:I:85:THR:HB	2:I:92:TYR:CD2	2.52	0.45
3:J:74:LEU:HD22	3:J:162:LYS:HG2	1.98	0.45
1:O:27:VAL:HA	1:O:39:GLN:O	2.17	0.45
2:S:167:LEU:HB3	2:S:201:ILE:HG23	1.99	0.45
1:U:93:LEU:O	1:U:95:ASP:N	2.49	0.45
2:V:119:THR:O	2:V:210:LYS:HE3	2.16	0.45
2:Y:137:MET:SD	2:Y:201:ILE:HD11	2.57	0.45
1:C:148:ILE:HD12	3:L:51:TYR:HB3	1.99	0.45
1:K:116:PRO:HD3	14:K:405:HOH:O	2.16	0.45
2:S:41:TRP:CE2	2:S:77:LYS:HA	2.51	0.45
3:W:77:GLU:HG3	3:W:81:ARG:NH1	2.32	0.45
2:1:59:LYS:HD2	2:1:90:GLU:CG	2.47	0.45
2:7:25:LEU:HD21	2:7:28:VAL:HG23	1.99	0.45
3:8:59:LEU:HG	3:8:114:TYR:HB2	1.98	0.45
2:A:170:HIS:HB2	2:A:198:LEU:HB3	1.98	0.45
1:K:65:HIS:HE1	1:K:75:ASP:O	2.00	0.45
1:O:155:ARG:HD3	1:O:168:GLN:OE1	2.17	0.45
3:Q:51:TYR:O	3:Q:55:ARG:HG2	2.17	0.45
1:X:80:SER:HB2	1:X:85:TYR:OH	2.17	0.45
1:9:137:GLU:HG3	1:9:137:GLU:O	2.17	0.44
1:C:141:GLU:HB2	1:C:143:TRP:CD1	2.53	0.44
1:E:198:GLN:O	1:E:200:ARG:HG3	2.16	0.44
3:G:79:LEU:CD1	3:G:91:LEU:HD11	2.47	0.44
1:K:90:ARG:HD2	1:K:97:HIS:HB2	1.98	0.44
2:M:55:VAL:HG22	2:M:96:VAL:HG22	1.99	0.44
1:R:34:PHE:CZ	1:R:108:VAL:HA	2.52	0.44
3:T:84:SER:O	3:T:88:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:146:VAL:O	2:Y:154:LEU:HD22	2.17	0.44
2:1:169:LEU:HD12	2:1:169:LEU:HA	1.74	0.44
2:4:90:GLU:OE1	3:5:73:ARG:NH2	2.29	0.44
2:7:198:LEU:HA	2:7:198:LEU:HD23	1.83	0.44
2:M:130:PRO:HA	2:M:135:ILE:HD13	1.98	0.44
1:R:105:PHE:CE2	1:R:107:PRO:HG3	2.52	0.44
2:V:123:PRO:HG3	2:V:213:ALA:HB3	1.98	0.44
2:Y:99:VAL:HG12	2:Y:105:PRO:HB3	2.00	0.44
2:M:147:LEU:HD12	2:M:147:LEU:H	1.83	0.44
1:6:88:ARG:HD2	1:6:100:TRP:CG	2.53	0.44
2:B:28:VAL:HG12	2:B:110:THR:HG22	1.99	0.44
2:F:187:GLU:O	2:F:189:LEU:HD12	2.17	0.44
3:G:95:VAL:HG13	3:G:148:LEU:CD1	2.48	0.44
3:J:40:CYS:HB2	3:J:132:CYS:HB2	1.86	0.44
1:K:157:GLN:HA	1:K:167:PHE:O	2.17	0.44
1:U:24:PRO:HA	1:U:43:PRO:HG3	1.98	0.44
1:6:90:ARG:HB3	1:6:100:TRP:CE3	2.53	0.44
2:B:86:ARG:NH1	2:B:145:PRO:O	2.48	0.44
1:H:68:ARG:HD2	14:H:402:HOH:O	2.16	0.44
1:K:45:PHE:CE1	1:K:47:LYS:HD2	2.52	0.44
2:M:44:GLY:C	2:M:46:ALA:H	2.20	0.44
3:W:51:TYR:O	3:W:55:ARG:HG2	2.18	0.44
3:Z:56:THR:HA	3:Z:118:VAL:HG21	1.98	0.44
3:2:49:SER:HB3	3:2:52:ILE:HD11	2.00	0.44
2:A:139:VAL:HG12	2:A:184:ARG:HH11	1.83	0.44
2:B:95:LYS:HA	2:B:109:MET:HA	1.98	0.44
2:B:198:LEU:HD12	2:B:198:LEU:HA	1.71	0.44
2:F:50:ASP:HB3	2:F:101:ALA:HB2	1.98	0.44
2:F:90:GLU:HB3	2:F:92:TYR:CE1	2.53	0.44
2:M:97:THR:HG22	2:M:107:THR:CG2	2.47	0.44
1:R:118:MET:HB3	1:R:118:MET:HE2	1.77	0.44
1:R:136:ILE:CD1	1:R:148:ILE:HD11	2.48	0.44
2:S:168:GLU:HA	2:S:177:MET:O	2.18	0.44
1:X:177:VAL:HG22	1:X:179:ARG:HG3	2.00	0.44
2:Y:139:VAL:HG21	2:Y:165:TYR:CZ	2.52	0.44
2:1:51:THR:HG23	2:1:99:VAL:O	2.18	0.44
2:4:215:TYR:HE2	2:4:217:CYS:SG	2.40	0.44
3:5:152:VAL:HG23	3:5:159:GLY:C	2.38	0.44
2:7:122:LYS:HG3	14:7:402:HOH:O	2.18	0.44
1:9:186:THR:OG1	1:9:211:ARG:HA	2.18	0.44
2:1:147:LEU:HD12	2:1:151:GLY:C	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:134:ILE:HD12	3:2:134:ILE:HA	1.80	0.44
1:3:118:MET:HE3	1:3:131:PHE:HE1	1.83	0.44
2:4:24:LEU:HB2	2:4:46:ALA:HB3	1.99	0.44
2:4:169:LEU:HD12	2:4:169:LEU:HA	1.85	0.44
1:6:120:ILE:HD13	1:6:208:ILE:CG2	2.48	0.44
2:B:169:LEU:HD22	2:B:188:PHE:CB	2.47	0.44
1:C:135:GLN:HG3	1:C:143:TRP:O	2.18	0.44
2:F:24:LEU:HD13	2:F:24:LEU:HA	1.78	0.44
3:G:44:VAL:CG1	3:G:179:VAL:HG21	2.47	0.44
3:W:134:ILE:HG22	3:W:136:GLY:H	1.82	0.44
1:X:113:ILE:HD12	1:X:145:LEU:HD23	2.00	0.44
2:1:86:ARG:HG3	2:1:86:ARG:O	2.16	0.44
3:2:74:LEU:HB2	3:2:166:GLU:OE1	2.17	0.44
1:6:38:LEU:HD21	1:6:89:VAL:HG13	2.00	0.44
2:A:126:VAL:HG11	2:A:201:ILE:HD13	1.99	0.44
3:D:101:GLU:HA	3:D:105:LEU:HD22	2.00	0.44
2:F:148:SER:HB3	2:F:154:LEU:HD21	1.99	0.44
2:I:55:VAL:CG1	2:I:71:CYS:HB2	2.47	0.44
2:I:144:THR:CG2	2:I:146:VAL:H	2.24	0.44
1:O:55:GLN:HG2	1:O:64:ASP:HA	1.99	0.44
2:P:176:GLN:HE21	1:R:130:ARG:HH12	1.66	0.44
2:S:119:THR:O	2:S:210:LYS:HE3	2.17	0.44
2:Y:74:ILE:HB	2:Y:76:GLN:CD	2.38	0.44
2:Y:95:LYS:HB3	2:Y:109:MET:HB3	2.00	0.44
3:2:55:ARG:CD	3:2:114:TYR:HD1	2.31	0.43
3:2:104:LEU:HD13	3:2:119:VAL:CG1	2.48	0.43
1:3:59:TYR:HB3	1:3:60:ARG:H	1.75	0.43
2:4:52:VAL:O	2:4:98:ALA:HA	2.18	0.43
2:4:181:GLY:HA2	1:6:173:TYR:CZ	2.52	0.43
3:5:52:ILE:HG13	3:5:53:VAL:N	2.33	0.43
3:5:107:GLN:NE2	3:5:109:ASP:HB2	2.29	0.43
2:F:130:PRO:HA	2:F:135:ILE:HD13	2.00	0.43
1:H:184:TRP:CE3	1:H:213:GLY:HA2	2.53	0.43
2:I:162:ASP:HB2	2:I:206:PRO:HD2	1.99	0.43
3:J:84:SER:O	3:J:88:GLN:HG3	2.18	0.43
2:M:51:THR:HG23	2:M:99:VAL:O	2.18	0.43
1:O:45:PHE:O	1:O:47:LYS:N	2.51	0.43
2:P:126:VAL:HB	2:P:215:TYR:CE2	2.52	0.43
2:S:114:SER:CB	2:S:117:GLN:HG3	2.47	0.43
1:U:42:VAL:HG22	1:U:52:PHE:HZ	1.82	0.43
1:U:90:ARG:HD2	1:U:97:HIS:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:169:LEU:HD12	2:7:169:LEU:HA	1.88	0.43
3:8:79:LEU:HD22	3:8:144:ASN:HB3	1.99	0.43
2:B:56:GLU:HB2	2:B:95:LYS:HD2	2.00	0.43
2:B:126:VAL:HB	2:B:215:TYR:CE2	2.52	0.43
3:D:46:ASN:HB3	3:D:125:LEU:HD21	2.01	0.43
2:F:129:ILE:HD12	2:M:40:THR:HG21	1.99	0.43
2:M:169:LEU:HA	2:M:169:LEU:HD12	1.78	0.43
2:P:135:ILE:HG22	2:P:188:PHE:HB2	1.99	0.43
3:Z:98:PHE:CD1	3:Z:149:LYS:HG2	2.52	0.43
3:Z:99:THR:O	3:Z:103:VAL:HG13	2.19	0.43
3:5:40:CYS:O	3:5:40:CYS:SG	2.76	0.43
2:A:215:TYR:HE2	2:A:217:CYS:SG	2.41	0.43
1:E:158:TYR:HB3	1:E:189:ILE:HG12	1.99	0.43
3:G:78:LYS:HA	3:G:81:ARG:NH1	2.33	0.43
1:K:60:ARG:NH1	2:M:64:LYS:HD2	2.32	0.43
2:M:86:ARG:HE	2:M:147:LEU:HD21	1.84	0.43
1:O:135:GLN:HG2	1:O:144:THR:HG22	1.99	0.43
3:Q:134:ILE:HD13	3:Q:138:ASP:HB3	2.00	0.43
1:C:43:PRO:O	1:C:45:PHE:N	2.51	0.43
3:D:112:GLN:HB2	3:D:113:PRO:HA	2.01	0.43
1:K:93:LEU:HD12	1:K:94:ALA:N	2.34	0.43
1:O:88:ARG:HD3	1:O:100:TRP:CE3	2.54	0.43
2:1:59:LYS:HE3	2:1:59:LYS:HB2	1.75	0.43
2:4:34:ASN:OD1	2:4:121:ILE:HA	2.19	0.43
3:5:51:TYR:HB3	1:6:148:ILE:HG13	2.00	0.43
3:8:47:PHE:CD2	3:8:175:ARG:HG3	2.53	0.43
2:B:217:CYS:HB3	2:B:219:VAL:HG13	2.00	0.43
3:G:96:LEU:HD22	3:G:174:LEU:HD21	2.01	0.43
1:H:93:LEU:HD23	1:H:94:ALA:H	1.82	0.43
1:H:116:PRO:HD3	14:H:405:HOH:O	2.18	0.43
2:M:180:GLU:OE1	1:O:173:TYR:HB3	2.18	0.43
3:T:117:GLU:OE2	1:U:80:SER:HA	2.19	0.43
3:2:92:MET:HB3	3:2:174:LEU:HG	2.00	0.43
3:8:112:GLN:HG2	3:8:113:PRO:HA	2.00	0.43
3:J:59:LEU:HD13	3:J:114:TYR:HB2	2.01	0.43
3:L:43:HIS:ND1	3:L:45:ARG:HG2	2.33	0.43
1:R:88:ARG:HD2	1:R:100:TRP:CG	2.54	0.43
1:R:133:ALA:HB3	1:R:144:THR:HB	2.00	0.43
3:T:59:LEU:CD1	3:T:167:LEU:HD23	2.48	0.43
1:X:115:PRO:HA	1:X:116:PRO:HD3	1.88	0.43
2:4:55:VAL:HB	2:4:71:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:40:CYS:HB2	3:G:132:CYS:HB2	1.65	0.43
2:I:85:THR:HB	2:I:92:TYR:CE2	2.54	0.43
2:I:144:THR:HG23	2:I:146:VAL:N	2.22	0.43
3:L:100:LEU:O	3:L:105:LEU:HD23	2.19	0.43
2:M:119:THR:O	2:M:210:LYS:HE3	2.19	0.43
2:M:187:GLU:O	2:M:189:LEU:HD12	2.19	0.43
3:Q:59:LEU:HD11	3:Q:111:PHE:HB3	2.01	0.43
2:S:36:GLU:OE1	2:S:122:LYS:NZ	2.45	0.43
1:U:136:ILE:HD12	1:U:143:TRP:HB3	2.00	0.43
1:X:206:GLU:OE1	1:X:206:GLU:N	2.49	0.43
2:Y:68:LYS:HE2	2:Y:84:GLU:OE2	2.18	0.43
3:Z:74:LEU:HB2	3:Z:166:GLU:OE1	2.19	0.43
3:2:41:LYS:HG2	3:2:42:LEU:N	2.31	0.43
3:2:104:LEU:HD12	3:2:105:LEU:N	2.33	0.43
2:I:139:VAL:HG11	2:I:165:TYR:CE1	2.54	0.43
2:I:156:LEU:HD23	2:I:156:LEU:HA	1.78	0.43
3:J:112:GLN:HB2	3:J:113:PRO:HA	2.01	0.43
1:K:88:ARG:HD2	1:K:100:TRP:CG	2.54	0.43
2:M:29:LYS:O	2:M:39:LEU:HD12	2.19	0.43
2:M:42:ASP:OD1	2:M:43:GLY:N	2.52	0.43
2:M:208:LEU:CD1	12:M:305:GOL:H11	2.49	0.43
1:O:158:TYR:HA	1:O:188:CYS:O	2.19	0.43
3:W:134:ILE:HG22	3:W:136:GLY:N	2.34	0.43
2:Y:146:VAL:HG22	2:Y:154:LEU:CD2	2.48	0.43
1:0:21:ILE:HD13	1:0:21:ILE:HG21	1.72	0.43
3:2:99:THR:O	3:2:104:LEU:HG	2.19	0.43
2:4:148:SER:HB2	2:4:154:LEU:HD21	2.01	0.43
2:I:178:HIS:CD2	1:K:130:ARG:HD2	2.54	0.43
3:Q:40:CYS:HB3	3:Q:132:CYS:HB2	1.60	0.43
3:Q:79:LEU:HD21	3:Q:95:VAL:HG21	2.00	0.43
3:Q:121:PHE:HD1	1:R:82:TYR:CE2	2.37	0.43
3:Q:134:ILE:HG13	3:Q:135:SER:N	2.34	0.43
1:U:182:GLU:O	1:U:185:THR:HG22	2.19	0.43
2:1:60:TYR:OH	3:2:162:LYS:HD2	2.19	0.43
3:2:83:VAL:HG23	3:2:83:VAL:O	2.19	0.43
1:3:88:ARG:HD2	1:3:100:TRP:CD2	2.54	0.43
1:3:149:TYR:HD2	1:3:195:LEU:HD21	1.84	0.43
2:4:171:VAL:HG13	2:4:175:TYR:O	2.18	0.43
2:4:198:LEU:HD21	1:E:49:GLN:HA	2.00	0.43
3:8:155:LEU:HD12	3:8:155:LEU:HA	1.83	0.43
1:9:192:GLN:HB3	1:9:204:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:PRO:HA	2:B:135:ILE:HD13	2.01	0.43
1:C:31:SER:HA	1:C:35:LYS:O	2.19	0.43
3:G:69:ASN:OD1	3:G:72:VAL:HG22	2.19	0.43
3:G:74:LEU:HB2	3:G:166:GLU:OE1	2.19	0.43
3:J:52:ILE:HD12	3:J:52:ILE:HA	1.90	0.43
1:R:123:LEU:CD1	1:R:124:ALA:H	2.22	0.43
3:T:134:ILE:O	3:T:134:ILE:HG13	2.12	0.43
2:V:167:LEU:HD11	2:V:186:TYR:CB	2.48	0.43
3:2:67:ASP:OD1	3:2:162:LYS:HE2	2.19	0.42
3:2:104:LEU:HD13	3:2:119:VAL:HG13	2.01	0.42
3:2:110:ARG:CD	3:2:111:PHE:H	2.31	0.42
1:3:136:ILE:HG22	1:3:145:LEU:HD12	2.00	0.42
2:B:83:MET:HE3	2:B:86:ARG:HG3	2.00	0.42
3:G:149:LYS:HG2	3:G:149:LYS:H	1.60	0.42
2:I:119:THR:O	2:I:210:LYS:HE3	2.19	0.42
3:J:165:GLY:HA3	14:J:305:HOH:O	2.19	0.42
3:Q:87:ASP:HB3	3:Q:141:ILE:HD11	2.01	0.42
3:Q:98:PHE:HE1	3:Q:153:LYS:NZ	2.17	0.42
1:R:175:SER:HB2	14:R:307:HOH:O	2.19	0.42
2:1:99:VAL:HG22	2:1:105:PRO:HB3	2.01	0.42
3:2:98:PHE:CE1	3:2:149:LYS:HG2	2.53	0.42
1:6:106:CYS:SG	1:6:109:GLU:OE1	2.75	0.42
3:D:149:LYS:HA	3:D:152:VAL:HG12	2.02	0.42
1:H:47:LYS:NZ	1:H:49:GLN:H	2.16	0.42
2:I:132:VAL:HG23	2:I:133:ARG:N	2.33	0.42
1:O:65:HIS:CE1	1:O:78:HIS:CD2	3.07	0.42
1:R:136:ILE:HD11	1:R:148:ILE:HD11	2.00	0.42
3:T:160:GLU:O	3:T:164:ILE:HG13	2.19	0.42
2:Y:91:PHE:CE2	2:Y:114:SER:HB2	2.53	0.42
3:Z:105:LEU:HB2	3:Z:106:PRO:HD3	2.01	0.42
2:1:162:ASP:HB2	2:1:206:PRO:HD2	2.02	0.42
2:4:35:PHE:CE2	2:4:159:ILE:HD13	2.53	0.42
2:4:41:TRP:CE3	2:4:96:VAL:HG21	2.55	0.42
3:D:69:ASN:CG	3:D:72:VAL:HG22	2.39	0.42
1:H:47:LYS:HD2	1:H:47:LYS:HA	1.62	0.42
1:K:200:ARG:HE	1:K:200:ARG:HB2	1.51	0.42
3:L:74:LEU:HB2	3:L:166:GLU:OE1	2.19	0.42
3:L:96:LEU:HA	3:L:99:THR:HG22	2.01	0.42
2:M:51:THR:OG1	2:M:100:SER:HA	2.19	0.42
2:Y:41:TRP:CE2	2:Y:77:LYS:HA	2.54	0.42
2:1:29:LYS:O	2:1:39:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:39:ARG:HE	3:5:39:ARG:HA	1.83	0.42
3:8:49:SER:HB3	3:8:52:ILE:HG12	2.01	0.42
3:8:142:GLN:HA	3:8:145:VAL:HG12	2.02	0.42
2:A:200:SER:HA	2:A:215:TYR:O	2.19	0.42
1:C:113:ILE:HB	1:C:202:GLY:CA	2.50	0.42
3:J:149:LYS:O	3:J:153:LYS:HD3	2.19	0.42
1:K:142:THR:H	1:K:142:THR:HG23	1.52	0.42
3:T:91:LEU:O	3:T:95:VAL:HG23	2.19	0.42
2:V:95:LYS:HB3	2:V:109:MET:HB3	2.01	0.42
3:2:93:LYS:NZ	3:2:129:LEU:O	2.41	0.42
2:4:195:THR:HB	2:4:197:PHE:CE1	2.54	0.42
3:5:43:HIS:CE1	3:5:45:ARG:HG3	2.55	0.42
3:5:51:TYR:CB	1:6:148:ILE:HG13	2.48	0.42
2:A:166:ARG:HA	2:A:180:GLU:HG2	2.02	0.42
3:D:80:PHE:O	3:D:83:VAL:HG22	2.19	0.42
2:F:91:PHE:HD2	2:F:112:ARG:HG2	1.84	0.42
2:P:58:LYS:HD2	2:P:62:GLU:O	2.19	0.42
2:P:153:GLN:H	2:P:153:GLN:HG2	1.63	0.42
1:R:34:PHE:CE2	1:R:148:ILE:HD13	2.54	0.42
1:R:90:ARG:CD	1:R:97:HIS:HB2	2.49	0.42
1:X:22:PRO:HG2	1:X:43:PRO:HB2	2.01	0.42
3:Z:52:ILE:HD12	3:Z:52:ILE:HA	1.85	0.42
1:6:57:GLU:OE2	1:6:86:THR:N	2.40	0.42
3:8:91:LEU:O	3:8:95:VAL:HG23	2.20	0.42
2:I:62:GLU:HB2	14:I:403:HOH:O	2.20	0.42
2:I:127:THR:HA	14:I:404:HOH:O	2.19	0.42
2:I:131:LYS:HB2	2:I:134:SER:O	2.19	0.42
2:S:130:PRO:HA	2:S:135:ILE:HD13	2.02	0.42
2:V:167:LEU:N	2:V:167:LEU:HD23	2.34	0.42
3:W:48:GLN:NE2	1:X:150:ASP:OD2	2.49	0.42
1:9:90:ARG:HD2	1:9:97:HIS:HB3	2.02	0.42
1:9:113:ILE:HG23	1:9:145:LEU:HD23	2.02	0.42
1:E:55:GLN:HG2	1:E:64:ASP:HA	2.01	0.42
2:F:91:PHE:CE2	2:F:114:SER:HB2	2.54	0.42
3:N:115:MET:O	3:N:119:VAL:HG23	2.20	0.42
2:P:91:PHE:CD2	2:P:114:SER:HB2	2.55	0.42
2:Y:160:PHE:CD1	2:Y:205:THR:HG21	2.54	0.42
1:0:81:LYS:HE2	1:0:138:ASN:ND2	2.34	0.42
3:2:115:MET:HE3	3:2:115:MET:HB3	1.47	0.42
1:3:78:HIS:HA	1:3:138:ASN:ND2	2.35	0.42
1:9:144:THR:HG22	1:9:147:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:59:LEU:HD23	3:G:118:VAL:HG11	2.02	0.42
3:G:77:GLU:CD	3:G:81:ARG:HH12	2.20	0.42
3:Q:52:ILE:HD12	3:Q:52:ILE:HA	1.70	0.42
2:V:128:CYS:HB3	2:V:219:VAL:HG11	2.01	0.42
3:W:152:VAL:HG23	3:W:159:GLY:O	2.18	0.42
2:7:25:LEU:HD21	2:7:28:VAL:HG21	2.00	0.42
2:B:167:LEU:HD23	2:B:167:LEU:H	1.84	0.42
1:C:181:LEU:HB3	1:C:187:TYR:CE1	2.55	0.42
1:H:163:THR:HG22	1:H:164:ASN:H	1.85	0.42
3:L:88:GLN:O	3:L:92:MET:HG2	2.20	0.42
3:W:73:ARG:HB3	3:W:78:LYS:HZ2	1.85	0.42
2:Y:165:TYR:O	2:Y:180:GLU:HA	2.20	0.42
3:Z:42:LEU:HG	3:Z:129:LEU:HD21	2.02	0.42
1:6:120:ILE:HD11	1:6:189:ILE:HD11	2.00	0.42
1:6:155:ARG:HD2	1:6:192:GLN:OE1	2.20	0.42
1:9:198:GLN:HE21	1:9:198:GLN:HB2	1.65	0.42
2:A:86:ARG:HH21	2:A:147:LEU:HD21	1.84	0.42
1:C:153:ALA:HB2	1:C:196:LEU:HD11	2.02	0.42
1:K:146:LYS:NZ	1:K:174:ASP:OD1	2.46	0.42
3:N:114:TYR:O	3:N:118:VAL:HG23	2.20	0.42
2:P:169:LEU:HD12	2:P:169:LEU:HA	1.82	0.42
2:S:164:PHE:HE1	2:S:206:PRO:HG3	1.85	0.42
3:T:42:LEU:O	3:T:179:VAL:HG23	2.19	0.42
3:T:51:TYR:OH	3:T:117:GLU:HG2	2.19	0.42
3:T:52:ILE:HD13	1:U:82:TYR:CZ	2.55	0.42
2:V:58:LYS:HE3	2:V:65:TRP:HE1	1.84	0.42
2:Y:177:MET:CE	2:Y:188:PHE:HB3	2.50	0.42
2:1:91:PHE:CD2	2:1:114:SER:HB2	2.55	0.41
1:3:149:TYR:HB3	1:3:195:LEU:HD11	2.01	0.41
2:M:28:VAL:O	2:M:28:VAL:HG13	2.20	0.41
3:Q:90:TYR:O	3:Q:93:LYS:HB3	2.19	0.41
1:R:172:PRO:HG2	1:R:173:TYR:CE2	2.55	0.41
2:S:41:TRP:O	2:S:77:LYS:HB3	2.20	0.41
2:S:156:LEU:HD23	14:S:410:HOH:O	2.19	0.41
2:V:129:ILE:HB	2:V:136:GLN:HB3	2.01	0.41
1:X:185:THR:H	1:X:212:THR:CG2	2.25	0.41
2:Y:83:MET:SD	2:Y:86:ARG:NH1	2.92	0.41
3:Z:134:ILE:HA	3:Z:134:ILE:HD13	1.71	0.41
3:Z:142:GLN:HA	3:Z:145:VAL:HG22	2.02	0.41
3:2:113:PRO:HG2	3:2:114:TYR:CD2	2.55	0.41
1:3:32:VAL:HG22	1:3:112:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:77:GLU:O	3:5:81:ARG:HG3	2.19	0.41
1:6:185:THR:H	1:6:212:THR:CG2	2.28	0.41
2:7:63:ARG:HD3	2:7:63:ARG:C	2.41	0.41
2:7:148:SER:OG	2:7:149:GLU:N	2.52	0.41
1:9:198:GLN:O	1:9:200:ARG:HG3	2.20	0.41
1:C:90:ARG:CZ	1:C:92:GLU:OE2	2.68	0.41
2:I:169:LEU:HD12	2:I:169:LEU:HA	1.83	0.41
2:I:189:LEU:O	1:K:123:LEU:HD21	2.20	0.41
3:N:45:ARG:O	1:O:150:ASP:HB2	2.20	0.41
2:P:68:LYS:HG2	2:P:79:CYS:SG	2.61	0.41
2:P:190:GLY:HA3	1:R:123:LEU:HD11	2.00	0.41
2:S:177:MET:HE2	2:S:188:PHE:HD1	1.85	0.41
3:T:124:LYS:HD2	1:U:82:TYR:CD2	2.55	0.41
1:0:20:MET:CG	1:0:21:ILE:H	2.33	0.41
2:4:139:VAL:HG11	2:4:165:TYR:CZ	2.56	0.41
1:9:113:ILE:HB	1:9:202:GLY:HA2	2.02	0.41
2:B:164:PHE:HE1	2:B:206:PRO:HG3	1.86	0.41
3:J:44:VAL:HB	3:J:179:VAL:HG11	2.01	0.41
3:N:42:LEU:HD21	3:N:129:LEU:HG	2.01	0.41
1:O:146:LYS:NZ	1:O:174:ASP:OD1	2.51	0.41
1:R:51:THR:O	1:R:92:GLU:HG2	2.20	0.41
1:U:120:ILE:HD12	1:U:129:LEU:HD22	2.01	0.41
1:X:79:LEU:HB3	1:X:85:TYR:CE2	2.55	0.41
1:3:59:TYR:HD1	1:3:59:TYR:HA	1.71	0.41
2:4:91:PHE:HA	2:4:113:PHE:O	2.20	0.41
1:6:88:ARG:HD2	1:6:100:TRP:CD2	2.56	0.41
2:7:24:LEU:HD23	2:7:24:LEU:HA	1.64	0.41
3:D:59:LEU:HD12	3:D:59:LEU:HA	1.71	0.41
1:H:23:PRO:HB2	1:H:101:VAL:CG2	2.51	0.41
3:J:83:VAL:HG11	3:J:91:LEU:HD22	2.02	0.41
2:P:41:TRP:CE2	2:P:77:LYS:HA	2.55	0.41
2:P:134:SER:HA	2:P:191:LEU:HD12	2.01	0.41
2:S:50:ASP:OD2	2:S:101:ALA:HB2	2.20	0.41
1:U:93:LEU:HD23	1:U:93:LEU:HA	1.87	0.41
2:V:55:VAL:HG22	2:V:68:LYS:HB3	2.02	0.41
3:W:47:PHE:CE2	3:W:174:LEU:HB3	2.53	0.41
1:0:40:TRP:HZ2	1:0:71:SER:O	2.03	0.41
1:0:160:LYS:HB2	1:0:160:LYS:HE3	1.65	0.41
1:3:51:THR:OG1	1:3:68:ARG:HA	2.21	0.41
2:4:42:ASP:OD1	2:4:43:GLY:N	2.52	0.41
1:9:198:GLN:HB3	1:9:200:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:144:THR:HG21	2:A:159:ILE:HD11	2.03	0.41
1:H:115:PRO:HA	1:H:116:PRO:HD3	1.87	0.41
2:I:86:ARG:NH2	2:I:145:PRO:O	2.53	0.41
1:K:45:PHE:CZ	1:K:47:LYS:HB2	2.56	0.41
2:V:139:VAL:O	2:V:184:ARG:HD3	2.18	0.41
2:Y:162:ASP:HB2	2:Y:206:PRO:HD2	2.01	0.41
1:0:141:GLU:HB2	1:0:143:TRP:NE1	2.36	0.41
2:1:60:TYR:OH	3:2:166:GLU:OE2	2.26	0.41
2:A:55:VAL:O	2:A:72:GLN:NE2	2.53	0.41
2:I:49:SER:O	2:I:50:ASP:HB2	2.20	0.41
1:K:152:TRP:CZ2	1:K:193:GLY:HA3	2.56	0.41
3:L:103:VAL:HG11	3:L:163:ALA:CB	2.49	0.41
2:Y:134:SER:HB2	2:Y:188:PHE:O	2.20	0.41
2:Y:217:CYS:HB3	2:Y:219:VAL:HG13	2.01	0.41
3:2:55:ARG:HB2	3:2:55:ARG:CZ	2.51	0.41
3:2:124:LYS:O	3:2:128:LYS:HG3	2.20	0.41
1:3:123:LEU:HD23	1:3:123:LEU:HA	1.86	0.41
3:5:105:LEU:HD23	3:5:105:LEU:HA	1.96	0.41
2:A:216:VAL:CG1	1:H:46:PRO:HB2	2.51	0.41
2:B:91:PHE:CD2	2:B:114:SER:HB2	2.54	0.41
1:C:88:ARG:HD2	1:C:100:TRP:CG	2.56	0.41
2:I:55:VAL:CG1	2:I:68:LYS:HB3	2.50	0.41
1:K:88:ARG:HD2	1:K:100:TRP:CD2	2.56	0.41
1:K:184:TRP:CD1	1:K:213:GLY:HA2	2.55	0.41
1:U:56:TYR:HB3	1:U:87:VAL:HG12	2.01	0.41
2:1:37:ASN:OD1	2:1:85:THR:OG1	2.37	0.41
1:3:137:GLU:C	1:3:139:GLU:H	2.24	0.41
2:7:44:GLY:C	2:7:46:ALA:H	2.24	0.41
1:E:45:PHE:HA	1:E:46:PRO:HD3	1.87	0.41
3:L:90:TYR:CD1	3:L:134:ILE:HG13	2.56	0.41
2:M:192:THR:O	2:M:195:THR:OG1	2.39	0.41
3:Q:59:LEU:CD1	3:Q:111:PHE:HB3	2.50	0.41
3:Q:86:LYS:HD2	3:Q:86:LYS:HA	1.59	0.41
3:W:162:LYS:O	3:W:166:GLU:HG3	2.21	0.41
1:0:50:LEU:HD12	1:0:50:LEU:HA	1.83	0.41
1:0:80:SER:O	1:0:107:PRO:HG2	2.21	0.41
3:2:100:LEU:HA	3:2:104:LEU:HG	2.03	0.41
3:2:153:LYS:HE2	3:2:153:LYS:HB3	1.90	0.41
1:3:113:ILE:HB	1:3:202:GLY:HA2	2.02	0.41
1:3:197:ASP:OD1	1:3:198:GLN:N	2.54	0.41
3:5:39:ARG:HA	3:5:39:ARG:NE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:113:ILE:HB	1:6:202:GLY:HA2	2.03	0.41
2:7:39:LEU:HD21	2:7:96:VAL:HG13	2.03	0.41
2:7:217:CYS:HB3	2:7:219:VAL:HG13	2.02	0.41
3:8:96:LEU:CD1	3:8:122:LEU:HD22	2.51	0.41
3:8:99:THR:O	3:8:103:VAL:HG22	2.21	0.41
3:8:152:VAL:HG12	3:8:159:GLY:O	2.20	0.41
1:9:23:PRO:HB3	1:9:99:GLU:CG	2.50	0.41
1:9:40:TRP:CE2	1:9:72:THR:HA	2.56	0.41
2:A:121:ILE:HB	2:A:212:SER:HB3	2.03	0.41
2:A:164:PHE:HE1	2:A:206:PRO:HG3	1.86	0.41
2:B:54:SER:O	2:B:96:VAL:HA	2.21	0.41
2:B:154:LEU:N	14:B:401:HOH:O	2.20	0.41
3:D:74:LEU:HB2	3:D:166:GLU:OE1	2.21	0.41
2:F:68:LYS:HG2	2:F:79:CYS:SG	2.61	0.41
3:G:89:CYS:HB2	3:G:177:ALA:O	2.20	0.41
3:G:100:LEU:HD23	3:G:104:LEU:HD12	2.02	0.41
1:H:157:GLN:HA	1:H:167:PHE:O	2.21	0.41
3:Q:124:LYS:HE3	1:R:106:CYS:SG	2.60	0.41
2:S:168:GLU:HG2	2:S:200:SER:HB3	2.02	0.41
3:T:90:TYR:CD2	3:T:134:ILE:HB	2.56	0.41
2:V:42:ASP:HA	2:V:77:LYS:HD3	2.02	0.41
2:Y:66:LEU:HB3	14:Y:415:HOH:O	2.21	0.41
3:Z:125:LEU:HD23	3:Z:125:LEU:HA	1.92	0.41
2:1:215:TYR:HE2	2:1:217:CYS:SG	2.44	0.41
3:5:59:LEU:HG	3:5:114:TYR:HB2	2.03	0.41
1:9:46:PRO:HG2	1:9:50:LEU:HD11	2.03	0.41
2:B:143:LEU:HD23	2:B:143:LEU:HA	1.94	0.41
2:B:192:THR:O	2:B:195:THR:OG1	2.39	0.41
3:D:66:ALA:N	14:D:302:HOH:O	2.53	0.41
3:D:142:GLN:HA	3:D:145:VAL:HG22	2.02	0.41
3:D:154:LYS:HG3	3:D:155:LEU:CD1	2.51	0.41
3:G:118:VAL:O	3:G:122:LEU:HD13	2.21	0.41
1:K:126:SER:O	1:K:127:LEU:HD12	2.21	0.41
2:P:167:LEU:HD23	2:P:167:LEU:N	2.36	0.41
2:S:94:ALA:O	2:S:110:THR:HG23	2.21	0.41
1:X:136:ILE:CG2	1:X:145:LEU:HD12	2.50	0.41
1:0:21:ILE:CG1	1:0:98:SER:HB2	2.51	0.40
1:0:98:SER:OG	1:0:99:GLU:N	2.54	0.40
2:4:32:SER:HB2	2:4:113:PHE:CZ	2.55	0.40
2:4:88:HIS:HA	2:4:115:SER:OG	2.22	0.40
1:6:115:PRO:HA	1:6:116:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:90:TYR:CD1	3:8:93:LYS:HD3	2.57	0.40
2:B:139:VAL:O	2:B:184:ARG:HD3	2.21	0.40
3:D:70:THR:H	3:D:70:THR:HG23	1.63	0.40
2:F:218:ARG:HH22	1:U:93:LEU:CD1	2.34	0.40
2:I:205:THR:OG1	2:I:210:LYS:HB2	2.21	0.40
3:J:107:GLN:OE1	3:J:110:ARG:HD2	2.20	0.40
1:K:55:GLN:NE2	1:K:64:ASP:OD1	2.53	0.40
3:N:100:LEU:O	3:N:105:LEU:HD23	2.21	0.40
1:0:182:GLU:O	1:0:185:THR:OG1	2.40	0.40
3:2:69:ASN:OD1	3:2:72:VAL:HG23	2.21	0.40
1:6:81:LYS:NZ	1:6:139:GLU:OE2	2.37	0.40
3:8:78:LYS:HG3	3:8:81:ARG:NH2	2.36	0.40
2:A:95:LYS:HB3	2:A:109:MET:HB3	2.03	0.40
2:B:216:VAL:CG1	1:X:46:PRO:HB2	2.51	0.40
3:D:69:ASN:HB3	3:D:162:LYS:NZ	2.35	0.40
2:I:24:LEU:HA	2:I:24:LEU:HD13	1.83	0.40
2:I:55:VAL:HG12	2:I:71:CYS:O	2.21	0.40
2:I:217:CYS:HB3	2:I:219:VAL:HG13	2.02	0.40
2:P:139:VAL:CG2	2:P:184:ARG:HA	2.51	0.40
1:X:80:SER:O	1:X:107:PRO:HG2	2.21	0.40
2:Y:24:LEU:HD13	2:Y:24:LEU:N	2.37	0.40
1:0:150:ASP:OD1	3:Z:45:ARG:HG3	2.21	0.40
1:0:193:GLY:O	1:0:202:GLY:N	2.47	0.40
2:4:117:GLN:HG3	2:4:118:HIS:ND1	2.37	0.40
3:8:96:LEU:HD11	3:8:122:LEU:HD22	2.03	0.40
3:8:112:GLN:HG2	14:8:302:HOH:O	2.21	0.40
1:E:40:TRP:O	1:E:72:THR:HB	2.21	0.40
2:F:60:TYR:OH	3:G:162:LYS:HD2	2.22	0.40
3:G:98:PHE:HA	3:G:101:GLU:HG2	2.03	0.40
3:G:128:LYS:NZ	14:G:303:HOH:O	2.54	0.40
1:K:125:GLU:HG3	1:K:181:LEU:O	2.21	0.40
1:X:136:ILE:HG12	1:X:143:TRP:O	2.21	0.40
2:B:103:GLY:N	2:B:104:PRO:CD	2.84	0.40
1:C:88:ARG:HD2	1:C:100:TRP:CD2	2.56	0.40
3:D:168:ASP:OD1	3:D:169:LEU:N	2.54	0.40
3:J:90:TYR:HH	3:J:133:HIS:CD2	2.40	0.40
3:N:79:LEU:HG	3:N:91:LEU:HD21	2.03	0.40
3:Q:117:GLU:OE1	14:Q:302:HOH:O	2.22	0.40
1:R:48:THR:O	1:R:49:GLN:C	2.59	0.40
2:S:68:LYS:HG2	2:S:79:CYS:SG	2.61	0.40
2:V:170:HIS:HD1	2:V:176:GLN:HG2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:135:GLN:NE2	1:0:142:THR:HA	2.36	0.40
1:0:185:THR:O	1:0:212:THR:HG23	2.22	0.40
2:I:58:LYS:NZ	2:I:65:TRP:HE1	2.19	0.40
1:O:152:TRP:CH2	1:O:193:GLY:HA3	2.57	0.40
2:S:56:GLU:HG3	2:S:95:LYS:HG3	2.03	0.40
1:U:139:GLU:HG2	1:U:143:TRP:HD1	1.85	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	0	191/204 (94%)	178 (93%)	12 (6%)	1 (0%)	29	52
1	3	193/204 (95%)	176 (91%)	14 (7%)	3 (2%)	9	19
1	6	193/204 (95%)	178 (92%)	13 (7%)	2 (1%)	15	32
1	9	182/204 (89%)	168 (92%)	11 (6%)	3 (2%)	9	19
1	C	193/204 (95%)	183 (95%)	7 (4%)	3 (2%)	9	19
1	E	193/204 (95%)	184 (95%)	7 (4%)	2 (1%)	15	32
1	H	193/204 (95%)	184 (95%)	8 (4%)	1 (0%)	29	52
1	K	193/204 (95%)	178 (92%)	11 (6%)	4 (2%)	7	13
1	O	194/204 (95%)	179 (92%)	11 (6%)	4 (2%)	7	13
1	R	193/204 (95%)	182 (94%)	7 (4%)	4 (2%)	7	13
1	U	193/204 (95%)	176 (91%)	16 (8%)	1 (0%)	29	52
1	X	195/204 (96%)	184 (94%)	8 (4%)	3 (2%)	10	21
2	1	199/204 (98%)	191 (96%)	7 (4%)	1 (0%)	29	52
2	4	199/204 (98%)	193 (97%)	5 (2%)	1 (0%)	29	52
2	7	199/204 (98%)	194 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	199/204 (98%)	192 (96%)	6 (3%)	1 (0%)	29	52
2	B	199/204 (98%)	190 (96%)	6 (3%)	3 (2%)	10	21
2	F	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	I	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	M	199/204 (98%)	192 (96%)	6 (3%)	1 (0%)	29	52
2	P	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
2	S	199/204 (98%)	194 (98%)	5 (2%)	0	100	100
2	V	199/204 (98%)	195 (98%)	4 (2%)	0	100	100
2	Y	199/204 (98%)	192 (96%)	7 (4%)	0	100	100
3	2	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
3	5	139/149 (93%)	135 (97%)	4 (3%)	0	100	100
3	8	138/149 (93%)	130 (94%)	8 (6%)	0	100	100
3	D	139/149 (93%)	133 (96%)	6 (4%)	0	100	100
3	G	139/149 (93%)	134 (96%)	5 (4%)	0	100	100
3	J	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
3	L	139/149 (93%)	135 (97%)	3 (2%)	1 (1%)	22	43
3	N	138/149 (93%)	135 (98%)	3 (2%)	0	100	100
3	Q	140/149 (94%)	135 (96%)	3 (2%)	2 (1%)	11	22
3	T	140/149 (94%)	136 (97%)	4 (3%)	0	100	100
3	W	139/149 (93%)	133 (96%)	5 (4%)	1 (1%)	22	43
3	Z	139/149 (93%)	134 (96%)	5 (4%)	0	100	100
All	All	6360/6684 (95%)	6065 (95%)	253 (4%)	42 (1%)	22	43

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	6	142	THR
1	E	46	PRO
1	K	142	THR
1	O	125	GLU
1	X	125	GLU
1	3	49	GLN
2	4	103	GLY
2	A	103	GLY
1	C	49	GLN

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Mol	Chain	Res	Type
1	K	180	ASN
2	M	47	SER
1	O	199	GLN
1	3	199	GLN
1	6	180	ASN
1	9	46	PRO
1	C	125	GLU
1	O	44	ALA
1	U	199	GLN
1	X	180	ASN
1	3	138	ASN
1	9	47	LYS
1	9	199	GLN
2	B	49	SER
1	E	199	GLN
1	H	199	GLN
1	K	43	PRO
1	K	199	GLN
1	O	49	GLN
1	R	161	GLN
1	R	199	GLN
1	0	180	ASN
2	1	49	SER
2	B	102	GLY
1	C	199	GLN
1	R	94	ALA
1	R	125	GLU
3	W	84	SER
1	X	199	GLN
3	L	84	SER
3	Q	84	SER
2	B	103	GLY
3	Q	136	GLY

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	0	174/188 (93%)	168 (97%)	6 (3%)	37 63
1	3	176/188 (94%)	149 (85%)	27 (15%)	2 4
1	6	178/188 (95%)	152 (85%)	26 (15%)	3 5
1	9	167/188 (89%)	144 (86%)	23 (14%)	3 6
1	C	180/188 (96%)	171 (95%)	9 (5%)	24 47
1	E	175/188 (93%)	166 (95%)	9 (5%)	24 46
1	H	178/188 (95%)	162 (91%)	16 (9%)	9 18
1	K	177/188 (94%)	158 (89%)	19 (11%)	6 12
1	O	178/188 (95%)	163 (92%)	15 (8%)	11 21
1	R	179/188 (95%)	163 (91%)	16 (9%)	9 19
1	U	177/188 (94%)	160 (90%)	17 (10%)	8 16
1	X	179/188 (95%)	160 (89%)	19 (11%)	6 12
2	1	182/185 (98%)	166 (91%)	16 (9%)	10 19
2	4	181/185 (98%)	167 (92%)	14 (8%)	13 25
2	7	180/185 (97%)	166 (92%)	14 (8%)	12 25
2	A	180/185 (97%)	167 (93%)	13 (7%)	14 29
2	B	181/185 (98%)	166 (92%)	15 (8%)	11 22
2	F	181/185 (98%)	167 (92%)	14 (8%)	13 25
2	I	182/185 (98%)	168 (92%)	14 (8%)	13 25
2	M	181/185 (98%)	170 (94%)	11 (6%)	18 38
2	P	184/185 (100%)	170 (92%)	14 (8%)	13 26
2	S	183/185 (99%)	169 (92%)	14 (8%)	13 25
2	V	182/185 (98%)	167 (92%)	15 (8%)	11 22
2	Y	182/185 (98%)	161 (88%)	21 (12%)	5 10
3	2	121/135 (90%)	106 (88%)	15 (12%)	4 8
3	5	126/135 (93%)	115 (91%)	11 (9%)	10 20
3	8	123/135 (91%)	98 (80%)	25 (20%)	1 2
3	D	128/135 (95%)	120 (94%)	8 (6%)	18 36
3	G	125/135 (93%)	107 (86%)	18 (14%)	3 5
3	J	126/135 (93%)	110 (87%)	16 (13%)	4 8
3	L	126/135 (93%)	116 (92%)	10 (8%)	12 24
3	N	120/135 (89%)	108 (90%)	12 (10%)	7 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	Q	125/135 (93%)	118 (94%)	7 (6%)	21 42
3	T	128/135 (95%)	113 (88%)	15 (12%)	5 10
3	W	126/135 (93%)	111 (88%)	15 (12%)	5 9
3	Z	127/135 (94%)	114 (90%)	13 (10%)	7 14
All	All	5798/6096 (95%)	5256 (91%)	542 (9%)	9 17

All (542) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	81	LYS
1	0	93	LEU
1	0	142	THR
1	0	150	ASP
1	0	165	GLU
1	0	186	THR
2	1	30	PHE
2	1	48	THR
2	1	64	LYS
2	1	75	THR
2	1	86	ARG
2	1	97	THR
2	1	106	VAL
2	1	110	THR
2	1	117	GLN
2	1	122	LYS
2	1	142	THR
2	1	167	LEU
2	1	171	VAL
2	1	195	THR
2	1	204	LEU
2	1	207	ILE
3	2	41	LYS
3	2	43	HIS
3	2	52	ILE
3	2	65	LEU
3	2	70	THR
3	2	71	ASP
3	2	81	ARG
3	2	86	LYS
3	2	93	LYS
3	2	103	VAL

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Mol	Chain	Res	Type
3	2	105	LEU
3	2	110	ARG
3	2	123	THR
3	2	154	LYS
3	2	174	LEU
1	3	42	VAL
1	3	48	THR
1	3	51	THR
1	3	53	THR
1	3	59	TYR
1	3	78	HIS
1	3	80	SER
1	3	81	LYS
1	3	90	ARG
1	3	93	LEU
1	3	95	ASP
1	3	96	GLU
1	3	103	VAL
1	3	104	THR
1	3	108	VAL
1	3	123	LEU
1	3	137	GLU
1	3	144	THR
1	3	149	TYR
1	3	160	LYS
1	3	161	GLN
1	3	166	LYS
1	3	181	LEU
1	3	185	THR
1	3	189	ILE
1	3	195	LEU
1	3	214	ASN
2	4	28	VAL
2	4	48	THR
2	4	63	ARG
2	4	64	LYS
2	4	142	THR
2	4	167	LEU
2	4	171	VAL
2	4	174	THR
2	4	179	LEU
2	4	189	LEU

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Mol	Chain	Res	Type
2	4	191	LEU
2	4	192	THR
2	4	195	THR
2	4	202	THR
3	5	44	VAL
3	5	53	VAL
3	5	59	LEU
3	5	65	LEU
3	5	70	THR
3	5	86	LYS
3	5	87	ASP
3	5	93	LYS
3	5	103	VAL
3	5	123	THR
3	5	151	THR
1	6	20	MET
1	6	21	ILE
1	6	42	VAL
1	6	51	THR
1	6	53	THR
1	6	55	GLN
1	6	56	TYR
1	6	57	GLU
1	6	60	ARG
1	6	63	GLN
1	6	93	LEU
1	6	123	LEU
1	6	136	ILE
1	6	138	ASN
1	6	141	GLU
1	6	142	THR
1	6	144	THR
1	6	148	ILE
1	6	150	ASP
1	6	160	LYS
1	6	181	LEU
1	6	182	GLU
1	6	185	THR
1	6	186	THR
1	6	189	ILE
1	6	199	GLN
2	7	57	TYR

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Mol	Chain	Res	Type
2	7	63	ARG
2	7	64	LYS
2	7	75	THR
2	7	117	GLN
2	7	138	LEU
2	7	142	THR
2	7	147	LEU
2	7	154	LEU
2	7	157	GLU
2	7	167	LEU
2	7	174	THR
2	7	183	GLN
2	7	195	THR
3	8	41	LYS
3	8	42	LEU
3	8	44	VAL
3	8	45	ARG
3	8	53	VAL
3	8	59	LEU
3	8	62	GLU
3	8	65	LEU
3	8	71	ASP
3	8	86	LYS
3	8	103	VAL
3	8	104	LEU
3	8	112	GLN
3	8	119	VAL
3	8	123	THR
3	8	124	LYS
3	8	132	CYS
3	8	141	ILE
3	8	142	GLN
3	8	149	LYS
3	8	152	VAL
3	8	157	GLU
3	8	167	LEU
3	8	178	CYS
3	8	179	VAL
1	9	49	GLN
1	9	50	LEU
1	9	53	THR
1	9	58	SER

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Mol	Chain	Res	Type
1	9	72	THR
1	9	86	THR
1	9	97	HIS
1	9	100	TRP
1	9	123	LEU
1	9	129	LEU
1	9	138	ASN
1	9	142	THR
1	9	148	ILE
1	9	151	SER
1	9	158	TYR
1	9	170	VAL
1	9	177	VAL
1	9	182	GLU
1	9	185	THR
1	9	189	ILE
1	9	196	LEU
1	9	198	GLN
1	9	201	THR
2	A	28	VAL
2	A	50	ASP
2	A	75	THR
2	A	83	MET
2	A	99	VAL
2	A	100	SER
2	A	106	VAL
2	A	117	GLN
2	A	142	THR
2	A	144	THR
2	A	146	VAL
2	A	195	THR
2	A	216	VAL
2	B	40	THR
2	B	75	THR
2	B	86	ARG
2	B	95	LYS
2	B	96	VAL
2	B	97	THR
2	B	99	VAL
2	B	117	GLN
2	B	142	THR
2	B	144	THR

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Mol	Chain	Res	Type
2	B	154	LEU
2	B	167	LEU
2	B	174	THR
2	B	205	THR
2	B	216	VAL
1	C	20	MET
1	C	48	THR
1	C	60	ARG
1	C	67	LYS
1	C	87	VAL
1	C	96	GLU
1	C	104	THR
1	C	129	LEU
1	C	144	THR
3	D	52	ILE
3	D	70	THR
3	D	86	LYS
3	D	105	LEU
3	D	134	ILE
3	D	151	THR
3	D	172	MET
3	D	174	LEU
1	E	20	MET
1	E	49	GLN
1	E	81	LYS
1	E	141	GLU
1	E	142	THR
1	E	144	THR
1	E	150	ASP
1	E	196	LEU
1	E	212	THR
2	F	25	LEU
2	F	30	PHE
2	F	49	SER
2	F	63	ARG
2	F	66	LEU
2	F	83	MET
2	F	99	VAL
2	F	117	GLN
2	F	129	ILE
2	F	142	THR
2	F	147	LEU

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Mol	Chain	Res	Type
2	F	180	GLU
2	F	195	THR
2	F	204	LEU
3	G	52	ILE
3	G	65	LEU
3	G	70	THR
3	G	78	LYS
3	G	91	LEU
3	G	99	THR
3	G	103	VAL
3	G	110	ARG
3	G	118	VAL
3	G	119	VAL
3	G	143	LYS
3	G	148	LEU
3	G	151	THR
3	G	152	VAL
3	G	167	LEU
3	G	172	MET
3	G	173	SER
3	G	174	LEU
1	H	51	THR
1	H	80	SER
1	H	81	LYS
1	H	93	LEU
1	H	103	VAL
1	H	104	THR
1	H	120	ILE
1	H	123	LEU
1	H	127	LEU
1	H	130	ARG
1	H	136	ILE
1	H	141	GLU
1	H	144	THR
1	H	148	ILE
1	H	158	TYR
1	H	163	THR
2	I	28	VAL
2	I	30	PHE
2	I	40	THR
2	I	58	LYS
2	I	74	ILE

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Mol	Chain	Res	Type
2	I	97	THR
2	I	106	VAL
2	I	117	GLN
2	I	142	THR
2	I	144	THR
2	I	157	GLU
2	I	171	VAL
2	I	174	THR
2	I	179	LEU
3	J	52	ILE
3	J	53	VAL
3	J	58	MET
3	J	65	LEU
3	J	70	THR
3	J	71	ASP
3	J	74	LEU
3	J	86	LYS
3	J	95	VAL
3	J	105	LEU
3	J	133	HIS
3	J	134	ILE
3	J	151	THR
3	J	157	GLU
3	J	172	MET
3	J	174	LEU
1	K	25	GLU
1	K	47	LYS
1	K	51	THR
1	K	53	THR
1	K	55	GLN
1	K	61	SER
1	K	87	VAL
1	K	93	LEU
1	K	101	VAL
1	K	119	GLN
1	K	129	LEU
1	K	158	TYR
1	K	164	ASN
1	K	165	GLU
1	K	177	VAL
1	K	185	THR
1	K	198	GLN

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Mol	Chain	Res	Type
1	K	200	ARG
1	K	214	ASN
3	L	52	ILE
3	L	70	THR
3	L	71	ASP
3	L	77	GLU
3	L	79	LEU
3	L	119	VAL
3	L	134	ILE
3	L	141	ILE
3	L	150	GLU
3	L	174	LEU
2	M	30	PHE
2	M	83	MET
2	M	97	THR
2	M	99	VAL
2	M	115	SER
2	M	117	GLN
2	M	147	LEU
2	M	155	THR
2	M	174	THR
2	M	183	GLN
2	M	195	THR
3	N	41	LYS
3	N	45	ARG
3	N	65	LEU
3	N	70	THR
3	N	71	ASP
3	N	84	SER
3	N	103	VAL
3	N	112	GLN
3	N	123	THR
3	N	142	GLN
3	N	174	LEU
3	N	179	VAL
1	O	20	MET
1	O	21	ILE
1	O	27	VAL
1	O	32	VAL
1	O	42	VAL
1	O	47	LYS
1	O	49	GLN

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Mol	Chain	Res	Type
1	O	53	THR
1	O	81	LYS
1	O	123	LEU
1	O	129	LEU
1	O	136	ILE
1	O	142	THR
1	O	164	ASN
1	O	214	ASN
2	P	24	LEU
2	P	28	VAL
2	P	40	THR
2	P	117	GLN
2	P	132	VAL
2	P	154	LEU
2	P	167	LEU
2	P	168	GLU
2	P	174	THR
2	P	183	GLN
2	P	192	THR
2	P	195	THR
2	P	198	LEU
2	P	216	VAL
3	Q	52	ILE
3	Q	58	MET
3	Q	70	THR
3	Q	78	LYS
3	Q	83	VAL
3	Q	134	ILE
3	Q	172	MET
1	R	32	VAL
1	R	51	THR
1	R	56	TYR
1	R	58	SER
1	R	90	ARG
1	R	93	LEU
1	R	104	THR
1	R	123	LEU
1	R	142	THR
1	R	148	ILE
1	R	161	GLN
1	R	170	VAL
1	R	185	THR

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Mol	Chain	Res	Type
1	R	200	ARG
1	R	208	ILE
1	R	212	THR
2	S	40	THR
2	S	48	THR
2	S	56	GLU
2	S	74	ILE
2	S	75	THR
2	S	117	GLN
2	S	144	THR
2	S	167	LEU
2	S	174	THR
2	S	180	GLU
2	S	183	GLN
2	S	196	GLU
2	S	198	LEU
2	S	201	ILE
3	T	39	ARG
3	T	44	VAL
3	T	58	MET
3	T	59	LEU
3	T	65	LEU
3	T	71	ASP
3	T	93	LYS
3	T	134	ILE
3	T	151	THR
3	T	153	LYS
3	T	167	LEU
3	T	172	MET
3	T	173	SER
3	T	174	LEU
3	T	179	VAL
1	U	28	ARG
1	U	32	VAL
1	U	56	TYR
1	U	58	SER
1	U	61	SER
1	U	81	LYS
1	U	86	THR
1	U	93	LEU
1	U	96	GLU
1	U	105	PHE

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Mol	Chain	Res	Type
1	U	118	MET
1	U	148	ILE
1	U	161	GLN
1	U	169	VAL
1	U	186	THR
1	U	200	ARG
1	U	214	ASN
2	V	30	PHE
2	V	40	THR
2	V	48	THR
2	V	52	VAL
2	V	72	GLN
2	V	76	GLN
2	V	95	LYS
2	V	106	VAL
2	V	117	GLN
2	V	142	THR
2	V	147	LEU
2	V	167	LEU
2	V	174	THR
2	V	195	THR
2	V	204	LEU
3	W	44	VAL
3	W	52	ILE
3	W	70	THR
3	W	71	ASP
3	W	78	LYS
3	W	101	GLU
3	W	110	ARG
3	W	118	VAL
3	W	119	VAL
3	W	132	CYS
3	W	134	ILE
3	W	151	THR
3	W	153	LYS
3	W	167	LEU
3	W	174	LEU
1	X	51	THR
1	X	61	SER
1	X	67	LYS
1	X	80	SER
1	X	86	THR

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Mol	Chain	Res	Type
1	X	92	GLU
1	X	104	THR
1	X	123	LEU
1	X	142	THR
1	X	144	THR
1	X	150	ASP
1	X	158	TYR
1	X	163	THR
1	X	166	LYS
1	X	170	VAL
1	X	181	LEU
1	X	182	GLU
1	X	198	GLN
1	X	214	ASN
2	Y	24	LEU
2	Y	48	THR
2	Y	49	SER
2	Y	55	VAL
2	Y	58	LYS
2	Y	64	LYS
2	Y	86	ARG
2	Y	97	THR
2	Y	99	VAL
2	Y	127	THR
2	Y	142	THR
2	Y	146	VAL
2	Y	154	LEU
2	Y	166	ARG
2	Y	167	LEU
2	Y	179	LEU
2	Y	180	GLU
2	Y	183	GLN
2	Y	192	THR
2	Y	195	THR
2	Y	204	LEU
3	Z	52	ILE
3	Z	58	MET
3	Z	65	LEU
3	Z	71	ASP
3	Z	77	GLU
3	Z	96	LEU
3	Z	103	VAL

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Mol	Chain	Res	Type
3	Z	105	LEU
3	Z	123	THR
3	Z	134	ILE
3	Z	151	THR
3	Z	167	LEU
3	Z	174	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	65	HIS
1	0	102	GLN
2	1	178	HIS
2	4	118	HIS
3	5	107	GLN
1	6	65	HIS
1	6	199	GLN
2	7	118	HIS
2	7	170	HIS
1	9	128	HIS
3	D	48	GLN
1	H	190	GLN
1	K	102	GLN
1	K	198	GLN
3	L	48	GLN
3	L	68	GLN
2	S	176	GLN
1	U	39	GLN
1	X	190	GLN
3	Z	94	GLN
3	Z	107	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

67 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	a	1	4,2	14,14,15	0.29	0	17,19,21	0.94	2 (11%)
4	NAG	a	2	4	14,14,15	0.88	1 (7%)	17,19,21	1.56	2 (11%)
4	BMA	a	3	4	11,11,12	1.11	1 (9%)	15,15,17	1.93	4 (26%)
4	FUC	a	4	4	10,10,11	1.34	2 (20%)	14,14,16	1.19	1 (7%)
5	NAG	b	1	5,3	14,14,15	0.51	0	17,19,21	0.83	1 (5%)
5	NAG	b	2	5	14,14,15	0.30	0	17,19,21	0.80	0
5	FUC	b	3	5	10,10,11	1.94	3 (30%)	14,14,16	1.33	2 (14%)
4	NAG	c	1	4,2	14,14,15	0.47	0	17,19,21	1.17	1 (5%)
4	NAG	c	2	4	14,14,15	1.07	1 (7%)	17,19,21	1.46	4 (23%)
4	BMA	c	3	4	11,11,12	1.47	2 (18%)	15,15,17	1.42	2 (13%)
4	FUC	c	4	4	10,10,11	1.42	1 (10%)	14,14,16	1.19	2 (14%)
6	NAG	d	1	6,3	14,14,15	0.66	0	17,19,21	0.90	0
6	FUC	d	2	6	10,10,11	1.57	2 (20%)	14,14,16	1.22	2 (14%)
5	NAG	e	1	5,2	14,14,15	0.33	0	17,19,21	0.99	1 (5%)
5	NAG	e	2	5	14,14,15	0.45	0	17,19,21	0.97	1 (5%)
5	FUC	e	3	5	10,10,11	1.26	1 (10%)	14,14,16	1.10	0
7	NAG	f	1	7,3	14,14,15	1.06	1 (7%)	17,19,21	0.89	1 (5%)
7	FUC	f	2	7	10,10,11	0.87	0	14,14,16	0.83	0
8	NAG	g	1	8,2	14,14,15	0.60	0	17,19,21	0.73	0
8	NAG	g	2	8	14,14,15	0.33	0	17,19,21	0.52	0
8	BMA	g	3	8	11,11,12	1.37	2 (18%)	15,15,17	0.82	0
9	NAG	h	1	9,3	14,14,15	0.27	0	17,19,21	0.63	0
9	NAG	h	2	9	14,14,15	0.63	0	17,19,21	1.49	2 (11%)
9	BMA	h	3	9	11,11,12	0.64	0	15,15,17	1.45	2 (13%)
9	FUC	h	4	9	10,10,11	1.32	2 (20%)	14,14,16	1.37	2 (14%)
9	FUC	h	5	9	10,10,11	1.38	2 (20%)	14,14,16	1.58	4 (28%)
5	NAG	i	1	5,2	14,14,15	0.71	1 (7%)	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	i	2	5	14,14,15	0.58	0	17,19,21	0.67	0
5	FUC	i	3	5	10,10,11	1.30	1 (10%)	14,14,16	1.56	2 (14%)
5	NAG	j	1	5,3	14,14,15	0.40	0	17,19,21	0.73	0
5	NAG	j	2	5	14,14,15	0.43	0	17,19,21	0.67	0
5	FUC	j	3	5	10,10,11	1.38	2 (20%)	14,14,16	1.89	5 (35%)
9	NAG	k	1	9,2	14,14,15	0.44	0	17,19,21	0.69	0
9	NAG	k	2	9	14,14,15	0.24	0	17,19,21	0.48	0
9	BMA	k	3	9	11,11,12	1.30	2 (18%)	15,15,17	0.90	0
9	FUC	k	4	9	10,10,11	1.04	2 (20%)	14,14,16	1.01	0
9	FUC	k	5	9	10,10,11	1.12	1 (10%)	14,14,16	0.94	1 (7%)
5	NAG	l	1	5,3	14,14,15	0.90	1 (7%)	17,19,21	1.09	1 (5%)
5	NAG	l	2	5	14,14,15	0.87	1 (7%)	17,19,21	0.88	0
5	FUC	l	3	5	10,10,11	1.45	3 (30%)	14,14,16	2.28	4 (28%)
5	NAG	m	1	5,3	14,14,15	0.44	0	17,19,21	1.22	3 (17%)
5	NAG	m	2	5	14,14,15	0.37	0	17,19,21	0.65	0
5	FUC	m	3	5	10,10,11	2.31	3 (30%)	14,14,16	2.17	5 (35%)
4	NAG	n	1	4,2	14,14,15	0.44	0	17,19,21	0.52	0
4	NAG	n	2	4	14,14,15	0.44	0	17,19,21	0.49	0
4	BMA	n	3	4	11,11,12	1.13	1 (9%)	15,15,17	0.84	0
4	FUC	n	4	4	10,10,11	1.12	1 (10%)	14,14,16	1.05	1 (7%)
6	NAG	o	1	6,3	14,14,15	0.88	2 (14%)	17,19,21	1.11	1 (5%)
6	FUC	o	2	6	10,10,11	1.23	1 (10%)	14,14,16	1.33	2 (14%)
6	NAG	p	1	6,2	14,14,15	0.83	1 (7%)	17,19,21	0.51	0
6	FUC	p	2	6	10,10,11	1.42	2 (20%)	14,14,16	1.66	1 (7%)
10	NAG	q	1	10,3	14,14,15	0.64	1 (7%)	17,19,21	0.99	1 (5%)
10	NAG	q	2	10	14,14,15	0.35	0	17,19,21	0.58	0
6	NAG	r	1	6,2	14,14,15	0.89	1 (7%)	17,19,21	0.70	0
6	FUC	r	2	6	10,10,11	1.70	3 (30%)	14,14,16	1.46	2 (14%)
5	NAG	s	1	5,3	14,14,15	0.25	0	17,19,21	0.64	0
5	NAG	s	2	5	14,14,15	0.45	0	17,19,21	0.52	0
5	FUC	s	3	5	10,10,11	1.11	1 (10%)	14,14,16	0.76	0
6	NAG	t	1	6,2	14,14,15	0.83	1 (7%)	17,19,21	0.68	0
6	FUC	t	2	6	10,10,11	0.84	0	14,14,16	1.13	2 (14%)
6	NAG	u	1	6,3	14,14,15	0.83	1 (7%)	17,19,21	0.46	0
6	FUC	u	2	6	10,10,11	1.70	3 (30%)	14,14,16	1.36	0
6	NAG	v	1	6,2	14,14,15	0.77	0	17,19,21	0.72	0
6	FUC	v	2	6	10,10,11	1.07	1 (10%)	14,14,16	1.96	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	w	1	11,3	14,14,15	0.44	0	17,19,21	0.76	1 (5%)
11	FUC	w	2	11	10,10,11	0.56	0	14,14,16	0.92	0
11	FUC	w	3	11	10,10,11	1.23	1 (10%)	14,14,16	1.26	2 (14%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	j	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	2/6/23/26	0/1/1/1
5	FUC	j	3	5	-	-	0/1/1/1
9	NAG	k	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	k	2	9	-	1/6/23/26	0/1/1/1
9	BMA	k	3	9	-	0/2/19/22	0/1/1/1
9	FUC	k	4	9	-	-	0/1/1/1
9	FUC	k	5	9	-	-	0/1/1/1
5	NAG	l	1	5,3	-	4/6/23/26	0/1/1/1
5	NAG	l	2	5	-	2/6/23/26	0/1/1/1
5	FUC	l	3	5	-	-	0/1/1/1
5	NAG	m	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	4/6/23/26	0/1/1/1
5	FUC	m	3	5	-	-	0/1/1/1
4	NAG	n	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	n	2	4	-	2/6/23/26	0/1/1/1
4	BMA	n	3	4	-	0/2/19/22	0/1/1/1
4	FUC	n	4	4	-	-	0/1/1/1
6	NAG	o	1	6,3	-	2/6/23/26	0/1/1/1
6	FUC	o	2	6	-	-	0/1/1/1
6	NAG	p	1	6,2	-	2/6/23/26	0/1/1/1
6	FUC	p	2	6	-	-	0/1/1/1
10	NAG	q	1	10,3	-	2/6/23/26	0/1/1/1
10	NAG	q	2	10	-	1/6/23/26	0/1/1/1
6	NAG	r	1	6,2	-	4/6/23/26	0/1/1/1
6	FUC	r	2	6	-	-	0/1/1/1
5	NAG	s	1	5,3	-	0/6/23/26	0/1/1/1
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	FUC	s	3	5	-	-	0/1/1/1
6	NAG	t	1	6,2	-	2/6/23/26	0/1/1/1
6	FUC	t	2	6	-	-	0/1/1/1
6	NAG	u	1	6,3	-	2/6/23/26	0/1/1/1
6	FUC	u	2	6	-	-	0/1/1/1
6	NAG	v	1	6,2	-	0/6/23/26	0/1/1/1
6	FUC	v	2	6	-	-	0/1/1/1
11	NAG	w	1	11,3	-	0/6/23/26	0/1/1/1
11	FUC	w	2	11	-	-	0/1/1/1
11	FUC	w	3	11	-	-	0/1/1/1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	m	3	FUC	C1-C2	4.87	1.63	1.52
5	b	3	FUC	C2-C3	4.16	1.58	1.52
7	f	1	NAG	O5-C1	3.77	1.49	1.43
5	m	3	FUC	O5-C1	3.64	1.49	1.43
4	c	4	FUC	O5-C1	-3.62	1.37	1.43
6	r	2	FUC	C2-C3	3.46	1.57	1.52
5	i	3	FUC	C4-C5	3.31	1.60	1.52
6	u	2	FUC	C2-C3	3.29	1.57	1.52
5	e	3	FUC	C1-C2	3.27	1.59	1.52
4	c	3	BMA	C1-C2	3.26	1.59	1.52
6	p	2	FUC	C1-C2	3.20	1.59	1.52
9	h	4	FUC	O5-C5	3.10	1.50	1.43
5	l	2	NAG	C1-C2	3.00	1.56	1.52
5	l	1	NAG	O5-C1	2.99	1.48	1.43
4	c	2	NAG	C1-C2	2.97	1.56	1.52
6	u	2	FUC	C1-C2	2.94	1.58	1.52
4	a	4	FUC	C1-C2	2.93	1.58	1.52
4	c	3	BMA	C2-C3	2.83	1.56	1.52
9	k	5	FUC	O5-C1	-2.80	1.39	1.43
6	r	2	FUC	C1-C2	2.80	1.58	1.52
5	l	3	FUC	C4-C5	2.79	1.59	1.52
5	m	3	FUC	O5-C5	2.78	1.49	1.43
4	a	3	BMA	C1-C2	2.78	1.58	1.52
8	g	3	BMA	C4-C5	2.74	1.58	1.53
9	h	5	FUC	C1-C2	2.73	1.58	1.52
6	d	2	FUC	C4-C3	2.71	1.59	1.52
5	j	3	FUC	C1-C2	2.62	1.58	1.52
9	k	3	BMA	C1-C2	2.62	1.58	1.52
4	n	4	FUC	C2-C3	2.60	1.56	1.52
8	g	3	BMA	C4-C3	2.59	1.58	1.52
6	d	2	FUC	C4-C5	2.57	1.58	1.52
6	p	2	FUC	C2-C3	2.52	1.56	1.52
5	b	3	FUC	O5-C5	2.48	1.48	1.43
5	i	1	NAG	C1-C2	2.48	1.56	1.52
4	a	2	NAG	O5-C1	-2.46	1.39	1.43
6	o	2	FUC	C2-C3	2.43	1.56	1.52
6	p	1	NAG	O5-C1	2.43	1.47	1.43
11	w	3	FUC	C1-C2	2.42	1.57	1.52
5	b	3	FUC	C4-C5	2.41	1.58	1.52
6	v	2	FUC	C1-C2	2.37	1.57	1.52
5	s	3	FUC	C2-C3	2.34	1.56	1.52
6	u	1	NAG	O5-C1	2.34	1.47	1.43
10	q	1	NAG	O5-C1	2.32	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	r	1	NAG	C1-C2	2.30	1.55	1.52
9	h	5	FUC	O5-C5	2.29	1.48	1.43
5	l	3	FUC	O5-C5	2.24	1.48	1.43
5	j	3	FUC	O5-C5	2.24	1.48	1.43
9	h	4	FUC	C1-C2	2.23	1.57	1.52
9	k	4	FUC	C1-C2	2.20	1.57	1.52
6	r	2	FUC	O5-C5	2.17	1.48	1.43
6	o	1	NAG	C1-C2	2.15	1.55	1.52
6	t	1	NAG	O5-C1	2.15	1.47	1.43
6	u	2	FUC	O5-C1	-2.11	1.40	1.43
4	n	3	BMA	C4-C5	2.10	1.57	1.53
5	l	3	FUC	C2-C3	2.07	1.55	1.52
6	o	1	NAG	O5-C1	2.05	1.47	1.43
4	a	4	FUC	O5-C1	-2.05	1.40	1.43
9	k	3	BMA	C2-C3	2.03	1.55	1.52
9	k	4	FUC	O5-C5	2.01	1.47	1.43

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	a	3	BMA	C1-O5-C5	5.07	119.06	112.19
6	p	2	FUC	C1-C2-C3	5.01	115.83	109.67
4	a	2	NAG	C2-N2-C7	4.81	129.75	122.90
6	v	2	FUC	O5-C1-C2	4.72	118.05	110.77
5	l	3	FUC	O5-C5-C4	4.63	117.82	109.52
5	m	3	FUC	O5-C5-C4	4.57	117.73	109.52
5	j	3	FUC	C1-O5-C5	4.44	122.83	112.78
5	l	3	FUC	C3-C4-C5	4.36	116.57	109.77
9	h	2	NAG	C1-O5-C5	4.31	118.03	112.19
5	m	3	FUC	C1-O5-C5	4.22	122.35	112.78
4	c	1	NAG	O4-C4-C5	-3.96	99.45	109.30
4	c	2	NAG	C1-O5-C5	-3.86	106.96	112.19
6	r	2	FUC	C1-C2-C3	3.84	114.38	109.67
5	i	3	FUC	C1-C2-C3	-3.73	105.08	109.67
5	e	2	NAG	C1-O5-C5	3.66	117.15	112.19
4	c	3	BMA	C1-O5-C5	3.49	116.93	112.19
6	o	1	NAG	O3-C3-C2	3.45	116.60	109.47
9	h	3	BMA	C1-O5-C5	3.39	116.78	112.19
5	l	3	FUC	O3-C3-C4	-3.38	102.53	110.35
9	h	5	FUC	C2-C3-C4	-3.13	105.47	110.89
11	w	3	FUC	C1-C2-C3	3.13	113.51	109.67
4	a	4	FUC	O2-C2-C1	3.10	115.49	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	h	2	NAG	O4-C4-C5	3.06	116.89	109.30
5	e	1	NAG	O4-C4-C3	-3.01	103.39	110.35
5	m	3	FUC	C1-C2-C3	2.99	113.34	109.67
5	l	3	FUC	C1-O5-C5	2.87	119.29	112.78
9	h	5	FUC	O5-C5-C4	2.85	114.63	109.52
9	h	5	FUC	O2-C2-C1	2.82	114.92	109.15
5	l	1	NAG	O4-C4-C3	2.76	116.73	110.35
4	a	3	BMA	C1-C2-C3	2.74	113.04	109.67
5	b	3	FUC	O5-C5-C4	2.73	114.43	109.52
4	c	3	BMA	C1-C2-C3	2.72	113.01	109.67
4	c	4	FUC	C1-C2-C3	-2.71	106.34	109.67
5	j	3	FUC	O5-C5-C4	2.68	114.32	109.52
4	a	3	BMA	O5-C1-C2	2.67	114.89	110.77
5	j	3	FUC	O2-C2-C1	2.64	114.55	109.15
6	v	2	FUC	O5-C5-C6	-2.62	101.69	107.33
4	c	4	FUC	O2-C2-C1	2.60	114.48	109.15
6	o	2	FUC	C1-O5-C5	2.59	118.66	112.78
9	h	4	FUC	C1-O5-C5	2.55	118.56	112.78
9	h	4	FUC	O5-C5-C4	2.54	114.08	109.52
9	h	5	FUC	C1-O5-C5	2.47	118.39	112.78
4	n	4	FUC	C1-C2-C3	2.45	112.68	109.67
6	v	2	FUC	O3-C3-C2	-2.43	105.34	109.99
4	a	3	BMA	O2-C2-C3	-2.42	105.28	110.14
5	j	3	FUC	C2-C3-C4	-2.42	106.71	110.89
4	a	1	NAG	O4-C4-C3	-2.41	104.77	110.35
6	r	2	FUC	O5-C5-C4	2.41	113.85	109.52
9	h	3	BMA	O5-C1-C2	2.41	114.49	110.77
6	t	2	FUC	C1-O5-C5	2.41	118.24	112.78
6	d	2	FUC	O5-C5-C4	2.37	113.77	109.52
5	j	3	FUC	O5-C1-C2	2.37	114.42	110.77
6	o	2	FUC	O5-C5-C4	2.35	113.75	109.52
4	c	2	NAG	O4-C4-C5	-2.35	103.45	109.30
6	v	2	FUC	C1-O5-C5	2.34	118.08	112.78
5	m	3	FUC	O5-C1-C2	2.31	114.34	110.77
5	b	1	NAG	C1-C2-N2	2.30	114.42	110.49
4	a	1	NAG	O4-C4-C5	-2.30	103.58	109.30
4	c	2	NAG	C4-C3-C2	2.29	114.38	111.02
4	a	2	NAG	O4-C4-C5	2.28	114.97	109.30
9	k	5	FUC	O2-C2-C1	2.24	113.73	109.15
11	w	3	FUC	C1-O5-C5	2.24	117.85	112.78
6	t	2	FUC	O5-C5-C4	2.24	113.53	109.52
5	i	3	FUC	O5-C5-C4	2.17	113.41	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	w	1	NAG	C1-O5-C5	2.16	115.12	112.19
5	m	1	NAG	C6-C5-C4	2.15	118.03	113.00
6	d	2	FUC	C1-O5-C5	2.13	117.62	112.78
7	f	1	NAG	C1-O5-C5	2.13	115.08	112.19
5	b	3	FUC	C1-O5-C5	2.12	117.59	112.78
5	m	1	NAG	O3-C3-C4	2.10	115.20	110.35
10	q	1	NAG	C1-C2-N2	2.09	114.07	110.49
5	m	3	FUC	C6-C5-C4	-2.06	109.26	113.07
4	c	2	NAG	C2-N2-C7	2.06	125.84	122.90
5	m	1	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	l	2	NAG	C1-C2-N2-C7
5	m	1	NAG	C4-C5-C6-O6
6	r	1	NAG	C1-C2-N2-C7
5	b	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	n	2	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
6	o	1	NAG	O5-C5-C6-O6
4	c	3	BMA	O5-C5-C6-O6
6	u	1	NAG	O5-C5-C6-O6
10	q	1	NAG	O5-C5-C6-O6
5	l	1	NAG	O5-C5-C6-O6
4	a	3	BMA	O5-C5-C6-O6
5	i	2	NAG	O5-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
9	h	2	NAG	C4-C5-C6-O6
5	m	1	NAG	O5-C5-C6-O6
9	h	2	NAG	O5-C5-C6-O6
4	c	3	BMA	C4-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
6	p	1	NAG	O5-C5-C6-O6
4	n	2	NAG	C4-C5-C6-O6
6	d	1	NAG	C4-C5-C6-O6
6	u	1	NAG	C4-C5-C6-O6
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2

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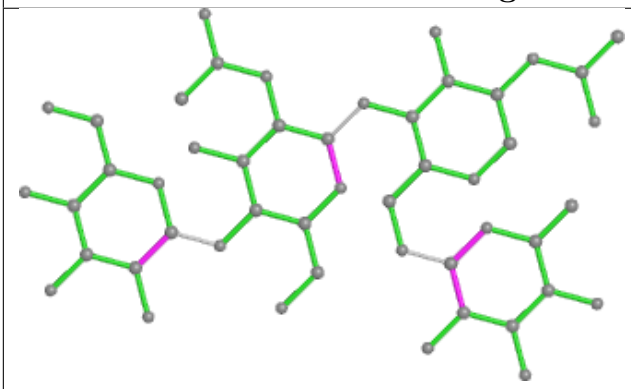
Mol	Chain	Res	Type	Atoms
5	e	1	NAG	C4-C5-C6-O6
6	o	1	NAG	C4-C5-C6-O6
10	q	1	NAG	C4-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
6	r	1	NAG	O5-C5-C6-O6
9	h	1	NAG	O5-C5-C6-O6
5	l	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
9	h	1	NAG	C4-C5-C6-O6
6	p	1	NAG	C4-C5-C6-O6
6	r	1	NAG	C4-C5-C6-O6
5	s	2	NAG	O5-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
9	h	3	BMA	O5-C5-C6-O6
5	s	2	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	c	2	NAG	O5-C5-C6-O6
5	j	2	NAG	C4-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
5	l	1	NAG	C1-C2-N2-C7
4	c	1	NAG	O5-C5-C6-O6
5	i	2	NAG	C4-C5-C6-O6
9	k	2	NAG	O5-C5-C6-O6
5	m	2	NAG	C4-C5-C6-O6
4	a	3	BMA	C4-C5-C6-O6
5	b	2	NAG	C3-C2-N2-C7
5	l	2	NAG	C3-C2-N2-C7
6	r	1	NAG	C3-C2-N2-C7
6	t	1	NAG	C3-C2-N2-C7
10	q	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C1-C2-N2-C7
4	c	2	NAG	C1-C2-N2-C7
5	b	2	NAG	C1-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
5	i	1	NAG	C3-C2-N2-C7
5	l	1	NAG	C3-C2-N2-C7
5	m	2	NAG	C3-C2-N2-C7
6	t	1	NAG	C4-C5-C6-O6
5	i	1	NAG	C1-C2-N2-C7
5	m	2	NAG	C1-C2-N2-C7

There are no ring outliers.

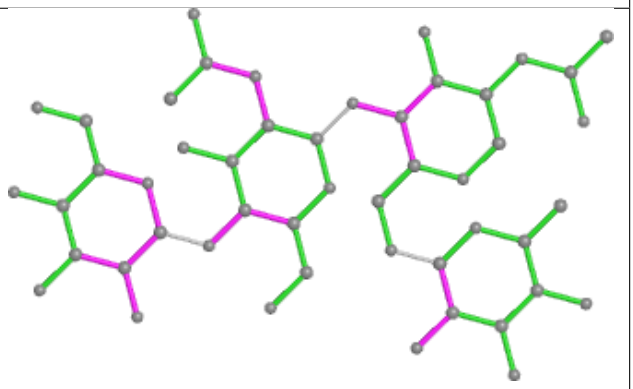
No monomer is involved in short contacts.

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

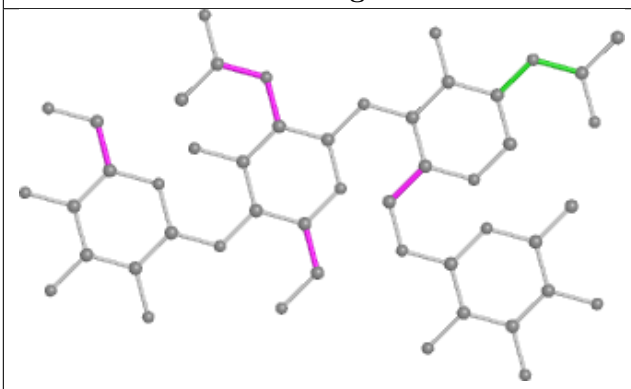
Oligosaccharide Chain a



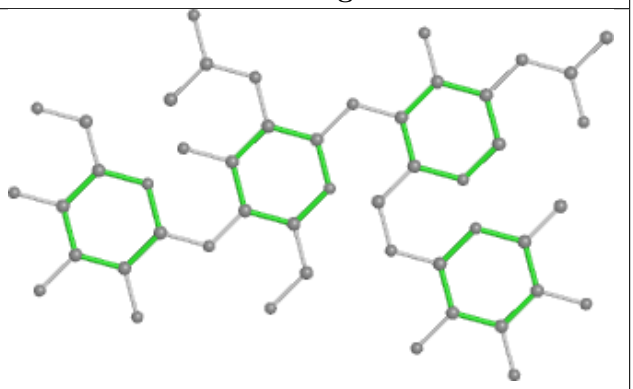
Bond lengths



Bond angles

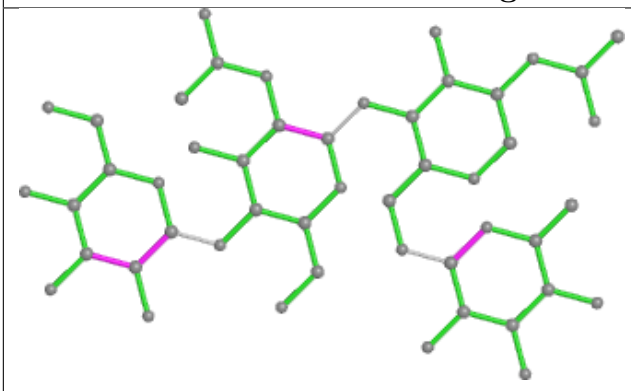


Torsions

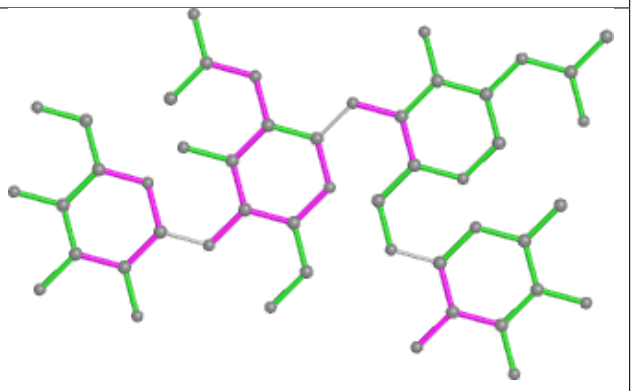


Rings

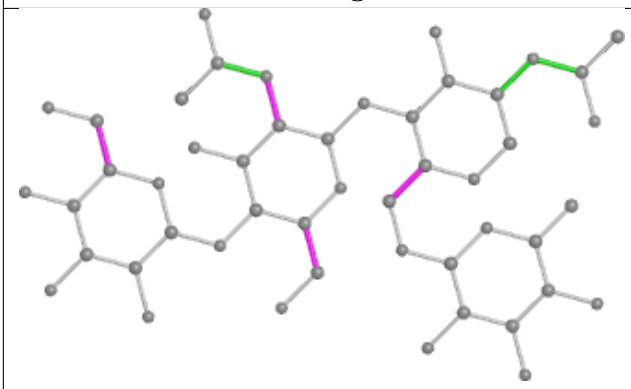
Oligosaccharide Chain c



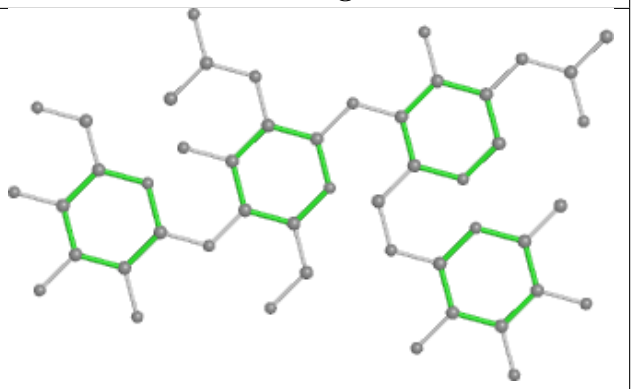
Bond lengths



Bond angles

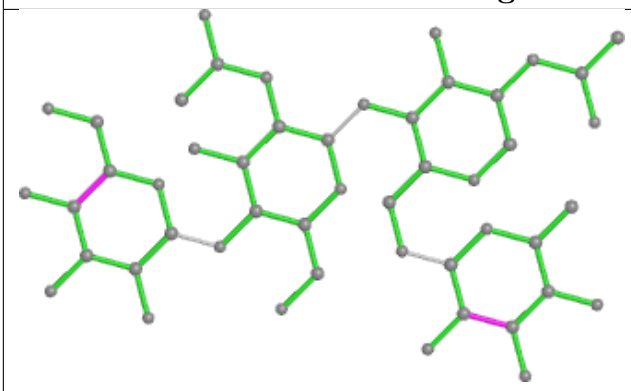


Torsions

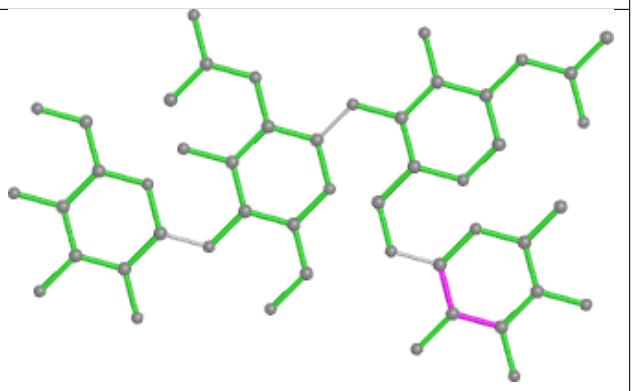


Rings

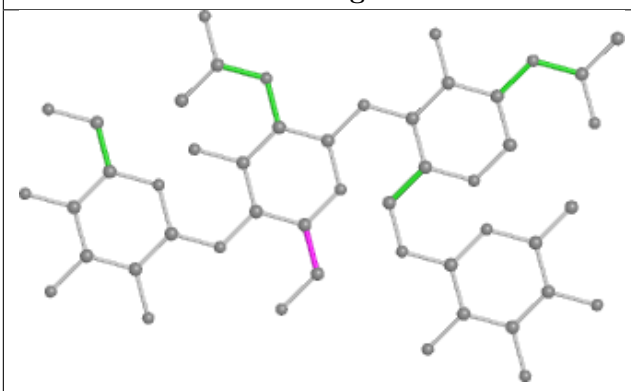
Oligosaccharide Chain n



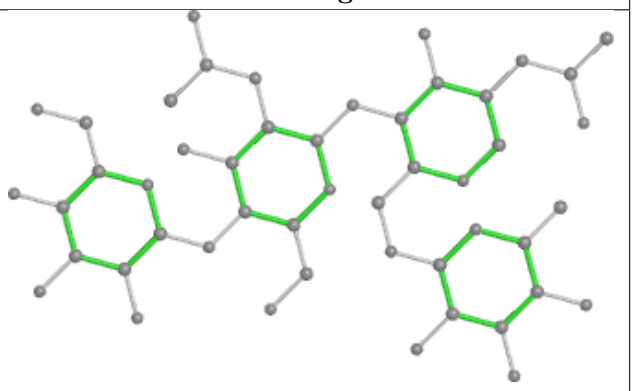
Bond lengths



Bond angles

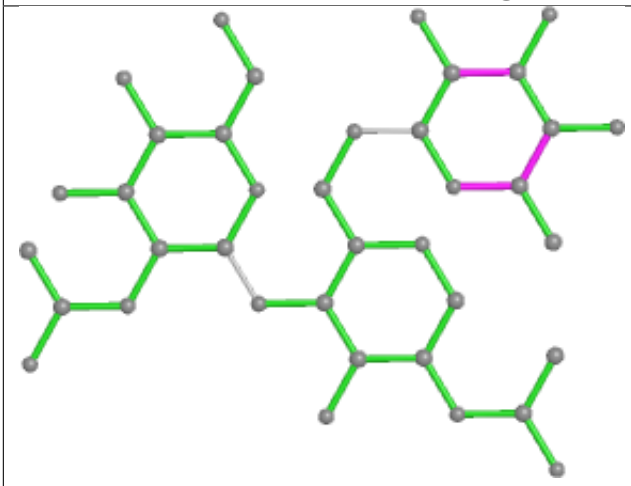


Torsions

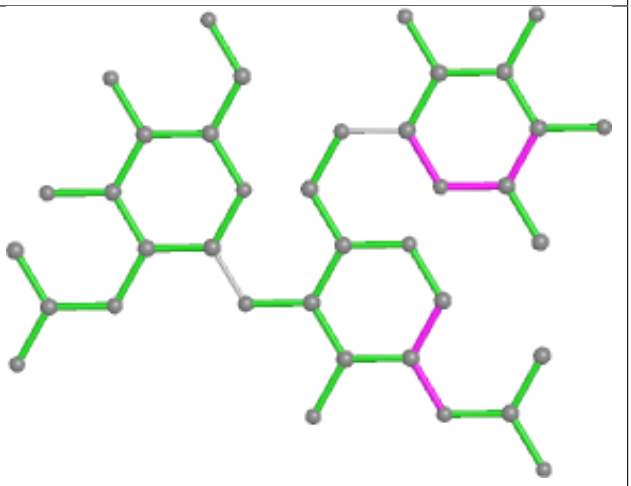


Rings

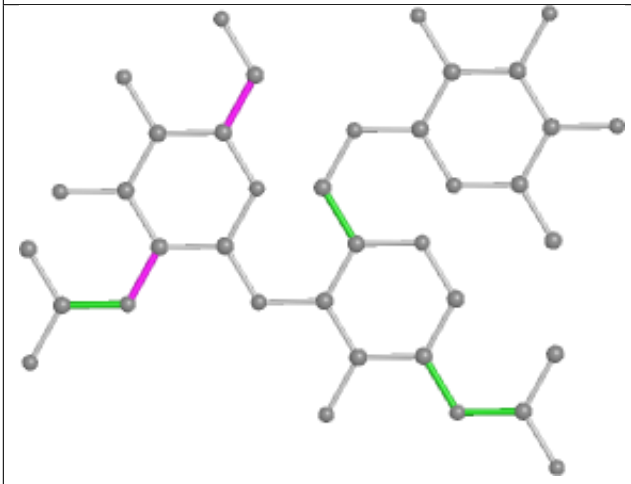
Oligosaccharide Chain b



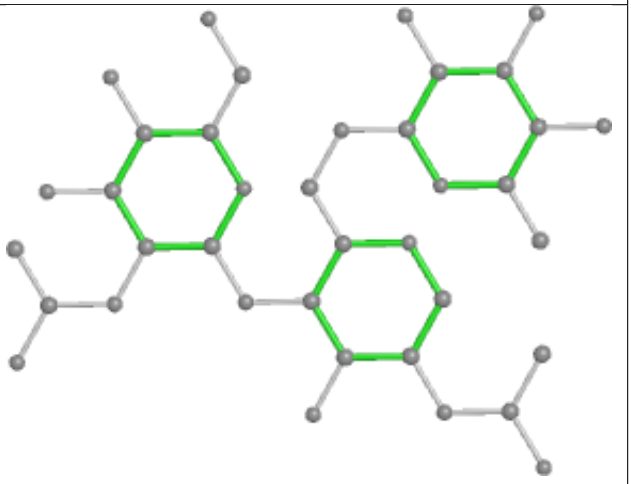
Bond lengths



Bond angles

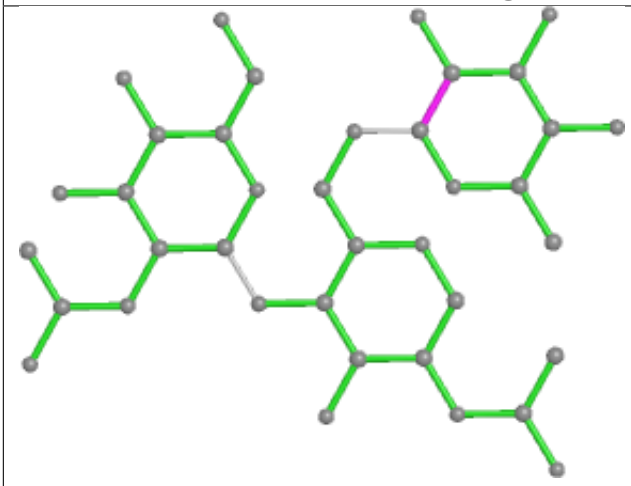


Torsions

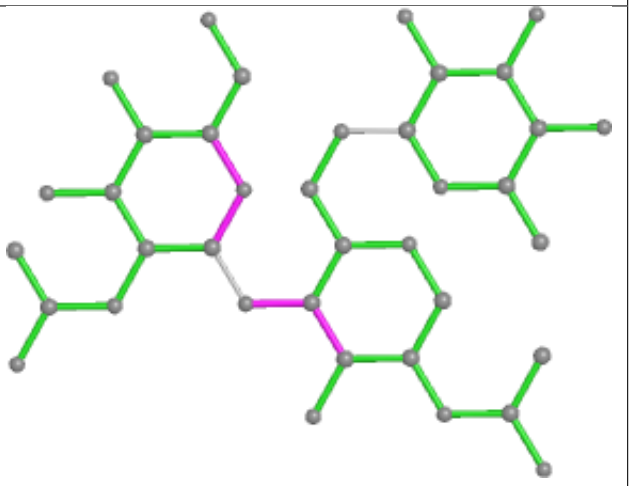


Rings

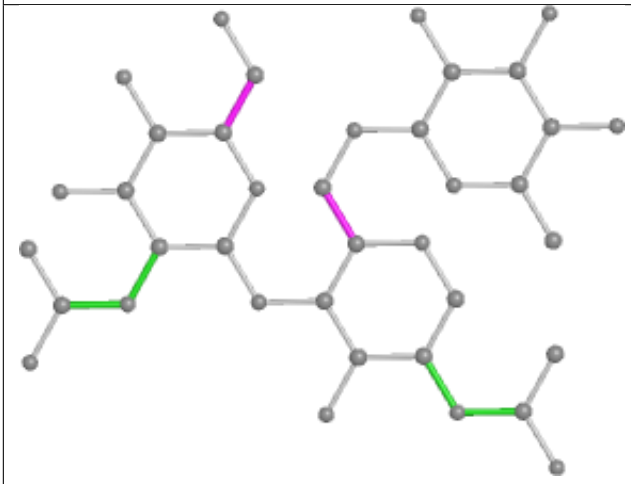
Oligosaccharide Chain e



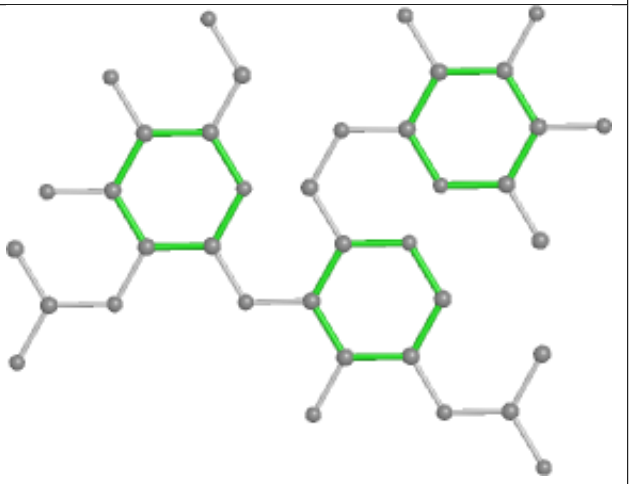
Bond lengths



Bond angles

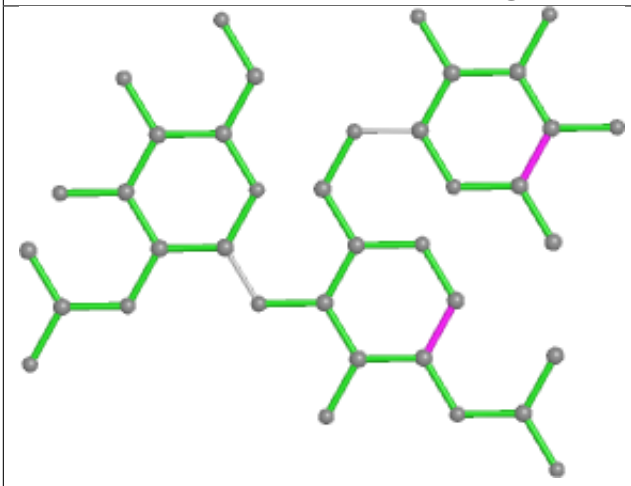


Torsions

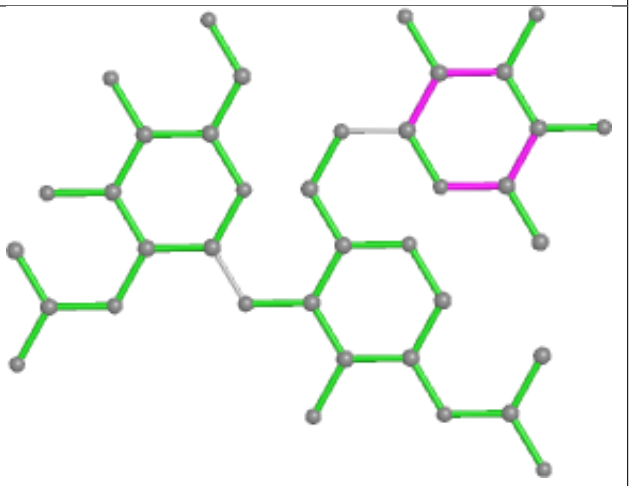


Rings

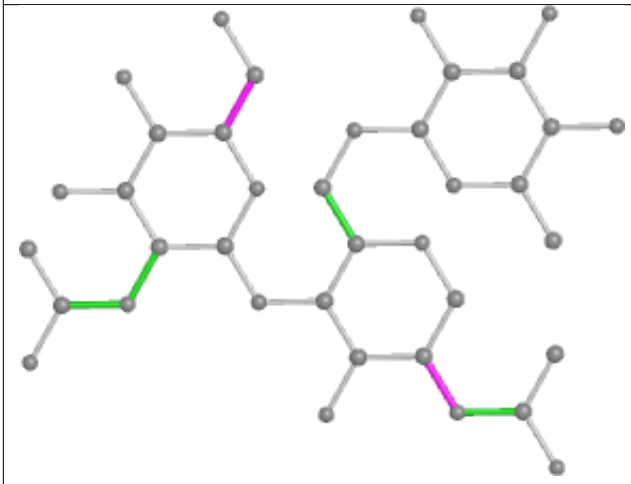
Oligosaccharide Chain i



Bond lengths



Bond angles



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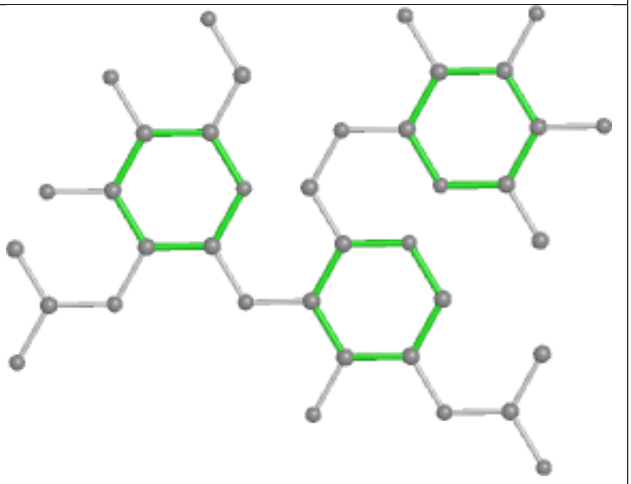
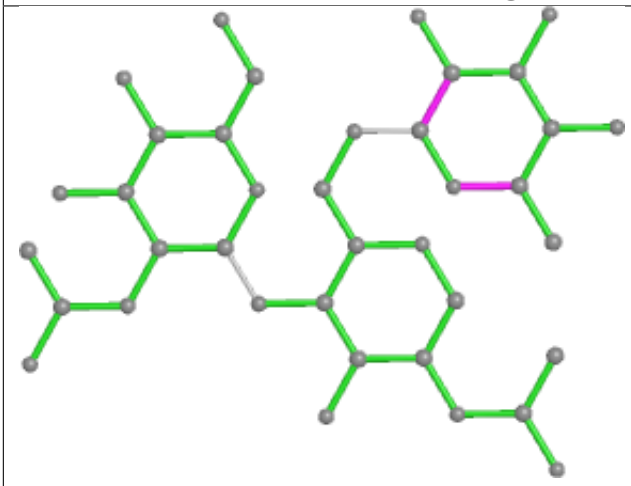
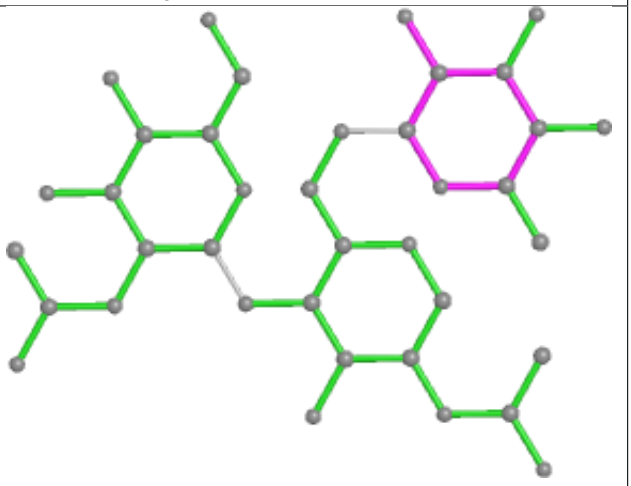


Rings

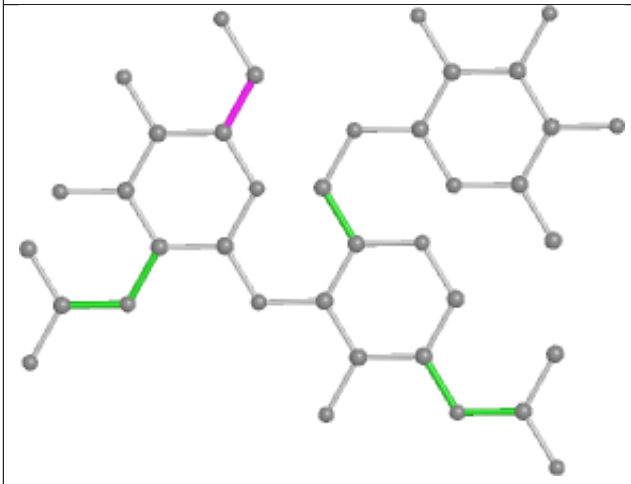
Oligosaccharide Chain j



Bond lengths



Bond angles



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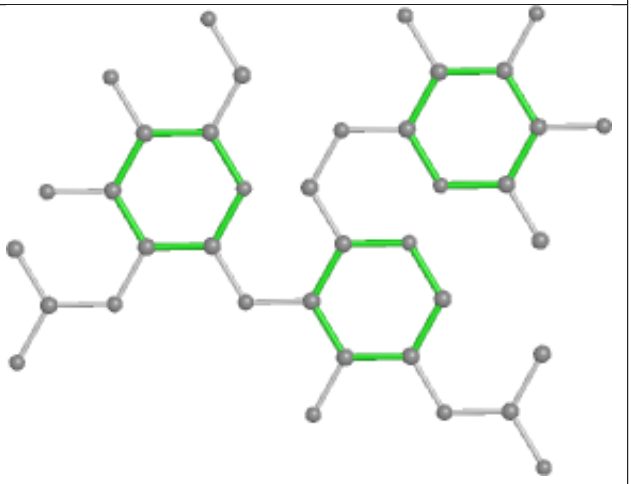
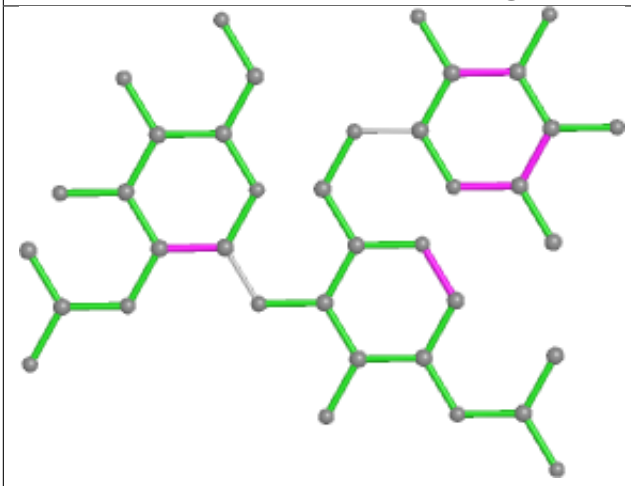
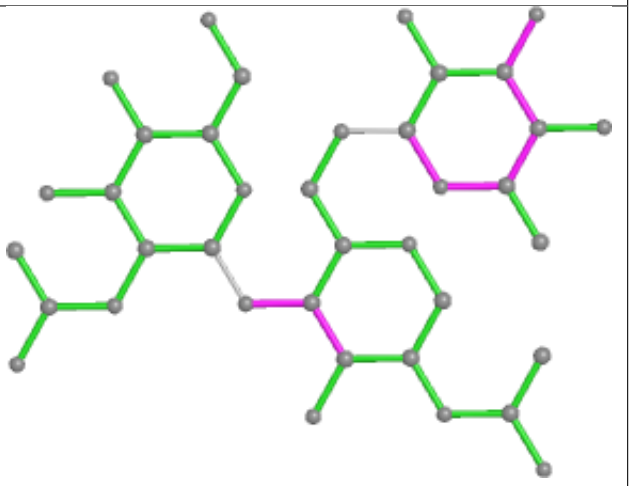


Rings

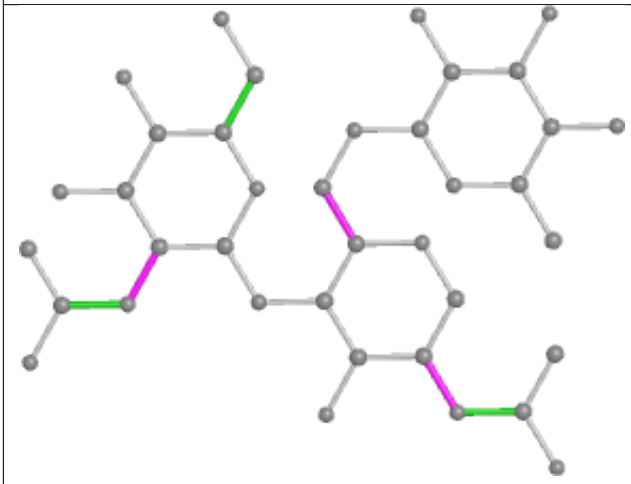
Oligosaccharide Chain l



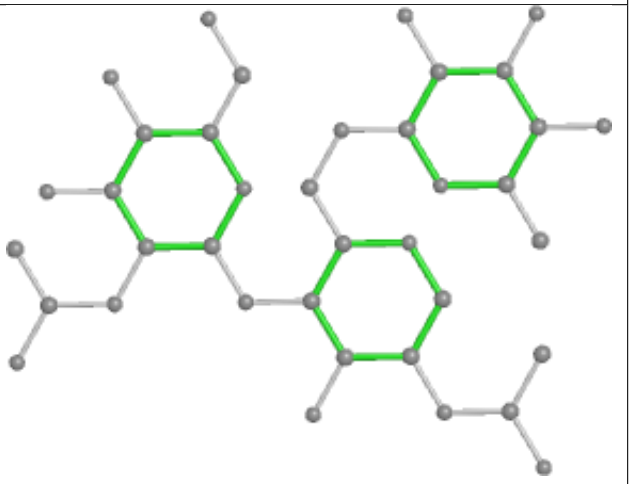
Bond lengths



Bond angles

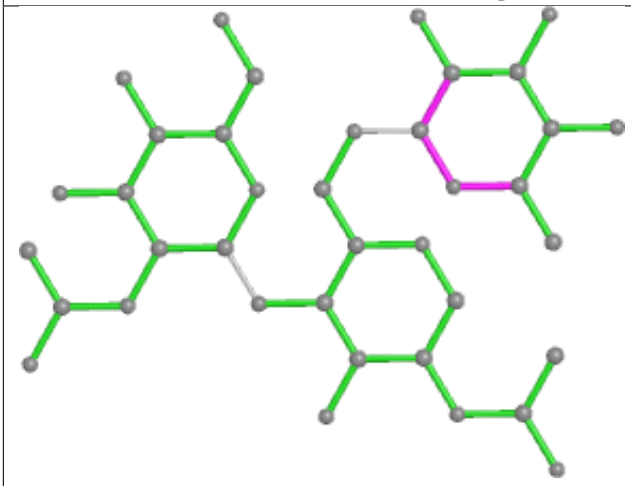


Torsions



Rings

Oligosaccharide Chain m



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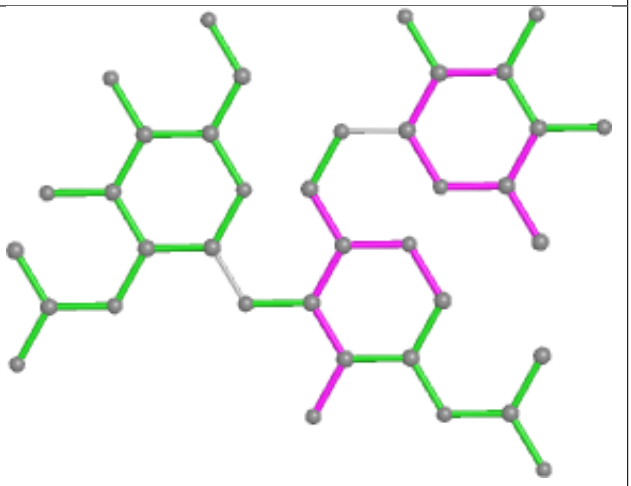

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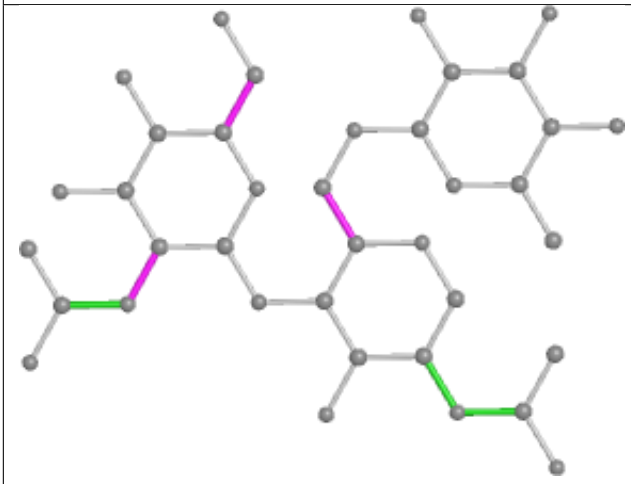
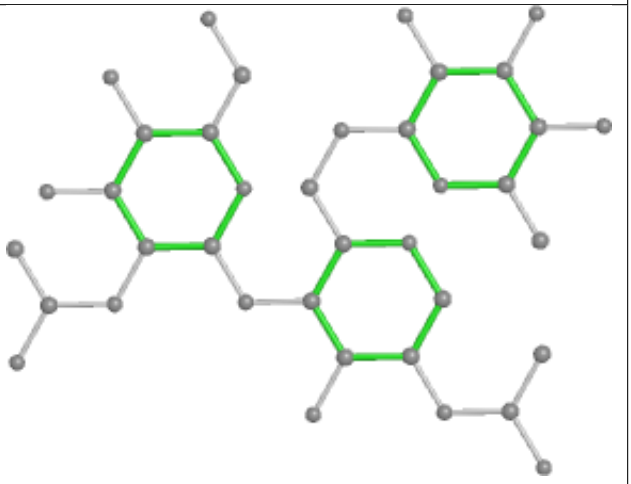
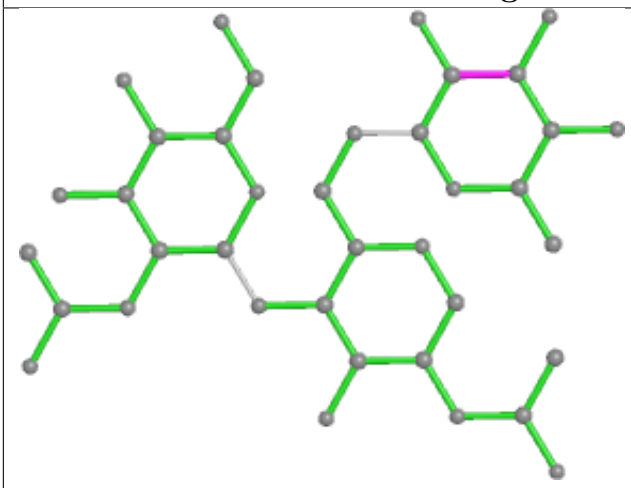


Torsions



Rings

Oligosaccharide Chain s



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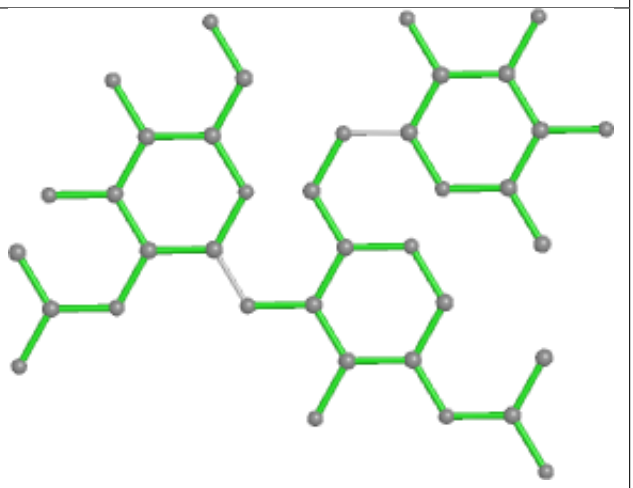

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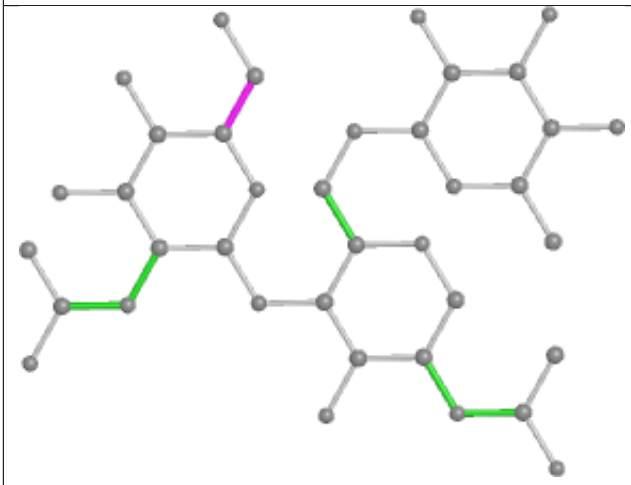

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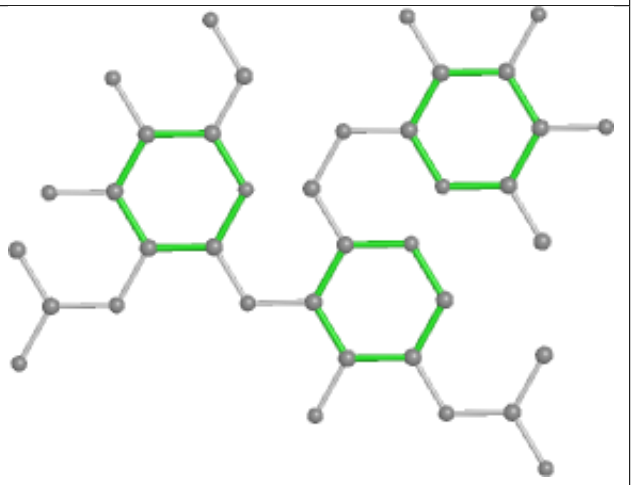
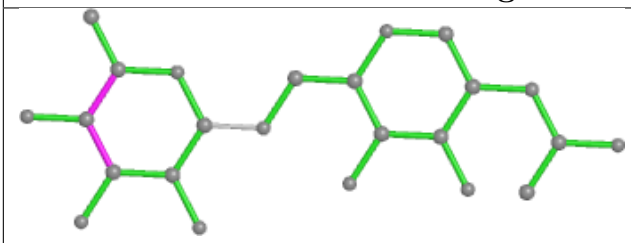


Rings

Oligosaccharide Chain d



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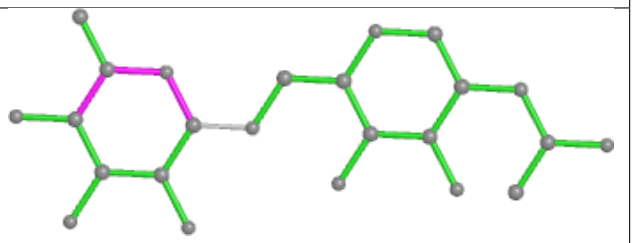
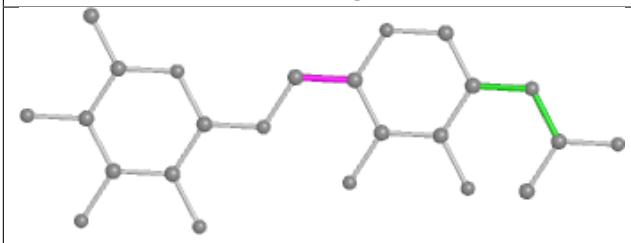
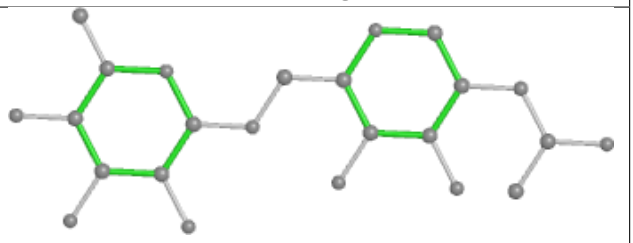


Bond angles

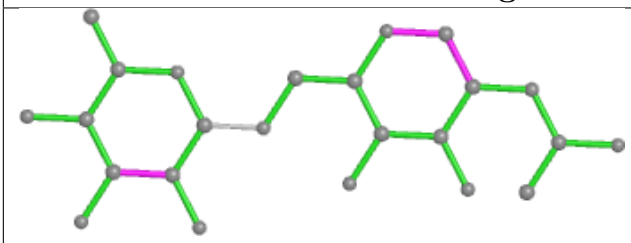


Torsions



Rings

Oligosaccharide Chain o



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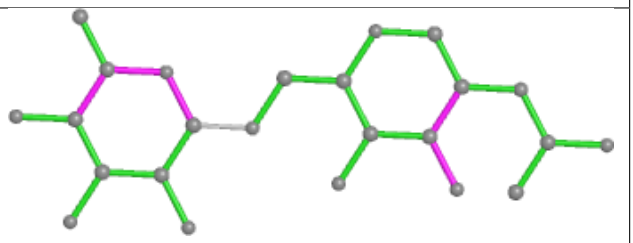
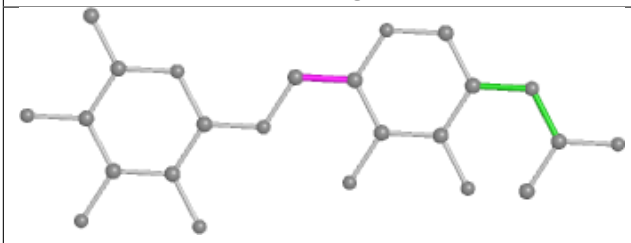


Bond angles



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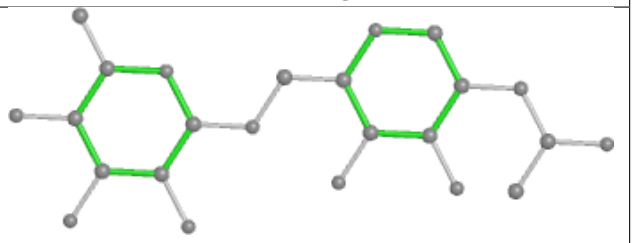
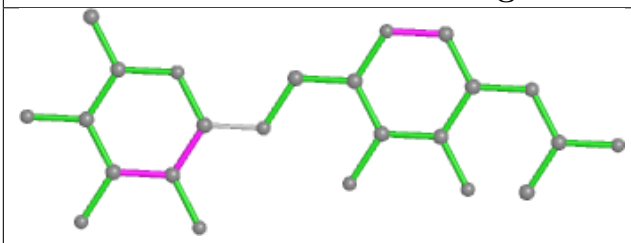


Rings

Oligosaccharide Chain p



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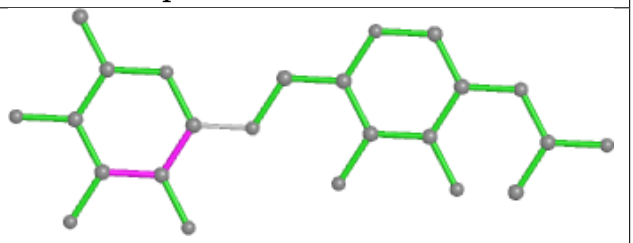
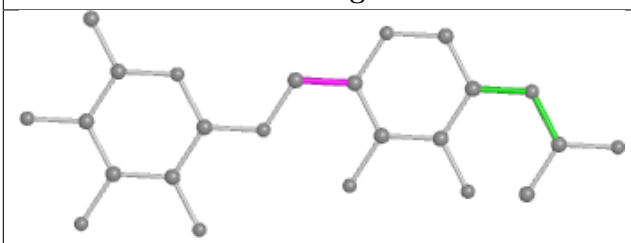


Bond angles



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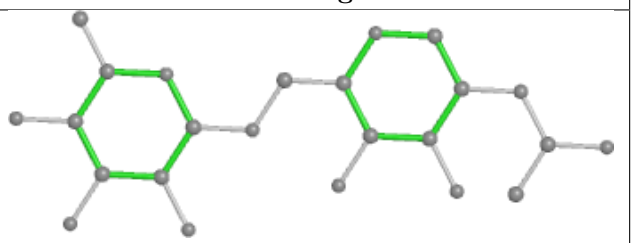
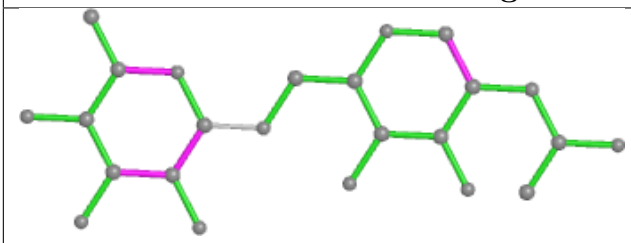


Rings

Oligosaccharide Chain r



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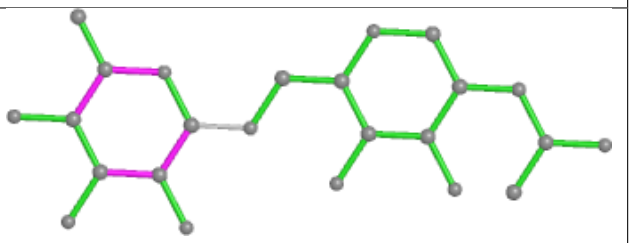
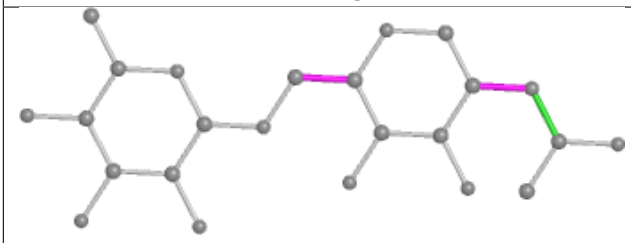


Bond angles



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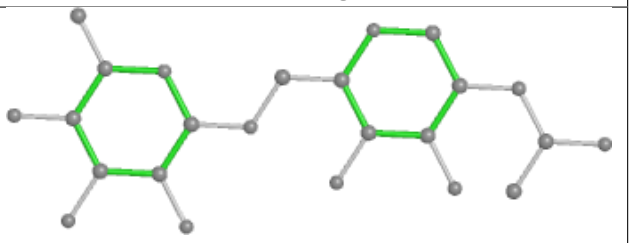
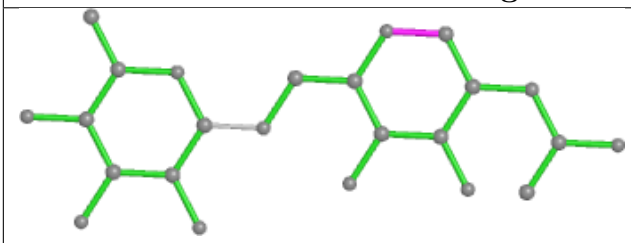


Rings

Oligosaccharide Chain t



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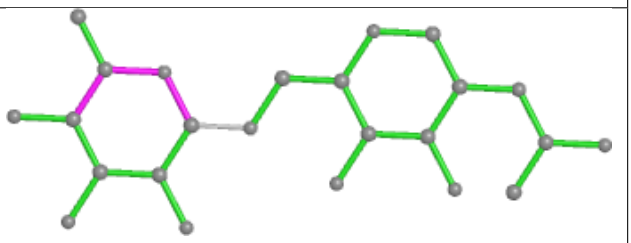
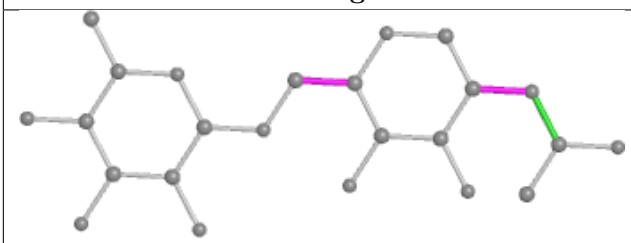
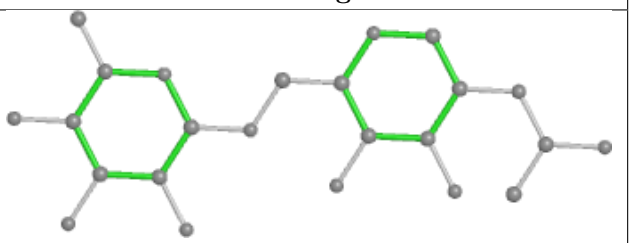


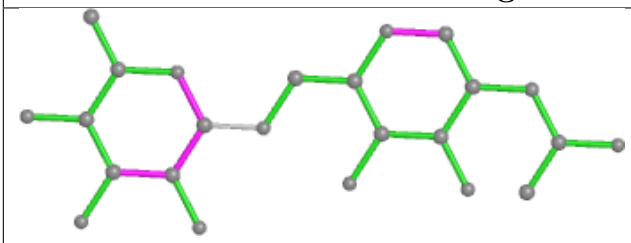
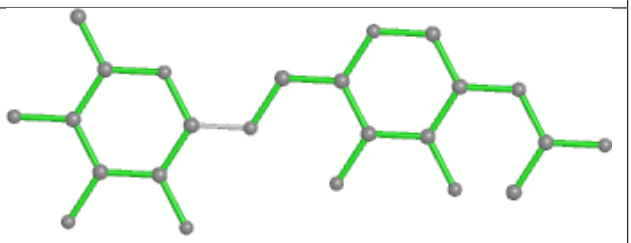
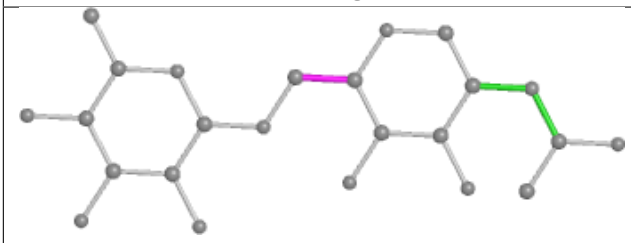
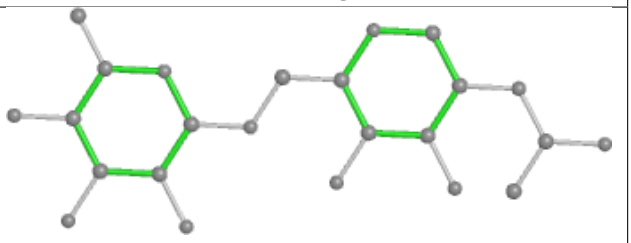
Bond angles

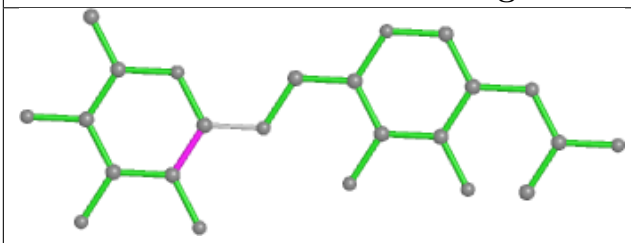
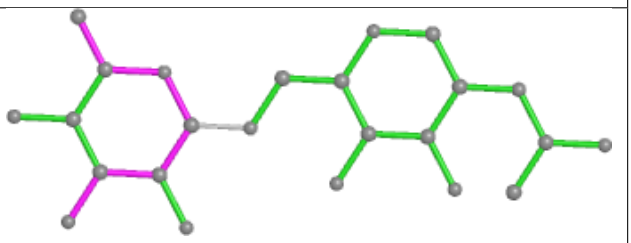
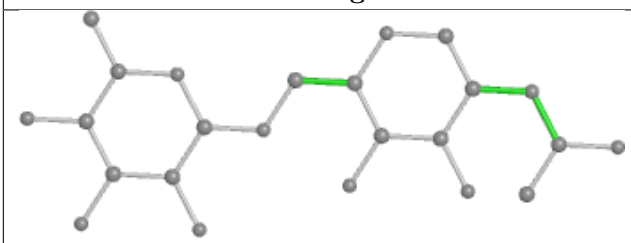
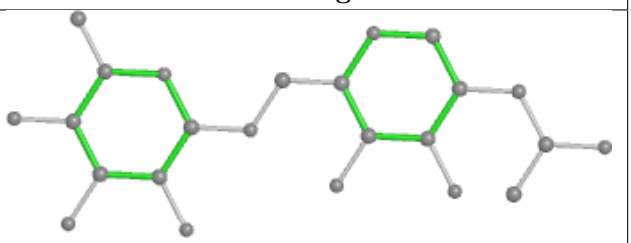


Torsions

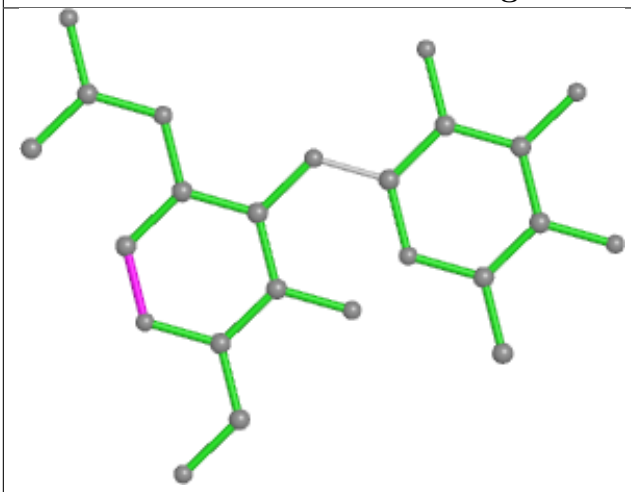


Rings

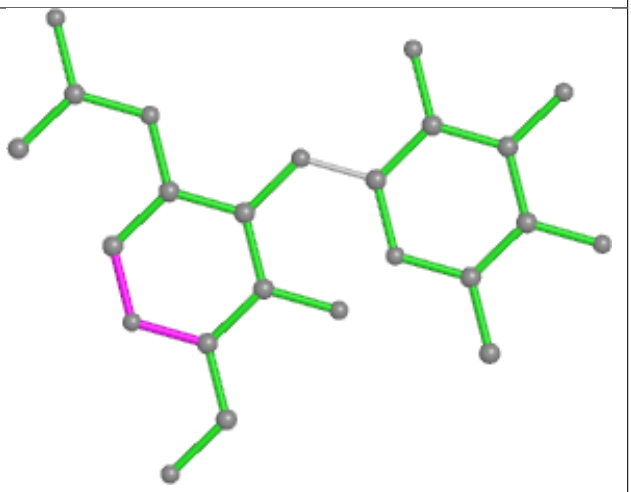
Oligosaccharide Chain u	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain v	
 Bond lengths	 Bond angles
 Torsions	 Rings

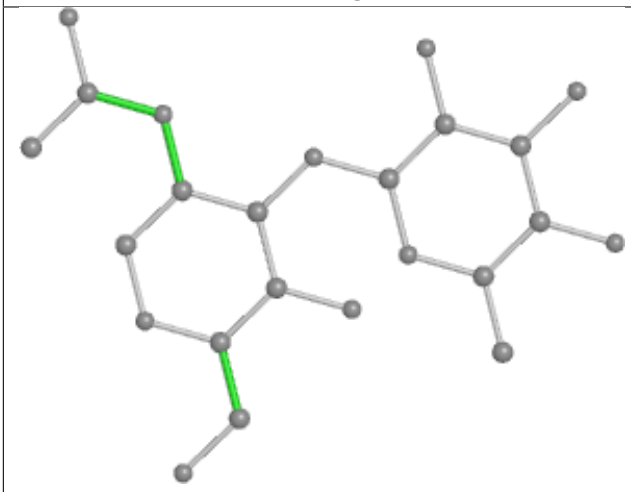
Oligosaccharide Chain f



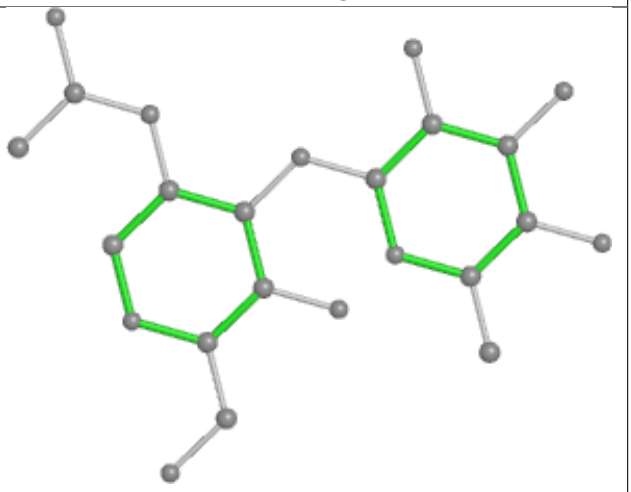
Bond lengths



Bond angles

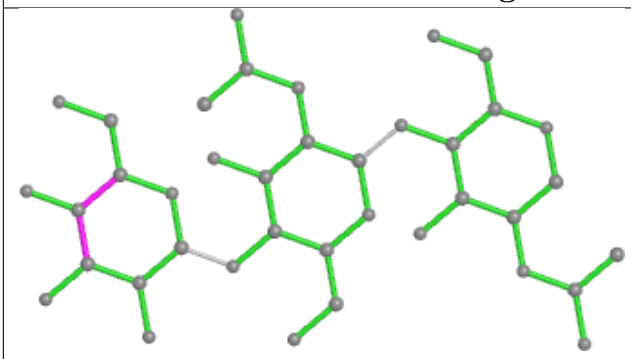


Torsions



Rings

Oligosaccharide Chain g



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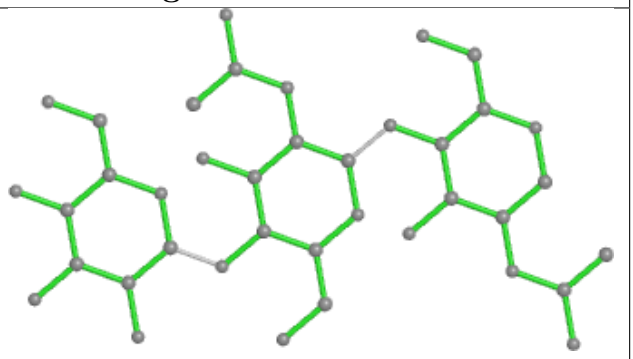
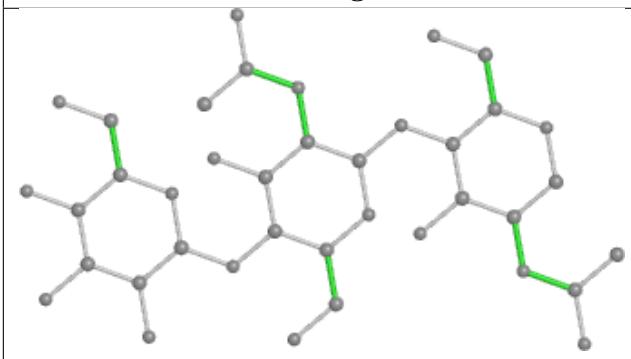


Bond angles



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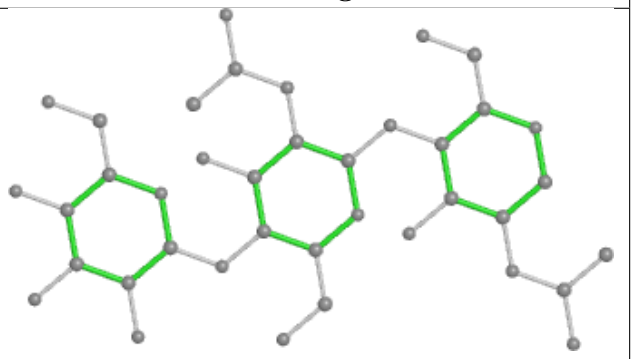
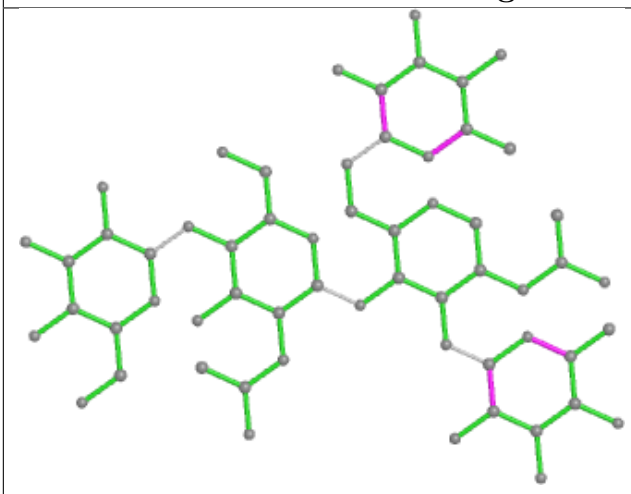
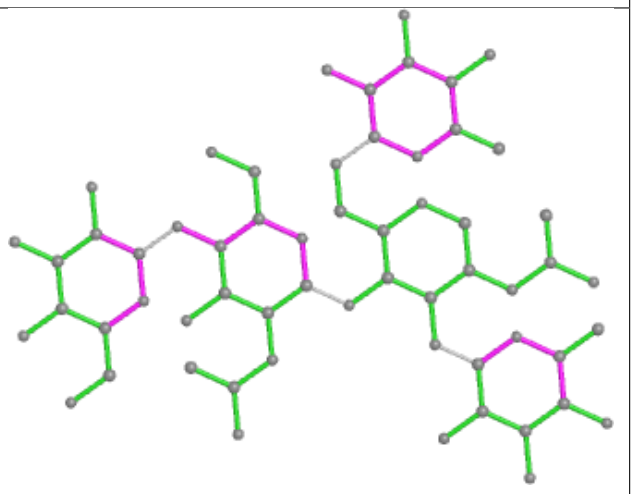


Rings

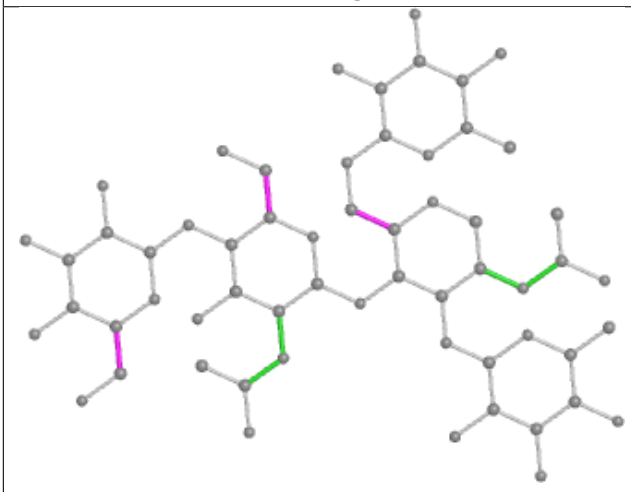
Oligosaccharide Chain h



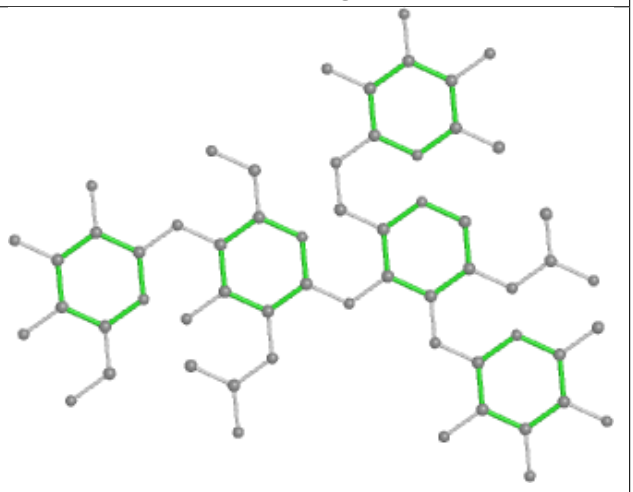
Bond lengths



Bond angles

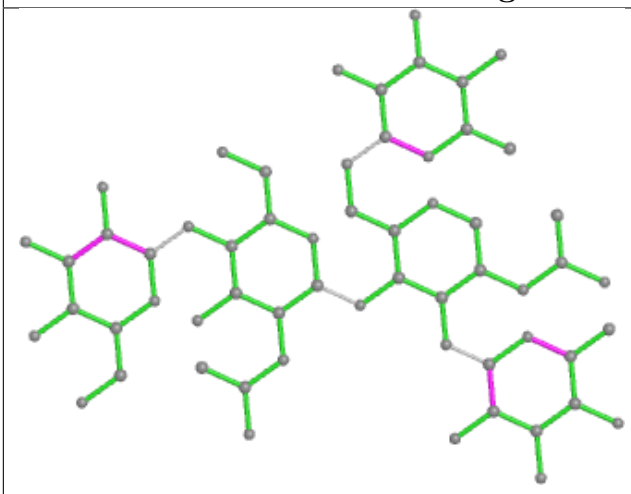


Torsions

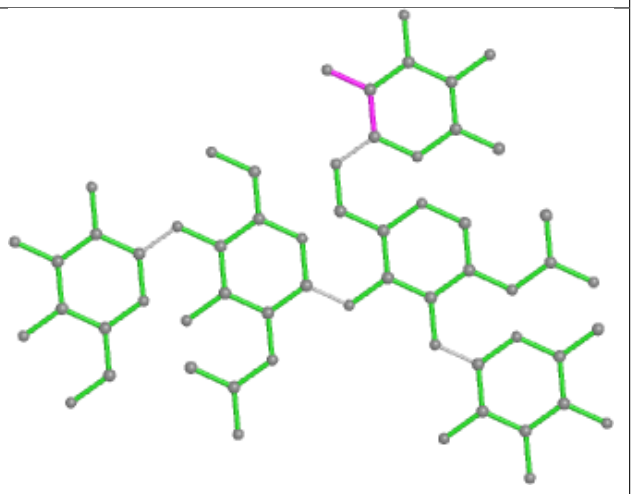


Rings

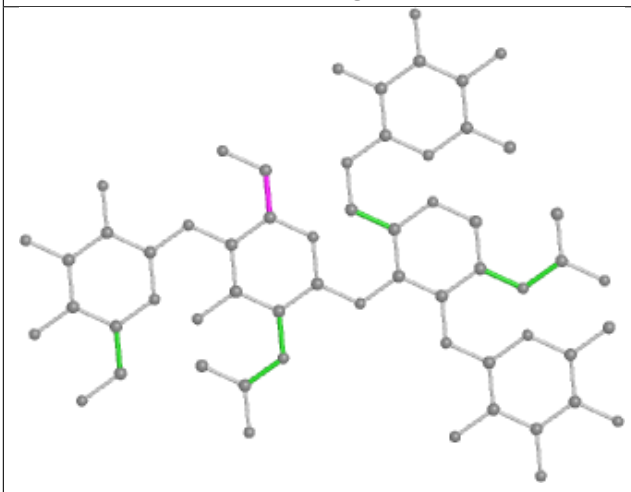
Oligosaccharide Chain k



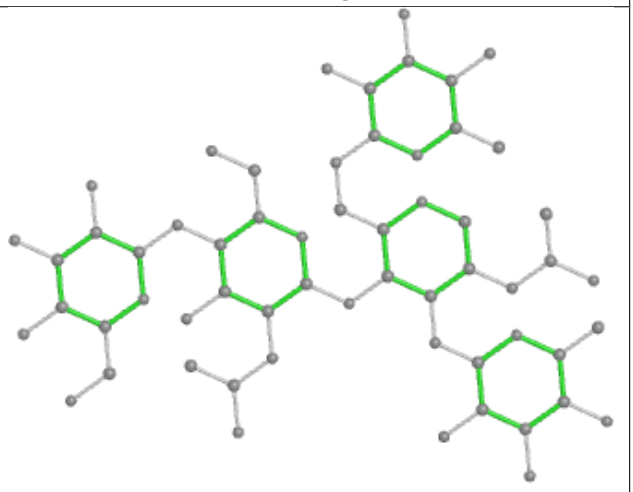
Bond lengths



Bond angles

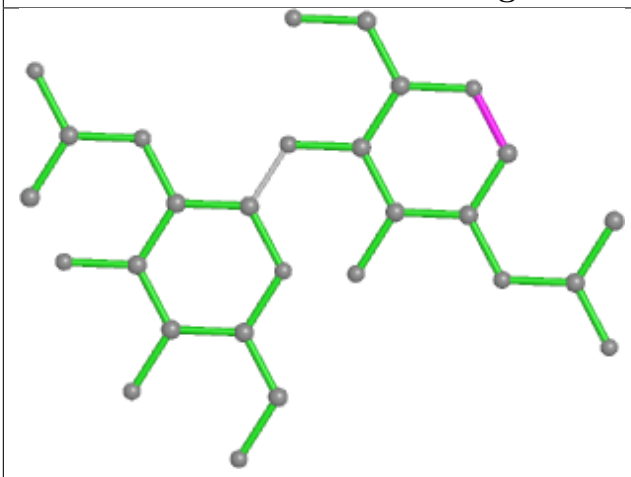


Torsions

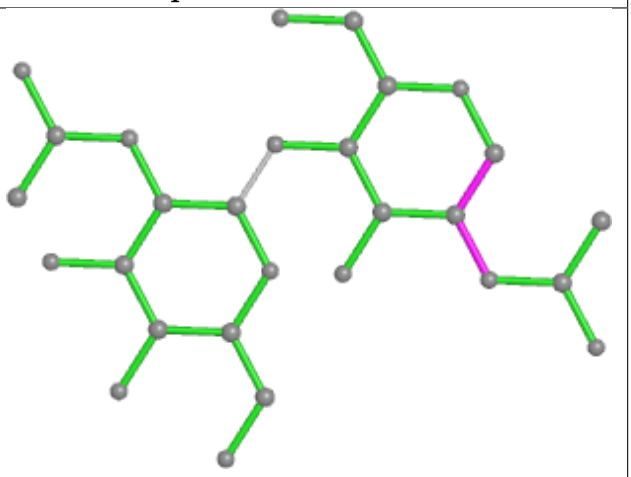


Rings

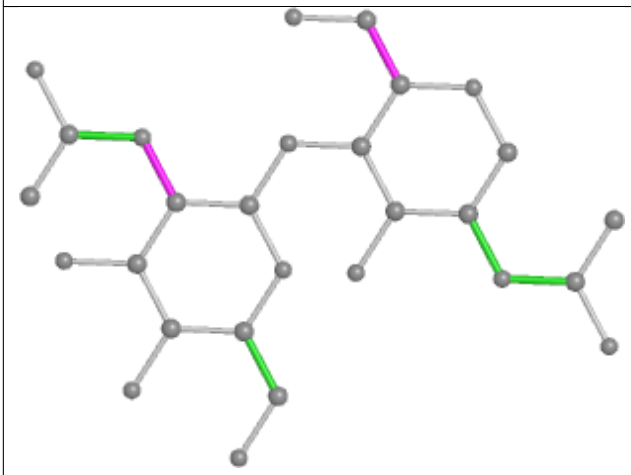
Oligosaccharide Chain q



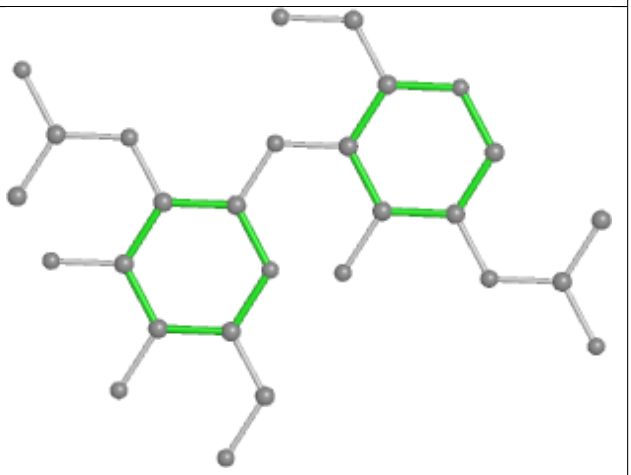
Bond lengths



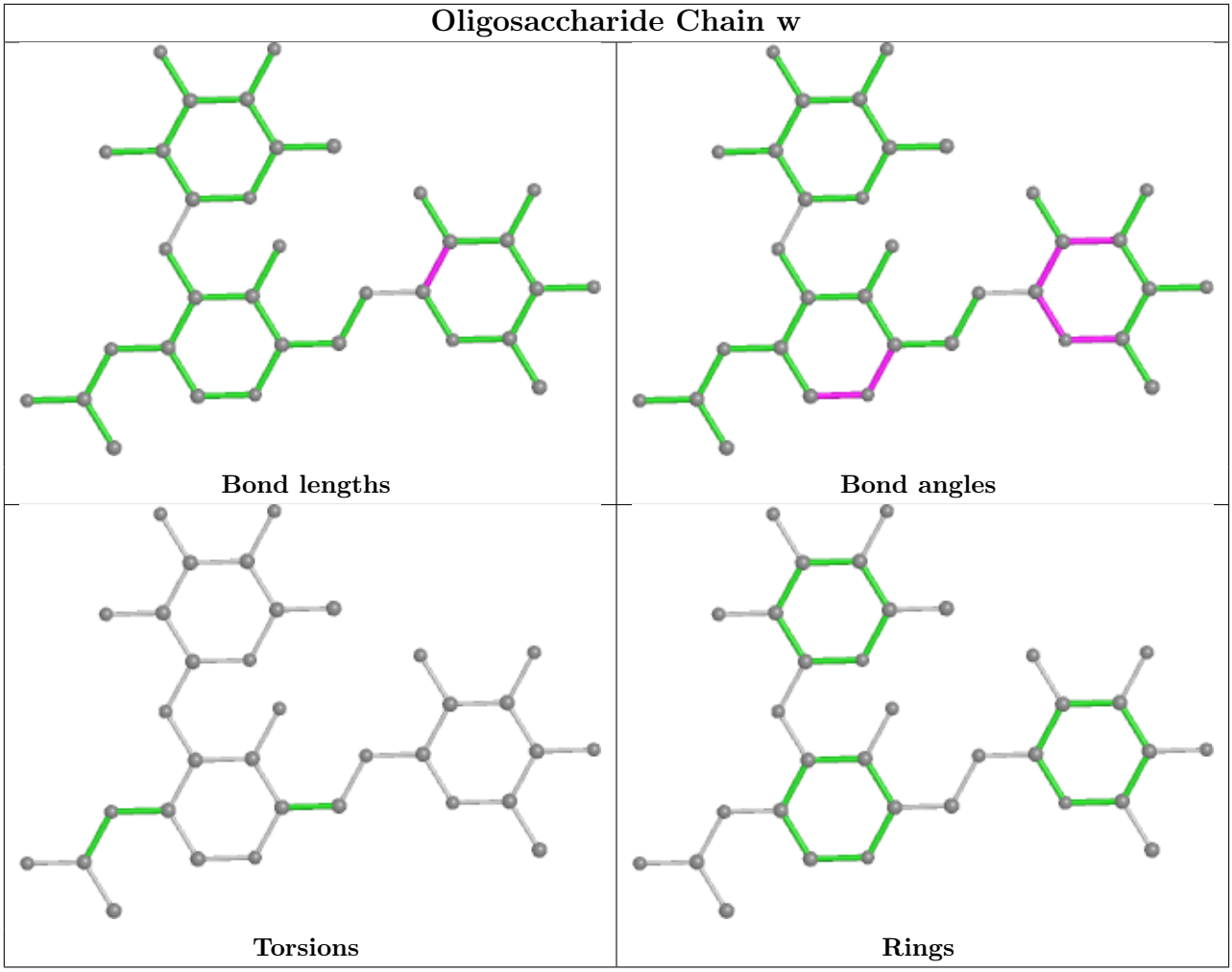
Bond angles



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	$\#\|Z\| > 2$
13	NAG	B	301	2	14,14,15	0.92	1 (7%)	17,19,21	0.57	0
12	GOL	Y	303	-	5,5,5	1.06	0	5,5,5	0.73	0
12	GOL	A	304	-	5,5,5	1.24	0	5,5,5	0.94	0
12	GOL	J	204	-	5,5,5	1.06	0	5,5,5	0.89	0
12	GOL	H	301	-	5,5,5	1.23	1 (20%)	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	GOL	K	301	-	5,5,5	0.97	0	5,5,5	0.99	0
12	GOL	M	305	-	5,5,5	1.63	1 (20%)	5,5,5	0.81	0
12	GOL	O	401	-	5,5,5	0.89	0	5,5,5	0.98	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
13	NAG	B	301	2	-	2/6/23/26	0/1/1/1
12	GOL	Y	303	-	-	2/4/4/4	-
12	GOL	A	304	-	-	4/4/4/4	-
12	GOL	J	204	-	-	2/4/4/4	-
12	GOL	H	301	-	-	2/4/4/4	-
12	GOL	K	301	-	-	2/4/4/4	-
12	GOL	M	305	-	-	4/4/4/4	-
12	GOL	O	401	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	305	GOL	C3-C2	2.81	1.63	1.51
13	B	301	NAG	O5-C1	2.76	1.48	1.43
12	H	301	GOL	C1-C2	2.44	1.61	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	304	GOL	C1-C2-C3-O3
12	H	301	GOL	C1-C2-C3-O3
12	Y	303	GOL	O1-C1-C2-O2
13	B	301	NAG	C4-C5-C6-O6
13	B	301	NAG	O5-C5-C6-O6
12	J	204	GOL	C1-C2-C3-O3
12	K	301	GOL	C1-C2-C3-O3
12	M	305	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	M	305	GOL	C1-C2-C3-O3
12	O	401	GOL	C1-C2-C3-O3
12	Y	303	GOL	O1-C1-C2-C3
12	A	304	GOL	O2-C2-C3-O3
12	H	301	GOL	O2-C2-C3-O3
12	M	305	GOL	O1-C1-C2-O2
12	J	204	GOL	O2-C2-C3-O3
12	M	305	GOL	O2-C2-C3-O3
12	O	401	GOL	O2-C2-C3-O3
12	A	304	GOL	O1-C1-C2-O2
12	K	301	GOL	O2-C2-C3-O3
12	A	304	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	Y	303	GOL	1	0
12	M	305	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.