Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 12:45 PM EDT

PDB ID	:	6CM3 / pdb_00006cm3
EMDB ID	:	EMD-7516
Title	:	BG505 SOSIP in complex with sCD4, 17b, 8ANC195
Authors	:	Wang, H.; Bjorkman, P.J.
Deposited on	:	2018-03-02
Resolution	:	3.54 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

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

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

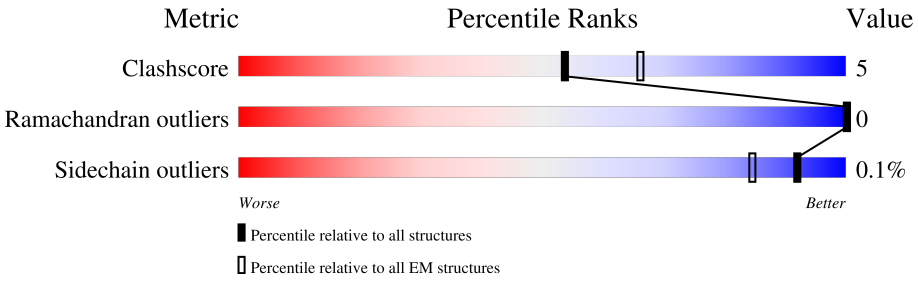
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 3.54 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	153	73% · 23%
1	B	153	75% · 23%
1	C	153	75% · · 23%
2	D	481	67% 10% 23%
2	E	481	67% 11% 23%
2	F	481	67% 10% 23%
3	G	192	43% 8% 49%
3	H	192	43% 8% 49%

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Mol	Chain	Length	Quality of chain
3	I	192	42% 8% 49%
4	J	214	13% 40% 10% 50%
4	L	214	12% 41% 9% 50%
4	N	214	13% 41% 9% 50%
5	K	229	7% 45% 10% 45%
5	M	229	6% 45% 10% 45%
5	O	229	7% 45% 10% 45%
6	P	244	44% 9% 46%
6	R	244	44% 9% 46%
6	T	244	45% 9% 46%
7	Q	215	44% 6% 50%
7	S	215	45% 5% 50%
7	U	215	45% 5% 50%
8	V	2	100%
8	W	2	100%
8	X	2	100%
8	b	2	100%
8	f	2	100%
8	j	2	100%
9	Y	10	80% 20%
9	c	10	80% 20%
9	g	10	90% 10%
10	Z	5	20% 80%
10	d	5	20% 60% 20%
10	h	5	20% 60% 20%

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Mol	Chain	Length	Quality of chain
11	a	5	40% 40% 20%
11	e	5	40% 20% 40%
11	i	5	40% 40% 20%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 25455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	118	Total	C	N	O	S	0	0
			897	575	154	163	5		
1	B	118	Total	C	N	O	S	0	0
			897	575	154	163	5		
1	C	118	Total	C	N	O	S	0	0
			897	575	154	163	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	conflict	UNP Q2N0S7
A	605	CYS	THR	conflict	UNP Q2N0S7
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
C	559	PRO	ILE	conflict	UNP Q2N0S7
C	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	372	Total	C	N	O	S	0	0
			2814	1779	488	523	24		
2	E	372	Total	C	N	O	S	0	0
			2814	1779	488	523	24		
2	F	372	Total	C	N	O	S	0	0
			2814	1779	488	523	24		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	332	ASN	THR	conflict	UNP Q2N0S5
D	501	CYS	ALA	conflict	UNP Q2N0S5
D	509	ARG	GLU	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	ARG	LYS	conflict	UNP Q2N0S5
D	512	ARG	-	expression tag	UNP Q2N0S5
D	513	ARG	-	expression tag	UNP Q2N0S5
E	332	ASN	THR	conflict	UNP Q2N0S5
E	501	CYS	ALA	conflict	UNP Q2N0S5
E	509	ARG	GLU	conflict	UNP Q2N0S5
E	510	ARG	LYS	conflict	UNP Q2N0S5
E	512	ARG	-	expression tag	UNP Q2N0S5
E	513	ARG	-	expression tag	UNP Q2N0S5
F	332	ASN	THR	conflict	UNP Q2N0S5
F	501	CYS	ALA	conflict	UNP Q2N0S5
F	509	ARG	GLU	conflict	UNP Q2N0S5
F	510	ARG	LYS	conflict	UNP Q2N0S5
F	512	ARG	-	expression tag	UNP Q2N0S5
F	513	ARG	-	expression tag	UNP Q2N0S5

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

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	183	ILE	-	expression tag	UNP P01730
G	184	ASP	-	expression tag	UNP P01730
G	185	GLY	-	expression tag	UNP P01730
G	186	ARG	-	expression tag	UNP P01730
G	187	HIS	-	expression tag	UNP P01730
G	188	HIS	-	expression tag	UNP P01730
G	189	HIS	-	expression tag	UNP P01730
G	190	HIS	-	expression tag	UNP P01730
G	191	HIS	-	expression tag	UNP P01730
G	192	HIS	-	expression tag	UNP P01730
H	183	ILE	-	expression tag	UNP P01730
H	184	ASP	-	expression tag	UNP P01730
H	185	GLY	-	expression tag	UNP P01730

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Chain	Residue	Modelled	Actual	Comment	Reference
H	186	ARG	-	expression tag	UNP P01730
H	187	HIS	-	expression tag	UNP P01730
H	188	HIS	-	expression tag	UNP P01730
H	189	HIS	-	expression tag	UNP P01730
H	190	HIS	-	expression tag	UNP P01730
H	191	HIS	-	expression tag	UNP P01730
H	192	HIS	-	expression tag	UNP P01730
I	183	ILE	-	expression tag	UNP P01730
I	184	ASP	-	expression tag	UNP P01730
I	185	GLY	-	expression tag	UNP P01730
I	186	ARG	-	expression tag	UNP P01730
I	187	HIS	-	expression tag	UNP P01730
I	188	HIS	-	expression tag	UNP P01730
I	189	HIS	-	expression tag	UNP P01730
I	190	HIS	-	expression tag	UNP P01730
I	191	HIS	-	expression tag	UNP P01730
I	192	HIS	-	expression tag	UNP P01730

- Molecule 4 is a protein called 17b Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	107	Total	C	N	O	S	0	0
			819	512	141	163	3		
4	L	107	Total	C	N	O	S	0	0
			819	512	141	163	3		
4	N	107	Total	C	N	O	S	0	0
			819	512	141	163	3		

- Molecule 5 is a protein called 17b Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	127	Total	C	N	O	S	0	0
			985	621	168	193	3		
5	M	127	Total	C	N	O	S	0	0
			985	621	168	193	3		
5	O	127	Total	C	N	O	S	0	0
			985	621	168	193	3		

- Molecule 6 is a protein called 8ANC195 Fab heavy chain.

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

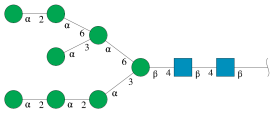
- Molecule 7 is a protein called 8ANC195 Fab light chain.

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

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

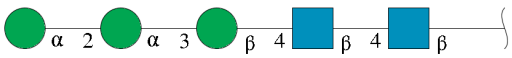
Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	2	Total	C	N	O	0	0
			28	16	2	10		
8	W	2	Total	C	N	O	0	0
			28	16	2	10		
8	X	2	Total	C	N	O	0	0
			28	16	2	10		
8	b	2	Total	C	N	O	0	0
			28	16	2	10		
8	f	2	Total	C	N	O	0	0
			28	16	2	10		
8	j	2	Total	C	N	O	0	0
			28	16	2	10		

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



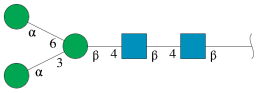
Mol	Chain	Residues	Atoms				AltConf	Trace
9	Y	10	Total	C	N	O	0	0
			116	64	2	50		
9	c	10	Total	C	N	O	0	0
			116	64	2	50		
9	g	10	Total	C	N	O	0	0
			116	64	2	50		

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



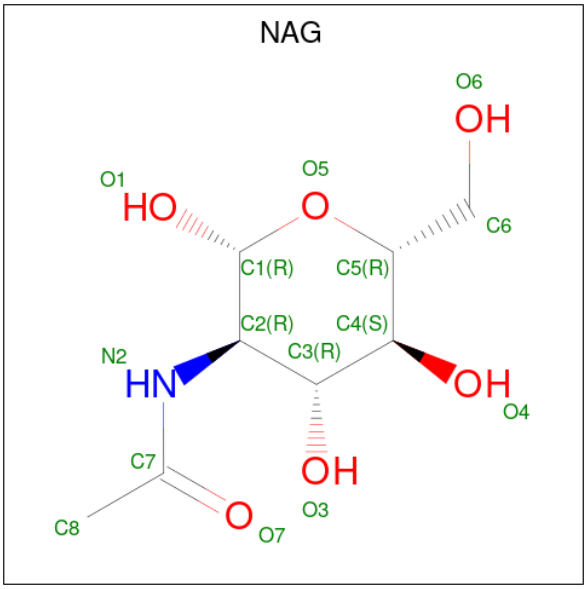
Mol	Chain	Residues	Atoms				AltConf	Trace
10	Z	5	Total	C	N	O	0	0
			61	34	2	25		
10	d	5	Total	C	N	O	0	0
			61	34	2	25		
10	h	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
11	a	5	Total	C	N	O	0	0
			61	34	2	25		
11	e	5	Total	C	N	O	0	0
			61	34	2	25		
11	i	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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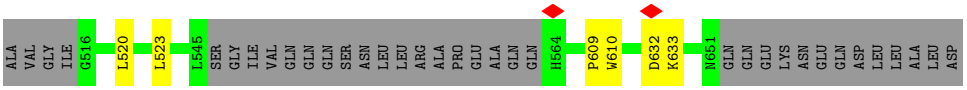
Mol	Chain	Residues	Atoms				AltConf
12	F	1	Total	C	N	O	0
			14	8	1	5	
12	F	1	Total	C	N	O	0
			14	8	1	5	
12	F	1	Total	C	N	O	0
			14	8	1	5	
12	F	1	Total	C	N	O	0
			14	8	1	5	
12	F	1	Total	C	N	O	0
			14	8	1	5	
12	F	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

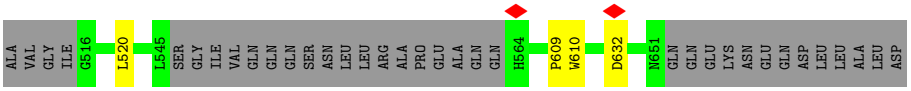
• Molecule 1: Envelope glycoprotein gp160

Chain A:



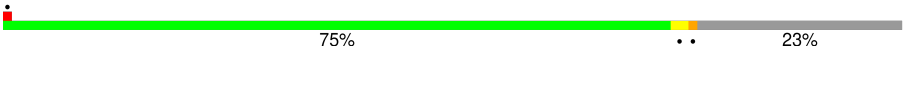
• Molecule 1: Envelope glycoprotein gp160

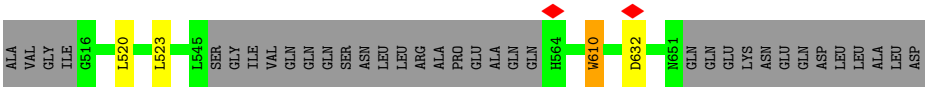
Chain B:



• Molecule 1: Envelope glycoprotein gp160

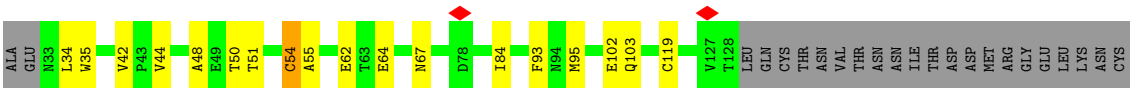
Chain C:

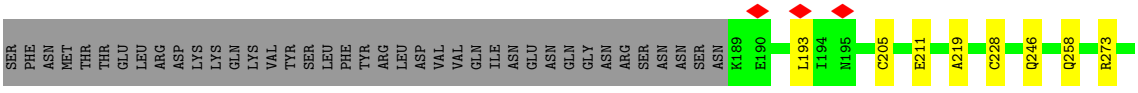


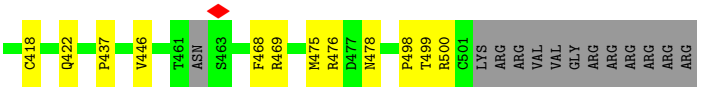


• Molecule 2: Envelope glycoprotein gp160

Chain D:

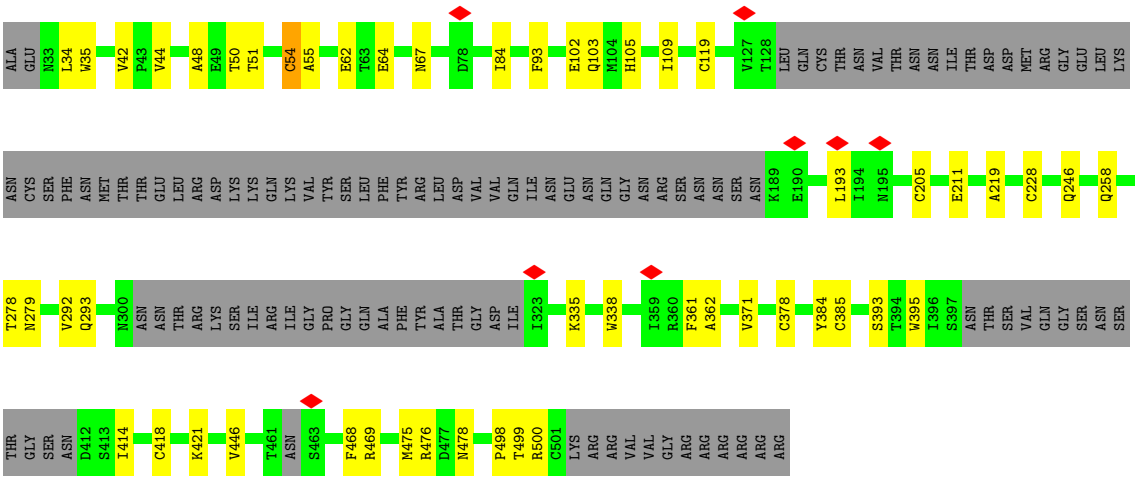






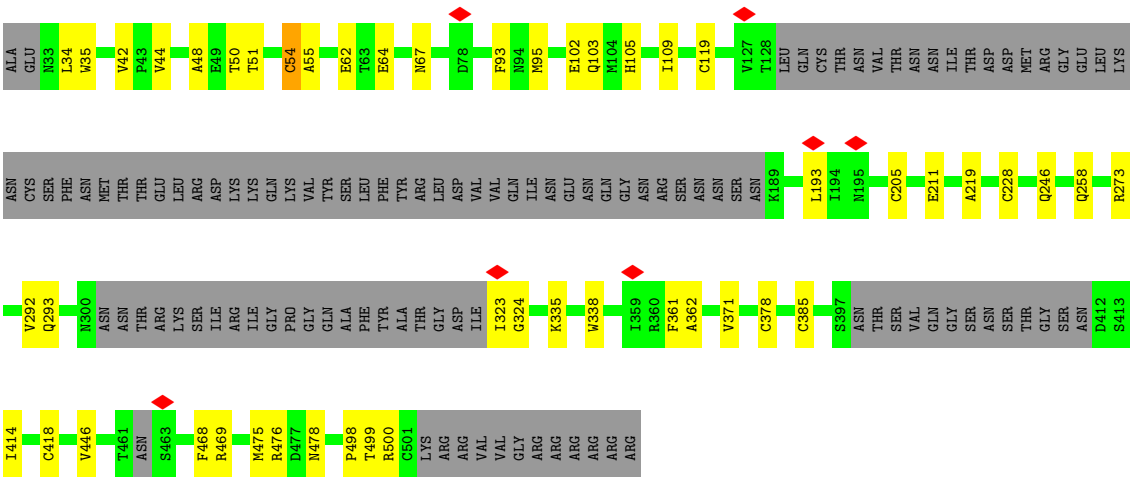
• Molecule 2: Envelope glycoprotein gp160

Chain E:



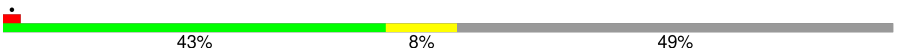
• Molecule 2: Envelope glycoprotein gp160

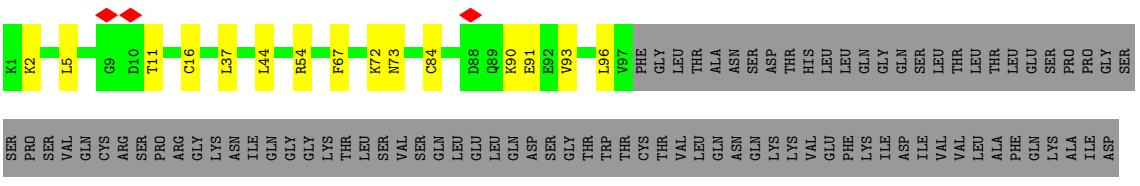
Chain F:



• Molecule 3: T-cell surface glycoprotein CD4

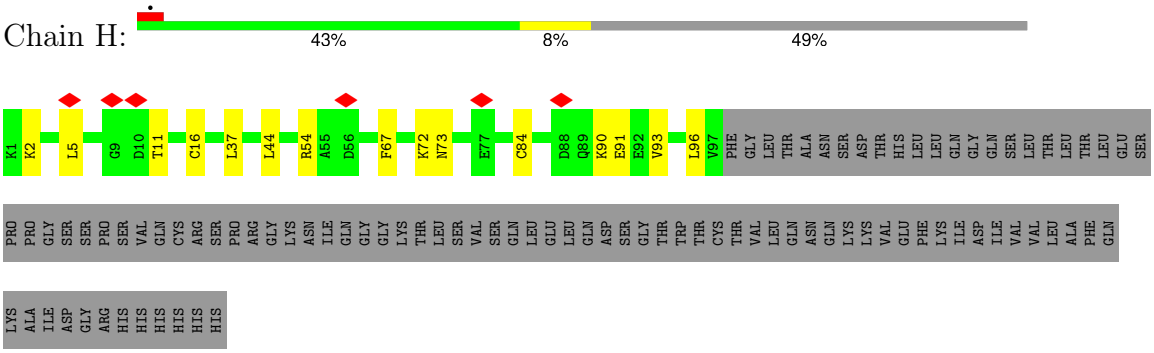
Chain G:





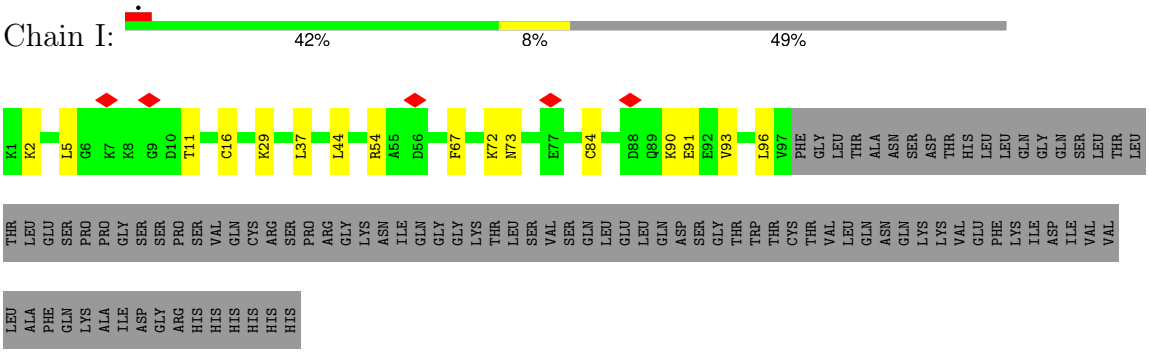
• Molecule 3: T-cell surface glycoprotein CD4

Chain H:



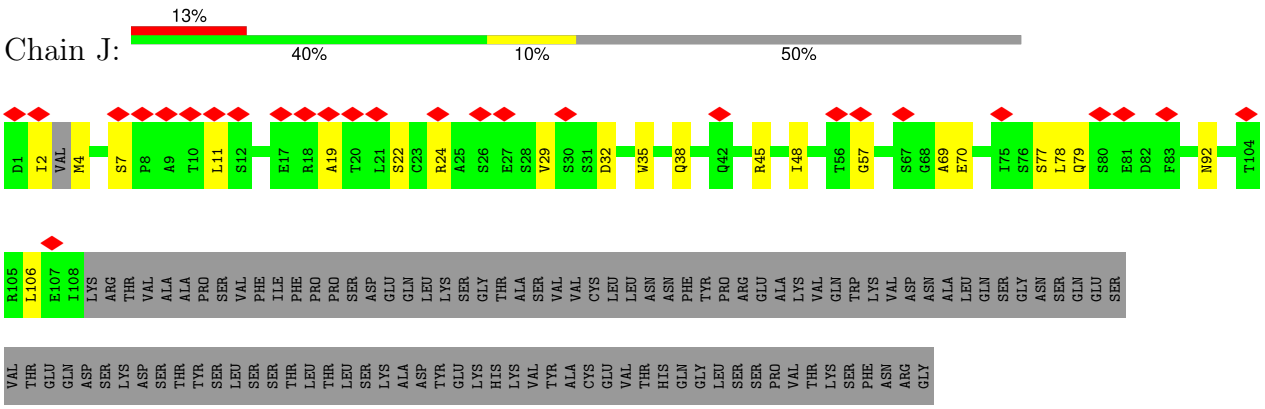
• Molecule 3: T-cell surface glycoprotein CD4

Chain I:



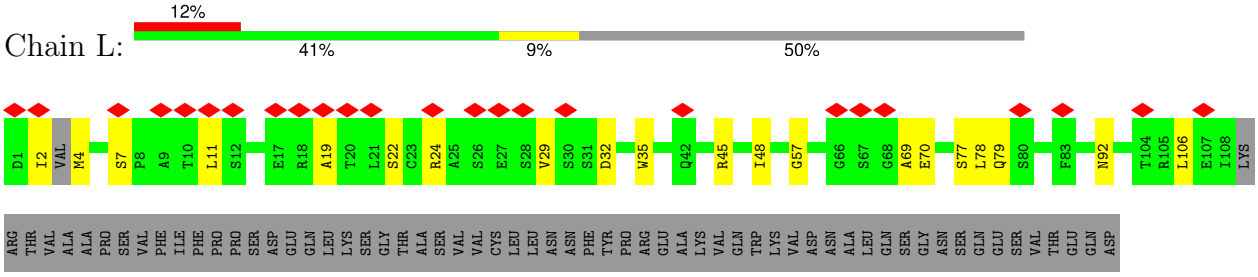
• Molecule 4: 17b Fab light chain

Chain J:



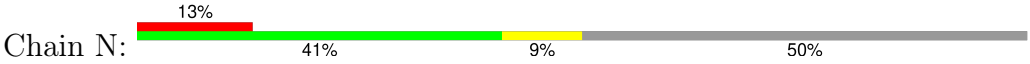
• Molecule 4: 17b Fab light chain

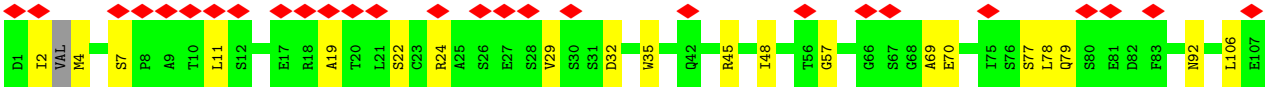
Chain L:



• Molecule 4: 17b Fab light chain

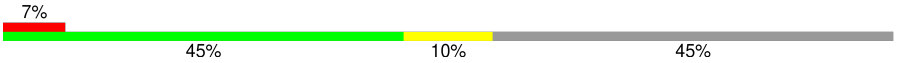
Chain N:

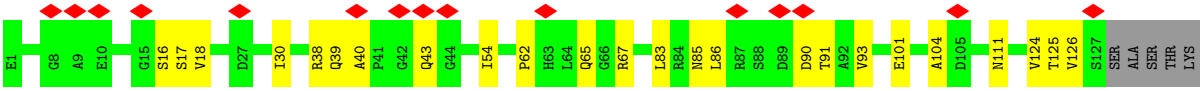




• Molecule 5: 17b Fab heavy chain

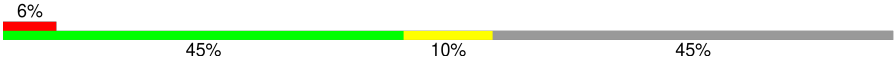
Chain K:

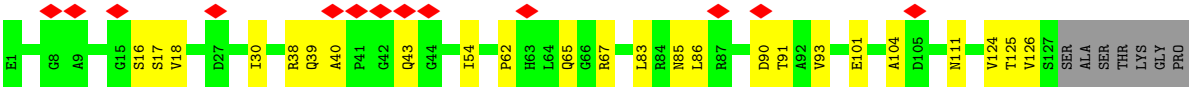




• Molecule 5: 17b Fab heavy chain

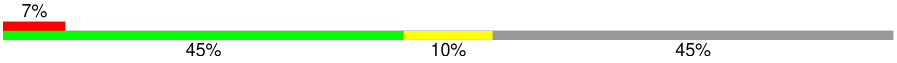
Chain M:

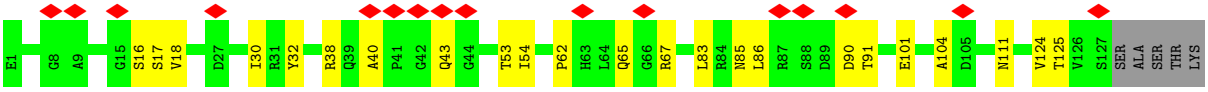




• Molecule 5: 17b Fab heavy chain

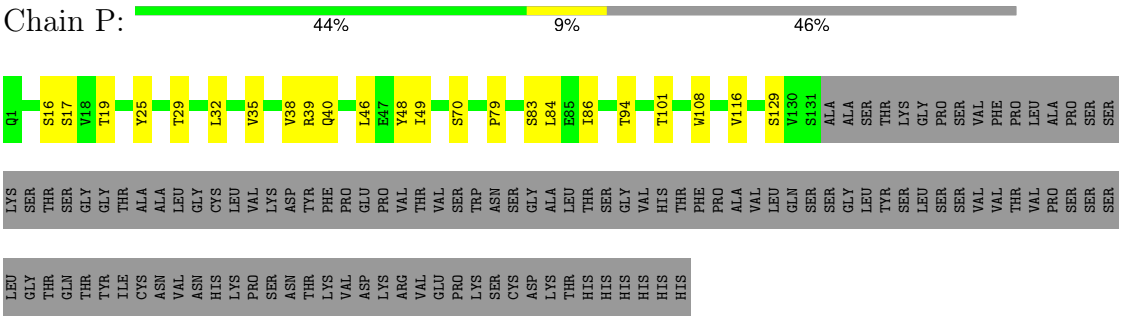
Chain O:





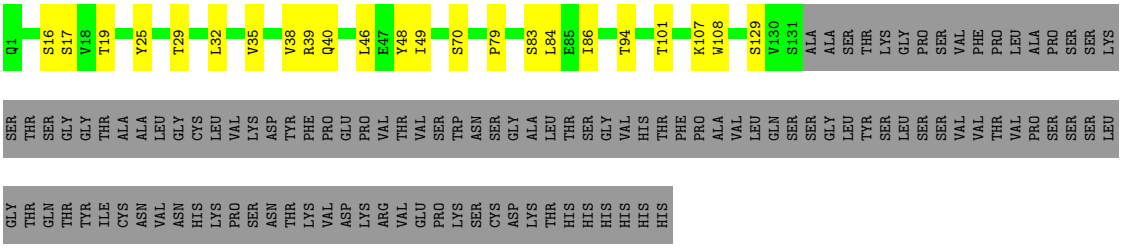
• Molecule 6: 8ANC195 Fab heavy chain

Chain P:



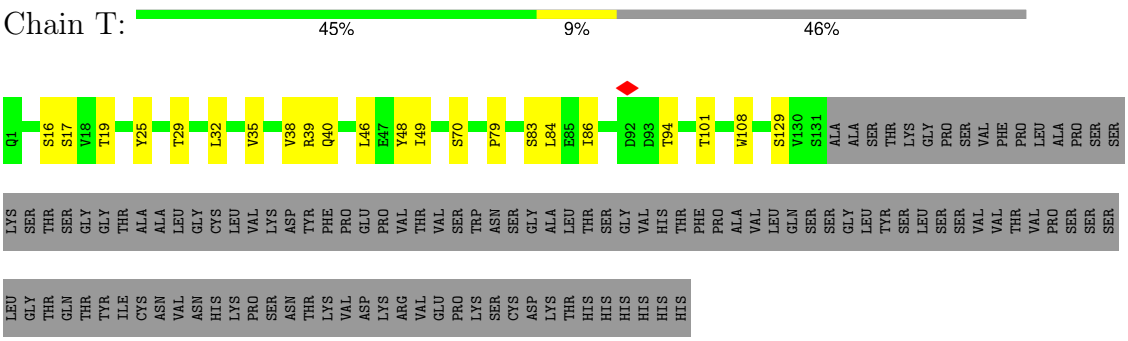
• Molecule 6: 8ANC195 Fab heavy chain

Chain R:



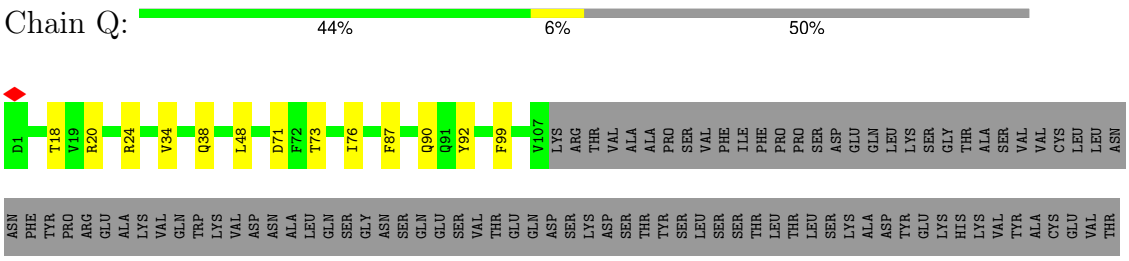
• Molecule 6: 8ANC195 Fab heavy chain

Chain T:



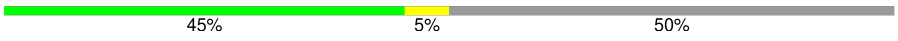
• Molecule 7: 8ANC195 Fab light chain

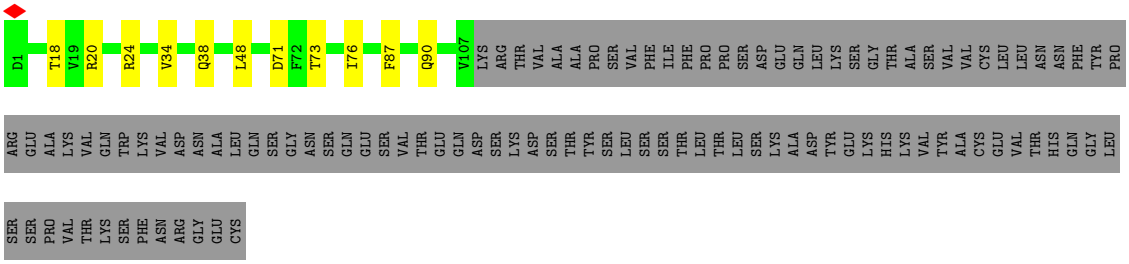
Chain Q:



• Molecule 7: 8ANC195 Fab light chain

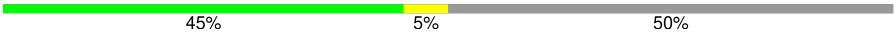
Chain S:

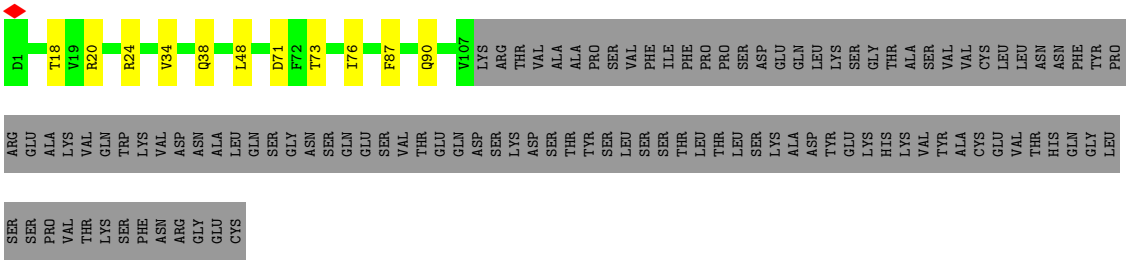




• Molecule 7: 8ANC195 Fab light chain

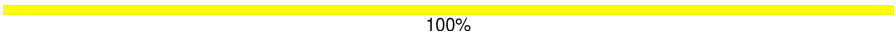
Chain U:





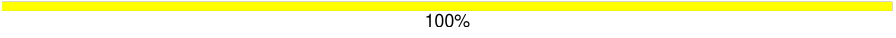
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



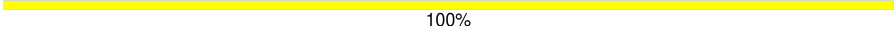
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



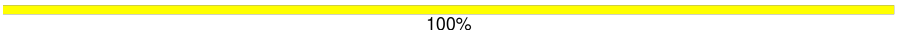
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



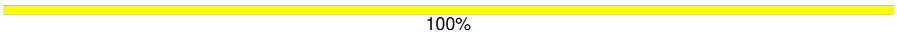
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



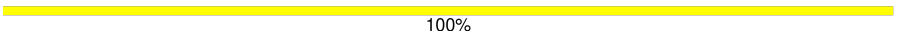
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain j:

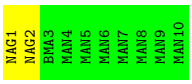


• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

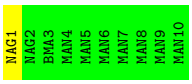
• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



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

Chain g:

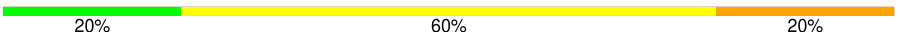


• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

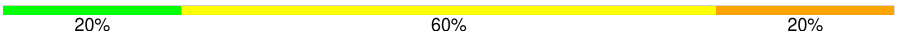
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain h:

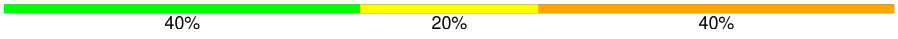


• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

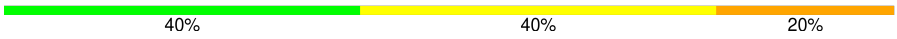
• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	143099	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	87.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0386	Depositor
Map size (Å)	392.99997, 392.99997, 392.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/915	0.52	0/1247
1	B	0.43	0/915	0.52	0/1247
1	C	0.43	0/915	0.52	0/1247
2	D	0.46	0/2878	0.65	2/3929 (0.1%)
2	E	0.46	0/2878	0.66	2/3929 (0.1%)
2	F	0.46	0/2878	0.66	2/3929 (0.1%)
3	G	0.34	0/785	0.50	0/1053
3	H	0.34	0/785	0.50	0/1053
3	I	0.34	0/785	0.50	0/1053
4	J	0.22	0/838	0.55	0/1139
4	L	0.22	0/838	0.55	0/1139
4	N	0.22	0/838	0.55	0/1139
5	K	0.23	0/1006	0.45	0/1365
5	M	0.23	0/1006	0.45	0/1365
5	O	0.23	0/1006	0.45	0/1365
6	P	0.41	0/1034	0.56	0/1408
6	R	0.41	0/1034	0.56	0/1408
6	T	0.41	0/1034	0.57	0/1408
7	Q	0.34	0/828	0.49	0/1125
7	S	0.34	0/828	0.49	0/1125
7	U	0.34	0/828	0.49	0/1125
All	All	0.38	0/24852	0.57	6/33798 (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
1	A	0	1
1	B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	54	CYS	CA-C-N	7.30	134.83	121.70
2	F	54	CYS	C-N-CA	7.30	134.83	121.70
2	D	54	CYS	CA-C-N	7.29	134.82	121.70
2	D	54	CYS	C-N-CA	7.29	134.82	121.70
2	E	54	CYS	CA-C-N	7.29	134.81	121.70
2	E	54	CYS	C-N-CA	7.29	134.81	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	610	TRP	Peptide
1	B	610	TRP	Peptide
1	C	610	TRP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	897	0	859	6	0
1	B	897	0	859	4	0
1	C	897	0	859	4	0
2	D	2814	0	2679	28	0
2	E	2814	0	2679	30	0
2	F	2814	0	2679	27	0
3	G	775	0	795	8	0
3	H	775	0	795	8	0
3	I	775	0	795	9	0
4	J	819	0	782	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	819	0	782	11	0
4	N	819	0	782	11	0
5	K	985	0	952	15	0
5	M	985	0	952	14	0
5	O	985	0	952	13	0
6	P	1007	0	979	16	0
6	R	1007	0	979	15	0
6	T	1007	0	979	14	0
7	Q	810	0	783	8	0
7	S	810	0	783	6	0
7	U	810	0	783	6	0
8	V	28	0	25	0	0
8	W	28	0	25	0	0
8	X	28	0	25	0	0
8	b	28	0	25	0	0
8	f	28	0	25	0	0
8	j	28	0	25	0	0
9	Y	116	0	97	0	0
9	c	116	0	97	0	0
9	g	116	0	97	0	0
10	Z	61	0	51	0	0
10	d	61	0	51	1	0
10	h	61	0	51	1	0
11	a	61	0	52	1	0
11	e	61	0	52	2	0
11	i	61	0	52	1	0
12	D	84	0	78	0	0
12	E	84	0	78	0	0
12	F	84	0	78	0	0
All	All	25455	0	24471	249	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 5.

All (249) 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:A:632:ASP:OD2	6:R:108:TRP:NE1	2.12	0.82
5:K:17:SER:HA	5:K:83:LEU:O	1.81	0.81
5:M:17:SER:HA	5:M:83:LEU:O	1.81	0.81
5:O:17:SER:HA	5:O:83:LEU:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:ASP:OD2	6:P:108:TRP:NE1	2.17	0.78
4:L:22:SER:OG	4:L:70:GLU:OE2	2.04	0.75
4:N:22:SER:OG	4:N:70:GLU:OE2	2.04	0.74
4:J:22:SER:OG	4:J:70:GLU:OE2	2.05	0.74
2:F:64:GLU:OE2	2:F:211:GLU:N	2.22	0.72
2:D:64:GLU:OE2	2:D:211:GLU:N	2.22	0.72
2:E:64:GLU:OE2	2:E:211:GLU:N	2.22	0.72
2:E:102:GLU:OE2	2:E:476:ARG:NH1	2.25	0.69
7:S:18:THR:HA	7:S:76:ILE:O	1.94	0.67
7:U:18:THR:HA	7:U:76:ILE:O	1.94	0.67
7:Q:18:THR:HA	7:Q:76:ILE:O	1.94	0.67
6:P:17:SER:HA	6:P:86:ILE:O	1.95	0.66
5:O:91:THR:HA	5:O:124:VAL:O	1.97	0.65
6:T:17:SER:HA	6:T:86:ILE:O	1.95	0.65
2:D:102:GLU:OE2	2:D:476:ARG:NH1	2.25	0.65
3:I:16:CYS:HB2	3:I:67:PHE:HB2	1.78	0.65
6:R:17:SER:HA	6:R:86:ILE:O	1.95	0.64
5:M:91:THR:HA	5:M:124:VAL:O	1.97	0.64
3:G:16:CYS:HB2	3:G:67:PHE:HB2	1.78	0.64
3:H:11:THR:HG22	3:H:72:LYS:HG2	1.80	0.64
3:H:16:CYS:HB2	3:H:67:PHE:HB2	1.78	0.64
5:K:91:THR:HA	5:K:124:VAL:O	1.97	0.64
3:G:11:THR:HG22	3:G:72:LYS:HG2	1.80	0.63
3:I:2:LYS:HB2	3:I:93:VAL:HG12	1.81	0.63
3:I:11:THR:HG22	3:I:72:LYS:HG2	1.80	0.63
2:E:35:TRP:H	2:E:499:THR:HG22	1.64	0.63
2:F:35:TRP:H	2:F:499:THR:HG22	1.64	0.63
2:D:35:TRP:H	2:D:499:THR:HG22	1.64	0.62
1:C:632:ASP:OD2	6:T:108:TRP:NE1	2.32	0.62
2:F:102:GLU:OE2	2:F:476:ARG:NH1	2.25	0.61
3:H:2:LYS:HB2	3:H:93:VAL:HG12	1.80	0.61
3:G:2:LYS:HB2	3:G:93:VAL:HG12	1.80	0.61
2:D:475:MET:SD	2:D:478:ASN:ND2	2.74	0.61
2:E:475:MET:SD	2:E:478:ASN:ND2	2.74	0.60
2:F:475:MET:SD	2:F:478:ASN:ND2	2.74	0.60
2:E:54:CYS:HB2	2:E:55:ALA:HB2	1.86	0.58
2:E:219:ALA:O	2:E:246:GLN:NE2	2.37	0.58
2:F:219:ALA:O	2:F:246:GLN:NE2	2.37	0.58
2:D:219:ALA:O	2:D:246:GLN:NE2	2.37	0.58
6:P:40:GLN:HB2	6:P:46:LEU:HD23	1.86	0.58
2:D:54:CYS:HB2	2:D:55:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:CYS:HB2	2:F:55:ALA:HB2	1.86	0.57
6:R:40:GLN:HB2	6:R:46:LEU:HD23	1.86	0.56
2:E:51:THR:HA	2:E:103:GLN:HE22	1.70	0.56
6:T:40:GLN:HB2	6:T:46:LEU:HD23	1.86	0.56
2:F:51:THR:HA	2:F:103:GLN:HE22	1.70	0.56
4:N:77:SER:OG	4:N:79:GLN:NE2	2.39	0.56
2:D:51:THR:HA	2:D:103:GLN:HE22	1.70	0.55
4:J:77:SER:OG	4:J:79:GLN:NE2	2.39	0.55
4:L:77:SER:OG	4:L:79:GLN:NE2	2.39	0.55
3:G:84:CYS:O	3:G:90:LYS:HA	2.08	0.54
3:H:84:CYS:O	3:H:90:LYS:HA	2.08	0.54
3:I:84:CYS:O	3:I:90:LYS:HA	2.08	0.54
1:A:520:LEU:HD11	2:E:246:GLN:HB2	1.90	0.53
6:R:70:SER:OG	6:R:83:SER:OG	2.27	0.53
6:T:70:SER:OG	6:T:83:SER:OG	2.27	0.52
2:E:362:ALA:HB3	2:E:469:ARG:HG2	1.92	0.52
5:K:67:ARG:NH2	5:K:85:ASN:O	2.43	0.52
5:O:67:ARG:NH2	5:O:85:ASN:O	2.43	0.52
5:M:67:ARG:NH2	5:M:85:ASN:O	2.43	0.52
5:M:62:PRO:HA	5:M:65:GLN:HE21	1.75	0.52
5:O:62:PRO:HA	5:O:65:GLN:HE21	1.75	0.51
7:S:24:ARG:NH1	7:S:71:ASP:OD1	2.44	0.51
2:D:362:ALA:HB3	2:D:469:ARG:HG2	1.92	0.51
6:P:70:SER:OG	6:P:83:SER:OG	2.27	0.51
6:R:25:TYR:HE1	6:R:79:PRO:HG3	1.76	0.51
7:Q:24:ARG:NH1	7:Q:71:ASP:OD1	2.44	0.51
5:O:16:SER:HB3	5:O:86:LEU:HD12	1.93	0.51
6:T:35:VAL:HG22	6:T:101:THR:HG22	1.93	0.51
2:F:362:ALA:HB3	2:F:469:ARG:HG2	1.92	0.50
7:U:24:ARG:NH1	7:U:71:ASP:OD1	2.44	0.50
6:P:25:TYR:HE1	6:P:79:PRO:HG3	1.76	0.50
5:K:62:PRO:HA	5:K:65:GLN:HE21	1.75	0.50
6:R:35:VAL:HG22	6:R:101:THR:HG22	1.93	0.50
2:D:62:GLU:OE1	2:D:67:ASN:ND2	2.45	0.50
6:T:25:TYR:HE1	6:T:79:PRO:HG3	1.76	0.50
4:J:38:GLN:HE22	5:K:39:GLN:HE22	1.60	0.49
5:K:16:SER:HB3	5:K:86:LEU:HD12	1.93	0.49
5:O:91:THR:HG23	5:O:125:THR:HA	1.95	0.49
6:P:35:VAL:HG22	6:P:101:THR:HG22	1.93	0.49
2:F:62:GLU:OE1	2:F:67:ASN:ND2	2.45	0.49
4:J:2:ILE:O	4:J:4:MET:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:29:VAL:HG13	4:J:92:ASN:HB2	1.95	0.49
5:M:16:SER:HB3	5:M:86:LEU:HD12	1.93	0.49
2:E:62:GLU:OE1	2:E:67:ASN:ND2	2.45	0.49
4:L:29:VAL:HG13	4:L:92:ASN:HB2	1.95	0.49
5:M:91:THR:HG23	5:M:125:THR:HA	1.95	0.49
4:L:2:ILE:O	4:L:4:MET:N	2.46	0.49
6:P:94:THR:HG23	6:P:129:SER:HA	1.95	0.49
6:R:94:THR:HG23	6:R:129:SER:HA	1.95	0.49
4:N:29:VAL:HG13	4:N:92:ASN:HB2	1.95	0.48
2:D:499:THR:OG1	2:D:500:ARG:N	2.46	0.48
4:N:2:ILE:O	4:N:4:MET:N	2.46	0.48
3:H:5:LEU:HG	3:H:96:LEU:HB2	1.95	0.48
5:K:91:THR:HG23	5:K:125:THR:HA	1.95	0.48
4:L:7:SER:HB2	4:L:22:SER:HB3	1.96	0.48
6:P:25:TYR:CE1	6:P:79:PRO:HG3	2.48	0.48
6:T:94:THR:HG23	6:T:129:SER:HA	1.95	0.48
3:I:5:LEU:HG	3:I:96:LEU:HB2	1.95	0.48
6:R:25:TYR:CE1	6:R:79:PRO:HG3	2.48	0.48
6:T:38:VAL:HG23	6:T:48:TYR:HA	1.96	0.48
4:J:19:ALA:HB2	4:J:78:LEU:HD12	1.96	0.48
5:O:30:ILE:HD12	5:O:54:ILE:HD12	1.96	0.48
6:P:38:VAL:HG23	6:P:48:TYR:HA	1.96	0.48
2:F:499:THR:OG1	2:F:500:ARG:N	2.46	0.48
3:G:5:LEU:HG	3:G:96:LEU:HB2	1.95	0.48
5:M:30:ILE:HD12	5:M:54:ILE:HD12	1.96	0.48
1:B:520:LEU:HD11	2:D:246:GLN:HB2	1.95	0.47
4:L:19:ALA:HB2	4:L:78:LEU:HD12	1.96	0.47
6:T:25:TYR:CE1	6:T:79:PRO:HG3	2.48	0.47
4:N:19:ALA:HB2	4:N:78:LEU:HD12	1.96	0.47
2:E:499:THR:OG1	2:E:500:ARG:N	2.46	0.47
4:J:7:SER:HB2	4:J:22:SER:HB3	1.96	0.47
3:H:84:CYS:HB2	3:H:91:GLU:HB2	1.97	0.47
4:J:45:ARG:NH2	4:J:57:GLY:O	2.48	0.47
4:N:45:ARG:NH2	4:N:57:GLY:O	2.48	0.47
6:P:39:ARG:HB3	6:P:49:ILE:HD11	1.97	0.47
6:R:39:ARG:HB3	6:R:49:ILE:HD11	1.97	0.47
4:N:7:SER:HB2	4:N:22:SER:HB3	1.96	0.47
4:L:45:ARG:NH2	4:L:57:GLY:O	2.48	0.46
2:E:335:LYS:HD3	2:E:414:ILE:HD11	1.98	0.46
3:G:84:CYS:HB2	3:G:91:GLU:HB2	1.97	0.46
6:T:39:ARG:HB3	6:T:49:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:GLN:NE2	2:D:371:VAL:O	2.49	0.46
2:D:292:VAL:HG11	2:D:338:TRP:HE3	1.80	0.46
5:O:18:VAL:HG12	5:O:83:LEU:HB2	1.98	0.46
6:R:38:VAL:HG23	6:R:48:TYR:HA	1.96	0.46
2:E:258:GLN:NE2	2:E:371:VAL:O	2.49	0.46
7:S:38:GLN:HB2	7:S:48:LEU:HD11	1.98	0.46
2:D:335:LYS:HD3	2:D:414:ILE:HD11	1.97	0.46
7:U:38:GLN:HB2	7:U:48:LEU:HD11	1.98	0.46
5:K:30:ILE:HD12	5:K:54:ILE:HD12	1.96	0.46
2:E:292:VAL:HG11	2:E:338:TRP:HE3	1.80	0.46
4:N:11:LEU:HB3	4:N:106:LEU:HG	1.98	0.46
1:A:609:PRO:HA	2:E:35:TRP:HB3	1.98	0.45
2:F:119:CYS:N	2:F:205:CYS:SG	2.89	0.45
5:M:18:VAL:HG12	5:M:83:LEU:HB2	1.98	0.45
5:M:91:THR:HG1	5:M:126:VAL:H	1.64	0.45
2:F:258:GLN:NE2	2:F:371:VAL:O	2.49	0.45
2:F:292:VAL:HG11	2:F:338:TRP:HE3	1.80	0.45
4:L:11:LEU:HB3	4:L:106:LEU:HG	1.97	0.45
2:D:119:CYS:N	2:D:205:CYS:SG	2.89	0.45
3:I:84:CYS:HB2	3:I:91:GLU:HB2	1.97	0.45
7:Q:38:GLN:HB2	7:Q:48:LEU:HD11	1.98	0.45
2:E:119:CYS:N	2:E:205:CYS:SG	2.89	0.45
2:E:279:ASN:O	3:I:29:LYS:NZ	2.42	0.45
2:E:278:THR:O	11:e:1:NAG:O6	2.35	0.45
4:J:11:LEU:HB3	4:J:106:LEU:HG	1.98	0.45
7:Q:76:ILE:HD11	7:Q:87:PHE:HE2	1.82	0.45
5:O:40:ALA:HB3	5:O:43:GLN:HB2	1.99	0.45
2:E:385:CYS:HA	2:E:418:CYS:HA	1.99	0.45
5:K:18:VAL:HG12	5:K:83:LEU:HB2	1.98	0.45
5:K:91:THR:HG1	5:K:126:VAL:H	1.63	0.45
6:R:25:TYR:HE2	11:e:3:BMA:H62	1.81	0.45
4:J:29:VAL:HG12	4:J:32:ASP:H	1.81	0.44
4:N:29:VAL:HG12	4:N:32:ASP:H	1.81	0.44
7:S:76:ILE:HD11	7:S:87:PHE:HE2	1.82	0.44
2:F:335:LYS:HD3	2:F:414:ILE:HD11	1.97	0.44
5:O:54:ILE:HG21	5:O:104:ALA:HB1	1.99	0.44
5:K:54:ILE:HG21	5:K:104:ALA:HB1	1.99	0.44
6:P:19:THR:HA	6:P:84:LEU:O	2.18	0.44
5:M:54:ILE:HG21	5:M:104:ALA:HB1	1.99	0.44
2:D:323:ILE:HA	2:D:324:GLY:HA2	1.82	0.44
2:E:393:SER:OG	2:E:395:TRP:NE1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:29:VAL:HG12	4:L:32:ASP:H	1.81	0.44
6:P:46:LEU:HB2	7:Q:99:PHE:CD2	2.51	0.44
1:C:520:LEU:HD11	2:F:246:GLN:HB2	2.00	0.44
2:F:34:LEU:HD12	2:F:498:PRO:HB3	2.00	0.43
5:K:38:ARG:HH22	5:K:90:ASP:HA	1.83	0.43
7:U:76:ILE:HD11	7:U:87:PHE:HE2	1.82	0.43
5:M:40:ALA:HB3	5:M:43:GLN:HB2	1.99	0.43
2:E:48:ALA:HB1	2:E:50:THR:HG23	2.00	0.43
5:K:40:ALA:HB3	5:K:43:GLN:HB2	1.99	0.43
6:R:19:THR:HA	6:R:84:LEU:O	2.18	0.43
2:D:393:SER:OG	2:D:395:TRP:NE1	2.47	0.43
2:F:385:CYS:HA	2:F:418:CYS:HA	1.99	0.43
5:M:38:ARG:HH22	5:M:90:ASP:HA	1.83	0.43
2:F:323:ILE:HA	2:F:324:GLY:HA2	1.82	0.43
5:K:39:GLN:N	5:K:93:VAL:O	2.50	0.43
5:O:38:ARG:HH22	5:O:90:ASP:HA	1.83	0.43
6:T:25:TYR:HE2	11:i:3:BMA:H62	1.83	0.43
3:G:37:LEU:HD22	3:G:44:LEU:HD11	2.01	0.43
7:Q:34:VAL:HA	7:Q:90:GLN:O	2.18	0.43
2:D:385:CYS:HA	2:D:418:CYS:HA	1.99	0.43
3:H:54:ARG:NH1	3:H:73:ASN:O	2.52	0.43
3:I:37:LEU:HD22	3:I:44:LEU:HD11	2.01	0.43
6:P:16:SER:OG	6:P:17:SER:N	2.51	0.43
2:D:48:ALA:HB1	2:D:50:THR:HG23	2.00	0.43
2:E:34:LEU:HD12	2:E:498:PRO:HB3	2.00	0.43
2:F:48:ALA:HB1	2:F:50:THR:HG23	2.00	0.43
3:G:54:ARG:NH1	3:G:73:ASN:O	2.52	0.43
3:H:37:LEU:HD22	3:H:44:LEU:HD11	2.01	0.43
3:I:54:ARG:NH1	3:I:73:ASN:O	2.52	0.43
7:U:34:VAL:HA	7:U:90:GLN:O	2.18	0.43
6:T:16:SER:OG	6:T:17:SER:N	2.51	0.42
2:F:378:CYS:SG	10:h:2:NAG:O6	2.77	0.42
7:S:34:VAL:HA	7:S:90:GLN:O	2.19	0.42
1:B:520:LEU:HB3	2:D:84:ILE:HD13	2.01	0.42
6:T:19:THR:HA	6:T:84:LEU:O	2.18	0.42
2:D:34:LEU:HD12	2:D:498:PRO:HB3	2.00	0.42
2:E:42:VAL:HG12	2:E:44:VAL:HG23	2.02	0.42
2:F:42:VAL:HG12	2:F:44:VAL:HG23	2.02	0.42
5:M:39:GLN:N	5:M:93:VAL:O	2.50	0.42
1:C:610:TRP:CZ3	2:F:498:PRO:HG3	2.54	0.42
2:E:293:GLN:HE21	2:E:446:VAL:HG13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:361:PHE:HE1	2:E:468:PHE:HD2	1.68	0.42
5:O:32:TYR:O	5:O:53:THR:OG1	2.34	0.42
2:D:293:GLN:HE21	2:D:446:VAL:HG13	1.84	0.41
4:L:35:TRP:HD1	4:L:48:ILE:HB	1.85	0.41
2:D:361:PHE:HE1	2:D:468:PHE:HD2	1.68	0.41
2:F:361:PHE:HE1	2:F:468:PHE:HD2	1.68	0.41
2:E:93:PHE:CE2	2:E:228:CYS:HB2	2.56	0.41
5:M:101:GLU:OE1	5:M:111:ASN:N	2.53	0.41
2:F:293:GLN:HE21	2:F:446:VAL:HG13	1.84	0.41
5:K:101:GLU:OE1	5:K:111:ASN:N	2.53	0.41
4:N:35:TRP:HD1	4:N:48:ILE:HB	1.85	0.41
6:P:116:VAL:HG12	7:Q:92:TYR:HB2	2.02	0.41
2:E:105:HIS:O	2:E:109:ILE:HG12	2.21	0.41
4:L:24:ARG:HH21	4:L:69:ALA:HB3	1.86	0.41
4:N:24:ARG:HH21	4:N:69:ALA:HB3	1.85	0.41
2:D:93:PHE:CE2	2:D:228:CYS:HB2	2.56	0.41
2:E:378:CYS:SG	10:d:2:NAG:O6	2.78	0.41
4:J:35:TRP:HD1	4:J:48:ILE:HB	1.85	0.41
6:P:25:TYR:HE2	11:a:3:BMA:H62	1.84	0.41
1:A:633:LYS:HE2	6:R:107:LYS:O	2.21	0.41
1:C:523:LEU:HD13	1:C:523:LEU:HA	1.82	0.41
5:O:101:GLU:OE1	5:O:111:ASN:N	2.53	0.41
7:Q:20:ARG:HG3	7:Q:73:THR:HG23	2.03	0.41
1:B:609:PRO:HA	2:D:35:TRP:HB3	2.03	0.40
7:U:20:ARG:HG3	7:U:73:THR:HG23	2.03	0.40
2:D:42:VAL:HG12	2:D:44:VAL:HG23	2.02	0.40
2:D:95:MET:HE1	2:D:273:ARG:HD3	2.03	0.40
2:E:384:TYR:HD2	2:E:421:LYS:HD2	1.86	0.40
4:J:24:ARG:HH21	4:J:69:ALA:HB3	1.86	0.40
6:R:16:SER:OG	6:R:17:SER:N	2.51	0.40
6:R:29:THR:HG23	6:R:32:LEU:H	1.86	0.40
6:T:29:THR:HG23	6:T:32:LEU:H	1.86	0.40
1:A:520:LEU:HB3	2:E:84:ILE:HD13	2.03	0.40
2:D:422:GLN:HE22	2:D:437:PRO:HA	1.87	0.40
2:F:105:HIS:O	2:F:109:ILE:HG12	2.21	0.40
7:S:20:ARG:HG3	7:S:73:THR:HG23	2.03	0.40
1:A:523:LEU:HD13	1:A:523:LEU:HA	1.82	0.40
2:F:93:PHE:CE2	2:F:228:CYS:HB2	2.56	0.40
2:F:95:MET:HE1	2:F:273:ARG:HD3	2.04	0.40
6:P:29:THR:HG23	6:P:32:LEU:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	114/153 (74%)	109 (96%)	5 (4%)	0	100	100
1	B	114/153 (74%)	109 (96%)	5 (4%)	0	100	100
1	C	114/153 (74%)	109 (96%)	5 (4%)	0	100	100
2	D	362/481 (75%)	324 (90%)	38 (10%)	0	100	100
2	E	362/481 (75%)	323 (89%)	39 (11%)	0	100	100
2	F	362/481 (75%)	323 (89%)	39 (11%)	0	100	100
3	G	95/192 (50%)	84 (88%)	11 (12%)	0	100	100
3	H	95/192 (50%)	84 (88%)	11 (12%)	0	100	100
3	I	95/192 (50%)	84 (88%)	11 (12%)	0	100	100
4	J	103/214 (48%)	94 (91%)	9 (9%)	0	100	100
4	L	103/214 (48%)	94 (91%)	9 (9%)	0	100	100
4	N	103/214 (48%)	94 (91%)	9 (9%)	0	100	100
5	K	125/229 (55%)	115 (92%)	10 (8%)	0	100	100
5	M	125/229 (55%)	114 (91%)	11 (9%)	0	100	100
5	O	125/229 (55%)	114 (91%)	11 (9%)	0	100	100
6	P	129/244 (53%)	118 (92%)	11 (8%)	0	100	100
6	R	129/244 (53%)	118 (92%)	11 (8%)	0	100	100
6	T	129/244 (53%)	118 (92%)	11 (8%)	0	100	100
7	Q	105/215 (49%)	97 (92%)	8 (8%)	0	100	100
7	S	105/215 (49%)	96 (91%)	9 (9%)	0	100	100
7	U	105/215 (49%)	97 (92%)	8 (8%)	0	100	100
All	All	3099/5184 (60%)	2818 (91%)	281 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/129 (70%)	90 (100%)	0	100	100
1	B	90/129 (70%)	90 (100%)	0	100	100
1	C	90/129 (70%)	90 (100%)	0	100	100
2	D	306/428 (72%)	305 (100%)	1 (0%)	91	96
2	E	306/428 (72%)	305 (100%)	1 (0%)	91	96
2	F	306/428 (72%)	305 (100%)	1 (0%)	91	96
3	G	89/173 (51%)	89 (100%)	0	100	100
3	H	89/173 (51%)	89 (100%)	0	100	100
3	I	89/173 (51%)	89 (100%)	0	100	100
4	J	88/184 (48%)	88 (100%)	0	100	100
4	L	88/184 (48%)	88 (100%)	0	100	100
4	N	88/184 (48%)	88 (100%)	0	100	100
5	K	105/193 (54%)	105 (100%)	0	100	100
5	M	105/193 (54%)	105 (100%)	0	100	100
5	O	105/193 (54%)	105 (100%)	0	100	100
6	P	112/210 (53%)	112 (100%)	0	100	100
6	R	112/210 (53%)	112 (100%)	0	100	100
6	T	112/210 (53%)	112 (100%)	0	100	100
7	Q	85/182 (47%)	85 (100%)	0	100	100
7	S	85/182 (47%)	85 (100%)	0	100	100
7	U	85/182 (47%)	85 (100%)	0	100	100
All	All	2625/4497 (58%)	2622 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	193	LEU

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Mol	Chain	Res	Type
2	E	193	LEU
2	F	193	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	611	ASN
1	B	611	ASN
1	C	611	ASN
2	D	66	HIS
2	D	103	GLN
2	D	279	ASN
2	D	293	GLN
2	E	66	HIS
2	E	103	GLN
2	E	279	ASN
2	F	66	HIS
2	F	67	ASN
2	F	103	GLN
2	F	258	GLN
2	F	279	ASN
2	F	293	GLN
3	G	39	ASN
3	H	39	ASN
3	I	39	ASN
4	J	38	GLN
4	J	79	GLN
4	J	102	GLN
5	K	39	GLN
5	K	65	GLN
4	L	37	GLN
4	L	79	GLN
4	L	102	GLN
5	M	65	GLN
4	N	79	GLN
4	N	102	GLN
5	O	63	HIS
5	O	65	GLN
7	Q	38	GLN
7	S	38	GLN
7	U	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

72 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	V	1	8,1	14,14,15	0.46	0	17,19,21	1.53	4 (23%)
8	NAG	V	2	8	14,14,15	0.24	0	17,19,21	1.58	3 (17%)
8	NAG	W	1	8,1	14,14,15	0.45	0	17,19,21	1.47	4 (23%)
8	NAG	W	2	8	14,14,15	0.24	0	17,19,21	1.58	4 (23%)
8	NAG	X	1	8,1	14,14,15	0.46	0	17,19,21	1.43	2 (11%)
8	NAG	X	2	8	14,14,15	0.25	0	17,19,21	1.60	4 (23%)
9	NAG	Y	1	9,2	14,14,15	0.57	0	17,19,21	1.09	1 (5%)
9	MAN	Y	10	9	11,11,12	0.22	0	15,15,17	0.77	0
9	NAG	Y	2	9	14,14,15	0.40	0	17,19,21	1.03	2 (11%)
9	BMA	Y	3	9	11,11,12	0.23	0	15,15,17	0.89	0
9	MAN	Y	4	9	11,11,12	0.20	0	15,15,17	0.87	0
9	MAN	Y	5	9	11,11,12	0.24	0	15,15,17	0.83	0
9	MAN	Y	6	9	11,11,12	0.20	0	15,15,17	0.74	0
9	MAN	Y	7	9	11,11,12	0.31	0	15,15,17	0.98	0
9	MAN	Y	8	9	11,11,12	0.20	0	15,15,17	0.88	0
9	MAN	Y	9	9	11,11,12	0.27	0	15,15,17	0.81	0
10	NAG	Z	1	10,2	14,14,15	0.51	0	17,19,21	1.44	3 (17%)
10	NAG	Z	2	10	14,14,15	0.37	0	17,19,21	1.21	2 (11%)
10	BMA	Z	3	10	11,11,12	0.20	0	15,15,17	1.02	1 (6%)
10	MAN	Z	4	10	11,11,12	0.20	0	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	Z	5	10	11,11,12	0.47	0	15,15,17	1.40	3 (20%)
11	NAG	a	1	11,2	14,14,15	0.55	0	17,19,21	1.48	3 (17%)
11	NAG	a	2	11	14,14,15	0.32	0	17,19,21	0.88	1 (5%)
11	BMA	a	3	11	11,11,12	0.16	0	15,15,17	1.07	1 (6%)
11	MAN	a	4	11	11,11,12	0.23	0	15,15,17	0.65	0
11	MAN	a	5	11	11,11,12	0.26	0	15,15,17	0.76	0
8	NAG	b	1	8,2	14,14,15	0.47	0	17,19,21	1.25	3 (17%)
8	NAG	b	2	8	14,14,15	0.51	0	17,19,21	1.61	4 (23%)
9	NAG	c	1	9,2	14,14,15	0.52	0	17,19,21	1.10	1 (5%)
9	MAN	c	10	9	11,11,12	0.22	0	15,15,17	0.76	0
9	NAG	c	2	9	14,14,15	0.43	0	17,19,21	0.99	1 (5%)
9	BMA	c	3	9	11,11,12	0.23	0	15,15,17	0.89	0
9	MAN	c	4	9	11,11,12	0.17	0	15,15,17	0.90	0
9	MAN	c	5	9	11,11,12	0.25	0	15,15,17	0.81	0
9	MAN	c	6	9	11,11,12	0.22	0	15,15,17	0.81	0
9	MAN	c	7	9	11,11,12	0.31	0	15,15,17	0.98	0
9	MAN	c	8	9	11,11,12	0.20	0	15,15,17	0.88	0
9	MAN	c	9	9	11,11,12	0.27	0	15,15,17	0.77	0
10	NAG	d	1	10,2	14,14,15	0.51	0	17,19,21	1.47	3 (17%)
10	NAG	d	2	10	14,14,15	0.37	0	17,19,21	1.18	2 (11%)
10	BMA	d	3	10	11,11,12	0.19	0	15,15,17	1.02	1 (6%)
10	MAN	d	4	10	11,11,12	0.21	0	15,15,17	0.92	0
10	MAN	d	5	10	11,11,12	0.47	0	15,15,17	1.38	3 (20%)
11	NAG	e	1	11,2	14,14,15	0.54	0	17,19,21	1.50	3 (17%)
11	NAG	e	2	11	14,14,15	0.32	0	17,19,21	0.87	1 (5%)
11	BMA	e	3	11	11,11,12	0.17	0	15,15,17	1.14	2 (13%)
11	MAN	e	4	11	11,11,12	0.22	0	15,15,17	0.67	0
11	MAN	e	5	11	11,11,12	0.27	0	15,15,17	0.76	0
8	NAG	f	1	8,2	14,14,15	0.45	0	17,19,21	1.22	2 (11%)
8	NAG	f	2	8	14,14,15	0.52	0	17,19,21	1.64	4 (23%)
9	NAG	g	1	9,2	14,14,15	0.55	0	17,19,21	1.10	1 (5%)
9	MAN	g	10	9	11,11,12	0.21	0	15,15,17	0.77	0
9	NAG	g	2	9	14,14,15	0.42	0	17,19,21	0.98	0
9	BMA	g	3	9	11,11,12	0.22	0	15,15,17	0.86	0
9	MAN	g	4	9	11,11,12	0.20	0	15,15,17	0.85	0
9	MAN	g	5	9	11,11,12	0.25	0	15,15,17	0.83	0
9	MAN	g	6	9	11,11,12	0.22	0	15,15,17	0.76	0
9	MAN	g	7	9	11,11,12	0.32	0	15,15,17	0.97	0
9	MAN	g	8	9	11,11,12	0.19	0	15,15,17	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	g	9	9	11,11,12	0.28	0	15,15,17	0.80	0
10	NAG	h	1	10,2	14,14,15	0.51	0	17,19,21	1.40	3 (17%)
10	NAG	h	2	10	14,14,15	0.37	0	17,19,21	1.18	2 (11%)
10	BMA	h	3	10	11,11,12	0.17	0	15,15,17	1.00	1 (6%)
10	MAN	h	4	10	11,11,12	0.20	0	15,15,17	0.92	0
10	MAN	h	5	10	11,11,12	0.46	0	15,15,17	1.37	3 (20%)
11	NAG	i	1	11,2	14,14,15	0.54	0	17,19,21	1.48	3 (17%)
11	NAG	i	2	11	14,14,15	0.33	0	17,19,21	0.87	1 (5%)
11	BMA	i	3	11	11,11,12	0.16	0	15,15,17	1.12	2 (13%)
11	MAN	i	4	11	11,11,12	0.23	0	15,15,17	0.67	0
11	MAN	i	5	11	11,11,12	0.26	0	15,15,17	0.76	0
8	NAG	j	1	8,2	14,14,15	0.45	0	17,19,21	1.28	3 (17%)
8	NAG	j	2	8	14,14,15	0.52	0	17,19,21	1.63	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	V	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	V	2	8	-	2/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	2/6/23/26	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
9	NAG	Y	1	9,2	-	0/6/23/26	0/1/1/1
9	MAN	Y	10	9	-	2/2/19/22	0/1/1/1
9	NAG	Y	2	9	-	0/6/23/26	0/1/1/1
9	BMA	Y	3	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	4	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	5	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	6	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	7	9	-	0/2/19/22	0/1/1/1
9	MAN	Y	8	9	-	1/2/19/22	0/1/1/1
9	MAN	Y	9	9	-	0/2/19/22	0/1/1/1
10	NAG	Z	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	Z	2	10	-	2/6/23/26	0/1/1/1
10	BMA	Z	3	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	Z	4	10	-	1/2/19/22	0/1/1/1
10	MAN	Z	5	10	-	1/2/19/22	0/1/1/1
11	NAG	a	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	a	2	11	-	0/6/23/26	0/1/1/1
11	BMA	a	3	11	-	2/2/19/22	0/1/1/1
11	MAN	a	4	11	-	1/2/19/22	0/1/1/1
11	MAN	a	5	11	-	0/2/19/22	0/1/1/1
8	NAG	b	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	b	2	8	-	2/6/23/26	0/1/1/1
9	NAG	c	1	9,2	-	0/6/23/26	0/1/1/1
9	MAN	c	10	9	-	2/2/19/22	0/1/1/1
9	NAG	c	2	9	-	0/6/23/26	0/1/1/1
9	BMA	c	3	9	-	0/2/19/22	0/1/1/1
9	MAN	c	4	9	-	0/2/19/22	0/1/1/1
9	MAN	c	5	9	-	1/2/19/22	0/1/1/1
9	MAN	c	6	9	-	2/2/19/22	0/1/1/1
9	MAN	c	7	9	-	0/2/19/22	0/1/1/1
9	MAN	c	8	9	-	2/2/19/22	0/1/1/1
9	MAN	c	9	9	-	0/2/19/22	0/1/1/1
10	NAG	d	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	d	2	10	-	2/6/23/26	0/1/1/1
10	BMA	d	3	10	-	0/2/19/22	0/1/1/1
10	MAN	d	4	10	-	1/2/19/22	0/1/1/1
10	MAN	d	5	10	-	1/2/19/22	0/1/1/1
11	NAG	e	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	e	2	11	-	0/6/23/26	0/1/1/1
11	BMA	e	3	11	-	2/2/19/22	0/1/1/1
11	MAN	e	4	11	-	1/2/19/22	0/1/1/1
11	MAN	e	5	11	-	0/2/19/22	0/1/1/1
8	NAG	f	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
9	NAG	g	1	9,2	-	0/6/23/26	0/1/1/1
9	MAN	g	10	9	-	2/2/19/22	0/1/1/1
9	NAG	g	2	9	-	0/6/23/26	0/1/1/1
9	BMA	g	3	9	-	0/2/19/22	0/1/1/1
9	MAN	g	4	9	-	0/2/19/22	0/1/1/1
9	MAN	g	5	9	-	0/2/19/22	0/1/1/1
9	MAN	g	6	9	-	0/2/19/22	0/1/1/1
9	MAN	g	7	9	-	0/2/19/22	0/1/1/1
9	MAN	g	8	9	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	g	9	9	-	0/2/19/22	0/1/1/1
10	NAG	h	1	10,2	-	0/6/23/26	0/1/1/1
10	NAG	h	2	10	-	2/6/23/26	0/1/1/1
10	BMA	h	3	10	-	0/2/19/22	0/1/1/1
10	MAN	h	4	10	-	1/2/19/22	0/1/1/1
10	MAN	h	5	10	-	1/2/19/22	0/1/1/1
11	NAG	i	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	i	2	11	-	0/6/23/26	0/1/1/1
11	BMA	i	3	11	-	2/2/19/22	0/1/1/1
11	MAN	i	4	11	-	1/2/19/22	0/1/1/1
11	MAN	i	5	11	-	0/2/19/22	0/1/1/1
8	NAG	j	1	8,2	-	0/6/23/26	0/1/1/1
8	NAG	j	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	2	NAG	C2-N2-C7	4.63	129.10	122.90
8	j	2	NAG	C2-N2-C7	4.59	129.05	122.90
8	b	2	NAG	C2-N2-C7	4.54	128.98	122.90
8	V	2	NAG	C2-N2-C7	4.06	128.34	122.90
8	X	2	NAG	C2-N2-C7	4.03	128.30	122.90
8	W	2	NAG	C2-N2-C7	3.99	128.25	122.90
10	d	1	NAG	C2-N2-C7	-3.48	118.24	122.90
10	Z	1	NAG	C2-N2-C7	-3.42	118.32	122.90
10	h	1	NAG	C2-N2-C7	-3.38	118.37	122.90
11	e	1	NAG	C2-N2-C7	-3.30	118.48	122.90
11	a	1	NAG	C2-N2-C7	-3.12	118.72	122.90
11	i	1	NAG	C2-N2-C7	-3.09	118.76	122.90
10	Z	2	NAG	C2-N2-C7	-2.98	118.90	122.90
10	h	2	NAG	C2-N2-C7	-2.89	119.03	122.90
8	X	1	NAG	C1-O5-C5	2.88	116.05	112.19
10	Z	1	NAG	C1-O5-C5	2.88	116.04	112.19
10	d	2	NAG	C2-N2-C7	-2.86	119.06	122.90
10	d	1	NAG	C1-O5-C5	2.85	116.00	112.19
11	a	1	NAG	C1-O5-C5	2.84	115.99	112.19
11	i	1	NAG	C1-O5-C5	2.82	115.96	112.19
8	W	1	NAG	C1-O5-C5	2.81	115.96	112.19
8	V	1	NAG	C1-C2-N2	-2.78	106.05	110.43
10	Z	1	NAG	O5-C1-C2	-2.78	106.99	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	V	1	NAG	O4-C4-C5	-2.77	102.51	109.32
10	Z	5	MAN	O4-C4-C3	-2.77	103.86	110.38
10	h	5	MAN	O4-C4-C3	-2.72	103.98	110.38
10	d	5	MAN	O4-C4-C3	-2.69	104.04	110.38
11	e	1	NAG	C1-O5-C5	2.67	115.76	112.19
10	d	1	NAG	O5-C1-C2	-2.66	107.17	111.29
10	h	1	NAG	C1-O5-C5	2.65	115.74	112.19
11	i	2	NAG	C1-O5-C5	2.62	115.70	112.19
8	V	1	NAG	C1-O5-C5	2.61	115.69	112.19
11	e	2	NAG	C1-O5-C5	2.60	115.67	112.19
10	Z	5	MAN	O4-C4-C5	-2.58	102.97	109.32
8	X	1	NAG	C2-N2-C7	-2.56	119.47	122.90
11	a	2	NAG	C1-O5-C5	2.56	115.61	112.19
10	Z	2	NAG	O5-C1-C2	-2.55	107.35	111.29
10	d	2	NAG	O5-C1-C2	-2.53	107.37	111.29
10	h	1	NAG	O5-C1-C2	-2.52	107.39	111.29
10	d	3	BMA	O3-C3-C2	-2.50	104.96	110.05
10	h	2	NAG	O5-C1-C2	-2.48	107.46	111.29
10	h	5	MAN	O4-C4-C5	-2.47	103.23	109.32
10	Z	3	BMA	O3-C3-C2	-2.45	105.06	110.05
10	d	5	MAN	O4-C4-C5	-2.44	103.31	109.32
8	j	2	NAG	C1-O5-C5	2.43	115.44	112.19
10	h	3	BMA	O3-C3-C2	-2.42	105.12	110.05
9	g	1	NAG	C1-O5-C5	-2.40	108.97	112.19
8	V	2	NAG	O5-C1-C2	-2.39	107.60	111.29
8	f	2	NAG	C1-O5-C5	2.37	115.37	112.19
8	f	1	NAG	C3-C4-C5	-2.37	105.94	110.23
8	b	2	NAG	O7-C7-N2	2.37	126.17	121.98
9	c	1	NAG	C1-O5-C5	-2.36	109.02	112.19
8	j	1	NAG	C3-C4-C5	-2.36	105.95	110.23
8	W	1	NAG	C2-N2-C7	-2.35	119.75	122.90
8	b	1	NAG	C3-C4-C5	-2.35	105.98	110.23
8	j	2	NAG	O7-C7-N2	2.33	126.09	121.98
11	e	3	BMA	O5-C5-C6	2.32	112.18	107.66
8	f	2	NAG	O7-C7-N2	2.32	126.08	121.98
8	b	2	NAG	C1-O5-C5	2.32	115.29	112.19
8	X	2	NAG	C1-O5-C5	2.28	115.24	112.19
11	i	1	NAG	O5-C1-C2	-2.28	107.77	111.29
8	W	2	NAG	O5-C1-C2	-2.27	107.78	111.29
8	V	1	NAG	C2-N2-C7	-2.27	119.86	122.90
10	Z	5	MAN	C1-C2-C3	-2.27	106.34	109.64
11	a	3	BMA	O5-C5-C6	2.25	112.04	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	d	5	MAN	C1-C2-C3	-2.22	106.41	109.64
11	i	3	BMA	O5-C5-C6	2.21	111.97	107.66
11	e	1	NAG	O5-C1-C2	-2.21	107.87	111.29
8	X	2	NAG	O5-C1-C2	-2.21	107.87	111.29
9	Y	1	NAG	C1-O5-C5	-2.21	109.23	112.19
10	h	5	MAN	C1-C2-C3	-2.17	106.48	109.64
8	W	2	NAG	C1-O5-C5	2.16	115.08	112.19
8	W	1	NAG	O4-C4-C5	-2.15	104.02	109.32
8	f	1	NAG	O4-C4-C3	-2.15	105.32	110.38
8	j	1	NAG	C4-C3-C2	2.14	114.16	111.02
8	j	1	NAG	O4-C4-C3	-2.14	105.33	110.38
11	a	1	NAG	O5-C1-C2	-2.12	108.00	111.29
9	Y	2	NAG	O4-C4-C3	-2.12	105.39	110.38
8	b	1	NAG	O4-C4-C3	-2.10	105.43	110.38
8	b	1	NAG	C4-C3-C2	2.07	114.06	111.02
9	Y	2	NAG	C1-O5-C5	2.07	114.96	112.19
8	f	2	NAG	O5-C1-C2	-2.07	108.09	111.29
8	j	2	NAG	O5-C1-C2	-2.06	108.10	111.29
9	c	2	NAG	O4-C4-C3	-2.06	105.52	110.38
11	i	3	BMA	O3-C3-C2	-2.06	105.85	110.05
11	e	3	BMA	O3-C3-C2	-2.04	105.89	110.05
8	V	2	NAG	C1-O5-C5	2.03	114.91	112.19
8	b	2	NAG	O5-C1-C2	-2.03	108.15	111.29
8	X	2	NAG	C1-C2-N2	2.03	113.63	110.43
8	W	1	NAG	C1-C2-N2	-2.02	107.25	110.43
8	W	2	NAG	C1-C2-N2	2.02	113.61	110.43

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	d	2	NAG	O5-C5-C6-O6
10	h	2	NAG	O5-C5-C6-O6
10	d	2	NAG	C4-C5-C6-O6
10	h	2	NAG	C4-C5-C6-O6
10	Z	2	NAG	O5-C5-C6-O6
11	a	1	NAG	C4-C5-C6-O6
11	e	1	NAG	C4-C5-C6-O6
11	i	1	NAG	C4-C5-C6-O6
11	a	1	NAG	O5-C5-C6-O6
11	e	1	NAG	O5-C5-C6-O6
11	i	1	NAG	O5-C5-C6-O6

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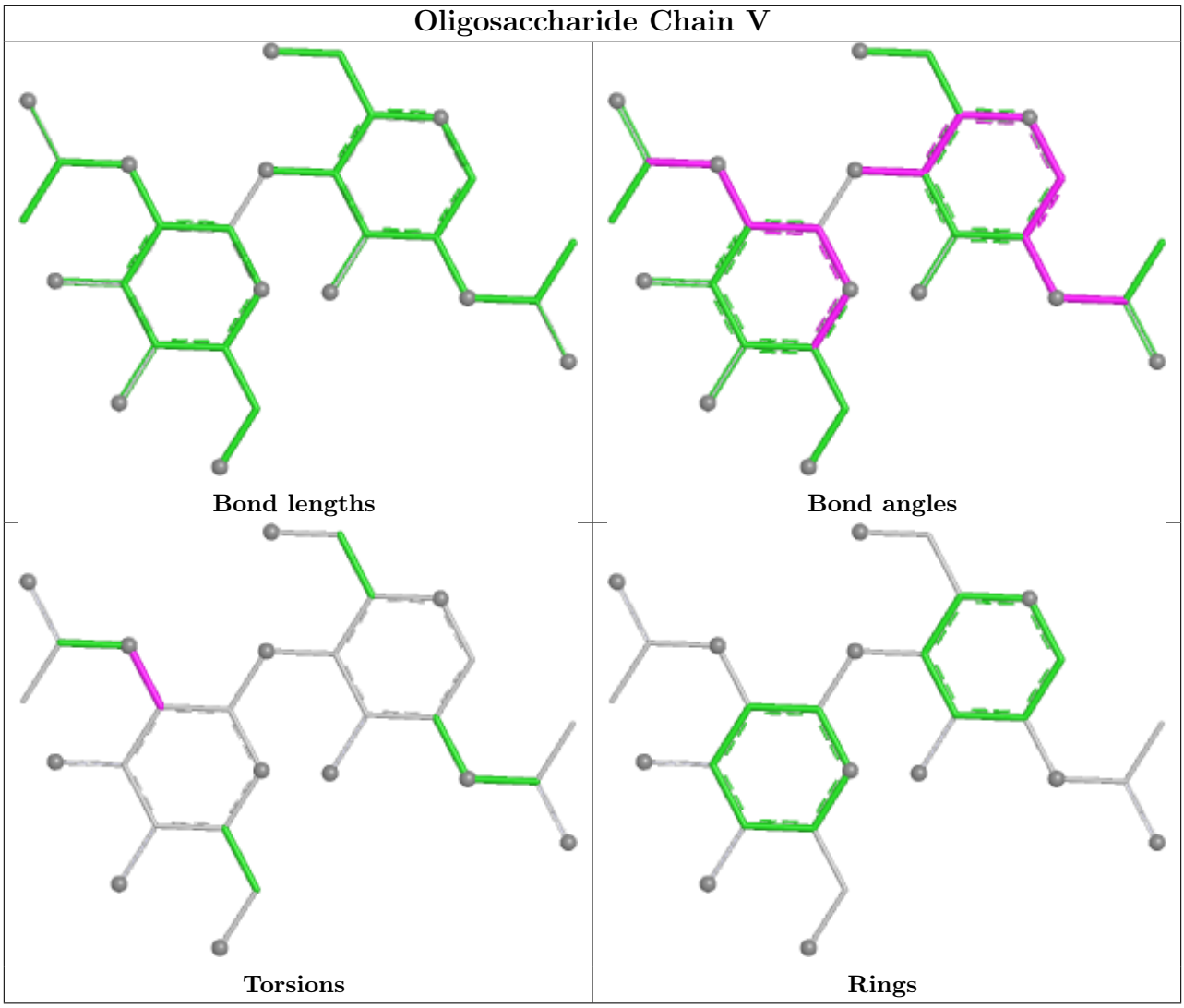
Mol	Chain	Res	Type	Atoms
10	Z	2	NAG	C4-C5-C6-O6
9	c	8	MAN	O5-C5-C6-O6
9	c	6	MAN	O5-C5-C6-O6
9	Y	10	MAN	O5-C5-C6-O6
9	Y	8	MAN	O5-C5-C6-O6
9	g	8	MAN	O5-C5-C6-O6
10	Z	5	MAN	O5-C5-C6-O6
10	d	5	MAN	O5-C5-C6-O6
10	h	5	MAN	O5-C5-C6-O6
11	a	4	MAN	O5-C5-C6-O6
10	Z	4	MAN	C4-C5-C6-O6
11	e	4	MAN	O5-C5-C6-O6
11	i	4	MAN	O5-C5-C6-O6
10	d	4	MAN	C4-C5-C6-O6
11	i	3	BMA	O5-C5-C6-O6
11	e	3	BMA	O5-C5-C6-O6
10	h	4	MAN	C4-C5-C6-O6
11	i	3	BMA	C4-C5-C6-O6
11	e	3	BMA	C4-C5-C6-O6
9	c	10	MAN	O5-C5-C6-O6
8	b	2	NAG	C1-C2-N2-C7
8	f	2	NAG	C1-C2-N2-C7
8	j	2	NAG	C1-C2-N2-C7
9	g	10	MAN	O5-C5-C6-O6
11	a	3	BMA	C4-C5-C6-O6
9	Y	10	MAN	C4-C5-C6-O6
11	a	3	BMA	O5-C5-C6-O6
9	c	8	MAN	C4-C5-C6-O6
9	c	6	MAN	C4-C5-C6-O6
9	c	5	MAN	O5-C5-C6-O6
8	V	2	NAG	C1-C2-N2-C7
8	W	2	NAG	C1-C2-N2-C7
8	X	2	NAG	C1-C2-N2-C7
8	V	2	NAG	C3-C2-N2-C7
8	W	2	NAG	C3-C2-N2-C7
8	X	2	NAG	C3-C2-N2-C7
8	b	2	NAG	C3-C2-N2-C7
8	f	2	NAG	C3-C2-N2-C7
8	j	2	NAG	C3-C2-N2-C7
9	c	10	MAN	C4-C5-C6-O6
9	g	10	MAN	C4-C5-C6-O6

There are no ring outliers.

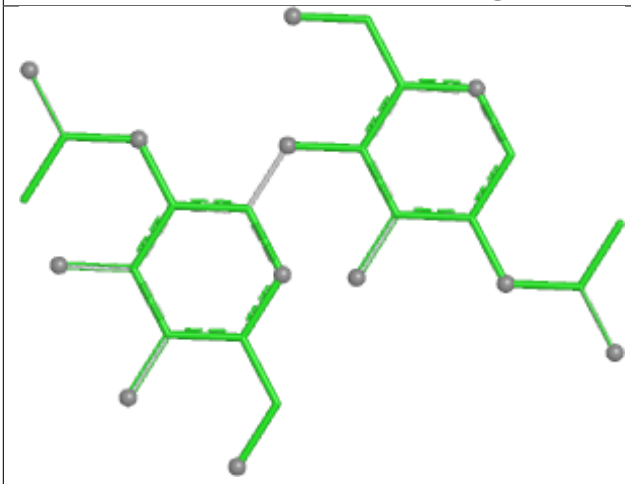
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	d	2	NAG	1	0
10	h	2	NAG	1	0
11	a	3	BMA	1	0
11	i	3	BMA	1	0
11	e	1	NAG	1	0
11	e	3	BMA	1	0

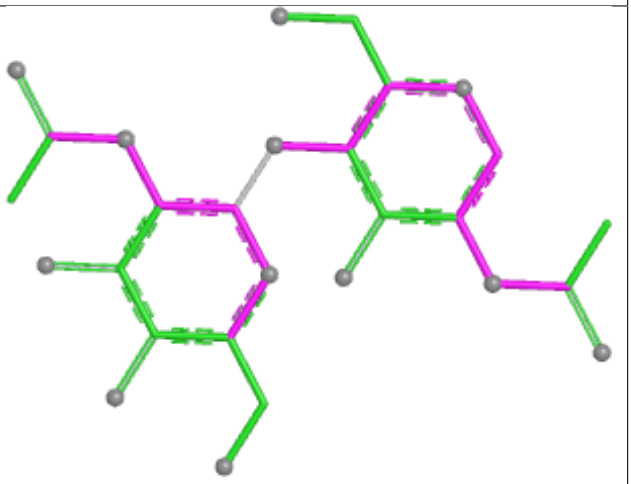
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



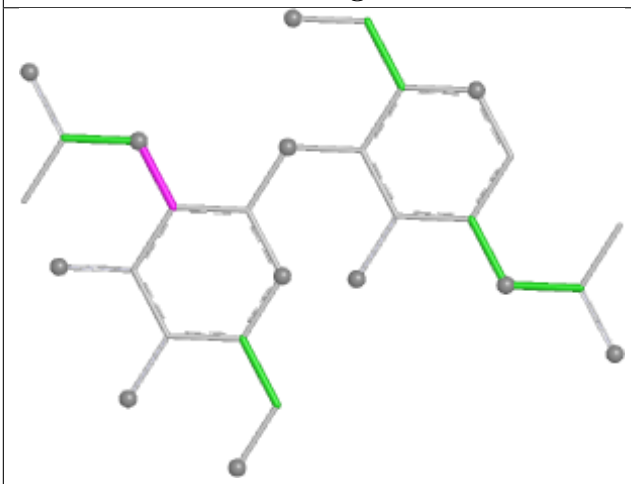
Oligosaccharide Chain W



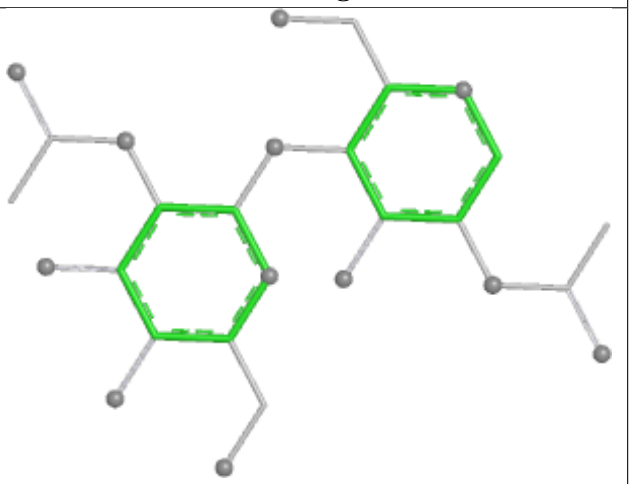
Bond lengths



Bond angles

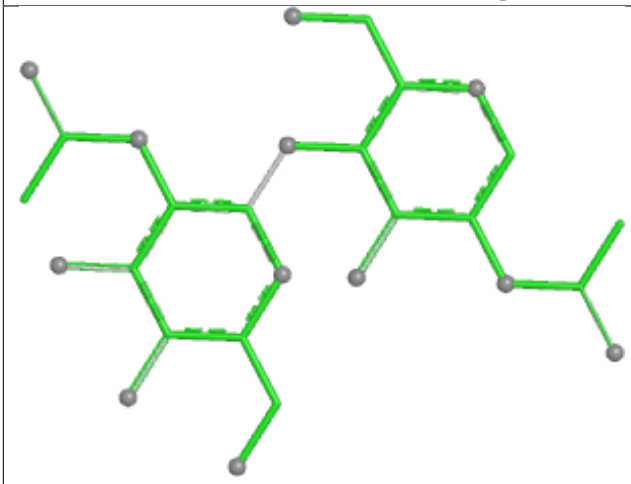


Torsions

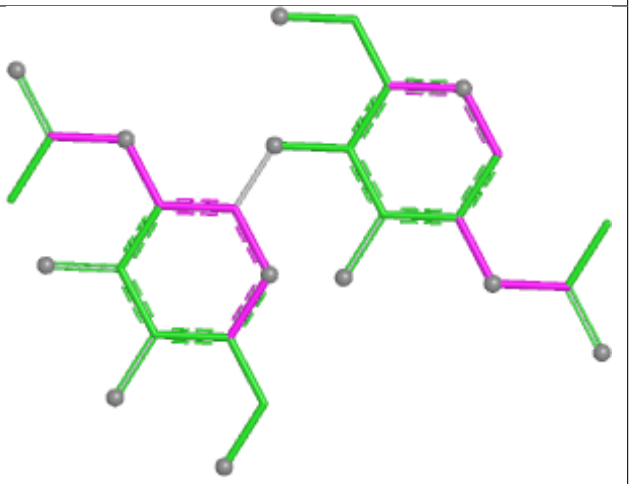


Rings

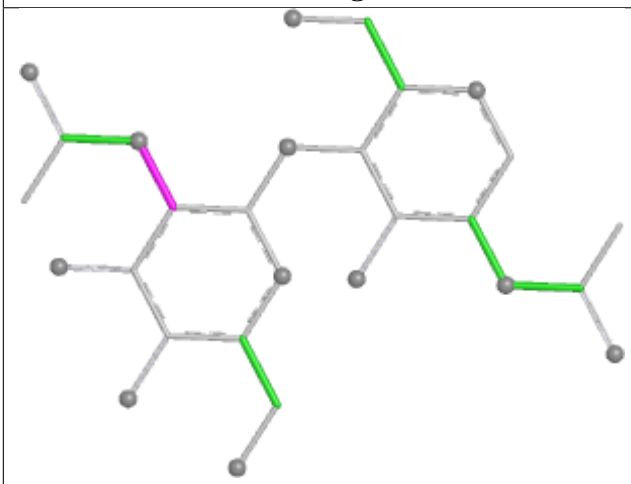
Oligosaccharide Chain X



Bond lengths



Bond angles



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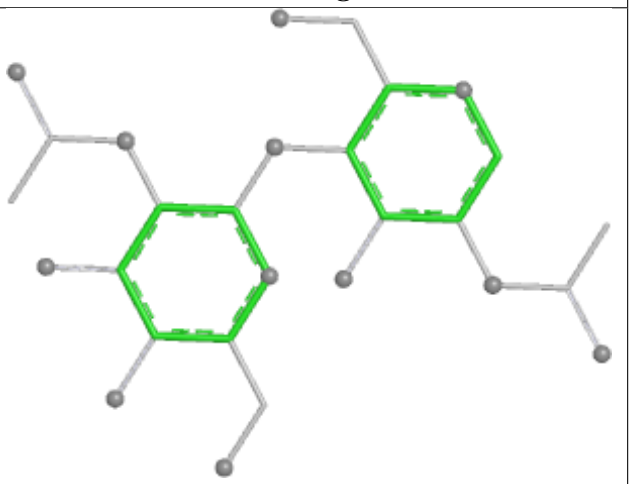
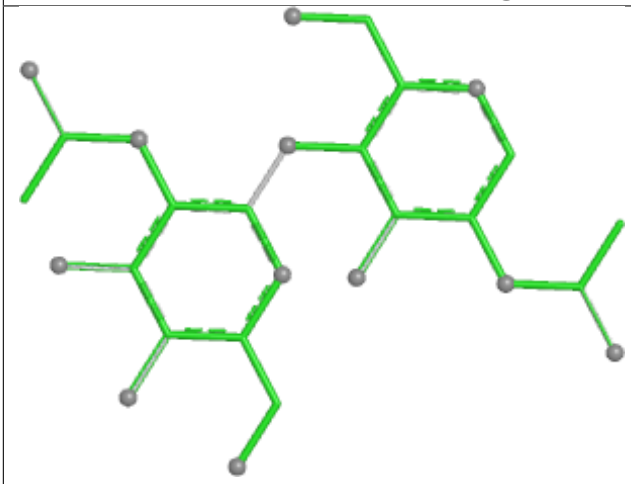
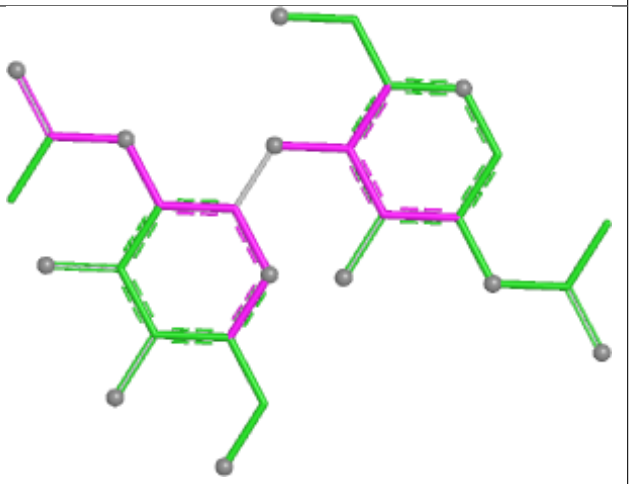


Rings

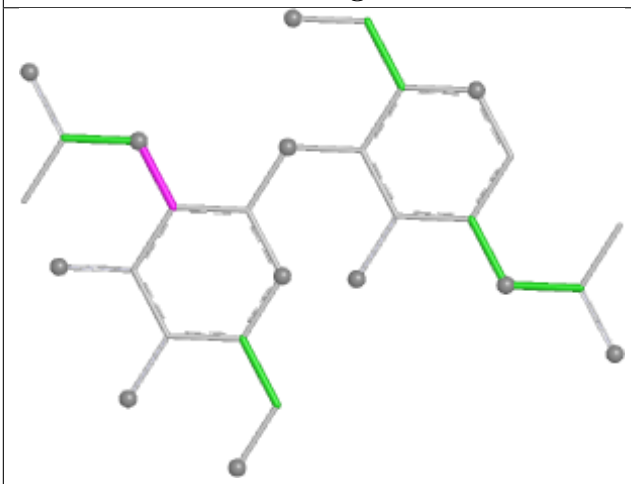
Oligosaccharide Chain b



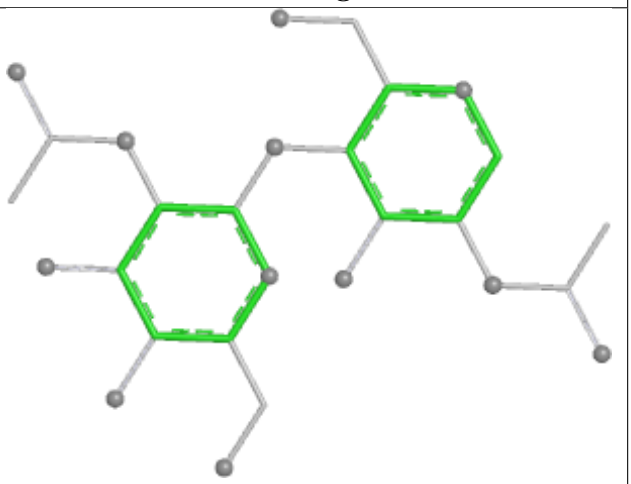
Bond lengths



Bond angles

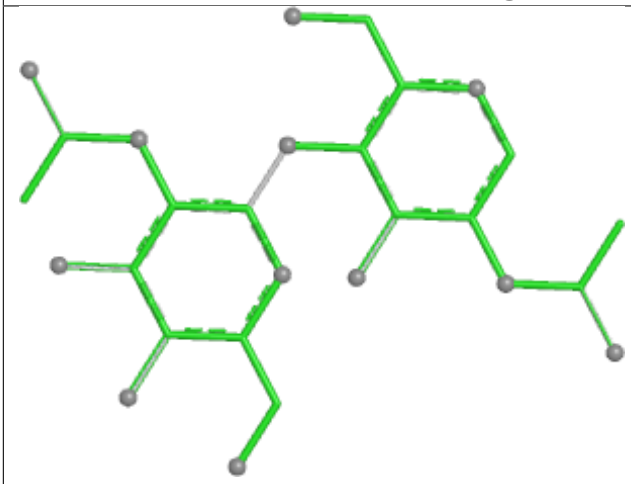


Torsions

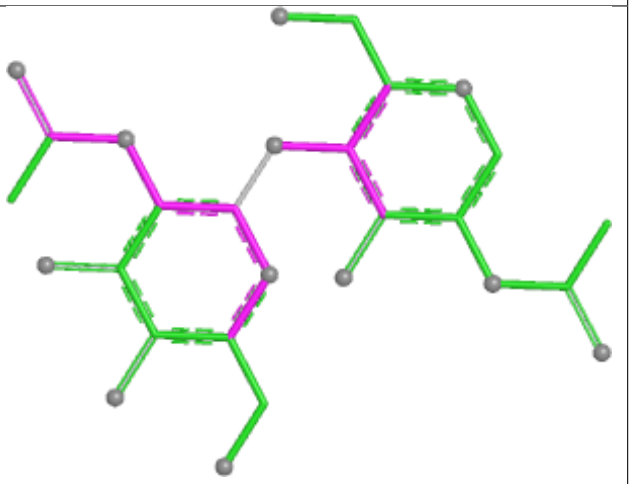


Rings

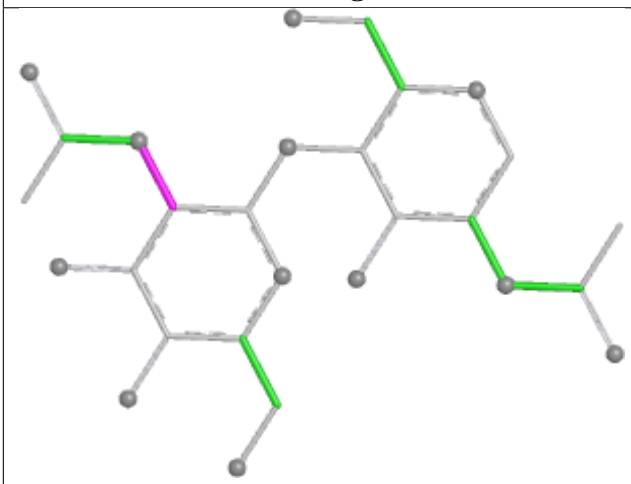
Oligosaccharide Chain f



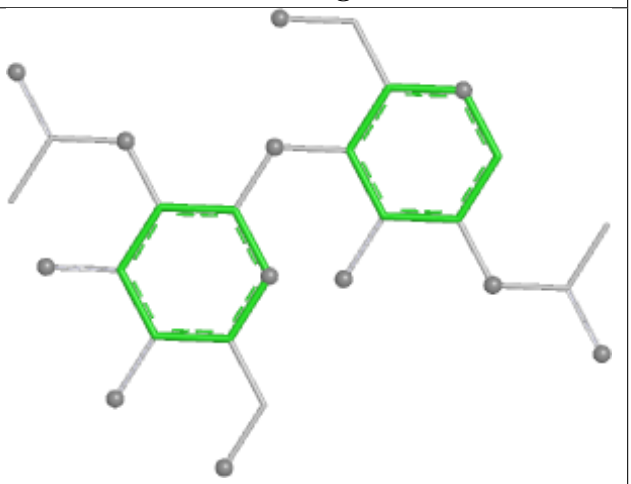
Bond lengths



Bond angles

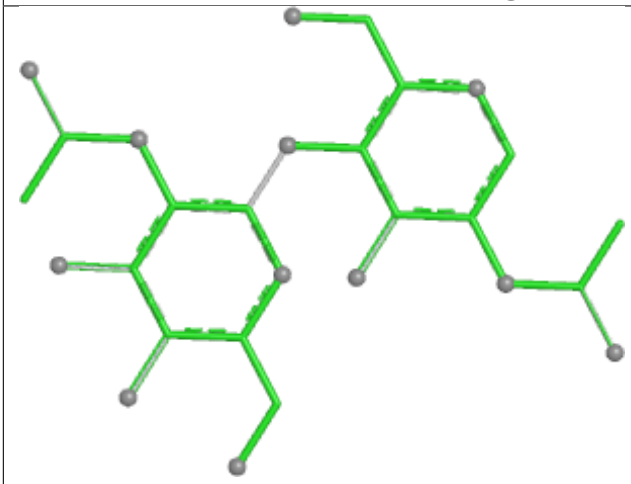


Torsions

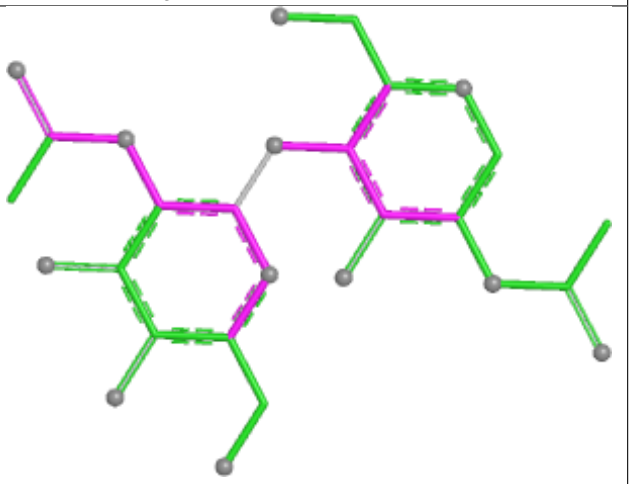


Rings

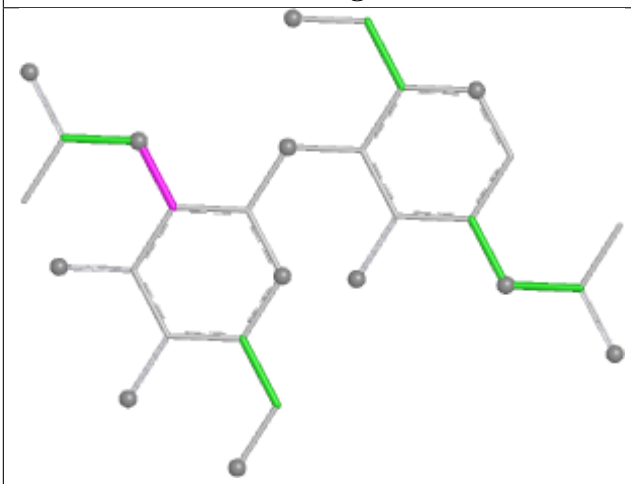
Oligosaccharide Chain j



Bond lengths



Bond angles



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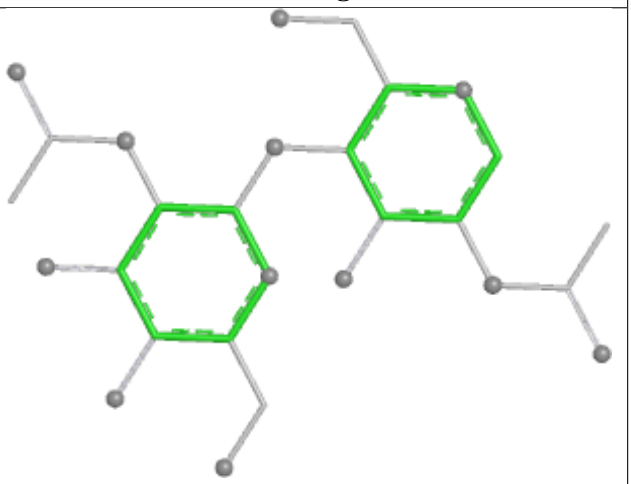
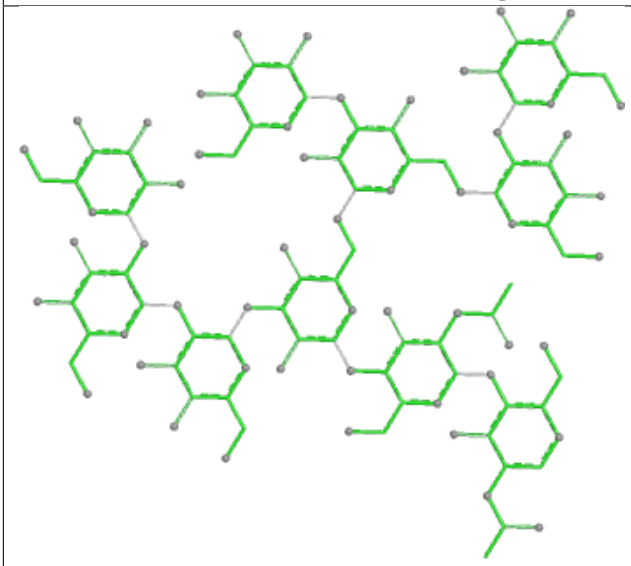
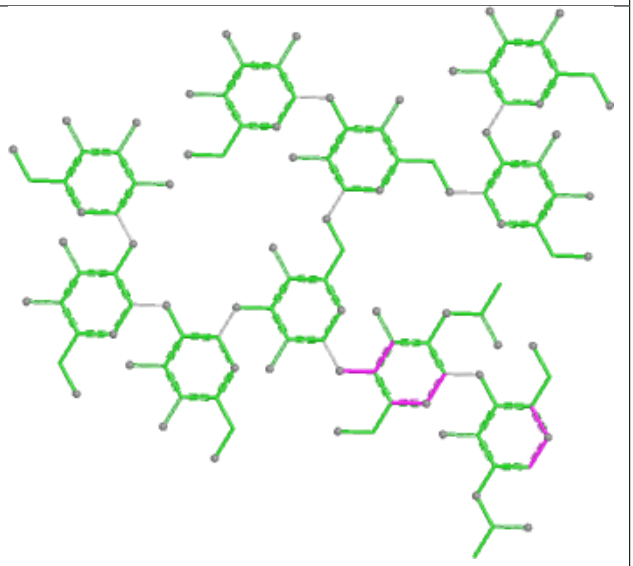


Rings

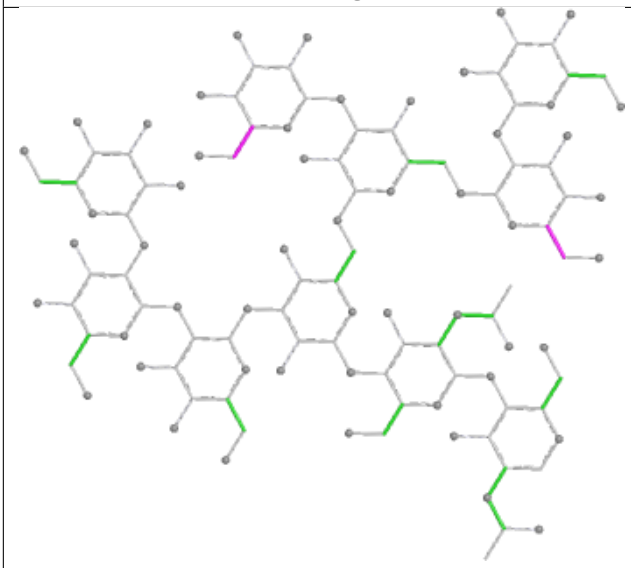
Oligosaccharide Chain Y



Bond lengths



Bond angles



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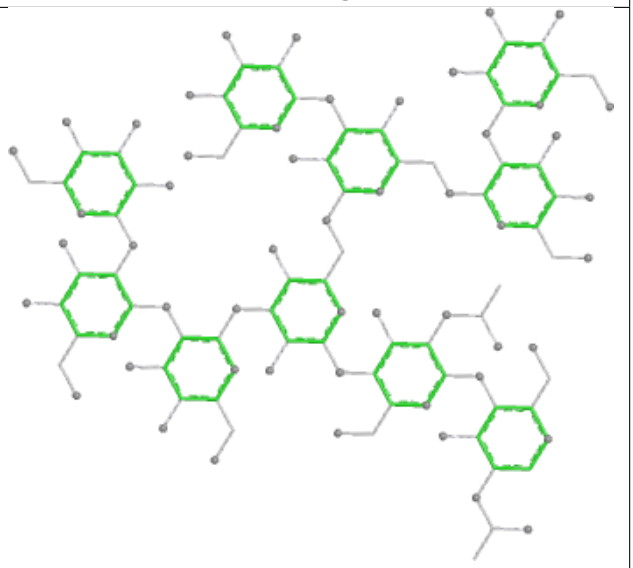
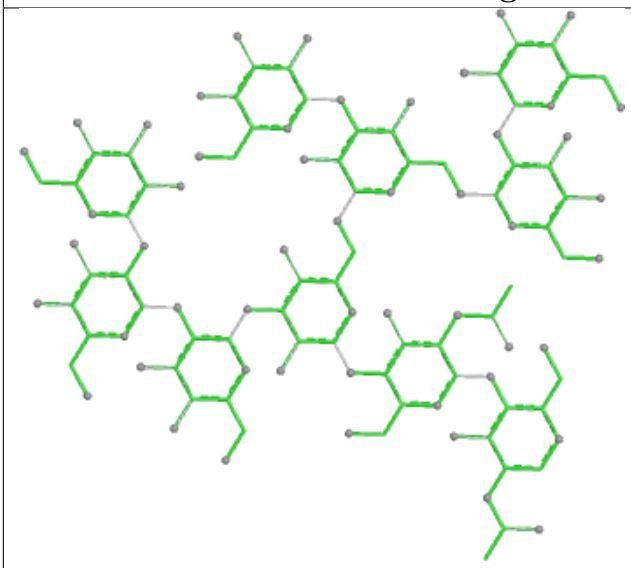


Rings

Oligosaccharide Chain c



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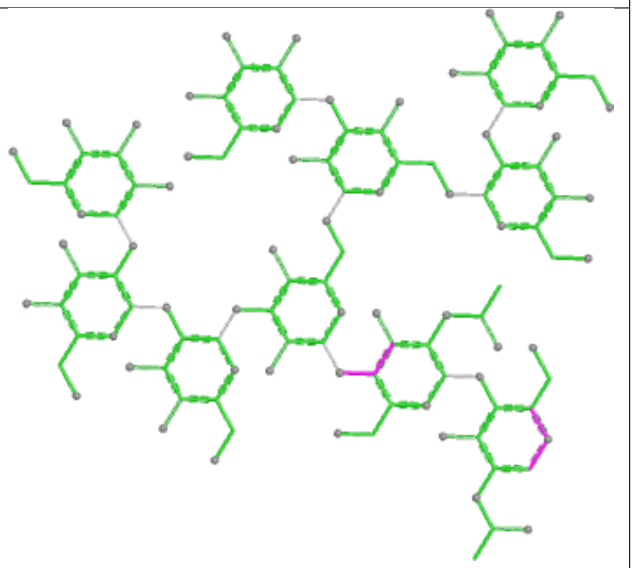
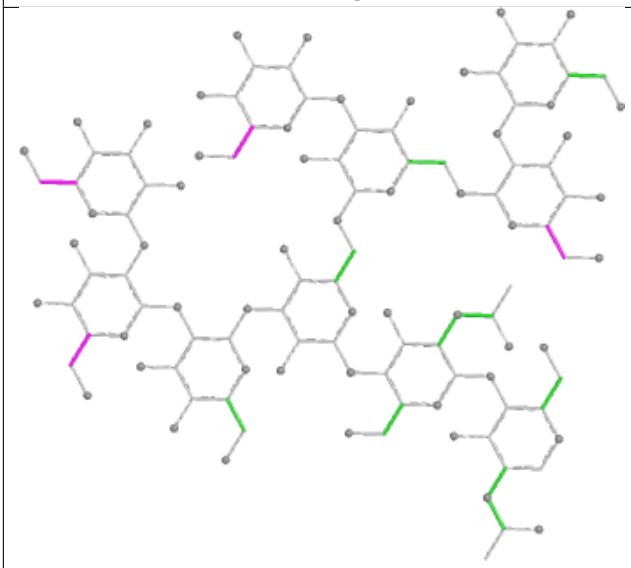


Bond angles



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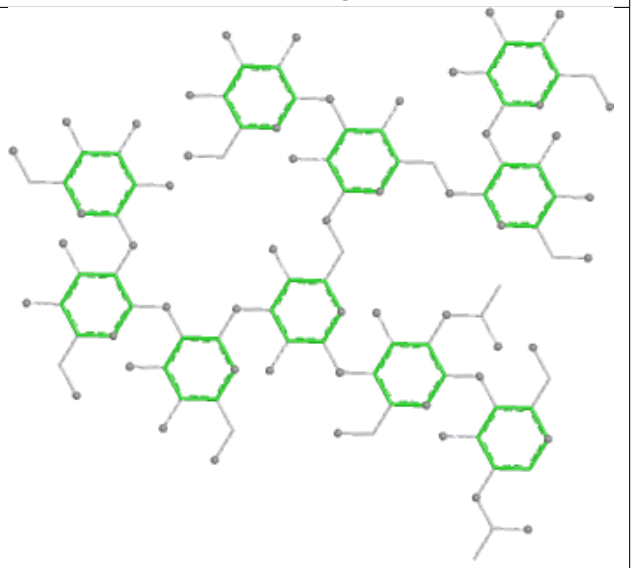
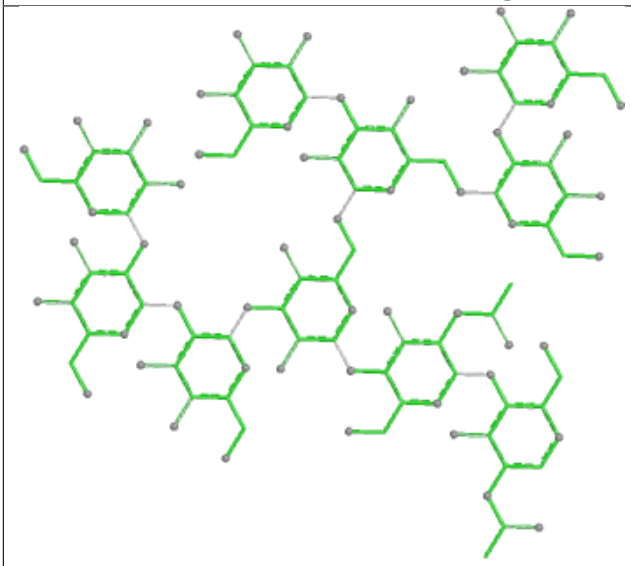
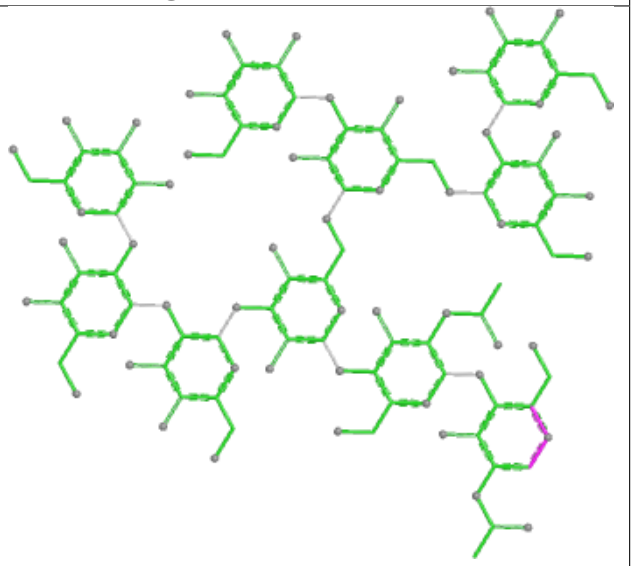


Rings

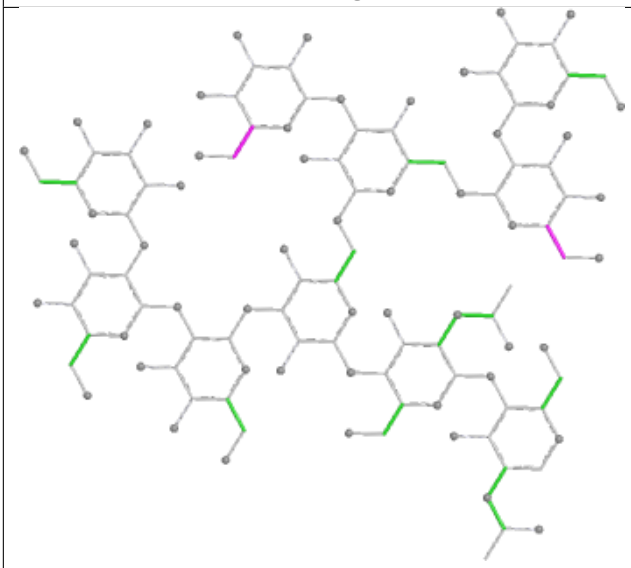
Oligosaccharide Chain g



Bond lengths



Bond angles



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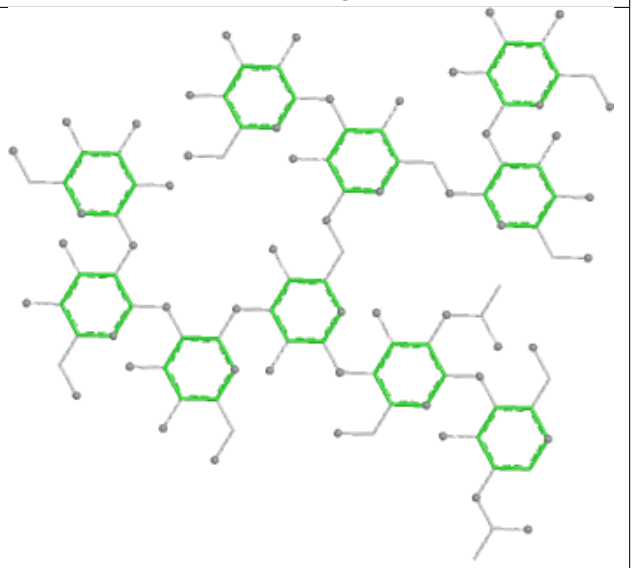
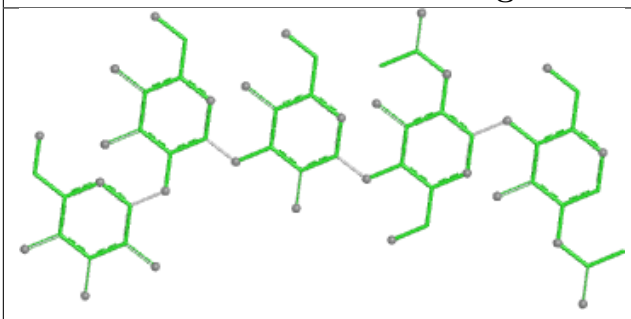
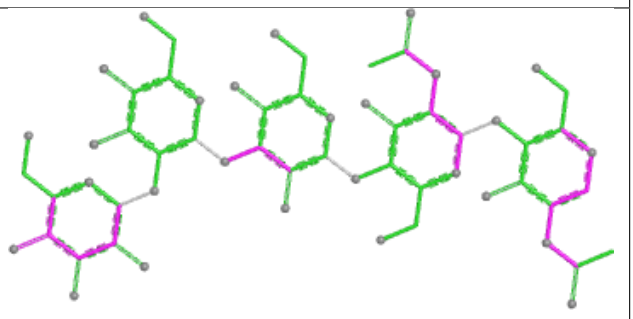


Rings

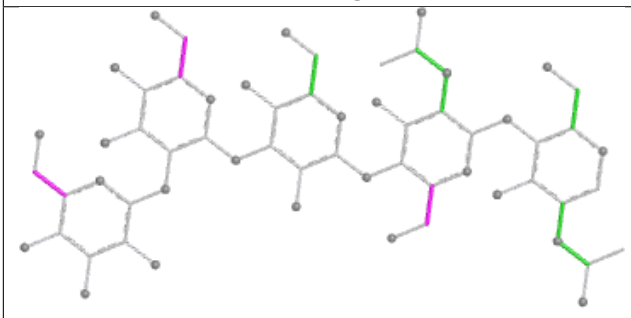
Oligosaccharide Chain Z



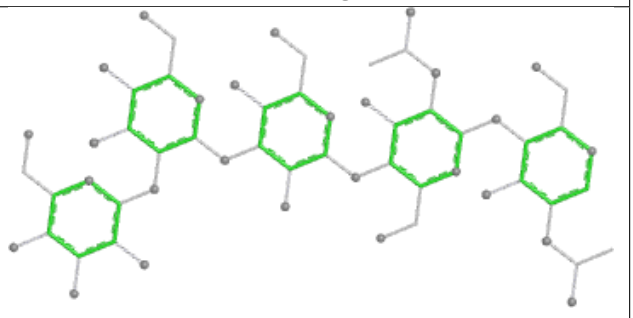
Bond lengths



Bond angles

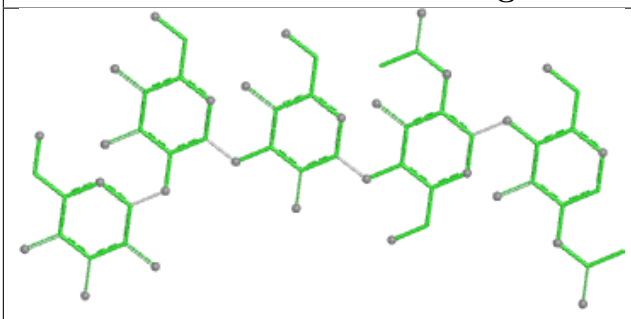


Torsions

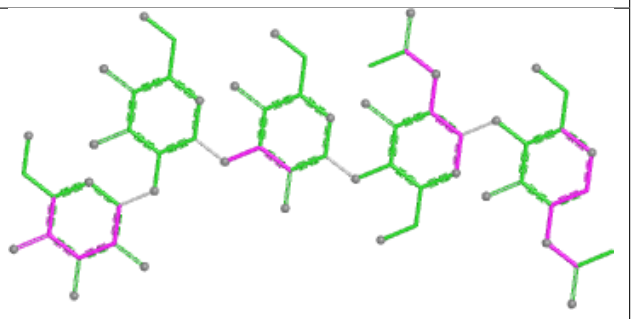


Rings

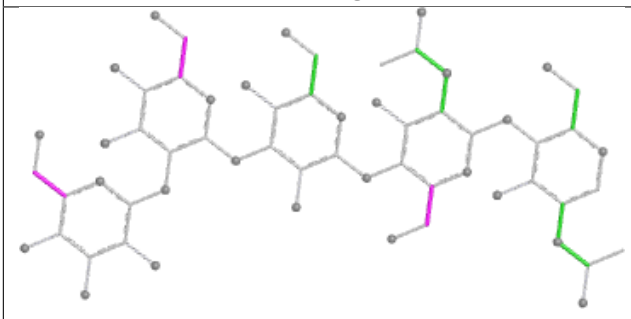
Oligosaccharide Chain d



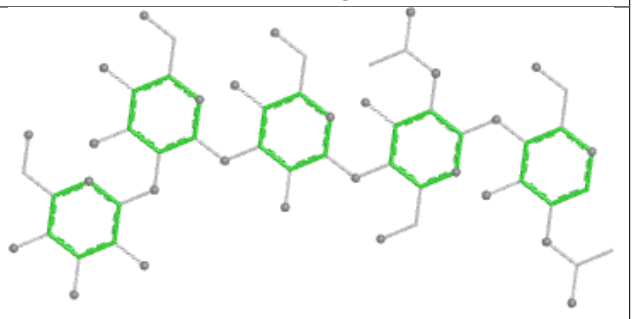
Bond lengths



Bond angles

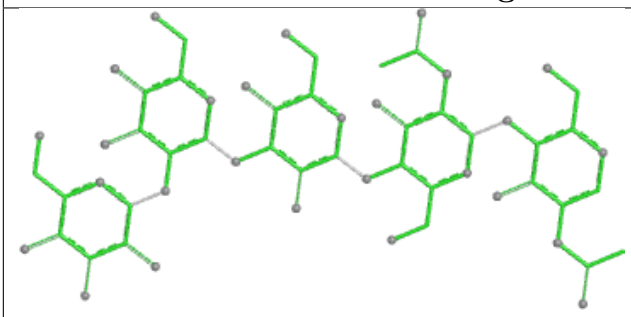


Torsions

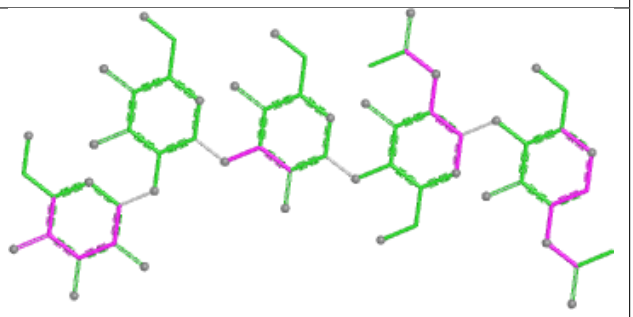


Rings

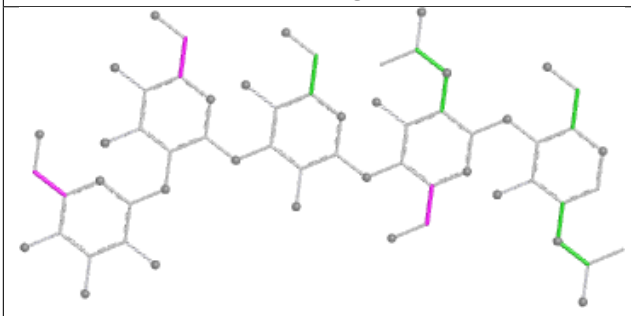
Oligosaccharide Chain h



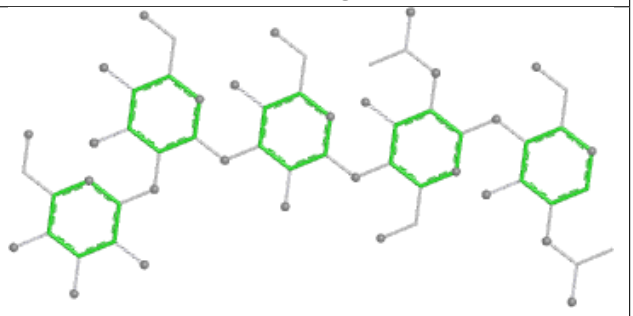
Bond lengths



Bond angles

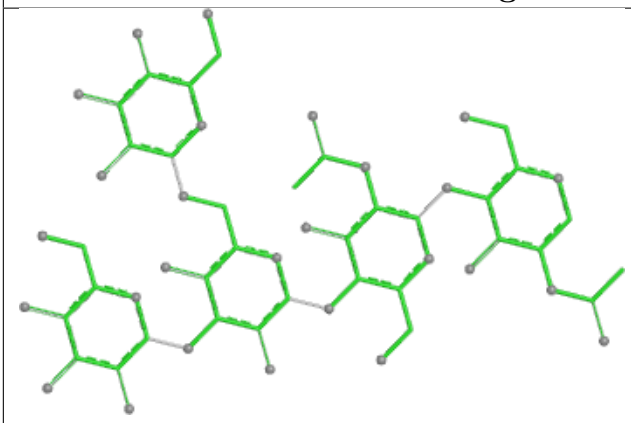


Torsions

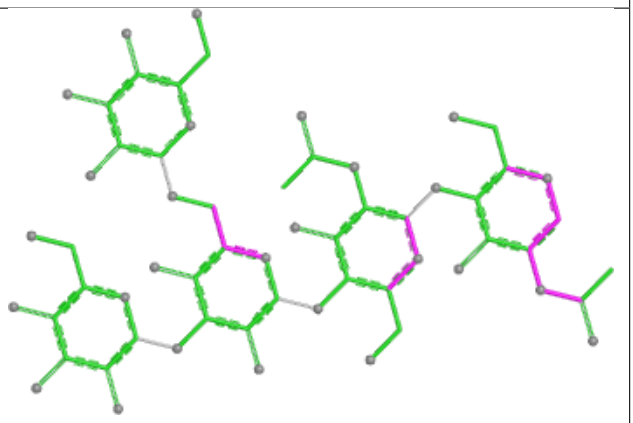


Rings

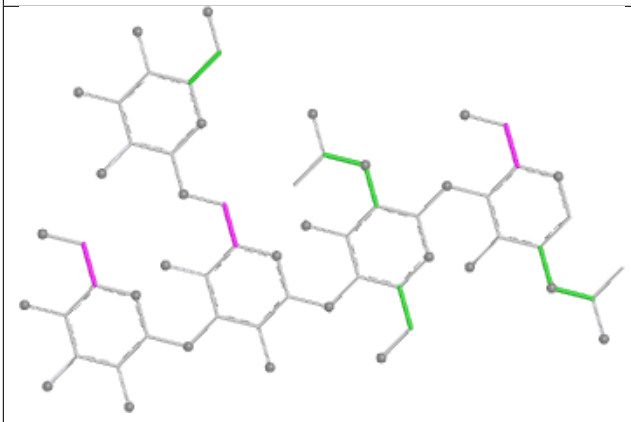
Oligosaccharide Chain a



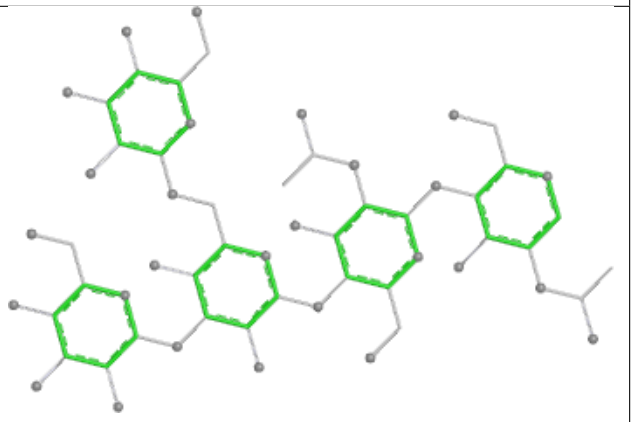
Bond lengths



Bond angles

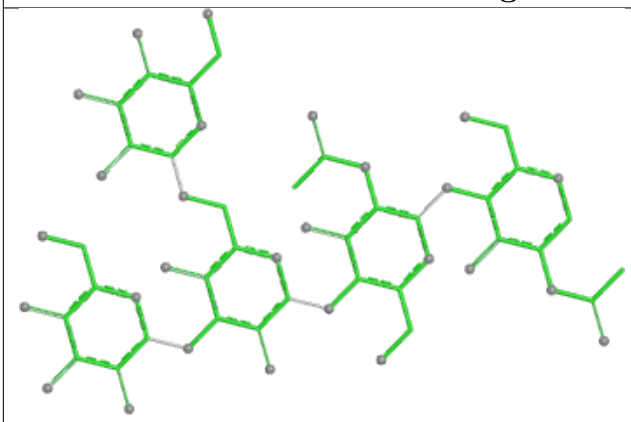


Torsions

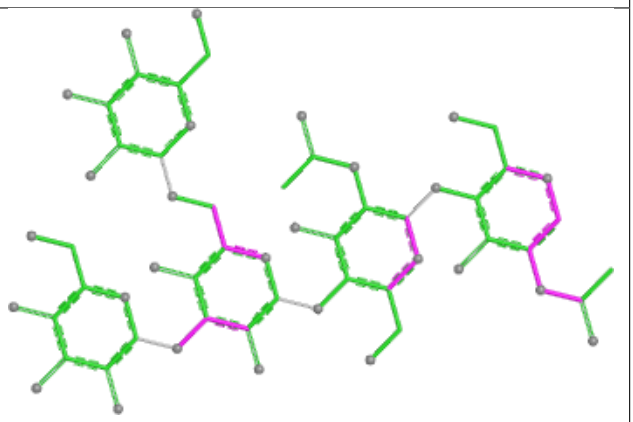


Rings

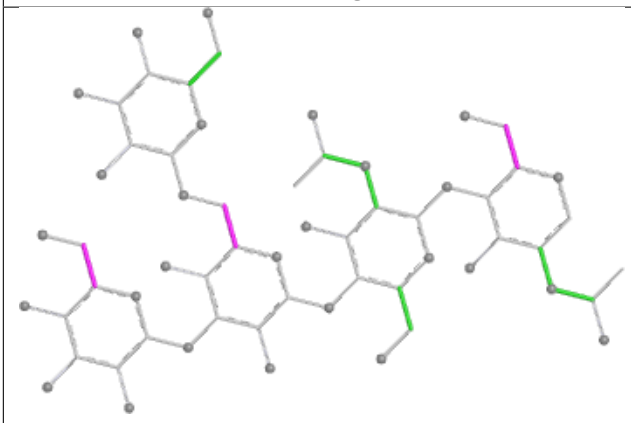
Oligosaccharide Chain e



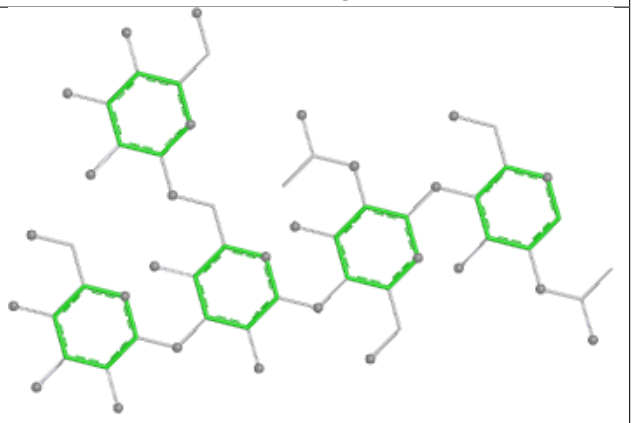
Bond lengths



Bond angles

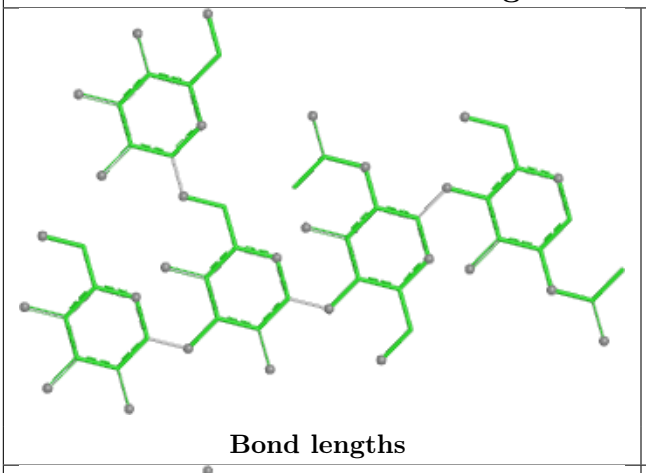


Torsions

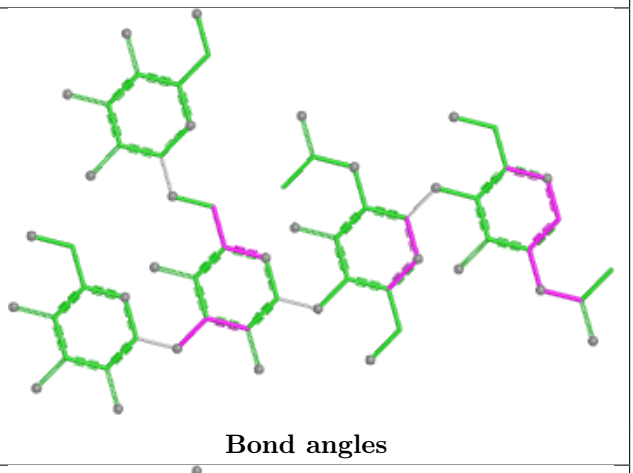


Rings

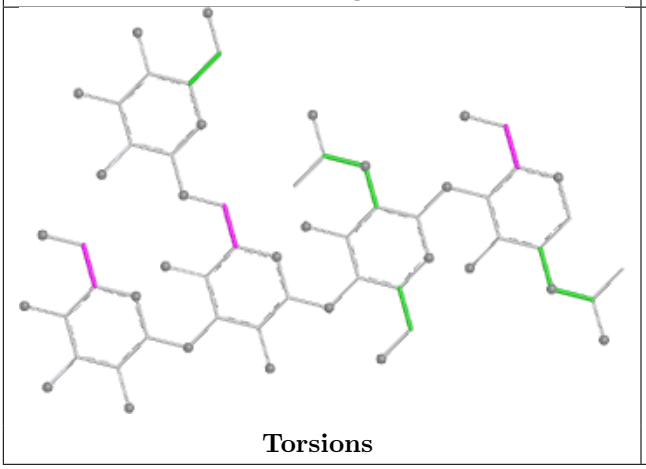
Oligosaccharide Chain i



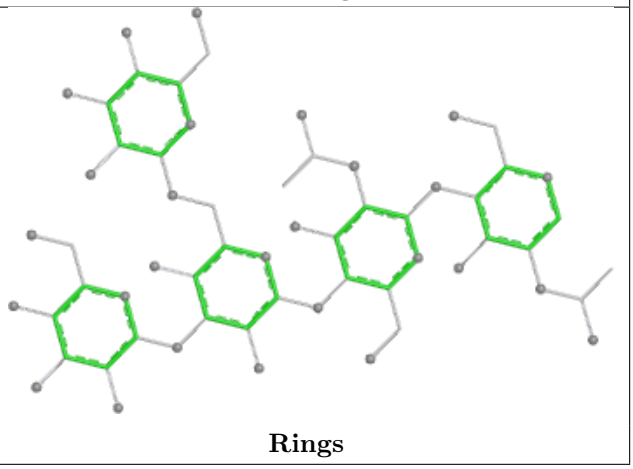
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
12	NAG	E	606	2	14,14,15	0.35	0	17,19,21	1.27	1 (5%)
12	NAG	F	601	2	14,14,15	0.30	0	17,19,21	0.85	1 (5%)
12	NAG	E	601	2	14,14,15	0.28	0	17,19,21	0.83	0
12	NAG	E	604	2	14,14,15	0.34	0	17,19,21	0.94	1 (5%)
12	NAG	D	605	2	14,14,15	0.38	0	17,19,21	0.77	0
12	NAG	D	604	2	14,14,15	0.34	0	17,19,21	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	NAG	D	603	2	14,14,15	0.41	0	17,19,21	0.76	0
12	NAG	F	605	2	14,14,15	0.39	0	17,19,21	0.76	0
12	NAG	F	603	2	14,14,15	0.41	0	17,19,21	0.74	0
12	NAG	F	606	2	14,14,15	0.34	0	17,19,21	1.24	1 (5%)
12	NAG	E	603	2	14,14,15	0.42	0	17,19,21	0.77	0
12	NAG	E	605	2	14,14,15	0.36	0	17,19,21	0.77	0
12	NAG	D	602	2	14,14,15	0.32	0	17,19,21	1.16	2 (11%)
12	NAG	E	602	2	14,14,15	0.33	0	17,19,21	1.11	2 (11%)
12	NAG	F	602	2	14,14,15	0.33	0	17,19,21	1.15	2 (11%)
12	NAG	F	604	2	14,14,15	0.34	0	17,19,21	0.96	1 (5%)
12	NAG	D	606	2	14,14,15	0.34	0	17,19,21	1.24	1 (5%)
12	NAG	D	601	2	14,14,15	0.29	0	17,19,21	0.86	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	E	606	2	-	3/6/23/26	0/1/1/1
12	NAG	F	601	2	-	2/6/23/26	0/1/1/1
12	NAG	E	601	2	-	2/6/23/26	0/1/1/1
12	NAG	E	604	2	-	2/6/23/26	0/1/1/1
12	NAG	D	605	2	-	0/6/23/26	0/1/1/1
12	NAG	D	604	2	-	2/6/23/26	0/1/1/1
12	NAG	D	603	2	-	2/6/23/26	0/1/1/1
12	NAG	F	605	2	-	0/6/23/26	0/1/1/1
12	NAG	F	603	2	-	2/6/23/26	0/1/1/1
12	NAG	F	606	2	-	3/6/23/26	0/1/1/1
12	NAG	E	603	2	-	2/6/23/26	0/1/1/1
12	NAG	E	605	2	-	0/6/23/26	0/1/1/1
12	NAG	D	602	2	-	0/6/23/26	0/1/1/1
12	NAG	E	602	2	-	0/6/23/26	0/1/1/1
12	NAG	F	602	2	-	0/6/23/26	0/1/1/1
12	NAG	F	604	2	-	2/6/23/26	0/1/1/1
12	NAG	D	606	2	-	3/6/23/26	0/1/1/1
12	NAG	D	601	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	606	NAG	C1-O5-C5	3.53	116.91	112.19
12	D	606	NAG	C1-O5-C5	3.39	116.74	112.19
12	F	606	NAG	C1-O5-C5	3.39	116.73	112.19
12	D	602	NAG	C1-O5-C5	2.95	116.14	112.19
12	E	602	NAG	C1-O5-C5	2.91	116.09	112.19
12	F	602	NAG	C1-O5-C5	2.85	116.01	112.19
12	F	602	NAG	O5-C1-C2	-2.28	107.77	111.29
12	D	602	NAG	O5-C1-C2	-2.22	107.86	111.29
12	F	604	NAG	C2-N2-C7	2.18	125.81	122.90
12	E	604	NAG	C2-N2-C7	2.14	125.77	122.90
12	E	602	NAG	O5-C1-C2	-2.13	107.99	111.29
12	F	601	NAG	C1-O5-C5	2.00	114.87	112.19
12	D	601	NAG	C1-O5-C5	2.00	114.87	112.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	D	606	NAG	C8-C7-N2-C2
12	D	606	NAG	O7-C7-N2-C2
12	E	606	NAG	C8-C7-N2-C2
12	E	606	NAG	O7-C7-N2-C2
12	F	606	NAG	C8-C7-N2-C2
12	F	606	NAG	O7-C7-N2-C2
12	F	606	NAG	O5-C5-C6-O6
12	E	606	NAG	O5-C5-C6-O6
12	D	606	NAG	O5-C5-C6-O6
12	E	601	NAG	O5-C5-C6-O6
12	F	601	NAG	O5-C5-C6-O6
12	F	603	NAG	O5-C5-C6-O6
12	E	601	NAG	C4-C5-C6-O6
12	F	604	NAG	O5-C5-C6-O6
12	F	601	NAG	C4-C5-C6-O6
12	E	603	NAG	O5-C5-C6-O6
12	F	604	NAG	C4-C5-C6-O6
12	D	603	NAG	O5-C5-C6-O6
12	E	604	NAG	O5-C5-C6-O6
12	E	604	NAG	C4-C5-C6-O6
12	D	601	NAG	O5-C5-C6-O6
12	D	601	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	D	604	NAG	C4-C5-C6-O6
12	D	604	NAG	O5-C5-C6-O6
12	F	603	NAG	C4-C5-C6-O6
12	E	603	NAG	C4-C5-C6-O6
12	D	603	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

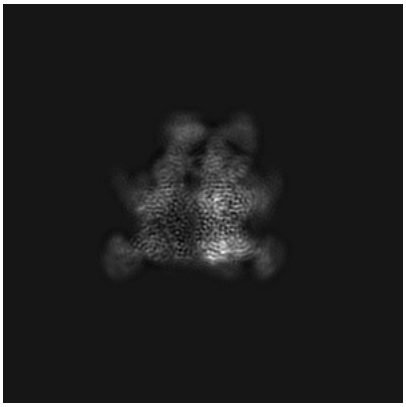
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7516. These allow visual inspection of the internal detail of the map and identification of artifacts.

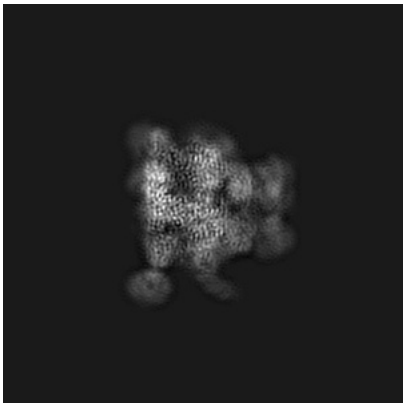
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

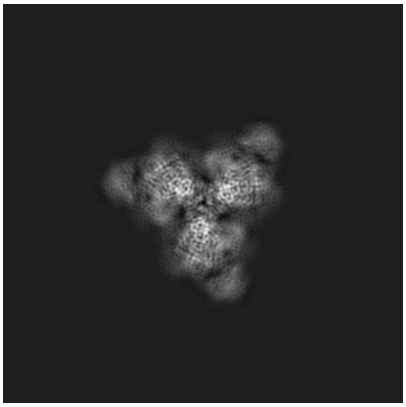
6.1.1 Primary map



X



Y

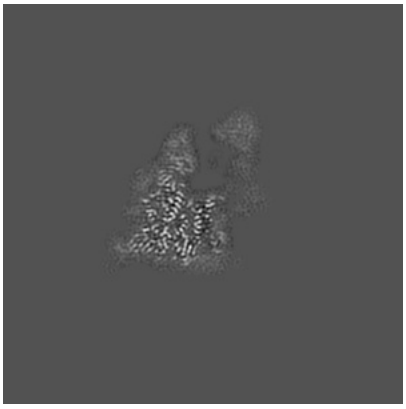


Z

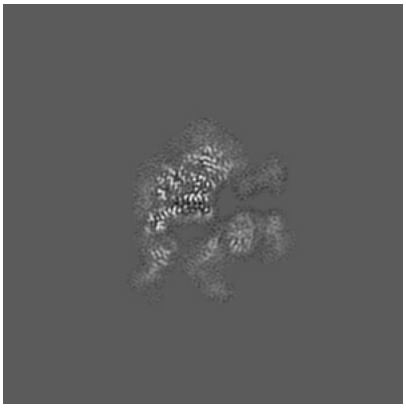
The images above show the map projected in three orthogonal directions.

6.2 Central slices

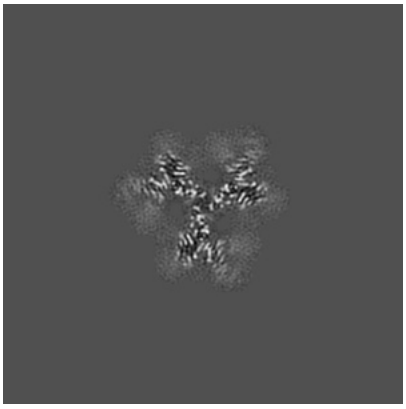
6.2.1 Primary map



X Index: 150



Y Index: 150

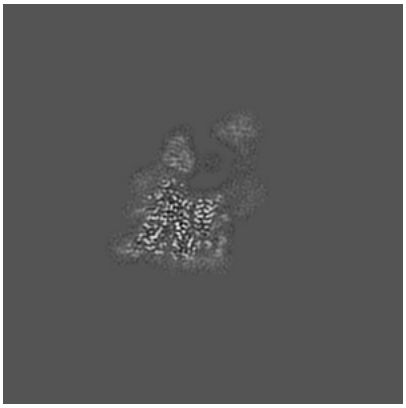


Z Index: 150

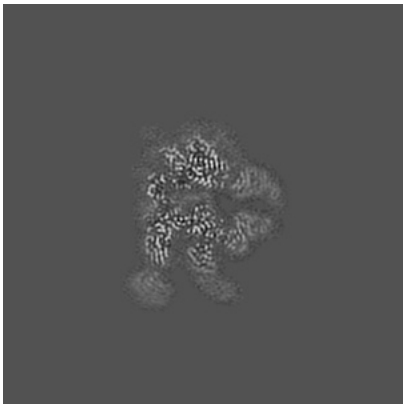
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 148



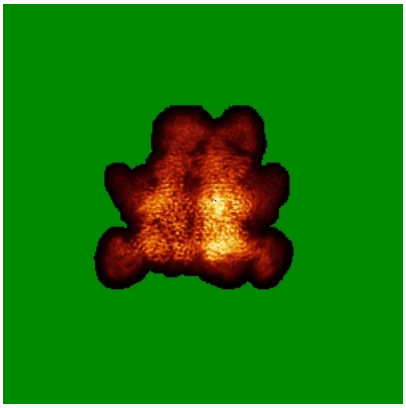
Y Index: 160

Z Index: 119

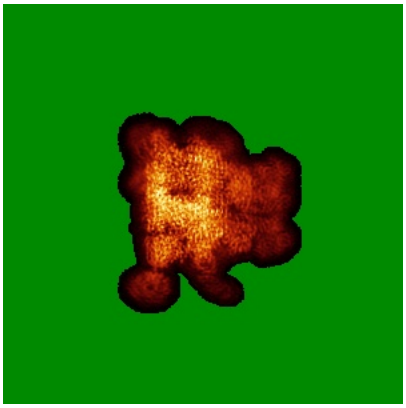
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

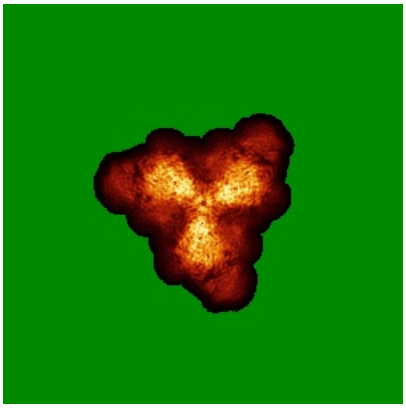
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0386. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

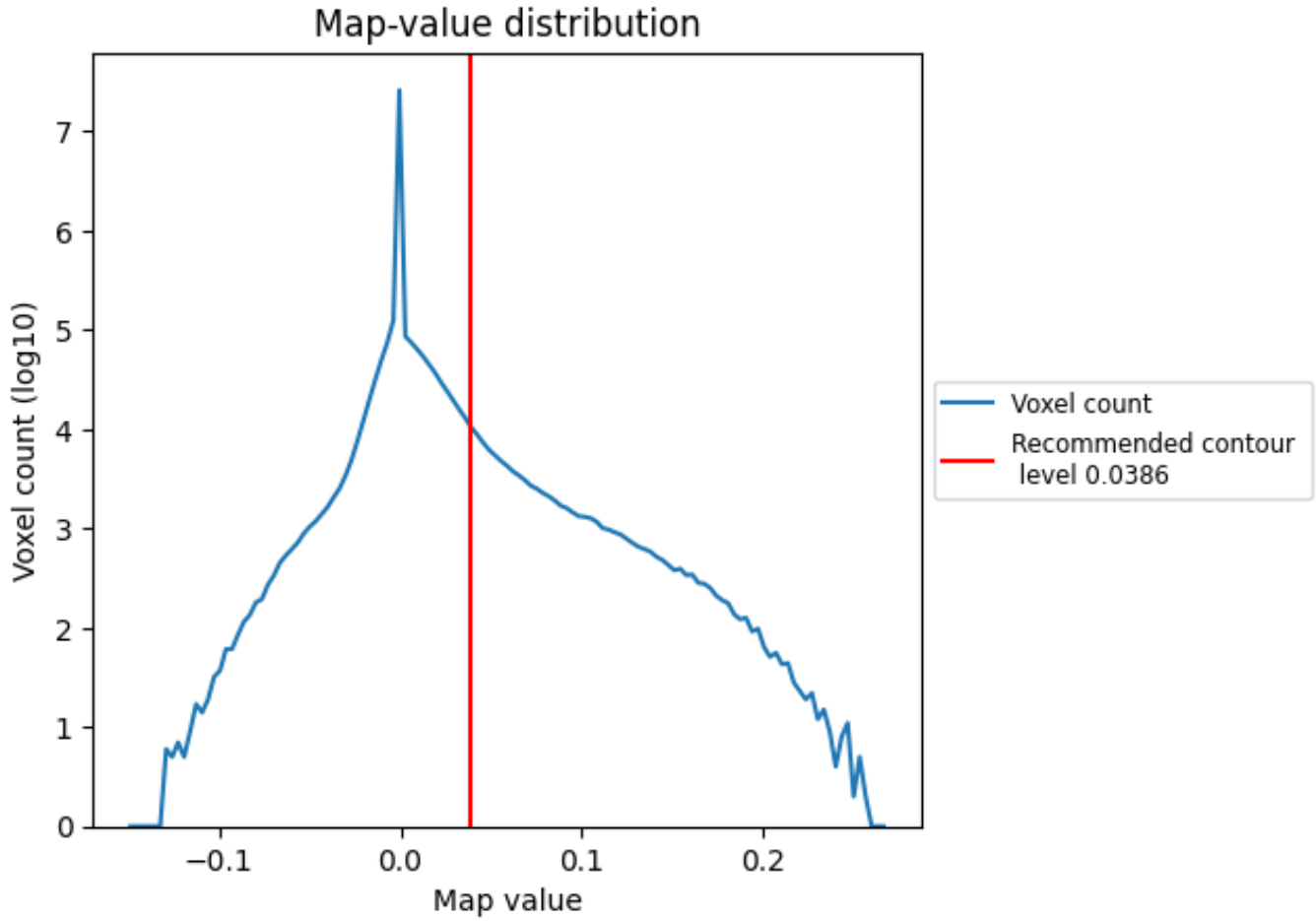
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

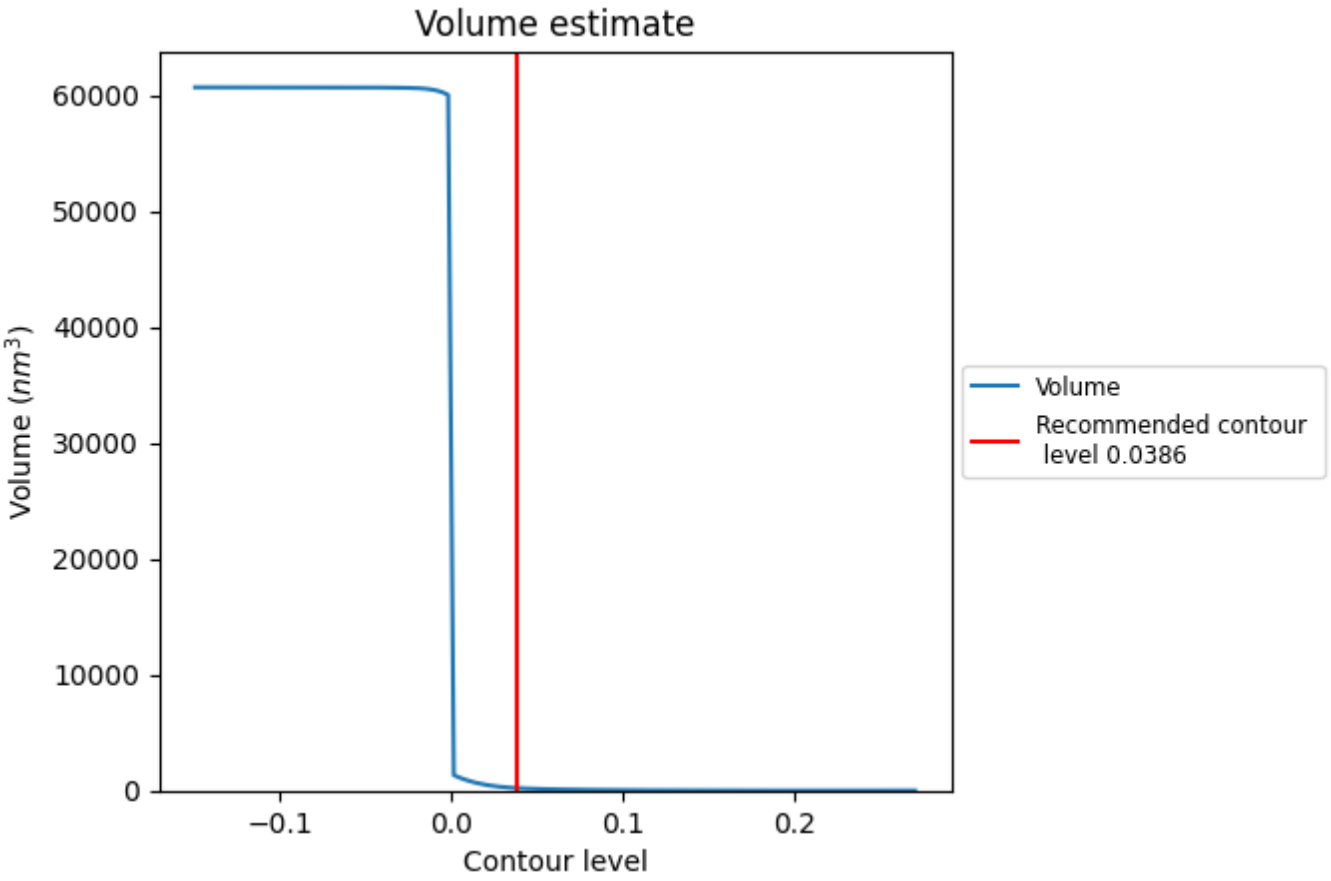
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

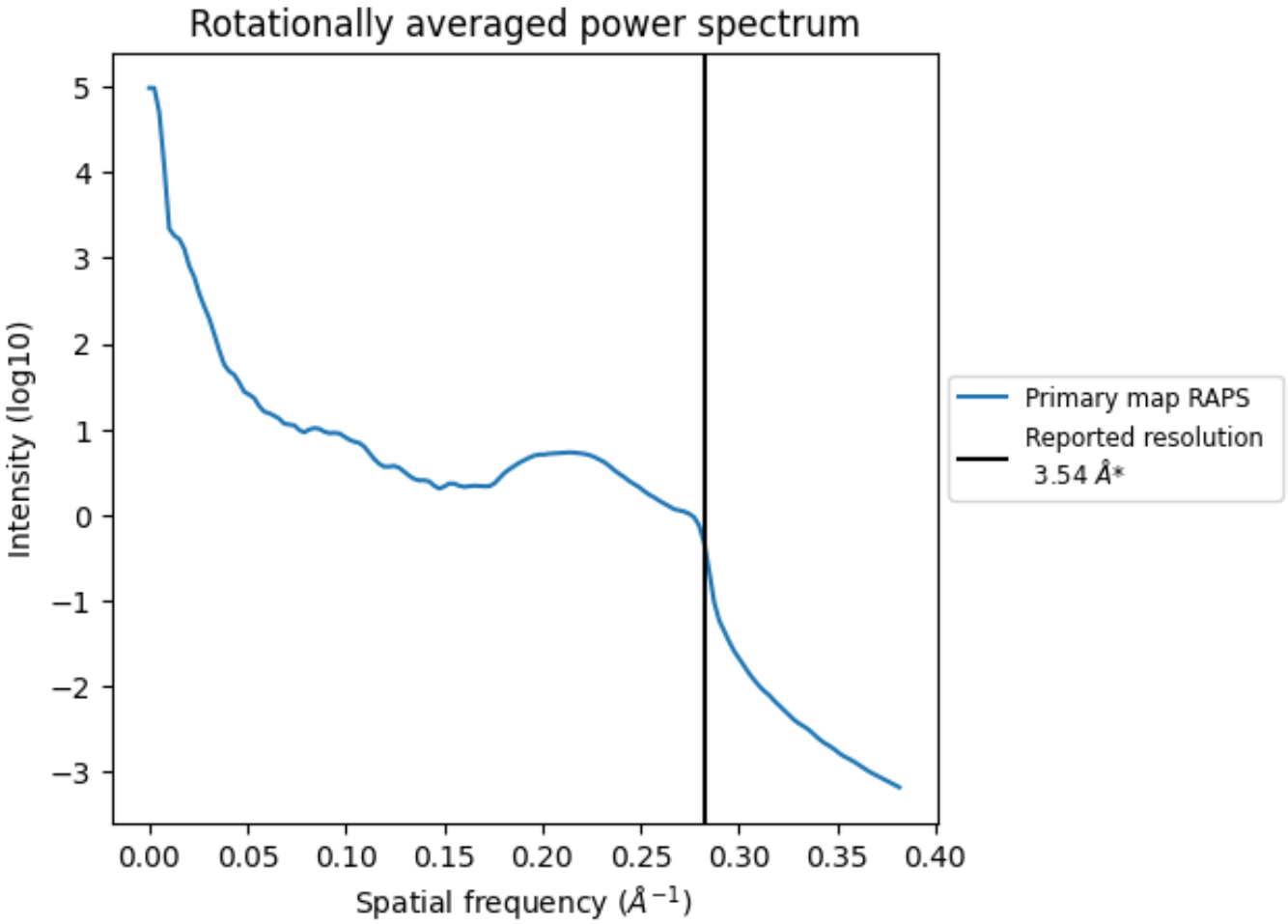
7.2 Volume estimate



The volume at the recommended contour level is 210 nm^3; this corresponds to an approximate mass of 190 kDa.

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

7.3 Rotationally averaged power spectrum (i)

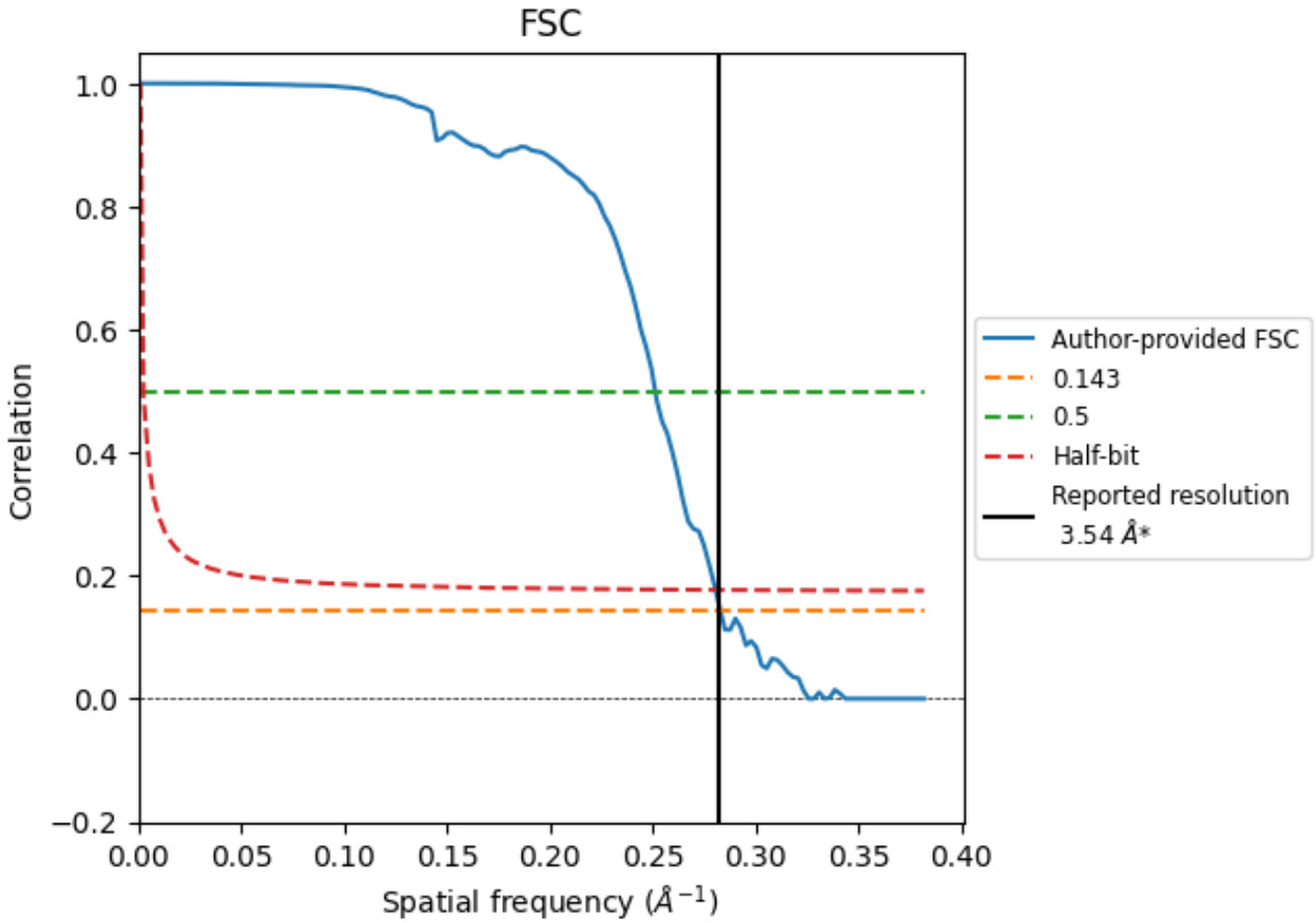


*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.282 Å^{-1}

8.2 Resolution estimates (i)

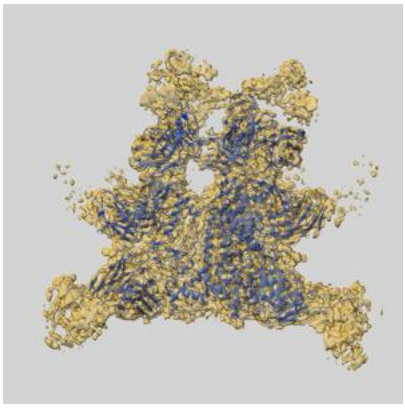
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.54	-	-
Author-provided FSC curve	3.54	3.98	3.57
Unmasked-calculated*	-	-	-

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

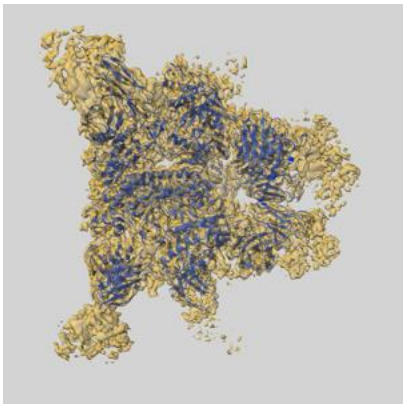
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7516 and PDB model 6CM3. Per-residue inclusion information can be found in section 3 on page 12.

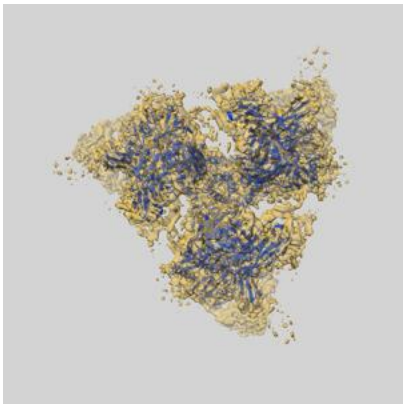
9.1 Map-model overlay



X



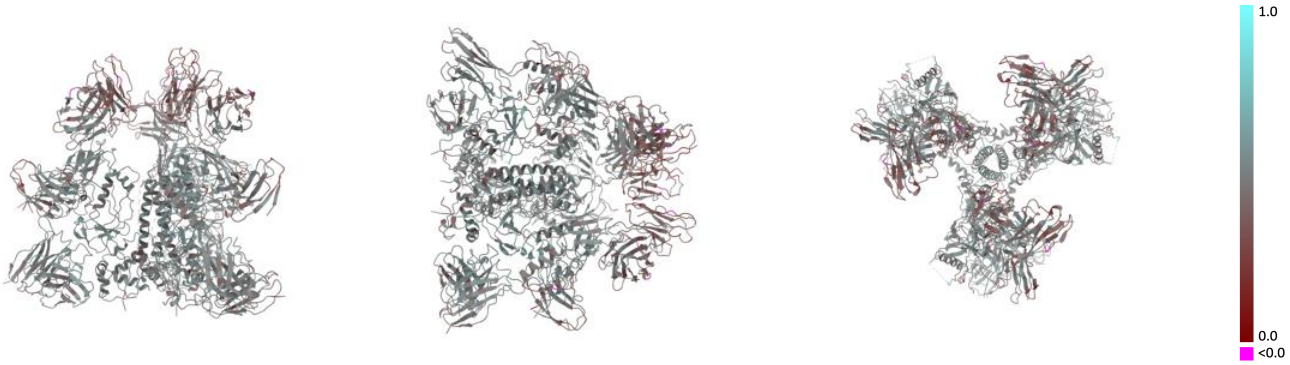
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0386 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

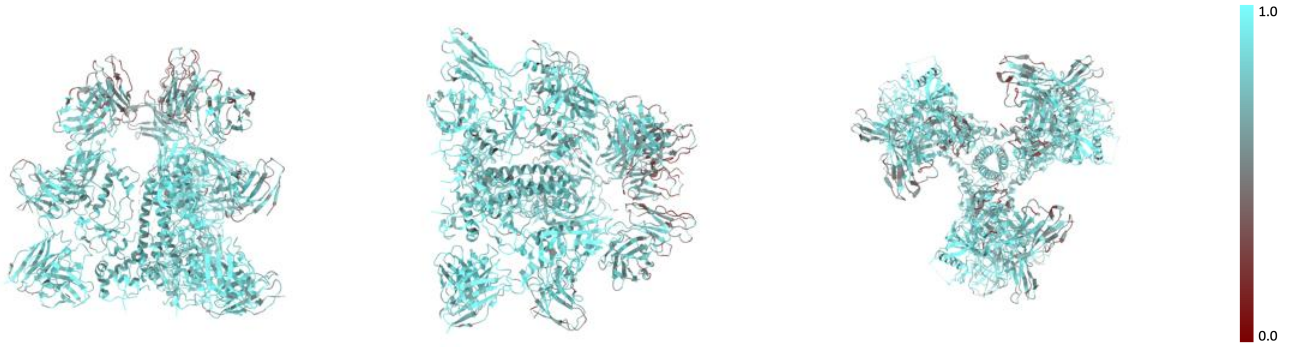
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

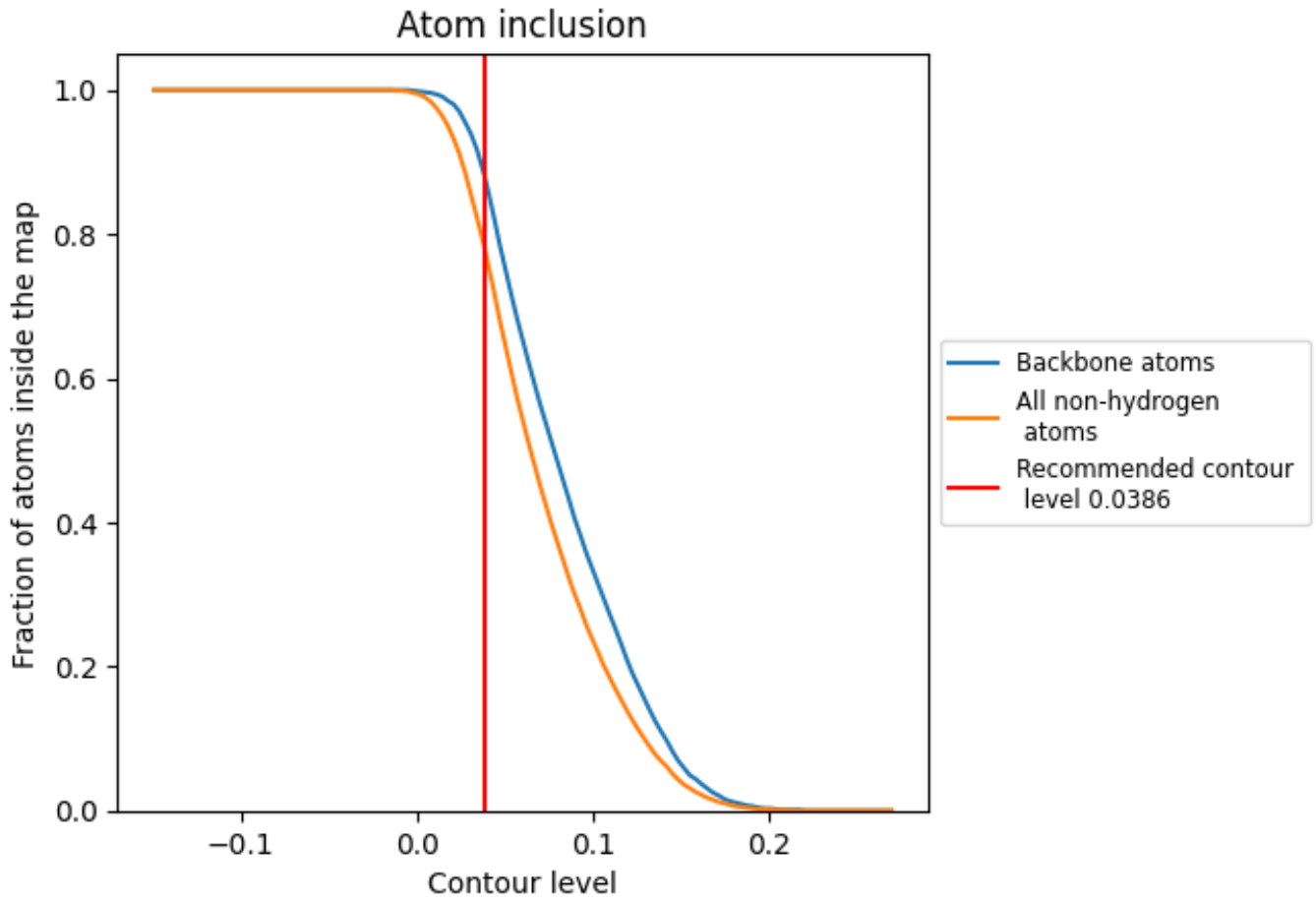
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0386).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0386) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.4650
A	0.8460	0.4960
B	0.8540	0.5010
C	0.8420	0.4980
D	0.8370	0.4920
E	0.8360	0.4940
F	0.8380	0.4930
G	0.7100	0.4450
H	0.7040	0.4470
I	0.7000	0.4450
J	0.5970	0.3600
K	0.6850	0.4140
L	0.6040	0.3650
M	0.6810	0.4120
N	0.5950	0.3620
O	0.6770	0.4090
P	0.8420	0.4990
Q	0.8140	0.4710
R	0.8410	0.4910
S	0.8100	0.4740
T	0.8360	0.5000
U	0.8100	0.4740
V	0.7500	0.4620
W	0.7860	0.4690
X	0.7860	0.4510
Y	0.8360	0.4750
Z	0.8360	0.5080
a	0.7540	0.4640
b	0.8210	0.4640
c	0.8280	0.4700
d	0.8200	0.5170
e	0.7540	0.4520
f	0.8570	0.4720
g	0.8450	0.4710
h	0.8360	0.5180

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Chain	Atom inclusion	Q-score
i	0.7540	0.4530
j	0.8570	0.4820