Full wwPDB EM Validation Report ⓘ

Jun 27, 2024 – 12:22 AM JST

PDB ID	:	8XUR
EMDB ID	:	EMD-38681
Title	:	BA.2.86 Spike Trimer in complex with heparan sulfate
Authors	:	Yue, C.; Liu, P.
Deposited on	:	2024-01-14
Resolution	:	3.85 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:

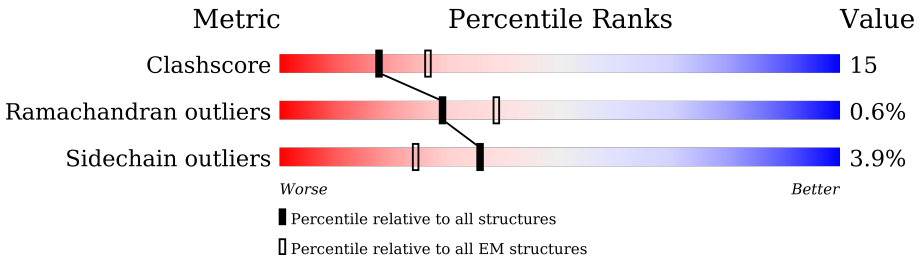
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.85 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	1206	13% 56% 30% • 12%
1	B	1206	21% 58% 29% • 12%
1	C	1206	9% 57% 30% • 12%
2	D	2	50% 50% 50%
3	E	2	100% 100%
3	F	2	100%
3	G	2	100%
3	H	2	50% 100%

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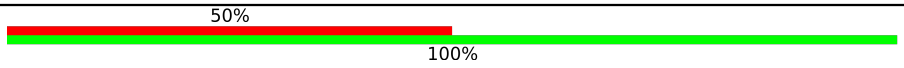
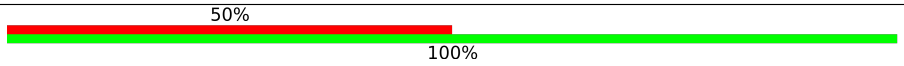
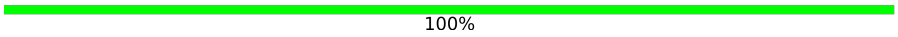
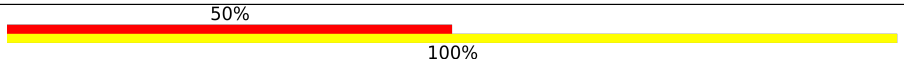
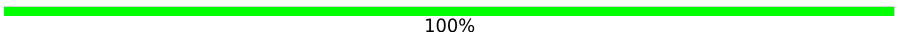
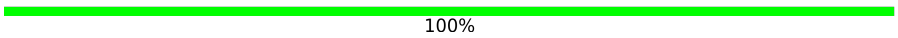
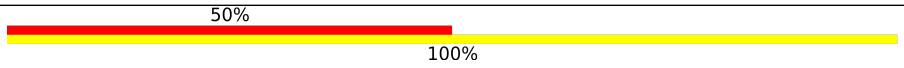
Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
1	B	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		
1	C	1063	Total	C	N	O	S	0	0
			8316	5322	1383	1573	38		

There are 219 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P0DTC2
A	-1	THR	-	expression tag	UNP P0DTC2
A	16	MET	-	insertion	UNP P0DTC2
A	17	PRO	-	insertion	UNP P0DTC2
A	18	LEU	-	insertion	UNP P0DTC2
A	19	PHE	-	insertion	UNP P0DTC2
A	22	ILE	THR	conflict	UNP P0DTC2
A	24	THR	ARG	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	143	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	216	PHE	LEU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	554	LYS	GLU	conflict	UNP P0DTC2
A	570	VAL	ALA	conflict	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	621	SER	PRO	conflict	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	ARG	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	conflict	UNP P0DTC2
A	685	ALA	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	-2	ALA	-	expression tag	UNP P0DTC2
B	-1	THR	-	expression tag	UNP P0DTC2
B	16	MET	-	insertion	UNP P0DTC2
B	17	PRO	-	insertion	UNP P0DTC2
B	18	LEU	-	insertion	UNP P0DTC2
B	19	PHE	-	insertion	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	143	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	216	PHE	LEU	variant	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	554	LYS	GLU	conflict	UNP P0DTC2
B	570	VAL	ALA	conflict	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	621	SER	PRO	conflict	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	ARG	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	conflict	UNP P0DTC2
B	685	ALA	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	-2	ALA	-	expression tag	UNP P0DTC2
C	-1	THR	-	expression tag	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	insertion	UNP P0DTC2
C	19	PHE	-	insertion	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	143	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	216	PHE	LEU	variant	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	ARG	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

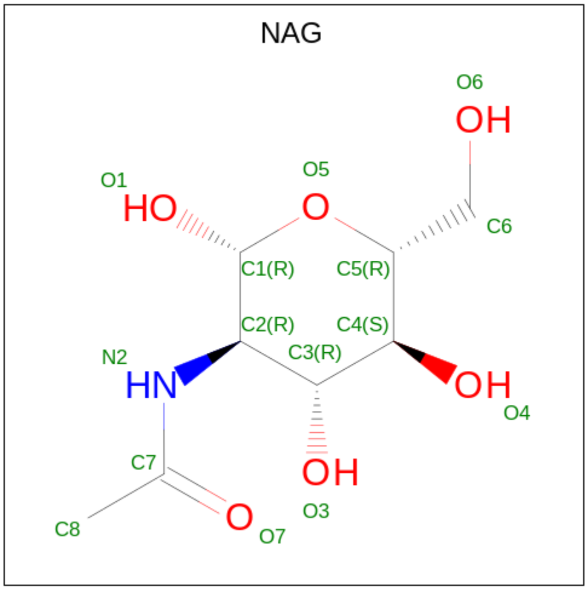
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

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

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



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

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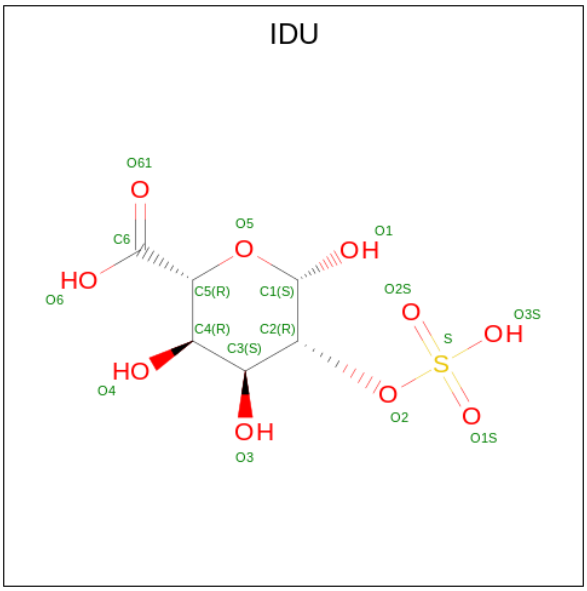
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total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

- Molecule 5 is 2-O-sulfo-beta-L-altropyranuronic acid (three-letter code: IDU) (formula: $C_6H_{10}O_{10}S$) (labeled as "Ligand of Interest" by depositor).

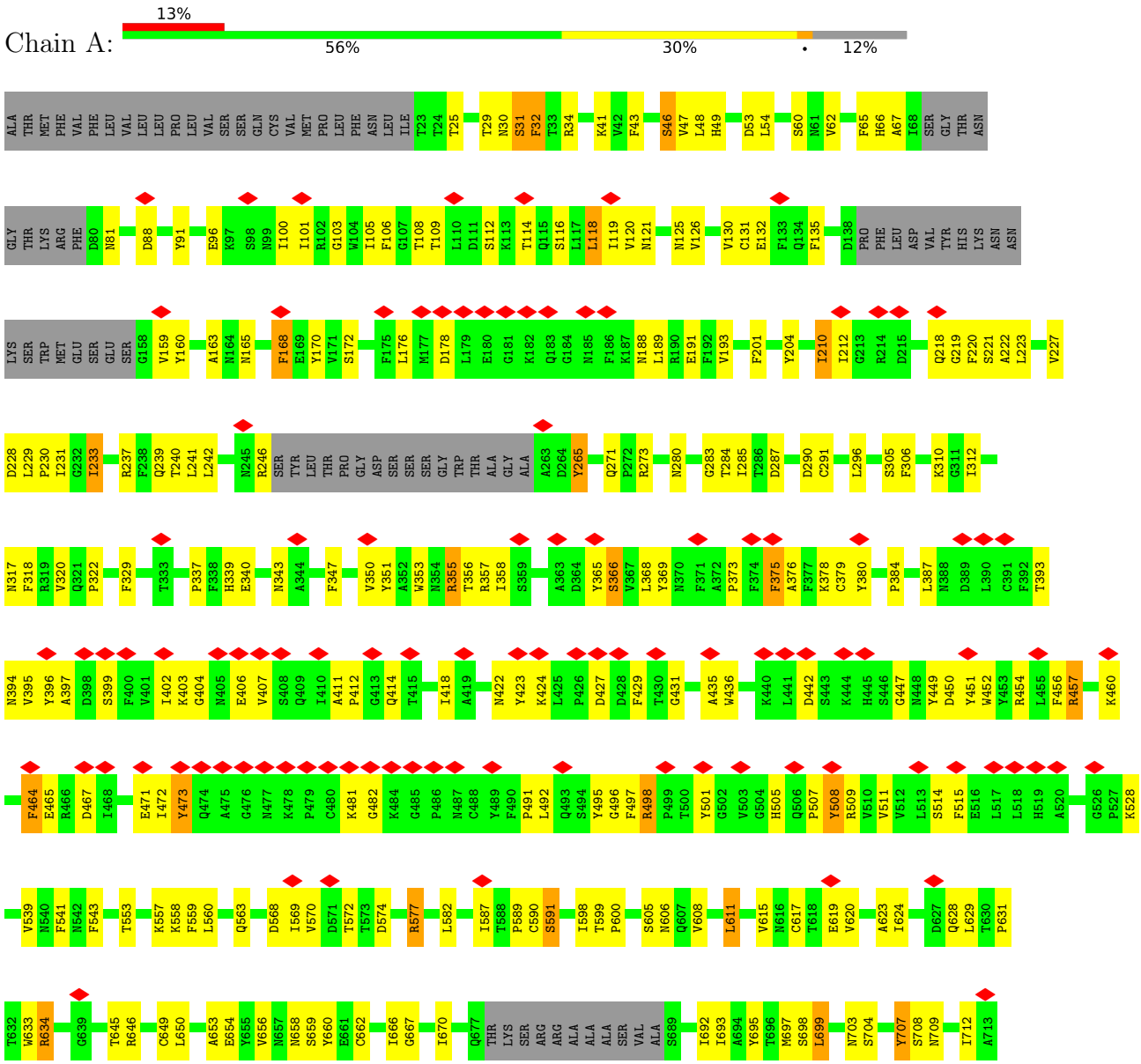


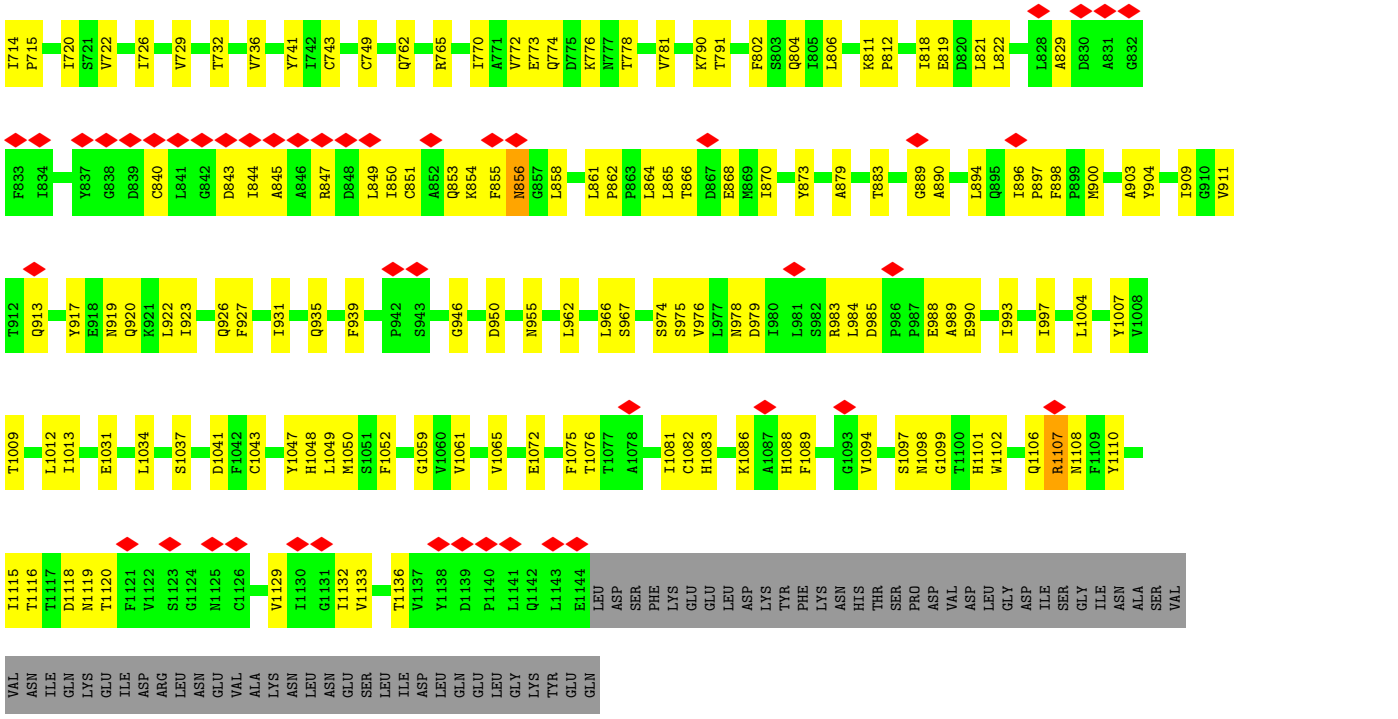
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
5	C	1	15	6	8	1	0

3 Residue-property plots (i)

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

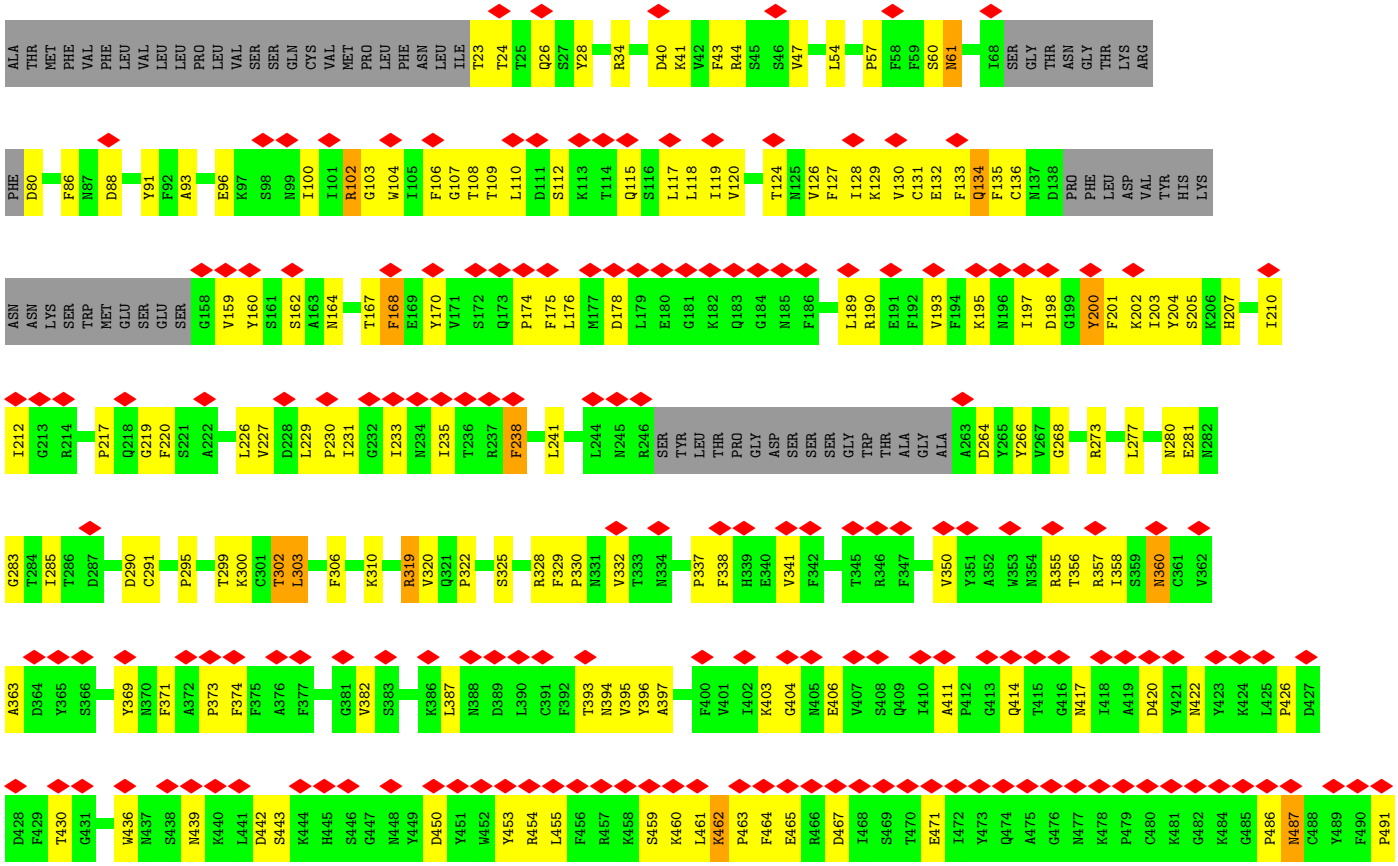
- Molecule 1: Spike glycoprotein

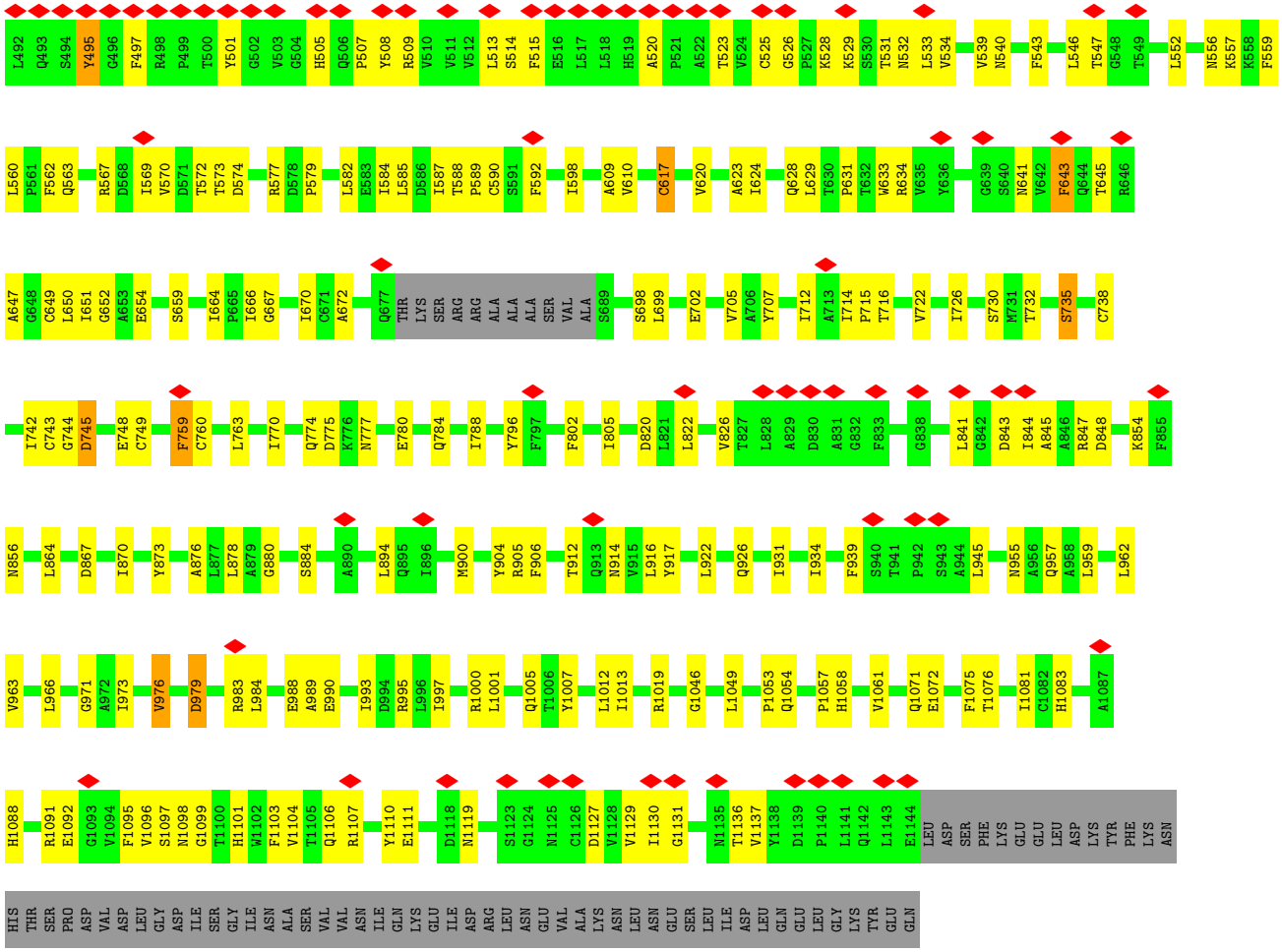




• Molecule 1: Spike glycoprotein

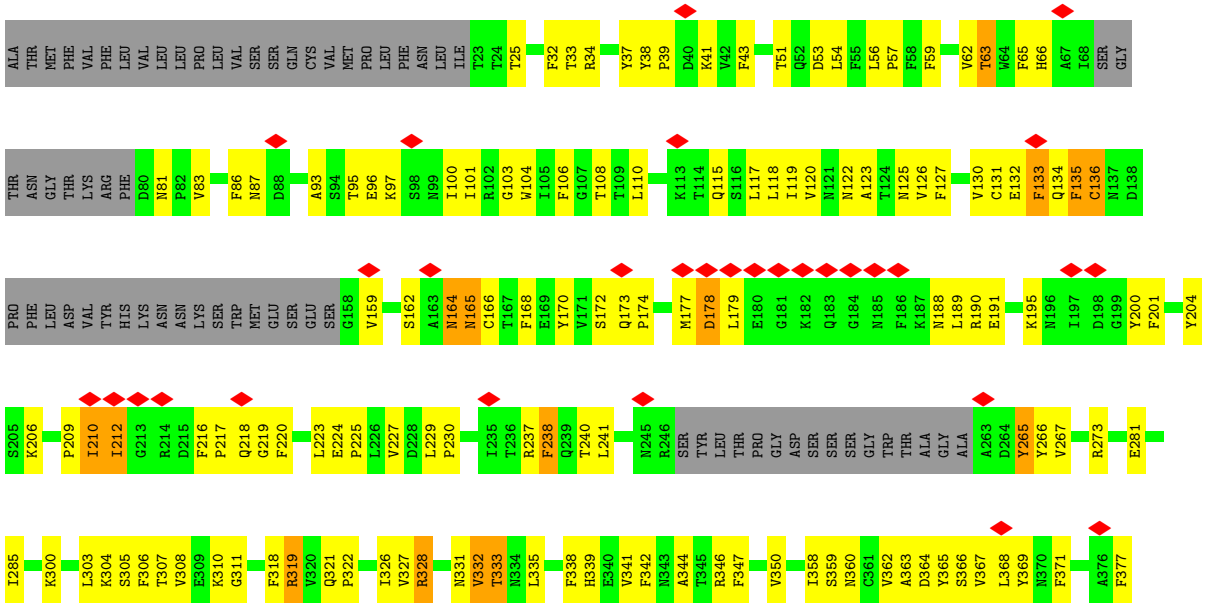
Chain B:

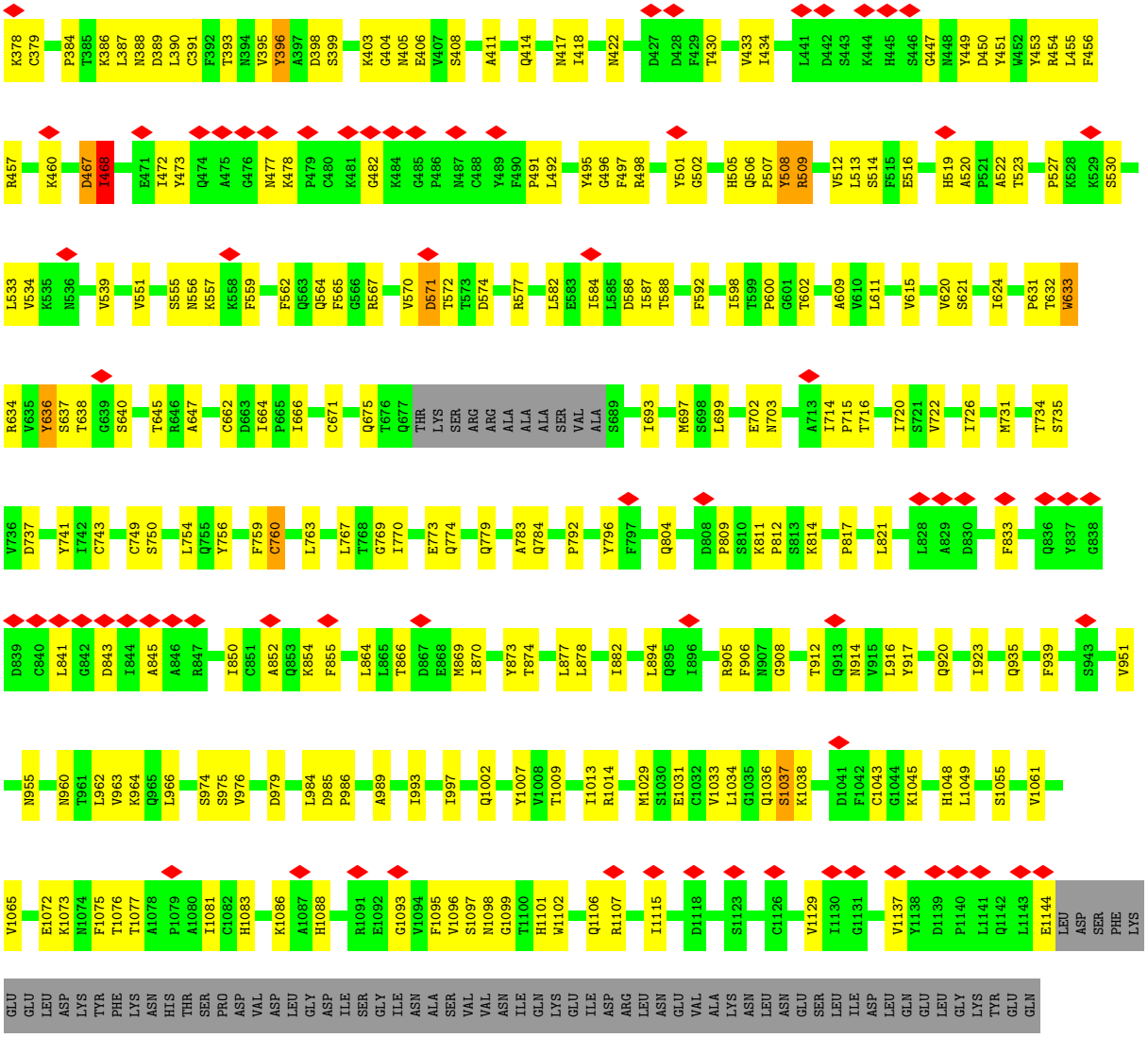




• Molecule 1: Spike glycoprotein

Chain C:





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

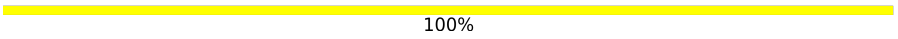
Chain D:

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

Chain E:

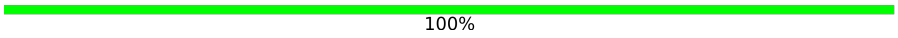
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



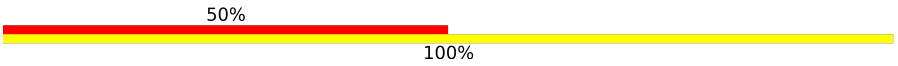
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



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

Chain H:

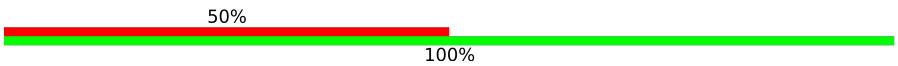


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

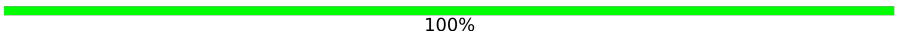
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



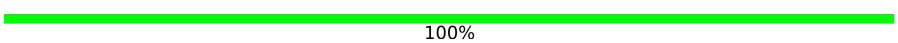
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



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

Chain L:

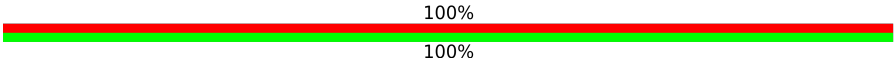


• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

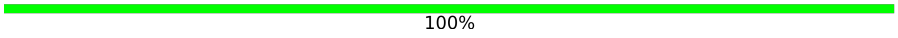
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



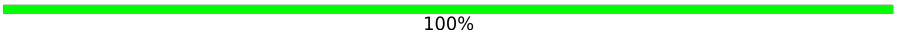
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



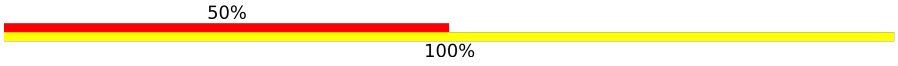
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215534	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.442	Depositor
Minimum map value	-0.643	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	321.00003, 321.00003, 321.00003	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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, IDU

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	0.33	0/8516	0.53	0/11591
1	B	0.32	0/8516	0.53	0/11591
1	C	0.34	0/8516	0.55	0/11591
All	All	0.33	0/25548	0.53	0/34773

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	2
1	B	0	1
1	C	0	4
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	ARG	Sidechain
1	A	577	ARG	Sidechain
1	B	319	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	457	ARG	Sidechain
1	C	509	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8316	0	8102	274	0
1	B	8316	0	8100	264	0
1	C	8316	0	8104	271	0
2	D	28	0	25	1	0
3	E	25	0	22	0	0
3	F	25	0	22	2	0
3	G	25	0	22	0	0
3	H	25	0	22	0	0
3	I	25	0	22	0	0
3	J	25	0	22	0	0
3	K	25	0	22	0	0
3	L	25	0	22	0	0
3	M	25	0	22	0	0
3	N	25	0	22	0	0
3	O	25	0	22	0	0
3	P	25	0	22	0	0
3	Q	25	0	22	0	0
4	A	154	0	143	1	0
4	B	154	0	143	4	0
4	C	168	0	156	3	0
5	C	15	0	4	0	0
All	All	25792	0	25063	764	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 15.

All (764) 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:C:328:ARG:HA	1:C:530:SER:HA	1.29	1.09
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.50	0.92
1:A:896:ILE:HD13	1:B:712:ILE:HD13	1.53	0.89
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.55	0.87
1:B:645:THR:HG22	1:B:647:ALA:H	1.40	0.87
1:B:532:ASN:OD1	1:B:533:LEU:N	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:SER:HB3	1:A:698:SER:HB3	1.58	0.85
1:A:917:TYR:HB3	1:B:1129:VAL:HG22	1.61	0.82
1:A:498:ARG:H	1:A:501:TYR:HE1	1.28	0.82
1:C:347:PHE:HD2	1:C:399:SER:HB2	1.45	0.81
1:C:173:GLN:NE2	1:C:174:PRO:O	2.14	0.80
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.64	0.80
1:B:788:ILE:HD11	1:C:699:LEU:HB2	1.64	0.79
1:A:699:LEU:HB3	1:C:873:TYR:HE2	1.48	0.78
1:B:300:LYS:HE3	1:B:306:PHE:HA	1.66	0.78
1:B:40:ASP:OD1	1:B:41:LYS:N	2.16	0.78
1:C:519:HIS:HD1	1:C:565:PHE:HE1	1.30	0.77
1:B:659:SER:HB3	1:B:698:SER:HB3	1.65	0.77
1:B:61:ASN:HB2	4:B:1302:NAG:N2	2.00	0.76
1:A:976:VAL:HG12	1:A:979:ASP:H	1.49	0.76
1:A:159:VAL:HG11	1:A:241:LEU:HD11	1.69	0.75
1:C:338:PHE:HB3	1:C:342:PHE:CZ	2.21	0.75
1:A:109:THR:H	1:A:237:ARG:HD3	1.49	0.74
1:B:462:LYS:HD2	1:B:465:GLU:HB2	1.69	0.74
1:A:53:ASP:OD2	1:A:54:LEU:N	2.20	0.74
1:B:108:THR:HG21	4:B:1304:NAG:H62	1.68	0.74
1:B:96:GLU:OE1	1:B:100:ILE:N	2.21	0.73
1:B:193:VAL:HB	1:B:204:TYR:HD2	1.51	0.73
1:C:433:VAL:HG23	1:C:512:VAL:HG12	1.70	0.73
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.72	0.71
1:A:866:THR:HG22	1:A:868:GLU:H	1.56	0.71
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.72	0.70
1:B:200:TYR:O	1:B:202:LYS:NZ	2.23	0.70
1:A:707:TYR:HD1	1:C:792:PRO:HG2	1.56	0.70
1:A:896:ILE:HD12	1:A:897:PRO:HD2	1.73	0.70
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.55	0.70
1:C:53:ASP:OD1	1:C:195:LYS:NZ	2.24	0.70
1:A:108:THR:HG22	1:A:109:THR:HG23	1.74	0.70
1:A:802:PHE:HB3	1:A:806:LEU:HD23	1.74	0.69
1:A:317:ASN:ND2	1:C:737:ASP:OD2	2.26	0.69
1:A:1129:VAL:HG12	1:C:917:TYR:HB3	1.73	0.69
1:A:355:ARG:H	2:D:1:NAG:H82	1.58	0.68
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.26	0.68
1:A:903:ALA:HB1	1:A:913:GLN:HB2	1.76	0.68
1:A:577:ARG:HD3	1:A:582:LEU:HD13	1.76	0.68
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.76	0.68
1:C:783:ALA:HA	1:C:873:TYR:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LYS:HB3	1:C:223:LEU:HD13	1.76	0.67
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.76	0.67
1:C:1038:LYS:HE3	1:C:1038:LYS:HA	1.77	0.67
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.76	0.67
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.27	0.67
1:A:178:ASP:HA	1:A:188:ASN:HD21	1.58	0.67
1:C:319:ARG:HB3	1:C:592:PHE:HD1	1.60	0.67
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.76	0.67
1:B:164:ASN:HB2	4:B:1303:NAG:H2	1.76	0.66
1:B:201:PHE:HB2	1:B:231:ILE:HG12	1.75	0.66
1:A:108:THR:HB	1:A:114:THR:HG21	1.76	0.66
1:A:599:THR:HB	1:A:608:VAL:HG12	1.76	0.66
1:C:131:CYS:SG	1:C:132:GLU:N	2.69	0.66
1:B:330:PRO:HA	1:B:579:PRO:HB2	1.77	0.66
1:C:731:MET:HE1	1:C:1014:ARG:HB3	1.77	0.66
1:C:769:GLY:O	1:C:773:GLU:HG3	1.97	0.65
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.30	0.65
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.77	0.65
1:C:347:PHE:CD2	1:C:399:SER:HB2	2.28	0.65
1:C:360:ASN:H	1:C:523:THR:HB	1.62	0.65
1:A:890:ALA:HA	1:B:1046:GLY:HA2	1.78	0.65
1:B:131:CYS:SG	1:B:132:GLU:N	2.69	0.65
1:B:763:LEU:HD21	1:B:1005:GLN:HE22	1.62	0.65
1:C:188:ASN:HB3	1:C:209:PRO:HB3	1.79	0.65
1:A:736:VAL:HG11	1:A:1004:LEU:HD11	1.78	0.64
1:B:486:PRO:O	1:B:487:ASN:ND2	2.29	0.64
1:A:347:PHE:HD2	1:A:399:SER:HB2	1.63	0.64
1:B:867:ASP:HA	1:B:870:ILE:HD12	1.80	0.64
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.79	0.64
1:B:760:CYS:HA	1:B:763:LEU:HG	1.79	0.64
1:A:699:LEU:HD12	1:A:699:LEU:H	1.63	0.64
1:A:864:LEU:HA	1:B:667:GLY:HA2	1.80	0.64
1:C:96:GLU:OE1	1:C:100:ILE:N	2.30	0.64
1:A:454:ARG:NH1	1:A:467:ASP:O	2.29	0.64
1:B:104:TRP:HB2	1:B:119:ILE:HD11	1.80	0.64
1:C:393:THR:HA	1:C:522:ALA:HA	1.81	0.63
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.80	0.63
1:C:460:LYS:HE3	1:C:460:LYS:HA	1.81	0.63
1:A:447:GLY:HA2	1:A:498:ARG:HG3	1.81	0.63
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.64	0.62
1:B:195:LYS:HB3	1:B:202:LYS:HE2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.32	0.62
1:B:34:ARG:NH2	1:B:219:GLY:O	2.32	0.62
1:B:629:LEU:HG	1:B:631:PRO:HD2	1.80	0.62
1:A:396:TYR:HB2	1:A:514:SER:HB3	1.82	0.62
1:C:451:TYR:HB2	1:C:495:TYR:HB3	1.80	0.62
1:A:773:GLU:HA	1:A:776:LYS:HE2	1.82	0.62
1:A:844:ILE:HG23	1:B:556:ASN:HB2	1.81	0.61
1:C:311:GLY:HA2	1:C:664:ILE:HD12	1.82	0.61
1:B:454:ARG:NH1	1:B:467:ASP:O	2.32	0.61
1:A:861:LEU:HD12	1:A:862:PRO:HD2	1.82	0.61
1:C:322:PRO:HB3	1:C:539:VAL:HA	1.82	0.61
1:C:86:PHE:HD1	1:C:238:PHE:HB2	1.65	0.61
1:C:303:LEU:HD11	1:C:308:VAL:HG12	1.83	0.61
1:C:104:TRP:HA	1:C:240:THR:HA	1.82	0.61
1:C:519:HIS:ND1	1:C:565:PHE:CE1	2.66	0.61
1:B:23:THR:N	1:B:80:ASP:OD1	2.34	0.61
1:A:1075:PHE:O	1:A:1076:THR:OG1	2.18	0.60
1:C:178:ASP:OD2	1:C:190:ARG:NH2	2.34	0.60
1:B:552:LEU:HD13	1:B:585:LEU:HD13	1.83	0.60
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.01	0.60
1:C:976:VAL:HG12	1:C:979:ASP:H	1.67	0.60
1:A:34:ARG:NH2	1:A:219:GLY:O	2.34	0.60
1:B:210:ILE:HG21	1:B:217:PRO:HG3	1.83	0.60
1:B:330:PRO:HB2	1:B:332:VAL:HG12	1.83	0.60
1:A:189:LEU:HD21	1:A:191:GLU:HG3	1.84	0.60
1:C:328:ARG:HA	1:C:530:SER:CA	2.19	0.60
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.84	0.60
1:C:645:THR:HG23	1:C:647:ALA:H	1.65	0.60
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.84	0.59
1:A:729:VAL:HG12	1:A:781:VAL:HG21	1.85	0.59
1:B:369:TYR:HA	1:B:374:PHE:HZ	1.67	0.59
1:C:367:VAL:HG23	1:C:371:PHE:HD1	1.67	0.59
1:C:874:THR:HG21	1:C:1055:SER:HB3	1.84	0.59
1:A:91:TYR:HD1	1:A:193:VAL:HG12	1.66	0.59
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.83	0.59
1:A:617:CYS:HB2	1:A:620:VAL:HG12	1.83	0.59
1:B:844:ILE:HG23	1:C:556:ASN:HB2	1.85	0.59
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.85	0.59
1:A:456:PHE:HB3	1:A:473:TYR:HD2	1.68	0.59
1:B:189:LEU:HD22	1:B:210:ILE:HD12	1.84	0.59
1:B:805:ILE:HD12	1:B:878:LEU:HD11	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:HB2	4:B:1302:NAG:HN2	1.68	0.58
1:B:107:GLY:H	1:B:235:ILE:HG23	1.68	0.58
1:B:735:SER:O	1:B:735:SER:OG	2.22	0.58
1:C:310:LYS:HG2	1:C:664:ILE:HD11	1.83	0.58
1:C:406:GLU:OE1	1:C:406:GLU:N	2.35	0.58
1:B:338:PHE:HE1	1:B:358:ILE:HD13	1.69	0.58
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.85	0.58
1:A:553:THR:HG21	1:C:841:LEU:HB2	1.84	0.58
1:C:749:CYS:SG	1:C:997:ILE:HD11	2.44	0.58
1:C:809:PRO:O	1:C:814:LYS:NZ	2.36	0.58
1:C:908:GLY:HA3	1:C:1036:GLN:HE22	1.69	0.58
1:C:1083:HIS:HB2	1:C:1137:VAL:HG12	1.86	0.58
1:A:619:GLU:OE1	1:A:619:GLU:N	2.37	0.57
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.86	0.57
1:C:188:ASN:HA	1:C:209:PRO:HA	1.85	0.57
1:A:983:ARG:HG3	1:A:984:LEU:HG	1.85	0.57
1:B:900:MET:SD	1:C:1077:THR:OG1	2.57	0.57
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.86	0.57
1:C:350:VAL:HG22	1:C:422:ASN:HB3	1.87	0.57
1:C:760:CYS:HA	1:C:763:LEU:HG	1.86	0.57
1:C:767:LEU:HA	1:C:770:ILE:HG22	1.86	0.57
1:B:290:ASP:OD1	1:B:291:CYS:N	2.38	0.57
1:C:170:TYR:HE2	1:C:227:VAL:HG21	1.69	0.57
1:A:563:GLN:HB3	1:C:43:PHE:HB2	1.85	0.57
1:B:560:LEU:HB2	1:B:563:GLN:HG2	1.86	0.57
1:B:641:ASN:HB3	1:B:652:GLY:H	1.68	0.57
1:C:577:ARG:HA	1:C:584:ILE:HA	1.85	0.57
1:A:210:ILE:HG22	1:A:212:ILE:H	1.69	0.57
1:C:133:PHE:HA	1:C:162:SER:HB2	1.87	0.57
1:A:337:PRO:HG2	1:A:358:ILE:HD12	1.86	0.57
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.05	0.56
1:C:398:ASP:HB2	1:C:512:VAL:HG22	1.86	0.56
1:A:376:ALA:HB3	1:A:435:ALA:HB3	1.87	0.56
1:B:624:ILE:HG23	1:B:634:ARG:HD2	1.87	0.56
1:B:976:VAL:HG23	1:B:979:ASP:HB3	1.86	0.56
1:B:990:GLU:N	1:B:990:GLU:OE1	2.39	0.56
1:C:577:ARG:HH21	1:C:582:LEU:HD22	1.71	0.56
1:A:984:LEU:HB2	1:A:989:ALA:HB2	1.88	0.56
1:B:200:TYR:HA	1:B:230:PRO:HA	1.87	0.56
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.88	0.56
1:C:1093:GLY:H	1:C:1107:ARG:HH12	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:TYR:HA	1:A:368:LEU:CD1	2.36	0.56
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	1.87	0.56
1:C:326:ILE:HD13	1:C:533:LEU:HA	1.87	0.56
1:C:393:THR:OG1	1:C:516:GLU:OE1	2.24	0.56
1:B:577:ARG:HD3	1:B:582:LEU:HD13	1.87	0.56
1:C:404:GLY:HA2	1:C:508:TYR:CD2	2.41	0.56
1:C:559:PHE:HB2	1:C:584:ILE:HD11	1.87	0.56
1:A:456:PHE:HB2	1:A:491:PRO:HA	1.86	0.56
1:A:853:GLN:HB3	1:A:858:LEU:HB3	1.87	0.56
1:B:102:ARG:HE	1:B:241:LEU:HB3	1.69	0.55
1:B:178:ASP:OD1	1:B:178:ASP:N	2.39	0.55
1:A:358:ILE:HB	1:A:395:VAL:HB	1.88	0.55
1:A:631:PRO:O	1:A:634:ARG:NH1	2.28	0.55
1:B:513:LEU:HB3	1:B:515:PHE:HE1	1.70	0.55
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	1.88	0.55
1:A:160:TYR:HE2	1:A:163:ALA:HB2	1.70	0.55
1:A:919:ASN:HB3	1:A:922:LEU:HD12	1.88	0.55
1:B:748:GLU:OE1	1:B:748:GLU:N	2.32	0.55
1:A:624:ILE:HG13	1:A:634:ARG:HD2	1.88	0.55
1:B:917:TYR:HB3	1:C:1129:VAL:HG23	1.89	0.55
1:C:1075:PHE:O	1:C:1076:THR:OG1	2.17	0.55
1:A:412:PRO:HG3	1:A:429:PHE:HB3	1.89	0.55
1:A:589:PRO:HG3	1:C:855:PHE:HA	1.89	0.55
1:B:666:ILE:HD12	1:B:670:ILE:HG22	1.89	0.55
1:C:567:ARG:NH1	1:C:571:ASP:OD1	2.40	0.55
1:B:103:GLY:HA3	1:B:120:VAL:HA	1.88	0.54
1:C:662:CYS:HB2	1:C:697:MET:HG3	1.89	0.54
1:B:1075:PHE:O	1:B:1076:THR:OG1	2.17	0.54
1:A:30:ASN:HB3	1:A:32:PHE:CE1	2.43	0.54
1:A:343:ASN:HB3	4:A:1301:NAG:N2	2.22	0.54
1:C:358:ILE:HD13	1:C:395:VAL:HG12	1.90	0.54
1:A:320:VAL:H	1:A:591:SER:HB2	1.73	0.54
1:A:373:PRO:HD2	1:A:436:TRP:CD1	2.42	0.54
1:A:43:PHE:HE1	1:B:557:LYS:HD2	1.71	0.54
1:B:328:ARG:NH1	1:B:531:THR:O	2.40	0.54
1:C:41:LYS:HE3	1:C:225:PRO:HG2	1.88	0.54
1:C:63:THR:HG23	1:C:267:VAL:HG13	1.90	0.54
1:C:750:SER:O	1:C:754:LEU:HG	2.08	0.54
1:C:741:TYR:HE1	1:C:966:LEU:HD11	1.72	0.54
1:A:697:MET:HE3	1:A:697:MET:HA	1.89	0.54
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ARG:NH2	1:C:217:PRO:O	2.41	0.54
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.90	0.54
1:A:384:PRO:O	1:A:387:LEU:HG	2.08	0.54
1:A:569:ILE:O	1:C:964:LYS:NZ	2.41	0.54
1:C:200:TYR:HA	1:C:230:PRO:HA	1.89	0.54
1:B:570:VAL:HG23	1:B:572:THR:HG23	1.91	0.53
1:B:973:ILE:HG22	1:B:983:ARG:HH22	1.73	0.53
1:C:666:ILE:HD12	1:C:671:CYS:HA	1.89	0.53
1:C:332:VAL:HG22	1:C:333:THR:H	1.73	0.53
1:A:570:VAL:HG21	1:C:852:ALA:HB1	1.91	0.53
1:C:307:THR:HA	1:C:602:THR:HG21	1.90	0.53
1:A:43:PHE:HA	1:B:563:GLN:NE2	2.24	0.53
1:B:567:ARG:HG2	1:B:573:THR:HA	1.89	0.53
1:B:176:LEU:H	1:B:176:LEU:HD23	1.74	0.53
1:B:44:ARG:HB3	1:B:47:VAL:HG11	1.90	0.53
1:B:732:THR:OG1	1:B:955:ASN:OD1	2.26	0.53
1:A:811:LYS:HZ2	1:A:812:PRO:HD2	1.74	0.53
1:C:364:ASP:N	1:C:364:ASP:OD1	2.41	0.53
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.91	0.53
1:B:190:ARG:HD3	1:B:207:HIS:CE1	2.44	0.53
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.90	0.53
1:B:329:PHE:CG	1:B:528:LYS:HB3	2.44	0.53
1:C:53:ASP:OD1	1:C:54:LEU:N	2.37	0.52
1:C:93:ALA:HB3	1:C:266:TYR:HB2	1.91	0.52
1:A:350:VAL:HG11	1:A:418:ILE:HD12	1.91	0.52
1:A:699:LEU:HD21	1:C:869:MET:HB2	1.90	0.52
1:B:360:ASN:H	1:B:523:THR:HG22	1.74	0.52
1:A:623:ALA:HA	1:A:628:GLN:HE21	1.74	0.52
1:A:168:PHE:HZ	1:A:229:LEU:HB2	1.75	0.52
1:A:909:ILE:HD13	1:A:1047:TYR:HB3	1.92	0.52
1:B:744:GLY:O	1:B:745:ASP:C	2.48	0.52
1:C:434:ILE:HD13	1:C:513:LEU:HD23	1.90	0.52
1:A:818:ILE:O	1:A:822:LEU:HG	2.09	0.52
1:C:1031:GLU:HG2	1:C:1037:SER:HB2	1.91	0.52
1:C:422:ASN:ND2	1:C:454:ARG:O	2.38	0.52
1:B:320:VAL:O	1:B:590:CYS:SG	2.68	0.52
1:C:405:ASN:O	1:C:408:SER:OG	2.25	0.52
1:A:442:ASP:HB3	1:A:451:TYR:HE2	1.74	0.51
1:B:501:TYR:HB3	1:B:505:HIS:HB3	1.92	0.51
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.91	0.51
1:A:105:ILE:HG13	1:A:239:GLN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:GLN:N	1:B:1106:GLN:OE1	2.43	0.51
1:B:439:ASN:O	1:B:443:SER:OG	2.28	0.51
1:A:65:PHE:HB2	1:A:265:TYR:HB2	1.92	0.51
1:A:666:ILE:HB	1:A:670:ILE:O	2.11	0.51
1:B:126:VAL:HG13	1:B:174:PRO:HA	1.92	0.51
1:B:295:PRO:HG3	1:B:633:TRP:HD1	1.75	0.51
1:C:389:ASP:OD1	1:C:389:ASP:N	2.42	0.51
1:C:633:TRP:HD1	1:C:633:TRP:H	1.58	0.51
1:A:600:PRO:HD3	1:A:692:ILE:HD11	1.93	0.51
1:A:699:LEU:HB3	1:C:873:TYR:CE2	2.38	0.51
1:B:91:TYR:N	1:B:268:GLY:O	2.38	0.51
1:C:33:THR:O	1:C:33:THR:OG1	2.29	0.51
1:A:1075:PHE:HB3	1:A:1097:SER:O	2.11	0.51
1:A:320:VAL:O	1:A:590:CYS:SG	2.69	0.51
1:A:356:THR:OG1	1:A:397:ALA:HB3	2.10	0.51
1:B:231:ILE:HG22	1:B:233:ILE:HG12	1.93	0.51
1:C:720:ILE:HD12	1:C:923:ILE:HD11	1.93	0.51
1:A:1116:THR:OG1	1:A:1118:ASP:OD1	2.29	0.50
1:B:984:LEU:HB3	1:B:989:ALA:HB2	1.93	0.50
1:C:564:GLN:OE1	1:C:577:ARG:NH1	2.45	0.50
1:C:714:ILE:HD12	1:C:1096:VAL:HG21	1.92	0.50
1:A:126:VAL:HG22	1:A:172:SER:H	1.76	0.50
1:C:342:PHE:CZ	1:C:368:LEU:HB2	2.47	0.50
1:B:197:ILE:HG22	1:B:202:LYS:HE3	1.92	0.50
1:B:382:VAL:HG21	1:B:387:LEU:HD21	1.94	0.50
1:C:95:THR:HB	1:C:189:LEU:HG	1.93	0.50
1:A:118:LEU:C	1:A:119:ILE:HD13	2.32	0.50
1:B:569:ILE:HD12	1:B:569:ILE:H	1.77	0.50
1:A:25:THR:HG23	1:A:66:HIS:HB3	1.93	0.50
1:A:894:LEU:HD13	1:B:715:PRO:HD3	1.93	0.50
1:B:102:ARG:HG3	1:B:120:VAL:HG23	1.94	0.50
1:B:134:GLN:HB2	1:B:162:SER:HB2	1.92	0.50
1:A:791:THR:HG21	1:A:806:LEU:HD11	1.93	0.50
1:B:119:ILE:HG22	1:B:128:ILE:HG23	1.94	0.50
1:C:636:TYR:HD1	1:C:637:SER:N	2.10	0.50
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	1.93	0.50
1:A:34:ARG:HD2	1:A:191:GLU:OE2	2.12	0.50
1:A:365:TYR:HA	1:A:368:LEU:HD12	1.93	0.50
1:A:422:ASN:ND2	1:A:454:ARG:O	2.30	0.50
1:B:403:LYS:HE3	1:B:495:TYR:HE1	1.77	0.50
1:B:971:GLY:O	1:B:995:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.94	0.50
1:B:847:ARG:NE	1:C:574:ASP:OD1	2.35	0.50
1:B:959:LEU:O	1:B:963:VAL:HG23	2.12	0.50
1:B:1092:GLU:OE1	1:B:1092:GLU:N	2.45	0.50
1:C:335:LEU:HD13	1:C:362:VAL:HB	1.93	0.49
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.47	0.49
1:C:811:LYS:HD2	1:C:812:PRO:HD2	1.94	0.49
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.94	0.49
1:B:914:ASN:ND2	1:B:1111:GLU:OE1	2.42	0.49
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.46	0.49
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.94	0.49
1:A:985:ASP:OD1	1:A:985:ASP:N	2.44	0.49
1:B:57:PRO:HB2	1:B:60:SER:HB3	1.93	0.49
1:C:631:PRO:HB3	1:C:633:TRP:NE1	2.28	0.49
1:A:843:ASP:O	1:A:845:ALA:N	2.44	0.49
1:B:210:ILE:HG22	1:B:212:ILE:H	1.76	0.49
1:B:369:TYR:HA	1:B:374:PHE:CZ	2.47	0.49
1:C:404:GLY:HA2	1:C:508:TYR:HD2	1.76	0.49
1:A:168:PHE:CZ	1:A:229:LEU:HB2	2.47	0.49
1:A:449:TYR:HA	1:A:496:GLY:HA2	1.93	0.49
1:B:777:ASN:HD21	1:B:1019:ARG:HA	1.78	0.49
1:C:555:SER:HB3	1:C:584:ILE:HG22	1.93	0.49
1:C:912:THR:OG1	1:C:914:ASN:OD1	2.30	0.49
1:A:563:GLN:HG3	1:C:43:PHE:HD2	1.77	0.49
1:A:927:PHE:HZ	1:A:1052:PHE:HE2	1.61	0.49
1:B:912:THR:OG1	1:B:914:ASN:OD1	2.30	0.49
1:C:417:ASN:O	1:C:422:ASN:ND2	2.46	0.49
1:C:843:ASP:O	1:C:845:ALA:N	2.45	0.49
1:C:974:SER:OG	1:C:975:SER:N	2.45	0.49
1:A:1129:VAL:HG21	1:A:1132:ILE:HD12	1.95	0.49
1:B:124:THR:O	1:B:174:PRO:HD3	2.13	0.49
1:B:454:ARG:HH22	1:B:467:ASP:HB3	1.77	0.49
1:B:843:ASP:O	1:B:845:ALA:N	2.45	0.49
1:C:328:ARG:CA	1:C:530:SER:HA	2.20	0.49
1:A:452:TRP:HB3	1:A:492:LEU:HD13	1.95	0.49
1:B:118:LEU:HD22	1:B:129:LYS:HD2	1.94	0.49
1:B:167:THR:HG23	1:B:168:PHE:HB3	1.94	0.49
1:B:742:ILE:HG22	1:B:997:ILE:HD12	1.94	0.49
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.12	0.49
1:C:218:GLN:OE1	1:C:218:GLN:N	2.46	0.49
1:C:406:GLU:HG3	1:C:418:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:817:PRO:O	1:C:821:LEU:HG	2.13	0.49
1:A:112:SER:HA	1:A:132:GLU:HG2	1.95	0.48
1:A:720:ILE:HG13	1:A:923:ILE:HG13	1.94	0.48
1:A:865:LEU:HB3	1:A:870:ILE:HD11	1.94	0.48
1:B:873:TYR:CE2	1:C:699:LEU:HD13	2.47	0.48
1:A:904:TYR:HE1	1:B:1107:ARG:HD3	1.78	0.48
1:C:1098:ASN:OD1	1:C:1099:GLY:N	2.46	0.48
1:A:762:GLN:HA	1:A:765:ARG:NH1	2.29	0.48
1:A:1072:GLU:OE1	1:A:1072:GLU:N	2.46	0.48
1:C:165:ASN:H	1:C:165:ASN:HD22	1.61	0.48
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.94	0.48
1:B:357:ARG:HE	1:B:394:ASN:HD21	1.60	0.48
1:B:990:GLU:HA	1:B:993:ILE:HG22	1.95	0.48
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.95	0.48
1:C:559:PHE:H	1:C:584:ILE:HD11	1.77	0.48
1:A:34:ARG:NH1	1:A:221:SER:OG	2.47	0.48
1:C:83:VAL:HG21	1:C:237:ARG:HE	1.78	0.48
1:C:570:VAL:O	1:C:570:VAL:HG23	2.14	0.48
1:A:732:THR:OG1	1:A:955:ASN:OD1	2.31	0.48
1:B:28:TYR:HD2	1:B:61:ASN:HD21	1.61	0.48
1:C:131:CYS:HB3	1:C:133:PHE:CZ	2.49	0.48
1:C:170:TYR:CE1	1:C:172:SER:HB3	2.47	0.48
1:C:621:SER:O	1:C:624:ILE:HG22	2.13	0.48
1:A:403:LYS:HE3	1:A:495:TYR:CZ	2.49	0.48
1:B:559:PHE:HB3	1:B:577:ARG:NH2	2.29	0.48
1:C:220:PHE:HE2	1:C:285:ILE:HG22	1.77	0.48
1:C:779:GLN:O	1:C:783:ALA:HB3	2.14	0.48
1:B:210:ILE:HD13	1:B:217:PRO:HG3	1.96	0.48
1:B:497:PHE:HA	1:B:501:TYR:HE2	1.79	0.48
1:B:880:GLY:O	1:B:884:SER:OG	2.28	0.48
1:C:123:ALA:HB3	4:C:1306:NAG:C7	2.44	0.48
1:C:418:ILE:H	1:C:418:ILE:HD12	1.79	0.48
1:C:632:THR:HA	1:C:634:ARG:HH21	1.78	0.48
1:A:312:ILE:HD12	1:A:666:ILE:HD13	1.95	0.48
1:B:320:VAL:HG13	1:B:628:GLN:CG	2.44	0.48
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.54	0.48
1:B:1072:GLU:N	1:B:1072:GLU:OE1	2.47	0.48
1:C:586:ASP:OD1	1:C:587:ILE:N	2.47	0.48
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.95	0.48
1:C:638:THR:HG23	1:C:640:SER:H	1.78	0.48
1:C:1098:ASN:CG	1:C:1101:HIS:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ASN:OD1	1:B:281:GLU:N	2.47	0.47
1:B:759:PHE:HZ	1:C:1002:GLN:HG3	1.78	0.47
1:C:117:LEU:HD12	1:C:118:LEU:N	2.29	0.47
1:C:716:THR:HG21	1:C:1073:LYS:HD3	1.96	0.47
1:C:962:LEU:HD22	1:C:1007:TYR:CG	2.49	0.47
1:A:993:ILE:O	1:A:997:ILE:HG12	2.15	0.47
1:B:325:SER:HB2	1:B:540:ASN:HD22	1.78	0.47
1:A:667:GLY:HA2	1:C:864:LEU:HA	1.97	0.47
1:B:355:ARG:HH12	1:B:464:PHE:HB3	1.79	0.47
1:B:450:ASP:OD1	1:B:450:ASP:N	2.46	0.47
1:B:738:CYS:HB3	1:B:760:CYS:HB2	1.65	0.47
1:B:993:ILE:O	1:B:997:ILE:HG12	2.14	0.47
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.96	0.47
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.39	0.47
1:C:363:ALA:HB1	1:C:365:TYR:CE1	2.49	0.47
1:A:271:GLN:OE1	1:A:271:GLN:N	2.48	0.47
1:A:329:PHE:HE2	1:A:528:LYS:HG3	1.79	0.47
1:A:729:VAL:HG11	1:A:781:VAL:HG11	1.97	0.47
1:C:631:PRO:O	1:C:634:ARG:NE	2.46	0.47
1:A:559:PHE:HB3	1:A:577:ARG:NH2	2.29	0.47
1:A:889:GLY:HA3	1:A:1034:LEU:HD11	1.96	0.47
1:A:922:LEU:O	1:A:926:GLN:HG2	2.14	0.47
1:B:118:LEU:HD21	1:B:120:VAL:HG12	1.97	0.47
1:B:203:ILE:HB	1:B:227:VAL:HG22	1.96	0.47
1:B:404:GLY:HA2	1:B:508:TYR:HD2	1.80	0.47
1:B:620:VAL:HA	1:B:623:ALA:HB3	1.95	0.47
1:C:379:CYS:HB2	1:C:384:PRO:HD3	1.97	0.47
1:C:1107:ARG:HH11	1:C:1107:ARG:HG3	1.79	0.47
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.95	0.47
1:A:598:ILE:HG12	1:A:666:ILE:HD11	1.96	0.47
1:C:81:ASN:ND2	1:C:240:THR:O	2.35	0.47
1:C:633:TRP:N	1:C:633:TRP:CD1	2.82	0.47
1:C:1081:ILE:O	1:C:1088:HIS:N	2.43	0.47
1:C:502:GLY:O	1:C:506:GLN:HG2	2.13	0.47
1:A:305:SER:OG	1:A:306:PHE:N	2.48	0.47
1:A:366:SER:HA	1:A:369:TYR:HD1	1.79	0.47
1:A:560:LEU:HB2	1:A:563:GLN:HG2	1.96	0.47
1:A:570:VAL:HG23	1:A:572:THR:HG23	1.96	0.47
1:A:889:GLY:HA3	1:A:1034:LEU:HD21	1.96	0.47
1:B:848:ASP:OD1	1:B:848:ASP:N	2.40	0.47
1:C:367:VAL:HG23	1:C:371:PHE:CD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:HG2	1:A:418:ILE:HG13	1.96	0.46
1:B:195:LYS:HD2	1:B:202:LYS:HE3	1.97	0.46
1:C:1144:GLU:OE1	1:C:1144:GLU:N	2.47	0.46
1:A:741:TYR:CZ	1:A:966:LEU:HD21	2.50	0.46
1:A:985:ASP:OD1	1:A:988:GLU:HB3	2.15	0.46
1:A:1031:GLU:OE1	1:A:1037:SER:OG	2.26	0.46
1:B:894:LEU:HD13	1:C:715:PRO:HD3	1.98	0.46
1:C:305:SER:OG	1:C:306:PHE:N	2.48	0.46
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.96	0.46
1:C:878:LEU:O	1:C:882:ILE:HG23	2.15	0.46
1:C:1098:ASN:OD1	1:C:1101:HIS:N	2.36	0.46
1:A:168:PHE:CZ	1:A:230:PRO:HD2	2.51	0.46
1:B:201:PHE:N	1:B:229:LEU:O	2.48	0.46
1:B:299:THR:O	1:B:302:THR:HG22	2.15	0.46
1:B:337:PRO:O	1:B:341:VAL:HG23	2.15	0.46
1:C:783:ALA:HA	1:C:873:TYR:CE1	2.44	0.46
1:A:339:HIS:CE1	1:A:340:GLU:HG3	2.50	0.46
1:A:633:TRP:O	1:A:634:ARG:NH1	2.49	0.46
1:C:97:LYS:O	1:C:97:LYS:NZ	2.48	0.46
1:C:126:VAL:HG22	1:C:172:SER:H	1.79	0.46
1:A:31:SER:O	1:A:32:PHE:HB2	2.16	0.46
1:A:231:ILE:HG13	1:A:233:ILE:HB	1.98	0.46
1:B:363:ALA:N	1:B:525:CYS:O	2.39	0.46
1:C:188:ASN:HD21	1:C:190:ARG:HH21	1.63	0.46
1:C:384:PRO:HA	1:C:387:LEU:HD22	1.97	0.46
1:C:770:ILE:O	1:C:774:GLN:HG2	2.14	0.46
1:A:436:TRP:HZ3	1:A:511:VAL:HG12	1.81	0.46
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.41	0.46
1:A:560:LEU:O	1:A:577:ARG:NH2	2.48	0.46
1:B:417:ASN:HD22	1:B:455:LEU:HD23	1.80	0.46
1:B:422:ASN:ND2	1:B:454:ARG:O	2.29	0.46
1:B:471:GLU:H	1:B:491:PRO:HG3	1.81	0.46
1:B:712:ILE:HG13	1:B:714:ILE:HG13	1.97	0.46
1:B:856:ASN:ND2	1:B:966:LEU:HD13	2.29	0.46
1:A:967:SER:O	1:A:967:SER:OG	2.32	0.46
1:B:633:TRP:HE3	1:B:633:TRP:H	1.63	0.46
1:A:48:LEU:HD11	1:A:306:PHE:CE1	2.51	0.46
1:A:791:THR:HG22	1:A:879:ALA:HB2	1.96	0.46
1:B:525:CYS:SG	1:B:526:GLY:N	2.87	0.46
1:C:319:ARG:HH12	1:C:321:GLN:HA	1.81	0.46
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:THR:O	1:C:430:THR:OG1	2.33	0.45
1:A:81:ASN:OD1	1:A:239:GLN:NE2	2.50	0.45
1:B:997:ILE:HG22	1:B:1001:LEU:HD23	1.98	0.45
1:A:106:PHE:O	1:A:116:SER:HB3	2.16	0.45
1:A:598:ILE:HD11	1:A:650:LEU:HD11	1.98	0.45
1:B:108:THR:C	1:B:110:LEU:H	2.20	0.45
1:A:765:ARG:NE	1:B:957:GLN:OE1	2.49	0.45
1:A:791:THR:HG21	1:A:806:LEU:CD1	2.47	0.45
1:B:560:LEU:HB2	1:B:563:GLN:CG	2.46	0.45
1:B:722:VAL:HG12	1:B:934:ILE:HD12	1.97	0.45
1:C:115:GLN:OE1	1:C:130:VAL:HG12	2.16	0.45
1:A:962:LEU:HD22	1:A:1007:TYR:CG	2.51	0.45
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.49	0.45
1:B:131:CYS:HB3	1:B:133:PHE:CE1	2.52	0.45
1:B:420:ASP:O	1:B:461:LEU:N	2.50	0.45
1:B:777:ASN:ND2	1:B:1019:ARG:HA	2.32	0.45
1:C:34:ARG:NH2	1:C:219:GLY:O	2.49	0.45
1:C:393:THR:HG21	1:C:520:ALA:HB3	1.97	0.45
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.52	0.45
1:A:239:GLN:HE21	1:A:240:THR:H	1.63	0.45
1:B:406:GLU:N	1:B:406:GLU:OE1	2.48	0.45
1:B:931:ILE:O	1:B:934:ILE:HG22	2.17	0.45
1:C:106:PHE:HE1	1:C:201:PHE:HZ	1.63	0.45
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.49	0.45
1:A:617:CYS:HB2	1:A:620:VAL:CG1	2.46	0.45
1:A:850:ILE:O	1:A:854:LYS:HG2	2.17	0.45
1:C:32:PHE:HA	1:C:59:PHE:CD1	2.51	0.45
1:C:472:ILE:HG12	1:C:482:GLY:O	2.16	0.45
1:A:189:LEU:HB2	1:A:210:ILE:HD11	1.99	0.45
1:A:1107:ARG:HG2	1:A:1107:ARG:HH11	1.82	0.45
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.52	0.45
1:B:322:PRO:HB3	1:B:539:VAL:HA	1.98	0.45
1:C:358:ILE:HD12	1:C:358:ILE:N	2.32	0.45
1:C:388:ASN:O	1:C:527:PRO:HD2	2.17	0.45
1:B:131:CYS:HB3	1:B:133:PHE:CZ	2.52	0.45
1:A:121:ASN:HD22	1:A:176:LEU:HD23	1.82	0.45
1:B:529:LYS:HB2	1:B:529:LYS:HE2	1.74	0.45
1:B:775:ASP:OD2	1:B:864:LEU:HB3	2.16	0.45
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.35	0.45
1:C:454:ARG:HG2	1:C:492:LEU:HB3	1.98	0.45
1:A:365:TYR:CD2	1:A:368:LEU:HD13	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:NE	1:A:501:TYR:OH	2.50	0.44
1:A:821:LEU:HD13	1:A:939:PHE:HD2	1.82	0.44
1:A:1115:ILE:HA	1:A:1119:ASN:HD21	1.82	0.44
1:C:281:GLU:HB3	4:C:1309:NAG:H82	1.99	0.44
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.98	0.44
1:A:790:LYS:HD3	1:B:702:GLU:OE2	2.17	0.44
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.52	0.44
1:A:774:GLN:O	1:A:778:THR:HG22	2.17	0.44
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.99	0.44
1:C:906:PHE:CD2	1:C:916:LEU:HB2	2.52	0.44
1:A:125:ASN:HB2	1:A:172:SER:O	2.18	0.44
1:A:605:SER:OG	1:A:606:ASN:N	2.51	0.44
1:A:855:PHE:HE2	1:B:587:ILE:HG22	1.81	0.44
1:C:675:GLN:HG3	1:C:693:ILE:HD11	1.99	0.44
1:A:43:PHE:CE1	1:B:557:LYS:HD2	2.51	0.44
1:A:290:ASP:OD1	1:A:291:CYS:N	2.51	0.44
1:B:130:VAL:O	1:B:167:THR:HG22	2.17	0.44
1:C:1029:MET:SD	1:C:1033:VAL:HG21	2.58	0.44
1:C:1106:GLN:OE1	1:C:1106:GLN:N	2.51	0.44
1:A:96:GLU:OE1	1:A:100:ILE:N	2.44	0.44
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.82	0.44
1:B:41:LYS:HG3	1:C:562:PHE:CE1	2.53	0.44
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.53	0.44
1:C:702:GLU:OE1	1:C:703:ASN:N	2.50	0.44
1:A:46:SER:O	1:A:46:SER:OG	2.34	0.44
1:A:280:ASN:HB2	1:A:284:THR:O	2.18	0.44
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.52	0.44
1:B:229:LEU:H	1:B:229:LEU:HD23	1.83	0.44
1:B:560:LEU:H	1:B:560:LEU:HD22	1.82	0.44
1:B:826:VAL:HB	1:B:1057:PRO:HG2	2.00	0.44
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.53	0.44
1:A:375:PHE:CE2	1:A:407:VAL:HG11	2.52	0.44
1:A:904:TYR:CE1	1:B:1107:ARG:HD3	2.51	0.44
1:B:430:THR:O	1:B:430:THR:OG1	2.35	0.44
1:B:1098:ASN:CG	1:B:1101:HIS:H	2.20	0.44
1:C:378:LYS:O	1:C:433:VAL:HG12	2.18	0.44
1:C:456:PHE:HB3	1:C:473:TYR:CD2	2.53	0.44
1:A:54:LEU:HD11	1:A:88:ASP:HB3	1.99	0.44
1:A:375:PHE:HE2	1:A:407:VAL:HG11	1.83	0.44
1:A:541:PHE:CZ	1:A:587:ILE:HD12	2.53	0.44
1:A:708:SER:OG	1:A:709:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LYS:HE3	1:C:304:LYS:HB2	1.57	0.44
1:A:650:LEU:HD23	1:A:653:ALA:HB3	1.98	0.43
1:A:896:ILE:HD12	1:A:896:ILE:HA	1.87	0.43
1:A:1098:ASN:CG	1:A:1101:HIS:H	2.21	0.43
1:C:134:GLN:HG3	1:C:135:PHE:H	1.82	0.43
1:C:179:LEU:HD21	1:C:209:PRO:HG3	2.00	0.43
1:C:870:ILE:O	1:C:874:THR:HG23	2.18	0.43
1:A:322:PRO:HB3	1:A:539:VAL:HA	2.00	0.43
1:C:101:ILE:HG23	1:C:241:LEU:O	2.18	0.43
1:C:338:PHE:HB3	1:C:342:PHE:CE1	2.53	0.43
1:B:356:THR:OG1	1:B:397:ALA:HB3	2.18	0.43
1:B:922:LEU:O	1:B:926:GLN:HG3	2.18	0.43
1:A:574:ASP:O	1:A:587:ILE:N	2.50	0.43
1:B:650:LEU:HD12	1:B:650:LEU:HA	1.89	0.43
1:C:132:GLU:HB3	1:C:164:ASN:HD21	1.83	0.43
1:C:136:CYS:SG	1:C:159:VAL:HA	2.58	0.43
1:C:326:ILE:HD11	1:C:534:VAL:HG23	2.00	0.43
1:A:170:TYR:CE1	1:A:227:VAL:HG21	2.53	0.43
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.81	0.43
1:B:471:GLU:N	1:B:491:PRO:HG3	2.33	0.43
1:B:574:ASP:O	1:B:587:ILE:N	2.48	0.43
1:B:796:TYR:CD2	4:C:1303:NAG:H5	2.54	0.43
1:C:391:CYS:HB3	1:C:522:ALA:CB	2.49	0.43
1:A:402:ILE:HG13	1:A:403:LYS:H	1.83	0.43
1:A:714:ILE:HD11	1:A:1110:TYR:CD1	2.54	0.43
1:B:528:LYS:H	1:B:528:LYS:HD2	1.84	0.43
1:B:1083:HIS:HB2	1:B:1137:VAL:HG13	2.00	0.43
1:B:1083:HIS:ND1	1:B:1137:VAL:HG22	2.34	0.43
1:A:620:VAL:HA	1:A:623:ALA:HB3	2.00	0.43
1:C:456:PHE:HB2	1:C:491:PRO:HA	2.00	0.43
1:A:393:THR:OG1	1:A:394:ASN:N	2.51	0.43
1:A:611:LEU:HD11	1:A:666:ILE:HG23	2.00	0.43
1:A:829:ALA:O	1:A:850:ILE:HD11	2.18	0.43
1:A:1043:CYS:HB2	1:A:1048:HIS:CG	2.53	0.43
1:B:610:VAL:HB	1:B:651:ILE:HG22	2.01	0.43
1:C:984:LEU:HB3	1:C:989:ALA:HB2	2.01	0.43
1:C:108:THR:C	1:C:110:LEU:H	2.22	0.43
1:A:558:LYS:HD3	1:A:558:LYS:HA	1.89	0.43
1:A:656:VAL:HG12	1:A:658:ASN:H	1.84	0.43
1:B:86:PHE:HD1	1:B:238:PHE:HB2	1.84	0.43
1:B:459:SER:OG	1:B:460:LYS:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:ILE:HG23	1:B:876:ALA:HB2	2.01	0.43
1:C:229:LEU:HD23	1:C:229:LEU:H	1.84	0.43
1:A:611:LEU:HD23	1:A:649:CYS:O	2.18	0.42
1:A:990:GLU:HA	1:A:993:ILE:HG22	2.01	0.42
1:A:1102:TRP:NE1	1:A:1133:VAL:HG11	2.33	0.42
1:B:200:TYR:O	1:B:202:LYS:HG3	2.19	0.42
1:B:231:ILE:CG2	1:B:233:ILE:HG12	2.49	0.42
1:B:299:THR:O	1:B:303:LEU:HG	2.18	0.42
1:B:617:CYS:HB3	1:B:649:CYS:HB2	1.57	0.42
1:C:985:ASP:OD1	1:C:986:PRO:HD2	2.19	0.42
1:C:993:ILE:O	1:C:997:ILE:HG12	2.18	0.42
1:A:464:PHE:CG	1:A:464:PHE:O	2.71	0.42
1:A:904:TYR:HE1	1:B:1107:ARG:CD	2.32	0.42
1:B:319:ARG:NH2	1:B:590:CYS:SG	2.92	0.42
1:B:403:LYS:HE3	1:B:495:TYR:CE1	2.53	0.42
1:A:974:SER:OG	1:A:975:SER:N	2.52	0.42
1:A:1089:PHE:O	1:A:1120:THR:OG1	2.25	0.42
1:A:1107:ARG:HB3	1:A:1108:ASN:OD1	2.19	0.42
1:B:41:LYS:N	1:B:41:LYS:HD3	2.35	0.42
1:B:115:GLN:OE1	1:B:130:VAL:HG12	2.19	0.42
1:B:357:ARG:HE	1:B:394:ASN:ND2	2.17	0.42
1:B:426:PRO:HD3	1:B:463:PRO:HB3	2.01	0.42
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.54	0.42
1:B:643:PHE:O	1:B:649:CYS:HA	2.19	0.42
1:B:1130:ILE:HD12	1:B:1131:GLY:H	1.84	0.42
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.19	0.42
1:A:357:ARG:HA	1:A:357:ARG:NE	2.34	0.42
1:A:471:GLU:HA	1:A:481:LYS:HZ1	1.85	0.42
1:A:472:ILE:HG12	1:A:482:GLY:O	2.19	0.42
1:A:707:TYR:OH	1:C:796:TYR:O	2.37	0.42
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.60	0.42
1:A:772:VAL:O	1:A:776:LYS:HG3	2.19	0.42
1:A:1086:LYS:HE3	1:A:1086:LYS:HB2	1.85	0.42
1:B:226:LEU:HG	1:B:227:VAL:HG13	2.01	0.42
1:C:877:LEU:HD23	1:C:877:LEU:HA	1.84	0.42
1:B:1081:ILE:O	1:B:1088:HIS:N	2.42	0.42
1:C:359:SER:O	1:C:360:ASN:ND2	2.52	0.42
1:C:866:THR:OG1	1:C:869:MET:HG2	2.20	0.42
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.94	0.42
1:B:136:CYS:HB2	1:B:159:VAL:O	2.19	0.42
1:C:118:LEU:HD23	1:C:118:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG13	1:A:49:HIS:H	1.85	0.42
1:A:222:ALA:HB2	1:A:285:ILE:HB	2.02	0.42
1:A:660:TYR:HB2	1:A:695:TYR:CZ	2.54	0.42
1:A:840:CYS:HB2	1:B:588:THR:HG23	2.00	0.42
1:A:883:THR:OG1	1:B:705:VAL:HG11	2.20	0.42
1:B:962:LEU:HD22	1:B:1007:TYR:CG	2.54	0.42
1:B:1081:ILE:HG12	1:B:1095:PHE:CE2	2.55	0.42
1:C:367:VAL:O	1:C:371:PHE:HB2	2.20	0.42
1:C:449:TYR:HA	1:C:496:GLY:HA2	2.02	0.42
1:C:450:ASP:N	1:C:450:ASP:OD1	2.39	0.42
1:C:735:SER:O	1:C:735:SER:OG	2.28	0.42
1:A:1083:HIS:CD2	1:A:1136:THR:HA	2.54	0.42
1:A:1098:ASN:OD1	1:A:1101:HIS:N	2.47	0.42
1:B:589:PRO:HB3	1:B:592:PHE:CD2	2.55	0.42
1:B:780:GLU:O	1:B:784:GLN:NE2	2.50	0.42
1:B:1096:VAL:O	1:B:1103:PHE:N	2.47	0.42
1:C:131:CYS:HB2	1:C:166:CYS:HB3	1.71	0.42
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.85	0.42
1:C:975:SER:O	1:C:975:SER:OG	2.32	0.42
1:A:204:TYR:C	1:A:223:LEU:HD11	2.40	0.42
1:A:378:LYS:HD2	1:A:380:TYR:OH	2.20	0.42
1:A:559:PHE:HA	1:C:43:PHE:CD2	2.55	0.42
1:A:819:GLU:H	1:A:819:GLU:HG3	1.67	0.42
1:A:1081:ILE:O	1:A:1088:HIS:N	2.46	0.42
1:B:699:LEU:H	1:B:699:LEU:HG	1.72	0.42
1:B:988:GLU:OE2	1:B:988:GLU:N	2.52	0.42
1:C:363:ALA:HB1	1:C:365:TYR:HE1	1.84	0.42
1:C:551:VAL:HB	1:C:588:THR:OG1	2.20	0.42
3:F:1:NAG:H62	3:F:2:BMA:H2	2.02	0.42
1:A:729:VAL:HG22	1:A:1059:GLY:CA	2.50	0.42
1:A:854:LYS:HA	1:A:854:LYS:HD2	1.88	0.42
1:A:931:ILE:HD12	1:A:931:ILE:HA	1.81	0.42
1:B:350:VAL:HG22	1:B:422:ASN:HB3	2.02	0.42
1:B:966:LEU:O	1:B:966:LEU:HD23	2.20	0.42
1:C:210:ILE:HB	1:C:212:ILE:H	1.66	0.42
1:C:960:ASN:HA	1:C:963:VAL:HG22	2.01	0.42
1:A:645:THR:HG23	1:A:649:CYS:HA	2.02	0.41
1:B:44:ARG:HB3	1:B:47:VAL:CG1	2.49	0.41
1:B:220:PHE:HE1	1:B:285:ILE:HG22	1.84	0.41
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.01	0.41
1:B:543:PHE:O	1:B:546:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LYS:HB2	1:B:584:ILE:HG21	2.02	0.41
1:C:25:THR:HG23	1:C:66:HIS:HB2	2.01	0.41
1:C:39:PRO:HG2	1:C:51:THR:HG21	2.02	0.41
1:C:122:ASN:HB3	1:C:125:ASN:O	2.19	0.41
1:C:174:PRO:HG2	1:C:177:MET:HE3	2.02	0.41
1:C:300:LYS:HD3	1:C:306:PHE:HA	2.02	0.41
1:C:456:PHE:HB3	1:C:473:TYR:HD2	1.84	0.41
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.78	0.41
1:A:920:GLN:HA	1:A:923:ILE:HG22	2.01	0.41
1:A:329:PHE:CE2	1:A:528:LYS:HG3	2.55	0.41
1:A:366:SER:HA	1:A:369:TYR:CD1	2.54	0.41
1:A:662:CYS:HB2	1:A:697:MET:CE	2.50	0.41
1:B:106:PHE:HD1	1:B:235:ILE:HG21	1.86	0.41
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.92	0.41
1:B:770:ILE:O	1:B:774:GLN:HG2	2.20	0.41
1:B:904:TYR:CE2	1:C:1107:ARG:HG2	2.55	0.41
1:C:87:ASN:OD1	1:C:87:ASN:N	2.53	0.41
1:C:165:ASN:H	1:C:165:ASN:ND2	2.18	0.41
1:C:366:SER:HA	1:C:369:TYR:CD1	2.56	0.41
1:A:379:CYS:HB2	1:A:384:PRO:HD3	2.01	0.41
1:A:715:PRO:HD3	1:C:894:LEU:HD13	2.02	0.41
1:A:1082:CYS:HB2	1:A:1132:ILE:HD13	2.01	0.41
1:B:104:TRP:CD1	1:B:238:PHE:HE1	2.38	0.41
1:B:1001:LEU:O	1:B:1005:GLN:HG2	2.20	0.41
1:B:1091:ARG:HB3	1:B:1092:GLU:OE1	2.20	0.41
1:C:37:TYR:HB3	1:C:223:LEU:HB2	2.03	0.41
1:C:38:TYR:CE2	1:C:224:GLU:HG3	2.55	0.41
1:A:188:ASN:OD1	1:A:188:ASN:N	2.52	0.41
1:A:427:ASP:N	1:A:427:ASP:OD1	2.53	0.41
1:A:557:LYS:HD2	1:A:559:PHE:HE1	1.85	0.41
1:B:338:PHE:CE1	1:B:358:ILE:HD13	2.53	0.41
1:B:598:ILE:HG13	1:B:609:ALA:HB3	2.01	0.41
1:B:841:LEU:HB3	1:C:588:THR:HG21	2.02	0.41
1:B:1013:ILE:HD13	1:B:1013:ILE:HA	1.80	0.41
1:C:25:THR:O	1:C:65:PHE:HA	2.20	0.41
1:C:467:ASP:O	1:C:468:ILE:C	2.59	0.41
1:C:574:ASP:O	1:C:587:ILE:N	2.50	0.41
1:A:634:ARG:HD3	1:A:634:ARG:HA	1.90	0.41
1:B:24:THR:O	1:B:26:GLN:NE2	2.54	0.41
1:C:850:ILE:O	1:C:854:LYS:HG2	2.20	0.41
1:C:920:GLN:HA	1:C:923:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ILE:HD12	1:A:101:ILE:HA	1.98	0.41
1:A:168:PHE:HZ	1:A:230:PRO:HD2	1.86	0.41
1:A:404:GLY:HA2	1:A:508:TYR:CD2	2.56	0.41
1:A:457:ARG:NH1	1:A:467:ASP:OD2	2.47	0.41
1:B:654:GLU:N	1:B:654:GLU:OE2	2.53	0.41
1:A:280:ASN:HB2	1:A:284:THR:H	1.84	0.41
1:A:646:ARG:HG2	1:C:833:PHE:HB2	2.02	0.41
1:B:417:ASN:ND2	1:B:455:LEU:HD23	2.36	0.41
1:B:854:LYS:HD2	1:B:854:LYS:HA	1.87	0.41
1:C:188:ASN:HA	1:C:209:PRO:CA	2.51	0.41
1:C:478:LYS:HE3	1:C:478:LYS:HB2	1.89	0.41
1:A:424:LYS:HB2	1:A:424:LYS:HE3	1.91	0.41
1:A:431:GLY:HA2	1:A:515:PHE:CD2	2.56	0.41
1:A:703:ASN:OD1	1:A:704:SER:N	2.54	0.41
1:A:855:PHE:HB3	1:A:856:ASN:OD1	2.20	0.41
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.56	0.41
1:B:120:VAL:HG13	1:B:127:PHE:HD2	1.84	0.41
1:B:373:PRO:HD2	1:B:436:TRP:NE1	2.36	0.41
1:B:1075:PHE:HB3	1:B:1097:SER:O	2.20	0.41
1:C:134:GLN:O	1:C:135:PHE:HB2	2.20	0.41
1:A:501:TYR:HB3	1:A:505:HIS:HB3	2.01	0.41
1:A:804:GLN:OE1	3:F:1:NAG:O6	2.25	0.41
1:A:849:LEU:HD22	1:A:849:LEU:H	1.86	0.41
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.90	0.41
1:A:66:HIS:ND1	1:A:67:ALA:N	2.63	0.40
1:A:418:ILE:HG23	1:A:422:ASN:HB2	2.03	0.40
1:A:450:ASP:OD1	1:A:450:ASP:N	2.52	0.40
1:B:320:VAL:HG13	1:B:628:GLN:HG2	2.03	0.40
1:B:730:SER:O	1:B:1058:HIS:HB3	2.21	0.40
1:A:48:LEU:CD1	1:A:306:PHE:CE1	3.04	0.40
1:A:271:GLN:O	1:A:273:ARG:HG3	2.21	0.40
1:A:946:GLY:O	1:A:950:ASP:HB2	2.22	0.40
1:C:191:GLU:HB2	1:C:223:LEU:HD11	2.03	0.40
1:C:338:PHE:O	1:C:339:HIS:C	2.58	0.40
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.55	0.40
1:C:570:VAL:O	1:C:572:THR:HG23	2.21	0.40
1:C:784:GLN:HG3	1:C:1034:LEU:HD11	2.03	0.40
1:C:1086:LYS:HE3	1:C:1086:LYS:HB2	1.88	0.40
1:A:847:ARG:HB2	1:A:851:CYS:HB2	2.04	0.40
1:B:716:THR:HA	1:B:1110:TYR:HB3	2.03	0.40
1:B:1071:GLN:H	1:B:1071:GLN:HG3	1.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HD12	1:C:57:PRO:HD2	2.02	0.40
1:C:204:TYR:HD1	1:C:225:PRO:HA	1.86	0.40
1:C:951:VAL:O	1:C:955:ASN:ND2	2.54	0.40
1:A:41:LYS:HB3	1:B:562:PHE:O	2.21	0.40
1:A:1049:LEU:HB2	1:A:1065:VAL:O	2.22	0.40
1:B:54:LEU:HD21	1:B:88:ASP:O	2.22	0.40
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.03	0.40
1:B:358:ILE:HD12	1:B:395:VAL:HG12	2.04	0.40
1:B:979:ASP:O	1:B:983:ARG:HG3	2.22	0.40
1:C:331:ASN:O	1:C:332:VAL:HB	2.22	0.40
1:C:1081:ILE:HG13	1:C:1095:PHE:CD2	2.56	0.40
1:A:201:PHE:O	1:A:228:ASP:HA	2.21	0.40
1:A:337:PRO:HA	1:A:339:HIS:CE1	2.56	0.40
1:A:460:LYS:HA	1:A:460:LYS:HD3	1.77	0.40
1:A:471:GLU:HA	1:A:481:LYS:NZ	2.36	0.40
1:B:358:ILE:HD11	1:B:397:ALA:HB2	2.03	0.40
1:C:159:VAL:O	1:C:159:VAL:HG12	2.22	0.40
1:C:338:PHE:O	1:C:341:VAL:HG22	2.22	0.40
1:C:734:THR:O	1:C:767:LEU:HD12	2.22	0.40
1:C:1043:CYS:HB2	1:C:1048:HIS:CG	2.56	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	1053/1206 (87%)	960 (91%)	87 (8%)	6 (1%)	25	62
1	B	1053/1206 (87%)	973 (92%)	77 (7%)	3 (0%)	41	74
1	C	1053/1206 (87%)	963 (92%)	81 (8%)	9 (1%)	17	53
All	All	3159/3618 (87%)	2896 (92%)	245 (8%)	18 (1%)	29	62

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	210	ILE
1	A	591	SER
1	C	332	VAL
1	C	467	ASP
1	B	109	THR
1	B	745	ASP
1	C	135	PHE
1	A	283	GLY
1	A	1106	GLN
1	C	210	ILE
1	C	212	ILE
1	C	468	ILE
1	A	32	PHE
1	C	164	ASN
1	B	534	VAL
1	C	136	CYS
1	C	327	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	925/1054 (88%)	881 (95%)	44 (5%)	25	54
1	B	925/1054 (88%)	892 (96%)	33 (4%)	35	61
1	C	925/1054 (88%)	894 (97%)	31 (3%)	37	62
All	All	2775/3162 (88%)	2667 (96%)	108 (4%)	36	59

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

Mol	Chain	Res	Type
1	A	29	THR
1	A	31	SER
1	A	46	SER

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Mol	Chain	Res	Type
1	A	60	SER
1	A	62	VAL
1	A	118	LEU
1	A	130	VAL
1	A	131	CYS
1	A	135	PHE
1	A	168	PHE
1	A	218	GLN
1	A	220	PHE
1	A	233	ILE
1	A	242	LEU
1	A	246	ARG
1	A	265	TYR
1	A	287	ASP
1	A	296	LEU
1	A	351	TYR
1	A	353	TRP
1	A	366	SER
1	A	375	PHE
1	A	423	TYR
1	A	457	ARG
1	A	464	PHE
1	A	465	GLU
1	A	473	TYR
1	A	498	ARG
1	A	508	TYR
1	A	543	PHE
1	A	568	ASP
1	A	611	LEU
1	A	634	ARG
1	A	699	LEU
1	A	707	TYR
1	A	856	ASN
1	A	873	TYR
1	A	898	PHE
1	A	900	MET
1	A	911	VAL
1	A	978	ASN
1	A	1041	ASP
1	A	1050	MET
1	A	1107	ARG
1	B	61	ASN

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	112	SER
1	B	134	GLN
1	B	135	PHE
1	B	160	TYR
1	B	168	PHE
1	B	198	ASP
1	B	200	TYR
1	B	205	SER
1	B	238	PHE
1	B	264	ASP
1	B	277	LEU
1	B	302	THR
1	B	303	LEU
1	B	360	ASN
1	B	371	PHE
1	B	453	TYR
1	B	462	LYS
1	B	487	ASN
1	B	495	TYR
1	B	547	THR
1	B	617	CYS
1	B	643	PHE
1	B	707	TYR
1	B	735	SER
1	B	759	PHE
1	B	820	ASP
1	B	939	PHE
1	B	976	VAL
1	B	979	ASP
1	B	1000	ARG
1	B	1127	ASP
1	C	62	VAL
1	C	63	THR
1	C	119	ILE
1	C	127	PHE
1	C	133	PHE
1	C	165	ASN
1	C	168	PHE
1	C	178	ASP
1	C	216	PHE
1	C	238	PHE

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Mol	Chain	Res	Type
1	C	265	TYR
1	C	328	ARG
1	C	333	THR
1	C	377	PHE
1	C	386	LYS
1	C	390	LEU
1	C	396	TYR
1	C	455	LEU
1	C	468	ILE
1	C	477	ASN
1	C	508	TYR
1	C	571	ASP
1	C	620	VAL
1	C	633	TRP
1	C	636	TYR
1	C	756	TYR
1	C	759	PHE
1	C	760	CYS
1	C	939	PHE
1	C	1037	SER
1	C	1045	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	628	GLN
1	B	321	GLN
1	B	394	ASN
1	B	1005	GLN
1	C	173	GLN
1	C	360	ASN

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)

28 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	$\#\|Z\| > 2$
2	NAG	D	1	2,1	14,14,15	0.41	0	17,19,21	0.62	0
2	NAG	D	2	2	14,14,15	0.42	0	17,19,21	0.50	0
3	NAG	E	1	3,1	14,14,15	0.19	0	17,19,21	0.41	0
3	BMA	E	2	3	11,11,12	0.59	0	15,15,17	0.78	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.43	0
3	BMA	F	2	3	11,11,12	0.62	0	15,15,17	0.71	0
3	NAG	G	1	3,1	14,14,15	0.25	0	17,19,21	0.41	0
3	BMA	G	2	3	11,11,12	0.58	0	15,15,17	0.73	0
3	NAG	H	1	3,1	14,14,15	1.05	1 (7%)	17,19,21	1.00	1 (5%)
3	BMA	H	2	3	11,11,12	0.56	0	15,15,17	1.11	1 (6%)
3	NAG	I	1	3,1	14,14,15	0.22	0	17,19,21	0.38	0
3	BMA	I	2	3	11,11,12	0.61	0	15,15,17	0.74	0
3	NAG	J	1	3,1	14,14,15	0.20	0	17,19,21	0.41	0
3	BMA	J	2	3	11,11,12	0.57	0	15,15,17	0.71	0
3	NAG	K	1	3,1	14,14,15	0.30	0	17,19,21	0.46	0
3	BMA	K	2	3	11,11,12	0.62	0	15,15,17	0.68	0
3	NAG	L	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	L	2	3	11,11,12	0.61	0	15,15,17	0.73	0
3	NAG	M	1	3,1	14,14,15	1.01	1 (7%)	17,19,21	0.99	1 (5%)
3	BMA	M	2	3	11,11,12	0.61	0	15,15,17	1.45	3 (20%)
3	NAG	N	1	3,1	14,14,15	0.22	0	17,19,21	0.43	0
3	BMA	N	2	3	11,11,12	0.61	0	15,15,17	0.71	0
3	NAG	O	1	3,1	14,14,15	0.26	0	17,19,21	0.45	0
3	BMA	O	2	3	11,11,12	0.65	0	15,15,17	0.67	0
3	NAG	P	1	3,1	14,14,15	0.21	0	17,19,21	0.42	0
3	BMA	P	2	3	11,11,12	0.59	0	15,15,17	0.74	0
3	NAG	Q	1	3,1	14,14,15	1.14	1 (7%)	17,19,21	1.11	1 (5%)
3	BMA	Q	2	3	11,11,12	0.62	0	15,15,17	1.34	3 (20%)

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
2	NAG	D	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	E	2	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	G	2	3	-	0/2/19/22	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	H	2	3	-	0/2/19/22	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	I	2	3	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	J	2	3	-	0/2/19/22	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	K	2	3	-	1/2/19/22	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	L	2	3	-	1/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	M	2	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	N	2	3	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	O	2	3	-	0/2/19/22	0/1/1/1
3	NAG	P	1	3,1	-	0/6/23/26	0/1/1/1
3	BMA	P	2	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	BMA	Q	2	3	-	2/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	1	NAG	O5-C1	-3.96	1.37	1.43
3	H	1	NAG	O5-C1	-3.66	1.37	1.43
3	M	1	NAG	O5-C1	-3.54	1.38	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	2	BMA	C1-O5-C5	3.14	116.44	112.19
3	Q	1	NAG	C3-C4-C5	3.02	115.63	110.24
3	Q	2	BMA	C1-O5-C5	2.92	116.15	112.19
3	M	2	BMA	O5-C1-C2	2.65	114.86	110.77
3	H	1	NAG	C3-C4-C5	2.62	114.91	110.24
3	H	2	BMA	C1-O5-C5	2.58	115.68	112.19
3	M	1	NAG	C3-C4-C5	2.46	114.62	110.24
3	M	2	BMA	C1-C2-C3	2.45	112.68	109.67
3	Q	2	BMA	O5-C1-C2	2.30	114.32	110.77
3	Q	2	BMA	C1-C2-C3	2.24	112.42	109.67

There are no chirality outliers.

All (26) torsion outliers are listed below:

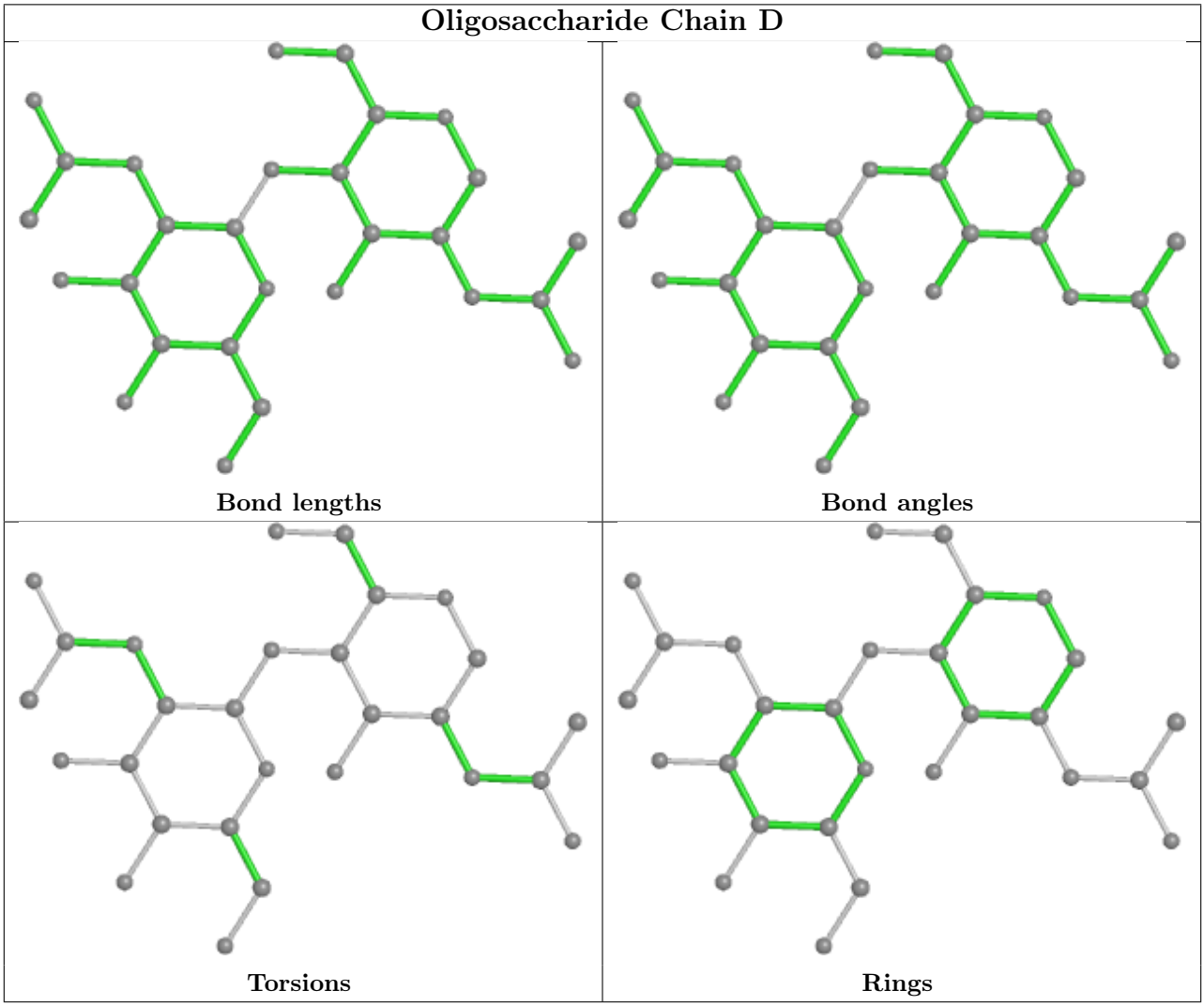
Mol	Chain	Res	Type	Atoms
3	M	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	2	BMA	O5-C5-C6-O6
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	M	2	BMA	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
3	Q	2	BMA	O5-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	Q	2	BMA	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	K	2	BMA	O5-C5-C6-O6
3	L	2	BMA	O5-C5-C6-O6

There are no ring outliers.

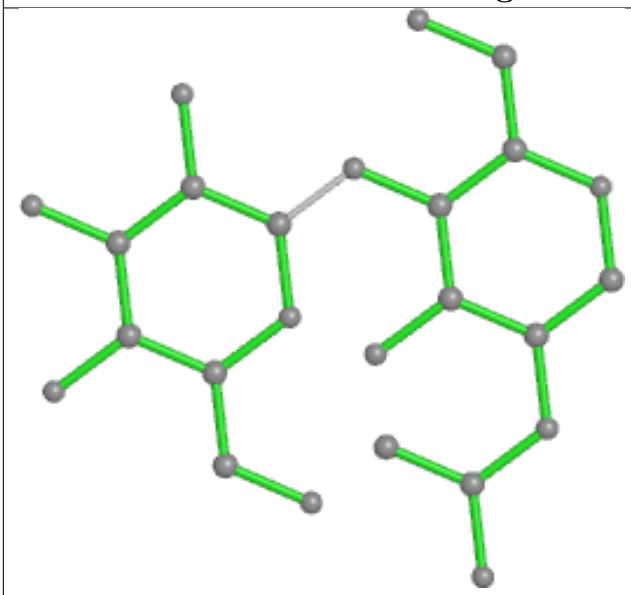
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	F	2	BMA	1	0
2	D	1	NAG	1	0

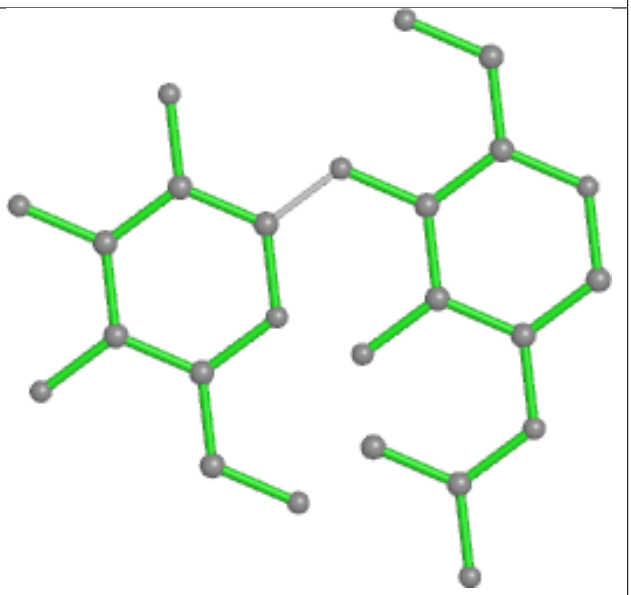
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



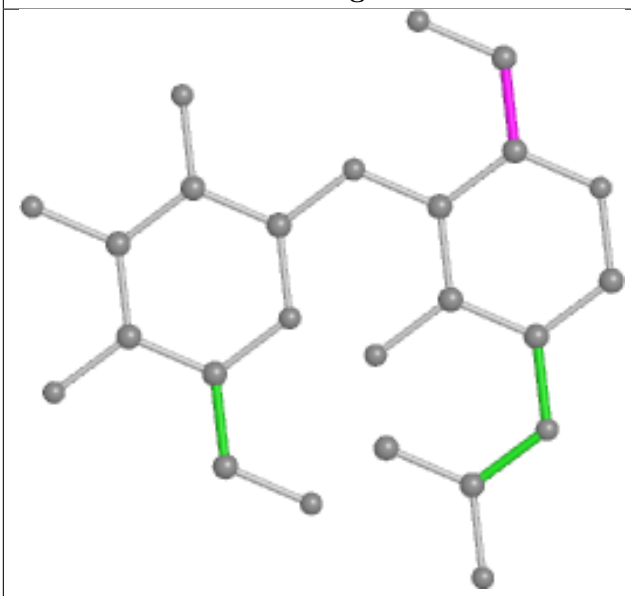
Oligosaccharide Chain E



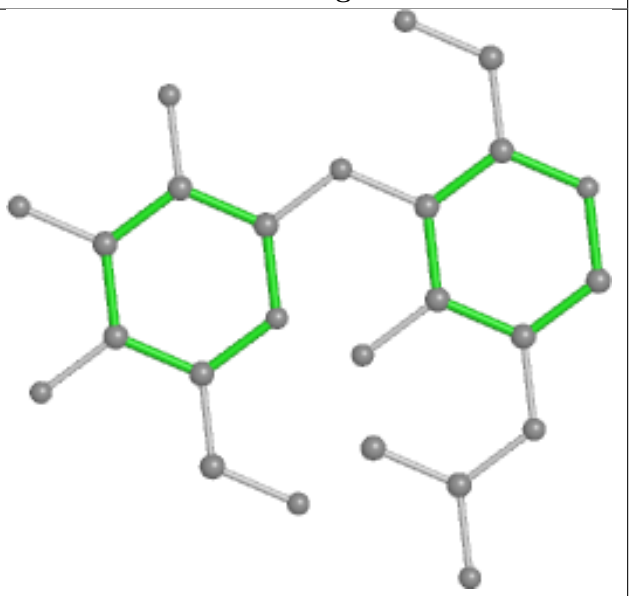
Bond lengths



Bond angles

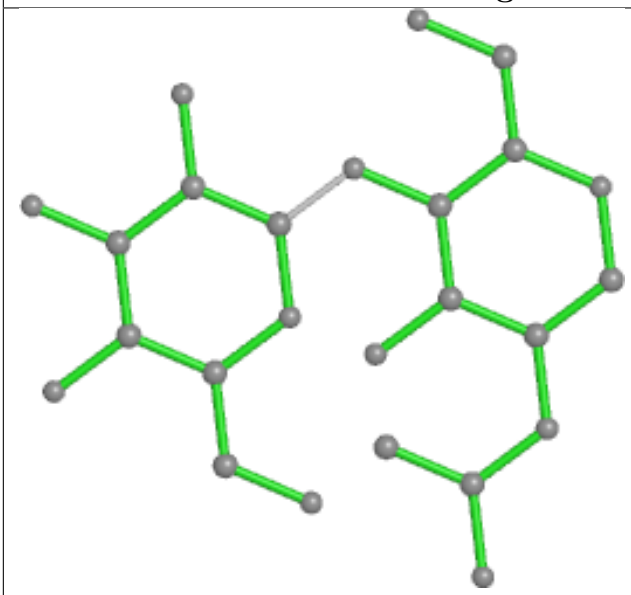


Torsions

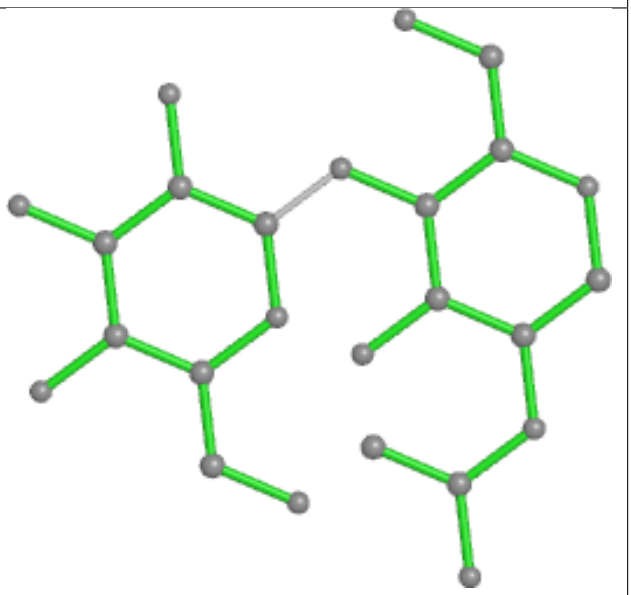


Rings

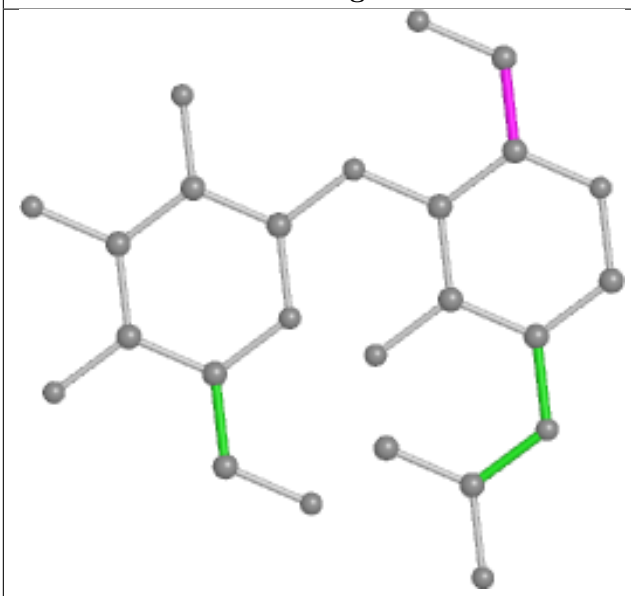
Oligosaccharide Chain F



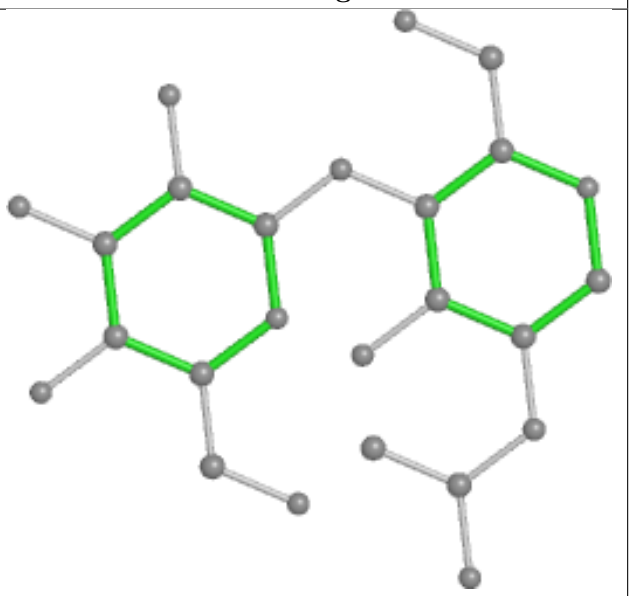
Bond lengths



Bond angles

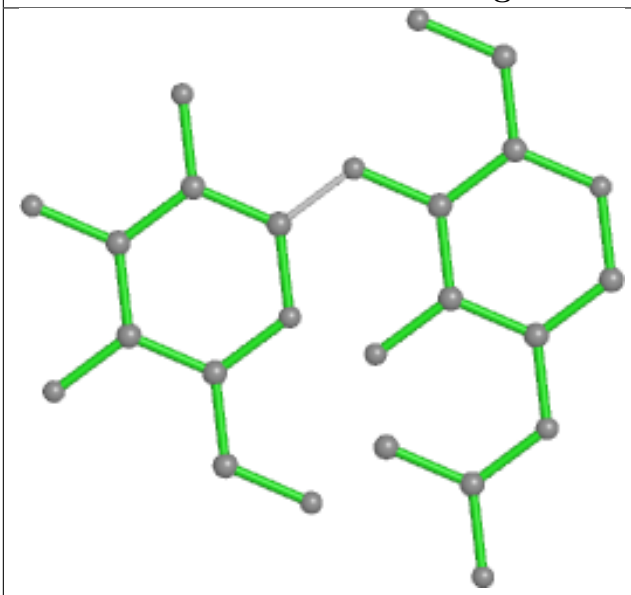


Torsions

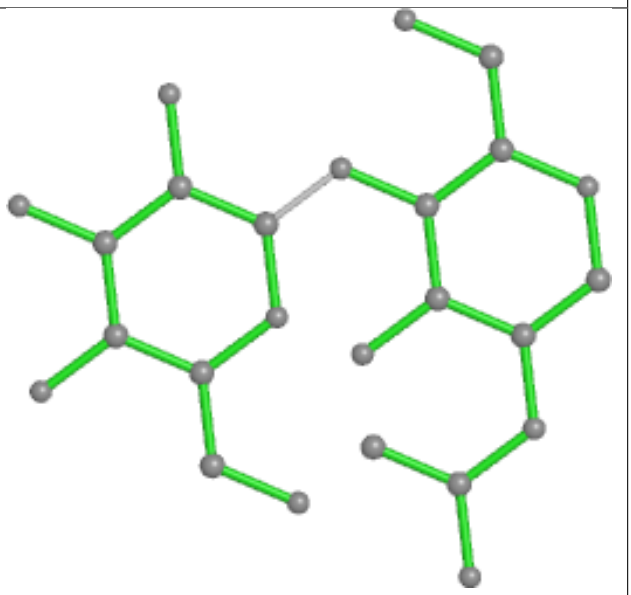


Rings

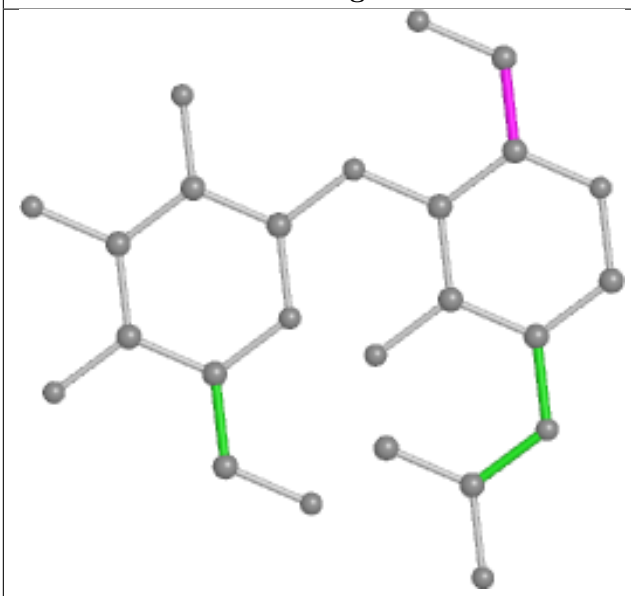
Oligosaccharide Chain G



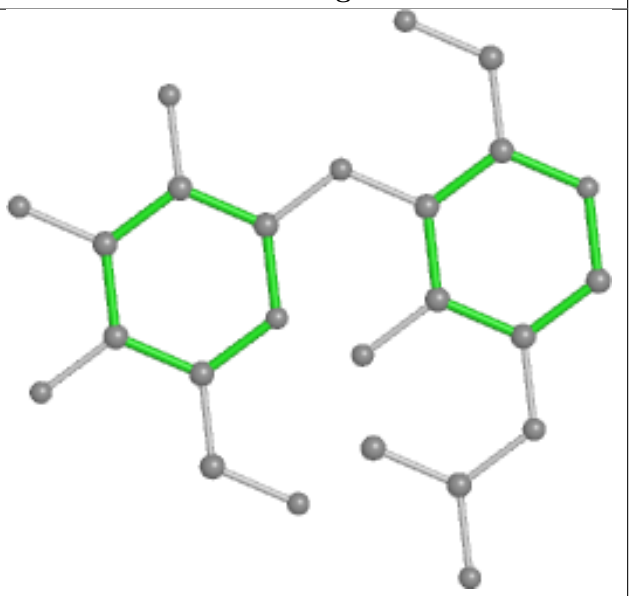
Bond lengths



Bond angles

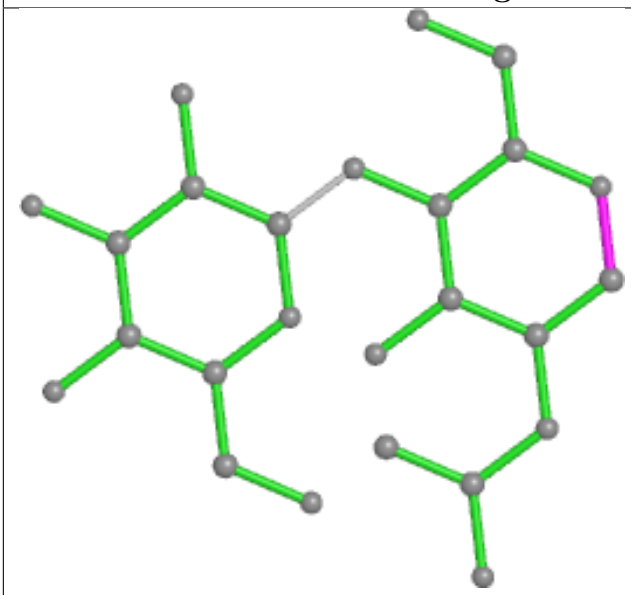


Torsions

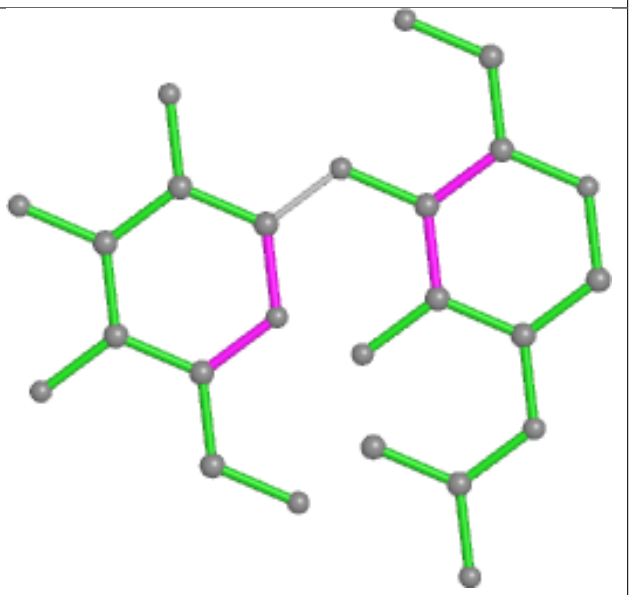


Rings

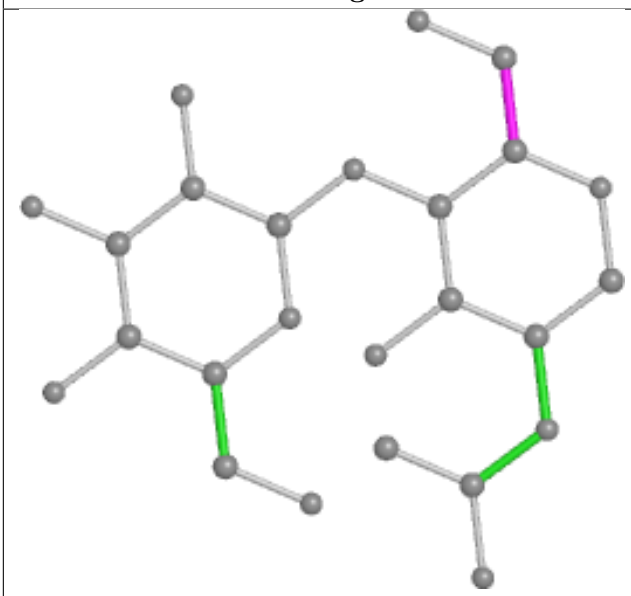
Oligosaccharide Chain H



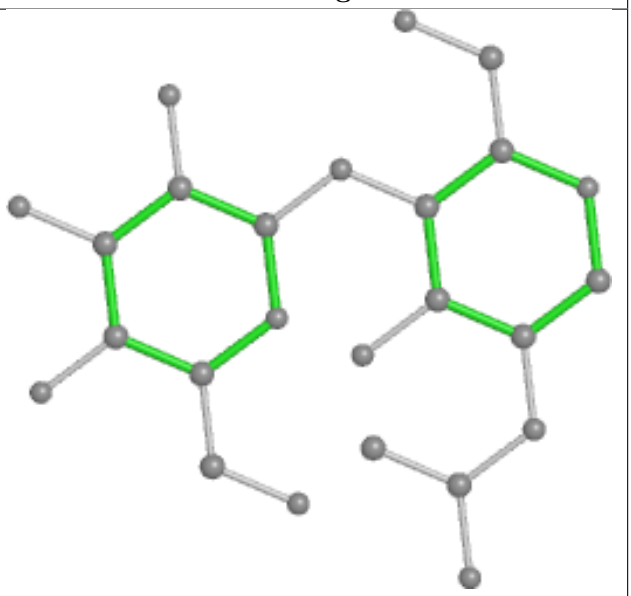
Bond lengths



Bond angles

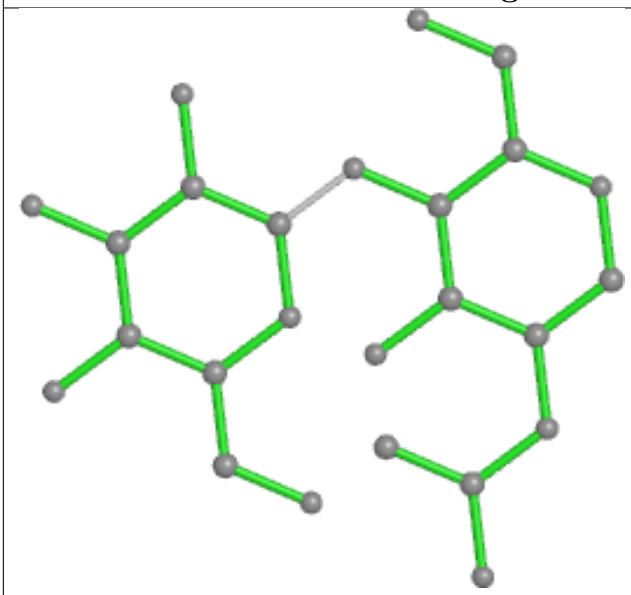


Torsions

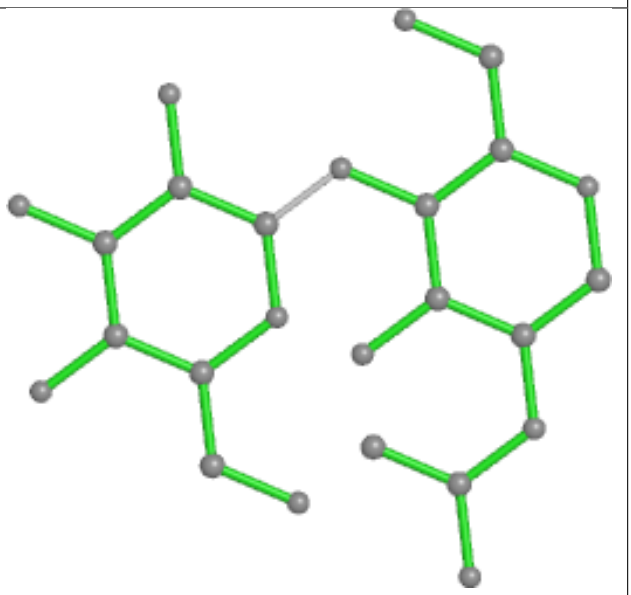


Rings

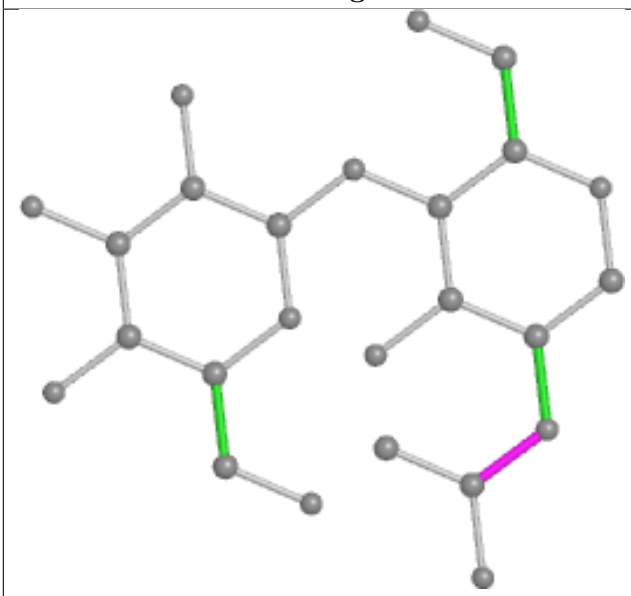
Oligosaccharide Chain I



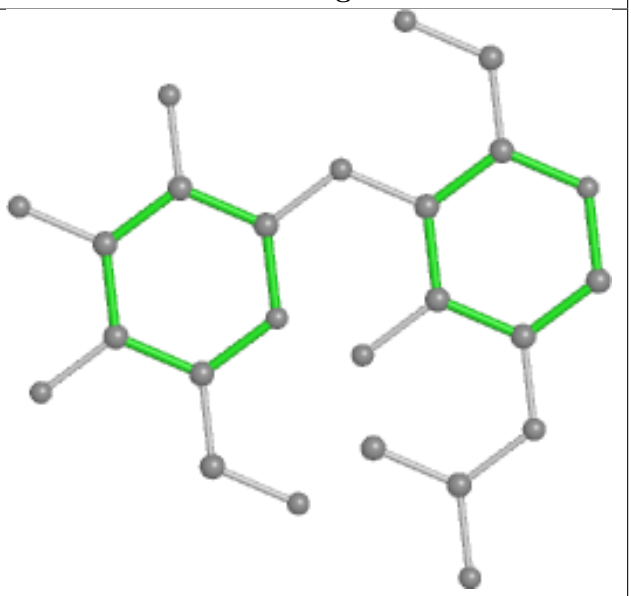
Bond lengths



Bond angles

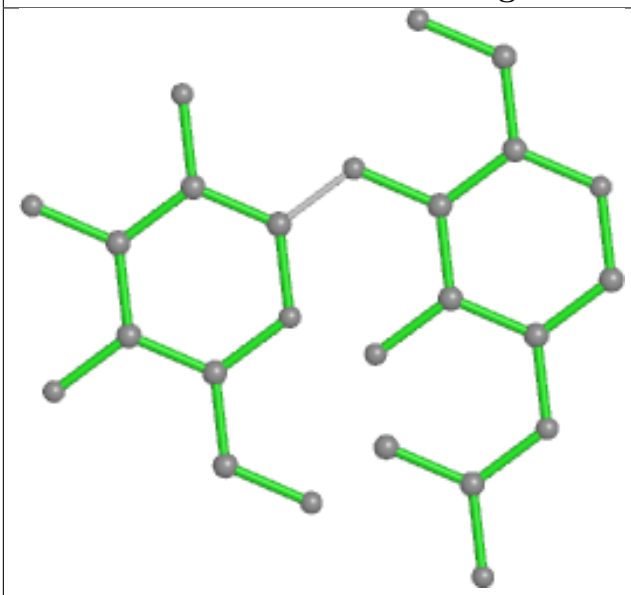


Torsions

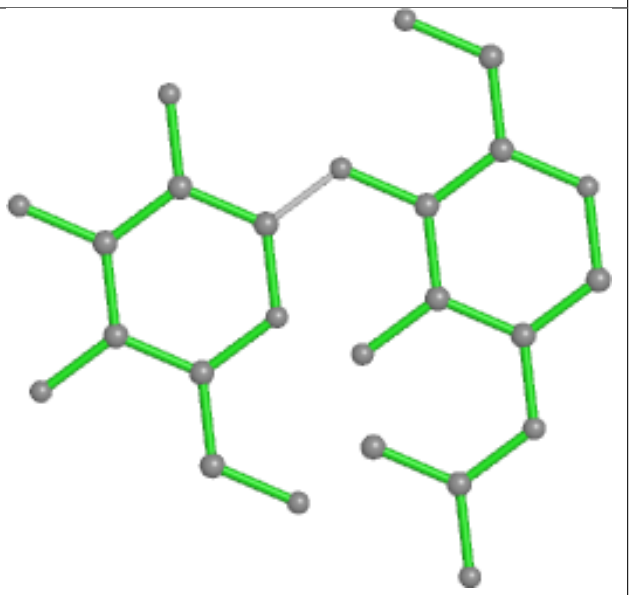


Rings

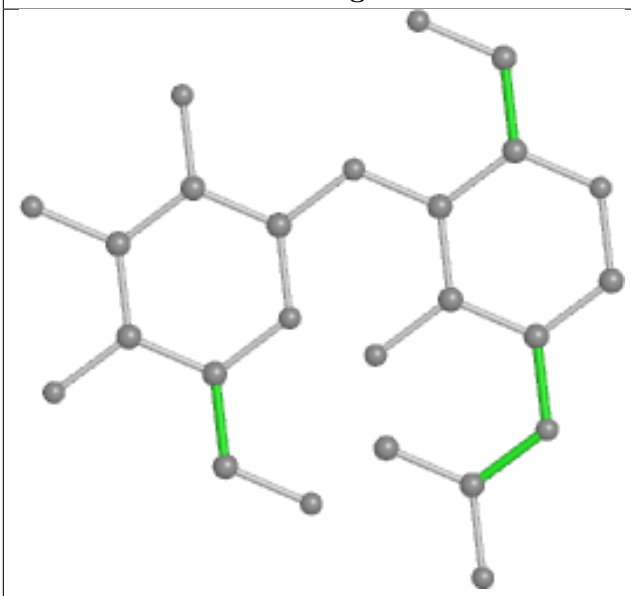
Oligosaccharide Chain J



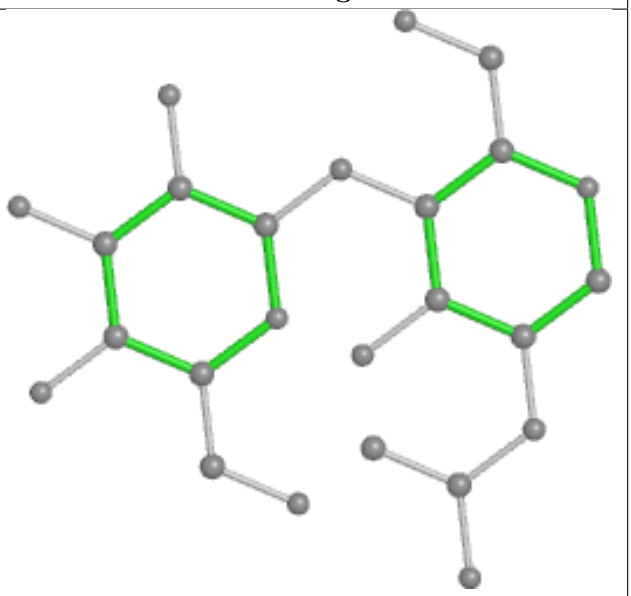
Bond lengths



Bond angles

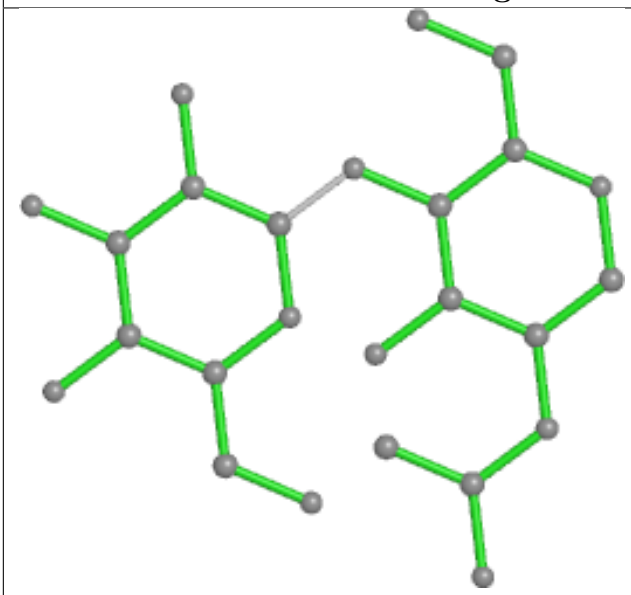


Torsions

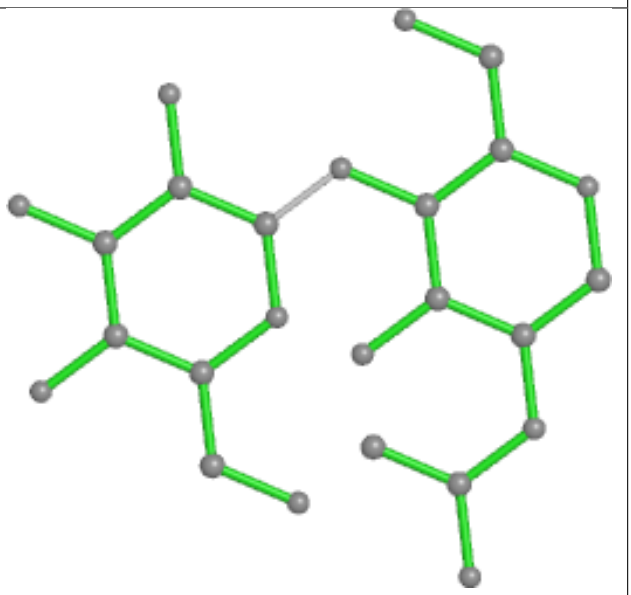


Rings

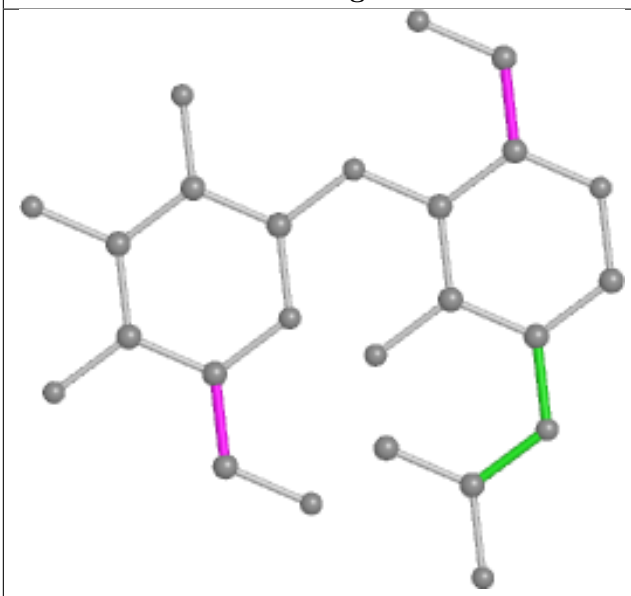
Oligosaccharide Chain K



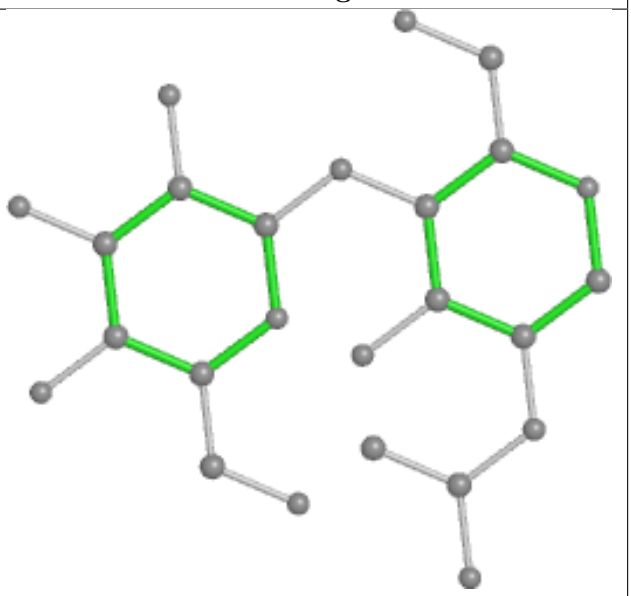
Bond lengths



Bond angles

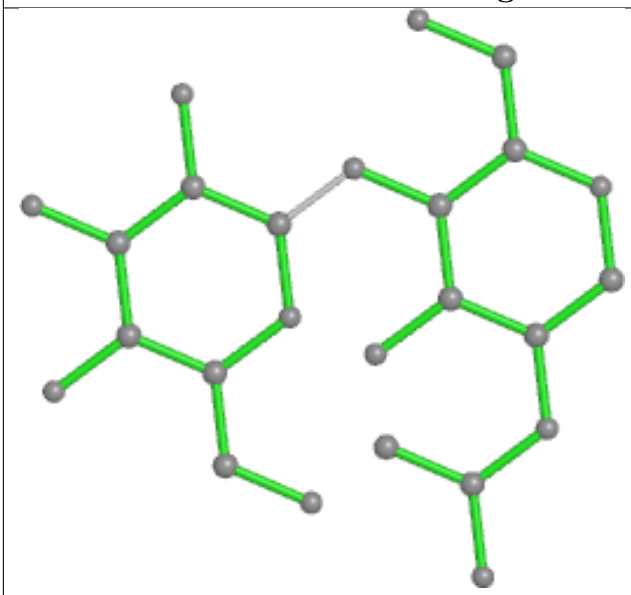


Torsions

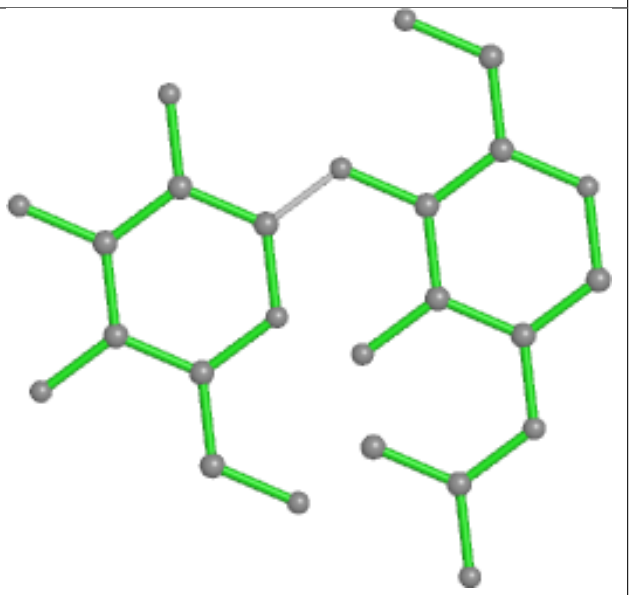


Rings

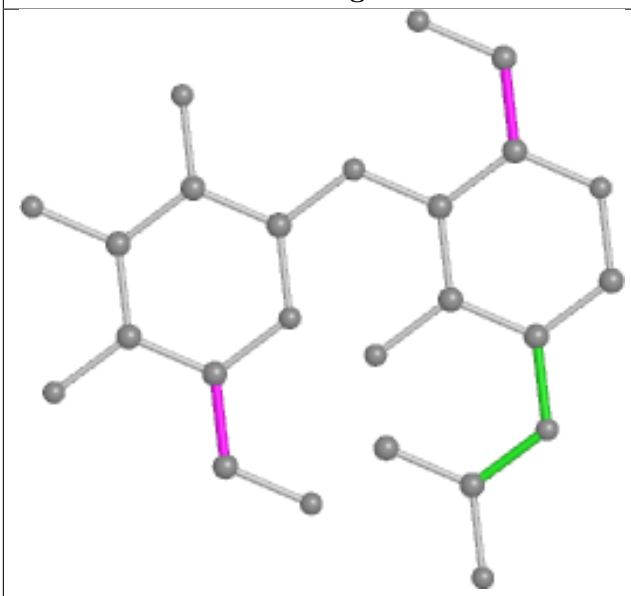
Oligosaccharide Chain L



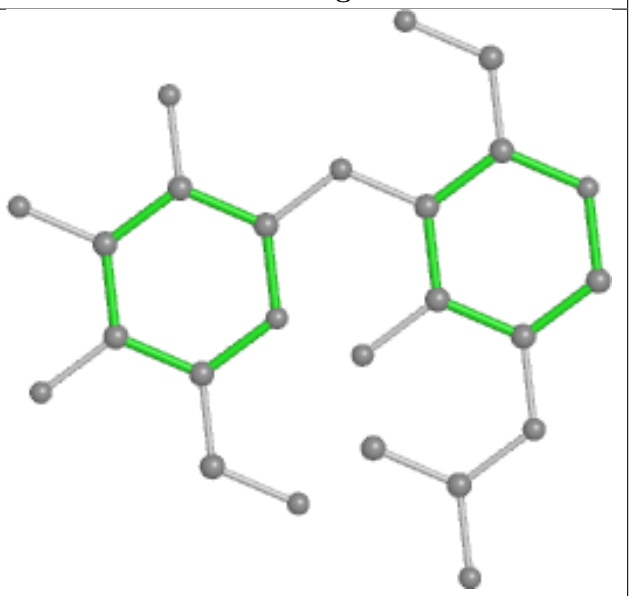
Bond lengths



Bond angles

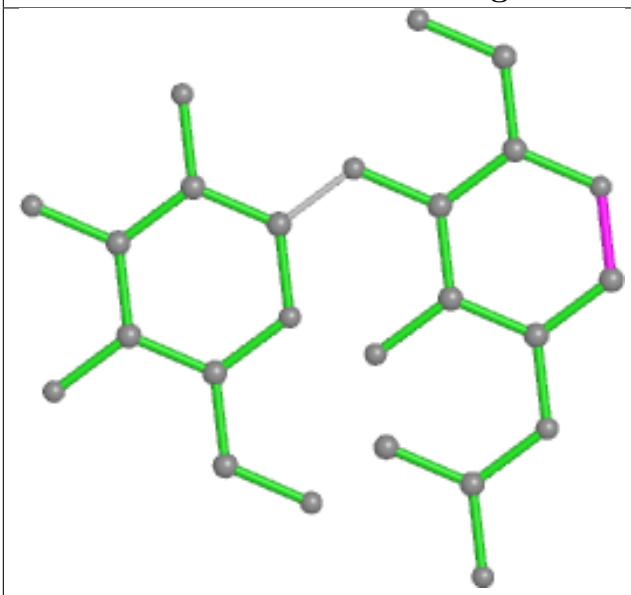


Torsions

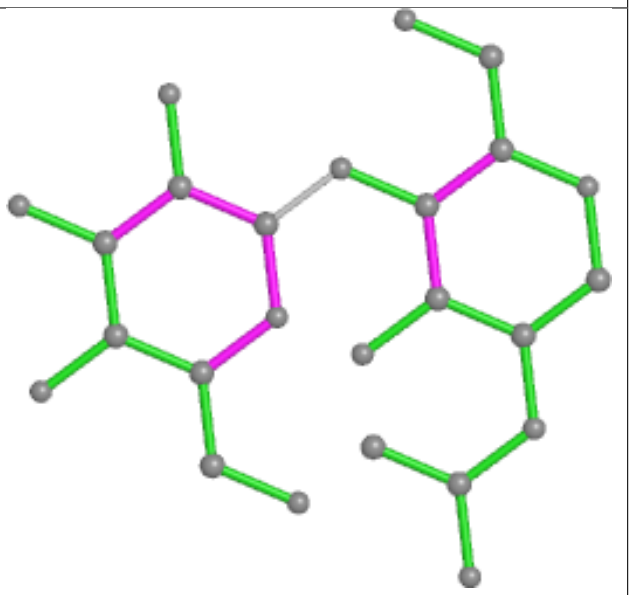


Rings

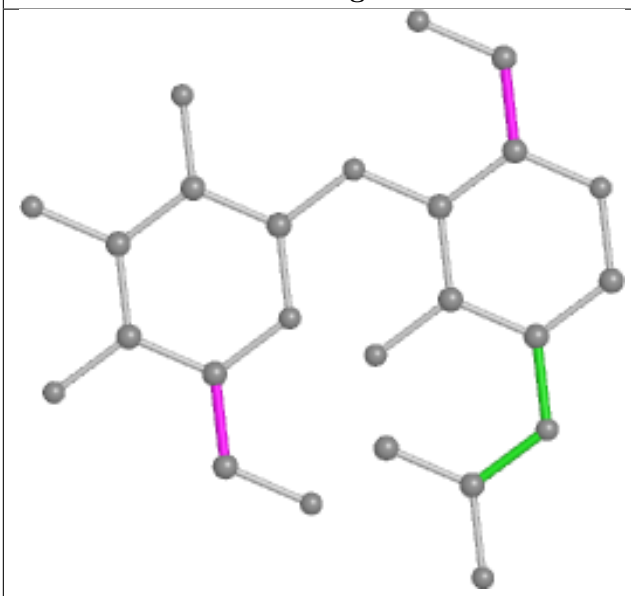
Oligosaccharide Chain M



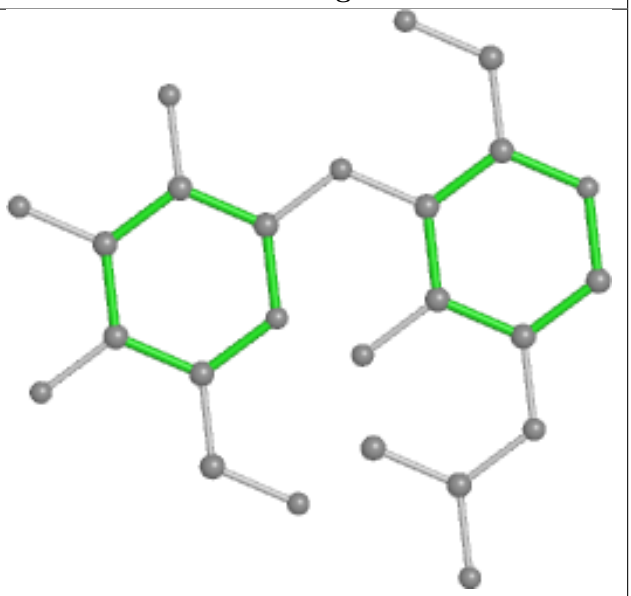
Bond lengths



Bond angles

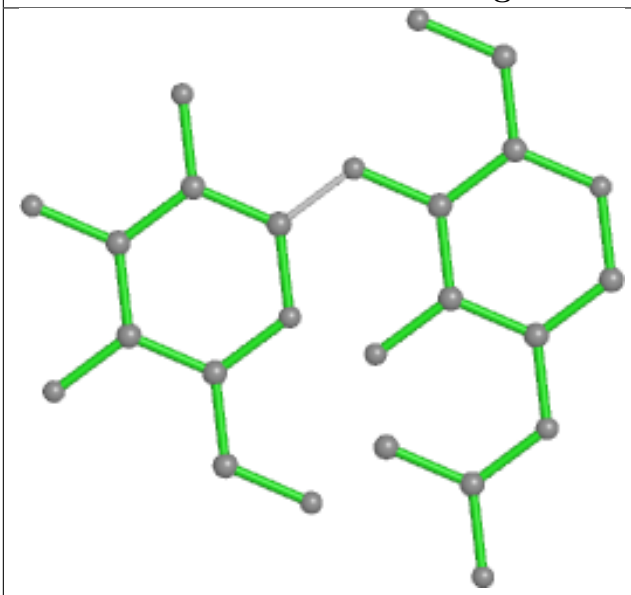


Torsions

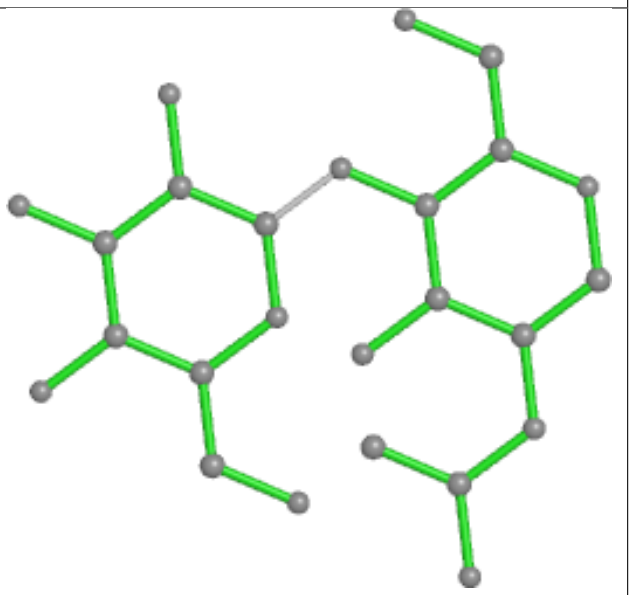


Rings

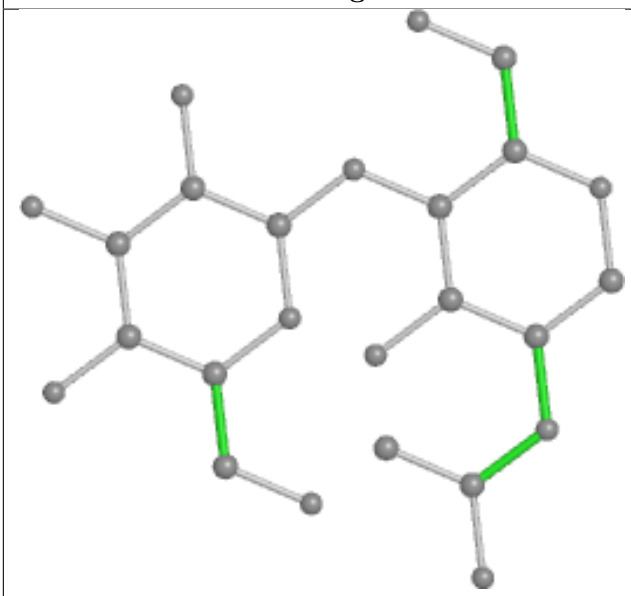
Oligosaccharide Chain N



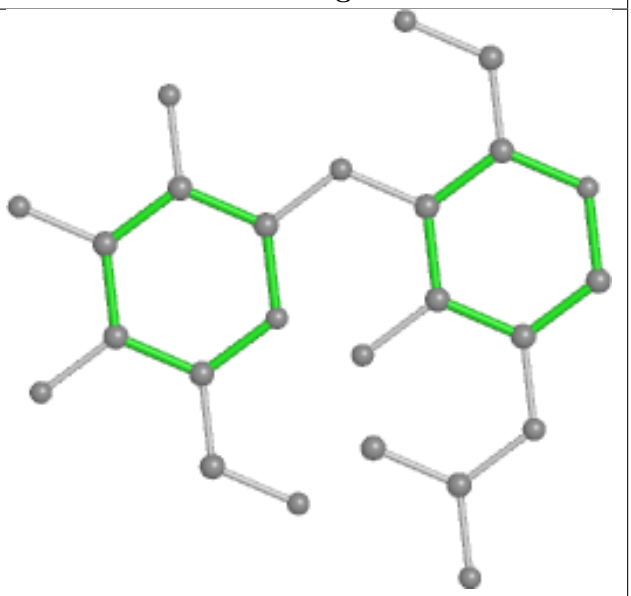
Bond lengths



Bond angles

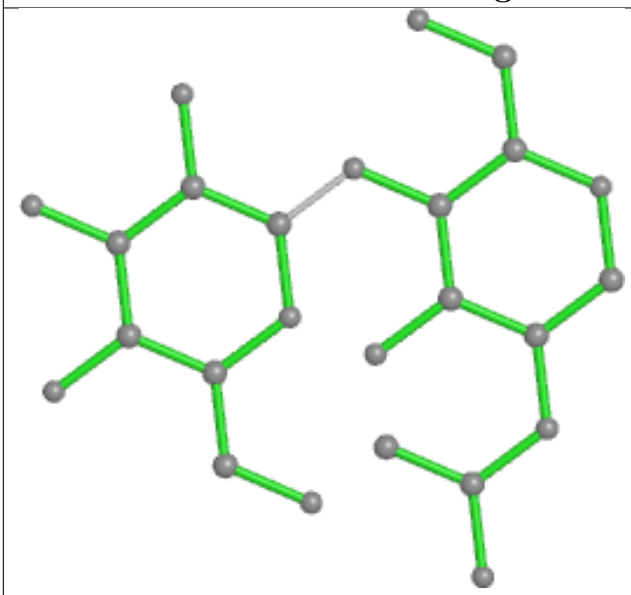


Torsions

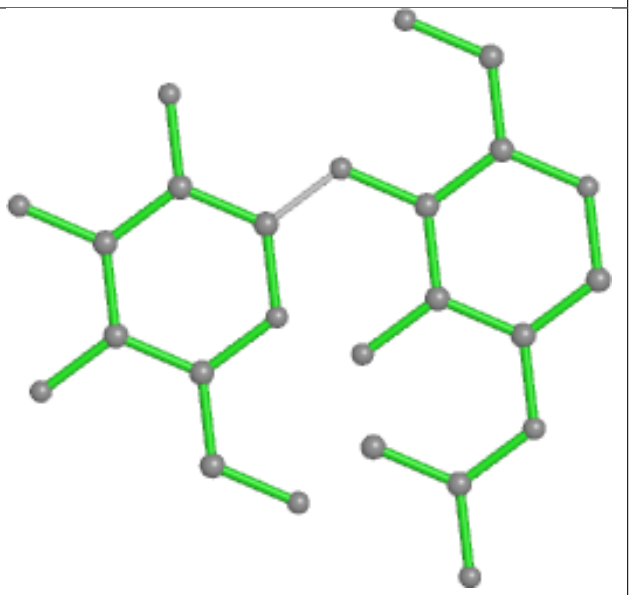


Rings

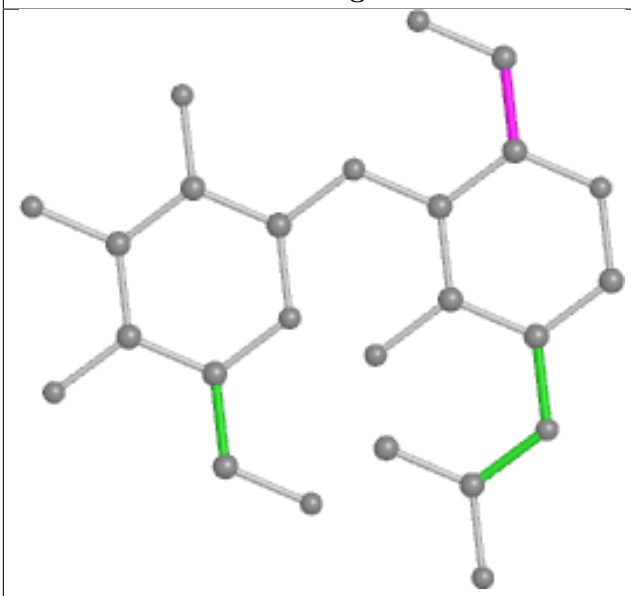
Oligosaccharide Chain O



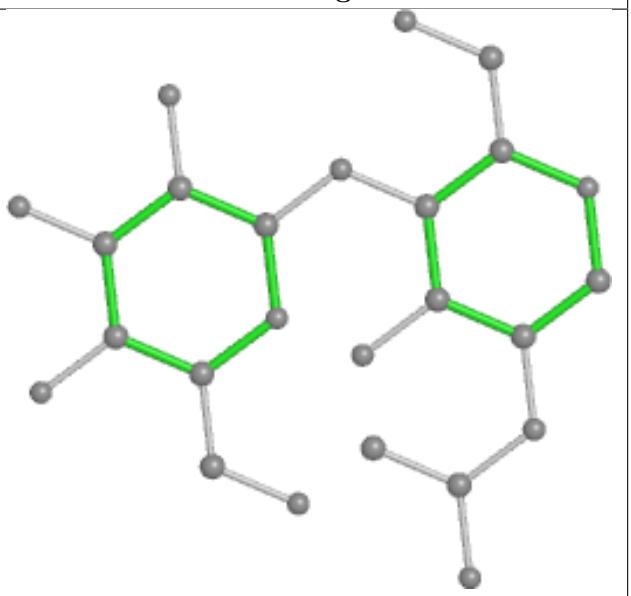
Bond lengths



Bond angles

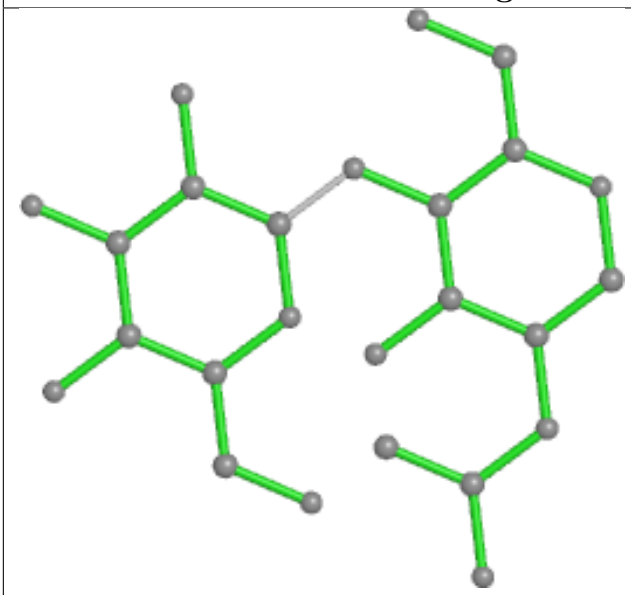


Torsions

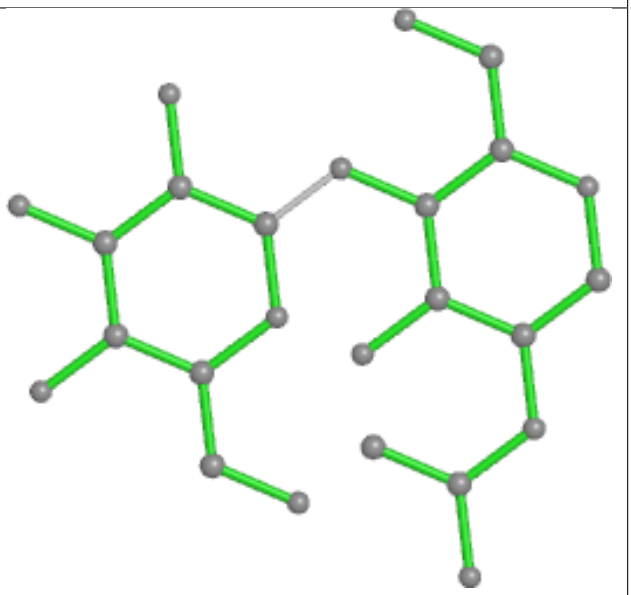


Rings

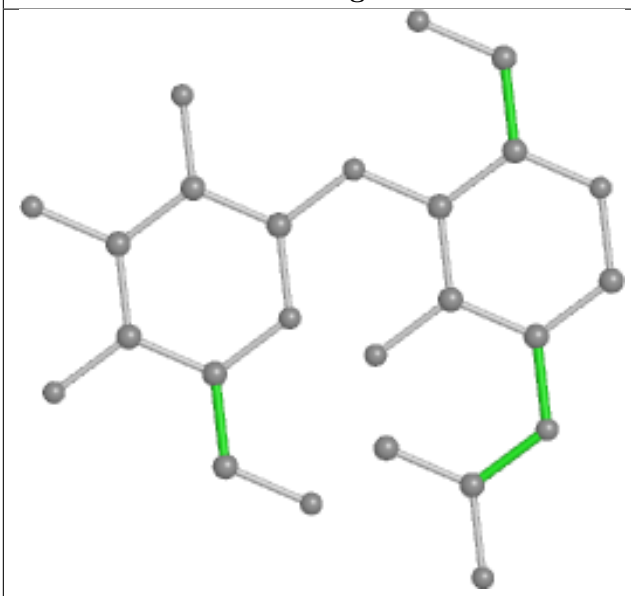
Oligosaccharide Chain P



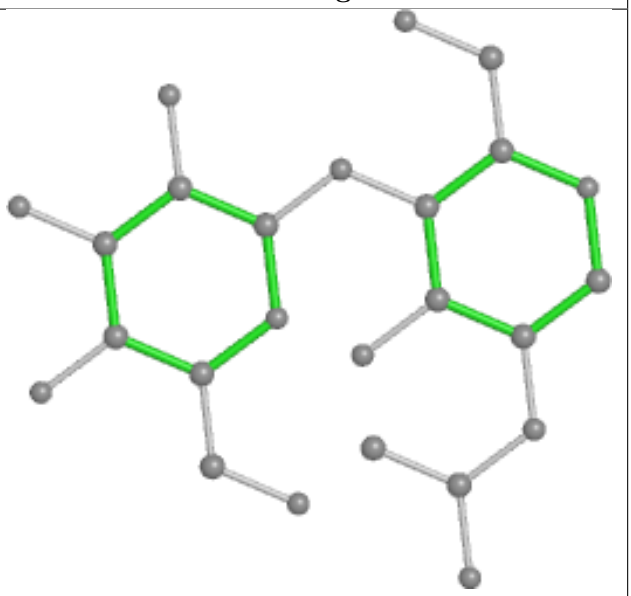
Bond lengths



Bond angles

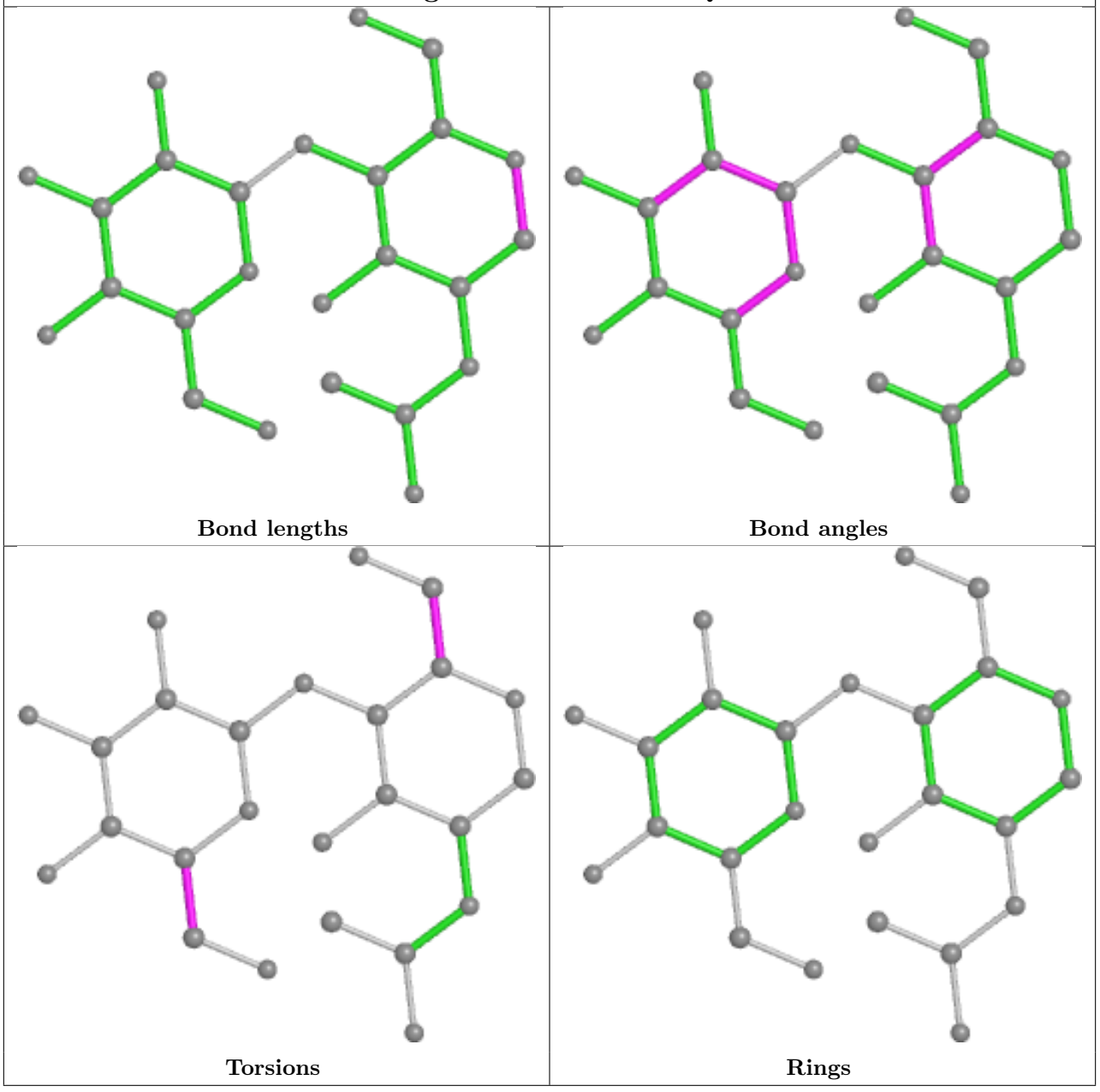


Torsions



Rings

Oligosaccharide Chain Q



5.6 Ligand geometry (i)

35 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	$\#\|Z\|>2$
4	NAG	C	1306	1	14,14,15	0.39	0	17,19,21	0.65	0
4	NAG	B	1310	1	14,14,15	0.27	0	17,19,21	0.44	0
4	NAG	B	1302	1	14,14,15	0.72	1 (7%)	17,19,21	0.73	1 (5%)
4	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	A	1309	1	14,14,15	0.39	0	17,19,21	0.53	0
4	NAG	A	1308	1	14,14,15	0.39	0	17,19,21	0.44	0
4	NAG	B	1309	1	14,14,15	0.27	0	17,19,21	0.58	0
4	NAG	B	1303	1	14,14,15	0.40	0	17,19,21	0.91	1 (5%)
4	NAG	B	1308	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1312	1	14,14,15	0.41	0	17,19,21	0.82	0
4	NAG	A	1305	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	1.37	1 (5%)
4	NAG	C	1310	1	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	B	1307	1	14,14,15	0.34	0	17,19,21	0.38	0
4	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.63	0
4	NAG	B	1305	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	A	1307	1	14,14,15	0.38	0	17,19,21	0.58	0
4	NAG	C	1309	1	14,14,15	0.40	0	17,19,21	0.70	0
4	NAG	C	1307	1	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
4	NAG	C	1308	1	14,14,15	0.39	0	17,19,21	0.56	1 (5%)
4	NAG	C	1305	1	14,14,15	0.38	0	17,19,21	1.10	2 (11%)
4	NAG	B	1304	1	14,14,15	0.39	0	17,19,21	0.70	1 (5%)
4	NAG	A	1304	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	A	1311	1	14,14,15	0.40	0	17,19,21	0.69	1 (5%)
4	NAG	A	1306	1	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	A	1310	1	14,14,15	0.39	0	17,19,21	0.39	0
4	NAG	A	1303	1	14,14,15	0.33	0	17,19,21	1.36	1 (5%)
4	NAG	B	1306	1	14,14,15	0.32	0	17,19,21	1.38	1 (5%)
5	IDU	C	1313	-	15,15,17	1.01	1 (6%)	15,22,26	1.33	2 (13%)
4	NAG	A	1301	1	14,14,15	0.53	0	17,19,21	0.59	0
4	NAG	B	1301	1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	NAG	C	1302	1	14,14,15	0.37	0	17,19,21	0.44	0
4	NAG	C	1311	1	14,14,15	0.39	0	17,19,21	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
5	IDU	C	1313	-	-	3/9/22/29	1/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1313	IDU	O6-C6	-2.98	1.20	1.30
4	B	1302	NAG	C1-C2	2.36	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1306	NAG	C1-O5-C5	5.04	119.03	112.19
4	C	1301	NAG	C1-O5-C5	5.01	118.97	112.19
4	A	1303	NAG	C1-O5-C5	5.00	118.96	112.19
5	C	1313	IDU	C2-O2-S	3.66	122.68	117.91
4	C	1305	NAG	C2-N2-C7	3.15	127.39	122.90
4	B	1301	NAG	C2-N2-C7	2.85	126.96	122.90
4	C	1307	NAG	C2-N2-C7	2.84	126.95	122.90
4	B	1303	NAG	C2-N2-C7	2.72	126.77	122.90
4	B	1302	NAG	C1-O5-C5	2.58	115.69	112.19
4	C	1305	NAG	C1-C2-N2	2.47	114.71	110.49
4	A	1311	NAG	C1-O5-C5	2.30	115.31	112.19
5	C	1313	IDU	O6-C6-C5	2.22	119.37	113.03
4	B	1304	NAG	C1-C2-N2	2.15	114.15	110.49
4	C	1308	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	C8-C7-N2-C2
4	A	1307	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2
4	C	1305	NAG	C3-C2-N2-C7
5	C	1313	IDU	C1-C2-O2-S
4	C	1303	NAG	O5-C5-C6-O6
4	C	1306	NAG	C8-C7-N2-C2
4	C	1306	NAG	O7-C7-N2-C2
4	A	1306	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	A	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O5-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1306	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	C	1310	NAG	C8-C7-N2-C2
4	B	1308	NAG	C4-C5-C6-O6
4	A	1306	NAG	C8-C7-N2-C2
4	A	1306	NAG	O7-C7-N2-C2
4	A	1308	NAG	O7-C7-N2-C2
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1309	NAG	C8-C7-N2-C2
4	B	1309	NAG	O7-C7-N2-C2
4	C	1304	NAG	C8-C7-N2-C2
4	C	1304	NAG	O7-C7-N2-C2
4	C	1310	NAG	O7-C7-N2-C2
4	B	1305	NAG	O5-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1303	NAG	C1-C2-N2-C7
4	A	1301	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	C	1306	NAG	C1-C2-N2-C7
4	B	1311	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
5	C	1313	IDU	C3-C2-O2-S
4	C	1302	NAG	O5-C5-C6-O6
5	C	1313	IDU	O5-C5-C6-O61
4	C	1305	NAG	C1-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	C	1307	NAG	C1-C2-N2-C7
4	B	1303	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7

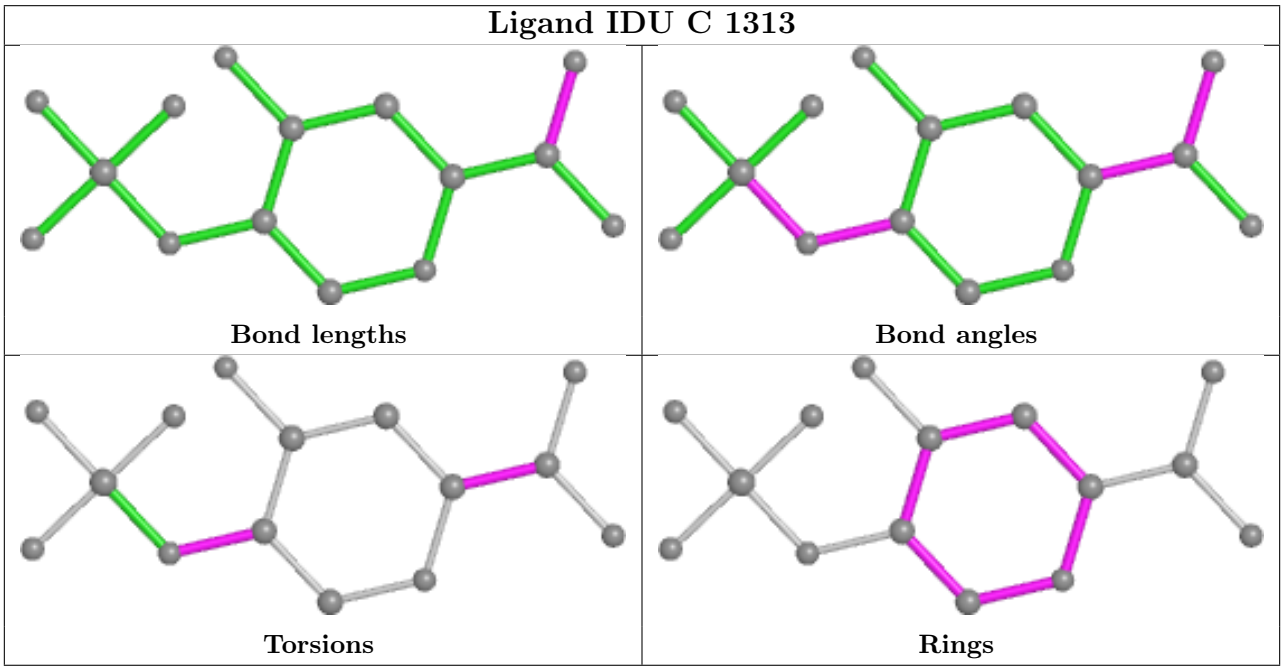
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1313	IDU	C1-C2-C3-C4-C5-O5

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1306	NAG	1	0
4	B	1302	NAG	2	0
4	B	1303	NAG	1	0
4	C	1303	NAG	1	0
4	C	1309	NAG	1	0
4	B	1304	NAG	1	0
4	A	1301	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

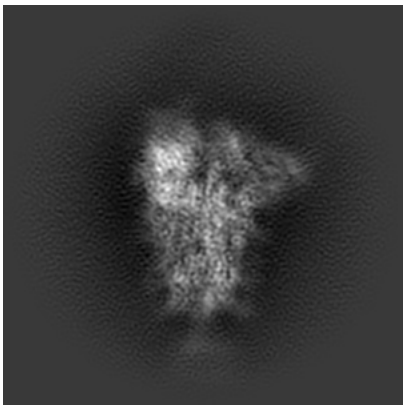
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38681. These allow visual inspection of the internal detail of the map and identification of artifacts.

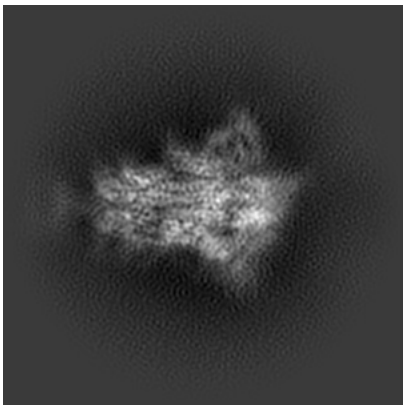
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

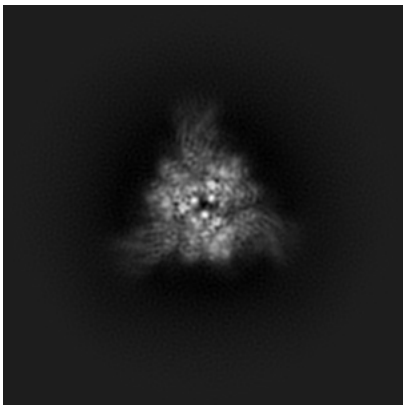
6.1.1 Primary map



X

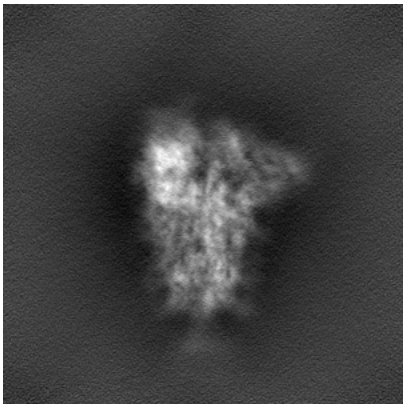


Y

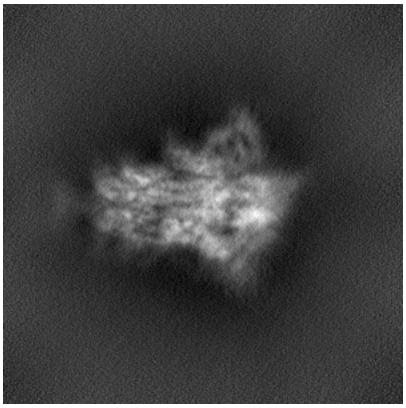


Z

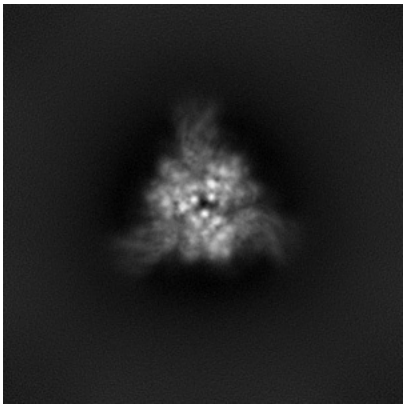
6.1.2 Raw map



X



Y

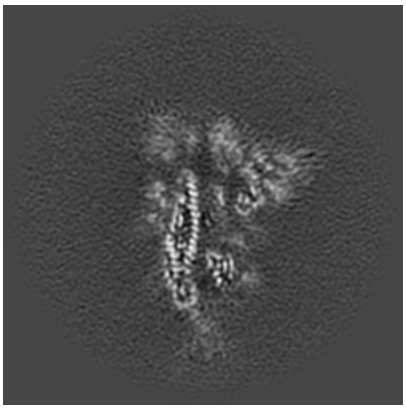


Z

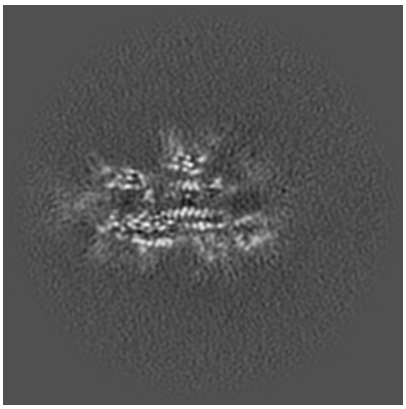
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

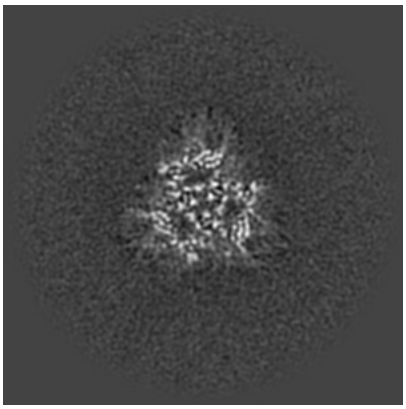
6.2.1 Primary map



X Index: 150

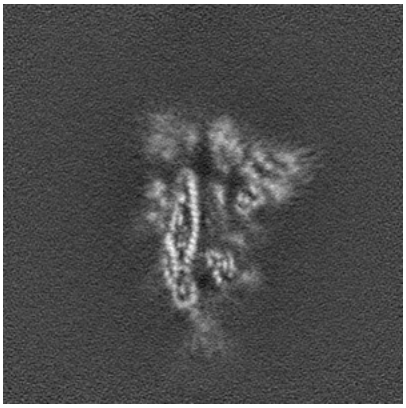


Y Index: 150

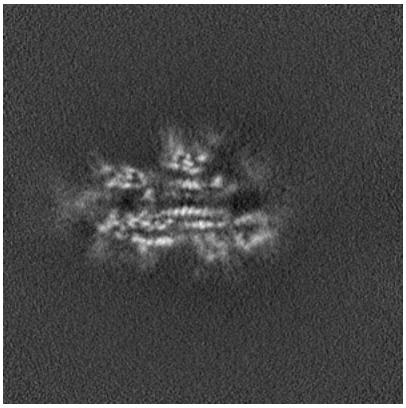


Z Index: 150

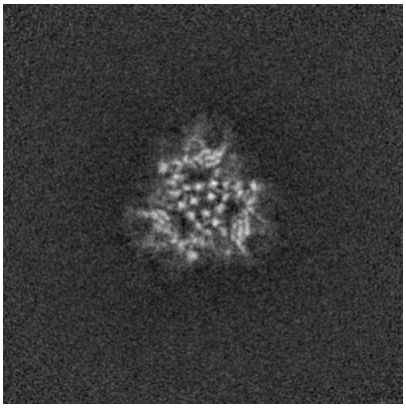
6.2.2 Raw map



X Index: 150



Y Index: 150

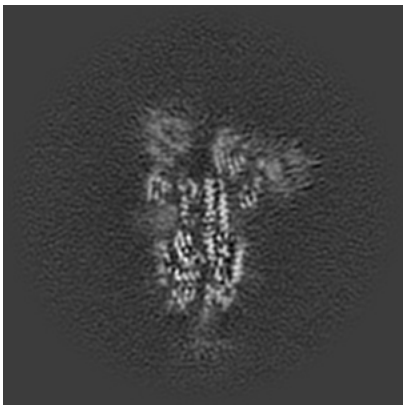


Z Index: 150

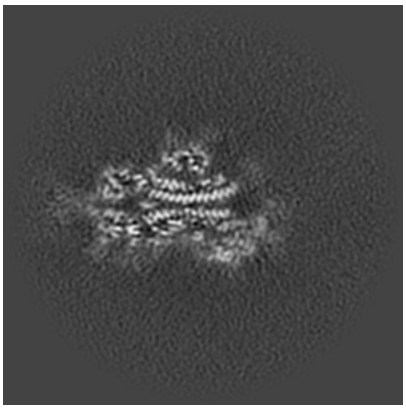
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

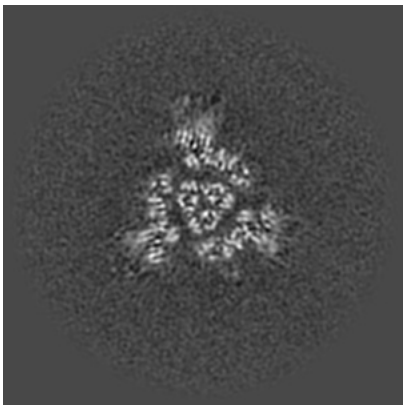
6.3.1 Primary map



X Index: 157

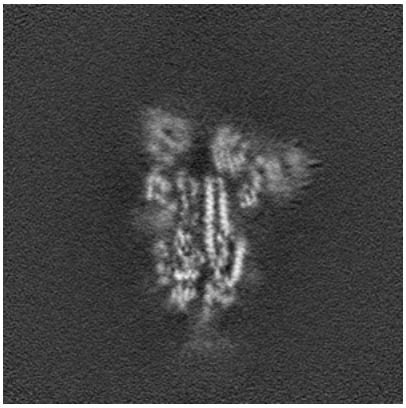


Y Index: 154

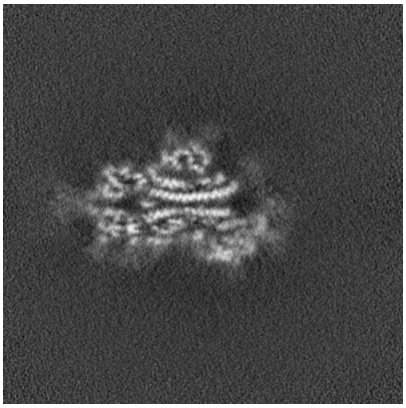


Z Index: 162

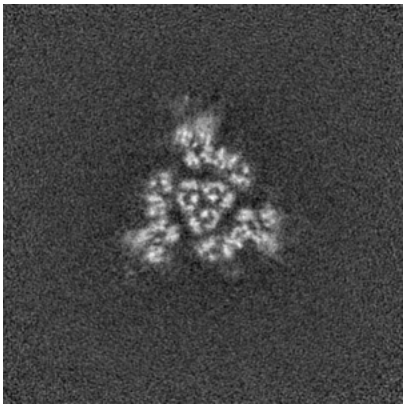
6.3.2 Raw map



X Index: 156



Y Index: 154

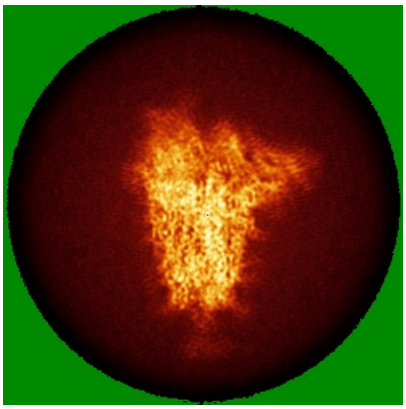


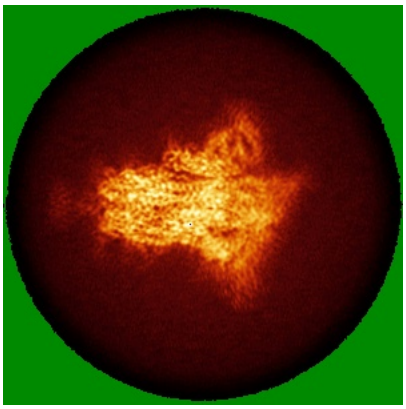
Z Index: 162

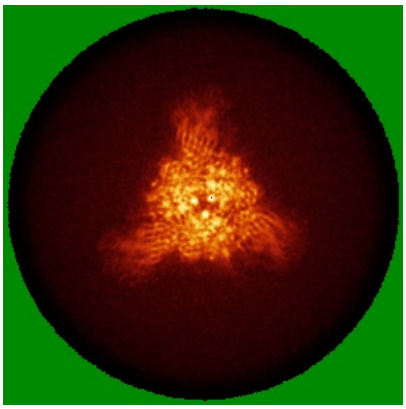
The images above show the largest variance slices of the map in three orthogonal directions.

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

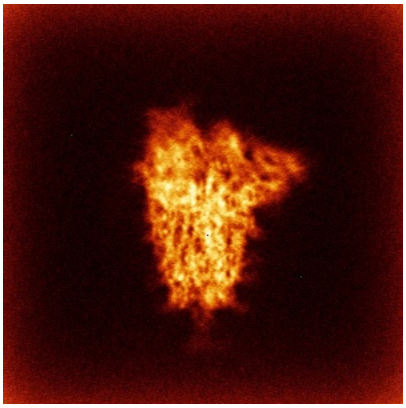
6.4.1 Primary map

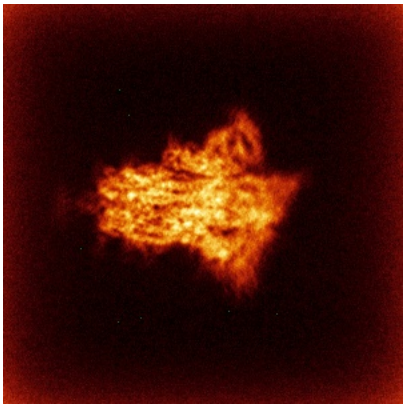

X

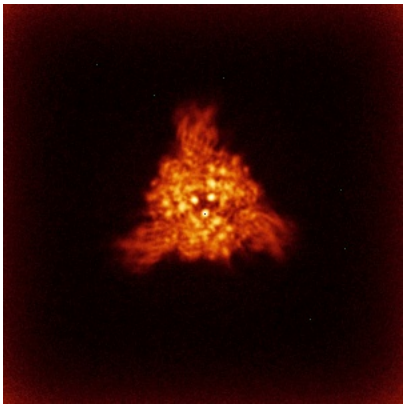

Y


Z

6.4.2 Raw 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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

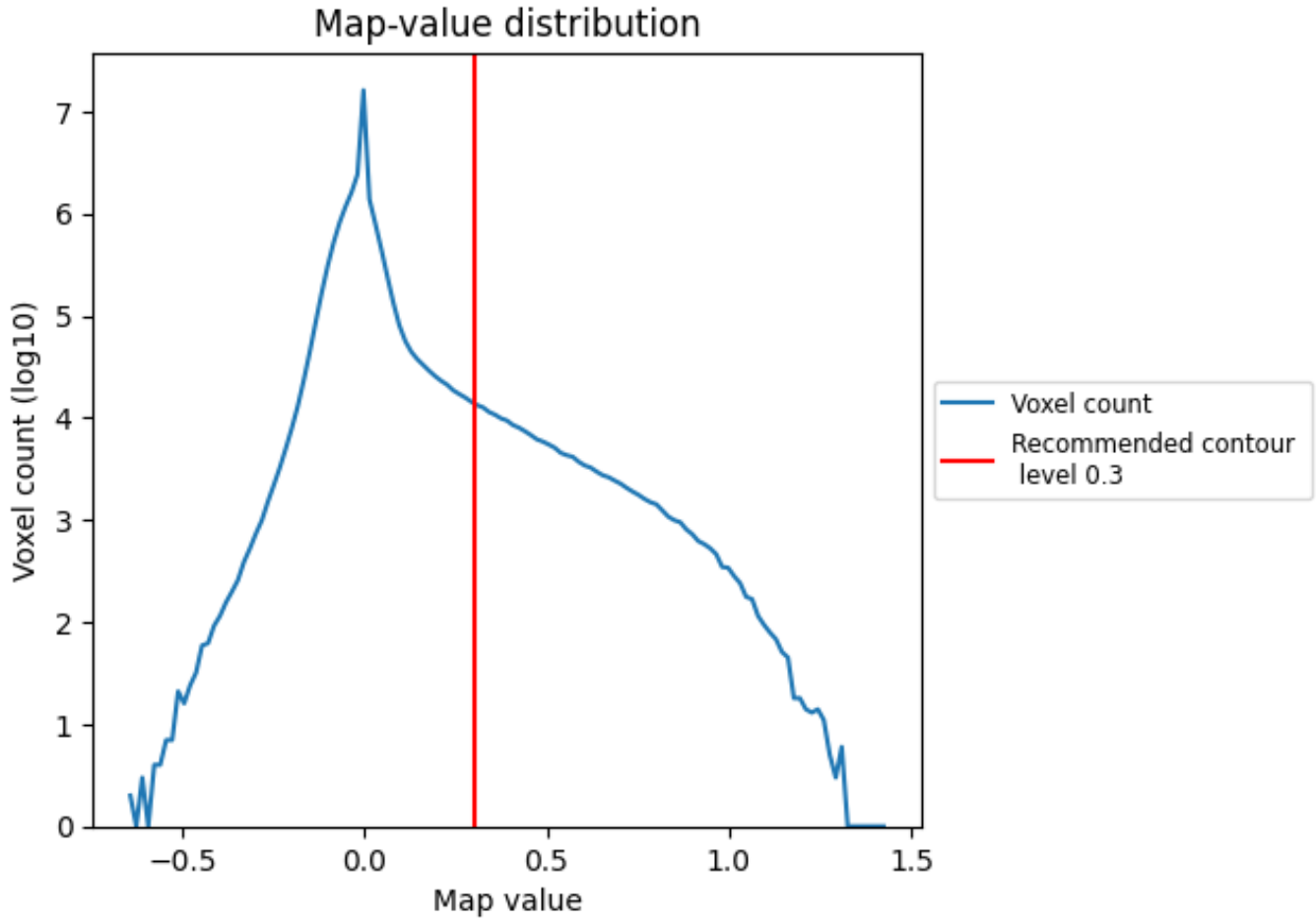
6.6 Mask visualisation (i)

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

7 Map analysis

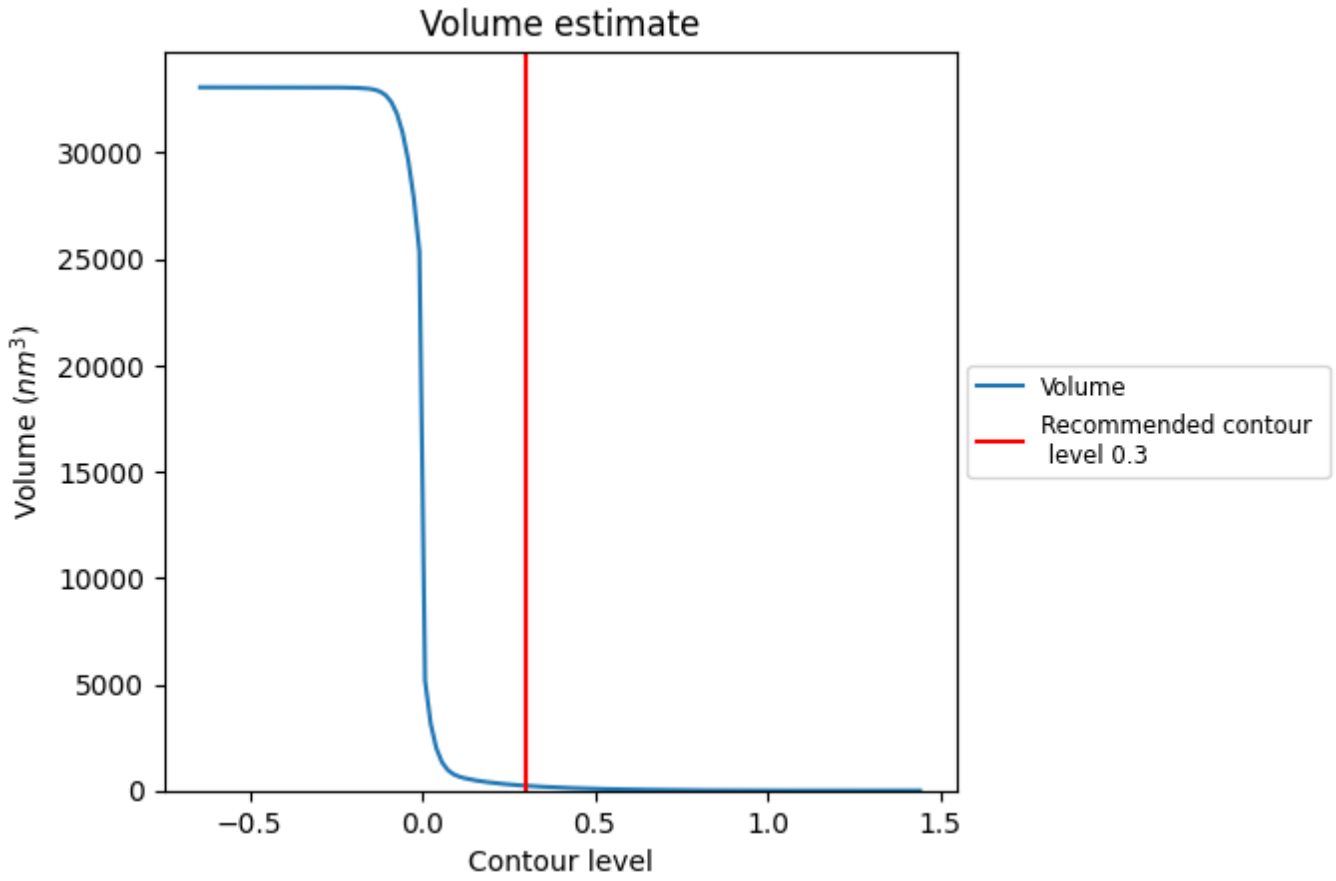
This section contains the results of statistical analysis of the map.

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.

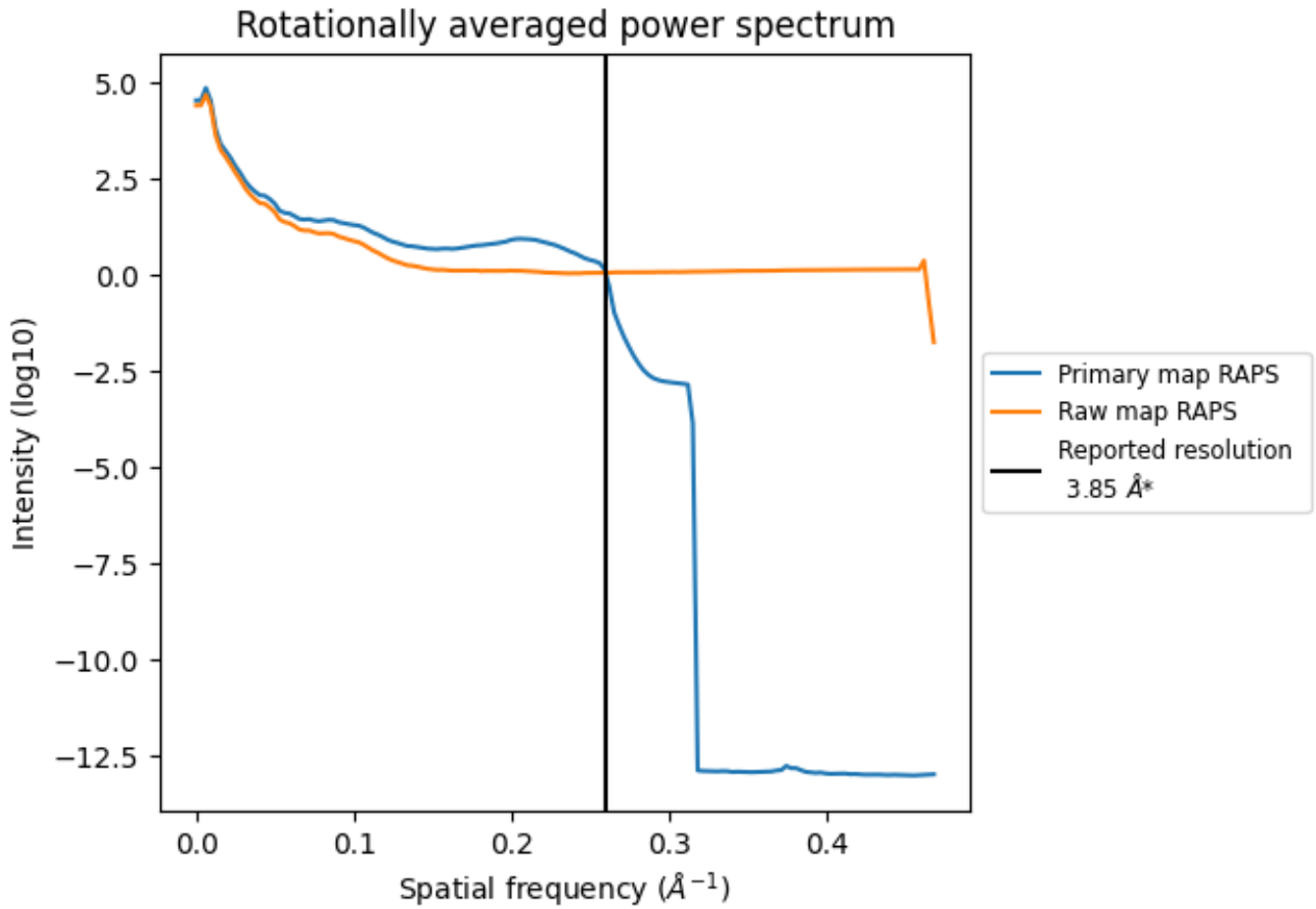
7.2 Volume estimate



The volume at the recommended contour level is 227 nm^3; this corresponds to an approximate mass of 205 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)

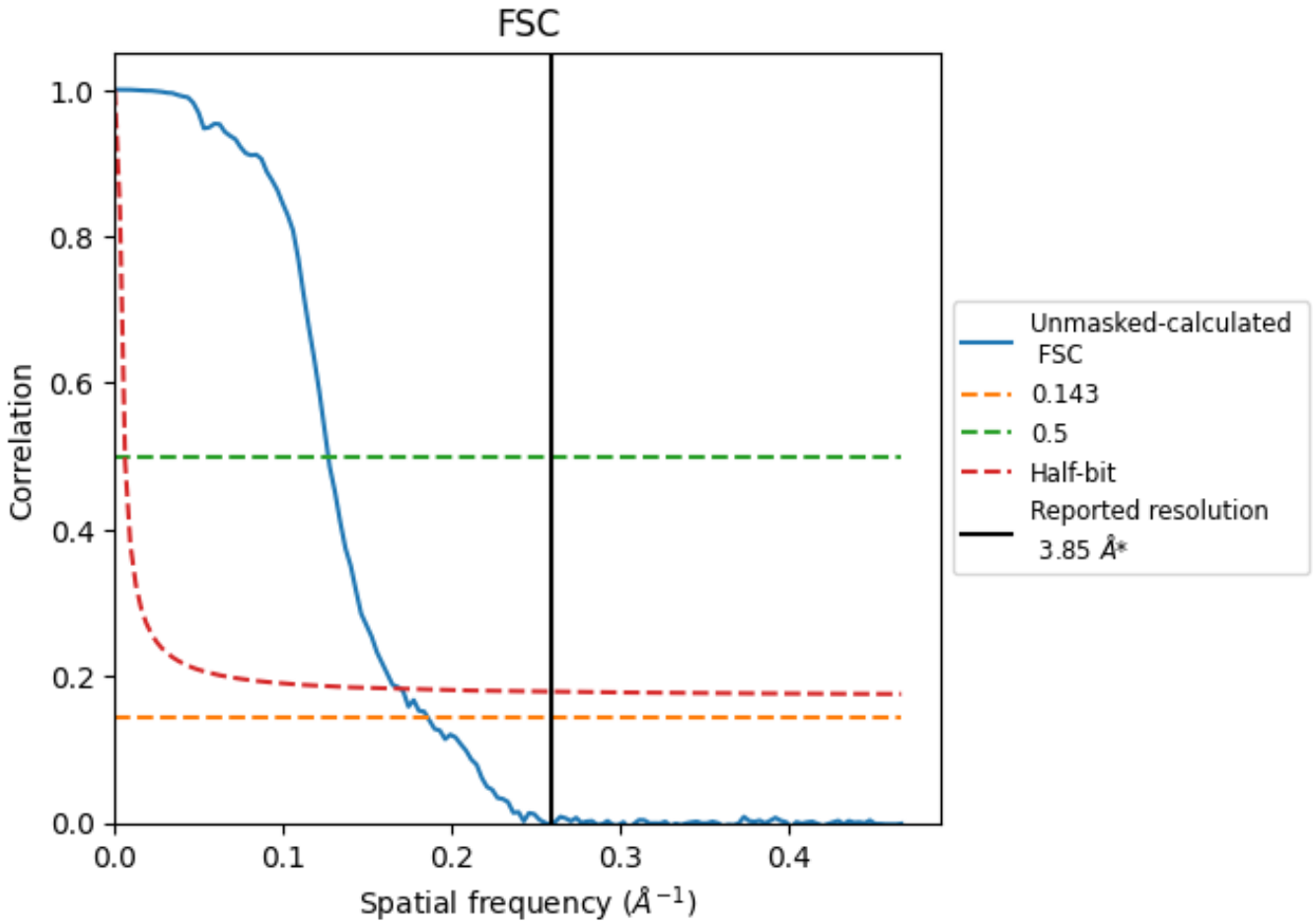


*Reported resolution corresponds to spatial frequency of 0.260 $Å^{-1}$

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 0.260 Å^{-1}

8.2 Resolution estimates (i)

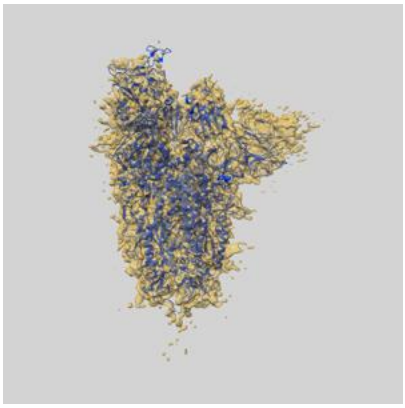
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.85	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.38	7.88	5.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.38 differs from the reported value 3.85 by more than 10 %

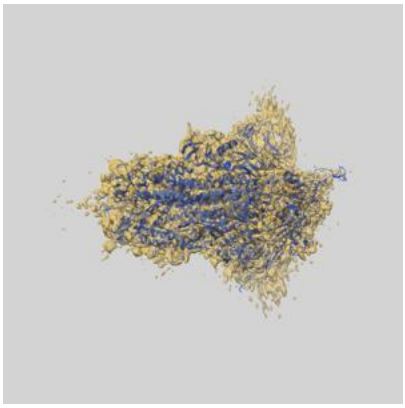
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38681 and PDB model 8XUR. Per-residue inclusion information can be found in section 3 on page 14.

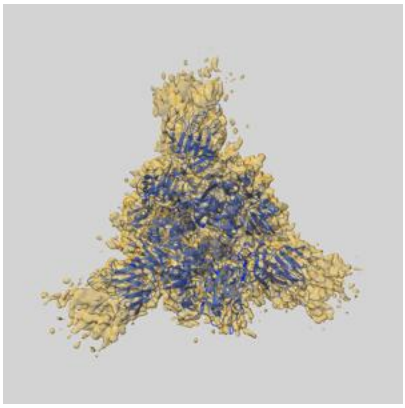
9.1 Map-model overlay



X



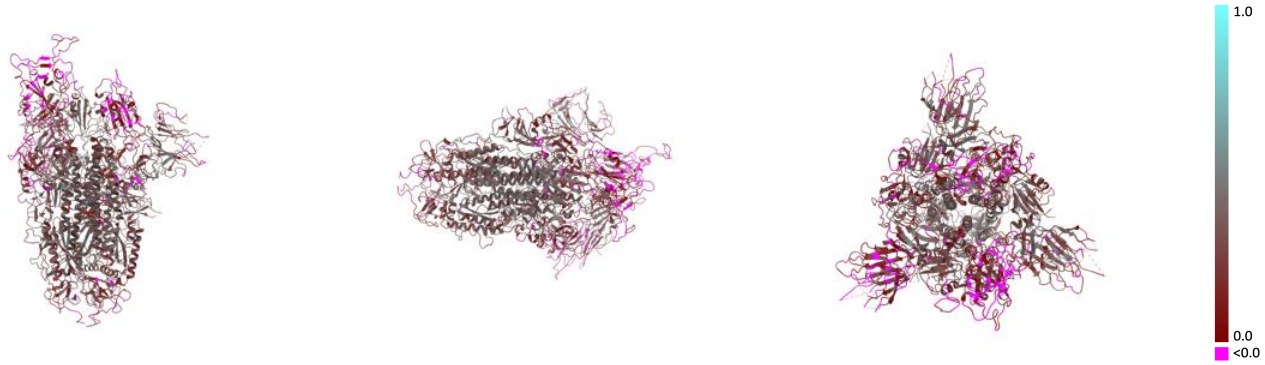
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

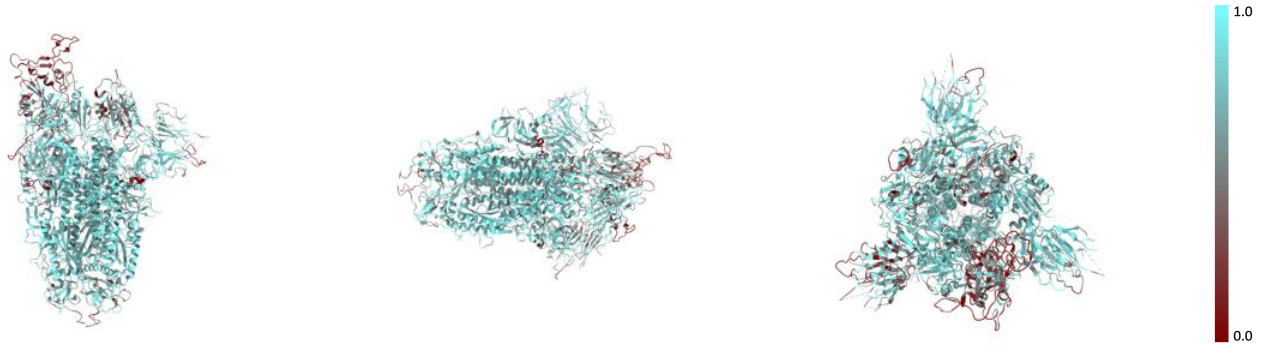
9.2 Q-score mapped to coordinate model (i)



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.

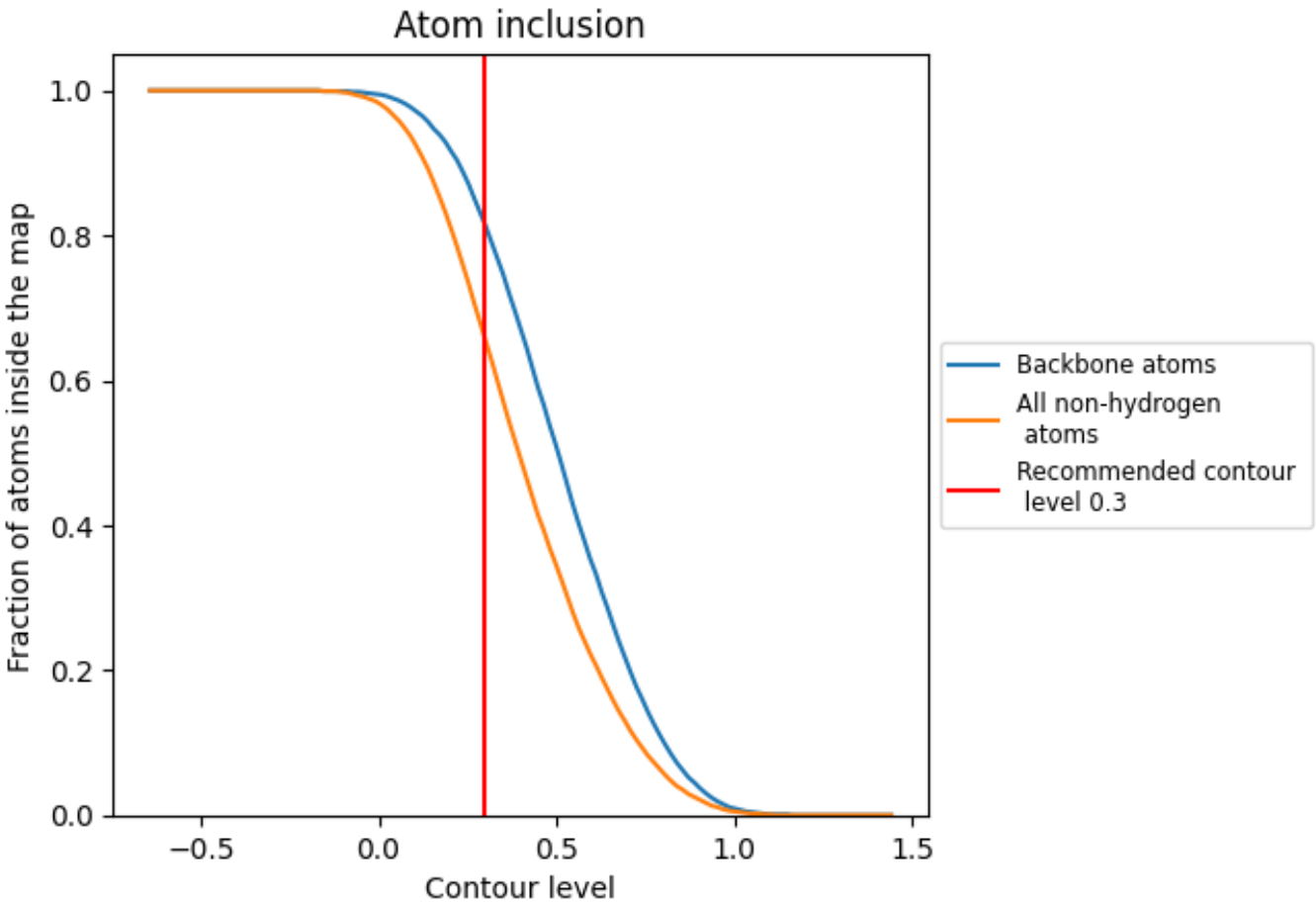
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 66% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.2470
A	0.6630	0.2430
B	0.6020	0.2100
C	0.7110	0.2890
D	0.5000	0.3390
E	0.2400	0.1740
F	0.7200	0.3310
G	0.7600	0.3430
H	0.4000	0.1640
I	0.2800	0.1130
J	0.2400	0.0890
K	0.7200	0.3550
L	0.6400	0.3300
M	0.3600	0.0640
N	0.2000	0.1290
O	0.6800	0.2960
P	0.7200	0.3480
Q	0.4400	0.1350