Full wwPDB EM Validation Report ⓘ

Sep 3, 2024 – 08:25 PM JST

PDB ID	:	8Y4A
EMDB ID	:	EMD-38914
Title	:	BA.2.86 S-trimer in complex with Nab XG2v046
Authors	:	Zhu, Q.; Liu, P.
Deposited on	:	2024-01-30
Resolution	:	3.40 Å(reported)

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

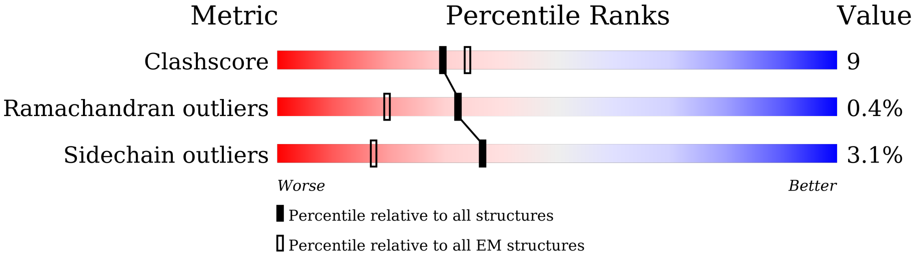
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance ⓘ

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

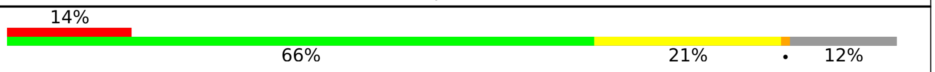
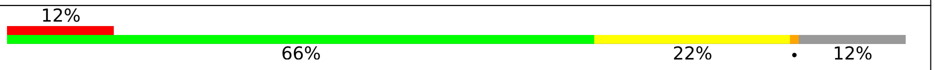
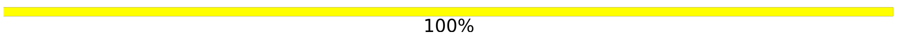
The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1204	
1	B	1204	
1	C	1204	
2	D	122	
2	H	122	
3	E	108	
3	L	108	
4	F	2	

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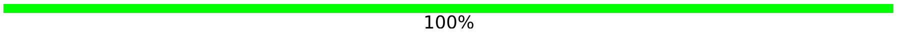
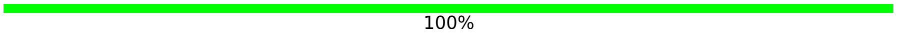
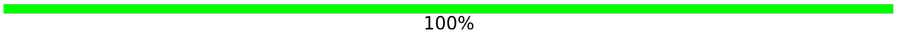
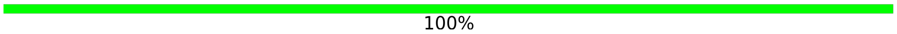
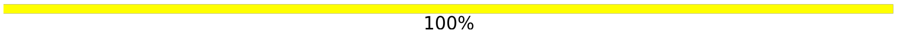
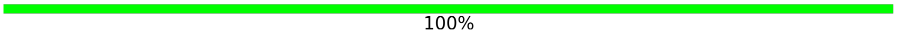
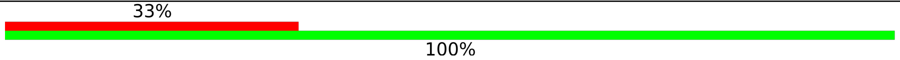
Mol	Chain	Length	Quality of chain
4	G	2	
4	I	2	
4	M	2	
4	N	2	
4	O	2	
4	R	2	
4	S	2	
4	T	2	
5	J	2	
5	P	2	
5	Q	2	
5	U	2	
6	K	3	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 29416 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
			Total	C	N	O	S		
1	B	1063	8316	5322	1383	1573	38	0	0
1	C	1063	8316	5322	1383	1573	38	0	0
1	A	1063	8316	5322	1383	1573	38	0	0

There are 213 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	variant	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	213	GLY	VAL	conflict	UNP P0DTC2
B	216	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	16	MET	-	insertion	UNP P0DTC2
C	17	PRO	-	insertion	UNP P0DTC2
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	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	variant	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	213	GLY	VAL	conflict	UNP P0DTC2
C	216	PHE	LEU	conflict	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	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	484	LYS	GLU	conflict	UNP P0DTC2
C	486	PRO	PHE	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	554	LYS	GLU	conflict	UNP P0DTC2
C	570	VAL	ALA	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	621	SER	PRO	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	PRO	conflict	UNP P0DTC2
C	683	ALA	ARG	conflict	UNP P0DTC2
C	685	ALA	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	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	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2
C	1143	LEU	PRO	conflict	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	variant	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	213	GLY	VAL	conflict	UNP P0DTC2
A	216	PHE	LEU	conflict	UNP P0DTC2
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	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	486	PRO	PHE	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2

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

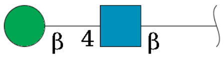
- Molecule 2 is a protein called XG2v046 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	122	Total 955	C 610	N 162	O 179	S 4	0	0
2	D	122	Total 955	C 610	N 162	O 179	S 4	0	0

- Molecule 3 is a protein called XG2v046 Light chain.

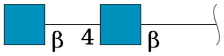
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	108	Total 818	C 515	N 140	O 160	S 3	0	0
3	E	108	Total 818	C 515	N 140	O 160	S 3	0	0

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



Mol	Chain	Residues	Atoms	AltConf	Trace
4	F	2	Total C N O 25 14 1 10	0	0
4	G	2	Total C N O 25 14 1 10	0	0
4	I	2	Total C N O 25 14 1 10	0	0
4	M	2	Total C N O 25 14 1 10	0	0
4	N	2	Total C N O 25 14 1 10	0	0
4	O	2	Total C N O 25 14 1 10	0	0
4	R	2	Total C N O 25 14 1 10	0	0
4	S	2	Total C N O 25 14 1 10	0	0
4	T	2	Total C N O 25 14 1 10	0	0

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

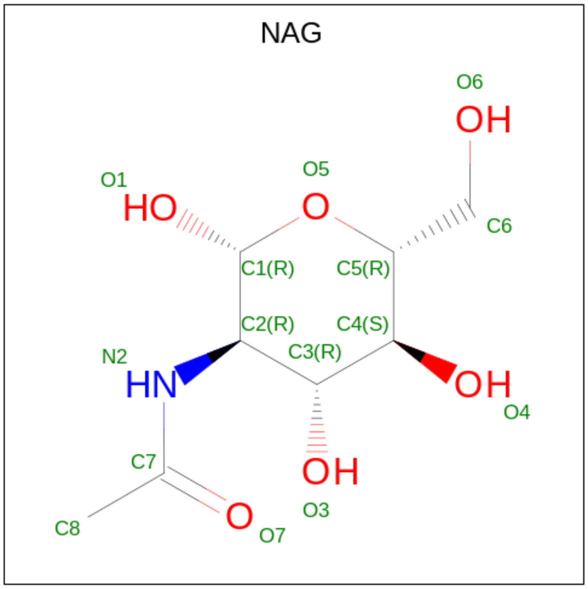


Mol	Chain	Residues	Atoms	AltConf	Trace
5	J	2	Total C N O 28 16 2 10	0	0
5	P	2	Total C N O 28 16 2 10	0	0
5	Q	2	Total C N O 28 16 2 10	0	0
5	U	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(8-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	K	3	39	22	2	15	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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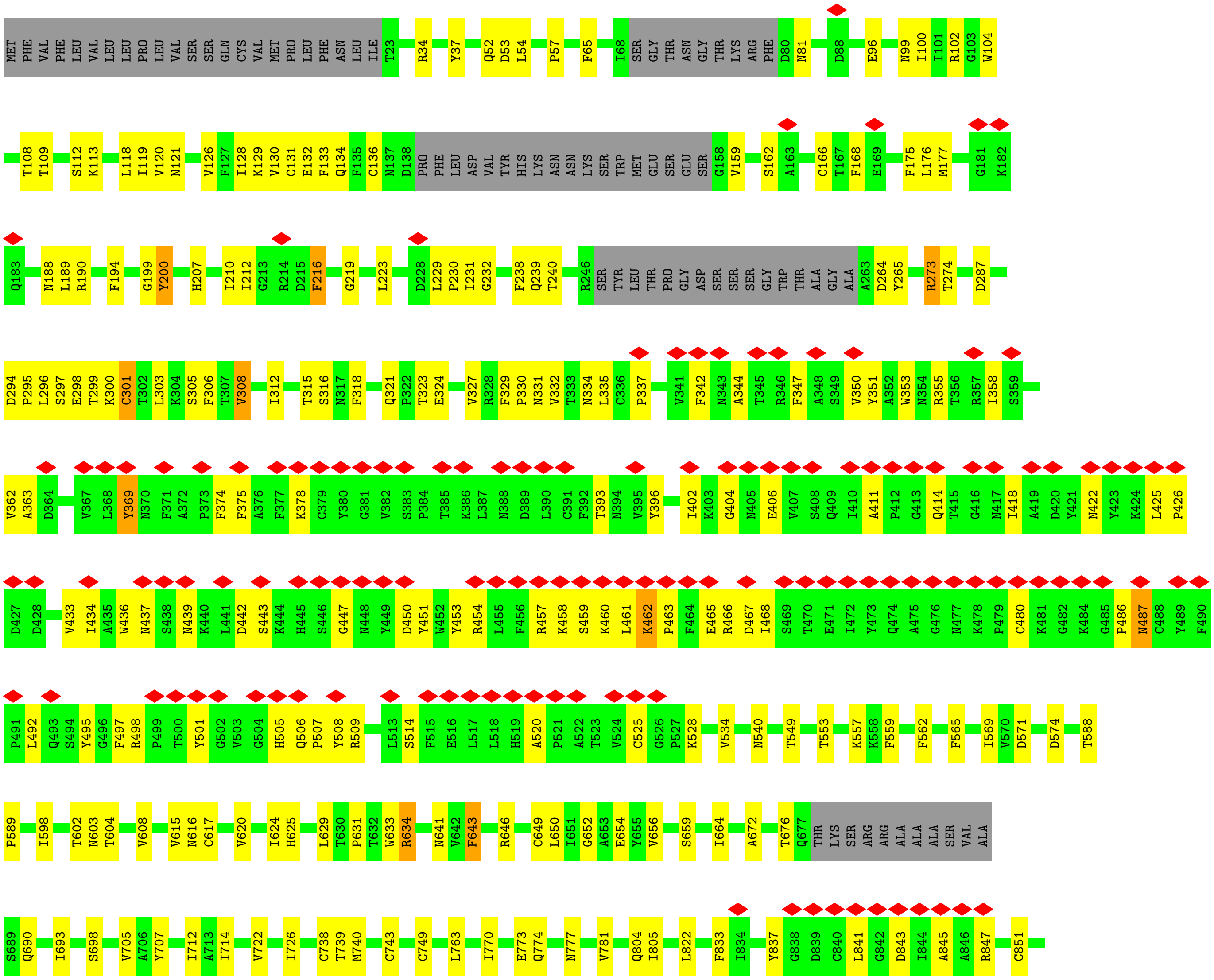
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0
7	A	1	Total C N O 14 8 1 5	0

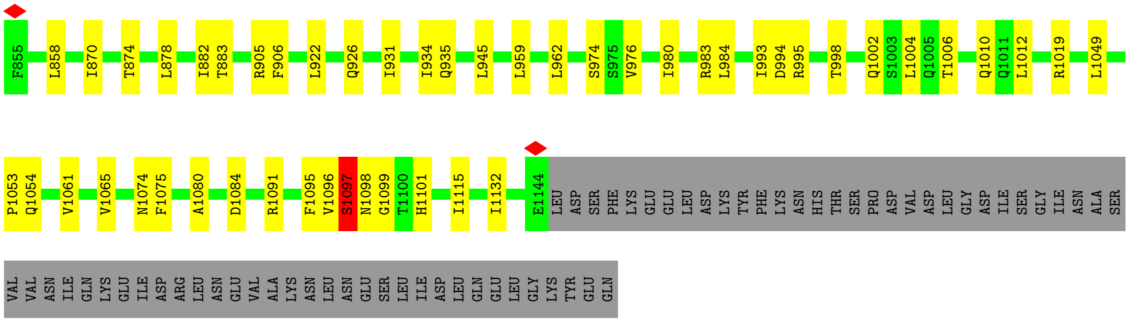
3 Residue-property plots

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.

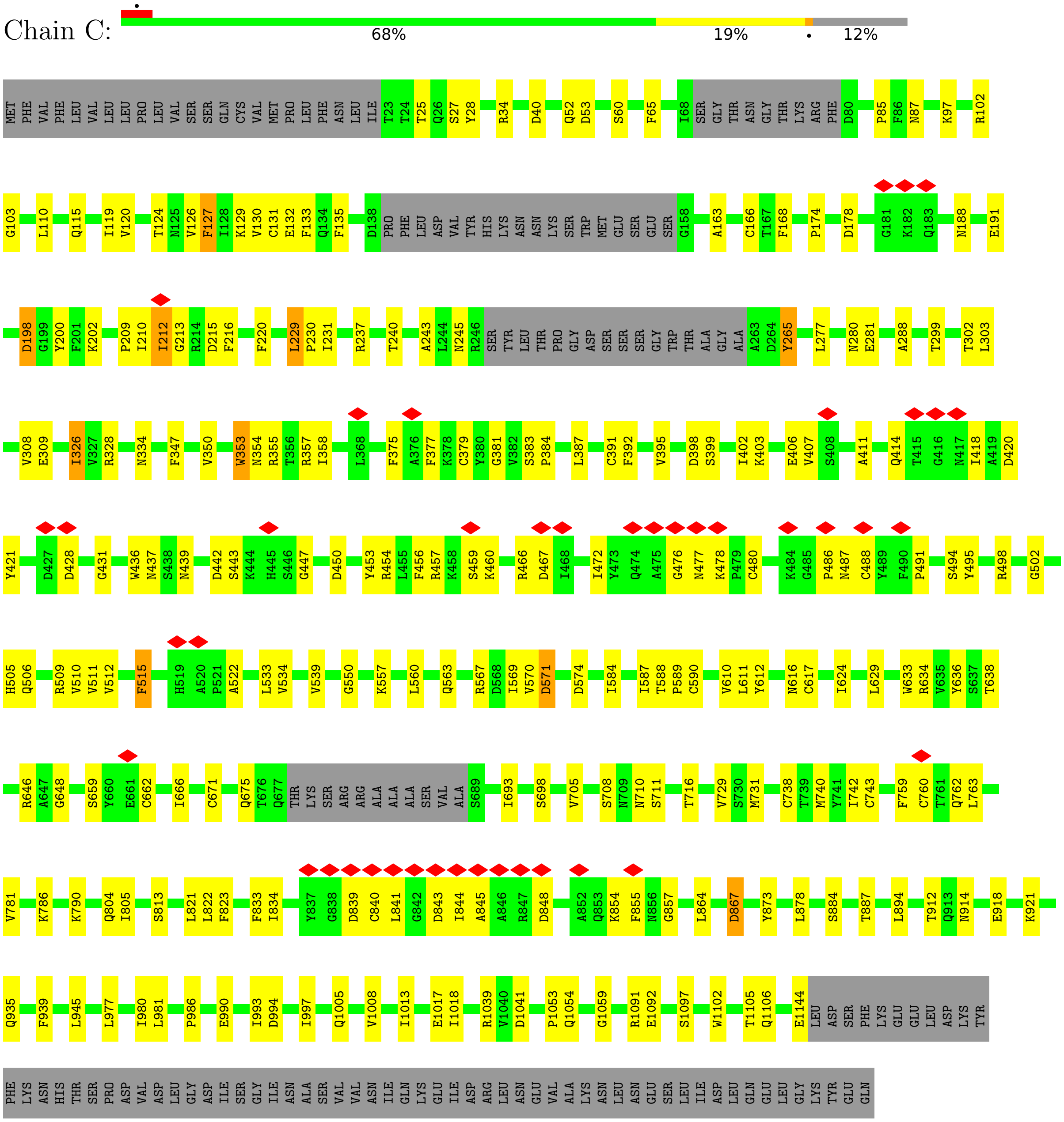
- Molecule 1: Spike glycoprotein

Chain B:



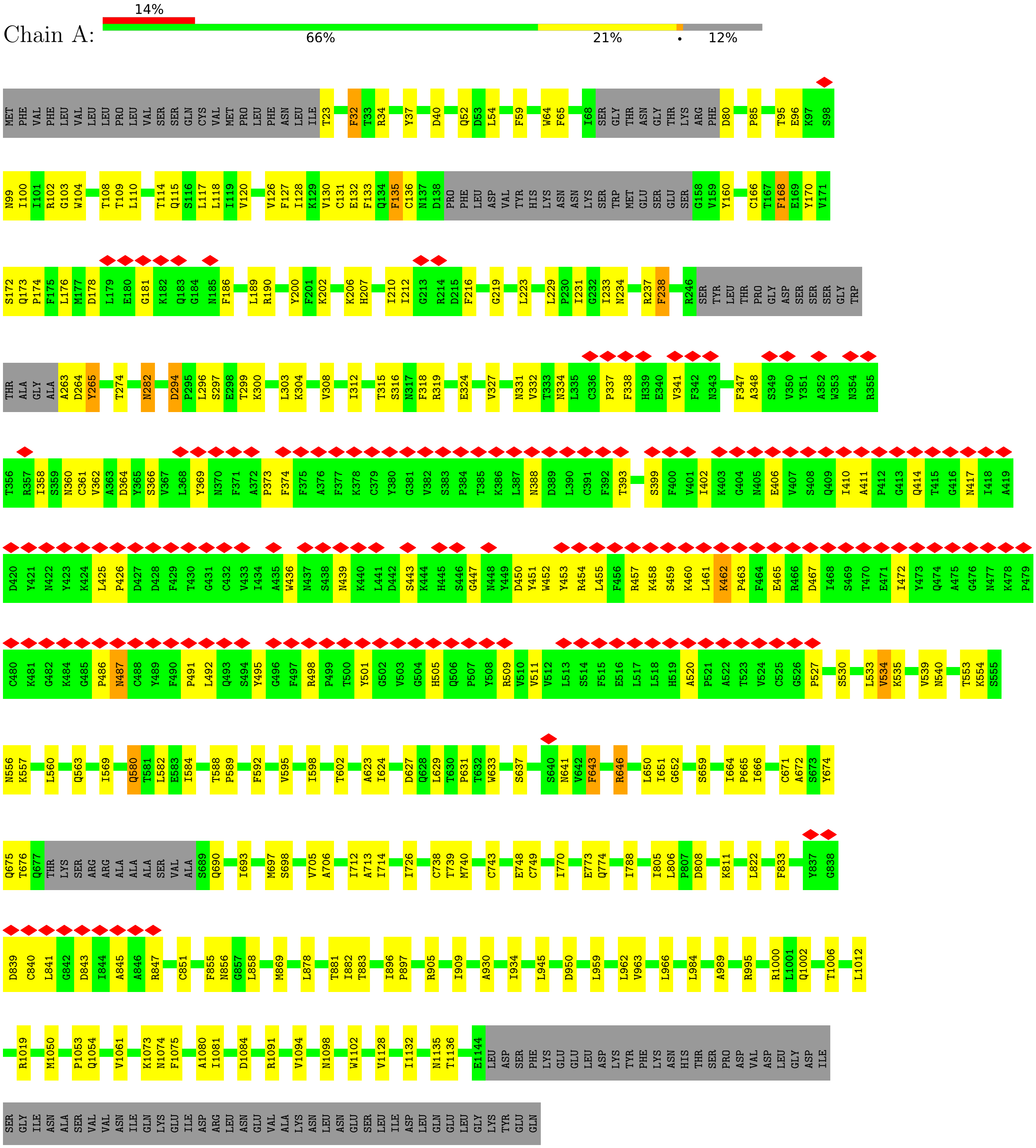


- Molecule 1: Spike glycoprotein



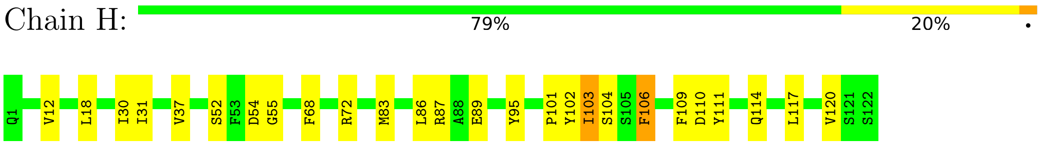
- Molecule 1: Spike glycoprotein

Chain A:



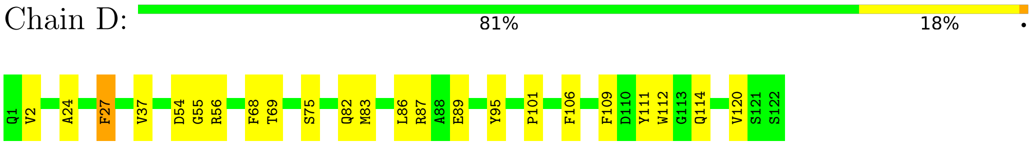
- Molecule 2: XG2v046 Heavy chain

Chain H:



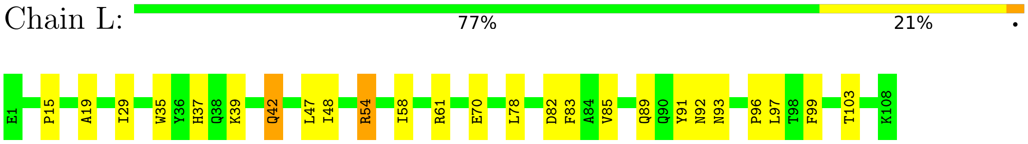
- Molecule 2: XG2v046 Heavy chain

Chain D:



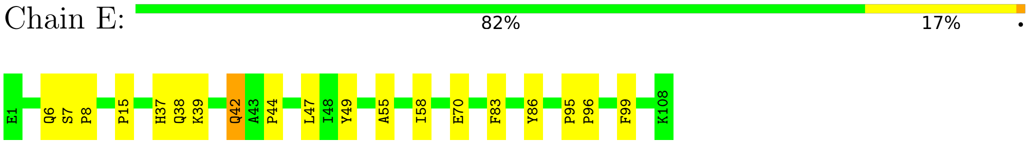
- Molecule 3: XG2v046 Light chain

Chain L:



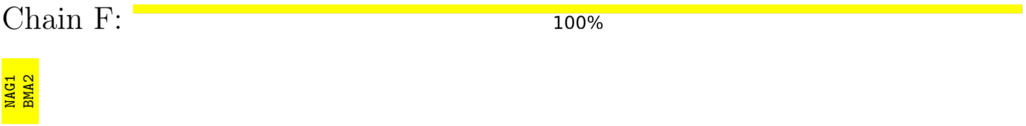
- Molecule 3: XG2v046 Light chain

Chain E:



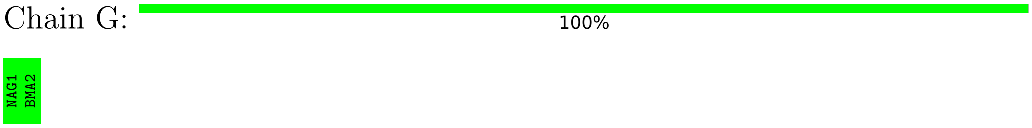
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



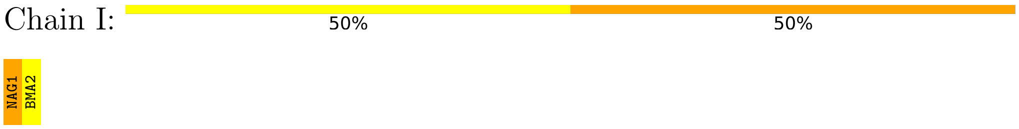
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



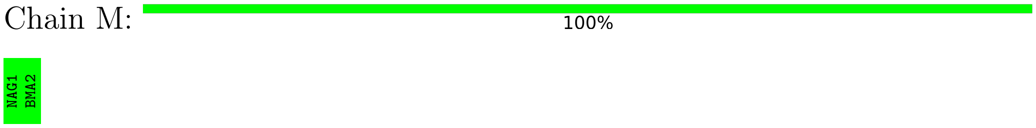
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



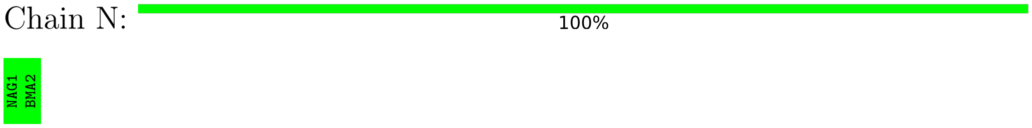
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



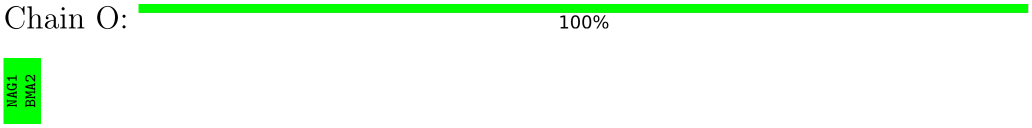
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



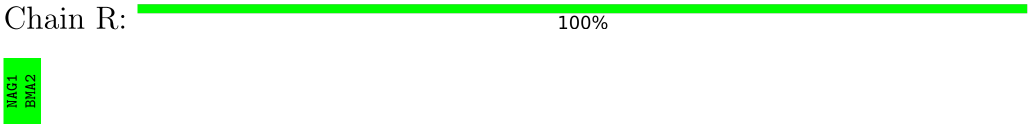
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



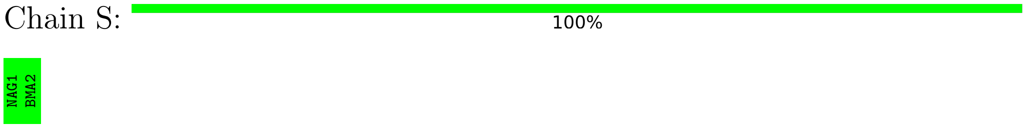
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



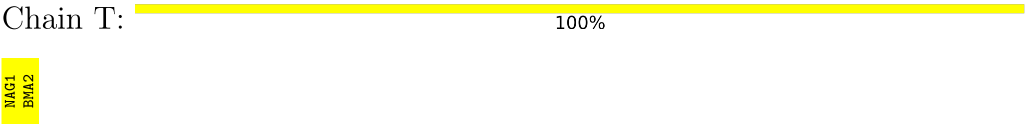
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



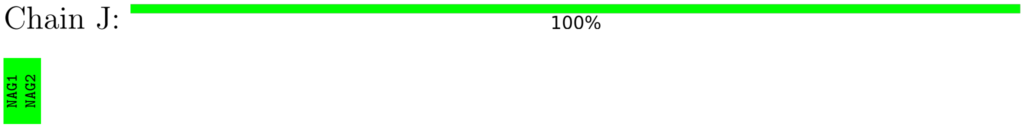
- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



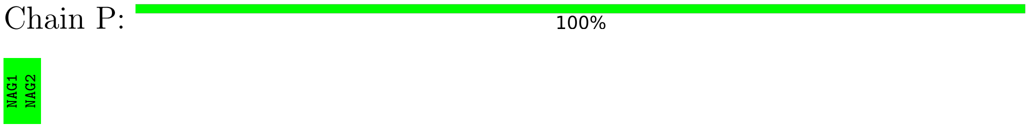
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



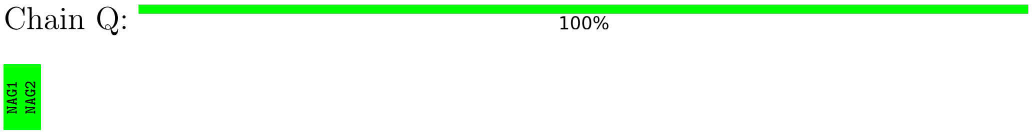
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



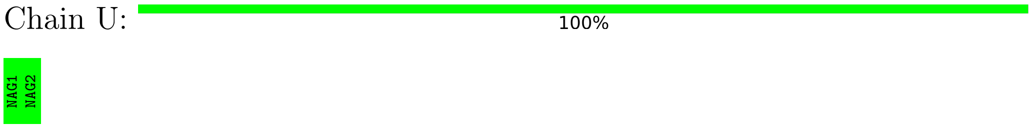
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



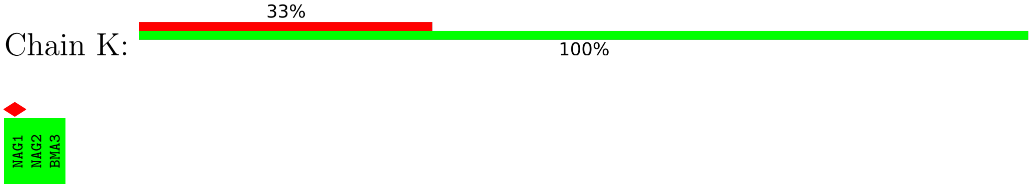
- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(8-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	712822	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	60	Depositor
Electron dose $(e^-/\text{Å}^2)$	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	3.233	Depositor
Minimum map value	-1.923	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.079	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	385.2, 385.2, 385.2	wwPDB
Map dimensions	360, 360, 360	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: NAG, BMA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.28	0/8516	0.51	0/11591
1	B	0.30	1/8516 (0.0%)	0.52	1/11591 (0.0%)
1	C	0.28	0/8516	0.51	1/11591 (0.0%)
2	D	0.31	0/979	0.54	0/1328
2	H	0.31	0/979	0.57	0/1328
3	E	0.36	0/838	0.57	0/1140
3	L	0.33	0/838	0.58	0/1140
All	All	0.29	1/29182 (0.0%)	0.52	2/39709 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1097	SER	CA-CB	-5.09	1.45	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	198	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	571	ASP	CB-CG-OD1	5.50	123.25	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	B	273	ARG	Sidechain
1	C	466	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	8103	180	0
1	B	8316	0	8104	170	0
1	C	8316	0	8104	146	0
2	D	955	0	923	15	0
2	H	955	0	923	16	0
3	E	818	0	798	10	0
3	L	818	0	798	15	0
4	F	25	0	22	1	0
4	G	25	0	22	0	0
4	I	25	0	22	1	0
4	M	25	0	22	0	0
4	N	25	0	22	0	0
4	O	25	0	22	0	0
4	R	25	0	22	0	0
4	S	25	0	22	0	0
4	T	25	0	22	0	0
5	J	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	U	28	0	25	0	0
6	K	39	0	32	0	0
7	A	196	0	182	3	0
7	B	182	0	169	2	0
7	C	168	0	156	1	0
All	All	29416	0	28590	521	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 9.

All (521) 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:85:PRO:HB3	2:H:101:PRO:HG2	1.46	0.97
1:A:452:TRP:HB3	1:A:492:LEU:HD21	1.62	0.79
1:B:323:THR:HG22	1:B:324:GLU:H	1.48	0.79
1:A:85:PRO:HB3	2:D:101:PRO:HG2	1.65	0.79
1:A:233:ILE:HG13	1:A:234:ASN:H	1.49	0.78
1:B:308:VAL:HG23	1:B:602:THR:HB	1.65	0.77
1:B:833:PHE:HB2	1:C:646:ARG:HD3	1.67	0.77
1:B:131:CYS:SG	1:B:132:GLU:N	2.58	0.76
1:C:659:SER:HB3	1:C:698:SER:HB2	1.67	0.76
2:D:83:MET:HB3	2:D:86:LEU:HD11	1.67	0.75
1:A:454:ARG:NH1	1:A:467:ASP:O	2.20	0.74
1:C:65:PHE:HB2	1:C:265:TYR:HB3	1.68	0.74
1:C:326:ILE:HD12	1:C:539:VAL:HG21	1.69	0.72
3:L:35:TRP:HD1	3:L:48:ILE:HB	1.55	0.71
1:C:188:ASN:HA	1:C:209:PRO:HA	1.72	0.71
1:B:589:PRO:HG3	1:A:855:PHE:HD1	1.56	0.70
1:B:462:LYS:HD2	1:B:465:GLU:HB2	1.74	0.70
3:E:95:PRO:HB2	3:E:96:PRO:HD3	1.73	0.70
1:A:659:SER:HB3	1:A:698:SER:HB2	1.74	0.69
1:A:1098:ASN:N	1:A:1098:ASN:OD1	2.25	0.69
3:E:37:HIS:HB2	3:E:47:LEU:HD21	1.75	0.69
1:B:705:VAL:HG11	1:A:883:THR:HG21	1.75	0.68
3:L:29:ILE:HA	3:L:92:ASN:HD22	1.58	0.68
1:B:659:SER:HB3	1:B:698:SER:HB3	1.76	0.67
1:A:462:LYS:HD2	1:A:465:GLU:HB2	1.76	0.67
1:C:102:ARG:HD3	1:C:243:ALA:HB2	1.77	0.67
1:B:96:GLU:OE1	1:B:100:ILE:N	2.27	0.67
1:B:454:ARG:NH1	1:B:467:ASP:O	2.27	0.67
1:C:229:LEU:HD12	1:C:231:ILE:HD11	1.78	0.66
3:L:54:ARG:NH1	3:L:58:ILE:O	2.29	0.66
1:C:840:CYS:HB2	1:A:588:THR:HG23	1.77	0.66
1:A:65:PHE:HB2	1:A:265:TYR:HB3	1.77	0.66
1:A:131:CYS:SG	1:A:132:GLU:N	2.70	0.65
1:A:486:PRO:O	1:A:487:ASN:ND2	2.28	0.65
1:A:369:TYR:HA	1:A:374:PHE:HZ	1.62	0.65
1:C:212:ILE:HG13	1:C:213:GLY:H	1.62	0.65
2:H:54:ASP:OD1	2:H:55:GLY:N	2.30	0.65
1:C:347:PHE:HD2	1:C:399:SER:HB2	1.60	0.65
1:A:117:LEU:HD21	1:A:231:ILE:HG21	1.79	0.64
1:A:858:LEU:HD23	1:A:959:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ASN:HB3	1:B:362:VAL:H	1.62	0.64
1:B:486:PRO:O	1:B:487:ASN:ND2	2.31	0.64
2:D:37:VAL:HG23	2:D:95:TYR:HB2	1.78	0.64
1:C:131:CYS:HA	1:C:166:CYS:HB3	1.80	0.64
1:A:176:LEU:HA	1:A:207:HIS:HE1	1.63	0.63
1:A:847:ARG:HD2	1:A:851:CYS:HB3	1.79	0.63
1:C:403:LYS:HG2	1:C:505:HIS:HA	1.81	0.63
1:C:358:ILE:HB	1:C:395:VAL:HB	1.80	0.62
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.81	0.62
1:B:121:ASN:HD22	1:B:126:VAL:HG22	1.65	0.62
3:E:55:ALA:HB3	3:E:58:ILE:HD12	1.81	0.61
1:B:858:LEU:HD21	1:B:962:LEU:HD23	1.83	0.61
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.82	0.61
1:C:918:GLU:HG3	1:A:1128:VAL:HG21	1.83	0.61
1:B:130:VAL:HG21	1:B:231:ILE:HD12	1.82	0.61
1:B:301:CYS:O	1:B:301:CYS:SG	2.58	0.61
1:B:294:ASP:HB2	1:B:295:PRO:HD2	1.83	0.61
1:B:629:LEU:HB3	1:B:631:PRO:HD2	1.83	0.60
1:B:998:THR:O	1:B:1002:GLN:HG2	2.00	0.60
1:C:731:MET:HB3	1:C:1018:ILE:HD13	1.82	0.60
1:A:641:ASN:HB3	1:A:652:GLY:H	1.65	0.60
1:B:375:PHE:HA	1:C:486:PRO:HA	1.82	0.60
1:C:420:ASP:HB2	1:C:460:LYS:HD2	1.83	0.60
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.67	0.59
1:C:855:PHE:HD1	1:A:589:PRO:HG3	1.67	0.59
1:B:451:TYR:HB2	1:B:495:TYR:HB2	1.85	0.59
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.84	0.59
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.35	0.59
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.83	0.59
1:A:533:LEU:HD23	1:A:535:LYS:HE3	1.83	0.59
1:A:439:ASN:O	1:A:443:SER:OG	2.21	0.58
1:B:296:LEU:HG	1:B:297:SER:H	1.67	0.58
1:C:456:PHE:HB2	1:C:491:PRO:HA	1.85	0.58
1:B:858:LEU:HD23	1:B:959:LEU:HD22	1.85	0.58
1:B:112:SER:HB2	1:B:134:GLN:HG2	1.84	0.58
1:B:369:TYR:HA	1:B:374:PHE:HZ	1.68	0.58
1:B:108:THR:HG22	1:B:109:THR:HG23	1.86	0.58
1:C:178:ASP:N	1:C:178:ASP:OD1	2.37	0.58
1:A:103:GLY:HA3	1:A:120:VAL:HA	1.84	0.58
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.36	0.58
1:A:554:LYS:NZ	1:A:556:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:HG2	1:B:216:PHE:HE1	1.69	0.57
1:B:773:GLU:OE1	1:B:774:GLN:NE2	2.37	0.57
1:C:398:ASP:HB2	1:C:512:VAL:HG12	1.86	0.57
1:A:294:ASP:N	1:A:294:ASP:OD2	2.36	0.57
1:A:178:ASP:N	1:A:178:ASP:OD1	2.38	0.57
1:A:133:PHE:HB3	1:A:160:TYR:HB2	1.87	0.57
1:A:773:GLU:OE1	1:A:774:GLN:NE2	2.38	0.57
2:D:54:ASP:OD1	2:D:55:GLY:N	2.37	0.57
1:C:406:GLU:OE1	1:C:406:GLU:N	2.38	0.56
1:C:379:CYS:HB2	1:C:384:PRO:HD3	1.86	0.56
1:A:334:ASN:HD22	1:A:362:VAL:HG23	1.70	0.56
1:B:176:LEU:HA	1:B:207:HIS:HE1	1.70	0.56
1:B:200:TYR:HA	1:B:230:PRO:HA	1.88	0.56
1:B:976:VAL:O	1:B:980:ILE:HG23	2.05	0.56
1:A:808:ASP:HB3	1:A:811:LYS:HG3	1.86	0.56
1:A:1102:TRP:HD1	1:A:1135:ASN:HD22	1.51	0.56
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.86	0.56
1:C:200:TYR:O	1:C:202:LYS:HD2	2.04	0.56
1:A:930:ALA:O	1:A:934:ILE:HG23	2.06	0.56
1:B:363:ALA:N	1:B:525:CYS:O	2.35	0.56
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.88	0.56
1:C:762:GLN:OE1	1:C:762:GLN:N	2.37	0.56
1:A:334:ASN:HB3	1:A:362:VAL:HB	1.88	0.56
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.42	0.55
1:C:119:ILE:HG22	1:C:119:ILE:O	2.06	0.55
1:C:442:ASP:OD1	1:C:509:ARG:NH2	2.39	0.55
1:A:454:ARG:HG2	1:A:492:LEU:HG	1.87	0.55
1:B:393:THR:HG21	1:B:520:ALA:HB3	1.89	0.55
1:A:712:ILE:HG22	1:A:1075:PHE:HB2	1.88	0.55
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.89	0.55
1:A:447:GLY:HA2	1:A:498:ARG:HG2	1.89	0.55
1:B:134:GLN:HG3	1:B:162:SER:HB2	1.89	0.54
1:A:135:PHE:CD2	1:A:136:CYS:N	2.75	0.54
2:H:102:TYR:O	2:H:104:SER:N	2.39	0.54
1:A:200:TYR:O	1:A:202:LYS:HD2	2.06	0.54
1:C:986:PRO:O	1:C:990:GLU:HG2	2.07	0.54
1:A:172:SER:OG	1:A:173:GLN:N	2.41	0.54
2:H:89:GLU:OE2	2:H:89:GLU:N	2.26	0.54
1:C:391:CYS:HB3	1:C:522:ALA:HB2	1.89	0.54
1:B:190:ARG:HD3	1:B:207:HIS:CE1	2.42	0.54
1:B:712:ILE:HG22	1:B:1075:PHE:HB2	1.90	0.54

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:C:384:PRO:HA	1:C:387:LEU:HD22	1.89	0.54
1:C:912:THR:OG1	1:C:914:ASN:OD1	2.23	0.54
1:C:993:ILE:O	1:C:997:ILE:HG12	2.08	0.54
1:B:337:PRO:HD2	1:B:358:ILE:HG23	1.90	0.53
2:H:37:VAL:O	2:H:95:TYR:N	2.36	0.53
1:A:843:ASP:O	1:A:845:ALA:N	2.40	0.53
1:B:296:LEU:HD13	1:B:608:VAL:HG11	1.91	0.53
2:D:109:PHE:HE2	3:E:99:PHE:HZ	1.57	0.53
1:B:81:ASN:OD1	1:B:239:GLN:NE2	2.42	0.53
1:B:439:ASN:O	1:B:443:SER:OG	2.21	0.53
1:B:1084:ASP:N	1:B:1084:ASP:OD1	2.41	0.53
1:A:176:LEU:HA	1:A:207:HIS:CE1	2.44	0.53
1:B:442:ASP:OD1	1:B:509:ARG:NH2	2.41	0.53
1:A:451:TYR:HB2	1:A:495:TYR:HB2	1.88	0.53
1:A:839:ASP:O	1:A:843:ASP:N	2.42	0.53
1:B:99:ASN:OD1	1:B:102:ARG:NH1	2.42	0.53
1:B:501:TYR:HB3	1:B:505:HIS:HB3	1.91	0.53
1:C:131:CYS:SG	1:C:163:ALA:HA	2.49	0.53
1:C:729:VAL:HG23	1:C:1059:GLY:HA2	1.91	0.53
1:C:738:CYS:O	1:C:742:ILE:HG22	2.08	0.53
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.91	0.53
1:B:369:TYR:OH	1:C:477:ASN:OD1	2.27	0.53
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.90	0.53
1:A:190:ARG:HD3	1:A:207:HIS:CE1	2.44	0.53
1:B:738:CYS:O	1:B:740:MET:N	2.40	0.52
1:A:23:THR:N	1:A:80:ASP:OD1	2.42	0.52
1:A:598:ILE:HG21	1:A:666:ILE:HD11	1.91	0.52
1:A:637:SER:HB3	1:A:651:ILE:HD11	1.90	0.52
1:B:210:ILE:HG22	1:B:212:ILE:H	1.74	0.52
1:C:855:PHE:CD1	1:A:589:PRO:HG3	2.44	0.52
1:A:99:ASN:OD1	1:A:102:ARG:NH1	2.42	0.52
1:B:450:ASP:OD1	1:B:450:ASP:N	2.42	0.52
1:B:676:THR:HG22	1:B:690:GLN:HE22	1.75	0.52
1:C:126:VAL:HG13	1:C:174:PRO:HA	1.89	0.52
1:B:353:TRP:HE1	1:B:466:ARG:HA	1.74	0.52
1:B:355:ARG:HD2	1:B:396:TYR:HB3	1.92	0.52
1:C:1097:SER:HB3	1:C:1102:TRP:CD2	2.45	0.52
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.75	0.52
1:B:369:TYR:HA	1:B:374:PHE:CZ	2.45	0.52
1:A:206:LYS:HB3	1:A:223:LEU:HD23	1.92	0.52
3:E:49:TYR:HE2	3:E:55:ALA:HA	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.31	0.52
3:E:7:SER:HB2	3:E:8:PRO:HD3	1.92	0.52
1:A:738:CYS:O	1:A:740:MET:N	2.42	0.51
1:A:1084:ASP:OD1	1:A:1084:ASP:N	2.43	0.51
1:B:327:VAL:HG12	1:B:327:VAL:O	2.10	0.51
1:B:422:ASN:ND2	1:B:454:ARG:O	2.35	0.51
1:B:553:THR:HG21	1:A:841:LEU:HD22	1.92	0.51
1:B:337:PRO:HG2	1:B:358:ILE:HG12	1.92	0.51
1:A:96:GLU:OE1	1:A:100:ILE:N	2.43	0.51
1:B:454:ARG:HG2	1:B:492:LEU:HB3	1.92	0.51
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.92	0.51
1:C:841:LEU:HB2	1:A:553:THR:HG21	1.92	0.51
1:A:210:ILE:HG22	1:A:212:ILE:H	1.75	0.51
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.91	0.51
1:A:501:TYR:HB3	1:A:505:HIS:HB3	1.93	0.51
1:A:580:GLN:C	1:A:582:LEU:H	2.14	0.51
2:D:24:ALA:HB1	2:D:27:PHE:HE2	1.74	0.51
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.10	0.51
1:A:299:THR:O	1:A:303:LEU:HD23	2.10	0.51
1:A:324:GLU:O	1:A:540:ASN:ND2	2.43	0.50
1:A:337:PRO:HD2	1:A:358:ILE:HG23	1.93	0.50
1:A:623:ALA:O	1:A:627:ASP:N	2.45	0.50
1:B:296:LEU:C	1:B:298:GLU:H	2.13	0.50
1:A:705:VAL:HG12	1:A:706:ALA:H	1.76	0.50
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.93	0.50
1:B:305:SER:OG	1:B:306:PHE:N	2.45	0.50
1:B:646:ARG:HH21	1:A:833:PHE:HB2	1.75	0.50
1:C:103:GLY:HA3	1:C:120:VAL:HA	1.94	0.50
1:C:439:ASN:O	1:C:443:SER:OG	2.22	0.50
1:C:215:ASP:N	1:C:215:ASP:OD2	2.43	0.50
1:B:34:ARG:NH2	1:B:219:GLY:O	2.45	0.50
1:B:378:LYS:HG2	1:B:433:VAL:HG22	1.94	0.50
1:B:57:PRO:HG3	1:B:273:ARG:HD2	1.92	0.49
1:B:177:MET:O	1:B:188:ASN:ND2	2.45	0.49
1:B:189:LEU:HD23	1:B:210:ILE:HD12	1.94	0.49
1:C:610:VAL:HG21	1:C:633:TRP:HH2	1.77	0.49
1:A:337:PRO:O	1:A:341:VAL:HG23	2.12	0.49
1:A:788:ILE:O	1:A:788:ILE:HG13	2.12	0.49
1:C:188:ASN:OD1	1:C:188:ASN:N	2.44	0.49
1:C:115:GLN:HG2	1:C:132:GLU:HG2	1.93	0.49
1:C:299:THR:O	1:C:302:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:39:LYS:HB2	3:E:42:GLN:HG2	1.93	0.49
1:B:643:PHE:HB3	1:B:650:LEU:HG	1.94	0.49
1:C:411:ALA:HB3	1:C:414:GLN:HG3	1.94	0.49
1:A:338:PHE:HE1	1:A:358:ILE:HD13	1.77	0.49
1:C:843:ASP:O	1:C:845:ALA:N	2.44	0.49
1:C:894:LEU:HB3	1:A:713:ALA:HB3	1.95	0.49
1:A:131:CYS:HB3	1:A:133:PHE:CE2	2.47	0.49
1:B:447:GLY:HA2	1:B:498:ARG:HG2	1.94	0.49
1:C:406:GLU:HG3	1:C:418:ILE:HD13	1.95	0.49
1:A:459:SER:OG	1:A:460:LYS:N	2.46	0.49
1:B:712:ILE:HD11	1:A:896:ILE:HG12	1.94	0.49
1:B:847:ARG:HD2	1:B:851:CYS:HB3	1.95	0.49
1:C:200:TYR:HA	1:C:230:PRO:HA	1.95	0.48
1:B:707:TYR:HE2	1:A:897:PRO:HA	1.78	0.48
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.94	0.48
1:A:189:LEU:HD22	1:A:210:ILE:HD12	1.96	0.48
1:C:354:ASN:OD1	1:C:355:ARG:N	2.46	0.48
1:B:588:THR:HG23	1:A:840:CYS:HB2	1.94	0.48
1:A:104:TRP:HD1	1:A:238:PHE:HE1	1.62	0.48
1:A:233:ILE:HG13	1:A:234:ASN:N	2.23	0.48
1:C:25:THR:O	1:C:65:PHE:HA	2.14	0.48
1:C:418:ILE:H	1:C:418:ILE:HD12	1.78	0.48
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.95	0.48
1:B:569:ILE:HD12	1:B:569:ILE:H	1.78	0.48
1:C:34:ARG:NH1	1:C:191:GLU:OE2	2.47	0.48
1:C:567:ARG:HD3	1:C:571:ASP:HA	1.94	0.48
1:C:821:LEU:HD11	1:C:935:GLN:HE21	1.79	0.48
1:A:714:ILE:HD11	1:A:1094:VAL:HG21	1.96	0.48
1:B:240:THR:HB	1:B:265:TYR:OH	2.14	0.47
1:A:399:SER:HB3	1:A:511:VAL:HG22	1.95	0.47
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.14	0.47
1:B:436:TRP:CD1	1:B:509:ARG:HB3	2.49	0.47
1:B:1101:HIS:ND1	4:I:1:NAG:H5	2.29	0.47
1:C:616:ASN:OD1	1:C:617:CYS:N	2.45	0.47
1:B:983:ARG:NH1	1:C:381:GLY:O	2.47	0.47
3:L:39:LYS:HB2	3:L:42:GLN:HG2	1.96	0.47
1:C:760:CYS:HA	1:C:763:LEU:HG	1.97	0.47
1:C:884:SER:O	1:C:887:THR:OG1	2.31	0.47
1:C:1013:ILE:O	1:C:1017:GLU:HG3	2.15	0.47
1:C:210:ILE:O	1:C:212:ILE:HB	2.14	0.47
1:C:454:ARG:NH1	1:C:467:ASP:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:TRP:O	1:C:634:ARG:HD3	2.14	0.47
1:C:841:LEU:HB3	1:A:588:THR:OG1	2.14	0.47
2:H:109:PHE:HE2	3:L:99:PHE:HZ	1.61	0.47
1:B:603:ASN:OD1	1:B:604:THR:N	2.48	0.47
1:C:1091:ARG:HB3	1:C:1092:GLU:OE2	2.15	0.47
1:A:52:GLN:HG2	1:A:274:THR:HG22	1.96	0.47
1:A:569:ILE:HD12	1:A:569:ILE:H	1.79	0.47
1:B:308:VAL:H	1:B:602:THR:HG21	1.79	0.47
1:C:611:LEU:HD22	1:C:666:ILE:HG23	1.96	0.47
1:B:335:LEU:HD23	1:B:335:LEU:H	1.80	0.47
1:B:980:ILE:HD11	1:B:993:ILE:HG12	1.96	0.47
1:C:569:ILE:HG23	1:C:570:VAL:H	1.79	0.47
2:H:110:ASP:OD1	2:H:111:TYR:N	2.48	0.47
1:B:350:VAL:HG22	1:B:422:ASN:HB3	1.97	0.46
1:A:65:PHE:HB2	1:A:265:TYR:CB	2.44	0.46
1:A:595:VAL:HG11	1:A:633:TRP:CZ2	2.49	0.46
1:B:457:ARG:HD3	1:B:458:LYS:N	2.30	0.46
1:B:656:VAL:HG13	1:B:693:ILE:HD11	1.97	0.46
1:A:675:GLN:HG2	1:A:693:ILE:HG12	1.98	0.46
3:L:19:ALA:HB2	3:L:78:LEU:HD11	1.97	0.46
1:B:459:SER:OG	1:B:460:LYS:N	2.47	0.46
1:B:805:ILE:HD12	1:B:878:LEU:HD11	1.95	0.46
1:A:95:THR:HB	1:A:189:LEU:HD12	1.97	0.46
1:B:588:THR:OG1	1:A:841:LEU:HB3	2.15	0.46
1:B:1095:PHE:HE1	1:B:1115:ILE:HG12	1.81	0.46
1:C:1105:THR:OG1	1:C:1106:GLN:N	2.49	0.46
1:A:308:VAL:H	1:A:602:THR:HG21	1.80	0.46
3:E:15:PRO:HG3	3:E:83:PHE:HZ	1.81	0.46
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.97	0.46
1:A:878:LEU:O	1:A:882:ILE:HG23	2.15	0.46
1:A:1074:ASN:OD1	7:A:1305:NAG:N2	2.49	0.46
1:A:1081:ILE:HG23	1:A:1135:ASN:HB3	1.98	0.46
1:B:230:PRO:O	1:C:357:ARG:NH1	2.49	0.46
1:A:905:ARG:O	1:A:909:ILE:HG23	2.16	0.46
2:H:103:ILE:HG23	2:H:104:SER:H	1.80	0.46
1:B:104:TRP:HE3	1:B:119:ILE:HD12	1.81	0.46
1:B:321:GLN:OE1	1:B:321:GLN:HA	2.16	0.46
1:B:323:THR:HG22	1:B:324:GLU:N	2.24	0.46
1:B:334:ASN:HB3	1:B:362:VAL:N	2.30	0.46
1:A:32:PHE:HA	1:A:59:PHE:HD1	1.81	0.46
1:A:181:GLY:H	1:A:186:PHE:HD2	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HG	1:A:297:SER:H	1.80	0.46
1:A:118:LEU:HB2	1:A:133:PHE:HE1	1.80	0.46
1:A:856:ASN:HD22	1:A:966:LEU:HD12	1.80	0.46
1:A:331:ASN:HB2	7:A:1301:NAG:HN2	1.80	0.46
1:A:1073:LYS:HE2	1:A:1073:LYS:HB3	1.71	0.46
1:A:369:TYR:HA	1:A:374:PHE:CZ	2.48	0.45
3:L:93:ASN:O	3:L:96:PRO:HD2	2.15	0.45
1:B:65:PHE:HD2	1:B:265:TYR:HD1	1.63	0.45
1:B:351:TYR:HE2	1:B:468:ILE:HG23	1.81	0.45
1:A:595:VAL:HG11	1:A:633:TRP:HZ2	1.81	0.45
3:L:37:HIS:HB2	3:L:47:LEU:HD11	1.97	0.45
1:B:777:ASN:O	1:B:781:VAL:HG23	2.17	0.45
1:C:124:THR:HG23	7:C:1308:NAG:HN2	1.81	0.45
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	1.97	0.45
1:C:921:LYS:HA	1:C:921:LYS:HD3	1.73	0.45
1:B:763:LEU:HD23	1:B:1004:LEU:HG	1.98	0.45
1:C:131:CYS:SG	1:C:132:GLU:N	2.87	0.45
1:C:326:ILE:HD11	1:C:534:VAL:HG12	1.99	0.45
1:C:447:GLY:HA2	1:C:498:ARG:HG2	1.99	0.45
1:A:364:ASP:HB3	1:A:527:PRO:HB3	1.97	0.45
1:B:437:ASN:HD21	1:B:506:GLN:HB2	1.81	0.45
1:C:833:PHE:C	1:C:834:ILE:HD13	2.36	0.45
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.97	0.45
1:A:436:TRP:CD1	1:A:509:ARG:HB3	2.51	0.45
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.98	0.45
1:A:856:ASN:ND2	1:A:963:VAL:HG13	2.32	0.45
1:B:65:PHE:HB2	1:B:265:TYR:HB3	1.99	0.45
1:B:297:SER:HA	1:B:300:LYS:CB	2.46	0.45
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.99	0.45
1:A:856:ASN:ND2	1:A:966:LEU:HD12	2.30	0.45
1:C:977:LEU:HA	1:C:980:ILE:HG22	1.98	0.45
2:H:52:SER:O	2:H:72:ARG:NH1	2.48	0.45
1:B:843:ASP:O	1:B:845:ALA:N	2.44	0.45
1:B:870:ILE:O	1:B:874:THR:HG23	2.17	0.45
1:C:97:LYS:O	1:C:97:LYS:NZ	2.46	0.45
1:C:350:VAL:O	1:C:353:TRP:HD1	1.99	0.45
1:C:790:LYS:HE2	1:C:790:LYS:HB3	1.70	0.45
1:A:411:ALA:HB3	1:A:414:GLN:HG3	1.99	0.45
1:A:966:LEU:HD23	1:A:966:LEU:HA	1.84	0.45
1:B:108:THR:O	1:B:109:THR:OG1	2.35	0.45
1:B:404:GLY:HA2	1:B:508:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:PRO:HB3	1:B:633:TRP:CE2	2.52	0.45
1:B:984:LEU:HD12	1:B:984:LEU:HA	1.85	0.45
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.41	0.45
1:B:841:LEU:HB3	1:C:588:THR:HG21	1.99	0.44
1:B:878:LEU:O	1:B:882:ILE:HG23	2.17	0.44
1:A:366:SER:HA	1:A:369:TYR:HB3	1.99	0.44
1:A:402:ILE:HD13	1:A:410:ILE:HD11	1.99	0.44
1:A:676:THR:HA	1:A:690:GLN:OE1	2.16	0.44
1:B:931:ILE:O	1:B:934:ILE:HG22	2.17	0.44
1:C:502:GLY:O	1:C:506:GLN:HG2	2.17	0.44
1:A:773:GLU:OE2	1:A:1019:ARG:HB2	2.17	0.44
3:E:70:GLU:N	3:E:70:GLU:OE1	2.50	0.44
1:B:743:CYS:HB3	1:B:749:CYS:HB3	1.75	0.44
1:B:1096:VAL:CG1	1:B:1097:SER:N	2.80	0.44
1:C:436:TRP:CZ3	1:C:511:VAL:HG12	2.52	0.44
1:B:229:LEU:H	1:B:229:LEU:HD23	1.83	0.44
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.51	0.44
1:C:328:ARG:HH21	1:C:533:LEU:HB2	1.83	0.44
1:C:821:LEU:HD11	1:C:935:GLN:NE2	2.32	0.44
1:A:34:ARG:NH2	1:A:219:GLY:O	2.50	0.44
1:B:131:CYS:HB2	1:B:166:CYS:HB3	1.74	0.44
1:C:120:VAL:HG13	1:C:127:PHE:HB3	1.99	0.44
1:A:417:ASN:HD22	1:A:455:LEU:HD23	1.83	0.44
2:D:114:GLN:OE1	2:D:114:GLN:N	2.51	0.44
1:B:426:PRO:HD3	1:B:463:PRO:HB3	1.99	0.44
1:C:87:ASN:OD1	1:C:87:ASN:N	2.49	0.44
1:C:303:LEU:HD21	1:C:308:VAL:HG12	1.99	0.44
1:A:360:ASN:O	1:A:360:ASN:ND2	2.50	0.44
2:H:87:ARG:O	2:H:120:VAL:HG11	2.17	0.44
2:D:112:TRP:CZ3	3:E:44:PRO:HG2	2.53	0.44
1:A:282:ASN:N	1:A:282:ASN:OD1	2.51	0.44
2:H:18:LEU:HB3	2:H:83:MET:HE3	2.00	0.44
1:B:34:ARG:HE	1:B:34:ARG:HB2	1.65	0.43
1:B:329:PHE:CE2	1:B:528:LYS:HG3	2.53	0.43
1:B:342:PHE:HZ	1:B:434:ILE:HD13	1.83	0.43
1:C:480:CYS:HB3	1:C:488:CYS:HB3	1.84	0.43
1:B:641:ASN:HB3	1:B:652:GLY:H	1.83	0.43
1:C:27:SER:OG	1:C:28:TYR:N	2.51	0.43
1:C:129:LYS:HD3	1:C:133:PHE:HZ	1.83	0.43
1:B:113:LYS:HE2	1:B:113:LYS:HB3	1.69	0.43
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603:ASN:OD1	1:B:603:ASN:C	2.57	0.43
1:C:40:ASP:OD2	1:C:40:ASP:N	2.49	0.43
1:C:472:ILE:HG21	1:C:488:CYS:HB2	2.00	0.43
2:D:54:ASP:OD1	2:D:56:ARG:HG2	2.18	0.43
1:C:421:TYR:CD1	1:C:457:ARG:HB3	2.54	0.43
1:C:478:LYS:NZ	1:C:487:ASN:HD21	2.16	0.43
1:C:708:SER:HB3	1:C:711:SER:HB3	2.00	0.43
1:C:854:LYS:HA	1:C:854:LYS:HD2	1.77	0.43
1:A:806:LEU:HD23	1:A:806:LEU:HA	1.90	0.43
2:H:68:PHE:CE1	2:H:83:MET:HG2	2.53	0.43
1:C:240:THR:HB	1:C:265:TYR:OH	2.18	0.43
1:A:327:VAL:O	1:A:327:VAL:HG12	2.18	0.43
1:B:1074:ASN:OD1	7:B:1304:NAG:N2	2.52	0.43
1:B:714:ILE:HD11	1:B:1096:VAL:HG21	2.00	0.43
1:B:773:GLU:OE2	1:B:1019:ARG:HB2	2.17	0.43
2:H:30:ILE:HG13	2:H:31:ILE:HG23	2.00	0.43
1:B:53:ASP:OD1	1:B:54:LEU:N	2.52	0.43
1:B:883:THR:HG21	1:C:705:VAL:HG11	2.00	0.43
1:C:740:MET:SD	1:A:319:ARG:NH1	2.92	0.43
1:A:674:TYR:CZ	1:A:690:GLN:HB3	2.54	0.43
3:L:35:TRP:CD1	3:L:48:ILE:HB	2.44	0.43
2:D:87:ARG:O	2:D:120:VAL:HG11	2.19	0.43
1:B:315:THR:OG1	1:B:316:SER:N	2.52	0.43
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.91	0.43
1:C:662:CYS:HB2	1:C:671:CYS:HB2	1.60	0.43
1:A:406:GLU:N	1:A:406:GLU:OE1	2.51	0.43
1:A:426:PRO:HD3	1:A:463:PRO:HB3	2.01	0.43
1:A:457:ARG:HD3	1:A:458:LYS:N	2.34	0.43
4:F:1:NAG:H62	4:F:2:BMA:H2	1.99	0.43
1:B:136:CYS:HB2	1:B:159:VAL:O	2.18	0.43
1:B:404:GLY:HA2	1:B:508:TYR:HD2	1.84	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.01	0.43
1:A:135:PHE:HD2	1:A:136:CYS:H	1.67	0.43
1:A:557:LYS:HG3	1:A:584:ILE:HG21	2.01	0.43
1:A:334:ASN:OD1	1:A:361:CYS:HA	2.18	0.42
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.90	0.42
1:A:643:PHE:HB3	1:A:650:LEU:HG	2.01	0.42
1:B:104:TRP:CD1	1:B:240:THR:HG23	2.54	0.42
1:B:129:LYS:HB3	1:B:129:LYS:HE2	1.88	0.42
1:C:550:GLY:HA2	1:C:589:PRO:O	2.19	0.42
1:A:300:LYS:H	1:A:300:LYS:HG3	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:VAL:HG23	1:A:539:VAL:HG11	2.00	0.42
1:A:748:GLU:OE1	1:A:748:GLU:N	2.43	0.42
1:B:312:ILE:HB	1:B:598:ILE:HG22	2.00	0.42
1:C:437:ASN:OD1	1:C:439:ASN:ND2	2.52	0.42
1:C:675:GLN:HG3	1:C:693:ILE:HD11	2.00	0.42
1:C:710:ASN:N	1:C:710:ASN:OD1	2.52	0.42
1:C:805:ILE:HB	1:C:878:LEU:HD11	2.00	0.42
1:C:387:LEU:HA	1:C:387:LEU:HD12	1.79	0.42
1:C:839:ASP:O	1:C:843:ASP:N	2.53	0.42
1:A:108:THR:O	1:A:114:THR:OG1	2.36	0.42
1:A:312:ILE:HB	1:A:598:ILE:HG22	2.00	0.42
1:A:315:THR:OG1	1:A:316:SER:N	2.53	0.42
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	2.00	0.42
1:C:131:CYS:HB3	1:C:133:PHE:CE1	2.54	0.42
1:A:560:LEU:H	1:A:563:GLN:HG3	1.84	0.42
1:A:1080:ALA:HB3	1:A:1132:ILE:HG13	2.01	0.42
1:C:624:ILE:HG13	1:C:629:LEU:HD12	2.00	0.42
1:A:641:ASN:HB3	1:A:652:GLY:N	2.33	0.42
1:B:52:GLN:HB2	1:B:274:THR:HG22	2.01	0.42
1:B:406:GLU:OE1	1:B:406:GLU:N	2.52	0.42
1:C:277:LEU:HD23	1:C:288:ALA:HB2	2.01	0.42
1:C:457:ARG:NE	1:C:459:SER:O	2.53	0.42
1:A:130:VAL:HG12	1:A:168:PHE:HB3	2.02	0.42
1:A:450:ASP:OD1	1:A:450:ASP:N	2.51	0.42
1:A:472:ILE:HA	1:A:491:PRO:HD3	2.01	0.42
3:L:15:PRO:HG3	3:L:83:PHE:CZ	2.55	0.42
2:D:69:THR:HB	2:D:82:GLN:HB3	2.01	0.42
1:B:199:GLY:HA2	1:B:232:GLY:HA2	2.02	0.42
1:B:299:THR:O	1:B:303:LEU:HB2	2.20	0.42
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.37	0.42
1:A:131:CYS:HA	1:A:166:CYS:CB	2.50	0.42
1:A:822:LEU:HD22	1:A:945:LEU:HD21	2.00	0.42
2:H:114:GLN:H	2:H:114:GLN:HG2	1.66	0.42
2:D:68:PHE:CE1	2:D:83:MET:HG2	2.54	0.42
1:B:620:VAL:O	1:B:624:ILE:HG12	2.19	0.42
1:B:664:ILE:HG12	1:B:672:ALA:O	2.20	0.42
1:C:212:ILE:HG13	1:C:213:GLY:N	2.32	0.42
1:C:612:TYR:O	1:C:648:GLY:HA3	2.20	0.42
3:L:29:ILE:HA	3:L:92:ASN:ND2	2.31	0.41
2:D:89:GLU:H	2:D:89:GLU:CD	2.23	0.41
1:B:402:ILE:HD11	1:B:418:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ASN:OD1	1:B:549:THR:HG22	2.20	0.41
1:B:922:LEU:O	1:B:926:GLN:HG3	2.21	0.41
1:C:716:THR:O	1:C:716:THR:OG1	2.35	0.41
1:C:742:ILE:HG12	1:C:743:CYS:SG	2.60	0.41
1:C:844:ILE:HD13	1:A:556:ASN:HB2	2.02	0.41
1:C:867:ASP:C	1:C:867:ASP:OD1	2.58	0.41
1:A:373:PRO:HD2	1:A:436:TRP:CE3	2.55	0.41
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.83	0.41
1:B:332:VAL:HB	7:B:1311:NAG:H82	2.02	0.41
1:A:337:PRO:HG2	1:A:358:ILE:HG12	2.01	0.41
1:A:743:CYS:HB3	1:A:749:CYS:HB3	1.84	0.41
1:B:1080:ALA:HB3	1:B:1132:ILE:HG13	2.01	0.41
1:C:560:LEU:H	1:C:563:GLN:HG3	1.86	0.41
1:C:1144:GLU:OE1	1:C:1144:GLU:N	2.53	0.41
1:A:64:TRP:HE1	1:A:263:ALA:N	2.18	0.41
1:A:624:ILE:HD13	1:A:624:ILE:HA	1.85	0.41
1:A:674:TYR:OH	1:A:690:GLN:HB3	2.20	0.41
1:A:869:MET:H	1:A:869:MET:HG2	1.70	0.41
1:B:128:ILE:HD11	1:B:175:PHE:CZ	2.55	0.41
1:B:905:ARG:HD2	1:B:1049:LEU:O	2.21	0.41
1:C:428:ASP:OD1	1:C:428:ASP:N	2.48	0.41
1:C:636:TYR:CZ	1:C:638:THR:HB	2.56	0.41
1:A:37:TYR:OH	1:A:54:LEU:O	2.32	0.41
3:L:85:VAL:HA	3:L:103:THR:O	2.20	0.41
1:B:297:SER:HA	1:B:300:LYS:HB3	2.02	0.41
1:C:402:ILE:HD11	1:C:510:VAL:HG21	2.02	0.41
1:C:857:GLY:HA2	1:A:592:PHE:CE1	2.55	0.41
1:A:664:ILE:HG12	1:A:672:ALA:O	2.20	0.41
1:B:118:LEU:HG	1:B:120:VAL:HG23	2.03	0.41
1:A:348:ALA:HB2	7:A:1306:NAG:H5	2.02	0.41
1:A:534:VAL:HG23	1:A:534:VAL:O	2.20	0.41
1:A:671:CYS:SG	1:A:697:MET:HG2	2.60	0.41
1:A:878:LEU:HA	1:A:881:THR:HG22	2.02	0.41
1:B:624:ILE:HG23	1:B:634:ARG:HD2	2.02	0.41
1:B:654:GLU:OE1	1:B:654:GLU:N	2.53	0.41
1:B:770:ILE:HD11	1:B:1012:LEU:HD23	2.02	0.41
1:C:375:PHE:HE2	1:C:407:VAL:HG11	1.85	0.41
1:C:402:ILE:HD12	1:C:406:GLU:HB3	2.03	0.41
1:C:574:ASP:O	1:C:587:ILE:N	2.54	0.41
1:C:638:THR:O	1:C:638:THR:OG1	2.30	0.41
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:LEU:HD11	1:A:665:PRO:HB3	2.01	0.41
1:B:974:SER:HB3	1:B:980:ILE:HG22	2.03	0.41
1:C:848:ASP:OD1	1:C:848:ASP:N	2.54	0.41
1:A:115:GLN:HB3	1:A:233:ILE:HD13	2.03	0.41
1:A:347:PHE:HD2	1:A:399:SER:HB2	1.86	0.41
1:B:411:ALA:HB3	1:B:414:GLN:HG3	2.03	0.40
1:C:431:GLY:HA2	1:C:515:PHE:CD1	2.56	0.40
1:C:453:TYR:CD1	1:C:495:TYR:HD1	2.39	0.40
1:A:304:LYS:HB2	1:A:304:LYS:HE3	1.84	0.40
2:H:106:PHE:HD1	2:H:106:PHE:O	2.03	0.40
2:D:2:VAL:HG11	2:D:111:TYR:CE2	2.56	0.40
1:C:981:LEU:HD23	1:C:981:LEU:HA	1.88	0.40
1:A:417:ASN:ND2	1:A:455:LEU:HD23	2.36	0.40
1:A:631:PRO:HB3	1:A:633:TRP:CE2	2.57	0.40
1:A:646:ARG:HA	1:A:646:ARG:HD2	1.89	0.40
1:B:344:ALA:HB3	1:B:347:PHE:CE1	2.56	0.40
1:B:369:TYR:CE1	1:C:476:GLY:HA3	2.55	0.40
1:A:108:THR:HG22	1:A:109:THR:HG23	2.04	0.40
1:A:984:LEU:HD23	1:A:989:ALA:HA	2.03	0.40
3:L:70:GLU:N	3:L:70:GLU:OE1	2.54	0.40
3:L:89:GLN:NE2	3:L:91:TYR:HB3	2.37	0.40
1:B:176:LEU:HA	1:B:207:HIS:CE1	2.54	0.40
1:C:450:ASP:OD1	1:C:450:ASP:N	2.53	0.40
1:A:34:ARG:HE	1:A:34:ARG:HB2	1.68	0.40
1:A:629:LEU:HB3	1:A:631:PRO:HD2	2.04	0.40
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.57	0.40
1:B:557:LYS:HD2	1:B:559:PHE:HE1	1.86	0.40
1:C:280:ASN:OD1	1:C:281:GLU:N	2.50	0.40
1:A:847:ARG:HH11	1:A:851:CYS:HB3	1.87	0.40
2:D:37:VAL:HG21	2:D:112:TRP:CZ3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1053/1204 (88%)	963 (92%)	86 (8%)	4 (0%)	30	60
1	B	1053/1204 (88%)	957 (91%)	92 (9%)	4 (0%)	30	60
1	C	1053/1204 (88%)	972 (92%)	76 (7%)	5 (0%)	25	54
2	D	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
2	H	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16	44
3	E	106/108 (98%)	99 (93%)	7 (7%)	0	100	100
3	L	106/108 (98%)	100 (94%)	5 (5%)	1 (1%)	14	41
All	All	3611/4072 (89%)	3319 (92%)	277 (8%)	15 (0%)	32	60

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	ILE
1	C	590	CYS
2	H	103	ILE
1	C	326	ILE
1	A	534	VAL
1	B	739	THR
1	A	110	LEU
1	B	1098	ASN
1	A	739	THR
1	B	534	VAL
1	C	571	ASP
1	B	1099	GLY
1	C	110	LEU
3	L	97	LEU
1	A	332	VAL

5.3.2 Protein sidechains ⓘ

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	925/1053 (88%)	900 (97%)	25 (3%)	40	63
1	B	925/1053 (88%)	895 (97%)	30 (3%)	34	59
1	C	925/1053 (88%)	893 (96%)	32 (4%)	31	56
2	D	101/101 (100%)	98 (97%)	3 (3%)	36	61
2	H	101/101 (100%)	99 (98%)	2 (2%)	50	70
3	E	89/89 (100%)	85 (96%)	4 (4%)	23	50
3	L	89/89 (100%)	87 (98%)	2 (2%)	47	68
All	All	3155/3539 (89%)	3057 (97%)	98 (3%)	37	60

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	168	PHE
1	B	194	PHE
1	B	200	TYR
1	B	216	PHE
1	B	238	PHE
1	B	264	ASP
1	B	287	ASP
1	B	301	CYS
1	B	308	VAL
1	B	331	ASN
1	B	369	TYR
1	B	453	TYR
1	B	462	LYS
1	B	480	CYS
1	B	487	ASN
1	B	562	PHE
1	B	565	PHE
1	B	574	ASP
1	B	616	ASN
1	B	617	CYS
1	B	625	HIS
1	B	634	ARG
1	B	643	PHE
1	B	649	CYS
1	B	837	TYR
1	B	906	PHE
1	B	994	ASP
1	B	995	ARG
1	B	1091	ARG

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Mol	Chain	Res	Type
1	B	1097	SER
1	C	52	GLN
1	C	53	ASP
1	C	60	SER
1	C	127	PHE
1	C	135	PHE
1	C	168	PHE
1	C	198	ASP
1	C	216	PHE
1	C	220	PHE
1	C	229	LEU
1	C	237	ARG
1	C	245	ASN
1	C	265	TYR
1	C	309	GLU
1	C	334	ASN
1	C	353	TRP
1	C	377	PHE
1	C	383	SER
1	C	392	PHE
1	C	494	SER
1	C	515	PHE
1	C	759	PHE
1	C	786	LYS
1	C	813	SER
1	C	823	PHE
1	C	867	ASP
1	C	873	TYR
1	C	939	PHE
1	C	994	ASP
1	C	1005	GLN
1	C	1039	ARG
1	C	1041	ASP
1	A	32	PHE
1	A	40	ASP
1	A	127	PHE
1	A	135	PHE
1	A	168	PHE
1	A	216	PHE
1	A	229	LEU
1	A	238	PHE
1	A	264	ASP

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Mol	Chain	Res	Type
1	A	265	TYR
1	A	282	ASN
1	A	294	ASP
1	A	318	PHE
1	A	453	TYR
1	A	462	LYS
1	A	487	ASN
1	A	530	SER
1	A	580	GLN
1	A	643	PHE
1	A	646	ARG
1	A	950	ASP
1	A	995	ARG
1	A	1000	ARG
1	A	1050	MET
1	A	1091	ARG
2	H	106	PHE
2	H	117	LEU
3	L	42	GLN
3	L	54	ARG
2	D	27	PHE
2	D	75	SER
2	D	106	PHE
3	E	6	GLN
3	E	38	GLN
3	E	42	GLN
3	E	86	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	121	ASN
1	B	207	HIS
1	B	506	GLN
1	C	81	ASN
1	A	207	HIS
1	A	506	GLN
1	A	856	ASN
1	A	1083	HIS
3	L	92	ASN
3	E	6	GLN
3	E	32	ASN

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Mol	Chain	Res	Type
3	E	92	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

29 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	F	1	4,1	14,14,15	0.26	0	17,19,21	0.46	0
4	BMA	F	2	4	11,11,12	0.57	0	15,15,17	0.71	0
4	NAG	G	1	4,1	14,14,15	0.24	0	17,19,21	0.41	0
4	BMA	G	2	4	11,11,12	0.54	0	15,15,17	0.72	0
4	NAG	I	1	4,1	14,14,15	0.42	0	17,19,21	0.92	1 (5%)
4	BMA	I	2	4	11,11,12	0.97	0	15,15,17	1.04	2 (13%)
5	NAG	J	1	5,1	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	J	2	5	14,14,15	0.24	0	17,19,21	0.44	0
6	NAG	K	1	6,1	14,14,15	0.26	0	17,19,21	0.43	0
6	NAG	K	2	6,1	14,14,15	0.29	0	17,19,21	0.40	0
6	BMA	K	3	6	11,11,12	0.54	0	15,15,17	0.74	0
4	NAG	M	1	4,1	14,14,15	0.29	0	17,19,21	0.49	0
4	BMA	M	2	4	11,11,12	0.64	0	15,15,17	0.71	0
4	NAG	N	1	4,1	14,14,15	0.30	0	17,19,21	0.47	0
4	BMA	N	2	4	11,11,12	0.57	0	15,15,17	0.73	0
4	NAG	O	1	4,1	14,14,15	0.19	0	17,19,21	0.41	0
4	BMA	O	2	4	11,11,12	0.59	0	15,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	NAG	P	1	5,1	14,14,15	0.23	0	17,19,21	0.48	0
5	NAG	P	2	5	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	Q	1	5,1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	Q	2	5	14,14,15	0.26	0	17,19,21	0.39	0
4	NAG	R	1	4,1	14,14,15	0.26	0	17,19,21	0.44	0
4	BMA	R	2	4	11,11,12	0.55	0	15,15,17	0.68	0
4	NAG	S	1	4,1	14,14,15	0.21	0	17,19,21	0.44	0
4	BMA	S	2	4	11,11,12	0.51	0	15,15,17	0.73	0
4	NAG	T	1	4,1	14,14,15	1.11	1 (7%)	17,19,21	1.07	2 (11%)
4	BMA	T	2	4	11,11,12	0.50	0	15,15,17	1.02	1 (6%)
5	NAG	U	1	5,1	14,14,15	0.16	0	17,19,21	0.49	0
5	NAG	U	2	5	14,14,15	0.27	0	17,19,21	0.41	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	F	1	4,1	-	2/6/23/26	0/1/1/1
4	BMA	F	2	4	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	1/6/23/26	0/1/1/1
4	BMA	G	2	4	-	0/2/19/22	0/1/1/1
4	NAG	I	1	4,1	-	1/6/23/26	0/1/1/1
4	BMA	I	2	4	-	1/2/19/22	0/1/1/1
5	NAG	J	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6,1	-	2/6/23/26	0/1/1/1
6	BMA	K	3	6	-	0/2/19/22	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	BMA	M	2	4	-	0/2/19/22	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	BMA	N	2	4	-	0/2/19/22	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	BMA	O	2	4	-	0/2/19/22	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	R	2	4	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	BMA	S	2	4	-	0/2/19/22	0/1/1/1
4	NAG	T	1	4,1	-	2/6/23/26	0/1/1/1
4	BMA	T	2	4	-	0/2/19/22	0/1/1/1
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-3.95	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	1	NAG	C3-C4-C5	2.65	114.97	110.24
4	T	2	BMA	C1-O5-C5	2.46	115.52	112.19
4	I	1	NAG	O5-C1-C2	2.36	115.01	111.29
4	T	1	NAG	O4-C4-C5	-2.22	103.79	109.30
4	I	2	BMA	O2-C2-C3	-2.17	105.79	110.14
4	I	2	BMA	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	U	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
5	J	1	NAG	O5-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	N	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C8-C7-N2-C2
4	M	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	J	1	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	I	2	BMA	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6

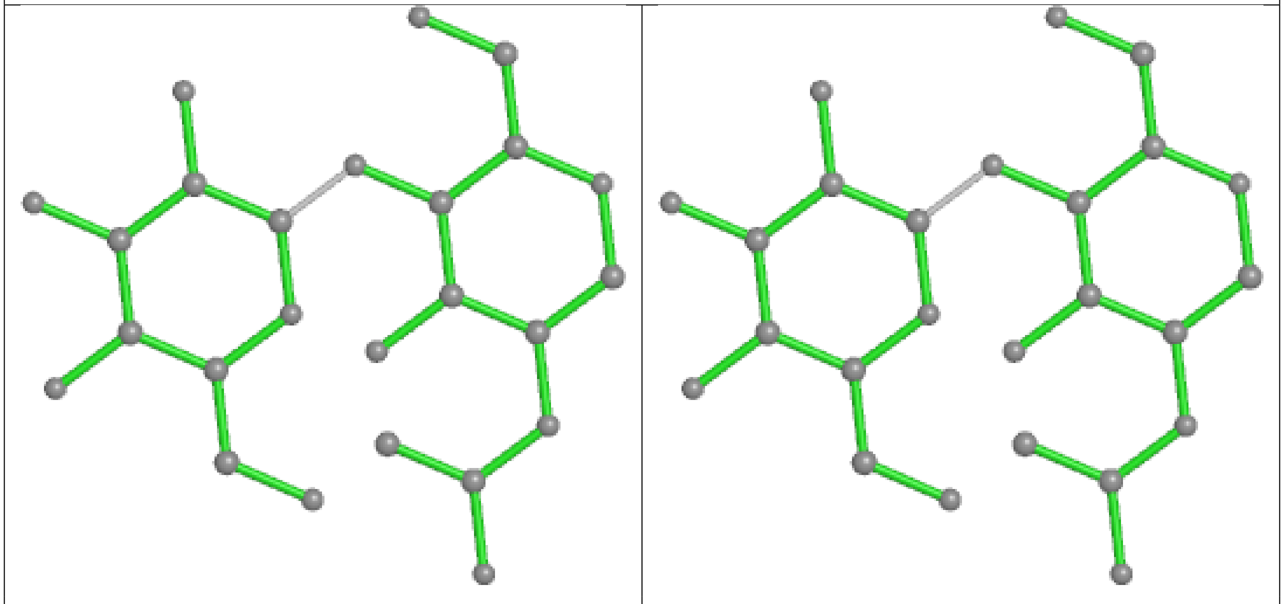
There are no ring outliers.

3 monomers are involved in 2 short contacts:

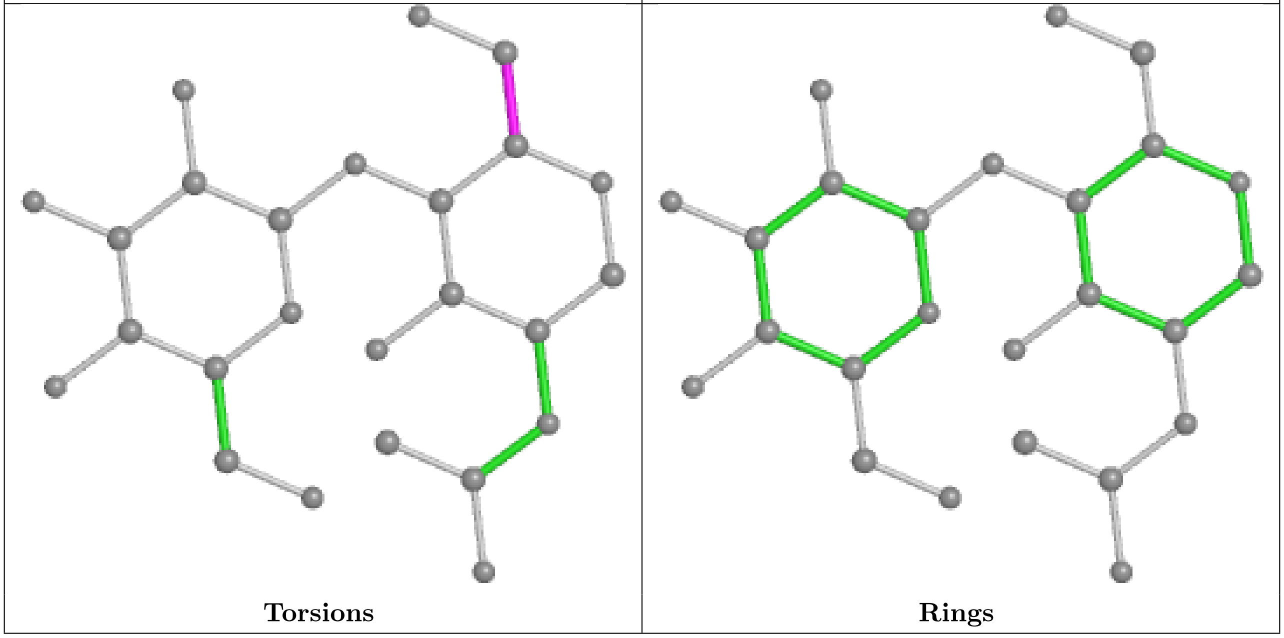
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	NAG	1	0
4	F	2	BMA	1	0
4	I	1	NAG	1	0

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 F

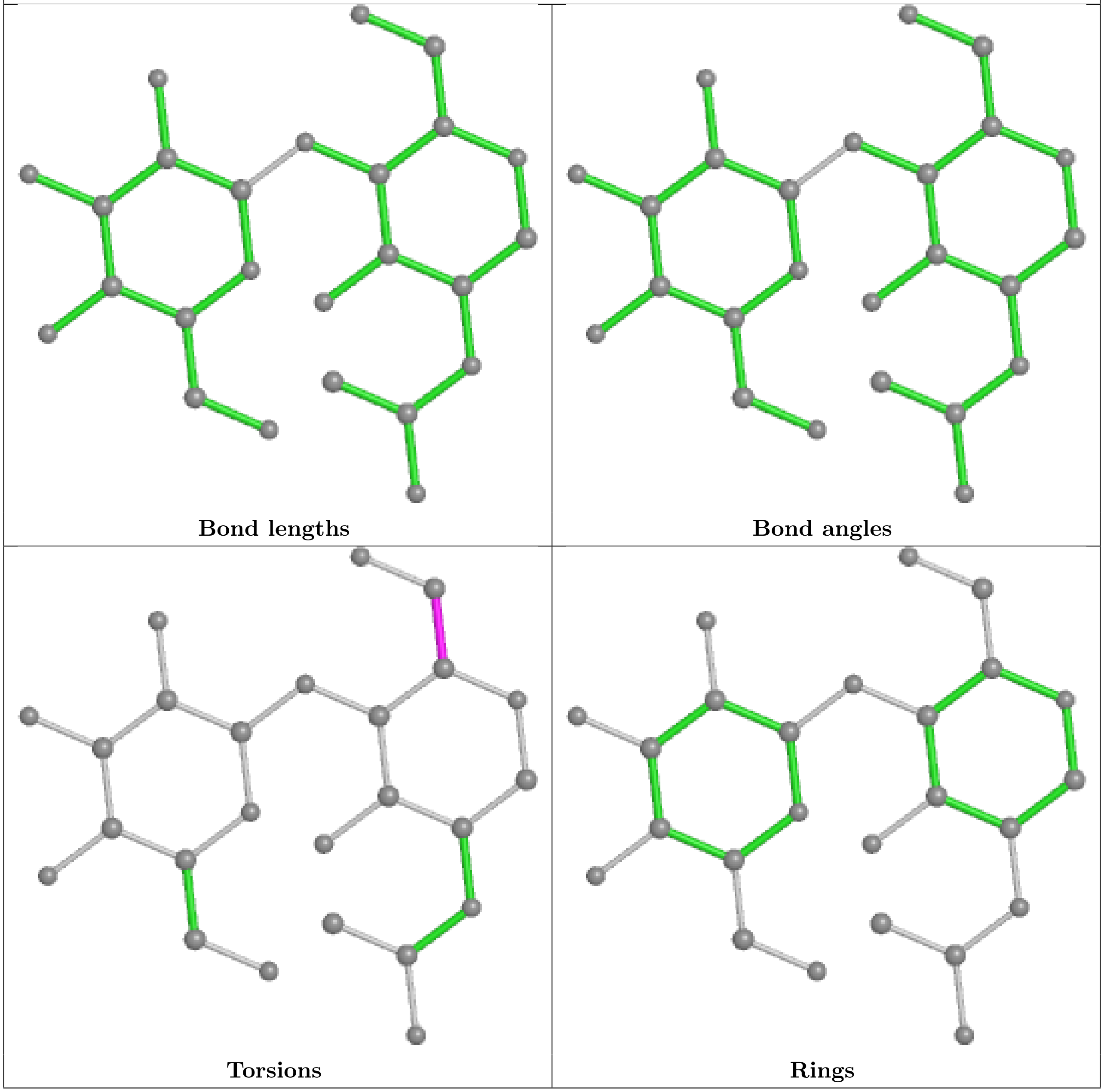


Bond lengths **Bond angles**



Torsions **Rings**

Oligosaccharide Chain G



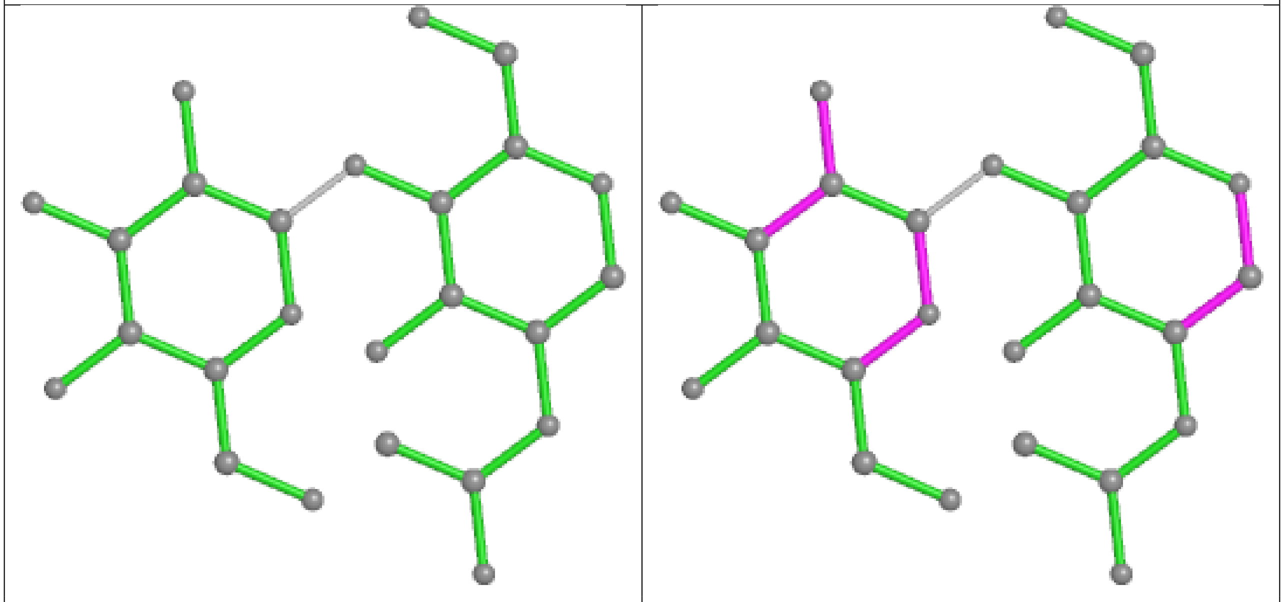
Bond lengths

Bond angles

Torsions

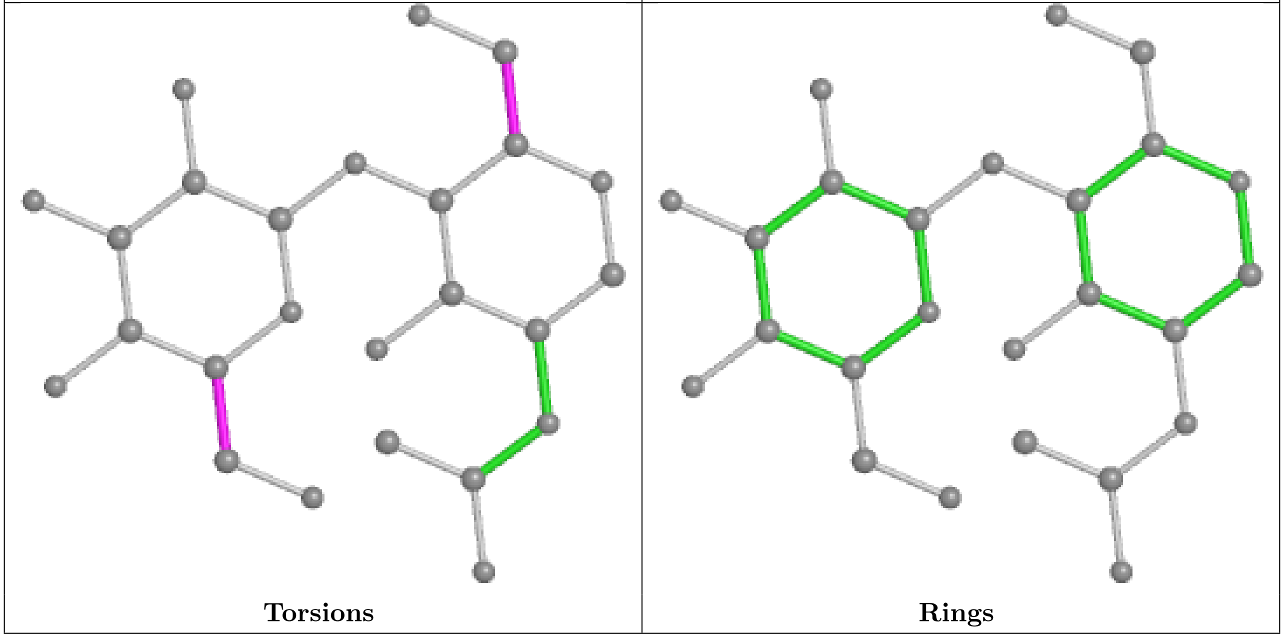
Rings

Oligosaccharide Chain I



Bond lengths

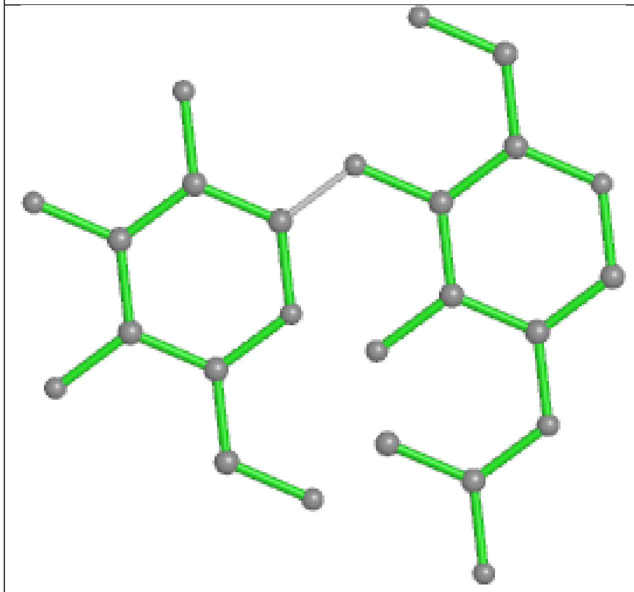
Bond angles



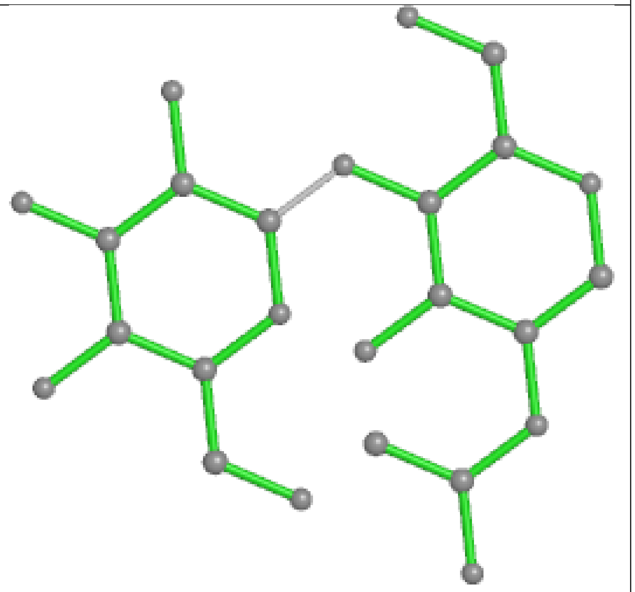
Torsions

Rings

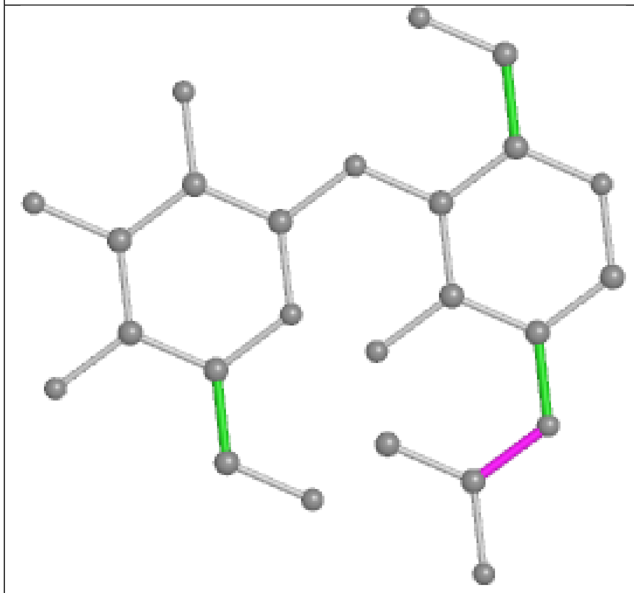
Oligosaccharide Chain M



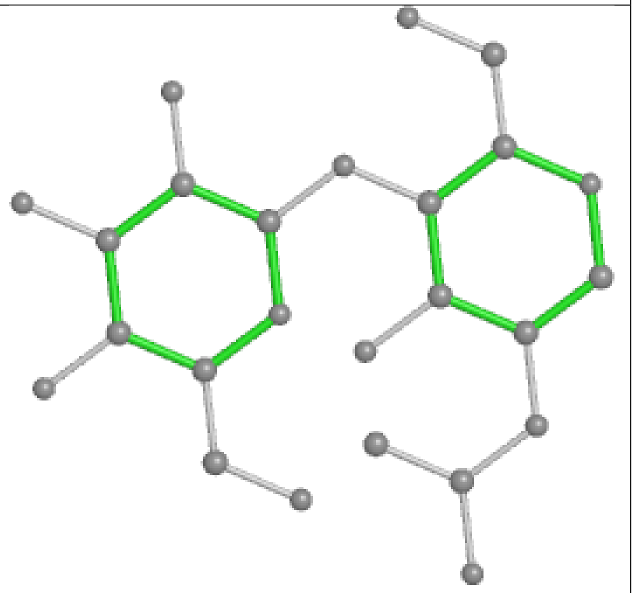
Bond lengths



Bond angles

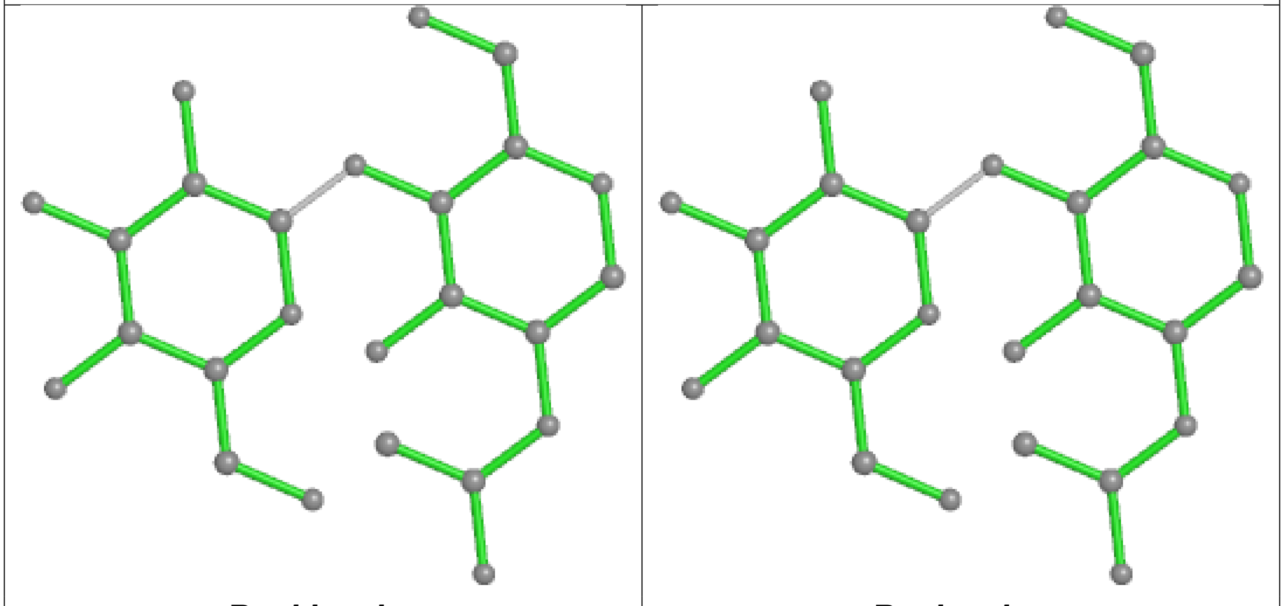


Torsions



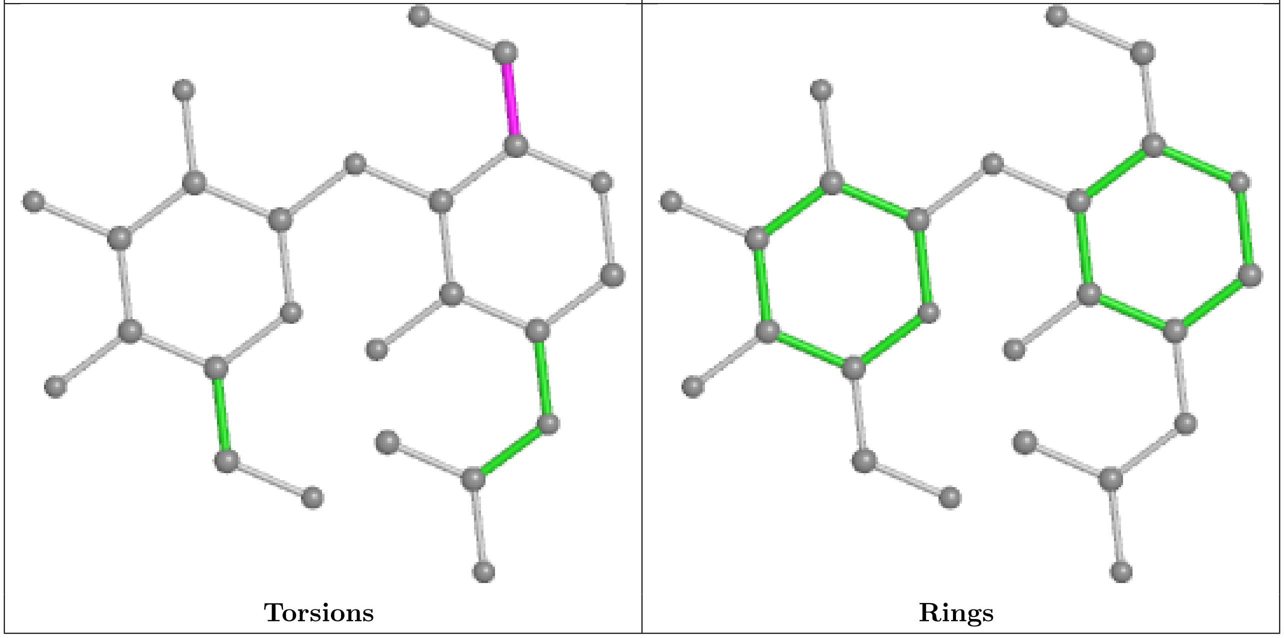
Rings

Oligosaccharide Chain N



Bond lengths

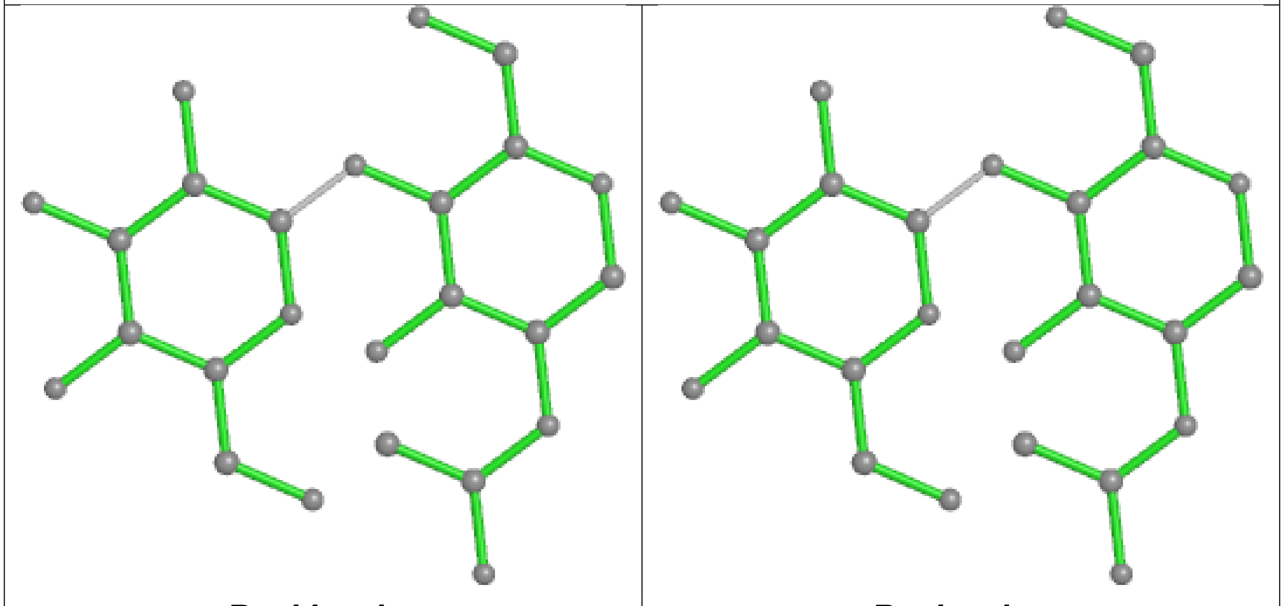
Bond angles



Torsions

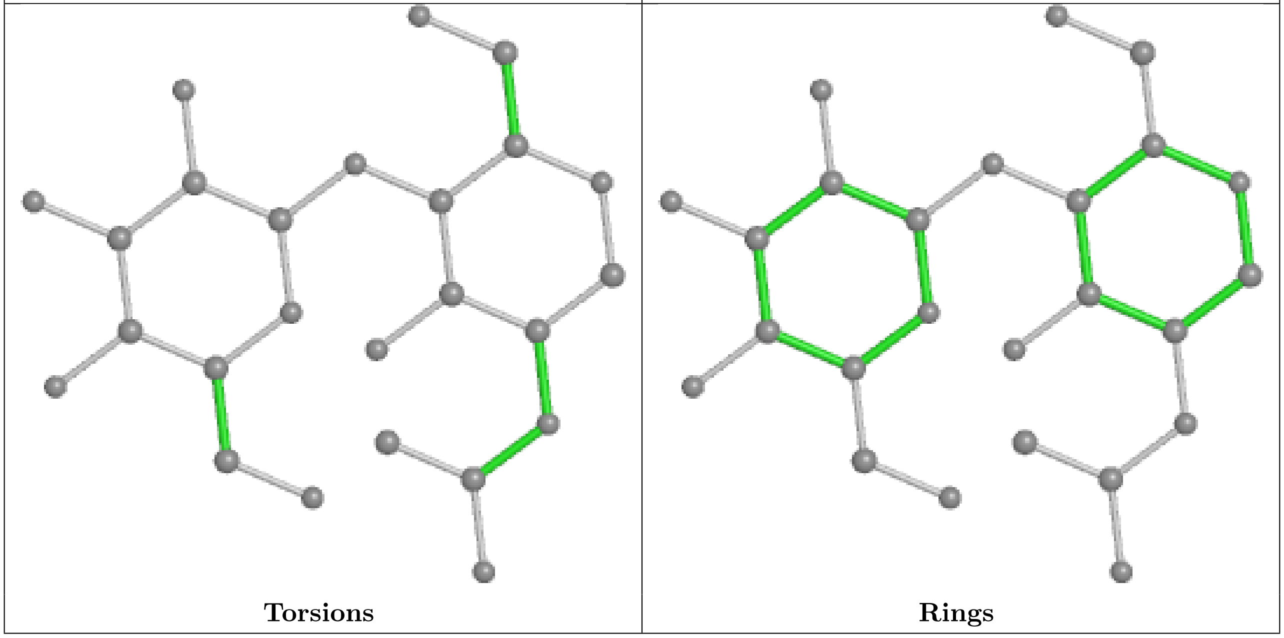
Rings

Oligosaccharide Chain O



Bond lengths

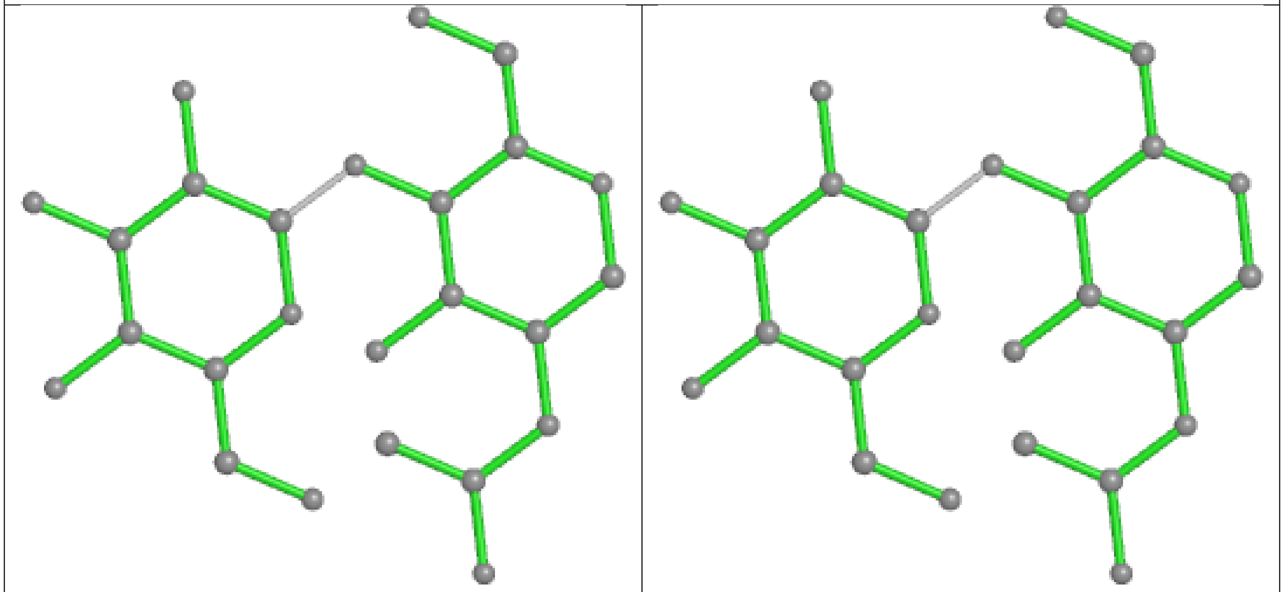
Bond angles



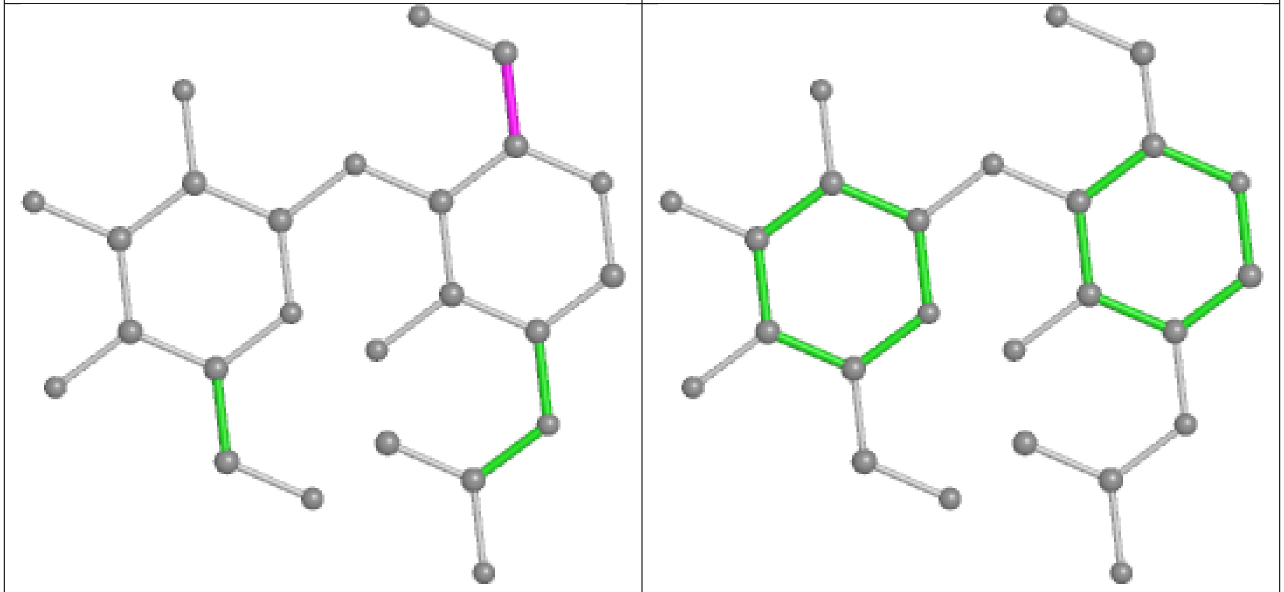
Torsions

Rings

Oligosaccharide Chain R

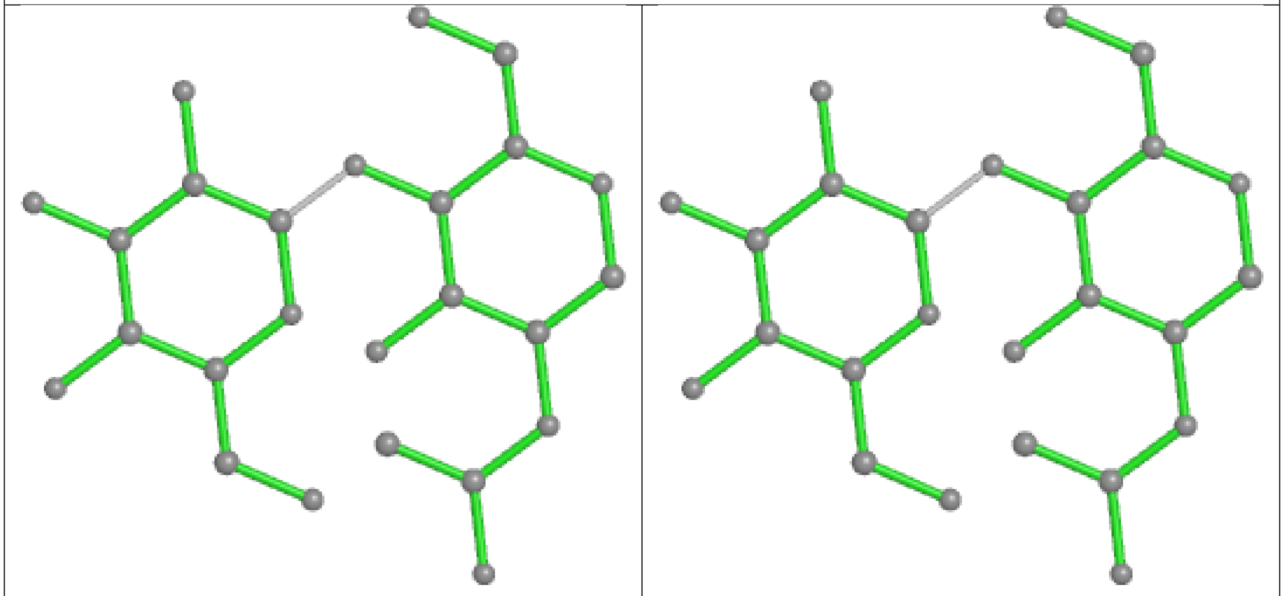


Bond lengths **Bond angles**



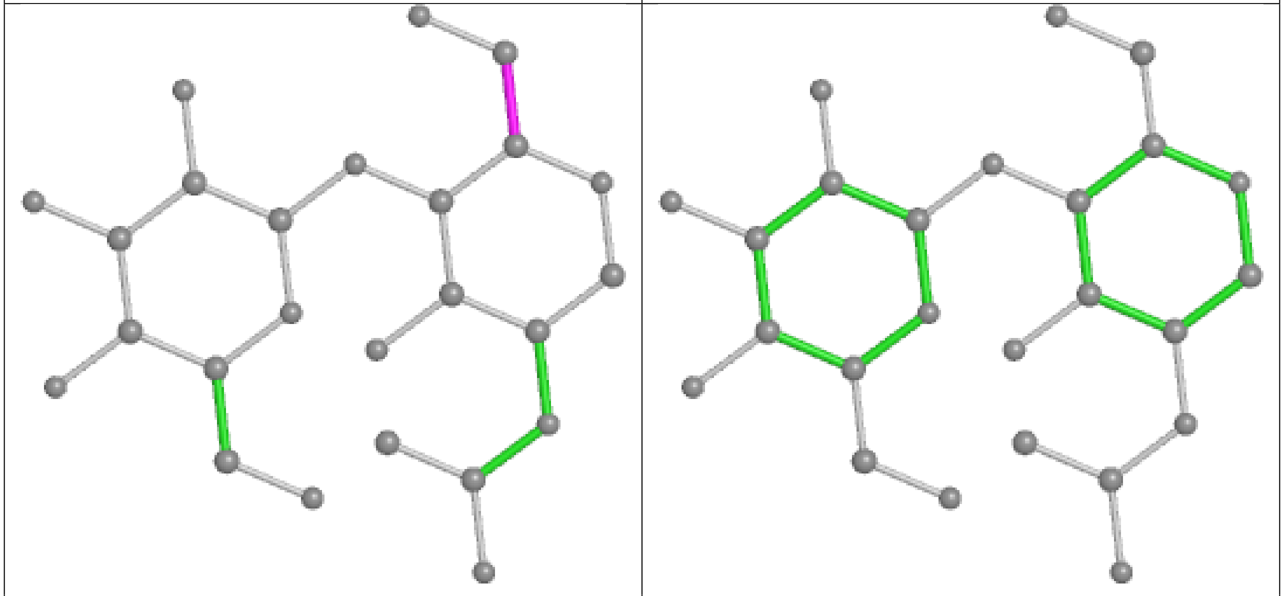
Torsions **Rings**

Oligosaccharide Chain S



Bond lengths

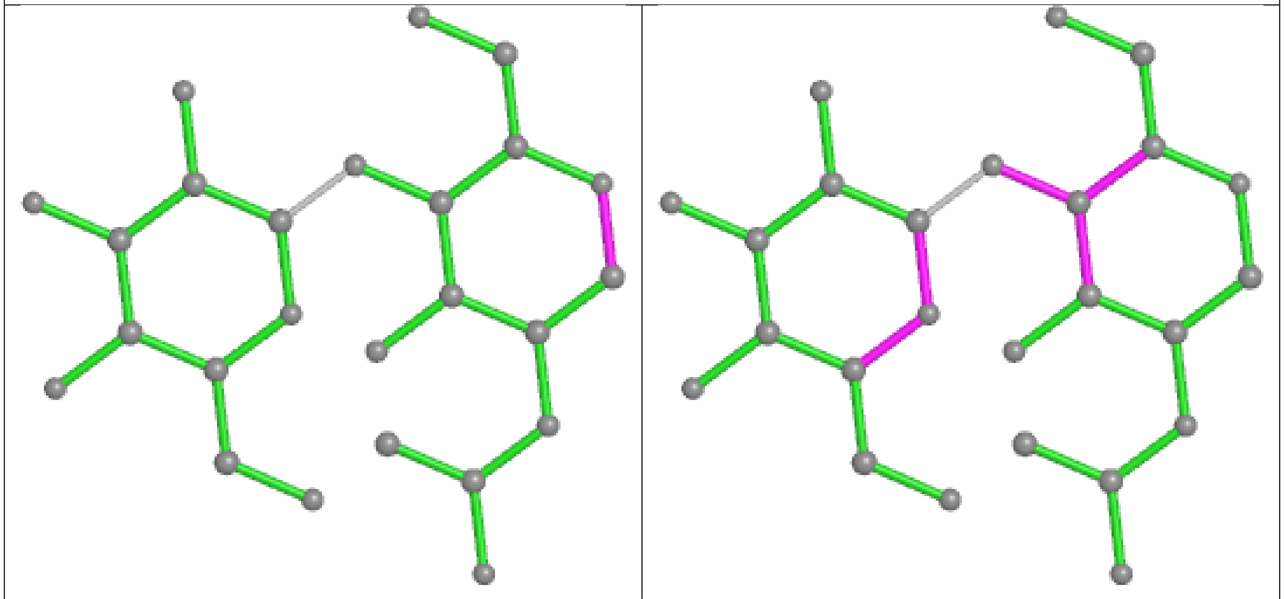
Bond angles



Torsions

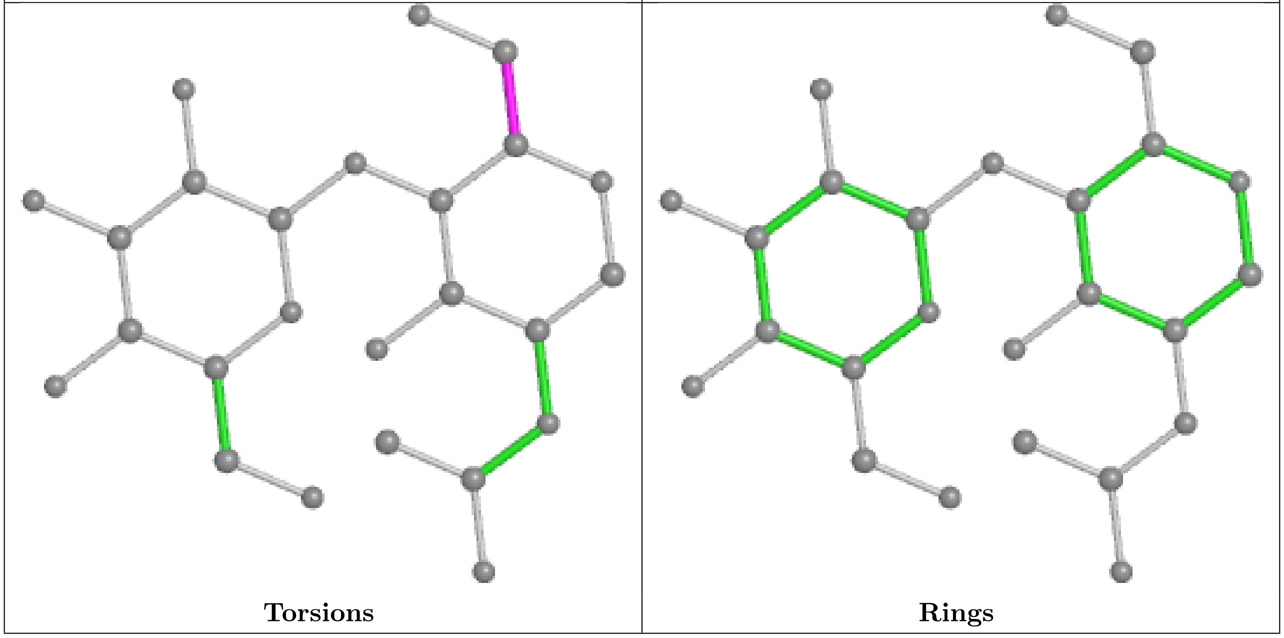
Rings

Oligosaccharide Chain T



Bond lengths

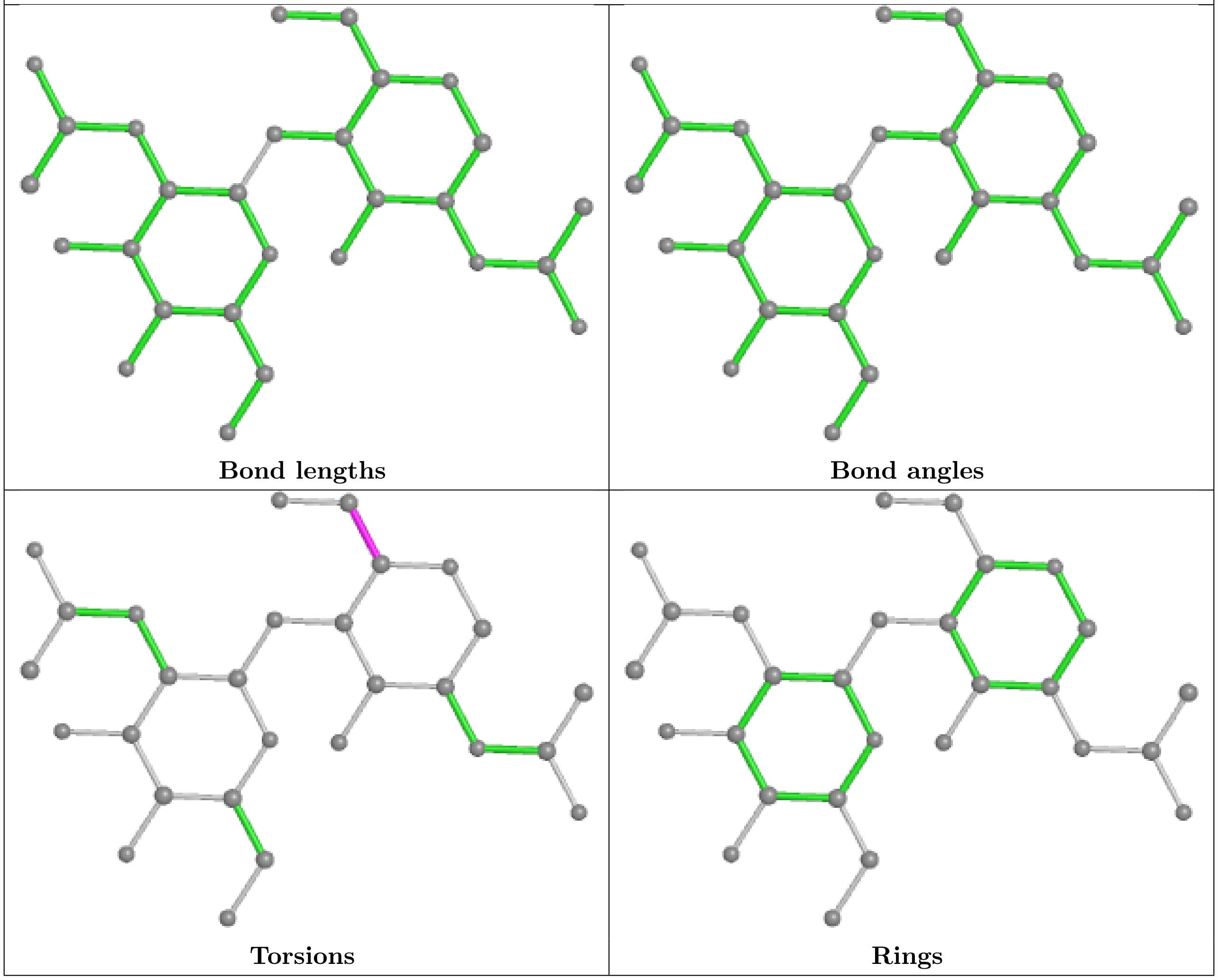
Bond angles



Torsions

Rings

Oligosaccharide Chain J



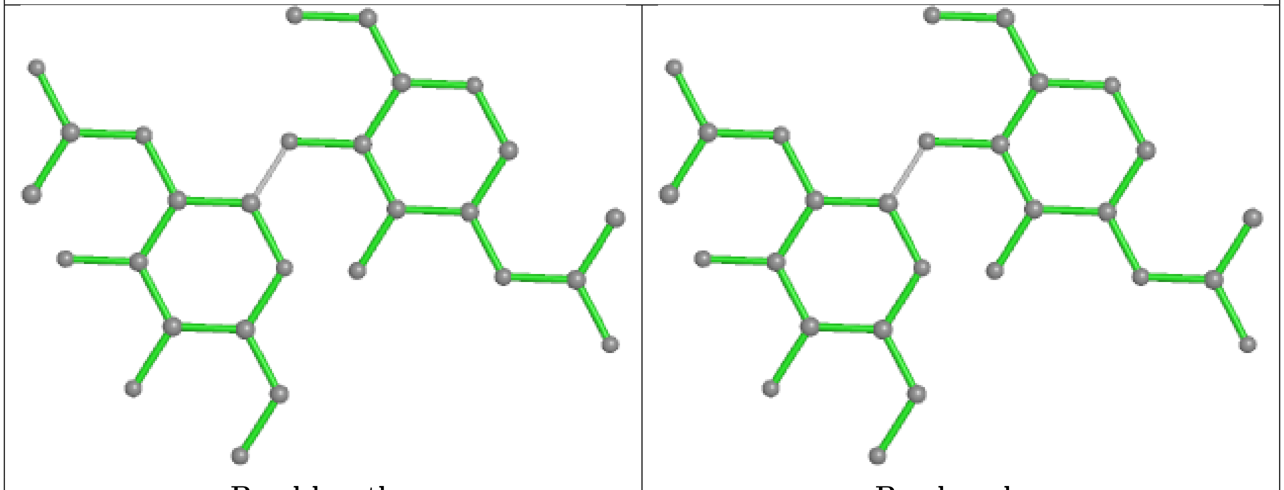
Bond lengths

Bond angles

Torsions

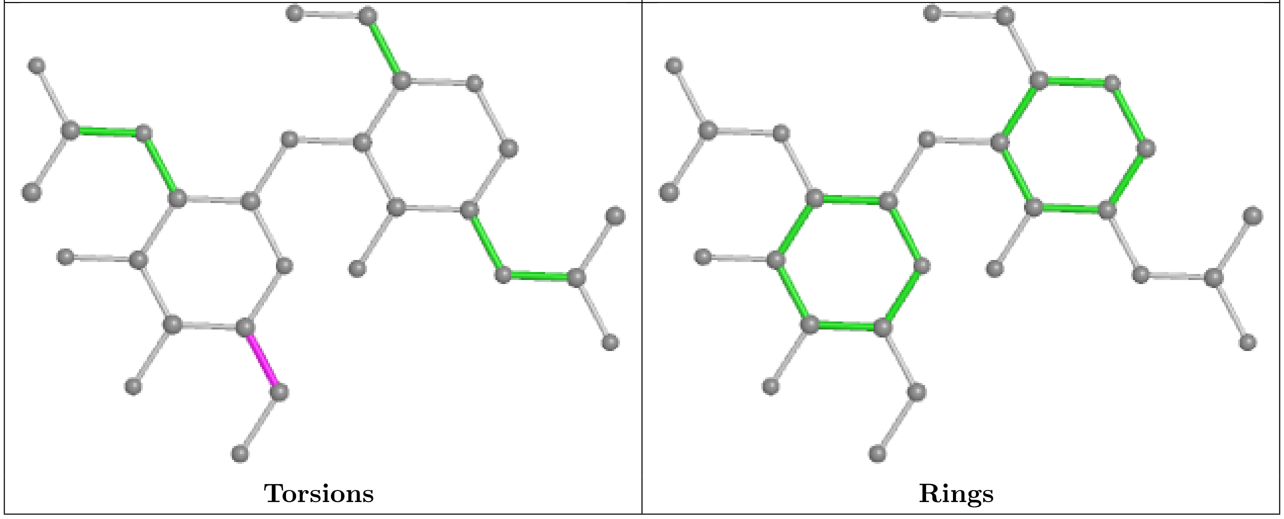
Rings

Oligosaccharide Chain P



Bond lengths

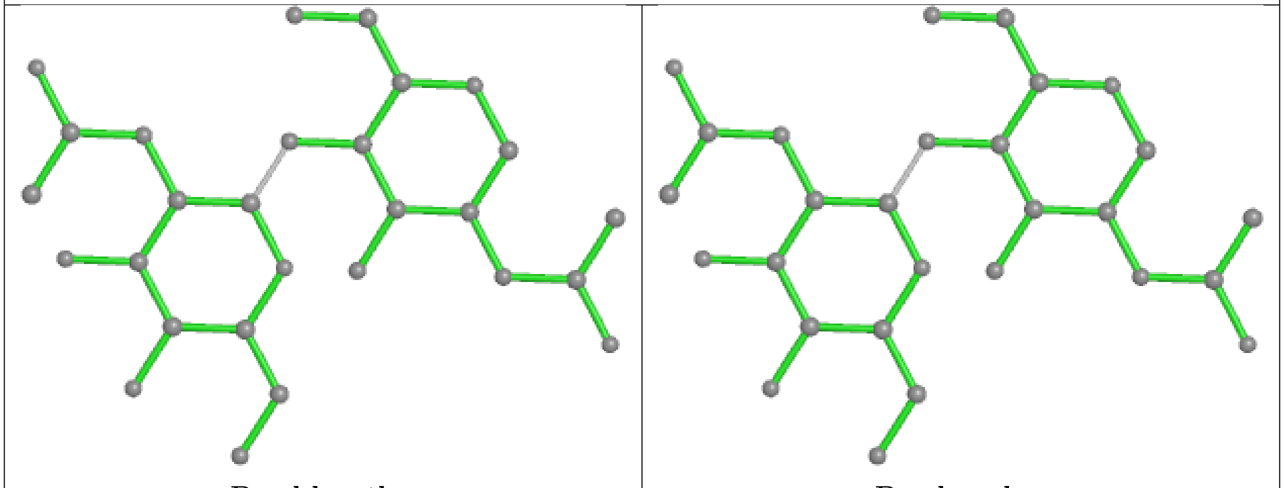
Bond angles



Torsions

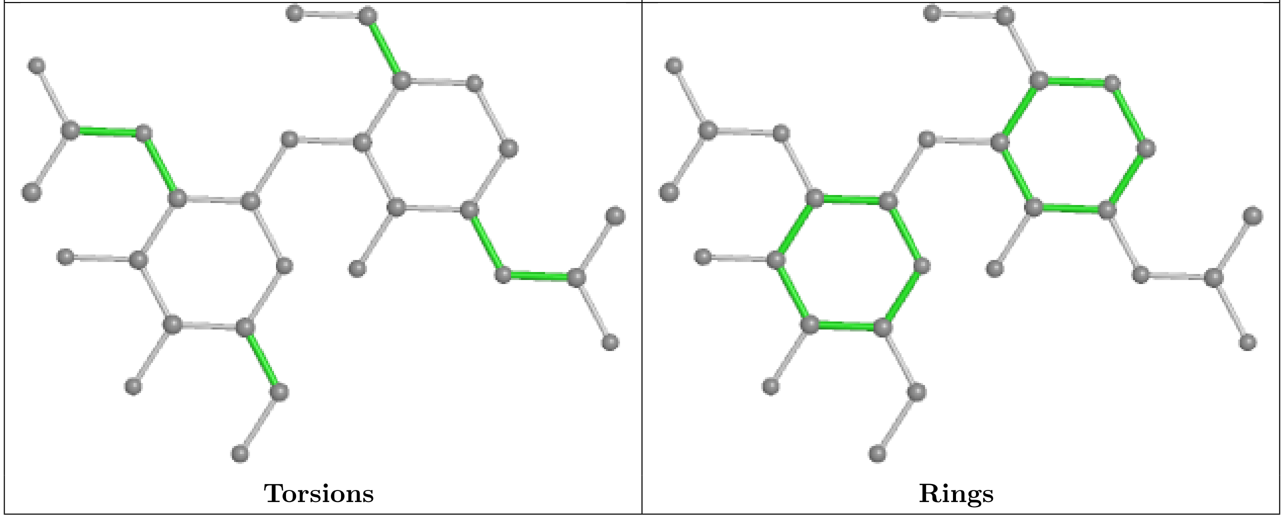
Rings

Oligosaccharide Chain Q



Bond lengths

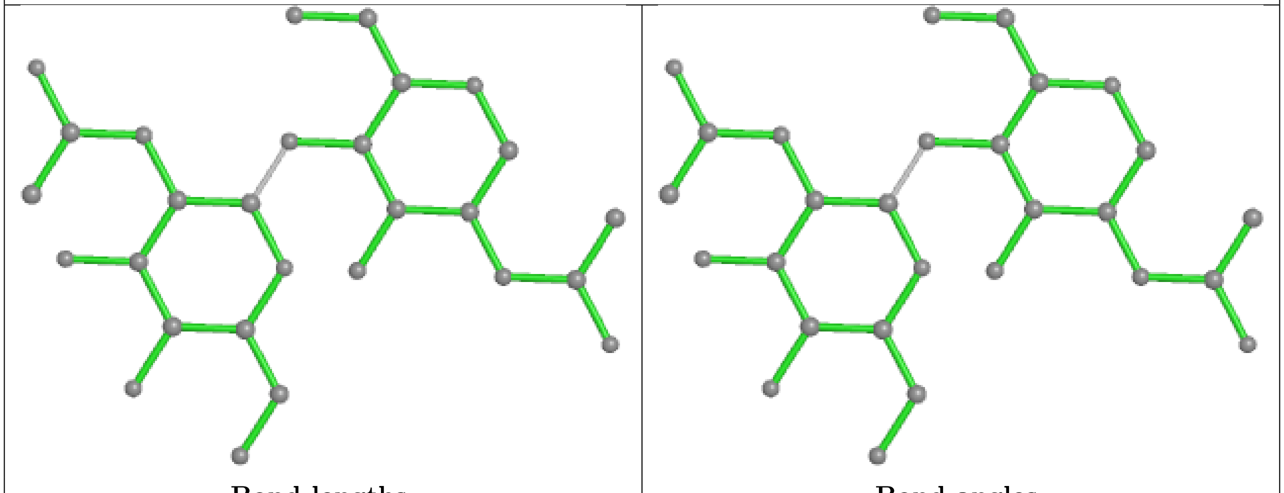
Bond angles



Torsions

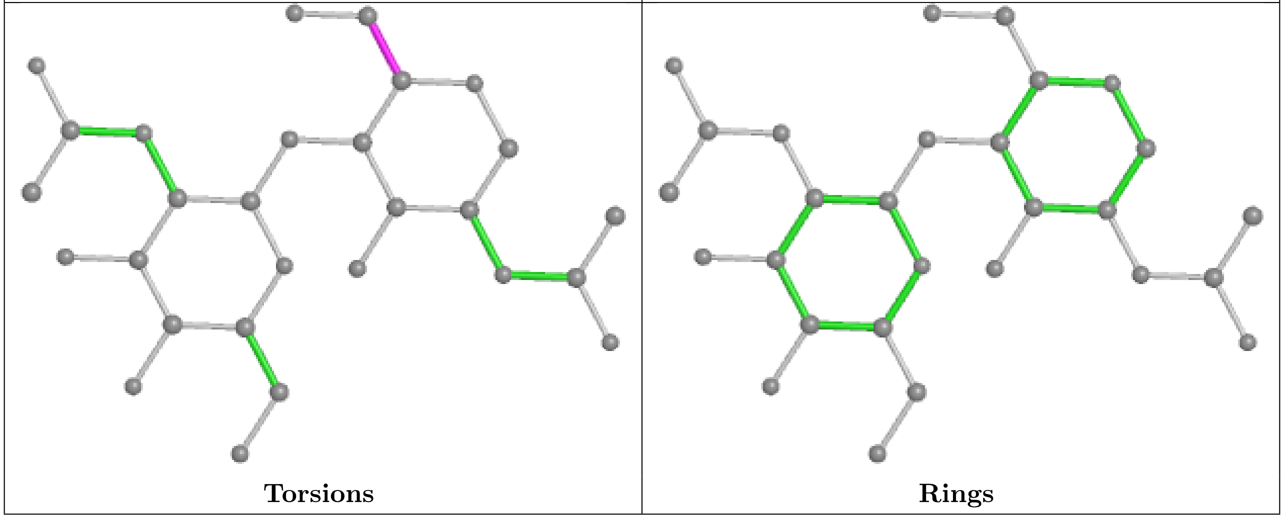
Rings

Oligosaccharide Chain U



Bond lengths

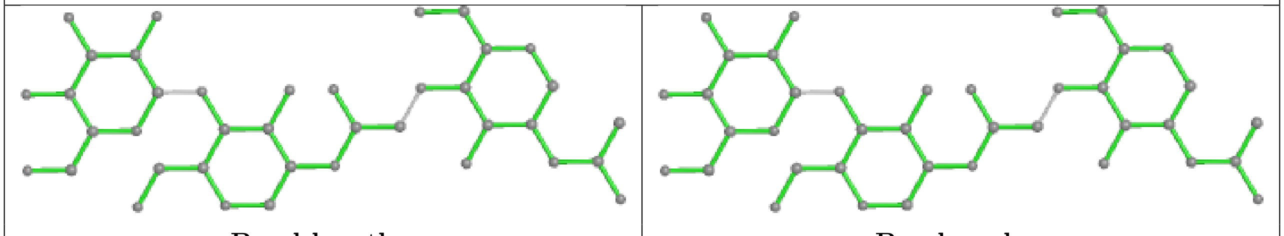
Bond angles



Torsions

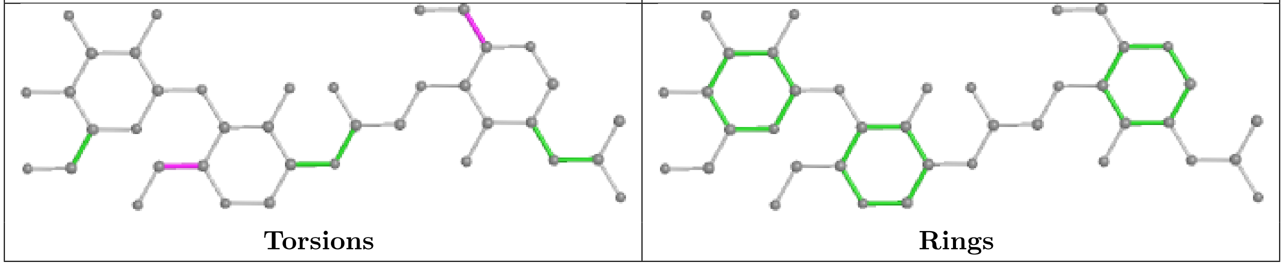
Rings

Oligosaccharide Chain K



Bond lengths

Bond angles



Torsions

Rings

5.6 Ligand geometry ⓘ

39 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	$\#\|Z\| > 2$
7	NAG	A	1309	1	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.44	0
7	NAG	A	1313	1	14,14,15	0.19	0	17,19,21	0.44	0
7	NAG	B	1305	1	14,14,15	0.26	0	17,19,21	0.42	0
7	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	C	1312	1	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	A	1301	1	14,14,15	0.41	0	17,19,21	0.50	0
7	NAG	C	1309	1	14,14,15	0.26	0	17,19,21	0.45	0
7	NAG	B	1313	1	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	A	1304	1	14,14,15	0.24	0	17,19,21	0.40	0
7	NAG	B	1308	1	14,14,15	0.39	0	17,19,21	0.44	0
7	NAG	A	1311	1	14,14,15	0.18	0	17,19,21	0.43	0
7	NAG	B	1306	1	14,14,15	0.18	0	17,19,21	0.42	0
7	NAG	A	1305	1	14,14,15	0.31	0	17,19,21	0.49	0
7	NAG	A	1306	1	14,14,15	0.24	0	17,19,21	0.45	0
7	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.38	0
7	NAG	A	1303	1	14,14,15	0.21	0	17,19,21	0.37	0
7	NAG	C	1301	1	14,14,15	0.41	0	17,19,21	0.35	0
7	NAG	A	1310	1	14,14,15	0.20	0	17,19,21	0.41	0
7	NAG	B	1309	1	14,14,15	0.24	0	17,19,21	0.44	0
7	NAG	C	1302	1	14,14,15	0.27	0	17,19,21	0.44	0
7	NAG	C	1304	1	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	A	1302	1	14,14,15	0.35	0	17,19,21	0.35	0
7	NAG	C	1306	1	14,14,15	0.57	0	17,19,21	0.52	0
7	NAG	A	1314	1	14,14,15	0.20	0	17,19,21	0.43	0
7	NAG	C	1307	1	14,14,15	0.19	0	17,19,21	0.45	0
7	NAG	C	1305	1	14,14,15	0.31	0	17,19,21	0.48	0
7	NAG	B	1310	1	14,14,15	0.43	0	17,19,21	0.78	1 (5%)
7	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	C	1311	1	14,14,15	0.21	0	17,19,21	0.42	0
7	NAG	B	1302	1	14,14,15	0.21	0	17,19,21	0.36	0
7	NAG	B	1304	1	14,14,15	0.33	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	1307	1	14,14,15	0.23	0	17,19,21	0.43	0
7	NAG	B	1301	1	14,14,15	0.28	0	17,19,21	1.37	2 (11%)
7	NAG	A	1312	1	14,14,15	0.23	0	17,19,21	0.44	0
7	NAG	B	1312	1	14,14,15	0.27	0	17,19,21	0.43	0
7	NAG	B	1303	1	14,14,15	0.19	0	17,19,21	0.43	0
7	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.48	0
7	NAG	B	1311	1	14,14,15	0.20	0	17,19,21	0.47	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
7	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1305	1	-	1/6/23/26	0/1/1/1
7	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1313	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1304	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
7	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1304	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
7	NAG	A	1314	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
7	NAG	C	1305	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
7	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1303	1	-	1/6/23/26	0/1/1/1
7	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1311	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	1301	NAG	C1-O5-C5	4.94	118.88	112.19
7	B	1310	NAG	C1-O5-C5	2.66	115.80	112.19
7	B	1301	NAG	C3-C4-C5	2.00	113.81	110.24

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1307	NAG	C4-C5-C6-O6
7	B	1307	NAG	O5-C5-C6-O6
7	C	1304	NAG	C4-C5-C6-O6
7	C	1311	NAG	C4-C5-C6-O6
7	A	1305	NAG	C4-C5-C6-O6
7	A	1308	NAG	C4-C5-C6-O6
7	C	1301	NAG	O5-C5-C6-O6
7	C	1311	NAG	O5-C5-C6-O6
7	B	1304	NAG	O5-C5-C6-O6
7	C	1306	NAG	O5-C5-C6-O6
7	C	1304	NAG	O5-C5-C6-O6
7	A	1308	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	1304	NAG	C4-C5-C6-O6
7	A	1305	NAG	O5-C5-C6-O6
7	A	1310	NAG	C4-C5-C6-O6
7	B	1306	NAG	O5-C5-C6-O6
7	B	1306	NAG	C4-C5-C6-O6
7	A	1309	NAG	O5-C5-C6-O6
7	B	1304	NAG	C8-C7-N2-C2
7	B	1304	NAG	O7-C7-N2-C2
7	C	1304	NAG	C8-C7-N2-C2
7	C	1304	NAG	O7-C7-N2-C2
7	A	1305	NAG	C8-C7-N2-C2
7	A	1305	NAG	O7-C7-N2-C2
7	A	1306	NAG	C8-C7-N2-C2
7	A	1306	NAG	O7-C7-N2-C2
7	C	1301	NAG	C4-C5-C6-O6
7	B	1310	NAG	C4-C5-C6-O6
7	A	1309	NAG	C4-C5-C6-O6
7	B	1305	NAG	O5-C5-C6-O6
7	C	1306	NAG	C4-C5-C6-O6
7	B	1311	NAG	O5-C5-C6-O6
7	A	1310	NAG	O5-C5-C6-O6
7	B	1310	NAG	O5-C5-C6-O6
7	B	1303	NAG	O5-C5-C6-O6
7	A	1301	NAG	C1-C2-N2-C7
7	B	1308	NAG	C1-C2-N2-C7
7	A	1304	NAG	O5-C5-C6-O6
7	B	1312	NAG	C4-C5-C6-O6
7	A	1306	NAG	O5-C5-C6-O6
7	B	1312	NAG	O5-C5-C6-O6
7	C	1302	NAG	C4-C5-C6-O6
7	A	1307	NAG	C4-C5-C6-O6
7	C	1302	NAG	O5-C5-C6-O6
7	C	1310	NAG	C4-C5-C6-O6
7	C	1308	NAG	C4-C5-C6-O6
7	C	1310	NAG	O5-C5-C6-O6
7	A	1307	NAG	O5-C5-C6-O6
7	B	1308	NAG	C3-C2-N2-C7
7	A	1301	NAG	C3-C2-N2-C7
7	C	1308	NAG	O5-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1308	NAG	1	0
7	A	1301	NAG	1	0
7	A	1305	NAG	1	0
7	A	1306	NAG	1	0
7	B	1304	NAG	1	0
7	B	1311	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

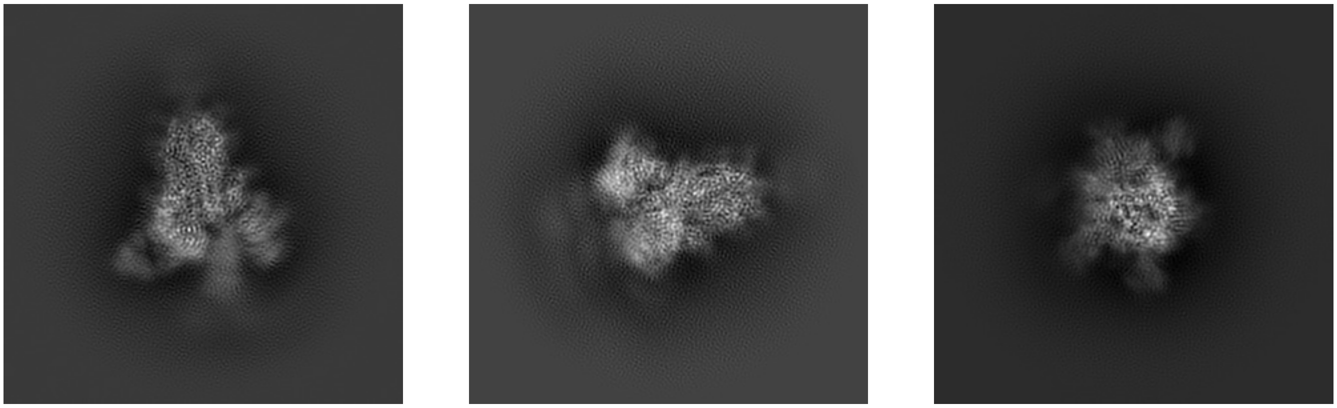
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-38914. 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.

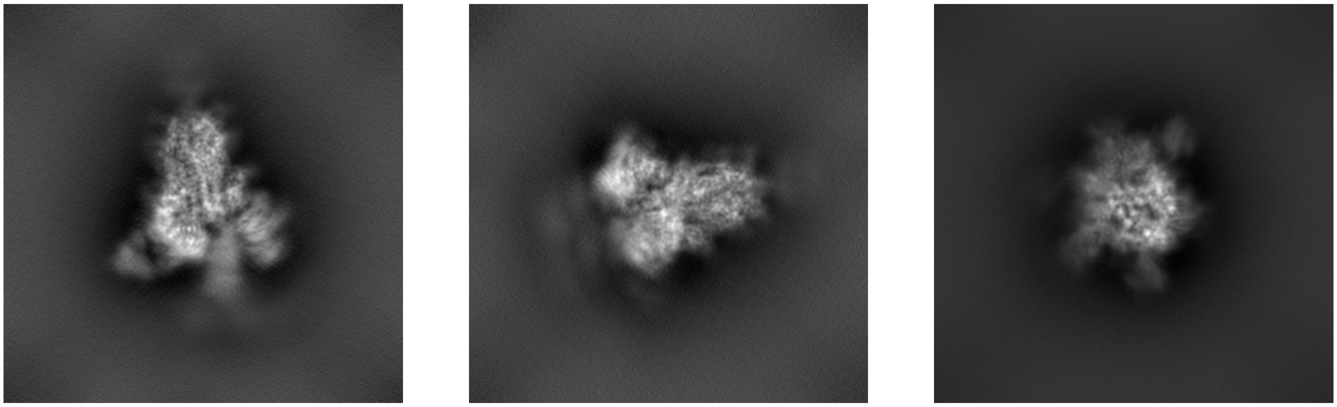
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

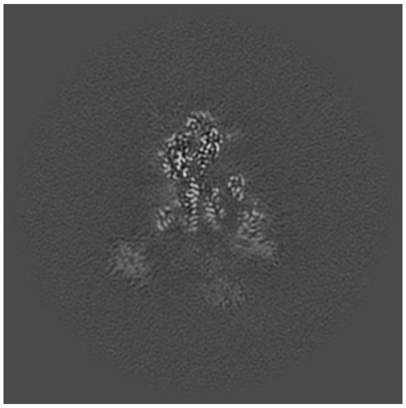


X Y Z

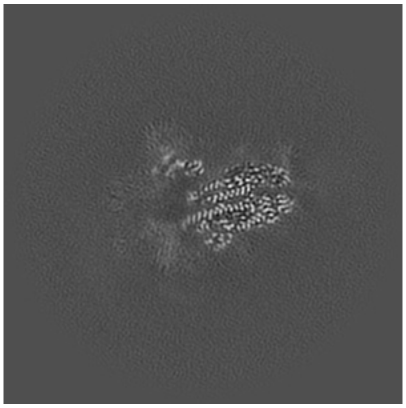
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

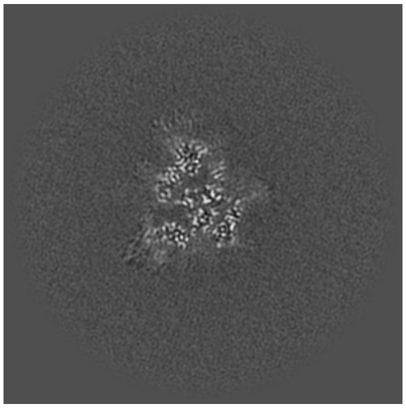
6.2.1 Primary map



X Index: 180

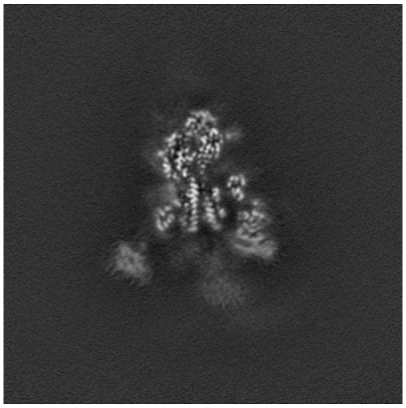


Y Index: 180

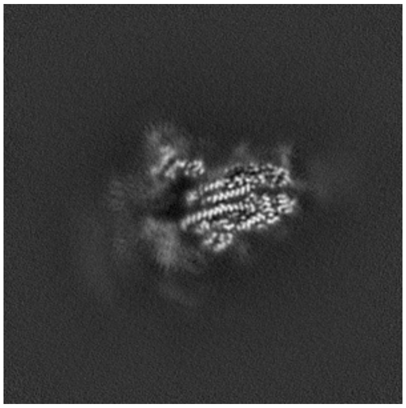


Z Index: 180

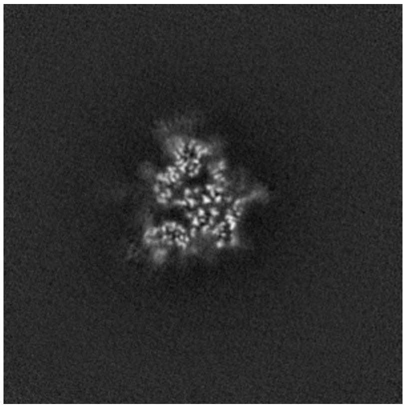
6.2.2 Raw map



X Index: 180



Y Index: 180

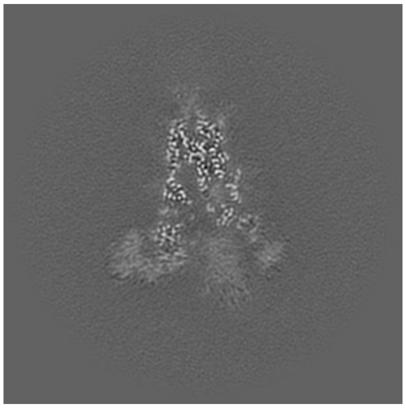


Z Index: 180

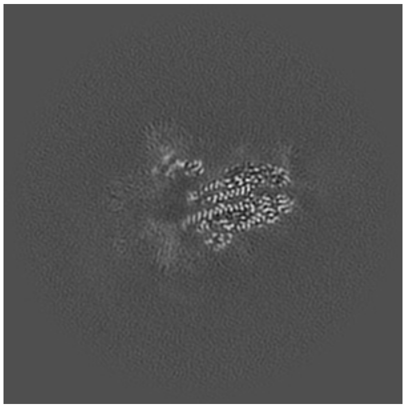
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

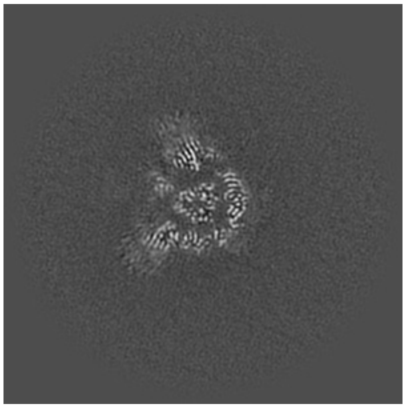
6.3.1 Primary map



X Index: 200

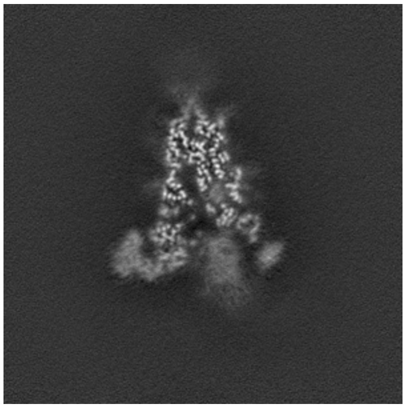


Y Index: 180

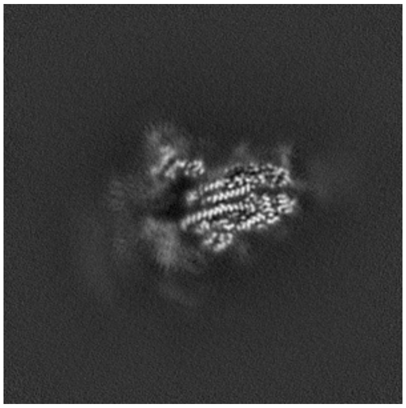


Z Index: 174

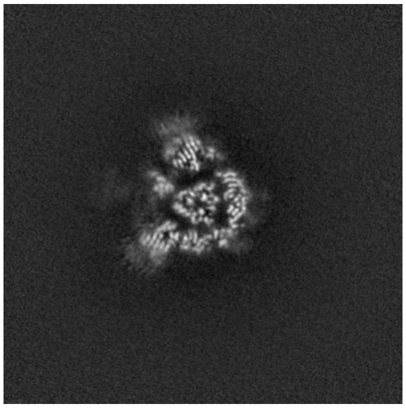
6.3.2 Raw map



X Index: 200



Y Index: 180

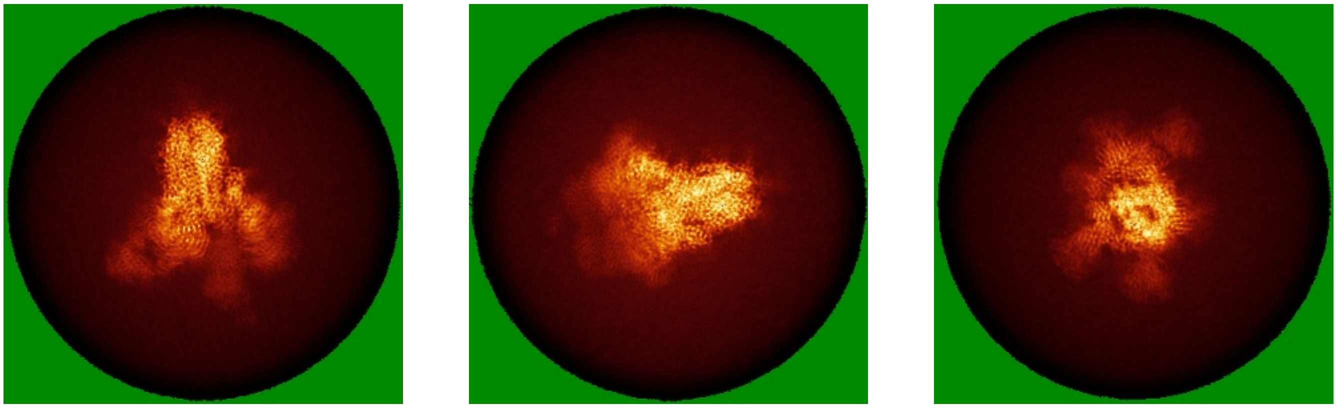


Z Index: 174

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

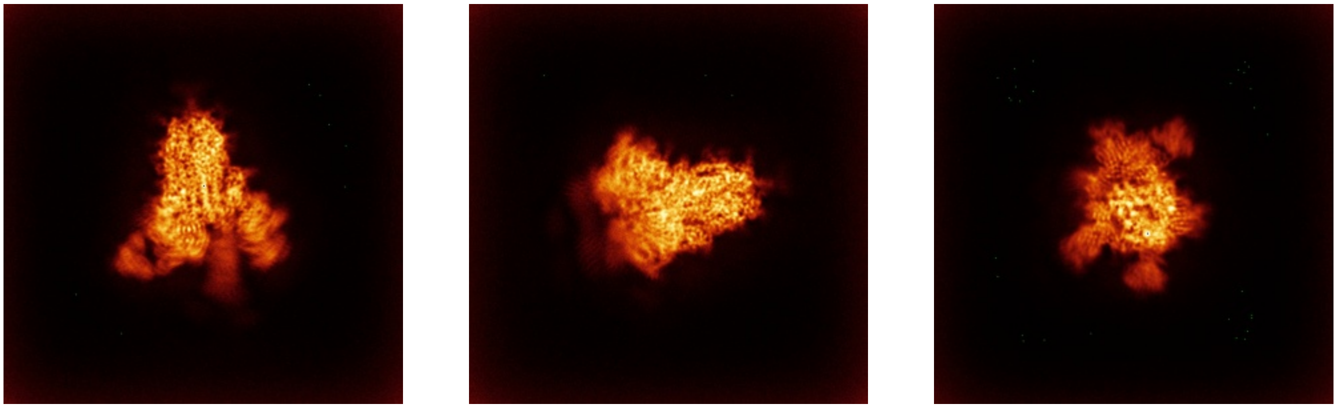
6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

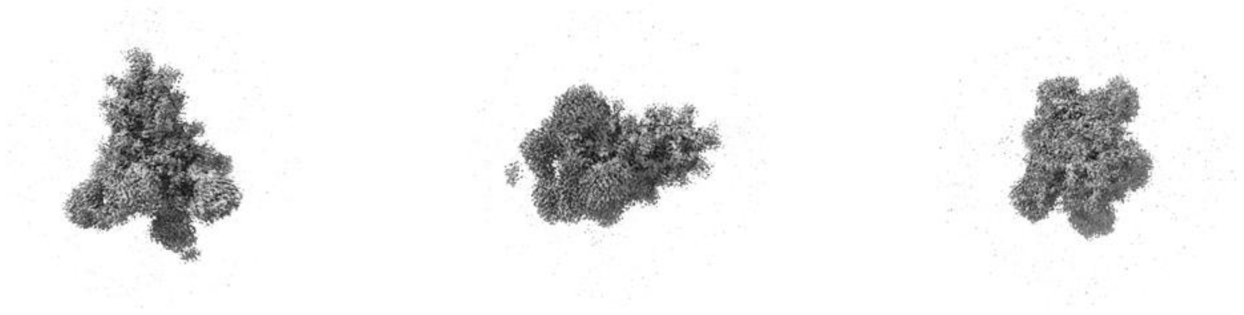


X Y Z

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

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. 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.

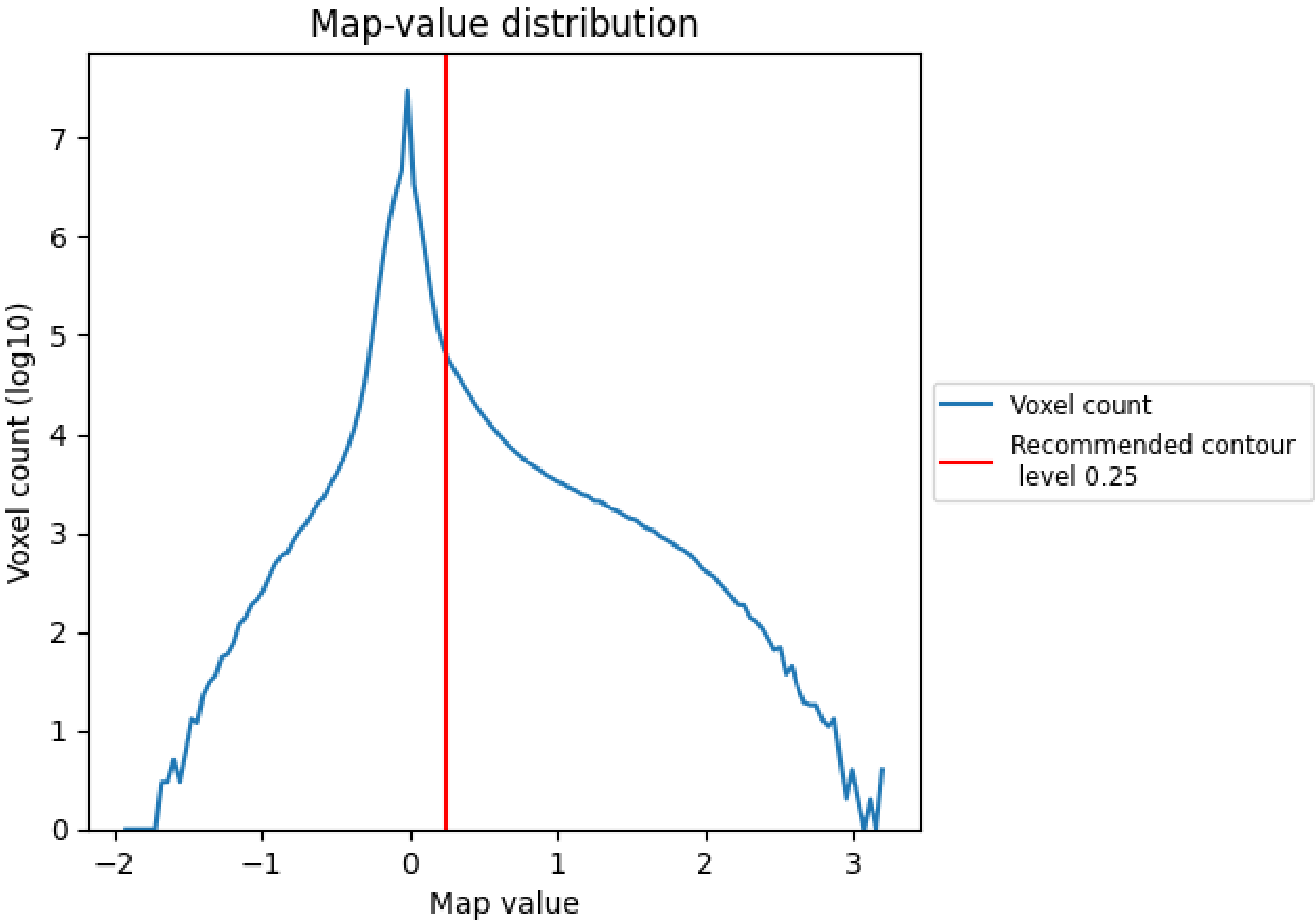
6.6 Mask visualisation

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

7 Map analysis ⓘ

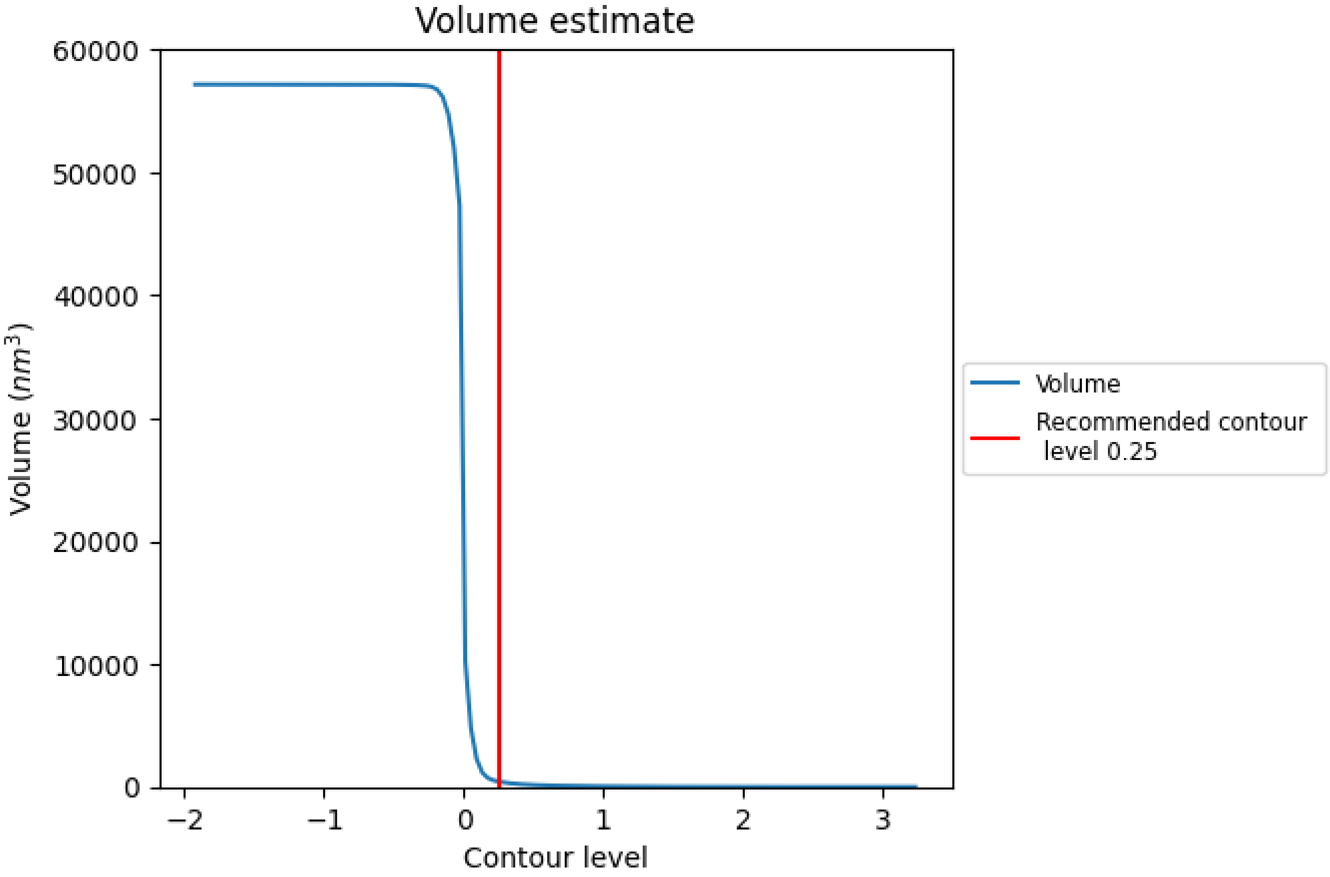
This section contains the results of statistical analysis of the map.

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.

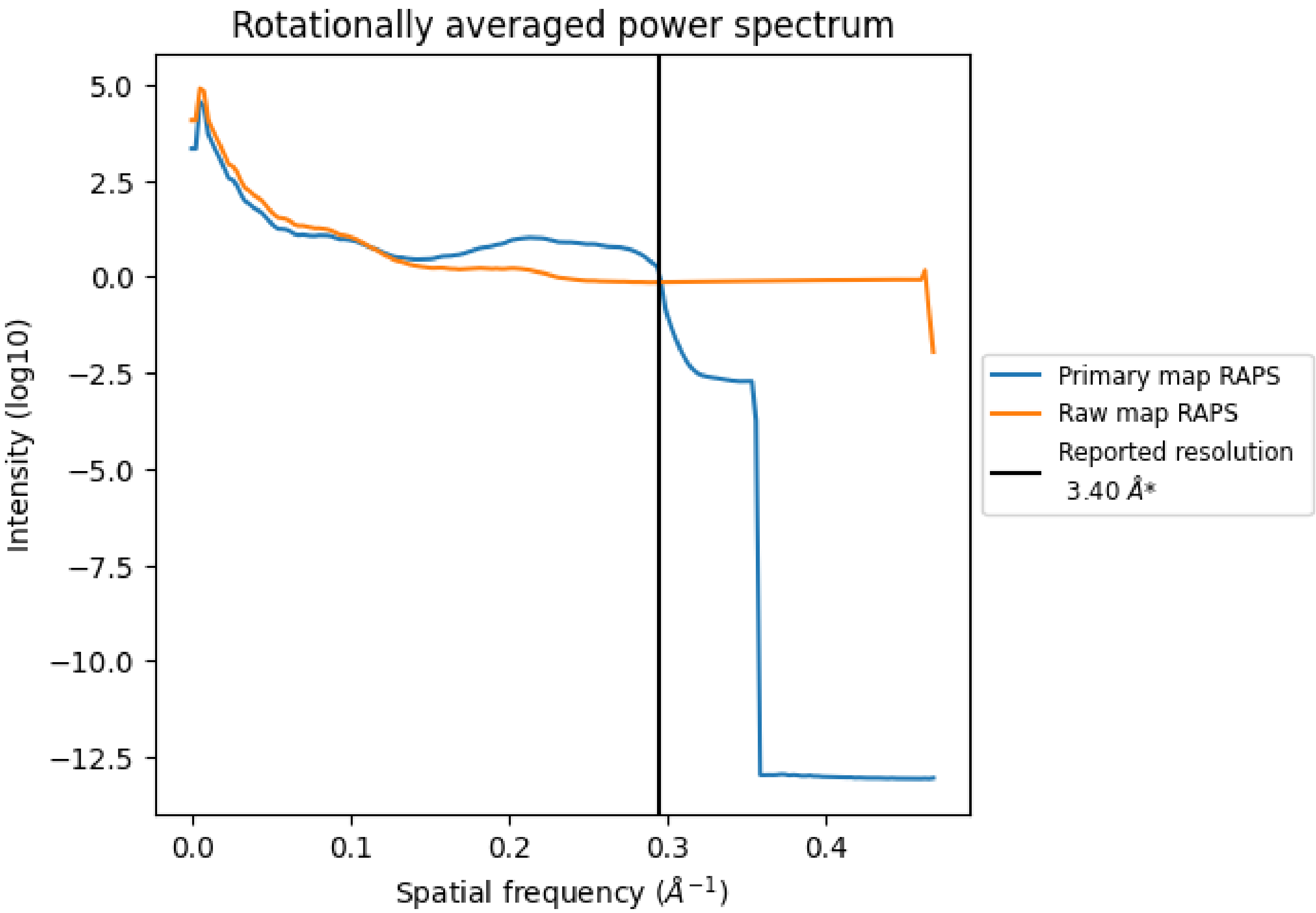
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 436 nm^3; this corresponds to an approximate mass of 394 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 ⓘ

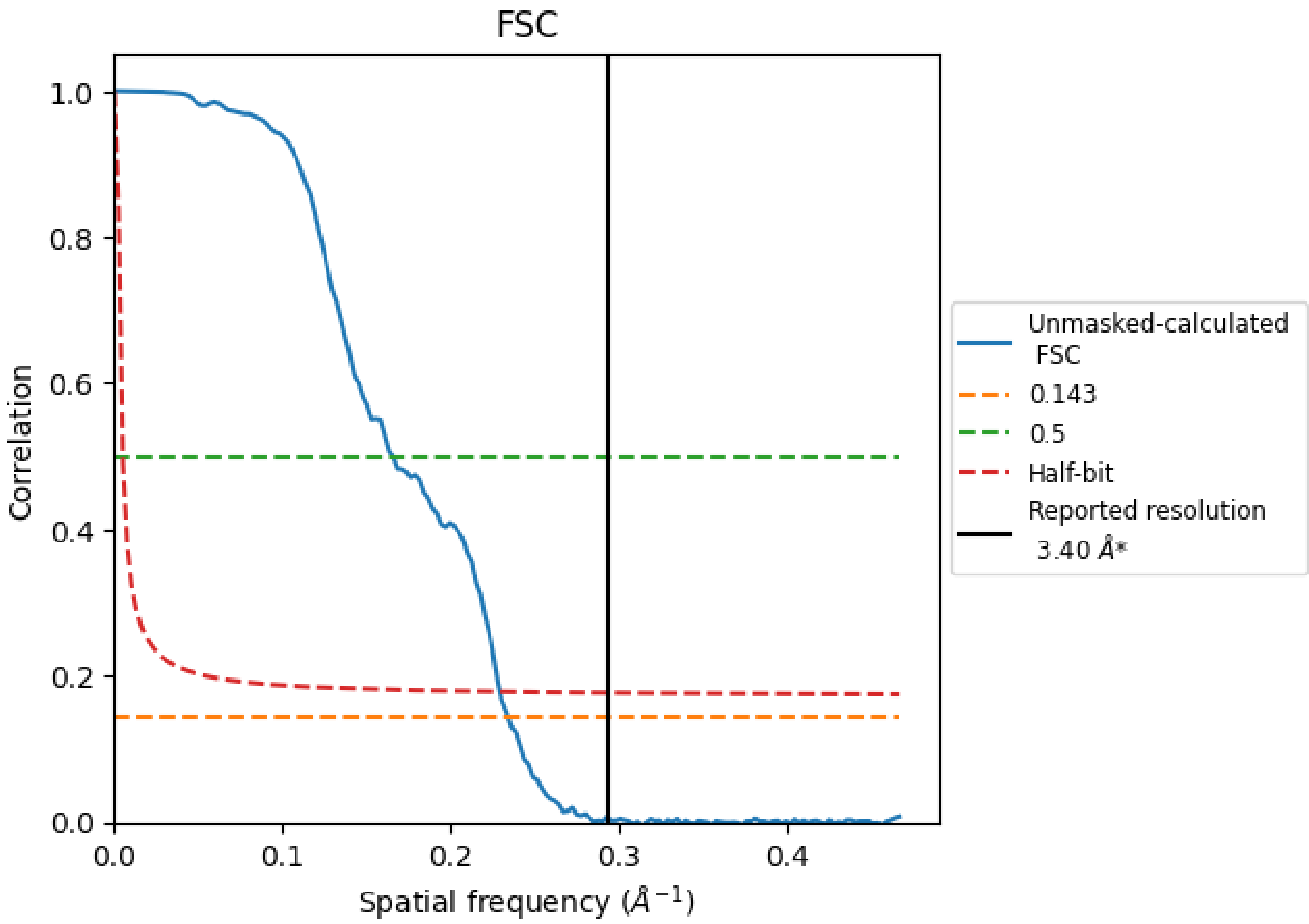


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates ⓘ

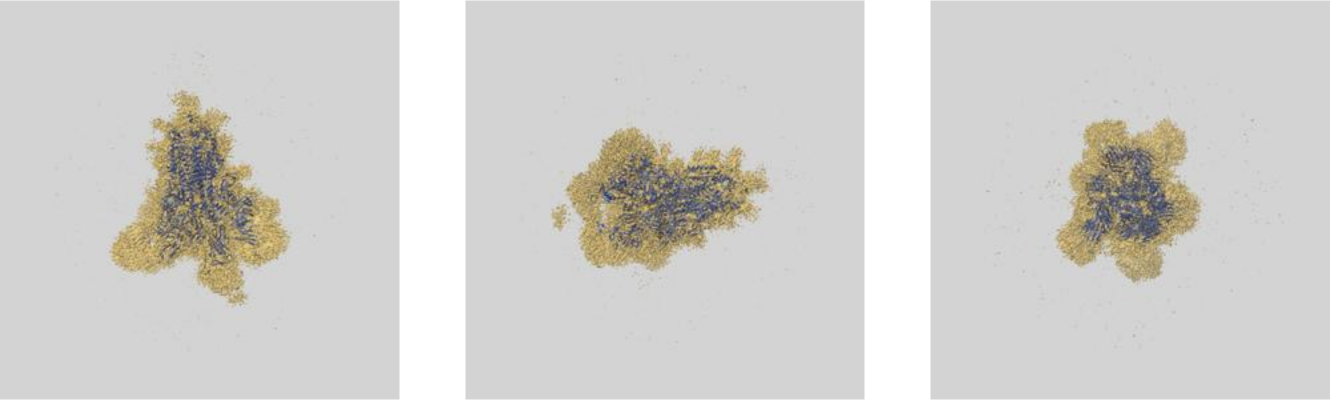
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.26	6.02	4.36

*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 4.26 differs from the reported value 3.4 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-38914 and PDB model 8Y4A. Per-residue inclusion information can be found in section 3 on page 14.

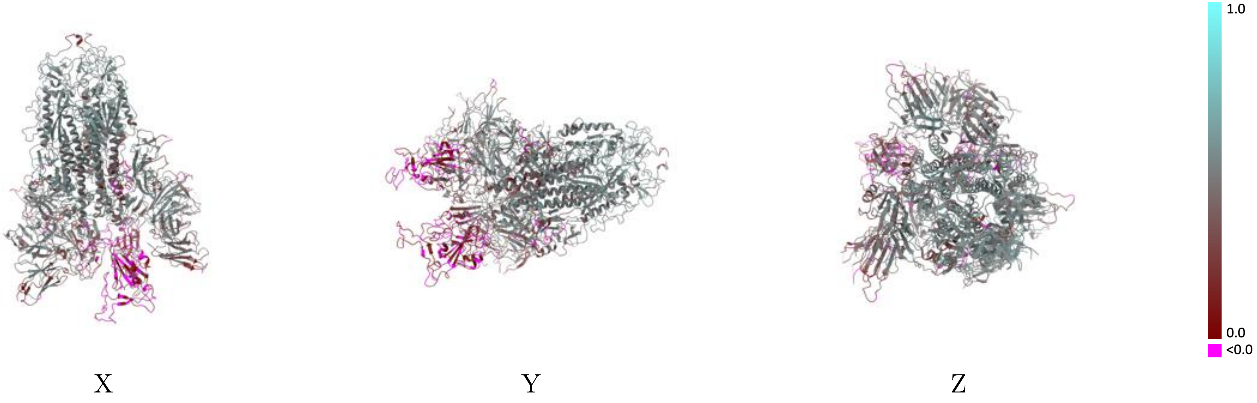
9.1 Map-model overlay (i)



X Y Z

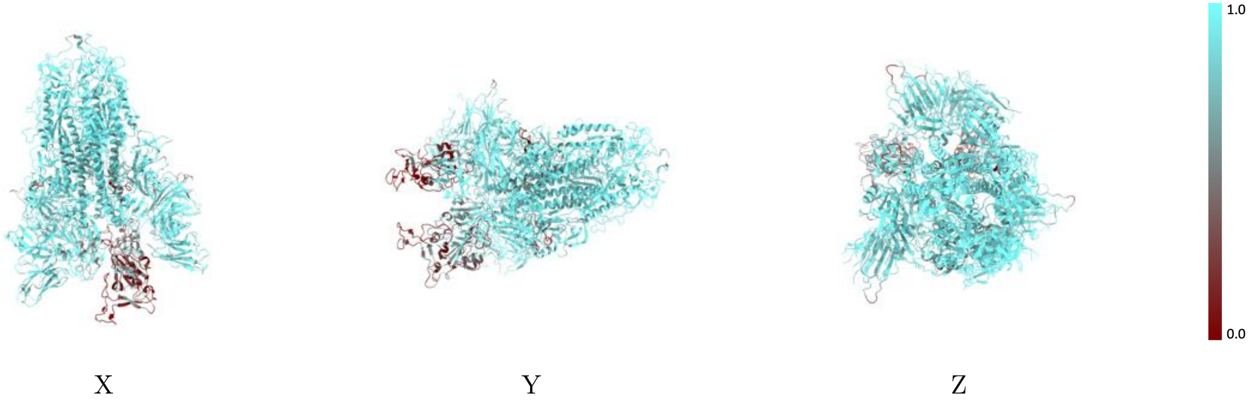
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



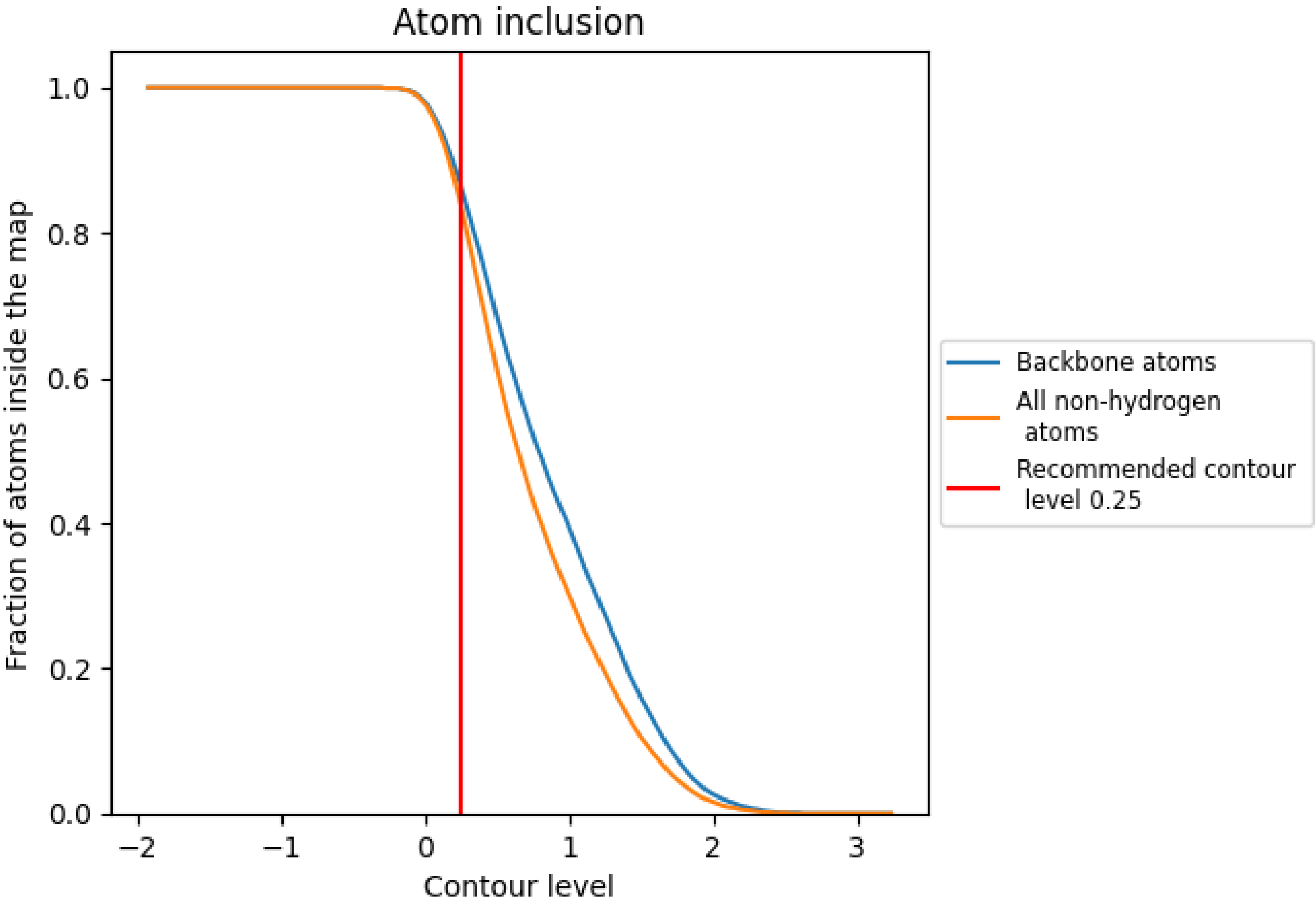
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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 (0.25).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.3970
A	0.7860	0.3820
B	0.7970	0.3670
C	0.8860	0.4270
D	0.9390	0.4760
E	0.8860	0.3670
F	0.9200	0.4010
G	0.9600	0.4260
H	0.9610	0.4880
I	0.9200	0.3620
J	0.7140	0.2940
K	0.3850	0.0360
L	0.8890	0.3890
M	0.8800	0.3470
N	0.9200	0.4340
O	0.9600	0.5110
P	0.8570	0.3900
Q	0.8210	0.4480
R	1.0000	0.4410
S	1.0000	0.4750
T	0.9200	0.4210
U	0.8570	0.4050