Full wwPDB EM Validation Report ⓘ

Aug 31, 2024 – 02:16 PM EDT

PDB ID	:	8UPX
EMDB ID	:	EMD-42456
Title	:	Omicron-S-MERS-RBD
Authors	:	Bu, F.; Li, F.; Liu, B.
Deposited on	:	2023-10-23
Resolution	:	3.40 Å(reported)
Based on initial model	:	7TGW

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:

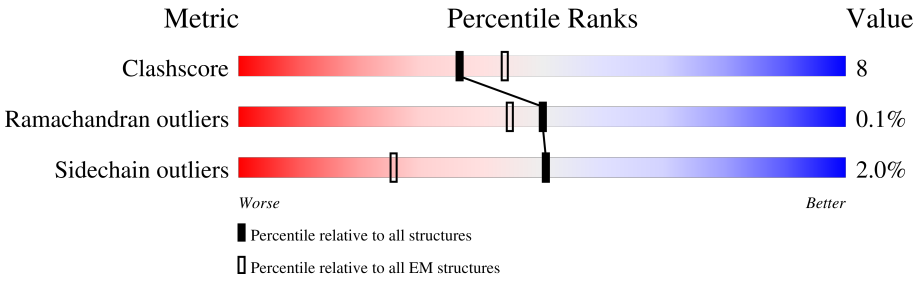
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.3

1 Overall quality at a glance (i)

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	1249	58% 14% 27%
1	B	1249	69% 18% 13%
1	C	1249	60% 12% 27%
2	D	2	100%
2	E	2	50% 50%
2	F	2	50% 50%
2	G	2	50% 50%
2	H	2	50% 50%

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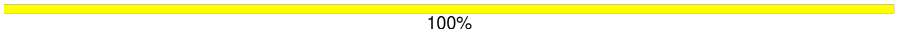
Mol	Chain	Length	Quality of chain
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23232 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,SARS-CoV-2 omicron spike with MERS RBD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	906	Total	C	N	O	S	2	0
			7082	4523	1180	1347	32		
1	B	1092	Total	C	N	O	S	2	0
			8530	5453	1408	1628	41		
1	C	906	Total	C	N	O	S	2	0
			7088	4529	1180	1347	32		

There are 201 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP A0A7T8KZF1
A	93	ILE	THR	conflict	UNP A0A7T8KZF1
A	140	ASP	GLY	conflict	UNP A0A7T8KZF1
A	?	-	VAL	deletion	UNP A0A7T8KZF1
A	?	-	TYR	deletion	UNP A0A7T8KZF1
A	?	-	ASN	deletion	UNP A0A7T8KZF1
A	206	ILE	LEU	conflict	UNP A0A7T8KZF1
A	209	GLU	-	insertion	UNP A0A7T8KZF1
A	210	PRO	-	insertion	UNP A0A7T8KZF1
A	211	GLU	-	insertion	UNP A0A7T8KZF1
A	328	GLN	-	linker	UNP A0A7T8KZF1
A	329	ALA	-	linker	UNP A0A7T8KZF1
A	330	GLU	-	linker	UNP A0A7T8KZF1
A	331	GLY	-	linker	UNP A0A7T8KZF1
A	332	VAL	-	linker	UNP A0A7T8KZF1
A	333	GLU	-	linker	UNP A0A7T8KZF1
A	334	CYS	-	linker	UNP A0A7T8KZF1
A	335	ASP	-	linker	UNP A0A7T8KZF1
A	336	PHE	-	linker	UNP A0A7T8KZF1
A	337	SER	-	linker	UNP A0A7T8KZF1
A	338	PRO	-	linker	UNP A0A7T8KZF1
A	339	LEU	-	linker	UNP A0A7T8KZF1
A	340	LEU	-	linker	UNP A0A7T8KZF1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	540	CYS	-	linker	UNP A0A0U2MMB6
A	541	GLY	-	linker	UNP A0A0U2MMB6
A	542	PRO	-	linker	UNP A0A0U2MMB6
A	543	LYS	-	linker	UNP A0A0U2MMB6
A	544	LYS	-	linker	UNP A0A0U2MMB6
A	545	SER	-	linker	UNP A0A0U2MMB6
A	546	THR	-	linker	UNP A0A0U2MMB6
A	547	ASN	-	linker	UNP A0A0U2MMB6
A	548	LEU	-	linker	UNP A0A0U2MMB6
A	549	VAL	-	linker	UNP A0A0U2MMB6
A	550	LYS	-	linker	UNP A0A0U2MMB6
A	551	ASN	-	linker	UNP A0A0U2MMB6
A	552	LYS	-	linker	UNP A0A0U2MMB6
A	562	LYS	THR	conflict	UNP A0A8B1J577
A	670	TYR	HIS	conflict	UNP A0A8B1J577
A	696	HIS	PRO	conflict	UNP A0A8B1J577
A	697	GLY	ARG	conflict	UNP A0A8B1J577
A	698	SER	ARG	conflict	UNP A0A8B1J577
A	700	SER	ARG	conflict	UNP A0A8B1J577
A	779	LYS	ASN	conflict	UNP A0A8B1J577
A	811	TYR	ASP	conflict	UNP A0A8B1J577
A	832	PRO	PHE	conflict	UNP A0A8B1J577
A	871	LYS	ASN	conflict	UNP A0A8B1J577
A	907	PRO	ALA	conflict	UNP A0A8B1J577
A	914	PRO	ALA	conflict	UNP A0A8B1J577
A	957	PRO	ALA	conflict	UNP A0A8B1J577
A	969	HIS	GLN	conflict	UNP A0A8B1J577
A	984	LYS	ASN	conflict	UNP A0A8B1J577
A	996	PHE	LEU	conflict	UNP A0A8B1J577
A	1001	PRO	LYS	conflict	UNP A0A8B1J577
A	1002	PRO	VAL	conflict	UNP A0A8B1J577
A	1227	GLY	-	linker	UNP A0A8B1J577
A	1228	SER	-	linker	UNP A0A8B1J577
A	1229	GLY	-	linker	UNP A0A8B1J577
A	1230	TYR	-	linker	UNP A0A8B1J577
A	1231	ILE	-	linker	UNP A0A8B1J577
A	1232	PRO	-	linker	UNP A0A8B1J577
A	1233	GLU	-	linker	UNP A0A8B1J577
A	1234	ALA	-	linker	UNP A0A8B1J577
A	1235	PRO	-	linker	UNP A0A8B1J577
A	1236	ARG	-	linker	UNP A0A8B1J577
A	1237	ASP	-	linker	UNP A0A8B1J577

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1238	GLY	-	linker	UNP A0A8B1J577
A	1239	GLN	-	linker	UNP A0A8B1J577
B	67	VAL	ALA	conflict	UNP A0A7T8KZF1
B	93	ILE	THR	conflict	UNP A0A7T8KZF1
B	140	ASP	GLY	conflict	UNP A0A7T8KZF1
B	?	-	VAL	deletion	UNP A0A7T8KZF1
B	?	-	TYR	deletion	UNP A0A7T8KZF1
B	?	-	ASN	deletion	UNP A0A7T8KZF1
B	206	ILE	LEU	conflict	UNP A0A7T8KZF1
B	209	GLU	-	insertion	UNP A0A7T8KZF1
B	210	PRO	-	insertion	UNP A0A7T8KZF1
B	211	GLU	-	insertion	UNP A0A7T8KZF1
B	328	GLN	-	linker	UNP A0A7T8KZF1
B	329	ALA	-	linker	UNP A0A7T8KZF1
B	330	GLU	-	linker	UNP A0A7T8KZF1
B	331	GLY	-	linker	UNP A0A7T8KZF1
B	332	VAL	-	linker	UNP A0A7T8KZF1
B	333	GLU	-	linker	UNP A0A7T8KZF1
B	334	CYS	-	linker	UNP A0A7T8KZF1
B	335	ASP	-	linker	UNP A0A7T8KZF1
B	336	PHE	-	linker	UNP A0A7T8KZF1
B	337	SER	-	linker	UNP A0A7T8KZF1
B	338	PRO	-	linker	UNP A0A7T8KZF1
B	339	LEU	-	linker	UNP A0A7T8KZF1
B	340	LEU	-	linker	UNP A0A7T8KZF1
B	540	CYS	-	linker	UNP A0A0U2MMB6
B	541	GLY	-	linker	UNP A0A0U2MMB6
B	542	PRO	-	linker	UNP A0A0U2MMB6
B	543	LYS	-	linker	UNP A0A0U2MMB6
B	544	LYS	-	linker	UNP A0A0U2MMB6
B	545	SER	-	linker	UNP A0A0U2MMB6
B	546	THR	-	linker	UNP A0A0U2MMB6
B	547	ASN	-	linker	UNP A0A0U2MMB6
B	548	LEU	-	linker	UNP A0A0U2MMB6
B	549	VAL	-	linker	UNP A0A0U2MMB6
B	550	LYS	-	linker	UNP A0A0U2MMB6
B	551	ASN	-	linker	UNP A0A0U2MMB6
B	552	LYS	-	linker	UNP A0A0U2MMB6
B	562	LYS	THR	conflict	UNP A0A8B1J577
B	670	TYR	HIS	conflict	UNP A0A8B1J577
B	696	HIS	PRO	conflict	UNP A0A8B1J577
B	697	GLY	ARG	conflict	UNP A0A8B1J577

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Chain	Residue	Modelled	Actual	Comment	Reference
B	698	SER	ARG	conflict	UNP A0A8B1J577
B	700	SER	ARG	conflict	UNP A0A8B1J577
B	779	LYS	ASN	conflict	UNP A0A8B1J577
B	811	TYR	ASP	conflict	UNP A0A8B1J577
B	832	PRO	PHE	conflict	UNP A0A8B1J577
B	871	LYS	ASN	conflict	UNP A0A8B1J577
B	907	PRO	ALA	conflict	UNP A0A8B1J577
B	914	PRO	ALA	conflict	UNP A0A8B1J577
B	957	PRO	ALA	conflict	UNP A0A8B1J577
B	969	HIS	GLN	conflict	UNP A0A8B1J577
B	984	LYS	ASN	conflict	UNP A0A8B1J577
B	996	PHE	LEU	conflict	UNP A0A8B1J577
B	1001	PRO	LYS	conflict	UNP A0A8B1J577
B	1002	PRO	VAL	conflict	UNP A0A8B1J577
B	1227	GLY	-	linker	UNP A0A8B1J577
B	1228	SER	-	linker	UNP A0A8B1J577
B	1229	GLY	-	linker	UNP A0A8B1J577
B	1230	TYR	-	linker	UNP A0A8B1J577
B	1231	ILE	-	linker	UNP A0A8B1J577
B	1232	PRO	-	linker	UNP A0A8B1J577
B	1233	GLU	-	linker	UNP A0A8B1J577
B	1234	ALA	-	linker	UNP A0A8B1J577
B	1235	PRO	-	linker	UNP A0A8B1J577
B	1236	ARG	-	linker	UNP A0A8B1J577
B	1237	ASP	-	linker	UNP A0A8B1J577
B	1238	GLY	-	linker	UNP A0A8B1J577
B	1239	GLN	-	linker	UNP A0A8B1J577
C	67	VAL	ALA	conflict	UNP A0A7T8KZF1
C	93	ILE	THR	conflict	UNP A0A7T8KZF1
C	140	ASP	GLY	conflict	UNP A0A7T8KZF1
C	?	-	VAL	deletion	UNP A0A7T8KZF1
C	?	-	TYR	deletion	UNP A0A7T8KZF1
C	?	-	ASN	deletion	UNP A0A7T8KZF1
C	206	ILE	LEU	conflict	UNP A0A7T8KZF1
C	209	GLU	-	insertion	UNP A0A7T8KZF1
C	210	PRO	-	insertion	UNP A0A7T8KZF1
C	211	GLU	-	insertion	UNP A0A7T8KZF1
C	328	GLN	-	linker	UNP A0A7T8KZF1
C	329	ALA	-	linker	UNP A0A7T8KZF1
C	330	GLU	-	linker	UNP A0A7T8KZF1
C	331	GLY	-	linker	UNP A0A7T8KZF1
C	332	VAL	-	linker	UNP A0A7T8KZF1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	333	GLU	-	linker	UNP A0A7T8KZF1
C	334	CYS	-	linker	UNP A0A7T8KZF1
C	335	ASP	-	linker	UNP A0A7T8KZF1
C	336	PHE	-	linker	UNP A0A7T8KZF1
C	337	SER	-	linker	UNP A0A7T8KZF1
C	338	PRO	-	linker	UNP A0A7T8KZF1
C	339	LEU	-	linker	UNP A0A7T8KZF1
C	340	LEU	-	linker	UNP A0A7T8KZF1
C	540	CYS	-	linker	UNP A0A0U2MMB6
C	541	GLY	-	linker	UNP A0A0U2MMB6
C	542	PRO	-	linker	UNP A0A0U2MMB6
C	543	LYS	-	linker	UNP A0A0U2MMB6
C	544	LYS	-	linker	UNP A0A0U2MMB6
C	545	SER	-	linker	UNP A0A0U2MMB6
C	546	THR	-	linker	UNP A0A0U2MMB6
C	547	ASN	-	linker	UNP A0A0U2MMB6
C	548	LEU	-	linker	UNP A0A0U2MMB6
C	549	VAL	-	linker	UNP A0A0U2MMB6
C	550	LYS	-	linker	UNP A0A0U2MMB6
C	551	ASN	-	linker	UNP A0A0U2MMB6
C	552	LYS	-	linker	UNP A0A0U2MMB6
C	562	LYS	THR	conflict	UNP A0A8B1J577
C	670	TYR	HIS	conflict	UNP A0A8B1J577
C	696	HIS	PRO	conflict	UNP A0A8B1J577
C	697	GLY	ARG	conflict	UNP A0A8B1J577
C	698	SER	ARG	conflict	UNP A0A8B1J577
C	700	SER	ARG	conflict	UNP A0A8B1J577
C	779	LYS	ASN	conflict	UNP A0A8B1J577
C	811	TYR	ASP	conflict	UNP A0A8B1J577
C	832	PRO	PHE	conflict	UNP A0A8B1J577
C	871	LYS	ASN	conflict	UNP A0A8B1J577
C	907	PRO	ALA	conflict	UNP A0A8B1J577
C	914	PRO	ALA	conflict	UNP A0A8B1J577
C	957	PRO	ALA	conflict	UNP A0A8B1J577
C	969	HIS	GLN	conflict	UNP A0A8B1J577
C	984	LYS	ASN	conflict	UNP A0A8B1J577
C	996	PHE	LEU	conflict	UNP A0A8B1J577
C	1001	PRO	LYS	conflict	UNP A0A8B1J577
C	1002	PRO	VAL	conflict	UNP A0A8B1J577
C	1227	GLY	-	linker	UNP A0A8B1J577
C	1228	SER	-	linker	UNP A0A8B1J577
C	1229	GLY	-	linker	UNP A0A8B1J577

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1230	TYR	-	linker	UNP A0A8B1J577
C	1231	ILE	-	linker	UNP A0A8B1J577
C	1232	PRO	-	linker	UNP A0A8B1J577
C	1233	GLU	-	linker	UNP A0A8B1J577
C	1234	ALA	-	linker	UNP A0A8B1J577
C	1235	PRO	-	linker	UNP A0A8B1J577
C	1236	ARG	-	linker	UNP A0A8B1J577
C	1237	ASP	-	linker	UNP A0A8B1J577
C	1238	GLY	-	linker	UNP A0A8B1J577
C	1239	GLN	-	linker	UNP A0A8B1J577

- 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		

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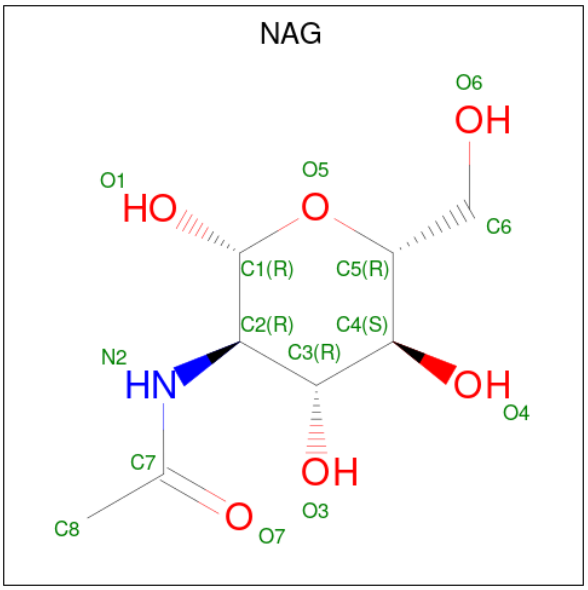
Mol	Chain	Residues	Atoms				AltConf	Trace
2	O	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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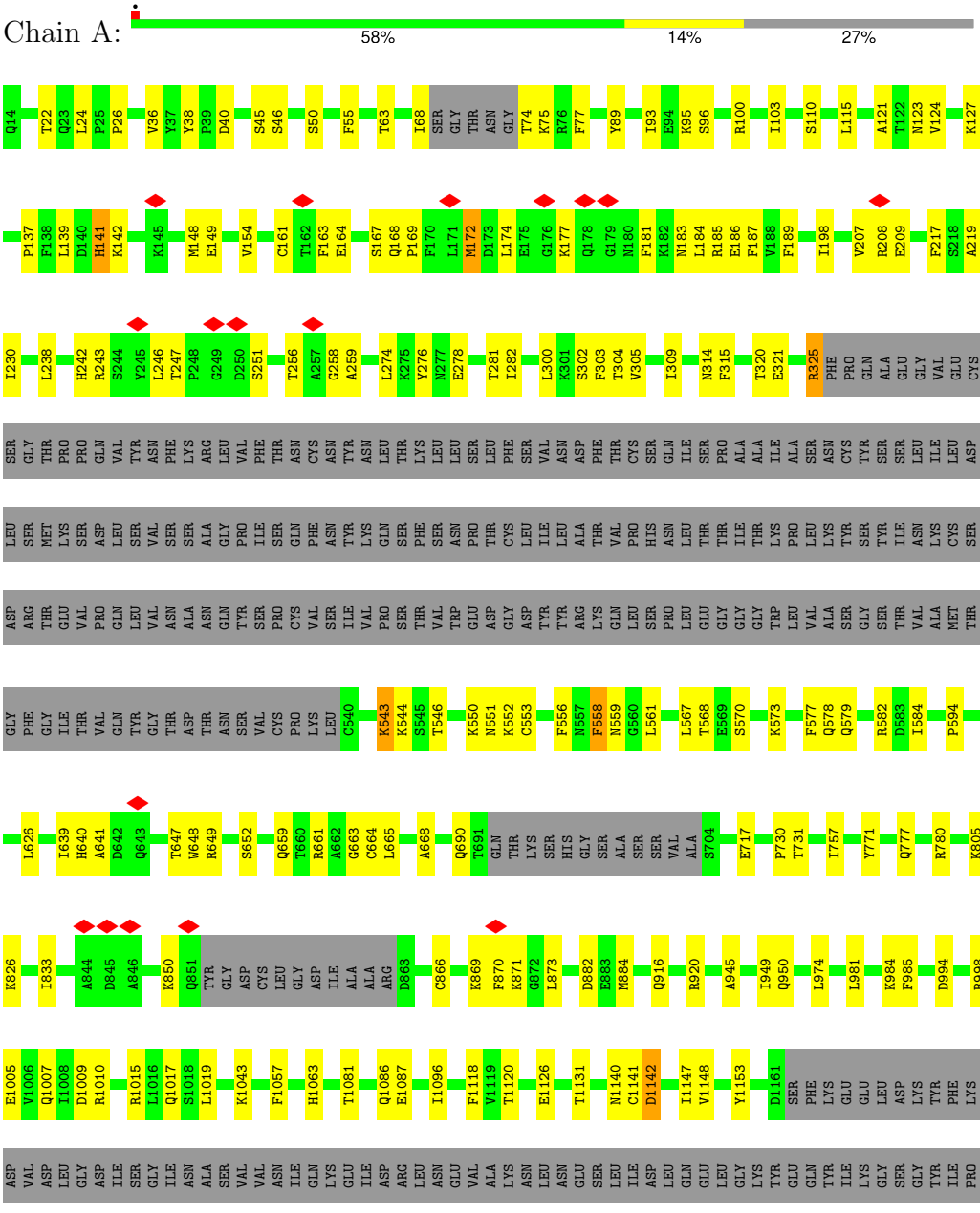
Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

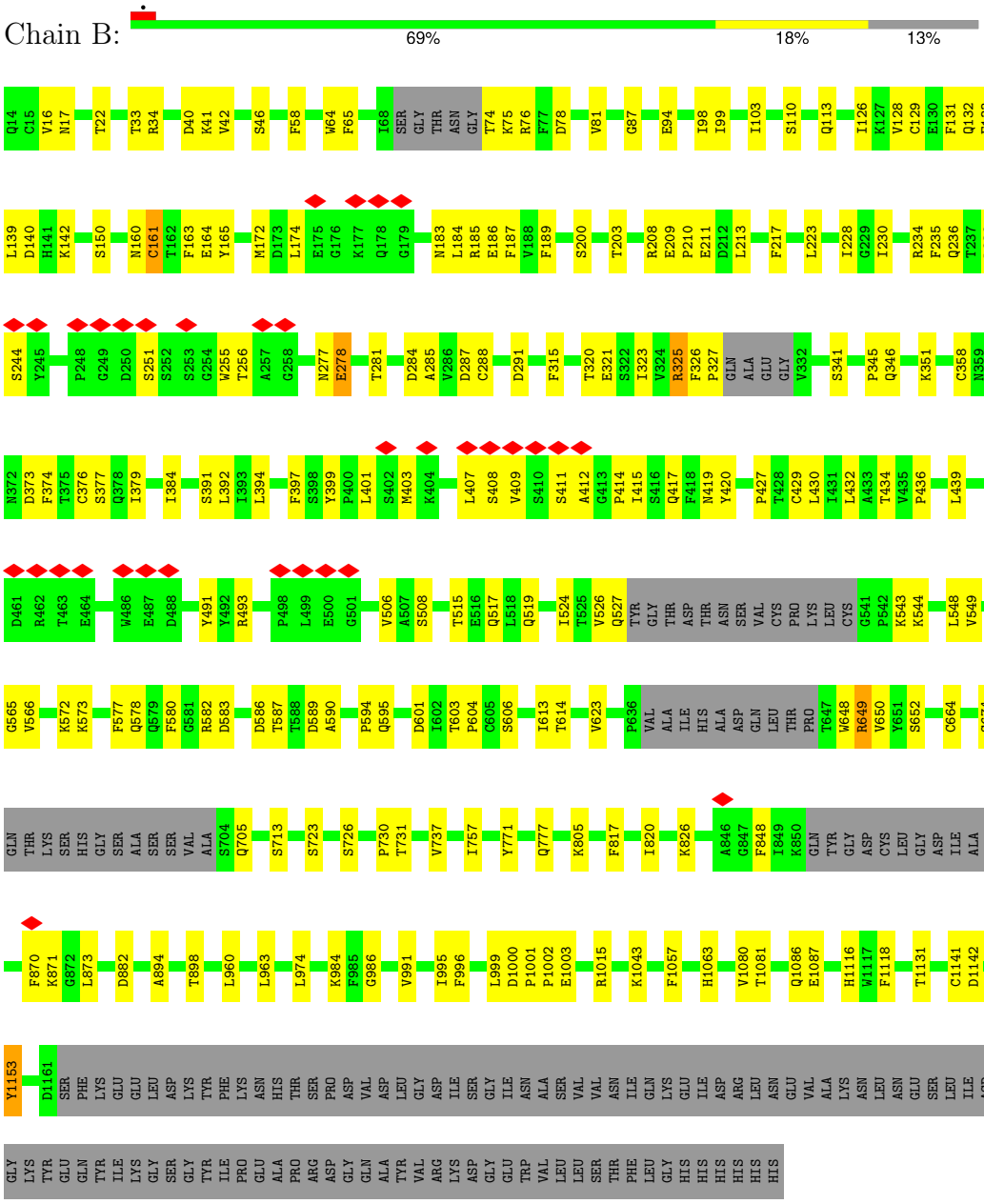
- Molecule 1: Spike glycoprotein,SARS-CoV-2 omicron spike with MERS RBD

Chain A:



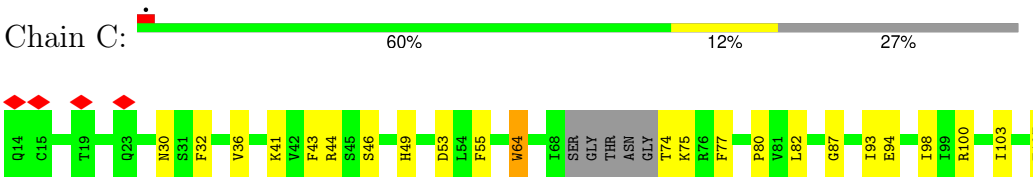
• Molecule 1: Spike glycoprotein,SARS-CoV-2 omicron spike with MERS RBD

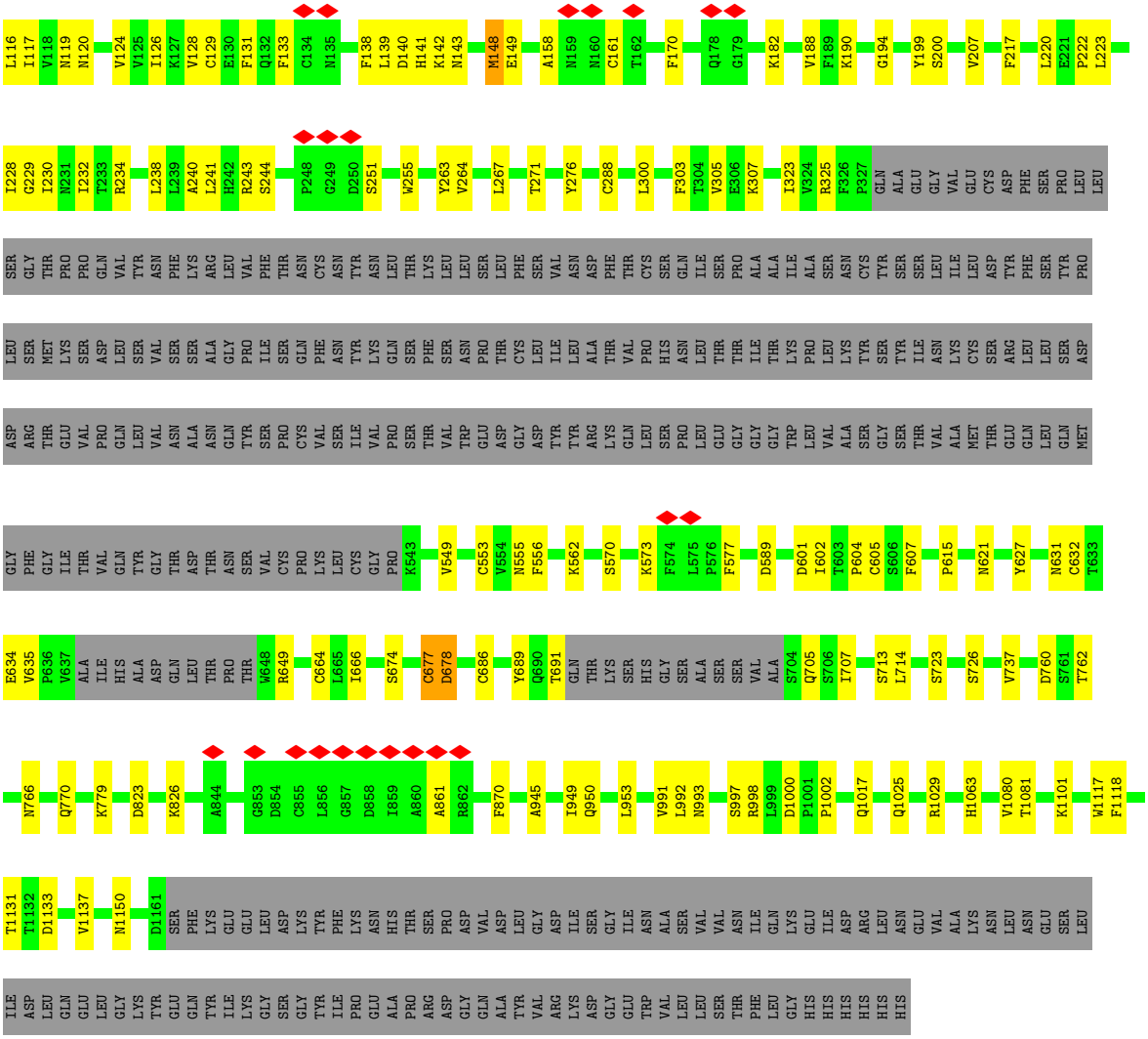
Chain B:



• Molecule 1: Spike glycoprotein,SARS-CoV-2 omicron spike with MERS RBD

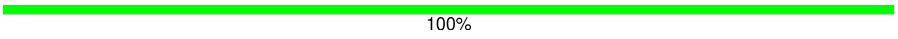
Chain C:





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

Chain D:



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

Chain E:

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

Chain F:

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

Chain G:

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

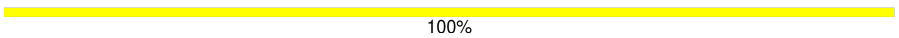
Chain H:

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

Chain I:

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

Chain J:



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

Chain K:

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

Chain L:

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

Chain M:

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

Chain N:

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

Chain O:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	192374	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.955	Depositor
Minimum map value	-0.406	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.103	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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

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	0.26	0/7249	0.50	2/9863 (0.0%)
1	B	0.27	0/8733	0.50	2/11886 (0.0%)
1	C	0.26	0/7255	0.50	0/9868
All	All	0.26	0/23237	0.50	4/31617 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	CYS	CA-CB-SG	6.28	125.30	114.00
1	B	594	PRO	N-CD-CG	-6.09	94.06	103.20
1	A	1142	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	55	PHE	C-N-CA	5.10	134.46	121.70

There are no chirality outliers.

There are no planarity outliers.

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	7082	0	6975	115	0
1	B	8530	0	8389	153	0
1	C	7088	0	6973	93	0
2	D	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	1	0
2	L	28	0	25	3	0
2	M	28	0	25	0	0
2	N	28	0	25	2	0
2	O	28	0	25	1	0
3	A	56	0	52	1	0
3	B	84	0	78	2	0
3	C	56	0	52	0	0
All	All	23232	0	22819	346	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 8.

All (346) 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:631:ASN:HB3	1:C:634:GLU:HG2	1.60	0.84
1:B:453:LYS:HB3	1:B:508:SER:HB3	1.62	0.79
1:B:986:GLY:H	1:C:770:GLN:HE22	1.34	0.76
1:C:634:GLU:HG3	1:C:635:VAL:HG22	1.70	0.74
1:A:314:ASN:HA	1:A:609:GLY:HA2	1.73	0.71
1:A:142:LYS:HD2	1:A:242:HIS:HA	1.73	0.71
1:B:392:LEU:HD11	1:B:524:ILE:HD11	1.73	0.71
1:B:580:PHE:HE2	1:B:582:ARG:HH21	1.39	0.70
1:B:315:PHE:HA	1:B:648:TRP:HB3	1.71	0.70
1:A:819:GLN:NE2	1:A:950:GLN:OE1	2.25	0.70
1:C:1131:THR:HG23	1:C:1133:ASP:H	1.55	0.69
1:B:548:LEU:HD11	1:B:558:PHE:HE2	1.59	0.67
1:A:1118:PHE:HZ	2:G:1:NAG:H62	1.59	0.67
1:A:302:SER:OG	1:A:304:THR:O	2.12	0.67
1:C:194:GLY:HA2	1:C:229:GLY:HA2	1.75	0.67
1:B:140:ASP:HB3	1:B:142:LYS:HE3	1.76	0.66
1:A:999:LEU:HD11	1:A:1003:GLU:HB2	1.76	0.66
1:A:1141:CYS:HB2	1:A:1147:ILE:HG12	1.77	0.65
1:C:46:SER:HA	1:C:276:TYR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:HB2	1:A:256:THR:HB	1.79	0.64
1:B:582:ARG:NH1	1:B:586:ASP:OD1	2.31	0.64
1:A:665:LEU:HD21	1:A:668:ALA:HB3	1.78	0.64
1:B:129:CYS:HA	1:B:161:CYS:HB3	1.78	0.64
1:B:412:ALA:O	1:B:417:GLN:NE2	2.29	0.64
1:B:113:GLN:HE21	1:B:128:VAL:HG12	1.61	0.64
1:B:553:CYS:HB3	1:B:566:VAL:HB	1.80	0.64
1:C:1063:HIS:HA	1:C:1081:THR:HG22	1.79	0.64
1:A:757:ILE:O	1:A:1015:ARG:NH1	2.32	0.63
1:B:650:VAL:HG12	1:B:652:SER:H	1.63	0.63
1:A:325:ARG:NH1	1:A:546:THR:O	2.32	0.63
1:B:94:GLU:O	1:B:183:ASN:HB2	2.00	0.62
1:B:777:GLN:N	1:B:777:GLN:OE1	2.32	0.61
1:A:1131:THR:HG22	1:A:1153:TYR:HB3	1.82	0.61
1:B:1063:HIS:HA	1:B:1081:THR:HG22	1.83	0.60
1:C:138:PHE:HE2	1:C:241:LEU:HD11	1.66	0.60
1:A:129:CYS:HA	1:A:161:CYS:HB3	1.84	0.60
1:A:103:ILE:HG23	1:A:238:LEU:HD11	1.84	0.60
1:B:583:ASP:OD1	1:B:587:THR:N	2.31	0.60
1:A:95:LYS:HB3	1:A:177:LYS:HB3	1.82	0.60
1:A:1017:GLN:NE2	1:C:1017:GLN:OE1	2.34	0.60
1:A:661:ARG:HH12	1:B:848:PHE:H	1.50	0.59
1:A:1096:ILE:HD13	1:A:1148:VAL:HG23	1.83	0.59
1:C:120:ASN:ND2	1:C:149:GLU:OE1	2.34	0.59
1:B:415:ILE:HA	1:B:419:ASN:HB2	1.84	0.59
1:A:172:MET:HG2	1:A:174:LEU:HD22	1.85	0.59
1:C:74:THR:OG1	1:C:75:LYS:N	2.35	0.58
1:C:243:ARG:NH2	1:C:251:SER:OG	2.36	0.58
1:A:1003:GLU:OE1	1:A:1003:GLU:N	2.36	0.58
1:B:391:SER:HB2	1:B:527:GLN:HB3	1.85	0.58
1:A:224:VAL:HG13	1:A:226:LEU:HD13	1.86	0.57
1:A:639:ILE:HG23	1:A:640:HIS:H	1.70	0.57
1:A:649:ARG:HA	1:A:652:SER:HB3	1.86	0.57
1:B:649:ARG:HE	1:B:650:VAL:CG2	2.18	0.57
1:B:986:GLY:H	1:C:770:GLN:NE2	2.03	0.57
1:C:1118:PHE:HZ	2:N:1:NAG:H62	1.70	0.57
1:B:379:ILE:HB	1:B:427:PRO:HB3	1.86	0.57
1:C:1025:GLN:OE1	1:C:1029:ARG:NH1	2.37	0.57
1:B:74:THR:OG1	1:B:75:LYS:N	2.37	0.57
1:A:647:THR:HG22	1:A:649:ARG:HH21	1.69	0.56
1:B:1118:PHE:HZ	2:K:1:NAG:H62	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ALA:HA	1:B:601:ASP:HA	1.86	0.56
1:A:850:LYS:HD2	1:A:869:LYS:HD3	1.86	0.56
1:B:1149:ASN:OD1	2:L:1:NAG:N2	2.39	0.56
1:B:142:LYS:HB2	1:B:150:SER:HB2	1.88	0.56
1:C:139:LEU:HD13	1:C:149:GLU:HG3	1.88	0.56
1:A:172:MET:SD	1:A:172:MET:N	2.78	0.55
1:B:325:ARG:HD3	1:B:548:LEU:HD13	1.88	0.55
1:A:659:GLN:NE2	1:A:663:GLY:O	2.40	0.55
2:O:2:NAG:H83	2:O:2:NAG:H3	1.88	0.55
2:H:2:NAG:H3	2:H:2:NAG:H83	1.89	0.55
1:A:777:GLN:OE1	1:A:780:ARG:NH2	2.40	0.55
1:A:1120:THR:HG23	1:A:1126:GLU:H	1.70	0.55
1:A:110:SER:HB2	1:A:132:GLN:HB2	1.88	0.55
1:C:762:THR:O	1:C:766:ASN:ND2	2.39	0.55
1:B:368:LEU:HB3	1:B:439:LEU:HD11	1.89	0.55
1:C:117:ILE:HG13	1:C:126:ILE:HG23	1.89	0.55
1:C:691:THR:HA	1:C:705:GLN:HA	1.89	0.55
1:A:243:ARG:NH2	1:A:251:SER:O	2.40	0.54
1:B:208:ARG:NH1	1:B:209:GLU:O	2.41	0.54
1:B:757:ILE:O	1:B:1015:ARG:NH1	2.40	0.54
1:B:403:MET:N	1:B:403:MET:SD	2.81	0.54
2:L:2:NAG:H83	2:L:2:NAG:H3	1.88	0.54
1:A:247:THR:O	1:A:247:THR:OG1	2.26	0.54
1:B:242:HIS:CE1	1:B:244:SER:HB3	2.43	0.54
1:B:376:CYS:HB3	1:B:379:ILE:HG23	1.90	0.54
1:A:38:TYR:HE1	1:A:219:ALA:HB1	1.72	0.53
1:A:89:TYR:OH	1:A:186:GLU:OE1	2.26	0.53
1:B:691:THR:HA	1:B:705:GLN:HA	1.90	0.53
1:B:94:GLU:OE2	1:B:98:ILE:N	2.41	0.53
1:B:399:TYR:OH	1:B:403:MET:O	2.25	0.53
1:C:46:SER:CA	1:C:276:TYR:O	2.57	0.53
1:B:578:GLN:HA	1:C:41:LYS:HZ2	1.73	0.53
1:A:1063:HIS:HA	1:A:1081:THR:HG22	1.90	0.53
1:B:126:ILE:HD13	1:B:165:TYR:HD2	1.74	0.53
1:A:578:GLN:NE2	1:B:40:ASP:O	2.42	0.53
1:A:121:ALA:HB2	1:A:149:GLU:HB3	1.89	0.53
1:A:207:VAL:HG13	1:A:208:ARG:H	1.74	0.53
1:B:185:ARG:HB3	1:B:187:PHE:CZ	2.44	0.53
1:C:140:ASP:OD2	1:C:142:LYS:NZ	2.41	0.53
1:A:242:HIS:HE2	1:A:258:GLY:HA3	1.74	0.53
1:B:139:LEU:HG	1:B:239:LEU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PHE:HB2	1:A:207:VAL:HG11	1.90	0.52
1:B:321:GLU:HG2	1:B:554:VAL:HG11	1.90	0.52
1:A:167:SER:OG	1:A:168:GLN:N	2.42	0.52
1:B:110:SER:HB3	1:B:132:GLN:HB2	1.92	0.52
1:B:291:ASP:OD1	1:B:291:ASP:N	2.43	0.52
1:B:1141:CYS:HB2	1:B:1147:ILE:HD13	1.92	0.52
1:B:33:THR:HG22	1:B:58:PHE:HE2	1.74	0.52
1:B:730:PRO:HA	1:B:1087:GLU:HA	1.92	0.52
1:B:164:GLU:OE1	1:B:164:GLU:N	2.42	0.52
1:A:242:HIS:O	1:A:256:THR:N	2.36	0.52
1:C:93:ILE:HG12	1:C:263:TYR:HE1	1.75	0.52
1:B:128:VAL:HB	1:B:163:PHE:HB3	1.93	0.52
1:B:366:LEU:HD12	1:B:371:VAL:HG22	1.91	0.52
1:B:817:PHE:HD1	1:B:820:ILE:HD11	1.74	0.52
1:A:320:THR:OG1	1:A:321:GLU:N	2.43	0.51
1:B:22:THR:O	1:B:76:ARG:NH1	2.43	0.51
1:B:34:ARG:NH1	1:B:186:GLU:OE2	2.43	0.51
1:B:320:THR:OG1	1:B:321:GLU:OE1	2.28	0.51
1:A:985:PHE:HA	1:B:771:TYR:HE1	1.75	0.51
1:B:213:LEU:HD23	1:B:213:LEU:H	1.76	0.51
1:B:326:PHE:CB	1:B:543:LYS:HD2	2.40	0.51
1:C:108:LEU:HB3	1:C:133:PHE:HB2	1.91	0.51
1:A:228:ILE:HD12	1:A:230:ILE:HG12	1.92	0.51
1:A:582:ARG:HG3	1:B:42:VAL:HG11	1.92	0.51
1:A:771:TYR:OH	1:A:1009:ASP:OD1	2.26	0.51
1:C:100:ARG:NH2	1:C:119:ASN:O	2.44	0.51
1:C:271:THR:HG23	1:C:288:CYS:HB3	1.91	0.51
1:B:867:ALA:HA	1:B:870:PHE:CZ	2.45	0.51
1:B:565:GLY:HA2	1:B:604:PRO:HA	1.93	0.50
1:C:300:LEU:HD22	1:C:305:VAL:HG12	1.93	0.50
1:B:326:PHE:HB2	1:B:543:LYS:HD2	1.93	0.50
1:B:582:ARG:HG3	1:B:583:ASP:H	1.77	0.50
1:C:36:VAL:HG11	1:C:217:PHE:CZ	2.46	0.50
1:C:128:VAL:HG11	1:C:228:ILE:HG23	1.94	0.50
1:A:167:SER:OG	1:A:168:GLN:OE1	2.29	0.50
1:A:315:PHE:HB2	1:A:639:ILE:HG13	1.93	0.50
1:A:945:ALA:O	1:A:949:ILE:HG22	2.12	0.50
1:A:320:THR:OG1	1:A:552:LYS:NZ	2.44	0.50
1:B:103:ILE:HG12	1:B:236:GLN:HB3	1.94	0.50
1:C:100:ARG:O	1:C:119:ASN:HB3	2.11	0.50
1:A:22:THR:HB	1:A:24:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:TYR:HB2	1:B:493:ARG:NH1	2.26	0.50
1:B:894:ALA:O	1:B:898:THR:OG1	2.22	0.50
1:C:200:SER:HB3	1:C:223:LEU:HD22	1.94	0.50
1:B:392:LEU:CD1	1:B:524:ILE:HD11	2.42	0.50
1:B:434:THR:HG23	1:B:519:GLN:HG2	1.94	0.50
1:B:649:ARG:HE	1:B:650:VAL:HG22	1.77	0.50
1:A:274:LEU:HD22	1:A:282:ILE:HD13	1.94	0.49
1:B:209:GLU:HG3	1:B:211:GLU:HG2	1.94	0.49
1:B:64:TRP:HD1	1:B:65:PHE:N	2.10	0.49
1:C:124:VAL:HG23	1:C:170:PHE:CZ	2.47	0.49
1:A:884:MET:HB3	1:C:714:LEU:HD21	1.95	0.49
1:B:407:LEU:HG	1:B:430:LEU:HD23	1.94	0.49
1:C:107:THR:HG21	1:C:111:LYS:HB3	1.94	0.49
1:A:984:LYS:HA	1:A:984:LYS:HD3	1.65	0.49
1:B:172:MET:SD	1:B:174:LEU:HB2	2.53	0.49
1:A:730:PRO:HA	1:A:1087:GLU:HA	1.94	0.49
1:B:17:ASN:OD1	1:B:135:ASN:ND2	2.45	0.49
1:B:999:LEU:HD13	1:B:1003:GLU:HG2	1.95	0.49
1:C:138:PHE:CE2	1:C:241:LEU:HD11	2.48	0.49
1:B:614:THR:HB	1:B:623:VAL:HG12	1.95	0.48
1:A:659:GLN:NE2	3:A:1301:NAG:H82	2.28	0.48
1:A:717:GLU:OE2	1:B:805:LYS:NZ	2.35	0.48
1:B:94:GLU:OE2	1:B:99:ILE:N	2.34	0.48
1:A:183:ASN:HB3	1:A:185:ARG:HE	1.77	0.48
1:B:323:ILE:HD11	1:B:549:VAL:O	2.14	0.48
1:A:100:ARG:HG3	1:A:139:LEU:HD13	1.96	0.48
1:A:26:PRO:HB3	1:A:63:THR:HG23	1.95	0.48
1:C:148:MET:SD	1:C:148:MET:N	2.87	0.48
1:A:129:CYS:HB2	1:A:131:PHE:CE2	2.49	0.48
1:A:543:LYS:HD3	1:A:544:LYS:HB2	1.94	0.48
1:A:604:PRO:HG3	1:B:870:PHE:HB3	1.95	0.48
1:B:723:SER:HB3	1:B:726:SER:HB3	1.96	0.48
1:A:74:THR:OG1	1:A:75:LYS:N	2.48	0.47
1:C:553:CYS:HB3	1:C:605:CYS:HB3	1.75	0.47
1:A:1000:ASP:OD1	1:A:1000:ASP:N	2.43	0.47
1:B:737:VAL:HG22	1:B:1080:VAL:HG22	1.96	0.47
1:B:373:ASP:HB2	1:B:432:LEU:HD13	1.95	0.47
1:B:674:SER:HB3	1:B:713:SER:HB3	1.95	0.47
1:C:555:ASN:HB3	1:C:562:LYS:HZ1	1.78	0.47
1:A:805:LYS:HE3	1:A:805:LYS:HB3	1.73	0.47
1:B:287:ASP:OD1	1:B:288:CYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB2	1:B:409:VAL:HG21	1.97	0.47
1:C:44:ARG:HH12	1:C:49:HIS:CG	2.32	0.47
1:C:82:LEU:HD23	1:C:264:VAL:HG11	1.97	0.47
1:B:129:CYS:HA	1:B:161:CYS:CB	2.43	0.47
1:B:826:LYS:HB3	1:B:826:LYS:HE3	1.78	0.47
1:C:103:ILE:HG23	1:C:116:LEU:HG	1.97	0.47
1:C:634:GLU:HG3	1:C:635:VAL:N	2.30	0.47
1:A:552:LYS:NZ	1:A:553:CYS:O	2.48	0.47
1:B:81:VAL:HG11	1:B:234:ARG:NH2	2.30	0.47
1:C:677:CYS:HB2	1:C:686:CYS:HB2	1.60	0.47
1:C:945:ALA:O	1:C:949:ILE:HG22	2.14	0.47
1:A:46:SER:HA	1:A:276:TYR:O	2.15	0.46
1:B:345:PRO:HG3	1:B:351:LYS:HG3	1.97	0.46
1:B:873:LEU:HD13	1:B:974:LEU:HD22	1.97	0.46
1:B:991:VAL:O	1:B:995:ILE:HG12	2.15	0.46
1:B:242:HIS:O	1:B:256:THR:N	2.43	0.46
1:C:44:ARG:HH12	1:C:49:HIS:CE1	2.33	0.46
1:C:627:TYR:HE2	1:C:666:ILE:HD12	1.80	0.46
1:C:723:SER:HB3	1:C:726:SER:HB3	1.96	0.46
1:C:108:LEU:HD21	1:C:234:ARG:HD2	1.95	0.46
1:B:1131:THR:HG22	1:B:1153:TYR:HB3	1.97	0.46
1:B:566:VAL:N	1:B:603:THR:O	2.35	0.46
1:C:1117:TRP:HB2	1:C:1150:ASN:ND2	2.30	0.46
1:A:207:VAL:HG22	1:A:209:GLU:H	1.81	0.46
1:A:1043:LYS:NZ	1:A:1057:PHE:O	2.48	0.46
1:B:228:ILE:HG22	1:B:230:ILE:HG23	1.98	0.46
1:A:994:ASP:HB3	1:A:998:ARG:HH22	1.81	0.45
1:B:415:ILE:O	1:B:420:TYR:N	2.37	0.45
1:A:123:ASN:HB3	1:A:169:PRO:HA	1.99	0.45
1:B:1001:PRO:N	1:B:1002:PRO:HD2	2.31	0.45
1:A:300:LEU:HD12	1:A:305:VAL:HG12	1.97	0.45
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.45
1:A:96:SER:OG	1:A:96:SER:O	2.33	0.45
1:B:139:LEU:HD11	1:B:238:LEU:HB3	1.99	0.45
1:B:243:ARG:HH12	1:B:251:SER:HA	1.81	0.45
1:B:1000:ASP:OD1	1:B:1002:PRO:HD2	2.17	0.45
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.52	0.45
1:B:1043:LYS:NZ	1:B:1057:PHE:O	2.49	0.45
1:C:124:VAL:HG23	1:C:170:PHE:CE2	2.52	0.45
1:C:141:HIS:HB2	1:C:240:ALA:HB1	1.98	0.45
1:C:87:GLY:HA3	1:C:267:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLU:CD	1:C:98:ILE:H	2.20	0.45
1:C:129:CYS:HB2	1:C:131:PHE:CE2	2.52	0.45
1:A:731:THR:N	1:A:1086:GLN:O	2.39	0.45
1:A:871:LYS:HD3	1:A:981:LEU:HD12	1.98	0.45
3:B:1303:NAG:H3	3:B:1303:NAG:H83	1.99	0.45
1:C:307:LYS:HG3	1:C:615:PRO:HA	1.99	0.45
1:B:543:LYS:HG2	1:B:544:LYS:H	1.82	0.45
1:C:1101:LYS:HD2	1:C:1137:VAL:HG11	1.97	0.45
1:B:138:PHE:O	1:B:139:LEU:HD13	2.17	0.45
1:C:678:ASP:OD1	1:C:678:ASP:N	2.50	0.45
1:A:68:ILE:HD13	1:A:259:ALA:HA	1.99	0.45
1:A:1001:PRO:N	1:A:1002:PRO:HD2	2.32	0.45
1:B:392:LEU:HD13	1:B:526:VAL:HG12	1.99	0.45
1:A:137:PRO:HB3	1:A:154:VAL:HA	1.98	0.44
1:C:689:TYR:HB2	1:C:707:ILE:HD13	2.00	0.44
1:B:129:CYS:CA	1:B:161:CYS:HB3	2.45	0.44
1:B:129:CYS:HB2	1:B:131:PHE:CE2	2.52	0.44
1:B:613:ILE:HG23	1:B:679:ILE:HG21	1.98	0.44
1:C:190:LYS:HE3	1:C:199:TYR:CE1	2.53	0.44
1:B:603:THR:HG23	1:C:870:PHE:CZ	2.52	0.44
1:B:394:LEU:HB2	1:B:524:ILE:HD13	1.99	0.44
1:C:182:LYS:HD3	1:C:207:VAL:HG22	2.00	0.44
1:C:573:LYS:HA	1:C:573:LYS:HD3	1.76	0.44
1:C:737:VAL:HG22	1:C:1080:VAL:HG22	2.00	0.44
1:C:823:ASP:OD2	1:C:826:LYS:NZ	2.45	0.44
1:A:36:VAL:HG11	1:A:217:PHE:CZ	2.53	0.44
1:A:568:THR:HG23	1:A:601:ASP:HB3	2.00	0.44
1:C:94:GLU:OE1	1:C:98:ILE:N	2.46	0.44
1:B:572:LYS:HE3	1:C:43:PHE:CZ	2.53	0.43
1:C:143:ASN:HB3	1:C:244:SER:HA	1.99	0.43
1:C:80:PRO:HB2	1:C:82:LEU:HD12	1.99	0.43
1:B:184:LEU:HB3	1:B:203:THR:HG23	1.98	0.43
1:B:327:PRO:C	1:B:595:GLN:HE22	2.18	0.43
1:A:187:PHE:HB3	1:A:189:PHE:CE1	2.53	0.43
1:A:578:GLN:HG2	1:B:41:LYS:HA	2.00	0.43
1:B:87:GLY:HA2	1:B:189:PHE:O	2.18	0.43
1:A:544:LYS:HD3	1:A:544:LYS:HA	1.74	0.43
1:B:346:GLN:NE2	1:B:447:LYS:O	2.51	0.43
1:B:493:ARG:NH1	1:B:506:VAL:HG13	2.33	0.43
1:B:589:ASP:OD1	1:C:861:ALA:HB3	2.18	0.43
1:B:408:SER:O	1:B:411:SER:OG	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:THR:OG1	1:B:517:GLN:O	2.35	0.43
1:A:141:HIS:HB3	1:A:142:LYS:H	1.57	0.43
1:C:103:ILE:HD11	1:C:238:LEU:HG	2.01	0.43
1:A:550:LYS:HA	1:A:550:LYS:HE3	2.01	0.43
1:A:584:ILE:HD12	1:A:584:ILE:H	1.83	0.43
1:B:379:ILE:HD11	1:B:384:ILE:HG13	2.00	0.43
1:C:556:PHE:CZ	1:C:602:ILE:HD13	2.53	0.43
1:A:127:LYS:HG2	1:A:164:GLU:HG2	2.00	0.43
1:B:200:SER:OG	1:B:223:LEU:HD22	2.19	0.43
1:C:570:SER:OG	1:C:601:ASP:N	2.52	0.43
1:A:93:ILE:HG12	1:A:184:LEU:HD13	2.01	0.42
3:B:1305:NAG:H3	3:B:1305:NAG:H83	2.01	0.42
1:A:556:PHE:HB3	1:A:567:LEU:HD11	2.00	0.42
1:B:984:LYS:HG3	1:C:770:GLN:HE21	1.84	0.42
1:A:38:TYR:OH	1:A:281:THR:HA	2.18	0.42
1:A:823:ASP:OD2	1:A:826:LYS:NZ	2.52	0.42
1:B:16:VAL:HB	1:B:138:PHE:HZ	1.83	0.42
1:C:1000:ASP:HB3	1:C:1002:PRO:HD2	2.01	0.42
1:A:577:PHE:CD2	1:A:578:GLN:HG3	2.55	0.42
1:B:543:LYS:HE2	1:B:543:LYS:HB3	1.76	0.42
1:B:87:GLY:CA	1:B:189:PHE:O	2.68	0.42
1:B:649:ARG:HD2	1:B:649:ARG:HA	1.82	0.42
1:A:1001:PRO:O	1:A:1005:GLU:HG2	2.20	0.42
1:B:397:PHE:CE2	1:B:399:TYR:HB2	2.55	0.42
1:B:414:PRO:HB3	1:B:452:ASN:HA	2.00	0.42
1:B:436:PRO:HA	1:B:517:GLN:HB3	2.02	0.42
1:A:558:PHE:O	1:A:561:LEU:HB2	2.18	0.42
1:C:779:LYS:HB3	1:C:779:LYS:HE2	1.78	0.42
1:A:1140:ASN:OD1	1:A:1142:ASP:HB3	2.20	0.42
1:A:309:ILE:HD11	1:A:626:LEU:HD21	2.01	0.42
1:A:559:ASN:HB2	1:A:594:PRO:HG3	2.01	0.42
1:A:833:ILE:HG12	1:A:950:GLN:HG3	2.02	0.42
1:C:41:LYS:HA	1:C:41:LYS:HE2	2.02	0.42
1:B:871:LYS:HA	1:B:871:LYS:HD3	1.79	0.42
1:A:198:ILE:HB	1:A:224:VAL:HB	2.02	0.41
1:B:984:LYS:HG3	1:C:770:GLN:NE2	2.35	0.41
1:B:731:THR:N	1:B:1086:GLN:O	2.40	0.41
1:A:115:LEU:HD12	1:A:228:ILE:HG21	2.03	0.41
1:A:916:GLN:O	1:A:920:ARG:HG3	2.20	0.41
1:A:974:LEU:HD23	1:A:974:LEU:HA	1.95	0.41
1:B:399:TYR:CZ	1:B:407:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:LEU:HD12	1:B:963:LEU:HD12	2.03	0.41
1:B:1149:ASN:OD1	2:L:1:NAG:C7	2.69	0.41
1:C:632:CYS:HB2	1:C:664:CYS:HB2	1.45	0.41
1:C:997:SER:OG	1:C:998:ARG:N	2.53	0.41
1:A:573:LYS:HA	1:A:573:LYS:HD3	1.97	0.41
1:C:230:ILE:HD11	1:C:232:ILE:HD11	2.03	0.41
1:A:95:LYS:HG3	1:A:181:PHE:CE1	2.55	0.41
1:A:1019:LEU:HD23	1:A:1019:LEU:HA	1.92	0.41
1:B:209:GLU:HA	1:B:210:PRO:HD3	1.82	0.41
1:B:277:ASN:OD1	1:B:281:THR:N	2.46	0.41
1:C:30:ASN:HB3	1:C:32:PHE:CE1	2.55	0.41
1:C:188:VAL:HG23	1:C:220:LEU:HD12	2.02	0.41
1:C:323:ILE:HD13	1:C:549:VAL:HG12	2.01	0.41
1:B:46:SER:OG	1:B:278:GLU:HB3	2.20	0.41
1:B:160:ASN:OD1	1:B:160:ASN:N	2.52	0.41
1:B:239:LEU:HD23	1:B:240:ALA:N	2.35	0.41
1:C:1118:PHE:CZ	2:N:1:NAG:H62	2.52	0.41
1:B:320:THR:OG1	1:B:321:GLU:N	2.53	0.41
1:B:326:PHE:N	1:B:327:PRO:HD2	2.36	0.41
1:B:401:LEU:HD23	1:B:401:LEU:O	2.20	0.41
1:B:577:PHE:CD2	1:C:222:PRO:HG2	2.56	0.41
1:B:128:VAL:HG21	1:B:228:ILE:HD12	2.03	0.41
1:B:429:CYS:HB2	1:B:524:ILE:HG23	2.03	0.41
1:A:45:SER:HB2	1:A:278:GLU:HA	2.03	0.41
1:A:869:LYS:HA	1:A:873:LEU:O	2.20	0.41
1:A:870:PHE:CE1	1:C:604:PRO:HD2	2.56	0.41
1:A:985:PHE:HA	1:B:771:TYR:CE1	2.55	0.41
1:B:284:ASP:OD1	1:B:285:ALA:N	2.52	0.41
1:C:115:LEU:HD22	1:C:228:ILE:HG21	2.02	0.41
1:C:992:LEU:HD12	1:C:992:LEU:HA	1.96	0.41
1:B:572:LYS:HE2	1:B:573:LYS:O	2.21	0.41
1:C:158:ALA:HB1	1:C:161:CYS:SG	2.60	0.41
1:A:1007:GLN:HA	1:A:1010:ARG:HD3	2.02	0.40
1:C:64:TRP:CD1	1:C:64:TRP:C	2.94	0.40
1:A:124:VAL:HB	1:A:167:SER:HB3	2.04	0.40
1:B:649:ARG:HG3	1:B:650:VAL:HG23	2.04	0.40
1:C:991:VAL:HG12	1:C:993:ASN:H	1.87	0.40
1:A:570:SER:HB2	1:A:601:ASP:HB2	2.03	0.40
1:B:139:LEU:CD1	1:B:238:LEU:HB3	2.51	0.40
1:C:674:SER:HB3	1:C:713:SER:HB3	2.03	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	898/1249 (72%)	831 (92%)	64 (7%)	3 (0%)	37 66
1	B	1080/1249 (86%)	1019 (94%)	61 (6%)	0	100 100
1	C	898/1249 (72%)	835 (93%)	63 (7%)	0	100 100
All	All	2876/3747 (77%)	2685 (93%)	188 (6%)	3 (0%)	50 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	641	ALA
1	A	141	HIS
1	A	543	LYS

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	797/1097 (73%)	781 (98%)	16 (2%)	50 70
1	B	968/1097 (88%)	948 (98%)	20 (2%)	48 69
1	C	796/1097 (73%)	780 (98%)	16 (2%)	50 70
All	All	2561/3291 (78%)	2509 (98%)	52 (2%)	50 70

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	77	PHE
1	A	148	MET
1	A	163	PHE
1	A	172	MET
1	A	246	LEU
1	A	303	PHE
1	A	325	ARG
1	A	551	ASN
1	A	558	PHE
1	A	579	GLN
1	A	648	TRP
1	A	664	CYS
1	A	690	GLN
1	A	866	CYS
1	A	882	ASP
1	B	78	ASP
1	B	133	PHE
1	B	217	PHE
1	B	235	PHE
1	B	255	TRP
1	B	278	GLU
1	B	325	ARG
1	B	341	SER
1	B	358	CYS
1	B	360	TYR
1	B	374	PHE
1	B	562	LYS
1	B	606	SER
1	B	649	ARG
1	B	664	CYS
1	B	882	ASP
1	B	996	PHE
1	B	1116	HIS
1	B	1142	ASP
1	B	1153	TYR
1	C	64	TRP
1	C	77	PHE
1	C	148	MET
1	C	255	TRP
1	C	303	PHE
1	C	325	ARG
1	C	577	PHE

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Mol	Chain	Res	Type
1	C	589	ASP
1	C	607	PHE
1	C	621	ASN
1	C	649	ARG
1	C	677	CYS
1	C	678	ASP
1	C	760	ASP
1	C	950	GLN
1	C	953	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	202	HIS
1	B	113	GLN
1	C	770	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

24 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	0.37	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	D	2	2	14,14,15	0.46	0	17,19,21	0.36	0
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.53	0
2	NAG	E	2	2	14,14,15	1.01	1 (7%)	17,19,21	1.42	1 (5%)
2	NAG	F	1	2,1	14,14,15	0.79	1 (7%)	17,19,21	0.58	0
2	NAG	F	2	2	14,14,15	0.32	0	17,19,21	0.57	0
2	NAG	G	1	2,1	14,14,15	0.25	0	17,19,21	0.43	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.44	0
2	NAG	H	1	2,1	14,14,15	0.36	0	17,19,21	0.57	0
2	NAG	H	2	2	14,14,15	0.50	0	17,19,21	1.33	2 (11%)
2	NAG	I	1	2,1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	I	2	2	14,14,15	0.48	0	17,19,21	0.99	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.72	1 (7%)	17,19,21	0.71	1 (5%)
2	NAG	J	2	2	14,14,15	0.48	0	17,19,21	0.99	2 (11%)
2	NAG	K	1	2,1	14,14,15	0.24	0	17,19,21	0.43	0
2	NAG	K	2	2	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	L	1	2,1	14,14,15	0.74	1 (7%)	17,19,21	0.77	1 (5%)
2	NAG	L	2	2	14,14,15	0.47	0	17,19,21	1.36	2 (11%)
2	NAG	M	1	2,1	14,14,15	0.59	0	17,19,21	0.97	1 (5%)
2	NAG	M	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	N	1	2,1	14,14,15	0.49	0	17,19,21	0.66	1 (5%)
2	NAG	N	2	2	14,14,15	0.33	0	17,19,21	0.39	0
2	NAG	O	1	2,1	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	O	2	2	14,14,15	0.49	0	17,19,21	1.33	2 (11%)

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	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	0/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	H	2	2	-	6/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	NAG	J	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	L	2	2	-	5/6/23/26	0/1/1/1
2	NAG	M	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	O	2	2	-	6/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	NAG	O5-C1	3.69	1.49	1.43
2	J	1	NAG	O5-C1	-2.39	1.39	1.43
2	L	1	NAG	O5-C1	2.31	1.47	1.43
2	F	1	NAG	O5-C1	-2.15	1.40	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	5.58	119.67	112.19
2	H	2	NAG	C2-N2-C7	4.58	129.03	122.90
2	O	2	NAG	C2-N2-C7	4.56	129.02	122.90
2	L	2	NAG	C2-N2-C7	4.54	128.99	122.90
2	I	2	NAG	C1-O5-C5	2.73	115.85	112.19
2	J	2	NAG	C1-O5-C5	2.47	115.49	112.19
2	L	2	NAG	C1-C2-N2	2.46	114.31	110.43
2	J	2	NAG	C3-C4-C5	2.42	114.61	110.23
2	M	1	NAG	C1-O5-C5	2.37	115.37	112.19
2	L	1	NAG	C1-O5-C5	2.35	115.34	112.19
2	I	2	NAG	C3-C4-C5	2.25	114.31	110.23
2	H	2	NAG	C1-C2-N2	2.25	113.97	110.43
2	O	2	NAG	C1-C2-N2	2.16	113.84	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	1	NAG	C1-O5-C5	2.16	115.08	112.19
2	J	1	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	N	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	L	2	NAG	C8-C7-N2-C2
2	L	2	NAG	O7-C7-N2-C2
2	O	1	NAG	C8-C7-N2-C2
2	O	1	NAG	O7-C7-N2-C2
2	O	2	NAG	C8-C7-N2-C2
2	O	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	M	1	NAG	C3-C2-N2-C7
2	I	2	NAG	O5-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	J	1	NAG	C1-C2-N2-C7
2	N	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	J	1	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C1-C2-N2-C7
2	H	2	NAG	C1-C2-N2-C7
2	L	2	NAG	C1-C2-N2-C7
2	O	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7
2	L	2	NAG	C3-C2-N2-C7
2	O	2	NAG	C3-C2-N2-C7
2	G	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

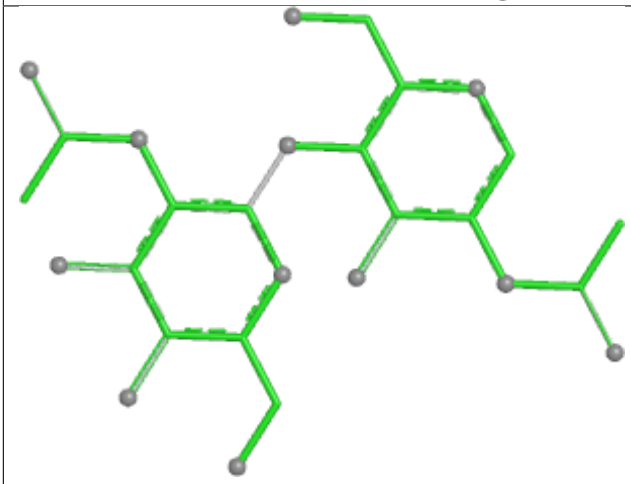
There are no ring outliers.

7 monomers are involved in 9 short contacts:

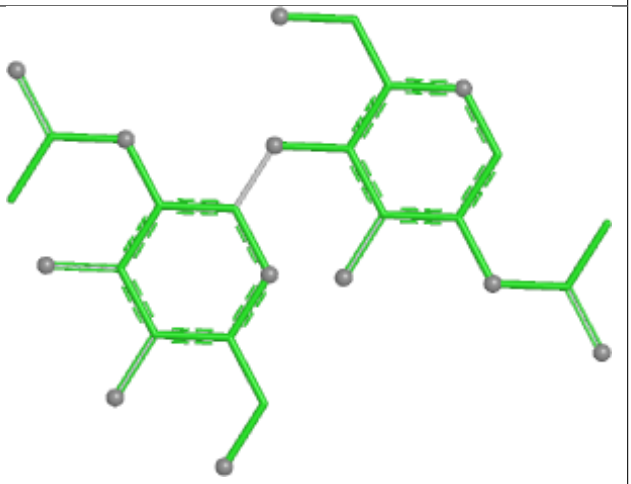
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	NAG	2	0
2	H	2	NAG	1	0
2	G	1	NAG	1	0
2	L	2	NAG	1	0
2	O	2	NAG	1	0
2	N	1	NAG	2	0
2	K	1	NAG	1	0

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

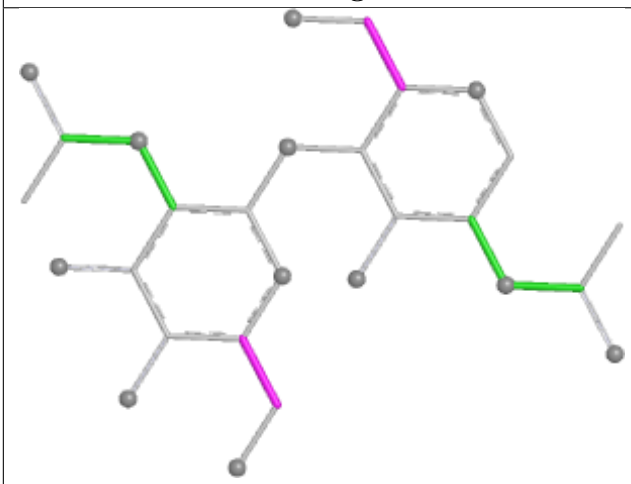
Oligosaccharide Chain D



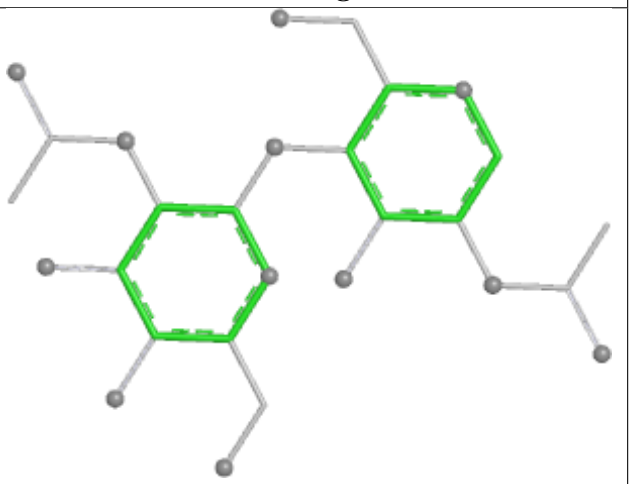
Bond lengths



Bond angles

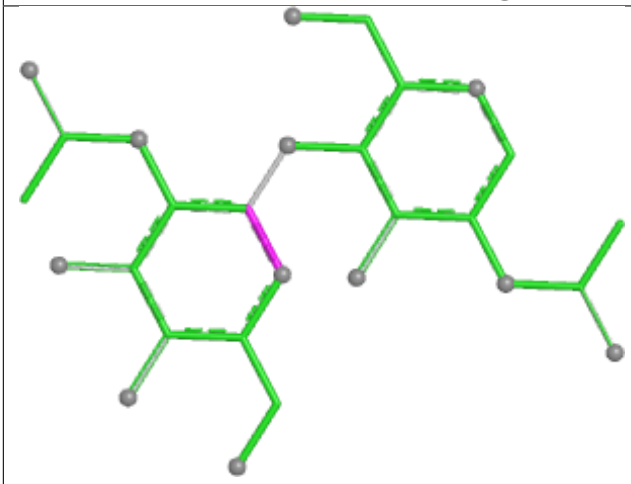


Torsions

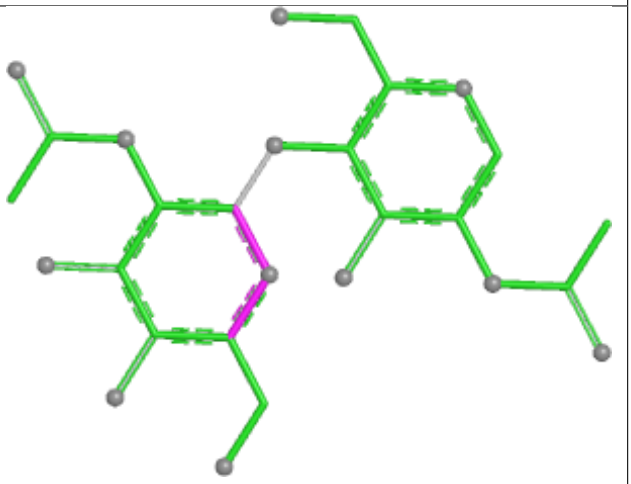


Rings

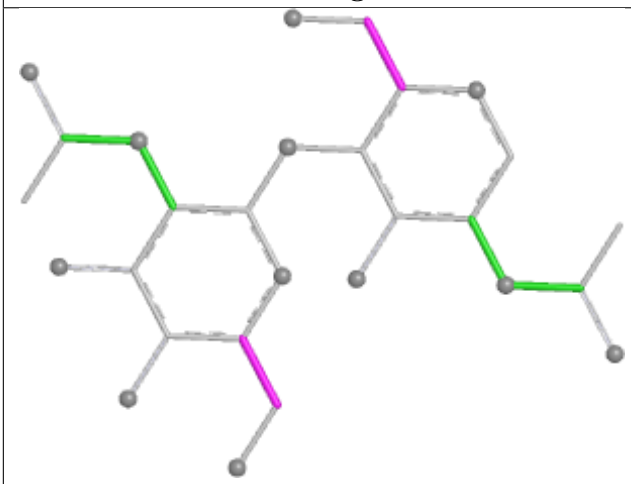
Oligosaccharide Chain E



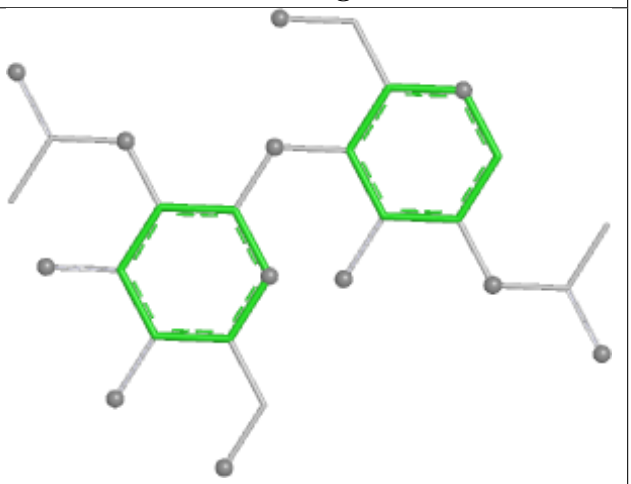
Bond lengths



Bond angles

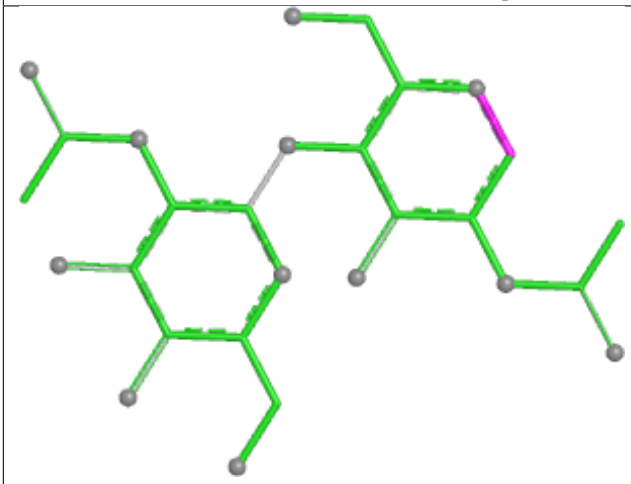


Torsions

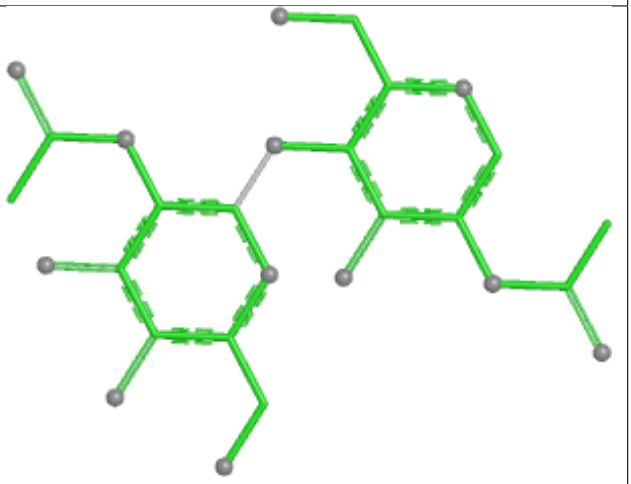


Rings

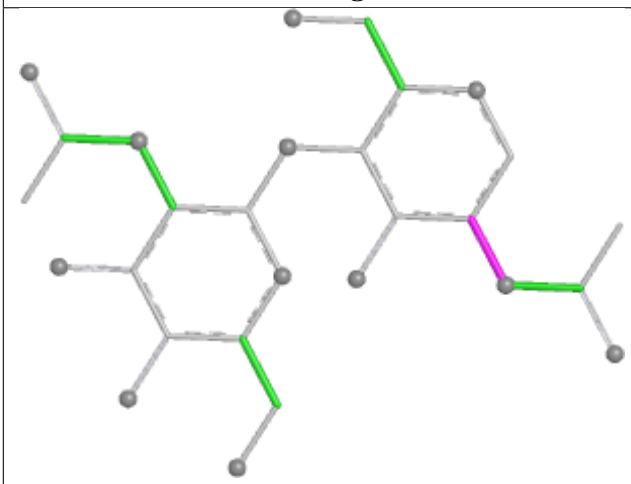
Oligosaccharide Chain F



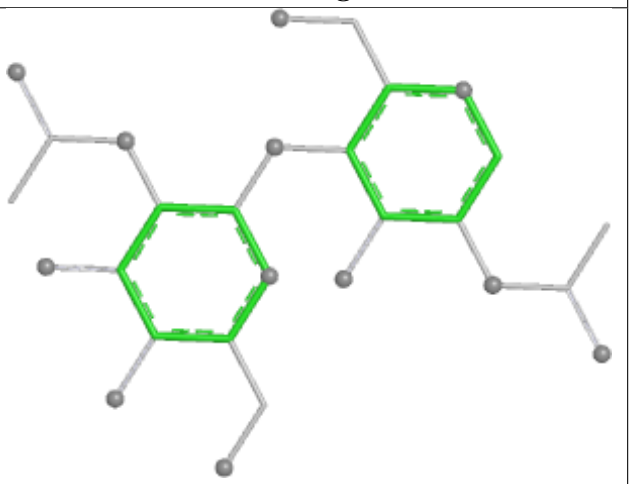
Bond lengths



Bond angles

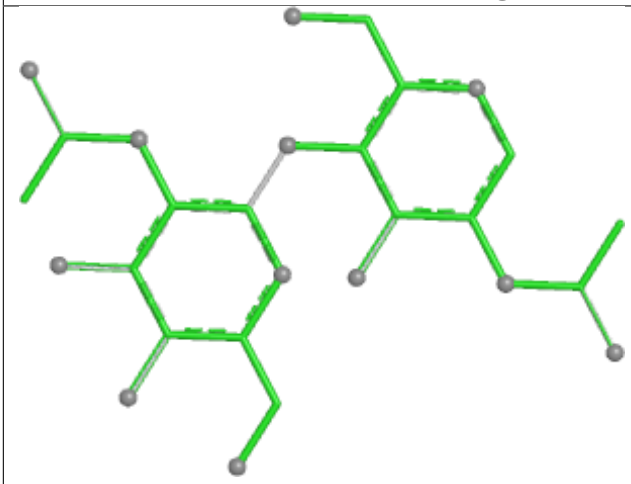


Torsions

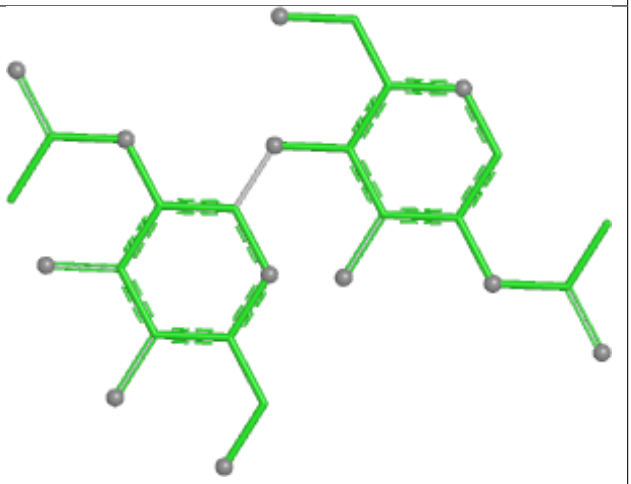


Rings

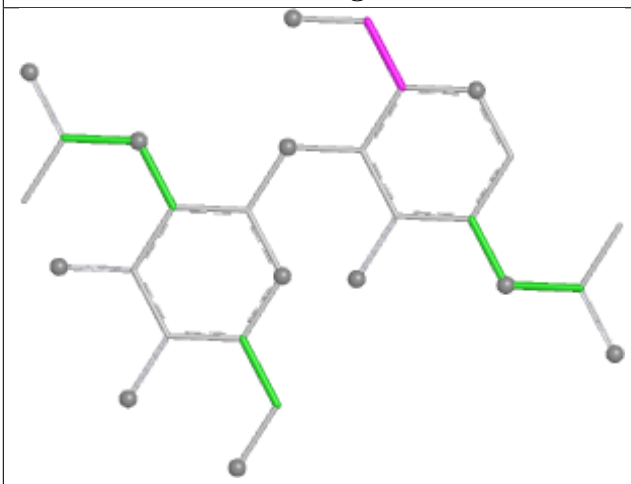
Oligosaccharide Chain G



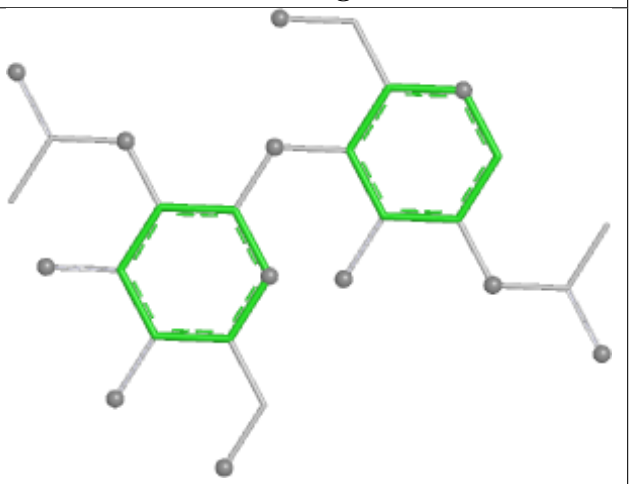
Bond lengths



Bond angles

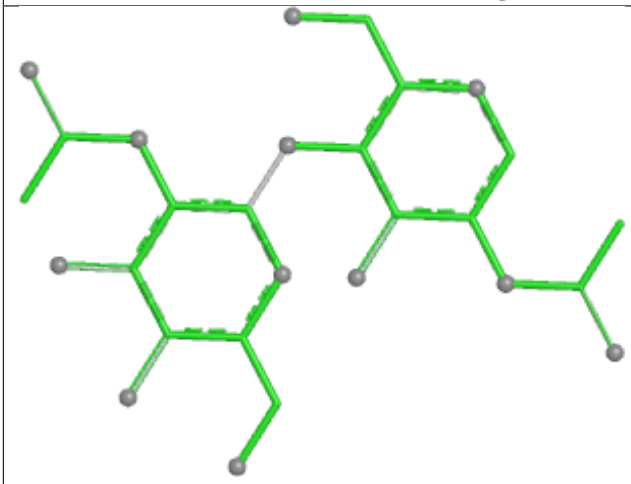


Torsions

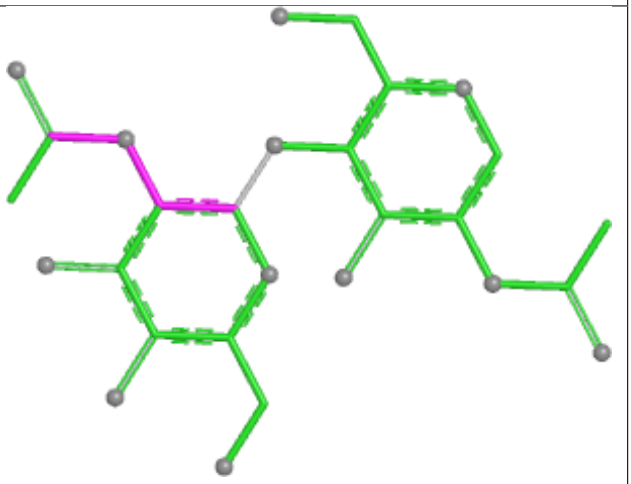


Rings

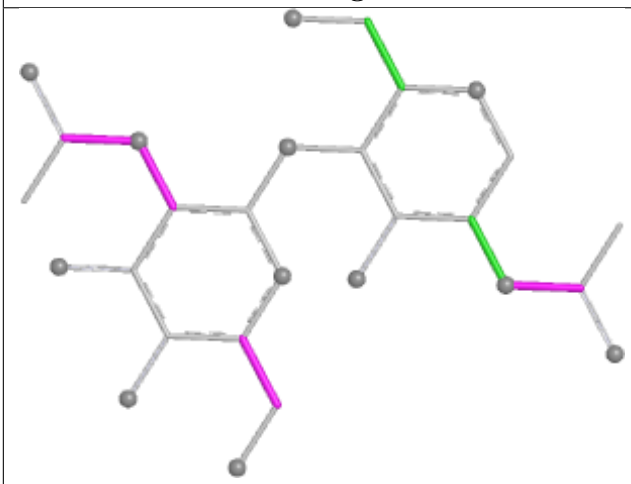
Oligosaccharide Chain H



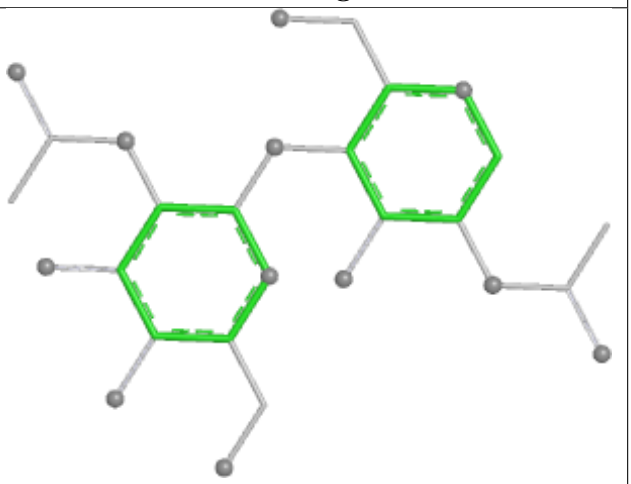
Bond lengths



Bond angles

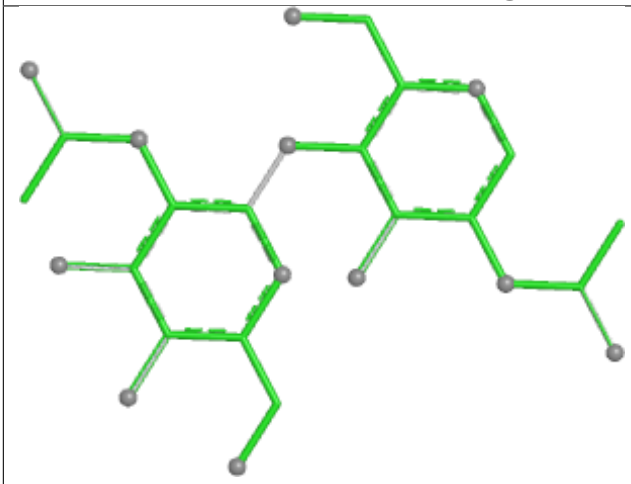


Torsions

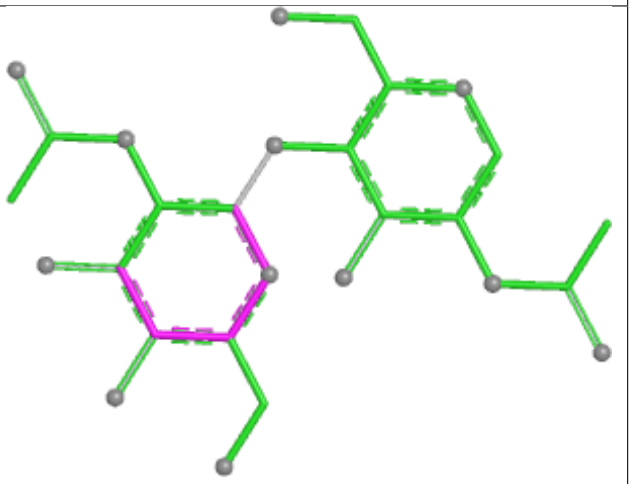


Rings

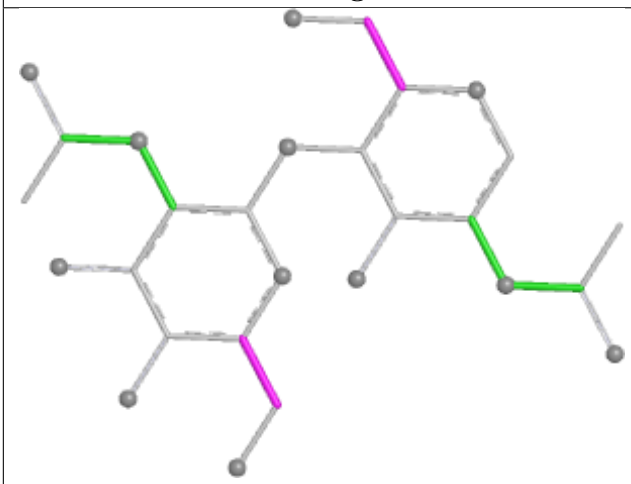
Oligosaccharide Chain I



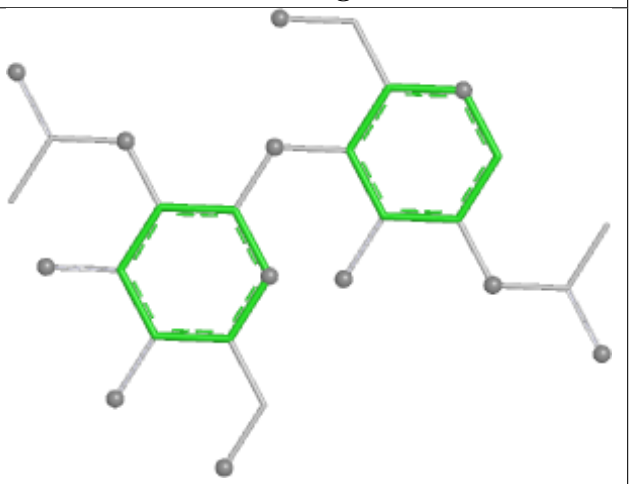
Bond lengths



Bond angles

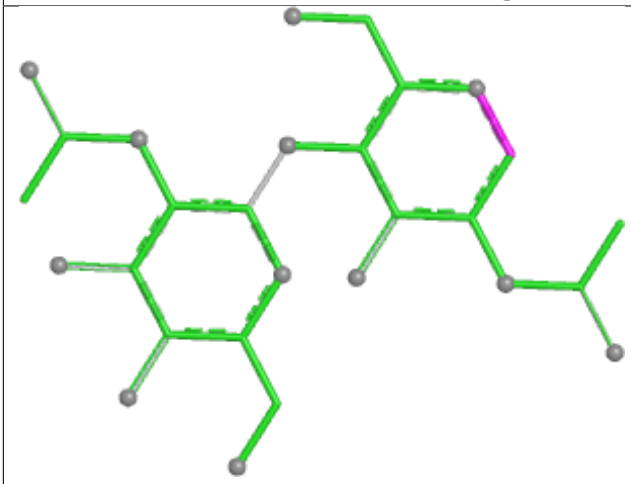


Torsions

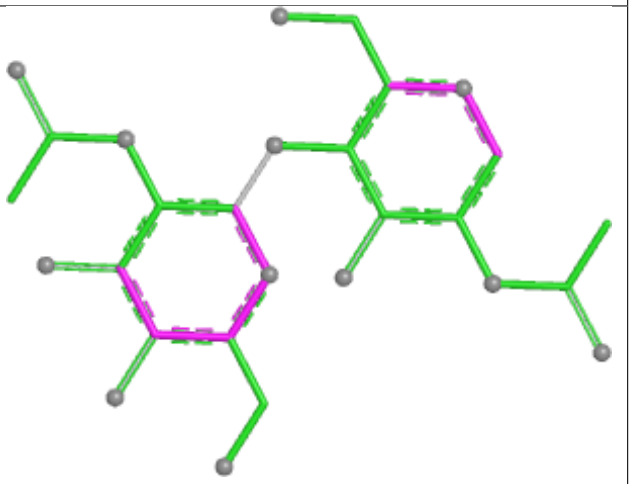


Rings

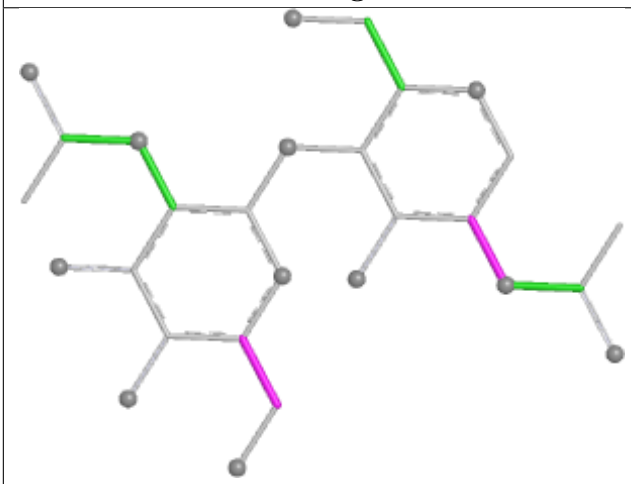
Oligosaccharide Chain J



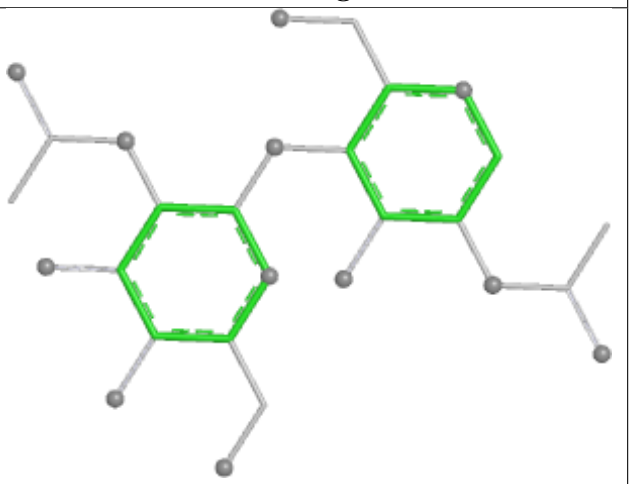
Bond lengths



Bond angles

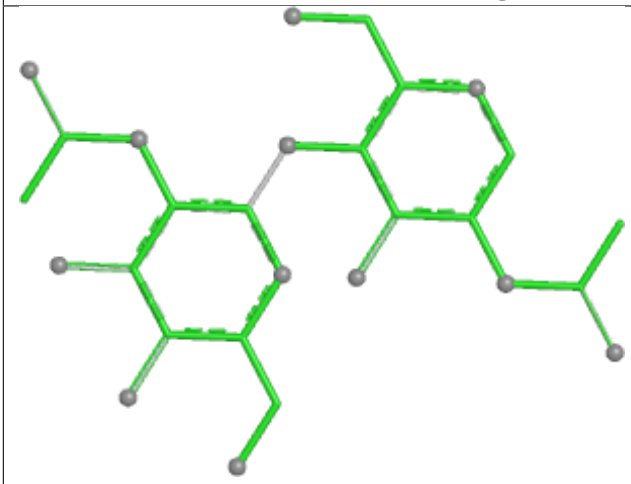


Torsions

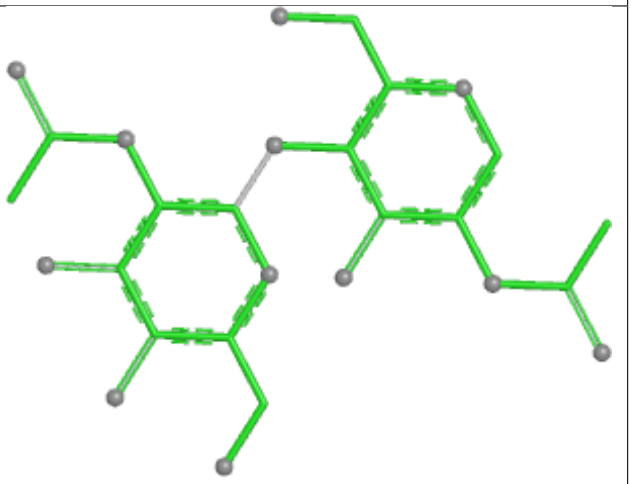


Rings

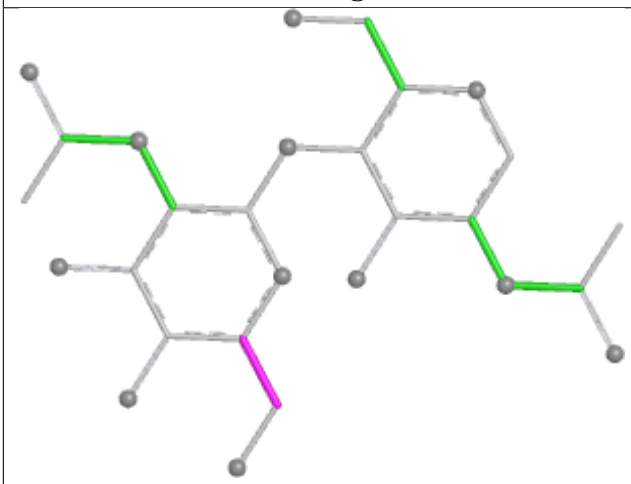
Oligosaccharide Chain K



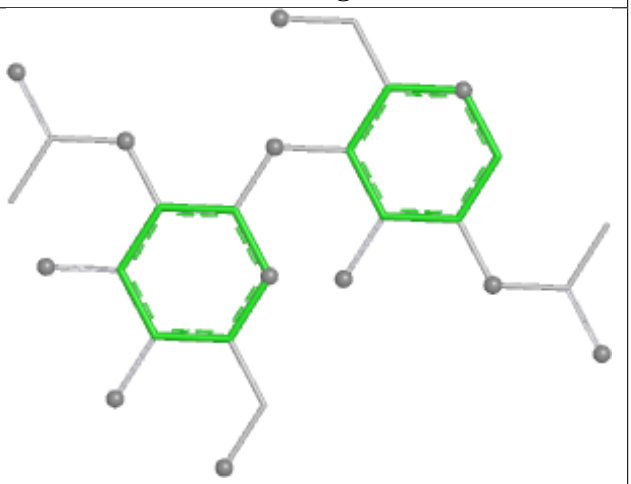
Bond lengths



Bond angles

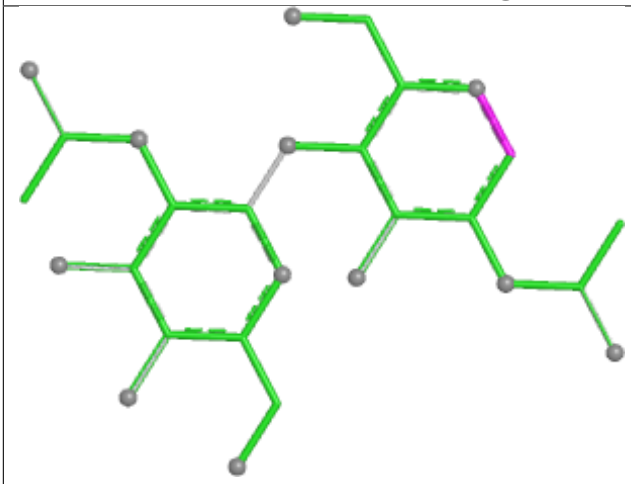


Torsions

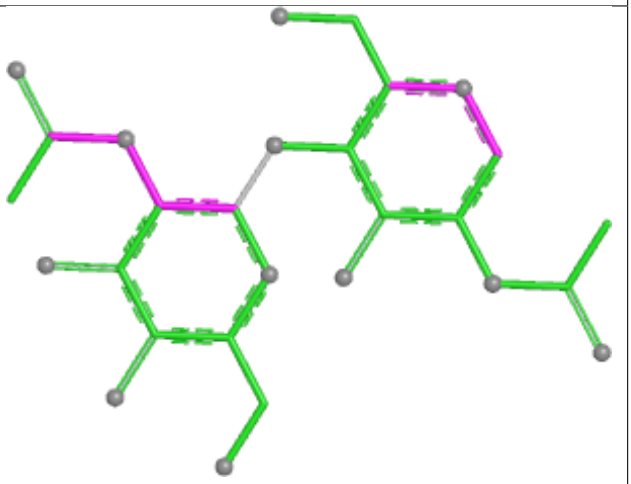


Rings

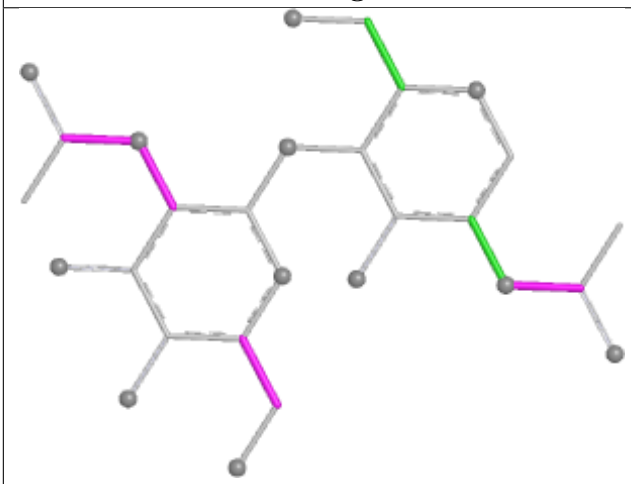
Oligosaccharide Chain L



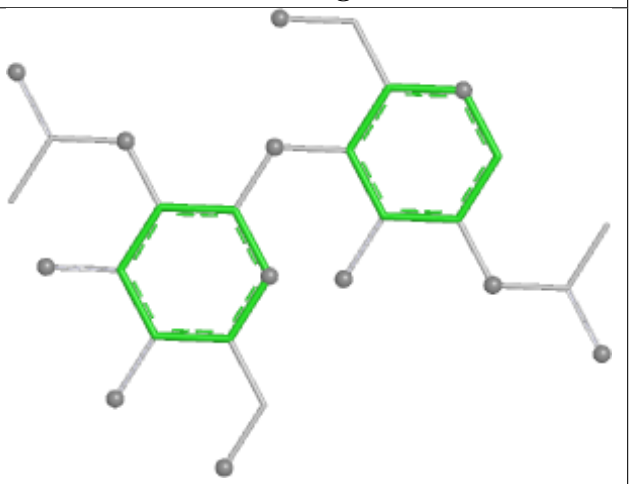
Bond lengths



Bond angles

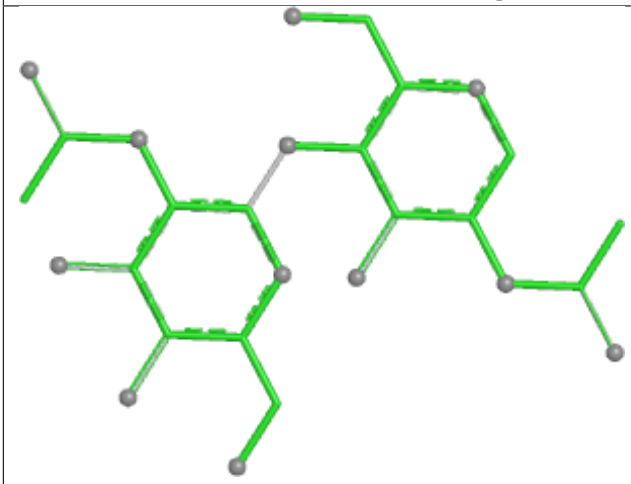


Torsions

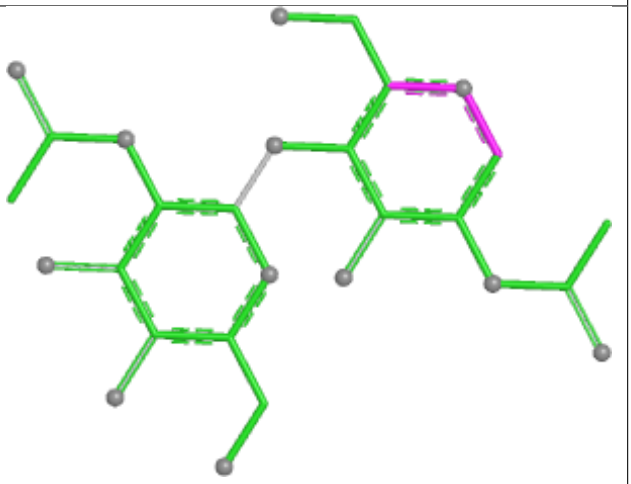


Rings

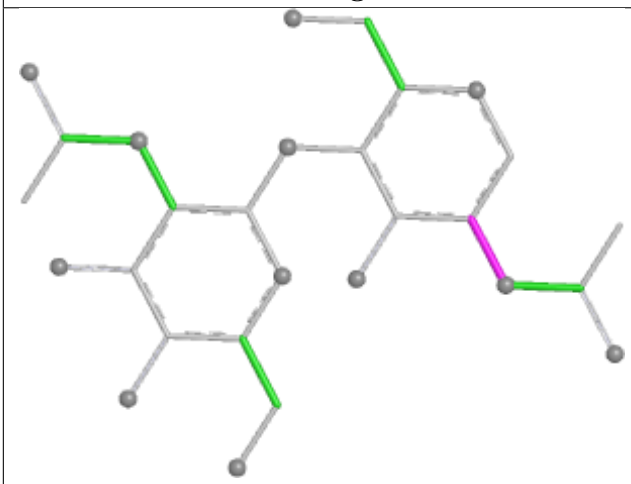
Oligosaccharide Chain M



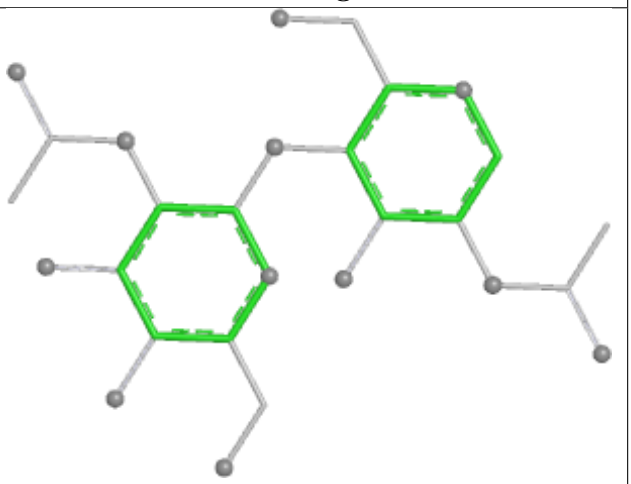
Bond lengths



Bond angles

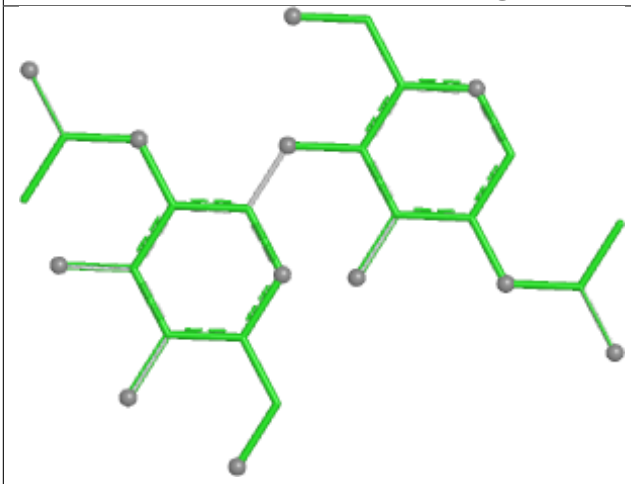


Torsions

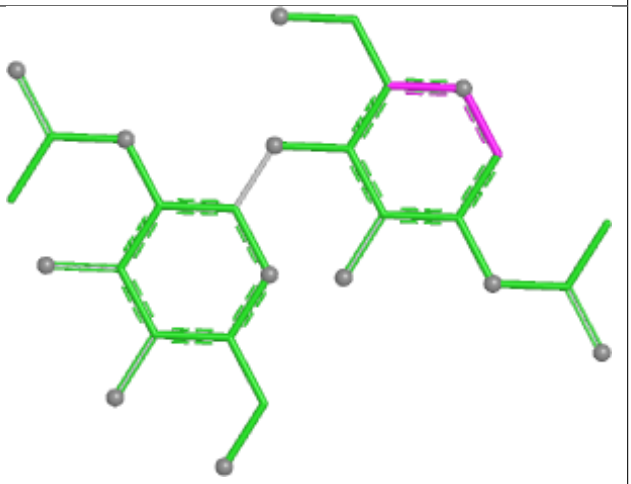


Rings

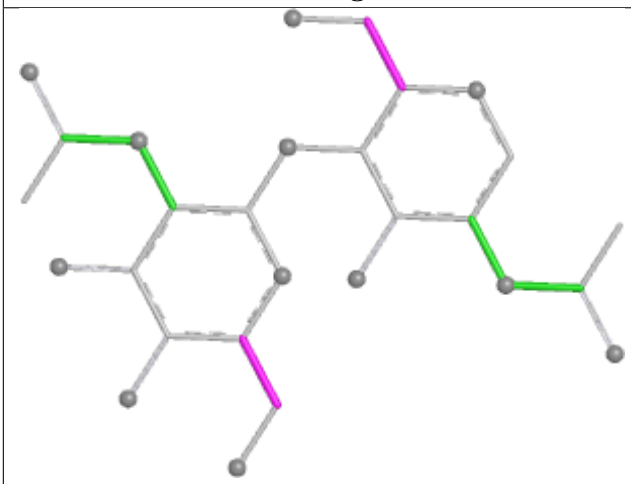
Oligosaccharide Chain N



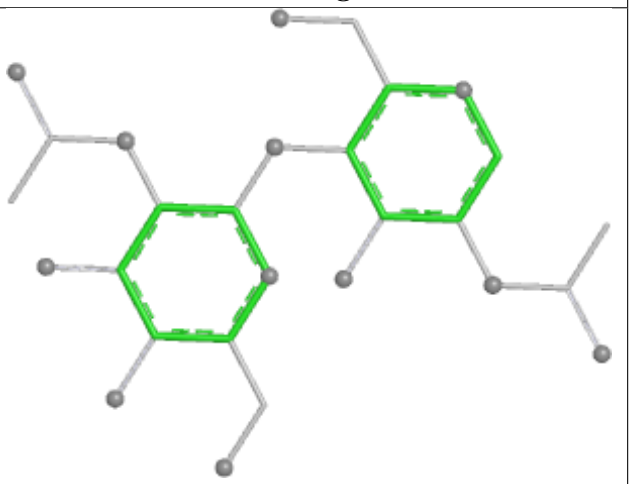
Bond lengths



Bond angles

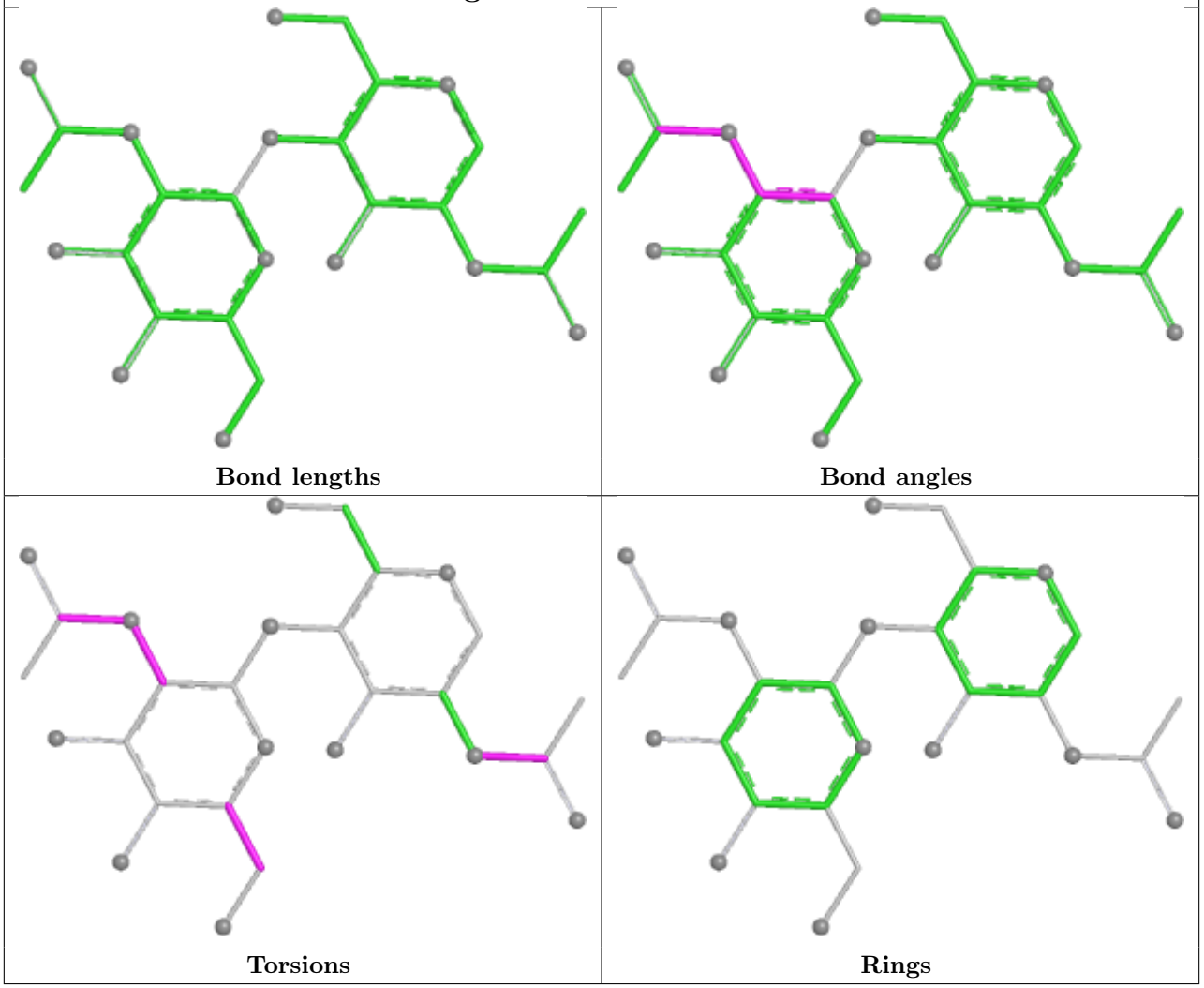


Torsions



Rings

Oligosaccharide Chain O



5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
3	NAG	B	1303	1	14,14,15	0.60	0	17,19,21	1.71	4 (23%)
3	NAG	B	1305	1	14,14,15	0.69	1 (7%)	17,19,21	1.60	3 (17%)
3	NAG	C	1302	1	14,14,15	0.42	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	B	1301	1	14,14,15	0.28	0	17,19,21	0.79	0
3	NAG	C	1303	1	14,14,15	0.48	0	17,19,21	0.50	0
3	NAG	A	1304	1	14,14,15	0.41	0	17,19,21	0.54	0
3	NAG	B	1304	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	A	1301	1	14,14,15	0.40	0	17,19,21	0.43	0
3	NAG	A	1303	1	14,14,15	0.25	0	17,19,21	0.38	0
3	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.46	0
3	NAG	C	1304	1	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	A	1302	1	14,14,15	0.43	0	17,19,21	0.54	0
3	NAG	B	1302	1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	B	1306	1	14,14,15	0.20	0	17,19,21	0.40	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
3	NAG	B	1303	1	-	6/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	5/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1306	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1305	NAG	O5-C1	-2.21	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1305	NAG	C2-N2-C7	4.73	129.24	122.90
3	B	1303	NAG	C2-N2-C7	4.65	129.13	122.90
3	B	1303	NAG	C1-O5-C5	3.19	116.47	112.19
3	B	1305	NAG	C3-C4-C5	2.67	115.08	110.23
3	B	1303	NAG	C1-C2-N2	2.53	114.42	110.43
3	B	1305	NAG	C1-C2-N2	2.31	114.07	110.43
3	B	1303	NAG	C3-C4-C5	2.20	114.22	110.23

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	B	1304	NAG	O5-C5-C6-O6
3	B	1303	NAG	C4-C5-C6-O6
3	A	1301	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	A	1301	NAG	O5-C5-C6-O6
3	A	1304	NAG	O5-C5-C6-O6
3	B	1304	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	B	1303	NAG	C8-C7-N2-C2
3	B	1303	NAG	O7-C7-N2-C2
3	B	1305	NAG	C8-C7-N2-C2
3	B	1305	NAG	O7-C7-N2-C2
3	C	1302	NAG	C8-C7-N2-C2
3	C	1302	NAG	O7-C7-N2-C2
3	B	1302	NAG	O5-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1303	NAG	O5-C5-C6-O6
3	B	1305	NAG	O5-C5-C6-O6
3	B	1306	NAG	O5-C5-C6-O6
3	B	1301	NAG	O5-C5-C6-O6
3	B	1301	NAG	C1-C2-N2-C7
3	A	1304	NAG	C4-C5-C6-O6
3	B	1302	NAG	C4-C5-C6-O6
3	B	1301	NAG	C3-C2-N2-C7
3	B	1303	NAG	C1-C2-N2-C7
3	B	1305	NAG	C1-C2-N2-C7
3	A	1301	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	B	1303	NAG	C3-C2-N2-C7
3	B	1305	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1303	NAG	1	0
3	B	1305	NAG	1	0
3	A	1301	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

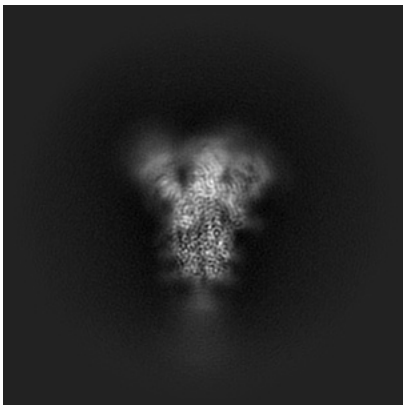
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42456. These allow visual inspection of the internal detail of the map and identification of artifacts.

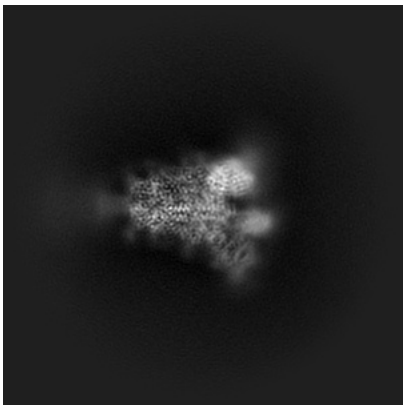
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

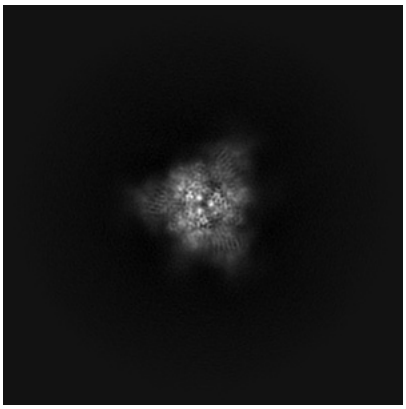
6.1.1 Primary map



X

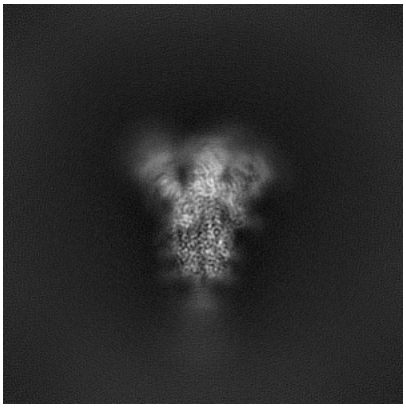


Y

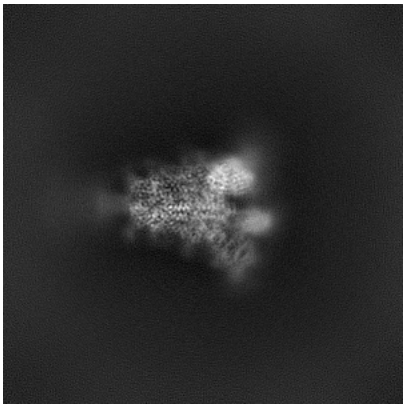


Z

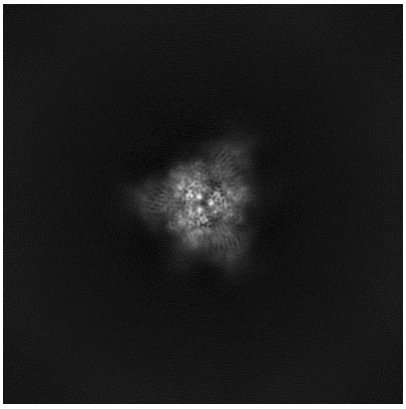
6.1.2 Raw map



X



Y

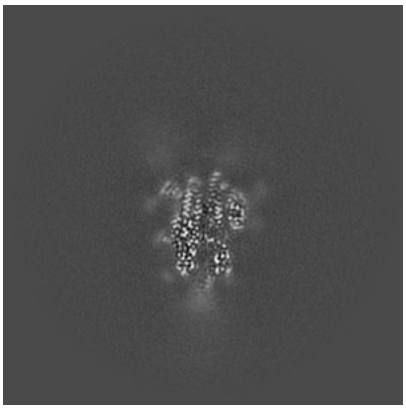


Z

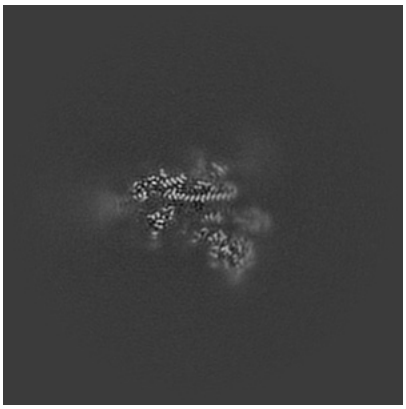
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

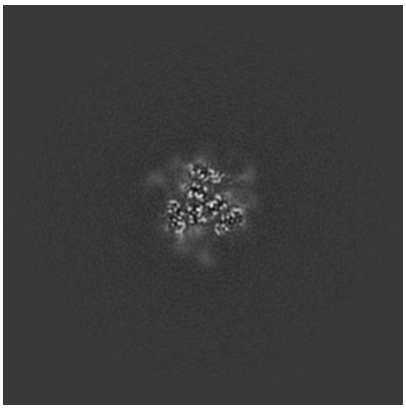
6.2.1 Primary map



X Index: 192

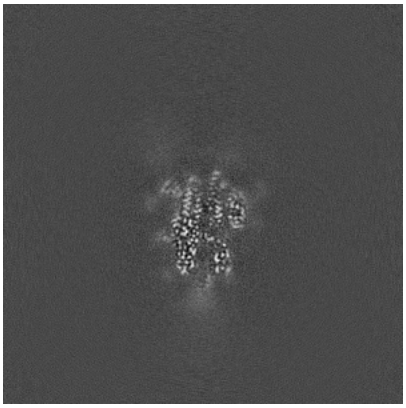


Y Index: 192

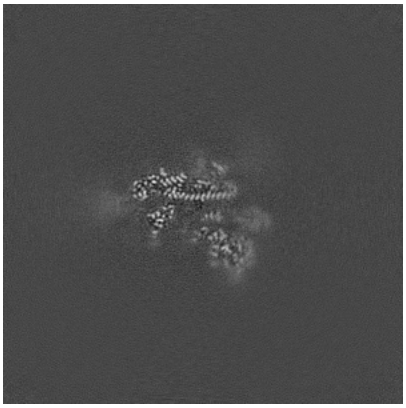


Z Index: 192

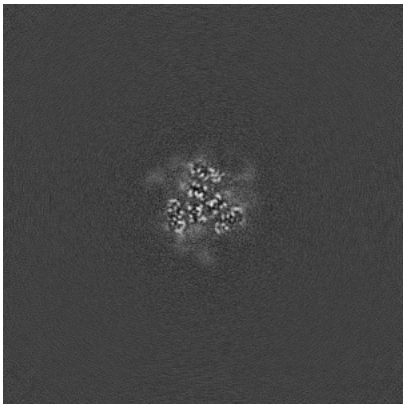
6.2.2 Raw map



X Index: 192



Y Index: 192

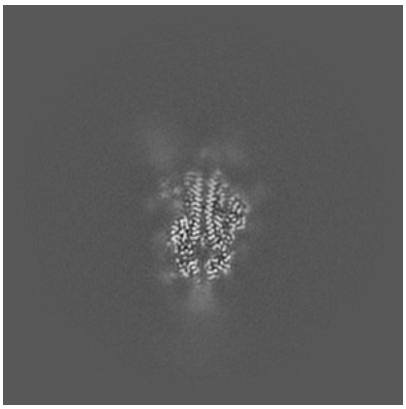


Z Index: 192

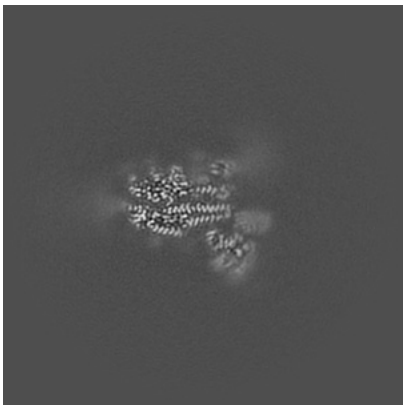
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

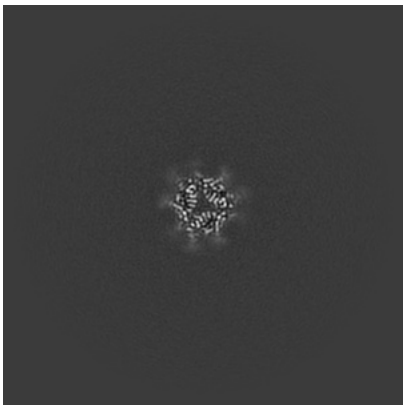
6.3.1 Primary map



X Index: 188

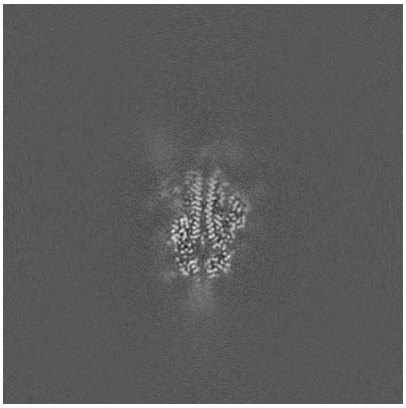


Y Index: 199

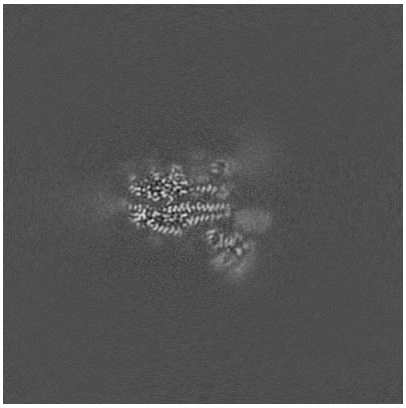


Z Index: 145

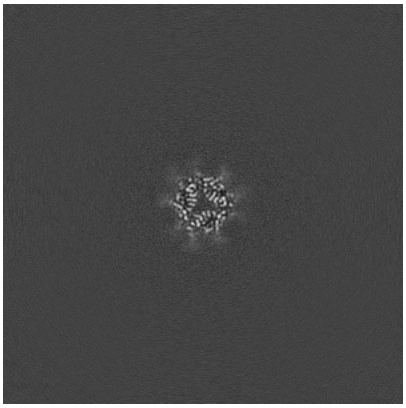
6.3.2 Raw map



X Index: 188



Y Index: 199

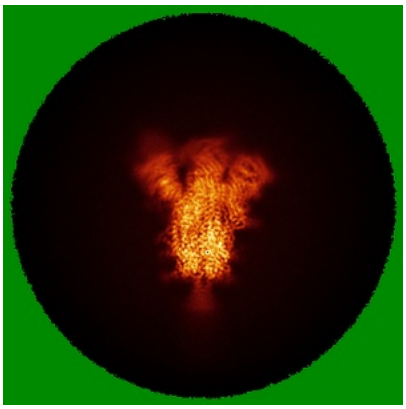


Z Index: 145

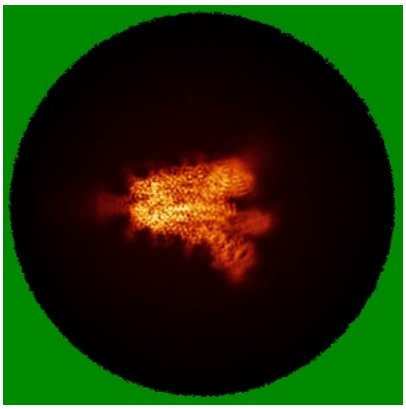
The images above show the largest variance slices of the map in three orthogonal directions.

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

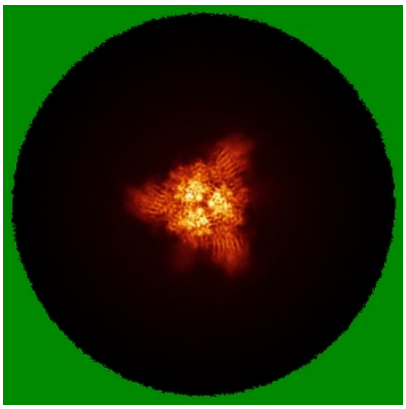
6.4.1 Primary map



X

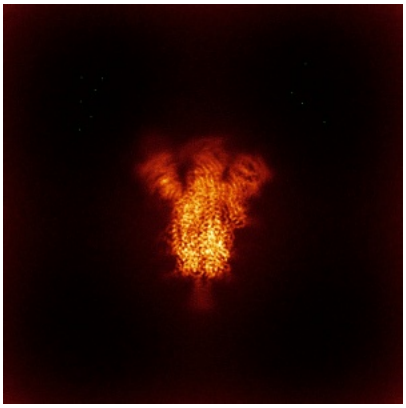


Y

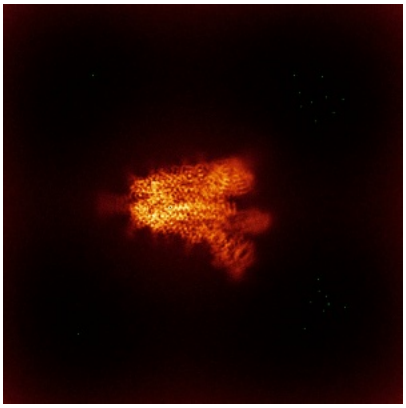


Z

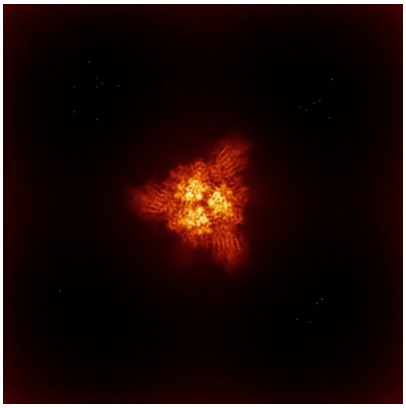
6.4.2 Raw map



X



Y

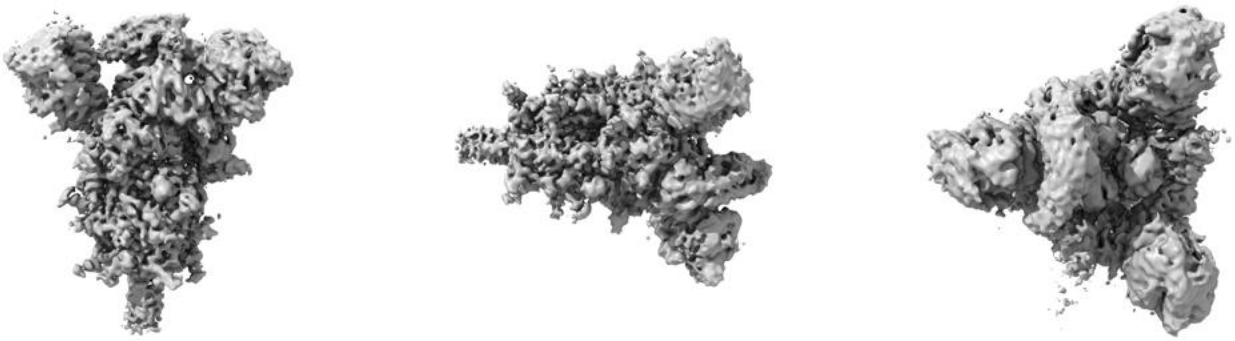


Z

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 0.103. 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.

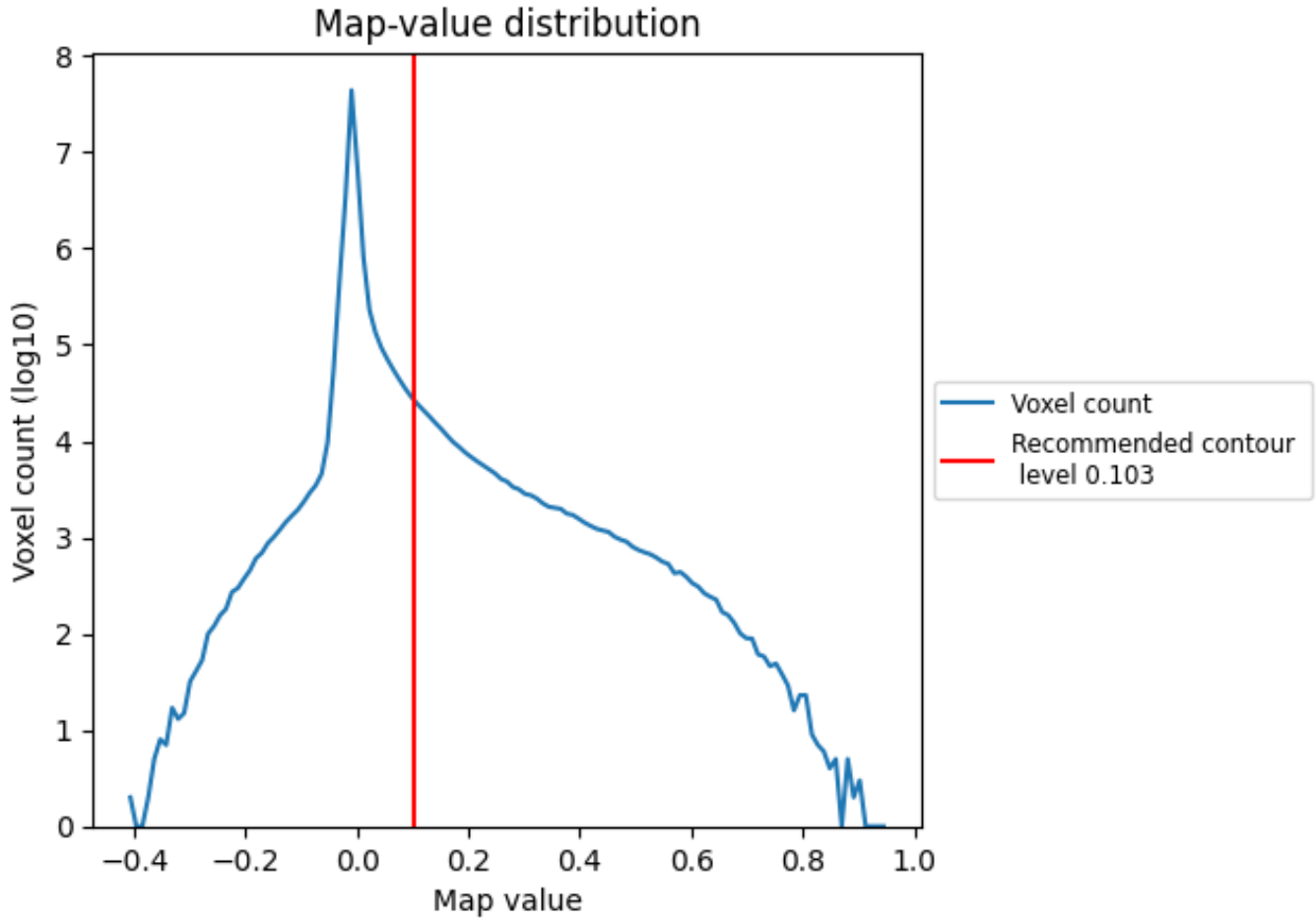
6.6 Mask visualisation (i)

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

7 Map analysis

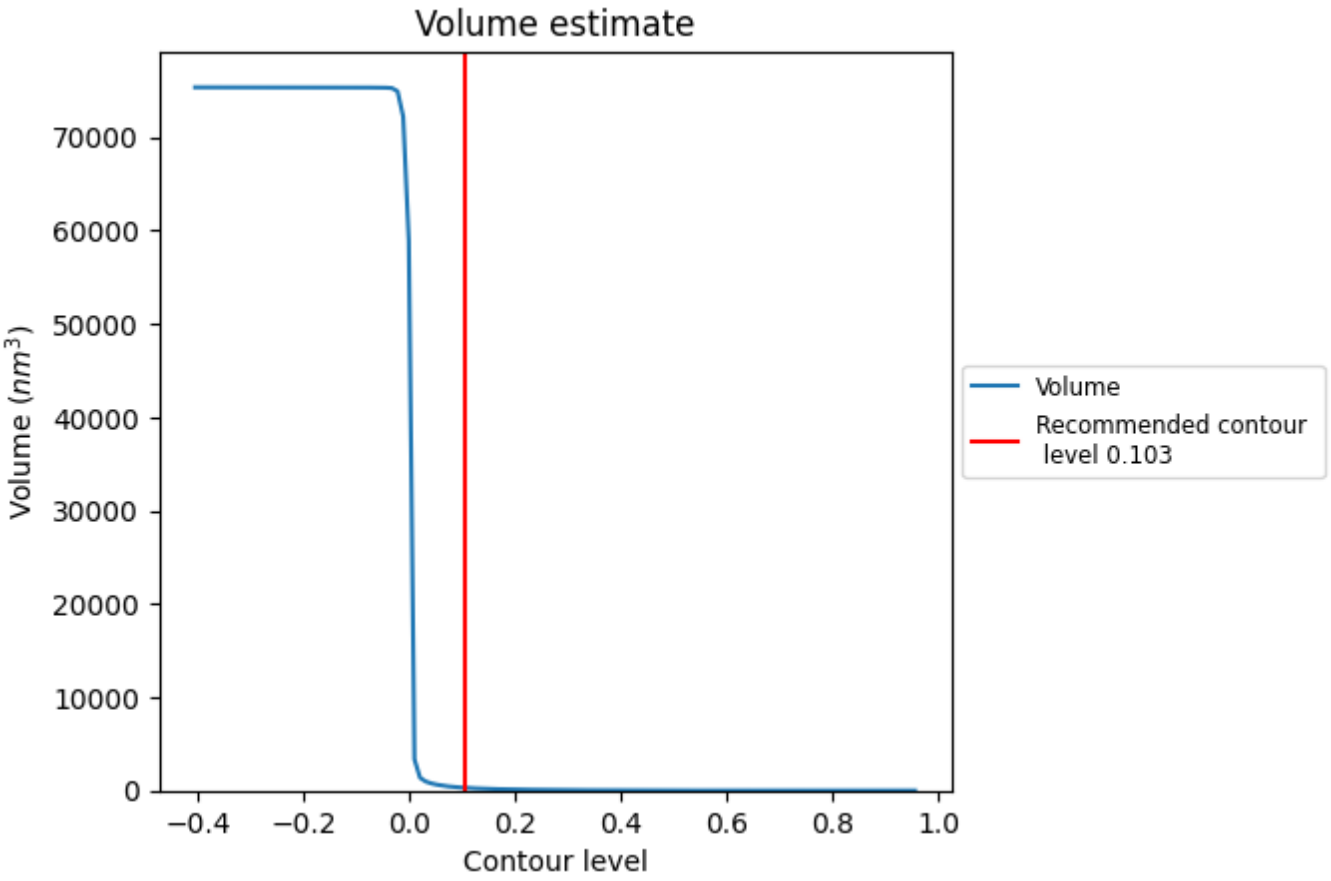
This section contains the results of statistical analysis of the map.

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.

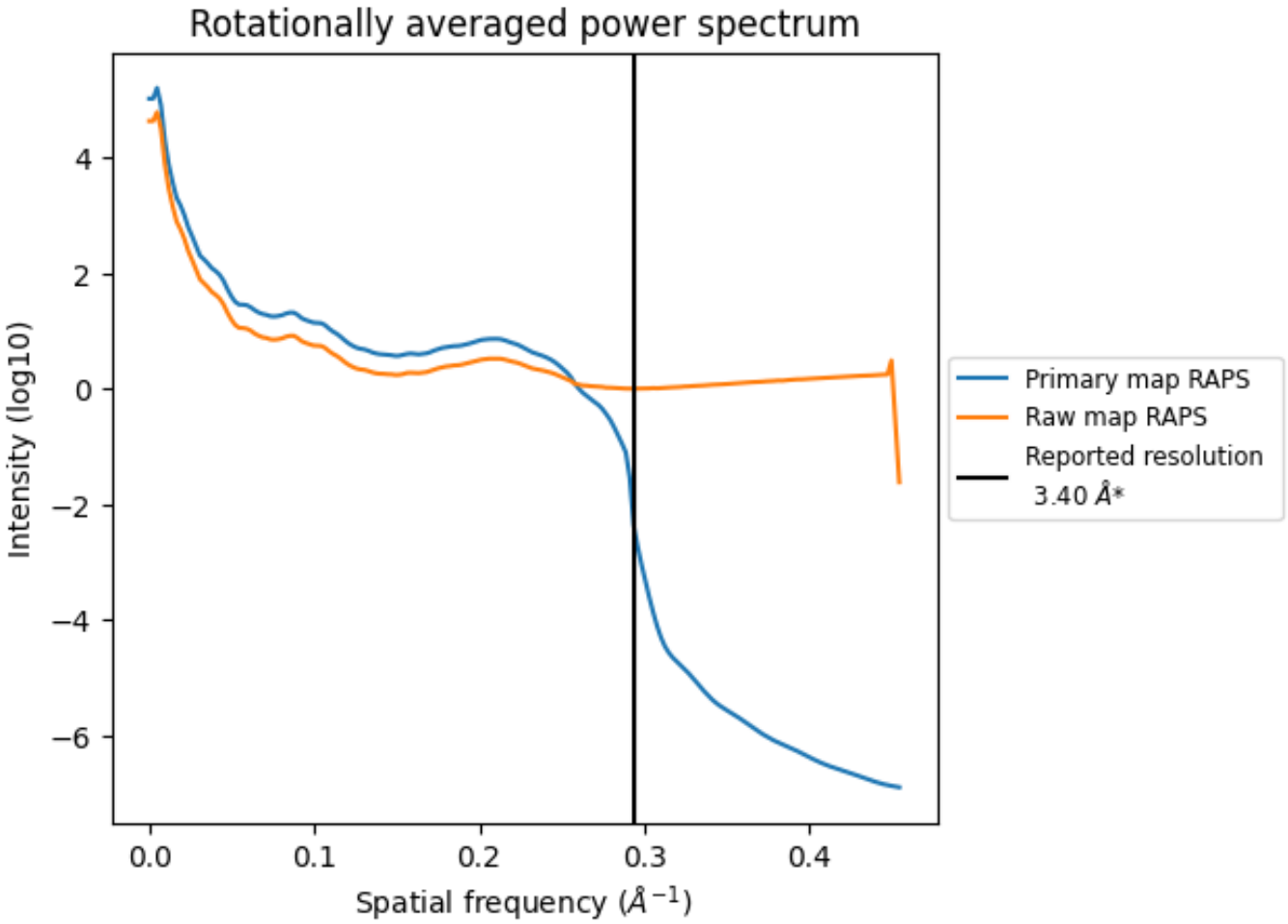
7.2 Volume estimate



The volume at the recommended contour level is 301 nm^3; this corresponds to an approximate mass of 272 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)

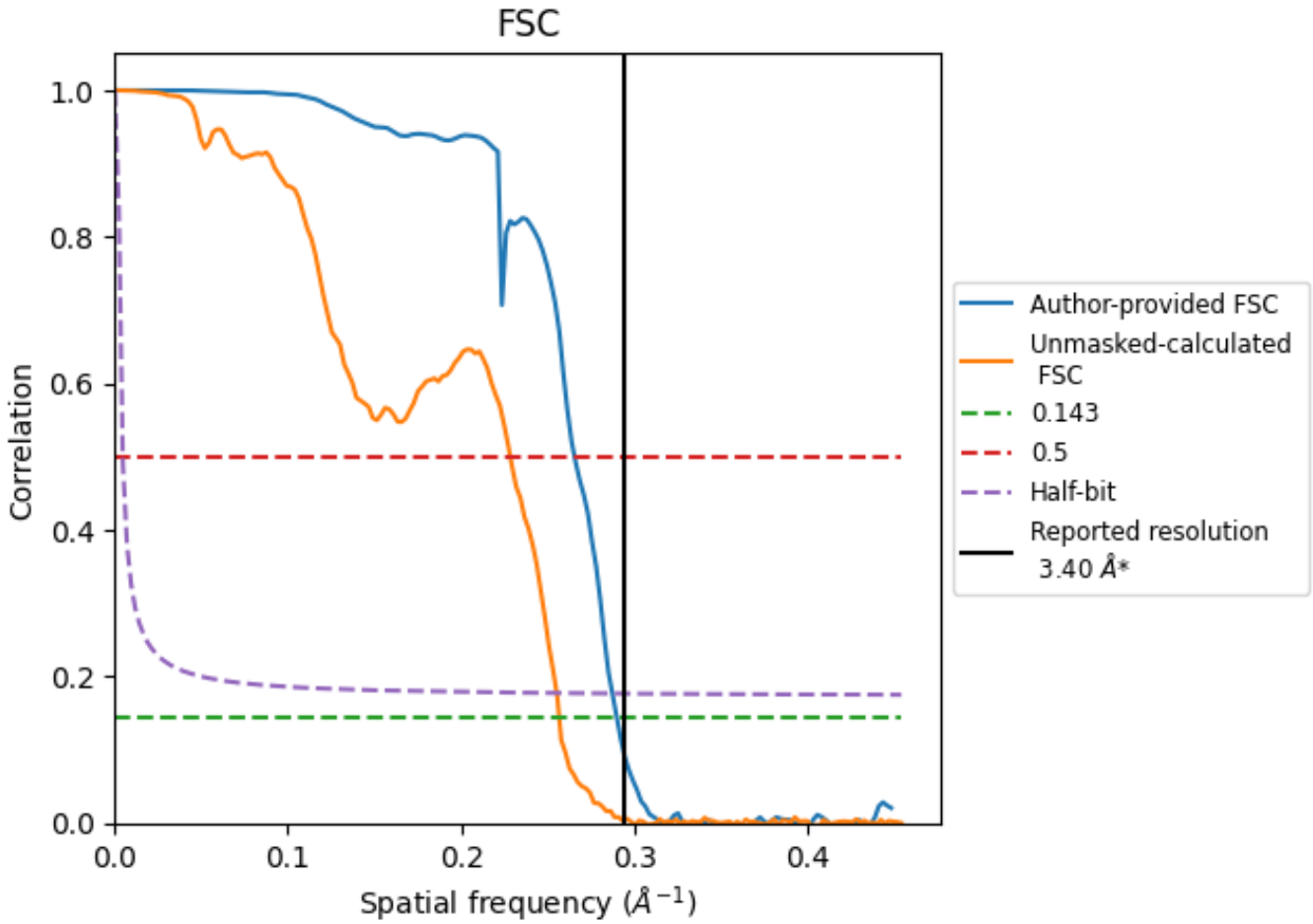


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 (i)

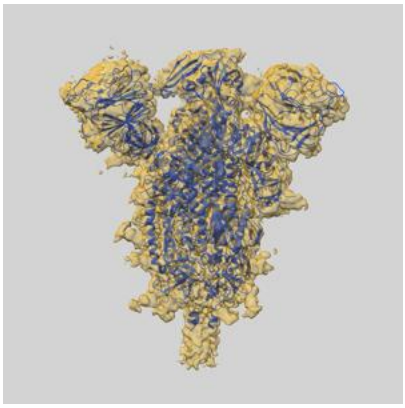
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.45	3.76	3.48
Unmasked-calculated*	3.89	4.38	3.92

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

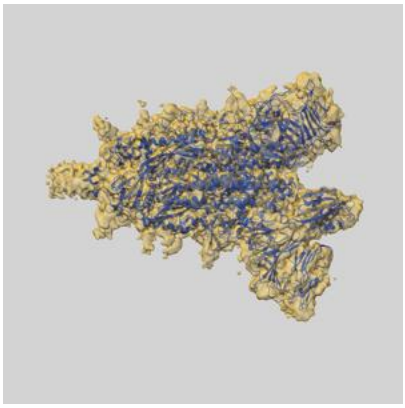
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42456 and PDB model 8UPX. Per-residue inclusion information can be found in section 3 on page 12.

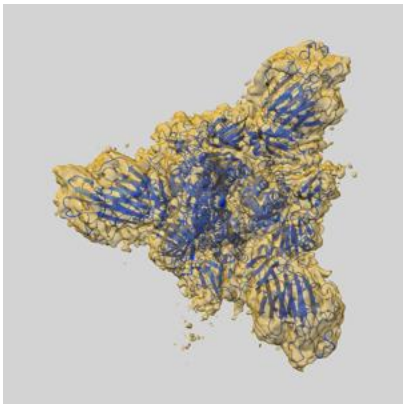
9.1 Map-model overlay



X



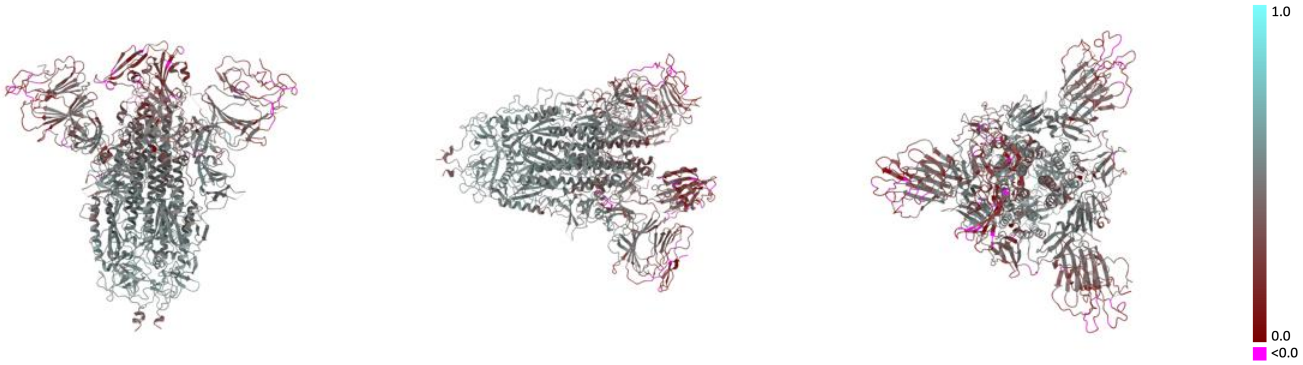
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.103 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.

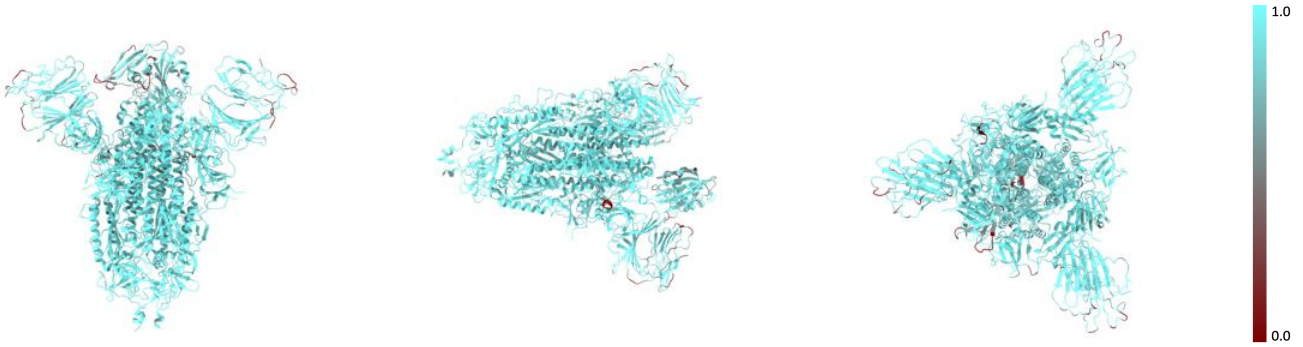
9.2 Q-score mapped to coordinate model (i)



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.

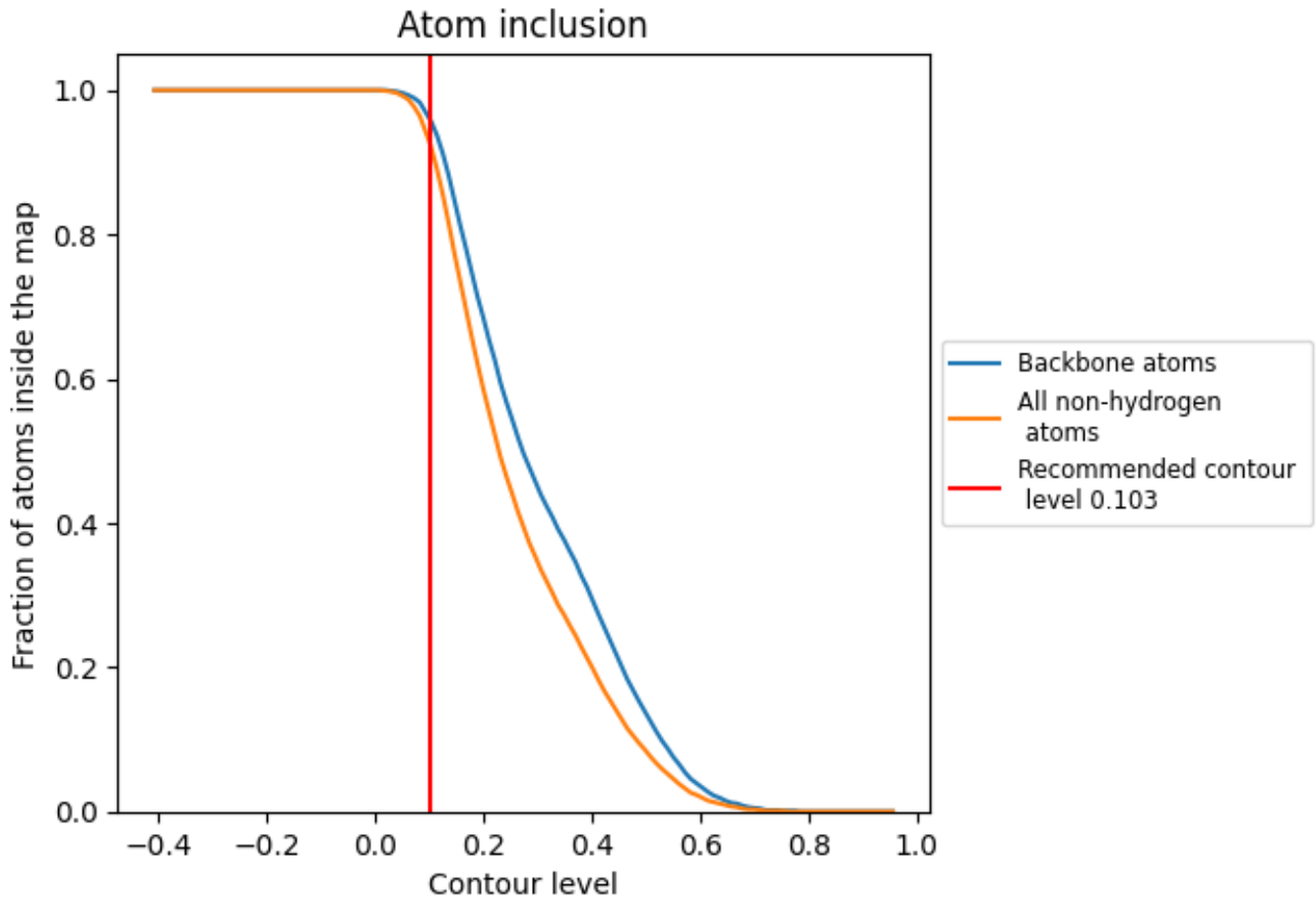
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.103).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.103) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.4180
A	0.9340	0.4290
B	0.9140	0.3970
C	0.9250	0.4300
D	0.9640	0.4320
E	1.0000	0.5070
F	0.8930	0.3630
G	0.9640	0.4570
H	0.9290	0.4170
I	1.0000	0.4990
J	1.0000	0.4410
K	0.9640	0.4710
L	0.8930	0.4000
M	0.9640	0.4760
N	0.9290	0.4600
O	0.9290	0.4450