Full wwPDB EM Validation Report

Oct 1, 2024 – 12:40 PM JST

PDB ID	:	7WGB
EMDB ID	:	EMD-32482
Title	:	Neutral Omicron Spike Trimer in complex with ACE2
Authors	:	Cui, Z.
Deposited on	:	2021-12-28
Resolution	:	3.50 Å(reported)

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

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

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

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

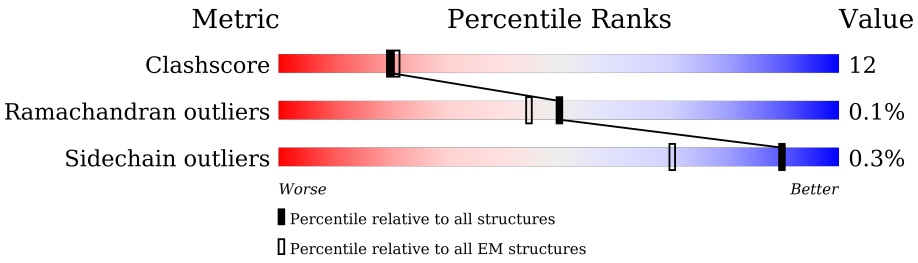
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.50 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	1270	66% 20% 14%
1	B	1270	5% 65% 22% 14%
1	C	1270	7% 62% 24% 14%
2	D	594	65% 61% 39%
2	F	594	81% 67% 33%
3	E	2	100% 100%
3	G	2	50% 100%
3	H	2	100%

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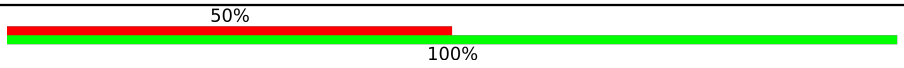
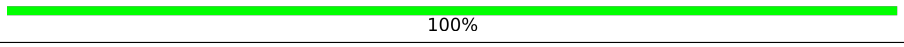
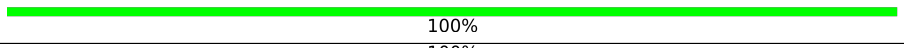
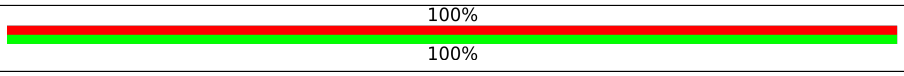
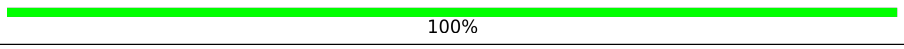
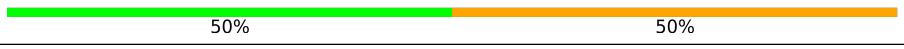
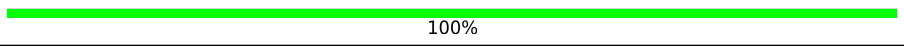
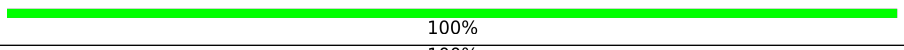
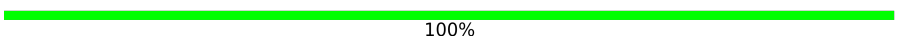
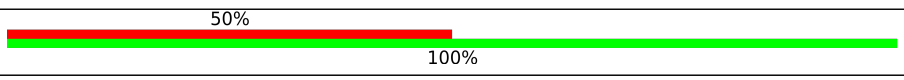
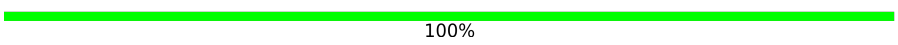
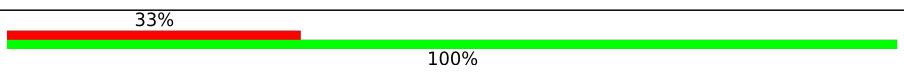
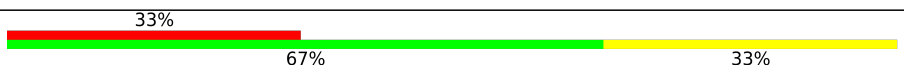
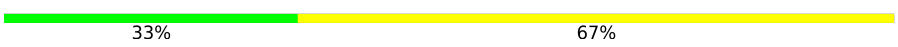
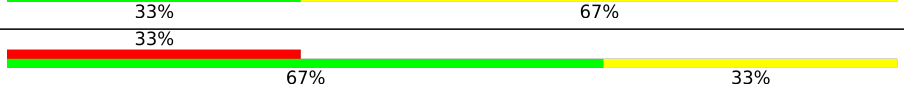
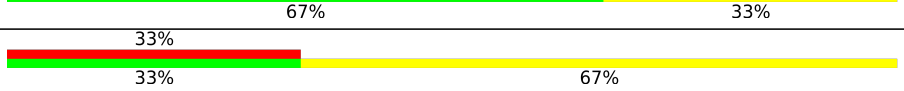
Mol	Chain	Length	Quality of chain
3	I	2	
3	J	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
4	K	3	
4	Q	3	
4	R	3	
4	Y	3	
4	Z	3	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 36719 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	B	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		
1	C	1098	Total	C	N	O	S	0	0
			8632	5525	1439	1629	39		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	211	ILE	-	insertion	UNP P0DTC2
A	212	VAL	-	insertion	UNP P0DTC2
A	213	ARG	ASN	conflict	UNP P0DTC2
A	214	GLU	LEU	conflict	UNP P0DTC2
A	215	PRO	VAL	conflict	UNP P0DTC2
A	216	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	683	ALA	ARG	variant	UNP P0DTC2
A	685	ALA	ARG	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
B	67	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	208	ILE	-	insertion	UNP P0DTC2
B	209	VAL	-	insertion	UNP P0DTC2
B	210	ARG	ASN	conflict	UNP P0DTC2
B	211	GLU	LEU	conflict	UNP P0DTC2
B	212	PRO	VAL	conflict	UNP P0DTC2
B	213	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	variant	UNP P0DTC2
B	685	ALA	ARG	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
C	67	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	211	ILE	-	insertion	UNP P0DTC2
C	212	VAL	-	insertion	UNP P0DTC2
C	213	ARG	ASN	conflict	UNP P0DTC2
C	214	GLU	LEU	conflict	UNP P0DTC2
C	215	PRO	VAL	conflict	UNP P0DTC2
C	216	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	547	LYS	THR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	variant	UNP P0DTC2
C	685	ALA	ARG	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	856	LYS	ASN	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	981	PHE	LEU	variant	UNP P0DTC2

- Molecule 2 is a protein called Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	594	Total	C	N	O	S	1	0
			4852	3104	805	914	29		
2	F	594	Total	C	N	O	S	1	0
			4852	3104	805	914	29		

- Molecule 3 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
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		

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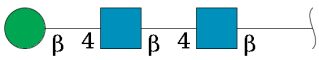
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	3	Total	C	N	O	0	0
			39	22	2	15		
4	Q	3	Total	C	N	O	0	0
			39	22	2	15		
4	R	3	Total	C	N	O	0	0
			39	22	2	15		
4	Y	3	Total	C	N	O	0	0
			39	22	2	15		

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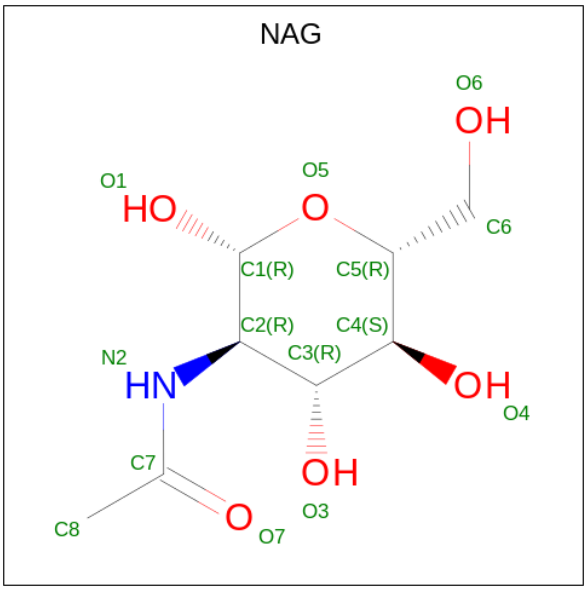
Mol	Chain	Residues	Atoms				AltConf	Trace
4	Z	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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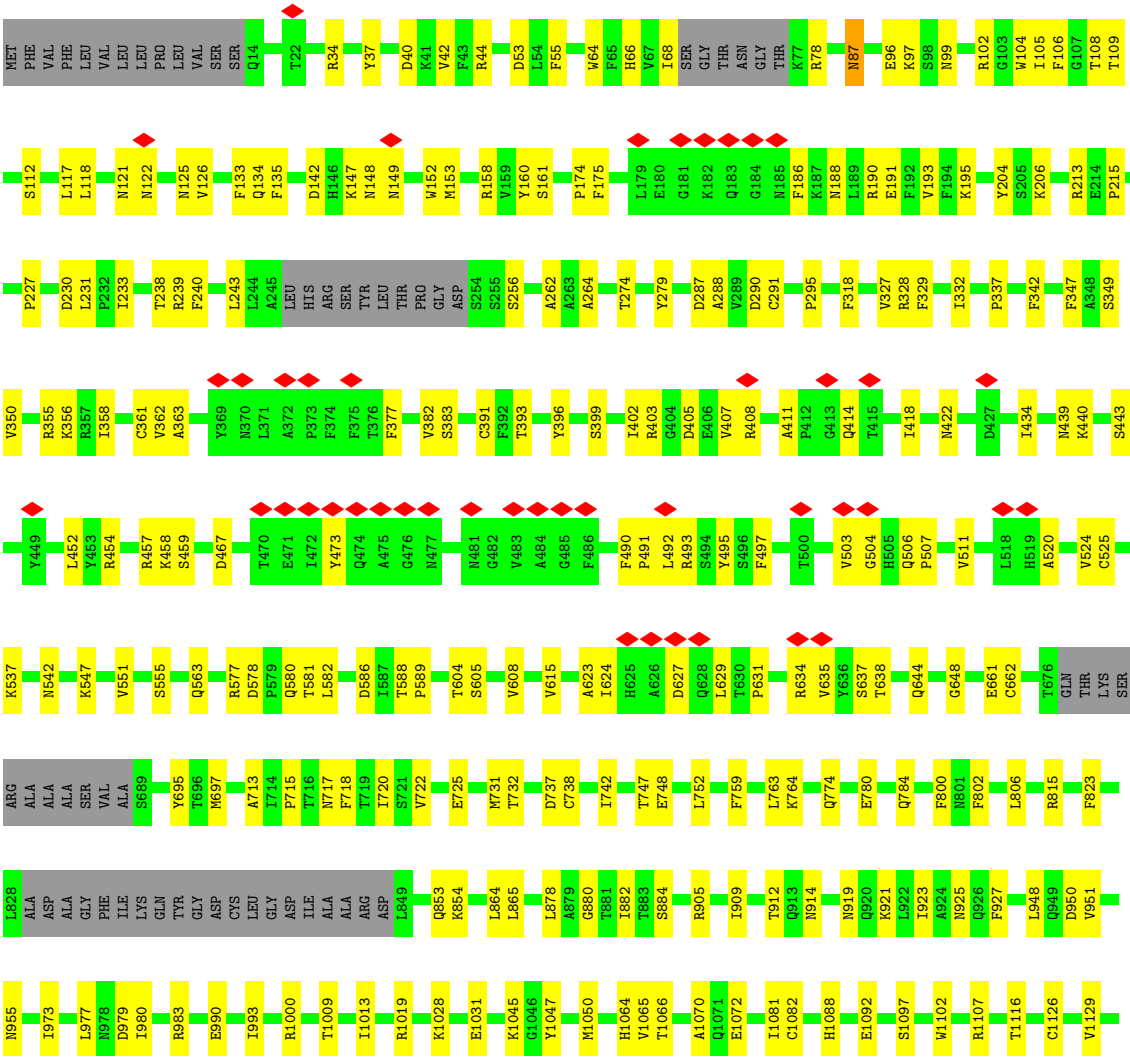
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	

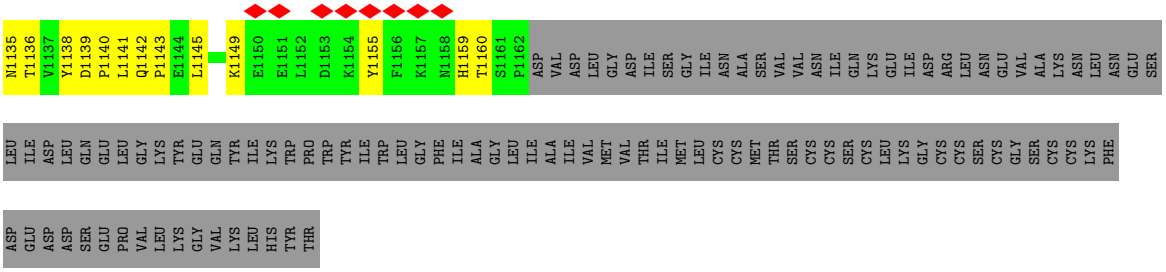
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

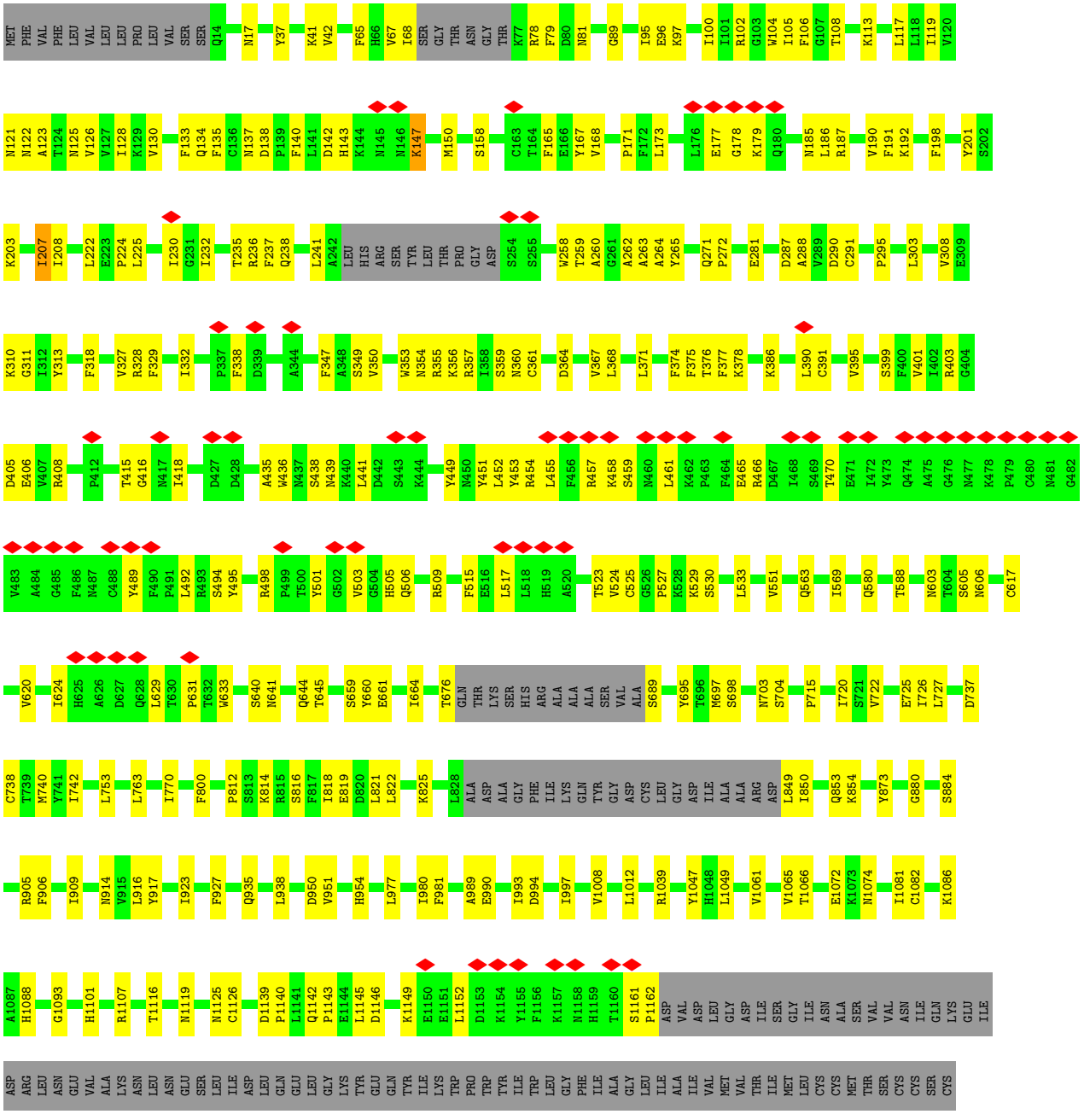
Chain A:





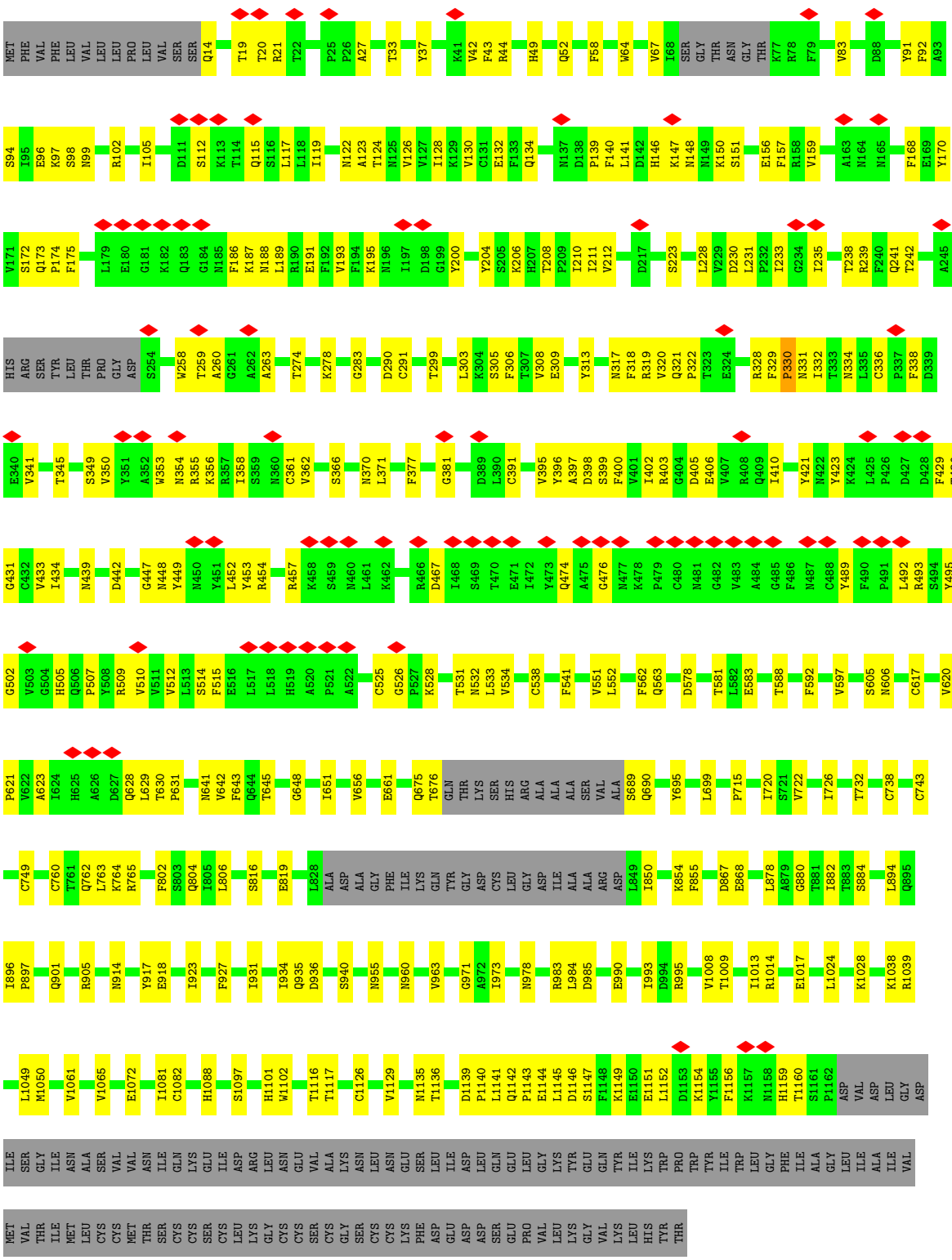
• Molecule 1: Spike glycoprotein

Chain B:



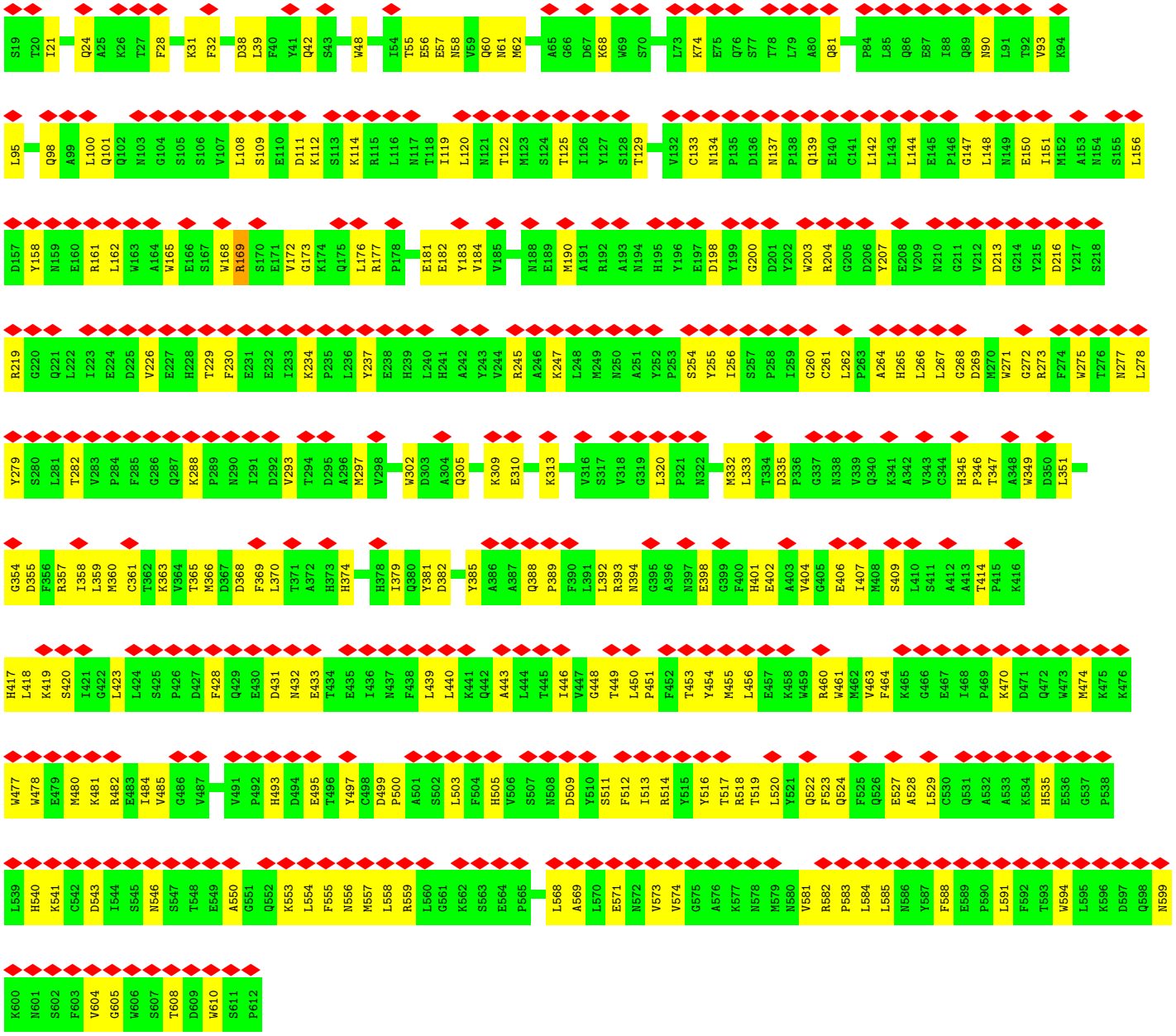
• Molecule 1: Spike glycoprotein

Chain C:



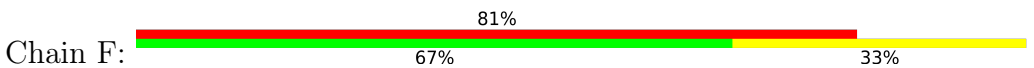
• Molecule 2: Processed angiotensin-converting enzyme 2

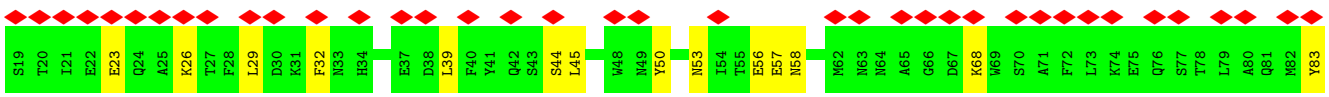
Chain D:

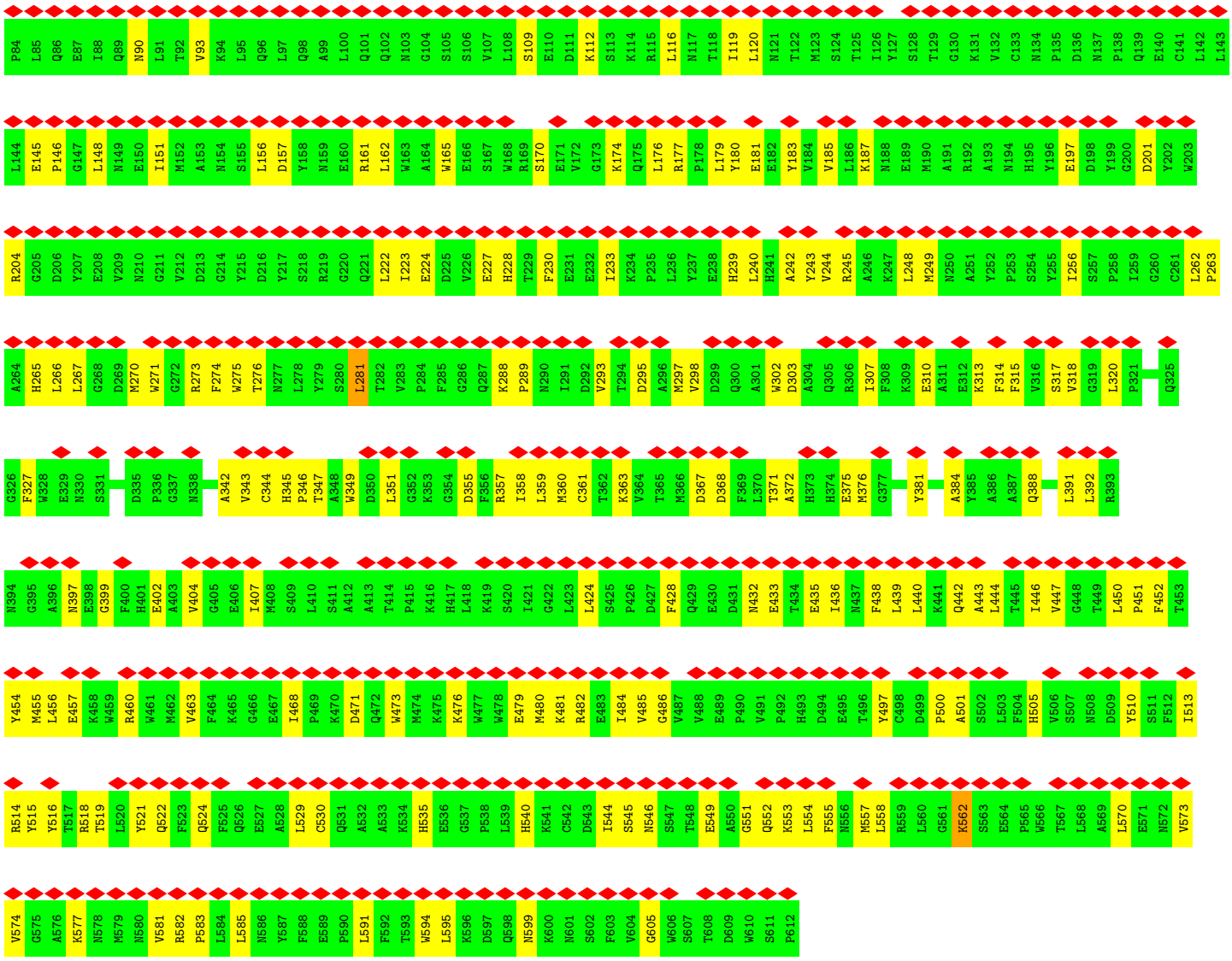


• Molecule 2: Processed angiotensin-converting enzyme 2

Chain F:

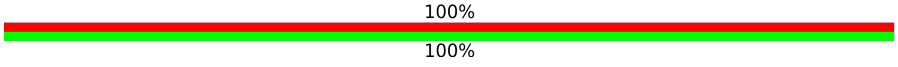






• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

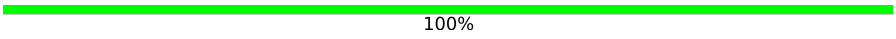


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

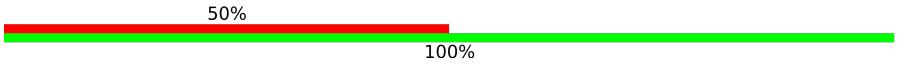
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



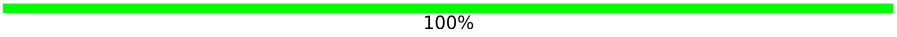
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



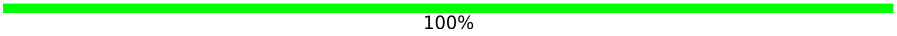
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain L:

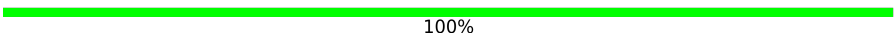


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain N:

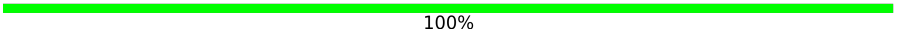


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

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

Chain P:

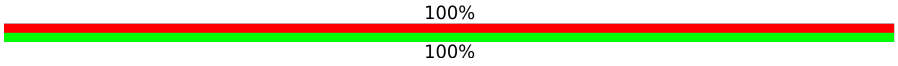


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

Chain T:

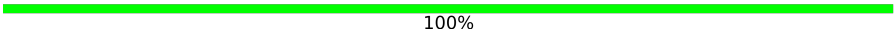


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

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

Chain V:

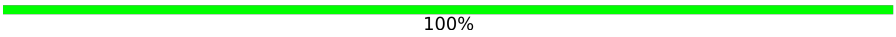


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

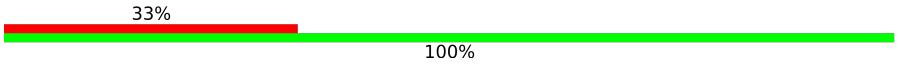
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



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

Chain K:

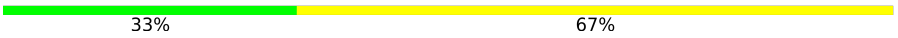


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain Y:

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

Chain Z:

NAG1
NAG2
BMA3

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	293334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.706	Depositor
Minimum map value	-1.037	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.404	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	0/8837	0.49	0/12019
1	B	0.28	0/8837	0.49	0/12019
1	C	0.28	0/8837	0.50	0/12019
2	D	0.25	0/4992	0.46	0/6782
2	F	0.26	0/4992	0.47	1/6782 (0.0%)
All	All	0.27	0/36495	0.49	1/49621 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	281	LEU	CA-CB-CG	5.42	127.76	115.30

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	8632	0	8451	181	0
1	B	8632	0	8450	185	0
1	C	8632	0	8451	204	0
2	D	4852	0	4628	180	0
2	F	4852	0	4628	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	2	0
3	P	28	0	25	0	0
3	S	28	0	25	0	0
3	T	28	0	24	0	0
3	U	28	0	25	1	0
3	V	28	0	25	0	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
4	K	39	0	34	0	0
4	Q	39	0	34	1	0
4	R	39	0	34	1	0
4	Y	39	0	34	1	0
4	Z	39	0	34	1	0
5	A	112	0	102	2	0
5	B	126	0	115	2	0
5	C	126	0	113	0	0
5	D	56	0	52	1	0
5	F	56	0	52	1	0
All	All	36719	0	35611	883	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 12.

All (883) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.55	0.89
1:C:358:ILE:O	1:C:395:VAL:HB	1.74	0.88
1:A:126:VAL:HG23	1:A:174:PRO:HA	1.57	0.86
2:D:573:VAL:HG13	2:D:574:VAL:HG23	1.61	0.82
1:A:604:THR:HG22	1:A:605:SER:H	1.49	0.78
1:C:732:THR:OG1	1:C:955:ASN:ND2	2.17	0.77
1:A:1081:ILE:HD11	1:A:1135:ASN:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:LEU:HG	1:C:631:PRO:HD2	1.68	0.75
2:F:457:GLU:HG3	2:F:513:ILE:HB	1.67	0.75
2:D:247:LYS:HG2	2:D:282:THR:HA	1.68	0.75
1:A:408:ARG:O	1:A:414:GLN:NE2	2.18	0.75
1:C:96:GLU:O	1:C:188:ASN:HB2	1.86	0.75
1:B:186:LEU:HB2	1:B:208:ILE:HD11	1.67	0.75
1:B:489:TYR:HH	2:F:83:TYR:HH	1.32	0.74
1:C:642:VAL:HG22	1:C:651:ILE:HG12	1.70	0.73
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.70	0.73
1:C:457:ARG:HE	1:C:467:ASP:HB3	1.53	0.73
2:D:173:GLY:HA2	2:D:176:LEU:HB2	1.70	0.73
1:B:1139:ASP:HB3	1:B:1142:GLN:HG2	1.71	0.73
1:A:411:ALA:HB3	1:A:414:GLN:HE22	1.53	0.73
1:C:623:ALA:HA	1:C:628:GLN:HE22	1.54	0.73
1:B:360:ASN:H	1:B:523:THR:HB	1.53	0.72
2:F:450:LEU:HD12	2:F:516:TYR:HD1	1.54	0.72
2:F:381:TYR:HB2	2:F:404:VAL:HG11	1.71	0.72
1:A:644:GLN:NE2	1:A:648:GLY:O	2.22	0.72
1:C:27:ALA:HB3	1:C:64:TRP:O	1.89	0.72
2:F:288:LYS:HE3	2:F:433:GLU:HB2	1.73	0.71
2:F:521:TYR:HE2	2:F:570:LEU:HD21	1.55	0.71
1:C:274:THR:HG23	1:C:291:CYS:HB3	1.72	0.71
1:A:732:THR:OG1	1:A:955:ASN:ND2	2.24	0.70
1:B:17:ASN:OD1	1:B:137:ASN:ND2	2.24	0.70
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.72	0.70
2:F:161:ARG:HH12	2:F:266:LEU:HD23	1.54	0.70
1:A:213:ARG:HG3	1:A:215:PRO:HD3	1.73	0.70
2:D:142:LEU:HB2	2:D:147:GLY:HA3	1.74	0.70
1:B:190:VAL:HG12	1:B:201:TYR:HB2	1.73	0.69
2:D:493:HIS:NE2	2:D:499:ASP:OD2	2.24	0.69
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.74	0.69
1:B:763:LEU:HD12	1:B:1008:VAL:HG21	1.74	0.69
1:C:804:GLN:NE2	1:C:935:GLN:OE1	2.26	0.69
2:D:404:VAL:HA	2:D:407:ILE:HD12	1.72	0.69
2:F:170:SER:HB2	2:F:174:LYS:HE3	1.75	0.69
1:A:1141:LEU:HD23	1:A:1145:LEU:HD23	1.75	0.69
1:A:950:ASP:OD2	1:A:951:VAL:N	2.27	0.68
1:B:659:SER:HB2	1:B:698:SER:HB3	1.75	0.68
2:F:443:ALA:HA	2:F:446:ILE:HG22	1.74	0.68
1:A:193:VAL:HG12	1:A:204:TYR:HB2	1.74	0.68
2:D:527:GLU:HB2	2:D:583:PRO:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1116:THR:HB	1:C:1140:PRO:HD3	1.75	0.67
1:B:1093:GLY:O	1:B:1107:ARG:NH1	2.27	0.67
2:D:109:SER:OG	2:D:111:ASP:OD1	2.13	0.67
1:C:474:GLN:NE2	1:C:476:GLY:O	2.28	0.67
1:B:96:GLU:O	1:B:185:ASN:HB2	1.93	0.67
2:F:256:ILE:HD12	2:F:263:PRO:HG3	1.75	0.67
2:F:460:ARG:NH1	2:F:500:PRO:O	2.26	0.67
2:F:148:LEU:HB3	2:F:270:MET:HG2	1.77	0.67
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.28	0.66
1:B:350:VAL:HG11	1:B:418:ILE:HG22	1.76	0.66
1:B:67:VAL:O	1:B:263:ALA:N	2.29	0.66
1:A:563:GLN:NE2	1:C:42:VAL:O	2.28	0.66
2:D:310:GLU:HA	2:D:313:LYS:HE2	1.78	0.66
1:B:950:ASP:O	1:B:954:HIS:ND1	2.28	0.66
1:B:909:ILE:HD12	1:B:1047:TYR:HB3	1.77	0.66
1:C:1141:LEU:HD23	1:C:1145:LEU:HD23	1.78	0.65
2:D:169:ARG:HH21	2:D:493:HIS:HE1	1.43	0.65
2:D:460:ARG:HA	2:D:463:VAL:HG12	1.78	0.65
1:A:439:ASN:HB3	1:A:506:GLN:HB3	1.78	0.65
2:D:177:ARG:NH1	2:D:470:LYS:O	2.30	0.65
1:B:147:LYS:HB3	1:B:259:THR:HB	1.79	0.65
2:D:55:THR:OG1	2:D:58:ASN:OD1	2.15	0.65
2:D:439:LEU:HD12	2:D:591:LEU:HB2	1.78	0.65
2:F:177:ARG:NH2	2:F:497:TYR:O	2.30	0.64
2:F:519:THR:O	2:F:522:GLN:HG2	1.97	0.64
1:C:14:GLN:HE22	1:C:156:GLU:HA	1.63	0.64
2:D:402:GLU:HB2	2:D:518:ARG:HG3	1.80	0.64
1:B:68:ILE:HA	1:B:262:ALA:HA	1.80	0.64
1:C:905:ARG:HH12	1:C:1050:MET:HB3	1.62	0.64
2:F:109:SER:OG	2:F:112:LYS:NZ	2.31	0.64
1:B:130:VAL:HB	1:B:165:PHE:HB3	1.80	0.63
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.30	0.63
1:B:338:PHE:HZ	1:B:395:VAL:HG11	1.62	0.63
1:C:328:ARG:NH2	1:C:531:THR:O	2.28	0.63
1:A:629:LEU:HG	1:A:631:PRO:HD2	1.81	0.63
1:B:81:ASN:O	1:B:238:GLN:NE2	2.31	0.63
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.81	0.63
1:C:37:TYR:OH	1:C:195:LYS:NZ	2.32	0.63
1:C:150:LYS:HB3	1:C:259:THR:HB	1.81	0.63
1:A:99:ASN:O	1:A:102:ARG:NH1	2.31	0.63
2:D:388:GLN:HB3	2:D:392:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:SER:OG	1:A:452:LEU:O	2.17	0.62
2:D:524:GLN:HB3	2:D:574:VAL:HG21	1.79	0.62
2:F:347:THR:HG1	2:F:349:TRP:HE1	1.47	0.62
1:A:990:GLU:HA	1:A:993:ILE:HG12	1.80	0.62
2:D:453:THR:HA	2:D:512:PHE:HE2	1.63	0.62
2:F:243:TYR:HD1	2:F:599:ASN:HD21	1.47	0.62
1:B:644:GLN:NE2	1:B:645:THR:O	2.29	0.62
1:A:977:LEU:HA	1:A:980:ILE:HD12	1.81	0.62
1:B:126:VAL:HG13	1:B:171:PRO:HA	1.80	0.62
1:B:470:THR:HG21	1:B:492:LEU:HD23	1.80	0.62
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.31	0.62
1:B:386:LYS:HG3	1:B:390:LEU:HD11	1.82	0.62
1:C:1144:GLU:O	1:C:1147:SER:OG	2.18	0.62
2:D:245:ARG:NH2	2:D:605:GLY:O	2.32	0.62
2:D:365:THR:O	2:D:369:PHE:N	2.27	0.62
1:A:457:ARG:NH1	1:A:459:SER:OG	2.33	0.62
2:F:381:TYR:HA	2:F:558:LEU:HD11	1.80	0.62
1:A:105:ILE:HG12	1:A:118:LEU:HD22	1.82	0.61
2:F:446:ILE:O	2:F:450:LEU:HD23	2.00	0.61
2:F:314:PHE:HZ	2:F:544:ILE:HB	1.64	0.61
1:B:311:GLY:HA2	1:B:664:ILE:HD12	1.80	0.61
1:C:115:GLN:HG2	1:C:132:GLU:HG3	1.83	0.61
1:A:454:ARG:HA	1:A:492:LEU:HG	1.82	0.61
1:A:661:GLU:O	1:A:695:TYR:OH	2.18	0.61
1:A:290:ASP:OD1	1:A:291:CYS:N	2.31	0.61
1:A:327:VAL:HG12	1:A:542:ASN:HB3	1.83	0.61
1:B:917:TYR:HB3	1:C:1129:VAL:HG23	1.83	0.61
1:C:905:ARG:NH1	1:C:1049:LEU:O	2.34	0.61
1:A:328:ARG:NH2	1:A:580:GLN:OE1	2.33	0.61
1:B:332:ILE:HG21	1:B:527:PRO:HB3	1.81	0.61
2:D:57:GLU:O	2:D:61:ASN:ND2	2.33	0.61
1:C:452:LEU:HG	1:C:492:LEU:HB3	1.82	0.60
2:D:108:LEU:HD21	2:D:190:MET:HA	1.81	0.60
2:D:234:LYS:HZ1	2:D:484:ILE:HA	1.66	0.60
1:B:449:TYR:OH	1:B:498:ARG:NH2	2.33	0.60
2:D:511:SER:OG	2:D:514:ARG:NE	2.34	0.60
1:A:34:ARG:NH1	1:A:223:SER:OG	2.35	0.60
1:A:42:VAL:O	1:B:563:GLN:NE2	2.32	0.60
1:C:206:LYS:NZ	1:C:223:SER:OG	2.30	0.60
2:D:261:CYS:SG	2:D:262:LEU:N	2.73	0.60
1:B:89:GLY:CA	1:B:191:PHE:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:TRP:HZ3	2:D:310:GLU:HG2	1.67	0.60
2:D:453:THR:HA	2:D:512:PHE:CE2	2.36	0.60
1:C:238:THR:OG1	1:C:239:ARG:NH1	2.34	0.60
2:F:267:LEU:HG	2:F:275:TRP:HE1	1.67	0.60
2:F:346:PRO:HA	2:F:359:LEU:O	2.00	0.60
2:F:482:ARG:HA	2:F:486:GLY:HA2	1.84	0.60
2:F:582:ARG:HD2	2:F:585:LEU:HD12	1.83	0.60
1:A:921:LYS:NZ	1:A:925:ASN:OD1	2.34	0.60
2:D:133:CYS:SG	2:D:134:ASN:N	2.71	0.59
2:D:183:TYR:OH	2:D:509:ASP:OD1	2.20	0.59
2:F:346:PRO:HD2	2:F:371:THR:HG21	1.83	0.59
1:C:67:VAL:HB	1:C:263:ALA:HB3	1.84	0.59
1:C:331:ASN:HB3	1:C:332:ILE:HA	1.83	0.59
1:C:581:THR:OG1	1:C:583:GLU:OE1	2.17	0.59
1:C:1141:LEU:HA	1:C:1144:GLU:HB2	1.83	0.59
2:D:90:ASN:HB3	2:D:93:VAL:HB	1.84	0.59
2:F:371:THR:O	2:F:375:GLU:HG2	2.02	0.59
1:C:97:LYS:HB2	1:C:186:PHE:HA	1.85	0.59
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	1.84	0.59
2:F:32:PHE:HE2	2:F:391:LEU:HD21	1.66	0.59
1:A:108:THR:O	1:A:239:ARG:NH1	2.36	0.59
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.38	0.59
1:C:403:ARG:NH2	1:C:405:ASP:OD2	2.35	0.59
2:D:48:TRP:HB2	2:D:351:LEU:HD11	1.85	0.59
2:F:242:ALA:HB2	2:F:605:GLY:H	1.68	0.59
2:F:524:GLN:HG2	2:F:583:PRO:HG2	1.85	0.59
1:C:355:ARG:NH2	1:C:398:ASP:OD2	2.36	0.58
1:C:1139:ASP:HB3	1:C:1142:GLN:HB2	1.85	0.58
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.34	0.58
1:C:52:GLN:OE1	1:C:274:THR:HB	2.04	0.58
1:A:87:ASN:O	1:A:87:ASN:ND2	2.34	0.58
1:A:912:THR:OG1	1:A:914:ASN:OD1	2.22	0.58
1:A:1047:TYR:O	1:A:1066:THR:OG1	2.19	0.58
1:B:106:PHE:CD1	1:B:237:PHE:HB2	2.38	0.58
2:F:456:LEU:O	2:F:460:ARG:HG2	2.03	0.58
1:A:133:PHE:HB3	1:A:160:TYR:HB2	1.86	0.58
1:A:909:ILE:HD12	1:A:1047:TYR:HB3	1.86	0.58
1:B:42:VAL:O	1:C:563:GLN:NE2	2.35	0.58
1:B:121:ASN:HB3	1:B:126:VAL:HG12	1.85	0.58
1:C:661:GLU:O	1:C:695:TYR:OH	2.21	0.58
1:C:290:ASP:OD1	1:C:291:CYS:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:GLY:HA3	1:C:430:THR:HG23	1.85	0.58
1:C:403:ARG:HG2	1:C:505:HIS:HA	1.85	0.58
1:A:1145:LEU:O	1:A:1149:LYS:HG2	2.04	0.58
1:C:366:SER:O	1:C:370:ASN:ND2	2.36	0.58
2:F:514:ARG:HB2	2:F:518:ARG:HH21	1.68	0.58
1:A:68:ILE:H	1:A:78:ARG:HB3	1.68	0.57
1:A:1081:ILE:HG23	1:A:1088:HIS:HB2	1.86	0.57
1:C:453:TYR:HB3	1:C:495:TYR:HE1	1.69	0.57
2:F:327:PHE:HE1	2:F:358:ILE:H	1.51	0.57
1:C:971:GLY:HA3	1:C:995:ARG:HH22	1.68	0.57
2:D:279:TYR:HE1	2:D:440:LEU:HD23	1.70	0.57
1:B:173:LEU:O	1:B:187:ARG:NH2	2.33	0.57
1:B:353:TRP:O	1:B:466:ARG:NH2	2.31	0.57
1:C:320:VAL:HG13	1:C:628:GLN:HE21	1.70	0.57
2:D:137:ASN:OD1	2:D:139:GLN:NE2	2.38	0.57
2:D:503:LEU:HD23	2:D:505:HIS:H	1.69	0.57
1:B:1101:HIS:CE1	4:Q:1:NAG:H5	2.39	0.57
1:B:816:SER:N	1:B:819:GLU:OE1	2.37	0.57
1:A:1116:THR:HB	1:A:1140:PRO:HD3	1.86	0.57
1:A:979:ASP:HB3	1:A:983:ARG:HH12	1.70	0.57
2:D:297:MET:HA	2:D:302:TRP:CD1	2.40	0.56
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.87	0.56
1:C:914:ASN:O	1:C:918:GLU:HG2	2.05	0.56
2:F:367:ASP:OD1	2:F:368:ASP:N	2.38	0.56
1:B:1081:ILE:HG23	1:B:1088:HIS:HB2	1.88	0.56
1:C:331:ASN:HD21	3:U:1:NAG:HN2	1.53	0.56
1:C:802:PHE:HB3	1:C:806:LEU:HD23	1.88	0.56
2:F:245:ARG:HH12	2:F:249:MET:HG2	1.70	0.56
1:B:177:GLU:HG2	1:B:178:GLY:H	1.70	0.56
2:D:528:ALA:HB2	2:D:574:VAL:HG22	1.87	0.56
1:A:37:TYR:OH	1:A:195:LYS:NZ	2.32	0.56
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.70	0.56
1:A:355:ARG:NH2	1:C:200:TYR:OH	2.39	0.56
1:B:327:VAL:HG23	1:B:530:SER:HA	1.88	0.56
1:C:317:ASN:OD1	1:C:318:PHE:N	2.39	0.56
2:D:269:ASP:HB2	2:D:272:GLY:H	1.70	0.56
1:B:980:ILE:HG22	1:B:989:ALA:HB1	1.88	0.55
1:C:230:ASP:OD1	1:C:231:LEU:N	2.38	0.55
2:F:116:LEU:HD11	2:F:187:LYS:HD3	1.88	0.55
1:C:330:PRO:HB2	1:C:332:ILE:HB	1.88	0.55
2:D:417:HIS:HA	2:D:420:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1:NAG:H3	3:O:1:NAG:H83	1.88	0.55
1:B:1143:PRO:HA	1:B:1146:ASP:HB2	1.88	0.55
1:C:623:ALA:HB1	1:C:629:LEU:HD22	1.88	0.55
1:C:973:ILE:HG21	1:C:983:ARG:HH12	1.70	0.55
1:A:147:LYS:HG2	1:A:153:MET:HB3	1.88	0.55
1:A:802:PHE:HE1	1:A:927:PHE:HE2	1.54	0.55
1:B:376:THR:HB	1:B:435:ALA:HB3	1.88	0.55
1:B:990:GLU:HA	1:B:993:ILE:HG12	1.87	0.55
1:C:396:TYR:HB2	1:C:514:SER:HB3	1.89	0.55
2:D:394:ASN:OD1	2:D:401:HIS:NE2	2.30	0.55
2:F:399:GLY:HA3	2:F:518:ARG:HB3	1.88	0.55
1:C:173:GLN:OE1	1:C:174:PRO:HD2	2.07	0.55
1:C:489:TYR:HE2	2:D:28:PHE:HA	1.71	0.55
1:A:439:ASN:O	1:A:443:SER:OG	2.24	0.55
1:A:880:GLY:O	1:A:884:SER:OG	2.21	0.55
1:A:1139:ASP:HB3	1:A:1142:GLN:HG3	1.87	0.55
1:C:189:LEU:HB2	1:C:211:ILE:HG13	1.89	0.55
1:C:439:ASN:HA	1:C:507:PRO:HG2	1.89	0.55
1:C:1139:ASP:OD2	1:C:1142:GLN:N	2.40	0.55
1:C:1143:PRO:HA	1:C:1146:ASP:HB2	1.89	0.55
2:F:271:TRP:HE1	2:F:273:ARG:HD2	1.72	0.55
2:F:530:CYS:O	2:F:535:HIS:ND1	2.39	0.55
1:B:303:LEU:HD12	1:B:308:VAL:HG12	1.89	0.55
2:D:165:TRP:O	2:D:169:ARG:NH1	2.40	0.55
2:D:200:GLY:HA3	2:D:461:TRP:HZ3	1.72	0.55
2:D:478:TRP:HE1	2:D:493:HIS:HD2	1.55	0.54
2:F:468:ILE:HD12	2:F:473:TRP:HE1	1.72	0.54
1:B:290:ASP:OD1	1:B:291:CYS:N	2.41	0.54
1:B:368:LEU:O	1:B:374:PHE:HE2	1.91	0.54
1:B:676:THR:HG23	1:B:689:SER:HB2	1.89	0.54
2:D:293:VAL:HG11	2:D:423:LEU:HD13	1.89	0.54
1:C:973:ILE:HD12	1:C:984:LEU:HD11	1.90	0.54
2:D:335:ASP:HB3	2:D:361:CYS:HA	1.88	0.54
2:F:545:SER:HB3	5:F:701:NAG:H82	1.89	0.54
1:B:403:ARG:NH1	1:B:406:GLU:OE2	2.41	0.54
1:B:403:ARG:HG2	1:B:405:ASP:H	1.72	0.54
1:C:532:ASN:OD1	1:C:533:LEU:N	2.40	0.54
2:F:438:PHE:O	2:F:442:GLN:HG2	2.08	0.54
1:B:880:GLY:O	1:B:884:SER:OG	2.20	0.54
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.90	0.54
1:A:108:THR:HA	1:A:238:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:275:TRP:NE1	2:D:448:GLY:O	2.41	0.54
1:C:309:GLU:N	1:C:309:GLU:OE1	2.41	0.54
1:A:752:LEU:HD22	1:A:993:ILE:HD11	1.89	0.54
1:B:449:TYR:O	1:B:494:SER:OG	2.25	0.54
2:F:363:LYS:N	2:F:368:ASP:OD2	2.41	0.53
2:F:230:PHE:HA	2:F:233:ILE:HG22	1.90	0.53
1:A:490:PHE:HB3	1:A:493:ARG:HH12	1.71	0.53
1:B:37:TYR:OH	1:B:192:LYS:NZ	2.35	0.53
1:C:141:LEU:HD21	1:C:157:PHE:HA	1.89	0.53
2:F:440:LEU:HD13	2:F:591:LEU:HD11	1.90	0.53
2:D:320:LEU:HD22	2:D:555:PHE:HD1	1.72	0.53
2:F:148:LEU:HA	2:F:151:ILE:HG22	1.90	0.53
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.57	0.53
1:C:187:LYS:HD2	1:C:210:ILE:HA	1.91	0.53
2:D:177:ARG:NE	2:D:495:GLU:O	2.41	0.53
1:A:393:THR:HG21	1:A:520:ALA:HB3	1.91	0.53
1:C:502:GLY:HA3	2:D:354:GLY:HA3	1.90	0.53
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.89	0.53
1:A:175:PHE:HB3	1:A:190:ARG:HH22	1.74	0.53
1:B:703:ASN:OD1	1:B:704:SER:N	2.42	0.53
1:C:816:SER:N	1:C:819:GLU:OE1	2.40	0.53
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.41	0.53
1:B:401:VAL:HB	1:B:451:TYR:HE2	1.74	0.53
1:C:1081:ILE:O	1:C:1088:HIS:N	2.42	0.53
2:F:176:LEU:O	2:F:180:TYR:N	2.39	0.53
2:F:303:ASP:N	2:F:303:ASP:OD1	2.41	0.53
2:F:392:LEU:HD23	2:F:562:LYS:HE3	1.91	0.53
2:D:234:LYS:HZ3	2:D:484:ILE:HG23	1.73	0.52
2:D:119:ILE:HD13	2:D:182:GLU:HG2	1.91	0.52
2:F:45:LEU:HD22	2:F:351:LEU:HD12	1.91	0.52
1:A:350:VAL:HG12	1:A:402:ILE:HG22	1.91	0.52
1:A:382:VAL:HG12	1:C:983:ARG:HB3	1.90	0.52
1:B:89:GLY:HA3	1:B:191:PHE:O	2.09	0.52
1:B:354:ASN:O	1:B:356:LYS:NZ	2.42	0.52
2:D:293:VAL:HB	2:D:423:LEU:HD22	1.92	0.52
2:D:366:MET:O	2:D:369:PHE:HB3	2.10	0.52
1:A:328:ARG:HH11	1:A:533:LEU:HG	1.74	0.52
1:A:329:PHE:O	1:A:580:GLN:NE2	2.42	0.52
1:A:780:GLU:O	1:A:784:GLN:NE2	2.42	0.52
2:D:81:GLN:HA	2:D:101:GLN:HE21	1.73	0.52
2:D:382:ASP:HA	2:D:385:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PHE:HE2	1:C:170:TYR:HB2	1.73	0.52
1:A:102:ARG:HD3	1:A:122:ASN:HA	1.90	0.52
1:B:661:GLU:O	1:B:695:TYR:OH	2.19	0.52
1:A:121:ASN:HB3	1:A:126:VAL:HG22	1.92	0.52
1:A:193:VAL:CG1	1:A:204:TYR:HB2	2.39	0.52
1:A:578:ASP:HB3	1:A:581:THR:O	2.10	0.52
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.90	0.52
2:D:269:ASP:OD2	2:D:273:ARG:N	2.42	0.52
2:D:351:LEU:HB2	2:D:355:ASP:HB3	1.92	0.52
1:C:187:LYS:HE2	1:C:212:VAL:HG12	1.90	0.52
1:B:1116:THR:HB	1:B:1140:PRO:HD3	1.91	0.52
1:C:92:PHE:CZ	1:C:94:SER:HB3	2.44	0.52
1:C:402:ILE:HD12	1:C:406:GLU:HB2	1.92	0.52
2:F:342:ALA:HB1	2:F:359:LEU:HD21	1.91	0.52
1:A:503:VAL:HA	1:A:506:GLN:HE22	1.74	0.51
1:B:375:PHE:HB2	1:B:436:TRP:HA	1.92	0.51
2:D:455:MET:HE1	2:D:481:LYS:HA	1.92	0.51
2:D:599:ASN:HB3	2:D:604:VAL:HG11	1.92	0.51
1:A:504:GLY:N	1:A:506:GLN:OE1	2.44	0.51
1:B:405:ASP:OD2	1:B:505:HIS:ND1	2.43	0.51
1:C:493:ARG:HH22	2:D:31:LYS:HA	1.75	0.51
2:F:165:TRP:HH2	2:F:270:MET:HA	1.74	0.51
1:C:1151:GLU:HA	1:C:1154:LYS:HE3	1.93	0.51
1:A:402:ILE:HD11	1:A:407:VAL:HG22	1.93	0.51
1:B:753:LEU:HD13	1:B:997:ILE:HD11	1.92	0.51
2:F:273:ARG:HG3	2:F:274:PHE:CD2	2.46	0.51
1:A:403:ARG:HG3	1:A:495:TYR:HE2	1.76	0.51
1:A:878:LEU:O	1:A:882:ILE:HG12	2.11	0.51
2:D:108:LEU:HD11	2:D:190:MET:HB2	1.92	0.51
2:D:265:HIS:CD2	2:D:266:LEU:HG	2.45	0.51
2:F:263:PRO:HG2	2:F:266:LEU:HD12	1.92	0.51
1:A:274:THR:HG23	1:A:291:CYS:HB2	1.91	0.51
1:A:623:ALA:HB1	1:A:629:LEU:HD13	1.93	0.51
2:F:455:MET:SD	2:F:484:ILE:HB	2.50	0.51
1:A:191:GLU:HG3	1:A:206:LYS:HB3	1.92	0.50
1:A:948:LEU:O	1:A:951:VAL:HB	2.11	0.50
1:B:117:LEU:HD12	1:B:230:ILE:HD12	1.93	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG3	1.92	0.50
1:B:1086:LYS:HA	1:B:1125:ASN:HA	1.92	0.50
2:D:111:ASP:OD1	2:D:112:LYS:N	2.44	0.50
2:D:389:PRO:O	2:D:393:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HG12	1:B:232:ILE:HG12	1.93	0.50
2:D:443:ALA:HB2	2:D:591:LEU:HD21	1.94	0.50
2:F:451:PRO:HB2	2:F:484:ILE:HD11	1.93	0.50
1:A:457:ARG:NH2	1:A:467:ASP:OD2	2.37	0.50
1:A:577:ARG:HH11	1:A:582:LEU:HD12	1.76	0.50
2:D:451:PRO:HB3	2:D:484:ILE:HG22	1.93	0.50
1:B:329:PHE:O	1:B:580:GLN:NE2	2.43	0.50
1:B:452:LEU:HD23	1:B:492:LEU:HD13	1.92	0.50
2:D:48:TRP:CZ2	2:D:357:ARG:HD2	2.47	0.50
2:D:108:LEU:HD13	2:D:112:LYS:HD2	1.92	0.50
2:F:32:PHE:CE2	2:F:391:LEU:HD21	2.47	0.50
2:F:156:LEU:O	2:F:161:ARG:NH2	2.45	0.50
1:B:137:ASN:OD1	1:B:138:ASP:N	2.38	0.50
1:C:354:ASN:OD1	1:C:399:SER:OG	2.20	0.50
2:D:39:LEU:HD13	2:D:68:LYS:HD3	1.93	0.50
2:D:48:TRP:HZ3	2:D:349:TRP:CD1	2.30	0.50
1:A:96:GLU:OE1	1:A:99:ASN:N	2.31	0.50
1:A:713:ALA:HB3	1:C:894:LEU:HB3	1.94	0.50
1:B:133:PHE:HB3	1:B:135:PHE:CE1	2.47	0.50
1:B:873:TYR:CE1	1:C:699:LEU:HD22	2.46	0.50
2:D:381:TYR:CD1	2:D:558:LEU:HB2	2.47	0.50
2:F:343:VAL:HG12	2:F:345:HIS:H	1.77	0.50
1:A:105:ILE:HG13	1:A:243:LEU:HD11	1.93	0.50
1:B:68:ILE:O	1:B:78:ARG:N	2.36	0.50
2:D:345:HIS:O	2:D:347:THR:HG23	2.12	0.50
2:F:402:GLU:HB2	2:F:518:ARG:HH11	1.76	0.50
1:A:328:ARG:NH2	1:A:580:GLN:HB2	2.27	0.50
1:A:717:ASN:OD1	1:A:718:PHE:N	2.45	0.50
1:A:1116:THR:HA	1:A:1138:TYR:O	2.12	0.50
1:B:515:PHE:HE2	1:B:517:LEU:HD21	1.76	0.50
1:B:849:LEU:O	1:B:853:GLN:HG2	2.12	0.50
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.93	0.50
1:A:142:ASP:OD1	1:A:152:TRP:NE1	2.44	0.49
1:B:1145:LEU:O	1:B:1149:LYS:HG2	2.12	0.49
1:B:461:LEU:HD13	1:B:465:GLU:HB3	1.94	0.49
1:A:134:GLN:O	1:A:161:SER:N	2.44	0.49
1:A:439:ASN:OD1	1:A:440:LYS:NZ	2.39	0.49
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.46	0.49
1:C:377:PHE:HD1	1:C:434:ILE:HG12	1.78	0.49
2:D:529:LEU:HD22	2:D:550:ALA:HB1	1.93	0.49
2:D:213:ASP:N	2:D:213:ASP:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ASP:OD1	1:A:738:CYS:N	2.45	0.49
1:A:1019:ARG:HH11	1:A:1019:ARG:HG3	1.77	0.49
1:C:362:VAL:HG13	1:C:526:GLY:HA2	1.93	0.49
2:F:244:VAL:O	2:F:248:LEU:HG	2.13	0.49
1:B:108:THR:HA	1:B:235:THR:HG22	1.95	0.49
2:D:440:LEU:HD13	2:D:594:TRP:HZ3	1.78	0.49
2:F:451:PRO:O	2:F:454:TYR:HB3	2.12	0.49
1:B:128:ILE:HB	1:B:167:TYR:HB3	1.95	0.49
2:D:147:GLY:O	2:D:150:GLU:HG3	2.12	0.49
2:D:446:ILE:HG21	2:D:523:PHE:CE2	2.47	0.49
1:A:328:ARG:HH21	1:A:580:GLN:HB2	1.77	0.49
2:F:44:SER:HB3	2:F:351:LEU:HD13	1.93	0.49
1:C:449:TYR:HE1	1:C:497:PHE:H	1.61	0.49
1:C:1117:THR:HB	1:C:1139:ASP:OD1	2.12	0.49
2:F:23:GLU:HA	2:F:26:LYS:HE2	1.95	0.49
1:A:1160:THR:HA	1:C:1159:HIS:CE1	2.48	0.49
1:C:743:CYS:HB3	1:C:749:CYS:HB3	1.65	0.49
2:F:347:THR:OG1	2:F:349:TRP:NE1	2.43	0.49
2:D:271:TRP:NE1	2:D:273:ARG:HB2	2.28	0.48
2:F:161:ARG:NH1	2:F:265:HIS:O	2.45	0.48
2:F:351:LEU:HB2	2:F:355:ASP:O	2.13	0.48
2:F:484:ILE:HG12	2:F:485:VAL:HG23	1.94	0.48
1:A:458:LYS:HB3	1:A:473:TYR:HE1	1.77	0.48
1:B:349:SER:OG	1:B:350:VAL:N	2.46	0.48
1:B:994:ASP:HA	1:B:997:ILE:HG22	1.95	0.48
1:C:990:GLU:HA	1:C:993:ILE:HG12	1.95	0.48
1:A:491:PRO:HB2	1:A:492:LEU:HD12	1.95	0.48
1:C:233:ILE:HG13	1:C:235:ILE:HG12	1.94	0.48
1:C:880:GLY:O	1:C:884:SER:OG	2.23	0.48
2:F:233:ILE:HD13	2:F:581:VAL:HG11	1.95	0.48
1:A:337:PRO:HD2	1:A:358:ILE:HG23	1.94	0.48
2:D:381:TYR:CD1	2:D:404:VAL:HG11	2.48	0.48
2:F:230:PHE:CD2	2:F:454:TYR:CD1	3.02	0.48
1:A:148:ASN:HA	1:A:149:ASN:HA	1.55	0.48
1:A:356:LYS:HZ2	1:A:358:ILE:HG13	1.78	0.48
1:B:439:ASN:HD22	1:B:506:GLN:HG2	1.79	0.48
2:F:201:ASP:HA	2:F:204:ARG:HB2	1.96	0.48
2:F:307:ILE:O	2:F:310:GLU:HG3	2.13	0.48
1:B:125:ASN:HB3	1:B:168:VAL:HG23	1.95	0.48
2:D:32:PHE:CE2	2:D:100:LEU:HD13	2.49	0.48
1:A:256:SER:HB2	5:A:1301:NAG:H3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:358:ILE:HD11	2:D:379:ILE:HG13	1.95	0.48
2:D:455:MET:HE2	2:D:484:ILE:HB	1.95	0.48
1:A:204:TYR:CD1	1:A:227:PRO:HA	2.48	0.48
1:B:812:PRO:O	1:B:814:LYS:NZ	2.46	0.48
1:B:1116:THR:OG1	1:B:1119:ASN:OD1	2.31	0.48
2:D:556:ASN:HA	2:D:559:ARG:HE	1.77	0.48
1:B:134:GLN:HB3	1:B:158:SER:OG	2.14	0.48
1:B:737:ASP:OD1	1:B:738:CYS:N	2.46	0.48
2:D:347:THR:HB	2:D:349:TRP:CD1	2.49	0.48
2:D:347:THR:HB	2:D:349:TRP:NE1	2.28	0.48
2:D:365:THR:HB	2:D:368:ASP:HB2	1.95	0.48
2:D:406:GLU:OE1	2:D:409:SER:OG	2.26	0.48
2:F:521:TYR:CE2	2:F:570:LEU:HD21	2.44	0.48
1:B:328:ARG:HA	1:B:530:SER:HB2	1.96	0.47
1:C:322:PRO:HA	1:C:538:CYS:HB3	1.96	0.47
1:C:421:TYR:HD1	1:C:457:ARG:HB3	1.78	0.47
2:D:95:LEU:O	2:D:98:GLN:HG3	2.14	0.47
2:F:315:PHE:HD1	2:F:320:LEU:HD12	1.79	0.47
1:A:747:THR:OG1	1:A:748:GLU:OE1	2.32	0.47
1:A:1155:TYR:O	1:A:1159:HIS:HB2	2.14	0.47
1:B:454:ARG:HA	1:B:492:LEU:HA	1.96	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.47	0.47
1:B:770:ILE:HD11	1:B:1012:LEU:HD13	1.95	0.47
1:B:1139:ASP:O	1:B:1143:PRO:HD2	2.14	0.47
1:A:53:ASP:HB3	1:A:55:PHE:CE2	2.50	0.47
1:A:534:VAL:HG11	1:A:537:LYS:HE2	1.96	0.47
1:A:547:LYS:O	1:C:978:ASN:ND2	2.47	0.47
1:C:170:TYR:CE2	1:C:172:SER:HB3	2.49	0.47
1:C:317:ASN:ND2	1:C:592:PHE:O	2.44	0.47
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.49	0.47
1:B:825:LYS:NZ	1:B:938:LEU:O	2.46	0.47
1:B:1082:CYS:HB2	1:B:1126:CYS:HB3	1.76	0.47
1:C:675:GLN:O	1:C:690:GLN:HA	2.15	0.47
2:D:39:LEU:HB3	2:D:68:LYS:HZ2	1.79	0.47
2:D:370:LEU:HB3	2:D:409:SER:HB2	1.97	0.47
2:F:245:ARG:NH1	2:F:249:MET:HG2	2.29	0.47
1:A:979:ASP:O	1:A:983:ARG:NH1	2.47	0.47
1:A:1019:ARG:HG3	1:A:1019:ARG:NH1	2.29	0.47
1:B:281:GLU:OE1	1:B:281:GLU:N	2.44	0.47
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.50	0.47
2:F:549:GLU:OE2	2:F:552:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.97	0.47
1:A:495:TYR:HD2	1:A:497:PHE:CZ	2.33	0.47
1:B:97:LYS:HG2	1:B:179:LYS:HB3	1.96	0.47
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.50	0.47
1:B:201:TYR:CD1	1:B:224:PRO:HA	2.49	0.47
1:C:656:VAL:HG22	1:C:695:TYR:HB3	1.97	0.47
1:C:760:CYS:HA	1:C:763:LEU:HB2	1.96	0.47
2:D:277:ASN:OD1	2:D:278:LEU:N	2.47	0.47
2:D:516:TYR:O	2:D:520:LEU:HD23	2.14	0.47
2:F:314:PHE:O	2:F:318:VAL:HG23	2.14	0.47
2:F:407:ILE:HG21	2:F:529:LEU:HD21	1.97	0.47
2:F:446:ILE:HG23	2:F:447:VAL:N	2.29	0.47
2:F:573:VAL:HG23	2:F:574:VAL:HG23	1.96	0.47
1:C:353:TRP:NE1	1:C:423:TYR:HB2	2.30	0.47
1:C:495:TYR:HB3	1:C:497:PHE:HD2	1.80	0.47
2:D:226:VAL:HG21	2:D:513:ILE:HD11	1.96	0.47
2:F:223:ILE:HG13	2:F:224:GLU:H	1.80	0.47
2:D:456:LEU:HB3	2:D:512:PHE:CE2	2.49	0.47
2:F:180:TYR:OH	2:F:463:VAL:HG21	2.15	0.47
1:B:201:TYR:HA	1:B:225:LEU:H	1.79	0.46
1:B:617:CYS:O	1:B:620:VAL:HG12	2.15	0.46
1:B:620:VAL:O	1:B:624:ILE:N	2.48	0.46
2:D:229:THR:HB	2:D:581:VAL:HG13	1.97	0.46
2:D:535:HIS:NE2	2:D:543:ASP:O	2.49	0.46
2:F:181:GLU:O	2:F:185:VAL:HG13	2.14	0.46
2:F:360:MET:SD	2:F:361:CYS:N	2.88	0.46
1:A:106:PHE:CD1	1:A:240:PHE:HB2	2.50	0.46
1:A:973:ILE:HD11	1:A:980:ILE:HG23	1.96	0.46
1:B:720:ILE:HD12	1:B:923:ILE:HG23	1.97	0.46
1:C:676:THR:O	1:C:676:THR:OG1	2.32	0.46
2:D:297:MET:HA	2:D:302:TRP:HD1	1.79	0.46
2:F:288:LYS:HZ2	2:F:289:PRO:HD2	1.79	0.46
2:F:297:MET:HA	2:F:302:TRP:CD1	2.51	0.46
1:A:287:ASP:OD1	1:A:288:ALA:N	2.48	0.46
1:A:551:VAL:HG22	1:A:588:THR:O	2.15	0.46
1:B:742:ILE:HG21	1:B:997:ILE:HG13	1.97	0.46
1:C:454:ARG:HH21	1:C:457:ARG:HG3	1.80	0.46
2:D:273:ARG:O	2:D:449:THR:HB	2.15	0.46
2:D:585:LEU:HA	2:D:588:PHE:HB2	1.97	0.46
1:A:403:ARG:HG3	1:A:495:TYR:CE2	2.49	0.46
1:B:603:ASN:HB2	5:B:1306:NAG:O5	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.50	0.46
1:C:319:ARG:NH1	1:C:320:VAL:O	2.48	0.46
2:D:346:PRO:HA	2:D:360:MET:HG2	1.97	0.46
2:F:317:SER:OG	2:F:545:SER:OG	2.24	0.46
2:F:452:PHE:HE1	2:F:481:LYS:HE2	1.80	0.46
1:B:89:GLY:HA2	1:B:191:PHE:O	2.16	0.46
2:D:480:MET:HB3	2:D:484:ILE:HD12	1.97	0.46
1:A:377:PHE:HD1	1:A:434:ILE:HG13	1.81	0.46
1:B:950:ASP:OD1	1:B:951:VAL:N	2.49	0.46
1:C:1009:THR:O	1:C:1013:ILE:HG12	2.16	0.46
1:C:1101:HIS:ND1	4:Y:1:NAG:H5	2.31	0.46
2:F:594:TRP:HE3	2:F:595:LEU:HD22	1.80	0.46
1:A:97:LYS:HB2	1:A:186:PHE:HA	1.97	0.46
1:C:551:VAL:HG23	1:C:588:THR:OG1	2.16	0.46
2:D:203:TRP:HB3	2:D:511:SER:HB3	1.98	0.46
2:D:446:ILE:HG13	2:D:523:PHE:HZ	1.81	0.46
1:C:620:VAL:HG22	1:C:621:PRO:HD3	1.98	0.46
1:C:764:LYS:HB3	1:C:764:LYS:HE2	1.65	0.46
2:D:39:LEU:HD22	2:D:68:LYS:HZ3	1.81	0.46
2:F:570:LEU:HA	2:F:573:VAL:HG22	1.96	0.46
1:C:83:VAL:HG23	1:C:241:GLN:HB2	1.98	0.46
1:C:147:LYS:HD2	1:C:147:LYS:HA	1.73	0.46
2:F:119:ILE:HD11	2:F:179:LEU:HB3	1.98	0.46
2:F:549:GLU:O	2:F:552:GLN:HG3	2.16	0.46
1:A:604:THR:HG22	1:A:605:SER:N	2.27	0.46
2:D:230:PHE:CZ	2:D:454:TYR:HB2	2.50	0.46
2:D:456:LEU:HD13	2:D:500:PRO:HB3	1.98	0.46
2:F:271:TRP:NE1	2:F:273:ARG:HD2	2.30	0.46
2:F:281:LEU:HD23	2:F:281:LEU:O	2.16	0.46
2:F:553:LYS:O	2:F:557:MET:HG3	2.16	0.46
1:A:68:ILE:HA	1:A:262:ALA:HA	1.98	0.45
1:A:589:PRO:HG2	1:C:855:PHE:CD1	2.51	0.45
1:C:258:TRP:CD1	1:C:260:ALA:HB2	2.52	0.45
2:D:450:LEU:HD13	2:D:516:TYR:HE1	1.81	0.45
2:F:388:GLN:HB3	2:F:392:LEU:HB3	1.97	0.45
2:F:476:LYS:O	2:F:480:MET:HG2	2.16	0.45
1:B:128:ILE:HD13	1:B:167:TYR:HD2	1.81	0.45
1:C:58:PHE:HD2	1:C:290:ASP:HB2	1.80	0.45
1:C:126:VAL:HG23	1:C:174:PRO:HB3	1.98	0.45
1:C:305:SER:OG	1:C:306:PHE:N	2.49	0.45
1:C:578:ASP:HB3	1:C:581:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:145:GLU:HA	2:F:146:PRO:HA	1.78	0.45
1:A:40:ASP:OD1	1:A:40:ASP:N	2.49	0.45
1:A:497:PHE:CG	1:A:507:PRO:HD3	2.51	0.45
1:B:108:THR:O	1:B:236:ARG:NH1	2.49	0.45
1:C:189:LEU:HD23	1:C:208:THR:HB	1.98	0.45
1:C:299:THR:HB	1:C:597:VAL:HG21	1.98	0.45
1:C:356:LYS:HG2	1:C:397:ALA:HB3	1.98	0.45
2:D:120:LEU:HD21	2:D:183:TYR:HD1	1.81	0.45
2:D:264:ALA:HA	2:D:267:LEU:HD13	1.97	0.45
1:A:629:LEU:O	1:A:634:ARG:NH2	2.50	0.45
1:C:20:THR:O	1:C:21:ARG:NE	2.48	0.45
1:C:105:ILE:HG12	1:C:241:GLN:O	2.16	0.45
2:D:523:PHE:CE2	2:D:584:LEU:HD13	2.51	0.45
2:F:433:GLU:HA	2:F:436:ILE:HD12	1.97	0.45
1:B:67:VAL:HG13	1:B:79:PHE:HA	1.99	0.45
1:B:117:LEU:HD21	1:B:119:ILE:HG12	1.98	0.45
1:B:328:ARG:NH1	1:B:533:LEU:HB2	2.32	0.45
1:C:430:THR:HG22	1:C:515:PHE:HE1	1.82	0.45
2:D:156:LEU:H	2:D:156:LEU:HD23	1.80	0.45
2:F:161:ARG:NH2	2:F:265:HIS:HD2	2.14	0.45
1:A:318:PHE:HZ	1:A:615:VAL:HG21	1.82	0.45
1:B:68:ILE:H	1:B:78:ARG:HB3	1.81	0.45
1:B:850:ILE:O	1:B:854:LYS:HG2	2.17	0.45
2:F:240:LEU:HD13	2:F:447:VAL:HG11	1.98	0.45
1:A:635:VAL:O	1:A:638:THR:HG22	2.17	0.45
1:A:1139:ASP:O	1:A:1143:PRO:HD2	2.16	0.45
1:B:357:ARG:NH1	1:B:359:SER:HB3	2.32	0.45
2:F:471:ASP:OD1	2:F:471:ASP:N	2.50	0.45
2:F:505:HIS:ND1	2:F:510:TYR:HB2	2.32	0.45
1:A:117:LEU:HD21	1:A:233:ILE:HG21	1.99	0.45
1:A:624:ILE:HG12	1:A:637:SER:OG	2.17	0.45
1:B:100:ILE:O	1:B:102:ARG:HG2	2.17	0.45
1:B:605:SER:OG	1:B:606:ASN:N	2.50	0.45
1:C:99:ASN:O	1:C:102:ARG:NH2	2.50	0.45
2:D:203:TRP:CE3	2:D:511:SER:HA	2.51	0.45
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.52	0.45
1:B:287:ASP:OD1	1:B:288:ALA:N	2.48	0.45
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.52	0.45
2:D:519:THR:O	2:D:522:GLN:HG2	2.17	0.45
1:A:403:ARG:HH12	1:A:405:ASP:HB2	1.82	0.44
1:A:1092:GLU:OE2	1:A:1107:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:ASP:O	1:C:940:SER:OG	2.20	0.44
1:C:1082:CYS:HB2	1:C:1126:CYS:HB3	1.79	0.44
1:C:1139:ASP:O	1:C:1143:PRO:HD2	2.17	0.44
1:B:303:LEU:HD11	1:B:313:TYR:CE1	2.53	0.44
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.99	0.44
1:C:495:TYR:HB3	1:C:497:PHE:CD2	2.52	0.44
1:A:328:ARG:NH1	1:A:533:LEU:HG	2.33	0.44
1:A:919:ASN:O	1:A:923:ILE:HD12	2.17	0.44
1:A:1142:GLN:O	1:A:1145:LEU:HG	2.18	0.44
1:C:96:GLU:OE1	1:C:99:ASN:N	2.38	0.44
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.99	0.44
1:C:867:ASP:OD1	1:C:868:GLU:N	2.50	0.44
1:C:905:ARG:NH1	1:C:1050:MET:HB3	2.30	0.44
2:D:446:ILE:HG21	2:D:523:PHE:HE2	1.82	0.44
2:D:450:LEU:HD22	2:D:516:TYR:HD1	1.83	0.44
2:F:165:TRP:CH2	2:F:270:MET:HA	2.52	0.44
1:A:1031:GLU:OE2	1:B:1039:ARG:NH2	2.51	0.44
1:B:1074:ASN:HD21	3:O:1:NAG:H4	1.82	0.44
2:D:158:TYR:HA	2:D:161:ARG:HB2	2.00	0.44
2:D:431:ASP:OD1	2:D:431:ASP:N	2.51	0.44
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.53	0.44
1:A:715:PRO:HA	1:A:1072:GLU:HA	1.99	0.44
1:C:341:VAL:HG13	1:C:356:LYS:HD2	1.99	0.44
1:C:763:LEU:HG	1:C:1008:VAL:HG21	1.98	0.44
1:C:1142:GLN:O	1:C:1145:LEU:HG	2.17	0.44
2:D:119:ILE:HA	2:D:122:THR:HG22	2.00	0.44
2:D:511:SER:O	2:D:514:ARG:HG2	2.17	0.44
2:F:346:PRO:HB2	2:F:375:GLU:HG3	2.00	0.44
2:F:432:ASN:O	2:F:435:GLU:HG2	2.18	0.44
1:B:916:LEU:HD12	1:B:923:ILE:HD13	1.99	0.44
1:C:850:ILE:O	1:C:854:LYS:NZ	2.51	0.44
2:D:120:LEU:HD21	2:D:183:TYR:CD1	2.53	0.44
2:D:181:GLU:HA	2:D:184:VAL:HG12	1.99	0.44
2:D:546:ASN:HB2	5:D:701:NAG:HN2	1.83	0.44
1:A:96:GLU:O	1:A:188:ASN:HB2	2.17	0.44
1:A:355:ARG:HE	1:A:396:TYR:HD2	1.66	0.44
1:A:921:LYS:HD2	1:A:921:LYS:HA	1.78	0.44
1:C:896:ILE:HD12	1:C:897:PRO:HD2	1.99	0.44
1:B:143:HIS:HA	1:B:258:TRP:CH2	2.53	0.44
1:C:371:LEU:HD23	1:C:371:LEU:HA	1.91	0.44
2:D:144:LEU:HA	2:D:148:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:148:LEU:HA	2:D:151:ILE:HG22	2.00	0.44
2:F:53:ASN:O	2:F:58:ASN:ND2	2.51	0.44
1:B:105:ILE:C	1:B:106:PHE:HD1	2.21	0.43
1:B:258:TRP:CD1	1:B:260:ALA:HB2	2.53	0.43
1:B:258:TRP:HD1	1:B:260:ALA:HB2	1.83	0.43
1:C:33:THR:HA	1:C:58:PHE:HE1	1.82	0.43
2:D:168:TRP:CZ3	2:D:172:VAL:HG21	2.53	0.43
2:D:374:HIS:HE1	2:D:402:GLU:HA	1.82	0.43
2:F:245:ARG:HA	2:F:245:ARG:HH11	1.83	0.43
2:F:295:ASP:HA	2:F:298:VAL:HG22	1.99	0.43
1:A:64:TRP:CZ2	1:A:66:HIS:HB2	2.52	0.43
1:A:347:PHE:CE2	1:A:399:SER:HB2	2.53	0.43
1:A:627:ASP:H	1:A:634:ARG:CD	2.31	0.43
1:A:853:GLN:HE21	1:A:854:LYS:NZ	2.16	0.43
1:A:1009:THR:O	1:A:1013:ILE:HG12	2.18	0.43
1:C:802:PHE:HE1	1:C:927:PHE:HE2	1.65	0.43
2:D:260:GLY:HA2	2:D:610:TRP:HE1	1.83	0.43
2:D:363:LYS:HA	2:D:363:LYS:HD2	1.72	0.43
2:F:293:VAL:HG23	2:F:297:MET:HE3	2.00	0.43
2:F:344:CYS:HA	2:F:361:CYS:HB3	1.99	0.43
2:F:424:LEU:HD21	2:F:428:PHE:HB3	2.00	0.43
1:A:99:ASN:HB3	1:A:102:ARG:HH22	1.82	0.43
1:A:405:ASP:O	1:A:408:ARG:NH2	2.51	0.43
1:B:191:PHE:HB3	1:B:198:PHE:CZ	2.53	0.43
1:C:689:SER:HB3	1:C:690:GLN:H	1.65	0.43
2:D:198:ASP:HB2	2:D:464:PHE:HB3	2.00	0.43
2:D:474:MET:O	2:D:478:TRP:HB2	2.19	0.43
2:D:535:HIS:CD2	2:D:543:ASP:H	2.36	0.43
2:F:262:LEU:HD12	2:F:263:PRO:HD2	1.99	0.43
1:A:853:GLN:HE21	1:A:854:LYS:HZ3	1.66	0.43
1:C:139:PRO:HA	1:C:159:VAL:HG11	2.00	0.43
1:C:334:ASN:ND2	1:C:361:CYS:HA	2.33	0.43
2:D:21:ILE:HA	2:D:24:GLN:HG2	1.99	0.43
2:D:557:MET:SD	2:D:569:ALA:HB1	2.58	0.43
2:F:90:ASN:HB3	2:F:93:VAL:CG1	2.49	0.43
2:F:310:GLU:HA	2:F:313:LYS:HG2	1.99	0.43
2:F:439:LEU:HD21	2:F:540:HIS:CD2	2.53	0.43
2:F:551:GLY:O	2:F:554:LEU:HG	2.18	0.43
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.53	0.43
1:C:96:GLU:OE2	1:C:98:SER:OG	2.23	0.43
1:C:617:CYS:O	1:C:620:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1156:PHE:O	1:C:1160:THR:HG23	2.18	0.43
2:D:254:SER:OG	2:D:255:TYR:N	2.52	0.43
2:D:305:GLN:HA	2:D:333:LEU:HD11	2.00	0.43
1:A:905:ARG:NH1	1:A:1050:MET:HB3	2.33	0.43
1:B:122:ASN:OD1	1:B:123:ALA:N	2.44	0.43
2:D:268:GLY:HA3	2:D:278:LEU:HD11	2.01	0.43
1:A:332:ILE:HG23	1:A:362:VAL:HG22	2.01	0.43
1:B:328:ARG:HA	1:B:328:ARG:HD2	1.82	0.43
1:C:44:ARG:HH21	1:C:49:HIS:HB2	1.83	0.43
2:D:204:ARG:NH2	2:D:219:ARG:O	2.38	0.43
2:F:120:LEU:HD12	2:F:183:TYR:HE1	1.84	0.43
2:F:295:ASP:N	2:F:295:ASP:OD1	2.52	0.43
1:A:342:PHE:CE1	1:A:511:VAL:HG11	2.54	0.43
1:A:759:PHE:O	1:A:763:LEU:HD23	2.19	0.43
1:B:165:PHE:CE2	1:B:167:TYR:HB2	2.54	0.43
1:C:122:ASN:O	1:C:124:THR:N	2.52	0.43
1:C:336:CYS:N	1:C:362:VAL:O	2.41	0.43
2:D:335:ASP:OD1	2:D:335:ASP:N	2.52	0.43
2:D:568:LEU:O	2:D:571:GLU:HG2	2.18	0.43
2:F:50:TYR:HD1	2:F:58:ASN:HB3	1.84	0.43
2:F:245:ARG:NH1	2:F:248:LEU:HB2	2.34	0.43
2:F:384:ALA:HB1	2:F:555:PHE:HE1	1.83	0.43
1:A:149:ASN:N	1:A:149:ASN:OD1	2.52	0.43
1:B:415:THR:OG1	1:B:416:GLY:N	2.51	0.43
1:B:551:VAL:HG23	1:B:588:THR:HB	2.01	0.43
2:D:119:ILE:HG13	2:D:120:LEU:N	2.34	0.43
2:F:197:GLU:HB3	2:F:201:ASP:OD2	2.19	0.43
1:B:207:ILE:HG13	1:B:207:ILE:O	2.18	0.43
2:F:223:ILE:HG13	2:F:224:GLU:N	2.33	0.43
2:F:480:MET:O	2:F:484:ILE:HG22	2.19	0.43
1:B:123:ALA:HB3	5:B:1301:NAG:H82	2.00	0.42
1:B:438:SER:HB3	1:B:509:ARG:HB2	2.01	0.42
1:B:1161:SER:OG	1:B:1162:PRO:HD3	2.19	0.42
1:C:119:ILE:HD12	1:C:128:ILE:HD12	2.01	0.42
1:A:1045:LYS:HE2	1:A:1045:LYS:HB2	1.79	0.42
1:B:364:ASP:O	1:B:367:VAL:HG12	2.19	0.42
2:D:398:GLU:HG3	2:D:514:ARG:CZ	2.49	0.42
2:F:56:GLU:HG2	2:F:57:GLU:N	2.33	0.42
1:A:118:LEU:HD21	1:A:135:PHE:CE1	2.54	0.42
1:A:383:SER:HB2	1:C:985:ASP:N	2.34	0.42
1:B:503:VAL:HA	1:B:506:GLN:HE22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:HD3	1:C:306:PHE:HE2	1.83	0.42
1:C:605:SER:OG	1:C:606:ASN:N	2.52	0.42
1:C:1038:LYS:HE2	1:C:1038:LYS:HB3	1.93	0.42
2:D:355:ASP:OD2	2:D:357:ARG:NH2	2.53	0.42
2:F:479:GLU:HA	2:F:482:ARG:HE	1.85	0.42
4:R:1:NAG:H62	4:R:2:NAG:N2	2.34	0.42
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.84	0.42
1:C:19:THR:O	1:C:21:ARG:HG2	2.19	0.42
2:D:419:LYS:NZ	2:D:428:PHE:HB3	2.34	0.42
2:F:515:TYR:O	2:F:518:ARG:HG2	2.20	0.42
1:A:230:ASP:OD1	1:A:231:LEU:N	2.52	0.42
1:A:361:CYS:O	1:A:524:VAL:HG23	2.19	0.42
1:B:453:TYR:HB3	1:B:495:TYR:CE2	2.54	0.42
1:A:644:GLN:HG2	5:A:1307:NAG:H83	1.77	0.42
1:B:457:ARG:NH1	1:B:459:SER:OG	2.53	0.42
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	2.01	0.42
1:B:1047:TYR:O	1:B:1066:THR:OG1	2.29	0.42
1:C:1014:ARG:O	1:C:1017:GLU:HG2	2.19	0.42
2:D:56:GLU:O	2:D:60:GLN:HG2	2.19	0.42
2:D:111:ASP:HA	2:D:114:LYS:HG2	2.01	0.42
2:D:275:TRP:CE3	2:D:278:LEU:HD22	2.55	0.42
2:F:227:GLU:HA	2:F:454:TYR:CE1	2.54	0.42
1:A:87:ASN:HD22	1:A:87:ASN:C	2.13	0.42
1:A:815:ARG:CZ	1:A:823:PHE:HD2	2.32	0.42
1:B:95:ILE:HD11	1:B:264:ALA:HB3	2.01	0.42
1:B:725:GLU:OE2	1:B:727:LEU:HG	2.20	0.42
1:C:429:PHE:CZ	1:C:431:GLY:HA3	2.55	0.42
2:D:237:TYR:CE2	2:D:485:VAL:HA	2.54	0.42
2:D:493:HIS:HB3	2:D:497:TYR:HB2	2.00	0.42
2:F:90:ASN:HB3	2:F:93:VAL:HG12	2.02	0.42
1:B:128:ILE:HD13	1:B:167:TYR:CD2	2.54	0.42
1:B:371:LEU:HD12	1:B:371:LEU:HA	1.84	0.42
1:B:629:LEU:H	1:B:629:LEU:HD23	1.83	0.42
1:C:410:ILE:HD13	1:C:510:VAL:HG11	2.02	0.42
1:C:720:ILE:HD12	1:C:923:ILE:HG23	2.02	0.42
2:D:38:ASP:O	2:D:42:GLN:HG2	2.20	0.42
2:D:256:ILE:H	2:D:256:ILE:HD12	1.85	0.42
2:D:305:GLN:O	2:D:309:LYS:HG2	2.18	0.42
2:D:519:THR:HA	2:D:522:GLN:HG2	2.01	0.42
2:F:545:SER:OG	2:F:546:ASN:N	2.53	0.42
2:F:582:ARG:HD2	2:F:582:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PHE:HB3	1:A:806:LEU:HD23	2.01	0.42
1:B:41:LYS:HD2	1:C:562:PHE:O	2.19	0.42
1:B:361:CYS:H	1:B:524:VAL:HG12	1.85	0.42
1:C:447:GLY:HA2	1:C:497:PHE:O	2.20	0.42
2:D:516:TYR:CZ	2:D:520:LEU:HD21	2.55	0.42
1:A:1082:CYS:HB2	1:A:1126:CYS:HB3	1.93	0.42
1:B:401:VAL:HB	1:B:451:TYR:CE2	2.53	0.42
1:B:569:ILE:HD12	1:B:569:ILE:H	1.85	0.42
1:B:818:ILE:O	1:B:822:LEU:HD23	2.19	0.42
1:C:140:PHE:CE2	1:C:146:HIS:HB2	2.54	0.42
1:C:541:PHE:HB3	1:C:552:LEU:HD11	2.02	0.42
2:F:276:THR:HA	2:F:444:LEU:HD23	2.02	0.42
4:Z:1:NAG:H61	4:Z:2:NAG:HN2	1.85	0.42
1:A:109:THR:O	1:A:239:ARG:NH2	2.53	0.41
1:A:112:SER:HB3	1:A:134:GLN:HA	2.02	0.41
1:C:148:ASN:ND2	1:C:151:SER:OG	2.50	0.41
1:C:345:THR:O	1:C:509:ARG:NH2	2.52	0.41
1:C:349:SER:OG	1:C:350:VAL:N	2.52	0.41
1:C:403:ARG:HG3	1:C:497:PHE:CE1	2.55	0.41
2:D:216:ASP:OD1	2:D:216:ASP:N	2.53	0.41
2:F:119:ILE:HD12	2:F:119:ILE:HA	1.93	0.41
1:C:630:THR:HB	1:C:631:PRO:HD3	2.02	0.41
2:D:158:TYR:HD2	2:D:162:LEU:HD23	1.85	0.41
2:D:347:THR:OG1	2:D:359:LEU:O	2.33	0.41
2:D:432:ASN:OD1	2:D:433:GLU:N	2.53	0.41
1:B:203:LYS:HB2	1:B:222:LEU:HD12	2.03	0.41
1:B:498:ARG:HD2	1:B:501:TYR:CE1	2.56	0.41
1:C:193:VAL:HG12	1:C:204:TYR:HB2	2.02	0.41
1:C:303:LEU:HD11	1:C:313:TYR:CE2	2.55	0.41
1:C:1039:ARG:H	1:C:1039:ARG:HG3	1.68	0.41
2:D:125:THR:O	2:D:129:THR:HG22	2.21	0.41
2:D:230:PHE:CE1	2:D:454:TYR:HB2	2.54	0.41
2:D:347:THR:HB	2:D:349:TRP:HE1	1.85	0.41
2:D:529:LEU:HD11	2:D:554:LEU:HD22	2.01	0.41
1:A:764:LYS:HB3	1:A:764:LYS:HE2	1.91	0.41
1:B:529:LYS:HD3	1:B:529:LYS:HA	1.81	0.41
1:B:914:ASN:N	1:B:914:ASN:OD1	2.52	0.41
1:C:645:THR:OG1	1:C:648:GLY:O	2.21	0.41
1:C:1145:LEU:O	1:C:1149:LYS:HG2	2.20	0.41
2:F:39:LEU:HD22	2:F:68:LYS:HD3	2.02	0.41
2:F:397:ASN:OD1	2:F:397:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:577:LYS:HB3	2:F:577:LYS:HE3	1.85	0.41
1:A:158:ARG:HA	1:A:158:ARG:HD3	1.89	0.41
1:B:977:LEU:HG	1:B:981:PHE:HE2	1.85	0.41
1:B:1081:ILE:O	1:B:1088:HIS:N	2.54	0.41
1:C:175:PHE:CZ	1:C:228:LEU:HD21	2.55	0.41
1:C:318:PHE:HD2	1:C:629:LEU:HD11	1.85	0.41
1:C:762:GLN:OE1	1:C:765:ARG:NH1	2.54	0.41
1:C:960:ASN:HA	1:C:963:VAL:HG12	2.03	0.41
1:C:1024:LEU:O	1:C:1028:LYS:HG2	2.20	0.41
2:D:74:LYS:HA	2:D:74:LYS:HD2	1.72	0.41
2:D:443:ALA:HB2	2:D:591:LEU:CD2	2.50	0.41
2:F:245:ARG:HA	2:F:245:ARG:HD2	1.86	0.41
2:F:355:ASP:OD2	2:F:357:ARG:NH2	2.48	0.41
1:B:140:PHE:CE1	1:B:143:HIS:HB2	2.55	0.41
1:B:620:VAL:O	1:B:624:ILE:HG13	2.21	0.41
1:C:241:GLN:NE2	1:C:242:THR:O	2.52	0.41
1:C:1049:LEU:HA	1:C:1049:LEU:HD23	1.80	0.41
2:D:204:ARG:O	2:D:219:ARG:NH2	2.54	0.41
2:D:414:THR:O	2:D:418:LEU:HD13	2.21	0.41
2:F:162:LEU:HA	2:F:165:TRP:CD1	2.56	0.41
1:A:1129:VAL:HG23	1:C:917:TYR:HB3	2.02	0.41
1:B:737:ASP:OD2	1:B:740:MET:HG3	2.20	0.41
1:C:124:THR:HG22	1:C:124:THR:O	2.21	0.41
1:C:321:GLN:HB2	1:C:628:GLN:HA	2.02	0.41
2:F:204:ARG:HD2	2:F:222:LEU:HD13	2.02	0.41
2:F:227:GLU:HA	2:F:454:TYR:HE1	1.86	0.41
1:A:342:PHE:HE1	1:A:511:VAL:HG11	1.86	0.41
1:A:720:ILE:HD12	1:A:923:ILE:HG23	2.03	0.41
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.86	0.41
1:B:376:THR:N	1:B:435:ALA:O	2.53	0.41
1:B:1152:LEU:HD21	1:C:1152:LEU:HD13	2.02	0.41
1:C:641:ASN:HA	1:C:643:PHE:CE2	2.56	0.41
2:D:207:TYR:CE2	2:D:517:THR:HG21	2.55	0.41
2:F:310:GLU:O	2:F:313:LYS:HG2	2.20	0.41
2:F:372:ALA:O	2:F:376:MET:HG2	2.21	0.41
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.38	0.41
1:A:731:MET:N	1:A:774:GLN:OE1	2.53	0.41
1:A:800:PHE:HD2	1:A:927:PHE:HD2	1.68	0.41
1:B:113:LYS:HA	1:B:113:LYS:HD2	1.97	0.41
1:B:347:PHE:CE2	1:B:399:SER:HB2	2.56	0.41
1:B:377:PHE:C	1:B:378:LYS:HD2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.02	0.41
1:C:91:TYR:OH	1:C:191:GLU:OE2	2.27	0.41
1:C:878:LEU:O	1:C:882:ILE:HG23	2.20	0.41
1:C:901:GLN:O	1:C:905:ARG:HG2	2.20	0.41
1:C:931:ILE:O	1:C:934:ILE:HG22	2.21	0.41
2:D:419:LYS:NZ	2:D:428:PHE:O	2.54	0.41
2:D:553:LYS:HD3	2:D:573:VAL:HG23	2.03	0.41
2:F:176:LEU:HD21	2:F:501:ALA:HB3	2.03	0.41
2:F:239:HIS:CE1	2:F:599:ASN:HB2	2.56	0.41
2:F:399:GLY:HA2	2:F:518:ARG:NH1	2.35	0.41
1:A:1138:TYR:CZ	1:A:1143:PRO:HD3	2.56	0.41
1:B:130:VAL:HG11	1:B:230:ILE:HG13	2.03	0.41
1:B:140:PHE:HB2	1:B:142:ASP:OD1	2.21	0.41
1:B:318:PHE:HE1	1:B:629:LEU:HB2	1.85	0.41
1:B:660:TYR:HB2	1:B:695:TYR:CE2	2.56	0.41
1:C:112:SER:HB3	1:C:134:GLN:HB2	2.03	0.41
2:D:305:GLN:N	2:D:333:LEU:HD21	2.36	0.41
2:D:374:HIS:CE1	2:D:406:GLU:HG2	2.56	0.41
2:D:398:GLU:HG3	2:D:514:ARG:NE	2.36	0.41
2:D:540:HIS:HE1	2:D:541:LYS:HE2	1.85	0.41
2:F:358:ILE:HG22	2:F:360:MET:HB2	2.03	0.41
1:A:418:ILE:HD12	1:A:422:ASN:OD1	2.21	0.40
1:B:271:GLN:HB2	1:B:272:PRO:HD2	2.02	0.40
2:F:26:LYS:O	2:F:29:LEU:HG	2.20	0.40
1:A:44:ARG:NH2	1:A:279:TYR:OH	2.42	0.40
1:A:717:ASN:HB3	1:A:1070:ALA:HB3	2.02	0.40
1:C:738:CYS:HB3	1:C:760:CYS:HB2	1.80	0.40
2:D:477:TRP:CH2	2:D:499:ASP:HB2	2.56	0.40
2:D:516:TYR:HA	2:D:519:THR:HG22	2.03	0.40
1:A:363:ALA:HB2	1:A:524:VAL:HG22	2.03	0.40
1:A:662:CYS:HB2	1:A:697:MET:CE	2.51	0.40
1:B:631:PRO:HB3	1:B:633:TRP:CZ2	2.56	0.40
1:B:697:MET:SD	1:B:697:MET:N	2.92	0.40
1:C:355:ARG:NE	1:C:398:ASP:OD1	2.54	0.40
1:C:493:ARG:NH2	2:D:31:LYS:HA	2.35	0.40
2:D:503:LEU:HD23	2:D:505:HIS:N	2.34	0.40
2:F:230:PHE:CZ	2:F:454:TYR:HB2	2.56	0.40
2:F:381:TYR:CE1	2:F:558:LEU:HG	2.55	0.40
1:A:490:PHE:HA	1:A:491:PRO:HD3	1.95	0.40
1:A:864:LEU:HG	1:A:865:LEU:HD23	2.03	0.40
1:B:100:ILE:HG22	1:B:241:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HD3	1:B:633:TRP:CD1	2.57	0.40
1:B:441:LEU:H	1:B:441:LEU:HD23	1.85	0.40
1:C:33:THR:HA	1:C:58:PHE:CE1	2.56	0.40
1:C:329:PHE:CD2	1:C:528:LYS:HB3	2.55	0.40
1:C:338:PHE:HE1	1:C:358:ILE:HG21	1.86	0.40
1:C:353:TRP:HB3	1:C:400:PHE:HB3	2.02	0.40
1:C:442:ASP:O	1:C:448:ASN:ND2	2.52	0.40
2:D:332:MET:N	2:D:332:MET:SD	2.94	0.40
1:A:1139:ASP:N	1:A:1142:GLN:OE1	2.53	0.40
1:B:353:TRP:HE1	1:B:466:ARG:HA	1.87	0.40
1:B:821:LEU:HD11	1:B:935:GLN:HE21	1.86	0.40
2:D:58:ASN:O	2:D:62:MET:HG2	2.22	0.40
2:D:482:ARG:HG3	2:D:608:THR:HG22	2.04	0.40
2:D:524:GLN:HG2	2:D:583:PRO:HG2	2.03	0.40
2:F:157:ASP:O	2:F:161:ARG:NE	2.52	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	1088/1270 (86%)	998 (92%)	90 (8%)	0	100	100
1	B	1088/1270 (86%)	1012 (93%)	75 (7%)	1 (0%)	48	79
1	C	1088/1270 (86%)	1003 (92%)	82 (8%)	3 (0%)	37	68
2	D	593/594 (100%)	560 (94%)	33 (6%)	0	100	100
2	F	593/594 (100%)	568 (96%)	25 (4%)	0	100	100
All	All	4450/4998 (89%)	4141 (93%)	305 (7%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ILE
1	C	330	PRO
1	C	123	ALA
1	C	534	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	964/1110 (87%)	963 (100%)	1 (0%)	92 97
1	B	964/1110 (87%)	959 (100%)	5 (0%)	86 93
1	C	964/1110 (87%)	964 (100%)	0	100 100
2	D	526/525 (100%)	523 (99%)	3 (1%)	84 91
2	F	526/525 (100%)	523 (99%)	3 (1%)	84 91
All	All	3944/4380 (90%)	3932 (100%)	12 (0%)	90 96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	B	147	LYS
1	B	150	MET
1	B	310	LYS
1	B	408	ARG
1	B	458	LYS
2	D	169	ARG
2	D	288	LYS
2	D	582	ARG
2	F	228[A]	HIS
2	F	228[B]	HIS
2	F	562	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	644	GLN
1	A	853	GLN
1	A	955	ASN
1	A	1159	HIS
1	C	370	ASN
1	C	804	GLN
1	C	935	GLN
1	C	955	ASN
2	D	265	HIS
2	F	239	HIS
2	F	540	HIS

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)

47 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	$\#\|Z\| > 2$
3	NAG	E	1	3	14,14,15	0.26	0	17,19,21	0.38	0
3	NAG	E	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	NAG	G	1	1,3	14,14,15	0.28	0	17,19,21	0.40	0
3	NAG	G	2	3	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	H	1	1,3	14,14,15	0.18	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	I	1	1,3	14,14,15	0.24	0	17,19,21	0.38	0
3	NAG	I	2	3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	J	1	1,3	14,14,15	0.22	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	K	1	1,4	14,14,15	0.39	0	17,19,21	0.47	0
4	NAG	K	2	4	14,14,15	0.26	0	17,19,21	0.49	0
4	BMA	K	3	4	11,11,12	0.59	0	15,15,17	0.70	0
3	NAG	L	1	1,3	14,14,15	0.22	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	M	1	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	N	1	1,3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	N	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	O	1	3	14,14,15	0.40	0	17,19,21	1.28	2 (11%)
3	NAG	O	2	3	14,14,15	0.32	0	17,19,21	0.46	0
3	NAG	P	1	1,3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	P	2	3	14,14,15	0.24	0	17,19,21	0.39	0
4	NAG	Q	1	1,4	14,14,15	0.39	0	17,19,21	0.49	0
4	NAG	Q	2	4	14,14,15	0.23	0	17,19,21	0.34	0
4	BMA	Q	3	4	11,11,12	0.59	0	15,15,17	0.83	0
4	NAG	R	1	1,4	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	R	2	4	14,14,15	0.20	0	17,19,21	0.37	0
4	BMA	R	3	4	11,11,12	0.57	0	15,15,17	0.80	0
3	NAG	S	1	1,3	14,14,15	0.34	0	17,19,21	0.52	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	T	1	3	14,14,15	0.27	0	17,19,21	0.40	0
3	NAG	T	2	3	14,14,15	0.29	0	17,19,21	0.40	0
3	NAG	U	1	3	14,14,15	0.21	0	17,19,21	0.47	0
3	NAG	U	2	3	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	V	1	1,3	14,14,15	0.24	0	17,19,21	0.44	0
3	NAG	V	2	3	14,14,15	0.20	0	17,19,21	0.42	0
3	NAG	W	1	1,3	14,14,15	0.42	0	17,19,21	0.41	0
3	NAG	W	2	3	14,14,15	0.26	0	17,19,21	0.36	0
3	NAG	X	1	1,3	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	X	2	3	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	Y	1	1,4	14,14,15	0.44	0	17,19,21	0.49	0
4	NAG	Y	2	4	14,14,15	0.23	0	17,19,21	0.50	0
4	BMA	Y	3	4	11,11,12	0.59	0	15,15,17	0.72	0
4	NAG	Z	1	1,4	14,14,15	0.27	0	17,19,21	0.47	0
4	NAG	Z	2	4	14,14,15	0.21	0	17,19,21	0.39	0
4	BMA	Z	3	4	11,11,12	0.60	0	15,15,17	0.77	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	E	1	3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	1/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	3	-	5/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	BMA	Q	3	4	-	1/2/19/22	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	BMA	R	3	4	-	2/2/19/22	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3	-	2/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	2/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	1	NAG	C2-N2-C7	4.33	129.07	122.90
3	O	1	NAG	C1-C2-N2	2.06	114.00	110.49

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
4	K	3	BMA	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	X	2	NAG	C4-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	K	3	BMA	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Q	2	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
3	O	1	NAG	C8-C7-N2-C2
3	O	1	NAG	O7-C7-N2-C2
3	S	2	NAG	C8-C7-N2-C2
3	S	2	NAG	O7-C7-N2-C2
3	U	2	NAG	C8-C7-N2-C2
3	U	2	NAG	O7-C7-N2-C2
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
3	O	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
4	Q	3	BMA	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	K	1	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	Y	2	NAG	C3-C2-N2-C7
4	R	3	BMA	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
4	R	3	BMA	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C3-C2-N2-C7
3	V	2	NAG	O5-C5-C6-O6

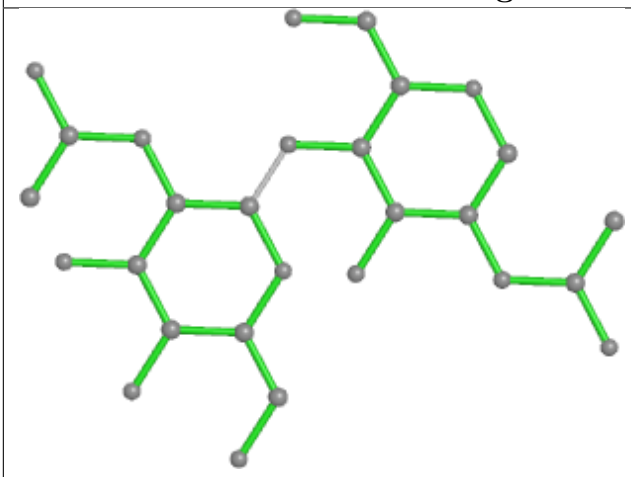
There are no ring outliers.

8 monomers are involved in 7 short contacts:

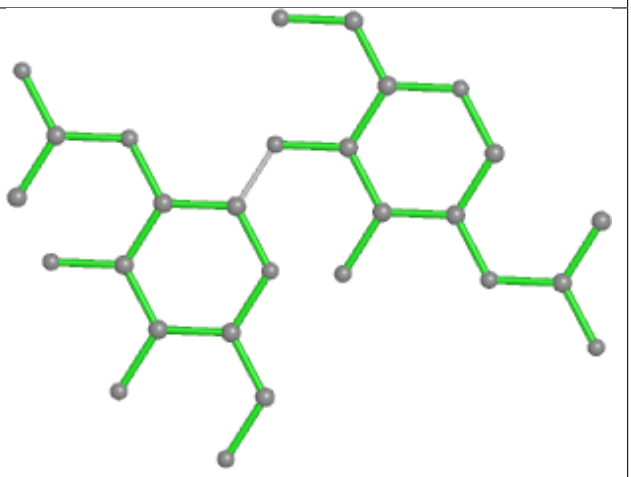
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	1	0
3	O	1	NAG	2	0
4	R	1	NAG	1	0
4	R	2	NAG	1	0
3	U	1	NAG	1	0
4	Y	1	NAG	1	0
4	Z	1	NAG	1	0
4	Z	2	NAG	1	0

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

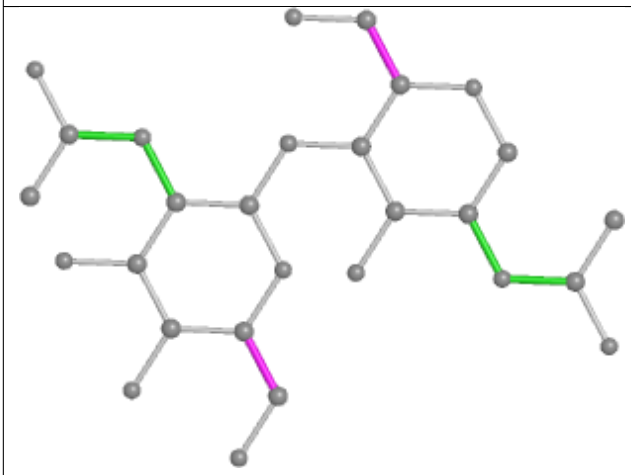
Oligosaccharide Chain E



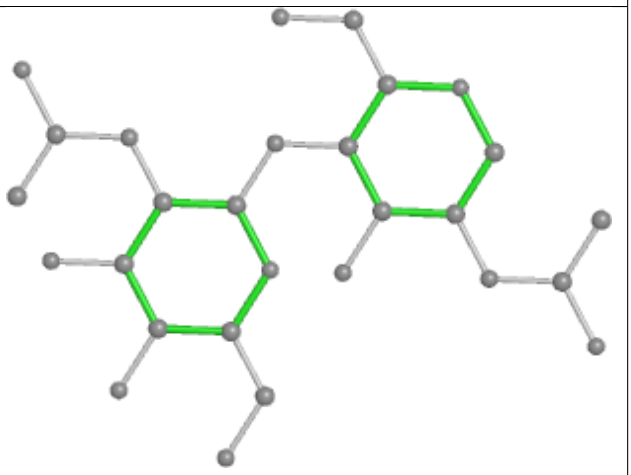
Bond lengths



Bond angles

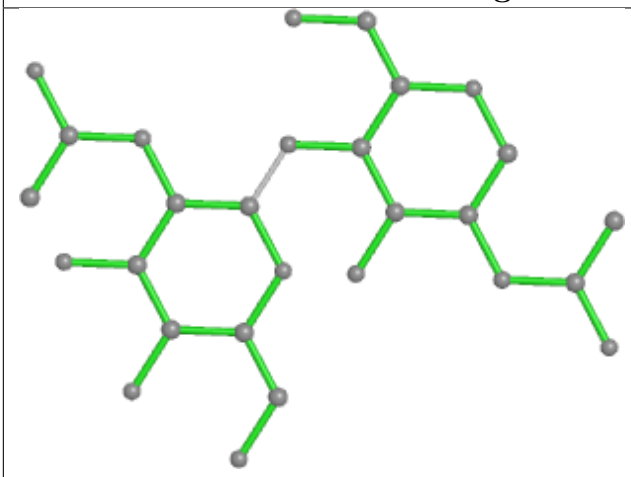


Torsions

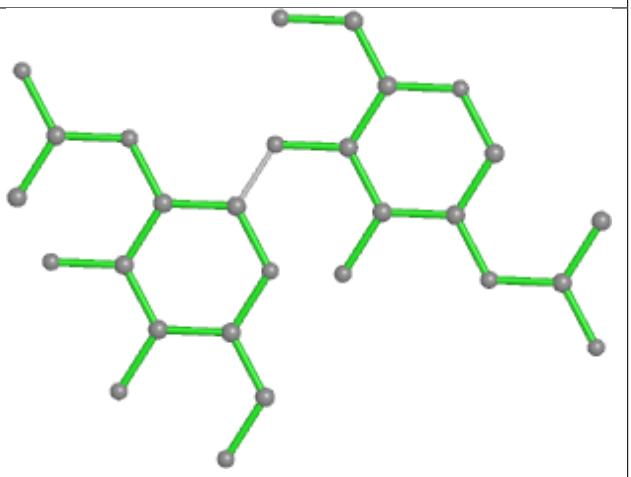


Rings

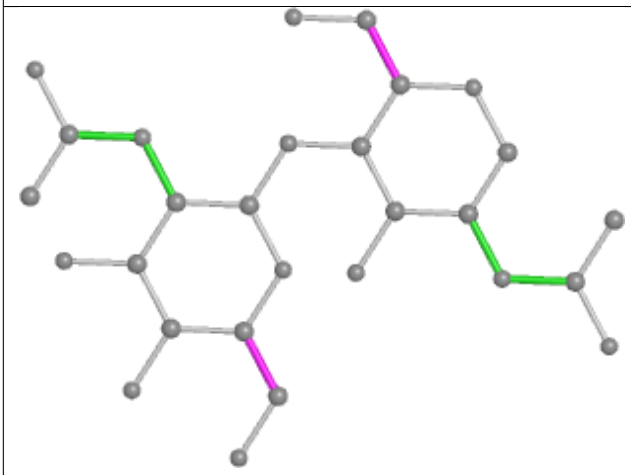
Oligosaccharide Chain G



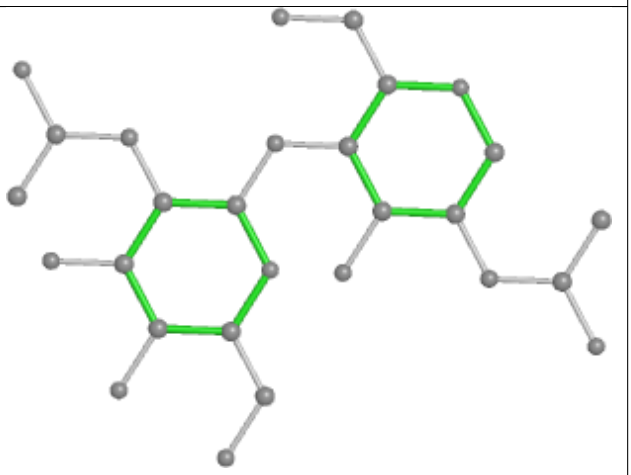
Bond lengths



Bond angles

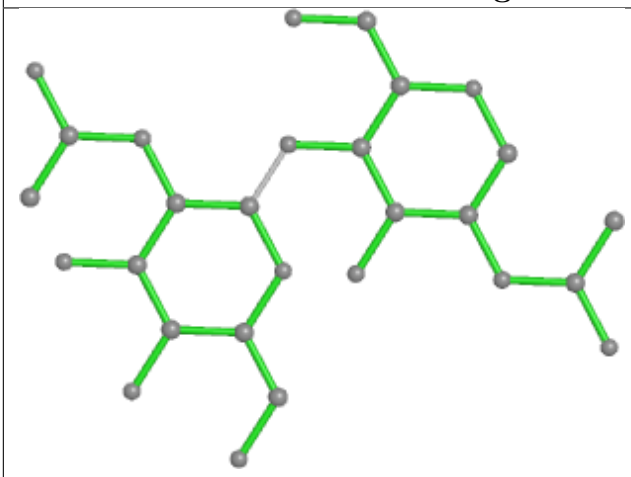


Torsions

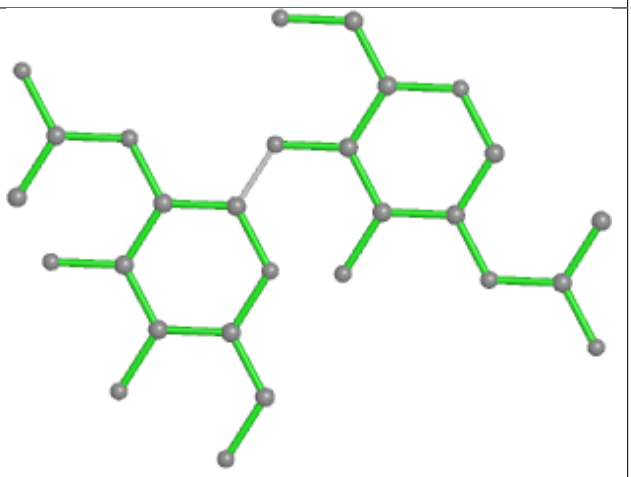


Rings

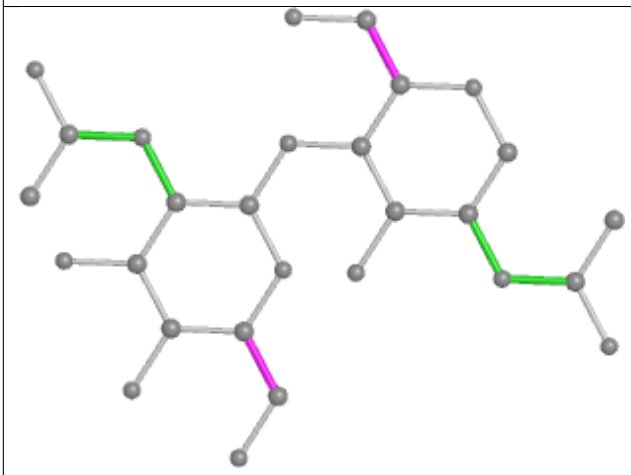
Oligosaccharide Chain H



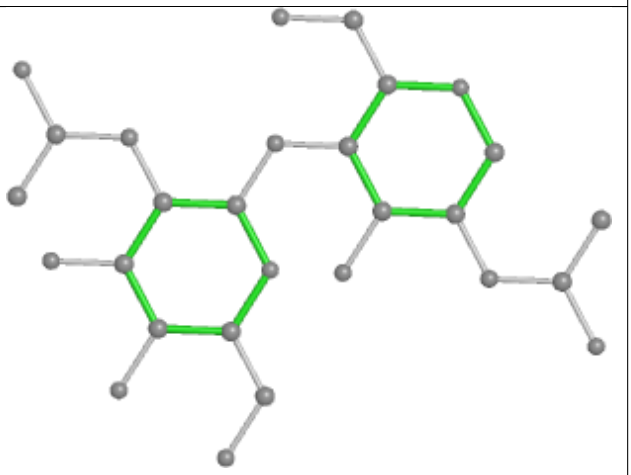
Bond lengths



Bond angles

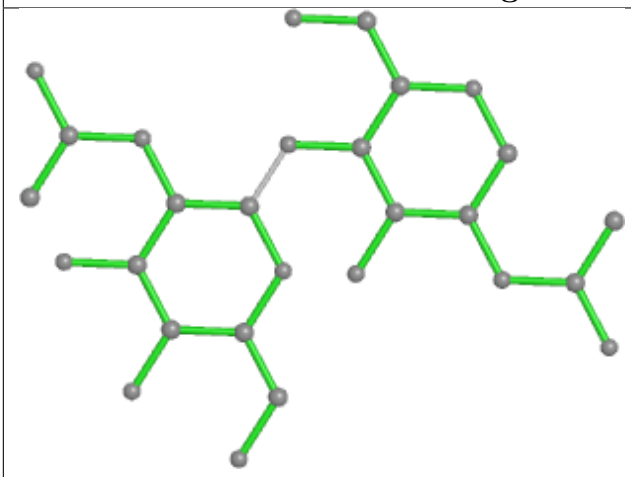


Torsions

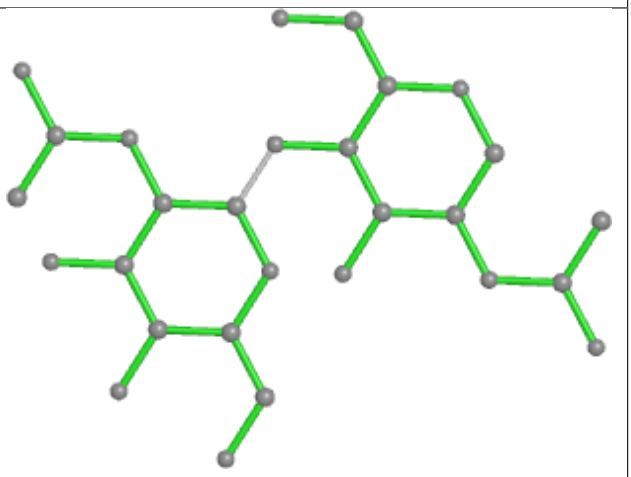


Rings

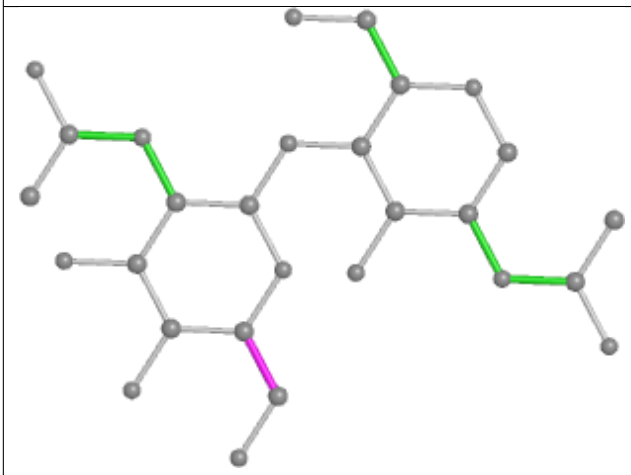
Oligosaccharide Chain I



Bond lengths



Bond angles



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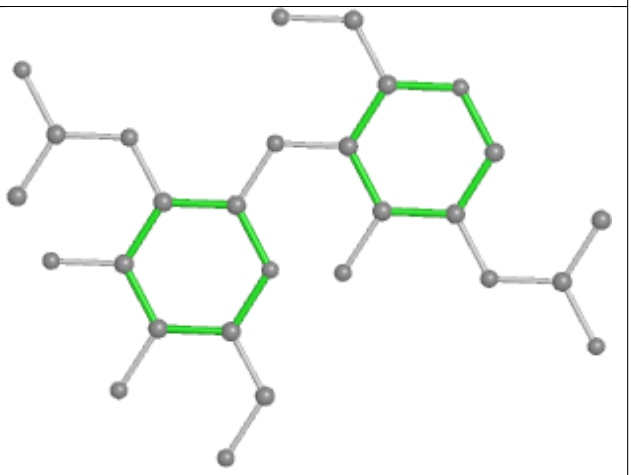
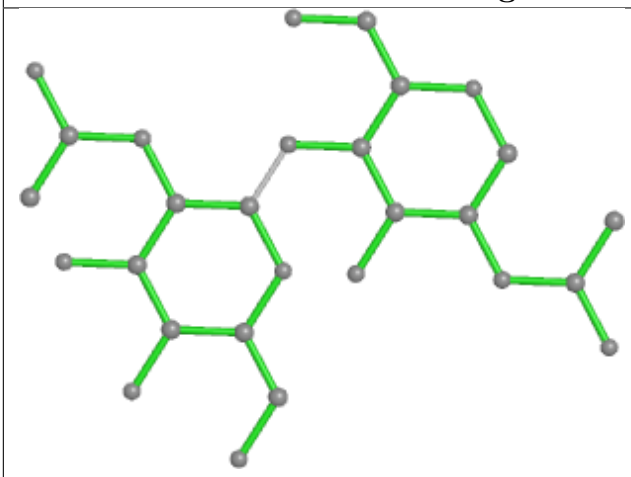


Rings

Oligosaccharide Chain J



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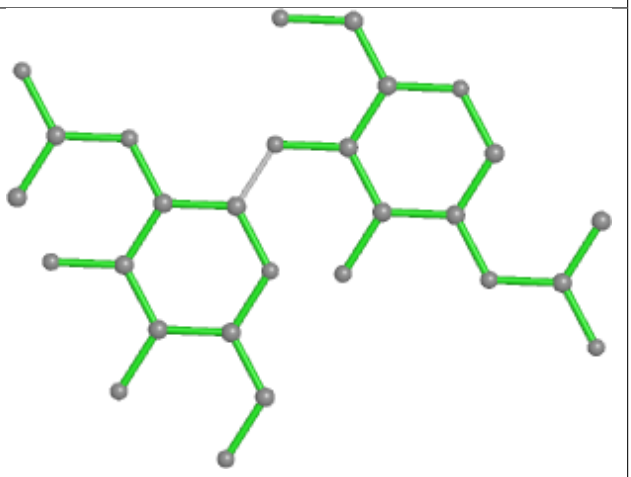
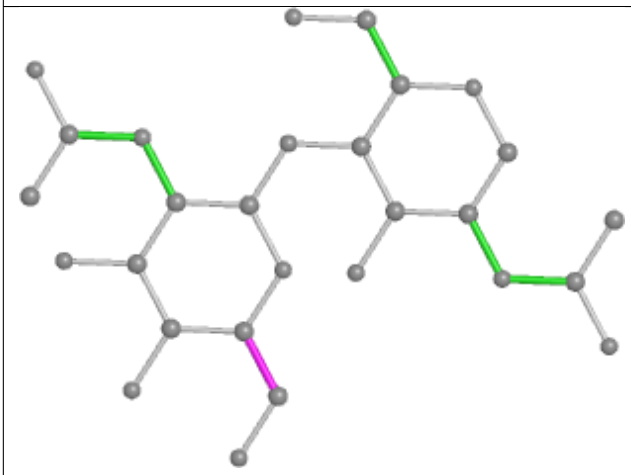


Bond angles



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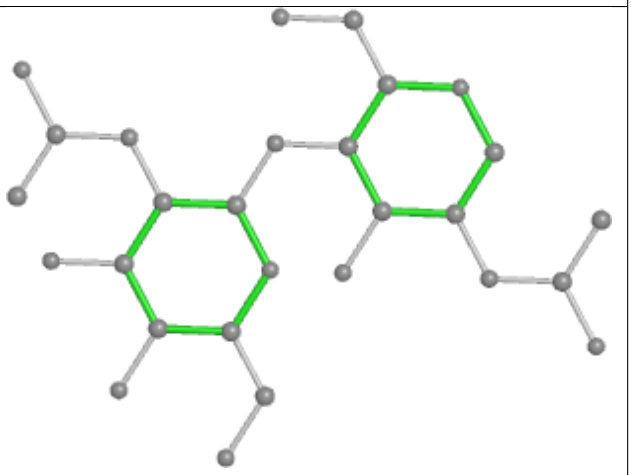
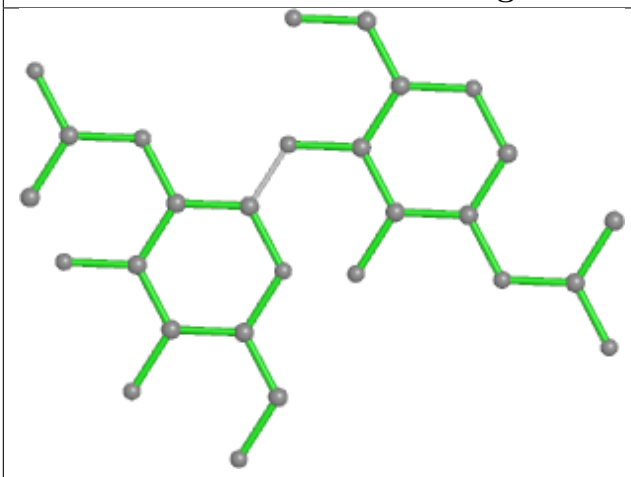
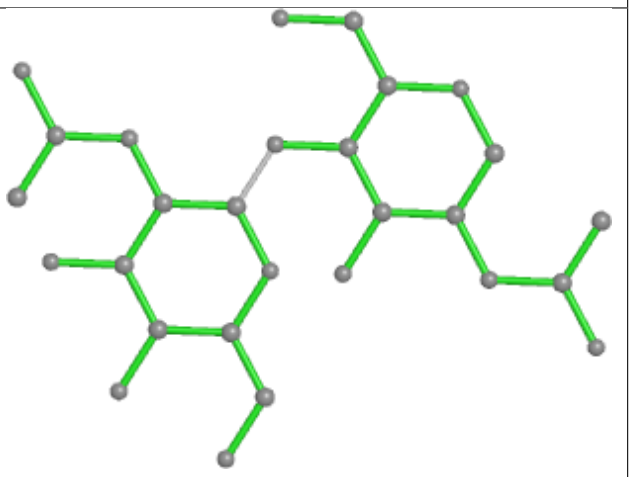
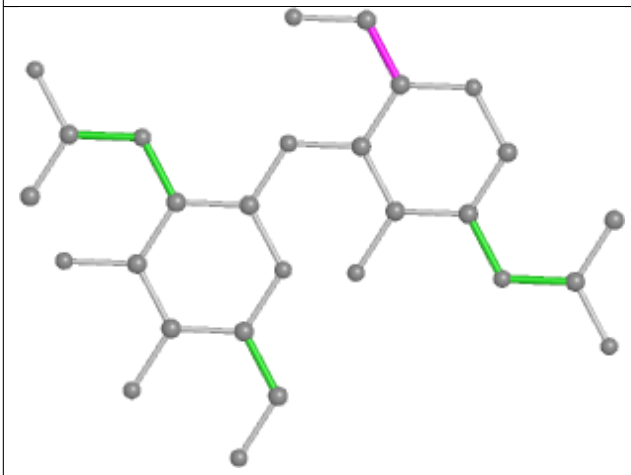
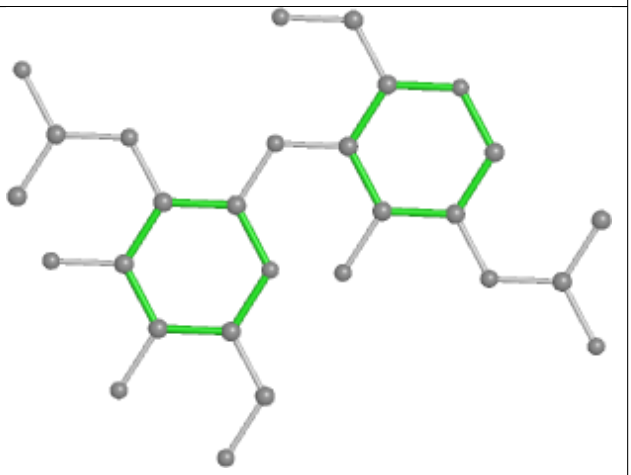
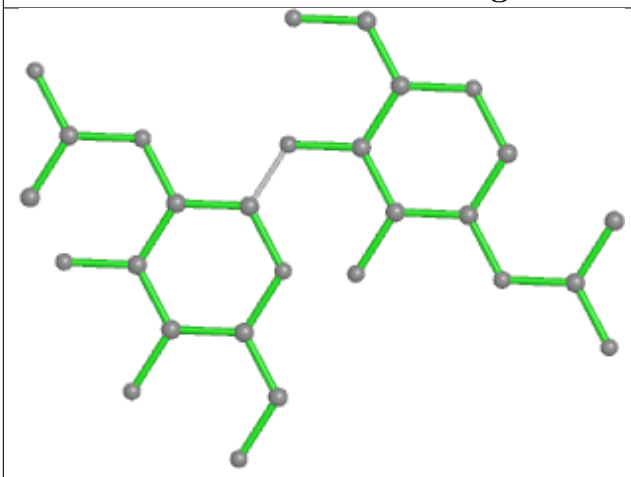


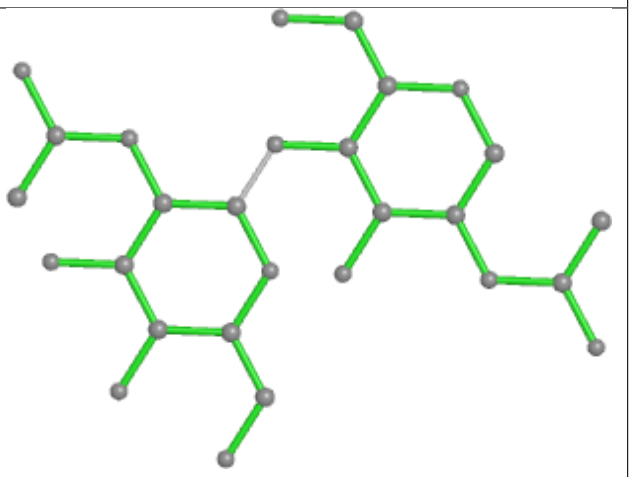
Rings

Oligosaccharide Chain L	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

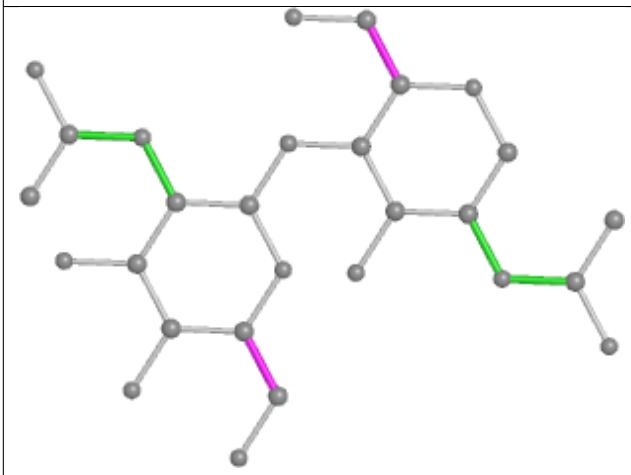
Oligosaccharide Chain M



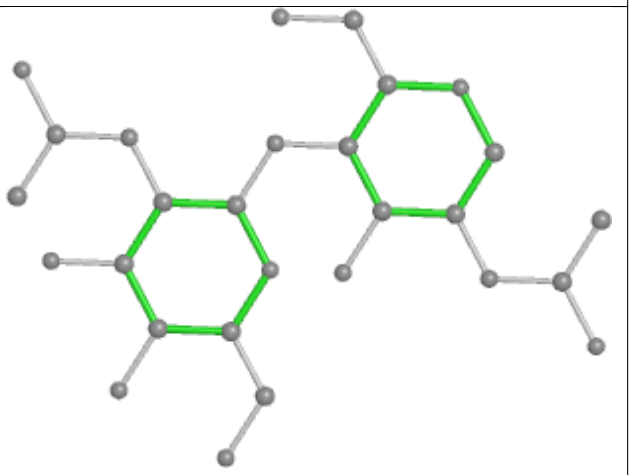
Bond lengths



Bond angles

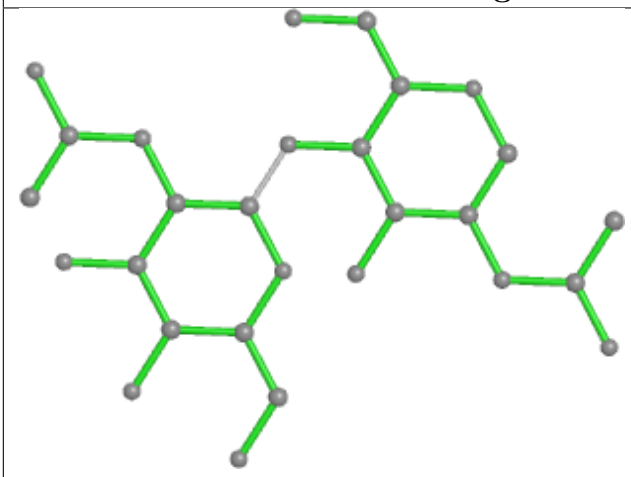


Torsions



Rings

Oligosaccharide Chain N



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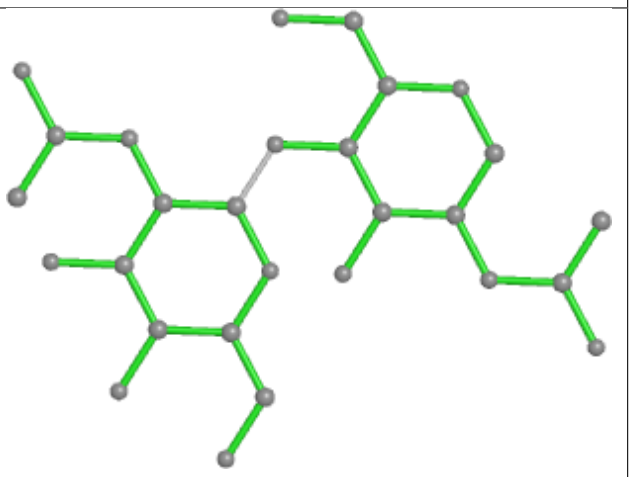
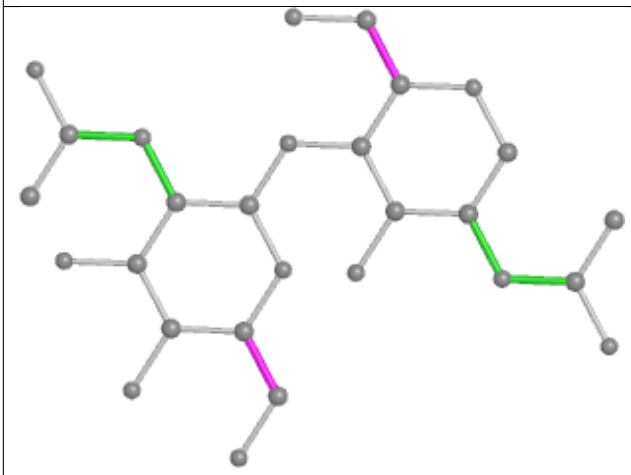
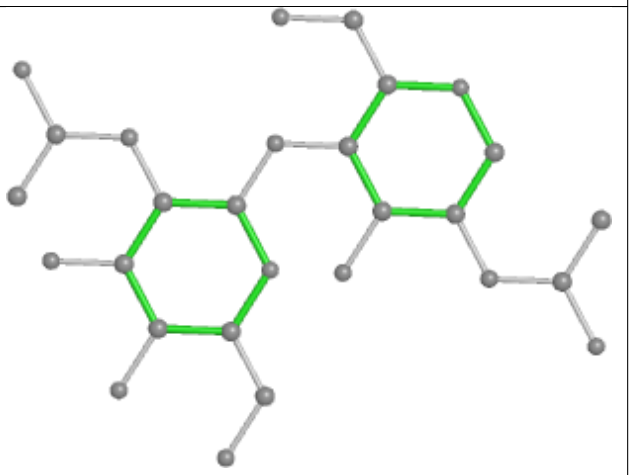


Bond angles

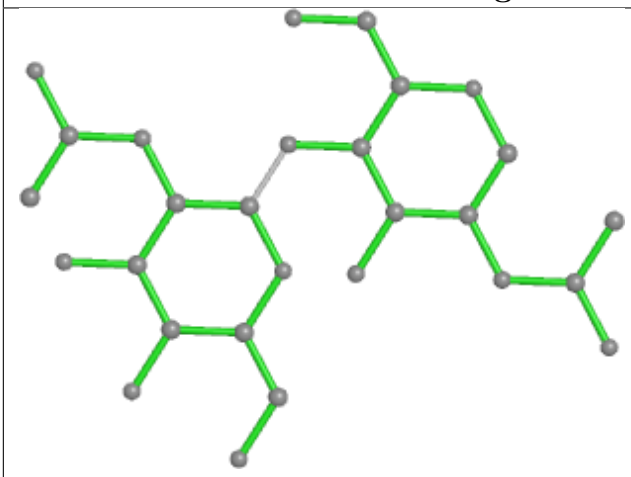


Torsions



Rings

Oligosaccharide Chain O



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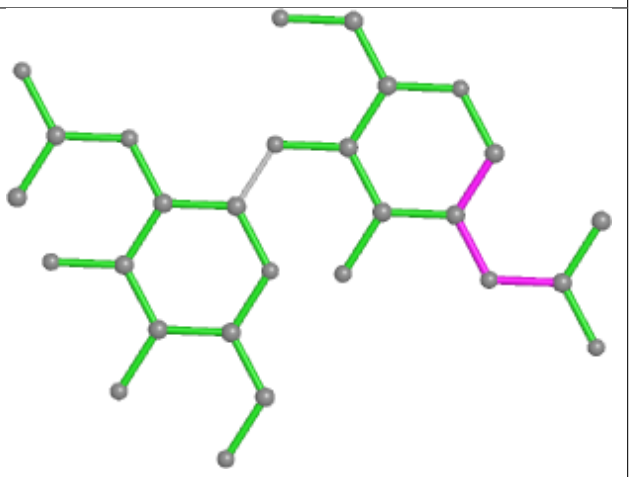
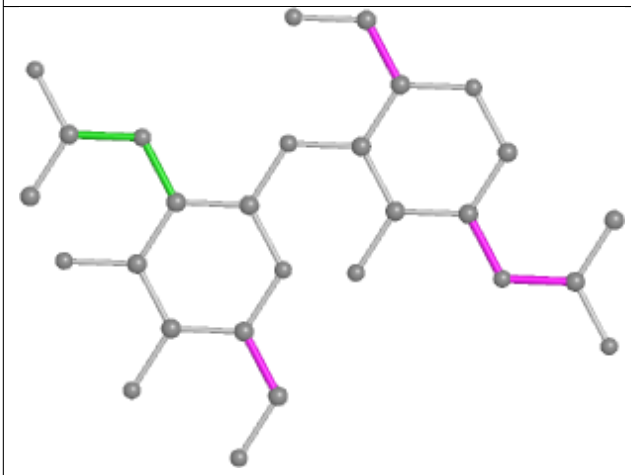


Bond angles



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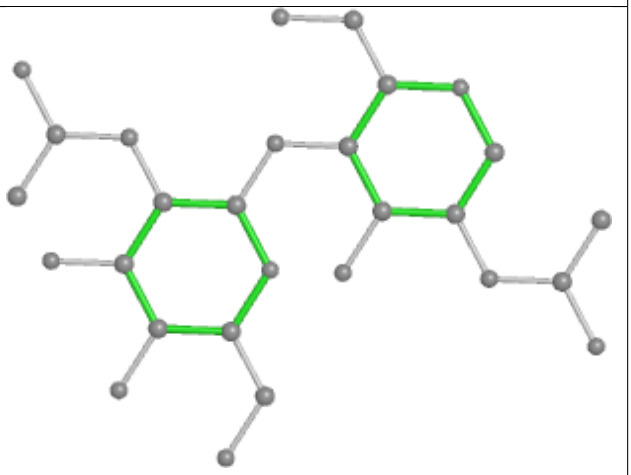
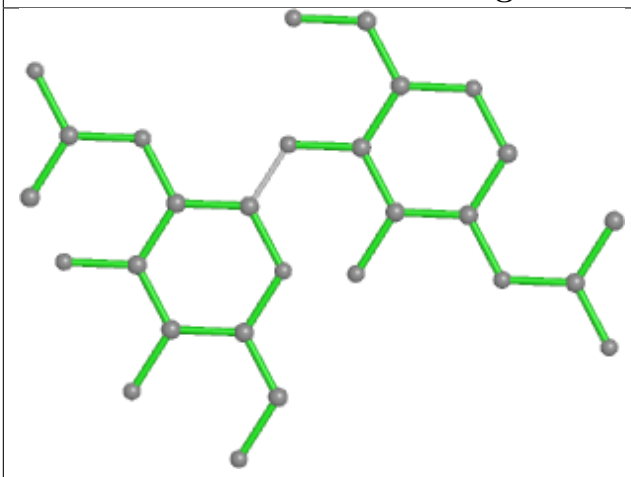


Rings

Oligosaccharide Chain P



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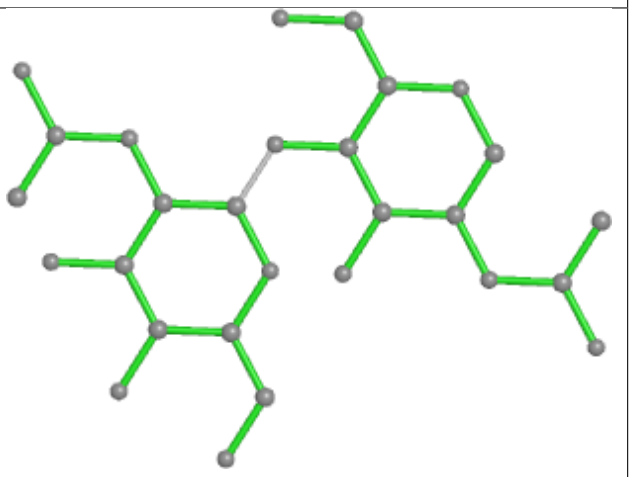

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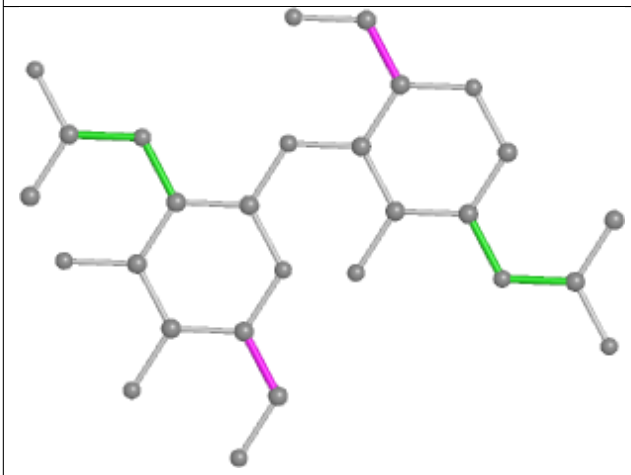

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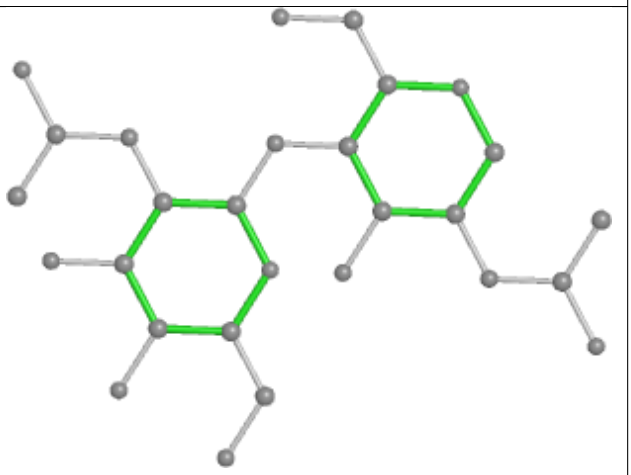
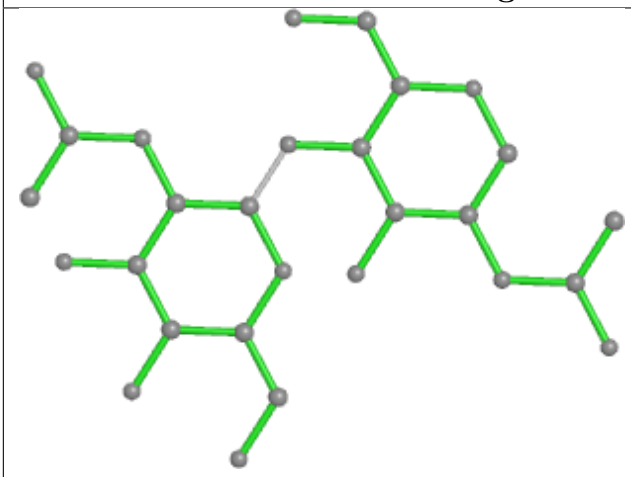


Rings

Oligosaccharide Chain S



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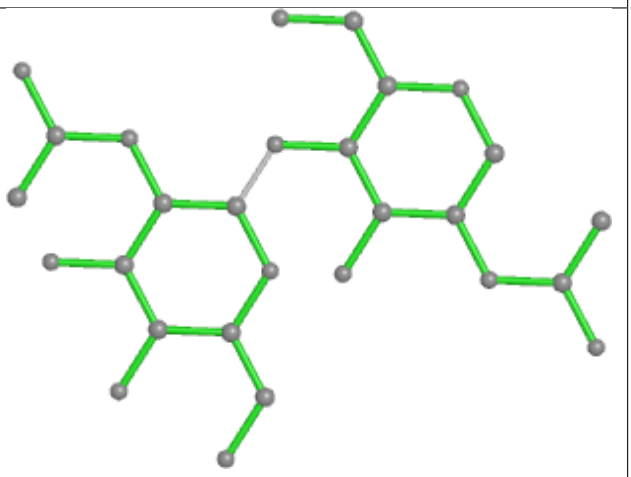
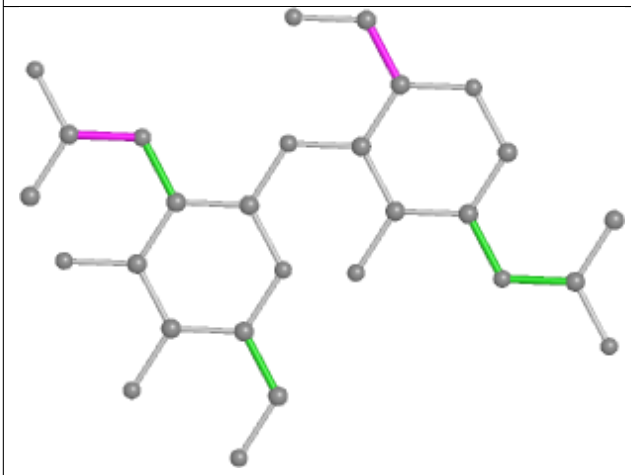


Bond angles



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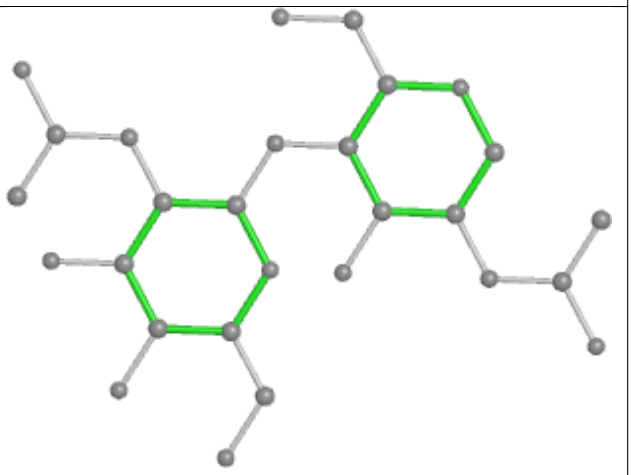
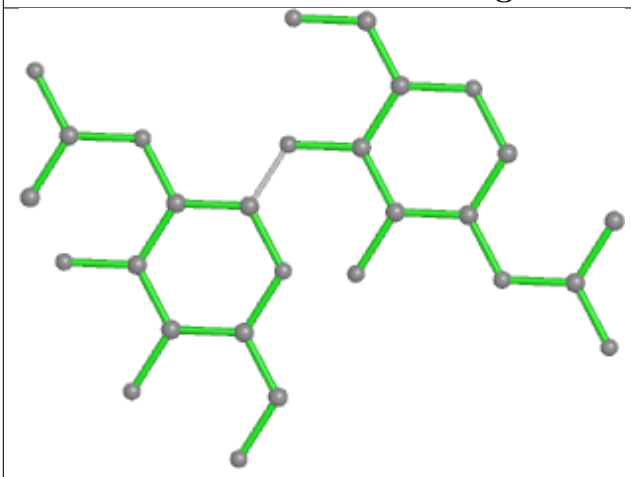
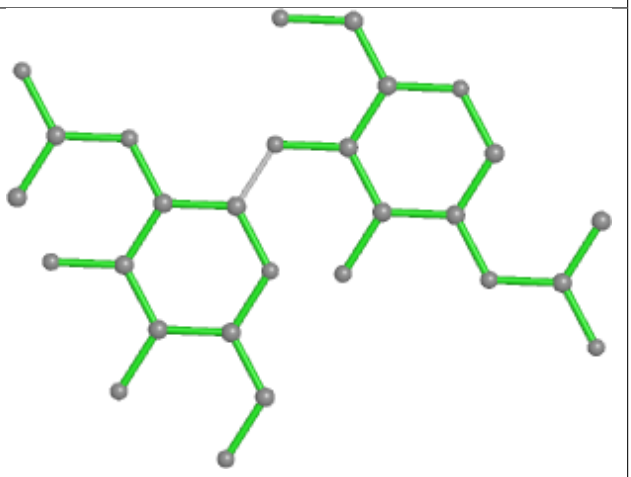


Rings

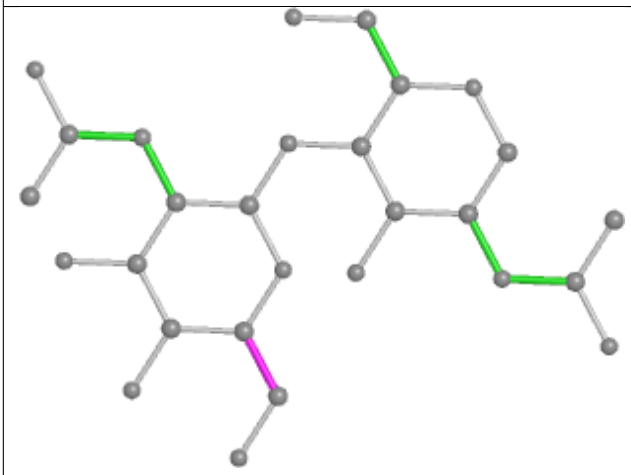
Oligosaccharide Chain T



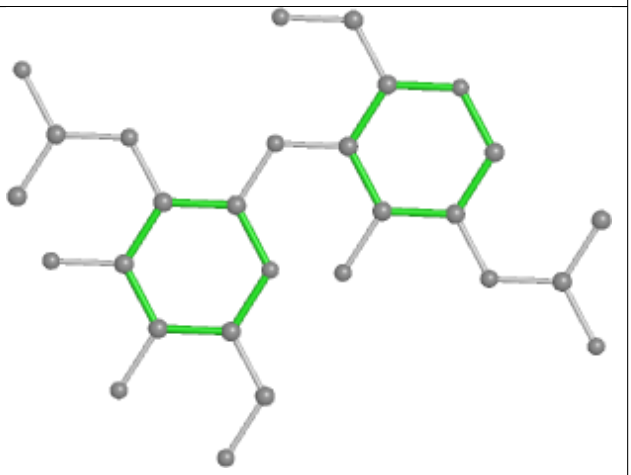
Bond lengths



Bond angles

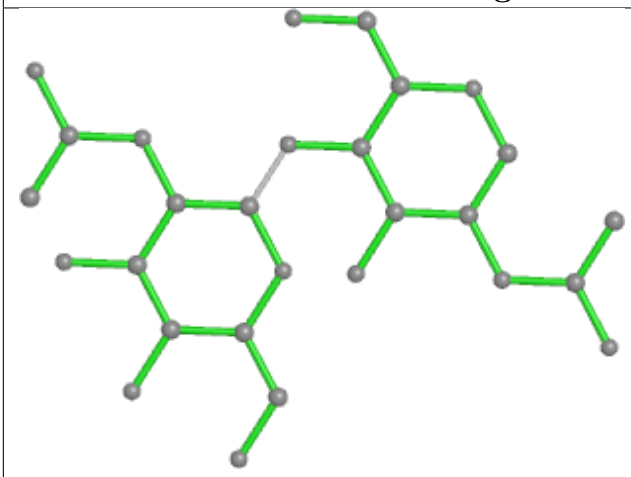


Torsions

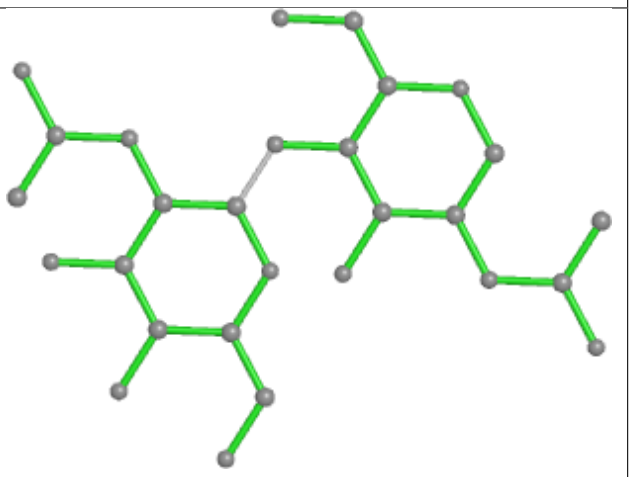


Rings

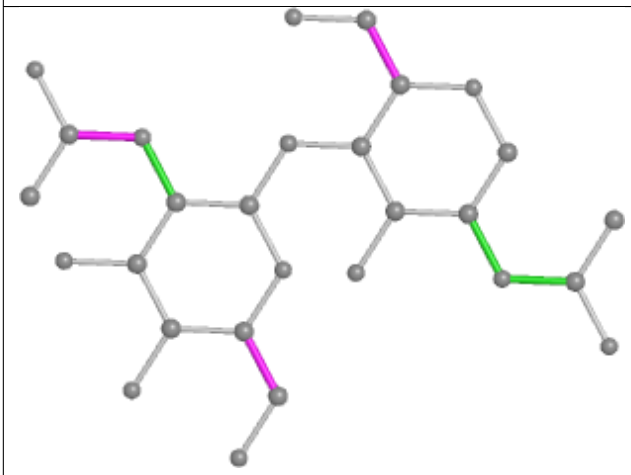
Oligosaccharide Chain U



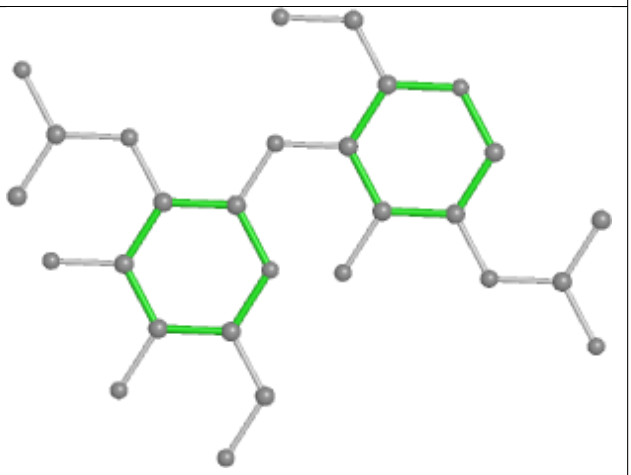
Bond lengths



Bond angles

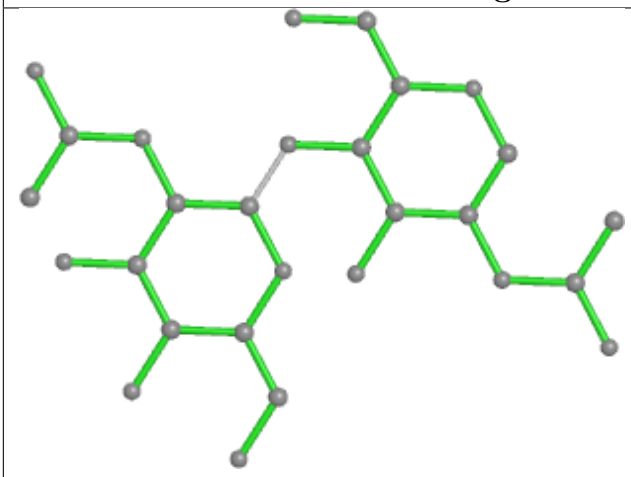


Torsions

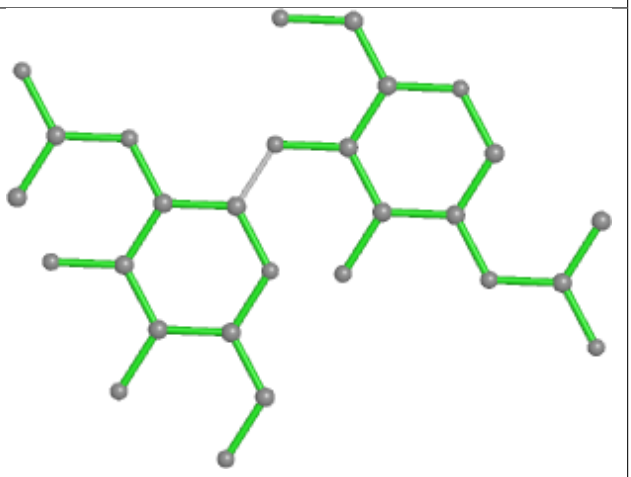


Rings

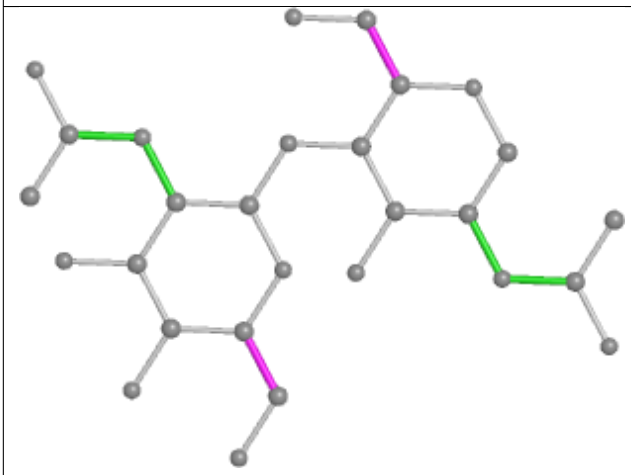
Oligosaccharide Chain V



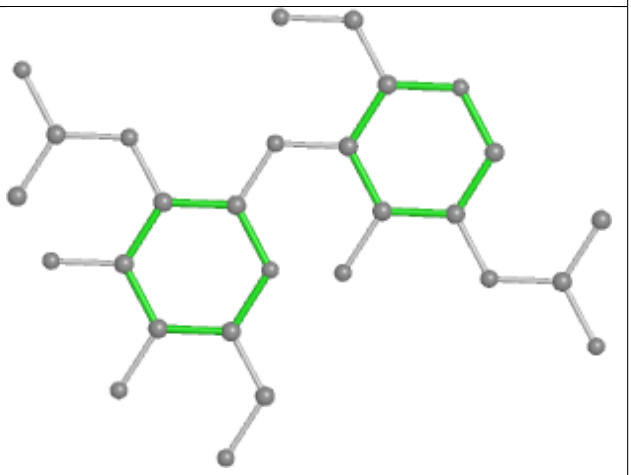
Bond lengths



Bond angles

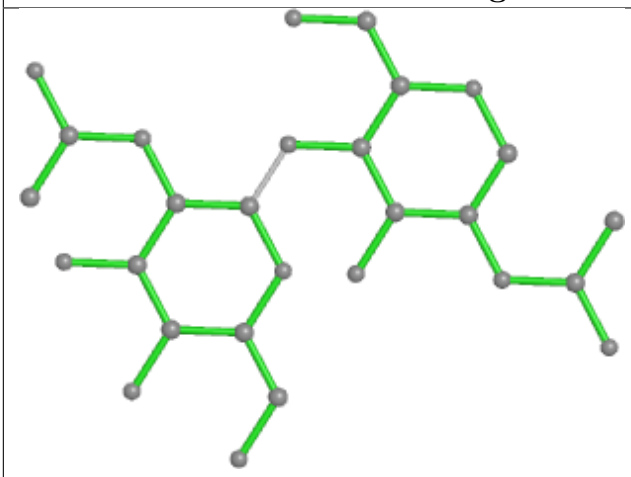


Torsions

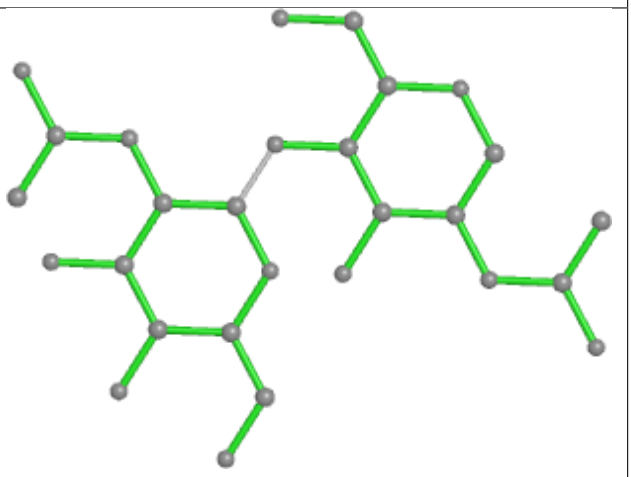


Rings

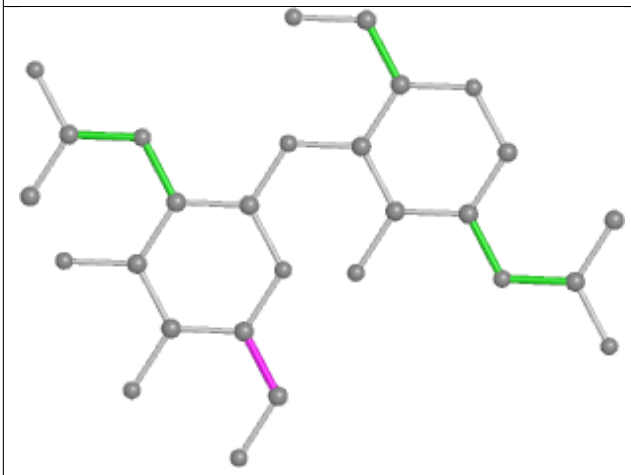
Oligosaccharide Chain W



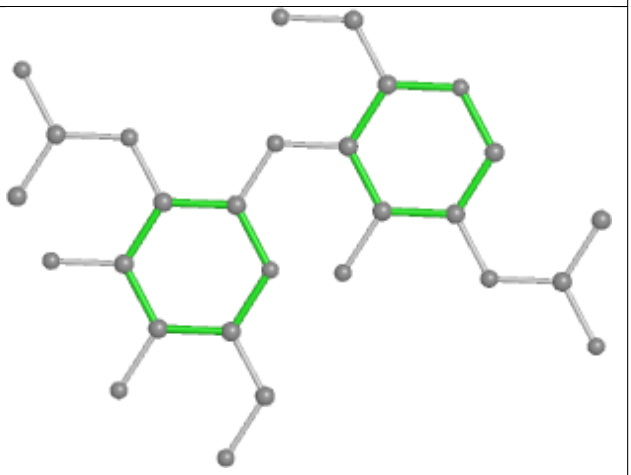
Bond lengths



Bond angles

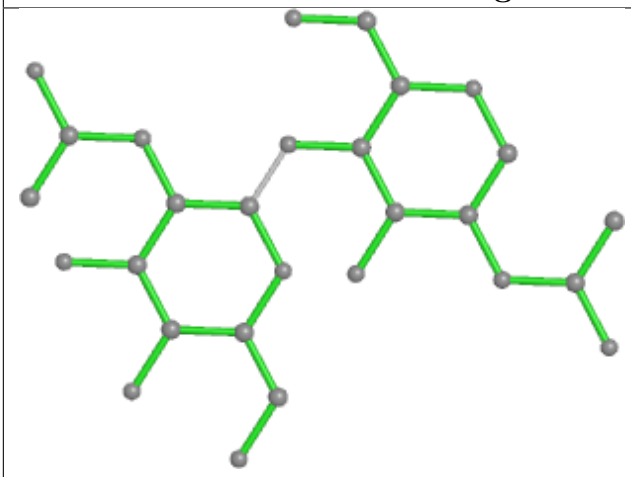


Torsions

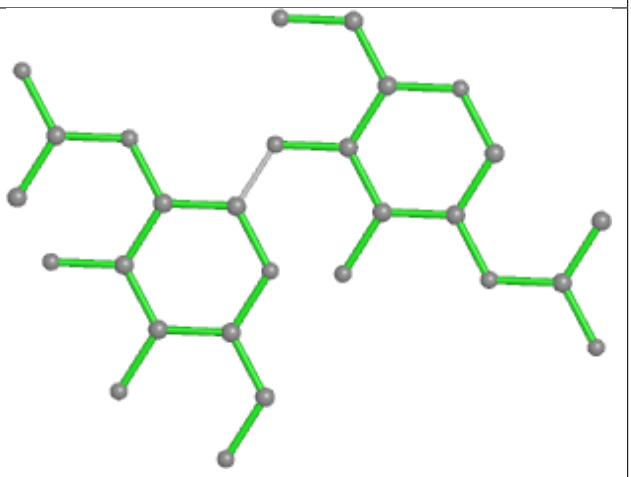


Rings

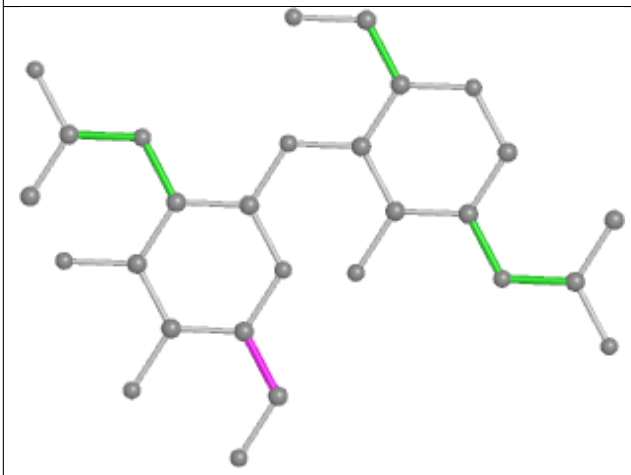
Oligosaccharide Chain X



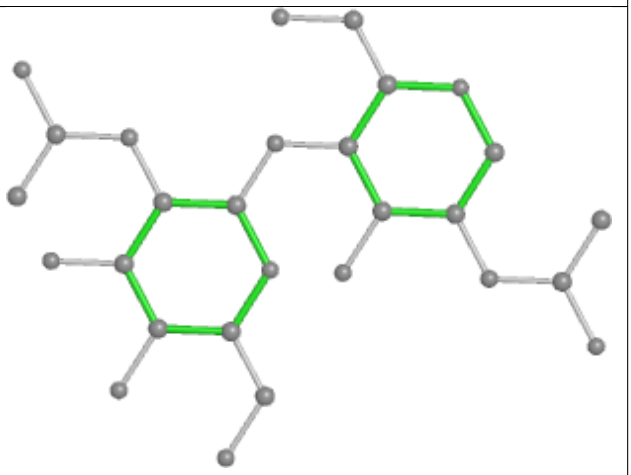
Bond lengths



Bond angles

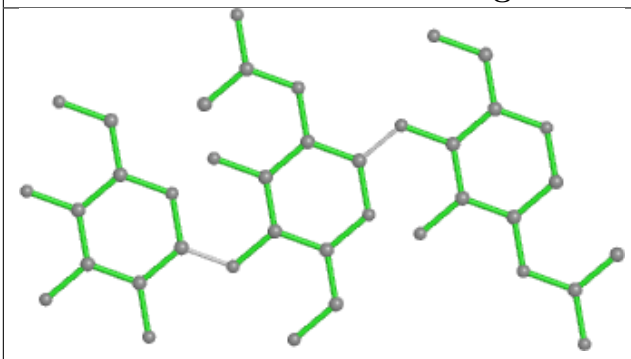


Torsions

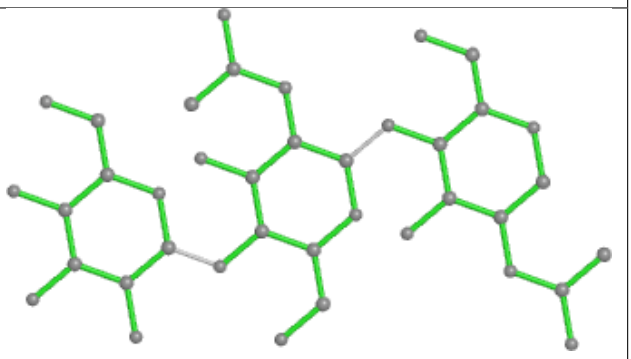


Rings

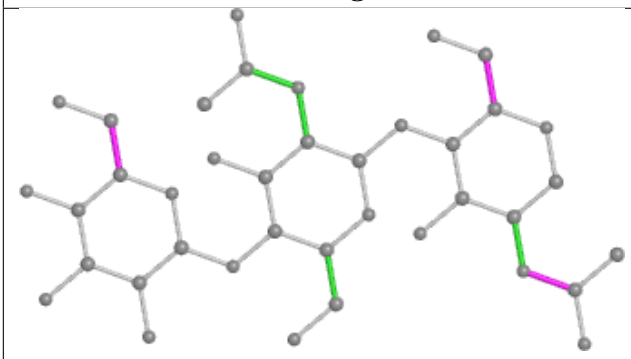
Oligosaccharide Chain K



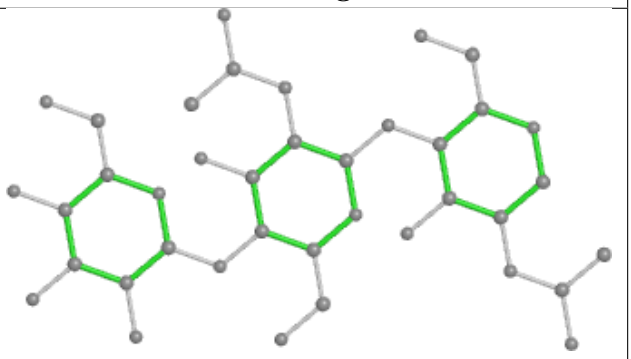
Bond lengths



Bond angles

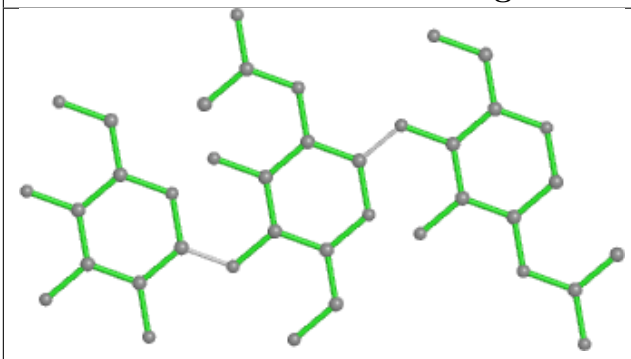


Torsions

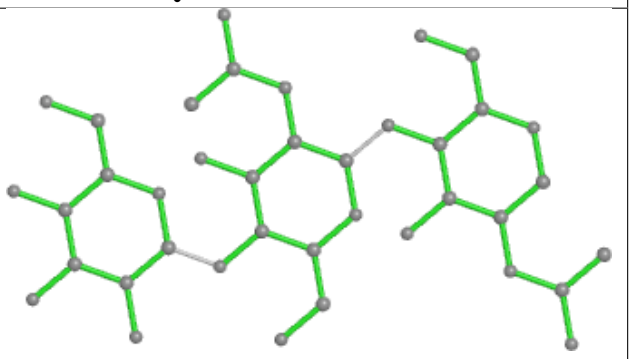


Rings

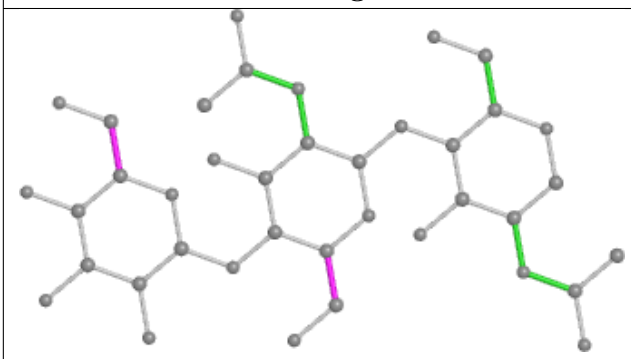
Oligosaccharide Chain Q



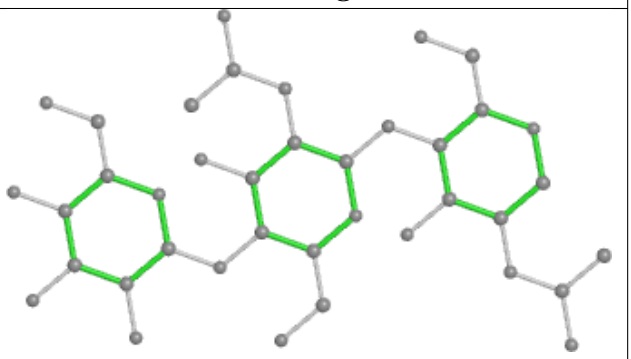
Bond lengths



Bond angles

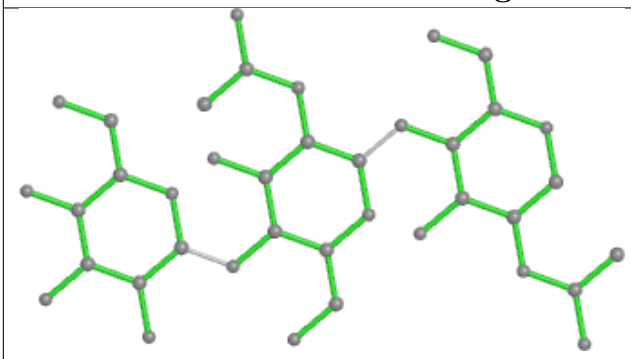


Torsions

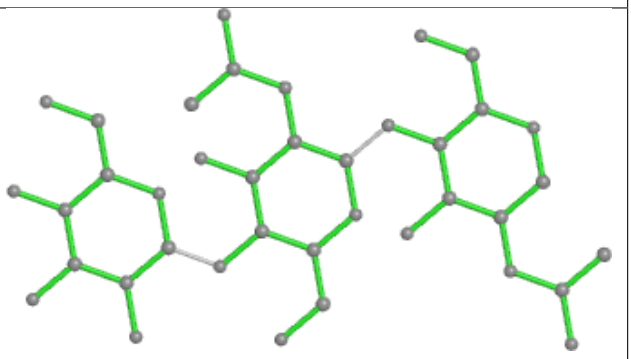


Rings

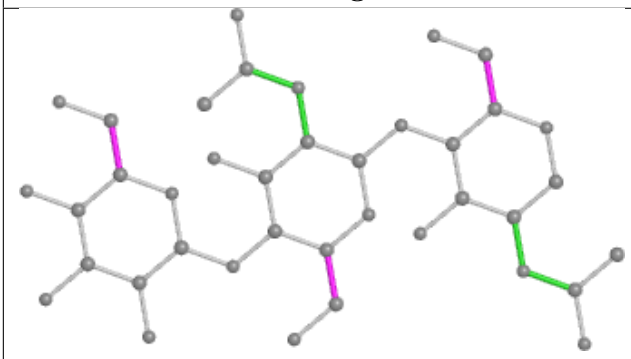
Oligosaccharide Chain R



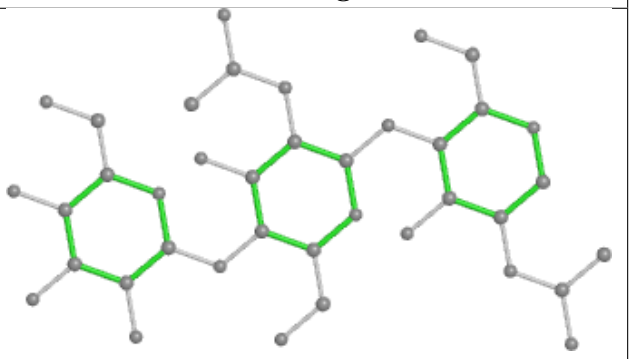
Bond lengths



Bond angles

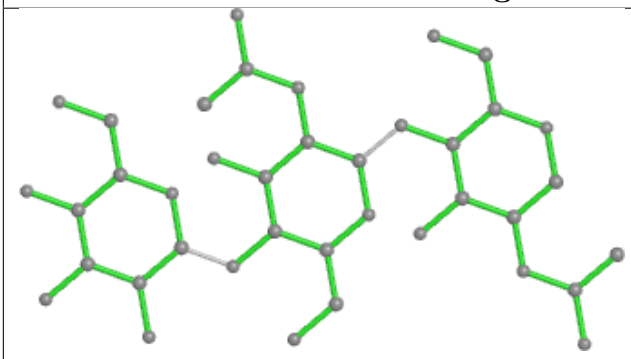


Torsions

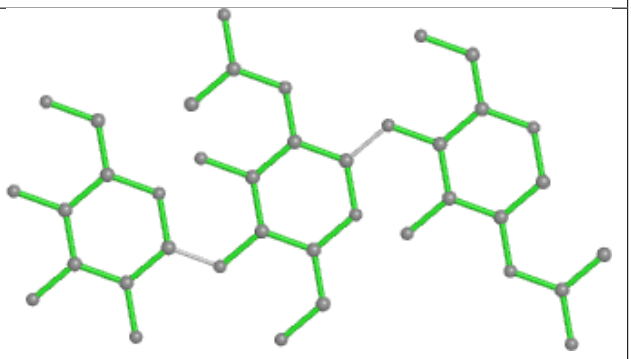


Rings

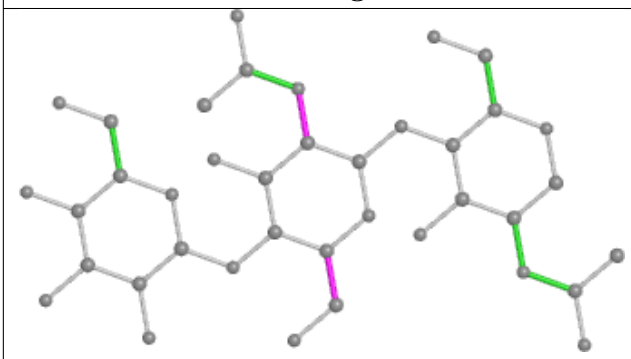
Oligosaccharide Chain Y



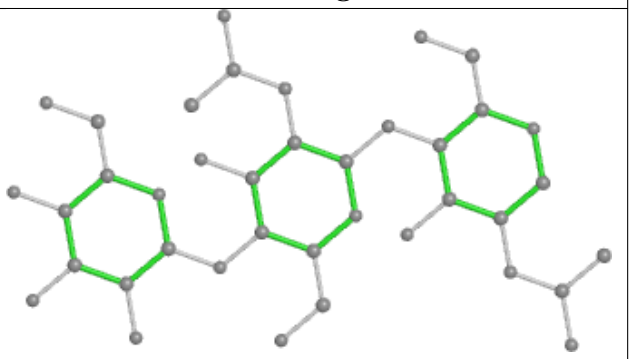
Bond lengths



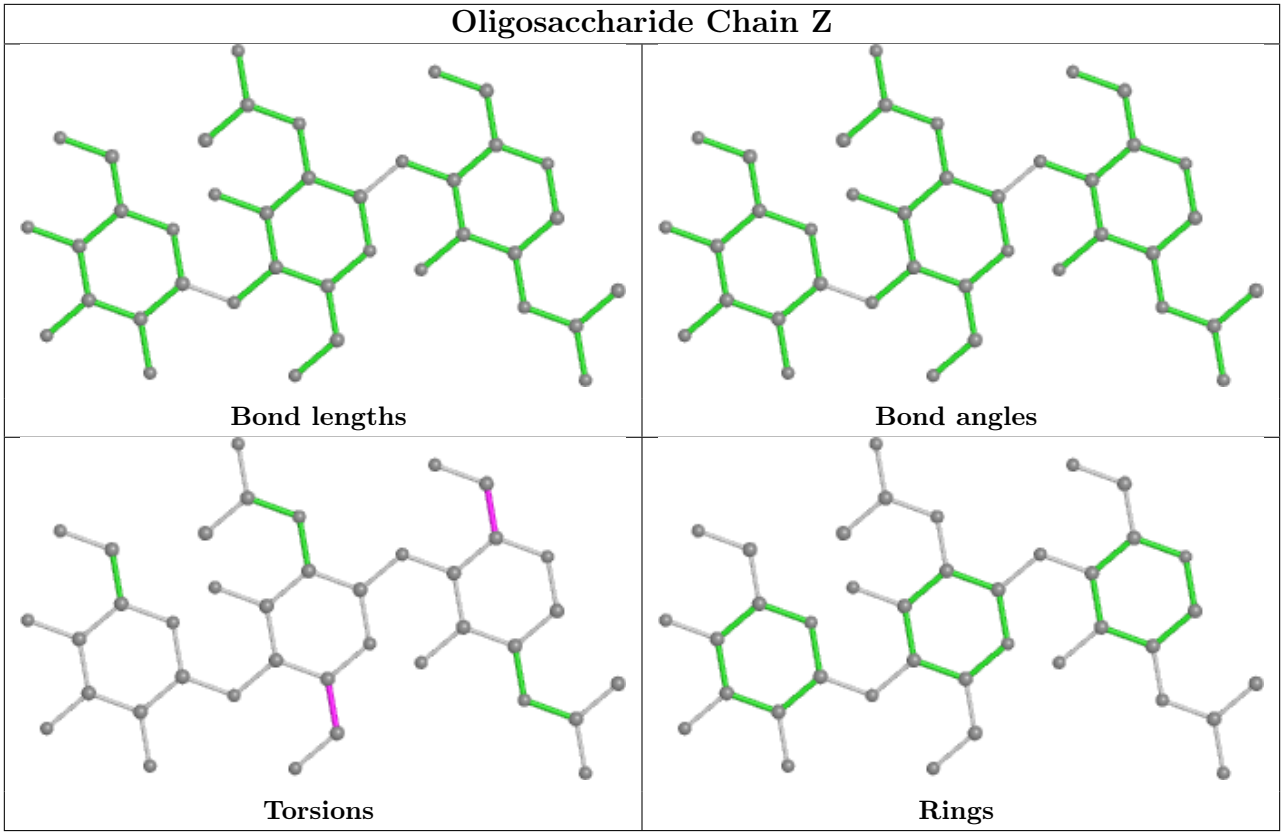
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

34 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	$\#\|Z\|>2$
5	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	A	1308	1	14,14,15	0.19	0	17,19,21	0.47	0
5	NAG	B	1303	-	14,14,15	0.19	0	17,19,21	0.45	0
5	NAG	D	701	2	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	F	701	2	14,14,15	0.22	0	17,19,21	0.44	0
5	NAG	A	1307	1	14,14,15	0.31	0	17,19,21	0.39	0
5	NAG	D	704	2	14,14,15	0.23	0	17,19,21	0.40	0
5	NAG	F	703	2	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	D	703	2	14,14,15	0.30	0	17,19,21	0.40	0
5	NAG	C	1306	1	14,14,15	0.19	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	1308	1	14,14,15	0.18	0	17,19,21	0.45	0
5	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.47	0
5	NAG	D	702	2	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	A	1304	-	14,14,15	0.18	0	17,19,21	0.45	0
5	NAG	C	1303	-	14,14,15	0.22	0	17,19,21	0.43	0
5	NAG	A	1303	1	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	A	1305	1	14,14,15	0.19	0	17,19,21	0.42	0
5	NAG	B	1306	1	14,14,15	0.22	0	17,19,21	0.36	0
5	NAG	C	1301	-	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	C	1308	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	F	704	2	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	A	1302	-	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	B	1305	1	14,14,15	0.20	0	17,19,21	0.42	0
5	NAG	A	1301	-	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	A	1306	-	14,14,15	0.20	0	17,19,21	0.46	0
5	NAG	C	1307	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	B	1302	1	14,14,15	0.17	0	17,19,21	0.43	0
5	NAG	B	1309	1	14,14,15	0.20	0	17,19,21	0.46	0
5	NAG	C	1304	-	14,14,15	0.18	0	17,19,21	0.48	0
5	NAG	C	1305	1	14,14,15	0.19	0	17,19,21	0.60	0
5	NAG	B	1304	-	14,14,15	0.31	0	17,19,21	0.38	0
5	NAG	F	702	2	14,14,15	0.28	0	17,19,21	0.50	0
5	NAG	B	1307	1	14,14,15	0.21	0	17,19,21	0.50	0
5	NAG	C	1309	1	14,14,15	0.16	0	17,19,21	0.50	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
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
5	NAG	D	701	2	-	2/6/23/26	0/1/1/1
5	NAG	F	701	2	-	2/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	D	704	2	-	2/6/23/26	0/1/1/1
5	NAG	F	703	2	-	0/6/23/26	0/1/1/1
5	NAG	D	703	2	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	D	702	2	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1303	-	-	2/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	F	704	2	-	0/6/23/26	0/1/1/1
5	NAG	A	1302	-	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	-	-	0/6/23/26	0/1/1/1
5	NAG	A	1306	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1304	-	-	2/6/23/26	0/1/1/1
5	NAG	F	702	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1305	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1304	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	D	704	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1304	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	D	704	NAG	C4-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	D	702	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	D	702	NAG	C4-C5-C6-O6
5	B	1303	NAG	C8-C7-N2-C2
5	B	1303	NAG	O7-C7-N2-C2
5	B	1306	NAG	C8-C7-N2-C2
5	B	1306	NAG	O7-C7-N2-C2
5	B	1308	NAG	C8-C7-N2-C2
5	B	1308	NAG	O7-C7-N2-C2
5	C	1306	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	F	701	NAG	O5-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	F	702	NAG	C4-C5-C6-O6
5	F	701	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	F	702	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1309	NAG	C4-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	D	701	NAG	O5-C5-C6-O6
5	B	1301	NAG	C4-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1305	NAG	C3-C2-N2-C7
5	D	701	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	701	NAG	1	0
5	F	701	NAG	1	0
5	A	1307	NAG	1	0
5	B	1301	NAG	1	0
5	B	1306	NAG	1	0
5	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.

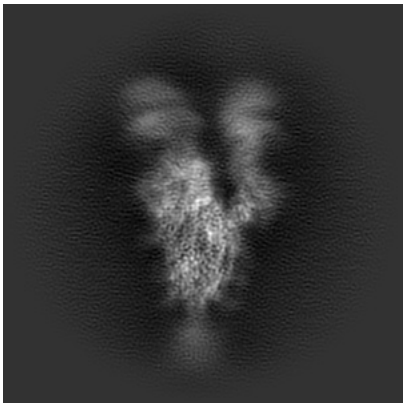
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32482. These allow visual inspection of the internal detail of the map and identification of artifacts.

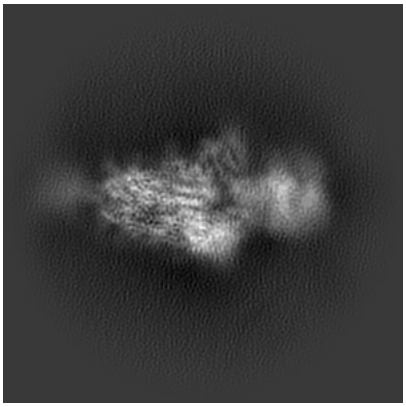
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

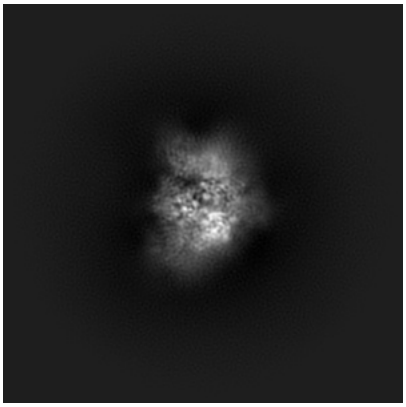
6.1.1 Primary map



X



Y



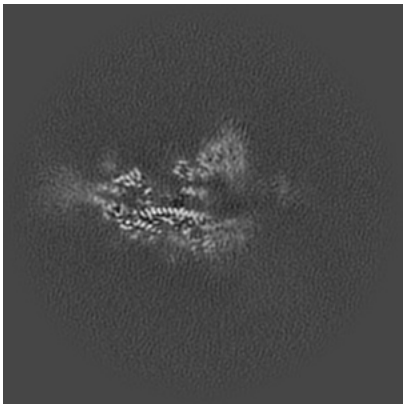
Z

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

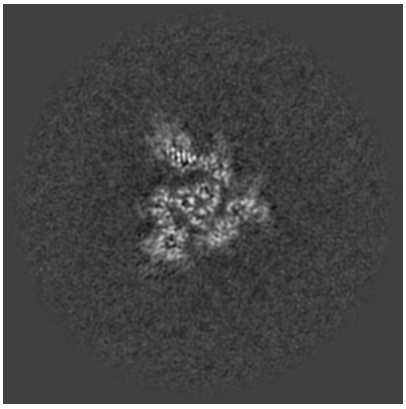
6.2 Central slices

6.2.1 Primary map

X Index: 180



Y Index: 180



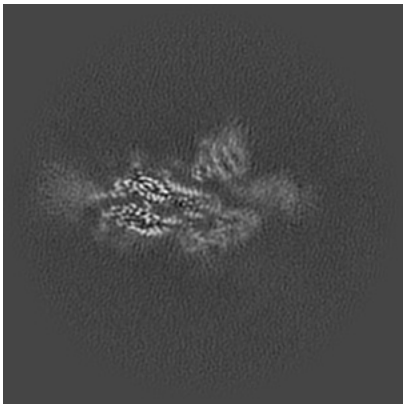
Z Index: 180

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

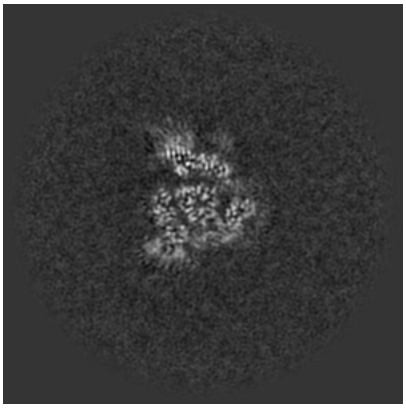
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 191



Y Index: 170

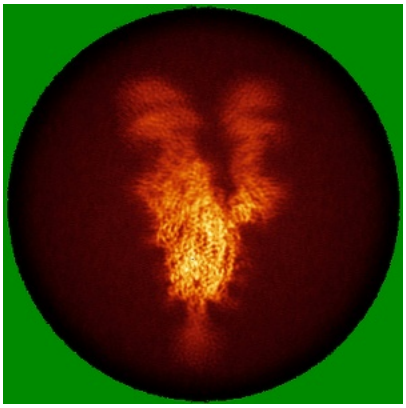


Z Index: 177

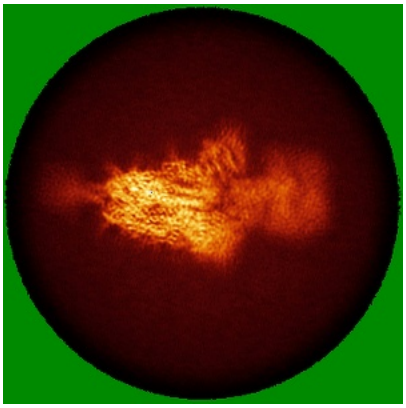
The images above show the largest variance slices of the map in three orthogonal directions.

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

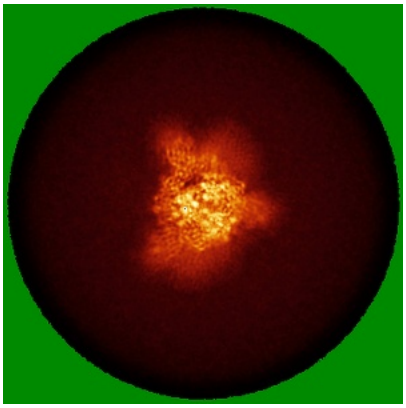
6.4.1 Primary map



X



Y

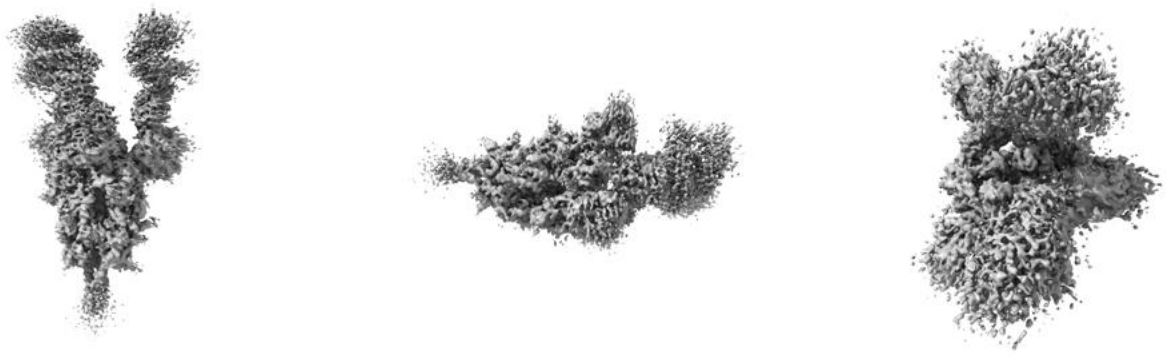


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.404. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

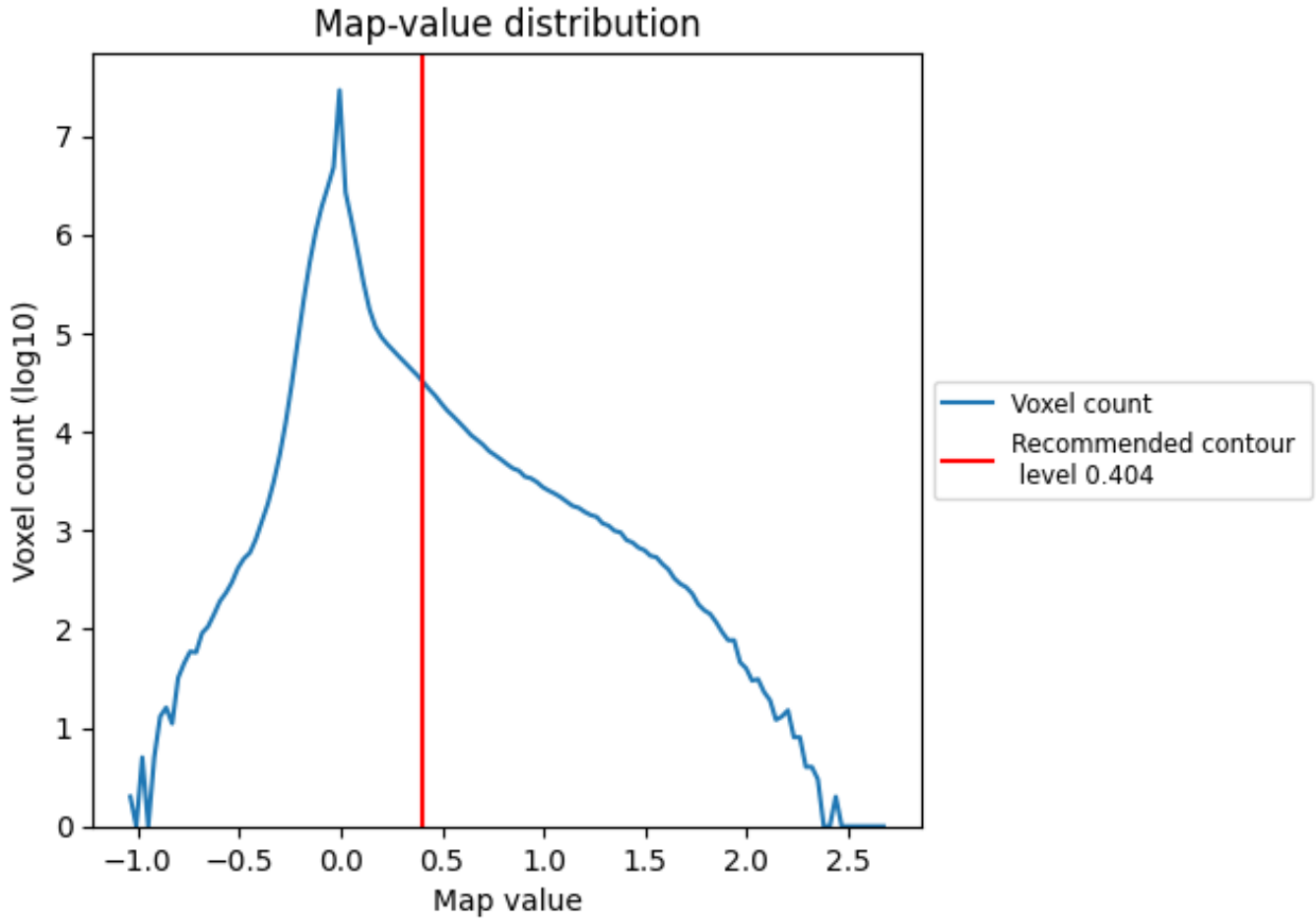
6.6 Mask visualisation (i)

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

7 Map analysis

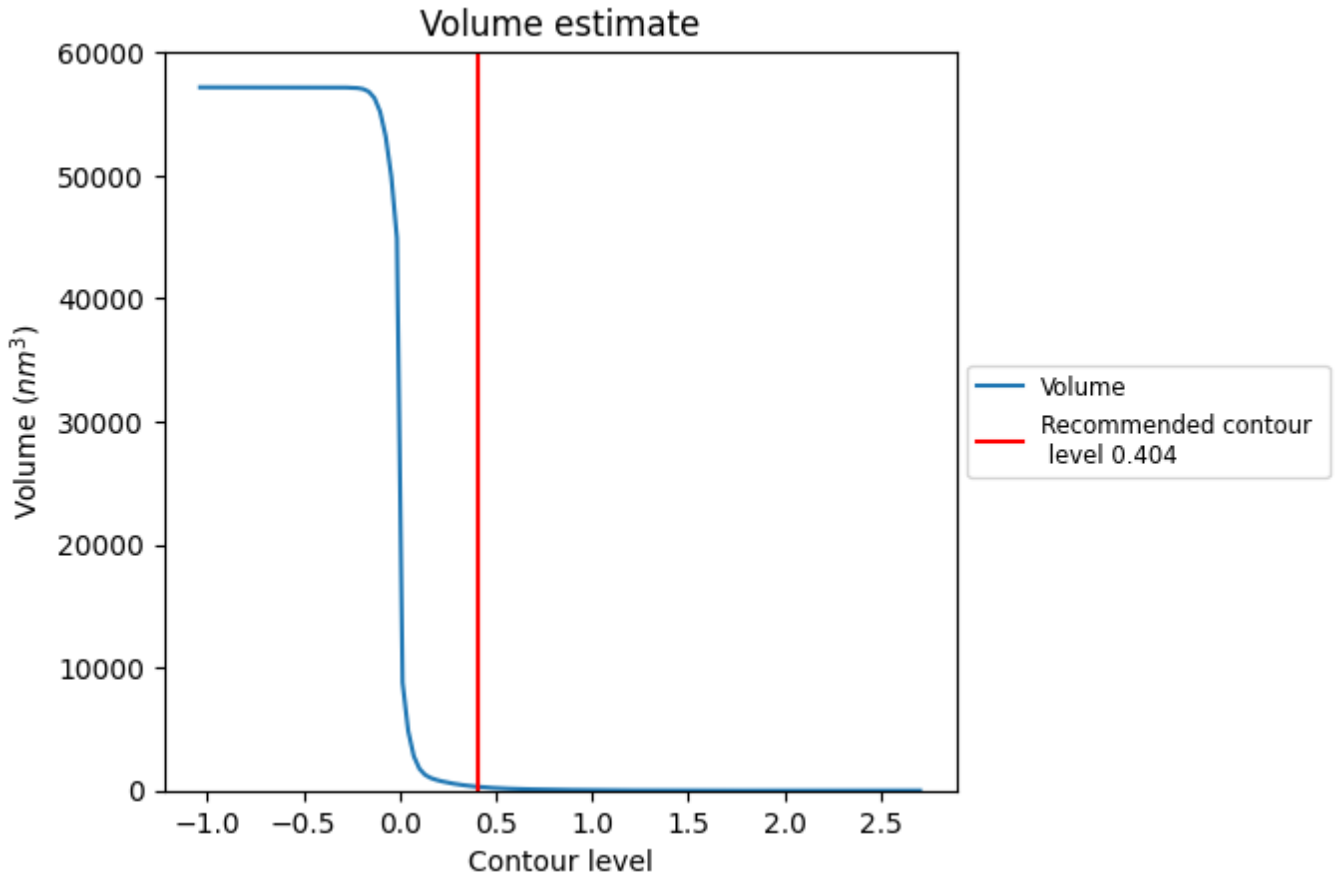
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

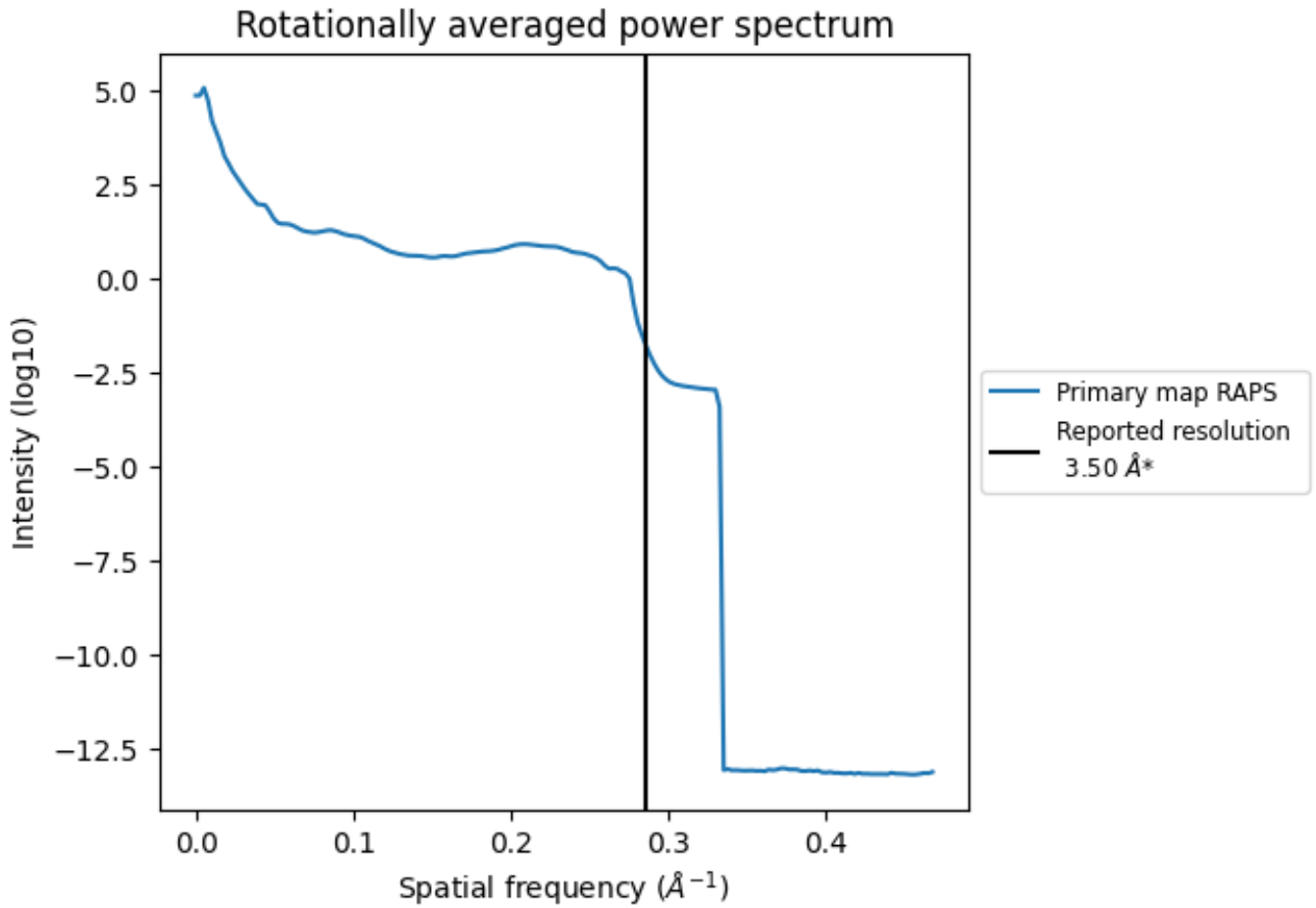
7.2 Volume estimate



The volume at the recommended contour level is 313 nm^3; this corresponds to an approximate mass of 283 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 0.286 $Å^{-1}$

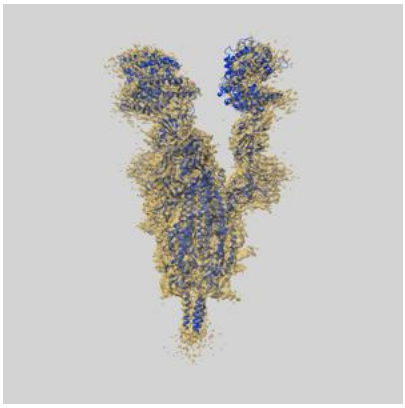
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

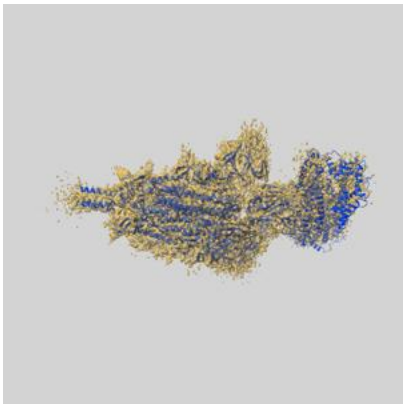
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32482 and PDB model 7WGB. Per-residue inclusion information can be found in section 3 on page 12.

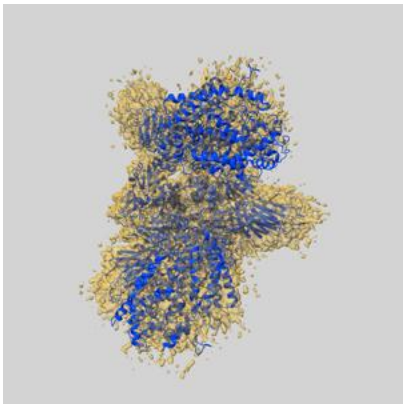
9.1 Map-model overlay



X



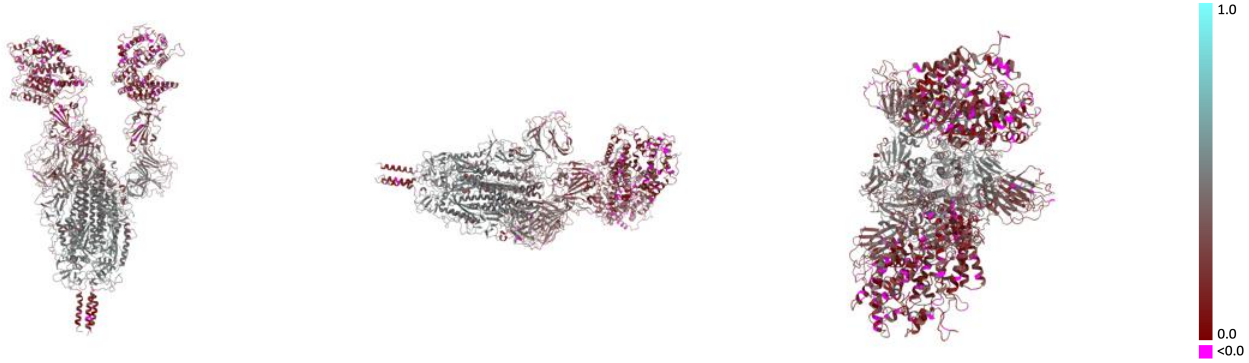
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.404 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.

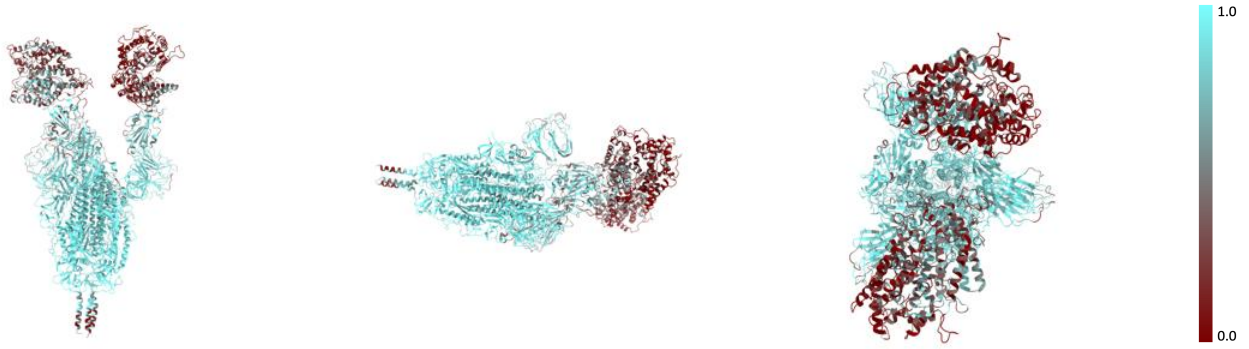
9.2 Q-score mapped to coordinate model



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.

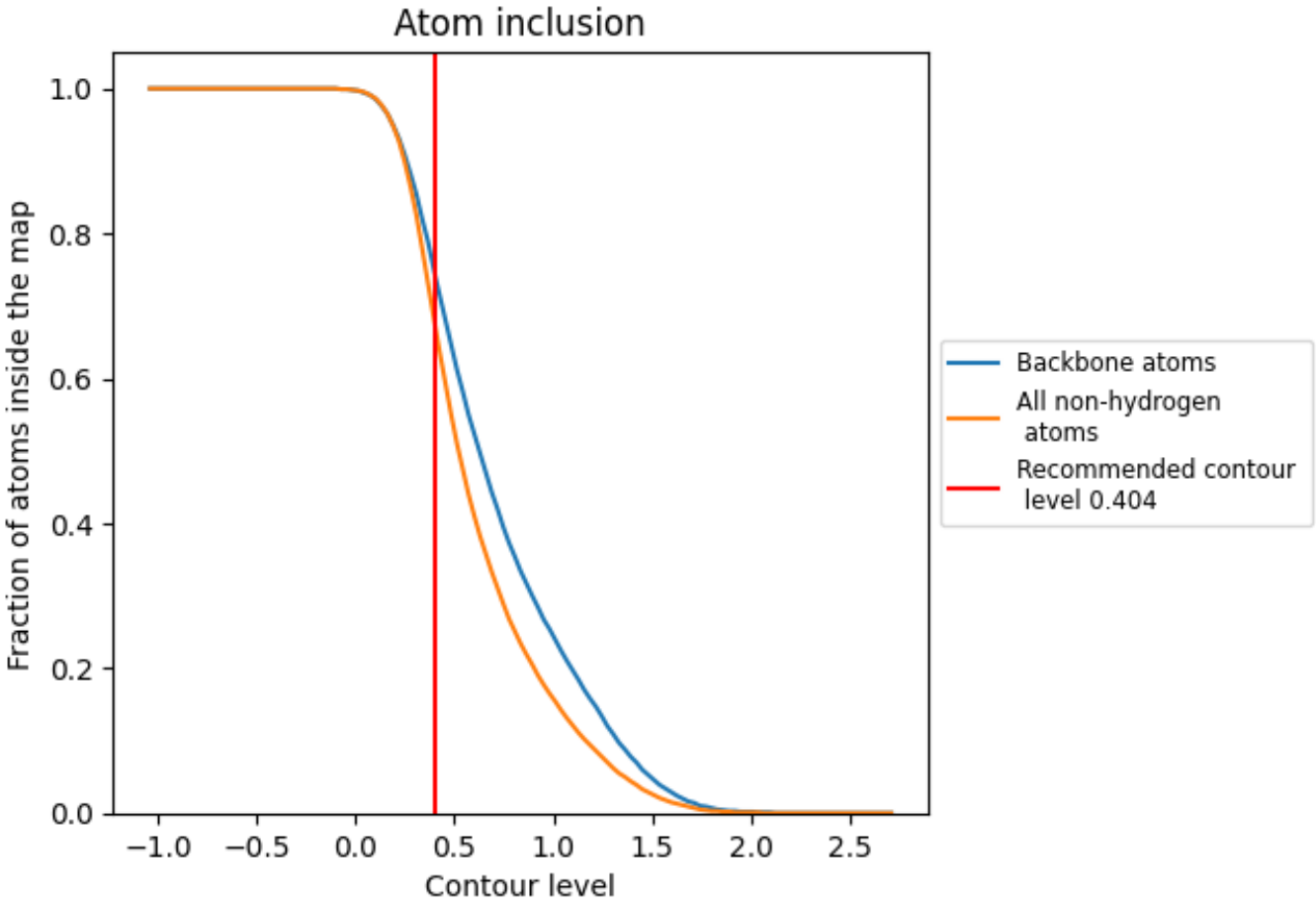
9.3 Atom inclusion mapped to coordinate model



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 (0.404).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.404) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6700	0.3410
A	0.8440	0.4120
B	0.8220	0.3870
C	0.8120	0.3740
D	0.3160	0.2020
E	0.0000	0.2900
F	0.1940	0.2010
G	0.2860	0.3630
H	0.9290	0.4670
I	0.5360	0.3620
J	0.9290	0.4570
K	0.6670	0.3490
L	0.7860	0.3970
M	0.1070	0.4080
N	0.8210	0.4260
O	0.5000	0.3690
P	0.8570	0.4660
Q	0.7690	0.3940
R	0.7180	0.4170
S	0.8210	0.3940
T	0.0000	0.4160
U	0.6070	0.3190
V	0.8570	0.4770
W	0.4290	0.3220
X	0.8570	0.4440
Y	0.7440	0.3620
Z	0.7180	0.4300