Full wwPDB EM Validation Report ⓘ

Sep 6, 2023 – 01:09 PM EDT

PDB ID	:	7U0Q
EMDB ID	:	EMD-26263
Title	:	SARS-Cov2 S protein structure in complex with neutralizing monoclonal antibody 002-02
Authors	:	Patel, A.; Ortlund, E.
Deposited on	:	2022-02-18
Resolution	:	3.86 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:

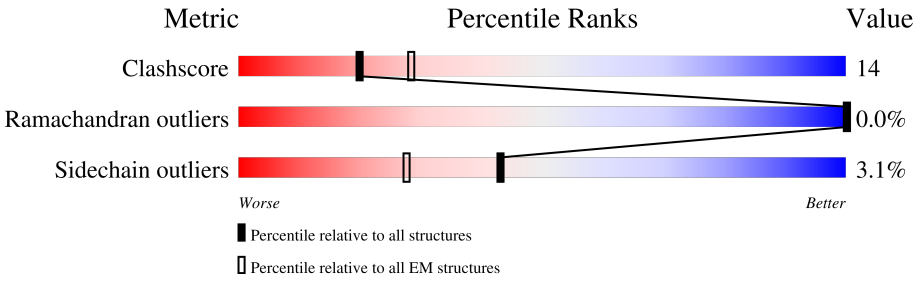
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.86 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1208	7% 73% 16% • 10%
1	B	1208	5% 70% 17% • 12%
1	C	1208	6% 68% 21% • 10%
2	F	214	78% 58% 39% •
2	I	214	65% 58% 38% •
3	G	447	31% 30% 19% 50%
3	J	447	33% 30% 17% • 50%
4	D	2	50% 50%

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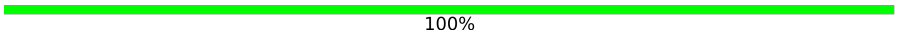
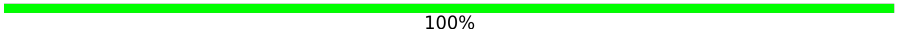
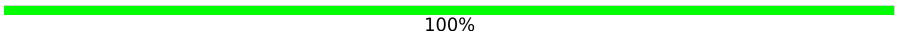
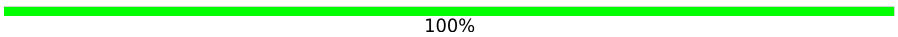
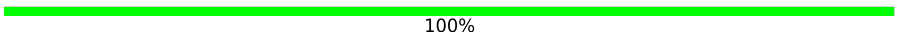
Mol	Chain	Length	Quality of chain
4	E	2	
4	H	2	
4	K	2	
4	L	2	
4	M	2	
4	N	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
5	V	3	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 32721 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	1084	Total	C	N	O	S	0	0
			8483	5414	1417	1614	38		
1	B	1063	Total	C	N	O	S	0	0
			8341	5333	1390	1581	37		
1	C	1087	Total	C	N	O	S	0	0
			8508	5432	1420	1618	38		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2

- Molecule 2 is a protein called mAb 002-02 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	214	Total	C	N	O	S	0	0
			1647	1028	280	334	5		
2	I	214	Total	C	N	O	S	0	0
			1647	1028	280	334	5		

- Molecule 3 is a protein called mAb 002-02 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	222	Total	C	N	O	S	0	0
			1671	1050	282	332	7		
3	J	222	Total	C	N	O	S	0	0
			1671	1050	282	332	7		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		

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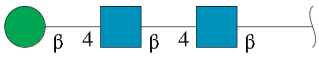
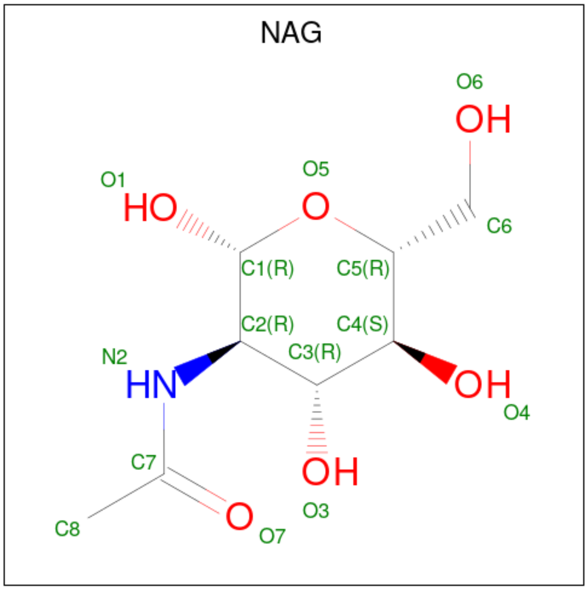
Mol	Chain	Residues	Atoms				AltConf	Trace
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	V	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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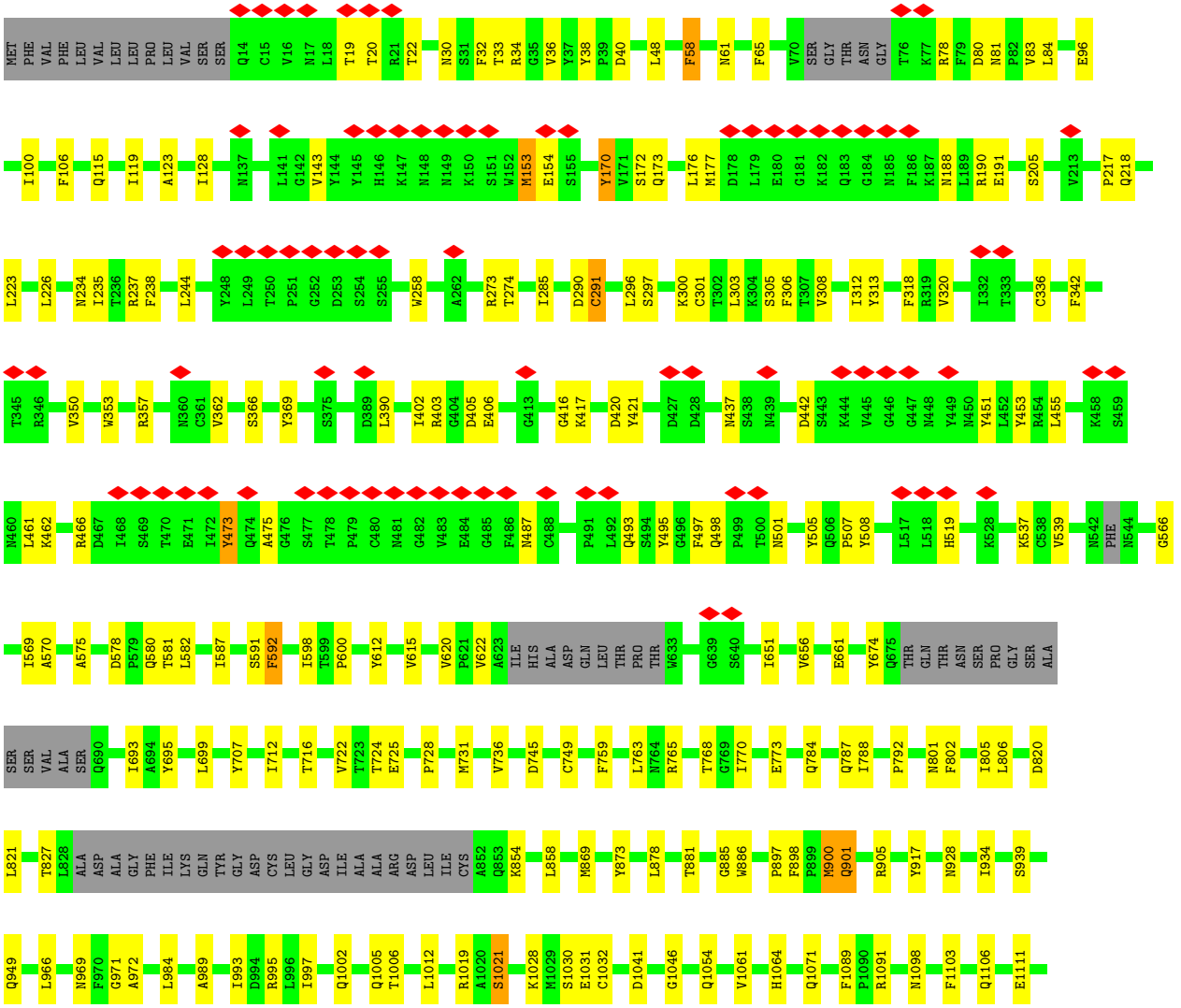
Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0
6	C	1	Total 14	C 8	N 1	O 5	0

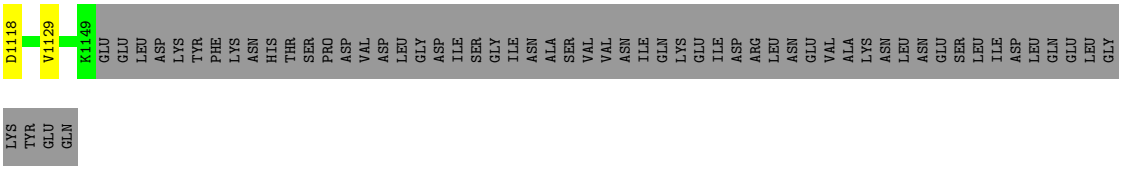
3 Residue-property plots (i)

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

- Molecule 1: Spike glycoprotein

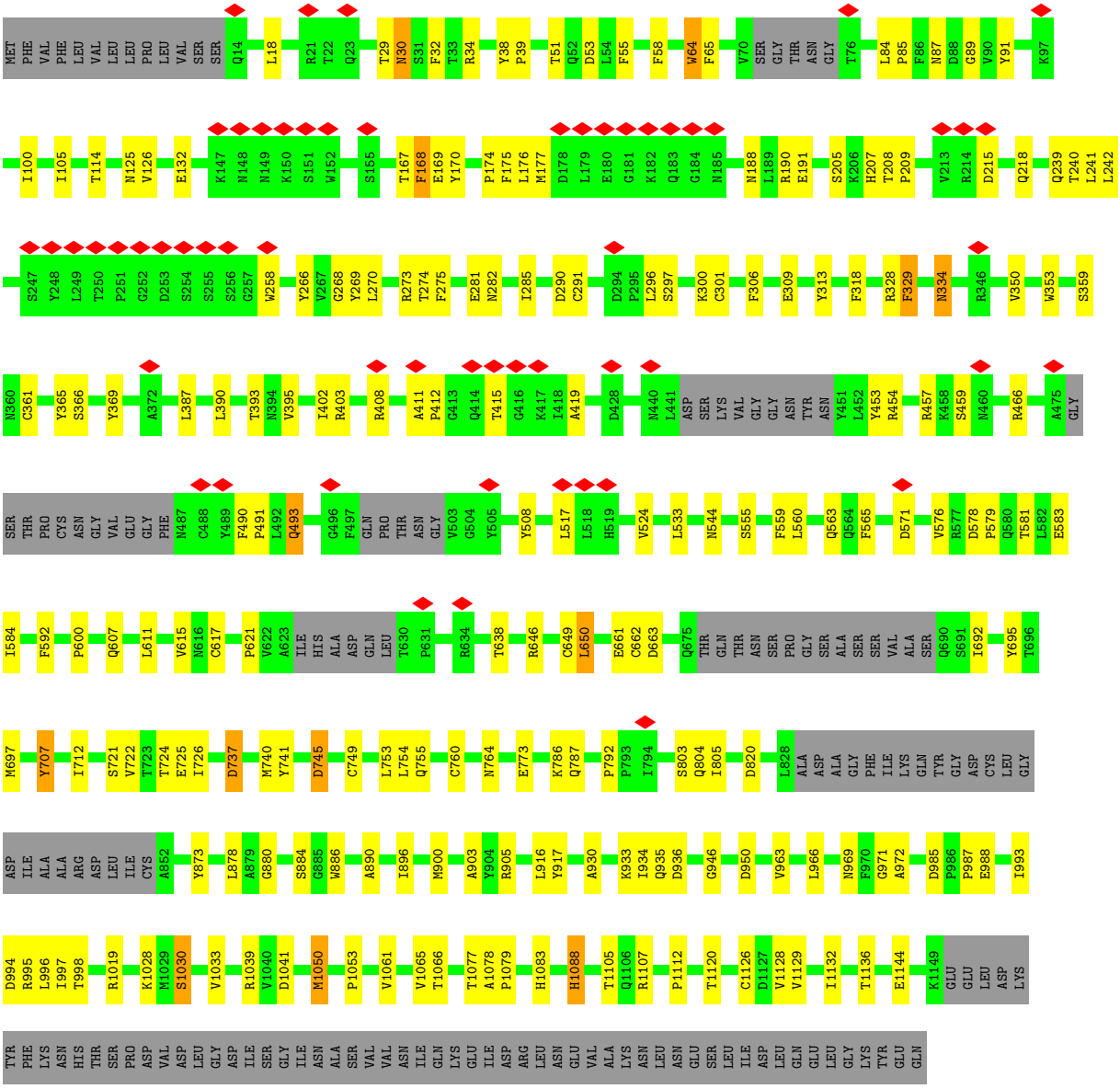
Chain A:





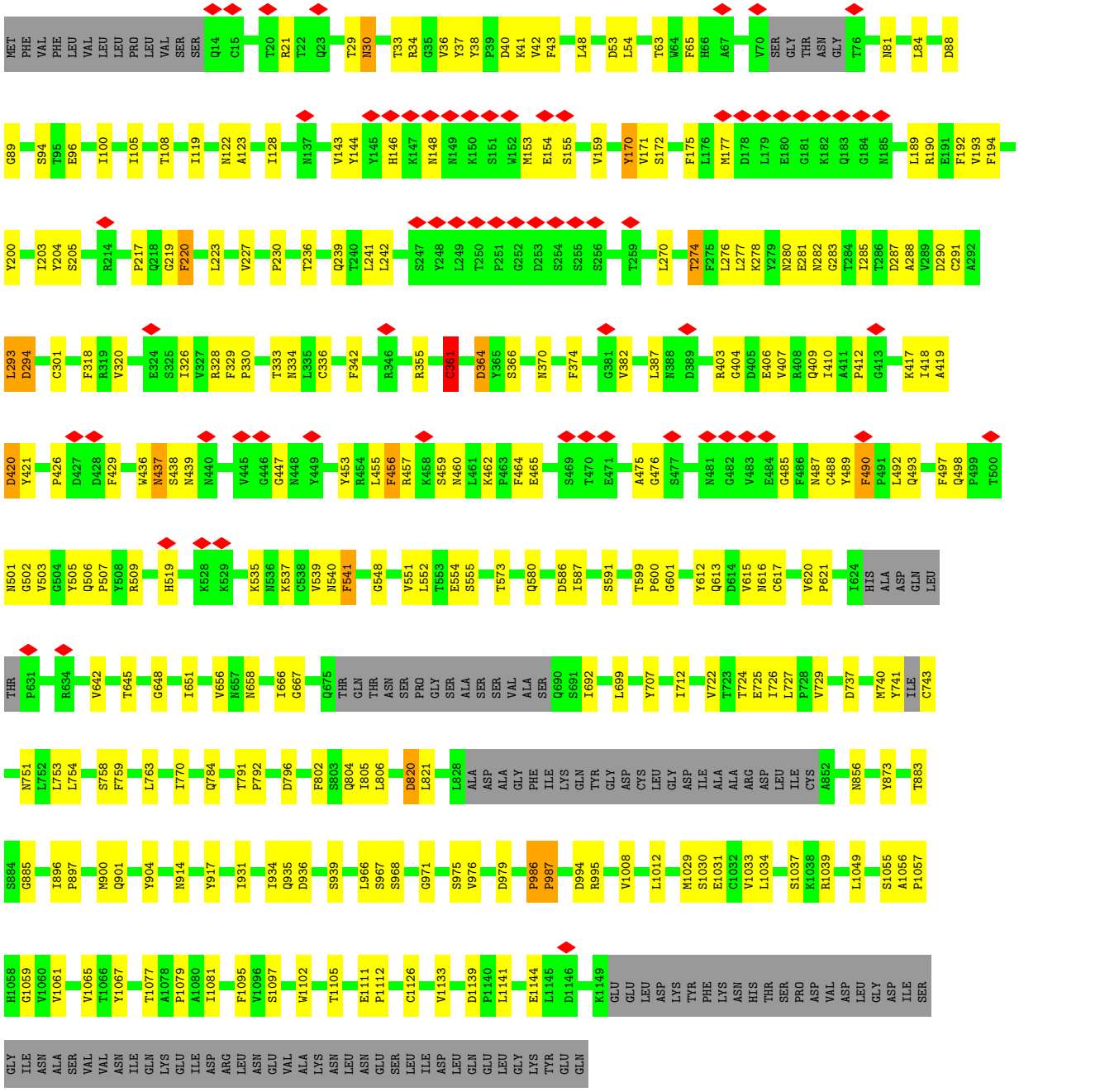
• Molecule 1: Spike glycoprotein

Chain B:



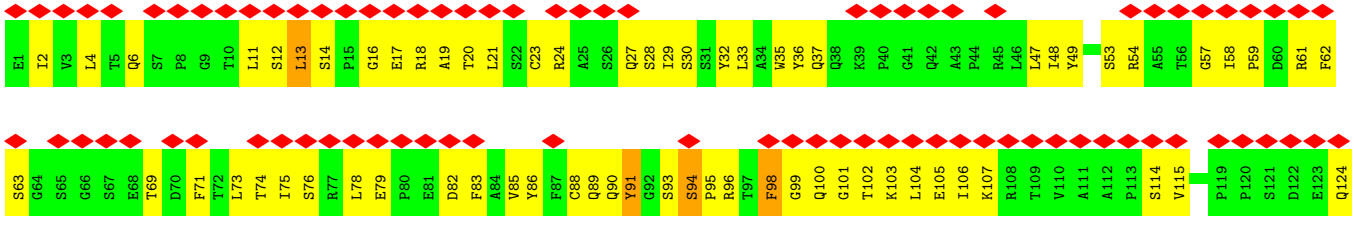
• Molecule 1: Spike glycoprotein

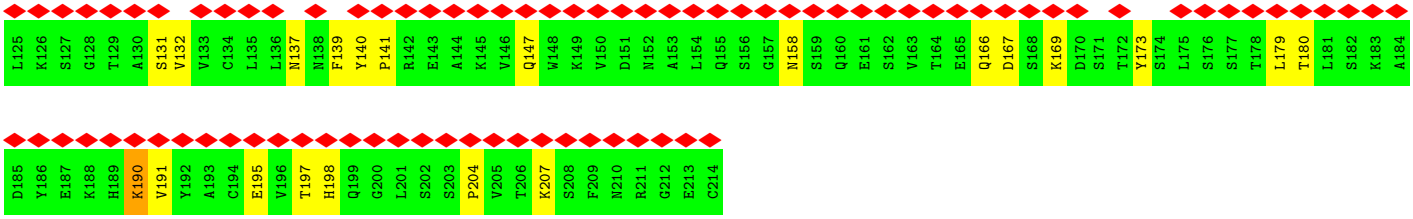
Chain C:



• Molecule 2: mAb 002-02 light chain

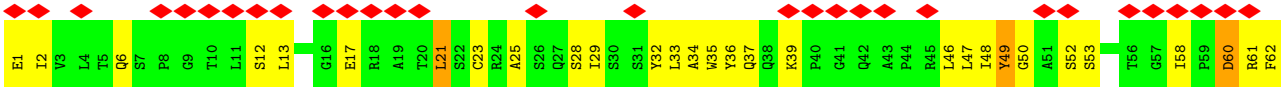
Chain F:

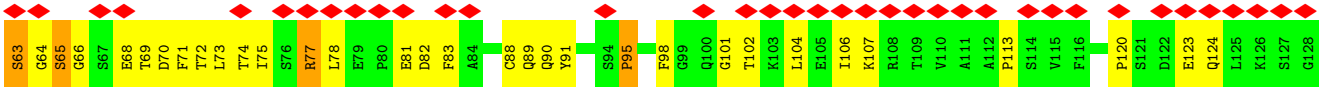


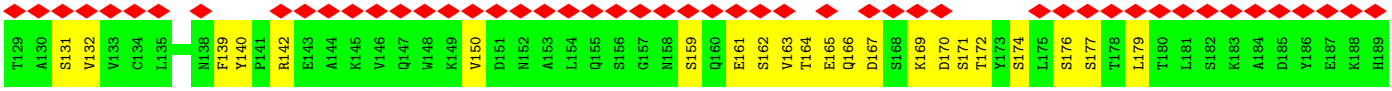


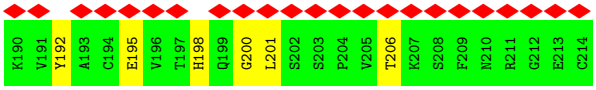
• Molecule 2: mAb 002-02 light chain

Chain I:



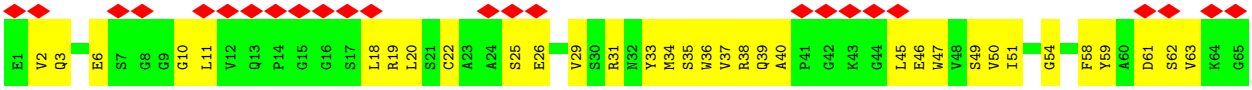


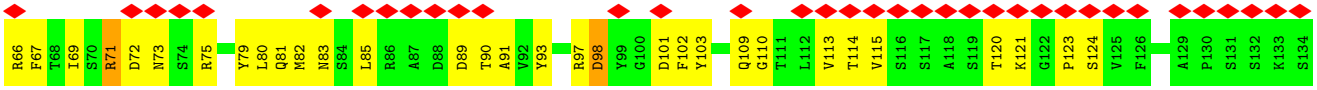


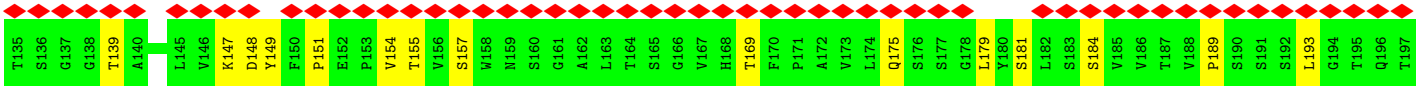


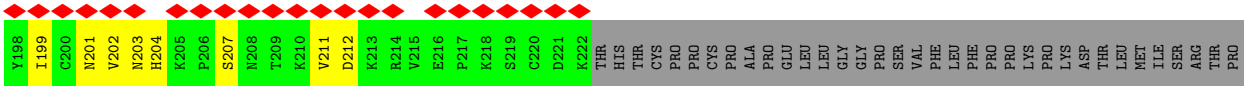
• Molecule 3: mAb 002-02 Heavy chain

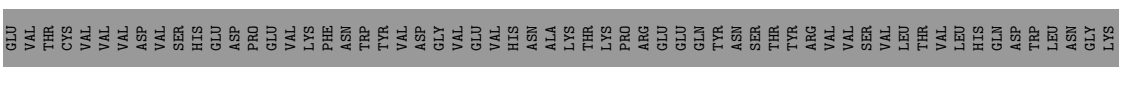
Chain G:

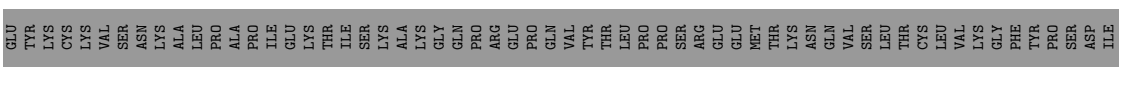


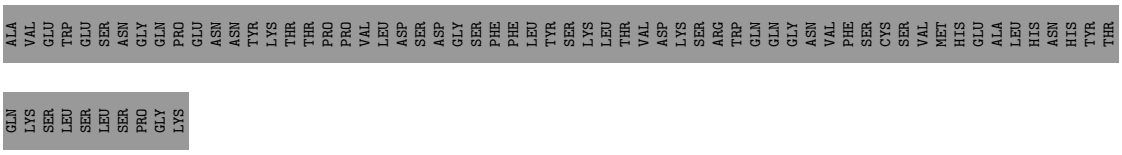






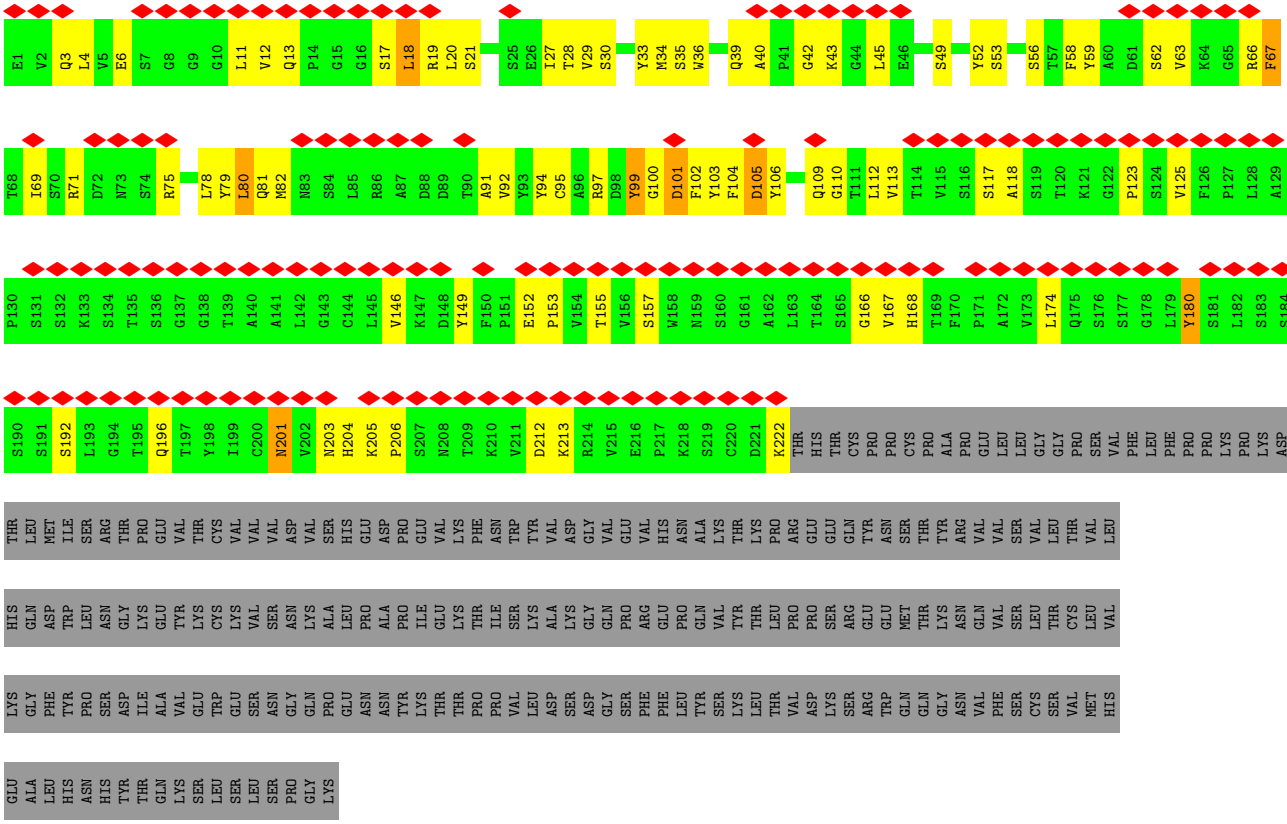






• Molecule 3: mAb 002-02 Heavy chain

Chain J:



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

Chain D:

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

Chain E:

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

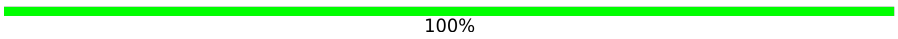
Chain H:

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

Chain K:

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

Chain L:

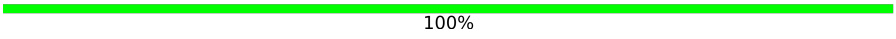


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

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

Chain N:

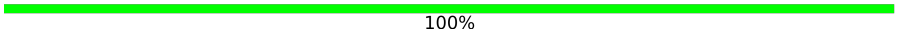


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

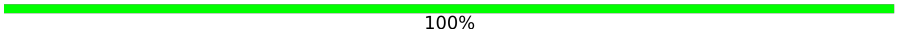
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



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

Chain Q:

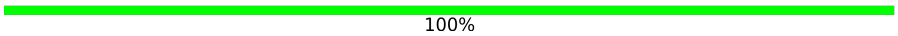


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

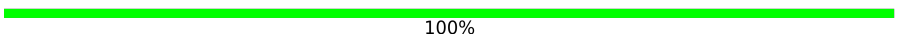
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



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

Chain T:



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

Chain U:

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

Chain V:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	452356	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	63.81	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.968	Depositor
Minimum map value	-2.959	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.29	Depositor
Map size (Å)	444.7456, 444.7456, 444.7456	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0691, 1.0691, 1.0691	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	0.31	2/8684 (0.0%)	0.50	1/11823 (0.0%)
1	B	0.31	0/8538	0.51	2/11623 (0.0%)
1	C	0.45	3/8711 (0.0%)	0.62	8/11860 (0.1%)
2	F	0.32	0/1682	0.57	0/2280
2	I	0.36	0/1682	0.58	1/2280 (0.0%)
3	G	0.29	0/1710	0.58	1/2328 (0.0%)
3	J	0.42	2/1710 (0.1%)	0.61	2/2328 (0.1%)
All	All	0.36	7/32717 (0.0%)	0.55	15/44522 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	987	PRO	CB-CG	20.15	2.50	1.50
1	C	987	PRO	CG-CD	-18.25	0.90	1.50
1	A	1032	CYS	CB-SG	-6.29	1.71	1.82
3	J	67	PHE	CD1-CE1	-5.91	1.27	1.39
1	A	291	CYS	CB-SG	-5.50	1.72	1.81
1	C	361	CYS	CB-SG	-5.49	1.72	1.81
3	J	67	PHE	CD2-CE2	-5.24	1.28	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	987	PRO	CB-CG-CD	-27.30	0.04	106.50
1	C	987	PRO	CA-N-CD	-11.93	94.80	111.50
1	C	987	PRO	N-CA-CB	-10.70	90.46	103.30
1	C	986	PRO	C-N-CD	8.93	147.15	128.40
1	C	293	LEU	CA-CB-CG	8.65	135.19	115.30
1	C	987	PRO	CA-CB-CG	-7.83	89.13	104.00
3	J	80	LEU	CB-CG-CD1	-7.13	98.88	111.00
1	B	745	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	364	ASP	CB-CG-OD1	6.47	124.13	118.30
1	B	301	CYS	CA-CB-SG	-6.44	102.40	114.00
3	J	18	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	587	ILE	C-N-CA	-6.01	106.67	121.70
1	C	820	ASP	CB-CG-OD2	5.43	123.19	118.30
3	G	193	LEU	CA-CB-CG	5.41	127.74	115.30
2	I	95	PRO	CA-N-CD	-5.08	104.39	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	J	101	ASP	Peptide
3	J	102	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8483	0	8289	151	0
1	B	8341	0	8171	154	0
1	C	8508	0	8318	250	0
2	F	1647	0	1606	106	0
2	I	1647	0	1606	96	0
3	G	1671	0	1629	91	0
3	J	1671	0	1629	95	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
4	H	28	0	25	3	0
4	K	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	28	0	25	0	0
4	M	28	0	25	1	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	1	0
5	V	39	0	34	1	0
6	A	126	0	117	1	0
6	B	98	0	91	0	0
6	C	98	0	91	0	0
All	All	32721	0	31931	891	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 14.

All (891) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:PRO:CG	1:C:987:PRO:N	1.86	1.34
2:F:166:GLN:HG2	2:F:173:TYR:CZ	1.74	1.21
1:C:987:PRO:CD	1:C:987:PRO:HG3	1.67	1.18
2:F:35:TRP:HB3	2:F:47:LEU:HD12	1.24	1.15
1:C:987:PRO:CD	1:C:987:PRO:HG2	1.67	1.11
2:F:166:GLN:CG	2:F:173:TYR:OH	1.98	1.11
3:J:18:LEU:HB3	3:J:82:MET:SD	1.92	1.10
2:F:166:GLN:HG2	2:F:173:TYR:OH	1.55	1.06
1:C:987:PRO:CG	1:C:987:PRO:HD3	1.56	1.06
2:F:37:GLN:HB2	2:F:47:LEU:HD21	1.36	1.05
1:C:987:PRO:CG	1:C:987:PRO:HD2	1.56	1.03
1:C:1139:ASP:OD1	1:C:1141:LEU:HD23	1.59	1.03
1:C:986:PRO:HB2	1:C:987:PRO:HG2	1.42	1.02
1:C:336:CYS:HA	1:C:361:CYS:SG	2.00	1.01
2:I:2:ILE:HB	2:I:90:GLN:HE22	1.23	1.01
1:C:455:LEU:HG	1:C:456:PHE:CE2	1.97	0.98
3:J:18:LEU:CB	3:J:82:MET:HE1	1.94	0.97
1:C:53:ASP:OD1	1:C:54:LEU:N	1.98	0.96
1:B:32:PHE:CE2	1:B:218:GLN:OE1	2.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ASP:OD2	1:C:460:ASN:ND2	2.00	0.93
1:C:437:ASN:HD21	1:C:439:ASN:HD22	1.16	0.92
2:F:35:TRP:CB	2:F:47:LEU:HD12	2.00	0.91
1:C:439:ASN:HD21	1:C:506:GLN:HB3	1.36	0.91
2:F:96:ARG:HH22	3:G:101:ASP:HB3	1.36	0.90
1:C:987:PRO:CG	1:C:987:PRO:CD	0.90	0.90
3:J:67:PHE:CE2	3:J:80:LEU:HD11	2.07	0.90
2:F:166:GLN:HG3	2:F:173:TYR:OH	1.72	0.89
1:B:176:LEU:O	1:B:190:ARG:NH2	2.06	0.88
1:C:220:PHE:CZ	1:C:287:ASP:HA	2.09	0.88
3:G:36:TRP:CD1	3:G:80:LEU:HD12	2.08	0.88
3:G:204:HIS:CE1	3:G:207:SER:H	1.92	0.88
1:C:455:LEU:HG	1:C:456:PHE:CD2	2.08	0.88
2:F:140:TYR:CD1	2:F:141:PRO:HA	2.08	0.87
1:B:175:PHE:O	1:B:190:ARG:NH2	2.07	0.87
3:G:204:HIS:ND1	3:G:207:SER:OG	2.08	0.87
2:F:29:ILE:HD13	2:F:32:TYR:HB2	1.55	0.86
1:C:293:LEU:HD23	1:C:294:ASP:OD1	1.76	0.85
3:J:18:LEU:HB3	3:J:82:MET:CE	2.07	0.84
2:I:12:SER:C	2:I:107:LYS:HZ3	1.81	0.84
3:J:67:PHE:HE2	3:J:80:LEU:HD11	1.41	0.83
1:C:462:LYS:N	1:C:465:GLU:OE1	2.12	0.82
1:C:426:PRO:HD3	1:C:464:PHE:HE2	1.44	0.82
1:C:456:PHE:HE1	1:C:489:TYR:HB2	1.43	0.82
3:J:18:LEU:HB2	3:J:82:MET:HE1	1.60	0.81
2:F:140:TYR:HD1	2:F:141:PRO:HA	1.41	0.81
1:B:176:LEU:HB2	1:B:190:ARG:HH21	1.44	0.81
2:F:37:GLN:HB2	2:F:47:LEU:CD2	2.11	0.80
2:F:27:GLN:NE2	2:F:28:SER:O	2.14	0.80
1:A:699:LEU:HD13	1:B:873:TYR:CE2	2.17	0.80
1:C:336:CYS:CA	1:C:361:CYS:SG	2.69	0.80
3:G:204:HIS:CE1	3:G:207:SER:N	2.49	0.80
1:B:32:PHE:CD2	1:B:218:GLN:OE1	2.34	0.80
1:C:436:TRP:HZ3	1:C:438:SER:HG	0.84	0.80
1:C:81:ASN:HD22	1:C:242:LEU:HD23	1.47	0.79
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.15	0.79
1:A:969:ASN:ND2	1:B:755:GLN:OE1	2.15	0.79
3:J:18:LEU:HB3	3:J:82:MET:HE1	1.63	0.79
3:J:36:TRP:CE2	3:J:80:LEU:HD22	2.18	0.79
1:C:421:TYR:OH	1:C:457:ARG:O	2.00	0.79
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:HE2	1:C:283:GLY:HA3	1.46	0.79
2:I:33:LEU:O	2:I:50:GLY:N	2.16	0.79
3:J:152:GLU:HB3	3:J:180:TYR:CD2	2.18	0.78
3:J:62:SER:O	3:J:66:ARG:NH2	2.17	0.77
1:B:985:ASP:OD2	1:B:988:GLU:HG2	1.84	0.77
1:A:123:ALA:HA	1:A:177:MET:HE1	1.67	0.77
1:C:318:PHE:HZ	1:C:615:VAL:HG21	1.49	0.77
2:I:37:GLN:NE2	2:I:39:LYS:HG3	2.01	0.76
1:B:176:LEU:O	1:B:190:ARG:CZ	2.34	0.76
3:G:34:MET:HE3	3:G:97:ARG:HA	1.68	0.76
1:C:48:LEU:HD23	1:C:276:LEU:HD21	1.67	0.75
1:B:578:ASP:OD1	1:B:581:THR:N	2.20	0.74
1:C:437:ASN:HD21	1:C:439:ASN:ND2	1.84	0.74
3:J:152:GLU:HB3	3:J:180:TYR:HD2	1.51	0.74
2:F:96:ARG:NH1	3:G:101:ASP:O	2.19	0.74
3:J:105:ASP:OD1	3:J:106:TYR:CD2	2.41	0.73
1:B:753:LEU:HD21	1:B:760:CYS:SG	2.28	0.73
1:B:555:SER:HB3	1:B:584:ILE:HG23	1.71	0.72
1:C:220:PHE:HE1	1:C:288:ALA:H	1.34	0.72
1:C:439:ASN:ND2	1:C:506:GLN:HB3	2.04	0.72
2:F:23:CYS:SG	2:F:35:TRP:HH2	2.12	0.72
3:J:67:PHE:HZ	3:J:80:LEU:HD21	1.54	0.72
1:B:565:PHE:HB3	1:B:576:VAL:HG23	1.69	0.72
1:C:439:ASN:HD21	1:C:506:GLN:CB	2.02	0.72
1:C:986:PRO:CB	1:C:987:PRO:HG2	2.19	0.72
2:I:13:LEU:N	2:I:107:LYS:HZ3	1.86	0.72
1:C:456:PHE:HE1	1:C:489:TYR:CB	2.02	0.72
3:G:202:VAL:HB	3:G:211:VAL:HB	1.72	0.72
1:B:274:THR:OG1	1:B:291:CYS:SG	2.48	0.71
1:A:699:LEU:HD13	1:B:873:TYR:CD2	2.25	0.71
1:C:355:ARG:HH22	1:C:464:PHE:HD1	1.38	0.71
3:J:36:TRP:NE1	3:J:80:LEU:HD13	2.04	0.71
3:J:174:LEU:HA	3:J:180:TYR:CD1	2.24	0.71
1:C:421:TYR:HE2	1:C:457:ARG:N	1.89	0.71
1:C:498:GLN:HB2	1:C:501:ASN:HD21	1.54	0.71
3:G:80:LEU:HD21	3:G:82:MET:SD	2.30	0.71
2:I:2:ILE:HB	2:I:90:GLN:NE2	2.03	0.71
3:J:6:GLU:OE2	3:J:109:GLN:N	2.24	0.71
3:G:175:GLN:NE2	3:G:181:SER:OG	2.23	0.71
1:A:969:ASN:OD1	1:A:972:ALA:N	2.22	0.70
2:I:13:LEU:CA	2:I:107:LYS:NZ	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:ILE:C	1:C:727:LEU:HD22	2.12	0.70
1:C:426:PRO:HD3	1:C:464:PHE:CE2	2.25	0.70
1:C:1029:MET:O	1:C:1033:VAL:HG12	1.92	0.70
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.25	0.70
3:J:152:GLU:CD	3:J:180:TYR:HE2	1.95	0.69
1:C:456:PHE:CE1	1:C:489:TYR:HB2	2.26	0.69
1:A:353:TRP:O	1:A:466:ARG:NH1	2.25	0.69
1:C:436:TRP:CZ3	1:C:438:SER:OG	2.41	0.69
3:G:71:ARG:NH1	3:G:73:ASN:OD1	2.25	0.69
1:C:293:LEU:CD2	1:C:294:ASP:OD1	2.40	0.69
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.75	0.69
2:I:64:GLY:HA2	2:I:73:LEU:HA	1.75	0.69
1:B:318:PHE:HZ	1:B:615:VAL:HG11	1.59	0.68
2:I:161:GLU:HA	2:I:177:SER:HA	1.76	0.68
1:C:537:LYS:C	1:C:551:VAL:HG23	2.14	0.68
3:G:155:THR:HB	3:G:203:ASN:HB3	1.74	0.68
1:C:417:LYS:HZ1	1:C:453:TYR:HE2	1.42	0.68
3:J:112:LEU:HD23	3:J:153:PRO:HD3	1.75	0.68
1:C:170:TYR:HD1	1:C:171:VAL:N	1.91	0.67
1:B:787:GLN:N	1:B:787:GLN:OE1	2.28	0.67
1:C:1141:LEU:HD23	1:C:1141:LEU:H	1.60	0.67
2:I:165:GLU:OE1	2:I:166:GLN:N	2.27	0.67
1:B:105:ILE:HG23	1:B:241:LEU:HD11	1.77	0.67
1:C:123:ALA:HA	1:C:177:MET:HE2	1.76	0.67
3:J:19:ARG:HG2	3:J:81:GLN:HG2	1.75	0.67
1:C:43:PHE:CE2	1:C:283:GLY:HA3	2.30	0.67
3:G:204:HIS:CE1	3:G:207:SER:HB3	2.30	0.67
1:C:586:ASP:OD1	1:C:587:ILE:N	2.28	0.66
2:F:32:TYR:HA	2:F:91:TYR:CE2	2.31	0.66
2:F:12:SER:HA	2:F:105:GLU:OE2	1.95	0.66
2:I:165:GLU:OE1	2:I:165:GLU:C	2.33	0.66
1:B:32:PHE:HD2	1:B:218:GLN:HB3	1.61	0.66
2:I:36:TYR:OH	3:J:104:PHE:N	2.25	0.66
1:C:220:PHE:CE1	1:C:287:ASP:HA	2.31	0.66
1:C:447:GLY:HA2	1:C:498:GLN:HE22	1.61	0.66
3:G:204:HIS:CE1	3:G:207:SER:CB	2.79	0.66
2:F:49:TYR:HB3	2:F:53:SER:HB3	1.78	0.66
3:J:174:LEU:HA	3:J:180:TYR:HD1	1.59	0.66
1:B:34:ARG:NH2	1:B:191:GLU:OE1	2.30	0.65
1:A:901:GLN:OE1	1:A:905:ARG:NE	2.30	0.65
1:C:436:TRP:HZ3	1:C:438:SER:OG	1.67	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:GLN:HG2	2:F:173:TYR:CE1	2.32	0.65
1:B:600:PRO:HD3	1:B:692:ILE:HD11	1.77	0.65
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.79	0.65
2:F:35:TRP:HD1	2:F:48:ILE:HD12	1.61	0.65
1:A:22:THR:O	1:A:78:ARG:NH1	2.29	0.65
1:C:724:THR:HB	1:C:934:ILE:HD11	1.78	0.64
2:I:162:SER:N	2:I:176:SER:O	2.27	0.64
3:J:63:VAL:HB	3:J:67:PHE:HB2	1.78	0.64
1:C:987:PRO:N	1:C:987:PRO:HG2	1.92	0.64
3:G:36:TRP:CG	3:G:80:LEU:HD12	2.32	0.64
2:I:91:TYR:HE2	3:J:101:ASP:HB3	1.62	0.64
1:C:896:ILE:HD13	1:C:904:TYR:CE2	2.32	0.64
2:F:18:ARG:NH1	2:F:20:THR:OG1	2.30	0.64
2:I:6:GLN:OE1	2:I:101:GLY:N	2.29	0.64
1:B:995:ARG:NH2	1:C:994:ASP:OD2	2.30	0.64
3:J:36:TRP:CD2	3:J:80:LEU:HD22	2.33	0.64
1:A:290:ASP:OD1	1:A:291:CYS:N	2.31	0.63
1:A:578:ASP:OD2	1:A:581:THR:HG22	1.97	0.63
1:C:976:VAL:HG23	1:C:979:ASP:H	1.63	0.63
1:C:580:GLN:NE2	5:V:1:NAG:O3	2.31	0.63
1:C:1139:ASP:OD1	1:C:1141:LEU:CD2	2.41	0.63
1:A:176:LEU:HB3	1:A:190:ARG:CD	2.29	0.63
1:C:791:THR:HG21	1:C:806:LEU:HD13	1.81	0.63
3:G:204:HIS:CG	3:G:207:SER:HG	2.16	0.63
2:I:83:PHE:HE2	2:I:165:GLU:OE2	1.82	0.63
2:I:28:SER:C	2:I:29:ILE:HD12	2.20	0.63
1:C:599:THR:HG22	1:C:601:GLY:H	1.63	0.62
1:B:29:THR:HG22	1:B:30:ASN:H	1.64	0.62
1:B:176:LEU:C	1:B:190:ARG:NH2	2.52	0.62
2:I:13:LEU:C	2:I:107:LYS:HZ2	2.01	0.62
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.32	0.62
2:F:49:TYR:N	2:F:53:SER:O	2.32	0.62
1:A:19:THR:O	1:A:78:ARG:NH2	2.31	0.62
1:C:421:TYR:HE2	1:C:456:PHE:C	2.03	0.62
1:A:402:ILE:HG22	1:A:406:GLU:OE1	2.00	0.62
3:G:6:GLU:OE2	3:G:110:GLY:N	2.32	0.62
2:I:1:GLU:OE2	2:I:95:PRO:HG2	1.99	0.62
1:B:985:ASP:OD1	1:B:987:PRO:HD2	2.00	0.62
3:G:154:VAL:HG22	3:G:204:HIS:HB2	1.80	0.62
1:C:290:ASP:OD1	1:C:293:LEU:HB2	2.00	0.62
1:C:455:LEU:CG	1:C:456:PHE:CE2	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:ARG:HH12	2:F:79:GLU:HB2	1.65	0.62
3:G:157:SER:OG	3:G:201:ASN:OD1	2.18	0.62
2:I:81:GLU:N	2:I:81:GLU:OE1	2.32	0.62
1:A:320:VAL:HG23	1:A:622:VAL:HG11	1.82	0.61
2:F:21:LEU:O	2:F:73:LEU:N	2.27	0.61
2:I:13:LEU:C	2:I:107:LYS:NZ	2.53	0.61
3:G:34:MET:HE1	3:G:97:ARG:HB2	1.82	0.61
1:B:91:TYR:OH	1:B:191:GLU:OE2	2.18	0.61
1:C:896:ILE:CD1	1:C:904:TYR:HE2	2.13	0.61
1:C:280:ASN:OD1	1:C:283:GLY:N	2.30	0.61
2:F:19:ALA:N	2:F:75:ILE:O	2.24	0.61
2:F:29:ILE:HD12	2:F:30:SER:N	2.15	0.61
3:G:204:HIS:HE1	3:G:207:SER:N	1.99	0.61
2:I:170:ASP:OD2	2:I:172:THR:OG1	2.18	0.61
1:C:642:VAL:HG12	1:C:651:ILE:HG22	1.83	0.61
3:J:174:LEU:HB2	3:J:180:TYR:HE1	1.65	0.60
1:C:821:LEU:HD11	1:C:939:SER:HB2	1.83	0.60
2:I:69:THR:CA	2:I:71:PHE:HE1	2.14	0.60
2:I:123:GLU:CD	2:I:123:GLU:H	2.02	0.60
2:I:65:SER:N	2:I:72:THR:O	2.31	0.60
1:C:503:VAL:HA	1:C:506:GLN:CD	2.20	0.60
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.83	0.60
1:C:421:TYR:OH	3:J:53:SER:OG	2.15	0.60
2:I:2:ILE:CB	2:I:90:GLN:HE22	2.07	0.60
1:A:153:MET:SD	1:A:154:GLU:N	2.75	0.60
3:J:12:VAL:HG11	3:J:82:MET:HE3	1.84	0.60
1:C:439:ASN:OD1	1:C:507:PRO:HD2	2.02	0.59
1:C:100:ILE:HG22	1:C:242:LEU:HD12	1.83	0.59
2:I:13:LEU:N	2:I:107:LYS:NZ	2.50	0.59
1:A:620:VAL:HG21	1:A:651:ILE:HD11	1.83	0.59
1:B:726:ILE:HD12	1:B:1061:VAL:HG22	1.83	0.59
1:C:281:GLU:OE2	1:C:281:GLU:N	2.35	0.59
1:C:537:LYS:O	1:C:539:VAL:HG13	2.02	0.59
2:I:83:PHE:CE2	2:I:165:GLU:OE2	2.55	0.59
3:G:38:ARG:HH12	3:G:89:ASP:HB3	1.67	0.59
1:B:712:ILE:HD11	1:C:896:ILE:HD12	1.83	0.59
3:J:17:SER:C	3:J:82:MET:HE2	2.22	0.59
1:A:712:ILE:HG13	1:B:896:ILE:HG13	1.84	0.59
1:A:773:GLU:OE2	1:A:1019:ARG:NE	2.32	0.59
1:C:436:TRP:CH2	1:C:509:ARG:HB3	2.38	0.59
1:B:457:ARG:NH1	1:B:459:SER:OG	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.43	0.59
1:A:403:ARG:HD2	1:A:405:ASP:HB2	1.84	0.59
2:F:13:LEU:HD22	2:F:17:GLU:OE1	2.02	0.59
2:F:37:GLN:CB	2:F:47:LEU:HD21	2.23	0.59
3:J:125:VAL:HG13	3:J:146:VAL:HG22	1.85	0.59
1:B:724:THR:HG23	1:B:934:ILE:HD12	1.85	0.58
1:B:946:GLY:O	1:B:950:ASP:HB2	2.02	0.58
3:J:36:TRP:HE1	3:J:80:LEU:HD13	1.68	0.58
1:A:312:ILE:HG13	1:A:598:ILE:CD1	2.33	0.58
2:F:100:GLN:OE1	2:F:100:GLN:HA	2.03	0.58
1:C:96:GLU:OE1	1:C:100:ILE:N	2.35	0.58
3:G:3:GLN:N	3:G:25:SER:OG	2.34	0.58
2:I:159:SER:HB3	2:I:179:LEU:HD13	1.85	0.58
3:G:34:MET:HE3	3:G:97:ARG:CA	2.31	0.58
3:J:17:SER:C	3:J:82:MET:CE	2.72	0.58
1:B:353:TRP:O	1:B:466:ARG:NH1	2.36	0.58
2:F:96:ARG:NH1	3:G:102:PHE:HB2	2.19	0.58
3:J:75:ARG:NH2	3:J:79:TYR:OH	2.37	0.58
1:B:611:LEU:HA	1:B:650:LEU:HA	1.85	0.58
1:C:791:THR:HG22	1:C:792:PRO:HD2	1.85	0.58
1:B:1041:ASP:HB3	1:C:1030:SER:HB3	1.85	0.57
3:G:204:HIS:ND1	3:G:207:SER:CB	2.66	0.57
1:B:1083:HIS:HD2	1:B:1136:THR:HA	1.69	0.57
1:A:995:ARG:HH11	1:A:995:ARG:HG2	1.68	0.57
3:G:33:TYR:HB2	3:G:98:ASP:OD1	2.04	0.57
1:B:726:ILE:CD1	1:B:1061:VAL:HG22	2.35	0.57
3:G:34:MET:HA	3:G:34:MET:CE	2.34	0.57
2:I:13:LEU:CA	2:I:107:LYS:HZ3	2.17	0.57
2:F:35:TRP:HB3	2:F:47:LEU:CD1	2.16	0.57
3:J:67:PHE:CZ	3:J:80:LEU:HD21	2.38	0.57
1:A:580:GLN:OE1	4:D:1:NAG:H5	2.04	0.57
1:B:581:THR:OG1	1:B:583:GLU:OE2	2.23	0.57
1:C:37:TYR:OH	1:C:53:ASP:OD1	2.23	0.57
1:B:661:GLU:O	1:B:695:TYR:OH	2.16	0.57
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.86	0.57
1:C:34:ARG:NE	1:C:219:GLY:HA3	2.19	0.57
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.86	0.56
1:A:869:MET:HG2	1:C:699:LEU:HD21	1.87	0.56
1:B:176:LEU:CB	1:B:190:ARG:HH21	2.17	0.56
1:B:583:GLU:N	1:B:583:GLU:OE1	2.38	0.56
1:C:277:LEU:HD23	1:C:285:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:TYR:CE2	1:C:457:ARG:N	2.72	0.56
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.68	0.56
1:B:721:SER:O	1:B:1066:THR:OG1	2.18	0.56
1:B:786:LYS:HB2	1:B:787:GLN:OE1	2.04	0.56
1:C:63:THR:HG1	1:C:65:PHE:HE2	1.51	0.56
1:C:436:TRP:CZ3	1:C:509:ARG:HB3	2.40	0.56
1:C:896:ILE:HG21	1:C:904:TYR:OH	2.06	0.56
3:G:35:SER:HA	3:G:50:VAL:HA	1.86	0.56
3:J:81:GLN:OE1	3:J:82:MET:N	2.38	0.56
1:A:291:CYS:SG	1:A:301:CYS:HB2	2.45	0.56
2:I:62:PHE:CD1	2:I:75:ILE:HG12	2.41	0.56
3:J:34:MET:HE3	3:J:97:ARG:HA	1.88	0.56
2:I:132:VAL:O	2:I:179:LEU:N	2.37	0.56
1:A:274:THR:HG23	1:A:291:CYS:HB2	1.88	0.56
1:B:987:PRO:HB2	1:B:988:GLU:OE2	2.06	0.56
1:C:751:ASN:HA	1:C:754:LEU:HD12	1.88	0.56
1:C:896:ILE:HD13	1:C:904:TYR:OH	2.06	0.56
1:B:215:ASP:OD2	1:B:266:TYR:OH	2.17	0.55
1:B:905:ARG:CZ	1:B:1050:MET:HB3	2.35	0.55
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.86	0.55
2:F:29:ILE:HD13	2:F:32:TYR:CB	2.33	0.55
2:I:37:GLN:HE22	2:I:39:LYS:HG3	1.70	0.55
2:I:169:LYS:O	2:I:169:LYS:NZ	2.31	0.55
1:C:40:ASP:HB3	1:C:42:VAL:HG22	1.88	0.55
1:C:537:LYS:O	1:C:551:VAL:HG23	2.06	0.55
2:F:89:GLN:HA	2:F:98:PHE:HA	1.89	0.55
1:B:707:TYR:HD2	1:C:883:THR:HG23	1.70	0.55
1:C:437:ASN:ND2	1:C:439:ASN:ND2	2.54	0.55
2:F:58:ILE:HG22	2:F:62:PHE:CD1	2.41	0.55
2:F:166:GLN:CG	2:F:173:TYR:CZ	2.62	0.55
3:J:36:TRP:CZ2	3:J:78:LEU:HD22	2.41	0.55
1:A:176:LEU:HD22	1:A:190:ARG:HD3	1.87	0.55
2:I:164:THR:HG21	2:I:174:SER:HB2	1.89	0.55
3:J:78:LEU:HD23	3:J:79:TYR:N	2.22	0.55
1:A:312:ILE:HG13	1:A:598:ILE:HD11	1.89	0.55
1:B:296:LEU:HD22	1:B:300:LYS:HE3	1.88	0.55
2:I:25:ALA:O	2:I:69:THR:OG1	2.24	0.55
1:A:971:GLY:HA3	1:A:995:ARG:HH21	1.72	0.55
3:G:49:SER:OG	3:G:50:VAL:N	2.39	0.55
1:A:33:THR:HG23	1:A:58:PHE:CE2	2.42	0.54
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:TYR:CE2	1:C:457:ARG:CB	2.90	0.54
1:C:555:SER:OG	1:C:586:ASP:N	2.40	0.54
2:F:94:SER:H	2:F:95:PRO:HA	1.72	0.54
3:G:6:GLU:OE2	3:G:109:GLN:N	2.40	0.54
1:C:896:ILE:HD13	1:C:904:TYR:HE2	1.69	0.54
3:J:21:SER:OG	3:J:78:LEU:O	2.15	0.54
3:G:75:ARG:NH1	3:G:79:TYR:OH	2.41	0.54
2:I:167:ASP:HB3	2:I:170:ASP:OD1	2.07	0.54
1:B:328:ARG:HH11	1:B:533:LEU:HD12	1.72	0.54
3:G:80:LEU:HD21	3:G:82:MET:CE	2.37	0.54
3:G:121:LYS:NZ	3:G:148:ASP:O	2.29	0.54
1:A:36:VAL:O	1:A:223:LEU:HD12	2.08	0.54
1:A:61:ASN:ND2	6:A:1306:NAG:O7	2.40	0.54
1:C:175:PHE:O	1:C:177:MET:HG3	2.07	0.54
1:C:971:GLY:O	1:C:995:ARG:NH1	2.39	0.54
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.90	0.54
1:C:455:LEU:HD11	3:J:100:GLY:HA2	1.89	0.54
2:I:165:GLU:CD	2:I:166:GLN:N	2.61	0.54
2:I:36:TYR:CE1	2:I:89:GLN:HG3	2.43	0.54
1:C:726:ILE:HG23	1:C:1061:VAL:HG22	1.90	0.54
1:A:115:GLN:CD	1:A:115:GLN:H	2.11	0.54
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.88	0.54
3:G:11:LEU:HA	3:G:114:THR:O	2.07	0.54
1:A:770:ILE:HD11	1:A:1012:LEU:HA	1.90	0.53
1:C:34:ARG:HH22	1:C:217:PRO:HG2	1.73	0.53
1:C:409:GLN:OE1	1:C:419:ALA:N	2.35	0.53
2:I:113:PRO:HB3	2:I:139:PHE:HB3	1.90	0.53
1:A:176:LEU:HB3	1:A:190:ARG:HD3	1.90	0.53
2:F:16:GLY:N	2:F:78:LEU:O	2.40	0.53
1:A:273:ARG:NH1	1:A:290:ASP:OD2	2.41	0.53
1:C:293:LEU:CG	1:C:294:ASP:OD1	2.56	0.53
1:C:726:ILE:O	1:C:727:LEU:HD22	2.08	0.53
2:F:59:PRO:HD2	2:F:62:PHE:CE1	2.43	0.53
1:A:342:PHE:HB2	4:M:1:NAG:H82	1.91	0.53
1:C:318:PHE:CZ	1:C:615:VAL:HG21	2.36	0.53
1:C:740:MET:CE	1:C:856:ASN:HB2	2.39	0.53
2:I:170:ASP:OD1	2:I:171:SER:N	2.42	0.53
1:B:712:ILE:CD1	1:C:896:ILE:HD12	2.39	0.53
1:B:745:ASP:OD1	1:B:745:ASP:O	2.27	0.53
1:A:65:PHE:CE2	1:A:84:LEU:HD21	2.43	0.53
2:F:147:GLN:O	2:F:195:GLU:N	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:150:VAL:HG13	2:I:192:TYR:CE1	2.43	0.53
3:J:30:SER:HA	3:J:71:ARG:CZ	2.39	0.53
1:A:96:GLU:OE1	1:A:100:ILE:N	2.42	0.53
1:A:1005:GLN:OE1	1:A:1005:GLN:HA	2.09	0.53
1:C:336:CYS:CB	1:C:361:CYS:SG	2.97	0.53
2:F:141:PRO:HD2	2:F:198:HIS:CE1	2.43	0.53
1:A:32:PHE:HB3	1:A:218:GLN:HB3	1.90	0.52
3:G:37:VAL:HG12	3:G:47:TRP:HA	1.91	0.52
1:C:729:VAL:HG22	1:C:1059:GLY:HA2	1.91	0.52
3:G:10:GLY:O	3:G:114:THR:N	2.38	0.52
1:C:456:PHE:CE1	1:C:489:TYR:CB	2.87	0.52
2:F:59:PRO:HD2	2:F:62:PHE:HE1	1.73	0.52
3:G:49:SER:HG	3:G:59:TYR:HD2	1.57	0.52
1:A:357:ARG:NH1	1:B:167:THR:O	2.42	0.52
1:B:1039:ARG:NE	1:C:1031:GLU:OE2	2.36	0.52
2:F:86:TYR:N	2:F:102:THR:O	2.39	0.52
2:I:61:ARG:NH1	2:I:77:ARG:O	2.43	0.52
1:B:53:ASP:HB3	1:B:55:PHE:HE2	1.74	0.52
1:C:885:GLY:HA2	1:C:901:GLN:OE1	2.08	0.52
3:G:6:GLU:OE1	3:G:6:GLU:N	2.42	0.52
1:B:754:LEU:HD12	1:B:754:LEU:O	2.10	0.52
3:G:51:ILE:HB	3:G:69:ILE:HD11	1.91	0.52
2:I:150:VAL:HG22	2:I:192:TYR:HE1	1.75	0.52
1:B:454:ARG:HD2	1:B:493:GLN:HB3	1.92	0.52
2:F:167:ASP:OD2	2:F:169:LYS:N	2.43	0.52
1:A:497:PHE:CD1	1:A:507:PRO:HD3	2.44	0.52
1:B:30:ASN:OD1	1:B:32:PHE:CD1	2.63	0.52
1:B:969:ASN:OD1	1:B:972:ALA:N	2.43	0.52
1:A:81:ASN:OD1	1:A:81:ASN:N	2.43	0.52
2:I:70:ASP:C	2:I:71:PHE:CD1	2.83	0.52
1:C:740:MET:HE1	1:C:856:ASN:HB2	1.92	0.51
2:F:197:THR:HG23	2:F:204:PRO:HG3	1.92	0.51
3:G:11:LEU:HD13	3:G:114:THR:HG22	1.91	0.51
1:C:89:GLY:HA3	1:C:270:LEU:HD12	1.93	0.51
1:C:502:GLY:O	1:C:506:GLN:HG3	2.09	0.51
1:C:612:TYR:HE1	1:C:651:ILE:HD11	1.75	0.51
2:F:35:TRP:NE1	2:F:73:LEU:HB2	2.25	0.51
2:F:105:GLU:OE1	2:F:106:ILE:C	2.49	0.51
1:A:453:TYR:HB3	1:A:495:TYR:HE1	1.76	0.51
1:A:537:LYS:O	1:A:539:VAL:HG13	2.11	0.51
1:A:656:VAL:HG21	1:A:693:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:784:GLN:NE2	1:C:1030:SER:OG	2.43	0.51
3:J:12:VAL:HG21	3:J:82:MET:HE3	1.92	0.51
3:J:19:ARG:C	3:J:20:LEU:HD23	2.31	0.51
1:B:366:SER:HA	1:B:369:TYR:CZ	2.45	0.51
1:B:880:GLY:O	1:B:884:SER:OG	2.24	0.51
1:C:220:PHE:HE1	1:C:288:ALA:N	2.07	0.51
2:F:82:ASP:O	2:F:104:LEU:HD23	2.10	0.51
1:B:571:ASP:OD2	1:C:967:SER:OG	2.21	0.50
1:C:40:ASP:OD1	1:C:41:LYS:N	2.36	0.50
1:C:65:PHE:CZ	1:C:84:LEU:HD21	2.46	0.50
1:A:296:LEU:HD22	1:A:300:LYS:HE3	1.92	0.50
1:C:291:CYS:HG	1:C:301:CYS:HG	1.58	0.50
1:C:421:TYR:HH	3:J:53:SER:HG	1.46	0.50
3:G:72:ASP:OD2	3:G:75:ARG:NH2	2.44	0.50
3:G:90:THR:OG1	3:G:115:VAL:N	2.37	0.50
3:J:13:GLN:HG2	3:J:117:SER:HA	1.94	0.50
1:C:190:ARG:HB3	1:C:192:PHE:HE1	1.77	0.50
3:G:11:LEU:HB2	3:G:114:THR:HB	1.92	0.50
1:B:65:PHE:CZ	1:B:84:LEU:HD11	2.46	0.50
1:B:350:VAL:HG12	1:B:453:TYR:HB2	1.93	0.50
2:F:11:LEU:HD23	2:F:104:LEU:HB2	1.92	0.50
2:F:37:GLN:N	2:F:47:LEU:HD21	2.26	0.50
2:F:85:VAL:HA	2:F:103:LYS:HA	1.94	0.50
2:F:12:SER:CA	2:F:105:GLU:OE2	2.59	0.50
1:A:1103:PHE:HZ	4:H:1:NAG:H61	1.77	0.50
1:B:18:LEU:HB3	1:B:258:TRP:CH2	2.47	0.50
1:B:1083:HIS:CD2	1:B:1136:THR:HA	2.47	0.50
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.47	0.50
2:F:13:LEU:HD13	2:F:17:GLU:OE1	2.11	0.50
2:F:62:PHE:HA	2:F:75:ILE:HG12	1.92	0.50
1:A:728:PRO:O	1:A:1021:SER:OG	2.30	0.50
1:B:188:ASN:HA	1:B:209:PRO:HA	1.94	0.50
1:C:143:VAL:HG12	1:C:154:GLU:HG2	1.94	0.50
3:G:139:THR:HA	3:G:189:PRO:HA	1.94	0.50
2:I:49:TYR:CD1	2:I:50:GLY:N	2.80	0.50
2:F:6:GLN:CD	2:F:101:GLY:H	2.15	0.50
2:I:29:ILE:HG22	2:I:32:TYR:H	1.77	0.50
3:J:12:VAL:HG21	3:J:82:MET:CE	2.41	0.50
1:A:749:CYS:SG	1:A:997:ILE:HD11	2.51	0.49
1:A:417:LYS:NZ	3:G:101:ASP:OD1	2.42	0.49
1:A:461:LEU:HD23	1:A:461:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:THR:H	1:A:949:GLN:NE2	2.10	0.49
1:C:476:GLY:HA2	3:J:28:THR:HG23	1.93	0.49
2:I:66:GLY:HA3	2:I:71:PHE:HA	1.93	0.49
1:C:497:PHE:CD1	1:C:507:PRO:HD3	2.47	0.49
3:G:38:ARG:NH1	3:G:89:ASP:HB3	2.26	0.49
1:A:173:GLN:OE1	1:A:173:GLN:N	2.26	0.49
1:A:366:SER:HA	1:A:369:TYR:CZ	2.48	0.49
1:B:741:TYR:CE1	1:B:966:LEU:HD21	2.48	0.49
2:I:83:PHE:HD1	2:I:104:LEU:O	1.95	0.49
1:B:994:ASP:O	1:B:998:THR:HG23	2.11	0.49
1:C:108:THR:HA	1:C:236:THR:HG22	1.94	0.49
2:F:23:CYS:N	2:F:71:PHE:O	2.41	0.49
3:G:199:ILE:HD11	3:G:212:ASP:HB3	1.94	0.49
1:C:541:PHE:CE2	1:C:587:ILE:HD11	2.48	0.49
3:G:39:GLN:NE2	3:G:40:ALA:O	2.45	0.49
2:I:21:LEU:HD11	2:I:102:THR:OG1	2.13	0.49
1:A:30:ASN:HB3	1:A:32:PHE:HE2	1.78	0.49
1:B:583:GLU:N	1:B:583:GLU:CD	2.66	0.49
1:C:294:ASP:OD1	1:C:294:ASP:N	2.46	0.49
1:A:661:GLU:O	1:A:695:TYR:OH	2.18	0.49
1:C:280:ASN:OD1	1:C:282:ASN:N	2.46	0.49
1:A:170:TYR:HE1	1:A:172:SER:HG	1.60	0.49
1:C:455:LEU:HD12	3:J:33:TYR:OH	2.12	0.49
1:A:421:TYR:OH	3:G:54:GLY:N	2.45	0.48
1:C:290:ASP:OD1	1:C:293:LEU:N	2.46	0.48
2:I:60:ASP:N	2:I:60:ASP:OD1	2.46	0.48
2:I:150:VAL:HG22	2:I:192:TYR:CE1	2.48	0.48
1:A:20:THR:HA	1:A:78:ARG:HH22	1.78	0.48
1:A:303:LEU:HD12	1:A:308:VAL:HG12	1.94	0.48
2:F:57:GLY:O	2:F:58:ILE:HD13	2.12	0.48
3:G:175:GLN:N	3:G:175:GLN:OE1	2.46	0.48
1:C:119:ILE:HG23	1:C:128:ILE:HG12	1.93	0.48
1:C:146:HIS:CE1	1:C:148:ASN:HB3	2.48	0.48
3:J:92:VAL:HG22	3:J:112:LEU:HB2	1.95	0.48
1:A:1129:VAL:HG13	1:B:917:TYR:HB3	1.94	0.48
2:F:59:PRO:O	2:F:62:PHE:HD1	1.96	0.48
3:G:124:SER:OG	3:G:147:LYS:O	2.30	0.48
3:J:29:VAL:HG12	3:J:71:ARG:HD2	1.94	0.48
3:J:152:GLU:HB3	3:J:180:TYR:CE2	2.48	0.48
2:F:29:ILE:CD1	2:F:32:TYR:H	2.26	0.48
3:G:34:MET:CE	3:G:97:ARG:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:81:GLN:NE2	3:G:82:MET:O	2.46	0.48
1:A:569:ILE:HD12	1:A:569:ILE:H	1.78	0.48
1:B:38:TYR:CE2	1:B:285:ILE:HG13	2.49	0.48
1:B:168:PHE:CD1	1:B:169:GLU:N	2.82	0.48
3:J:33:TYR:HD1	3:J:52:TYR:HA	1.77	0.48
1:A:821:LEU:HD11	1:A:939:SER:HB2	1.95	0.48
1:B:125:ASN:HA	1:B:174:PRO:HD3	1.96	0.48
1:B:268:GLY:O	1:B:269:TYR:HD2	1.97	0.48
1:C:200:TYR:CZ	1:C:230:PRO:HB3	2.48	0.48
1:A:592:PHE:CZ	1:B:740:MET:HE1	2.49	0.48
1:C:541:PHE:CE1	1:C:548:GLY:C	2.87	0.48
3:G:34:MET:HE3	3:G:34:MET:HA	1.95	0.48
2:F:139:PHE:O	2:F:173:TYR:N	2.47	0.48
2:I:6:GLN:NE2	2:I:102:THR:HG23	2.29	0.48
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.79	0.47
1:B:328:ARG:NH1	1:B:533:LEU:HD12	2.29	0.47
1:C:475:ALA:HB3	1:C:487:ASN:HB3	1.96	0.47
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.43	0.47
2:F:33:LEU:HD23	2:F:90:GLN:HA	1.96	0.47
2:F:35:TRP:CD1	2:F:48:ILE:HD12	2.45	0.47
1:A:318:PHE:CE2	1:A:615:VAL:HG11	2.49	0.47
1:B:365:TYR:CD1	1:B:387:LEU:HG	2.49	0.47
1:B:662:CYS:HB3	1:B:697:MET:SD	2.53	0.47
1:B:1077:THR:OG1	1:B:1078:ALA:N	2.47	0.47
1:B:1088:HIS:HB3	1:B:1120:THR:HG21	1.97	0.47
1:C:290:ASP:OD1	1:C:293:LEU:CB	2.62	0.47
1:C:896:ILE:HG13	1:C:897:PRO:HD2	1.96	0.47
2:F:23:CYS:SG	2:F:35:TRP:CH2	2.93	0.47
3:G:61:ASP:OD1	3:G:62:SER:N	2.47	0.47
3:G:91:ALA:O	3:G:113:VAL:N	2.31	0.47
2:I:98:PHE:CE2	3:J:45:LEU:HB2	2.49	0.47
2:I:195:GLU:OE1	2:I:206:THR:OG1	2.19	0.47
3:J:105:ASP:OD1	3:J:106:TYR:CG	2.67	0.47
1:A:119:ILE:HG12	1:A:128:ILE:HG23	1.96	0.47
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.97	0.47
1:B:395:VAL:HG23	1:B:524:VAL:HG21	1.96	0.47
1:B:905:ARG:NE	1:B:1050:MET:HB3	2.29	0.47
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.50	0.47
1:C:421:TYR:CE2	1:C:457:ARG:HB3	2.49	0.47
1:C:751:ASN:HA	1:C:754:LEU:CD1	2.43	0.47
1:A:736:VAL:HG12	1:A:858:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ILE:HG13	1:B:878:LEU:HD21	1.97	0.47
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.49	0.47
1:C:342:PHE:HB2	4:U:1:NAG:H82	1.97	0.47
1:C:382:VAL:HB	1:C:387:LEU:HD21	1.96	0.47
1:C:931:ILE:O	1:C:934:ILE:HG22	2.14	0.47
2:F:59:PRO:CD	2:F:62:PHE:HE1	2.28	0.47
2:I:17:GLU:O	2:I:78:LEU:HG	2.15	0.47
2:I:91:TYR:OH	3:J:101:ASP:O	2.16	0.47
3:J:123:PRO:HG3	3:J:204:HIS:HB2	1.95	0.47
1:B:559:PHE:CE1	1:C:43:PHE:HD1	2.33	0.47
1:B:903:ALA:HB2	1:B:916:LEU:HD22	1.95	0.47
1:C:320:VAL:HG12	1:C:591:SER:O	2.14	0.47
1:A:901:GLN:O	1:A:905:ARG:HG2	2.15	0.47
1:A:1031:GLU:OE2	1:C:1039:ARG:NE	2.39	0.47
1:B:334:ASN:HB2	1:B:361:CYS:SG	2.55	0.47
1:B:393:THR:OG1	1:B:517:LEU:O	2.25	0.47
2:F:62:PHE:HD2	2:F:75:ILE:HD11	1.79	0.47
3:G:19:ARG:HD2	3:G:81:GLN:HB2	1.96	0.47
2:I:1:GLU:HG2	2:I:95:PRO:CD	2.44	0.47
2:I:68:GLU:O	2:I:69:THR:HG22	2.14	0.47
2:I:73:LEU:HD12	2:I:74:THR:N	2.30	0.47
3:J:157:SER:O	3:J:201:ASN:N	2.31	0.47
1:B:281:GLU:HG3	1:B:282:ASN:N	2.30	0.47
1:C:374:PHE:CD1	1:C:436:TRP:HD1	2.33	0.47
1:C:741:TYR:CE1	1:C:966:LEU:HD21	2.50	0.47
3:G:120:THR:HG23	3:G:151:PRO:HD2	1.96	0.47
1:A:33:THR:O	1:A:33:THR:HG22	2.15	0.47
1:A:336:CYS:N	1:A:362:VAL:O	2.46	0.47
1:A:566:GLY:N	1:A:575:ALA:O	2.43	0.47
1:A:995:ARG:HG2	1:A:995:ARG:NH1	2.29	0.47
2:F:96:ARG:NH2	3:G:101:ASP:HB3	2.18	0.47
1:A:1089:PHE:HE2	1:B:917:TYR:HD2	1.62	0.47
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.96	0.47
1:B:411:ALA:O	1:B:415:THR:HG23	2.15	0.47
1:C:498:GLN:HB2	1:C:501:ASN:ND2	2.26	0.47
1:C:503:VAL:HA	1:C:506:GLN:NE2	2.30	0.47
2:F:36:TYR:C	2:F:47:LEU:HD11	2.36	0.47
2:I:33:LEU:HD12	2:I:71:PHE:CG	2.50	0.47
2:I:198:HIS:CE1	2:I:200:GLY:H	2.33	0.47
3:J:166:GLY:O	3:J:187:THR:N	2.48	0.47
1:C:34:ARG:HE	1:C:219:GLY:HA3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:THR:HA	1:A:885:GLY:HA2	1.97	0.46
1:B:309:GLU:O	1:B:313:TYR:OH	2.26	0.46
1:C:763:LEU:HD12	1:C:1008:VAL:HG21	1.97	0.46
2:F:18:ARG:HA	2:F:76:SER:HA	1.97	0.46
3:G:19:ARG:HA	3:G:81:GLN:HA	1.97	0.46
3:G:90:THR:HG23	3:G:114:THR:HA	1.96	0.46
2:I:58:ILE:HG13	2:I:62:PHE:HD2	1.79	0.46
2:I:113:PRO:HB3	2:I:139:PHE:CD2	2.50	0.46
3:J:192:SER:O	3:J:196:GLN:N	2.30	0.46
1:B:290:ASP:O	1:B:297:SER:HB3	2.15	0.46
2:F:63:SER:N	2:F:74:THR:O	2.47	0.46
2:I:69:THR:HA	2:I:71:PHE:HE1	1.79	0.46
3:J:18:LEU:HG	3:J:20:LEU:HD21	1.97	0.46
3:J:35:SER:OG	3:J:49:SER:O	2.12	0.46
1:A:290:ASP:O	1:A:297:SER:HB3	2.15	0.46
1:A:784:GLN:OE1	1:A:1030:SER:OG	2.23	0.46
1:C:366:SER:O	1:C:370:ASN:HB2	2.14	0.46
1:B:114:THR:C	1:B:132:GLU:HG2	2.36	0.46
1:C:896:ILE:HD13	1:C:904:TYR:CZ	2.51	0.46
3:G:2:VAL:HG22	3:G:26:GLU:HB2	1.96	0.46
3:G:39:GLN:O	3:G:91:ALA:HB1	2.16	0.46
1:B:415:THR:HB	1:B:419:ALA:HB2	1.97	0.46
1:A:475:ALA:HB3	1:A:487:ASN:HB3	1.97	0.46
1:A:984:LEU:HB3	1:A:989:ALA:HB2	1.98	0.46
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.16	0.46
1:B:1033:VAL:HG21	1:B:1053:PRO:HD3	1.98	0.46
1:A:897:PRO:HD2	1:A:900:MET:HE3	1.98	0.46
1:B:290:ASP:OD1	1:B:291:CYS:N	2.48	0.46
3:G:98:ASP:HA	3:G:103:TYR:O	2.15	0.46
1:B:85:PRO:O	1:B:269:TYR:OH	2.27	0.46
3:G:85:LEU:HB3	3:G:115:VAL:HG21	1.98	0.46
3:G:169:THR:HA	3:G:184:SER:HA	1.97	0.46
1:C:791:THR:HG22	1:C:792:PRO:CD	2.46	0.45
2:F:88:CYS:O	2:F:99:GLY:N	2.49	0.45
1:A:123:ALA:HA	1:A:177:MET:CE	2.42	0.45
1:B:933:LYS:O	1:B:936:ASP:OD2	2.34	0.45
2:F:14:SER:OG	2:F:17:GLU:OE2	2.20	0.45
3:G:179:LEU:N	3:G:179:LEU:HD22	2.31	0.45
3:J:18:LEU:HG	3:J:20:LEU:CD2	2.45	0.45
1:B:1144:GLU:OE1	1:B:1144:GLU:N	2.49	0.45
1:C:403:ARG:HH21	1:C:505:TYR:HD1	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:C	1:A:235:ILE:HD13	2.36	0.45
1:C:293:LEU:HD23	1:C:294:ASP:CG	2.35	0.45
1:C:645:THR:HG23	1:C:648:GLY:H	1.81	0.45
2:I:37:GLN:HB3	2:I:47:LEU:HD21	1.98	0.45
2:I:165:GLU:OE1	2:I:166:GLN:O	2.35	0.45
3:J:18:LEU:CB	3:J:82:MET:CE	2.70	0.45
1:B:32:PHE:CE2	1:B:218:GLN:CD	2.87	0.45
1:B:581:THR:HG23	1:B:583:GLU:OE1	2.17	0.45
2:F:124:GLN:NE2	2:F:131:SER:OG	2.49	0.45
1:A:119:ILE:HG23	1:A:128:ILE:HG12	1.99	0.45
1:B:707:TYR:CD2	1:C:883:THR:HG23	2.51	0.45
1:C:897:PRO:HD2	1:C:900:MET:HE3	1.99	0.45
1:A:802:PHE:HZ	1:A:898:PHE:CZ	2.35	0.45
1:B:737:ASP:HB3	1:B:740:MET:HB3	1.99	0.45
1:C:21:ARG:NH1	1:C:81:ASN:H	2.15	0.45
1:C:485:GLY:N	1:C:488:CYS:HB2	2.32	0.45
2:F:63:SER:OG	2:F:74:THR:HB	2.17	0.45
2:I:123:GLU:OE1	2:I:123:GLU:N	2.43	0.45
3:J:52:TYR:HB2	3:J:56:SER:OG	2.17	0.45
2:F:73:LEU:HD12	2:F:74:THR:N	2.32	0.45
1:A:971:GLY:HA3	1:A:995:ARG:NH2	2.32	0.45
1:C:573:THR:O	1:C:573:THR:OG1	2.32	0.45
3:G:49:SER:CB	3:G:59:TYR:HD2	2.30	0.45
3:G:66:ARG:C	3:G:67:PHE:HD1	2.19	0.45
2:I:124:GLN:NE2	2:I:131:SER:OG	2.49	0.45
1:A:303:LEU:HD11	1:A:313:TYR:CE1	2.52	0.45
1:C:616:ASN:OD1	1:C:617:CYS:N	2.50	0.45
3:G:6:GLU:HA	3:G:22:CYS:HA	1.99	0.45
3:G:19:ARG:HG3	3:G:80:LEU:O	2.17	0.45
3:J:20:LEU:HD11	3:J:113:VAL:HG21	1.99	0.45
1:A:716:THR:HG22	1:A:1071:GLN:O	2.17	0.44
1:A:1046:GLY:HA2	1:B:890:ALA:HB1	1.99	0.44
1:B:387:LEU:HD12	1:B:387:LEU:O	2.17	0.44
1:C:29:THR:HG22	1:C:30:ASN:N	2.32	0.44
1:C:412:PRO:HB3	1:C:426:PRO:O	2.17	0.44
3:G:80:LEU:C	3:G:80:LEU:HD23	2.37	0.44
2:I:46:LEU:C	2:I:47:LEU:HD23	2.37	0.44
1:B:712:ILE:HD13	1:B:712:ILE:HG21	1.61	0.44
2:F:114:SER:HB2	2:F:137:ASN:HB2	1.99	0.44
2:F:167:ASP:OD2	2:F:167:ASP:C	2.56	0.44
3:G:18:LEU:HG	3:G:20:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:63:SER:O	2:I:73:LEU:HD12	2.17	0.44
1:C:620:VAL:N	1:C:621:PRO:HD2	2.32	0.44
1:C:986:PRO:C	1:C:987:PRO:HG2	2.36	0.44
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.85	0.44
1:C:36:VAL:O	1:C:223:LEU:N	2.39	0.44
2:F:131:SER:HA	2:F:180:THR:HA	1.99	0.44
2:I:36:TYR:HA	2:I:47:LEU:HG	1.99	0.44
1:C:1049:LEU:HD11	1:C:1067:TYR:HB2	1.99	0.44
2:F:58:ILE:CG2	2:F:62:PHE:CE1	3.00	0.44
3:J:123:PRO:HA	3:J:149:TYR:HB3	1.98	0.44
1:C:737:ASP:OD1	1:C:737:ASP:N	2.47	0.44
3:G:36:TRP:NE1	3:G:80:LEU:HD12	2.33	0.44
1:A:498:GLN:HB2	1:A:501:ASN:OD1	2.17	0.44
1:A:1098:ASN:C	1:A:1098:ASN:OD1	2.56	0.44
1:B:176:LEU:C	1:B:190:ARG:HH21	2.21	0.44
1:C:753:LEU:HD12	1:C:753:LEU:O	2.17	0.44
2:F:132:VAL:N	2:F:179:LEU:O	2.40	0.44
3:G:81:GLN:NE2	3:G:83:ASN:OD1	2.50	0.44
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.52	0.44
1:B:168:PHE:CD1	1:B:168:PHE:C	2.90	0.44
1:B:773:GLU:OE2	1:B:1019:ARG:NH1	2.50	0.44
1:C:355:ARG:NH2	1:C:464:PHE:HD1	2.08	0.44
1:C:725:GLU:HG2	1:C:727:LEU:CD2	2.48	0.44
2:F:37:GLN:HG3	2:F:86:TYR:CE2	2.53	0.44
2:F:89:GLN:HG2	2:F:98:PHE:HB2	1.99	0.44
2:F:96:ARG:HH11	3:G:102:PHE:HB2	1.82	0.44
3:J:18:LEU:H	3:J:82:MET:HG2	1.82	0.44
3:J:92:VAL:HA	3:J:112:LEU:HA	2.00	0.44
1:A:30:ASN:HB3	1:A:32:PHE:CE2	2.53	0.44
1:A:495:TYR:CD2	1:A:497:PHE:CZ	3.06	0.44
1:B:1128:VAL:HG13	1:B:1129:VAL:HG13	2.00	0.44
1:C:291:CYS:SG	1:C:301:CYS:SG	3.13	0.44
2:F:19:ALA:HB3	2:F:75:ILE:HB	2.00	0.44
2:I:48:ILE:HD11	2:I:52:SER:HA	1.99	0.44
2:I:95:PRO:O	2:I:95:PRO:HD2	2.18	0.44
1:A:403:ARG:CD	1:A:405:ASP:HB2	2.48	0.43
1:A:498:GLN:H	1:A:501:ASN:ND2	2.16	0.43
1:A:505:TYR:OH	2:F:93:SER:N	2.51	0.43
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.98	0.43
1:C:278:LYS:HD3	1:C:287:ASP:HB2	1.99	0.43
1:C:1056:ALA:HB1	1:C:1057:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1102:TRP:CH2	1:C:1133:VAL:HG11	2.52	0.43
2:F:24:ARG:NE	2:F:69:THR:HG22	2.33	0.43
2:F:85:VAL:HG22	2:F:103:LYS:HE2	1.99	0.43
2:I:35:TRP:CZ3	2:I:88:CYS:HB2	2.53	0.43
1:B:64:TRP:HB2	1:B:266:TYR:CE2	2.53	0.43
1:B:578:ASP:OD2	1:B:579:PRO:HD2	2.18	0.43
1:C:105:ILE:HD11	1:C:239:GLN:HB3	2.00	0.43
1:C:293:LEU:HG	1:C:294:ASP:OD1	2.18	0.43
2:F:2:ILE:HG21	2:F:90:GLN:HE22	1.83	0.43
3:J:11:LEU:HD21	3:J:118:ALA:O	2.17	0.43
3:J:20:LEU:HD23	3:J:20:LEU:N	2.33	0.43
3:J:167:VAL:HG22	3:J:186:VAL:HG23	1.99	0.43
1:B:993:ILE:O	1:B:997:ILE:HG12	2.18	0.43
1:C:29:THR:HG22	1:C:30:ASN:H	1.83	0.43
1:C:144:TYR:HH	1:C:155:SER:HG	1.66	0.43
1:C:333:THR:HG22	1:C:334:ASN:OD1	2.18	0.43
3:J:212:ASP:O	3:J:213:LYS:HD2	2.19	0.43
1:A:416:GLY:O	1:A:420:ASP:N	2.39	0.43
1:A:917:TYR:CZ	1:C:1079:PRO:HB3	2.53	0.43
1:B:544:ASN:HD21	1:B:579:PRO:HB3	1.83	0.43
1:B:578:ASP:OD1	1:B:581:THR:CG2	2.67	0.43
1:C:896:ILE:HD11	1:C:904:TYR:HE2	1.84	0.43
2:F:61:ARG:NH1	2:F:79:GLU:HB2	2.31	0.43
3:G:3:GLN:HB3	3:G:25:SER:HB3	1.99	0.43
2:I:166:GLN:OE1	2:I:172:THR:N	2.50	0.43
3:J:27:ILE:HD12	3:J:27:ILE:HA	1.85	0.43
1:A:350:VAL:HB	1:A:402:ILE:HD11	2.00	0.43
1:A:1054:GLN:N	1:A:1061:VAL:O	2.50	0.43
1:A:1098:ASN:ND2	4:H:1:NAG:O7	2.52	0.43
1:B:32:PHE:CD2	1:B:218:GLN:HB3	2.49	0.43
1:B:89:GLY:C	1:B:270:LEU:HG	2.39	0.43
1:B:176:LEU:HD22	1:B:207:HIS:ND1	2.32	0.43
1:B:402:ILE:O	1:B:508:TYR:N	2.45	0.43
1:C:81:ASN:OD1	1:C:81:ASN:N	2.50	0.43
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.53	0.43
3:G:97:ARG:NH1	3:G:98:ASP:O	2.52	0.43
1:A:402:ILE:O	1:A:508:TYR:N	2.47	0.43
1:C:410:ILE:O	1:C:410:ILE:HG22	2.17	0.43
1:C:439:ASN:ND2	1:C:506:GLN:CD	2.72	0.43
1:C:455:LEU:CD1	3:J:100:GLY:HA2	2.49	0.43
2:F:58:ILE:HG22	2:F:62:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG11	1:A:237:ARG:HH21	1.84	0.43
1:A:805:ILE:HG13	1:A:878:LEU:HD21	2.00	0.43
1:C:505:TYR:CD2	1:C:505:TYR:N	2.86	0.43
2:F:47:LEU:HB2	2:F:48:ILE:HG13	2.01	0.43
1:A:966:LEU:O	1:A:966:LEU:HD12	2.18	0.43
1:B:177:MET:HG3	1:B:190:ARG:HH22	1.84	0.43
1:B:490:PHE:CG	1:B:491:PRO:HD2	2.54	0.43
1:C:170:TYR:CD1	1:C:170:TYR:C	2.91	0.43
1:C:417:LYS:NZ	1:C:453:TYR:HE2	2.15	0.43
3:G:204:HIS:HD1	3:G:207:SER:H	1.61	0.43
1:A:318:PHE:HE2	1:A:615:VAL:HG11	1.83	0.43
1:B:30:ASN:OD1	1:B:32:PHE:HD1	2.01	0.43
1:C:1081:ILE:HG13	1:C:1095:PHE:CE1	2.54	0.43
2:F:4:LEU:HD21	2:F:90:GLN:OE1	2.19	0.43
2:F:19:ALA:O	2:F:74:THR:HA	2.19	0.43
2:I:13:LEU:O	2:I:106:ILE:HA	2.19	0.43
2:I:120:PRO:HD3	2:I:132:VAL:HG22	2.01	0.43
1:A:1106:GLN:HE21	1:A:1111:GLU:HB3	1.84	0.42
1:B:1105:THR:HG22	1:B:1112:PRO:HA	2.00	0.42
1:C:21:ARG:NH2	1:C:81:ASN:OD1	2.51	0.42
1:C:404:GLY:O	1:C:407:VAL:HG12	2.18	0.42
2:F:13:LEU:HD23	2:F:13:LEU:HA	1.77	0.42
2:F:107:LYS:HG3	2:F:140:TYR:HE2	1.84	0.42
3:G:49:SER:OG	3:G:59:TYR:HD2	2.02	0.42
3:J:174:LEU:HA	3:J:180:TYR:CE1	2.53	0.42
1:A:350:VAL:HB	1:A:402:ILE:CD1	2.50	0.42
1:A:402:ILE:HG23	1:A:402:ILE:HD12	1.63	0.42
3:J:99:TYR:CE1	3:J:103:TYR:CD1	3.07	0.42
1:A:473:TYR:CZ	3:G:31:ARG:HB3	2.55	0.42
1:B:268:GLY:C	1:B:269:TYR:HD2	2.22	0.42
1:B:741:TYR:HE1	1:B:966:LEU:HD21	1.84	0.42
1:C:33:THR:O	1:C:33:THR:HG22	2.19	0.42
1:C:94:SER:O	1:C:189:LEU:HD12	2.19	0.42
1:C:122:ASN:C	1:C:177:MET:HE1	2.40	0.42
1:C:326:ILE:HA	1:C:540:ASN:O	2.20	0.42
1:C:804:GLN:OE1	1:C:935:GLN:NE2	2.45	0.42
2:I:62:PHE:HD1	2:I:75:ILE:HG12	1.81	0.42
1:B:560:LEU:HG	1:B:563:GLN:OE1	2.19	0.42
3:J:6:GLU:OE1	3:J:110:GLY:N	2.52	0.42
1:A:442:ASP:OD1	1:A:451:TYR:OH	2.33	0.42
1:A:765:ARG:O	1:A:768:THR:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:GLN:O	1:C:615:VAL:HG23	2.19	0.42
2:F:115:VAL:O	2:F:207:LYS:NZ	2.52	0.42
2:F:190:LYS:HD2	2:F:191:VAL:HG23	1.99	0.42
3:G:38:ARG:HA	3:G:93:TYR:HA	2.00	0.42
2:I:142:ARG:NH2	2:I:163:VAL:HG11	2.34	0.42
1:A:722:VAL:HA	1:A:1064:HIS:O	2.18	0.42
1:A:827:THR:H	1:A:949:GLN:HE21	1.68	0.42
1:A:993:ILE:HD13	1:A:993:ILE:HA	1.88	0.42
1:C:274:THR:O	1:C:291:CYS:HB2	2.19	0.42
1:A:763:LEU:HD21	1:A:1005:GLN:OE1	2.19	0.42
2:I:33:LEU:HD22	2:I:88:CYS:SG	2.60	0.42
3:J:17:SER:C	3:J:82:MET:HE1	2.40	0.42
1:A:34:ARG:NH2	1:A:191:GLU:OE1	2.52	0.42
2:I:13:LEU:CA	2:I:107:LYS:HZ2	2.27	0.42
2:I:34:ALA:O	2:I:88:CYS:HA	2.19	0.42
3:J:40:ALA:HB2	3:J:91:ALA:HB2	2.02	0.42
1:A:80:ASP:OD1	1:A:81:ASN:N	2.52	0.42
1:C:34:ARG:HH22	1:C:217:PRO:CG	2.32	0.42
1:C:278:LYS:HB3	1:C:287:ASP:HB2	2.02	0.42
1:C:666:ILE:HG22	1:C:667:GLY:H	1.84	0.42
2:I:37:GLN:OE1	2:I:39:LYS:NZ	2.47	0.42
2:I:161:GLU:HG2	2:I:177:SER:HB2	2.01	0.42
1:A:34:ARG:NH1	1:A:217:PRO:O	2.51	0.42
1:B:412:PRO:O	1:B:415:THR:OG1	2.28	0.42
1:C:177:MET:HB3	1:C:177:MET:HE3	1.78	0.42
1:C:455:LEU:HD12	1:C:455:LEU:O	2.20	0.42
1:B:239:GLN:HG3	1:B:240:THR:N	2.35	0.41
1:C:34:ARG:HA	1:C:34:ARG:HD3	1.67	0.41
1:C:170:TYR:OH	1:C:227:VAL:HG11	2.20	0.41
1:C:821:LEU:HD21	1:C:939:SER:HA	2.02	0.41
1:C:896:ILE:HD11	1:C:900:MET:HG2	2.01	0.41
2:F:105:GLU:CD	2:F:105:GLU:C	2.79	0.41
2:I:71:PHE:CD1	2:I:71:PHE:N	2.88	0.41
3:J:18:LEU:N	3:J:82:MET:HG2	2.35	0.41
1:A:22:THR:HB	1:A:78:ARG:HD2	2.02	0.41
1:C:220:PHE:CZ	1:C:287:ASP:CA	2.94	0.41
2:F:62:PHE:HD2	2:F:75:ILE:CD1	2.32	0.41
3:J:36:TRP:CZ2	3:J:80:LEU:HB2	2.55	0.41
3:J:42:GLY:HA3	3:J:43:LYS:NZ	2.35	0.41
1:C:170:TYR:CD1	1:C:171:VAL:N	2.81	0.41
1:C:170:TYR:HE1	1:C:172:SER:OG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HB3	1:C:418:ILE:HG13	2.02	0.41
2:F:32:TYR:HA	2:F:91:TYR:CD2	2.55	0.41
2:F:54:ARG:HD2	2:F:59:PRO:O	2.20	0.41
2:I:198:HIS:HB3	2:I:201:LEU:HD12	2.02	0.41
3:J:18:LEU:N	3:J:82:MET:CE	2.83	0.41
1:A:106:PHE:HD1	1:A:238:PHE:HB2	1.84	0.41
1:A:570:ALA:HB1	1:B:963:VAL:HG12	2.02	0.41
1:A:802:PHE:HB3	1:A:806:LEU:HD23	2.02	0.41
1:A:858:LEU:HD23	1:A:858:LEU:HA	1.86	0.41
1:B:722:VAL:HG12	1:B:1065:VAL:HA	2.02	0.41
1:B:971:GLY:HA3	1:B:995:ARG:NH2	2.35	0.41
1:C:820:ASP:OD2	1:C:820:ASP:C	2.59	0.41
3:G:29:VAL:O	3:G:71:ARG:NH2	2.53	0.41
2:I:61:ARG:HH22	2:I:82:ASP:CG	2.23	0.41
1:A:38:TYR:CE2	1:A:285:ILE:HD12	2.56	0.41
1:B:1107:ARG:NH2	1:C:904:TYR:HB3	2.36	0.41
1:B:1129:VAL:HG23	1:B:1132:ILE:HB	2.02	0.41
1:C:535:LYS:NZ	1:C:554:GLU:OE2	2.36	0.41
3:G:123:PRO:HA	3:G:149:TYR:HB3	2.01	0.41
2:I:90:GLN:HG3	2:I:91:TYR:N	2.35	0.41
3:J:33:TYR:CE1	3:J:52:TYR:CD2	3.09	0.41
3:J:222:LYS:HB3	3:J:222:LYS:HE2	1.91	0.41
1:A:48:LEU:HD13	1:A:48:LEU:HA	1.95	0.41
1:A:143:VAL:HG12	1:A:154:GLU:HB3	2.01	0.41
1:A:801:ASN:HB3	1:A:928:ASN:OD1	2.21	0.41
1:A:917:TYR:CE1	1:C:1079:PRO:HB3	2.55	0.41
1:C:421:TYR:CZ	1:C:457:ARG:HB3	2.56	0.41
2:F:33:LEU:HD23	2:F:33:LEU:HA	1.89	0.41
1:A:188:ASN:OD1	1:A:188:ASN:N	2.53	0.41
1:A:455:LEU:O	1:A:455:LEU:HD12	2.20	0.41
1:A:725:GLU:OE1	1:A:1028:LYS:NZ	2.41	0.41
1:A:1098:ASN:ND2	4:H:1:NAG:C7	2.84	0.41
1:C:194:PHE:HE1	1:C:203:ILE:HG23	1.85	0.41
1:C:712:ILE:HB	1:C:1077:THR:HG21	2.02	0.41
1:C:741:TYR:O	1:C:743:CYS:N	2.54	0.41
1:C:759:PHE:O	1:C:763:LEU:HD23	2.21	0.41
2:F:21:LEU:HD23	2:F:21:LEU:HA	1.96	0.41
2:F:98:PHE:CE2	3:G:45:LEU:N	2.88	0.41
3:G:63:VAL:HA	3:G:66:ARG:HD2	2.02	0.41
2:I:49:TYR:CD2	3:J:103:TYR:OH	2.57	0.41
3:J:3:GLN:O	3:J:4:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:12:VAL:HG11	3:J:82:MET:CE	2.49	0.41
3:J:59:TYR:CZ	3:J:69:ILE:HG22	2.56	0.41
1:A:170:TYR:CD1	1:A:170:TYR:C	2.94	0.41
1:A:244:LEU:HD23	1:A:258:TRP:HB3	2.03	0.41
1:A:724:THR:HG23	1:A:934:ILE:HD11	2.03	0.41
1:B:168:PHE:HE1	1:B:170:TYR:HB3	1.85	0.41
1:B:403:ARG:N	1:B:453:TYR:OH	2.54	0.41
1:C:159:VAL:HG21	1:C:241:LEU:HD13	2.02	0.41
1:C:656:VAL:HG22	1:C:658:ASN:H	1.86	0.41
1:C:1144:GLU:OE2	1:C:1144:GLU:HA	2.21	0.41
2:F:35:TRP:O	2:F:47:LEU:HG	2.20	0.41
2:F:98:PHE:CD2	3:G:45:LEU:HB2	2.56	0.41
2:I:89:GLN:HA	2:I:98:PHE:HB3	2.03	0.41
2:I:91:TYR:CE2	3:J:101:ASP:HB3	2.49	0.41
2:I:140:TYR:O	2:I:198:HIS:NE2	2.54	0.41
3:J:39:GLN:HB3	3:J:94:TYR:HE1	1.85	0.41
1:A:600:PRO:HB3	1:A:674:TYR:HB2	2.02	0.41
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.55	0.41
1:C:170:TYR:CE1	1:C:172:SER:OG	2.71	0.41
2:F:6:GLN:HG2	2:F:23:CYS:SG	2.62	0.41
3:G:49:SER:HB2	3:G:59:TYR:HD2	1.85	0.41
3:J:155:THR:HB	3:J:203:ASN:HB3	2.03	0.41
3:J:157:SER:OG	3:J:201:ASN:HB2	2.21	0.41
1:C:490:PHE:CZ	1:C:492:LEU:HB2	2.56	0.40
2:I:58:ILE:HG13	2:I:62:PHE:CD2	2.55	0.40
1:A:581:THR:O	1:A:582:LEU:HG	2.20	0.40
1:B:621:PRO:HA	1:B:638:THR:HA	2.04	0.40
1:B:646:ARG:NH1	1:B:646:ARG:HB3	2.37	0.40
1:B:1144:GLU:N	1:B:1144:GLU:CD	2.75	0.40
1:C:439:ASN:HD21	1:C:506:GLN:CD	2.25	0.40
1:C:1033:VAL:HG13	1:C:1034:LEU:HD13	2.03	0.40
3:J:205:LYS:N	3:J:206:PRO:HD2	2.36	0.40
1:A:320:VAL:HG12	1:A:591:SER:O	2.22	0.40
1:A:497:PHE:CG	1:A:507:PRO:HD3	2.56	0.40
1:A:787:GLN:O	1:A:788:ILE:HD13	2.21	0.40
1:A:969:ASN:OD1	1:A:969:ASN:C	2.60	0.40
1:B:168:PHE:CE1	1:B:170:TYR:HB3	2.56	0.40
1:B:329:PHE:HE1	1:B:544:ASN:HA	1.87	0.40
1:C:193:VAL:HB	1:C:204:TYR:HB2	2.03	0.40
1:C:552:LEU:HD23	1:C:552:LEU:N	2.36	0.40
3:J:18:LEU:HD21	3:J:20:LEU:HD21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TYR:CD2	1:A:497:PHE:HZ	2.40	0.40
1:A:1041:ASP:HB3	1:B:1030:SER:HB3	2.04	0.40
1:B:208:THR:HA	1:B:209:PRO:HD3	1.96	0.40
1:C:48:LEU:HD23	1:C:276:LEU:CD2	2.45	0.40
1:C:193:VAL:HG23	1:C:223:LEU:HD22	2.02	0.40
3:G:204:HIS:ND1	3:G:207:SER:N	2.63	0.40
2:I:49:TYR:HD2	2:I:53:SER:HB3	1.86	0.40
2:I:113:PRO:CB	2:I:139:PHE:HB3	2.51	0.40
3:J:166:GLY:HA3	3:J:187:THR:HB	2.03	0.40
1:C:38:TYR:CZ	1:C:285:ILE:HG13	2.57	0.40
3:G:19:ARG:HB2	3:G:81:GLN:OE1	2.22	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	1072/1208 (89%)	1021 (95%)	51 (5%)	0	100	100
1	B	1047/1208 (87%)	1003 (96%)	44 (4%)	0	100	100
1	C	1075/1208 (89%)	1036 (96%)	39 (4%)	0	100	100
2	F	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	29	66
2	I	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
3	G	220/447 (49%)	205 (93%)	15 (7%)	0	100	100
3	J	220/447 (49%)	204 (93%)	16 (7%)	0	100	100
All	All	4058/4946 (82%)	3870 (95%)	187 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	94	SER

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	950/1056 (90%)	924 (97%)	26 (3%)	44	67
1	B	935/1056 (88%)	903 (97%)	32 (3%)	37	62
1	C	953/1056 (90%)	924 (97%)	29 (3%)	41	64
2	F	186/186 (100%)	180 (97%)	6 (3%)	39	63
2	I	186/186 (100%)	179 (96%)	7 (4%)	33	59
3	G	188/396 (48%)	184 (98%)	4 (2%)	53	73
3	J	188/396 (48%)	181 (96%)	7 (4%)	34	60
All	All	3586/4332 (83%)	3475 (97%)	111 (3%)	43	64

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	58	PHE
1	A	153	MET
1	A	170	TYR
1	A	205	SER
1	A	305	SER
1	A	306	PHE
1	A	390	LEU
1	A	437	ASN
1	A	462	LYS
1	A	473	TYR
1	A	493	GLN
1	A	519	HIS
1	A	592	PHE
1	A	731	MET
1	A	745	ASP
1	A	759	PHE

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Mol	Chain	Res	Type
1	A	820	ASP
1	A	854	LYS
1	A	873	TYR
1	A	886	TRP
1	A	900	MET
1	A	901	GLN
1	A	1021	SER
1	A	1091	ARG
1	A	1118	ASP
1	B	30	ASN
1	B	58	PHE
1	B	64	TRP
1	B	87	ASN
1	B	168	PHE
1	B	205	SER
1	B	275	PHE
1	B	306	PHE
1	B	329	PHE
1	B	334	ASN
1	B	359	SER
1	B	390	LEU
1	B	408	ARG
1	B	493	GLN
1	B	592	PHE
1	B	607	GLN
1	B	617	CYS
1	B	649	CYS
1	B	650	LEU
1	B	663	ASP
1	B	707	TYR
1	B	737	ASP
1	B	764	ASN
1	B	803	SER
1	B	820	ASP
1	B	886	TRP
1	B	900	MET
1	B	996	LEU
1	B	1030	SER
1	B	1050	MET
1	B	1088	HIS
1	B	1126	CYS
1	C	30	ASN

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Mol	Chain	Res	Type
1	C	88	ASP
1	C	153	MET
1	C	170	TYR
1	C	205	SER
1	C	220	PHE
1	C	274	THR
1	C	294	ASP
1	C	328	ARG
1	C	361	CYS
1	C	364	ASP
1	C	420	ASP
1	C	437	ASN
1	C	456	PHE
1	C	459	SER
1	C	490	PHE
1	C	493	GLN
1	C	519	HIS
1	C	541	PHE
1	C	758	SER
1	C	796	ASP
1	C	873	TYR
1	C	936	ASP
1	C	968	SER
1	C	975	SER
1	C	1037	SER
1	C	1055	SER
1	C	1097	SER
1	C	1126	CYS
2	F	13	LEU
2	F	83	PHE
2	F	91	TYR
2	F	98	PHE
2	F	158	ASN
2	F	190	LYS
3	G	46	GLU
3	G	58	PHE
3	G	71	ARG
3	G	98	ASP
2	I	21	LEU
2	I	23	CYS
2	I	49	TYR
2	I	60	ASP

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Mol	Chain	Res	Type
2	I	63	SER
2	I	65	SER
2	I	77	ARG
3	J	58	PHE
3	J	95	CYS
3	J	99	TYR
3	J	105	ASP
3	J	168	HIS
3	J	180	TYR
3	J	201	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	955	ASN
1	C	439	ASN
1	C	498	GLN
1	C	501	ASN
1	C	580	GLN
1	C	655	HIS
3	G	175	GLN
2	I	90	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

31 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.54	0	17,19,21	1.09	1 (5%)
4	NAG	D	2	4	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	E	1	1,4	14,14,15	0.50	0	17,19,21	0.67	1 (5%)
4	NAG	E	2	4	14,14,15	0.18	0	17,19,21	0.38	0
4	NAG	H	1	1,4	14,14,15	0.35	0	17,19,21	0.43	0
4	NAG	H	2	4	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	K	1	1,4	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	K	2	4	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	L	1	1,4	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	L	2	4	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	M	1	1,4	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	M	2	4	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	N	1	1,4	14,14,15	0.15	0	17,19,21	0.56	0
4	NAG	N	2	4	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	O	1	1,4	14,14,15	0.59	0	17,19,21	1.05	1 (5%)
4	NAG	O	2	4	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	P	1	1,4	14,14,15	0.23	0	17,19,21	0.40	0
4	NAG	P	2	4	14,14,15	0.18	0	17,19,21	0.41	0
4	NAG	Q	1	1,4	14,14,15	0.27	0	17,19,21	0.52	0
4	NAG	Q	2	4	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	R	1	1,4	14,14,15	0.23	0	17,19,21	0.43	0
4	NAG	R	2	4	14,14,15	0.19	0	17,19,21	0.42	0
4	NAG	S	1	1,4	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	S	2	4	14,14,15	0.22	0	17,19,21	0.57	0
4	NAG	T	1	1,4	14,14,15	0.43	0	17,19,21	0.42	0
4	NAG	T	2	4	14,14,15	0.21	0	17,19,21	0.37	0
4	NAG	U	1	1,4	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	U	2	4	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	V	1	5,1	14,14,15	0.65	1 (7%)	17,19,21	0.90	1 (5%)
5	NAG	V	2	5	14,14,15	0.23	0	17,19,21	0.37	0
5	BMA	V	3	5	11,11,12	0.60	0	15,15,17	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	1/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
4	NAG	N	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	3/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	1/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	1/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	V	2	5	-	2/6/23/26	0/1/1/1
5	BMA	V	3	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	V	1	NAG	O5-C1	-2.23	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	NAG	C1-O5-C5	3.01	116.27	112.19
4	D	1	NAG	C2-N2-C7	2.34	126.24	122.90
4	E	1	NAG	C1-O5-C5	2.19	115.16	112.19
5	V	1	NAG	C3-C4-C5	2.02	113.84	110.24

There are no chirality outliers.

All (34) torsion outliers are listed below:

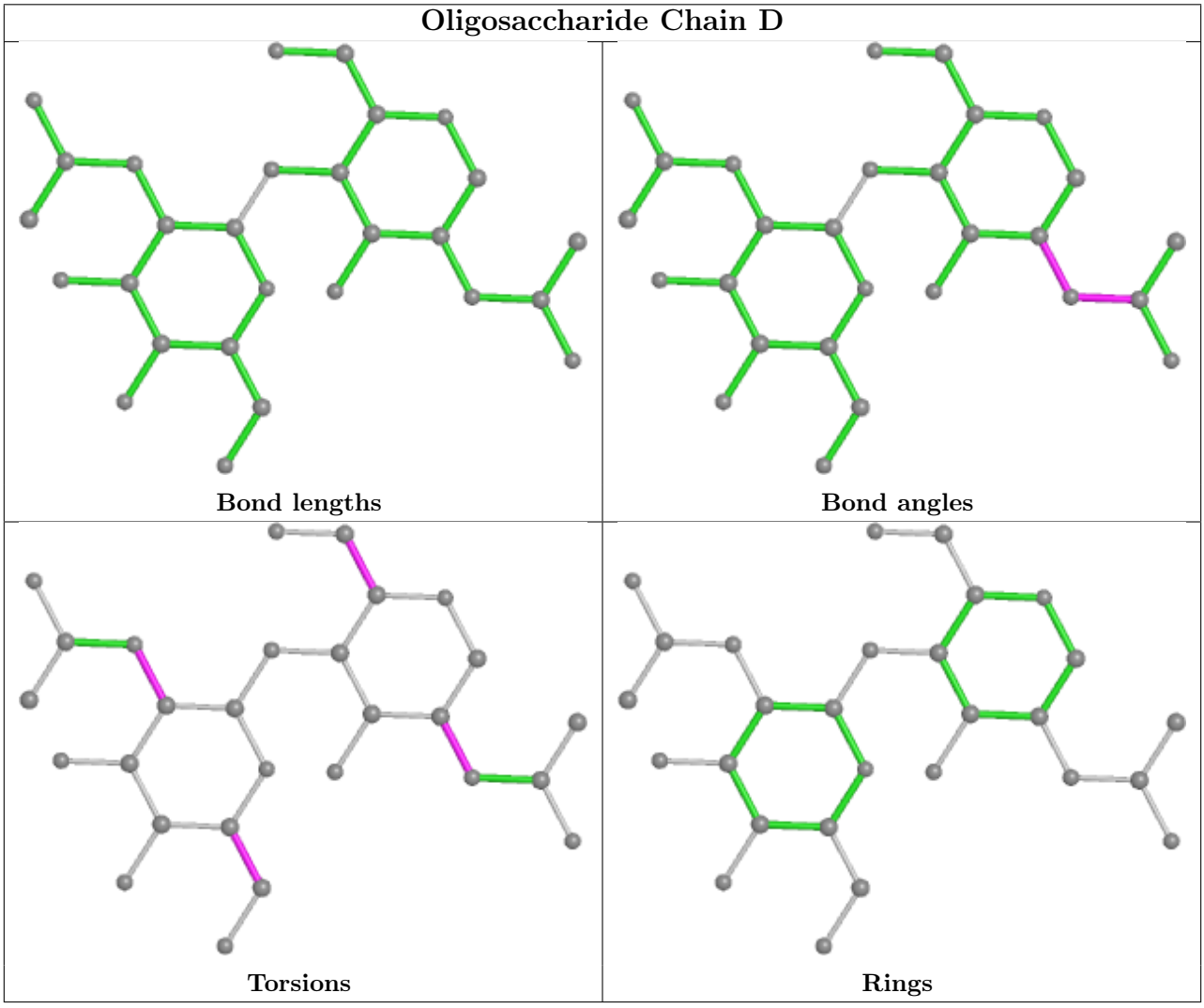
Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C3-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	O	1	NAG	C4-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C3-C2-N2-C7
4	N	1	NAG	C3-C2-N2-C7
4	Q	1	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6
4	N	2	NAG	C3-C2-N2-C7
4	O	1	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	S	1	NAG	C4-C5-C6-O6

There are no ring outliers.

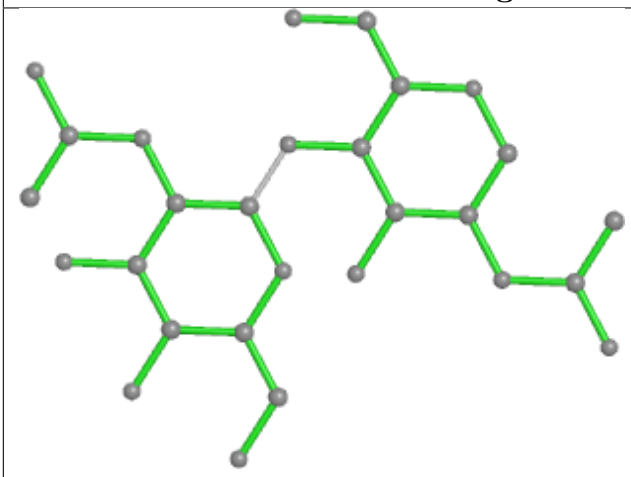
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	1	0
4	H	1	NAG	3	0
5	V	1	NAG	1	0
4	U	1	NAG	1	0
4	D	1	NAG	1	0

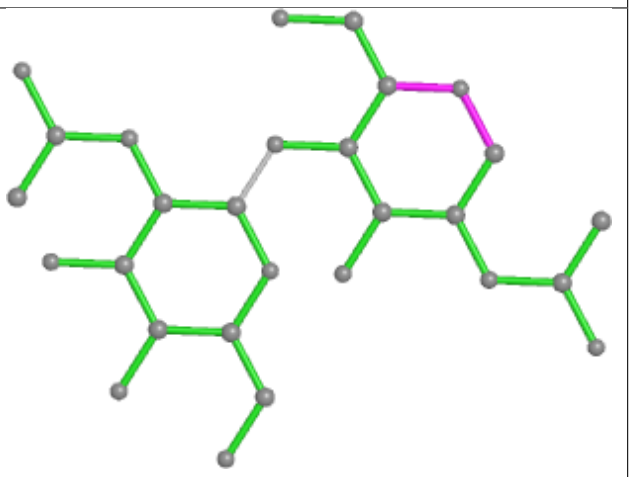
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



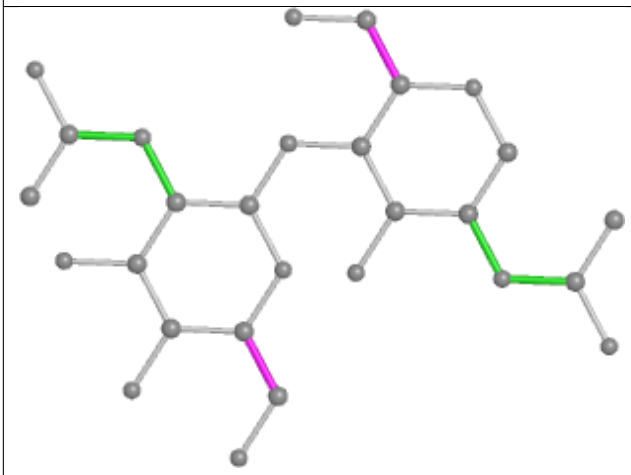
Oligosaccharide Chain E



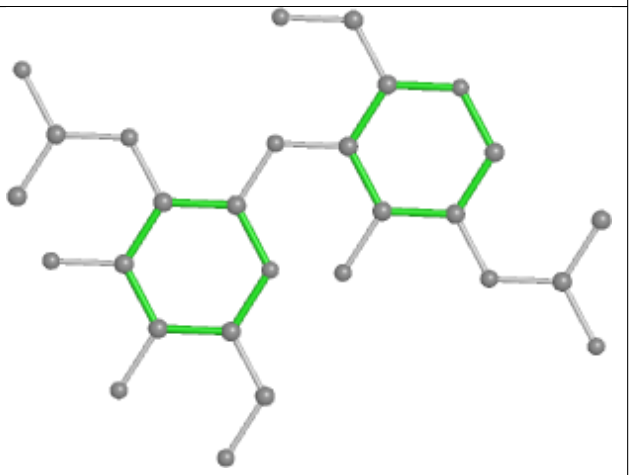
Bond lengths



Bond angles

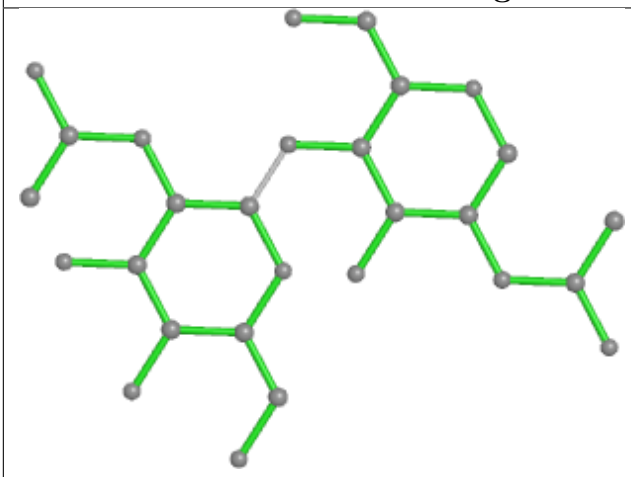


Torsions

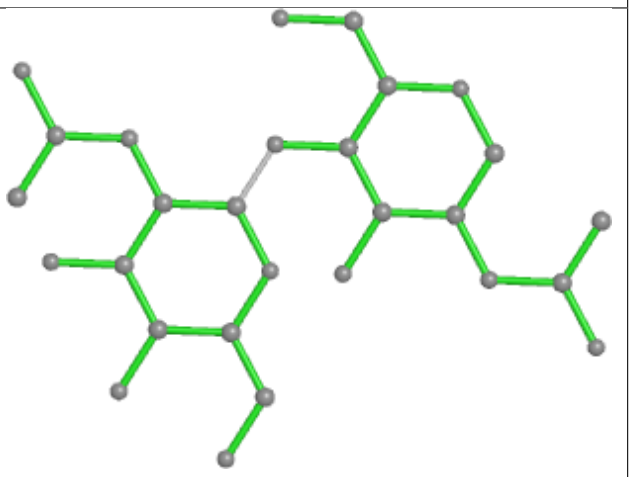


Rings

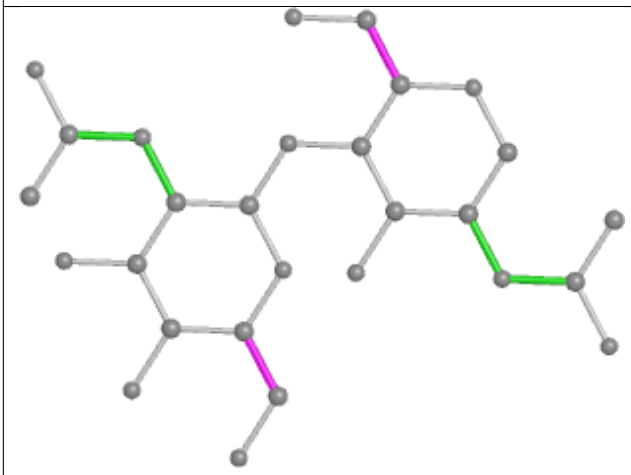
Oligosaccharide Chain H



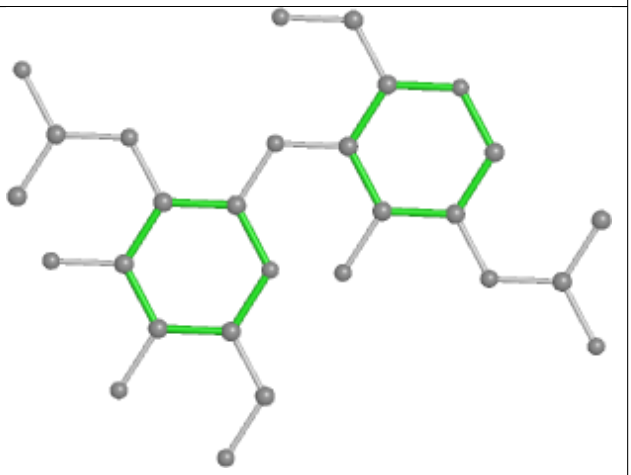
Bond lengths



Bond angles

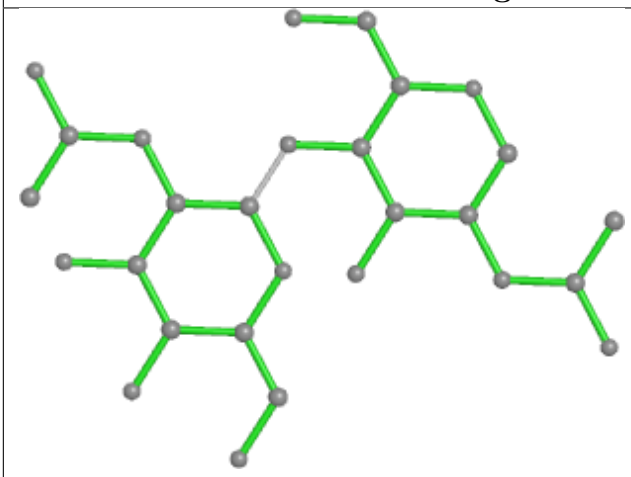


Torsions

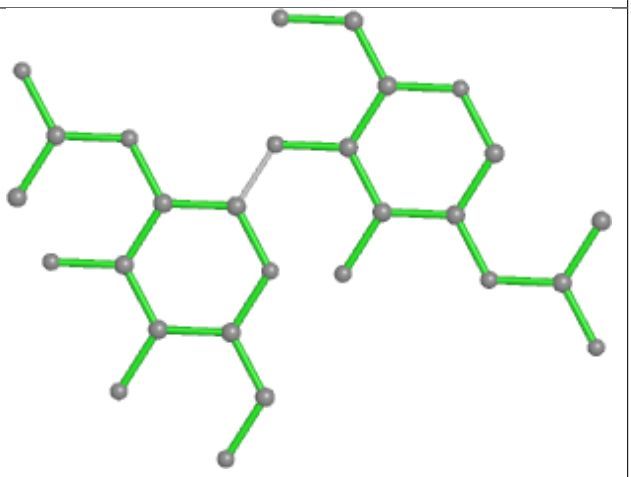


Rings

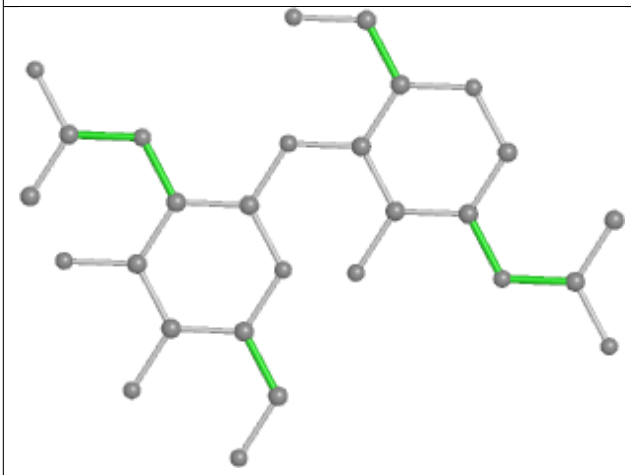
Oligosaccharide Chain K



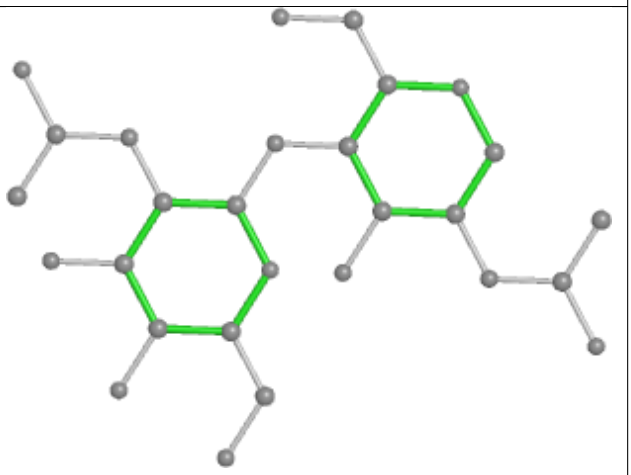
Bond lengths



Bond angles

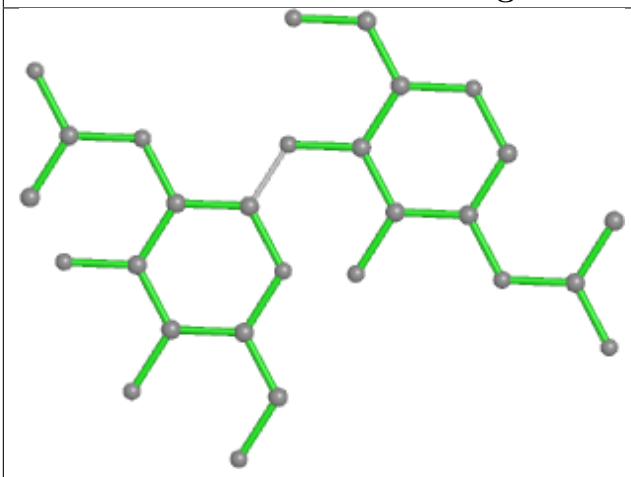


Torsions

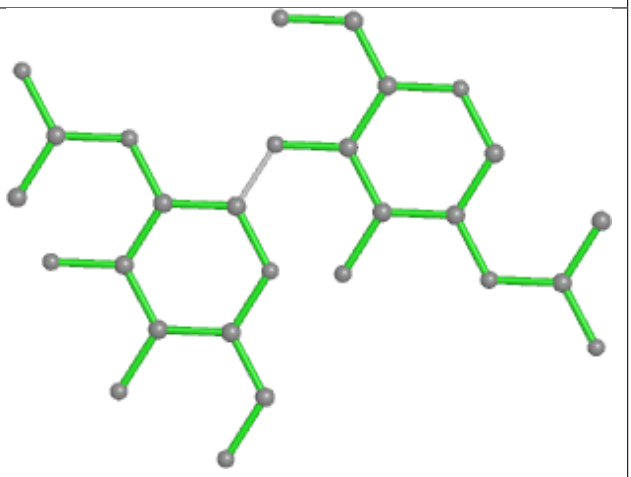


Rings

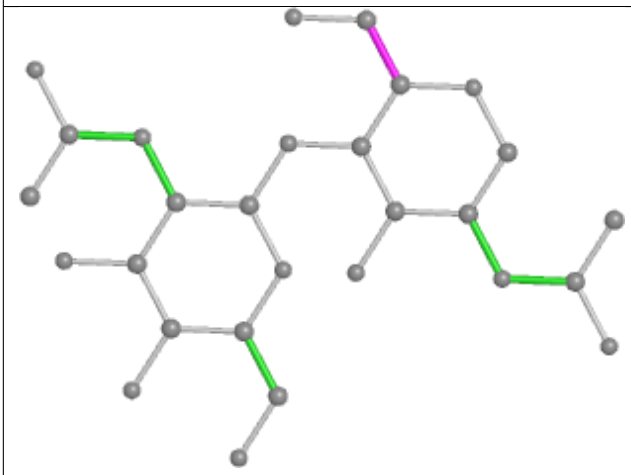
Oligosaccharide Chain L



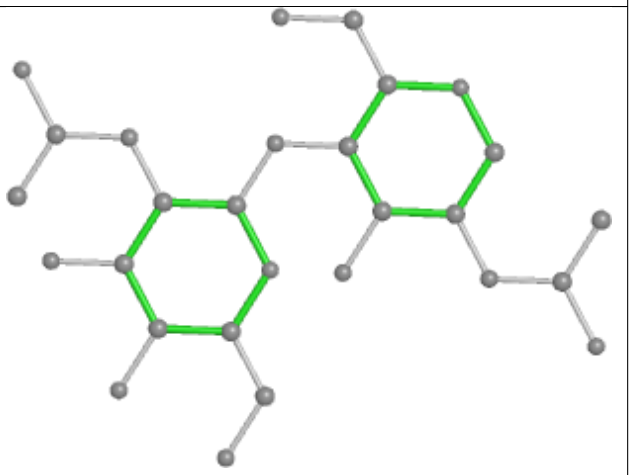
Bond lengths



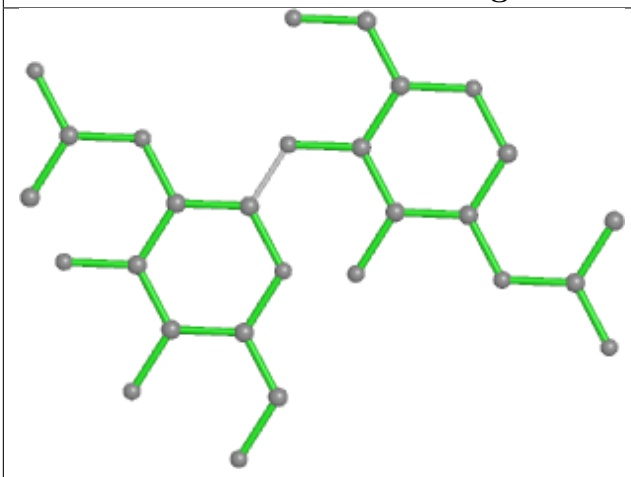
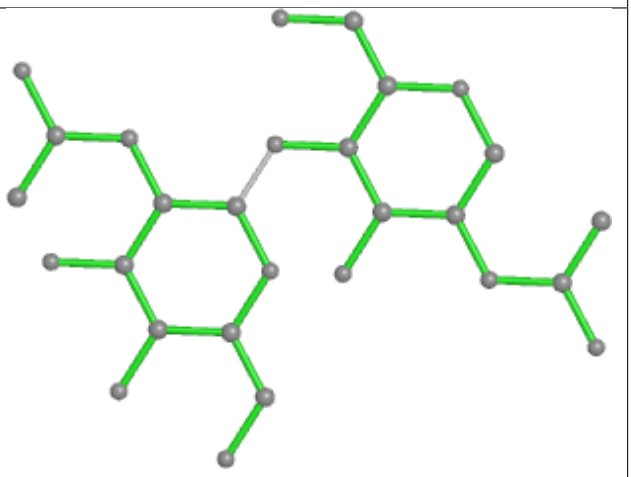
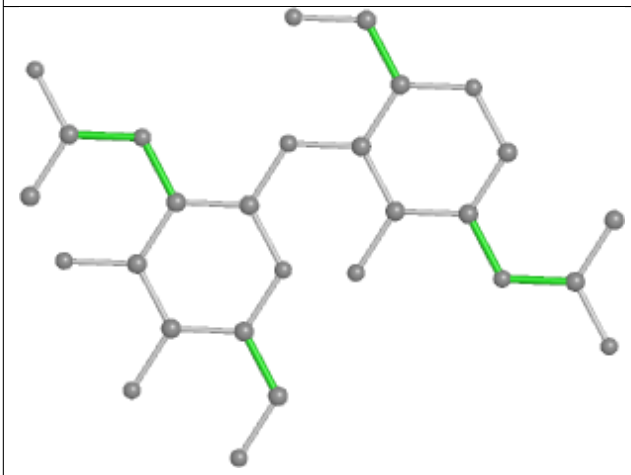
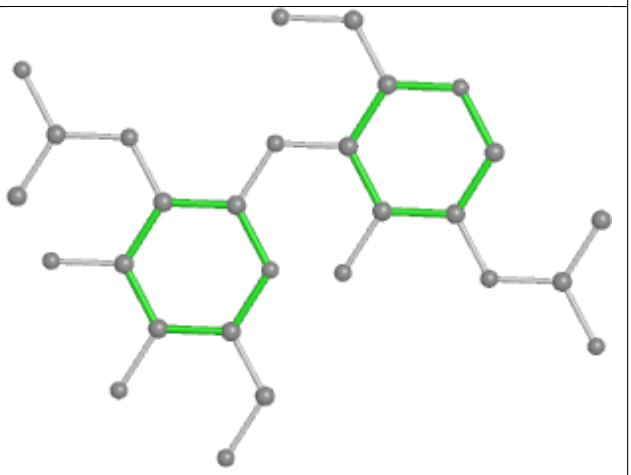
Bond angles



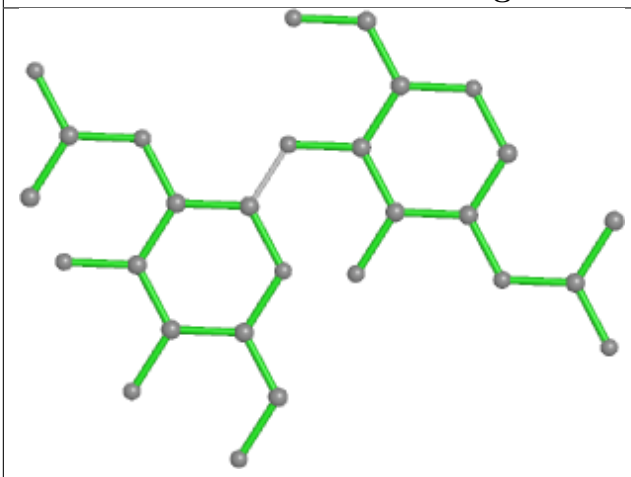
Torsions



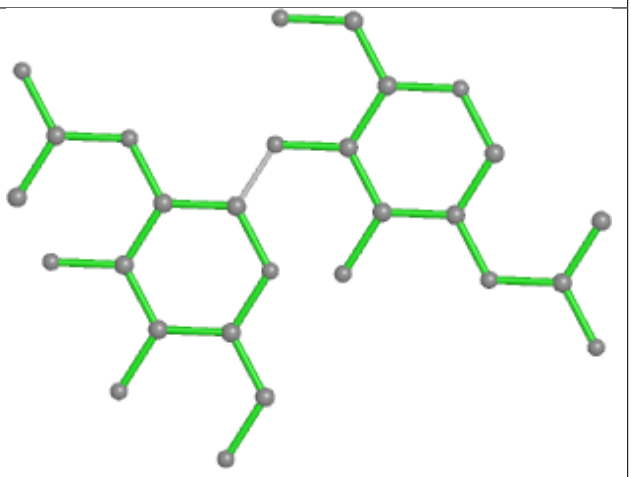
Rings

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

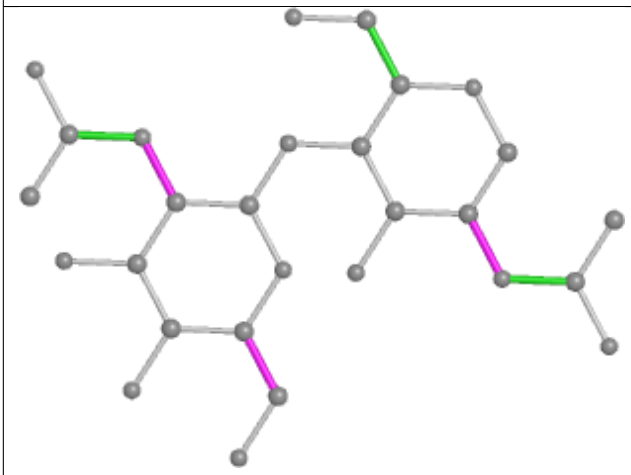
Oligosaccharide Chain N



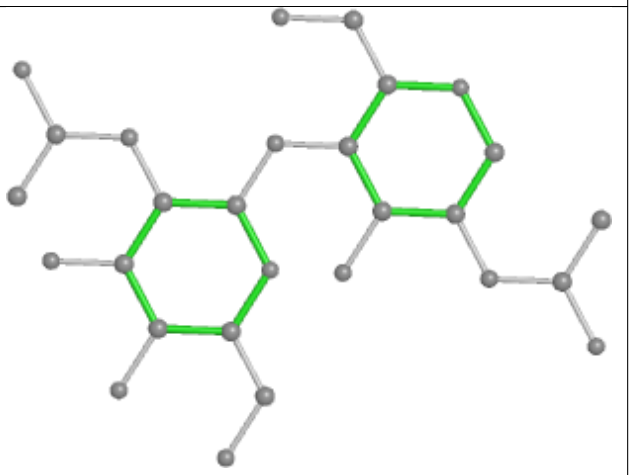
Bond lengths



Bond angles

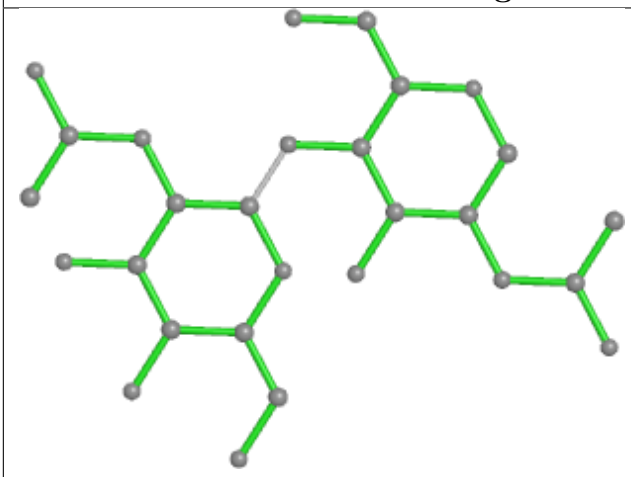


Torsions

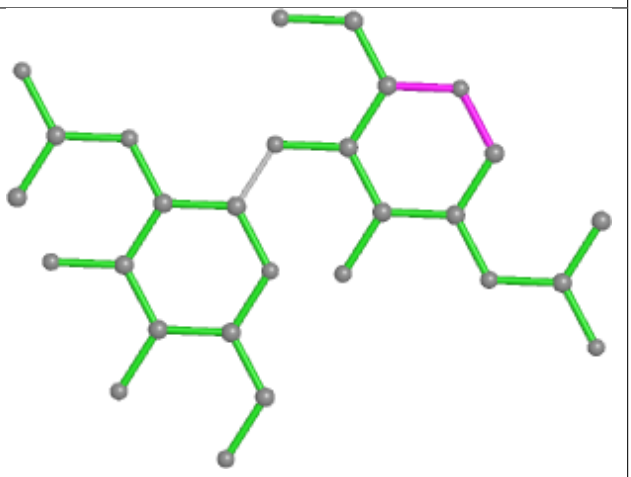


Rings

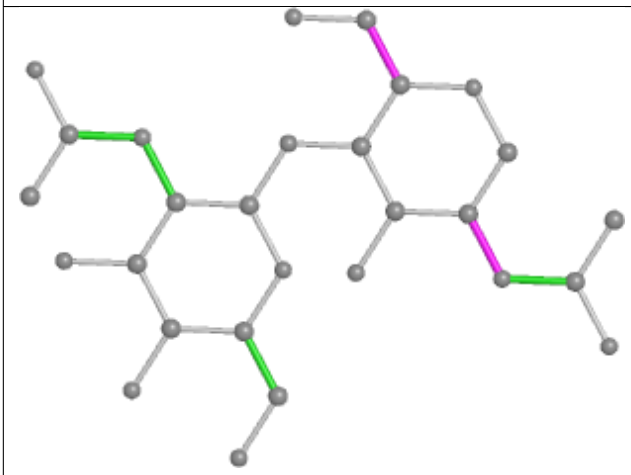
Oligosaccharide Chain O



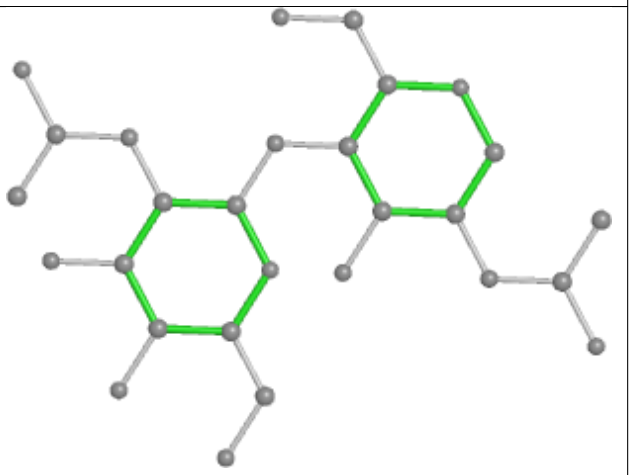
Bond lengths



Bond angles

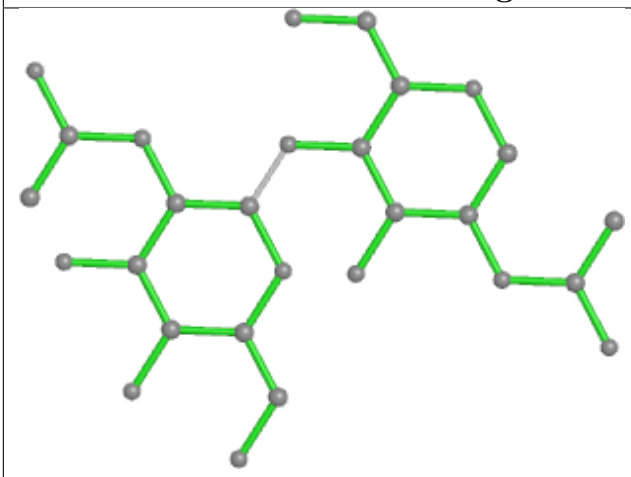


Torsions

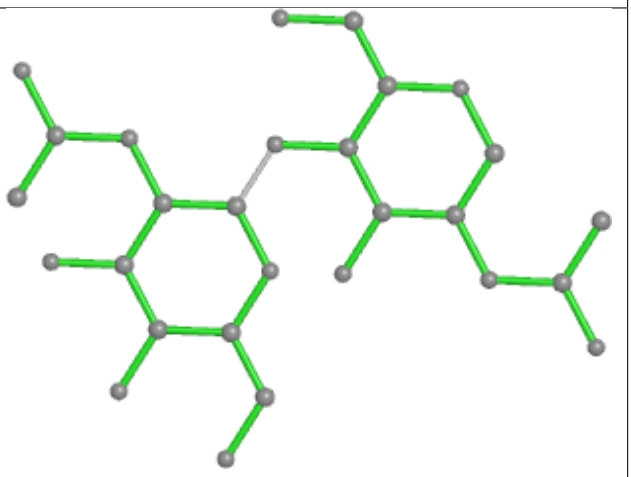


Rings

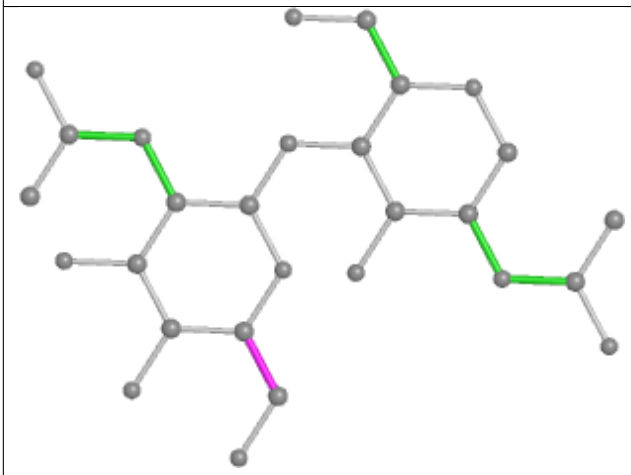
Oligosaccharide Chain P



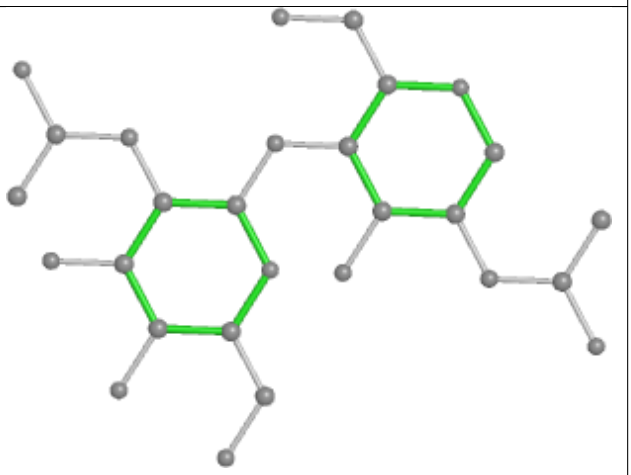
Bond lengths



Bond angles

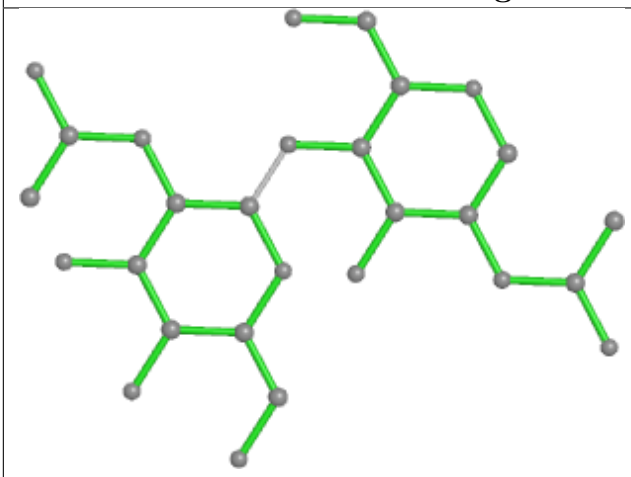


Torsions

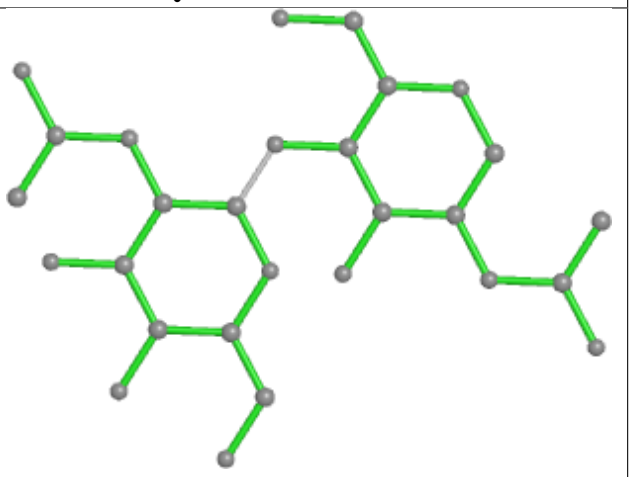


Rings

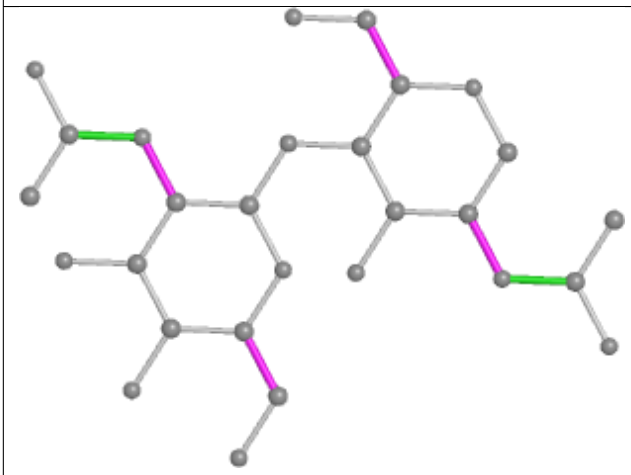
Oligosaccharide Chain Q



Bond lengths



Bond angles



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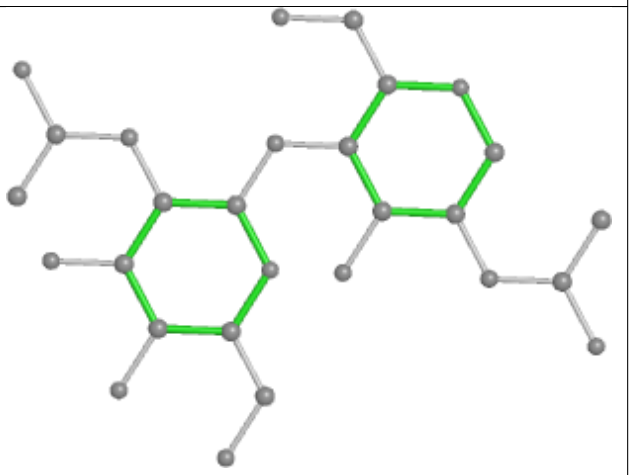
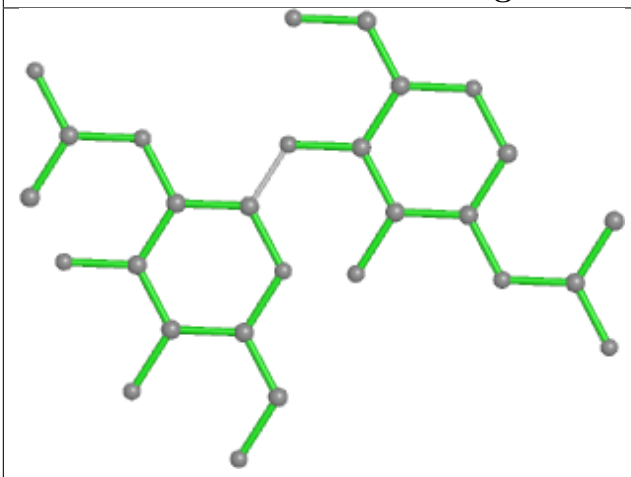
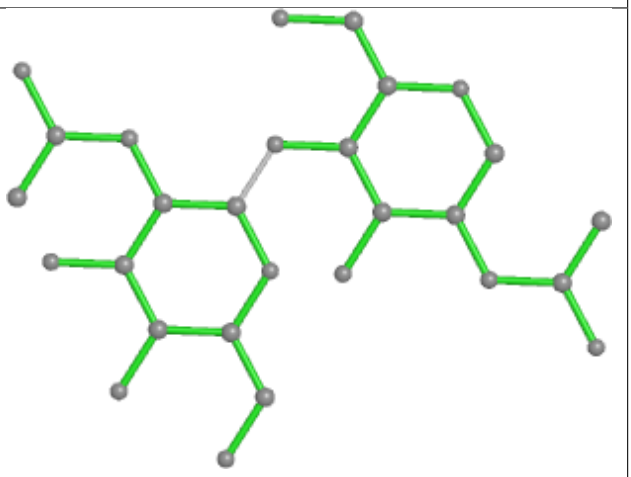


Rings

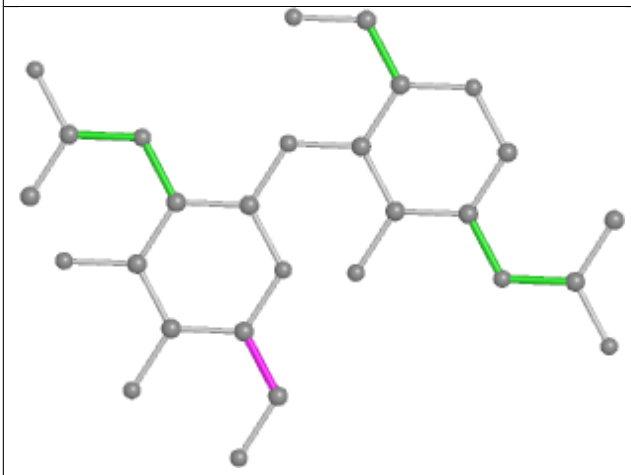
Oligosaccharide Chain R



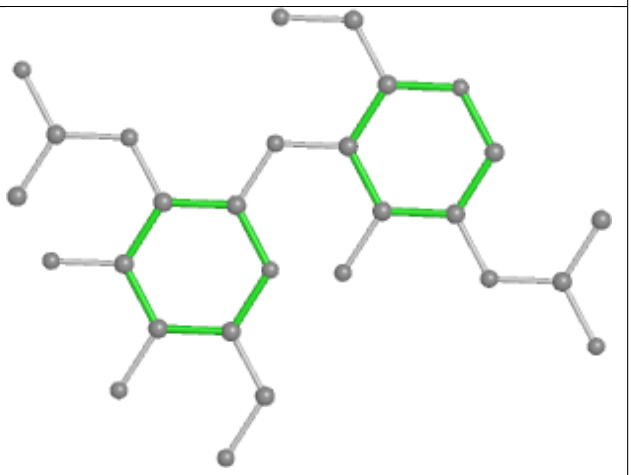
Bond lengths



Bond angles

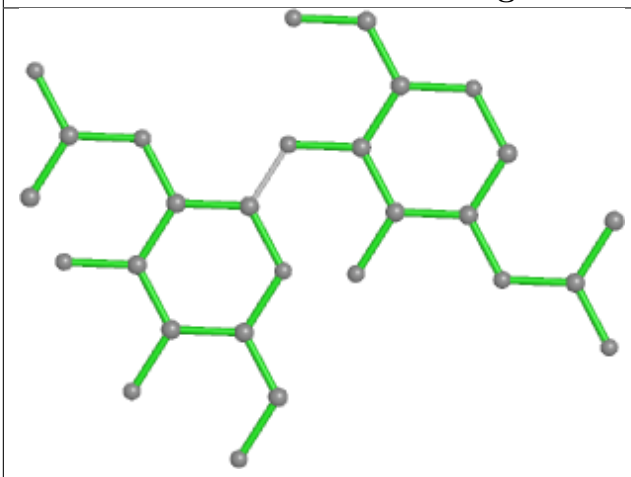


Torsions

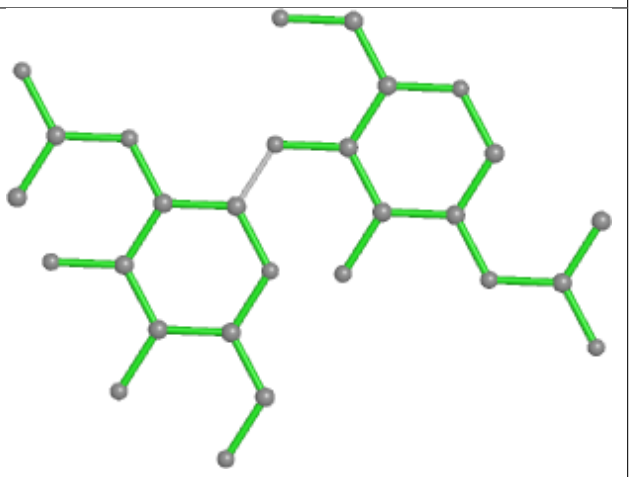


Rings

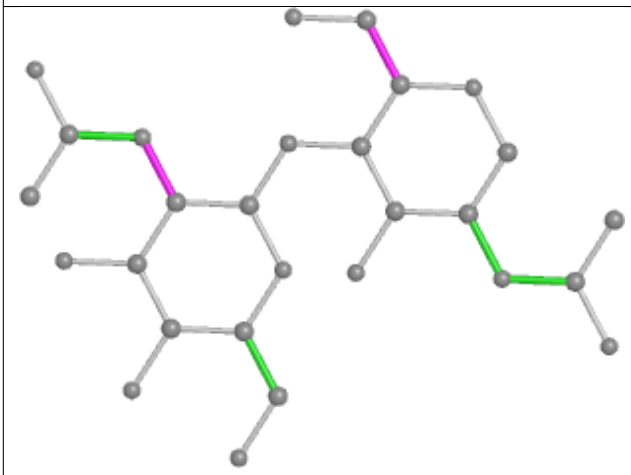
Oligosaccharide Chain S



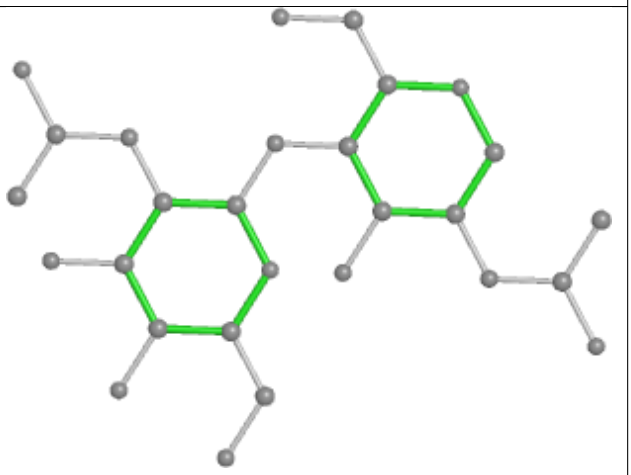
Bond lengths



Bond angles

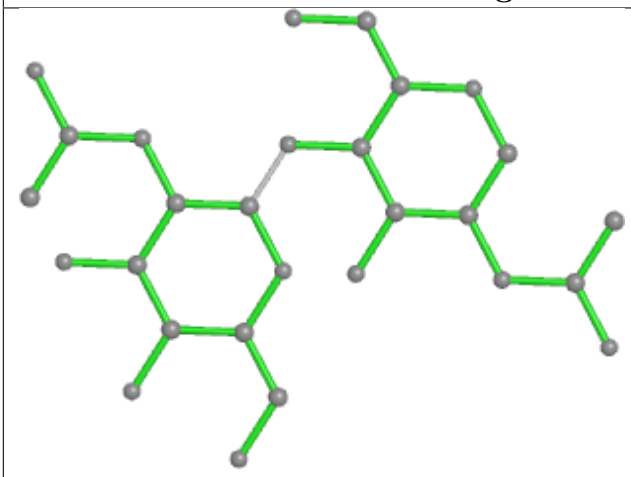


Torsions

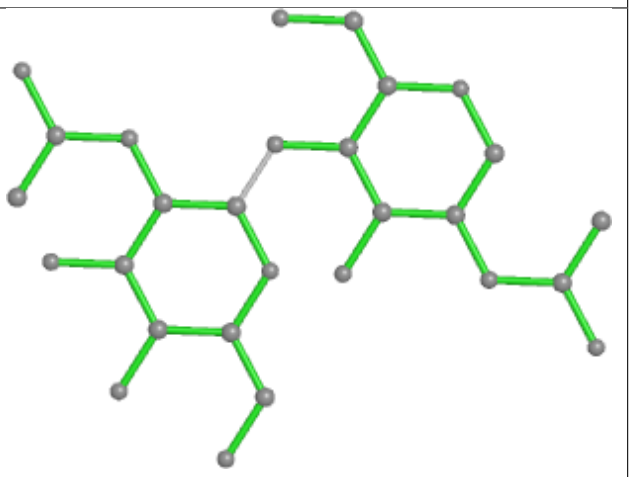


Rings

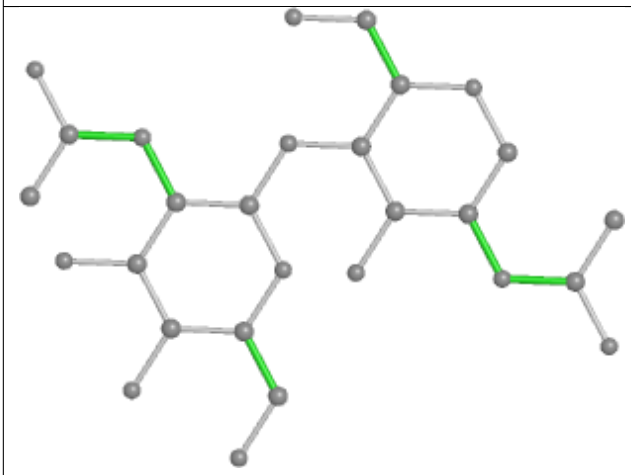
Oligosaccharide Chain T



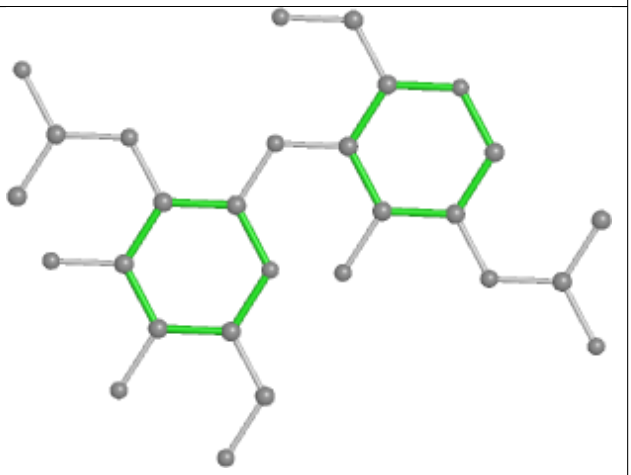
Bond lengths



Bond angles

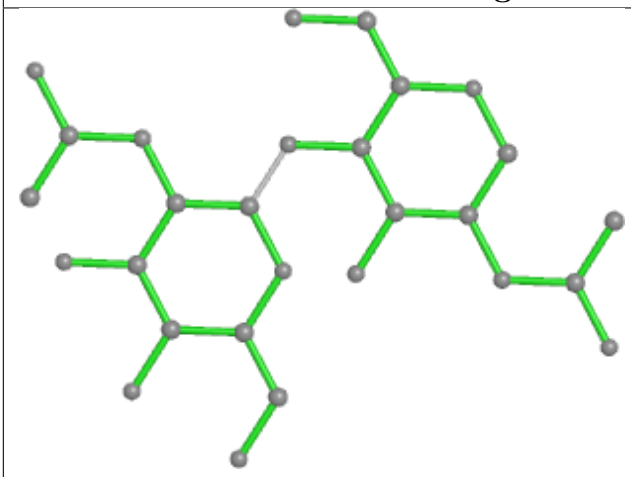


Torsions

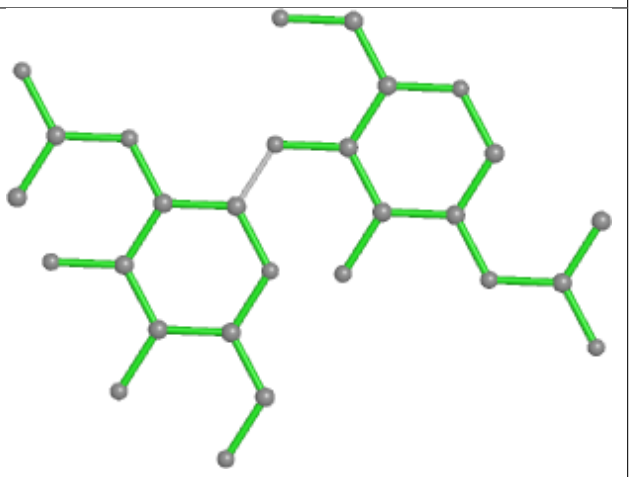


Rings

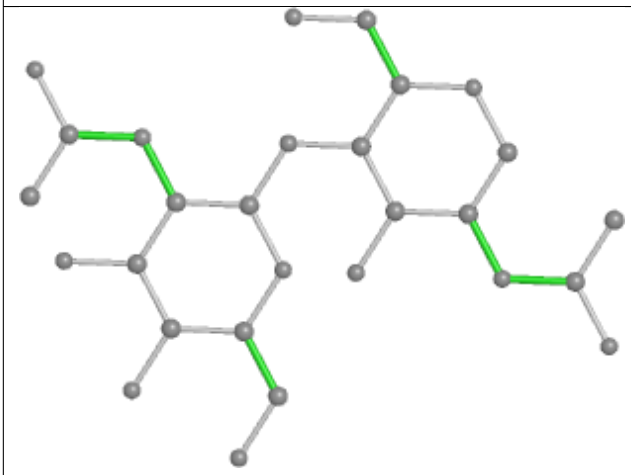
Oligosaccharide Chain U



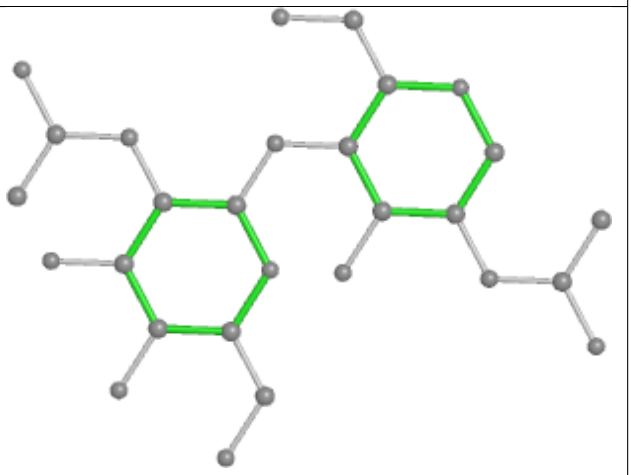
Bond lengths



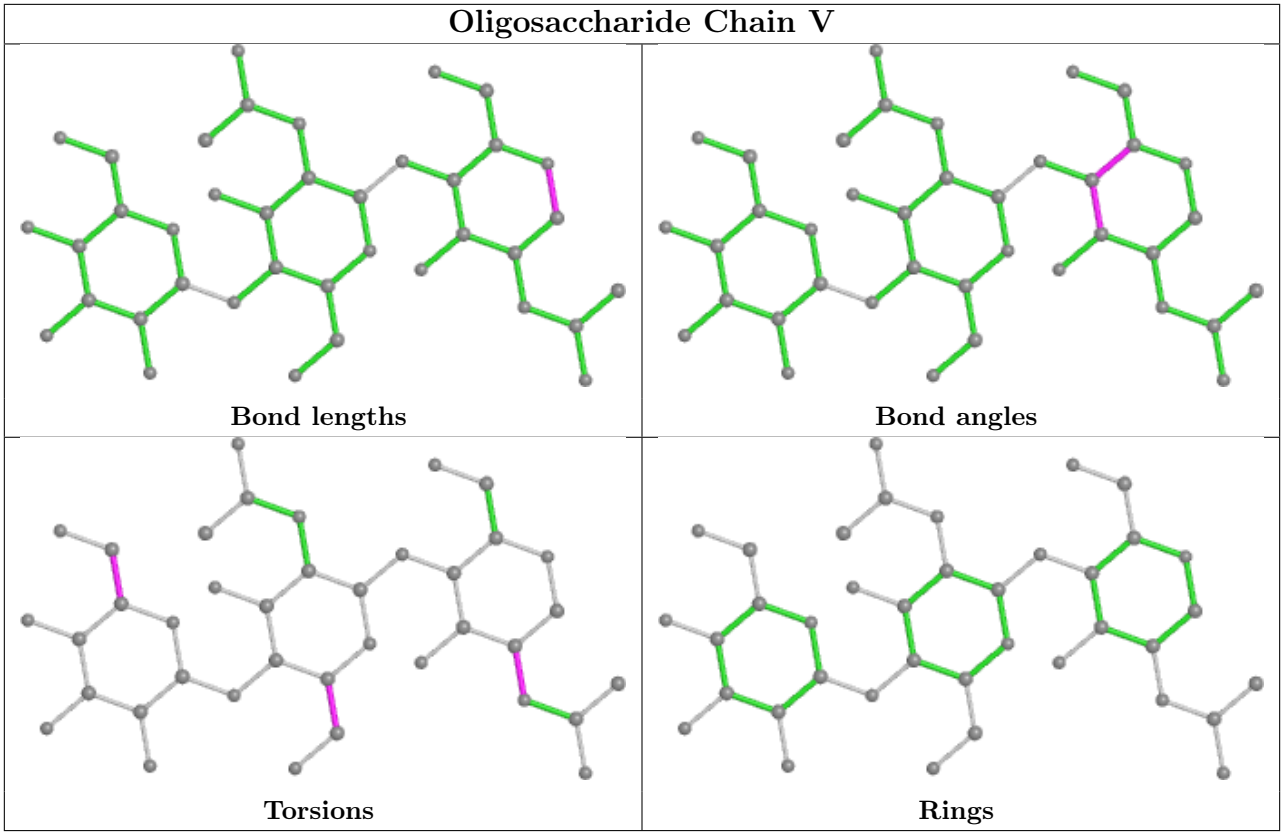
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

23 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	$\#\|Z\|>2$
6	NAG	C	1302	1	14,14,15	0.24	0	17,19,21	0.56	0
6	NAG	A	1309	1	14,14,15	0.31	0	17,19,21	0.46	0
6	NAG	B	1301	1	14,14,15	0.18	0	17,19,21	0.40	0
6	NAG	C	1306	1	14,14,15	0.17	0	17,19,21	0.42	0
6	NAG	B	1304	1	14,14,15	0.24	0	17,19,21	0.39	0
6	NAG	A	1302	1	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	C	1304	1	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	C	1305	1	14,14,15	0.39	0	17,19,21	0.47	0
6	NAG	C	1301	1	14,14,15	0.17	0	17,19,21	0.41	0
6	NAG	A	1308	1	14,14,15	0.26	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.32	0
6	NAG	A	1307	1	14,14,15	0.20	0	17,19,21	0.42	0
6	NAG	C	1307	1	14,14,15	0.30	0	17,19,21	0.51	0
6	NAG	C	1303	1	14,14,15	0.20	0	17,19,21	0.46	0
6	NAG	A	1301	1	14,14,15	0.16	0	17,19,21	0.39	0
6	NAG	A	1304	1	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	A	1305	1	14,14,15	0.35	0	17,19,21	0.45	0
6	NAG	A	1303	1	14,14,15	0.22	0	17,19,21	0.45	0
6	NAG	B	1302	1	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	A	1306	1	14,14,15	0.34	0	17,19,21	1.58	2 (11%)
6	NAG	B	1305	1	14,14,15	0.23	0	17,19,21	0.40	0
6	NAG	B	1303	1	14,14,15	0.20	0	17,19,21	0.50	0
6	NAG	B	1307	1	14,14,15	0.28	0	17,19,21	0.47	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	1/6/23/26	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})
6	A	1306	NAG	C2-N2-C7	4.01	128.62	122.90
6	A	1306	NAG	C1-C2-N2	3.82	117.01	110.49

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

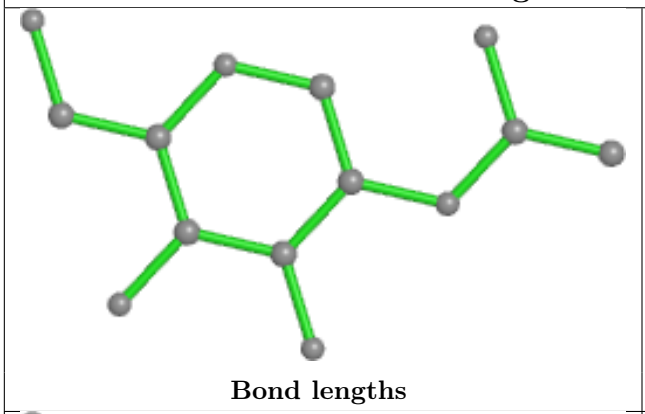
There are no ring outliers.

1 monomer is involved in 1 short contact:

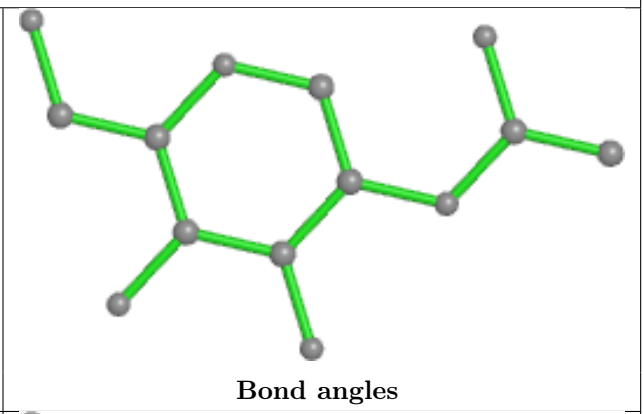
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1306	NAG	1	0

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

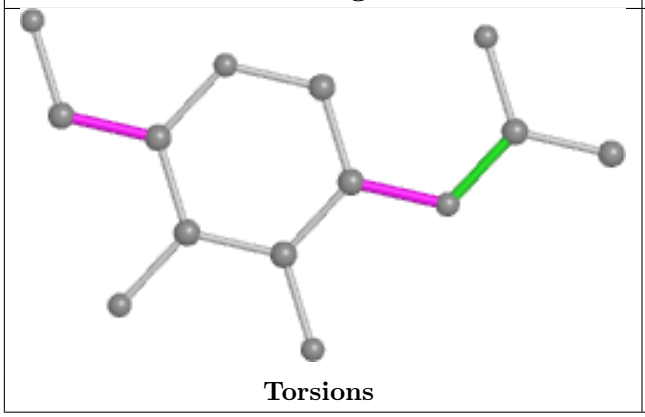
Ligand NAG C 1302



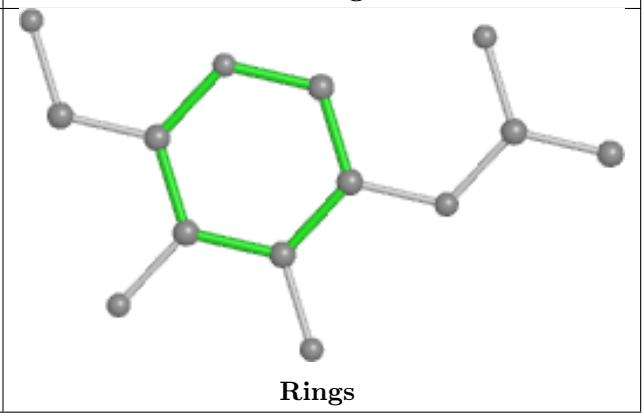
Bond lengths



Bond angles

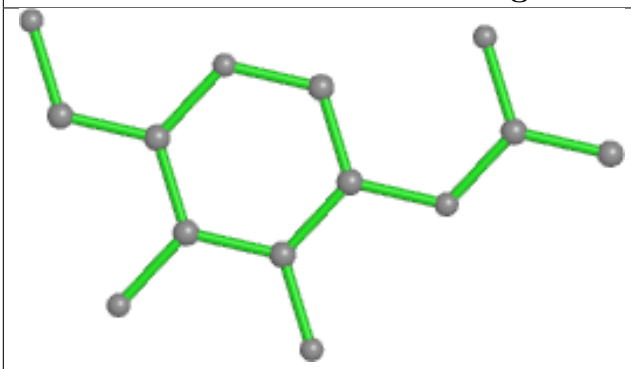


Torsions

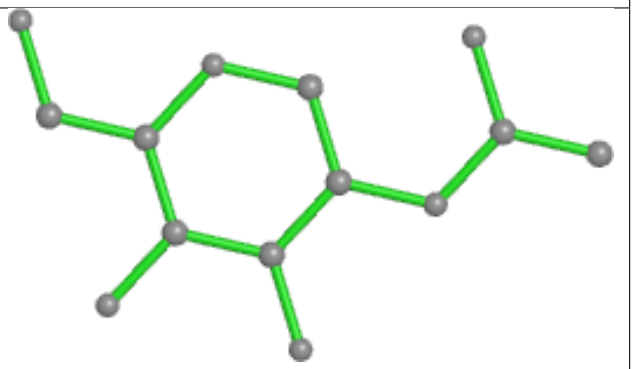


Rings

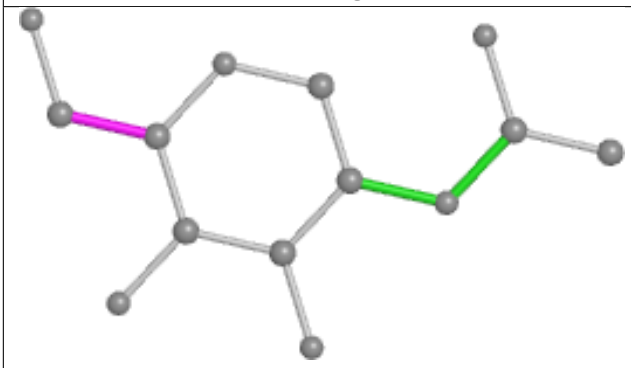
Ligand NAG A 1309



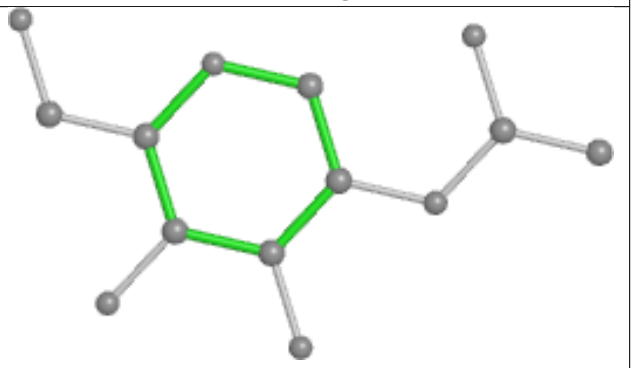
Bond lengths



Bond angles

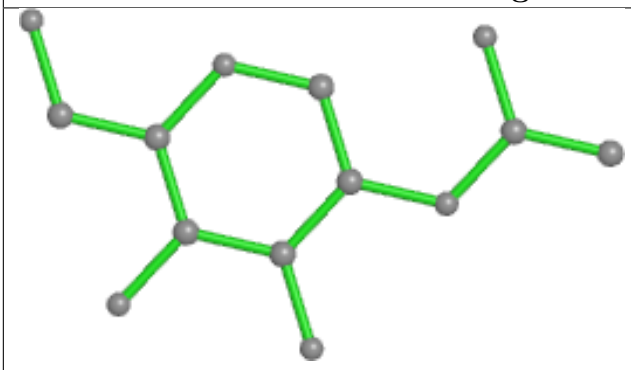


Torsions

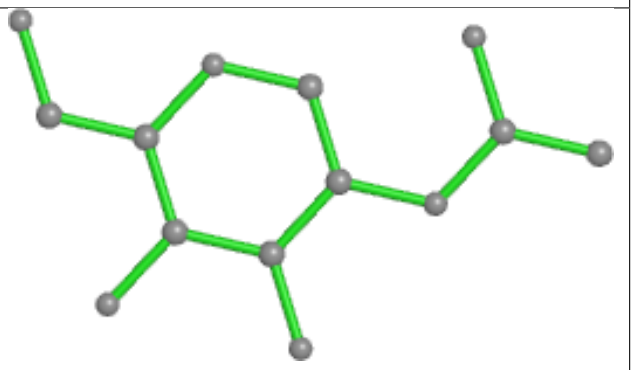


Rings

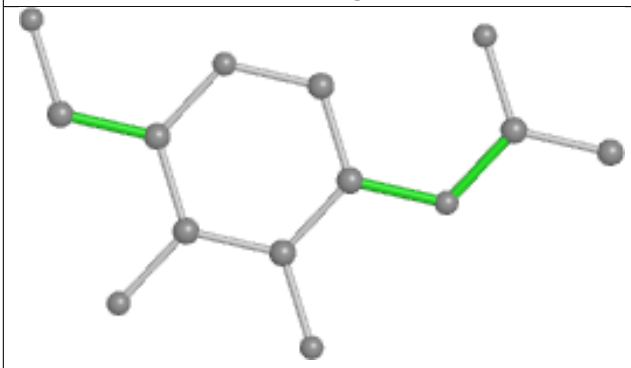
Ligand NAG B 1301



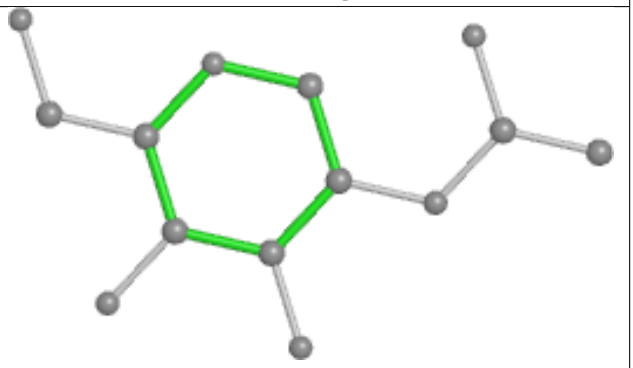
Bond lengths



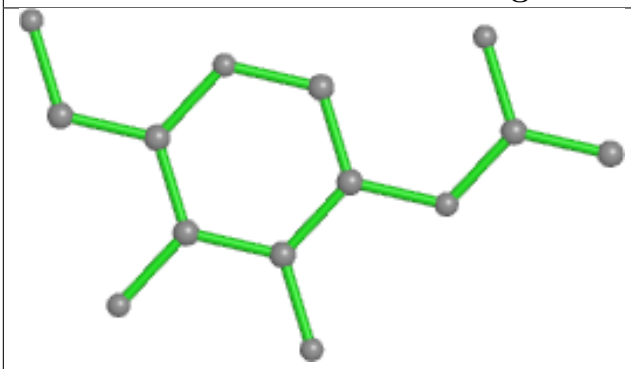
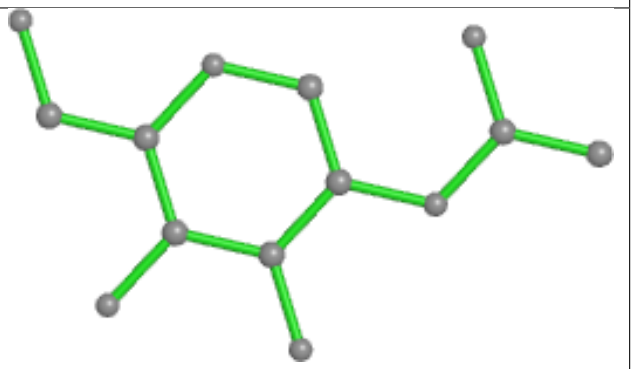
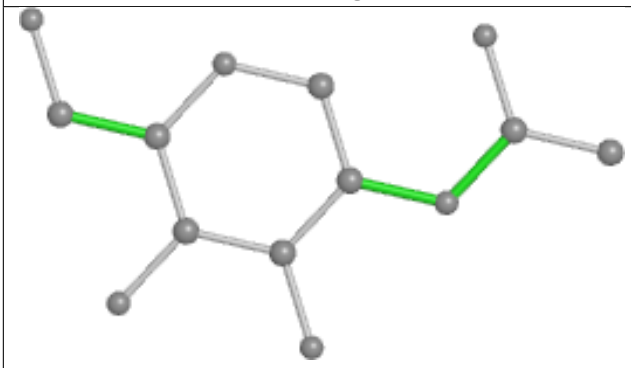
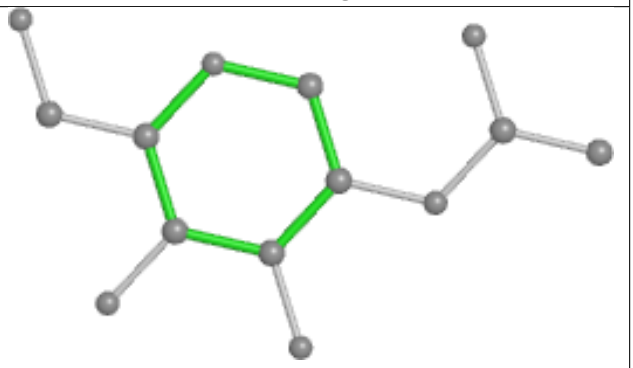
Bond angles

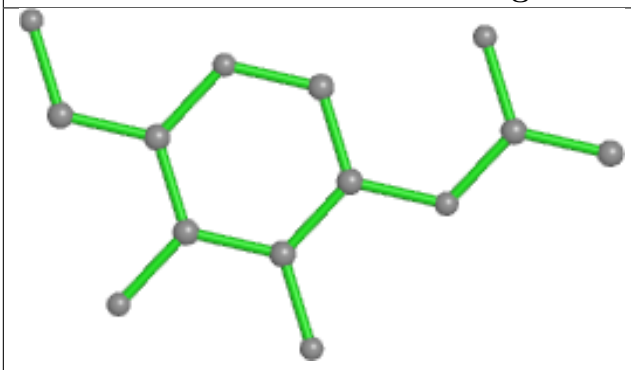
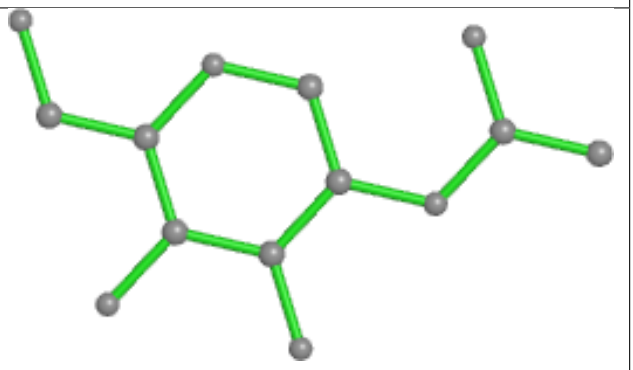
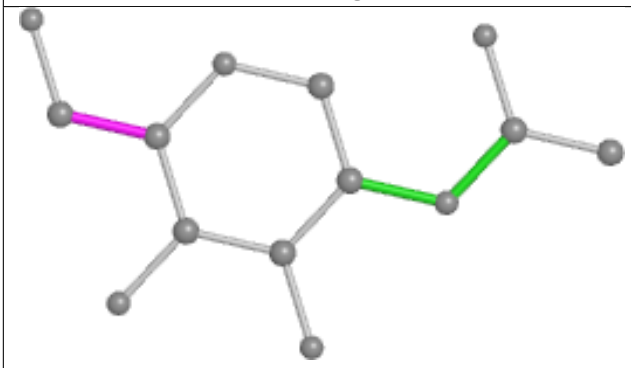
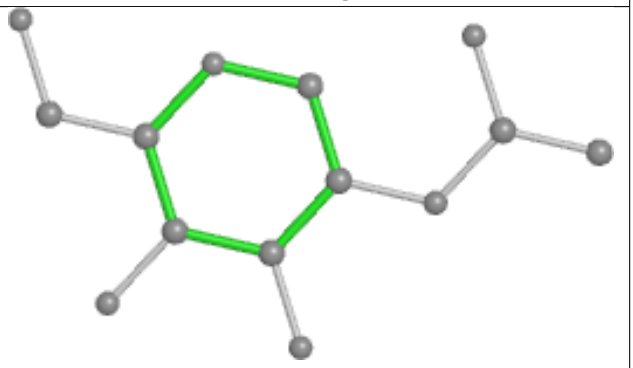


Torsions

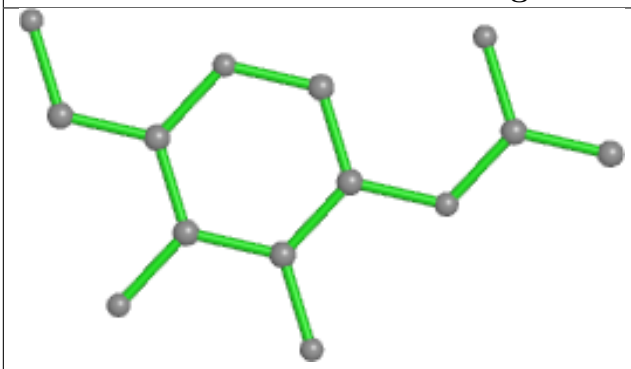


Rings

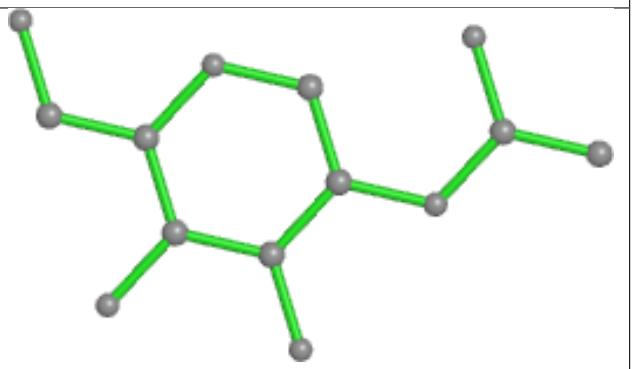
Ligand NAG C 1306	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NAG B 1304	
	
Bond lengths	Bond angles
	
Torsions	Rings

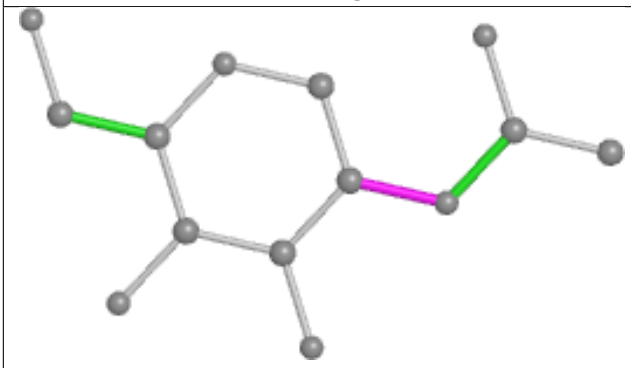
Ligand NAG A 1302



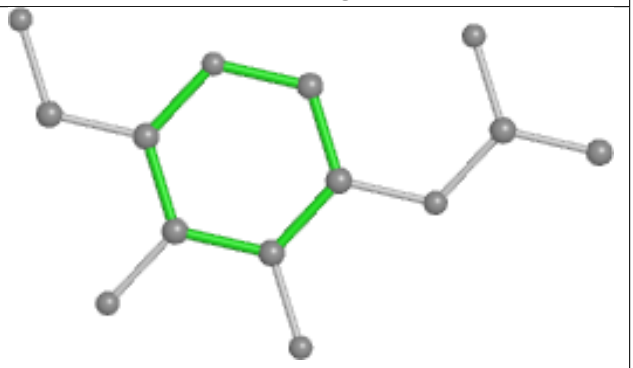
Bond lengths



Bond angles

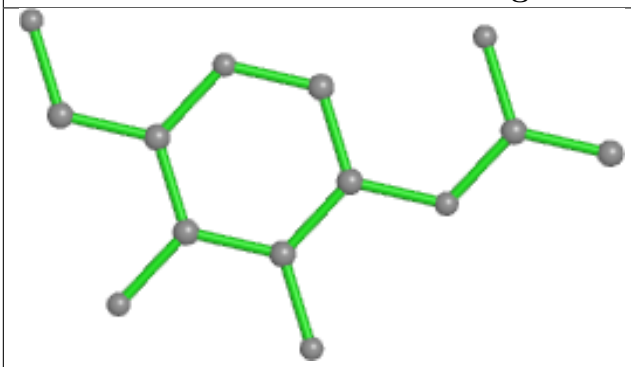


Torsions

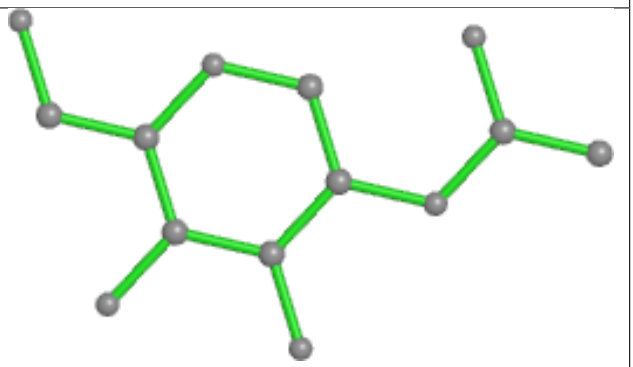


Rings

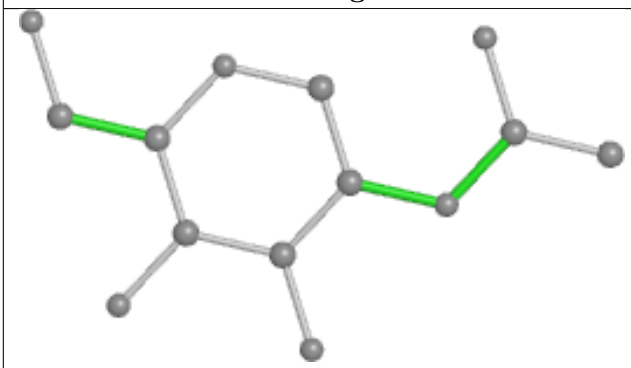
Ligand NAG C 1304



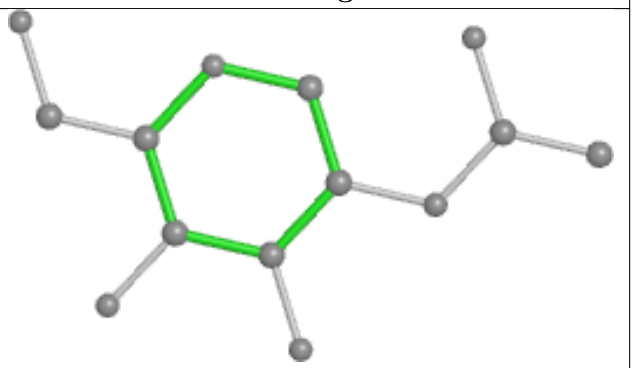
Bond lengths



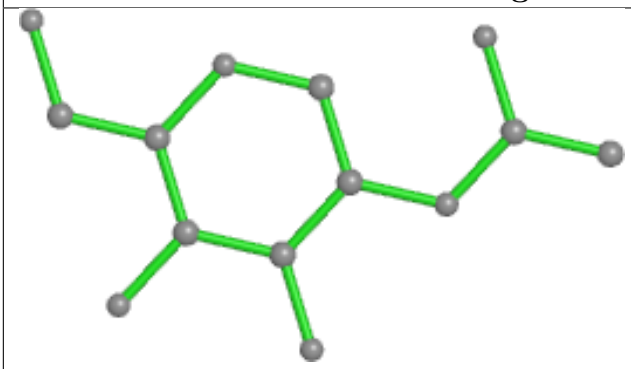
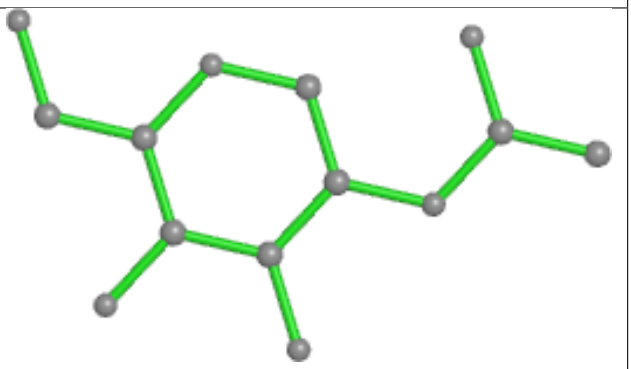
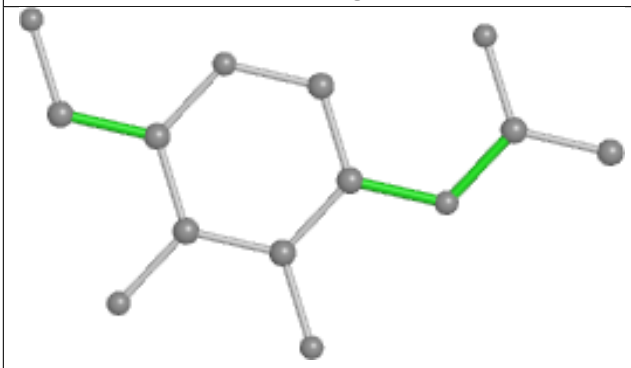
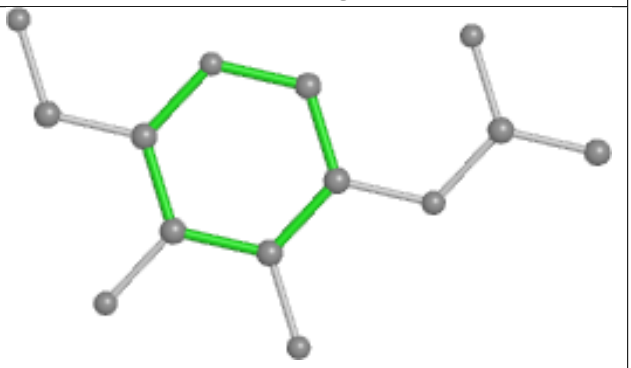
Bond angles

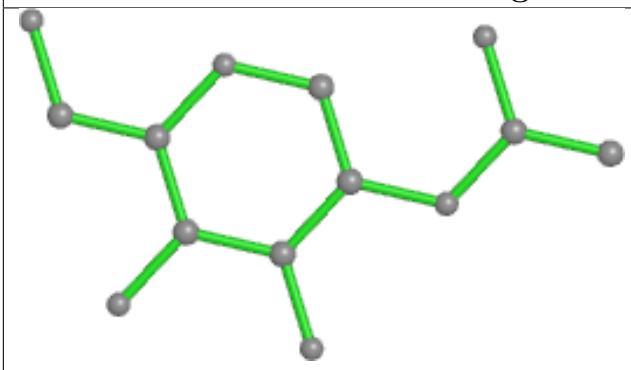
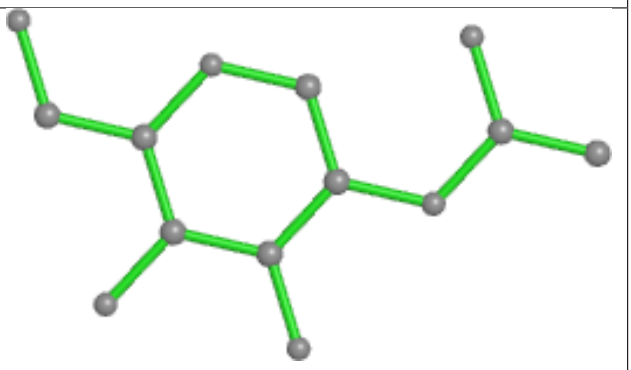
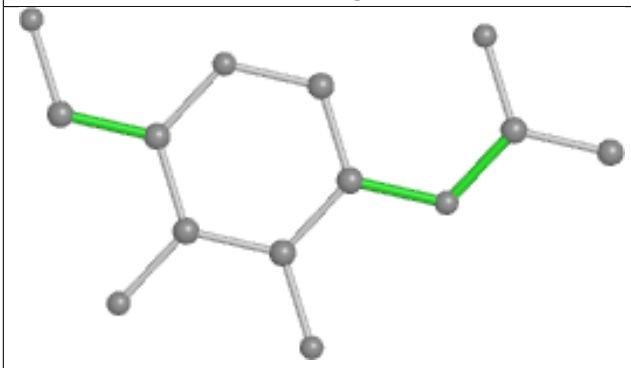
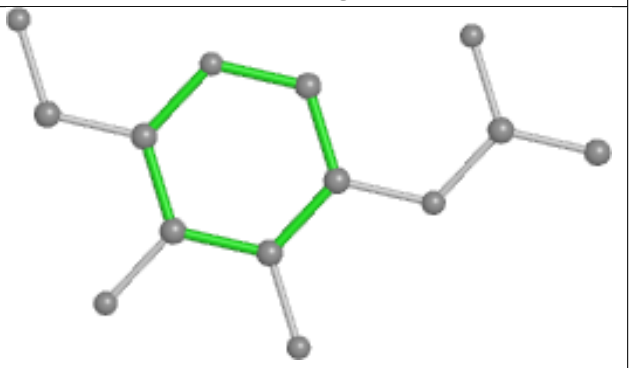


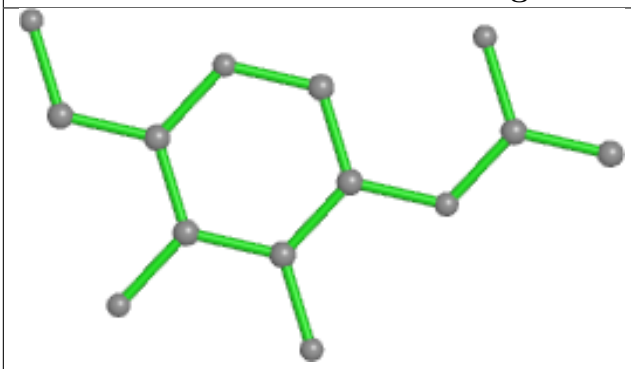
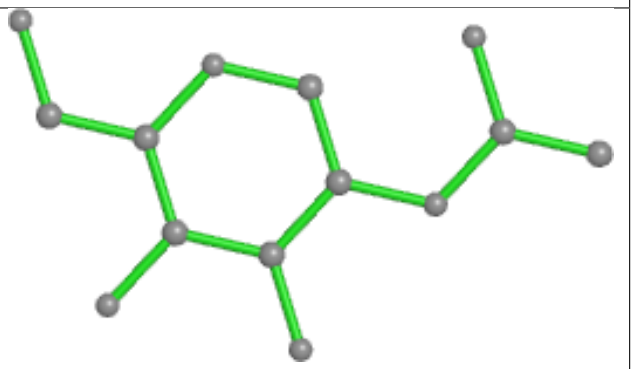
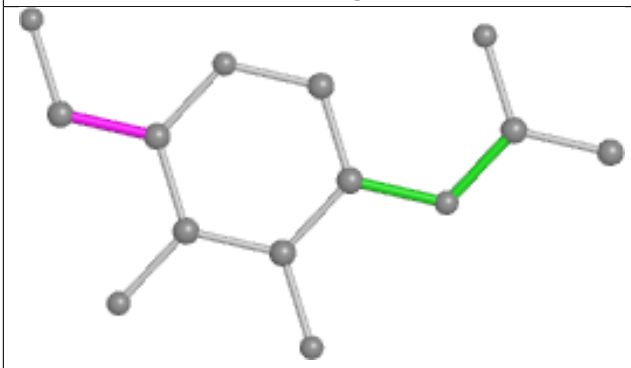
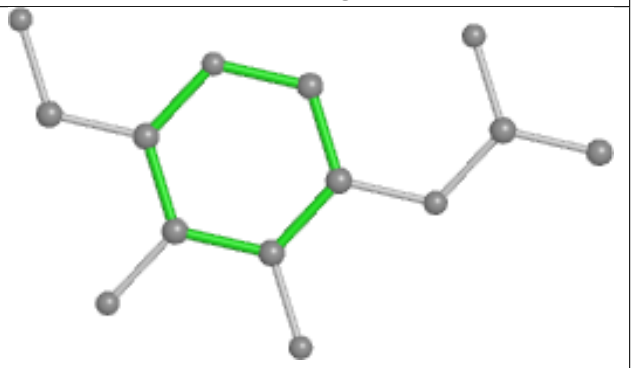
Torsions

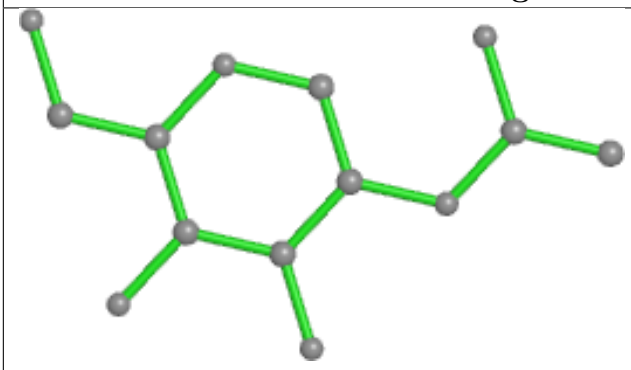
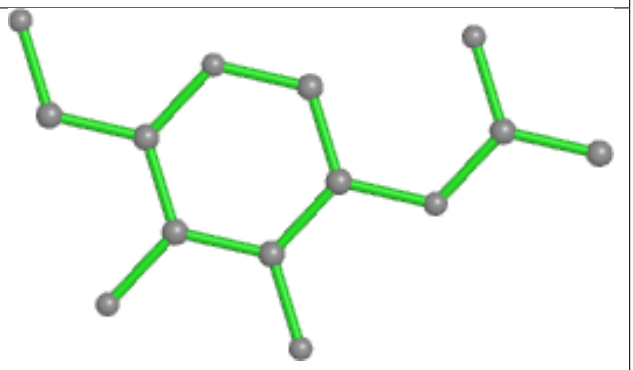
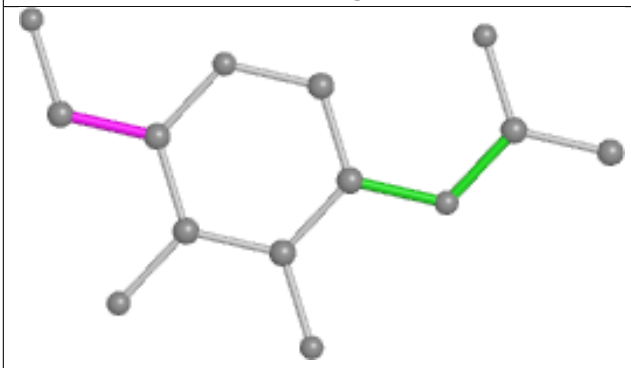
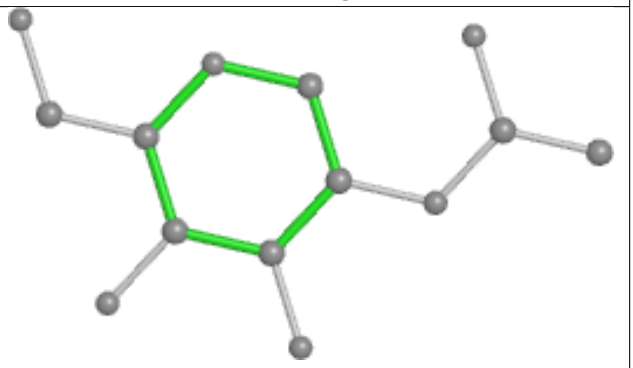


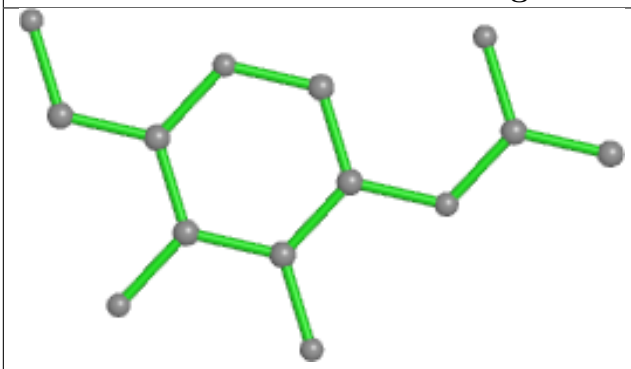
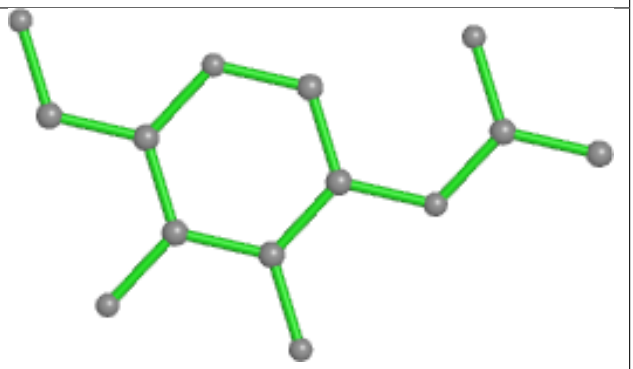
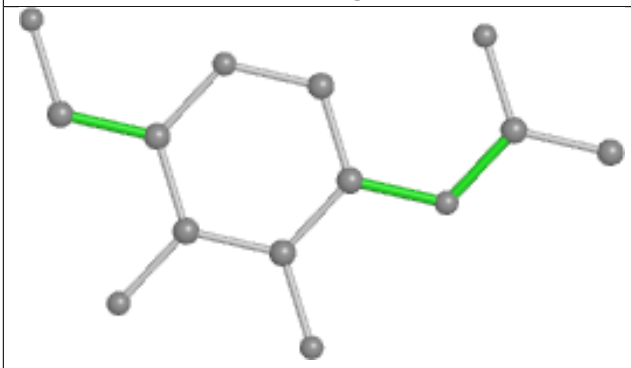
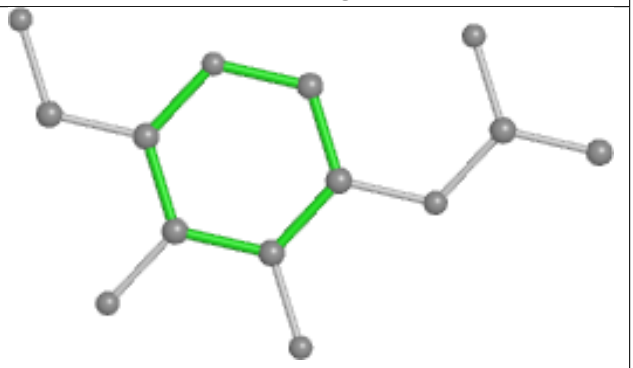
Rings

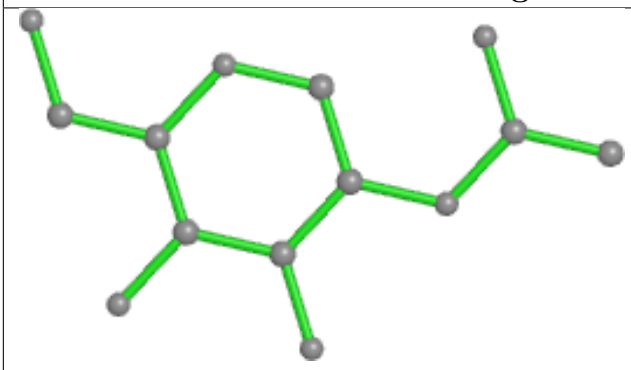
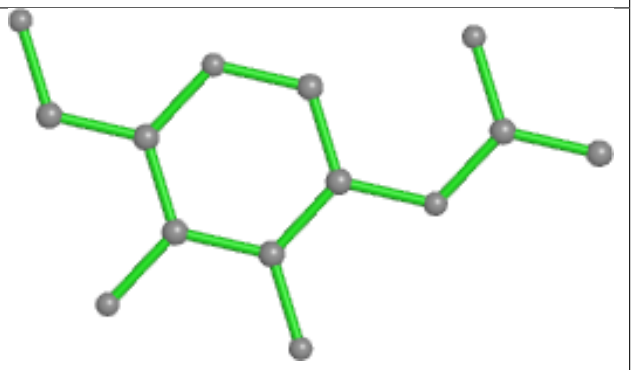
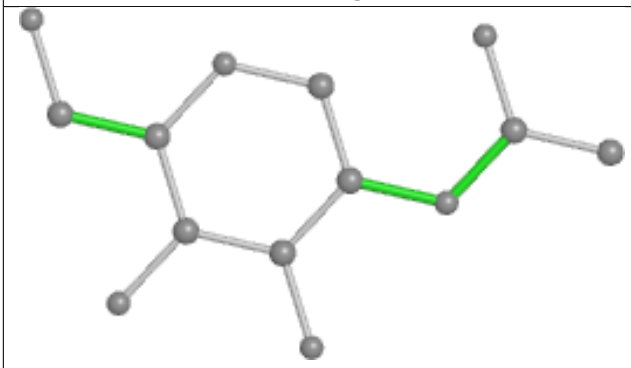
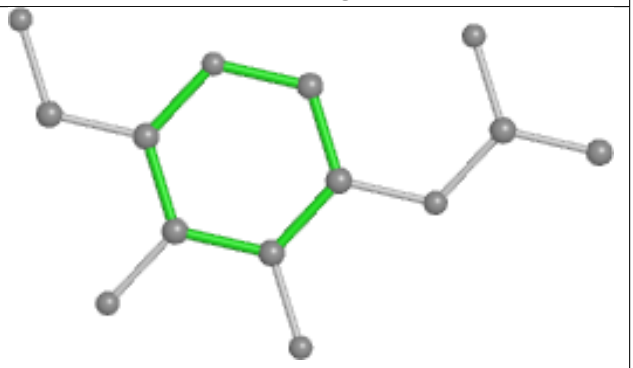
Ligand NAG C 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

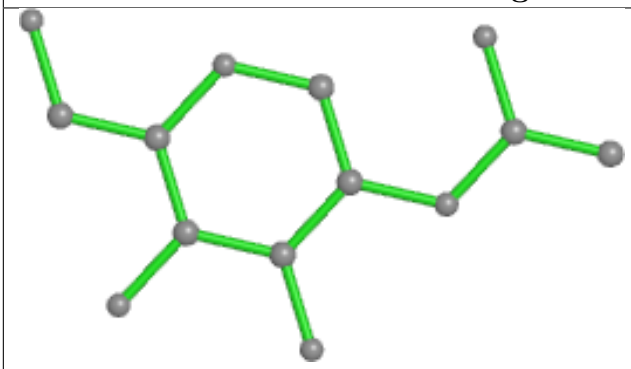
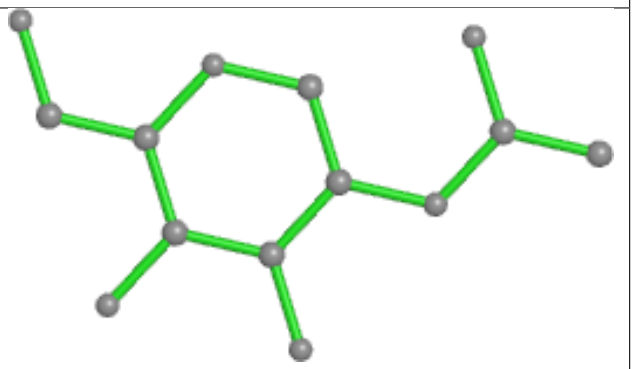
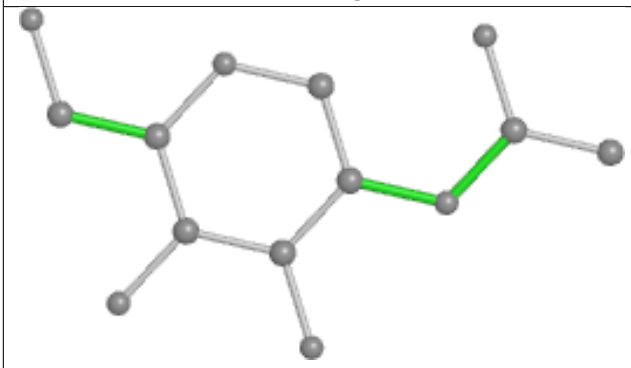
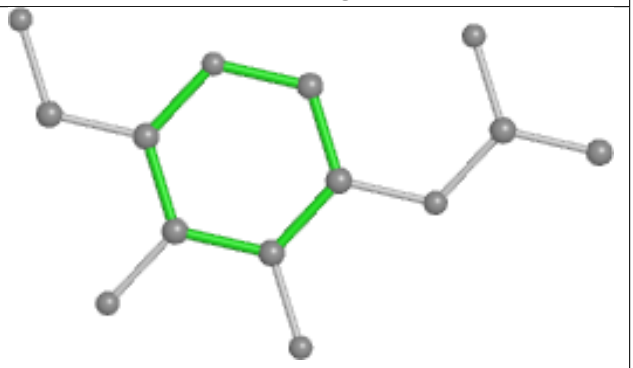
Ligand NAG C 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

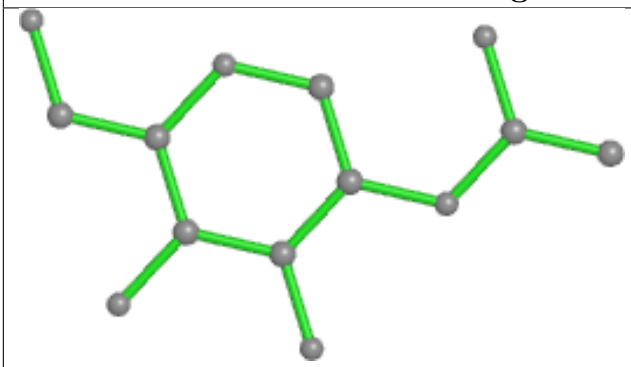
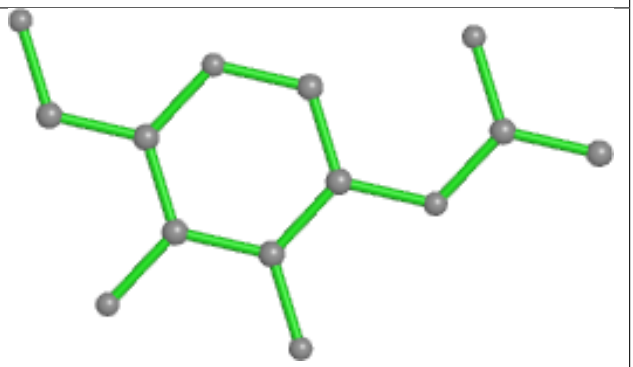
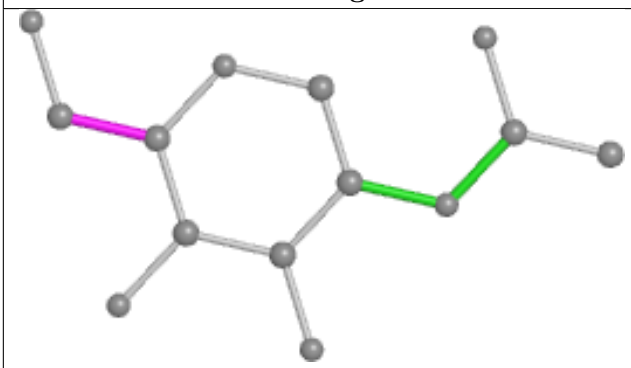
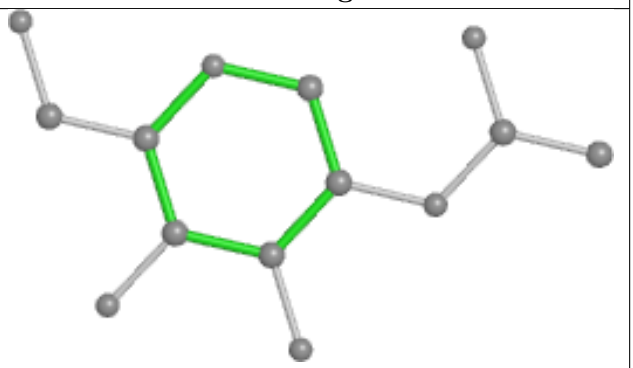
Ligand NAG A 1308	
	
Bond lengths	Bond angles
	
Torsions	Rings

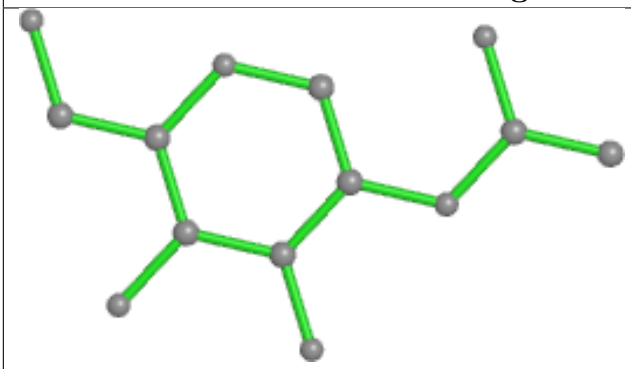
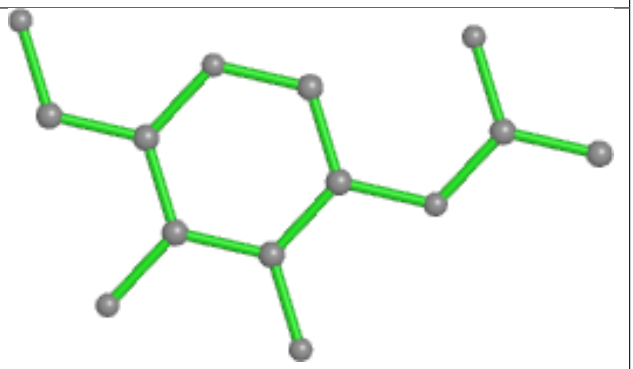
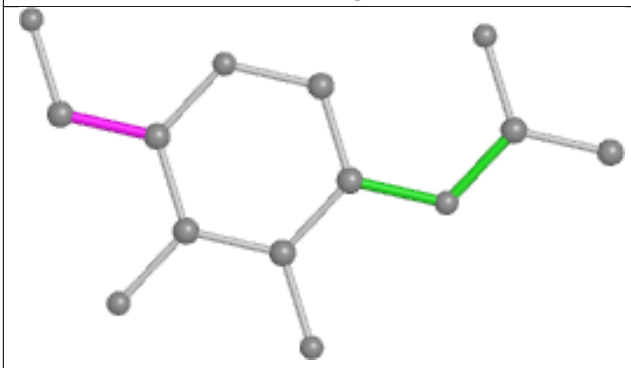
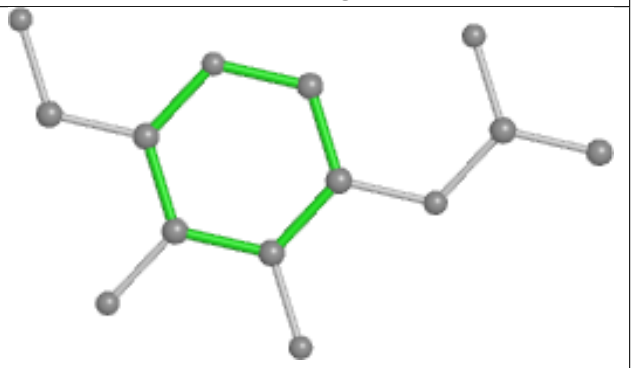
Ligand NAG B 1306	
	
Bond lengths	Bond angles
	
Torsions	Rings

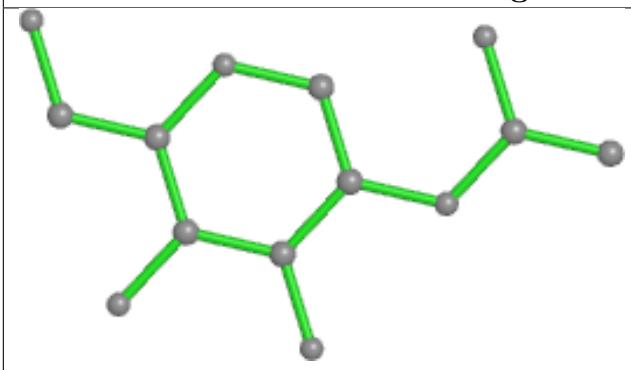
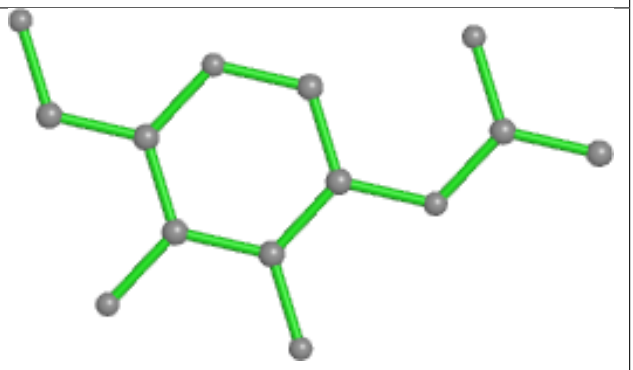
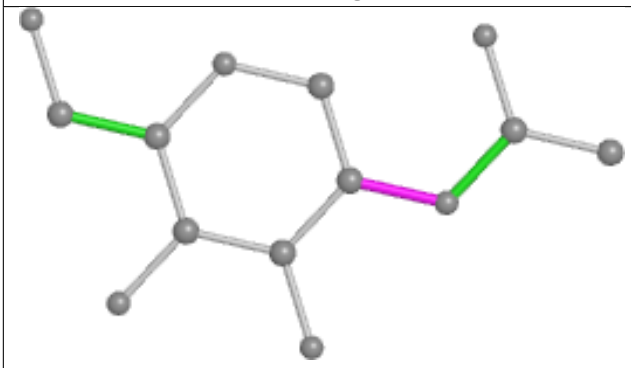
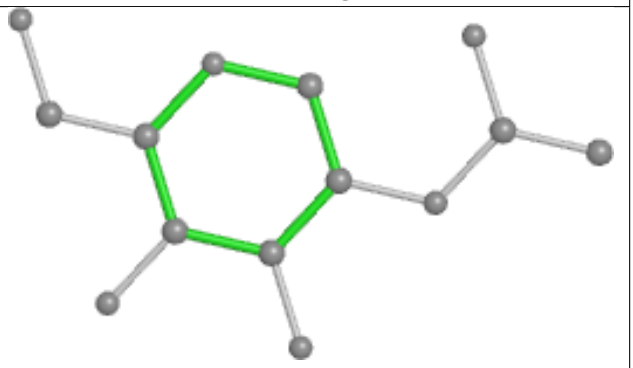
Ligand NAG A 1307	
	
Bond lengths	Bond angles
	
Torsions	Rings

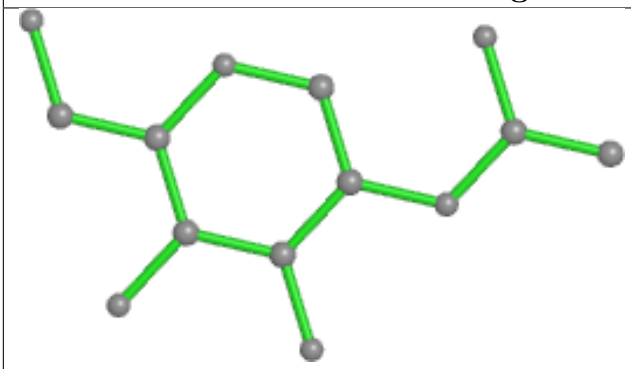
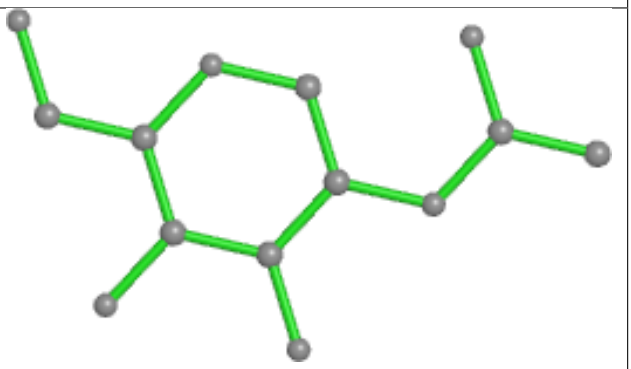
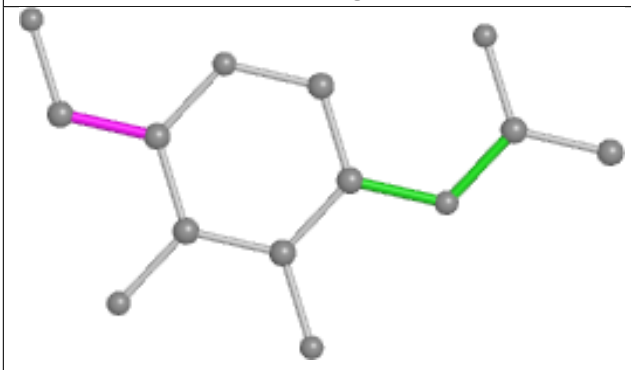
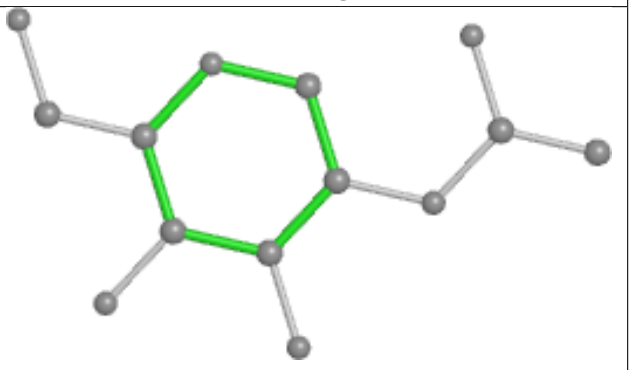
Ligand NAG C 1307	
	
Bond lengths	Bond angles
	
Torsions	Rings

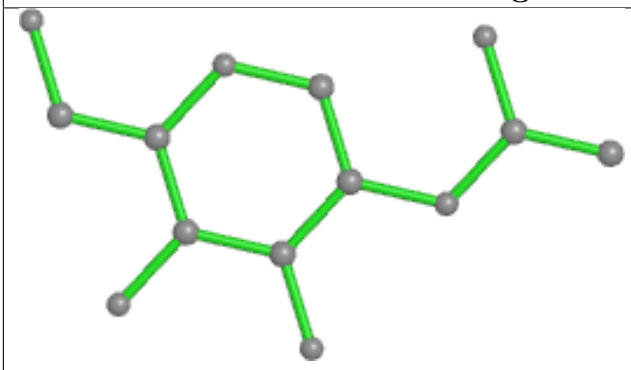
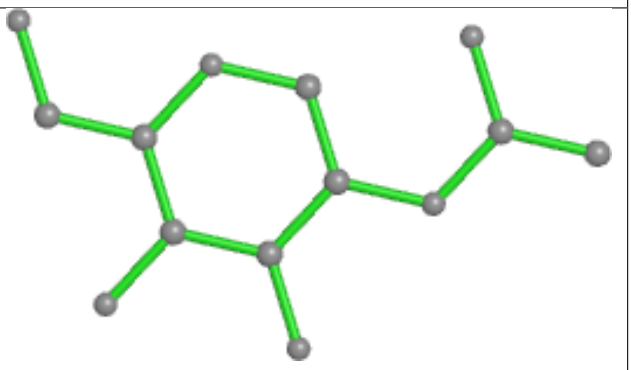
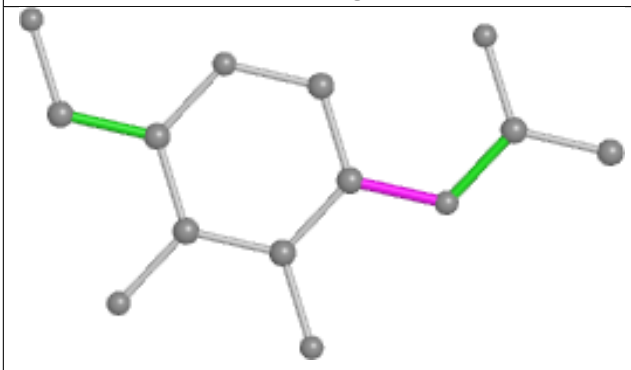
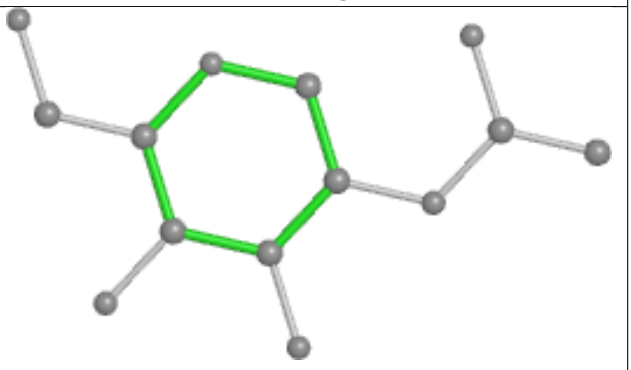
Ligand NAG C 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

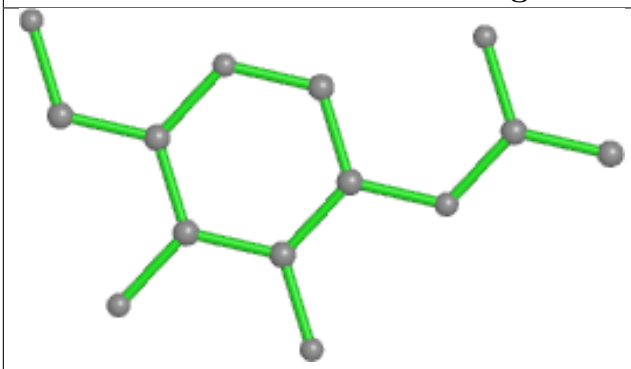
Ligand NAG A 1304	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1305	
 Bond lengths	 Bond angles
 Torsions	 Rings

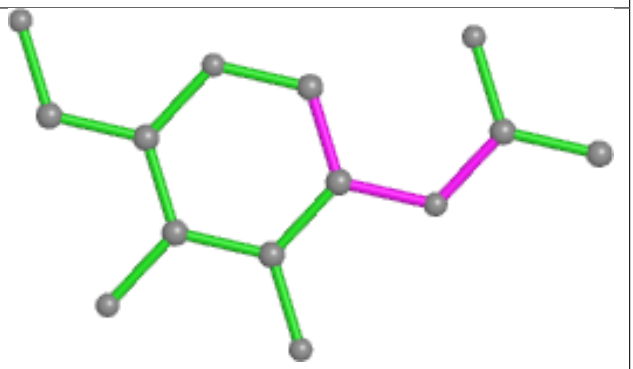
Ligand NAG A 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1302	
 Bond lengths	 Bond angles
 Torsions	 Rings

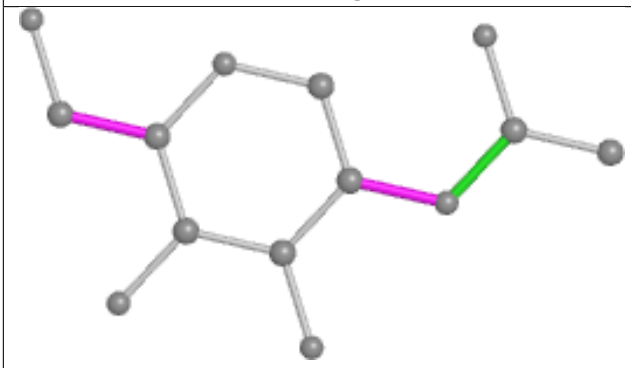
Ligand NAG A 1306



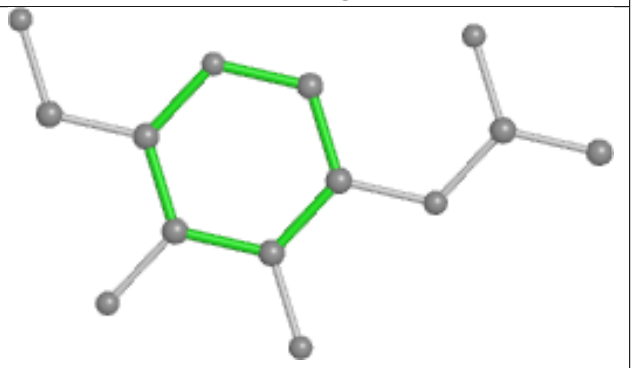
Bond lengths



Bond angles

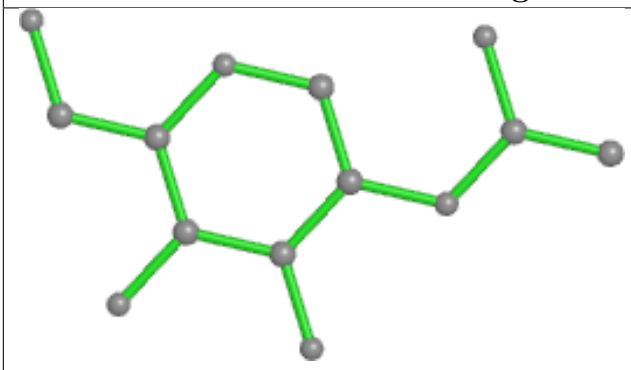


Torsions

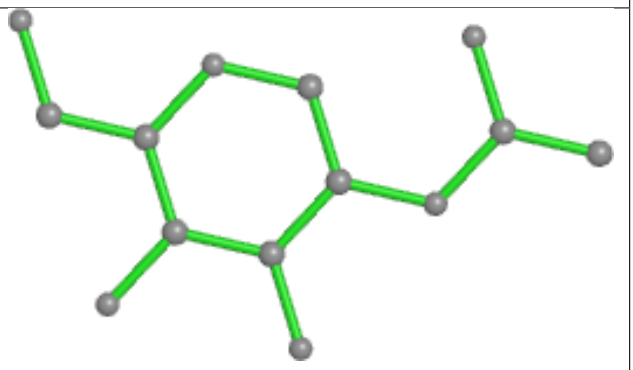


Rings

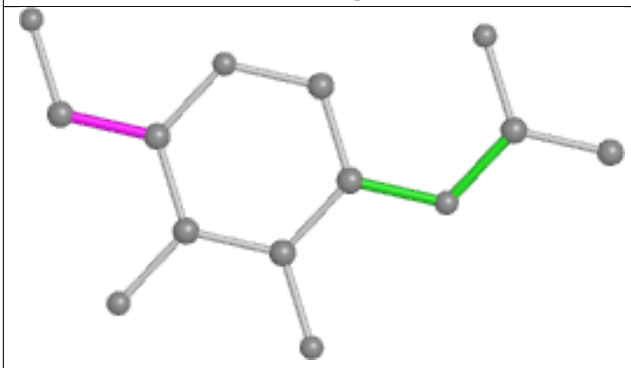
Ligand NAG B 1305



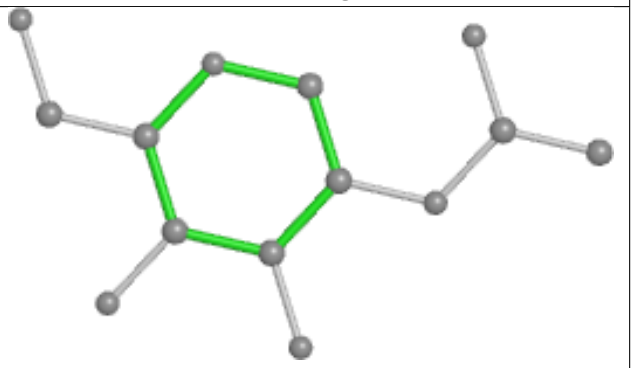
Bond lengths



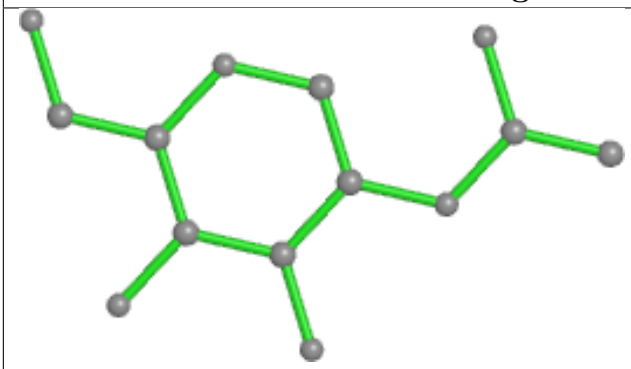
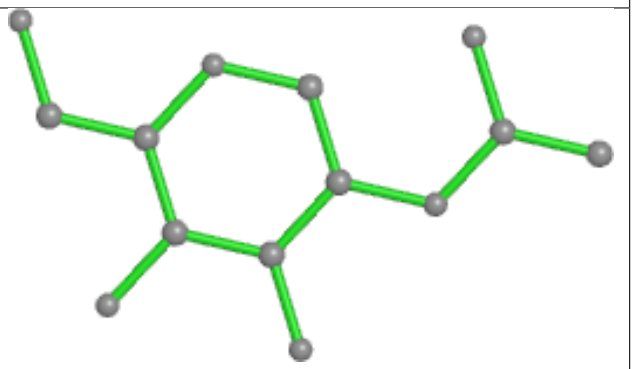
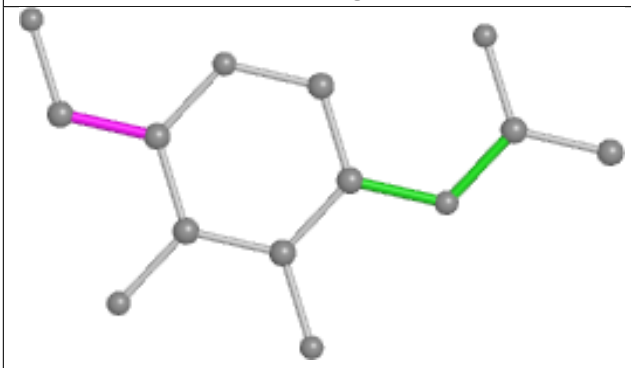
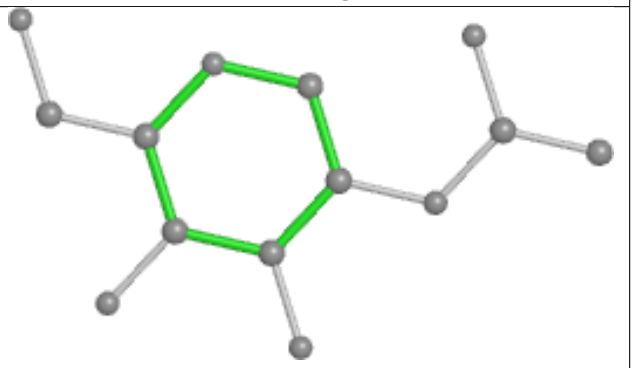
Bond angles

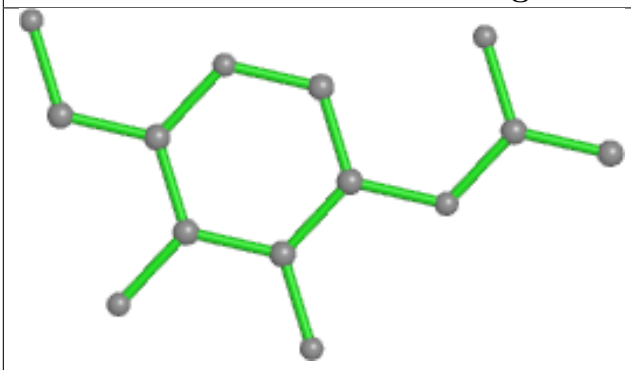
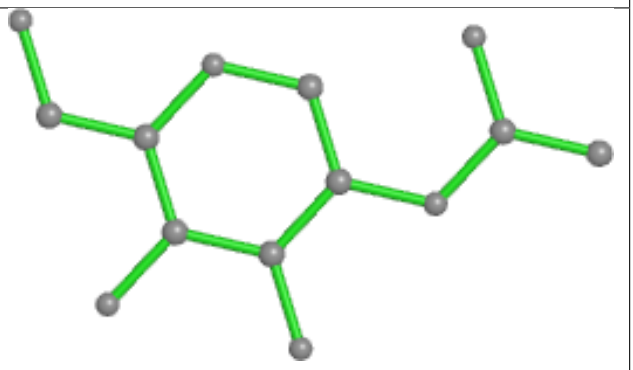
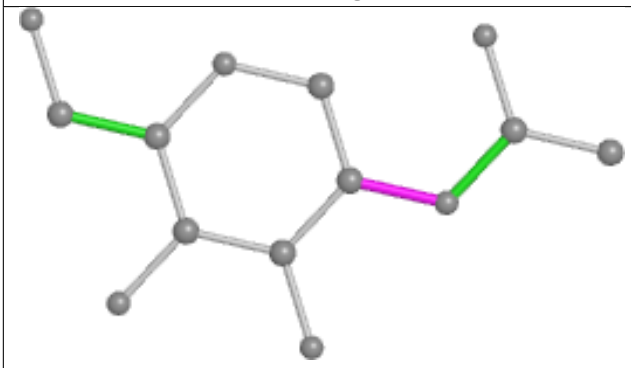
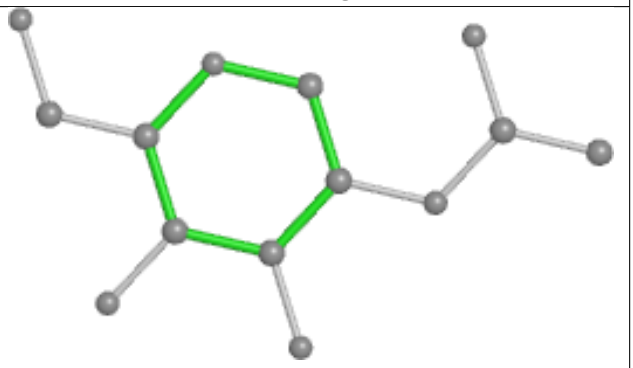


Torsions



Rings

Ligand NAG B 1303	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 1307	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

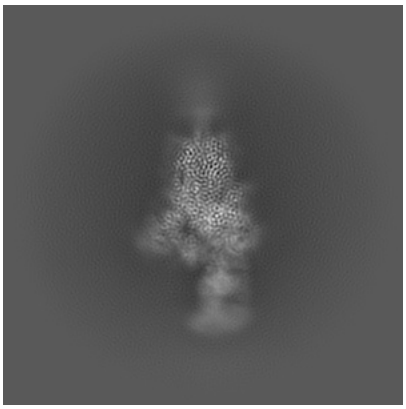
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26263. These allow visual inspection of the internal detail of the map and identification of artifacts.

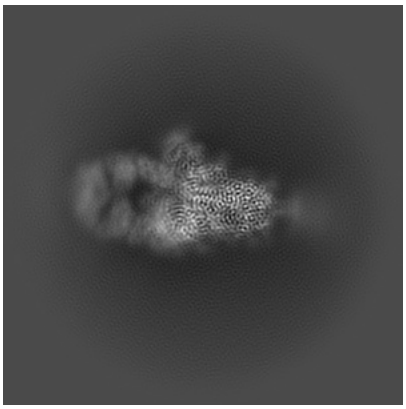
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

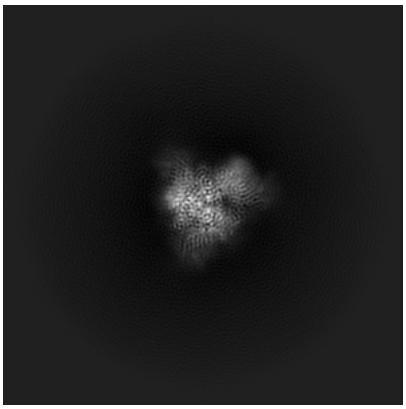
6.1.1 Primary map



X

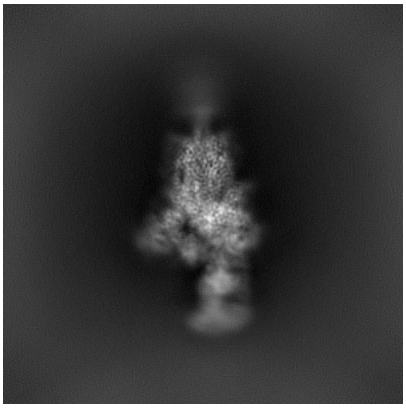


Y

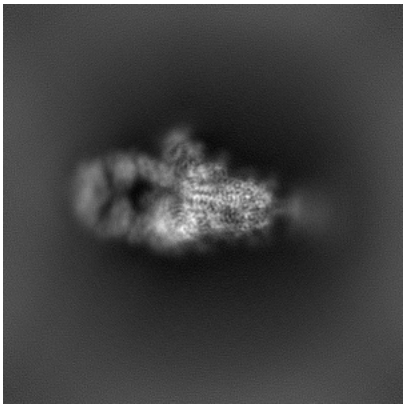


Z

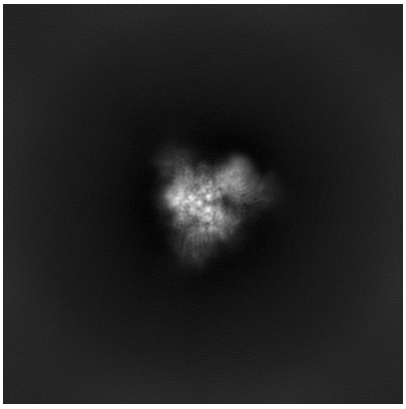
6.1.2 Raw map



X



Y

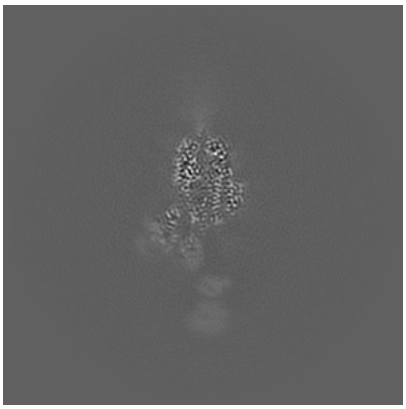


Z

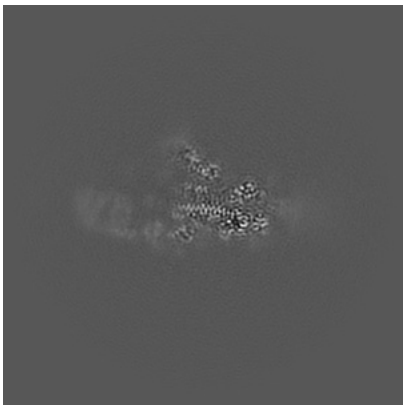
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

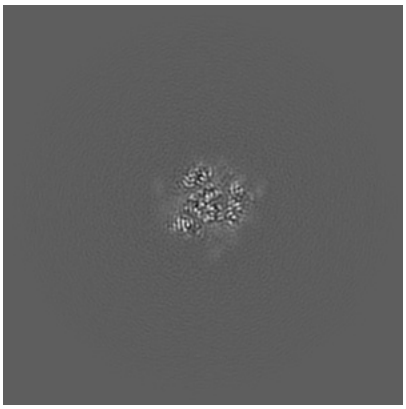
6.2.1 Primary map



X Index: 208

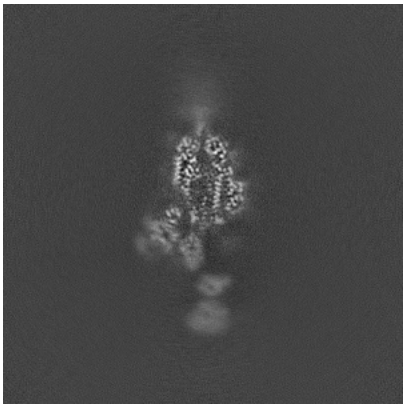


Y Index: 208

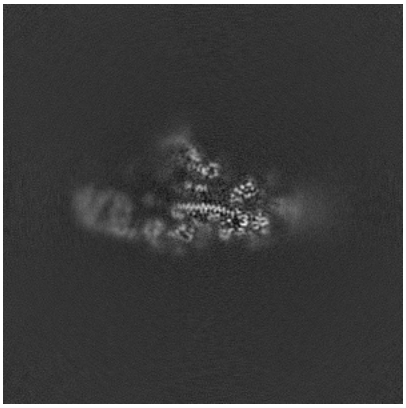


Z Index: 208

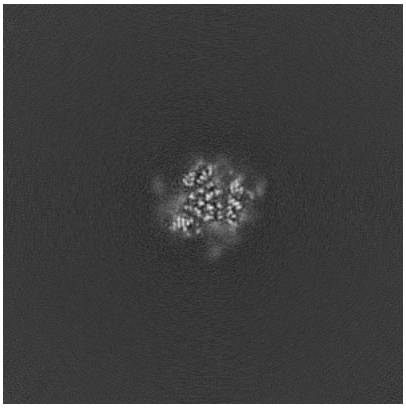
6.2.2 Raw map



X Index: 208



Y Index: 208



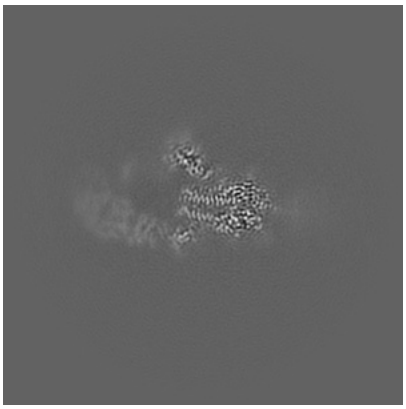
Z Index: 208

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

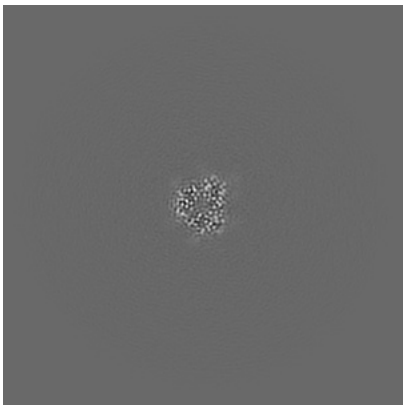
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 215

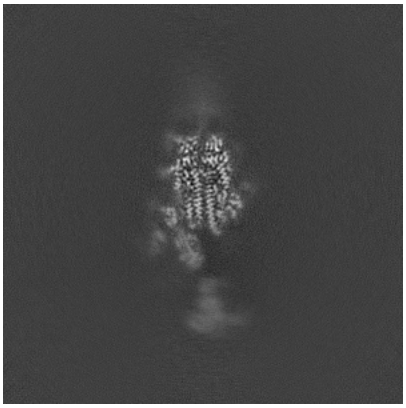


Y Index: 215

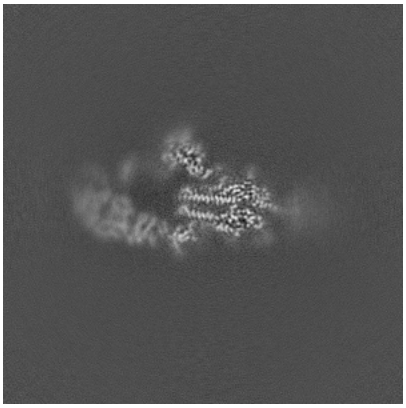


Z Index: 249

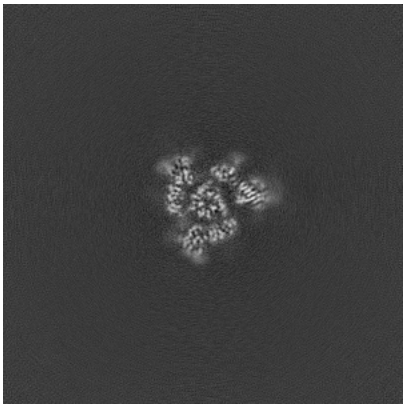
6.3.2 Raw map



X Index: 215



Y Index: 215

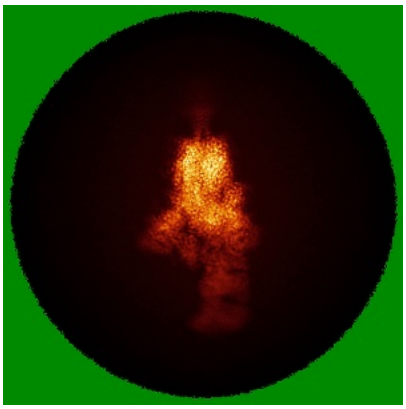


Z Index: 192

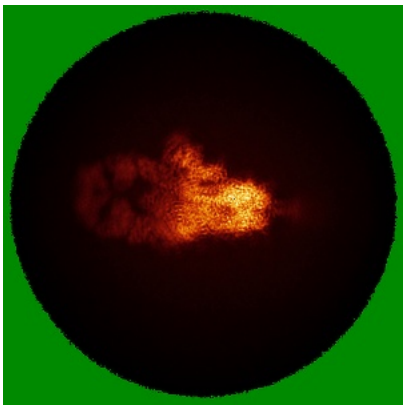
The images above show the largest variance slices of the map in three orthogonal directions.

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

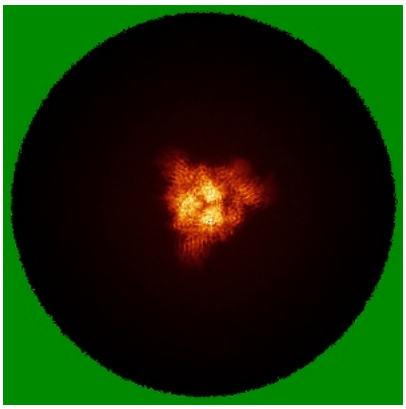
6.4.1 Primary map



X

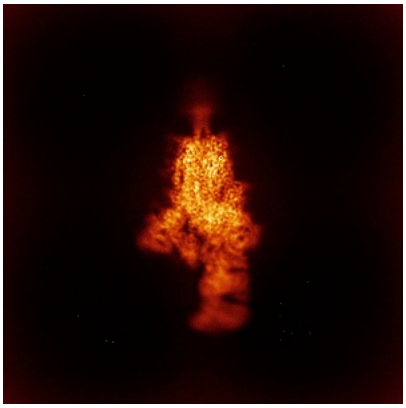


Y

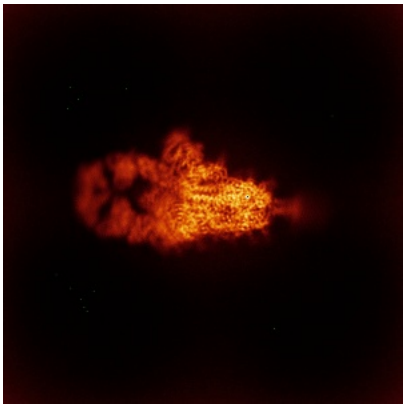


Z

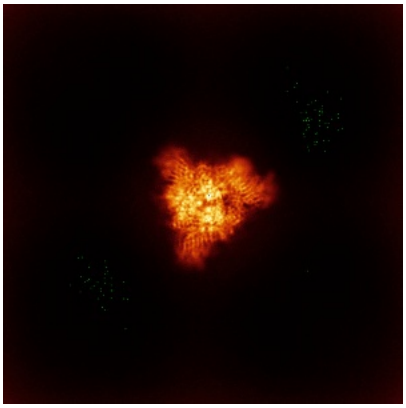
6.4.2 Raw map



X



Y

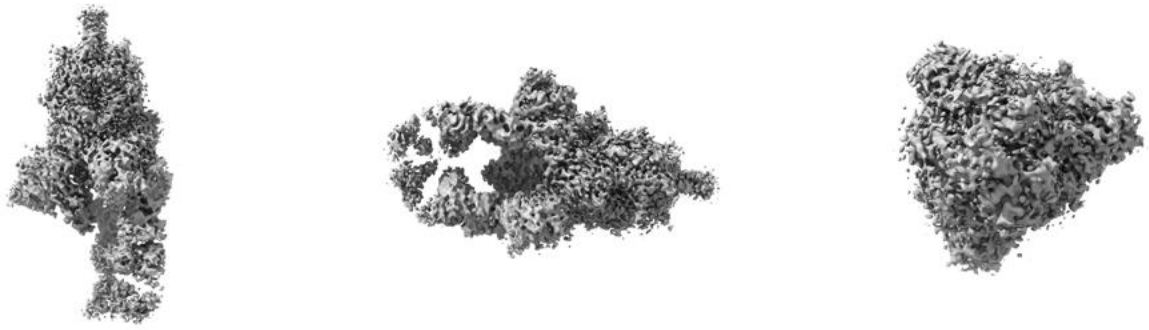


Z

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

6.5 Orthogonal surface views (i)

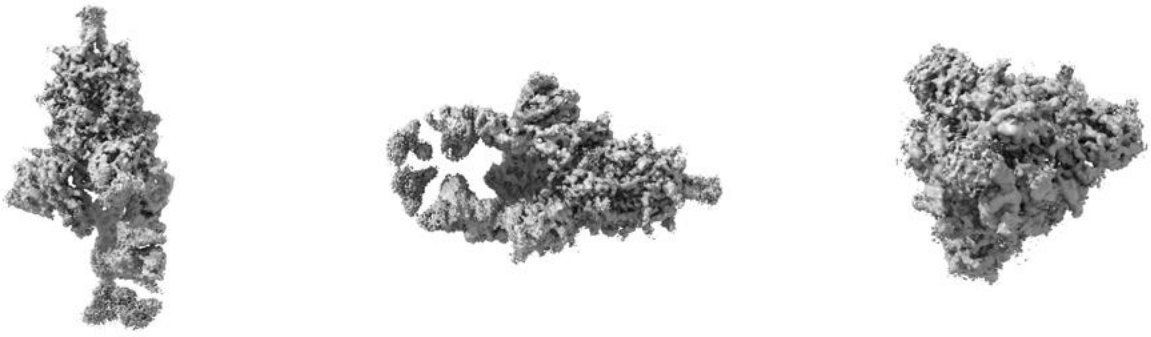
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.29. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

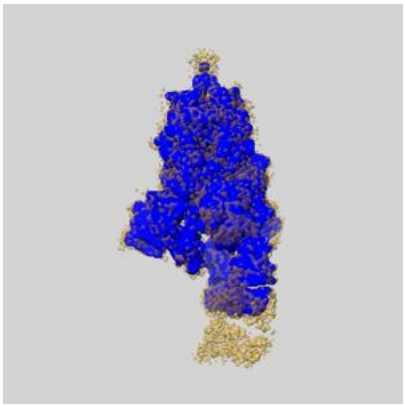
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

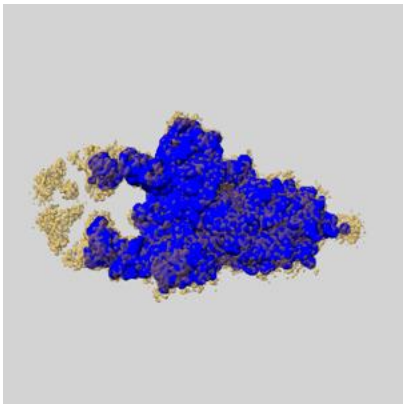
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

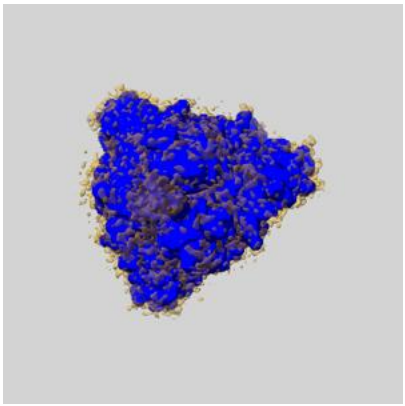
6.6.1 emd_26263_msk_1.map (i)



X



Y

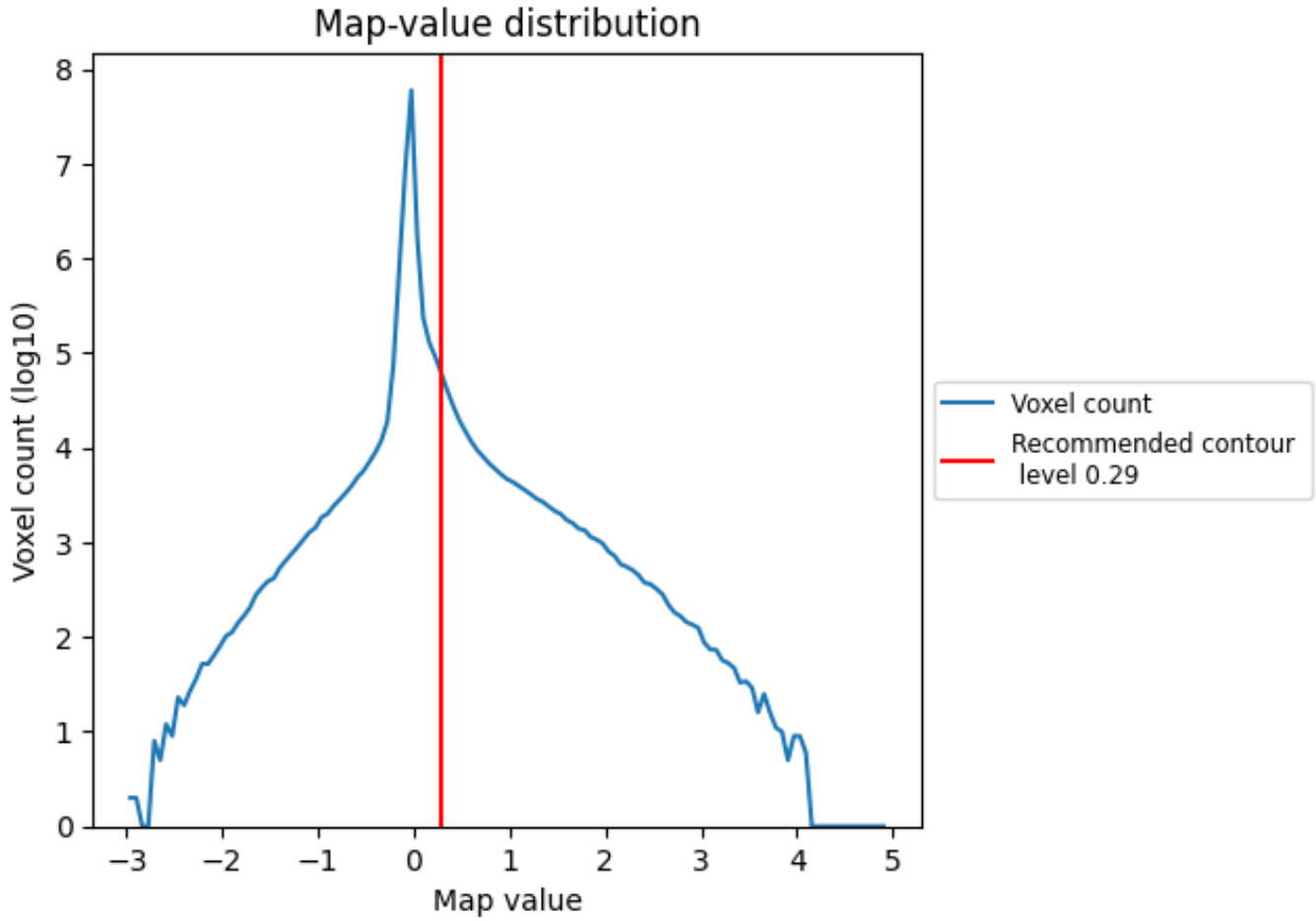


Z

7 Map analysis

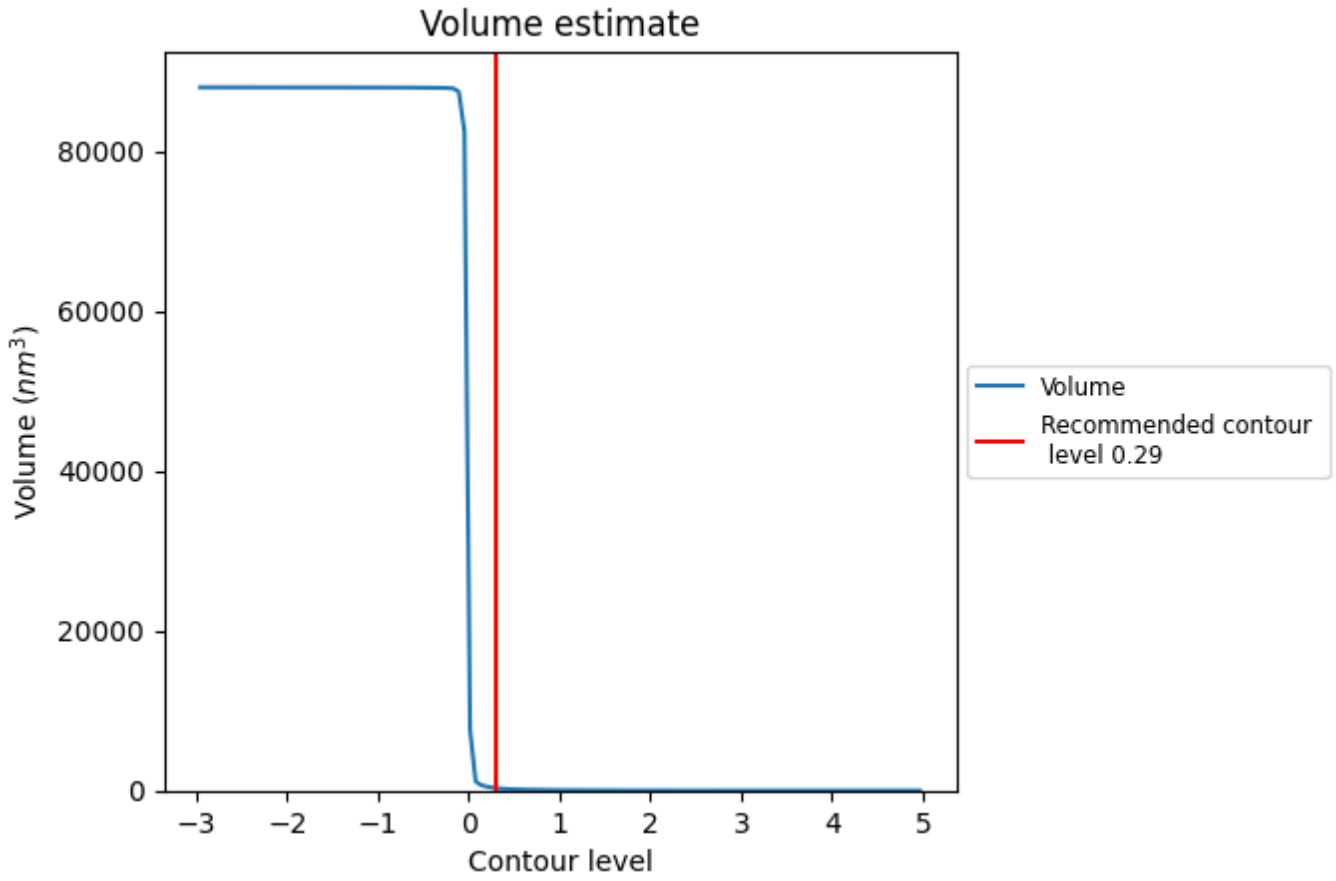
This section contains the results of statistical analysis of the map.

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.

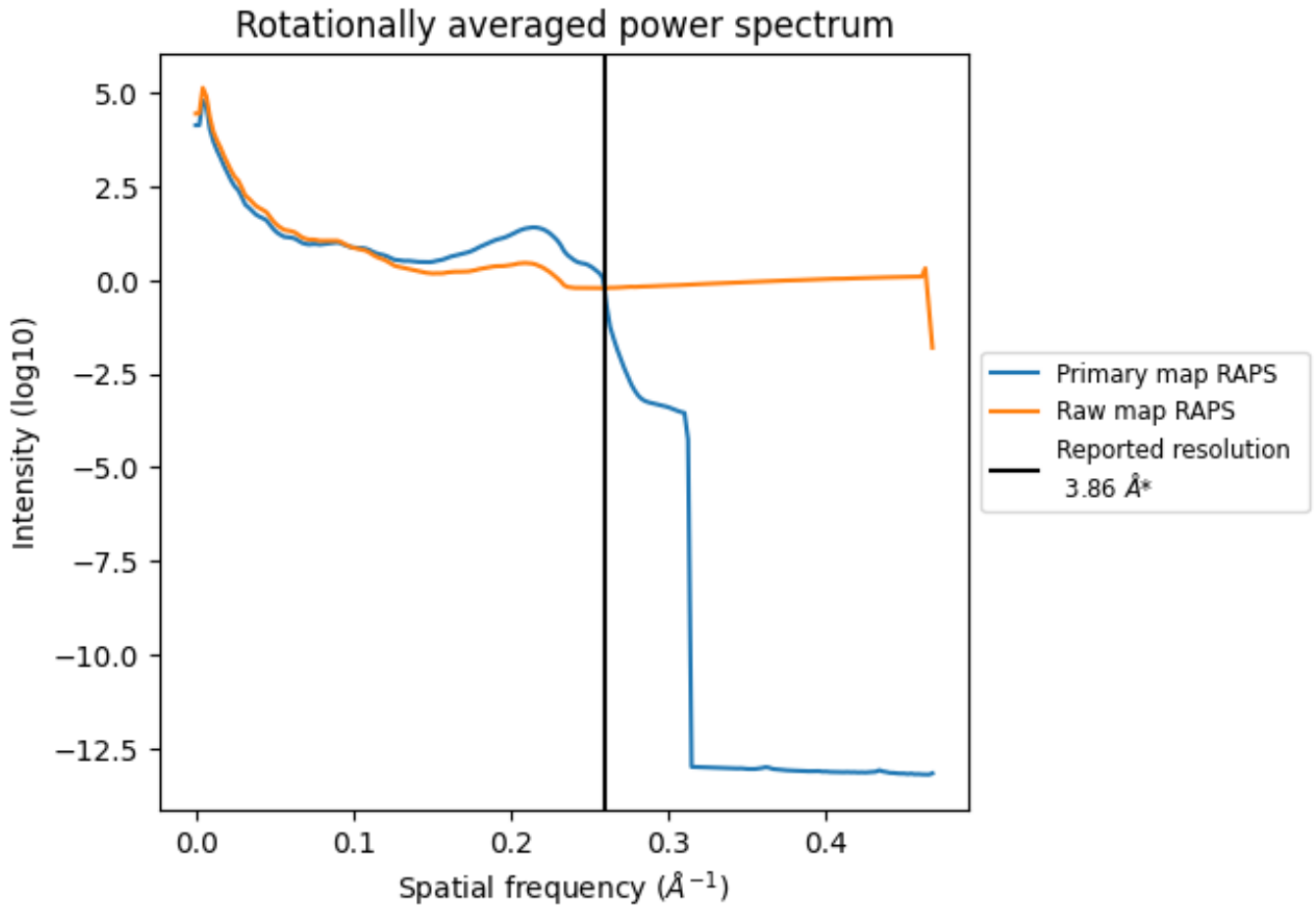
7.2 Volume estimate



The volume at the recommended contour level is 316 nm^3; this corresponds to an approximate mass of 285 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)

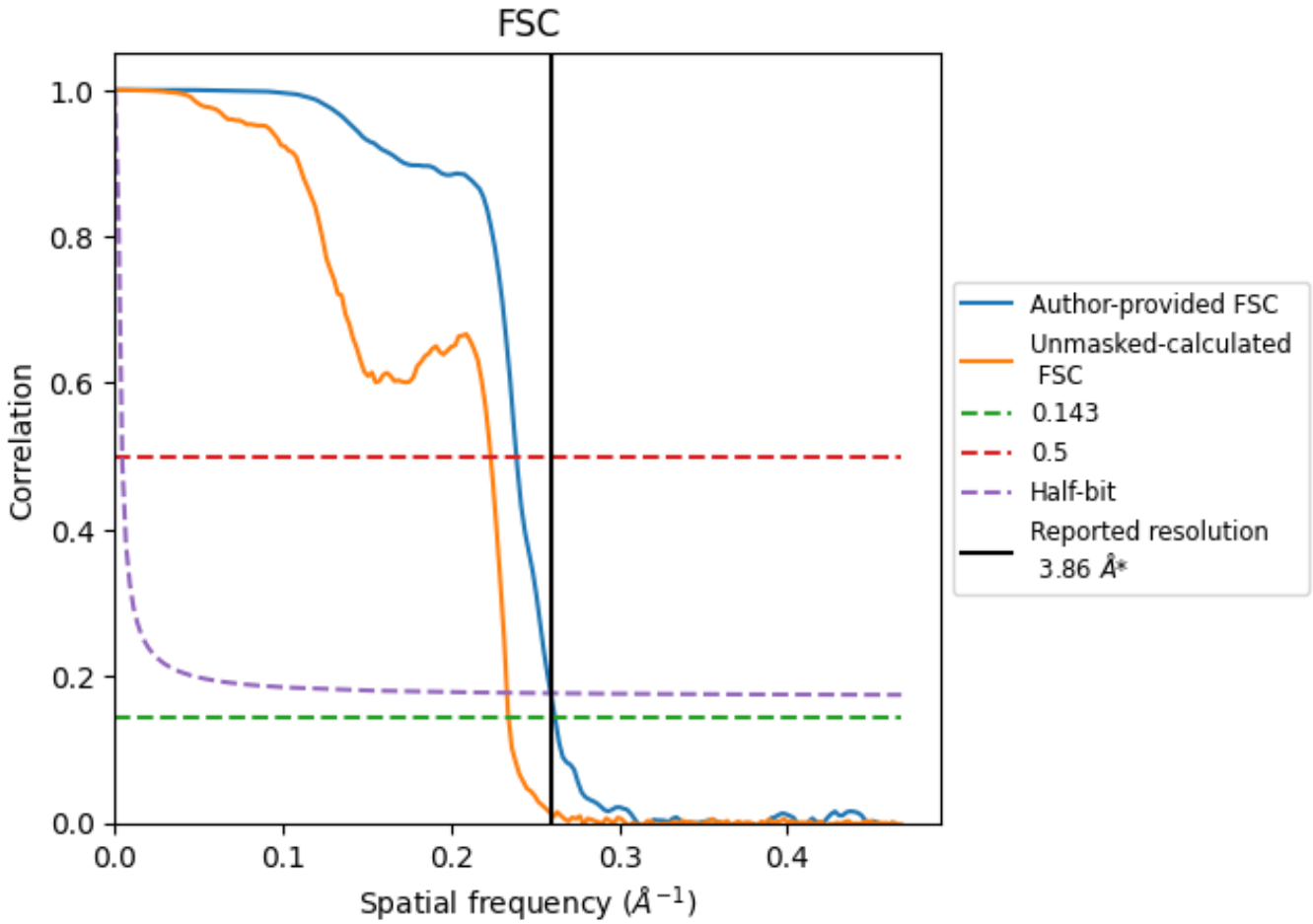


*Reported resolution corresponds to spatial frequency of 0.259 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.259 Å^{-1}

8.2 Resolution estimates (i)

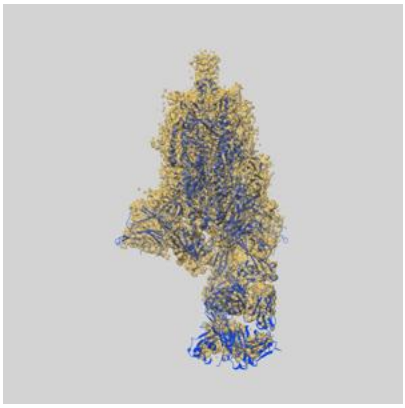
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.86	-	-
Author-provided FSC curve	3.82	4.19	3.86
Unmasked-calculated*	4.27	4.47	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.86 by more than 10 %

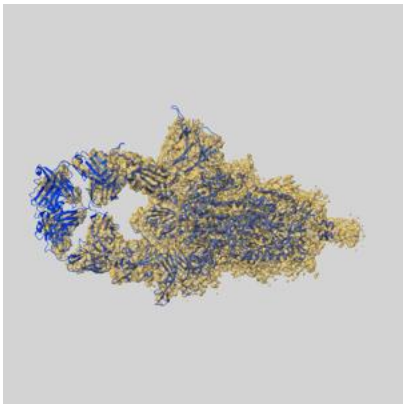
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26263 and PDB model 7U0Q. Per-residue inclusion information can be found in section 3 on page 9.

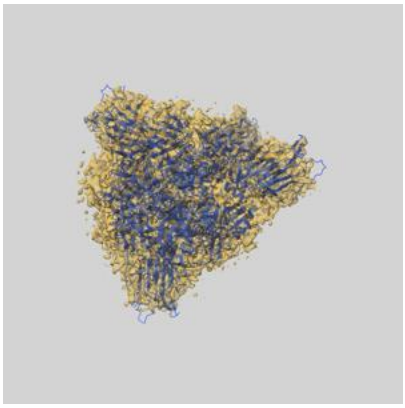
9.1 Map-model overlay



X



Y



Z

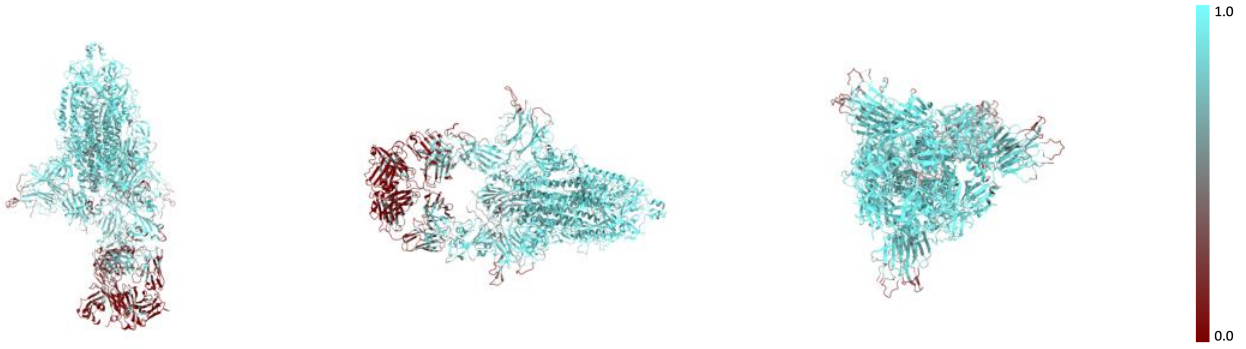
The images above show the 3D surface view of the map at the recommended contour level 0.29 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

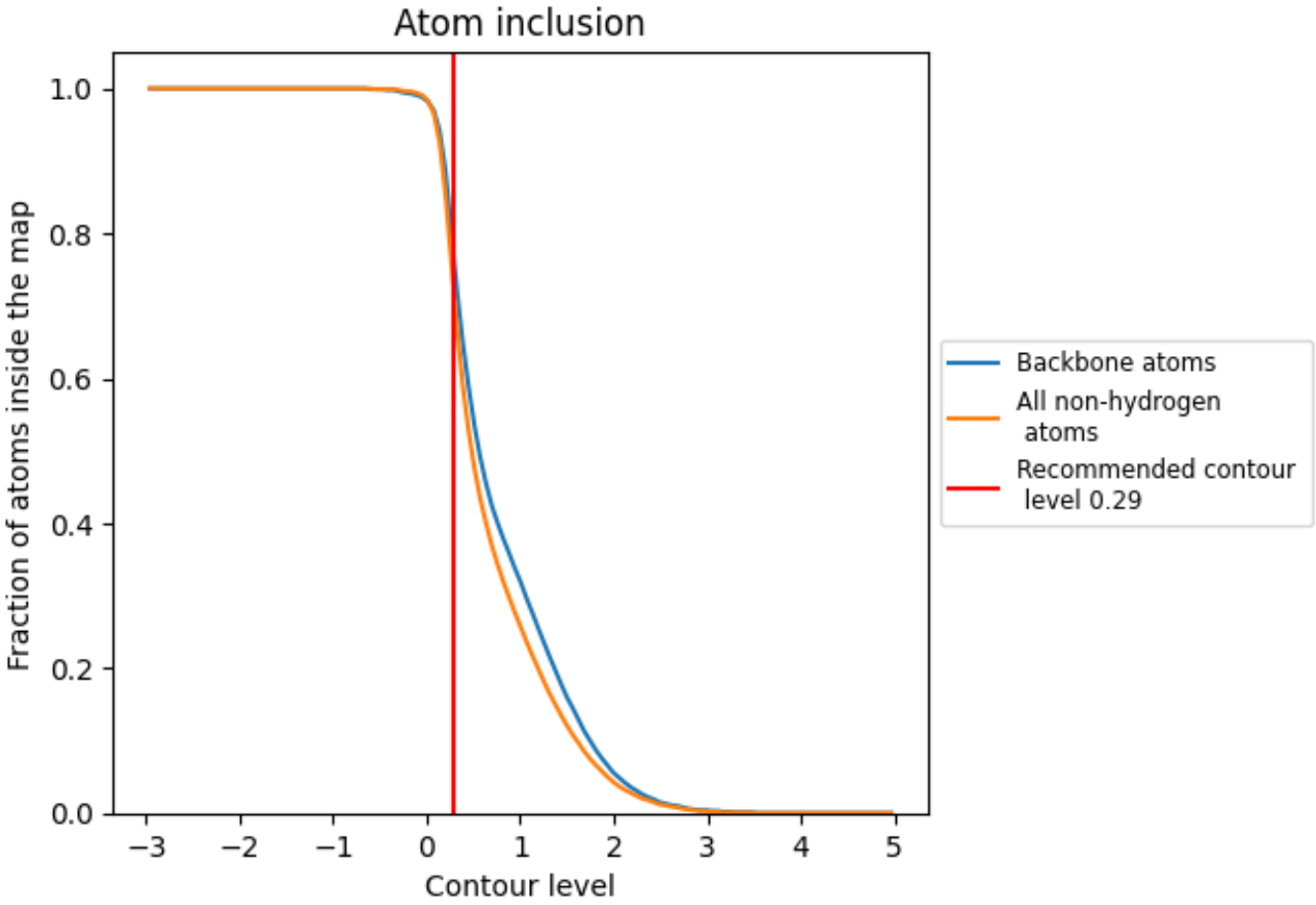
9.3 Atom inclusion mapped to coordinate model



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 (0.29).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 72% 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 (0.29) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7170	0.3240
A	0.8130	0.3800
B	0.8280	0.3860
C	0.8320	0.3830
D	0.8210	0.3020
E	0.8210	0.3660
F	0.2240	0.0840
G	0.3460	0.0960
H	0.8570	0.4250
I	0.3010	0.0800
J	0.3180	0.1090
K	0.9640	0.4720
L	0.7500	0.3600
M	0.4290	0.2190
N	0.7500	0.3530
O	0.7860	0.2810
P	0.8930	0.4480
Q	0.8210	0.3660
R	0.8210	0.4220
S	0.8570	0.3890
T	0.7500	0.2770
U	0.6070	0.3100
V	0.7690	0.3170