Full wwPDB EM Validation Report (i)

Nov 16, 2022 – 02:12 PM JST

PDB ID	:	6M17
EMDB ID	:	EMD-30039
Title	:	The 2019-nCoV RBD/ACE2-B0AT1 complex
Authors	:	Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Xia, L.; Guo, Y.Y.; Zhou, Q.
Deposited on	:	2020-02-24
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

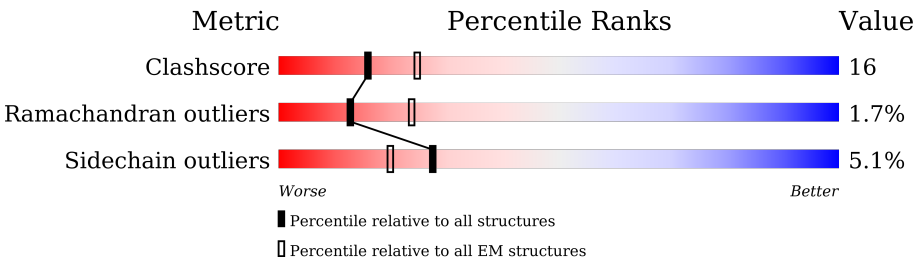
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.90 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	654	49%; 72%, 18%, •, 7%
1	C	654	49%; 71%, 19%, •, 7%
2	B	814	16%; 77%, 12%, •, 8%
2	D	814	16%; 77%, 12%, •, 8%
3	E	223	79%; 43%, 29%, 9%, 18%
3	F	223	79%; 43%, 29%, 9%, •, 18%
4	G	2	100%; 100%
4	H	2	100%; 50%, 50%

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Mol	Chain	Length	Quality of chain
4	I	2	100% 50% 50%
4	J	2	100% 100%
4	K	2	100% 100%
4	L	2	100% 50% 50%
4	M	2	100%
4	O	2	100% 100%
4	P	2	100% 50% 50%
4	Q	2	100% 50% 50%
4	R	2	100% 100%
4	S	2	100% 100%
4	T	2	100% 50% 50%
4	U	2	100%
5	N	3	100% 100%
5	V	3	100% 100%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25344 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 Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	605	4799	3171	744	854	30	0	0
1	C	605	4799	3171	744	854	30	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q695T7
A	-18	ALA	-	expression tag	UNP Q695T7
A	-17	ASP	-	expression tag	UNP Q695T7
A	-16	TYR	-	expression tag	UNP Q695T7
A	-15	LYS	-	expression tag	UNP Q695T7
A	-14	ASP	-	expression tag	UNP Q695T7
A	-13	ASP	-	expression tag	UNP Q695T7
A	-12	ASP	-	expression tag	UNP Q695T7
A	-11	ASP	-	expression tag	UNP Q695T7
A	-10	LYS	-	expression tag	UNP Q695T7
A	-9	SER	-	expression tag	UNP Q695T7
A	-8	GLY	-	expression tag	UNP Q695T7
A	-7	PRO	-	expression tag	UNP Q695T7
A	-6	ASP	-	expression tag	UNP Q695T7
A	-5	GLU	-	expression tag	UNP Q695T7
A	-4	VAL	-	expression tag	UNP Q695T7
A	-3	ASP	-	expression tag	UNP Q695T7
A	-2	ALA	-	expression tag	UNP Q695T7
A	-1	SER	-	expression tag	UNP Q695T7
A	0	GLY	-	expression tag	UNP Q695T7
A	1	ARG	-	expression tag	UNP Q695T7
C	-19	MET	-	initiating methionine	UNP Q695T7
C	-18	ALA	-	expression tag	UNP Q695T7
C	-17	ASP	-	expression tag	UNP Q695T7
C	-16	TYR	-	expression tag	UNP Q695T7
C	-15	LYS	-	expression tag	UNP Q695T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q695T7
C	-13	ASP	-	expression tag	UNP Q695T7
C	-12	ASP	-	expression tag	UNP Q695T7
C	-11	ASP	-	expression tag	UNP Q695T7
C	-10	LYS	-	expression tag	UNP Q695T7
C	-9	SER	-	expression tag	UNP Q695T7
C	-8	GLY	-	expression tag	UNP Q695T7
C	-7	PRO	-	expression tag	UNP Q695T7
C	-6	ASP	-	expression tag	UNP Q695T7
C	-5	GLU	-	expression tag	UNP Q695T7
C	-4	VAL	-	expression tag	UNP Q695T7
C	-3	ASP	-	expression tag	UNP Q695T7
C	-2	ALA	-	expression tag	UNP Q695T7
C	-1	SER	-	expression tag	UNP Q695T7
C	0	GLY	-	expression tag	UNP Q695T7
C	1	ARG	-	expression tag	UNP Q695T7

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	748	6089	3906	1018	1131	34	0	0
2	D	748	6089	3906	1018	1131	34	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	initiating methionine	UNP Q9BYF1
B	-7	ARG	-	expression tag	UNP Q9BYF1
B	10	TRP	-	insertion	UNP Q9BYF1
B	11	SER	-	insertion	UNP Q9BYF1
B	12	HIS	-	insertion	UNP Q9BYF1
B	13	PRO	-	insertion	UNP Q9BYF1
B	14	GLN	-	insertion	UNP Q9BYF1
B	15	PHE	-	insertion	UNP Q9BYF1
B	16	GLU	-	insertion	UNP Q9BYF1
B	17	LYS	-	insertion	UNP Q9BYF1
D	-8	MET	-	initiating methionine	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	183	1462	939	242	274	7	0	0
3	F	183	1462	939	242	274	7	0	0

- 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
			Total	C	N	O		
4	G	2	28	16	2	10	0	0
4	H	2	28	16	2	10	0	0
4	I	2	28	16	2	10	0	0
4	J	2	28	16	2	10	0	0
4	K	2	28	16	2	10	0	0
4	L	2	28	16	2	10	0	0
4	M	2	28	16	2	10	0	0
4	O	2	28	16	2	10	0	0
4	P	2	28	16	2	10	0	0

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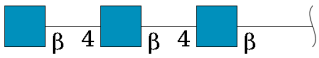
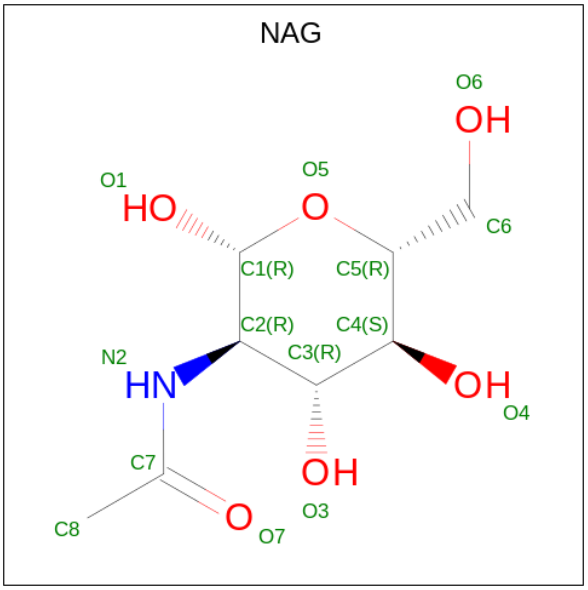
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	Q	2	28	16	2	10	0	0
			Total	C	N	O		
4	R	2	28	16	2	10	0	0
			Total	C	N	O		
4	S	2	28	16	2	10	0	0
			Total	C	N	O		
4	T	2	28	16	2	10	0	0
			Total	C	N	O		
4	U	2	28	16	2	10	0	0

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



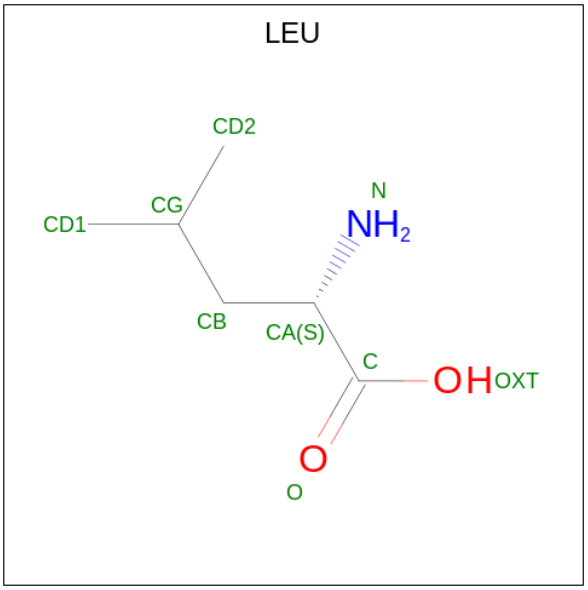
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	N	3	42	24	3	15	0	0
			Total	C	N	O		
5	V	3	42	24	3	15	0	0

- 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
			Total	C	N	O	
6	A	1	56	32	4	20	0
6	A	1	56	32	4	20	0
6	A	1	56	32	4	20	0
6	A	1	56	32	4	20	0
6	B	1	14	8	1	5	0
6	C	1	56	32	4	20	0
6	C	1	56	32	4	20	0
6	C	1	56	32	4	20	0
6	C	1	56	32	4	20	0
6	D	1	14	8	1	5	0

- Molecule 7 is LEUCINE (three-letter code: LEU) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	9	6	1	2	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	C	1	9	6	1	2	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
8	B	1	1	1	0
8	D	1	Total	Zn	0
			1	1	

- Molecule 9 is water.

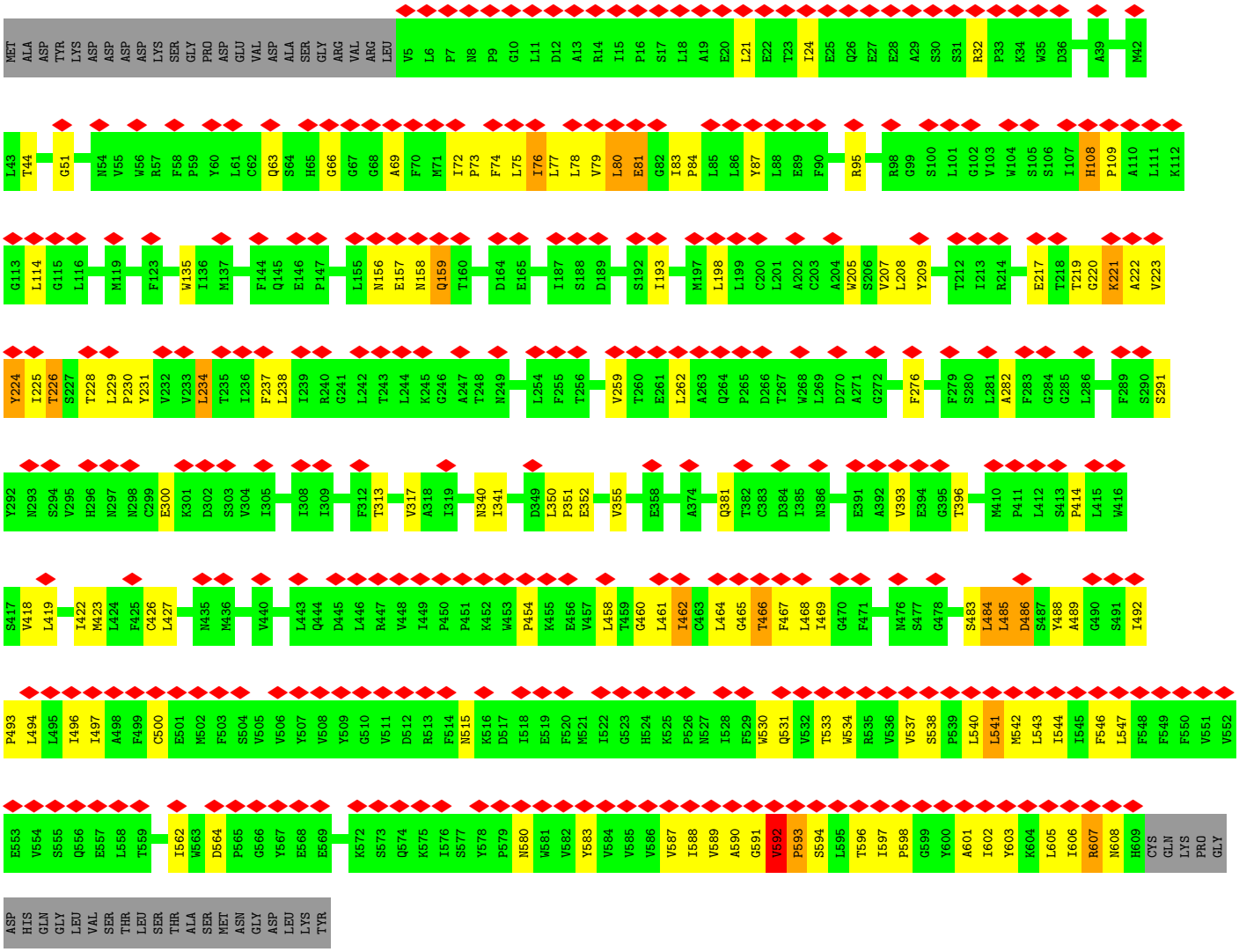
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
9	B	4	4	4	0
9	D	4	Total	O	0
			4	4	

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.

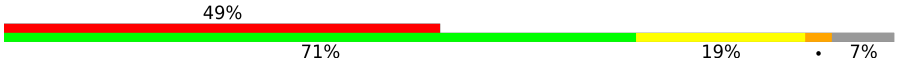
• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

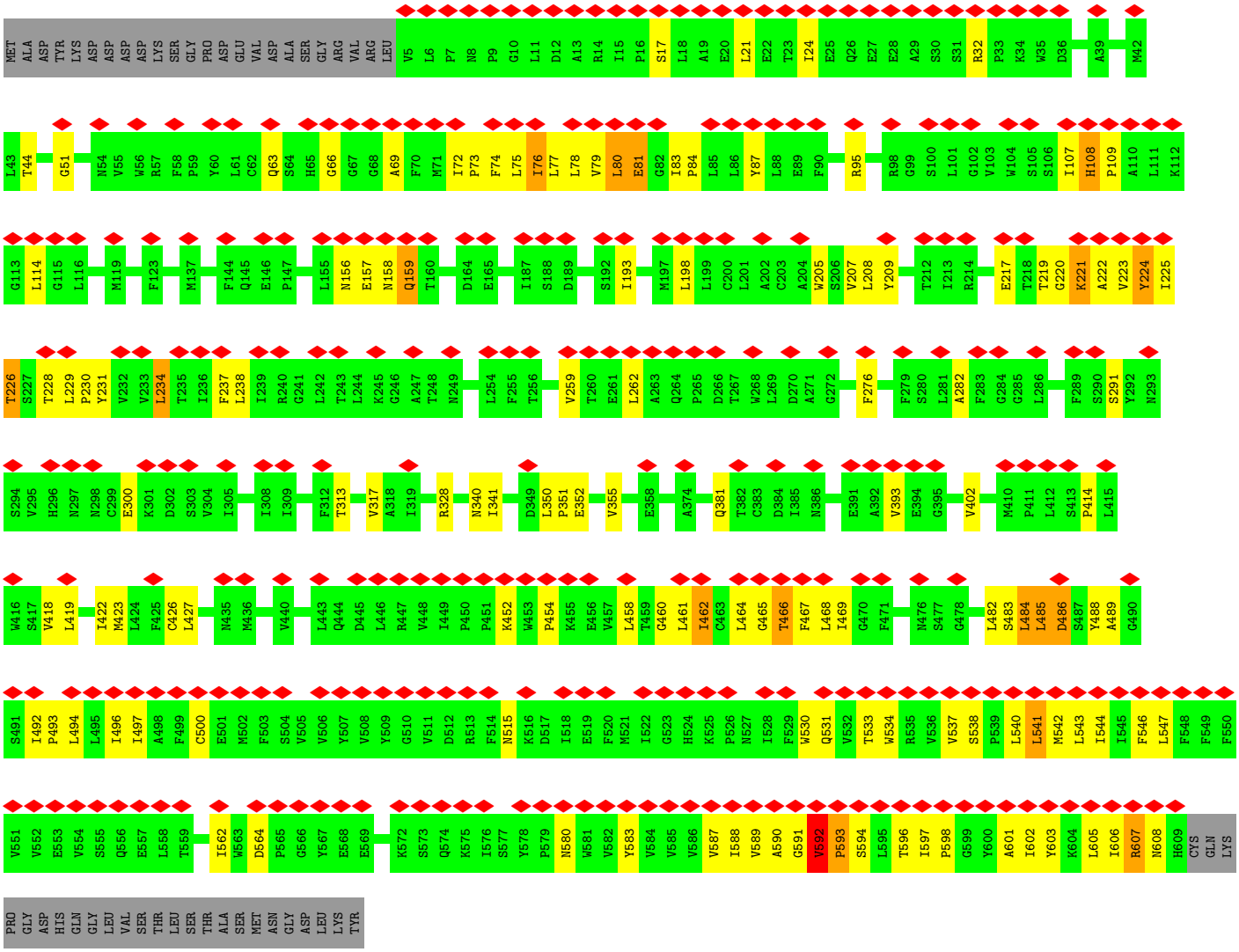
Chain A: 49% 72% 18% • 7%



• Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1

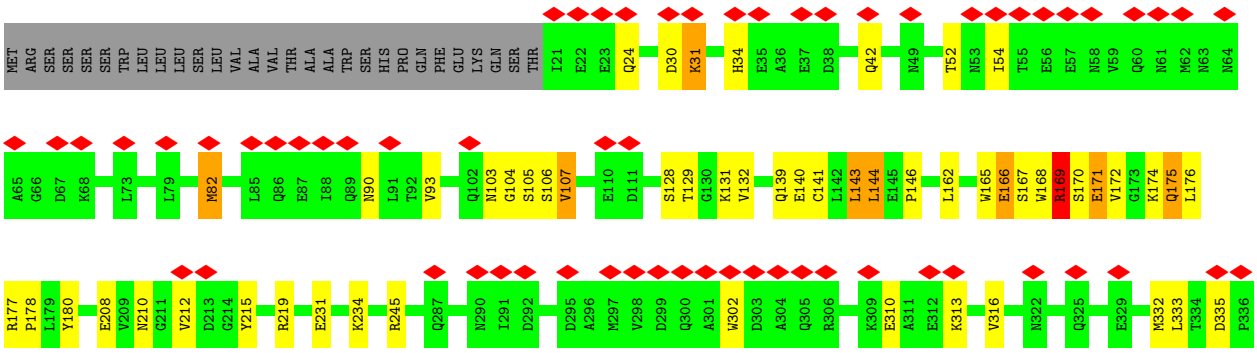
Chain C:

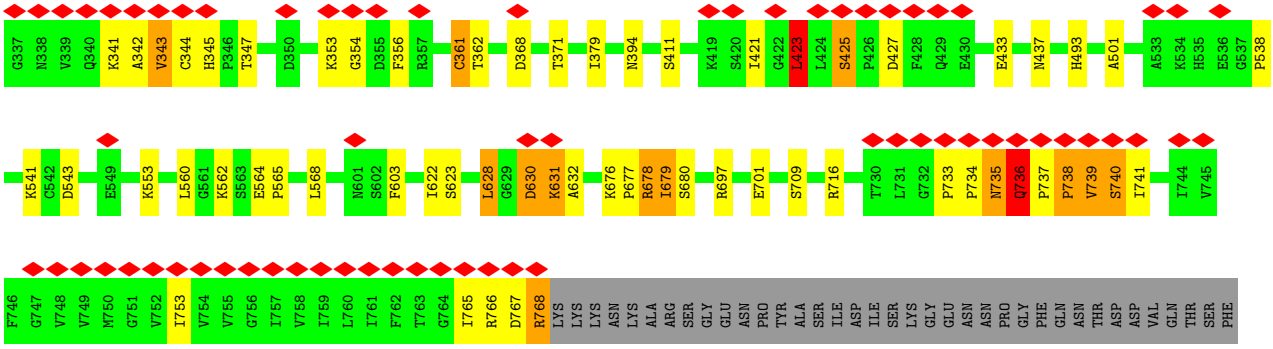




- Molecule 2: Angiotensin-converting enzyme 2

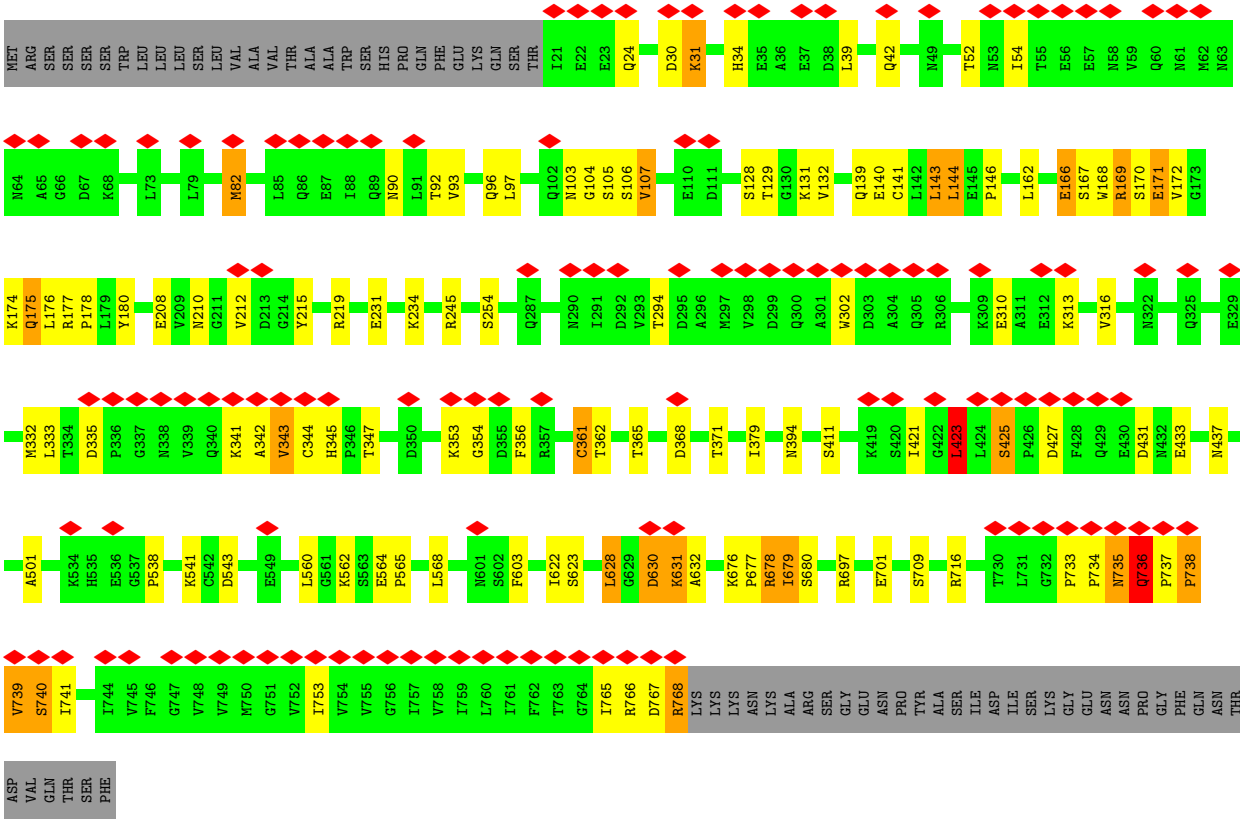
Chain B:





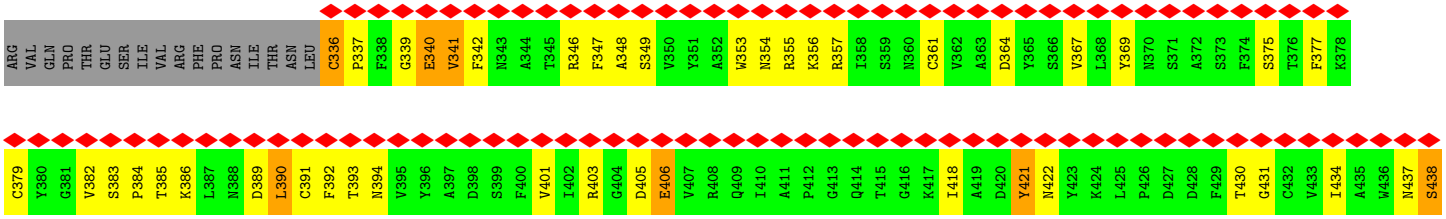
- Molecule 2: Angiotensin-converting enzyme 2

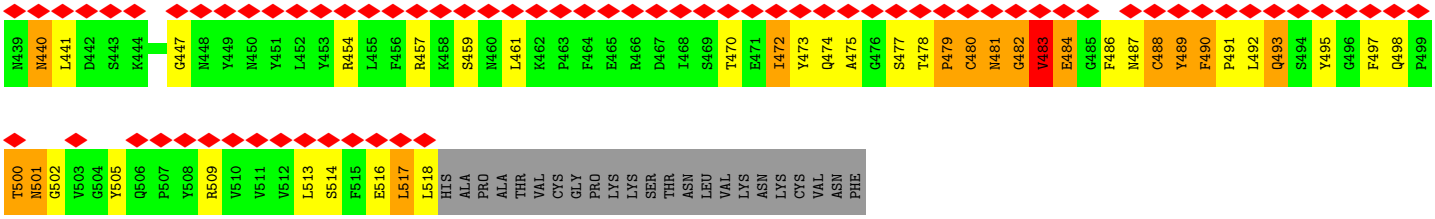
Chain D:



- Molecule 3: Spike protein S1

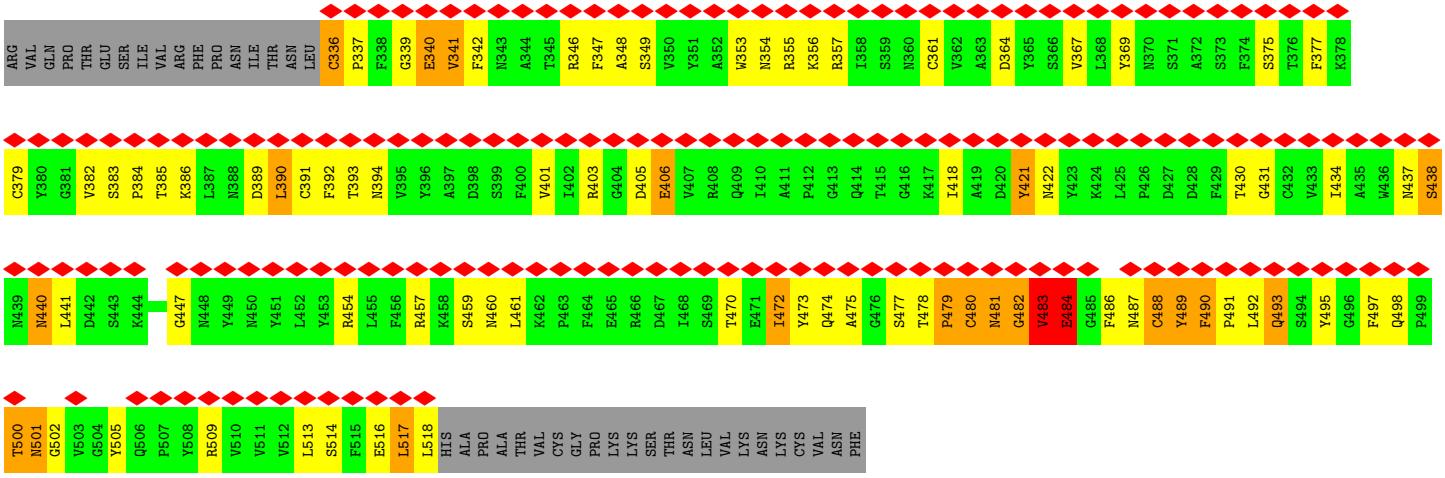
Chain E:





• Molecule 3: Spike protein S1

Chain F:

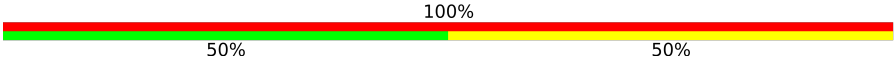


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

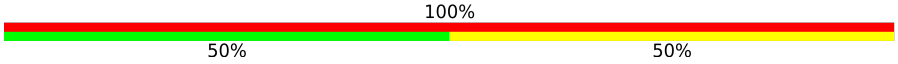
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

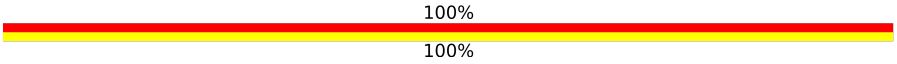


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

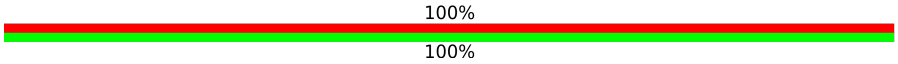
Chain I:



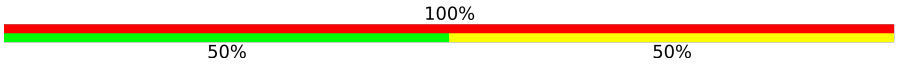
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

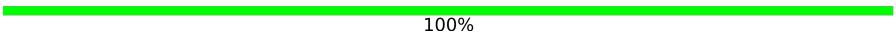
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 

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

Chain L: 

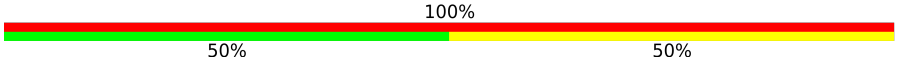
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M: 

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

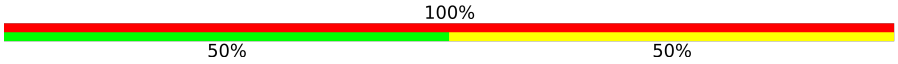
Chain O:

• 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

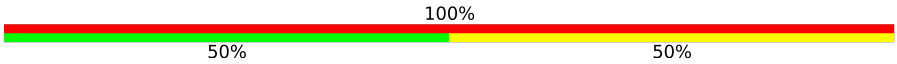
Chain R:

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

Chain S:

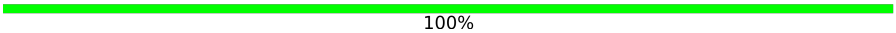
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



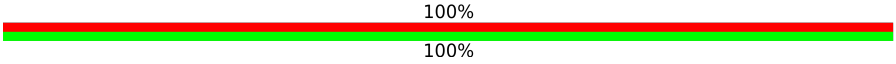
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain N:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(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, Not provided	
Number of particles used	301565	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.593	Depositor
Minimum map value	-1.869	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.66	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ZN

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	0.34	0/4940	0.56	0/6748
1	C	0.34	0/4940	0.56	0/6748
2	B	0.36	0/6252	0.52	0/8488
2	D	0.36	0/6252	0.52	0/8488
3	E	0.80	0/1503	0.56	0/2043
3	F	0.80	0/1503	0.56	0/2043
All	All	0.43	0/25390	0.54	0/34558

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4799	0	4762	155	0
1	C	4799	0	4762	156	0
2	B	6089	0	5901	148	0
2	D	6089	0	5901	152	0
3	E	1462	0	1385	127	0
3	F	1462	0	1385	131	0
4	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	6	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	M	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	6	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	N	42	0	37	0	0
5	V	42	0	37	0	0
6	A	56	0	52	0	0
6	B	14	0	13	0	0
6	C	56	0	52	0	0
6	D	14	0	13	0	0
7	A	9	0	10	0	0
7	C	9	0	10	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	B	4	0	0	0	0
9	D	4	0	0	0	0
All	All	25344	0	24670	801	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 16.

All (801) 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:205:TRP:CH2	1:C:466:THR:HG21	1.72	1.25
1:A:205:TRP:CH2	1:A:466:THR:HG21	1.72	1.25
3:E:341:VAL:CG2	3:E:356:LYS:HD3	1.83	1.09
2:B:34:HIS:CE1	3:E:493:GLN:HG3	1.88	1.08
2:D:82:MET:HG3	3:F:486:PHE:CE2	1.89	1.08
2:B:82:MET:HG3	3:E:486:PHE:CE2	1.89	1.08
1:A:81:GLU:OE2	1:A:541:LEU:HB3	1.51	1.08
1:C:81:GLU:OE2	1:C:541:LEU:HB3	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:HIS:CE1	3:F:493:GLN:HG3	1.88	1.07
3:E:475:ALA:HB1	3:E:487:ASN:HB3	1.35	1.07
3:E:392:PHE:HB3	3:E:517:LEU:HD21	1.34	1.07
3:F:341:VAL:CG2	3:F:356:LYS:HD3	1.83	1.07
3:F:392:PHE:HB3	3:F:517:LEU:HD21	1.34	1.06
1:A:221:LYS:H	1:A:221:LYS:HD2	1.19	1.06
4:R:1:NAG:H62	4:R:2:NAG:HN2	1.18	1.06
3:F:475:ALA:HB1	3:F:487:ASN:HB3	1.35	1.05
1:C:592:VAL:HG23	1:C:593:PRO:CD	1.87	1.04
3:F:392:PHE:HB3	3:F:517:LEU:CD2	1.88	1.04
1:A:592:VAL:HG23	1:A:593:PRO:CD	1.87	1.04
1:C:492:ILE:CG2	1:C:493:PRO:HD3	1.88	1.04
1:A:492:ILE:CG2	1:A:493:PRO:HD3	1.88	1.03
1:A:205:TRP:CZ2	1:A:466:THR:CG2	2.42	1.03
3:E:392:PHE:HB3	3:E:517:LEU:CD2	1.88	1.03
3:F:475:ALA:CB	3:F:487:ASN:HB3	1.88	1.03
1:C:221:LYS:H	1:C:221:LYS:HD2	1.19	1.02
3:E:475:ALA:CB	3:E:487:ASN:HB3	1.88	1.02
1:C:205:TRP:CZ2	1:C:466:THR:CG2	2.42	1.02
2:D:177:ARG:HB3	2:D:178:PRO:HD3	1.42	1.02
4:J:1:NAG:H62	4:J:2:NAG:HN2	1.18	1.02
1:C:492:ILE:HG23	1:C:493:PRO:CD	1.90	1.02
2:B:177:ARG:HB3	2:B:178:PRO:HD3	1.42	1.01
1:C:592:VAL:CG2	1:C:593:PRO:HD3	1.91	1.01
1:A:492:ILE:HG23	1:A:493:PRO:CD	1.90	1.00
1:A:592:VAL:CG2	1:A:593:PRO:HD3	1.91	1.00
2:B:736:GLN:H	2:B:737:PRO:HD2	1.25	1.00
3:E:392:PHE:CB	3:E:517:LEU:HD21	1.91	1.00
1:C:583:TYR:O	1:C:587:VAL:HG23	1.62	1.00
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.44	1.00
1:A:583:TYR:O	1:A:587:VAL:HG23	1.62	0.99
3:F:392:PHE:CB	3:F:517:LEU:HD21	1.91	0.99
1:A:454:PRO:HG3	2:B:768:ARG:NH2	1.77	0.99
1:C:454:PRO:HG3	2:D:768:ARG:NH2	1.77	0.99
3:F:341:VAL:HG22	3:F:356:LYS:HD3	1.44	0.99
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.98
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.44	0.97
2:B:34:HIS:ND1	3:E:493:GLN:HG3	1.78	0.97
2:B:34:HIS:CE1	3:E:493:GLN:CG	2.47	0.97
3:F:346:ARG:NH2	3:F:347:PHE:O	1.98	0.97
3:E:346:ARG:NH2	3:E:347:PHE:O	1.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:TRP:CZ2	1:A:466:THR:HG23	1.99	0.97
2:D:736:GLN:H	2:D:737:PRO:HD2	1.25	0.97
1:A:159:GLN:HE21	2:B:733:PRO:HB3	1.30	0.96
1:A:592:VAL:HG23	1:A:593:PRO:HD3	0.97	0.96
1:C:492:ILE:HG23	1:C:493:PRO:HD3	0.97	0.96
3:E:341:VAL:HG22	3:E:356:LYS:HD3	1.44	0.96
2:B:302:TRP:CH2	2:B:423:LEU:HD11	1.99	0.96
2:D:34:HIS:ND1	3:F:493:GLN:HG3	1.78	0.96
2:B:82:MET:HG3	3:E:486:PHE:CZ	2.01	0.96
1:C:159:GLN:HE21	2:D:733:PRO:HB3	1.30	0.96
2:D:34:HIS:CE1	3:F:493:GLN:CG	2.47	0.96
1:C:205:TRP:CZ2	1:C:466:THR:HG23	1.99	0.95
2:B:678:ARG:HH21	2:B:678:ARG:HG3	1.32	0.95
1:A:492:ILE:HG23	1:A:493:PRO:HD3	0.97	0.95
2:D:82:MET:HG3	3:F:486:PHE:CZ	2.01	0.94
1:C:592:VAL:HG23	1:C:593:PRO:HD3	0.97	0.94
2:D:34:HIS:ND1	3:F:493:GLN:CG	2.32	0.93
2:B:34:HIS:ND1	3:E:493:GLN:CG	2.32	0.93
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.33	0.93
2:D:678:ARG:HH21	2:D:678:ARG:HG3	1.32	0.93
1:A:205:TRP:CH2	1:A:466:THR:CG2	2.54	0.91
1:C:205:TRP:CH2	1:C:466:THR:CG2	2.54	0.91
1:C:205:TRP:CZ2	1:C:466:THR:HG21	2.05	0.91
3:F:336:CYS:N	3:F:361:CYS:HB2	1.86	0.91
1:A:205:TRP:CZ2	1:A:466:THR:HG21	2.05	0.91
3:F:340:GLU:OE1	3:F:340:GLU:N	2.03	0.90
3:E:340:GLU:N	3:E:340:GLU:OE1	2.03	0.90
1:A:492:ILE:HG21	1:A:590:ALA:HB1	1.53	0.90
1:C:588:ILE:O	1:C:592:VAL:HG22	1.71	0.90
1:C:492:ILE:HG21	1:C:590:ALA:HB1	1.53	0.90
3:E:336:CYS:N	3:E:361:CYS:HB2	1.86	0.89
1:C:489:ALA:HB2	1:C:589:VAL:CG1	2.03	0.88
1:A:489:ALA:HB2	1:A:589:VAL:CG1	2.03	0.88
1:A:588:ILE:O	1:A:592:VAL:HG22	1.71	0.88
2:B:302:TRP:HH2	2:B:423:LEU:HD11	1.33	0.88
3:E:475:ALA:CB	3:E:487:ASN:CB	2.52	0.87
3:F:475:ALA:CB	3:F:487:ASN:CB	2.52	0.87
1:A:220:GLY:O	1:A:223:VAL:HG12	1.75	0.86
1:C:220:GLY:O	1:C:223:VAL:HG12	1.75	0.86
3:F:392:PHE:CD2	3:F:517:LEU:HD21	2.11	0.86
2:D:34:HIS:CE1	3:F:493:GLN:HB3	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
2:B:105:SER:O	2:B:106:SER:OG	1.93	0.86
3:E:490:PHE:CD1	3:E:491:PRO:HD2	2.11	0.85
3:F:490:PHE:CD1	3:F:491:PRO:HD2	2.11	0.85
2:B:335:ASP:HB3	2:B:361:CYS:SG	2.16	0.85
3:E:392:PHE:CD2	3:E:517:LEU:HD21	2.11	0.85
1:A:83:ILE:HB	1:A:84:PRO:HD3	1.59	0.85
3:F:478:THR:HG23	3:F:479:PRO:HD2	1.55	0.85
2:B:34:HIS:CE1	3:E:493:GLN:HB3	2.11	0.85
3:E:478:THR:HG23	3:E:479:PRO:HD2	1.55	0.85
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.84
3:E:472:ILE:HD12	3:E:482:GLY:HA2	1.59	0.84
3:F:472:ILE:HD12	3:F:482:GLY:HA2	1.59	0.84
3:F:475:ALA:HB3	3:F:487:ASN:O	1.78	0.84
1:C:591:GLY:O	1:C:592:VAL:C	2.15	0.84
1:C:83:ILE:HB	1:C:84:PRO:HD3	1.59	0.84
1:C:221:LYS:HD2	1:C:221:LYS:N	1.93	0.84
1:A:591:GLY:O	1:A:592:VAL:C	2.15	0.83
3:E:516:GLU:O	3:E:517:LEU:HD22	1.78	0.83
1:A:221:LYS:HD2	1:A:221:LYS:N	1.93	0.83
3:F:516:GLU:O	3:F:517:LEU:HD22	1.78	0.82
2:D:170:SER:O	2:D:174:LYS:HG2	1.79	0.82
2:B:170:SER:O	2:B:174:LYS:HG2	1.79	0.82
1:C:72:ILE:O	1:C:76:ILE:HG23	1.80	0.82
2:B:144:LEU:HD22	2:B:168:TRP:CH2	2.15	0.82
3:E:475:ALA:HB3	3:E:487:ASN:O	1.78	0.82
3:E:486:PHE:CD1	3:E:487:ASN:ND2	2.49	0.81
2:D:736:GLN:N	2:D:737:PRO:HD2	1.95	0.81
1:A:229:LEU:HD23	1:A:426:CYS:SG	2.20	0.81
2:B:628:LEU:HD12	2:B:632:ALA:CB	2.10	0.81
1:A:72:ILE:O	1:A:76:ILE:HG23	1.80	0.80
2:B:736:GLN:N	2:B:737:PRO:HD2	1.95	0.80
2:D:628:LEU:HD12	2:D:632:ALA:CB	2.10	0.80
1:C:229:LEU:HD23	1:C:426:CYS:SG	2.20	0.80
3:F:486:PHE:CD1	3:F:487:ASN:ND2	2.49	0.80
2:D:144:LEU:HD22	2:D:168:TRP:CH2	2.15	0.80
1:A:597:ILE:HB	1:A:598:PRO:HD3	1.64	0.80
1:C:597:ILE:HB	1:C:598:PRO:HD3	1.64	0.80
1:A:81:GLU:OE2	1:A:541:LEU:CB	2.30	0.79
3:E:498:GLN:HB2	3:E:501:ASN:HD21	1.48	0.79
1:C:81:GLU:OE2	1:C:541:LEU:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:498:GLN:HB2	3:F:501:ASN:HD21	1.48	0.79
1:A:454:PRO:HG3	2:B:768:ARG:HH21	1.46	0.79
1:C:454:PRO:HG3	2:D:768:ARG:HH21	1.46	0.79
3:E:390:LEU:HD23	3:E:391:CYS:H	1.49	0.78
3:E:422:ASN:HD21	3:E:454:ARG:H	1.32	0.78
3:F:390:LEU:HD23	3:F:391:CYS:H	1.49	0.78
3:F:498:GLN:HB2	3:F:501:ASN:ND2	1.98	0.78
3:F:470:THR:CG2	3:F:490:PHE:CE1	2.68	0.77
3:E:498:GLN:HB2	3:E:501:ASN:ND2	1.98	0.77
1:A:492:ILE:HG21	1:A:590:ALA:CB	2.15	0.77
3:F:477:SER:O	3:F:478:THR:OG1	2.03	0.77
2:D:768:ARG:HG2	2:D:768:ARG:HH11	1.49	0.77
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
3:E:475:ALA:HB3	3:E:487:ASN:CB	2.16	0.76
3:E:470:THR:CG2	3:E:490:PHE:CE1	2.68	0.76
1:C:492:ILE:HG21	1:C:590:ALA:CB	2.15	0.76
2:D:34:HIS:CE1	3:F:493:GLN:CB	2.69	0.76
3:F:422:ASN:HD21	3:F:454:ARG:H	1.32	0.76
3:F:481:ASN:O	3:F:483:VAL:HG22	1.85	0.76
1:C:222:ALA:O	1:C:226:THR:HG23	1.86	0.76
2:B:768:ARG:HG2	2:B:768:ARG:HH11	1.49	0.76
1:A:418:VAL:O	1:A:422:ILE:HG23	1.86	0.75
3:E:481:ASN:O	3:E:483:VAL:HG22	1.85	0.75
1:C:159:GLN:HE21	2:D:733:PRO:CB	1.98	0.75
2:B:302:TRP:HH2	2:B:423:LEU:CD1	1.98	0.75
3:E:477:SER:O	3:E:478:THR:OG1	2.03	0.75
3:F:470:THR:HG22	3:F:490:PHE:HE1	1.51	0.75
3:E:470:THR:HG22	3:E:490:PHE:HE1	1.51	0.75
2:D:736:GLN:H	2:D:737:PRO:CD	1.99	0.75
1:A:222:ALA:O	1:A:226:THR:HG23	1.86	0.75
3:F:475:ALA:HB3	3:F:487:ASN:CB	2.16	0.75
1:A:78:LEU:HD23	1:A:79:VAL:N	2.02	0.74
2:B:736:GLN:H	2:B:737:PRO:CD	1.99	0.74
2:D:678:ARG:HG3	2:D:678:ARG:NH2	1.99	0.74
2:D:82:MET:CG	3:F:486:PHE:CZ	2.70	0.74
2:B:34:HIS:CE1	3:E:493:GLN:CB	2.69	0.74
2:B:335:ASP:CB	2:B:361:CYS:SG	2.75	0.74
1:C:418:VAL:O	1:C:422:ILE:HG23	1.86	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:C:78:LEU:HD23	1:C:79:VAL:N	2.02	0.74
2:B:82:MET:CG	3:E:486:PHE:CZ	2.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:MET:CG	3:F:486:PHE:CE2	2.71	0.74
1:A:159:GLN:HE21	2:B:733:PRO:CB	1.98	0.74
1:A:229:LEU:HB3	1:A:230:PRO:CD	2.17	0.74
3:E:392:PHE:HD2	3:E:517:LEU:HD21	1.53	0.73
2:B:172:VAL:CG1	2:B:176:LEU:HD11	2.18	0.73
2:D:172:VAL:CG1	2:D:176:LEU:HD11	2.18	0.73
2:D:172:VAL:HG13	2:D:176:LEU:HD11	1.71	0.73
1:A:205:TRP:CE2	1:A:466:THR:HG23	2.24	0.73
3:F:478:THR:CG2	3:F:479:PRO:HD2	2.18	0.73
3:F:486:PHE:CG	3:F:487:ASN:ND2	2.57	0.73
1:C:205:TRP:CE2	1:C:466:THR:HG23	2.24	0.72
3:F:392:PHE:HD2	3:F:517:LEU:HD21	1.53	0.72
2:B:82:MET:CG	3:E:486:PHE:CE2	2.71	0.72
3:E:478:THR:CG2	3:E:479:PRO:HD2	2.18	0.72
3:E:486:PHE:CG	3:E:487:ASN:ND2	2.57	0.72
1:C:229:LEU:HB3	1:C:230:PRO:CD	2.17	0.72
3:F:406:GLU:CD	3:F:418:ILE:HG13	2.10	0.72
1:C:209:TYR:HE2	1:C:460:GLY:CA	2.03	0.72
2:D:736:GLN:N	2:D:737:PRO:CD	2.53	0.72
2:B:172:VAL:CG1	2:B:176:LEU:CD1	2.68	0.72
3:E:406:GLU:CD	3:E:418:ILE:HG13	2.10	0.72
2:D:172:VAL:CG1	2:D:176:LEU:CD1	2.68	0.71
1:A:209:TYR:HE2	1:A:460:GLY:CA	2.03	0.71
2:B:172:VAL:HG13	2:B:176:LEU:HD11	1.71	0.71
2:B:736:GLN:N	2:B:737:PRO:CD	2.53	0.70
2:D:172:VAL:HG12	2:D:176:LEU:HD12	1.73	0.70
1:C:465:GLY:O	1:C:469:ILE:HG12	1.91	0.70
1:A:465:GLY:O	1:A:469:ILE:HG12	1.91	0.70
2:B:678:ARG:HG3	2:B:678:ARG:NH2	1.99	0.70
2:B:172:VAL:HG12	2:B:176:LEU:HD12	1.73	0.70
1:C:72:ILE:HD12	1:C:72:ILE:H	1.57	0.70
1:C:209:TYR:CE2	1:C:460:GLY:CA	2.75	0.70
3:E:487:ASN:O	3:E:488:CYS:HB2	1.91	0.69
1:A:209:TYR:CE2	1:A:460:GLY:CA	2.75	0.69
1:A:209:TYR:CE2	1:A:460:GLY:HA2	2.27	0.69
1:C:209:TYR:CE2	1:C:460:GLY:HA2	2.27	0.69
3:F:487:ASN:O	3:F:488:CYS:HB2	1.91	0.69
3:E:470:THR:HG22	3:E:490:PHE:CE1	2.28	0.69
1:A:72:ILE:H	1:A:72:ILE:HD12	1.57	0.69
3:F:492:LEU:C	3:F:493:GLN:NE2	2.47	0.68
1:C:454:PRO:CG	2:D:768:ARG:HH21	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:392:PHE:CG	3:E:517:LEU:HD21	2.29	0.68
3:E:403:ARG:HG3	3:E:495:TYR:CE1	2.29	0.68
3:F:403:ARG:HG3	3:F:495:TYR:CE1	2.29	0.68
1:A:454:PRO:CG	2:B:768:ARG:HH21	2.07	0.68
2:D:739:VAL:O	2:D:740:SER:HB2	1.94	0.68
2:B:34:HIS:ND1	3:E:493:GLN:HG2	2.09	0.67
3:E:492:LEU:C	3:E:493:GLN:NE2	2.47	0.67
3:F:470:THR:HG22	3:F:490:PHE:CE1	2.28	0.67
2:B:739:VAL:O	2:B:740:SER:HB2	1.94	0.67
3:E:482:GLY:O	3:E:483:VAL:HG13	1.95	0.67
3:F:482:GLY:O	3:F:483:VAL:HG13	1.95	0.67
3:F:340:GLU:O	3:F:342:PHE:N	2.28	0.67
1:A:350:LEU:O	2:B:678:ARG:HB2	1.96	0.66
3:F:392:PHE:CG	3:F:517:LEU:HD21	2.29	0.66
1:A:78:LEU:HD23	1:A:78:LEU:C	2.16	0.66
3:E:340:GLU:O	3:E:342:PHE:N	2.28	0.66
1:C:350:LEU:O	2:D:678:ARG:HB2	1.96	0.66
2:B:630:ASP:O	2:B:631:LYS:HB2	1.96	0.66
2:D:34:HIS:ND1	3:F:493:GLN:HG2	2.09	0.66
3:F:392:PHE:HD2	3:F:517:LEU:CD2	2.09	0.66
3:E:482:GLY:C	3:E:483:VAL:HG22	2.17	0.65
1:C:78:LEU:HD23	1:C:78:LEU:C	2.16	0.65
2:D:630:ASP:O	2:D:631:LYS:HB2	1.96	0.65
1:C:454:PRO:CG	2:D:768:ARG:NH2	2.58	0.65
4:R:1:NAG:H62	4:R:2:NAG:N2	2.02	0.65
1:A:594:SER:O	1:A:598:PRO:HD2	1.97	0.65
2:B:177:ARG:HB3	2:B:178:PRO:CD	2.22	0.65
2:D:734:PRO:O	2:D:735:ASN:HB2	1.96	0.65
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.79	0.65
2:D:177:ARG:HB3	2:D:178:PRO:CD	2.22	0.65
3:F:482:GLY:C	3:F:483:VAL:HG22	2.17	0.65
2:B:734:PRO:O	2:B:735:ASN:HB2	1.96	0.64
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.79	0.64
1:C:594:SER:O	1:C:598:PRO:HD2	1.97	0.64
3:E:392:PHE:HD2	3:E:517:LEU:CD2	2.09	0.64
1:C:72:ILE:HD12	1:C:72:ILE:N	2.13	0.64
1:C:543:LEU:HD12	1:C:543:LEU:O	1.97	0.64
2:D:766:ARG:O	2:D:766:ARG:HG2	1.98	0.64
1:A:72:ILE:HD12	1:A:72:ILE:N	2.13	0.64
2:D:177:ARG:CB	2:D:178:PRO:HD3	2.25	0.64
4:J:1:NAG:H62	4:J:2:NAG:N2	2.02	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HD2	3:E:505:TYR:HD2	1.63	0.64
1:C:276:PHE:O	1:C:494:LEU:HD13	1.98	0.63
1:C:454:PRO:HG3	2:D:768:ARG:HH22	1.62	0.63
1:C:583:TYR:O	1:C:587:VAL:CG2	2.42	0.63
2:B:310:GLU:OE1	2:B:421:ILE:HD11	1.97	0.63
1:A:543:LEU:O	1:A:543:LEU:HD12	1.97	0.63
2:B:335:ASP:N	2:B:361:CYS:SG	2.72	0.63
3:E:475:ALA:CB	3:E:487:ASN:C	2.67	0.63
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.63
1:A:276:PHE:O	1:A:494:LEU:HD13	1.98	0.63
2:B:302:TRP:CZ3	2:B:423:LEU:HD11	2.34	0.63
3:E:492:LEU:O	3:E:493:GLN:NE2	2.32	0.63
1:C:76:ILE:HG13	1:C:77:LEU:N	2.13	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
3:F:475:ALA:CB	3:F:487:ASN:C	2.67	0.63
2:B:766:ARG:O	2:B:766:ARG:HG2	1.98	0.62
1:A:76:ILE:HG13	1:A:77:LEU:N	2.13	0.62
2:D:353:LYS:HD2	3:F:505:TYR:HD2	1.63	0.62
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.62
3:F:492:LEU:O	3:F:493:GLN:NE2	2.32	0.62
1:A:454:PRO:HG3	2:B:768:ARG:HH22	1.62	0.62
2:D:143:LEU:O	2:D:146:PRO:HD2	2.00	0.62
2:B:143:LEU:O	2:B:146:PRO:HD2	2.00	0.61
2:D:768:ARG:HH11	2:D:768:ARG:CG	2.13	0.61
1:A:583:TYR:O	1:A:587:VAL:CG2	2.42	0.61
3:E:457:ARG:NH1	3:E:459:SER:O	2.33	0.61
3:E:475:ALA:CB	3:E:487:ASN:O	2.48	0.61
3:E:516:GLU:O	3:E:517:LEU:CD2	2.48	0.61
3:F:457:ARG:NH1	3:F:459:SER:O	2.33	0.61
3:F:470:THR:HG22	3:F:470:THR:O	2.00	0.61
2:B:353:LYS:HD2	3:E:505:TYR:CD2	2.36	0.61
3:E:470:THR:HG22	3:E:470:THR:O	2.00	0.61
2:D:628:LEU:HD12	2:D:632:ALA:HB1	1.82	0.61
1:C:607:ARG:NH2	1:C:607:ARG:HG3	2.15	0.61
2:D:735:ASN:ND2	2:D:737:PRO:HD2	2.15	0.61
2:D:353:LYS:HD2	3:F:505:TYR:CD2	2.36	0.61
3:F:357:ARG:HH12	3:F:394:ASN:HD21	1.49	0.61
2:B:768:ARG:HH11	2:B:768:ARG:CG	2.13	0.61
1:C:234:LEU:HD21	1:C:317:VAL:HG22	1.83	0.61
2:B:628:LEU:HD12	2:B:632:ALA:HB2	1.83	0.61
3:F:516:GLU:O	3:F:517:LEU:CD2	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:THR:HA	1:C:223:VAL:HG21	1.84	0.60
2:B:628:LEU:HD12	2:B:632:ALA:HB1	1.82	0.60
3:F:472:ILE:HG22	3:F:473:TYR:N	2.16	0.60
3:E:357:ARG:HH12	3:E:394:ASN:HD21	1.49	0.60
1:C:607:ARG:HH21	1:C:607:ARG:CG	2.15	0.60
2:B:735:ASN:ND2	2:B:737:PRO:HD2	2.15	0.60
3:E:472:ILE:HG22	3:E:473:TYR:N	2.16	0.60
3:E:486:PHE:CE1	3:E:487:ASN:ND2	2.69	0.60
3:F:486:PHE:CE1	3:F:487:ASN:ND2	2.69	0.60
3:F:406:GLU:OE1	3:F:418:ILE:HG12	2.02	0.60
1:A:205:TRP:CZ3	1:A:466:THR:HG21	2.36	0.60
2:D:628:LEU:HD12	2:D:632:ALA:HB2	1.83	0.60
1:C:159:GLN:NE2	2:D:733:PRO:HB3	2.11	0.60
3:F:392:PHE:HB3	3:F:517:LEU:HD22	1.82	0.60
1:C:51:GLY:HA2	1:C:427:LEU:HD13	1.84	0.59
1:A:607:ARG:NH2	1:A:607:ARG:HG3	2.15	0.59
2:B:129:THR:O	2:D:139:GLN:HG3	2.02	0.59
1:A:234:LEU:HD21	1:A:317:VAL:HG22	1.83	0.59
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.85	0.59
3:F:475:ALA:CB	3:F:487:ASN:O	2.48	0.59
1:A:44:THR:HA	1:A:223:VAL:HG21	1.84	0.59
1:A:607:ARG:HH21	1:A:607:ARG:CG	2.15	0.59
2:B:167:SER:O	2:B:171:GLU:HG2	2.03	0.59
3:E:406:GLU:OE1	3:E:418:ILE:HG12	2.02	0.59
2:D:167:SER:O	2:D:171:GLU:HG2	2.03	0.59
2:B:140:GLU:HG3	2:B:140:GLU:O	2.03	0.59
3:E:406:GLU:CD	3:E:418:ILE:CG1	2.71	0.59
2:B:736:GLN:NE2	2:B:736:GLN:O	2.35	0.58
3:E:392:PHE:HB3	3:E:517:LEU:HD22	1.82	0.58
1:A:51:GLY:HA2	1:A:427:LEU:HD13	1.84	0.58
2:B:172:VAL:HG13	2:B:176:LEU:CD1	2.32	0.58
2:D:736:GLN:O	2:D:736:GLN:NE2	2.35	0.58
1:A:605:LEU:O	1:A:608:ASN:HB3	2.03	0.58
2:D:140:GLU:HG3	2:D:140:GLU:O	2.03	0.58
2:B:139:GLN:HG3	2:D:129:THR:O	2.02	0.58
2:B:212:VAL:HG21	2:B:565:PRO:HG3	1.85	0.58
1:A:205:TRP:CZ3	1:A:208:LEU:HD23	2.39	0.58
1:C:605:LEU:O	1:C:608:ASN:HB3	2.03	0.58
2:D:131:LYS:HB3	2:D:141:CYS:HB3	1.86	0.58
1:C:205:TRP:CZ3	1:C:208:LEU:HD23	2.39	0.58
3:F:473:TYR:CG	3:F:474:GLN:N	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:PRO:CG	2:B:768:ARG:NH2	2.58	0.58
2:B:177:ARG:CB	2:B:178:PRO:HD3	2.25	0.58
3:E:475:ALA:HB2	3:E:487:ASN:C	2.25	0.58
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
1:C:87:TYR:HD2	1:C:534:TRP:HZ2	1.52	0.58
3:F:406:GLU:CD	3:F:418:ILE:CG1	2.71	0.58
1:A:87:TYR:HD2	1:A:534:TRP:HZ2	1.52	0.57
1:C:602:ILE:O	1:C:606:ILE:HG12	2.03	0.57
1:A:602:ILE:O	1:A:606:ILE:HG12	2.03	0.57
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.57
4:R:1:NAG:C6	4:R:2:NAG:HN2	2.06	0.57
1:A:159:GLN:NE2	2:B:733:PRO:HB3	2.11	0.57
1:C:87:TYR:CD2	1:C:534:TRP:HZ2	2.23	0.57
3:F:475:ALA:HB2	3:F:487:ASN:C	2.25	0.57
3:F:493:GLN:HE21	3:F:493:GLN:N	2.03	0.57
2:B:131:LYS:HB3	2:B:141:CYS:HB3	1.86	0.57
1:A:597:ILE:HB	1:A:598:PRO:CD	2.33	0.56
1:A:205:TRP:CE2	1:A:466:THR:CG2	2.87	0.56
1:A:483:SER:O	1:A:486:ASP:HB3	2.06	0.56
2:B:368:ASP:HA	2:B:371:THR:HG22	1.85	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.87	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
1:A:87:TYR:CD2	1:A:534:TRP:HZ2	2.23	0.56
2:B:167:SER:OG	2:B:168:TRP:N	2.39	0.56
2:D:735:ASN:O	2:D:736:GLN:HB3	2.05	0.56
1:A:492:ILE:CG2	1:A:590:ALA:HB1	2.34	0.56
2:B:425:SER:HB3	2:B:427:ASP:OD1	2.06	0.56
3:E:390:LEU:HD23	3:E:391:CYS:N	2.19	0.56
3:E:438:SER:O	3:E:438:SER:OG	2.21	0.56
3:E:493:GLN:N	3:E:493:GLN:HE21	2.03	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
3:E:341:VAL:HG21	3:E:356:LYS:HD3	1.84	0.56
2:B:538:PRO:HD2	2:B:541:LYS:HD2	1.88	0.56
1:C:108:HIS:ND1	1:C:109:PRO:HD2	2.21	0.56
3:F:341:VAL:HG21	3:F:356:LYS:HD3	1.84	0.56
1:A:489:ALA:HB2	1:A:589:VAL:HG12	1.88	0.55
1:C:483:SER:O	1:C:486:ASP:HB3	2.06	0.55
3:E:406:GLU:OE1	3:E:418:ILE:CG1	2.54	0.55
1:C:597:ILE:HB	1:C:598:PRO:CD	2.33	0.55
3:F:406:GLU:OE1	3:F:418:ILE:CG1	2.54	0.55
1:A:484:LEU:HG	1:A:485:LEU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:TRP:CZ3	1:C:466:THR:HG21	2.36	0.55
3:E:479:PRO:O	3:E:480:CYS:HB3	2.07	0.55
3:F:347:PHE:CE1	3:F:509:ARG:HD3	2.42	0.55
1:C:83:ILE:HB	1:C:84:PRO:CD	2.35	0.55
2:B:231:GLU:HA	2:B:234:LYS:HD3	1.88	0.55
3:E:347:PHE:CE1	3:E:509:ARG:HD3	2.42	0.55
3:F:392:PHE:HA	3:F:517:LEU:HD11	1.89	0.55
2:B:54:ILE:HD12	2:B:341:LYS:HG3	1.87	0.55
2:B:335:ASP:N	2:B:335:ASP:OD1	2.39	0.55
3:E:489:TYR:CD1	3:E:489:TYR:N	2.73	0.55
1:C:229:LEU:CB	1:C:230:PRO:HD3	2.29	0.55
3:F:489:TYR:CD1	3:F:489:TYR:N	2.73	0.55
1:A:83:ILE:HB	1:A:84:PRO:CD	2.35	0.55
2:B:735:ASN:O	2:B:736:GLN:HB3	2.05	0.55
2:D:167:SER:OG	2:D:168:TRP:N	2.39	0.55
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.55
2:B:739:VAL:O	2:B:740:SER:CB	2.56	0.54
1:C:414:PRO:O	1:C:418:VAL:HG23	2.07	0.54
1:C:484:LEU:HG	1:C:485:LEU:N	2.21	0.54
1:A:108:HIS:ND1	1:A:109:PRO:HD2	2.21	0.54
3:E:473:TYR:CG	3:E:474:GLN:N	2.72	0.54
1:A:414:PRO:O	1:A:418:VAL:HG23	2.07	0.54
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.54
4:J:1:NAG:C6	4:J:2:NAG:HN2	2.06	0.54
1:C:467:PHE:HD1	1:C:468:LEU:HD23	1.72	0.54
2:D:144:LEU:HD22	2:D:168:TRP:CZ2	2.43	0.54
3:F:492:LEU:C	3:F:493:GLN:HE21	2.10	0.54
1:A:607:ARG:HG3	1:A:607:ARG:HH21	1.72	0.54
1:C:205:TRP:CE2	1:C:466:THR:CG2	2.87	0.54
3:F:479:PRO:O	3:F:480:CYS:HB3	2.07	0.54
1:A:467:PHE:HD1	1:A:468:LEU:HD23	1.72	0.54
3:F:392:PHE:CD2	3:F:517:LEU:CD2	2.85	0.54
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.54
3:F:390:LEU:HD23	3:F:391:CYS:N	2.19	0.54
2:B:52:THR:OG1	2:B:332:MET:SD	2.66	0.54
1:A:209:TYR:HE2	1:A:460:GLY:N	2.07	0.53
1:C:593:PRO:O	1:C:596:THR:HB	2.09	0.53
2:B:697:ARG:NH1	2:B:701:GLU:OE2	2.41	0.53
3:E:392:PHE:HA	3:E:517:LEU:HD11	1.89	0.53
3:E:475:ALA:HB3	3:E:487:ASN:C	2.29	0.53
3:E:492:LEU:C	3:E:493:GLN:HE21	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:PRO:HG3	1:C:426:CYS:HB3	1.91	0.53
2:D:734:PRO:O	2:D:735:ASN:CB	2.56	0.53
3:F:475:ALA:HB3	3:F:487:ASN:HB2	1.89	0.53
3:F:478:THR:CG2	3:F:479:PRO:CD	2.86	0.53
1:A:230:PRO:HG3	1:A:426:CYS:HB3	1.91	0.53
3:F:482:GLY:O	3:F:483:VAL:HG22	2.08	0.53
2:B:144:LEU:HD22	2:B:168:TRP:CZ2	2.43	0.53
3:E:421:TYR:HA	3:E:461:LEU:HG	1.90	0.53
2:D:172:VAL:HG12	2:D:176:LEU:CD1	2.36	0.53
3:E:392:PHE:CD2	3:E:517:LEU:CD2	2.85	0.53
3:E:482:GLY:O	3:E:483:VAL:HG22	2.08	0.53
2:D:697:ARG:NH1	2:D:701:GLU:OE2	2.41	0.53
2:B:31:LYS:NZ	3:E:493:GLN:OE1	2.42	0.53
2:D:31:LYS:NZ	3:F:493:GLN:OE1	2.42	0.53
1:C:209:TYR:HE2	1:C:460:GLY:N	2.07	0.53
1:C:489:ALA:HB2	1:C:589:VAL:HG12	1.88	0.53
2:D:678:ARG:HH21	2:D:678:ARG:CG	2.13	0.53
2:D:739:VAL:O	2:D:740:SER:CB	2.56	0.53
1:A:598:PRO:O	1:A:602:ILE:HG12	2.09	0.53
2:B:741:ILE:HG22	2:B:741:ILE:O	2.09	0.52
1:A:231:TYR:HH	1:A:313:THR:HG1	1.55	0.52
2:B:622:ILE:HB	2:B:679:ILE:CG2	2.39	0.52
2:D:162:LEU:HD12	2:D:162:LEU:O	2.09	0.52
3:F:421:TYR:HA	3:F:461:LEU:HG	1.90	0.52
2:B:90:ASN:HB3	2:B:93:VAL:HG12	1.91	0.52
2:B:162:LEU:HD12	2:B:162:LEU:O	2.09	0.52
3:E:478:THR:CG2	3:E:479:PRO:CD	2.86	0.52
1:A:78:LEU:CD2	1:A:79:VAL:N	2.73	0.52
2:D:622:ILE:HB	2:D:679:ILE:CG2	2.39	0.52
1:A:593:PRO:O	1:A:596:THR:HB	2.09	0.52
1:A:607:ARG:NH2	1:A:607:ARG:CG	2.73	0.52
1:C:231:TYR:HH	1:C:313:THR:HG1	1.58	0.52
2:D:172:VAL:HG13	2:D:176:LEU:CD1	2.32	0.52
2:B:245:ARG:NH1	2:B:603:PHE:O	2.42	0.52
1:C:193:ILE:HG22	1:C:198:LEU:HD22	1.91	0.52
1:C:538:SER:O	1:C:542:MET:HE3	2.09	0.52
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.52
3:F:472:ILE:CG2	3:F:473:TYR:N	2.73	0.52
1:C:492:ILE:CG2	1:C:590:ALA:HB1	2.34	0.52
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.52
2:D:741:ILE:HG22	2:D:741:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LEU:HD13	2:B:501:ALA:O	2.10	0.52
3:E:472:ILE:CG2	3:E:473:TYR:N	2.73	0.52
3:E:493:GLN:NE2	3:E:493:GLN:CA	2.73	0.52
1:C:225:ILE:HG22	1:C:225:ILE:O	2.09	0.52
2:D:628:LEU:HB2	2:D:632:ALA:HB2	1.92	0.52
1:A:193:ILE:HG22	1:A:198:LEU:HD22	1.91	0.52
1:A:454:PRO:HB3	2:B:768:ARG:HH21	1.75	0.52
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
1:A:238:LEU:HD12	1:A:238:LEU:O	2.10	0.51
3:F:379:CYS:HB3	3:F:382:VAL:O	2.10	0.51
2:B:104:GLY:O	2:B:107:VAL:HG22	2.10	0.51
2:B:765:ILE:C	2:B:767:ASP:H	2.14	0.51
1:C:598:PRO:O	1:C:602:ILE:HG12	2.09	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
2:B:628:LEU:HB2	2:B:632:ALA:HB2	1.92	0.51
3:F:475:ALA:HB3	3:F:487:ASN:C	2.29	0.51
1:C:607:ARG:NH2	1:C:607:ARG:CG	2.73	0.51
1:A:66:GLY:HA3	1:A:69:ALA:HB3	1.93	0.51
3:E:490:PHE:CD1	3:E:491:PRO:CD	2.91	0.51
1:C:238:LEU:O	1:C:238:LEU:HD12	2.10	0.51
3:E:379:CYS:HB3	3:E:382:VAL:O	2.10	0.51
1:C:66:GLY:HA3	1:C:69:ALA:HB3	1.93	0.51
2:D:176:LEU:HD13	2:D:501:ALA:O	2.10	0.51
2:D:765:ILE:C	2:D:767:ASP:H	2.14	0.51
2:B:302:TRP:CH2	2:B:423:LEU:CD1	2.78	0.51
2:B:768:ARG:CG	2:B:768:ARG:NH1	2.73	0.51
3:E:348:ALA:HB2	3:E:354:ASN:ND2	2.26	0.51
1:C:454:PRO:HB3	2:D:768:ARG:HH21	1.75	0.51
1:A:225:ILE:HG22	1:A:225:ILE:O	2.09	0.50
1:C:454:PRO:CB	2:D:768:ARG:HH21	2.24	0.50
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.50
1:A:79:VAL:HG12	1:A:79:VAL:O	2.10	0.50
2:B:208:GLU:OE2	2:B:219:ARG:NH1	2.44	0.50
1:C:538:SER:O	1:C:542:MET:CE	2.59	0.50
3:E:475:ALA:HB3	3:E:487:ASN:HB2	1.89	0.50
1:A:538:SER:O	1:A:542:MET:CE	2.59	0.50
3:F:493:GLN:NE2	3:F:493:GLN:CA	2.73	0.50
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.50
3:F:479:PRO:HG2	3:F:480:CYS:H	1.77	0.50
1:A:80:LEU:HD13	1:A:537:VAL:HG11	1.94	0.50
2:B:335:ASP:CA	2:B:361:CYS:SG	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:403:ARG:NH1	3:E:405:ASP:OD1	2.43	0.50
1:C:78:LEU:CD2	1:C:79:VAL:N	2.73	0.50
1:C:80:LEU:HD13	1:C:537:VAL:HG11	1.94	0.50
3:F:348:ALA:HB2	3:F:354:ASN:ND2	2.26	0.50
2:B:394:ASN:HB2	2:B:562:LYS:HD2	1.92	0.50
3:E:401:VAL:HG22	3:E:509:ARG:HG2	1.94	0.50
2:B:433:GLU:O	2:B:437:ASN:ND2	2.44	0.49
2:B:564:GLU:HB3	2:B:568:LEU:HD23	1.95	0.49
3:F:401:VAL:HG22	3:F:509:ARG:HG2	1.94	0.49
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.49
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.49
1:A:207:VAL:HG22	2:B:753:ILE:HG13	1.94	0.49
2:B:734:PRO:O	2:B:735:ASN:CB	2.56	0.49
2:D:431:ASP:OD1	2:D:431:ASP:N	2.45	0.49
2:D:768:ARG:CG	2:D:768:ARG:NH1	2.73	0.49
2:B:342:ALA:O	2:B:343:VAL:C	2.50	0.49
3:F:475:ALA:CB	3:F:487:ASN:CA	2.91	0.49
3:E:475:ALA:CB	3:E:487:ASN:CA	2.91	0.49
3:F:437:ASN:OD1	3:F:438:SER:N	2.46	0.49
1:A:454:PRO:CB	2:B:768:ARG:HH21	2.24	0.49
2:B:678:ARG:O	2:B:679:ILE:HB	2.13	0.49
1:A:488:TYR:O	1:A:492:ILE:HG22	2.13	0.49
1:A:603:TYR:C	1:A:603:TYR:CD1	2.85	0.49
2:B:171:GLU:HG2	2:B:171:GLU:H	1.47	0.49
3:E:478:THR:HG22	3:E:479:PRO:N	2.28	0.49
1:C:352:GLU:OE2	2:D:623:SER:CB	2.61	0.49
3:E:488:CYS:C	3:E:489:TYR:CG	2.86	0.49
1:C:467:PHE:CD1	1:C:468:LEU:HD23	2.47	0.49
3:E:479:PRO:HG2	3:E:480:CYS:H	1.77	0.49
1:C:79:VAL:HG12	1:C:79:VAL:O	2.10	0.49
1:A:467:PHE:CD1	1:A:468:LEU:HD23	2.47	0.48
3:E:437:ASN:OD1	3:E:438:SER:N	2.46	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.95	0.48
2:B:34:HIS:HE1	3:E:493:GLN:HG3	1.66	0.48
1:C:488:TYR:O	1:C:492:ILE:HG22	2.13	0.48
1:C:591:GLY:O	1:C:593:PRO:N	2.46	0.48
1:C:607:ARG:HG3	1:C:607:ARG:HH21	1.72	0.48
3:F:431:GLY:HA3	3:F:513:LEU:O	2.12	0.48
3:E:431:GLY:HA3	3:E:513:LEU:O	2.12	0.48
3:E:501:ASN:N	3:E:501:ASN:HD22	2.11	0.48
2:D:676:LYS:HB3	2:D:677:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:478:THR:HG22	3:F:479:PRO:N	2.28	0.48
3:F:488:CYS:C	3:F:489:TYR:CG	2.86	0.48
1:A:352:GLU:OE2	2:B:623:SER:CB	2.61	0.48
3:E:486:PHE:CD2	3:E:487:ASN:ND2	2.82	0.48
2:D:631:LYS:HB2	2:D:631:LYS:HZ3	1.78	0.48
2:D:678:ARG:O	2:D:679:ILE:HB	2.13	0.48
3:F:501:ASN:N	3:F:501:ASN:HD22	2.11	0.48
1:A:340:ASN:HD21	1:A:381:GLN:HB2	1.79	0.48
3:F:438:SER:O	3:F:438:SER:OG	2.21	0.48
2:B:105:SER:C	2:B:106:SER:HG	2.07	0.48
2:B:421:ILE:HG13	2:B:421:ILE:O	2.14	0.48
1:C:340:ASN:HD21	1:C:381:GLN:HB2	1.79	0.48
1:C:603:TYR:CD1	1:C:603:TYR:C	2.85	0.48
1:A:591:GLY:O	1:A:593:PRO:N	2.46	0.48
1:A:540:LEU:O	1:A:544:ILE:HG12	2.14	0.47
2:D:175:GLN:O	2:D:178:PRO:HD2	2.14	0.47
2:B:676:LYS:HB3	2:B:677:PRO:HD2	1.95	0.47
3:E:516:GLU:C	3:E:517:LEU:CD2	2.82	0.47
3:F:516:GLU:C	3:F:517:LEU:CD2	2.82	0.47
1:A:341:ILE:HD12	1:A:355:VAL:HG12	1.97	0.47
2:D:421:ILE:HG13	2:D:421:ILE:O	2.14	0.47
2:D:735:ASN:CG	2:D:736:GLN:N	2.68	0.47
1:A:114:LEU:HD21	1:A:500:CYS:HB3	1.97	0.47
2:B:129:THR:O	2:D:139:GLN:CG	2.63	0.47
2:B:172:VAL:HG12	2:B:176:LEU:CD1	2.36	0.47
1:C:221:LYS:O	1:C:224:TYR:HB2	2.15	0.47
1:A:352:GLU:OE2	2:B:623:SER:HB3	2.14	0.47
1:C:207:VAL:HG22	2:D:753:ILE:HG13	1.94	0.47
3:F:385:THR:HG1	3:F:386:LYS:HZ3	1.59	0.47
1:A:156:ASN:HB2	1:A:158:ASN:O	2.15	0.47
1:A:229:LEU:CB	1:A:230:PRO:HD3	2.29	0.47
1:A:538:SER:O	1:A:542:MET:HE3	2.15	0.47
2:B:735:ASN:CG	2:B:736:GLN:N	2.68	0.47
2:B:175:GLN:O	2:B:178:PRO:HD2	2.14	0.47
2:B:333:LEU:O	2:B:362:THR:HG22	2.15	0.47
2:B:631:LYS:HB2	2:B:631:LYS:HZ3	1.80	0.47
3:E:369:TYR:CE2	3:E:384:PRO:HB2	2.50	0.47
1:C:341:ILE:HD12	1:C:355:VAL:HG12	1.97	0.47
1:C:352:GLU:OE2	2:D:623:SER:HB3	2.14	0.47
2:D:171:GLU:HG2	2:D:171:GLU:H	1.47	0.47
3:F:486:PHE:CD2	3:F:487:ASN:ND2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:SER:C	2:B:427:ASP:H	2.19	0.47
1:C:114:LEU:HD21	1:C:500:CYS:HB3	1.97	0.47
1:A:489:ALA:HB2	1:A:589:VAL:HG11	1.91	0.47
2:B:139:GLN:CG	2:D:129:THR:O	2.63	0.47
3:F:369:TYR:CE2	3:F:384:PRO:HB2	2.50	0.47
3:E:364:ASP:O	3:E:367:VAL:HG12	2.15	0.46
1:C:32:ARG:NH2	1:C:291:SER:OG	2.46	0.46
2:D:177:ARG:CB	2:D:178:PRO:CD	2.89	0.46
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.46
3:F:490:PHE:CD1	3:F:491:PRO:CD	2.91	0.46
1:A:221:LYS:O	1:A:224:TYR:HB2	2.15	0.46
1:A:159:GLN:HG2	2:B:733:PRO:HB3	1.98	0.46
1:A:592:VAL:CG2	1:A:593:PRO:CD	2.72	0.46
3:E:470:THR:CG2	3:E:490:PHE:CZ	2.98	0.46
1:C:540:LEU:O	1:C:544:ILE:HG12	2.14	0.46
3:F:364:ASP:O	3:F:367:VAL:HG12	2.15	0.46
4:R:2:NAG:C3	4:R:2:NAG:H83	2.45	0.46
1:A:74:PHE:CD2	1:A:75:LEU:HD23	2.51	0.46
3:E:500:THR:C	3:E:501:ASN:HD22	2.19	0.46
1:A:544:ILE:O	1:A:547:LEU:N	2.47	0.46
2:B:709:SER:OG	2:D:716:ARG:NH1	2.49	0.46
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.46
4:J:2:NAG:C3	4:J:2:NAG:H83	2.45	0.46
1:A:340:ASN:HD21	1:A:381:GLN:H	1.64	0.46
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.46
2:B:52:THR:HA	2:B:342:ALA:HB1	1.98	0.46
1:C:156:ASN:HB2	1:C:158:ASN:O	2.15	0.46
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.46
3:F:470:THR:CG2	3:F:490:PHE:CZ	2.98	0.46
1:C:467:PHE:CD1	1:C:467:PHE:C	2.89	0.46
2:D:34:HIS:HE1	3:F:493:GLN:HG3	1.66	0.46
2:B:356:PHE:HB3	2:B:379:ILE:HD12	1.98	0.45
2:B:716:ARG:NH1	2:D:709:SER:OG	2.49	0.45
3:F:403:ARG:NH1	3:F:405:ASP:OD1	2.43	0.45
3:F:500:THR:C	3:F:501:ASN:HD22	2.19	0.45
1:C:74:PHE:CD2	1:C:75:LEU:HD23	2.51	0.45
1:C:458:LEU:O	1:C:462:ILE:HD13	2.16	0.45
2:D:24:GLN:NE2	3:F:487:ASN:OD1	2.48	0.45
1:A:221:LYS:H	1:A:221:LYS:CD	2.08	0.45
3:F:493:GLN:NE2	3:F:493:GLN:N	2.65	0.45
1:A:467:PHE:CD1	1:A:467:PHE:C	2.89	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ILE:HD11	1:A:546:PHE:CE1	2.52	0.45
3:E:377:PHE:CD2	3:E:434:ILE:HG12	2.51	0.45
2:D:34:HIS:HE1	3:F:493:GLN:HB3	1.76	0.45
3:F:447:GLY:HA2	3:F:497:PHE:O	2.16	0.45
1:A:462:ILE:N	1:A:462:ILE:CD1	2.80	0.45
1:C:489:ALA:HB2	1:C:589:VAL:HG11	1.91	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
3:F:472:ILE:CD1	3:F:482:GLY:HA2	2.40	0.45
2:B:143:LEU:C	2:B:143:LEU:CD2	2.85	0.45
2:B:560:LEU:HD22	2:B:564:GLU:HG3	1.98	0.45
3:E:493:GLN:NE2	3:E:493:GLN:N	2.65	0.45
1:C:159:GLN:HG2	2:D:733:PRO:HB3	1.98	0.45
1:C:601:ALA:O	1:C:605:LEU:HG	2.17	0.45
1:A:562:ILE:HG22	1:A:564:ASP:HB2	1.99	0.45
1:C:462:ILE:CD1	1:C:462:ILE:N	2.80	0.45
1:A:458:LEU:O	1:A:462:ILE:HD13	2.16	0.45
1:C:340:ASN:HD21	1:C:381:GLN:H	1.64	0.45
3:F:377:PHE:CD2	3:F:434:ILE:HG12	2.51	0.45
1:C:74:PHE:HD2	1:C:75:LEU:HD23	1.82	0.45
2:D:132:VAL:O	2:D:141:CYS:HA	2.17	0.45
1:A:351:PRO:HD3	2:B:677:PRO:HG2	2.00	0.44
1:A:601:ALA:O	1:A:605:LEU:HG	2.17	0.44
2:B:176:LEU:O	2:B:180:TYR:HB2	2.17	0.44
3:E:447:GLY:HA2	3:E:497:PHE:O	2.16	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
3:F:440:ASN:ND2	3:F:441:LEU:HG	2.32	0.44
3:E:440:ASN:ND2	3:E:441:LEU:HG	2.32	0.44
1:A:74:PHE:HD2	1:A:75:LEU:HD23	1.82	0.44
1:C:496:ILE:HD11	1:C:546:PHE:CE1	2.52	0.44
2:D:143:LEU:C	2:D:143:LEU:CD2	2.85	0.44
3:E:472:ILE:CD1	3:E:482:GLY:HA2	2.40	0.44
1:C:351:PRO:HD3	2:D:677:PRO:HG2	2.00	0.44
2:D:174:LYS:HG2	2:D:174:LYS:H	1.54	0.44
2:D:176:LEU:O	2:D:180:TYR:HB2	2.17	0.44
2:B:166:GLU:OE1	2:B:493:HIS:HE1	2.01	0.44
3:E:472:ILE:HD12	3:E:482:GLY:CA	2.41	0.44
2:B:24:GLN:NE2	3:E:487:ASN:OD1	2.48	0.44
2:B:208:GLU:OE1	2:B:210:ASN:ND2	2.50	0.44
1:A:544:ILE:C	1:A:546:PHE:N	2.71	0.44
1:C:17:SER:O	1:C:17:SER:OG	2.33	0.44
1:C:230:PRO:HB3	1:C:427:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:ILE:C	1:C:546:PHE:N	2.71	0.44
1:A:32:ARG:NH2	1:A:291:SER:OG	2.46	0.43
1:C:229:LEU:HD12	1:C:229:LEU:HA	1.78	0.43
1:C:544:ILE:O	1:C:547:LEU:N	2.47	0.43
3:F:482:GLY:C	3:F:483:VAL:CG2	2.86	0.43
1:C:219:THR:HG22	1:C:219:THR:O	2.18	0.43
1:A:229:LEU:CB	1:A:230:PRO:CD	2.88	0.43
1:A:276:PHE:C	1:A:494:LEU:HD13	2.39	0.43
2:B:132:VAL:O	2:B:141:CYS:HA	2.17	0.43
2:B:353:LYS:HA	3:E:505:TYR:CE2	2.53	0.43
1:C:291:SER:OG	1:C:291:SER:O	2.37	0.43
3:F:472:ILE:HD12	3:F:482:GLY:CA	2.41	0.43
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.86	0.43
1:C:562:ILE:HG22	1:C:564:ASP:HB2	1.99	0.43
2:B:144:LEU:HD12	2:B:144:LEU:O	2.19	0.43
1:C:276:PHE:C	1:C:494:LEU:HD13	2.39	0.43
1:C:542:MET:HE3	1:C:542:MET:HB2	1.82	0.43
1:A:63:GLN:HE22	1:A:393:VAL:HG21	1.84	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
2:B:313:LYS:HA	2:B:316:VAL:HG12	2.00	0.43
1:C:515:ASN:HD21	1:C:531:GLN:HE22	1.67	0.43
2:D:353:LYS:HA	3:F:505:TYR:CE2	2.53	0.43
1:A:83:ILE:HG22	1:A:530:TRP:CZ3	2.54	0.43
1:A:230:PRO:HB3	1:A:427:LEU:CD2	2.48	0.43
1:C:205:TRP:CE3	1:C:208:LEU:HD23	2.54	0.43
1:C:464:LEU:HD12	1:C:464:LEU:HA	1.86	0.43
3:E:472:ILE:HD12	3:E:483:VAL:H	1.84	0.42
1:C:259:VAL:HA	1:C:262:LEU:HD13	2.01	0.42
2:D:738:PRO:HD2	2:D:739:VAL:HG12	2.01	0.42
1:A:282:ALA:HB1	1:A:497:ILE:HB	2.01	0.42
2:B:736:GLN:NE2	2:B:736:GLN:C	2.73	0.42
1:A:533:THR:HA	1:A:537:VAL:HB	2.02	0.42
3:E:478:THR:HG22	3:E:479:PRO:CD	2.49	0.42
2:D:736:GLN:NE2	2:D:736:GLN:C	2.73	0.42
3:F:516:GLU:C	3:F:517:LEU:HD23	2.39	0.42
1:A:422:ILE:HG13	1:A:423:MET:N	2.33	0.42
2:B:82:MET:HB3	3:E:486:PHE:CZ	2.55	0.42
1:C:544:ILE:O	1:C:546:PHE:N	2.53	0.42
2:D:144:LEU:HD12	2:D:144:LEU:O	2.19	0.42
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.42
3:F:472:ILE:HD12	3:F:483:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:219:THR:HG22	2.18	0.42
1:C:83:ILE:HG22	1:C:530:TRP:CZ3	2.54	0.42
2:D:82:MET:HB3	3:F:486:PHE:CZ	2.55	0.42
2:D:166:GLU:OE1	2:D:493:HIS:HE1	2.01	0.42
1:A:205:TRP:CE3	1:A:208:LEU:HD23	2.54	0.42
2:B:379:ILE:HD13	2:B:379:ILE:HA	1.92	0.42
2:B:425:SER:C	2:B:427:ASP:N	2.73	0.42
1:C:63:GLN:HE22	1:C:393:VAL:HG21	1.84	0.42
1:C:422:ILE:HG13	1:C:423:MET:N	2.33	0.42
1:C:592:VAL:CG2	1:C:593:PRO:CD	2.72	0.42
4:J:2:NAG:H83	4:J:2:NAG:H3	2.02	0.42
3:E:516:GLU:C	3:E:517:LEU:HD23	2.39	0.42
1:C:72:ILE:HB	1:C:73:PRO:CD	2.49	0.42
1:A:87:TYR:CD2	1:A:534:TRP:CZ2	3.06	0.42
1:A:515:ASN:HD21	1:A:531:GLN:HE22	1.67	0.42
2:B:174:LYS:HG2	2:B:174:LYS:H	1.54	0.42
3:E:340:GLU:H	3:E:340:GLU:CD	2.09	0.42
2:D:103:ASN:H	4:R:1:NAG:H82	1.85	0.42
2:B:678:ARG:HH21	2:B:678:ARG:CG	2.13	0.42
3:E:406:GLU:CG	3:E:418:ILE:HG13	2.50	0.42
3:E:473:TYR:CD2	3:E:474:GLN:N	2.72	0.42
2:D:354:GLY:O	3:F:502:GLY:HA3	2.20	0.42
3:F:406:GLU:CG	3:F:418:ILE:HG13	2.50	0.42
3:F:473:TYR:CD2	3:F:474:GLN:N	2.72	0.42
1:A:544:ILE:O	1:A:546:PHE:N	2.53	0.41
3:F:478:THR:HG22	3:F:479:PRO:CD	2.49	0.41
1:C:282:ALA:HB1	1:C:497:ILE:HB	2.01	0.41
2:D:254:SER:O	2:D:254:SER:OG	2.31	0.41
1:A:87:TYR:HE1	1:A:300:GLU:HA	1.84	0.41
1:A:259:VAL:HA	1:A:262:LEU:HD13	2.01	0.41
3:E:385:THR:HG1	3:E:386:LYS:HZ3	1.59	0.41
3:E:393:THR:H	3:E:517:LEU:HD22	1.85	0.41
4:R:2:NAG:H83	4:R:2:NAG:H3	2.02	0.41
2:B:738:PRO:HD2	2:B:739:VAL:HG12	2.01	0.41
1:C:87:TYR:HE1	1:C:300:GLU:HA	1.84	0.41
3:F:470:THR:HG21	3:F:490:PHE:CZ	2.56	0.41
2:B:212:VAL:HG23	2:B:215:TYR:HB2	2.02	0.41
2:B:354:GLY:O	3:E:502:GLY:HA3	2.20	0.41
2:B:411:SER:OG	2:B:543:ASP:OD1	2.38	0.41
1:C:606:ILE:C	1:C:608:ASN:N	2.74	0.41
3:F:393:THR:H	3:F:517:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:500:THR:O	3:F:500:THR:OG1	2.31	0.41
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.87	0.41
1:A:606:ILE:C	1:A:608:ASN:N	2.74	0.41
1:A:72:ILE:H	1:A:72:ILE:CD1	2.30	0.41
1:A:135:TRP:HZ3	1:A:396:THR:HG21	1.86	0.41
1:A:209:TYR:CD2	1:A:460:GLY:HA2	2.55	0.41
1:A:589:VAL:HG12	1:A:589:VAL:O	2.20	0.41
2:B:735:ASN:CG	2:B:736:GLN:H	2.24	0.41
1:C:107:ILE:O	1:C:108:HIS:CB	2.69	0.41
2:D:39:LEU:HD23	2:D:39:LEU:HA	1.93	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
1:C:209:TYR:CD2	1:C:460:GLY:HA2	2.55	0.41
1:C:589:VAL:HG12	1:C:589:VAL:O	2.20	0.41
2:B:103:ASN:H	4:J:1:NAG:H82	1.85	0.41
2:B:168:TRP:CH2	2:B:172:VAL:HG21	2.55	0.41
3:E:470:THR:HG21	3:E:490:PHE:CZ	2.56	0.41
3:E:480:CYS:SG	3:E:480:CYS:O	2.79	0.41
1:C:21:LEU:HA	1:C:24:ILE:HG22	2.03	0.41
1:C:492:ILE:CG2	1:C:493:PRO:CD	2.73	0.41
1:C:533:THR:HA	1:C:537:VAL:HB	2.02	0.41
2:D:168:TRP:CH2	2:D:172:VAL:HG21	2.55	0.41
2:D:739:VAL:O	2:D:739:VAL:HG22	2.21	0.41
3:F:480:CYS:O	3:F:480:CYS:SG	2.79	0.41
3:F:484:GLU:H	3:F:484:GLU:HG3	1.61	0.41
1:A:72:ILE:N	1:A:72:ILE:CD1	2.83	0.41
2:B:165:TRP:O	2:B:169:ARG:HB2	2.21	0.41
1:C:209:TYR:CD1	1:C:209:TYR:O	2.74	0.41
1:C:452:LYS:HE3	1:C:452:LYS:HB3	1.95	0.41
1:C:580:ASN:HD22	1:C:580:ASN:HA	1.64	0.41
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.41
2:B:553:LYS:HE3	2:B:553:LYS:HB3	1.89	0.40
2:B:677:PRO:C	2:B:679:ILE:N	2.75	0.40
1:C:81:GLU:OE2	1:C:541:LEU:HD23	2.21	0.40
1:A:580:ASN:HD22	1:A:580:ASN:HA	1.64	0.40
1:C:351:PRO:HD3	2:D:677:PRO:CG	2.51	0.40
2:D:97:LEU:HD23	2:D:97:LEU:HA	1.88	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
3:F:460:ASN:N	3:F:460:ASN:OD1	2.53	0.40
1:A:72:ILE:HB	1:A:73:PRO:CD	2.49	0.40
1:A:209:TYR:O	1:A:209:TYR:CD1	2.74	0.40
1:A:492:ILE:CG2	1:A:590:ALA:CB	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:472:ILE:CD1	3:E:483:VAL:N	2.84	0.40
3:F:472:ILE:CD1	3:F:483:VAL:N	2.84	0.40
1:A:21:LEU:HA	1:A:24:ILE:HG22	2.03	0.40
3:E:369:TYR:CZ	3:E:384:PRO:HB2	2.57	0.40
1:C:469:ILE:HG22	1:C:469:ILE:O	2.22	0.40
1:C:482:LEU:O	1:C:486:ASP:CB	2.69	0.40
2:D:735:ASN:CG	2:D:736:GLN:H	2.24	0.40
3:F:369:TYR:CZ	3:F:384:PRO:HB2	2.57	0.40
1:A:81:GLU:OE2	1:A:541:LEU:HD23	2.21	0.40
1:A:83:ILE:CB	1:A:84:PRO:HD3	2.40	0.40
1:A:469:ILE:O	1:A:469:ILE:HG22	2.22	0.40
2:B:170:SER:OG	2:B:171:GLU:N	2.55	0.40
1:C:328:ARG:HD3	1:C:402:VAL:HG13	2.04	0.40
2:D:92:THR:HG22	2:D:96:GLN:HE21	1.87	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	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	22	54
1	C	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	22	54
2	B	746/814 (92%)	684 (92%)	52 (7%)	10 (1%)	12	37
2	D	746/814 (92%)	684 (92%)	52 (7%)	10 (1%)	12	37
3	E	181/223 (81%)	135 (75%)	34 (19%)	12 (7%)	1	3
3	F	181/223 (81%)	135 (75%)	34 (19%)	12 (7%)	1	3
All	All	3060/3382 (90%)	2718 (89%)	290 (10%)	52 (2%)	13	31

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	LEU
2	B	631	LYS
2	B	736	GLN
3	E	341	VAL
3	E	479	PRO
3	E	483	VAL
2	D	144	LEU
2	D	631	LYS
2	D	736	GLN
3	F	341	VAL
3	F	479	PRO
3	F	483	VAL
2	B	343	VAL
2	B	679	ILE
2	B	735	ASN
2	B	739	VAL
3	E	339	GLY
3	E	481	ASN
3	E	482	GLY
3	E	484	GLU
3	E	488	CYS
2	D	343	VAL
2	D	679	ILE
2	D	735	ASN
2	D	739	VAL
3	F	339	GLY
3	F	481	ASN
3	F	482	GLY
3	F	484	GLU
3	F	488	CYS
1	A	486	ASP
2	B	169	ARG
2	B	423	LEU
1	C	486	ASP
2	D	169	ARG
2	D	423	LEU
1	A	108	HIS
1	A	592	VAL
3	E	349	SER
3	E	472	ILE
3	E	480	CYS
1	C	108	HIS
1	C	592	VAL

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Mol	Chain	Res	Type
3	F	349	SER
3	F	472	ILE
3	F	480	CYS
3	E	337	PRO
3	F	337	PRO
1	A	593	PRO
1	C	593	PRO
2	B	738	PRO
2	D	738	PRO

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	531/572 (93%)	509 (96%)	22 (4%)	30	64
1	C	531/572 (93%)	509 (96%)	22 (4%)	30	64
2	B	662/720 (92%)	638 (96%)	24 (4%)	35	69
2	D	662/720 (92%)	638 (96%)	24 (4%)	35	69
3	E	159/196 (81%)	136 (86%)	23 (14%)	3	9
3	F	159/196 (81%)	136 (86%)	23 (14%)	3	9
All	All	2704/2976 (91%)	2566 (95%)	138 (5%)	27	56

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ILE
1	A	80	LEU
1	A	81	GLU
1	A	95	ARG
1	A	157	GLU
1	A	159	GLN
1	A	217	GLU
1	A	221	LYS
1	A	224	TYR

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Mol	Chain	Res	Type
1	A	226	THR
1	A	228	THR
1	A	234	LEU
1	A	237	PHE
1	A	419	LEU
1	A	461	LEU
1	A	462	ILE
1	A	466	THR
1	A	484	LEU
1	A	485	LEU
1	A	541	LEU
1	A	592	VAL
1	A	607	ARG
2	B	30	ASP
2	B	31	LYS
2	B	42	GLN
2	B	82	MET
2	B	107	VAL
2	B	128	SER
2	B	143	LEU
2	B	166	GLU
2	B	169	ARG
2	B	171	GLU
2	B	175	GLN
2	B	344	CYS
2	B	345	HIS
2	B	347	THR
2	B	361	CYS
2	B	423	LEU
2	B	425	SER
2	B	628	LEU
2	B	630	ASP
2	B	678	ARG
2	B	680	SER
2	B	736	GLN
2	B	740	SER
2	B	768	ARG
3	E	336	CYS
3	E	340	GLU
3	E	353	TRP
3	E	355	ARG
3	E	375	SER

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Mol	Chain	Res	Type
3	E	383	SER
3	E	389	ASP
3	E	390	LEU
3	E	406	GLU
3	E	421	TYR
3	E	430	THR
3	E	438	SER
3	E	440	ASN
3	E	483	VAL
3	E	484	GLU
3	E	489	TYR
3	E	490	PHE
3	E	493	GLN
3	E	500	THR
3	E	501	ASN
3	E	514	SER
3	E	517	LEU
3	E	518	LEU
1	C	76	ILE
1	C	80	LEU
1	C	81	GLU
1	C	95	ARG
1	C	157	GLU
1	C	159	GLN
1	C	217	GLU
1	C	221	LYS
1	C	224	TYR
1	C	226	THR
1	C	228	THR
1	C	234	LEU
1	C	237	PHE
1	C	419	LEU
1	C	461	LEU
1	C	462	ILE
1	C	466	THR
1	C	484	LEU
1	C	485	LEU
1	C	541	LEU
1	C	592	VAL
1	C	607	ARG
2	D	30	ASP
2	D	31	LYS

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Mol	Chain	Res	Type
2	D	42	GLN
2	D	82	MET
2	D	107	VAL
2	D	128	SER
2	D	143	LEU
2	D	166	GLU
2	D	169	ARG
2	D	171	GLU
2	D	175	GLN
2	D	344	CYS
2	D	345	HIS
2	D	347	THR
2	D	361	CYS
2	D	423	LEU
2	D	425	SER
2	D	628	LEU
2	D	630	ASP
2	D	678	ARG
2	D	680	SER
2	D	736	GLN
2	D	740	SER
2	D	768	ARG
3	F	336	CYS
3	F	340	GLU
3	F	353	TRP
3	F	355	ARG
3	F	375	SER
3	F	383	SER
3	F	389	ASP
3	F	390	LEU
3	F	406	GLU
3	F	421	TYR
3	F	430	THR
3	F	438	SER
3	F	440	ASN
3	F	483	VAL
3	F	484	GLU
3	F	489	TYR
3	F	490	PHE
3	F	493	GLN
3	F	500	THR
3	F	501	ASN

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Mol	Chain	Res	Type
3	F	514	SER
3	F	517	LEU
3	F	518	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	194	GLN
1	A	310	ASN
1	A	340	ASN
1	A	515	ASN
1	A	580	ASN
1	A	609	HIS
2	B	58	ASN
2	B	96	GLN
2	B	159	ASN
2	B	175	GLN
2	B	239	HIS
2	B	277	ASN
2	B	378	HIS
2	B	472	GLN
2	B	493	HIS
2	B	505	HIS
2	B	586	ASN
2	B	735	ASN
2	B	736	GLN
3	E	354	ASN
3	E	360	ASN
3	E	394	ASN
3	E	422	ASN
3	E	440	ASN
3	E	501	ASN
1	C	159	GLN
1	C	194	GLN
1	C	310	ASN
1	C	340	ASN
1	C	515	ASN
1	C	580	ASN
1	C	609	HIS
2	D	58	ASN
2	D	96	GLN

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Mol	Chain	Res	Type
2	D	159	ASN
2	D	175	GLN
2	D	239	HIS
2	D	277	ASN
2	D	378	HIS
2	D	472	GLN
2	D	493	HIS
2	D	505	HIS
2	D	586	ASN
2	D	735	ASN
2	D	736	GLN
3	F	354	ASN
3	F	360	ASN
3	F	394	ASN
3	F	422	ASN
3	F	440	ASN
3	F	501	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

34 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	G	1	1,4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	G	2	4	14,14,15	0.32	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	H	1	2,4	14,14,15	0.61	1 (7%)	17,19,21	0.73	0
4	NAG	H	2	4	14,14,15	0.53	0	17,19,21	0.36	0
4	NAG	I	1	2,4	14,14,15	0.40	0	17,19,21	0.65	0
4	NAG	I	2	4	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
4	NAG	J	1	2,4	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	K	1	2,4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	K	2	4	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	L	1	2,4	14,14,15	0.23	0	17,19,21	0.61	0
4	NAG	L	2	4	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
4	NAG	M	1	2,4	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	M	2	4	14,14,15	0.22	0	17,19,21	0.57	0
5	NAG	N	1	5,3	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	N	2	5	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	N	3	5	14,14,15	0.29	0	17,19,21	0.61	0
4	NAG	O	1	1,4	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	O	2	4	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	P	1	2,4	14,14,15	0.61	1 (7%)	17,19,21	0.73	0
4	NAG	P	2	4	14,14,15	0.53	0	17,19,21	0.36	0
4	NAG	Q	1	2,4	14,14,15	0.40	0	17,19,21	0.65	0
4	NAG	Q	2	4	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
4	NAG	R	1	2,4	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	R	2	4	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	S	1	2,4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	S	2	4	14,14,15	0.35	0	17,19,21	0.47	0
4	NAG	T	1	2,4	14,14,15	0.23	0	17,19,21	0.61	0
4	NAG	T	2	4	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
4	NAG	U	1	2,4	14,14,15	0.25	0	17,19,21	0.56	0
4	NAG	U	2	4	14,14,15	0.22	0	17,19,21	0.57	0
5	NAG	V	1	5,3	14,14,15	0.28	0	17,19,21	0.62	0
5	NAG	V	2	5	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	V	3	5	14,14,15	0.29	0	17,19,21	0.61	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	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	O5-C1	-2.11	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	1	NAG	O5-C1	-2.11	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	2	NAG	C1-O5-C5	2.45	115.51	112.19
4	Q	2	NAG	C1-O5-C5	2.45	115.51	112.19
4	L	2	NAG	C1-O5-C5	2.05	114.97	112.19
4	T	2	NAG	C1-O5-C5	2.05	114.97	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	R	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	V	1	NAG	C8-C7-N2-C2
5	V	1	NAG	O7-C7-N2-C2
5	V	2	NAG	C8-C7-N2-C2
5	V	2	NAG	O7-C7-N2-C2
4	M	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	J	1	NAG	C8-C7-N2-C2
4	R	1	NAG	C8-C7-N2-C2
5	N	3	NAG	C8-C7-N2-C2
5	N	3	NAG	O7-C7-N2-C2
5	V	3	NAG	C8-C7-N2-C2
5	V	3	NAG	O7-C7-N2-C2
4	L	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	P	1	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	V	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	J	2	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
5	N	1	NAG	C1-C2-N2-C7
5	V	1	NAG	C1-C2-N2-C7
4	G	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
5	N	1	NAG	C3-C2-N2-C7
5	V	1	NAG	C3-C2-N2-C7
4	G	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6

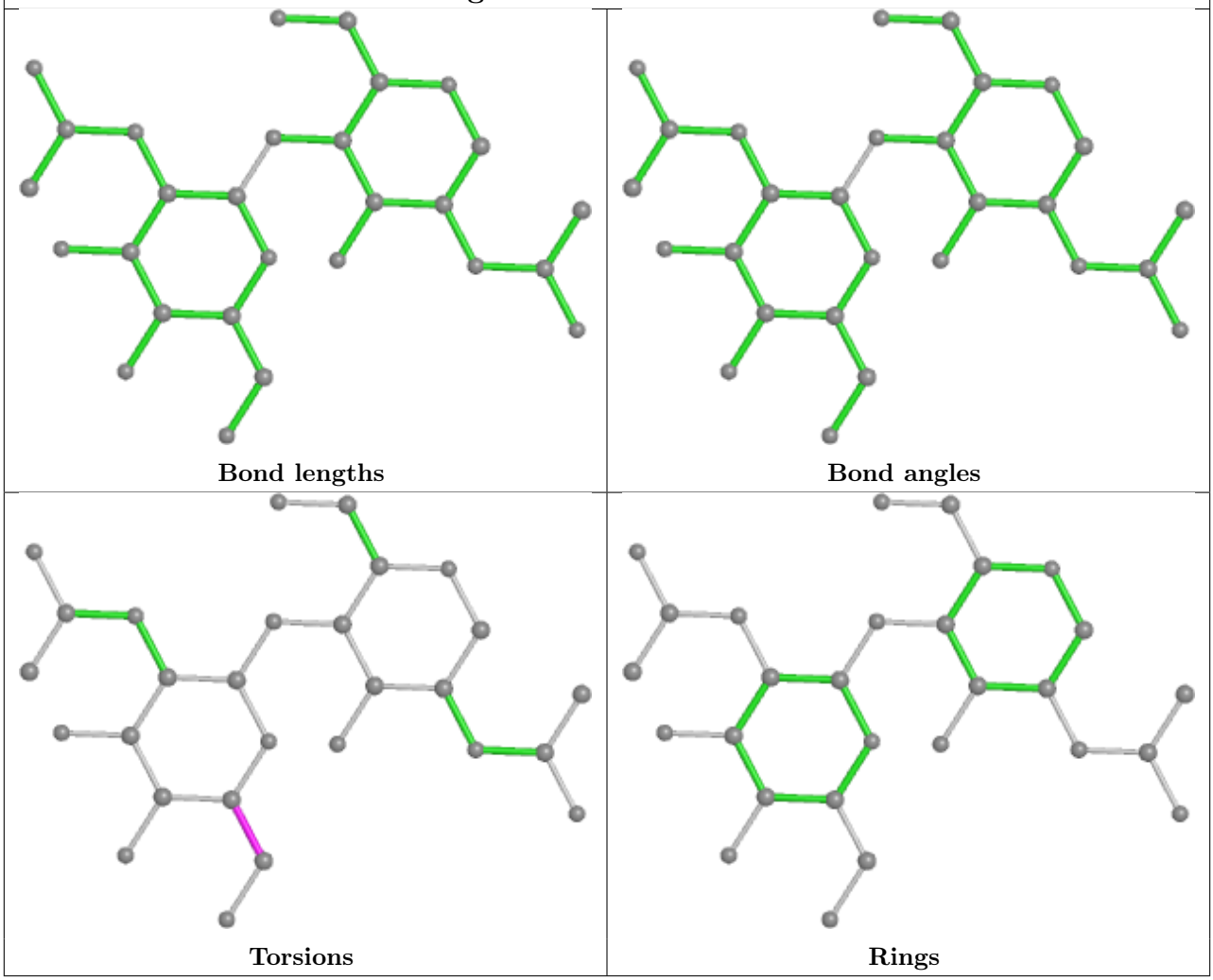
There are no ring outliers.

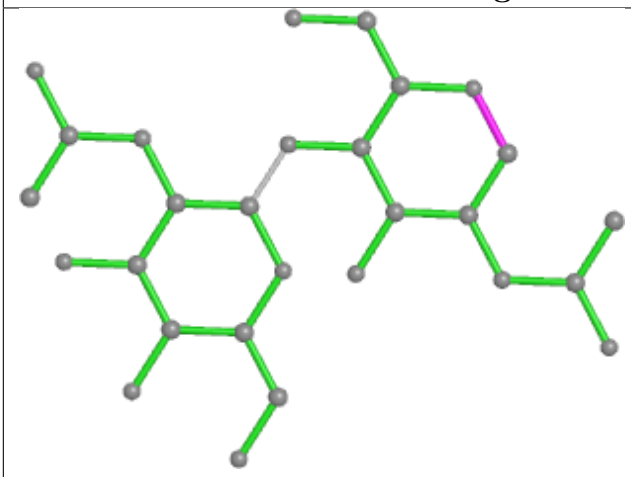
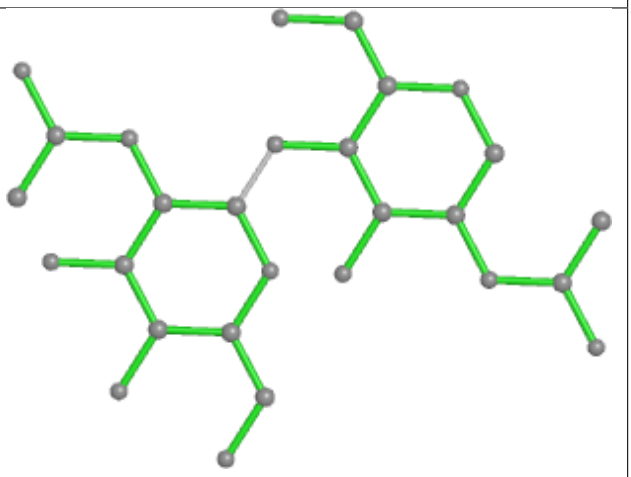
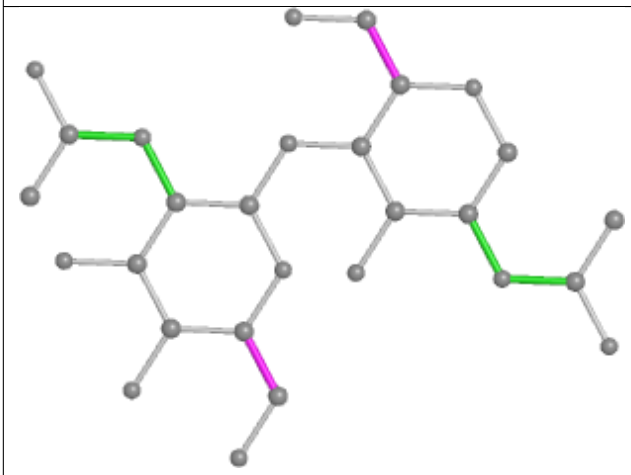
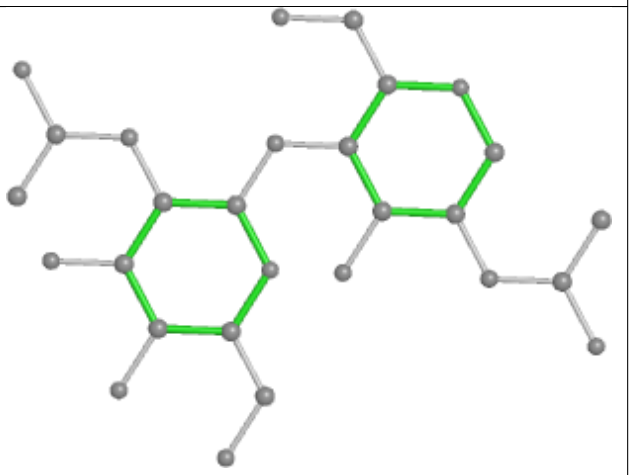
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	2	NAG	5	0
4	J	1	NAG	4	0
4	J	2	NAG	5	0
4	R	1	NAG	4	0

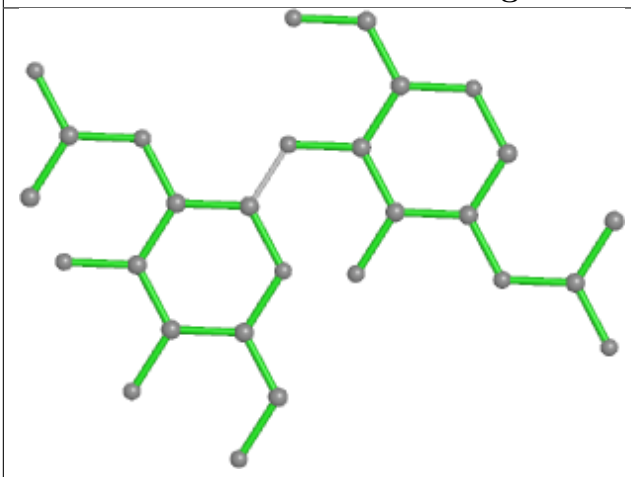
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain G

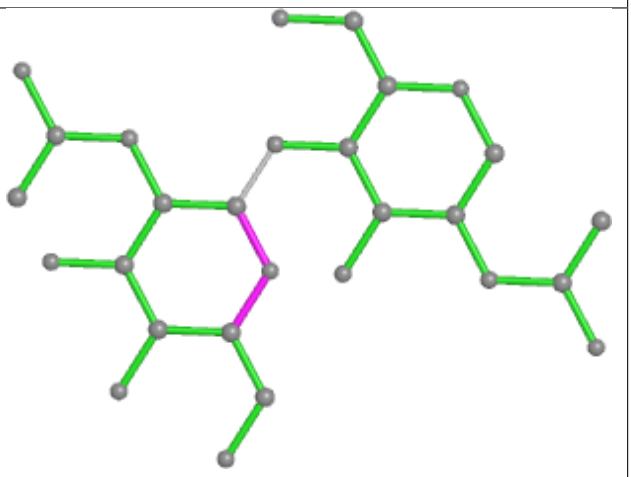


Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

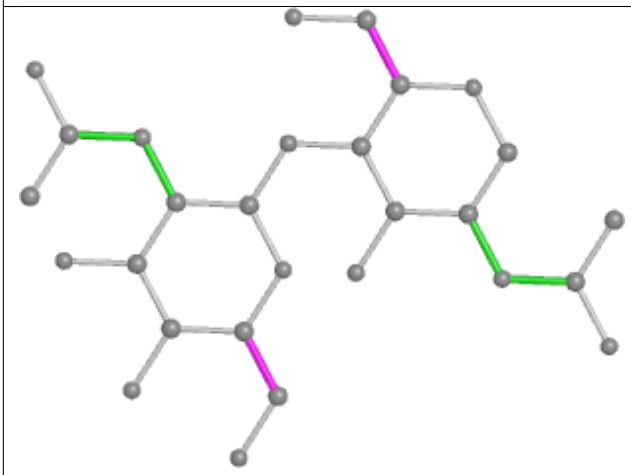
Oligosaccharide Chain I



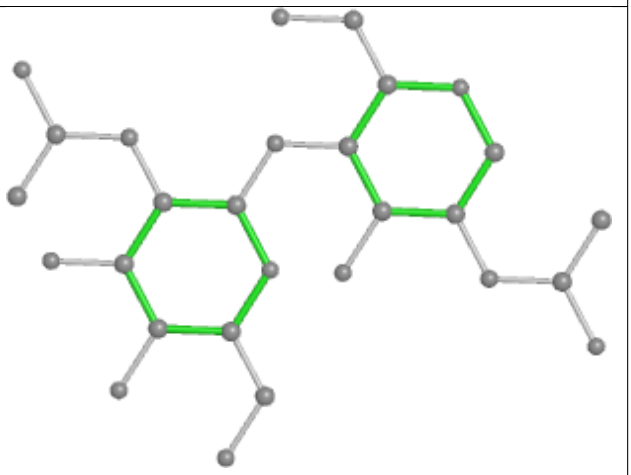
Bond lengths



Bond angles

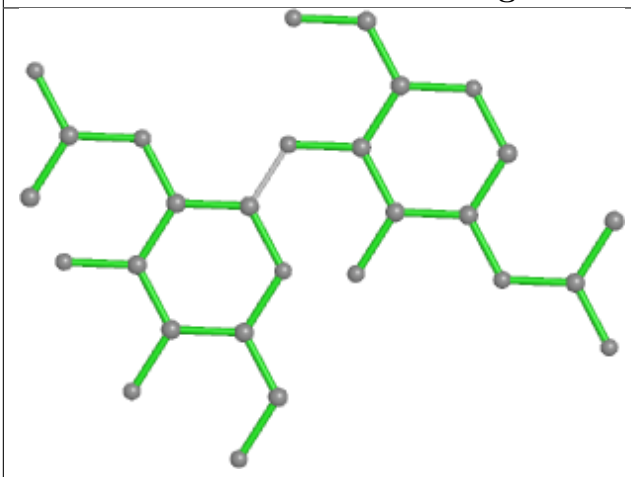


Torsions

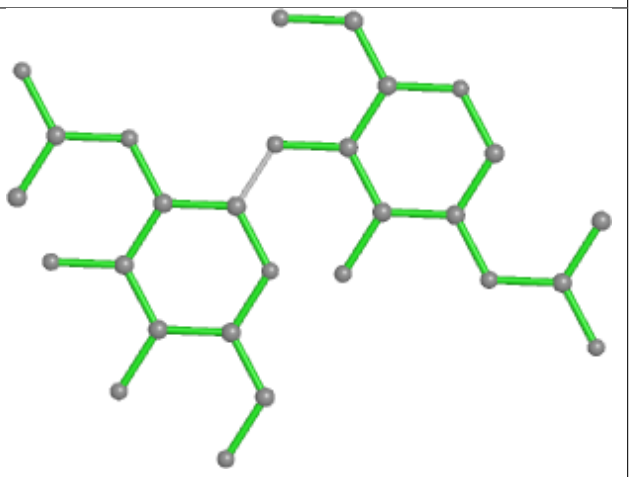


Rings

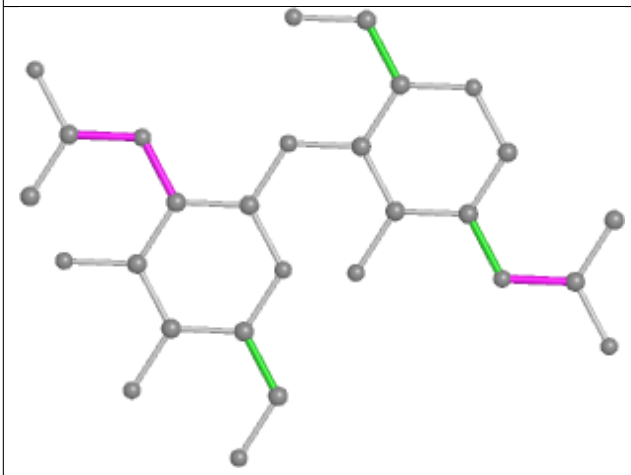
Oligosaccharide Chain J



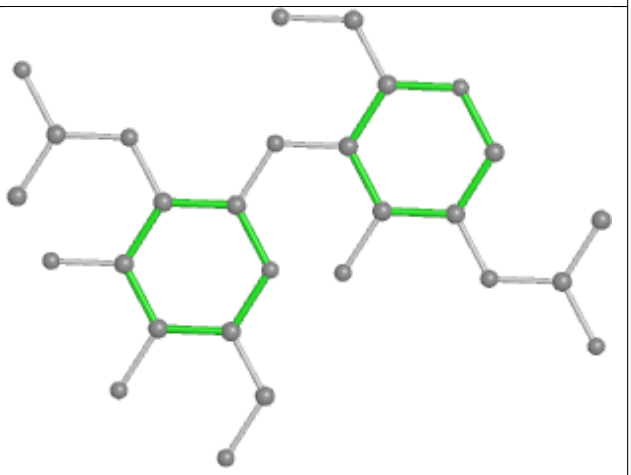
Bond lengths



Bond angles

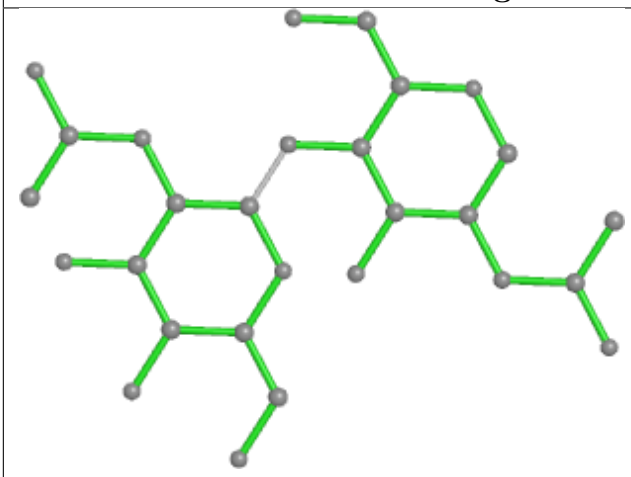


Torsions

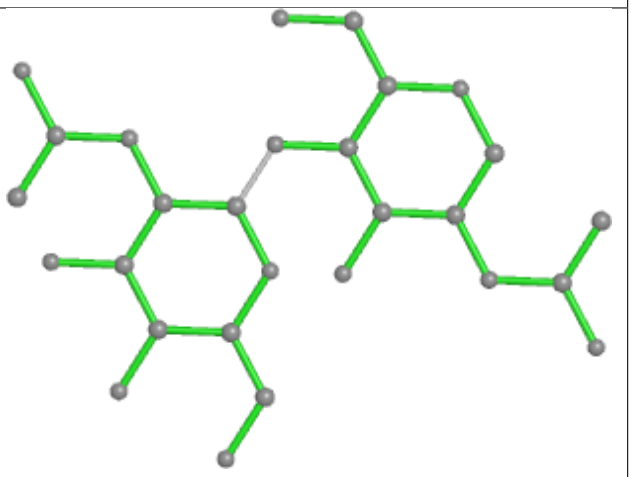


Rings

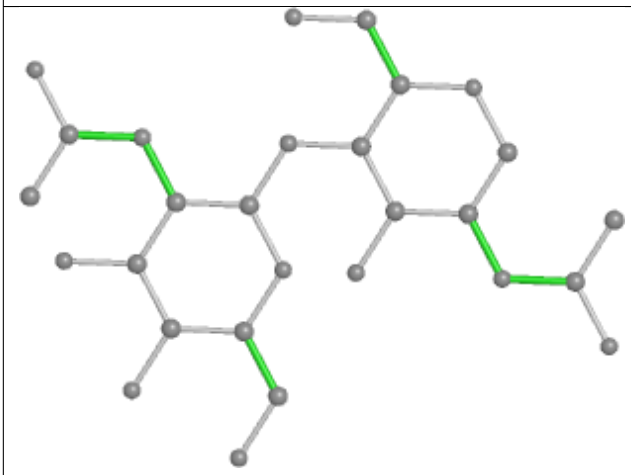
Oligosaccharide Chain K



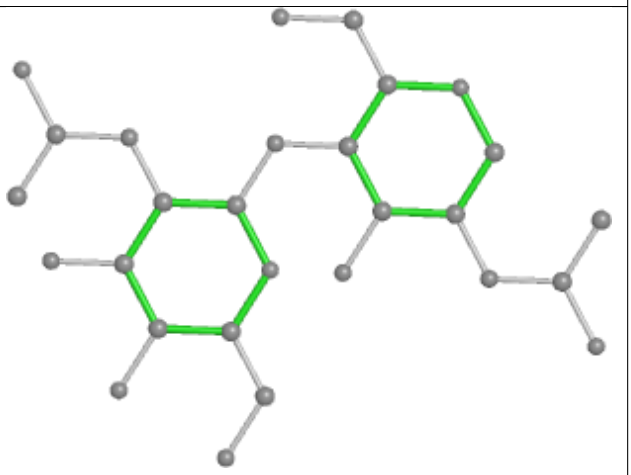
Bond lengths



Bond angles

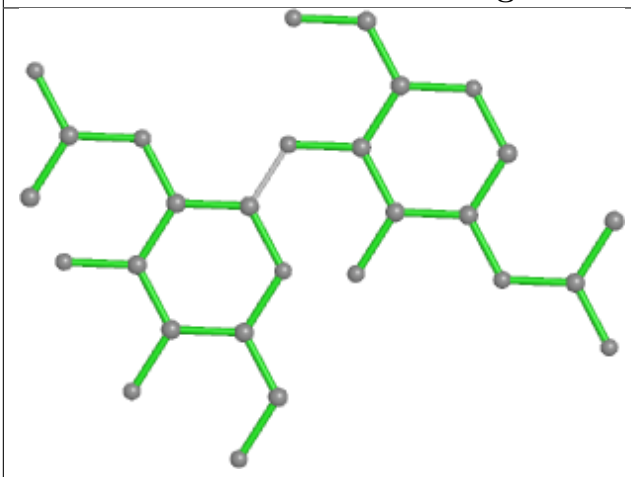


Torsions

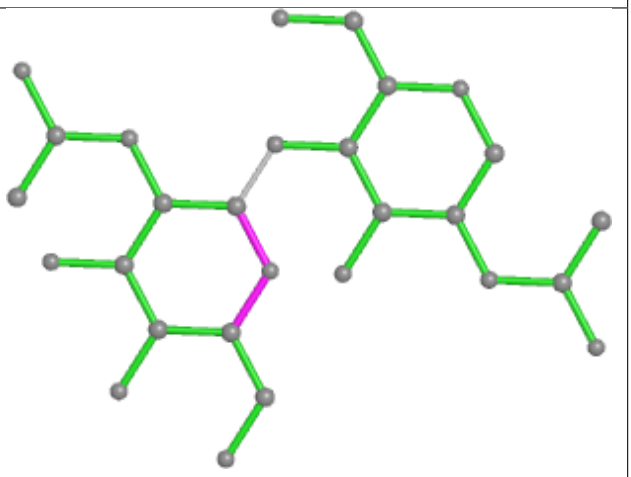


Rings

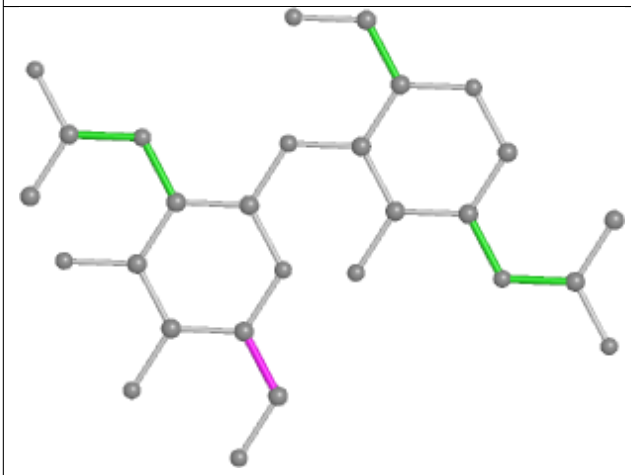
Oligosaccharide Chain L



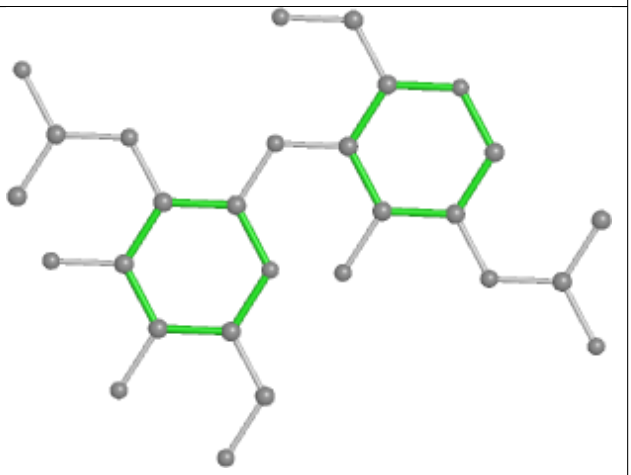
Bond lengths



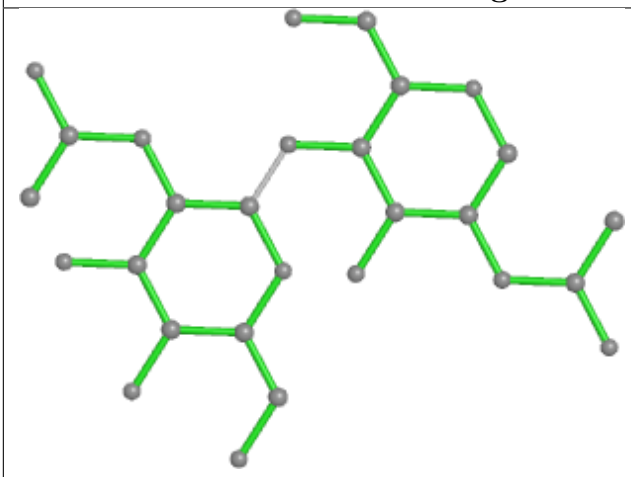
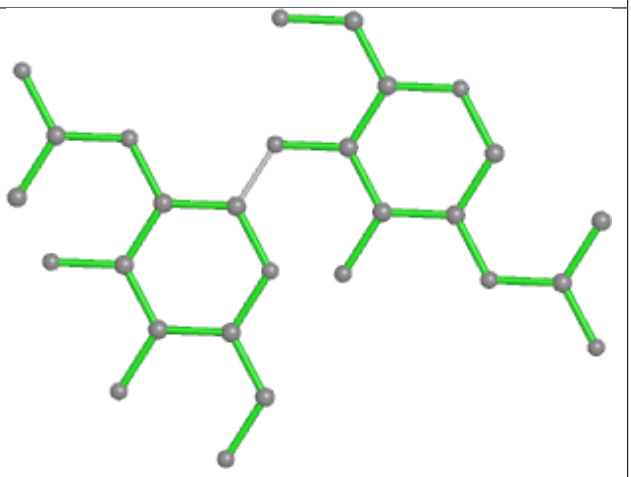
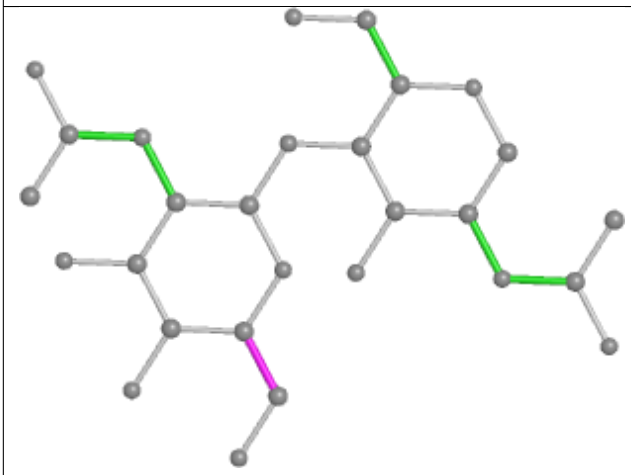
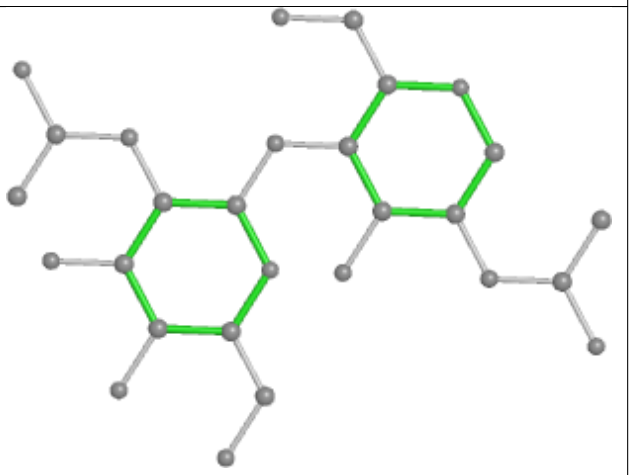
Bond angles



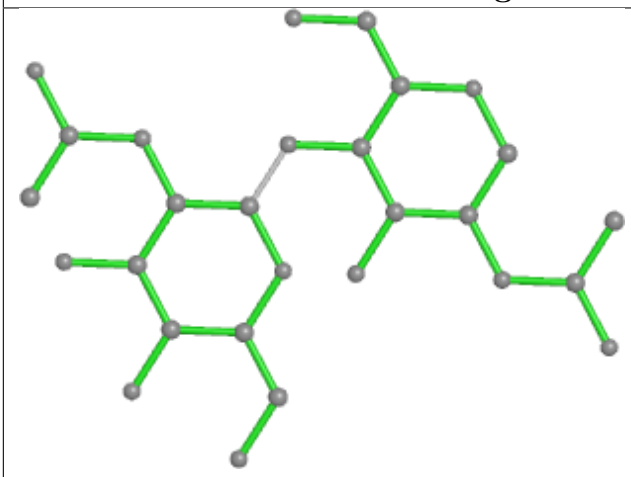
Torsions



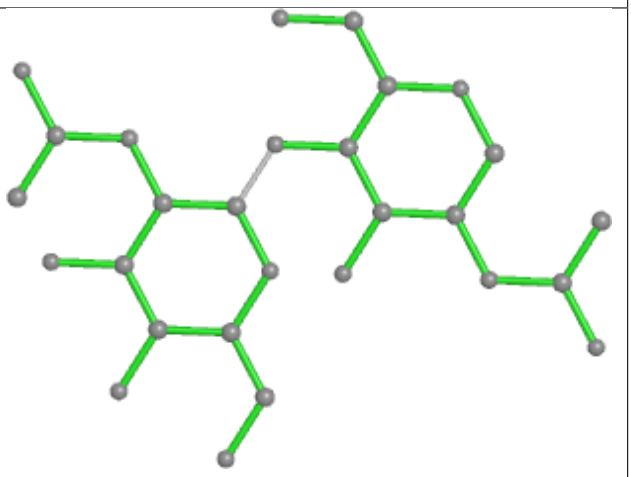
Rings

Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

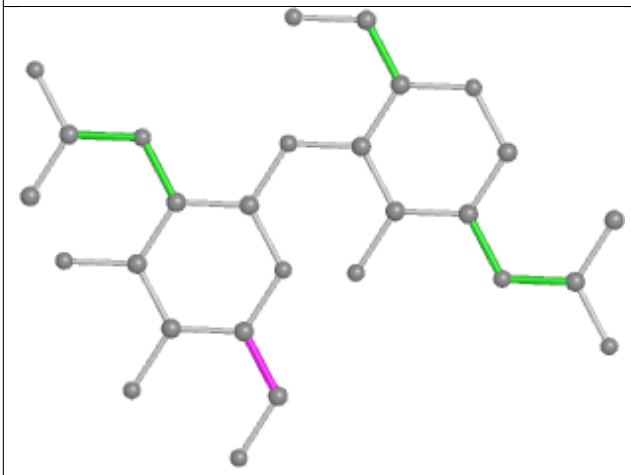
Oligosaccharide Chain O



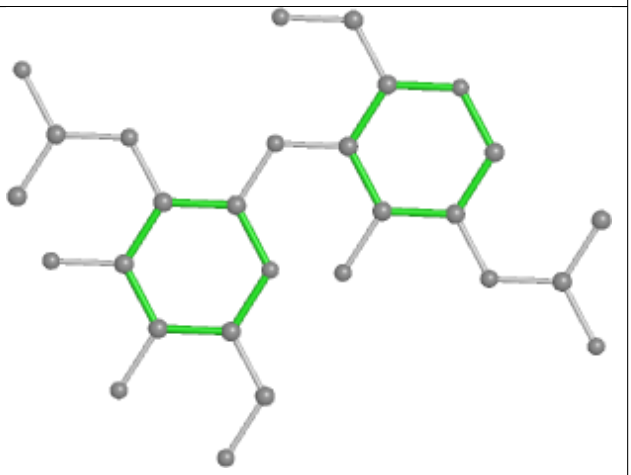
Bond lengths



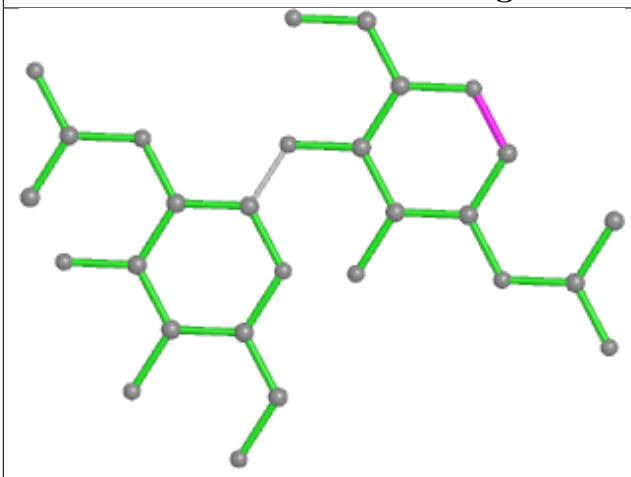
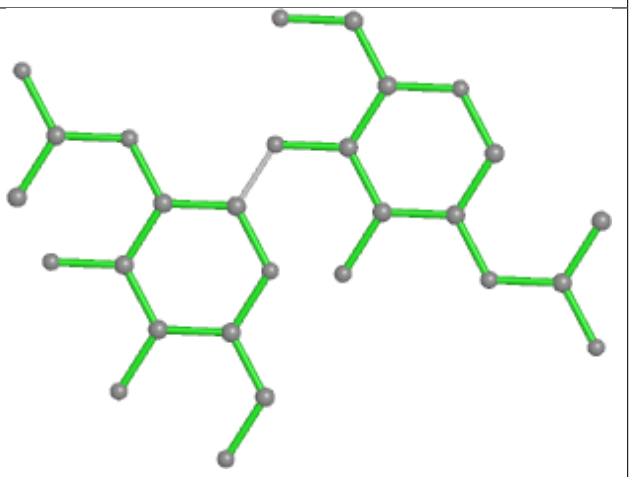
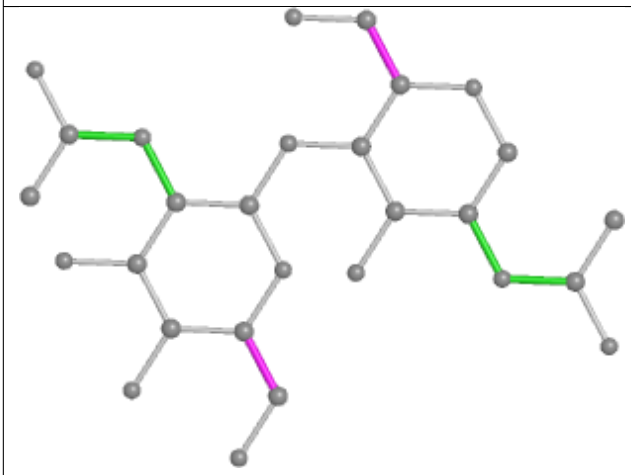
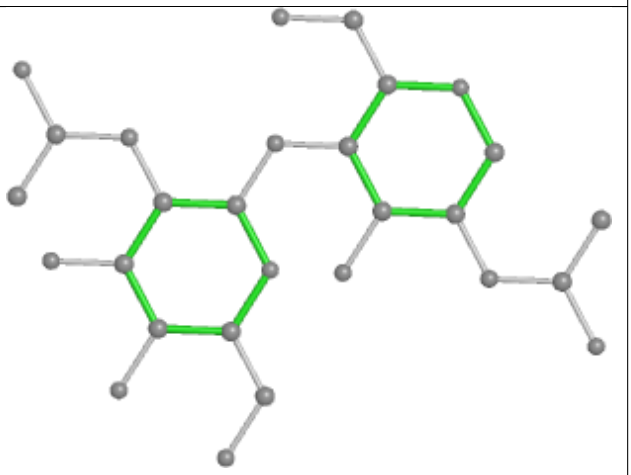
Bond angles



Torsions



Rings

Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

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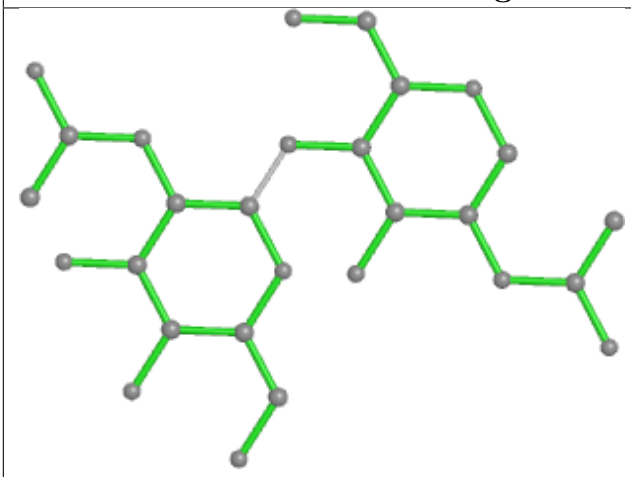
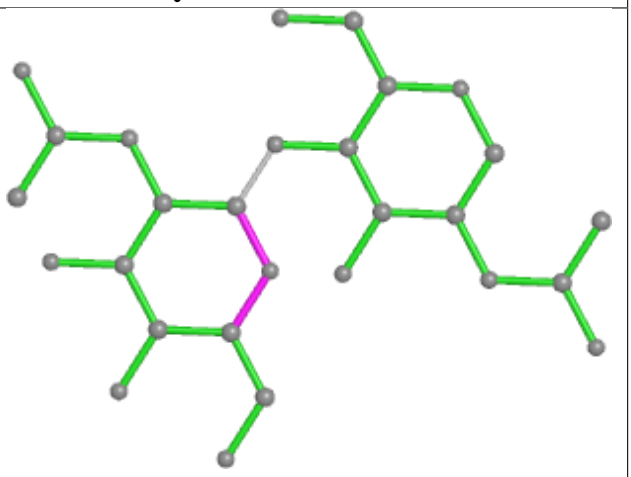
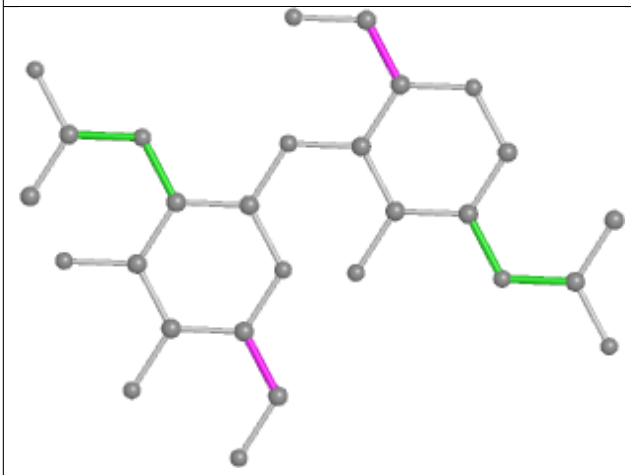
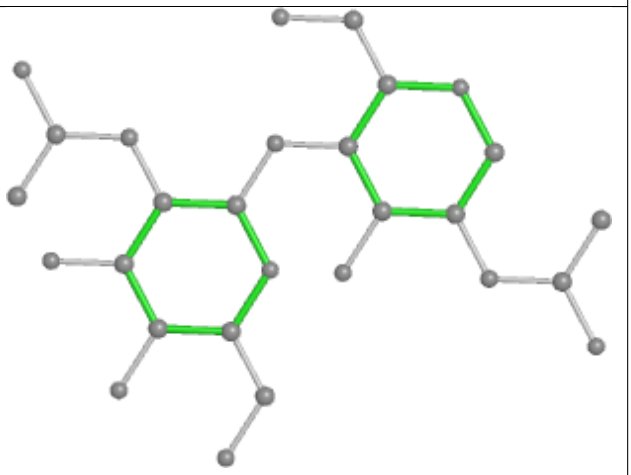
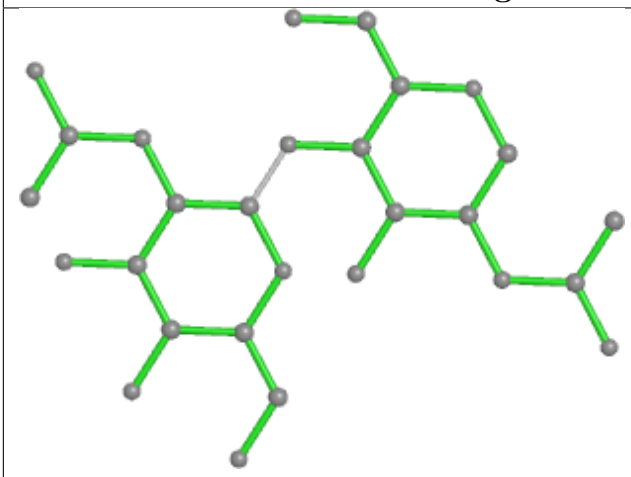
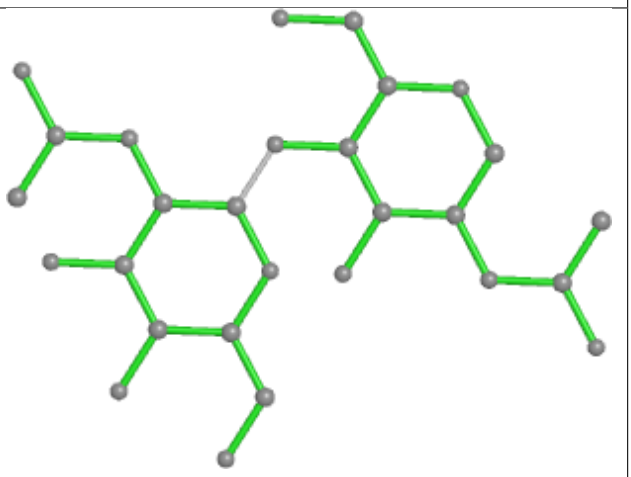
 Bond lengths	 Bond angles
 Torsions	 Rings

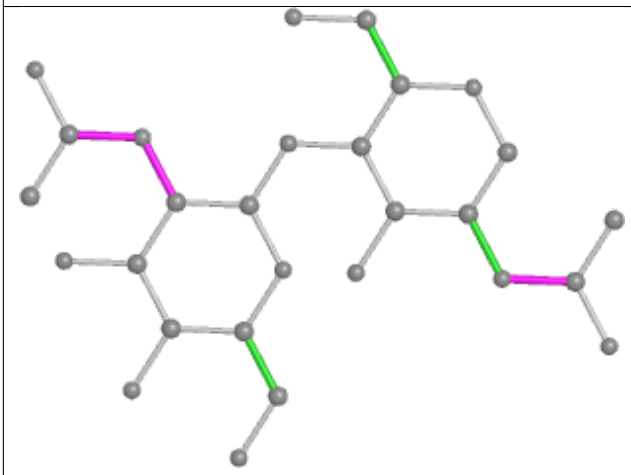
Oligosaccharide Chain R



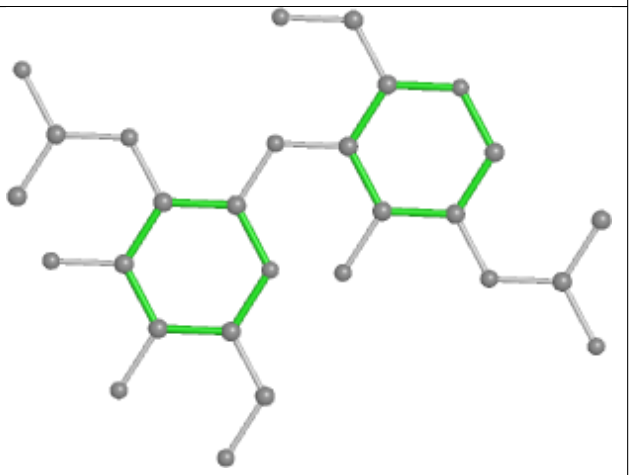
Bond lengths



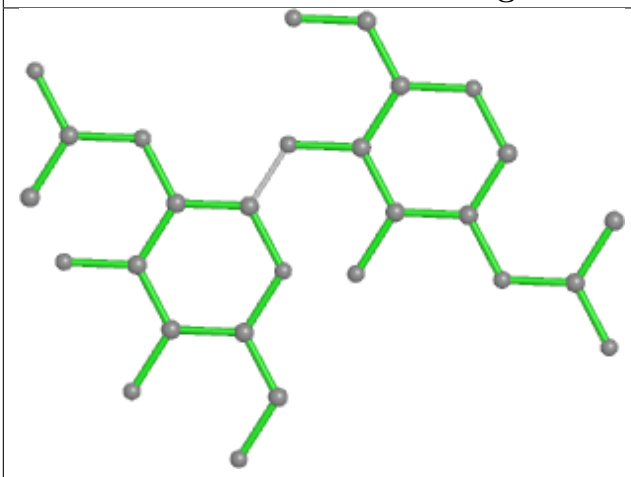
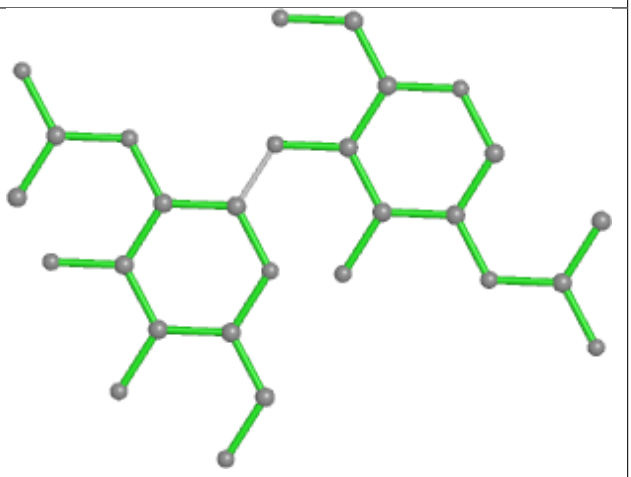
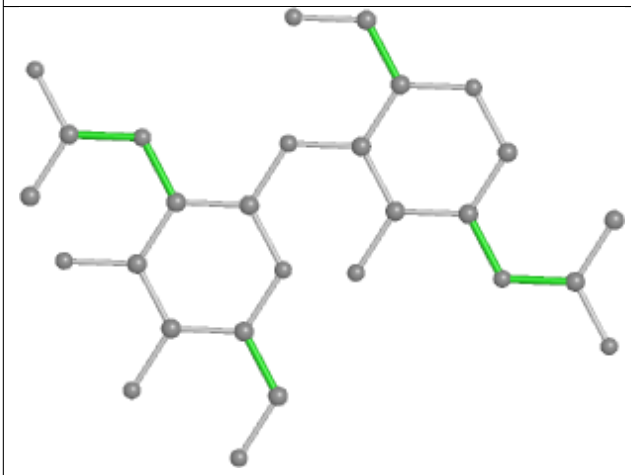
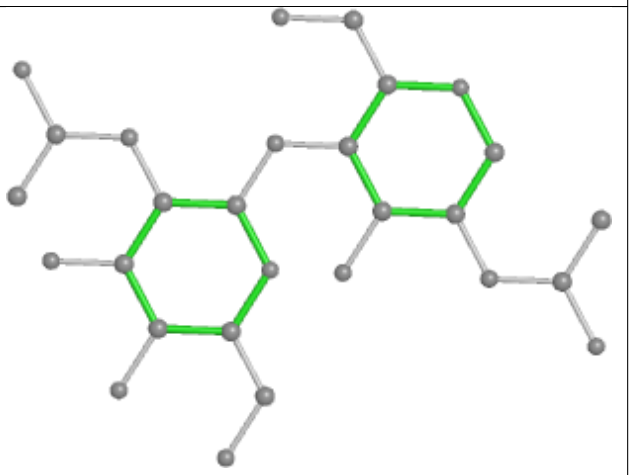
Bond angles



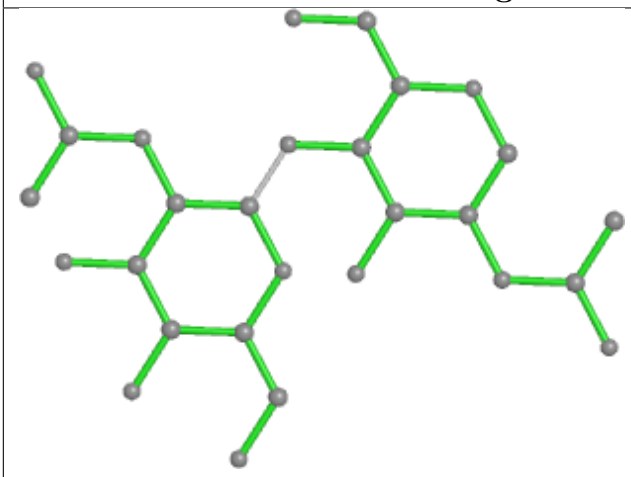
Torsions



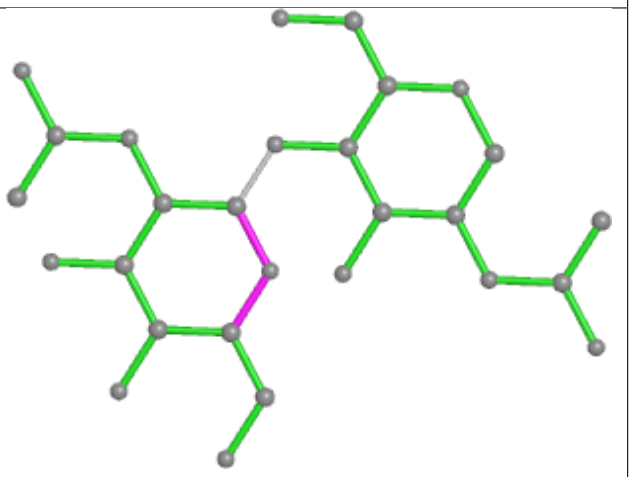
Rings

Oligosaccharide Chain S	
 Bond lengths	 Bond angles
 Torsions	 Rings

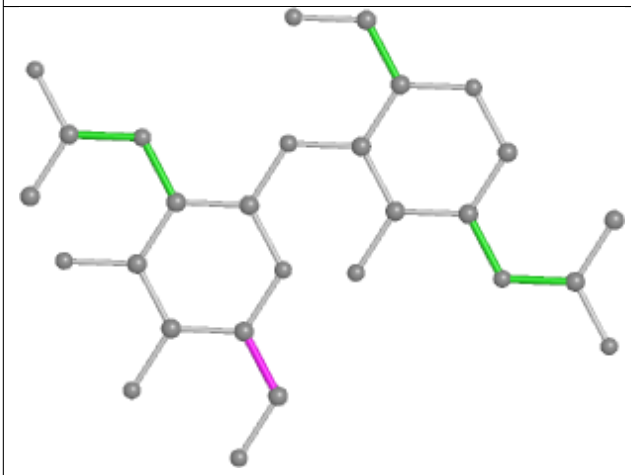
Oligosaccharide Chain T



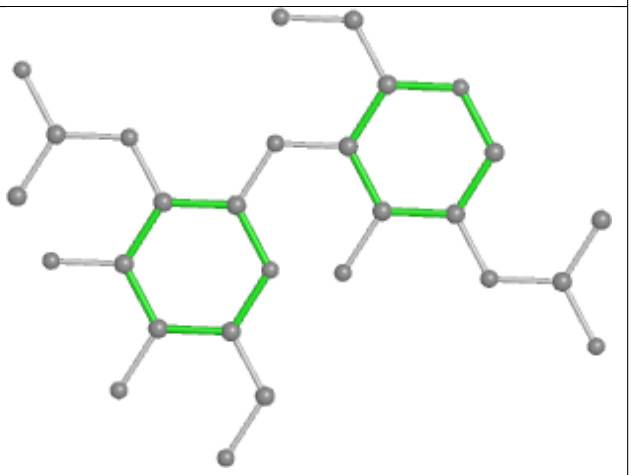
Bond lengths



Bond angles

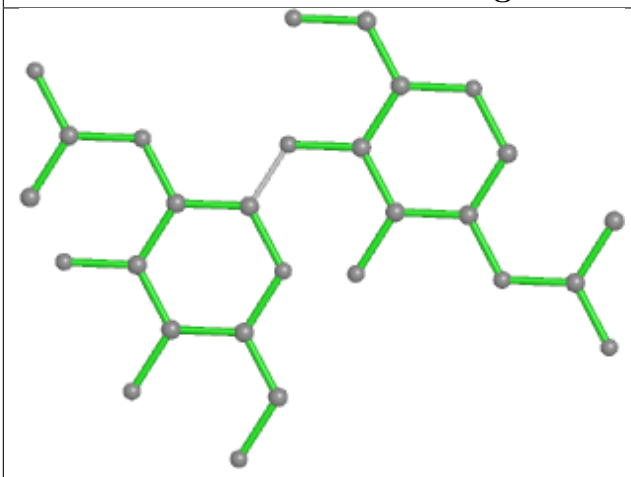


Torsions



Rings

Oligosaccharide Chain U



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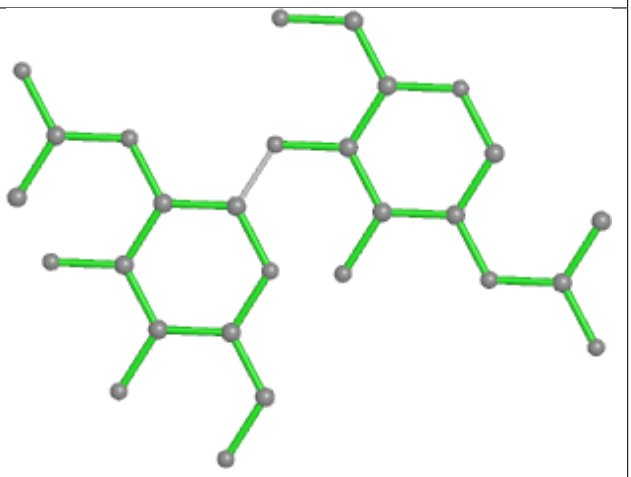
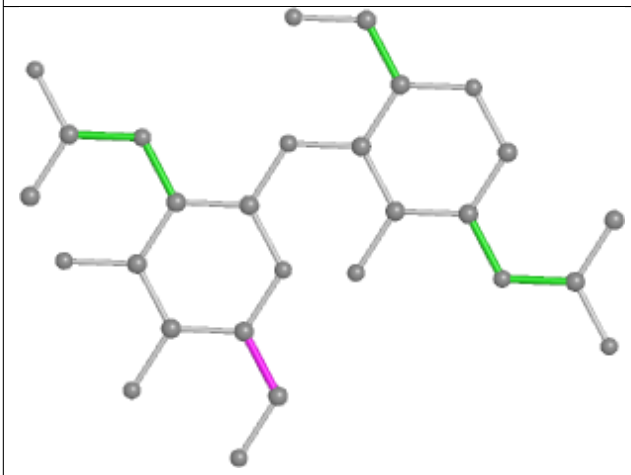
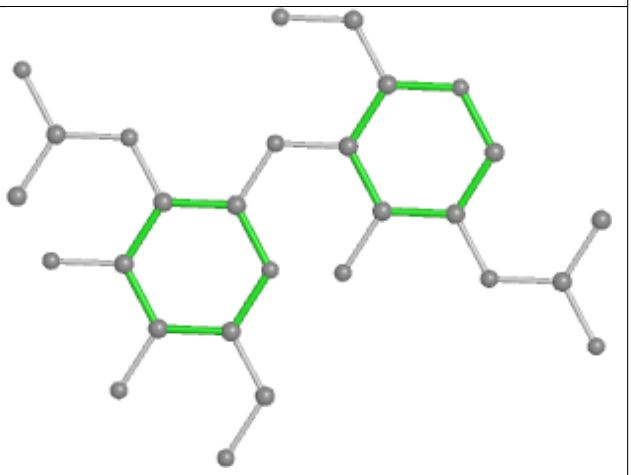


Bond angles

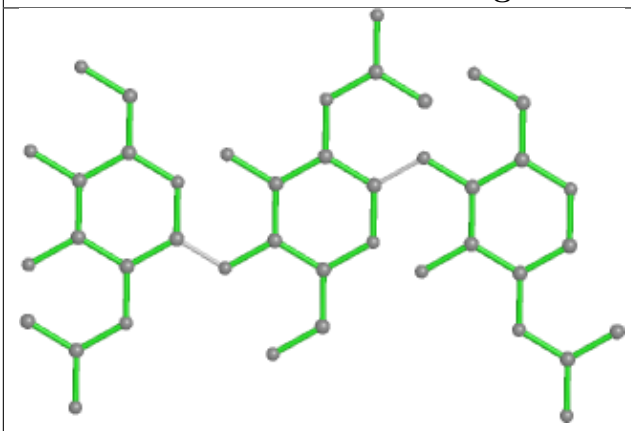


Torsions

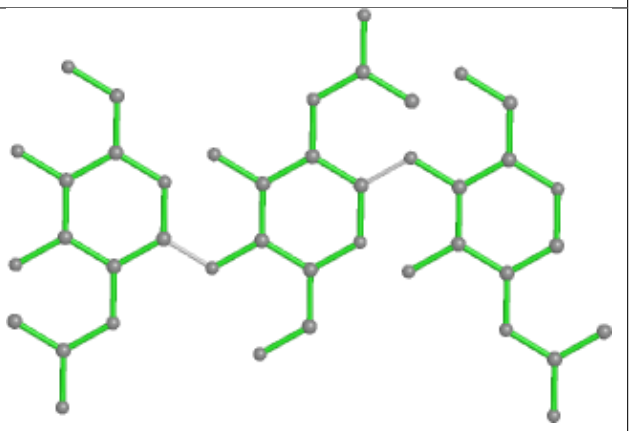


Rings

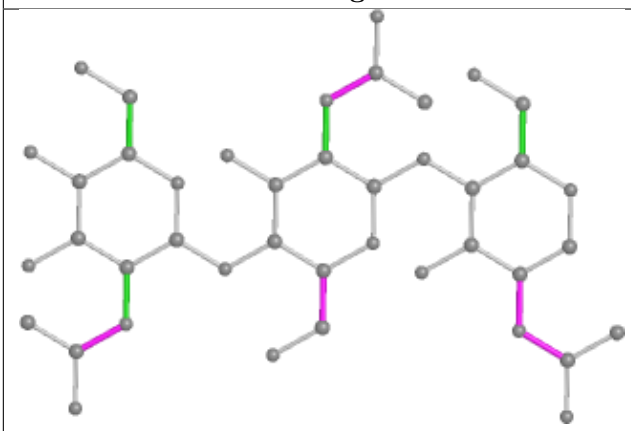
Oligosaccharide Chain N



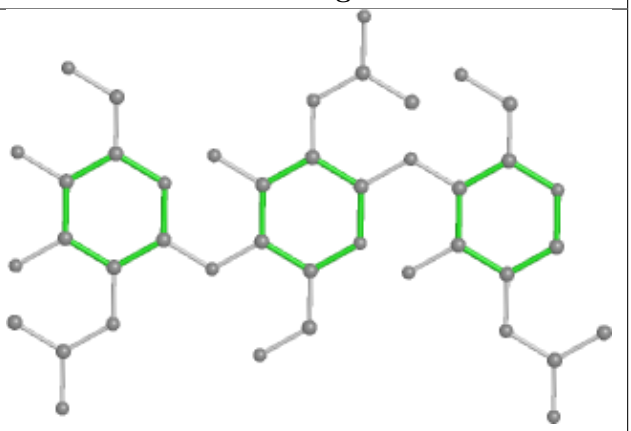
Bond lengths



Bond angles

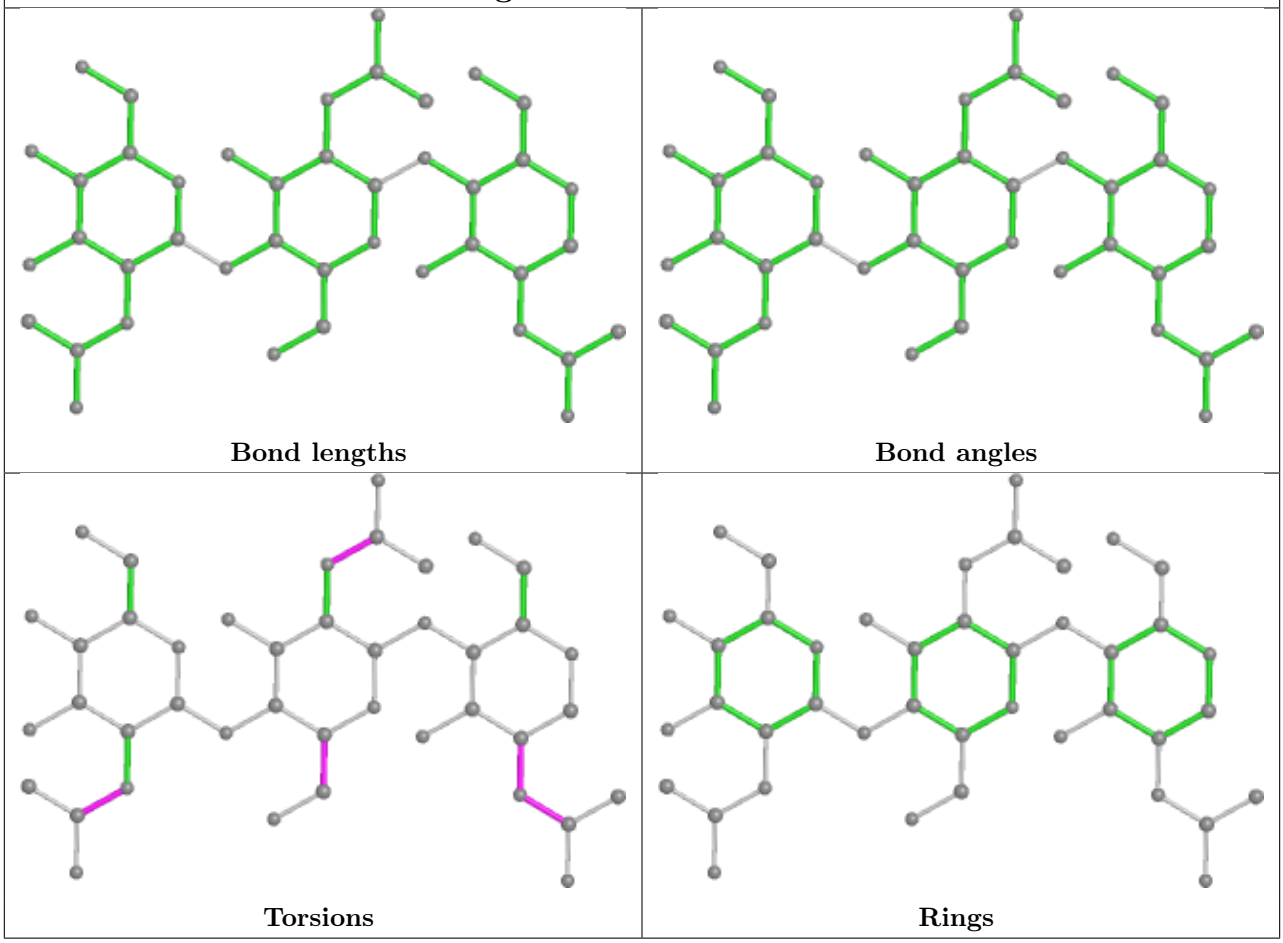


Torsions



Rings

Oligosaccharide Chain V



5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	A	702	1	14,14,15	0.36	0	17,19,21	0.40	0
6	NAG	A	703	1	14,14,15	0.40	0	17,19,21	0.64	1 (5%)
6	NAG	C	702	1	14,14,15	0.36	0	17,19,21	0.40	0
6	NAG	C	704	1	14,14,15	0.38	0	17,19,21	0.56	0
6	NAG	A	701	1	14,14,15	0.35	0	17,19,21	0.43	0
7	LEU	C	705	-	7,8,8	0.89	1 (14%)	9,10,10	1.25	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.56	0
7	LEU	A	705	-	7,8,8	0.89	1 (14%)	9,10,10	1.25	2 (22%)
6	NAG	C	703	1	14,14,15	0.40	0	17,19,21	0.64	1 (5%)
6	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.59	1 (5%)
6	NAG	B	901	2	14,14,15	0.39	0	17,19,21	0.59	1 (5%)
6	NAG	C	701	1	14,14,15	0.35	0	17,19,21	0.43	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	A	702	1	-	2/6/23/26	0/1/1/1
6	NAG	A	703	1	-	2/6/23/26	0/1/1/1
6	NAG	C	702	1	-	2/6/23/26	0/1/1/1
6	NAG	C	704	1	-	0/6/23/26	0/1/1/1
6	NAG	A	701	1	-	2/6/23/26	0/1/1/1
7	LEU	C	705	-	-	3/8/8/8	-
6	NAG	A	704	1	-	0/6/23/26	0/1/1/1
7	LEU	A	705	-	-	3/8/8/8	-
6	NAG	C	703	1	-	2/6/23/26	0/1/1/1
6	NAG	D	901	2	-	2/6/23/26	0/1/1/1
6	NAG	B	901	2	-	2/6/23/26	0/1/1/1
6	NAG	C	701	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	705	LEU	OXT-C	-2.23	1.23	1.30
7	C	705	LEU	OXT-C	-2.23	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	705	LEU	OXT-C-O	-2.80	117.73	124.09
7	C	705	LEU	OXT-C-O	-2.80	117.73	124.09
7	A	705	LEU	OXT-C-CA	2.43	121.67	113.38
7	C	705	LEU	OXT-C-CA	2.43	121.67	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	901	NAG	C1-O5-C5	2.03	114.95	112.19
6	D	901	NAG	C1-O5-C5	2.03	114.95	112.19
6	A	703	NAG	C1-O5-C5	2.02	114.93	112.19
6	C	703	NAG	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	705	LEU	N-CA-CB-CG
7	C	705	LEU	N-CA-CB-CG
6	A	701	NAG	O5-C5-C6-O6
6	C	701	NAG	O5-C5-C6-O6
6	A	701	NAG	C4-C5-C6-O6
6	C	701	NAG	C4-C5-C6-O6
6	A	703	NAG	C8-C7-N2-C2
6	A	703	NAG	O7-C7-N2-C2
6	C	703	NAG	C8-C7-N2-C2
6	C	703	NAG	O7-C7-N2-C2
6	A	702	NAG	O5-C5-C6-O6
6	C	702	NAG	O5-C5-C6-O6
6	B	901	NAG	O5-C5-C6-O6
6	D	901	NAG	O5-C5-C6-O6
6	A	702	NAG	C4-C5-C6-O6
6	C	702	NAG	C4-C5-C6-O6
6	B	901	NAG	C4-C5-C6-O6
6	D	901	NAG	C4-C5-C6-O6
7	A	705	LEU	O-C-CA-N
7	C	705	LEU	O-C-CA-N
7	A	705	LEU	OXT-C-CA-N
7	C	705	LEU	OXT-C-CA-N

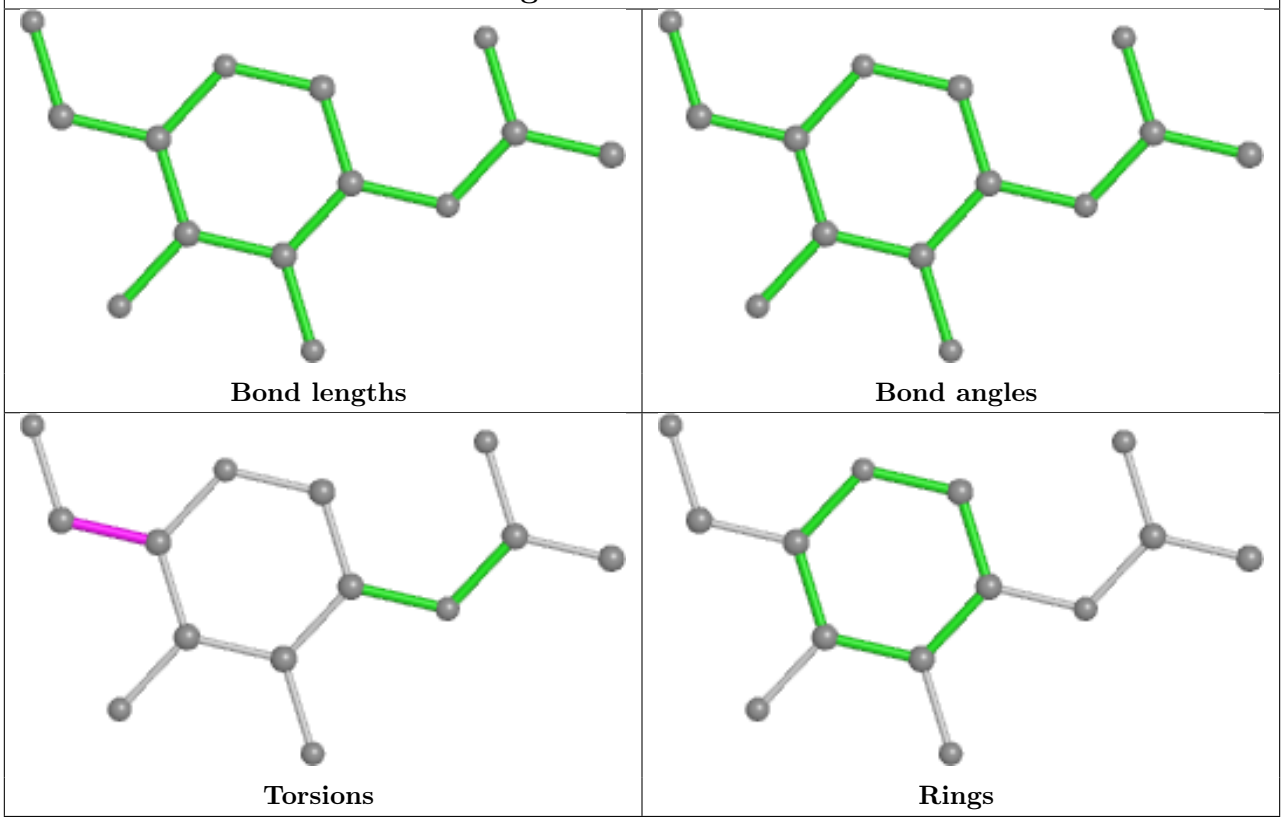
There are no ring outliers.

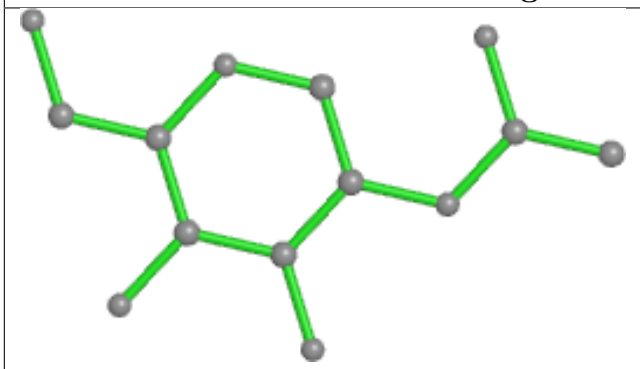
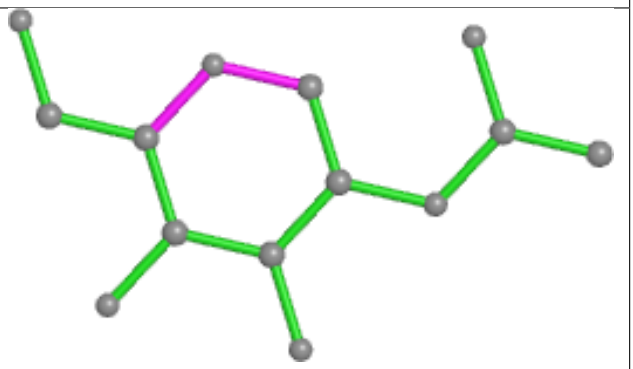
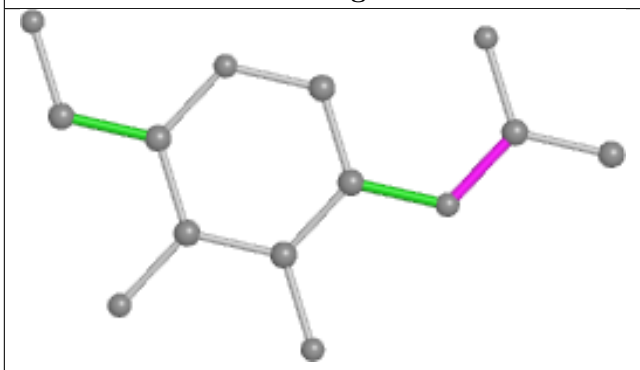
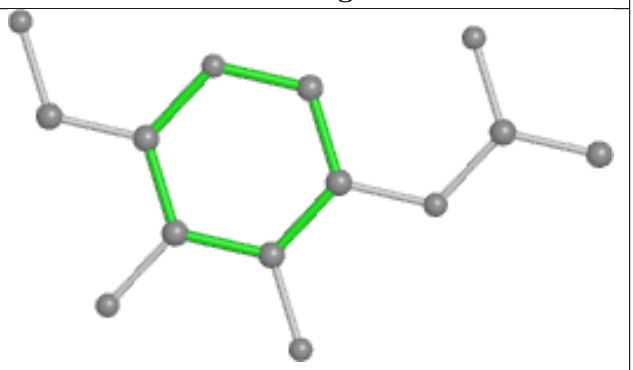
No monomer is involved in short contacts.

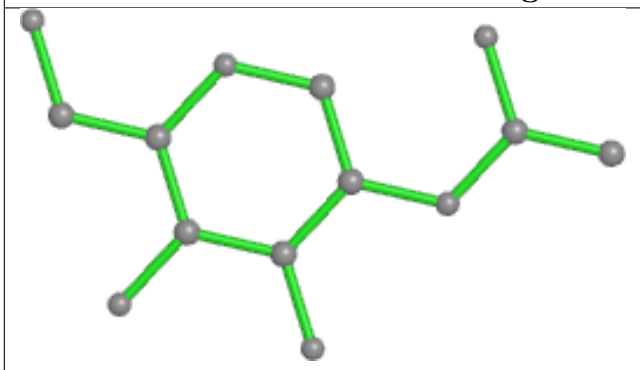
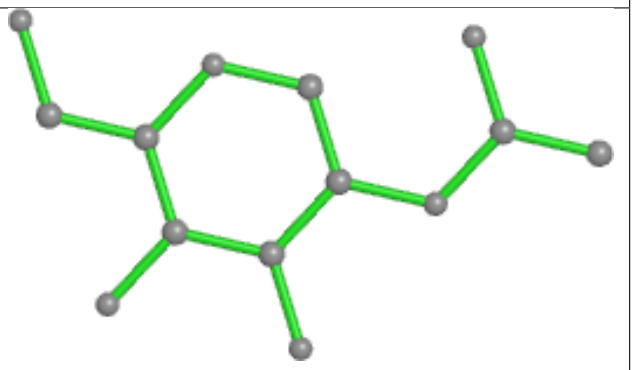
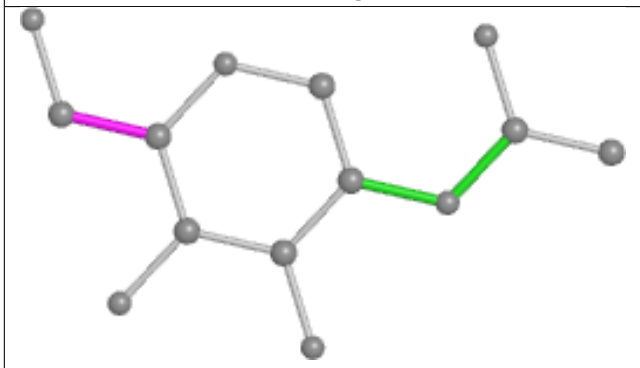
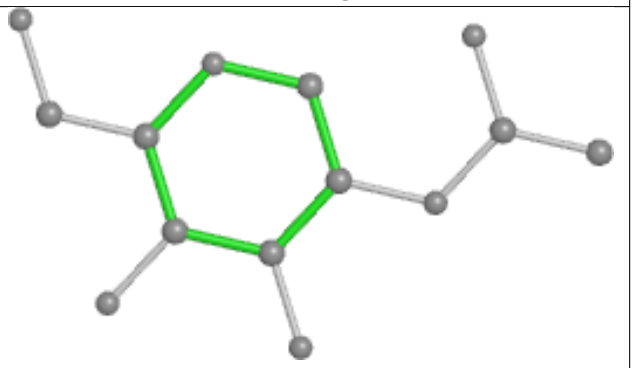
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

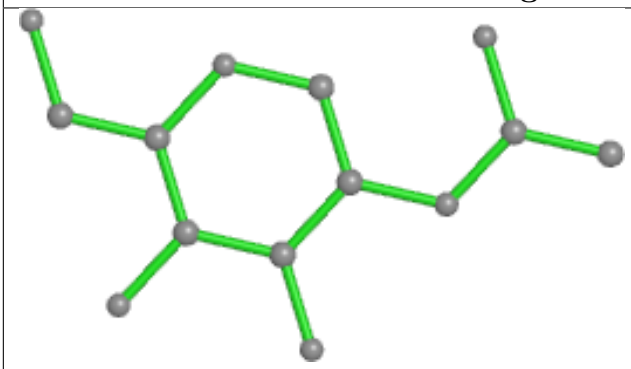
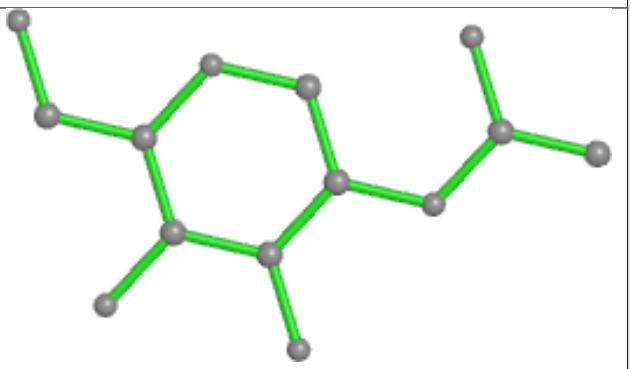
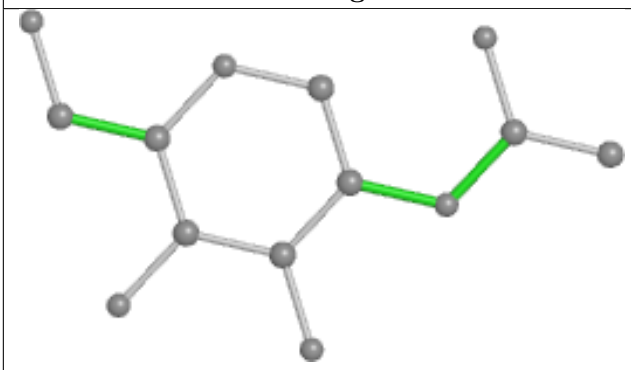
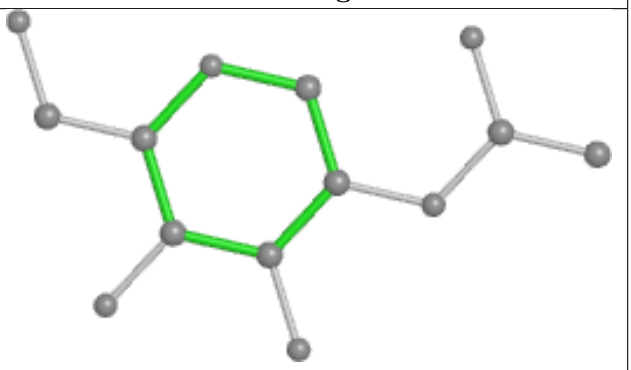
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

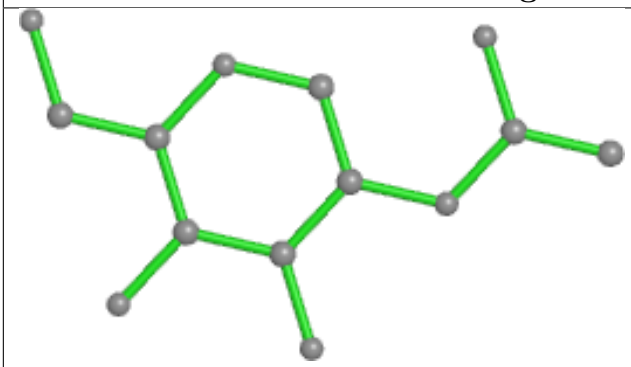
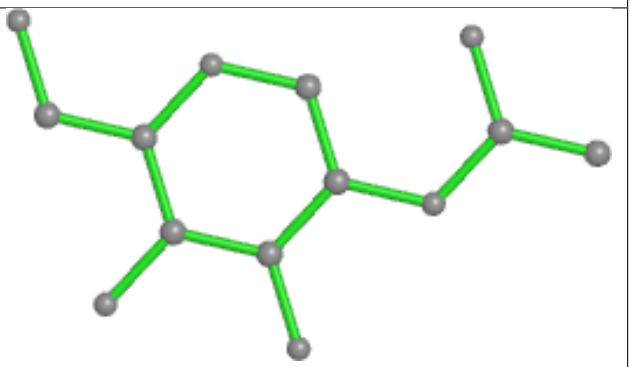
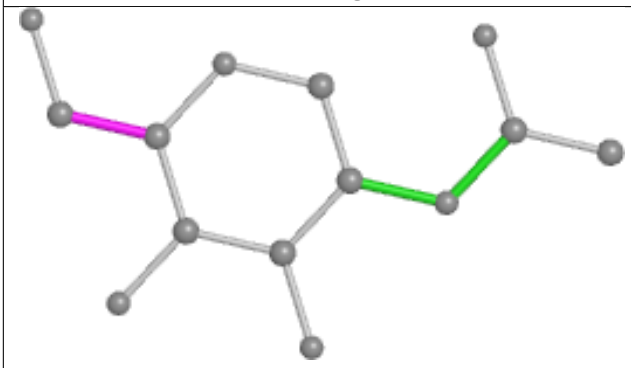
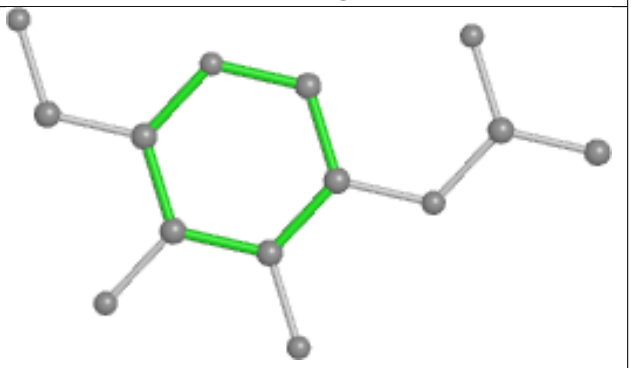
Ligand NAG A 702



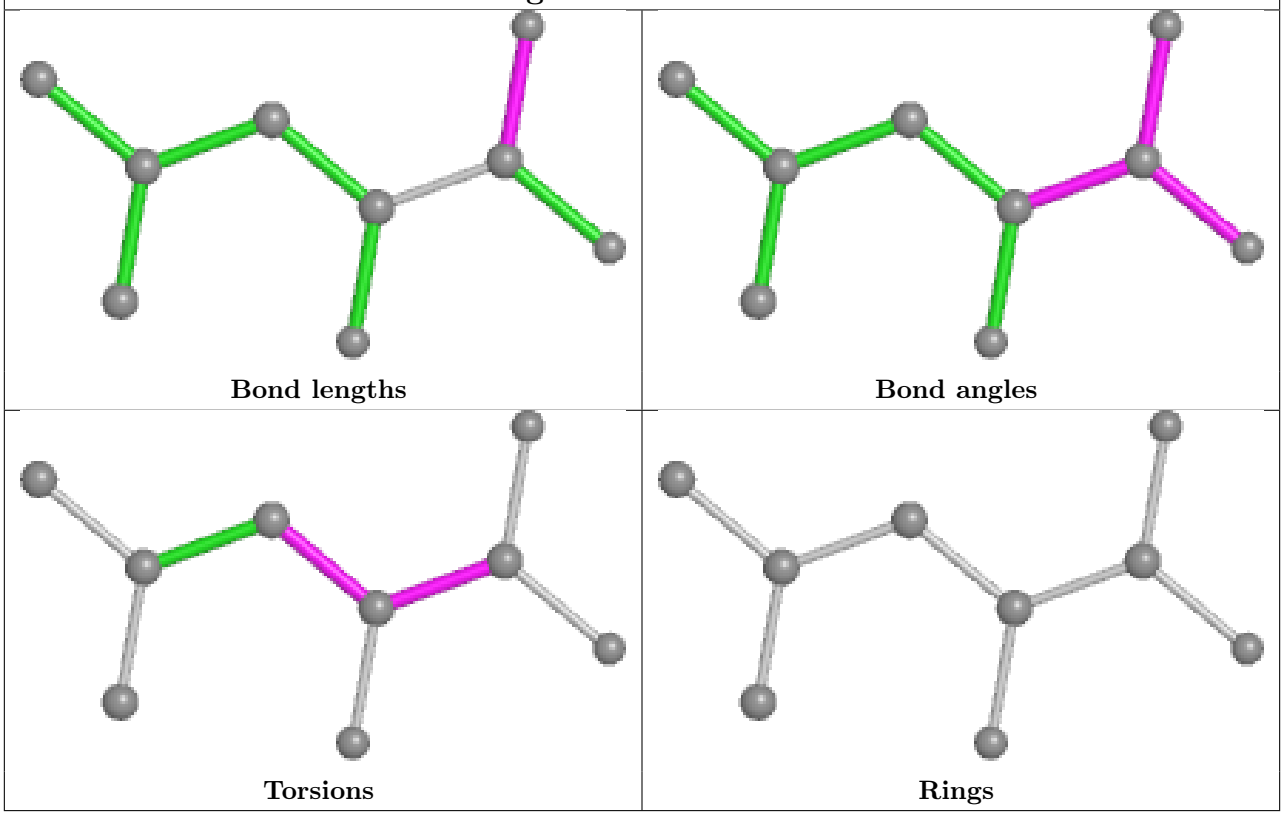
Ligand NAG A 703	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

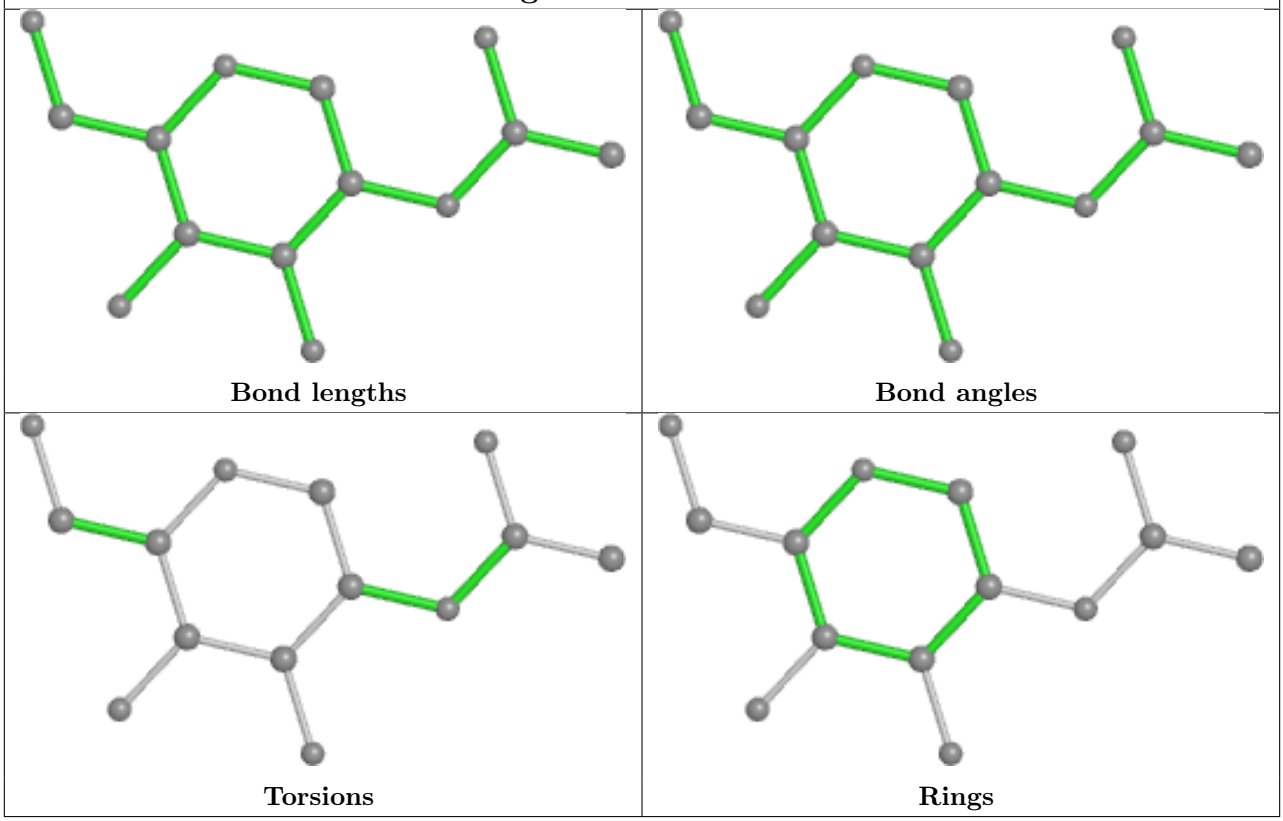
Ligand NAG C 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

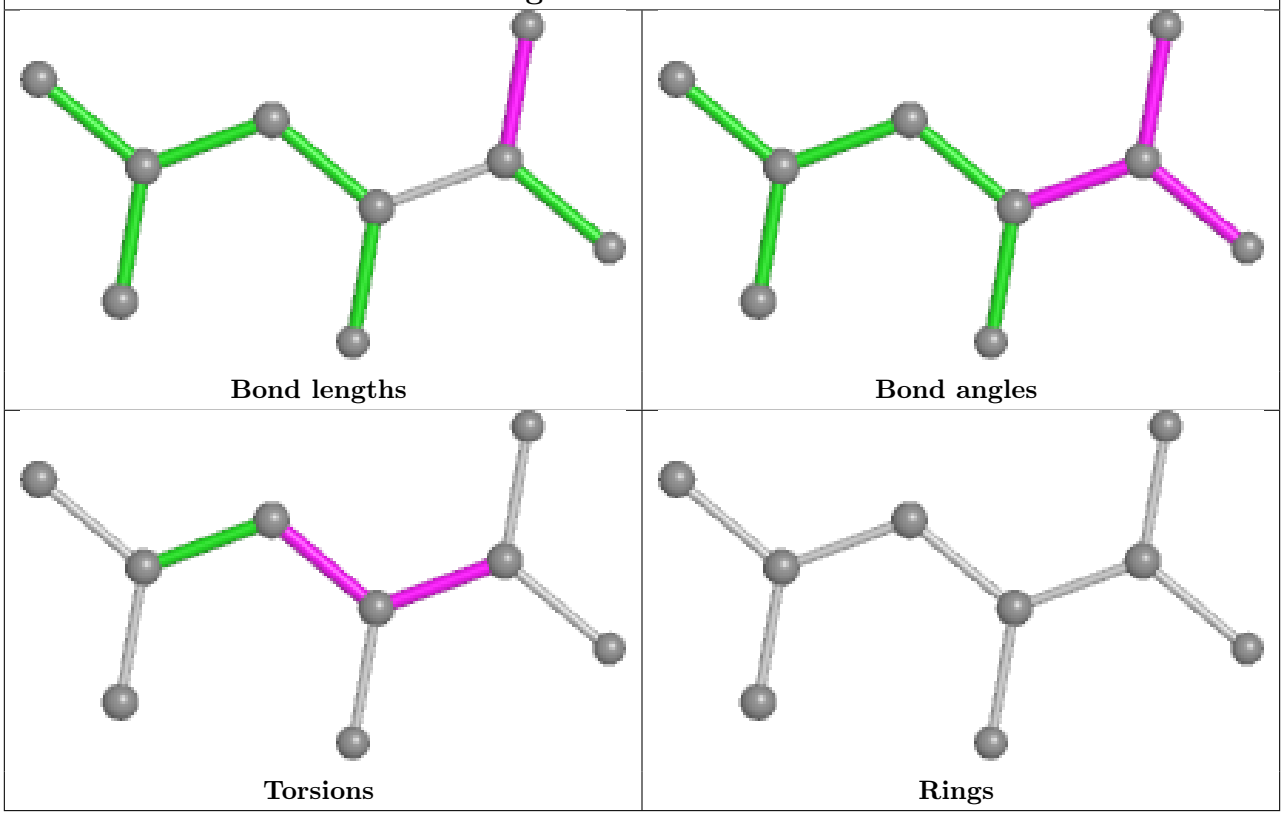
Ligand LEU C 705



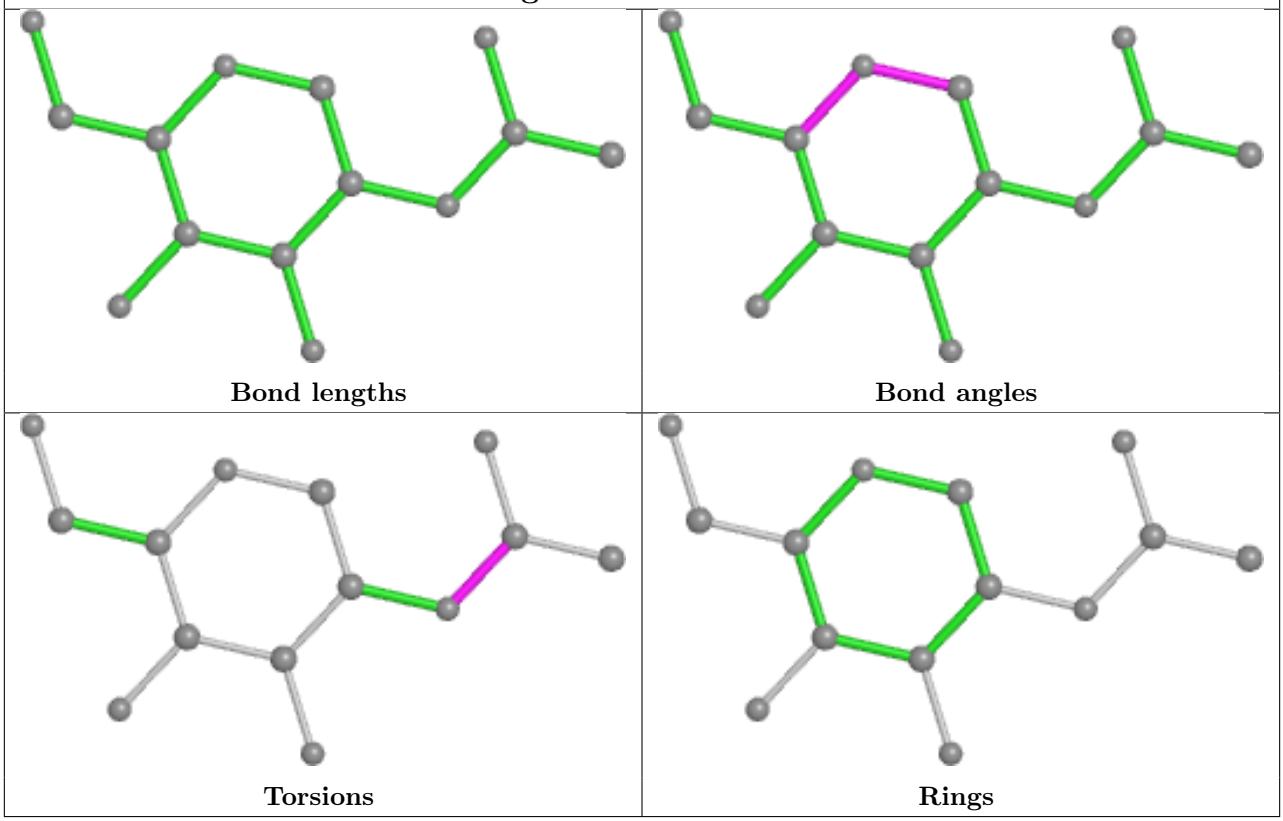
Ligand NAG A 704

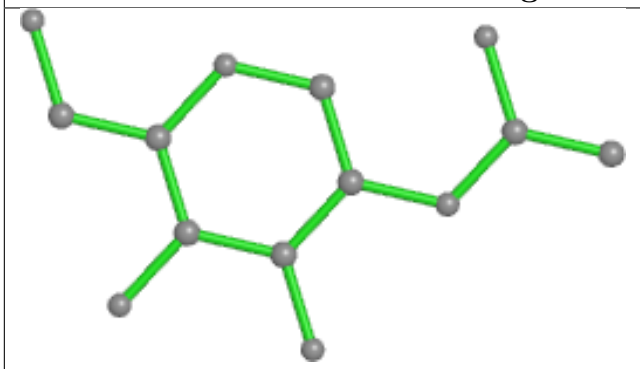
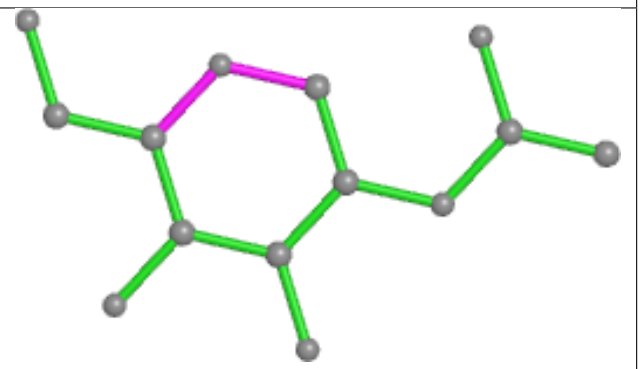
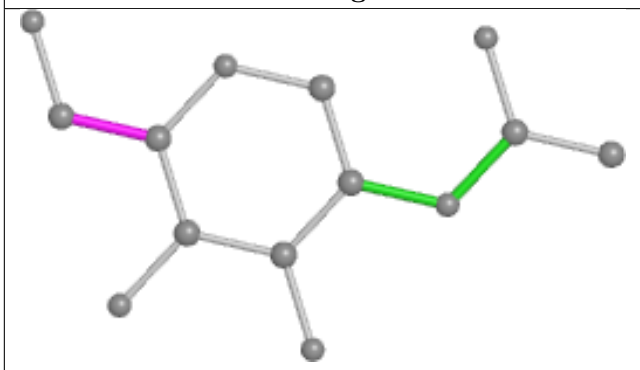
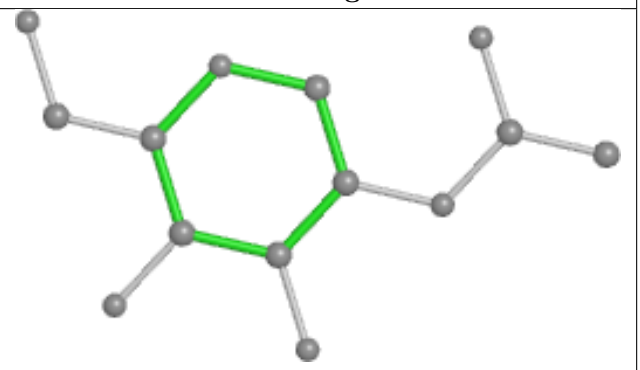


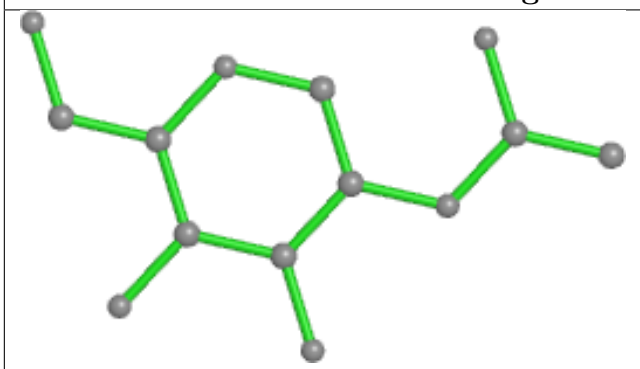
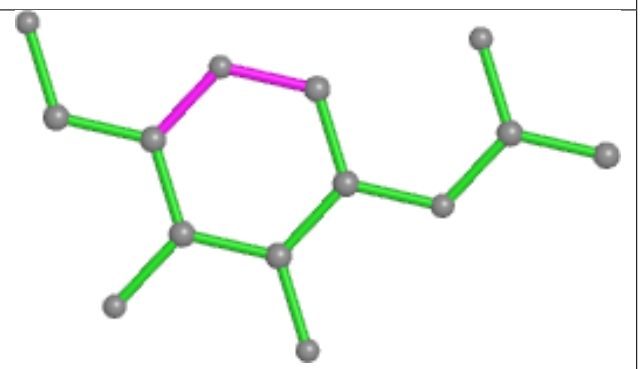
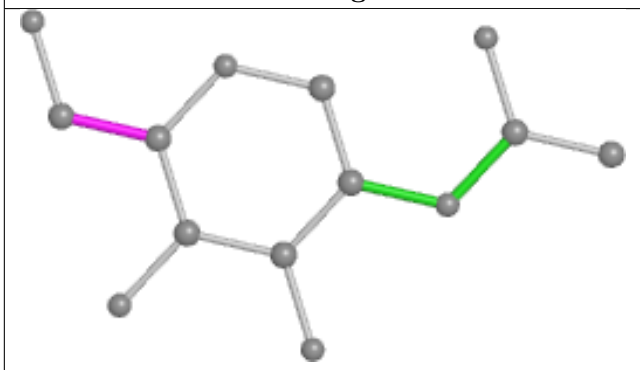
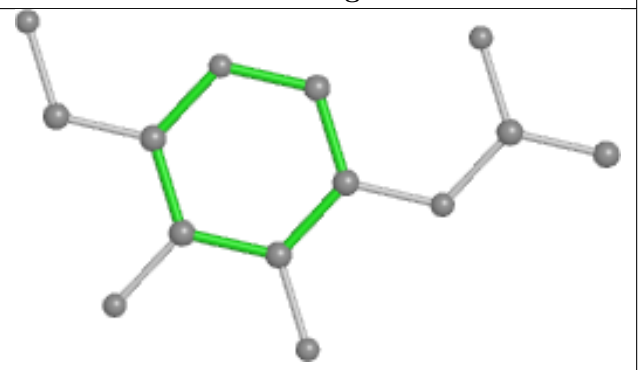
Ligand LEU A 705

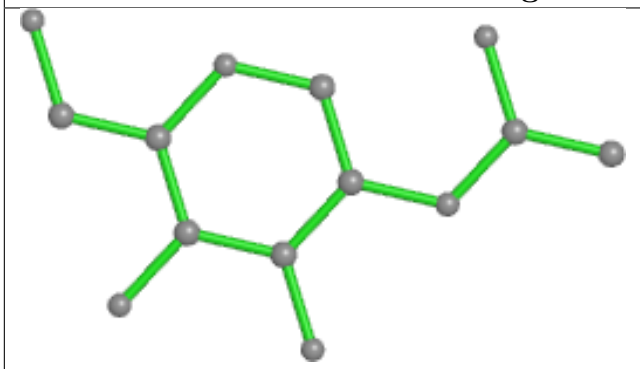
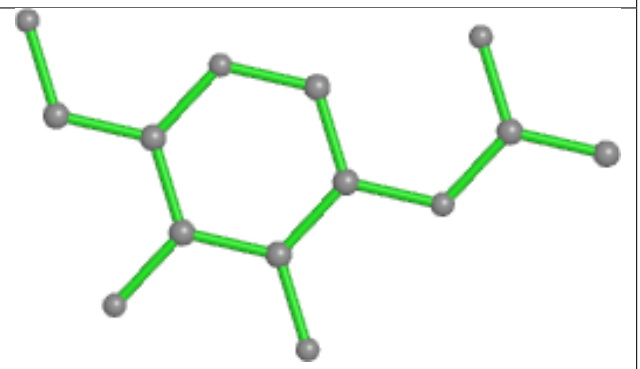
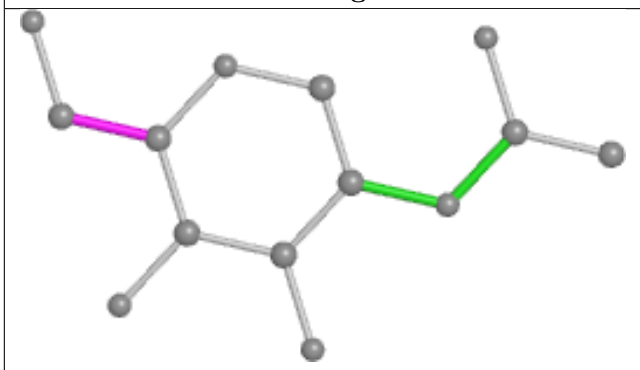
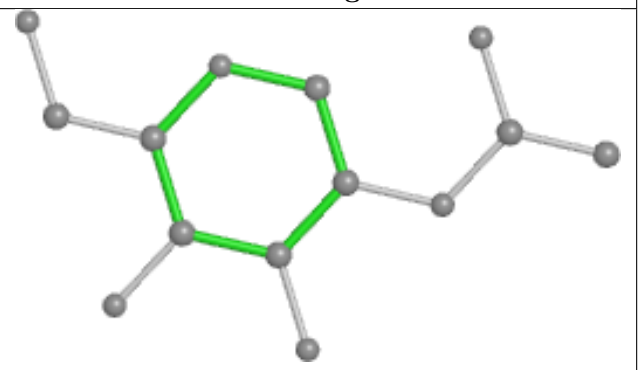


Ligand NAG C 703



Ligand NAG D 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG B 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG C 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

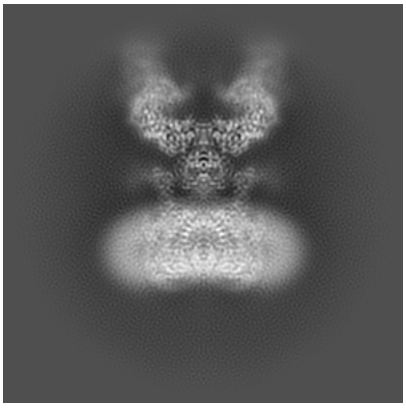
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30039. These allow visual inspection of the internal detail of the map and identification of artifacts.

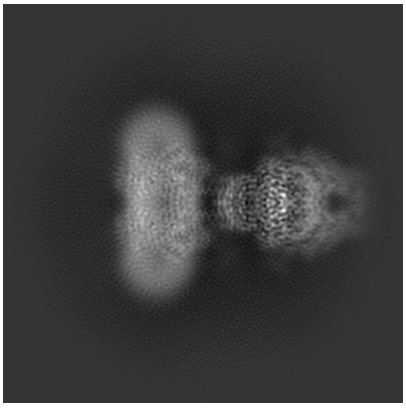
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

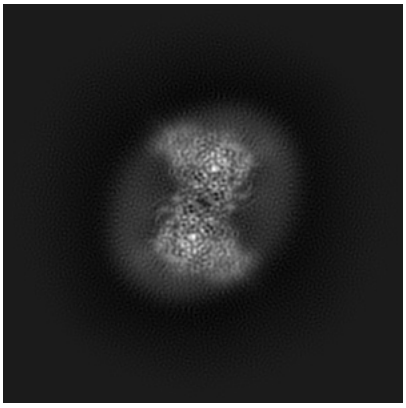
6.1.1 Primary map



X



Y

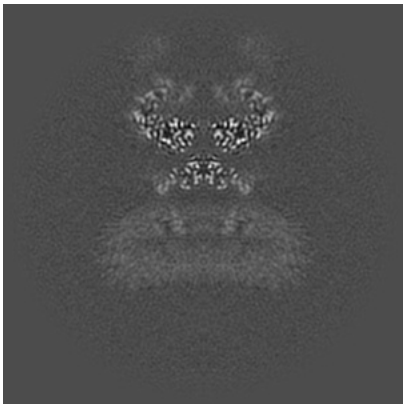


Z

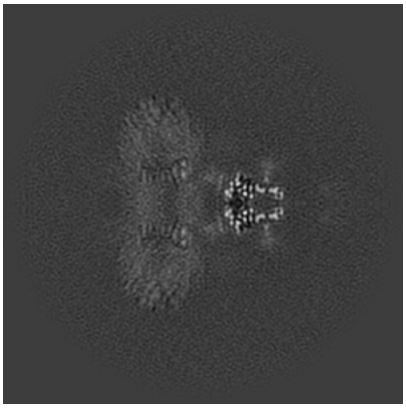
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

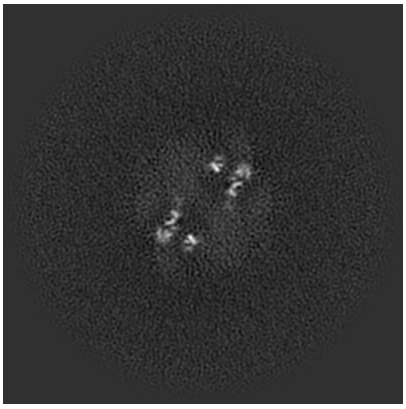
6.2.1 Primary map



X Index: 144



Y Index: 144

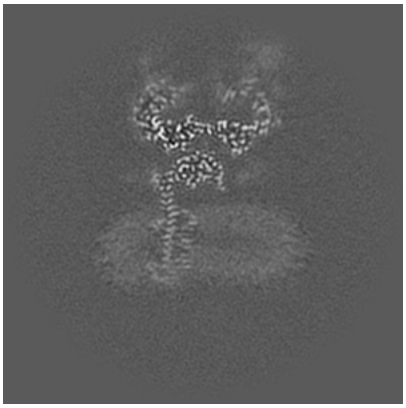


Z Index: 144

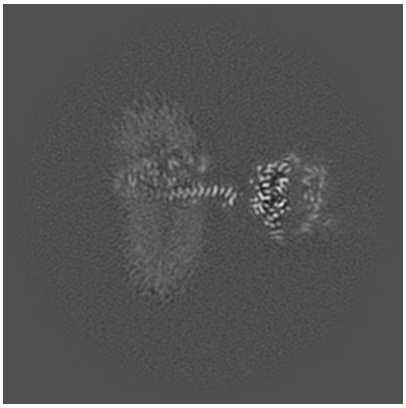
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

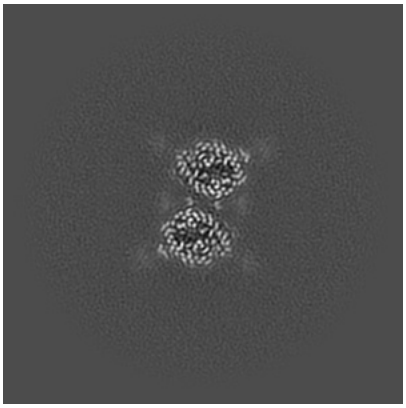
6.3.1 Primary map



X Index: 138



Y Index: 167



Z Index: 193

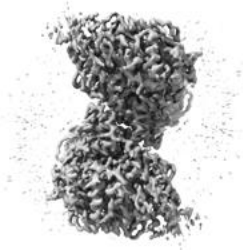
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

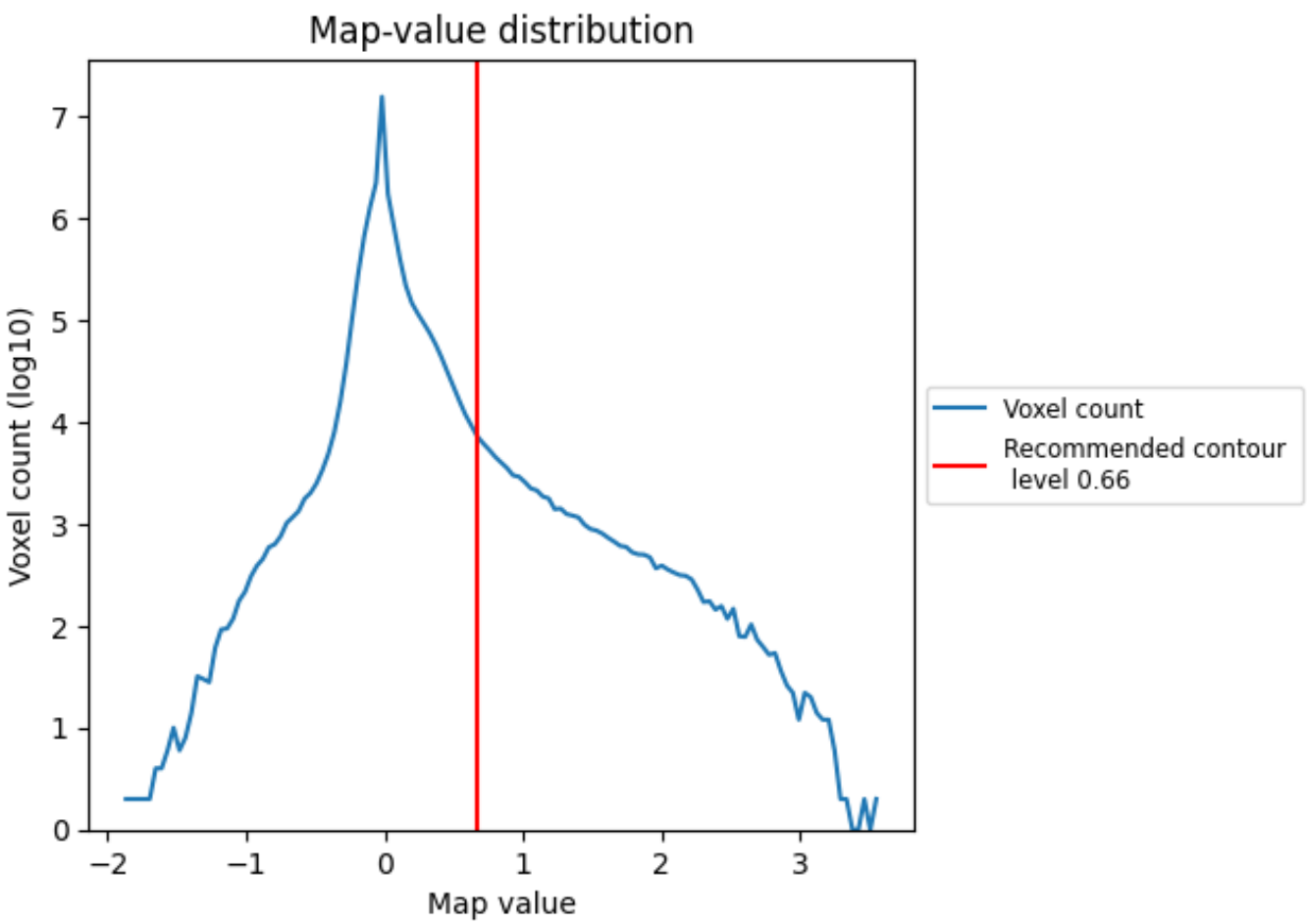
6.5 Mask visualisation (i)

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

7 Map analysis (i)

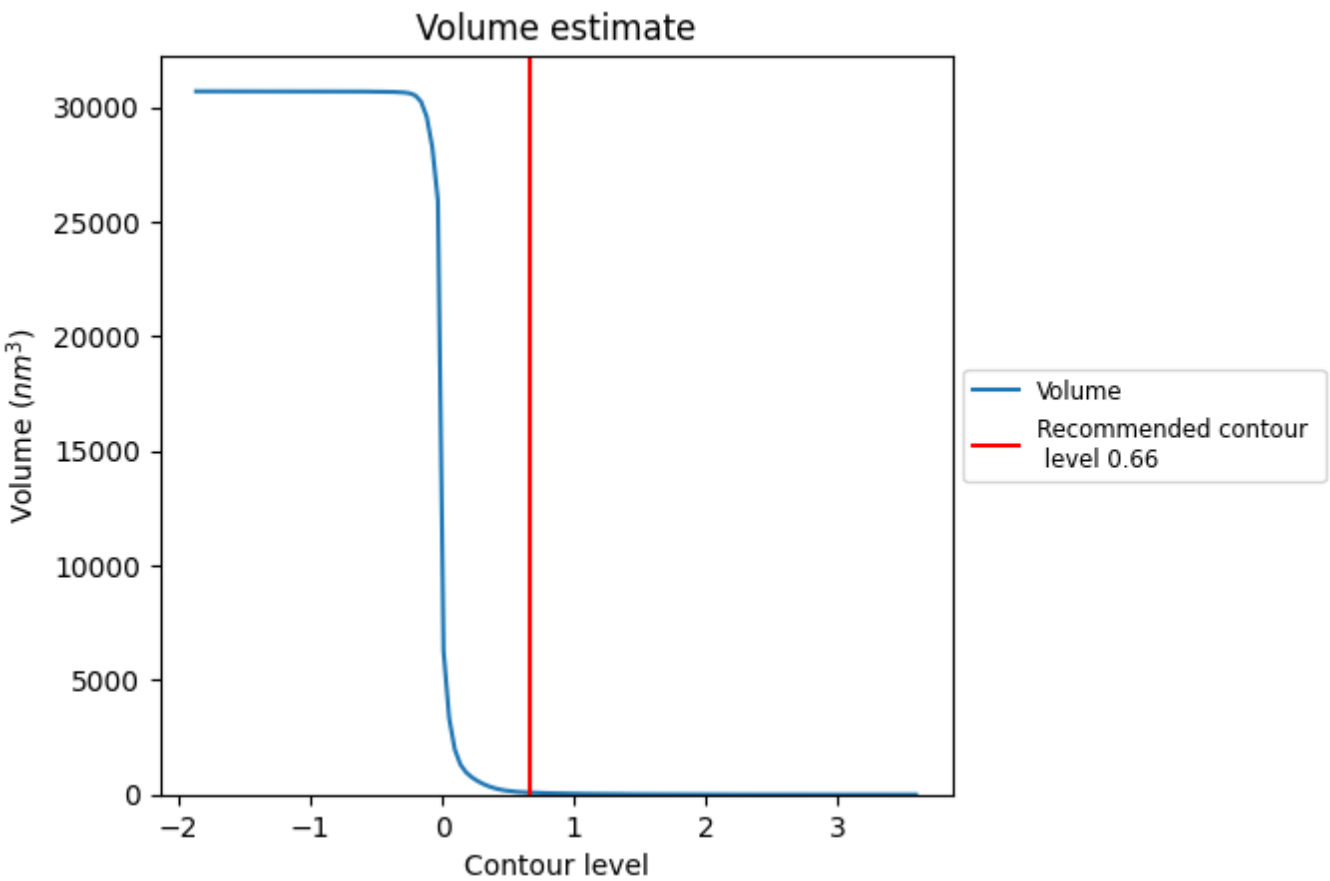
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

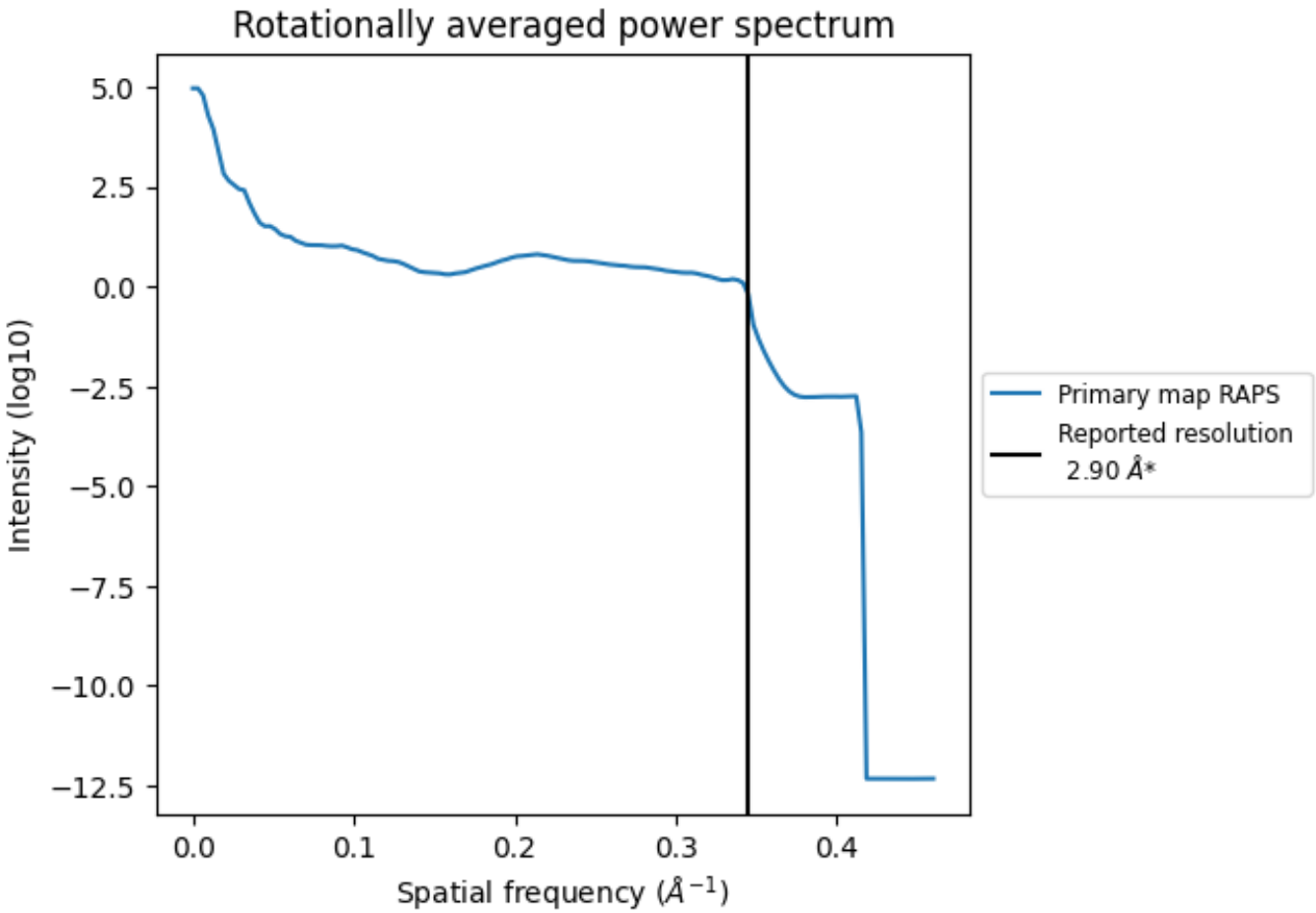
7.2 Volume estimate (i)



The volume at the recommended contour level is 87 nm^3; this corresponds to an approximate mass of 79 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 0.345 Å^{-1}

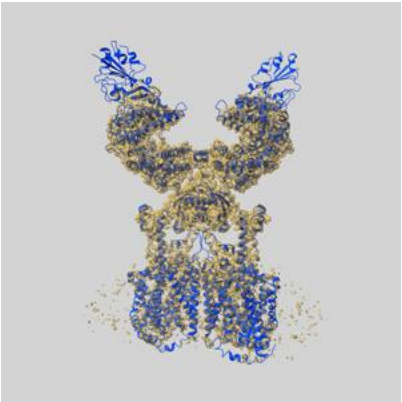
8 Fourier-Shell correlation (i)

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

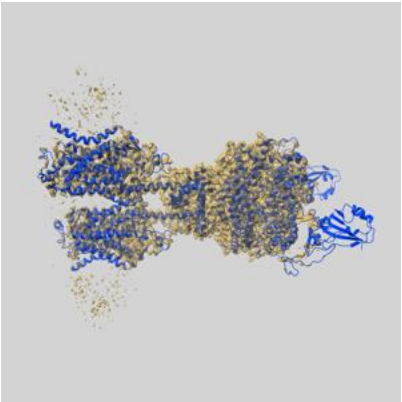
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30039 and PDB model 6M17. Per-residue inclusion information can be found in section 3 on page 10.

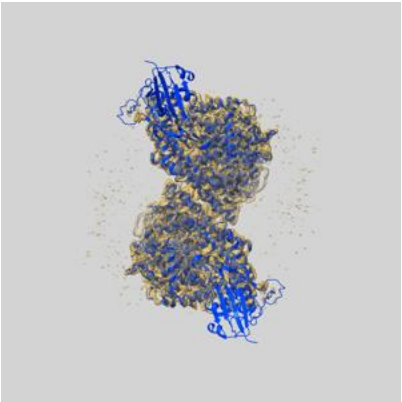
9.1 Map-model overlay (i)



X



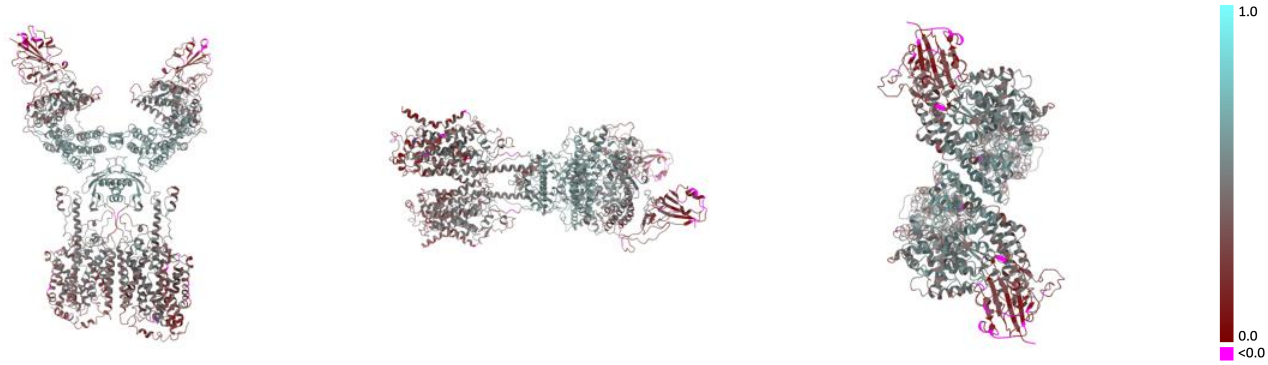
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

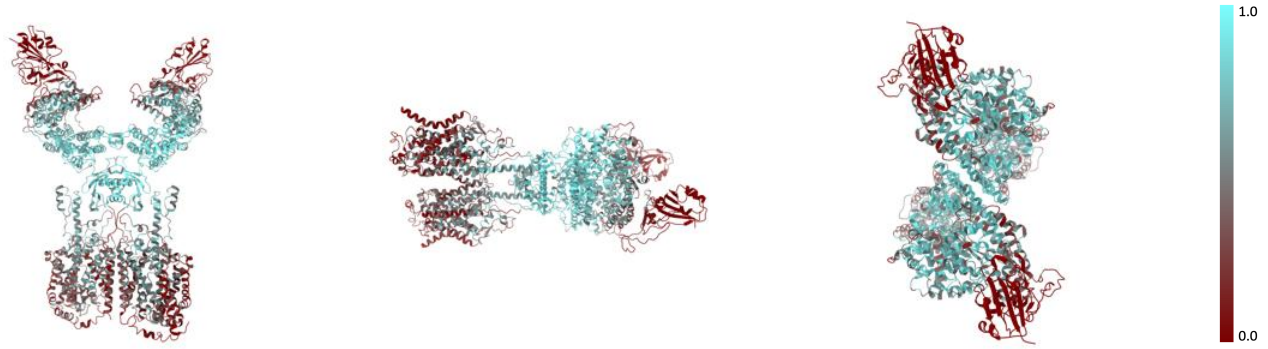
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

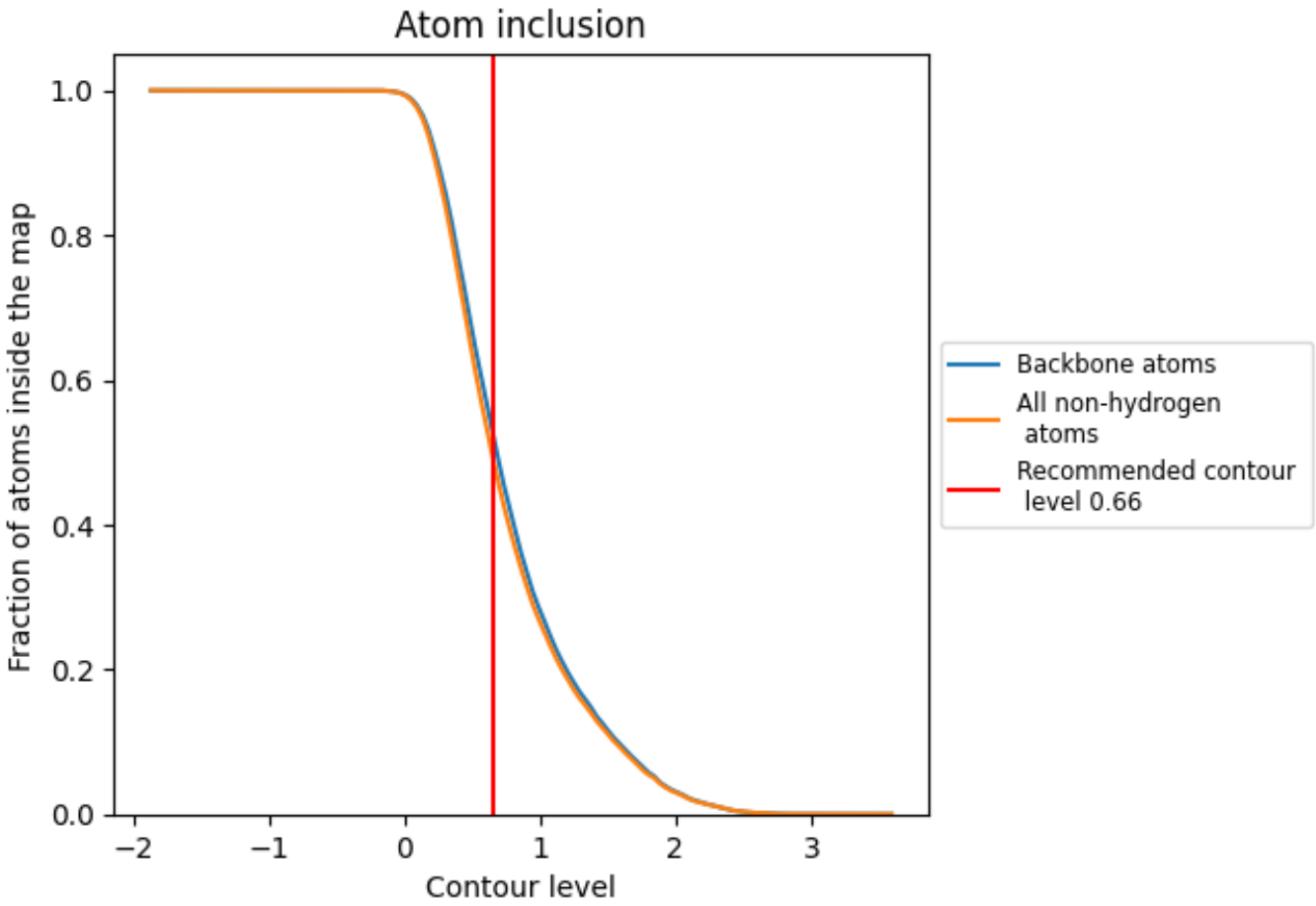
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.66).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4854	0.4200
A	0.3795	0.3780
B	0.6905	0.5080
C	0.3801	0.3770
D	0.6908	0.5050
E	0.0491	0.2330
F	0.0491	0.2270
G	0.0714	0.1940
H	0.0000	0.2040
I	0.1071	0.1140
J	0.0714	0.3000
K	0.1429	0.3390
L	0.0357	0.2420
M	0.5357	0.5240
N	0.0000	0.0450
O	0.0714	0.1980
P	0.0000	0.2170
Q	0.1071	0.1090
R	0.0714	0.2740
S	0.1429	0.3320
T	0.0357	0.2530
U	0.5357	0.5040
V	0.0000	0.0410