



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:20 AM UTC

PDB ID : 7FD2 / pdb\_00007fd2  
EMDB ID : EMD-31533  
Title : Cryo-EM structure of an alphavirus, Getah virus  
Authors : Liu, Z.; Liu, C.; Wang, A.  
Deposited on : 2021-07-15  
Resolution : 2.81 Å (reported)  
Based on initial model : 3J0C

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

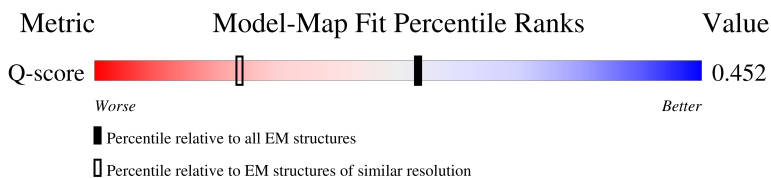
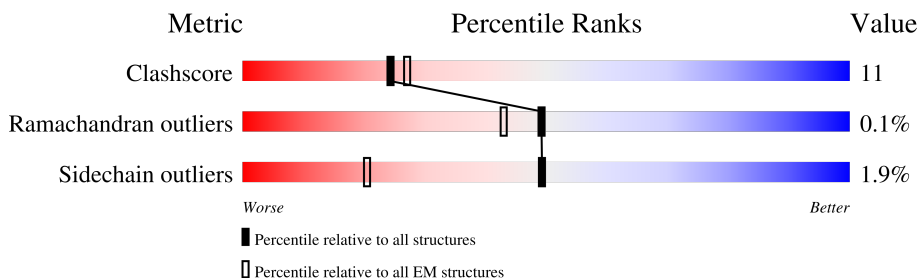
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.81 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11740 ( 2.31 - 3.31 )

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  $\geq 3$ , 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  $\leq 5\%$ . 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	438	77% (green), 23% (yellow)
1	E	438	78% (green), 21% (yellow)
1	I	438	78% (green), 21% (yellow), 1% (orange), 1% (red)
1	M	438	79% (green), 20% (yellow)

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Mol	Chain	Length	Quality of chain
2	B	419	77% 23%
2	F	419	75% 24%
2	J	419	72% 26%
2	N	419	77% 22%
3	C	268	41% 17% 41%
3	G	268	40% 18% 41%
3	K	268	41% 17% 41%
3	O	268	38% 19% 41%
4	D	4	75% 25%
4	P	4	25% 50% 25%
4	S	4	25% 75%
4	V	4	50% 50%
5	H	2	100%
5	Q	2	50% 50%
5	T	2	100%
5	W	2	50% 50%
6	L	3	67% 33%
6	R	3	67% 33%
6	U	3	67% 33%
6	X	3	67% 33%

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32613 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 Envelope glycoprotein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	438	3333	2101	567	640	25	0	0
1	E	438	3328	2098	565	640	25	0	0
1	I	438	3331	2099	567	640	25	0	0
1	M	438	3333	2101	567	640	25	0	0

- Molecule 2 is a protein called Envelope glycoprotein 2.

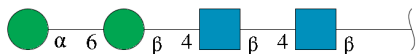
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	419	3239	2049	568	601	21	0	0
2	F	419	3239	2049	568	601	21	0	0
2	J	419	3239	2049	568	601	21	0	0
2	N	419	3239	2049	568	601	21	0	0

- Molecule 3 is a protein called capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	158	1220	769	214	228	9	0	0
3	G	158	1220	769	214	228	9	0	0
3	K	158	1220	769	214	228	9	0	0
3	O	158	1220	769	214	228	9	0	0

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos

e-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



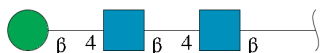
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	4	50	28	2	20	0	0
4	P	4	50	28	2	20	0	0
4	S	4	50	28	2	20	0	0
4	V	4	50	28	2	20	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	H	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	W	2	28	16	2	10	0	0

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



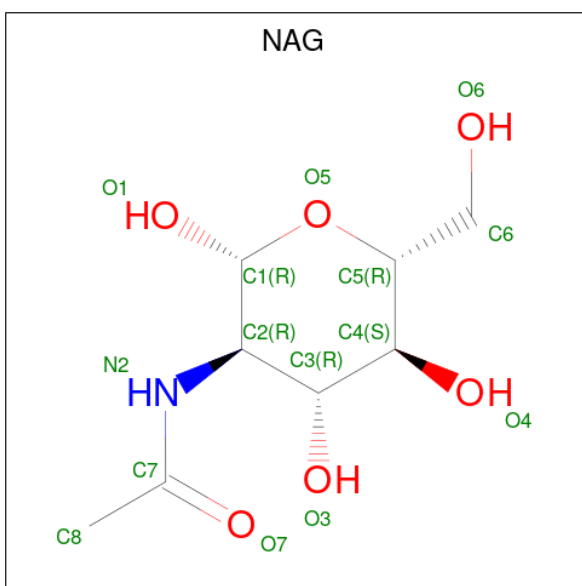
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	L	3	39	22	2	15	0	0

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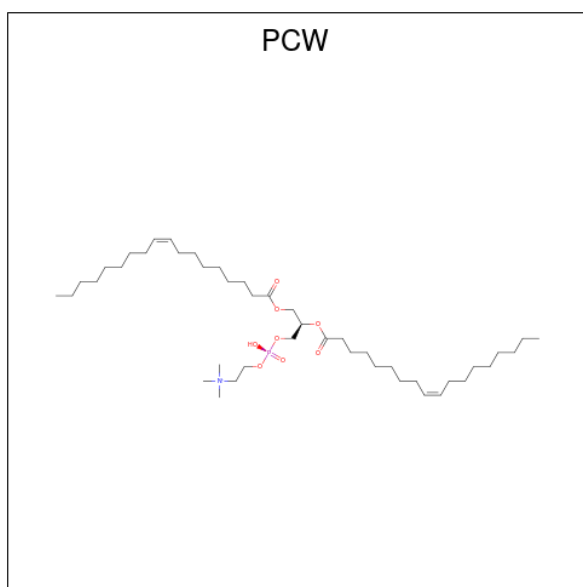
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	R	3	Total 39	C 22	N 2	O 15	0	0
6	U	3	Total 39	C 22	N 2	O 15	0	0
6	X	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



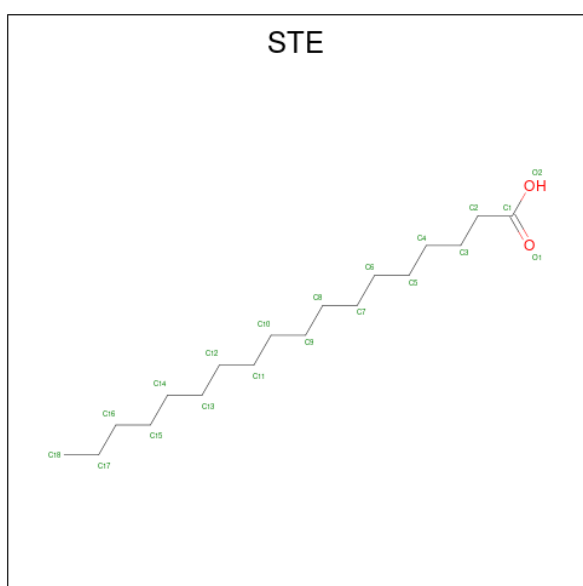
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	Total 14	C 8	N 1	O 5	0
7	E	1	Total 14	C 8	N 1	O 5	0
7	I	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0

- Molecule 8 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula:  $C_{44}H_{85}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



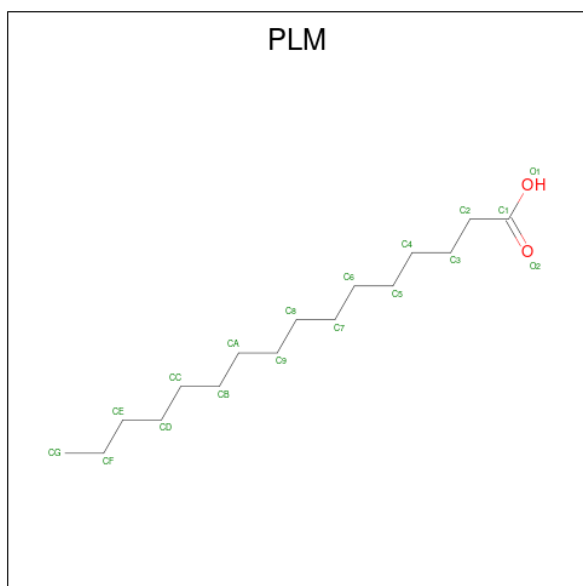
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 9 is STEARIC ACID (CCD ID: STE) (formula:  $C_{18}H_{36}O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
9	A	1	Total	C	O	0
			20	18	2	
9	B	1	Total	C	O	0
			20	18	2	
9	E	1	Total	C	O	0
			20	18	2	
9	F	1	Total	C	O	0
			20	18	2	
9	J	1	Total	C	O	0
			20	18	2	
9	J	1	Total	C	O	0
			20	18	2	
9	M	1	Total	C	O	0
			20	18	2	
9	N	1	Total	C	O	0
			20	18	2	

- Molecule 10 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



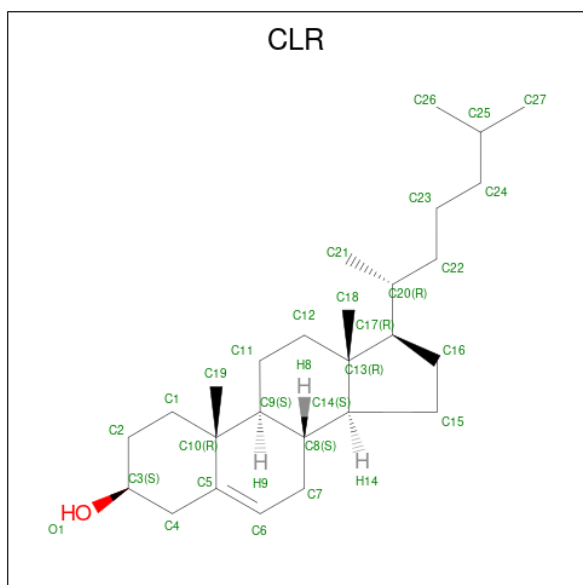
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			18	16	2	
10	B	1	Total	C	O	0
			18	16	2	
10	B	1	Total	C	O	0
			18	16	2	

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Mol	Chain	Residues	Atoms			AltConf
10	E	1	Total	C	O	0
			18	16	2	
10	F	1	Total	C	O	0
			18	16	2	
10	F	1	Total	C	O	0
			18	16	2	
10	I	1	Total	C	O	0
			18	16	2	
10	J	1	Total	C	O	0
			18	16	2	
10	J	1	Total	C	O	0
			18	16	2	
10	M	1	Total	C	O	0
			18	16	2	
10	N	1	Total	C	O	0
			18	16	2	
10	N	1	Total	C	O	0
			18	16	2	

- Molecule 11 is CHOLESTEROL (CCD ID: CLR) (formula:  $C_{27}H_{46}O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
11	B	1	Total	C	O	0
			28	27	1	
11	B	1	Total	C	O	0
			28	27	1	

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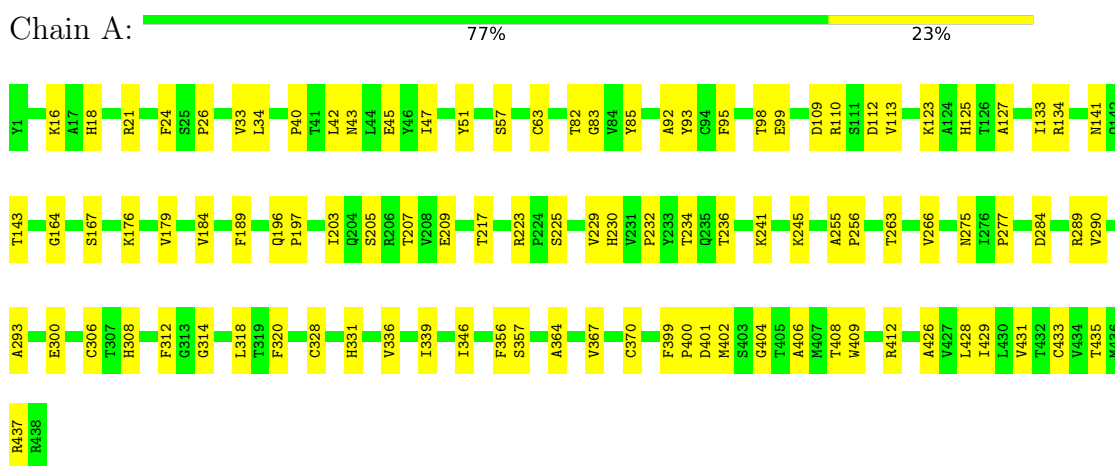
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>AltConf</b>
11	B	1	Total	C	O	0
			28	27	1	
11	F	1	Total	C	O	0
			28	27	1	
11	F	1	Total	C	O	0
			28	27	1	
11	F	1	Total	C	O	0
			28	27	1	
11	I	1	Total	C	O	0
			28	27	1	
11	J	1	Total	C	O	0
			28	27	1	
11	J	1	Total	C	O	0
			28	27	1	
11	N	1	Total	C	O	0
			28	27	1	
11	N	1	Total	C	O	0
			28	27	1	
11	N	1	Total	C	O	0
			28	27	1	

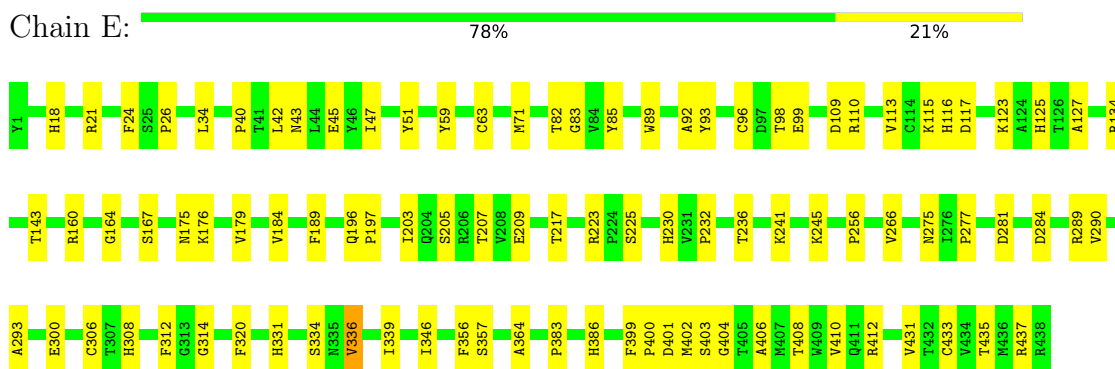
### 3 Residue-property plots [i](#)

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.

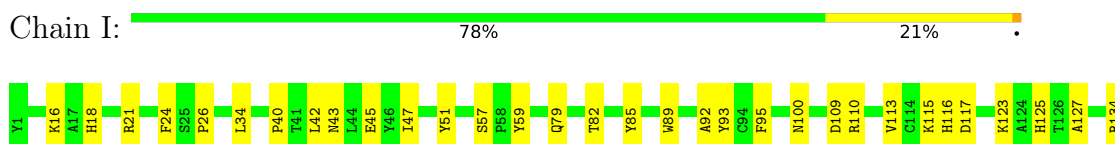
- Molecule 1: Envelope glycoprotein 1

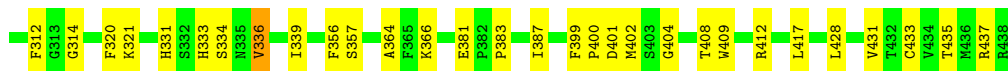
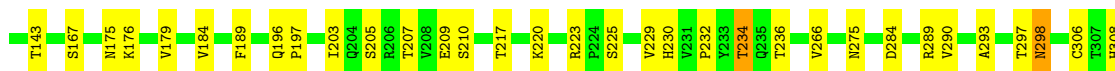


- Molecule 1: Envelope glycoprotein 1

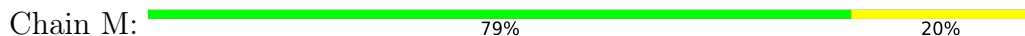


- Molecule 1: Envelope glycoprotein 1

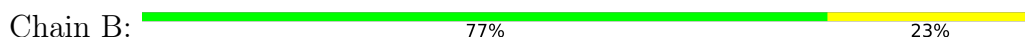




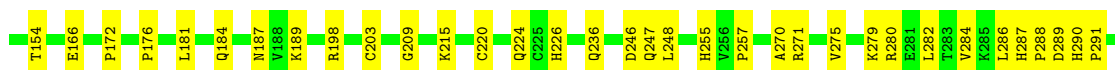
• Molecule 1: Envelope glycoprotein 1



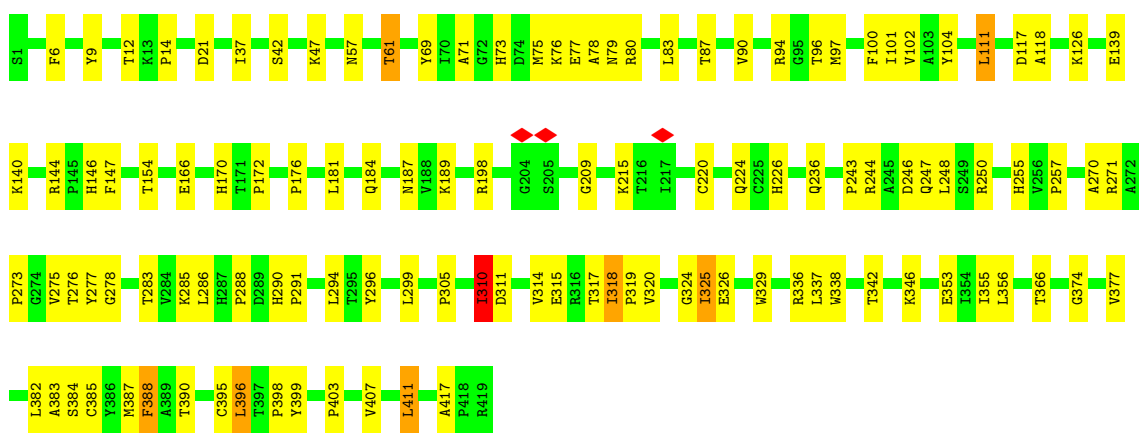
• Molecule 2: Envelope glycoprotein 2



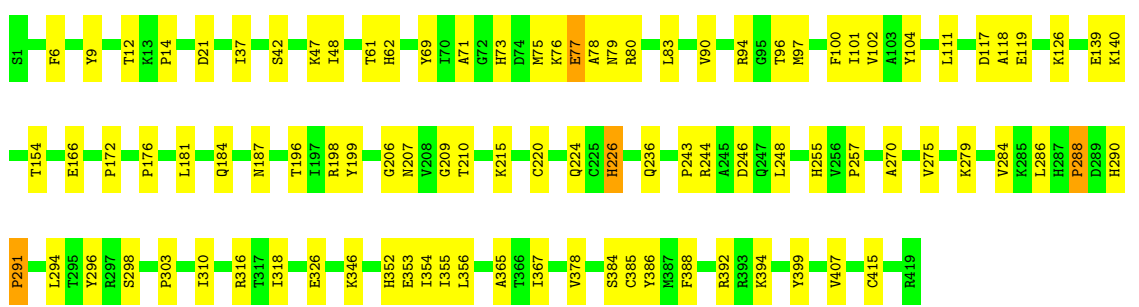
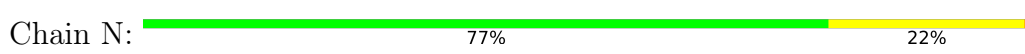
• Molecule 2: Envelope glycoprotein 2



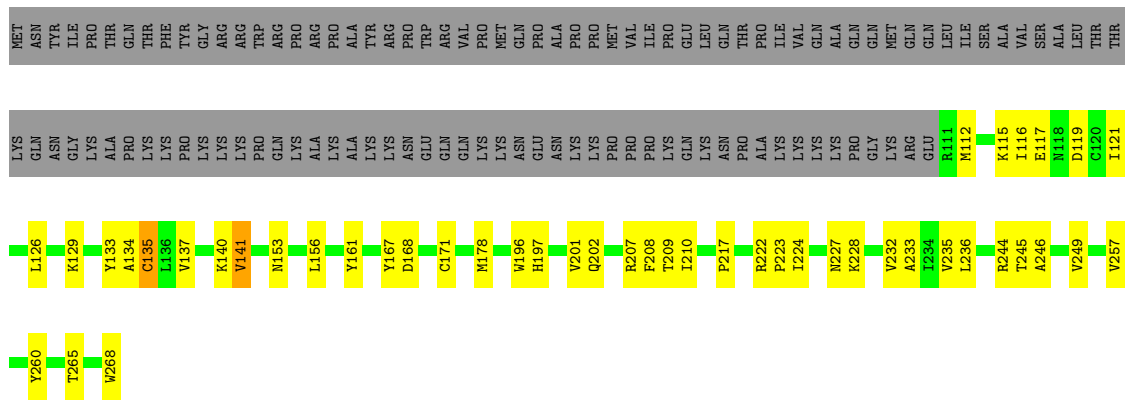
• Molecule 2: Envelope glycoprotein 2



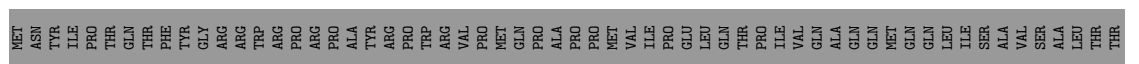
• Molecule 2: Envelope glycoprotein 2

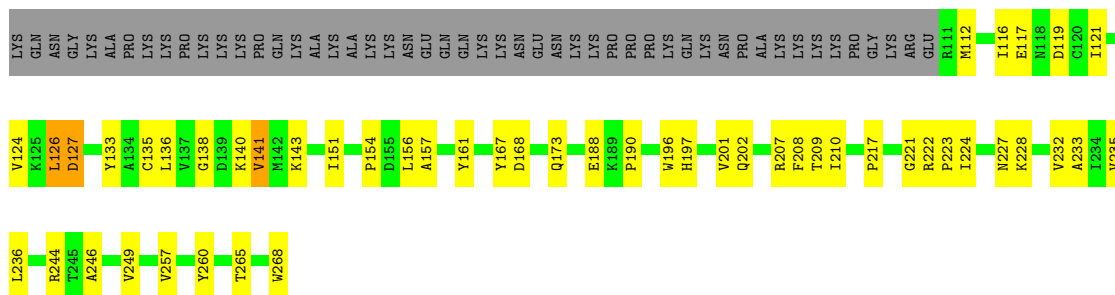


• Molecule 3: capsid protein



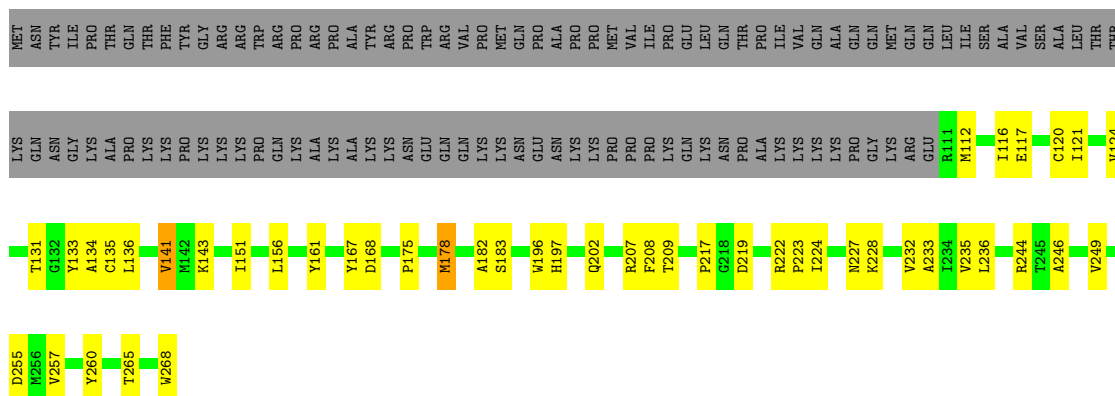
• Molecule 3: capsid protein





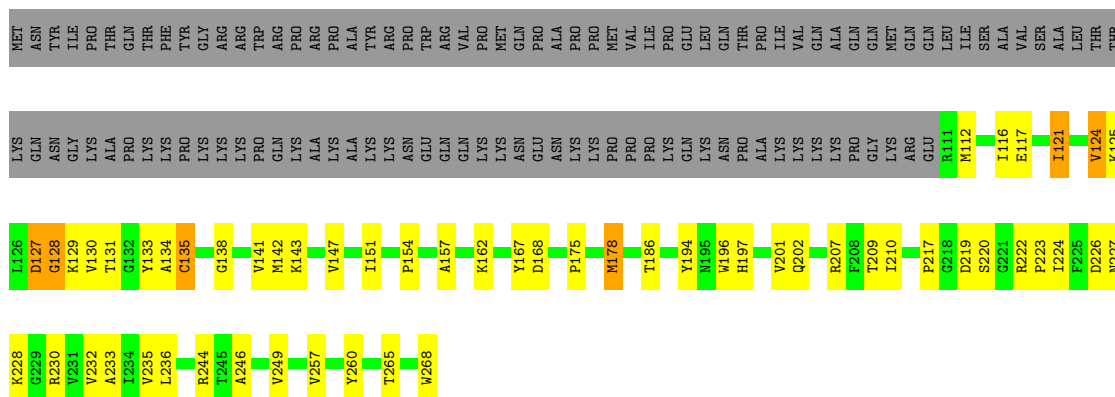
- Molecule 3: capsid protein

## Chain K:



- Molecule 3: capsid protein

## Chain O:

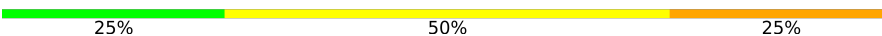


- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

## Chain D:

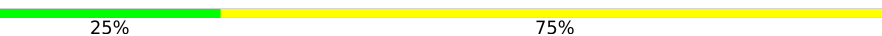


- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  25% 50% 25%



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

Chain S:  25% 75%



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

Chain V:  50% 50%



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

Chain H:  100%

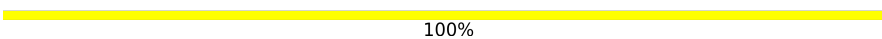


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50% 50%




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

Chain T:  100%




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

Chain W:  50% 50%


MAG1  
MAG2

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

Chain L:  67% 33%

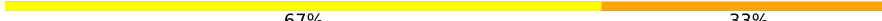
MAG1  
MAG2  
BMA3

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

Chain R:  67% 33%

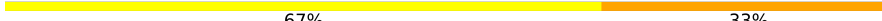
MAG1  
MAG2  
BMA3

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

Chain U:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain X:  67% 33%

MAG1  
MAG2  
BMA3

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2041957	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 ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	46.012	Depositor
Minimum map value	-32.611	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	849.92, 849.92, 849.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.66, 1.66, 1.66	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: MAN, CLR, NAG, BMA, PLM, STE, PCW

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	0.48	0/3417	0.67	0/4663
1	E	0.47	0/3411	0.65	0/4655
1	I	0.48	0/3415	0.67	0/4660
1	M	0.48	0/3417	0.66	0/4663
2	B	0.42	0/3326	0.61	0/4538
2	F	0.40	0/3326	0.60	0/4538
2	J	0.66	2/3326 (0.1%)	0.95	14/4538 (0.3%)
2	N	0.57	0/3326	0.80	4/4538 (0.1%)
3	C	0.64	0/1249	0.95	0/1687
3	G	0.63	0/1249	0.91	1/1687 (0.1%)
3	K	0.64	0/1249	0.95	0/1687
3	O	0.65	0/1249	0.96	3/1687 (0.2%)
All	All	0.53	2/31960 (0.0%)	0.75	22/43541 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	310	ILE	C-O	-5.55	1.17	1.24
2	J	273	PRO	C-O	-5.36	1.17	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	207	ASN	CB-CA-C	-8.01	107.34	116.63
2	J	319	PRO	CB-CA-C	-7.45	102.45	111.46
2	J	324	GLY	CA-C-O	-7.17	117.14	122.37
2	J	384	SER	CA-C-N	-6.56	111.12	122.79
2	J	384	SER	C-N-CA	-6.56	111.12	122.79
2	J	318	ILE	N-CA-CB	-6.00	103.83	111.39
2	J	403	PRO	N-CA-C	5.92	122.58	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	128	GLY	CA-C-N	-5.88	114.60	122.42
3	O	128	GLY	C-N-CA	-5.88	114.60	122.42
2	J	411	LEU	N-CA-C	-5.41	106.64	113.18
2	N	384	SER	N-CA-C	-5.41	105.39	111.28
3	G	127	ASP	N-CA-C	-5.37	106.68	113.23
2	J	384	SER	N-CA-C	-5.24	106.96	113.19
2	J	388	PHE	CB-CA-C	-5.23	102.67	110.88
3	O	127	ASP	CA-CB-CG	5.23	117.83	112.60
2	J	390	THR	CB-CA-C	-5.19	102.17	110.79
2	N	119	GLU	N-CA-C	-5.07	107.59	112.97
2	J	273	PRO	CA-C-O	-5.06	115.57	121.34
2	J	278	GLY	CA-C-N	-5.03	115.73	122.42
2	J	278	GLY	C-N-CA	-5.03	115.73	122.42
2	J	319	PRO	N-CA-CB	-5.02	98.94	103.36
2	N	367	ILE	N-CA-C	-5.01	105.51	110.62

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	3333	0	3236	75	0
1	E	3328	0	3230	78	0
1	I	3331	0	3228	77	0
1	M	3333	0	3235	70	0
2	B	3239	0	3191	63	0
2	F	3239	0	3191	76	0
2	J	3239	0	3191	78	0
2	N	3239	0	3190	60	0
3	C	1220	0	1204	30	0
3	G	1220	0	1204	31	0
3	K	1220	0	1204	33	0
3	O	1220	0	1204	39	0
4	D	50	0	43	1	0
4	P	50	0	43	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	50	0	43	0	0
4	V	50	0	43	0	0
5	H	28	0	25	6	0
5	Q	28	0	25	2	0
5	T	28	0	25	0	0
5	W	28	0	25	2	0
6	L	39	0	34	1	0
6	R	39	0	34	1	0
6	U	39	0	34	1	0
6	X	39	0	34	1	0
7	A	14	0	13	0	0
7	E	14	0	13	0	0
7	I	14	0	13	0	0
7	M	14	0	13	0	0
8	A	54	0	84	2	0
8	E	54	0	84	5	0
8	I	54	0	84	3	0
8	M	54	0	84	5	0
9	A	20	0	35	1	0
9	B	20	0	35	2	0
9	E	20	0	35	0	0
9	F	20	0	35	1	0
9	J	40	0	70	3	0
9	M	20	0	35	0	0
9	N	20	0	35	1	0
10	A	18	0	31	1	0
10	B	36	0	62	2	0
10	E	18	0	31	1	0
10	F	36	0	62	2	0
10	I	18	0	31	0	0
10	J	36	0	62	2	0
10	M	18	0	31	0	0
10	N	36	0	62	2	0
11	B	84	0	138	9	0
11	F	84	0	138	11	0
11	I	28	0	46	2	0
11	J	56	0	92	7	0
11	N	84	0	138	8	0
All	All	32613	0	32508	694	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 11.

All (694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HD21	5:H:1:NAG:C1	0.99	1.55
1:E:116:HIS:ND1	4:P:1:NAG:H83	1.59	1.17
1:E:116:HIS:ND1	4:P:1:NAG:C8	2.29	0.95
2:J:310:ILE:HD12	2:J:314:VAL:HG21	1.60	0.83
2:F:275:VAL:HG12	2:F:284:VAL:HG12	1.59	0.82
2:B:275:VAL:HG12	2:B:284:VAL:HG12	1.60	0.81
2:B:198:ARG:HA	2:B:209:GLY:HA3	1.68	0.76
2:J:198:ARG:HA	2:J:209:GLY:HA3	1.68	0.75
2:F:198:ARG:HA	2:F:209:GLY:HA3	1.68	0.75
2:N:198:ARG:HA	2:N:209:GLY:HA3	1.68	0.74
1:A:113:VAL:HG21	2:B:40:GLU:HG2	1.69	0.74
3:O:124:VAL:HG11	3:O:143:LYS:NZ	2.02	0.74
2:J:181:LEU:HD11	2:J:226:HIS:HA	1.72	0.70
2:B:181:LEU:HD11	2:B:226:HIS:HA	1.72	0.70
2:F:181:LEU:HD11	2:F:226:HIS:HA	1.72	0.70
1:M:93:TYR:HA	2:N:176:PRO:HG3	1.72	0.70
1:I:381:GLU:HB2	1:M:22:ASN:HD21	1.57	0.69
2:N:140:LYS:HD2	2:N:291:PRO:HB2	1.74	0.69
2:N:184:GLN:OE1	2:N:215:LYS:NZ	2.26	0.69
1:E:230:HIS:CD2	2:J:147:PHE:HB3	2.27	0.69
2:B:184:GLN:OE1	2:B:215:LYS:NZ	2.26	0.69
1:I:93:TYR:HA	2:J:176:PRO:HG3	1.73	0.68
8:E:502:PCW:H41	11:F:501:CLR:H41	1.74	0.68
2:F:282:LEU:HB3	2:F:318:ILE:HB	1.75	0.68
2:B:282:LEU:HB3	2:B:318:ILE:HB	1.75	0.67
2:F:346:LYS:HB3	2:F:353:GLU:HB3	1.76	0.67
3:O:124:VAL:HG13	3:O:151:ILE:HD13	1.76	0.67
2:F:184:GLN:OE1	2:F:215:LYS:NZ	2.26	0.66
2:N:355:ILE:HG21	11:N:502:CLR:H151	1.76	0.66
1:I:387:ILE:HD12	2:J:277:TYR:HD1	1.61	0.65
3:O:131:THR:HB	3:O:147:VAL:HG13	1.78	0.65
3:C:140:LYS:HD2	3:C:171:CYS:HB3	1.79	0.64
1:I:57:SER:HB2	2:J:244:ARG:HD2	1.80	0.64
2:F:351:PRO:HA	11:F:501:CLR:H262	1.80	0.63
1:E:21:ARG:HD3	1:E:24:PHE:HD2	1.64	0.63
2:J:184:GLN:OE1	2:J:215:LYS:NZ	2.26	0.63
2:J:288:PRO:HG3	2:J:310:ILE:HG22	1.81	0.63
3:O:124:VAL:HG21	3:O:143:LYS:HZ3	1.63	0.63
1:E:115:LYS:HE2	1:E:116:HIS:HE2	1.64	0.62
1:I:115:LYS:HE2	1:I:116:HIS:HE2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:121:ILE:HD11	3:K:223:PRO:HD3	1.82	0.62
1:A:21:ARG:HD3	1:A:24:PHE:HD2	1.64	0.62
3:C:134:ALA:HB1	3:C:141:VAL:CG2	2.30	0.62
1:E:93:TYR:HA	2:F:176:PRO:HG3	1.82	0.62
3:K:124:VAL:HG22	3:K:151:ILE:HD13	1.81	0.62
1:M:21:ARG:HD3	1:M:24:PHE:HD2	1.64	0.62
2:J:355:ILE:HG21	11:J:502:CLR:H151	1.83	0.61
1:I:21:ARG:HD3	1:I:24:PHE:HD2	1.64	0.61
2:B:359:TYR:CE2	11:B:503:CLR:H42	2.35	0.61
3:C:121:ILE:HD11	3:C:223:PRO:HD3	1.82	0.61
2:B:346:LYS:HB3	2:B:353:GLU:HB3	1.83	0.60
2:N:286:LEU:HD11	2:N:294:LEU:HD22	1.83	0.60
2:N:346:LYS:HB3	2:N:353:GLU:HB3	1.83	0.60
3:G:136:LEU:HA	3:G:141:VAL:HA	1.82	0.60
2:F:359:TYR:HA	2:F:366:THR:HG21	1.84	0.60
1:E:230:HIS:HD2	2:J:147:PHE:HB3	1.66	0.60
2:J:346:LYS:HB3	2:J:353:GLU:HB3	1.83	0.60
2:N:37:ILE:HD13	2:N:111:LEU:HD13	1.83	0.59
2:B:296:TYR:CE2	2:B:318:ILE:HG23	2.37	0.59
8:M:502:PCW:H362	2:N:365:ALA:HB1	1.83	0.59
3:G:121:ILE:HD11	3:G:223:PRO:HD3	1.83	0.59
1:M:401:ASP:OD1	1:M:402:MET:N	2.36	0.59
2:F:296:TYR:CE2	2:F:318:ILE:HG23	2.37	0.59
2:B:359:TYR:HA	2:B:366:THR:HG21	1.84	0.59
2:F:403:PRO:HA	3:G:140:LYS:HB2	1.85	0.59
1:A:401:ASP:OD1	1:A:402:MET:N	2.36	0.59
1:E:401:ASP:OD1	1:E:402:MET:N	2.36	0.58
3:O:227:ASN:OD1	3:O:228:LYS:N	2.36	0.58
1:A:112:ASP:HB3	2:B:165:GLU:HG2	1.84	0.58
1:I:401:ASP:OD1	1:I:402:MET:N	2.36	0.58
2:B:172:PRO:HG3	2:B:236:GLN:HG3	1.86	0.58
2:F:172:PRO:HG3	2:F:236:GLN:HG3	1.86	0.58
1:E:406:ALA:HB2	2:F:354:ILE:HG21	1.86	0.58
3:O:124:VAL:HG11	3:O:143:LYS:HZ3	1.68	0.58
2:B:370:VAL:CG1	11:B:503:CLR:H161	2.34	0.58
3:G:224:ILE:HB	3:G:233:ALA:HB3	1.86	0.58
2:N:199:TYR:HD1	2:N:206:GLY:HA2	1.69	0.58
1:E:134:ARG:HG3	1:E:143:THR:OG1	2.04	0.58
3:G:227:ASN:OD1	3:G:228:LYS:N	2.36	0.58
2:J:96:THR:HG22	2:J:101:ILE:HG23	1.85	0.58
2:N:187:ASN:HB3	2:N:215:LYS:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:THR:HG22	2:B:101:ILE:HG23	1.85	0.57
3:C:224:ILE:HB	3:C:233:ALA:HB3	1.86	0.57
2:F:96:THR:HG22	2:F:101:ILE:HG23	1.85	0.57
3:G:117:GLU:OE1	3:G:197:HIS:ND1	2.34	0.57
1:M:134:ARG:HG3	1:M:143:THR:OG1	2.04	0.57
1:M:134:ARG:NH1	5:W:1:NAG:H3	2.19	0.57
2:N:96:THR:HG22	2:N:101:ILE:HG23	1.85	0.57
3:K:133:TYR:HE2	3:K:219:ASP:HA	1.69	0.57
3:O:224:ILE:HB	3:O:233:ALA:HB3	1.86	0.57
2:J:172:PRO:HG3	2:J:236:GLN:HG3	1.86	0.57
2:J:140:LYS:HD2	2:J:291:PRO:HB2	1.87	0.57
1:I:134:ARG:HG3	1:I:143:THR:OG1	2.04	0.57
2:N:172:PRO:HG3	2:N:236:GLN:HG3	1.85	0.57
1:E:386:HIS:ND1	2:F:279:LYS:HA	2.20	0.57
2:F:355:ILE:CD1	11:F:501:CLR:H232	2.35	0.57
1:A:83:GLY:HA2	1:A:98:THR:O	2.05	0.56
2:N:275:VAL:HG12	2:N:284:VAL:HG12	1.86	0.56
2:B:187:ASN:HB3	2:B:215:LYS:HB3	1.86	0.56
2:N:199:TYR:CD1	2:N:206:GLY:HA2	2.40	0.56
1:A:134:ARG:HG3	1:A:143:THR:OG1	2.04	0.56
3:C:227:ASN:OD1	3:C:228:LYS:N	2.36	0.56
2:N:356:LEU:HD21	11:N:502:CLR:H6	1.86	0.56
3:K:227:ASN:OD1	3:K:228:LYS:N	2.36	0.56
1:E:43:ASN:OD1	1:E:125:HIS:NE2	2.37	0.56
2:J:187:ASN:HB3	2:J:215:LYS:HB3	1.86	0.56
2:N:288:PRO:HG3	2:N:310:ILE:HG22	1.86	0.56
3:K:175:PRO:HD2	3:K:178:MET:HG3	1.87	0.56
1:M:43:ASN:OD1	1:M:125:HIS:NE2	2.37	0.56
2:B:288:PRO:HG3	2:B:310:ILE:HG22	1.88	0.56
1:I:333:HIS:HB2	1:I:366:LYS:HG3	1.87	0.56
2:J:320:VAL:HG22	2:J:325:ILE:HG12	1.88	0.56
2:F:288:PRO:HG3	2:F:310:ILE:HG22	1.88	0.56
1:M:336:VAL:HG22	1:M:365:PHE:HB3	1.89	0.55
3:O:175:PRO:HD2	3:O:178:MET:HG3	1.87	0.55
3:G:188:GLU:HG2	3:G:190:PRO:HD3	1.87	0.55
3:K:224:ILE:HB	3:K:233:ALA:HB3	1.86	0.55
2:F:187:ASN:HB3	2:F:215:LYS:HB3	1.86	0.55
1:I:417:LEU:HD21	2:J:377:VAL:HA	1.88	0.55
1:M:47:ILE:N	1:M:205:SER:O	2.37	0.55
1:I:399:PHE:HD1	1:I:400:PRO:HD2	1.72	0.55
1:M:83:GLY:HA2	1:M:98:THR:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:406:ALA:HB2	2:N:354:ILE:HG21	1.89	0.55
3:O:121:ILE:HD11	3:O:223:PRO:HD3	1.89	0.55
3:C:117:GLU:OE1	3:C:197:HIS:ND1	2.34	0.55
2:F:355:ILE:HD13	11:F:501:CLR:H232	1.89	0.55
2:J:382:LEU:C	2:J:385:CYS:H	2.16	0.54
3:G:207:ARG:HH21	3:G:246:ALA:HB2	1.72	0.54
1:A:43:ASN:OD1	1:A:125:HIS:NE2	2.37	0.54
1:A:141:ASN:HD21	5:H:1:NAG:C2	2.04	0.54
3:C:209:THR:HG23	3:C:244:ARG:HH21	1.72	0.54
2:J:94:ARG:HH11	2:J:104:TYR:HE2	1.54	0.54
1:I:207:THR:HG22	1:I:209:GLU:H	1.73	0.54
2:N:94:ARG:HH11	2:N:104:TYR:HE2	1.55	0.54
1:E:207:THR:HG22	1:E:209:GLU:H	1.72	0.54
1:I:43:ASN:OD1	1:I:125:HIS:NE2	2.37	0.54
1:A:399:PHE:CD1	1:A:400:PRO:HD2	2.43	0.54
2:B:94:ARG:HH11	2:B:104:TYR:HE2	1.55	0.54
2:F:392:ARG:NE	2:F:415:CYS:O	2.39	0.54
3:K:209:THR:HG23	3:K:244:ARG:HH21	1.72	0.54
3:K:233:ALA:HB1	3:K:249:VAL:HG21	1.88	0.54
1:E:399:PHE:CD1	1:E:400:PRO:HD2	2.43	0.54
2:F:94:ARG:HH11	2:F:104:TYR:HE2	1.54	0.54
2:B:392:ARG:NE	2:B:415:CYS:O	2.39	0.54
1:E:179:VAL:HG22	1:E:184:VAL:HG22	1.90	0.54
8:E:502:PCW:H261	2:F:373:ALA:HB2	1.90	0.54
3:G:209:THR:HG23	3:G:244:ARG:HH21	1.72	0.54
1:M:399:PHE:CD1	1:M:400:PRO:HD2	2.43	0.54
1:E:47:ILE:N	1:E:205:SER:O	2.37	0.53
1:M:399:PHE:HD1	1:M:400:PRO:HD2	1.72	0.53
1:M:290:VAL:HA	1:M:293:ALA:HB3	1.90	0.53
3:O:207:ARG:HH21	3:O:246:ALA:HB2	1.72	0.53
1:A:47:ILE:N	1:A:205:SER:O	2.37	0.53
1:A:207:THR:HG22	1:A:209:GLU:H	1.73	0.53
3:K:121:ILE:HD12	3:K:133:TYR:HB3	1.90	0.53
3:O:209:THR:HG23	3:O:244:ARG:HH21	1.72	0.53
2:B:370:VAL:HG12	11:B:503:CLR:H161	1.91	0.53
1:A:290:VAL:HA	1:A:293:ALA:HB3	1.90	0.53
1:I:399:PHE:CD1	1:I:400:PRO:HD2	2.43	0.53
3:O:124:VAL:HG11	3:O:143:LYS:HZ1	1.74	0.53
3:C:207:ARG:HH21	3:C:246:ALA:HB2	1.72	0.53
1:M:179:VAL:HG22	1:M:184:VAL:HG22	1.90	0.53
1:A:399:PHE:HD1	1:A:400:PRO:HD2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PRO:HD2	2:B:75:MET:HE2	1.91	0.53
1:E:290:VAL:HA	1:E:293:ALA:HB3	1.90	0.53
1:M:207:THR:HG22	1:M:209:GLU:H	1.73	0.53
3:K:207:ARG:HH21	3:K:246:ALA:HB2	1.72	0.53
2:F:14:PRO:HD2	2:F:75:MET:HE2	1.91	0.52
1:I:85:TYR:HE1	1:I:92:ALA:HB1	1.74	0.52
2:J:399:TYR:HE1	3:K:255:ASP:HB3	1.73	0.52
1:A:85:TYR:HE1	1:A:92:ALA:HB1	1.74	0.52
1:I:179:VAL:HG22	1:I:184:VAL:HG22	1.90	0.52
3:K:120:CYS:HB2	3:K:183:SER:HB3	1.91	0.52
1:M:85:TYR:HE1	1:M:92:ALA:HB1	1.74	0.52
1:E:334:SER:HB3	1:E:336:VAL:HG23	1.91	0.52
1:E:399:PHE:HD1	1:E:400:PRO:HD2	1.72	0.52
1:I:220:LYS:HB2	1:I:234:THR:HG23	1.91	0.52
2:J:14:PRO:HD2	2:J:75:MET:HE2	1.91	0.52
1:A:179:VAL:HG22	1:A:184:VAL:HG22	1.90	0.52
2:J:356:LEU:HD21	11:J:502:CLR:H6	1.92	0.52
1:A:93:TYR:HA	2:B:176:PRO:HG3	1.90	0.52
1:E:63:CYS:HA	1:E:99:GLU:O	2.10	0.52
3:K:222:ARG:O	3:K:235:VAL:HG12	2.10	0.52
1:M:57:SER:HB2	2:N:244:ARG:HD2	1.90	0.52
3:C:202:GLN:HB3	3:C:209:THR:HG23	1.92	0.52
1:E:85:TYR:HE1	1:E:92:ALA:HB1	1.74	0.52
3:G:202:GLN:HB3	3:G:209:THR:HG23	1.92	0.52
11:J:502:CLR:H242	11:J:503:CLR:H232	1.92	0.52
2:N:14:PRO:HD2	2:N:75:MET:HE2	1.91	0.52
1:A:21:ARG:HH12	1:A:284:ASP:HA	1.75	0.51
3:C:207:ARG:HG2	3:C:260:TYR:CE2	2.46	0.51
1:E:408:THR:CG2	1:E:412:ARG:HE	2.24	0.51
1:A:408:THR:CG2	1:A:412:ARG:HE	2.24	0.51
1:I:290:VAL:HA	1:I:293:ALA:HB3	1.90	0.51
3:O:207:ARG:HG2	3:O:260:TYR:CE2	2.46	0.51
3:C:222:ARG:O	3:C:235:VAL:HG12	2.10	0.51
1:E:83:GLY:HA2	1:E:98:THR:O	2.10	0.51
1:I:334:SER:HB3	1:I:336:VAL:HG23	1.91	0.51
1:M:408:THR:CG2	1:M:412:ARG:HE	2.24	0.51
1:A:18:HIS:HD1	1:A:331:HIS:CB	2.24	0.51
11:B:502:CLR:H242	11:B:503:CLR:H232	1.90	0.51
2:F:286:LEU:C	2:F:287:HIS:HD1	2.18	0.51
1:I:21:ARG:HH12	1:I:284:ASP:HA	1.75	0.51
3:K:134:ALA:HB1	3:K:141:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:207:ARG:HG2	3:G:260:TYR:CE2	2.46	0.51
2:J:286:LEU:HD11	2:J:294:LEU:HD22	1.92	0.51
3:K:124:VAL:HG11	3:K:143:LYS:NZ	2.26	0.51
1:M:21:ARG:HH12	1:M:284:ASP:HA	1.76	0.51
3:O:222:ARG:O	3:O:235:VAL:HG12	2.10	0.51
2:B:71:ALA:HB3	2:B:76:LYS:HD3	1.93	0.51
1:E:21:ARG:HH12	1:E:284:ASP:HA	1.76	0.51
1:I:47:ILE:N	1:I:205:SER:O	2.37	0.51
3:O:202:GLN:HB3	3:O:209:THR:HG23	1.92	0.51
8:A:502:PCW:H19	11:B:501:CLR:H152	1.93	0.51
2:F:71:ALA:HB3	2:F:76:LYS:HD3	1.93	0.51
1:I:408:THR:CG2	1:I:412:ARG:HE	2.24	0.51
1:I:428:LEU:HD22	2:J:387:MET:HG3	1.92	0.51
1:M:18:HIS:HD1	1:M:331:HIS:CB	2.24	0.51
3:C:134:ALA:HB1	3:C:141:VAL:HG23	1.92	0.51
2:J:69:TYR:OH	2:J:117:ASP:OD1	2.21	0.51
1:A:57:SER:HB2	2:B:244:ARG:HD2	1.92	0.51
1:E:18:HIS:HD1	1:E:331:HIS:CB	2.24	0.51
1:E:51:TYR:HB3	1:E:203:ILE:HD13	1.93	0.51
1:E:308:HIS:NE2	2:F:357:TYR:OH	2.41	0.51
2:J:71:ALA:HB3	2:J:76:LYS:HD3	1.93	0.51
2:F:189:LYS:HB2	2:F:215:LYS:HZ2	1.75	0.50
2:F:356:LEU:HD21	11:F:502:CLR:H41	1.91	0.50
3:G:222:ARG:O	3:G:235:VAL:HG12	2.10	0.50
3:K:207:ARG:HG2	3:K:260:TYR:CE2	2.46	0.50
3:O:125:LYS:HA	3:O:130:VAL:HA	1.92	0.50
2:B:47:LYS:HG3	2:B:102:VAL:HG12	1.94	0.50
2:F:27:PHE:HB3	2:J:144:ARG:NH1	2.26	0.50
3:G:140:LYS:HE3	3:G:173:GLN:OE1	2.11	0.50
2:J:47:LYS:HG3	2:J:102:VAL:HG12	1.93	0.50
3:K:202:GLN:HB3	3:K:209:THR:HG23	1.92	0.50
2:N:392:ARG:NE	2:N:415:CYS:O	2.39	0.50
1:E:45:GLU:OE1	1:E:123:LYS:NZ	2.38	0.50
2:F:37:ILE:HG12	2:F:111:LEU:HD23	1.92	0.50
3:G:207:ARG:HG2	3:G:260:TYR:HE2	1.77	0.50
1:I:298:ASN:HD21	1:I:321:LYS:HD3	1.75	0.50
3:K:136:LEU:HD21	3:K:156:LEU:HD11	1.92	0.50
2:N:69:TYR:OH	2:N:117:ASP:OD1	2.22	0.50
1:A:51:TYR:HB3	1:A:203:ILE:HD13	1.93	0.50
2:B:37:ILE:HG21	2:B:129:TYR:CE2	2.47	0.50
2:B:37:ILE:HG12	2:B:111:LEU:HD23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:LYS:HG3	2:F:102:VAL:HG12	1.93	0.50
2:F:100:PHE:CD2	2:F:257:PRO:HD2	2.47	0.50
1:I:18:HIS:HD1	1:I:331:HIS:CB	2.24	0.50
1:I:45:GLU:OE1	1:I:123:LYS:NZ	2.38	0.50
2:J:399:TYR:CE1	3:K:255:ASP:HB3	2.47	0.50
1:E:34:LEU:HD11	1:E:134:ARG:HE	1.77	0.50
2:J:399:TYR:HB3	2:J:407:VAL:HG12	1.92	0.50
3:K:207:ARG:HG2	3:K:260:TYR:HE2	1.77	0.50
1:M:34:LEU:HD11	1:M:134:ARG:HE	1.77	0.50
1:A:34:LEU:HD11	1:A:134:ARG:HE	1.77	0.49
2:F:370:VAL:HG11	11:F:503:CLR:H161	1.94	0.49
3:G:217:PRO:HA	3:G:268:TRP:HB2	1.94	0.49
3:O:207:ARG:HG2	3:O:260:TYR:HE2	1.77	0.49
3:C:207:ARG:HG2	3:C:260:TYR:HE2	1.77	0.49
2:J:9:TYR:O	2:J:12:THR:OG1	2.26	0.49
3:K:217:PRO:HA	3:K:268:TRP:HB2	1.94	0.49
3:C:217:PRO:HA	3:C:268:TRP:HB2	1.94	0.49
2:F:403:PRO:HB2	3:G:138:GLY:HA3	1.93	0.49
2:J:388:PHE:CZ	10:J:506:PLM:H52	2.47	0.49
2:N:100:PHE:CD2	2:N:257:PRO:HD2	2.47	0.49
2:N:196:THR:HG23	2:N:210:THR:O	2.13	0.49
1:A:197:PRO:HB2	1:A:236:THR:HG21	1.95	0.49
2:B:100:PHE:CD2	2:B:257:PRO:HD2	2.47	0.49
2:B:189:LYS:HB2	2:B:215:LYS:HZ2	1.76	0.49
2:F:37:ILE:HG21	2:F:129:TYR:CE2	2.47	0.49
1:I:229:VAL:HG11	2:J:243:PRO:HG3	1.95	0.49
1:I:381:GLU:OE1	1:M:22:ASN:CG	2.56	0.49
1:M:51:TYR:HB3	1:M:203:ILE:HD13	1.93	0.49
1:I:408:THR:HG22	1:I:412:ARG:HE	1.77	0.49
2:J:246:ASP:OD1	2:J:248:LEU:HB2	2.13	0.49
2:N:47:LYS:HG3	2:N:102:VAL:HG12	1.93	0.49
2:B:6:PHE:CE1	2:B:97:MET:HG3	2.48	0.49
1:I:51:TYR:HB3	1:I:203:ILE:HD13	1.93	0.49
1:M:427:VAL:HG11	10:N:504:PLM:H22	1.95	0.49
2:N:6:PHE:CE1	2:N:97:MET:HG3	2.48	0.49
1:A:40:PRO:HA	1:A:127:ALA:HA	1.95	0.49
2:F:79:ASN:OD1	2:F:80:ARG:N	2.46	0.49
2:J:100:PHE:CD2	2:J:257:PRO:HD2	2.47	0.49
2:J:374:GLY:HA3	11:J:503:CLR:H272	1.95	0.49
1:M:408:THR:HG22	1:M:412:ARG:HE	1.77	0.49
2:N:246:ASP:OD1	2:N:248:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:THR:HG22	1:A:412:ARG:HE	1.77	0.49
1:I:34:LEU:HD11	1:I:134:ARG:HE	1.77	0.49
1:M:40:PRO:HA	1:M:127:ALA:HA	1.95	0.49
1:M:223:ARG:HG3	1:M:223:ARG:HH11	1.78	0.49
1:A:225:SER:H	1:A:230:HIS:CE1	2.31	0.48
2:N:71:ALA:HB3	2:N:76:LYS:HD3	1.93	0.48
2:B:246:ASP:OD1	2:B:248:LEU:HB2	2.13	0.48
3:C:135:CYS:SG	3:C:223:PRO:HG3	2.53	0.48
1:E:197:PRO:HB2	1:E:236:THR:HG21	1.95	0.48
2:F:6:PHE:CE1	2:F:97:MET:HG3	2.48	0.48
1:A:431:VAL:O	1:A:435:THR:HG23	2.13	0.48
8:E:502:PCW:H283	11:F:501:CLR:H231	1.93	0.48
2:F:246:ASP:OD1	2:F:248:LEU:HB2	2.13	0.48
2:N:79:ASN:OD1	2:N:80:ARG:N	2.46	0.48
3:O:217:PRO:HA	3:O:268:TRP:HB2	1.95	0.48
2:J:6:PHE:CE1	2:J:97:MET:HG3	2.48	0.48
1:M:113:VAL:O	1:M:117:ASP:N	2.33	0.48
8:E:502:PCW:H332	11:F:501:CLR:H192	1.95	0.48
1:I:40:PRO:HA	1:I:127:ALA:HA	1.95	0.48
1:I:223:ARG:HG3	1:I:223:ARG:HH11	1.78	0.48
1:I:431:VAL:O	1:I:435:THR:HG23	2.13	0.48
1:E:18:HIS:NE2	1:E:26:PRO:HB3	2.29	0.48
1:E:225:SER:H	1:E:230:HIS:CE1	2.31	0.48
2:J:79:ASN:OD1	2:J:80:ARG:N	2.46	0.48
2:N:290:HIS:O	2:N:291:PRO:C	2.57	0.48
3:G:126:LEU:HG	3:G:127:ASP:N	2.28	0.48
1:I:197:PRO:HB2	1:I:236:THR:HG21	1.95	0.48
1:I:225:SER:H	1:I:230:HIS:CE1	2.31	0.48
1:M:45:GLU:OE1	1:M:123:LYS:NZ	2.38	0.48
1:M:431:VAL:O	1:M:435:THR:HG23	2.13	0.48
3:O:133:TYR:HE2	3:O:219:ASP:HA	1.77	0.48
1:A:18:HIS:NE2	1:A:26:PRO:HB3	2.29	0.48
1:E:223:ARG:HG3	1:E:223:ARG:HH11	1.78	0.48
1:I:364:ALA:HB2	1:I:401:ASP:OD2	2.14	0.48
1:M:16:LYS:HE3	1:M:339:ILE:O	2.14	0.48
1:M:18:HIS:NE2	1:M:26:PRO:HB3	2.29	0.48
1:E:40:PRO:HA	1:E:127:ALA:HA	1.95	0.48
1:E:408:THR:HG22	1:E:412:ARG:HE	1.77	0.48
1:E:410:VAL:HG22	8:E:502:PCW:H271	1.96	0.48
2:J:283:THR:HG22	2:J:315:GLU:HG2	1.96	0.48
1:M:364:ALA:HB2	1:M:401:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LYS:HE3	1:A:339:ILE:O	2.14	0.47
1:A:21:ARG:HD3	1:A:24:PHE:CD2	2.48	0.47
2:B:42:SER:HB2	2:B:154:THR:H	1.79	0.47
1:E:230:HIS:HB2	2:J:146:HIS:CD2	2.48	0.47
2:J:285:LYS:HG2	2:J:315:GLU:HG3	1.95	0.47
1:M:63:CYS:HA	1:M:99:GLU:O	2.14	0.47
1:I:18:HIS:NE2	1:I:26:PRO:HB3	2.29	0.47
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.78	0.47
1:A:230:HIS:CD2	1:A:232:PRO:HG3	2.49	0.47
1:E:431:VAL:O	1:E:435:THR:HG23	2.13	0.47
1:I:230:HIS:CD2	1:I:232:PRO:HG3	2.50	0.47
2:J:42:SER:HB2	2:J:154:THR:H	1.80	0.47
2:N:140:LYS:O	2:N:290:HIS:HB2	2.14	0.47
1:A:164:GLY:O	1:A:277:PRO:HD2	2.14	0.47
1:A:364:ALA:HB2	1:A:401:ASP:OD2	2.14	0.47
2:F:308:GLU:CD	2:F:316:ARG:HH21	2.21	0.47
1:M:229:VAL:HG11	2:N:243:PRO:HG3	1.96	0.47
1:A:308:HIS:O	1:A:308:HIS:ND1	2.48	0.47
1:E:404:GLY:O	1:E:408:THR:N	2.45	0.47
2:F:42:SER:HB2	2:F:154:THR:H	1.79	0.47
1:M:230:HIS:CD2	1:M:232:PRO:HG3	2.50	0.47
2:B:79:ASN:OD1	2:B:80:ARG:N	2.46	0.47
2:B:355:ILE:HG21	11:B:502:CLR:H151	1.97	0.47
1:E:230:HIS:NE2	1:E:232:PRO:HG3	2.30	0.47
1:E:308:HIS:O	1:E:308:HIS:ND1	2.48	0.47
1:E:364:ALA:HB2	1:E:401:ASP:OD2	2.14	0.47
3:G:167:TYR:CE2	3:G:257:VAL:HG23	2.50	0.47
1:I:387:ILE:CG2	2:J:337:LEU:HB3	2.44	0.47
3:K:196:TRP:CD1	3:K:197:HIS:H	2.33	0.47
3:K:233:ALA:HB1	3:K:249:VAL:CG2	2.45	0.47
1:M:197:PRO:HB2	1:M:236:THR:HG21	1.95	0.47
2:N:42:SER:HB2	2:N:154:THR:H	1.79	0.47
3:O:168:ASP:OD2	3:O:236:LEU:HD13	2.15	0.47
1:E:383:PRO:HD2	2:F:341:LEU:O	2.15	0.47
2:J:189:LYS:HB2	2:J:215:LYS:HZ2	1.80	0.47
1:M:230:HIS:NE2	1:M:232:PRO:HG3	2.30	0.47
1:A:82:THR:O	1:A:223:ARG:NH2	2.48	0.47
2:B:308:GLU:CD	2:B:316:ARG:HH21	2.21	0.47
2:F:388:PHE:HZ	10:F:506:PLM:H21	1.80	0.47
1:I:59:TYR:CD2	2:J:247:GLN:HG3	2.50	0.47
2:J:220:CYS:HB2	2:J:224:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:225:SER:H	1:M:230:HIS:CE1	2.31	0.47
8:M:502:PCW:H242	11:N:501:CLR:H20	1.97	0.47
2:N:181:LEU:HD11	2:N:226:HIS:HA	1.95	0.47
3:K:208:PHE:CD2	3:K:249:VAL:HG11	2.50	0.47
1:I:308:HIS:ND1	1:I:308:HIS:O	2.48	0.46
2:J:388:PHE:HZ	10:J:506:PLM:H21	1.79	0.46
1:E:21:ARG:HD3	1:E:24:PHE:CD2	2.49	0.46
1:E:230:HIS:CD2	1:E:232:PRO:HG3	2.50	0.46
3:G:168:ASP:OD2	3:G:236:LEU:HD13	2.15	0.46
1:I:16:LYS:HE3	1:I:339:ILE:O	2.14	0.46
1:I:24:PHE:HE1	1:I:289:ARG:NH1	2.14	0.46
3:G:133:TYR:O	3:G:221:GLY:HA3	2.15	0.46
3:K:136:LEU:O	3:K:182:ALA:HB1	2.16	0.46
1:M:196:GLN:OE1	1:M:196:GLN:HA	2.15	0.46
2:N:220:CYS:HB2	2:N:224:GLN:HB2	1.97	0.46
1:A:409:TRP:HB2	11:B:501:CLR:H263	1.98	0.46
3:C:167:TYR:CE2	3:C:257:VAL:HG23	2.50	0.46
3:G:196:TRP:CD1	3:G:197:HIS:H	2.33	0.46
1:I:223:ARG:HG3	1:I:223:ARG:NH1	2.31	0.46
2:J:296:TYR:CE2	2:J:318:ILE:HG12	2.50	0.46
11:J:502:CLR:H222	11:J:502:CLR:H162	1.61	0.46
1:A:230:HIS:NE2	1:A:232:PRO:HG3	2.30	0.46
1:E:24:PHE:HE1	1:E:289:ARG:NH1	2.14	0.46
1:E:164:GLY:O	1:E:277:PRO:HD2	2.16	0.46
3:O:167:TYR:CE2	3:O:257:VAL:HG23	2.50	0.46
2:B:220:CYS:HB2	2:B:224:GLN:HB2	1.97	0.46
1:M:308:HIS:O	1:M:308:HIS:ND1	2.47	0.46
1:A:223:ARG:HG3	1:A:223:ARG:NH1	2.31	0.46
1:A:406:ALA:HB2	2:B:354:ILE:HG21	1.98	0.46
3:C:168:ASP:OD2	3:C:236:LEU:HD13	2.15	0.46
1:I:196:GLN:OE1	1:I:196:GLN:HA	2.15	0.46
1:I:230:HIS:NE2	1:I:232:PRO:HG3	2.30	0.46
1:M:24:PHE:HE1	1:M:289:ARG:NH1	2.14	0.46
6:R:2:NAG:H83	6:R:2:NAG:H2	1.81	0.46
2:B:80:ARG:O	2:B:80:ARG:HD3	2.16	0.46
3:C:196:TRP:CD1	3:C:197:HIS:H	2.33	0.46
1:E:223:ARG:HG3	1:E:223:ARG:NH1	2.31	0.46
2:J:396:LEU:HD11	2:J:417:ALA:HB2	1.97	0.46
3:O:196:TRP:CD1	3:O:197:HIS:H	2.33	0.46
2:B:9:TYR:O	2:B:12:THR:OG1	2.26	0.46
2:B:388:PHE:HZ	10:B:506:PLM:H21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:ILE:HG23	3:C:133:TYR:HB3	1.97	0.46
2:F:80:ARG:O	2:F:80:ARG:HD3	2.16	0.46
3:K:168:ASP:OD2	3:K:236:LEU:HD13	2.15	0.46
2:N:388:PHE:HZ	10:N:506:PLM:H21	1.80	0.46
1:A:24:PHE:HE1	1:A:289:ARG:NH1	2.14	0.45
3:K:167:TYR:CE2	3:K:257:VAL:HG23	2.50	0.45
2:N:69:TYR:HE1	2:N:78:ALA:HB2	1.81	0.45
2:N:80:ARG:O	2:N:80:ARG:HD3	2.16	0.45
1:A:63:CYS:HA	1:A:99:GLU:O	2.16	0.45
2:F:353:GLU:HA	2:F:356:LEU:HD12	1.97	0.45
2:F:365:ALA:HB3	11:F:501:CLR:H11	1.98	0.45
1:I:167:SER:HB3	1:I:275:ASN:H	1.81	0.45
2:N:385:CYS:O	2:N:386:TYR:C	2.59	0.45
1:A:196:GLN:OE1	1:A:196:GLN:HA	2.15	0.45
2:B:69:TYR:HE1	2:B:78:ALA:HB2	1.82	0.45
2:J:170:HIS:HD1	2:J:250:ARG:HA	1.80	0.45
2:N:352:HIS:HB2	11:N:502:CLR:H9	1.98	0.45
1:E:167:SER:HB3	1:E:275:ASN:H	1.81	0.45
2:F:69:TYR:HE1	2:F:78:ALA:HB2	1.82	0.45
3:O:143:LYS:HD2	3:O:151:ILE:HD11	1.99	0.45
11:J:502:CLR:H152	11:J:503:CLR:H17	1.98	0.45
3:O:112:MET:O	3:O:116:ILE:HG12	2.17	0.45
1:E:196:GLN:HA	1:E:196:GLN:OE1	2.15	0.45
2:N:9:TYR:O	2:N:12:THR:OG1	2.26	0.45
2:N:296:TYR:CE2	2:N:318:ILE:HG23	2.51	0.45
1:I:21:ARG:HD3	1:I:24:PHE:CD2	2.49	0.45
1:M:223:ARG:HG3	1:M:223:ARG:NH1	2.31	0.45
5:H:2:NAG:H83	5:H:2:NAG:H2	1.81	0.45
2:B:139:GLU:OE2	2:B:270:ALA:HB2	2.17	0.45
3:C:126:LEU:O	3:C:129:LYS:HG2	2.16	0.45
1:E:256:PRO:HB3	2:F:303:PRO:HD3	1.98	0.45
3:G:156:LEU:O	3:G:161:TYR:OH	2.25	0.45
2:N:139:GLU:OE2	2:N:270:ALA:HB2	2.17	0.45
1:A:167:SER:HB3	1:A:275:ASN:H	1.81	0.45
1:A:318:LEU:HD21	1:A:367:VAL:HG21	1.99	0.45
9:A:503:STE:H81	9:A:503:STE:H112	1.84	0.45
3:C:112:MET:O	3:C:116:ILE:HG12	2.17	0.45
2:F:139:GLU:OE2	2:F:270:ALA:HB2	2.17	0.45
3:G:143:LYS:HD2	3:G:151:ILE:HD11	1.99	0.45
2:J:80:ARG:O	2:J:80:ARG:HD3	2.16	0.45
2:J:139:GLU:OE2	2:J:270:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HB3	1:A:189:PHE:CE2	2.52	0.44
1:E:82:THR:O	1:E:223:ARG:NH2	2.50	0.44
1:I:82:THR:O	1:I:223:ARG:NH2	2.49	0.44
1:I:381:GLU:CB	1:M:22:ASN:HD21	2.26	0.44
1:M:176:LYS:HB3	1:M:189:PHE:CE2	2.53	0.44
2:B:140:LYS:HD2	2:B:291:PRO:HB2	1.99	0.44
2:F:220:CYS:HB2	2:F:224:GLN:HB2	1.97	0.44
3:G:112:MET:O	3:G:116:ILE:HG12	2.17	0.44
1:I:89:TRP:HH2	2:J:73:HIS:CD2	2.35	0.44
1:I:176:LYS:HB3	1:I:189:PHE:CE2	2.52	0.44
1:A:426:ALA:HA	1:A:429:ILE:HG12	1.99	0.44
3:C:153:ASN:ND2	3:C:178:MET:HE1	2.33	0.44
2:F:363:PRO:O	2:F:366:THR:HG22	2.18	0.44
11:J:502:CLR:H181	11:J:503:CLR:H213	2.00	0.44
2:B:363:PRO:O	2:B:366:THR:HG22	2.17	0.44
2:F:310:ILE:HD12	2:F:314:VAL:HG21	1.99	0.44
8:I:502:PCW:H412	8:I:502:PCW:H442	1.81	0.44
2:J:69:TYR:HE1	2:J:78:ALA:HB2	1.81	0.44
2:N:399:TYR:HD2	2:N:407:VAL:HG13	1.83	0.44
1:E:113:VAL:O	1:E:117:ASP:N	2.33	0.44
2:F:18:TYR:HE2	2:J:146:HIS:HB2	1.83	0.44
2:F:399:TYR:HD2	2:F:407:VAL:HG13	1.83	0.44
1:M:115:LYS:HE2	1:M:116:HIS:NE2	2.32	0.44
2:N:48:ILE:HG12	2:N:111:LEU:HD21	1.99	0.44
11:N:501:CLR:H213	11:N:501:CLR:H232	1.84	0.44
1:A:320:PHE:CD1	1:A:320:PHE:C	2.96	0.44
1:I:115:LYS:HE2	1:I:116:HIS:NE2	2.32	0.44
3:K:112:MET:O	3:K:116:ILE:HG12	2.17	0.44
2:B:326:GLU:O	2:B:326:GLU:HG3	2.18	0.44
1:E:320:PHE:CD1	1:E:320:PHE:C	2.96	0.44
3:K:124:VAL:HG22	3:K:151:ILE:CD1	2.47	0.44
8:M:502:PCW:H32	8:M:502:PCW:H122	1.63	0.44
4:D:3:BMA:H61	4:D:4:MAN:H2	1.42	0.44
2:B:287:HIS:CE1	2:B:313:TYR:CD1	3.06	0.43
1:E:176:LYS:HB3	1:E:189:PHE:CE2	2.53	0.43
1:E:401:ASP:OD1	1:E:403:SER:N	2.36	0.43
1:I:320:PHE:CD1	1:I:320:PHE:C	2.96	0.43
2:J:69:TYR:CE1	2:J:78:ALA:HB2	2.53	0.43
1:M:401:ASP:OD1	1:M:403:SER:N	2.36	0.43
1:A:134:ARG:NH1	5:H:1:NAG:H3	2.33	0.43
3:C:233:ALA:HB1	3:C:249:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:GLU:OE2	1:E:300:GLU:N	2.51	0.43
1:E:386:HIS:CG	2:F:279:LYS:HA	2.53	0.43
1:A:300:GLU:OE2	1:A:300:GLU:N	2.51	0.43
2:B:69:TYR:CE1	2:B:78:ALA:HB2	2.54	0.43
10:B:504:PLM:HG2	10:B:504:PLM:HD1	1.87	0.43
2:F:140:LYS:HD2	2:F:291:PRO:HB2	1.99	0.43
2:F:298:SER:HB3	2:F:303:PRO:HA	1.99	0.43
11:B:502:CLR:H162	11:B:502:CLR:H222	1.69	0.43
1:I:42:LEU:HD11	1:I:266:VAL:HB	2.00	0.43
1:M:320:PHE:CD1	1:M:320:PHE:C	2.96	0.43
2:N:298:SER:HB3	2:N:303:PRO:HA	1.99	0.43
2:B:280:ARG:HG2	2:B:339:ALA:HB1	2.01	0.43
1:E:63:CYS:SG	1:E:96:CYS:N	2.88	0.43
1:E:109:ASP:OD1	1:E:110:ARG:N	2.52	0.43
2:F:287:HIS:CE1	2:F:313:TYR:CD1	3.06	0.43
3:G:233:ALA:HB1	3:G:249:VAL:HG21	2.00	0.43
1:I:179:VAL:HG21	1:I:266:VAL:HG21	2.01	0.43
3:O:186:THR:HB	3:O:230:ARG:HB3	2.01	0.43
2:B:298:SER:HB3	2:B:303:PRO:HA	1.99	0.43
2:J:57:ASN:HD21	2:J:61:THR:HB	1.84	0.43
1:A:404:GLY:O	1:A:408:THR:N	2.45	0.43
1:E:179:VAL:HG21	1:E:266:VAL:HG21	2.01	0.43
1:A:109:ASP:OD1	1:A:110:ARG:N	2.52	0.43
2:F:69:TYR:CE1	2:F:78:ALA:HB2	2.54	0.43
3:G:201:VAL:HG22	3:G:210:ILE:HD11	2.00	0.43
1:I:297:THR:C	1:I:298:ASN:OD1	2.62	0.43
2:F:280:ARG:HG2	2:F:339:ALA:HB1	2.01	0.43
1:I:109:ASP:OD1	1:I:110:ARG:N	2.52	0.43
9:J:501:STE:H81	9:J:501:STE:H112	1.84	0.43
1:M:109:ASP:OD1	1:M:110:ARG:N	2.52	0.43
1:M:404:GLY:O	1:M:408:THR:N	2.45	0.43
2:N:326:GLU:O	2:N:326:GLU:HG3	2.18	0.43
3:O:233:ALA:HB1	3:O:249:VAL:HG21	2.00	0.43
1:A:428:LEU:HD22	2:B:387:MET:HG3	2.00	0.42
3:C:115:LYS:HE3	3:C:115:LYS:HB3	1.91	0.42
2:J:395:CYS:O	2:J:398:PRO:HD2	2.19	0.42
3:K:167:TYR:HE2	3:K:257:VAL:HG23	1.84	0.42
3:K:224:ILE:O	3:K:232:VAL:HG12	2.19	0.42
3:O:135:CYS:SG	3:O:223:PRO:HG3	2.59	0.42
3:O:224:ILE:O	3:O:232:VAL:HG12	2.19	0.42
2:B:310:ILE:HD12	2:B:314:VAL:HG21	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:E:504:PLM:HG2	10:E:504:PLM:HD2	1.88	0.42
1:M:300:GLU:OE2	1:M:300:GLU:N	2.51	0.42
9:N:505:STE:H72	9:N:505:STE:H41	1.87	0.42
3:O:125:LYS:HB3	3:O:130:VAL:HA	2.01	0.42
3:O:167:TYR:HE2	3:O:257:VAL:HG23	1.84	0.42
1:A:42:LEU:HD11	1:A:266:VAL:HB	2.00	0.42
1:A:197:PRO:HB3	1:A:217:THR:HA	2.01	0.42
3:C:135:CYS:HB3	3:C:137:VAL:HG23	2.00	0.42
9:F:505:STE:H132	9:F:505:STE:H161	1.89	0.42
1:E:71:MET:HE3	1:E:71:MET:HB2	1.90	0.42
1:E:197:PRO:HB3	1:E:217:THR:HA	2.02	0.42
3:G:154:PRO:O	3:G:157:ALA:N	2.51	0.42
3:G:224:ILE:O	3:G:232:VAL:HG12	2.19	0.42
1:I:95:PHE:HA	2:J:226:HIS:CE1	2.54	0.42
1:M:339:ILE:HD13	1:M:356:PHE:HB3	2.01	0.42
1:A:33:VAL:HA	1:A:133:ILE:HD13	2.00	0.42
2:F:326:GLU:O	2:F:326:GLU:HG3	2.18	0.42
1:M:89:TRP:HH2	2:N:73:HIS:CD2	2.37	0.42
1:A:229:VAL:HG21	2:B:243:PRO:HG3	2.00	0.42
1:A:312:PHE:CD1	1:A:357:SER:HB2	2.55	0.42
1:I:404:GLY:O	1:I:408:THR:N	2.45	0.42
8:M:502:PCW:H151	8:M:502:PCW:H121	1.71	0.42
3:O:201:VAL:HG22	3:O:210:ILE:HD11	2.02	0.42
2:B:21:ASP:OD1	2:B:126:LYS:HE2	2.20	0.42
1:I:57:SER:O	2:J:244:ARG:HB2	2.19	0.42
1:A:179:VAL:HG21	1:A:266:VAL:HG21	2.01	0.42
8:A:502:PCW:H152	8:A:502:PCW:H121	1.30	0.42
1:E:312:PHE:CD1	1:E:357:SER:HB2	2.55	0.42
1:I:197:PRO:HB3	1:I:217:THR:HA	2.02	0.42
2:J:271:ARG:H	2:J:271:ARG:HG3	1.71	0.42
1:M:134:ARG:HH11	5:W:1:NAG:H3	1.83	0.42
1:M:429:ILE:HD13	1:M:429:ILE:HA	1.91	0.42
3:O:124:VAL:CG1	3:O:151:ILE:HD13	2.48	0.42
3:O:133:TYR:N	3:O:220:SER:O	2.50	0.42
3:C:224:ILE:O	3:C:232:VAL:HG12	2.19	0.42
2:J:87:THR:HG22	2:J:111:LEU:HD22	2.02	0.42
9:J:505:STE:H132	9:J:505:STE:H161	1.89	0.42
1:M:21:ARG:HD3	1:M:24:PHE:CD2	2.49	0.42
2:N:69:TYR:CE1	2:N:78:ALA:HB2	2.53	0.42
1:E:116:HIS:ND1	4:P:1:NAG:H81	2.29	0.42
1:E:134:ARG:NH1	5:Q:1:NAG:H3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:ASP:OD1	2:F:126:LYS:HE2	2.20	0.42
2:F:297:ARG:NH2	2:F:326:GLU:OE2	2.52	0.42
1:M:306:CYS:HA	1:M:314:GLY:HA2	2.02	0.42
3:O:125:LYS:HD2	3:O:128:GLY:HA2	2.02	0.42
1:E:134:ARG:HH11	5:Q:1:NAG:H3	1.85	0.41
2:F:166:GLU:HA	2:F:255:HIS:HA	2.01	0.41
3:G:124:VAL:HG11	3:G:143:LYS:NZ	2.35	0.41
1:I:312:PHE:CD1	1:I:357:SER:HB2	2.55	0.41
2:J:326:GLU:HG3	2:J:336:ARG:HG2	2.02	0.41
1:M:51:TYR:OH	1:M:236:THR:O	2.38	0.41
1:M:95:PHE:CE2	6:X:1:NAG:H61	2.55	0.41
2:B:77:GLU:O	2:B:118:ALA:HB2	2.20	0.41
3:C:201:VAL:HG22	3:C:210:ILE:HD11	2.03	0.41
9:J:505:STE:H72	9:J:505:STE:H41	1.87	0.41
9:B:505:STE:H132	9:B:505:STE:H161	1.89	0.41
1:E:42:LEU:HD11	1:E:266:VAL:HB	2.01	0.41
1:E:433:CYS:O	1:E:437:ARG:HG2	2.20	0.41
2:F:77:GLU:O	2:F:118:ALA:HB2	2.20	0.41
2:F:362:TYR:HB3	11:F:501:CLR:H21	2.02	0.41
1:I:113:VAL:O	1:I:117:ASP:N	2.33	0.41
2:N:83:LEU:HD21	2:N:101:ILE:HD13	2.03	0.41
2:N:365:ALA:HB3	11:N:501:CLR:H11	2.01	0.41
1:A:51:TYR:OH	1:A:236:THR:O	2.38	0.41
1:A:255:ALA:O	2:B:297:ARG:NH1	2.50	0.41
11:B:503:CLR:H211	11:B:503:CLR:H231	1.79	0.41
2:F:271:ARG:NH2	2:F:289:ASP:OD1	2.53	0.41
1:I:339:ILE:HD13	1:I:356:PHE:HB3	2.01	0.41
1:I:387:ILE:HA	2:J:338:TRP:O	2.20	0.41
2:J:83:LEU:HD21	2:J:101:ILE:HD13	2.02	0.41
2:J:396:LEU:HD11	2:J:417:ALA:CB	2.50	0.41
2:N:77:GLU:O	2:N:118:ALA:HB2	2.20	0.41
6:U:2:NAG:H83	6:U:2:NAG:H2	1.85	0.41
1:A:141:ASN:CG	5:H:1:NAG:C1	2.77	0.41
1:A:306:CYS:HA	1:A:314:GLY:HA2	2.02	0.41
1:A:339:ILE:HD13	1:A:356:PHE:HB3	2.01	0.41
2:F:316:ARG:HD3	2:F:316:ARG:HA	1.94	0.41
1:I:409:TRP:HB2	11:I:503:CLR:H263	2.02	0.41
2:J:77:GLU:O	2:J:118:ALA:HB2	2.20	0.41
1:M:42:LEU:HD11	1:M:266:VAL:HB	2.02	0.41
1:M:197:PRO:HB3	1:M:217:THR:HA	2.01	0.41
3:O:154:PRO:O	3:O:157:ALA:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:CYS:HA	1:E:314:GLY:HA2	2.02	0.41
1:E:339:ILE:HD13	1:E:356:PHE:HB3	2.01	0.41
1:I:433:CYS:O	1:I:437:ARG:HG2	2.20	0.41
2:J:21:ASP:OD1	2:J:126:LYS:HE2	2.20	0.41
1:M:312:PHE:CD1	1:M:357:SER:HB2	2.55	0.41
2:N:100:PHE:HD2	2:N:257:PRO:HD2	1.86	0.41
11:N:502:CLR:H222	11:N:502:CLR:H162	1.55	0.41
1:A:320:PHE:CZ	1:A:346:ILE:HG23	2.56	0.41
2:B:83:LEU:HD21	2:B:101:ILE:HD13	2.03	0.41
2:B:320:VAL:HG12	2:B:339:ALA:HB2	2.03	0.41
1:I:79:GLN:HE21	1:I:79:GLN:HB3	1.72	0.41
8:I:502:PCW:H441	8:I:502:PCW:H471	1.91	0.41
2:J:311:ASP:OD1	2:J:311:ASP:N	2.52	0.41
3:K:202:GLN:HB3	3:K:209:THR:CG2	2.51	0.41
1:M:179:VAL:HG21	1:M:266:VAL:HG21	2.03	0.41
1:M:256:PRO:HB3	2:N:303:PRO:HD3	2.02	0.41
10:A:504:PLM:HG2	10:A:504:PLM:HD2	1.88	0.41
2:B:139:GLU:HB3	2:B:290:HIS:CD2	2.56	0.41
2:B:271:ARG:NH2	2:B:289:ASP:OD1	2.53	0.41
2:N:166:GLU:HA	2:N:255:HIS:HA	2.01	0.41
2:N:394:LYS:HE3	2:N:394:LYS:HB2	1.89	0.41
1:A:45:GLU:OE1	1:A:123:LYS:NZ	2.38	0.41
2:B:146:HIS:HD2	1:I:230:HIS:HD2	1.69	0.41
3:C:156:LEU:O	3:C:161:TYR:OH	2.25	0.41
2:F:203:CYS:HB2	2:F:220:CYS:HB3	2.02	0.41
2:F:279:LYS:NZ	2:F:280:ARG:HH21	2.19	0.41
2:F:296:TYR:CD2	2:F:318:ILE:HG23	2.56	0.41
2:F:320:VAL:HG12	2:F:339:ALA:HB2	2.03	0.41
10:F:506:PLM:HG2	10:F:506:PLM:HD2	1.79	0.41
1:I:306:CYS:HA	1:I:314:GLY:HA2	2.02	0.41
1:I:383:PRO:O	2:J:342:THR:HG22	2.21	0.41
2:J:286:LEU:HB3	2:J:329:TRP:CH2	2.56	0.41
2:N:21:ASP:OD1	2:N:126:LYS:HE2	2.20	0.41
2:N:316:ARG:HA	2:N:316:ARG:HD3	1.89	0.41
3:O:134:ALA:HA	3:O:142:MET:O	2.21	0.41
1:A:255:ALA:HA	1:A:256:PRO:HD3	1.96	0.41
1:A:433:CYS:O	1:A:437:ARG:HG2	2.20	0.41
2:B:297:ARG:NH2	2:B:326:GLU:OE2	2.52	0.41
1:E:59:TYR:CD2	2:F:247:GLN:HG3	2.56	0.41
2:J:299:LEU:HD21	2:J:326:GLU:HB2	2.03	0.41
1:A:95:PHE:CE2	6:L:1:NAG:H61	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:ND2	5:H:1:NAG:H83	2.36	0.40
2:B:279:LYS:NZ	2:B:280:ARG:HH21	2.19	0.40
1:E:230:HIS:CD2	2:J:146:HIS:HD2	2.39	0.40
2:N:37:ILE:HA	2:N:47:LYS:O	2.21	0.40
3:O:162:LYS:HB3	3:O:162:LYS:HE2	1.80	0.40
3:O:194:TYR:HD1	3:O:226:ASP:HA	1.86	0.40
1:A:229:VAL:O	2:B:241:PHE:HA	2.21	0.40
2:B:166:GLU:HA	2:B:255:HIS:HA	2.02	0.40
1:E:123:LYS:HA	1:E:175:ASN:O	2.21	0.40
8:I:502:PCW:H41	11:I:503:CLR:H41	2.02	0.40
2:J:383:ALA:C	2:J:385:CYS:N	2.76	0.40
1:M:320:PHE:CZ	1:M:346:ILE:HG23	2.56	0.40
1:M:333:HIS:HB2	1:M:366:LYS:HG3	2.03	0.40
9:B:505:STE:H72	9:B:505:STE:H41	1.87	0.40
3:C:208:PHE:CD2	3:C:249:VAL:HG11	2.57	0.40
1:E:160:ARG:HB2	1:E:281:ASP:HB3	2.03	0.40
1:E:241:LYS:O	1:E:245:LYS:HG2	2.22	0.40
3:G:208:PHE:CD2	3:G:249:VAL:HG11	2.57	0.40
1:I:123:LYS:HA	1:I:175:ASN:O	2.21	0.40
1:I:229:VAL:HG21	2:J:243:PRO:HG3	2.03	0.40
1:I:381:GLU:OE1	1:M:22:ASN:ND2	2.55	0.40
2:J:166:GLU:HA	2:J:255:HIS:HA	2.02	0.40
3:K:156:LEU:O	3:K:161:TYR:OH	2.25	0.40
8:M:502:PCW:H342	11:N:501:CLR:H22	2.02	0.40
3:O:202:GLN:HB3	3:O:209:THR:CG2	2.51	0.40
1:A:241:LYS:O	1:A:245:LYS:HG2	2.22	0.40
1:A:263:THR:HG22	1:A:266:VAL:HG22	2.03	0.40
1:A:328:CYS:HB3	1:A:370:CYS:H	1.87	0.40
1:E:89:TRP:HB3	2:F:29:TYR:CD2	2.56	0.40
2:F:83:LEU:HD21	2:F:101:ILE:HD13	2.03	0.40
2:F:402:THR:O	3:G:140:LYS:NZ	2.53	0.40
11:F:501:CLR:H232	11:F:501:CLR:H211	1.76	0.40
1:I:207:THR:N	1:I:210:SER:OG	2.54	0.40
2:J:37:ILE:HA	2:J:47:LYS:O	2.22	0.40
1:M:123:LYS:HA	1:M:175:ASN:O	2.21	0.40
3:C:210:ILE:O	3:C:245:THR:HG22	2.21	0.40
1:E:320:PHE:CZ	1:E:346:ILE:HG23	2.56	0.40
2:F:139:GLU:HB3	2:F:290:HIS:CD2	2.56	0.40
1:M:30:GLN:HE21	1:M:30:GLN:HB3	1.51	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	436/438 (100%)	425 (98%)	11 (2%)	0	100	100
1	E	436/438 (100%)	424 (97%)	12 (3%)	0	100	100
1	I	436/438 (100%)	423 (97%)	13 (3%)	0	100	100
1	M	436/438 (100%)	425 (98%)	11 (2%)	0	100	100
2	B	417/419 (100%)	396 (95%)	21 (5%)	0	100	100
2	F	417/419 (100%)	394 (94%)	23 (6%)	0	100	100
2	J	417/419 (100%)	398 (95%)	18 (4%)	1 (0%)	43	71
2	N	417/419 (100%)	394 (94%)	21 (5%)	2 (0%)	24	53
3	C	156/268 (58%)	148 (95%)	8 (5%)	0	100	100
3	G	156/268 (58%)	149 (96%)	7 (4%)	0	100	100
3	K	156/268 (58%)	149 (96%)	7 (4%)	0	100	100
3	O	156/268 (58%)	147 (94%)	8 (5%)	1 (1%)	21	48
All	All	4036/4500 (90%)	3872 (96%)	160 (4%)	4 (0%)	49	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	O	138	GLY
2	N	291	PRO
2	N	288	PRO
2	J	305	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	368/368 (100%)	366 (100%)	2 (0%)	81	93
1	E	367/368 (100%)	366 (100%)	1 (0%)	86	95
1	I	367/368 (100%)	363 (99%)	4 (1%)	65	86
1	M	368/368 (100%)	363 (99%)	5 (1%)	59	84
2	B	350/350 (100%)	344 (98%)	6 (2%)	53	81
2	F	350/350 (100%)	346 (99%)	4 (1%)	65	86
2	J	350/350 (100%)	338 (97%)	12 (3%)	32	66
2	N	350/350 (100%)	343 (98%)	7 (2%)	48	79
3	C	130/228 (57%)	126 (97%)	4 (3%)	35	69
3	G	130/228 (57%)	125 (96%)	5 (4%)	29	62
3	K	130/228 (57%)	124 (95%)	6 (5%)	24	56
3	O	130/228 (57%)	121 (93%)	9 (7%)	14	39
All	All	3390/3784 (90%)	3325 (98%)	65 (2%)	49	79

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	THR
1	A	336	VAL
2	B	61	THR
2	B	77	GLU
2	B	90	VAL
2	B	402	THR
2	B	406	VAL
2	B	414	LEU
3	C	119	ASP
3	C	135	CYS
3	C	141	VAL
3	C	265	THR
1	E	336	VAL
2	F	40	GLU
2	F	61	THR
2	F	77	GLU
2	F	90	VAL
3	G	119	ASP
3	G	126	LEU
3	G	135	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	G	141	VAL
3	G	265	THR
1	I	100	ASN
1	I	234	THR
1	I	298	ASN
1	I	336	VAL
2	J	61	THR
2	J	90	VAL
2	J	111	LEU
2	J	275	VAL
2	J	276	THR
2	J	290	HIS
2	J	310	ILE
2	J	317	THR
2	J	325	ILE
2	J	366	THR
2	J	396	LEU
2	J	411	LEU
3	K	117	GLU
3	K	131	THR
3	K	135	CYS
3	K	141	VAL
3	K	178	MET
3	K	265	THR
1	M	30	GLN
1	M	79	GLN
1	M	80	VAL
1	M	82	THR
1	M	336	VAL
2	N	61	THR
2	N	62	HIS
2	N	77	GLU
2	N	90	VAL
2	N	226	HIS
2	N	279	LYS
2	N	378	VAL
3	O	117	GLU
3	O	121	ILE
3	O	124	VAL
3	O	127	ASP
3	O	129	LYS
3	O	135	CYS

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Mol	Chain	Res	Type
3	O	141	VAL
3	O	178	MET
3	O	265	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	141	ASN
1	A	142	GLN
1	A	302	GLN
1	A	355	HIS
2	B	114	GLN
2	B	146	HIS
2	B	224	GLN
3	C	195	ASN
1	E	142	GLN
1	E	230	HIS
1	E	302	GLN
1	E	355	HIS
2	F	114	GLN
2	F	116	GLN
2	F	224	GLN
2	F	226	HIS
3	G	195	ASN
1	I	79	GLN
1	I	142	GLN
1	I	355	HIS
2	J	5	HIS
2	J	114	GLN
2	J	146	HIS
2	J	224	GLN
2	J	226	HIS
3	K	195	ASN
3	K	197	HIS
1	M	22	ASN
1	M	30	GLN
1	M	79	GLN
1	M	142	GLN
1	M	298	ASN
1	M	355	HIS
2	N	73	HIS

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Mol	Chain	Res	Type
2	N	114	GLN
2	N	226	HIS
2	N	287	HIS
3	O	195	ASN
3	O	197	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

36 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	D	1	4,2	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
4	NAG	D	2	4	14,14,15	0.67	0	17,19,21	1.16	3 (17%)
4	BMA	D	3	4	11,11,12	0.41	0	15,15,17	0.96	1 (6%)
4	MAN	D	4	4	11,11,12	0.30	0	15,15,17	0.84	0
5	NAG	H	1	1,5	14,14,15	0.77	0	17,19,21	1.56	3 (17%)
5	NAG	H	2	5	14,14,15	0.47	0	17,19,21	1.37	2 (11%)
6	NAG	L	1	2,6	14,14,15	0.89	0	17,19,21	2.62	5 (29%)
6	NAG	L	2	6	14,14,15	0.47	0	17,19,21	1.55	2 (11%)
6	BMA	L	3	6	11,11,12	0.37	0	15,15,17	1.42	1 (6%)
4	NAG	P	1	4,2	14,14,15	0.72	0	17,19,21	1.25	1 (5%)
4	NAG	P	2	4	14,14,15	0.58	0	17,19,21	1.98	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BMA	P	3	4	11,11,12	0.31	0	15,15,17	1.10	1 (6%)
4	MAN	P	4	4	11,11,12	0.21	0	15,15,17	0.46	0
5	NAG	Q	1	1,5	14,14,15	1.58	2 (14%)	17,19,21	1.80	4 (23%)
5	NAG	Q	2	5	14,14,15	0.45	0	17,19,21	0.74	0
6	NAG	R	1	2,6	14,14,15	1.04	1 (7%)	17,19,21	2.70	9 (52%)
6	NAG	R	2	6	14,14,15	0.45	0	17,19,21	1.65	6 (35%)
6	BMA	R	3	6	11,11,12	0.35	0	15,15,17	0.95	1 (6%)
4	NAG	S	1	4,2	14,14,15	2.10	1 (7%)	17,19,21	2.37	4 (23%)
4	NAG	S	2	4	14,14,15	0.52	0	17,19,21	1.37	1 (5%)
4	BMA	S	3	4	11,11,12	0.30	0	15,15,17	0.84	1 (6%)
4	MAN	S	4	4	11,11,12	0.21	0	15,15,17	0.80	0
5	NAG	T	1	1,5	14,14,15	0.85	0	17,19,21	2.17	5 (29%)
5	NAG	T	2	5	14,14,15	0.56	0	17,19,21	0.97	2 (11%)
6	NAG	U	1	2,6	14,14,15	1.56	1 (7%)	17,19,21	1.73	4 (23%)
6	NAG	U	2	6	14,14,15	0.56	0	17,19,21	0.92	1 (5%)
6	BMA	U	3	6	11,11,12	0.33	0	15,15,17	1.40	2 (13%)
4	NAG	V	1	4,2	14,14,15	1.37	1 (7%)	17,19,21	2.02	2 (11%)
4	NAG	V	2	4	14,14,15	0.78	0	17,19,21	1.16	2 (11%)
4	BMA	V	3	4	11,11,12	0.34	0	15,15,17	0.80	0
4	MAN	V	4	4	11,11,12	0.25	0	15,15,17	0.93	0
5	NAG	W	1	1,5	14,14,15	1.80	1 (7%)	17,19,21	1.62	4 (23%)
5	NAG	W	2	5	14,14,15	0.41	0	17,19,21	0.97	1 (5%)
6	NAG	X	1	2,6	14,14,15	1.00	1 (7%)	17,19,21	1.84	3 (17%)
6	NAG	X	2	6	14,14,15	0.55	0	17,19,21	1.43	2 (11%)
6	BMA	X	3	6	11,11,12	0.33	0	15,15,17	0.90	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	1/1/1/1
5	NAG	H	1	1,5	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	4/6/23/26	0/1/1/1
6	BMA	L	3	6	-	2/2/19/22	0/1/1/1
4	NAG	P	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	0/6/23/26	0/1/1/1
4	BMA	P	3	4	-	1/2/19/22	1/1/1/1
4	MAN	P	4	4	-	1/2/19/22	1/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	3/6/23/26	0/1/1/1
6	NAG	R	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	R	2	6	-	3/6/23/26	0/1/1/1
6	BMA	R	3	6	-	0/2/19/22	0/1/1/1
4	NAG	S	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	BMA	S	3	4	-	0/2/19/22	0/1/1/1
4	MAN	S	4	4	-	0/2/19/22	1/1/1/1
5	NAG	T	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
6	NAG	U	1	2,6	-	3/6/23/26	0/1/1/1
6	NAG	U	2	6	-	3/6/23/26	0/1/1/1
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
4	NAG	V	1	4,2	-	3/6/23/26	0/1/1/1
4	NAG	V	2	4	-	2/6/23/26	0/1/1/1
4	BMA	V	3	4	-	2/2/19/22	0/1/1/1
4	MAN	V	4	4	-	0/2/19/22	0/1/1/1
5	NAG	W	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	W	2	5	-	2/6/23/26	0/1/1/1
6	NAG	X	1	2,6	-	4/6/23/26	0/1/1/1
6	NAG	X	2	6	-	4/6/23/26	0/1/1/1
6	BMA	X	3	6	-	0/2/19/22	1/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	S	1	NAG	C1-C2	7.61	1.62	1.52
5	W	1	NAG	C1-C2	6.10	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	U	1	NAG	C1-C2	5.66	1.60	1.52
5	Q	1	NAG	C1-C2	4.87	1.59	1.52
4	V	1	NAG	C1-C2	4.10	1.57	1.52
6	R	1	NAG	C1-C2	3.39	1.57	1.52
6	X	1	NAG	C1-C2	3.00	1.56	1.52
5	Q	1	NAG	O5-C1	2.94	1.48	1.43

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	O5-C1-C2	-8.17	98.65	111.29
6	R	1	NAG	C1-O5-C5	7.41	122.11	112.19
4	S	1	NAG	C4-C3-C2	-5.81	102.50	111.02
5	T	1	NAG	O5-C1-C2	-5.78	102.35	111.29
6	X	1	NAG	O5-C1-C2	-5.77	102.36	111.29
4	V	1	NAG	O5-C1-C2	-5.38	102.96	111.29
5	Q	1	NAG	C1-O5-C5	5.33	119.33	112.19
6	L	2	NAG	O5-C1-C2	-5.22	103.22	111.29
4	P	2	NAG	C4-C3-C2	-5.07	103.59	111.02
4	S	1	NAG	O5-C1-C2	-4.97	103.60	111.29
4	S	2	NAG	O5-C1-C2	-4.75	103.94	111.29
4	S	1	NAG	C3-C4-C5	-4.55	101.98	110.23
6	L	3	BMA	C1-O5-C5	-4.30	106.42	112.19
6	U	1	NAG	C2-N2-C7	-4.19	117.29	122.90
6	X	2	NAG	C2-N2-C7	-4.07	117.44	122.90
6	L	1	NAG	C2-N2-C7	-3.85	117.74	122.90
6	L	1	NAG	C3-C4-C5	-3.78	103.38	110.23
4	P	2	NAG	C2-N2-C7	-3.76	117.86	122.90
5	H	1	NAG	O3-C3-C2	-3.72	101.68	109.40
6	U	1	NAG	C3-C4-C5	-3.71	103.51	110.23
5	W	1	NAG	O5-C1-C2	-3.70	105.56	111.29
4	V	1	NAG	C1-O5-C5	3.69	117.14	112.19
5	H	2	NAG	O5-C1-C2	-3.67	105.61	111.29
6	U	3	BMA	C1-O5-C5	3.65	117.08	112.19
6	R	1	NAG	C2-N2-C7	-3.53	118.16	122.90
5	T	1	NAG	C1-O5-C5	3.48	116.85	112.19
5	T	1	NAG	O5-C5-C4	-3.45	102.43	110.83
5	H	1	NAG	C3-C4-C5	-3.43	104.02	110.23
6	R	2	NAG	O5-C1-C2	-3.32	106.16	111.29
5	Q	1	NAG	O5-C1-C2	-3.29	106.19	111.29
6	R	2	NAG	C1-O5-C5	3.26	116.55	112.19
4	P	3	BMA	C1-O5-C5	3.21	116.49	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	1	NAG	O5-C1-C2	-3.09	106.51	111.29
6	R	1	NAG	O5-C5-C4	3.07	118.29	110.83
6	R	1	NAG	C1-C2-N2	3.01	115.18	110.43
4	P	2	NAG	C3-C4-C5	-2.86	105.05	110.23
5	W	1	NAG	C1-O5-C5	2.85	116.01	112.19
6	U	3	BMA	C1-C2-C3	2.85	113.80	109.64
5	T	2	NAG	C3-C4-C5	-2.84	105.09	110.23
4	P	2	NAG	C1-O5-C5	2.83	115.98	112.19
5	W	1	NAG	C3-C4-C5	-2.70	105.33	110.23
6	R	2	NAG	O4-C4-C3	-2.70	104.01	110.38
6	U	2	NAG	O5-C1-C2	-2.70	107.12	111.29
6	X	1	NAG	C3-C4-C5	-2.67	105.40	110.23
4	V	2	NAG	C4-C3-C2	2.66	114.92	111.02
6	X	1	NAG	C4-C3-C2	-2.65	107.13	111.02
5	W	1	NAG	O4-C4-C3	-2.63	104.19	110.38
4	P	1	NAG	O5-C1-C2	-2.60	107.26	111.29
6	R	1	NAG	C6-C5-C4	-2.54	106.77	113.02
6	R	1	NAG	O6-C6-C5	-2.54	102.67	111.33
6	L	2	NAG	O4-C4-C3	-2.54	104.40	110.38
6	X	3	BMA	C2-C3-C4	-2.53	106.42	110.86
6	L	1	NAG	O5-C5-C4	-2.52	104.69	110.83
4	D	2	NAG	O5-C1-C2	-2.52	107.39	111.29
6	U	1	NAG	O5-C5-C6	2.48	112.49	107.66
5	Q	1	NAG	C3-C4-C5	-2.47	105.75	110.23
6	X	2	NAG	O5-C5-C4	-2.45	104.86	110.83
6	R	1	NAG	O5-C5-C6	2.40	112.34	107.66
5	T	1	NAG	C4-C3-C2	2.33	114.44	111.02
4	S	3	BMA	C1-O5-C5	2.33	115.31	112.19
5	Q	1	NAG	O5-C5-C4	-2.31	105.21	110.83
4	S	1	NAG	C1-O5-C5	2.31	115.28	112.19
6	R	2	NAG	C1-C2-N2	2.26	114.00	110.43
5	H	2	NAG	C2-N2-C7	-2.22	119.92	122.90
4	V	2	NAG	O4-C4-C3	-2.22	105.14	110.38
5	T	1	NAG	C1-C2-N2	-2.21	106.95	110.43
4	D	2	NAG	C3-C4-C5	-2.20	106.24	110.23
5	T	2	NAG	O5-C5-C4	-2.19	105.49	110.83
6	R	2	NAG	O5-C5-C6	-2.19	103.41	107.66
4	D	2	NAG	C2-N2-C7	-2.15	120.02	122.90
6	R	1	NAG	O3-C3-C4	-2.13	105.35	110.38
6	R	3	BMA	C1-C2-C3	-2.10	106.59	109.64
5	H	1	NAG	O5-C1-C2	-2.10	108.05	111.29
6	U	1	NAG	O5-C5-C4	-2.09	105.74	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	2	NAG	C2-N2-C7	-2.08	120.11	122.90
6	L	1	NAG	C1-C2-N2	-2.08	107.16	110.43
4	D	1	NAG	O4-C4-C3	-2.07	105.49	110.38
5	W	2	NAG	O5-C1-C2	-2.07	108.09	111.29
4	D	3	BMA	O5-C5-C4	-2.03	105.89	110.83

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C8-C7-N2-C2
4	D	1	NAG	O7-C7-N2-C2
4	S	1	NAG	C1-C2-N2-C7
4	S	1	NAG	C8-C7-N2-C2
4	S	1	NAG	O7-C7-N2-C2
4	S	2	NAG	C8-C7-N2-C2
4	S	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C8-C7-N2-C2
4	V	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
5	H	1	NAG	C8-C7-N2-C2
5	H	2	NAG	C8-C7-N2-C2
5	H	2	NAG	O7-C7-N2-C2
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	T	1	NAG	C8-C7-N2-C2
5	T	1	NAG	O7-C7-N2-C2
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	W	1	NAG	C8-C7-N2-C2
5	W	1	NAG	O7-C7-N2-C2
5	W	2	NAG	C8-C7-N2-C2
5	W	2	NAG	O7-C7-N2-C2
6	L	1	NAG	C8-C7-N2-C2
6	L	1	NAG	O7-C7-N2-C2
6	R	1	NAG	C8-C7-N2-C2
6	R	1	NAG	O7-C7-N2-C2
6	R	2	NAG	C8-C7-N2-C2
6	R	2	NAG	O7-C7-N2-C2
6	U	1	NAG	C1-C2-N2-C7
6	U	1	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	U	1	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	X	2	NAG	C8-C7-N2-C2
6	X	2	NAG	O7-C7-N2-C2
5	H	1	NAG	O7-C7-N2-C2
6	L	2	NAG	O5-C5-C6-O6
6	X	1	NAG	O5-C5-C6-O6
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	L	3	BMA	O5-C5-C6-O6
4	V	3	BMA	O5-C5-C6-O6
6	X	1	NAG	C8-C7-N2-C2
4	P	3	BMA	O5-C5-C6-O6
6	R	2	NAG	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	X	1	NAG	O7-C7-N2-C2
6	R	1	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	L	2	NAG	C4-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
4	P	4	MAN	O5-C5-C6-O6
4	V	3	BMA	C4-C5-C6-O6
6	X	1	NAG	C4-C5-C6-O6
4	V	1	NAG	C1-C2-N2-C7
6	X	2	NAG	C4-C5-C6-O6
6	L	3	BMA	C4-C5-C6-O6
5	H	1	NAG	C1-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	P	4	MAN	C1-C2-C3-C4-C5-O5
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	S	4	MAN	C1-C2-C3-C4-C5-O5
6	X	3	BMA	C1-C2-C3-C4-C5-O5

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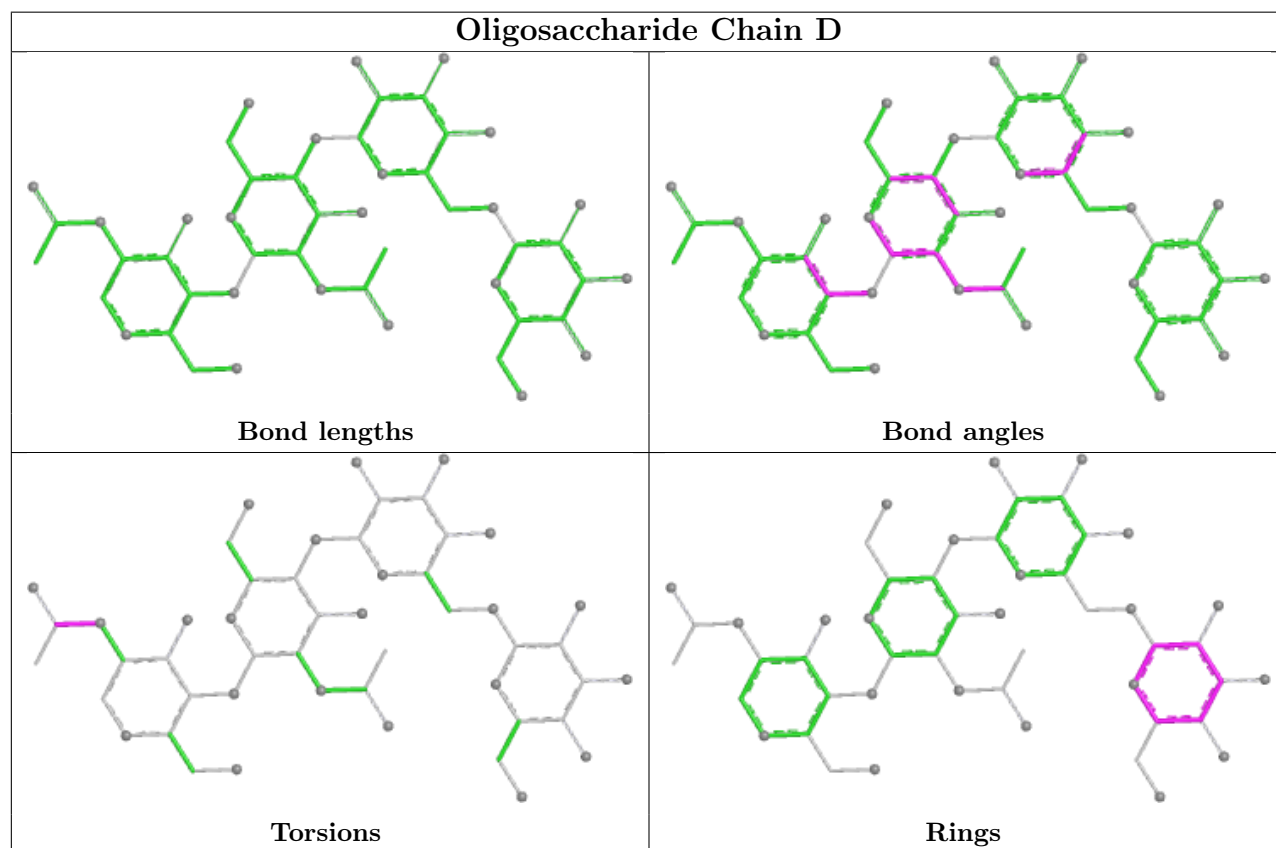
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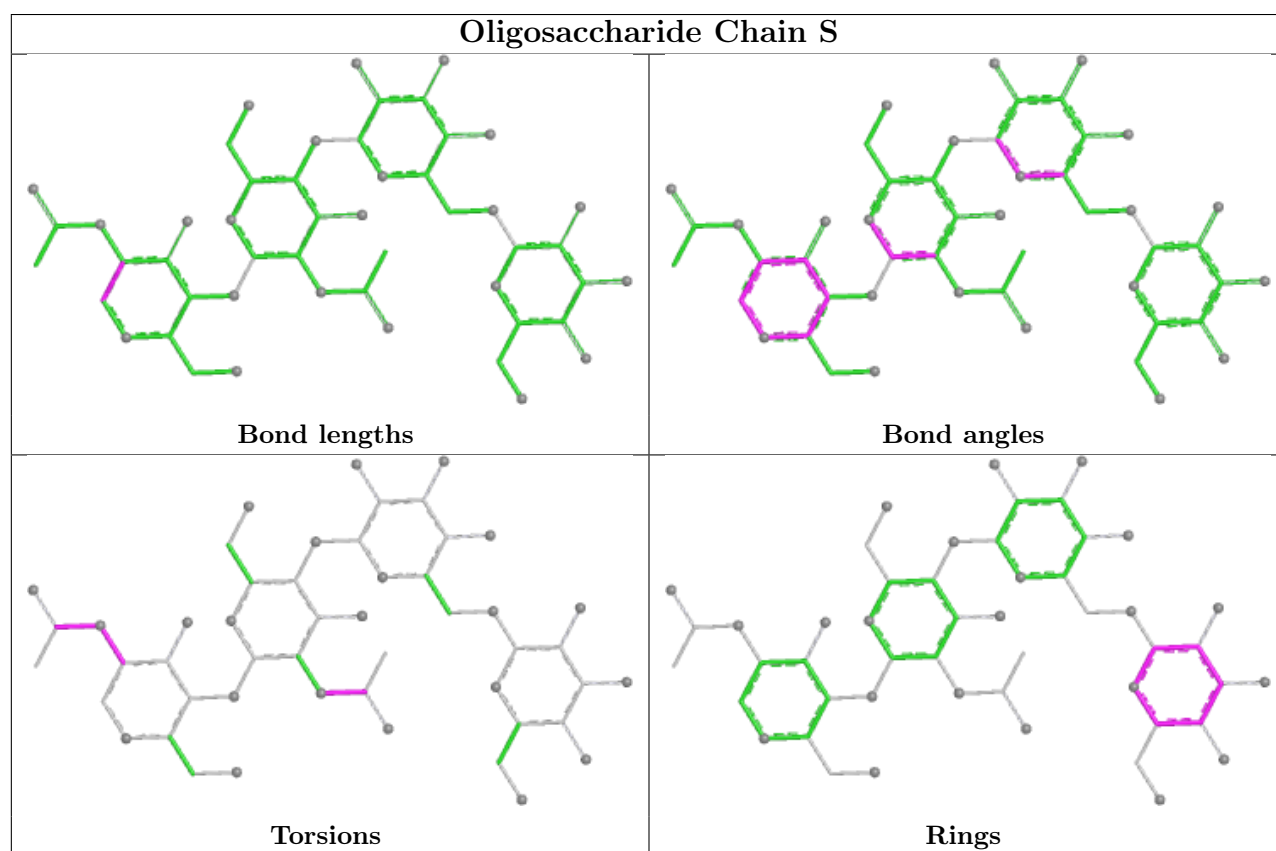
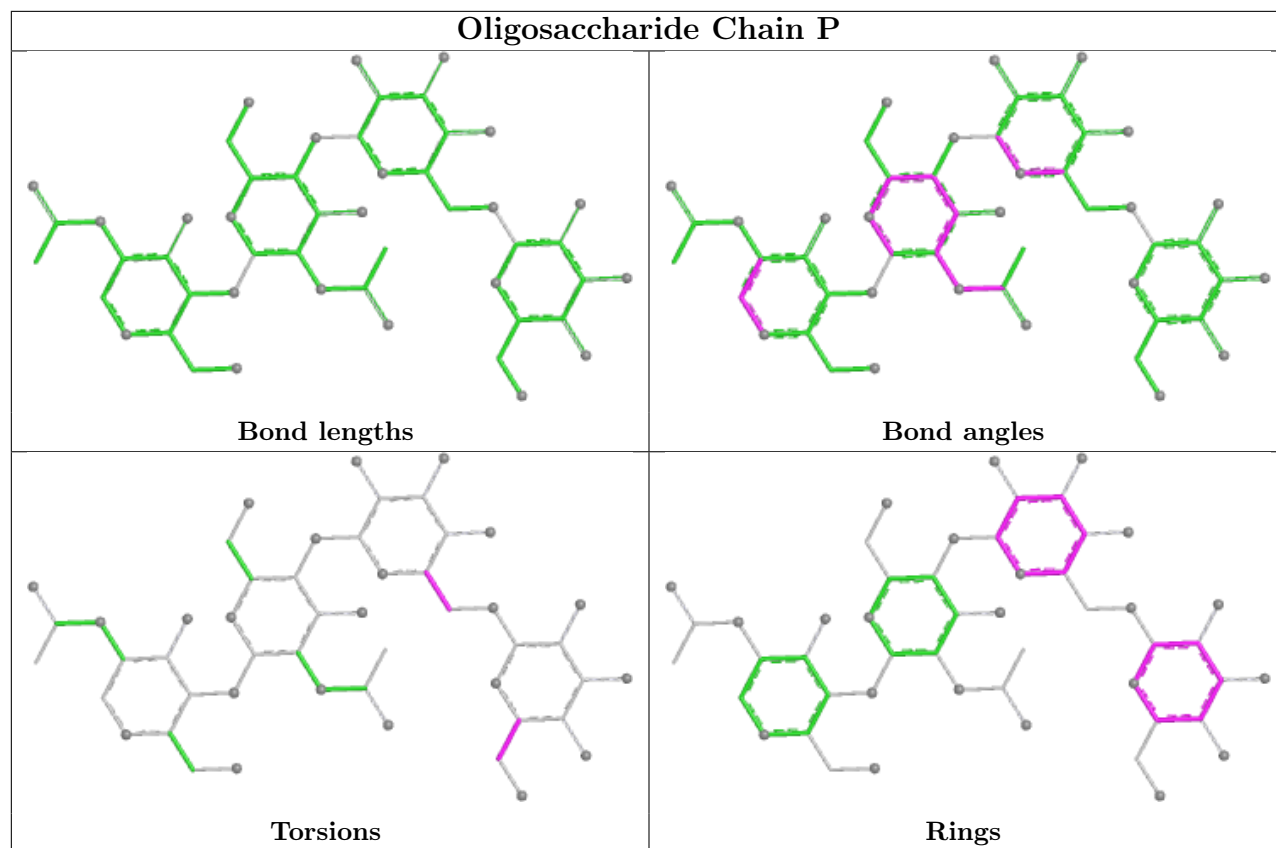
Mol	Chain	Res	Type	Atoms
4	P	3	BMA	C1-C2-C3-C4-C5-O5

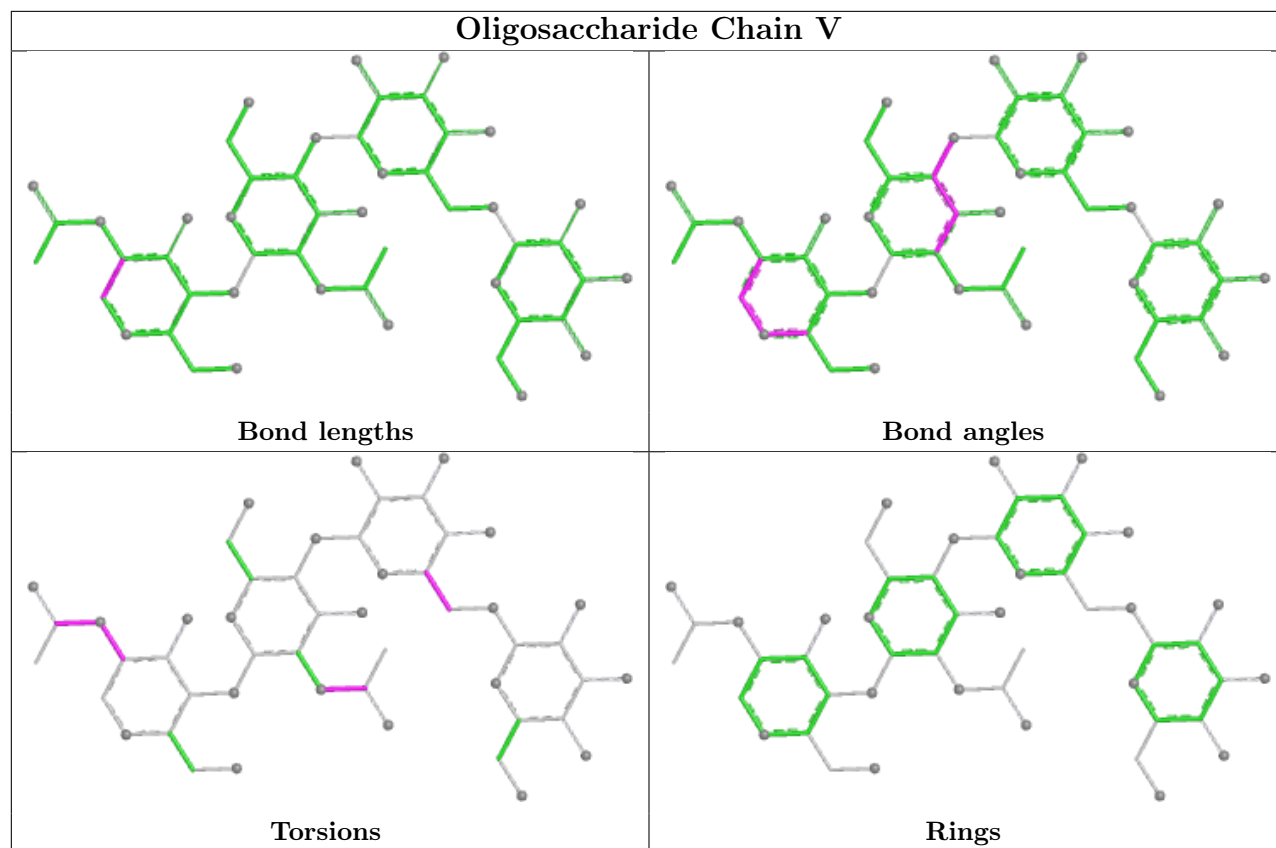
11 monomers are involved in 18 short contacts:

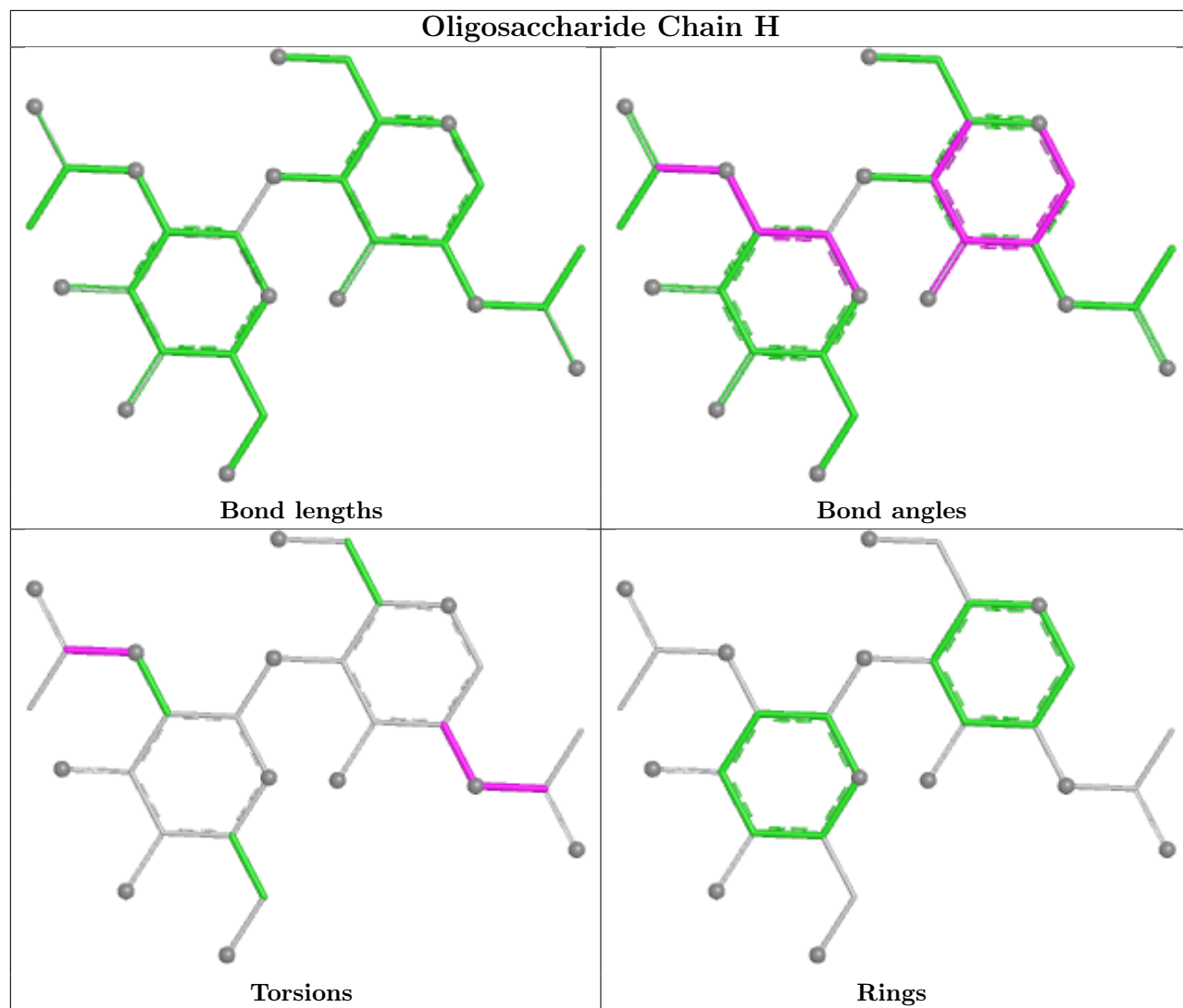
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	2	NAG	1	0
4	D	3	BMA	1	0
4	P	1	NAG	3	0
5	W	1	NAG	2	0
5	H	1	NAG	5	0
6	U	2	NAG	1	0
5	Q	1	NAG	2	0
6	X	1	NAG	1	0
6	R	2	NAG	1	0
6	L	1	NAG	1	0
4	D	4	MAN	1	0

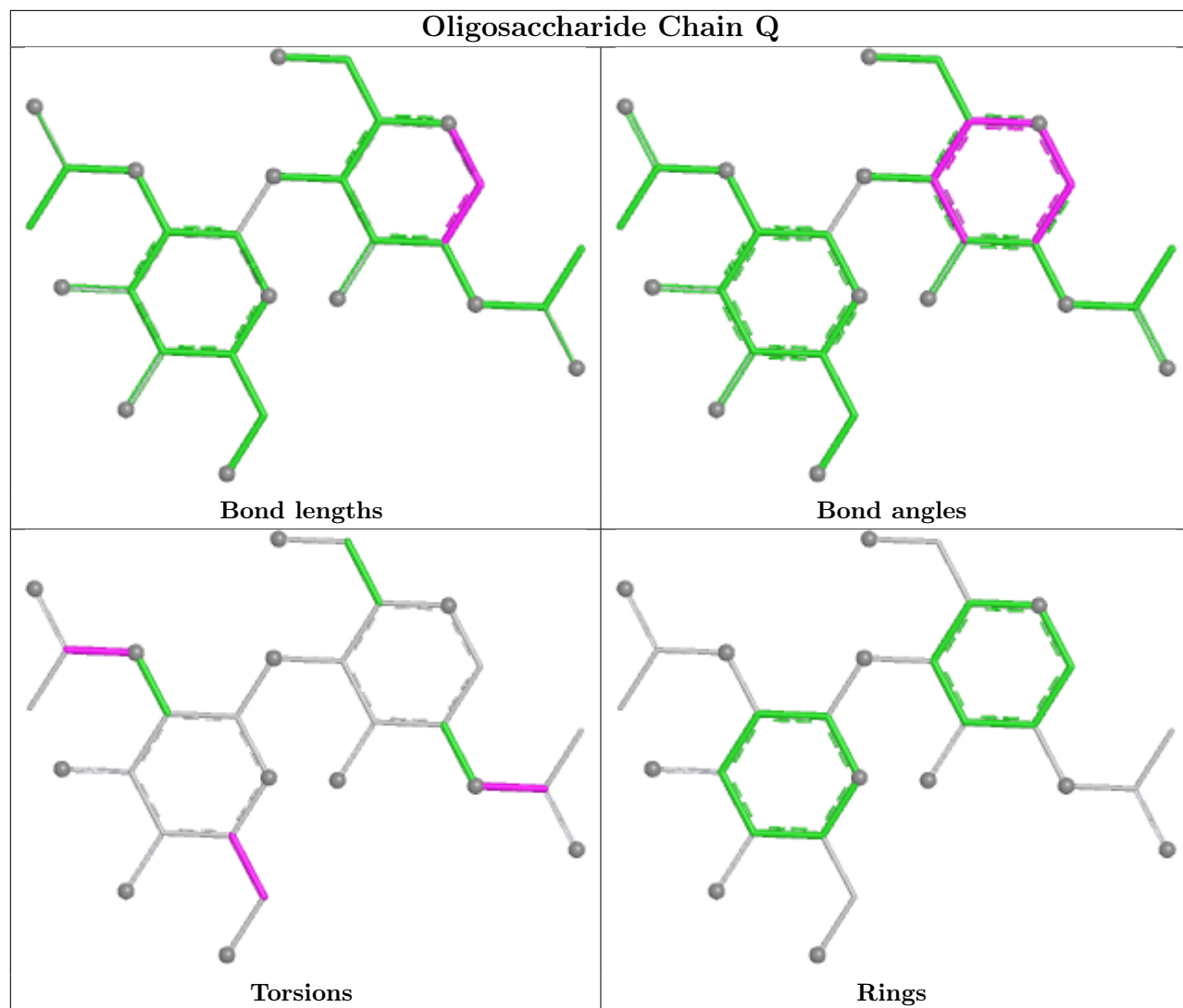
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

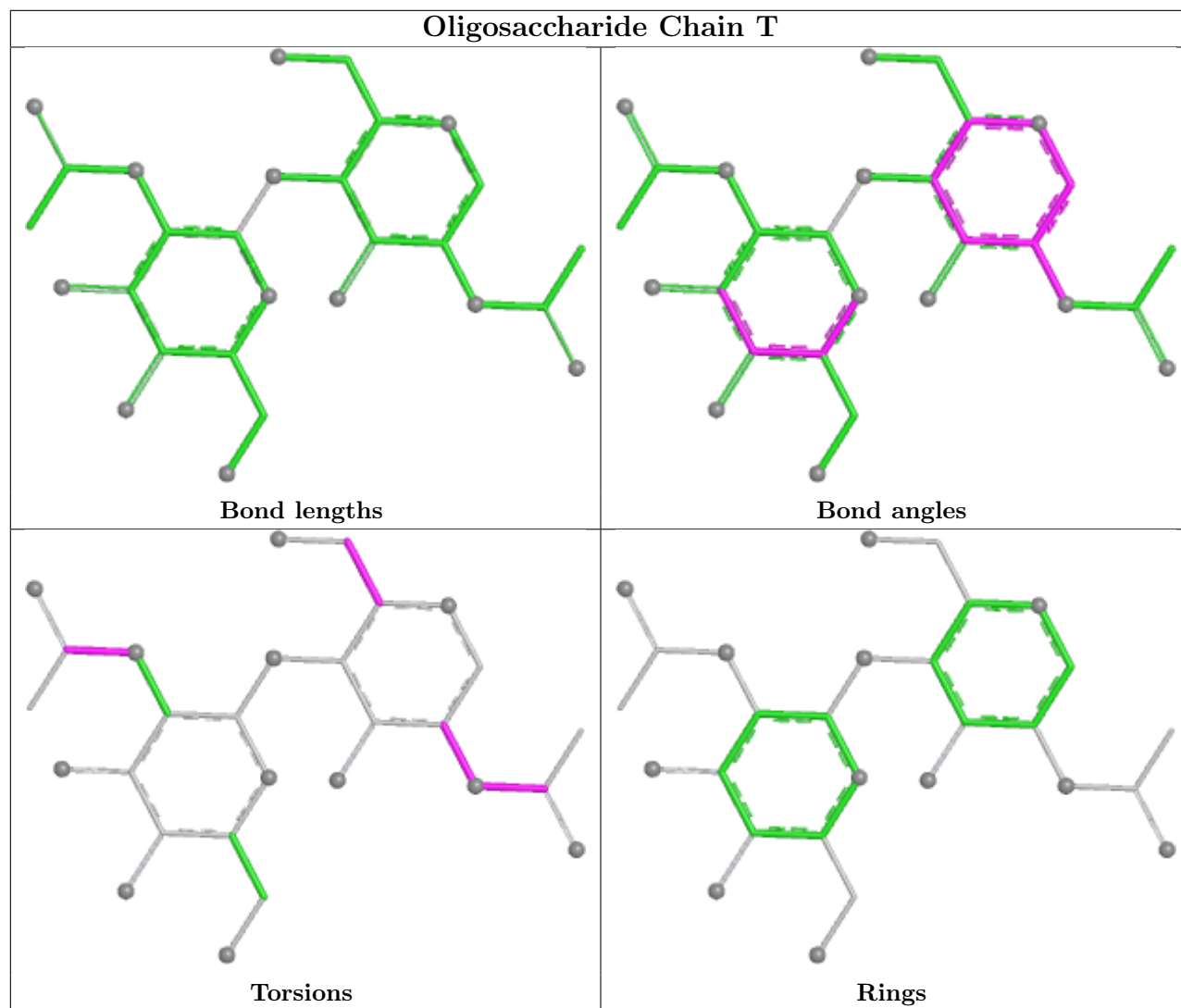


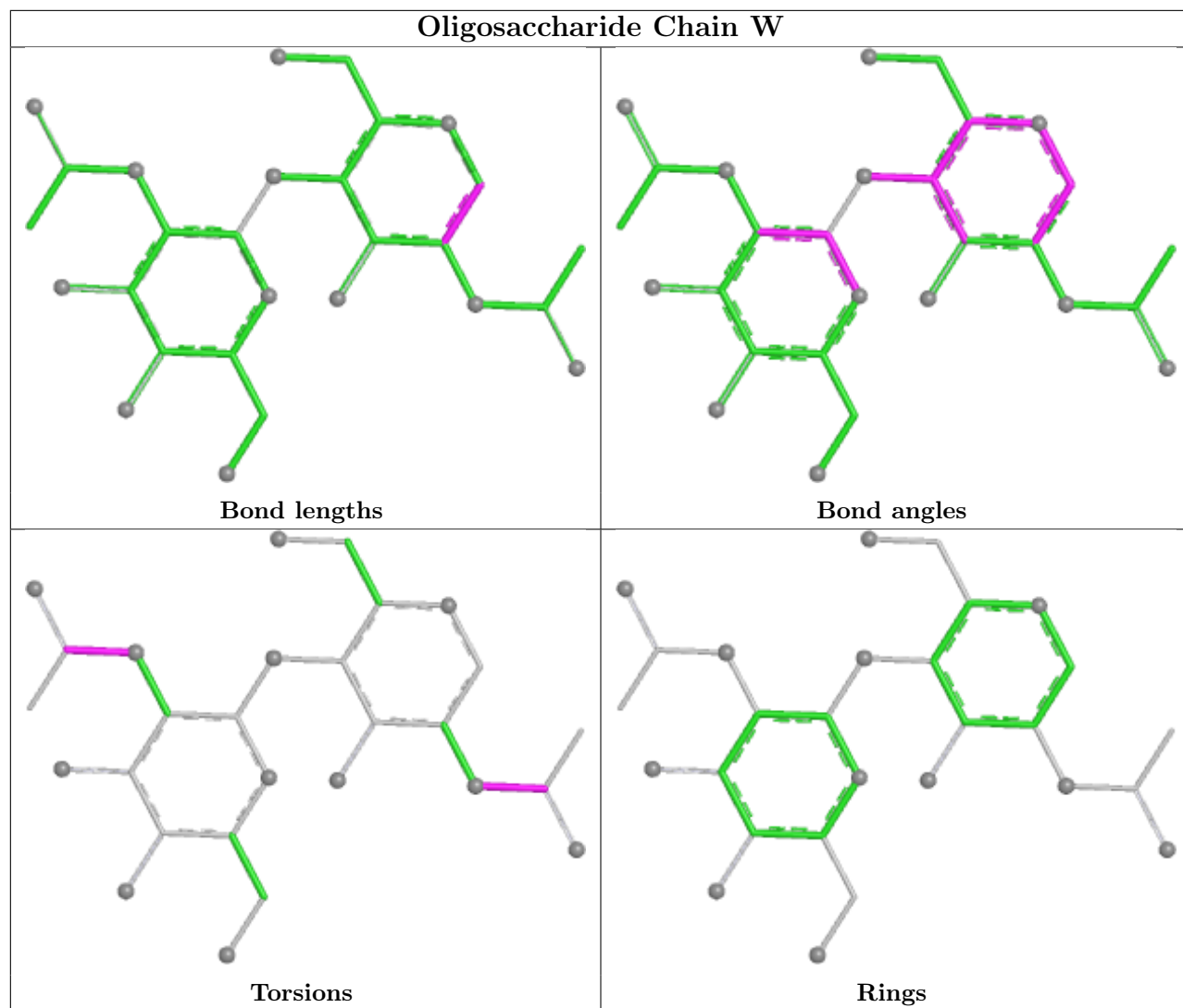


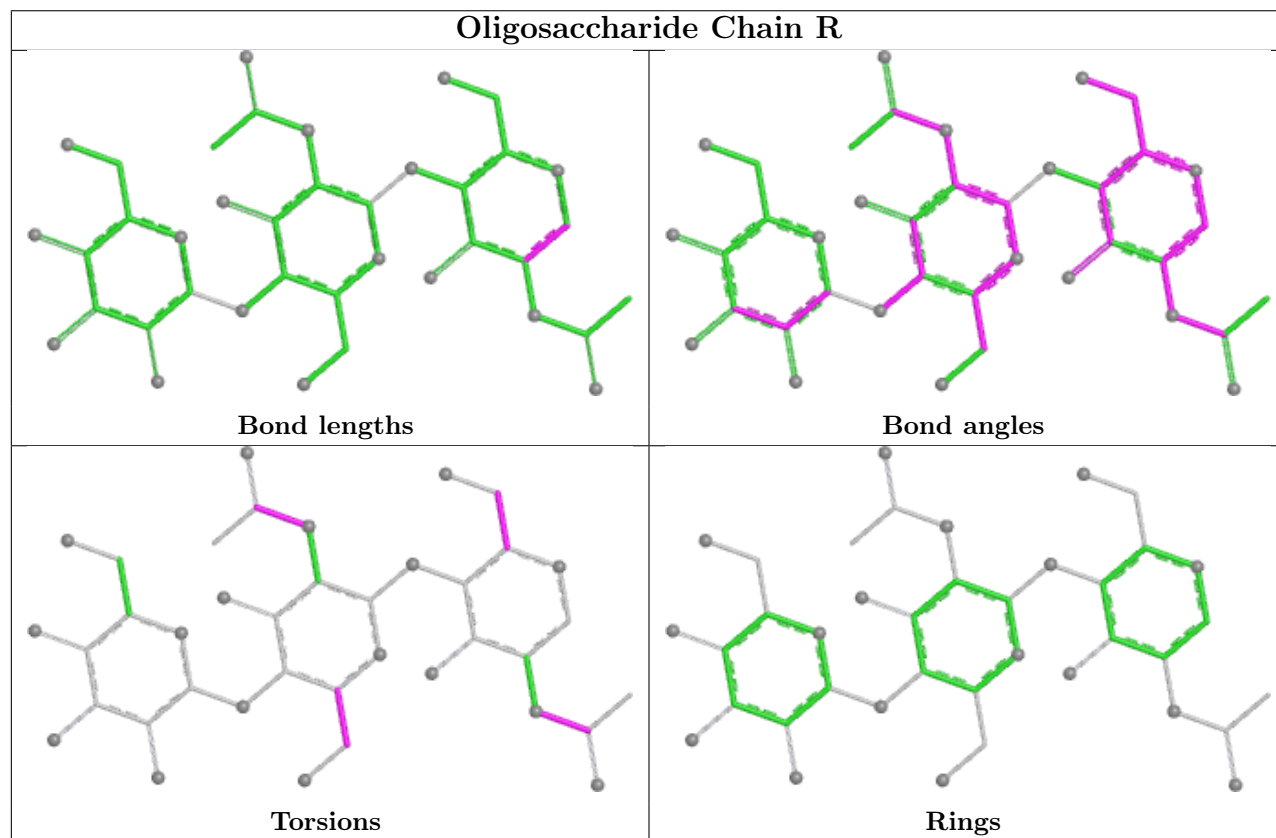
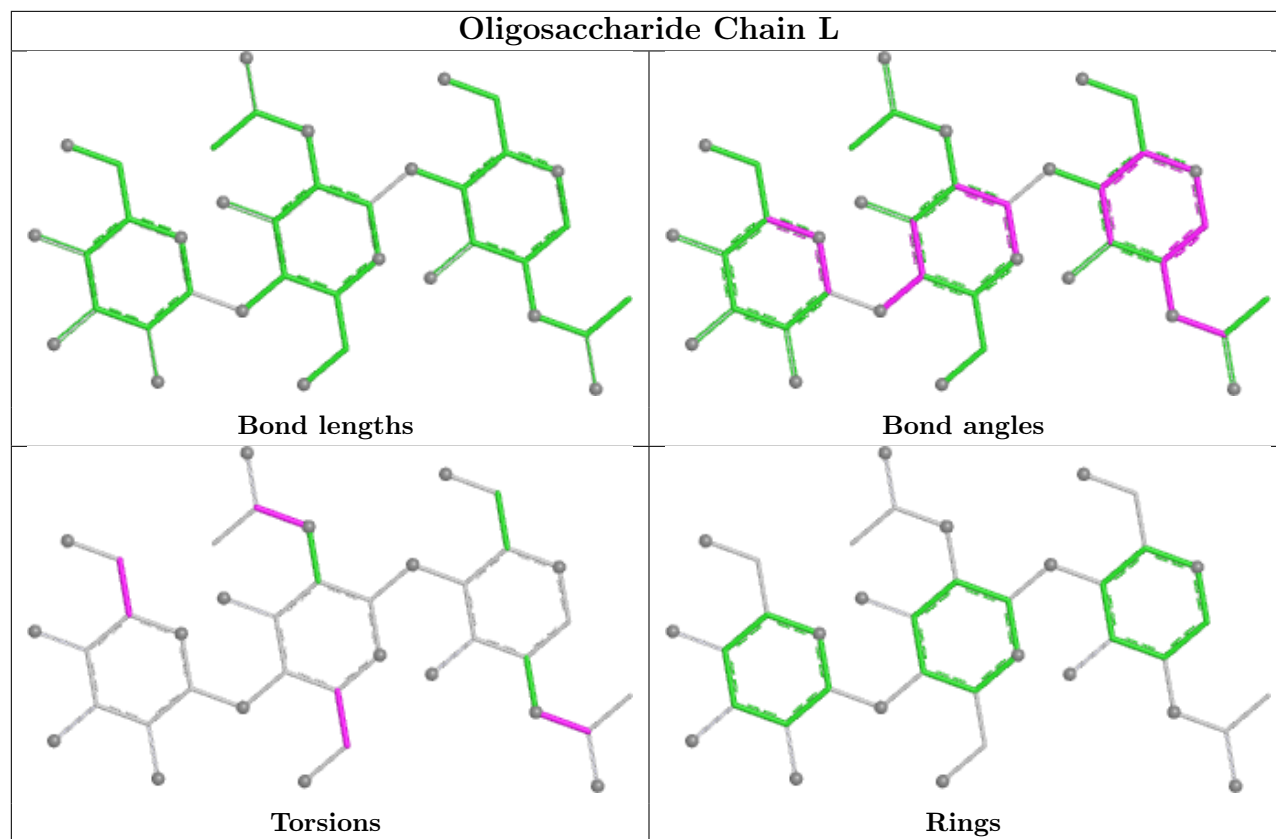


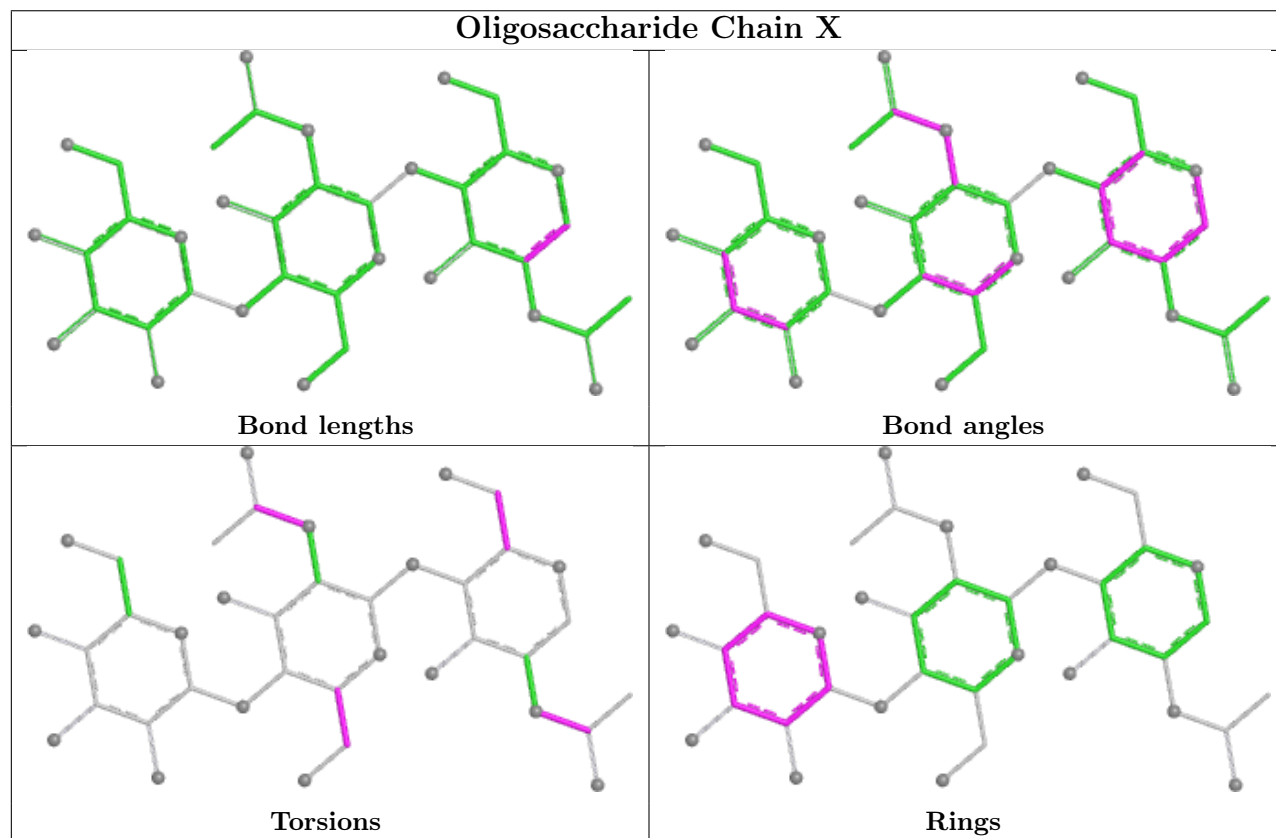
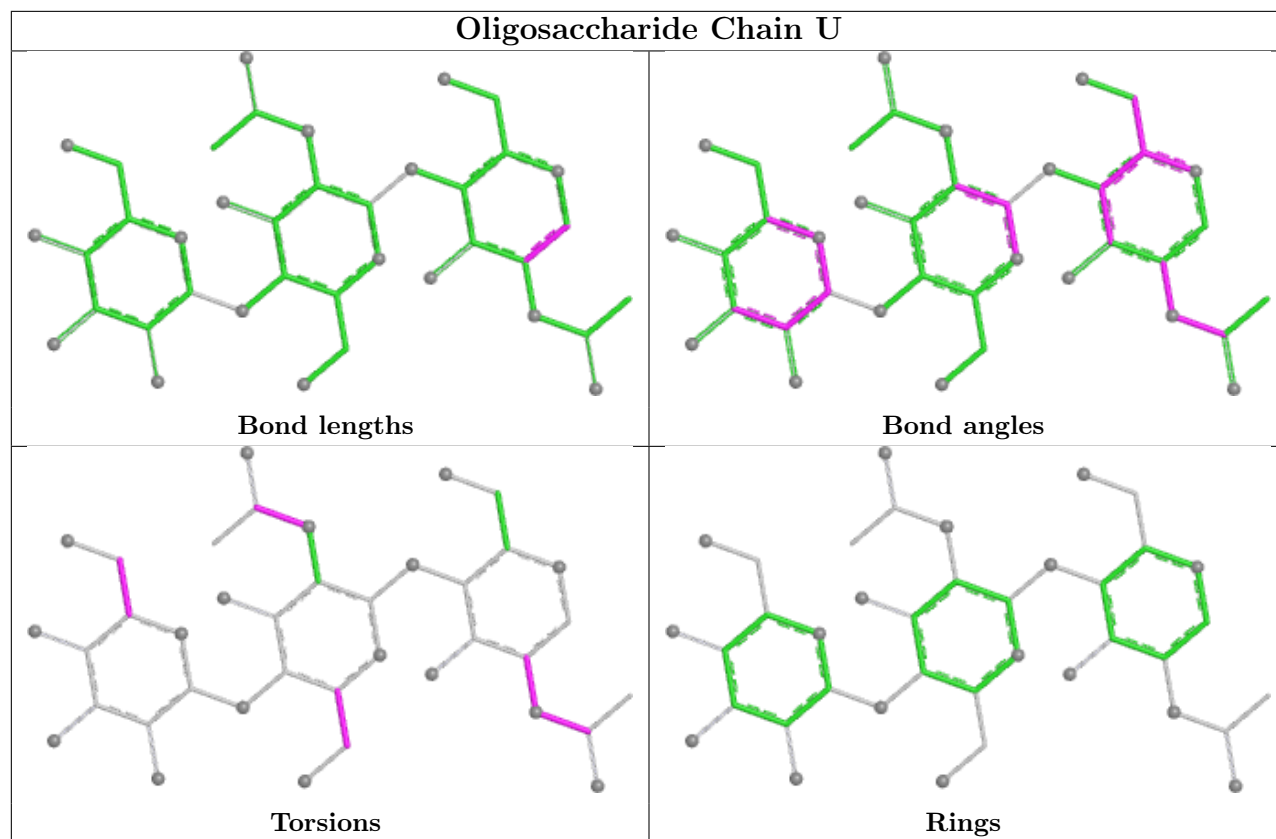












## 5.6 Ligand geometry

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	STE	E	503	-	19,19,19	0.56	0	19,19,19	0.67	0
11	CLR	N	503	-	31,31,31	0.30	0	48,48,48	0.48	0
9	STE	F	505	-	19,19,19	0.56	0	19,19,19	0.69	0
9	STE	N	505	-	19,19,19	0.56	0	19,19,19	0.69	0
10	PLM	N	504	-	17,17,17	0.59	0	17,17,17	0.68	0
10	PLM	F	504	-	17,17,17	0.59	0	17,17,17	0.67	0
11	CLR	F	503	-	31,31,31	0.27	0	48,48,48	0.45	0
7	NAG	A	501	1	14,14,15	0.55	0	17,19,21	1.46	3 (17%)
8	PCW	E	502	-	53,53,53	0.43	0	59,61,61	0.98	4 (6%)
10	PLM	B	504	-	17,17,17	0.58	0	17,17,17	0.68	0
8	PCW	A	502	-	53,53,53	0.31	0	59,61,61	0.31	0
10	PLM	E	504	-	17,17,17	0.59	0	17,17,17	0.70	0
7	NAG	E	501	1	14,14,15	0.56	0	17,19,21	1.45	3 (17%)
8	PCW	M	502	-	53,53,53	0.31	0	59,61,61	0.30	0
10	PLM	A	504	-	17,17,17	0.60	0	17,17,17	0.71	0
11	CLR	I	503	-	31,31,31	0.28	0	48,48,48	0.43	0
8	PCW	I	502	-	53,53,53	0.36	0	59,61,61	0.62	1 (1%)
9	STE	A	503	-	19,19,19	0.58	0	19,19,19	0.67	0
11	CLR	F	501	-	31,31,31	0.32	0	48,48,48	0.58	0
10	PLM	B	506	-	17,17,17	0.59	0	17,17,17	0.77	1 (5%)
9	STE	M	503	-	19,19,19	0.57	0	19,19,19	0.67	0
11	CLR	N	502	-	31,31,31	0.30	0	48,48,48	0.39	0
10	PLM	J	506	-	17,17,17	0.59	0	17,17,17	0.78	1 (5%)
11	CLR	N	501	-	31,31,31	0.36	0	48,48,48	0.64	1 (2%)
9	STE	J	501	-	19,19,19	0.57	0	19,19,19	0.67	0
11	CLR	B	503	-	31,31,31	0.26	0	48,48,48	0.58	1 (2%)
7	NAG	I	501	1	14,14,15	0.55	0	17,19,21	1.45	3 (17%)
10	PLM	J	504	-	17,17,17	0.59	0	17,17,17	0.68	0
11	CLR	J	503	-	31,31,31	0.29	0	48,48,48	0.70	1 (2%)
7	NAG	M	501	1	14,14,15	0.56	0	17,19,21	1.45	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	STE	J	505	-	19,19,19	0.56	0	19,19,19	0.69	0
10	PLM	I	504	-	17,17,17	0.59	0	17,17,17	0.71	0
9	STE	B	505	-	19,19,19	0.56	0	19,19,19	0.69	0
10	PLM	M	504	-	17,17,17	0.59	0	17,17,17	0.70	0
10	PLM	N	506	-	17,17,17	0.59	0	17,17,17	0.77	1 (5%)
11	CLR	B	501	-	31,31,31	0.29	0	48,48,48	0.51	0
11	CLR	B	502	-	31,31,31	0.28	0	48,48,48	0.42	0
11	CLR	J	502	-	31,31,31	0.29	0	48,48,48	0.39	0
10	PLM	F	506	-	17,17,17	0.58	0	17,17,17	0.77	1 (5%)
11	CLR	F	502	-	31,31,31	0.27	0	48,48,48	0.39	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
9	STE	E	503	-	-	10/17/17/17	-
11	CLR	N	503	-	-	8/10/68/68	0/4/4/4
9	STE	F	505	-	-	11/17/17/17	-
9	STE	N	505	-	-	11/17/17/17	-
10	PLM	N	504	-	-	11/15/15/15	-
10	PLM	F	504	-	-	11/15/15/15	-
11	CLR	F	503	-	-	4/10/68/68	0/4/4/4
7	NAG	A	501	1	-	4/6/23/26	0/1/1/1
8	PCW	E	502	-	-	30/57/57/57	-
10	PLM	B	504	-	-	11/15/15/15	-
8	PCW	A	502	-	-	27/57/57/57	-
10	PLM	E	504	-	-	9/15/15/15	-
7	NAG	E	501	1	-	4/6/23/26	0/1/1/1
8	PCW	M	502	-	-	30/57/57/57	-
10	PLM	A	504	-	-	9/15/15/15	-
11	CLR	I	503	-	-	7/10/68/68	0/4/4/4
8	PCW	I	502	-	-	27/57/57/57	-
9	STE	A	503	-	-	10/17/17/17	-
11	CLR	F	501	-	-	5/10/68/68	0/4/4/4
10	PLM	B	506	-	-	11/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	STE	M	503	-	-	10/17/17/17	-
11	CLR	N	502	-	-	5/10/68/68	0/4/4/4
10	PLM	J	506	-	-	11/15/15/15	-
11	CLR	N	501	-	-	8/10/68/68	0/4/4/4
9	STE	J	501	-	-	10/17/17/17	-
11	CLR	B	503	-	-	8/10/68/68	0/4/4/4
7	NAG	I	501	1	-	4/6/23/26	0/1/1/1
10	PLM	J	504	-	-	11/15/15/15	-
11	CLR	J	503	-	-	5/10/68/68	0/4/4/4
7	NAG	M	501	1	-	4/6/23/26	0/1/1/1
9	STE	J	505	-	-	11/17/17/17	-
10	PLM	I	504	-	-	9/15/15/15	-
9	STE	B	505	-	-	11/17/17/17	-
10	PLM	M	504	-	-	9/15/15/15	-
10	PLM	N	506	-	-	11/15/15/15	-
11	CLR	B	501	-	-	3/10/68/68	0/4/4/4
11	CLR	B	502	-	-	4/10/68/68	0/4/4/4
11	CLR	J	502	-	-	4/10/68/68	0/4/4/4
10	PLM	F	506	-	-	11/15/15/15	-
11	CLR	F	502	-	-	4/10/68/68	0/4/4/4

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	501	NAG	C1-O5-C5	4.50	118.21	112.19
7	A	501	NAG	C1-O5-C5	4.49	118.21	112.19
7	M	501	NAG	C1-O5-C5	4.49	118.20	112.19
7	I	501	NAG	C1-O5-C5	4.45	118.15	112.19
8	E	502	PCW	O4P-P-O2P	-4.19	92.32	108.94
8	E	502	PCW	O2-C31-C32	3.33	118.67	111.48
8	E	502	PCW	O2-C31-O31	-2.85	117.04	123.70
11	J	503	CLR	C17-C13-C14	-2.50	97.23	100.10
8	I	502	PCW	O2-C31-O31	-2.37	118.16	123.70
8	E	502	PCW	O3P-P-O2P	2.36	118.28	108.94
7	E	501	NAG	O5-C1-C2	2.34	114.90	111.29
7	A	501	NAG	O5-C1-C2	2.32	114.89	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	501	NAG	O5-C1-C2	2.32	114.88	111.29
7	M	501	NAG	O5-C1-C2	2.31	114.87	111.29
11	B	503	CLR	C16-C17-C13	-2.31	101.12	103.84
11	N	501	CLR	C11-C9-C10	-2.24	110.33	113.08
7	A	501	NAG	C4-C3-C2	-2.10	107.94	111.02
10	J	506	PLM	O1-C1-C2	2.07	120.54	114.00
10	B	506	PLM	O1-C1-C2	2.07	120.54	114.00
10	F	506	PLM	O1-C1-C2	2.05	120.49	114.00
7	I	501	NAG	C4-C3-C2	-2.05	108.01	111.02
10	N	506	PLM	O1-C1-C2	2.05	120.47	114.00
7	E	501	NAG	C4-C3-C2	-2.04	108.03	111.02
7	M	501	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (403) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	501	NAG	C8-C7-N2-C2
7	A	501	NAG	O7-C7-N2-C2
7	E	501	NAG	C8-C7-N2-C2
7	E	501	NAG	O7-C7-N2-C2
7	I	501	NAG	C8-C7-N2-C2
7	I	501	NAG	O7-C7-N2-C2
7	M	501	NAG	C8-C7-N2-C2
7	M	501	NAG	O7-C7-N2-C2
8	A	502	PCW	O2-C2-C3-O3
8	A	502	PCW	O4P-C4-C5-N
8	A	502	PCW	C1-O3P-P-O2P
8	A	502	PCW	C4-O4P-P-O1P
8	A	502	PCW	C4-O4P-P-O3P
8	E	502	PCW	O4P-C4-C5-N
8	E	502	PCW	C1-O3P-P-O1P
8	E	502	PCW	C1-O3P-P-O2P
8	E	502	PCW	C1-O3P-P-O4P
8	I	502	PCW	O2-C2-C3-O3
8	I	502	PCW	O4P-C4-C5-N
8	I	502	PCW	C1-O3P-P-O2P
8	I	502	PCW	C4-O4P-P-O3P
8	M	502	PCW	O3P-C1-C2-O2
8	M	502	PCW	O4P-C4-C5-N
8	M	502	PCW	C12-C11-O3-C3
8	M	502	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
8	M	502	PCW	C1-O3P-P-O1P
8	M	502	PCW	C4-O4P-P-O2P
8	M	502	PCW	C4-O4P-P-O3P
11	B	502	CLR	C13-C17-C20-C21
11	B	502	CLR	C16-C17-C20-C22
11	F	502	CLR	C13-C17-C20-C21
11	F	502	CLR	C16-C17-C20-C22
11	J	502	CLR	C13-C17-C20-C21
11	J	502	CLR	C16-C17-C20-C21
11	B	502	CLR	C16-C17-C20-C21
11	B	503	CLR	C16-C17-C20-C21
11	F	502	CLR	C16-C17-C20-C21
11	N	503	CLR	C16-C17-C20-C21
11	B	503	CLR	C13-C17-C20-C21
11	N	503	CLR	C13-C17-C20-C21
11	B	502	CLR	C13-C17-C20-C22
11	F	502	CLR	C13-C17-C20-C22
11	J	502	CLR	C13-C17-C20-C22
11	B	503	CLR	C21-C20-C22-C23
11	N	501	CLR	C21-C20-C22-C23
11	N	503	CLR	C21-C20-C22-C23
11	N	502	CLR	C16-C17-C20-C21
11	N	502	CLR	C13-C17-C20-C21
11	J	502	CLR	C16-C17-C20-C22
11	B	503	CLR	C13-C17-C20-C22
11	N	502	CLR	C13-C17-C20-C22
11	N	503	CLR	C13-C17-C20-C22
8	A	502	PCW	C38-C39-C40-C41
8	E	502	PCW	C18-C19-C20-C21
7	I	501	NAG	O5-C5-C6-O6
7	M	501	NAG	O5-C5-C6-O6
11	F	501	CLR	C21-C20-C22-C23
8	A	502	PCW	C12-C13-C14-C15
7	A	501	NAG	O5-C5-C6-O6
7	E	501	NAG	O5-C5-C6-O6
11	N	501	CLR	C17-C20-C22-C23
11	N	503	CLR	C17-C20-C22-C23
11	B	503	CLR	C17-C20-C22-C23
8	I	502	PCW	C41-C42-C43-C44
7	M	501	NAG	C4-C5-C6-O6
8	I	502	PCW	C12-C11-O3-C3
8	E	502	PCW	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
8	I	502	PCW	C44-C45-C46-C47
7	A	501	NAG	C4-C5-C6-O6
7	E	501	NAG	C4-C5-C6-O6
7	I	501	NAG	C4-C5-C6-O6
8	E	502	PCW	C4-C5-N-C7
8	E	502	PCW	C4-C5-N-C8
8	M	502	PCW	C4-C5-N-C7
8	I	502	PCW	O11-C11-O3-C3
8	M	502	PCW	C43-C44-C45-C46
11	B	503	CLR	C16-C17-C20-C22
11	N	502	CLR	C16-C17-C20-C22
11	N	503	CLR	C16-C17-C20-C22
8	A	502	PCW	C15-C16-C17-C18
8	A	502	PCW	C18-C19-C20-C21
8	A	502	PCW	C11-C12-C13-C14
8	A	502	PCW	C31-C32-C33-C34
8	E	502	PCW	C11-C12-C13-C14
9	A	503	STE	C11-C10-C9-C8
9	E	503	STE	C11-C10-C9-C8
9	J	501	STE	C11-C10-C9-C8
9	M	503	STE	C11-C10-C9-C8
8	M	502	PCW	C4-C5-N-C6
8	A	502	PCW	C22-C23-C24-C25
8	E	502	PCW	C31-C32-C33-C34
10	A	504	PLM	C1-C2-C3-C4
10	E	504	PLM	C1-C2-C3-C4
10	I	504	PLM	C1-C2-C3-C4
10	M	504	PLM	C1-C2-C3-C4
11	N	501	CLR	C13-C17-C20-C22
8	I	502	PCW	C38-C39-C40-C41
11	N	503	CLR	C20-C22-C23-C24
8	M	502	PCW	C22-C23-C24-C25
8	M	502	PCW	C32-C33-C34-C35
11	N	501	CLR	C22-C23-C24-C25
11	N	502	CLR	C20-C22-C23-C24
11	N	501	CLR	C13-C17-C20-C21
8	E	502	PCW	C4-C5-N-C6
8	M	502	PCW	C4-C5-N-C8
10	B	504	PLM	C6-C7-C8-C9
10	E	504	PLM	C9-CA-CB-CC
10	F	504	PLM	C6-C7-C8-C9
10	J	504	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
10	N	504	PLM	C6-C7-C8-C9
8	I	502	PCW	C18-C19-C20-C21
8	I	502	PCW	C32-C33-C34-C35
10	A	504	PLM	C9-CA-CB-CC
10	I	504	PLM	C9-CA-CB-CC
10	M	504	PLM	C9-CA-CB-CC
8	A	502	PCW	C32-C33-C34-C35
8	A	502	PCW	C44-C45-C46-C47
8	E	502	PCW	C23-C24-C25-C26
8	M	502	PCW	C41-C42-C43-C44
9	F	505	STE	C14-C15-C16-C17
9	N	505	STE	C14-C15-C16-C17
9	J	505	STE	C14-C15-C16-C17
10	A	504	PLM	C7-C8-C9-CA
10	M	504	PLM	C7-C8-C9-CA
9	B	505	STE	C14-C15-C16-C17
10	E	504	PLM	C7-C8-C9-CA
10	I	504	PLM	C7-C8-C9-CA
8	E	502	PCW	C44-C45-C46-C47
10	B	504	PLM	CC-CD-CE-CF
10	J	504	PLM	CC-CD-CE-CF
10	N	504	PLM	CC-CD-CE-CF
10	F	504	PLM	CC-CD-CE-CF
10	N	506	PLM	C7-C8-C9-CA
8	M	502	PCW	C13-C14-C15-C16
9	A	503	STE	C14-C15-C16-C17
9	E	503	STE	C14-C15-C16-C17
9	J	501	STE	C14-C15-C16-C17
9	M	503	STE	C14-C15-C16-C17
10	B	506	PLM	C7-C8-C9-CA
10	F	506	PLM	C7-C8-C9-CA
8	E	502	PCW	C13-C14-C15-C16
10	J	506	PLM	C7-C8-C9-CA
10	B	504	PLM	C3-C4-C5-C6
10	N	504	PLM	C3-C4-C5-C6
11	F	501	CLR	C22-C23-C24-C25
10	F	504	PLM	C3-C4-C5-C6
9	E	503	STE	C9-C10-C11-C12
10	J	504	PLM	C3-C4-C5-C6
9	A	503	STE	C9-C10-C11-C12
9	J	501	STE	C9-C10-C11-C12
9	M	503	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
8	M	502	PCW	C14-C15-C16-C17
10	A	504	PLM	C6-C7-C8-C9
10	E	504	PLM	C6-C7-C8-C9
10	I	504	PLM	C6-C7-C8-C9
10	M	504	PLM	C6-C7-C8-C9
8	M	502	PCW	C15-C16-C17-C18
9	B	505	STE	C5-C6-C7-C8
9	F	505	STE	C5-C6-C7-C8
9	J	505	STE	C5-C6-C7-C8
9	N	505	STE	C5-C6-C7-C8
8	I	502	PCW	C12-C13-C14-C15
9	A	503	STE	C4-C5-C6-C7
9	E	503	STE	C4-C5-C6-C7
9	J	501	STE	C4-C5-C6-C7
9	M	503	STE	C4-C5-C6-C7
10	A	504	PLM	C3-C4-C5-C6
10	E	504	PLM	C3-C4-C5-C6
8	I	502	PCW	C15-C16-C17-C18
10	I	504	PLM	C3-C4-C5-C6
10	M	504	PLM	C3-C4-C5-C6
8	E	502	PCW	C24-C25-C26-C27
8	E	502	PCW	C33-C34-C35-C36
9	A	503	STE	C3-C4-C5-C6
9	J	501	STE	C3-C4-C5-C6
9	M	503	STE	C3-C4-C5-C6
10	I	504	PLM	CC-CD-CE-CF
10	M	504	PLM	CC-CD-CE-CF
8	A	502	PCW	C13-C14-C15-C16
9	E	503	STE	C3-C4-C5-C6
10	A	504	PLM	CC-CD-CE-CF
10	E	504	PLM	CC-CD-CE-CF
11	N	501	CLR	C16-C17-C20-C21
8	M	502	PCW	C32-C31-O2-C2
8	M	502	PCW	O31-C31-O2-C2
8	M	502	PCW	C36-C37-C38-C39
9	M	503	STE	C10-C11-C12-C13
9	A	503	STE	C10-C11-C12-C13
9	E	503	STE	C10-C11-C12-C13
9	J	501	STE	C10-C11-C12-C13
8	E	502	PCW	C35-C36-C37-C38
10	B	506	PLM	C1-C2-C3-C4
10	F	506	PLM	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
10	J	506	PLM	C1-C2-C3-C4
10	N	506	PLM	C1-C2-C3-C4
8	A	502	PCW	C41-C42-C43-C44
9	B	505	STE	C11-C10-C9-C8
9	F	505	STE	C11-C10-C9-C8
9	J	505	STE	C11-C10-C9-C8
9	N	505	STE	C11-C10-C9-C8
8	M	502	PCW	C35-C36-C37-C38
8	A	502	PCW	C40-C41-C42-C43
8	I	502	PCW	C36-C37-C38-C39
8	M	502	PCW	C40-C41-C42-C43
9	A	503	STE	C11-C12-C13-C14
9	E	503	STE	C11-C12-C13-C14
9	J	501	STE	C11-C12-C13-C14
9	M	503	STE	C11-C12-C13-C14
8	E	502	PCW	C34-C35-C36-C37
9	F	505	STE	C10-C11-C12-C13
9	N	505	STE	C10-C11-C12-C13
9	B	505	STE	C10-C11-C12-C13
9	J	505	STE	C10-C11-C12-C13
10	B	504	PLM	C5-C6-C7-C8
10	F	504	PLM	C5-C6-C7-C8
10	F	504	PLM	C7-C8-C9-CA
10	J	504	PLM	C5-C6-C7-C8
10	N	504	PLM	C5-C6-C7-C8
10	N	504	PLM	C7-C8-C9-CA
10	B	504	PLM	C7-C8-C9-CA
10	J	504	PLM	C7-C8-C9-CA
8	M	502	PCW	C16-C17-C18-C19
10	B	506	PLM	C5-C6-C7-C8
10	J	506	PLM	C5-C6-C7-C8
8	M	502	PCW	O3P-C1-C2-C3
10	F	506	PLM	C5-C6-C7-C8
10	N	506	PLM	C5-C6-C7-C8
8	A	502	PCW	C1-C2-C3-O3
8	E	502	PCW	C16-C17-C18-C19
8	I	502	PCW	C33-C34-C35-C36
9	J	505	STE	C9-C10-C11-C12
9	N	505	STE	C9-C10-C11-C12
8	I	502	PCW	C22-C23-C24-C25
9	B	505	STE	C9-C10-C11-C12
11	J	503	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
8	E	502	PCW	C41-C42-C43-C44
9	F	505	STE	C9-C10-C11-C12
8	E	502	PCW	C40-C41-C42-C43
8	I	502	PCW	C20-C21-C22-C23
9	A	503	STE	C6-C7-C8-C9
9	J	501	STE	C6-C7-C8-C9
8	M	502	PCW	C12-C13-C14-C15
9	E	503	STE	C6-C7-C8-C9
9	M	503	STE	C6-C7-C8-C9
10	B	506	PLM	C9-CA-CB-CC
10	F	506	PLM	C9-CA-CB-CC
10	J	506	PLM	C9-CA-CB-CC
10	N	506	PLM	C9-CA-CB-CC
9	A	503	STE	C5-C6-C7-C8
9	E	503	STE	C5-C6-C7-C8
9	J	501	STE	C5-C6-C7-C8
9	M	503	STE	C5-C6-C7-C8
11	N	501	CLR	C16-C17-C20-C22
8	E	502	PCW	O2-C2-C3-O3
10	E	504	PLM	C2-C3-C4-C5
11	I	503	CLR	C16-C17-C20-C21
10	A	504	PLM	C2-C3-C4-C5
10	I	504	PLM	C2-C3-C4-C5
10	M	504	PLM	C2-C3-C4-C5
8	I	502	PCW	C37-C38-C39-C40
9	B	505	STE	C2-C3-C4-C5
9	F	505	STE	C2-C3-C4-C5
9	N	505	STE	C2-C3-C4-C5
8	A	502	PCW	C25-C26-C27-C28
9	J	505	STE	C2-C3-C4-C5
10	B	506	PLM	CC-CD-CE-CF
10	F	506	PLM	CC-CD-CE-CF
10	N	506	PLM	CC-CD-CE-CF
10	J	506	PLM	CC-CD-CE-CF
8	M	502	PCW	C45-C46-C47-C48
11	F	503	CLR	C13-C17-C20-C22
10	B	504	PLM	C9-CA-CB-CC
10	F	504	PLM	C9-CA-CB-CC
10	J	504	PLM	C9-CA-CB-CC
10	N	504	PLM	C9-CA-CB-CC
11	J	503	CLR	C20-C22-C23-C24
11	I	503	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
8	I	502	PCW	C25-C26-C27-C28
10	F	506	PLM	CD-CE-CF-CG
10	J	506	PLM	CD-CE-CF-CG
10	N	506	PLM	CD-CE-CF-CG
10	B	506	PLM	CD-CE-CF-CG
10	N	506	PLM	C3-C4-C5-C6
10	B	506	PLM	C3-C4-C5-C6
10	F	506	PLM	C3-C4-C5-C6
10	J	506	PLM	C3-C4-C5-C6
8	I	502	PCW	C39-C40-C41-C42
11	F	503	CLR	C13-C17-C20-C21
11	I	503	CLR	C16-C17-C20-C22
11	B	503	CLR	C22-C23-C24-C25
8	A	502	PCW	C14-C15-C16-C17
11	I	503	CLR	C13-C17-C20-C21
11	F	503	CLR	C16-C17-C20-C22
11	I	503	CLR	C13-C17-C20-C22
8	I	502	PCW	C1-C2-C3-O3
11	I	503	CLR	C23-C24-C25-C27
8	A	502	PCW	C17-C18-C19-C20
8	E	502	PCW	C12-C13-C14-C15
8	E	502	PCW	C36-C37-C38-C39
10	N	504	PLM	C4-C5-C6-C7
10	B	504	PLM	C4-C5-C6-C7
10	F	504	PLM	C4-C5-C6-C7
10	J	504	PLM	C4-C5-C6-C7
11	F	503	CLR	C16-C17-C20-C21
9	N	505	STE	C3-C4-C5-C6
9	B	505	STE	C3-C4-C5-C6
9	F	505	STE	C3-C4-C5-C6
9	J	505	STE	C3-C4-C5-C6
8	E	502	PCW	C1-C2-C3-O3
8	A	502	PCW	C43-C44-C45-C46
8	I	502	PCW	C4-O4P-P-O2P
8	M	502	PCW	C4-O4P-P-O1P
8	I	502	PCW	C2-C1-O3P-P
10	I	504	PLM	CD-CE-CF-CG
10	M	504	PLM	CD-CE-CF-CG
10	E	504	PLM	CD-CE-CF-CG
10	A	504	PLM	CD-CE-CF-CG
11	J	503	CLR	C16-C17-C20-C22
10	B	504	PLM	CD-CE-CF-CG

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Mol	Chain	Res	Type	Atoms
10	F	504	PLM	CD-CE-CF-CG
10	N	504	PLM	CD-CE-CF-CG
8	E	502	PCW	C25-C26-C27-C28
10	J	504	PLM	CD-CE-CF-CG
8	A	502	PCW	O3-C11-C12-C13
11	J	503	CLR	C13-C17-C20-C22
11	B	501	CLR	C23-C24-C25-C27
10	B	506	PLM	C8-C9-CA-CB
10	B	504	PLM	O1-C1-C2-C3
10	F	504	PLM	O1-C1-C2-C3
10	J	504	PLM	O1-C1-C2-C3
10	N	504	PLM	O1-C1-C2-C3
10	N	506	PLM	C8-C9-CA-CB
10	F	506	PLM	C8-C9-CA-CB
10	J	506	PLM	C8-C9-CA-CB
9	A	503	STE	C2-C3-C4-C5
9	M	503	STE	C2-C3-C4-C5
9	E	503	STE	C2-C3-C4-C5
9	J	501	STE	C2-C3-C4-C5
10	E	504	PLM	CB-CC-CD-CE
8	I	502	PCW	C19-C20-C21-C22
10	A	504	PLM	CB-CC-CD-CE
10	M	504	PLM	CB-CC-CD-CE
10	I	504	PLM	CB-CC-CD-CE
10	B	504	PLM	O2-C1-C2-C3
10	F	504	PLM	O2-C1-C2-C3
10	J	504	PLM	O2-C1-C2-C3
10	N	504	PLM	O2-C1-C2-C3
10	J	506	PLM	O2-C1-C2-C3
10	N	506	PLM	O2-C1-C2-C3
10	B	506	PLM	O2-C1-C2-C3
10	F	506	PLM	O2-C1-C2-C3
9	B	505	STE	O1-C1-C2-C3
9	B	505	STE	C1-C2-C3-C4
9	F	505	STE	O1-C1-C2-C3
9	J	505	STE	O1-C1-C2-C3
9	N	505	STE	O1-C1-C2-C3
8	A	502	PCW	C34-C35-C36-C37
9	J	505	STE	C1-C2-C3-C4
9	F	505	STE	C1-C2-C3-C4
9	N	505	STE	C1-C2-C3-C4
10	B	506	PLM	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	B	501	CLR	C16-C17-C20-C22
10	F	506	PLM	O1-C1-C2-C3
10	J	506	PLM	O1-C1-C2-C3
10	N	506	PLM	O1-C1-C2-C3
11	F	501	CLR	C20-C22-C23-C24
11	N	501	CLR	C20-C22-C23-C24
11	J	503	CLR	C13-C17-C20-C21
8	E	502	PCW	C2-C1-O3P-P
11	I	503	CLR	C23-C24-C25-C26
9	B	505	STE	O2-C1-C2-C3
9	F	505	STE	O2-C1-C2-C3
9	J	505	STE	O2-C1-C2-C3
9	N	505	STE	O2-C1-C2-C3
11	B	501	CLR	C13-C17-C20-C21
8	M	502	PCW	C19-C20-C21-C22
8	E	502	PCW	C19-C20-C21-C22
8	M	502	PCW	C17-C18-C19-C20
8	E	502	PCW	C37-C38-C39-C40
9	F	505	STE	C11-C12-C13-C14
9	J	505	STE	C11-C12-C13-C14
9	N	505	STE	C11-C12-C13-C14
9	B	505	STE	C11-C12-C13-C14
8	I	502	PCW	C43-C44-C45-C46
8	E	502	PCW	C45-C46-C47-C48
8	A	502	PCW	C39-C40-C41-C42
8	I	502	PCW	O3P-C1-C2-C3
10	F	504	PLM	CB-CC-CD-CE
10	B	504	PLM	CB-CC-CD-CE
11	B	503	CLR	C20-C22-C23-C24
10	J	504	PLM	CB-CC-CD-CE
11	N	503	CLR	C23-C24-C25-C27
10	N	504	PLM	CB-CC-CD-CE
10	B	506	PLM	C2-C3-C4-C5
11	F	501	CLR	C17-C20-C22-C23
8	A	502	PCW	C24-C25-C26-C27
10	F	506	PLM	C2-C3-C4-C5
10	N	506	PLM	C2-C3-C4-C5
10	J	506	PLM	C2-C3-C4-C5
8	A	502	PCW	C2-C1-O3P-P
8	M	502	PCW	C39-C40-C41-C42
8	I	502	PCW	O2-C31-C32-C33
11	F	501	CLR	C13-C17-C20-C21

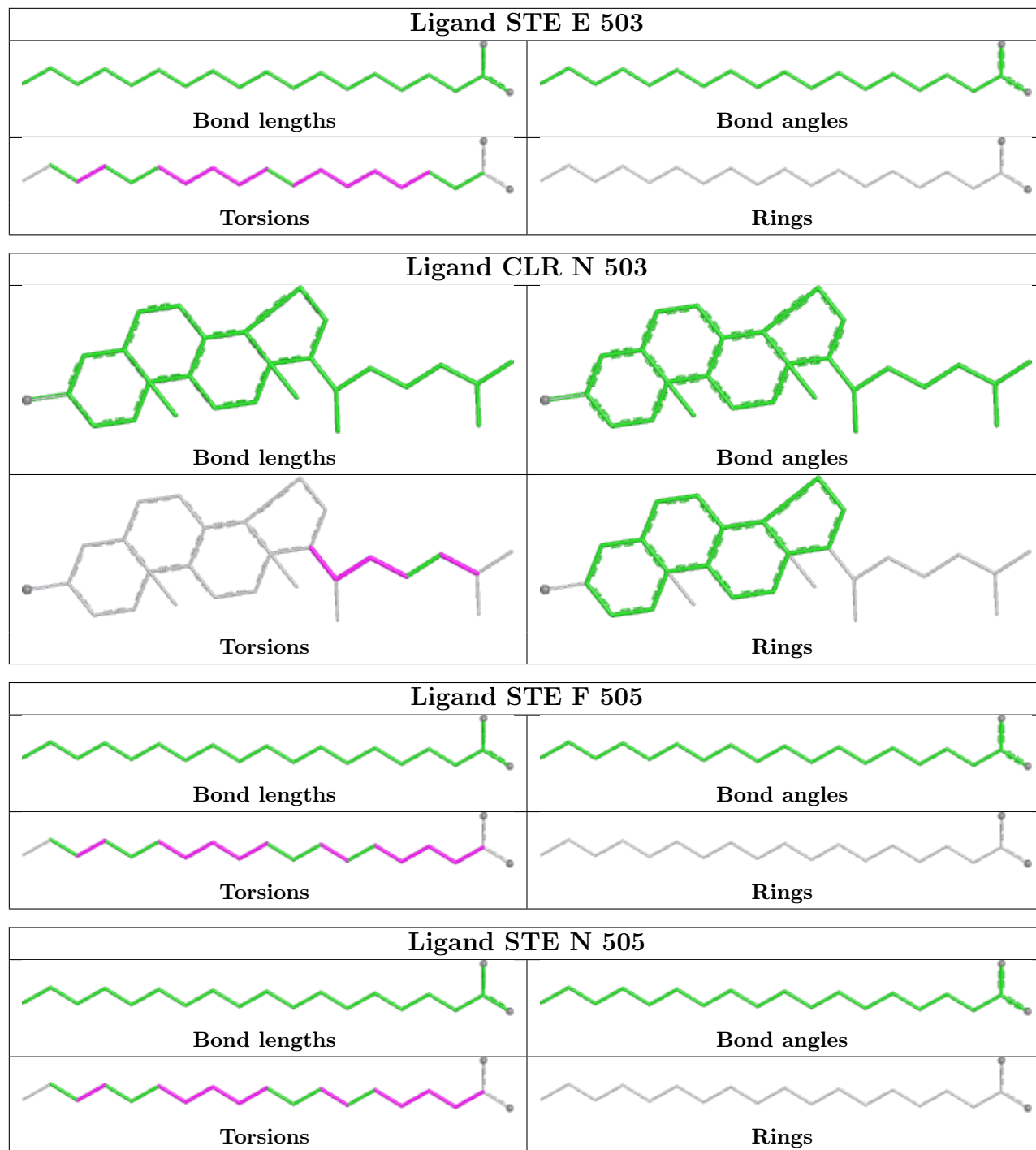
There are no ring outliers.

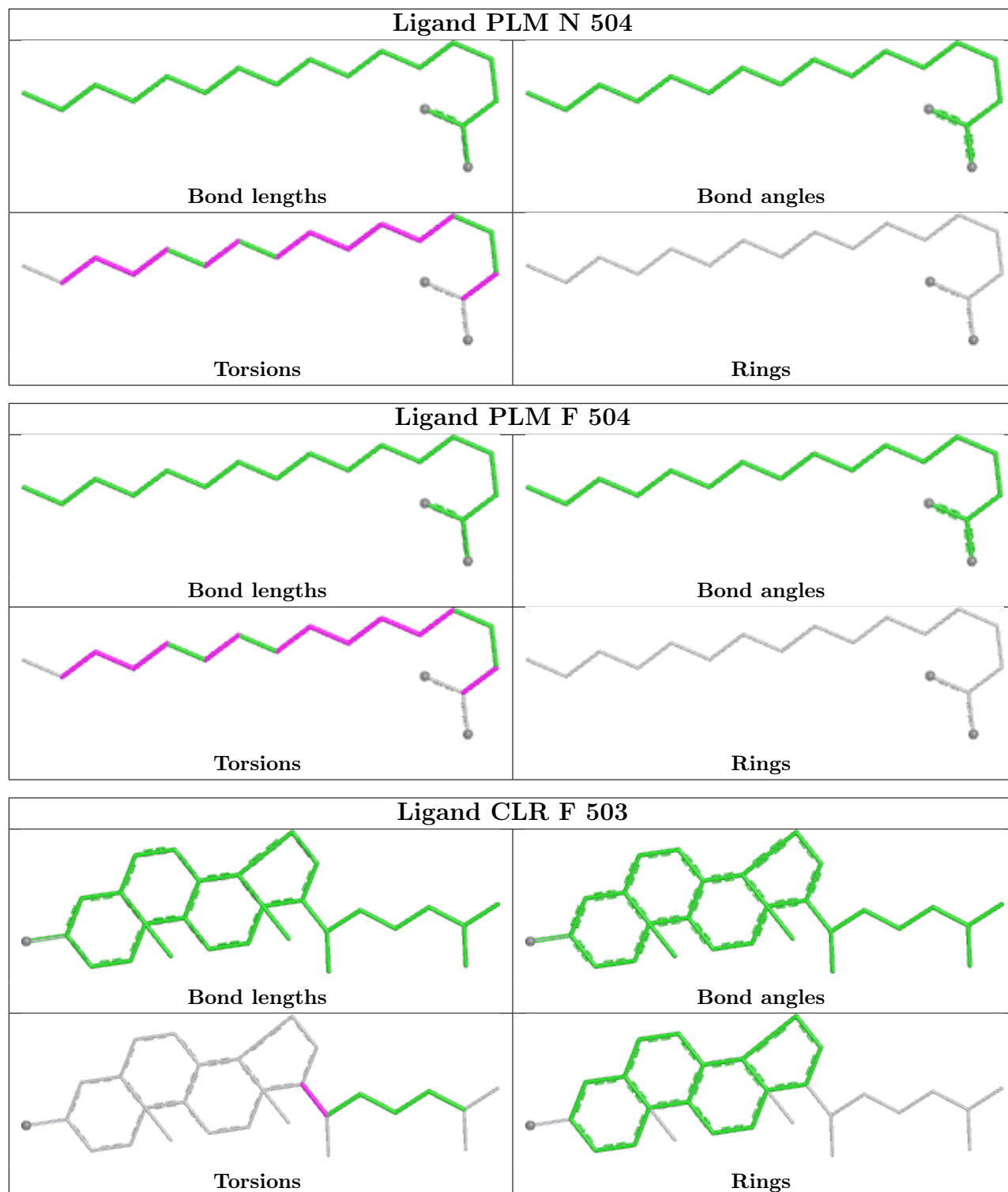
29 monomers are involved in 63 short contacts:

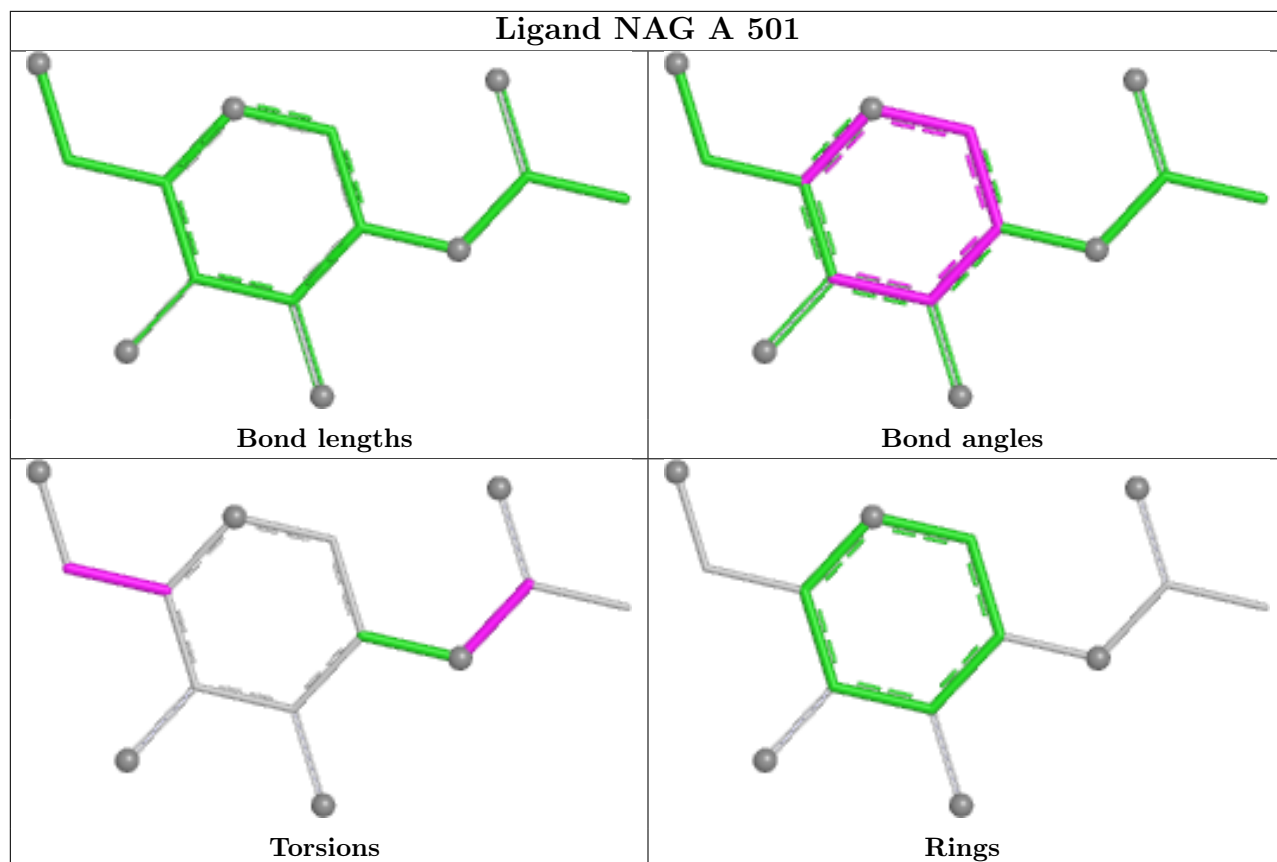
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	505	STE	1	0
9	N	505	STE	1	0
10	N	504	PLM	1	0
11	F	503	CLR	1	0
8	E	502	PCW	5	0
10	B	504	PLM	1	0
8	A	502	PCW	2	0
10	E	504	PLM	1	0
8	M	502	PCW	5	0
10	A	504	PLM	1	0
11	I	503	CLR	2	0
8	I	502	PCW	3	0
9	A	503	STE	1	0
11	F	501	CLR	9	0
10	B	506	PLM	1	0
11	N	502	CLR	4	0
10	J	506	PLM	2	0
11	N	501	CLR	4	0
9	J	501	STE	1	0
11	B	503	CLR	5	0
11	J	503	CLR	4	0
9	J	505	STE	2	0
9	B	505	STE	2	0
10	N	506	PLM	1	0
11	B	501	CLR	2	0
11	B	502	CLR	3	0
11	J	502	CLR	6	0
10	F	506	PLM	2	0
11	F	502	CLR	1	0

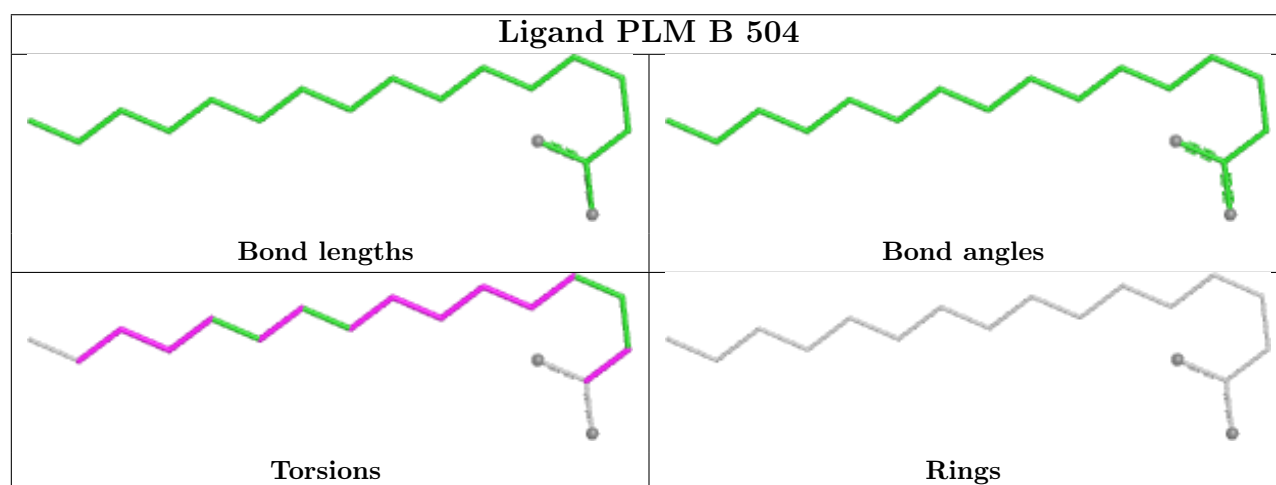
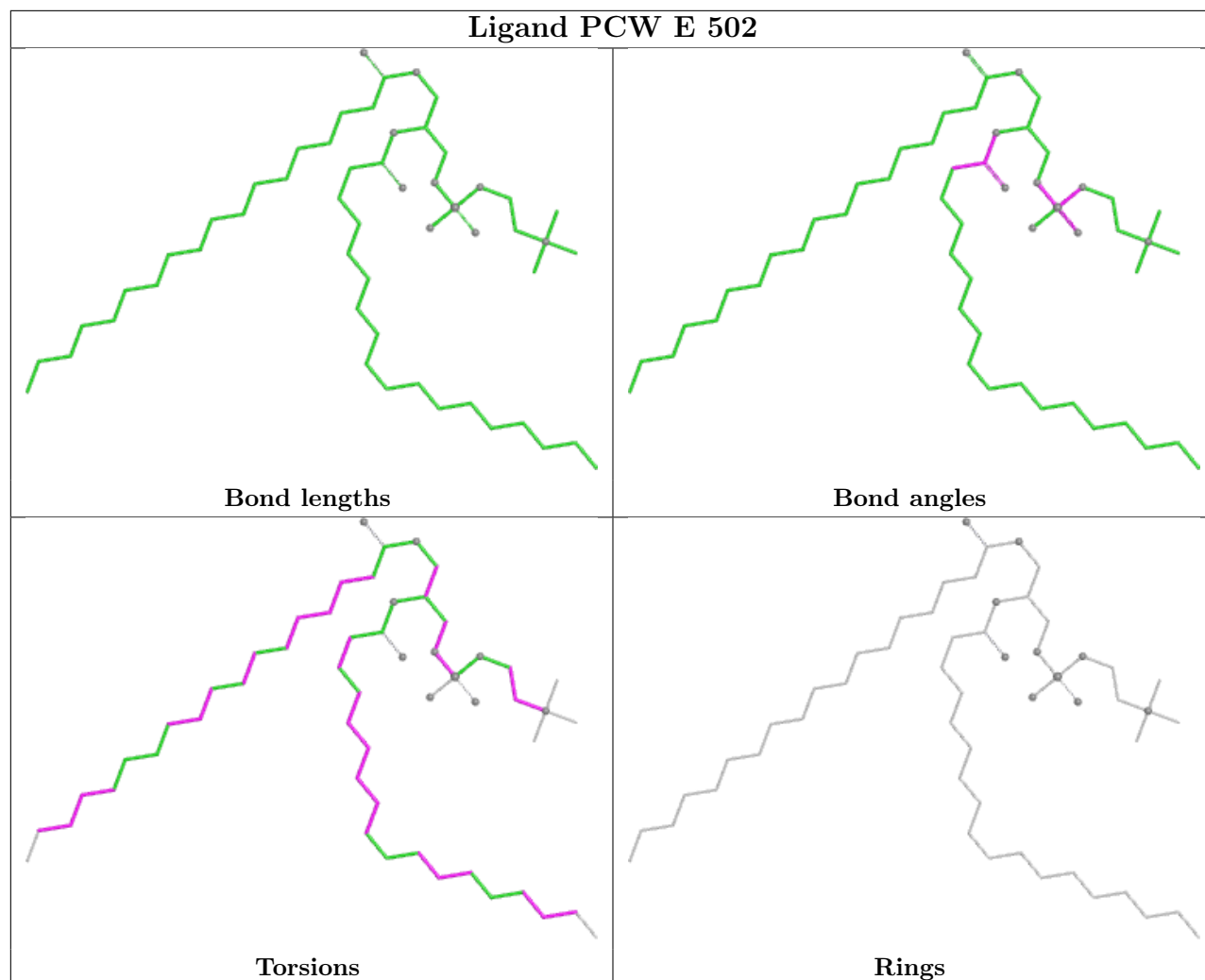
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

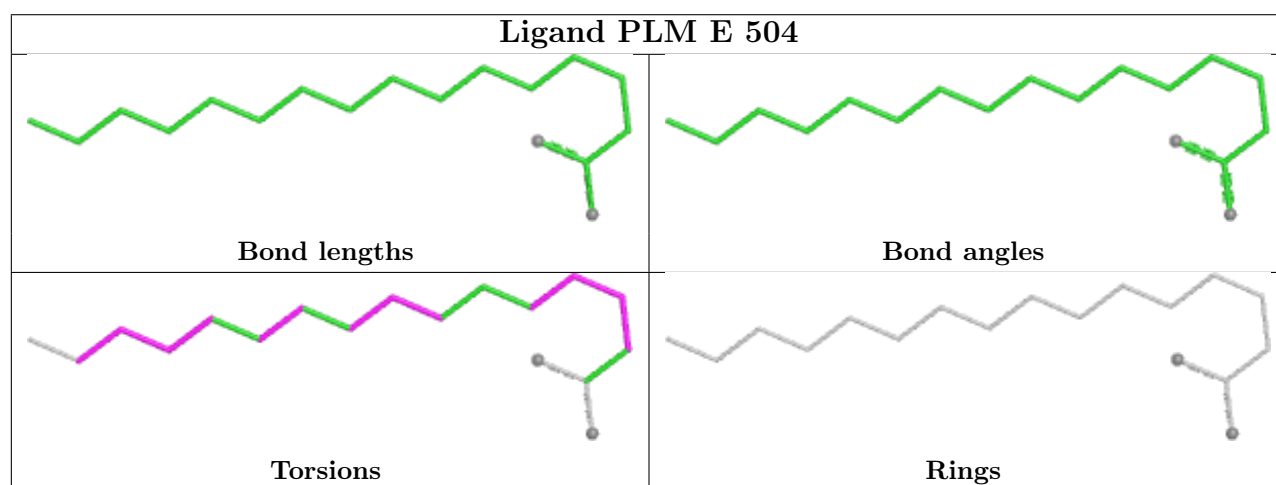
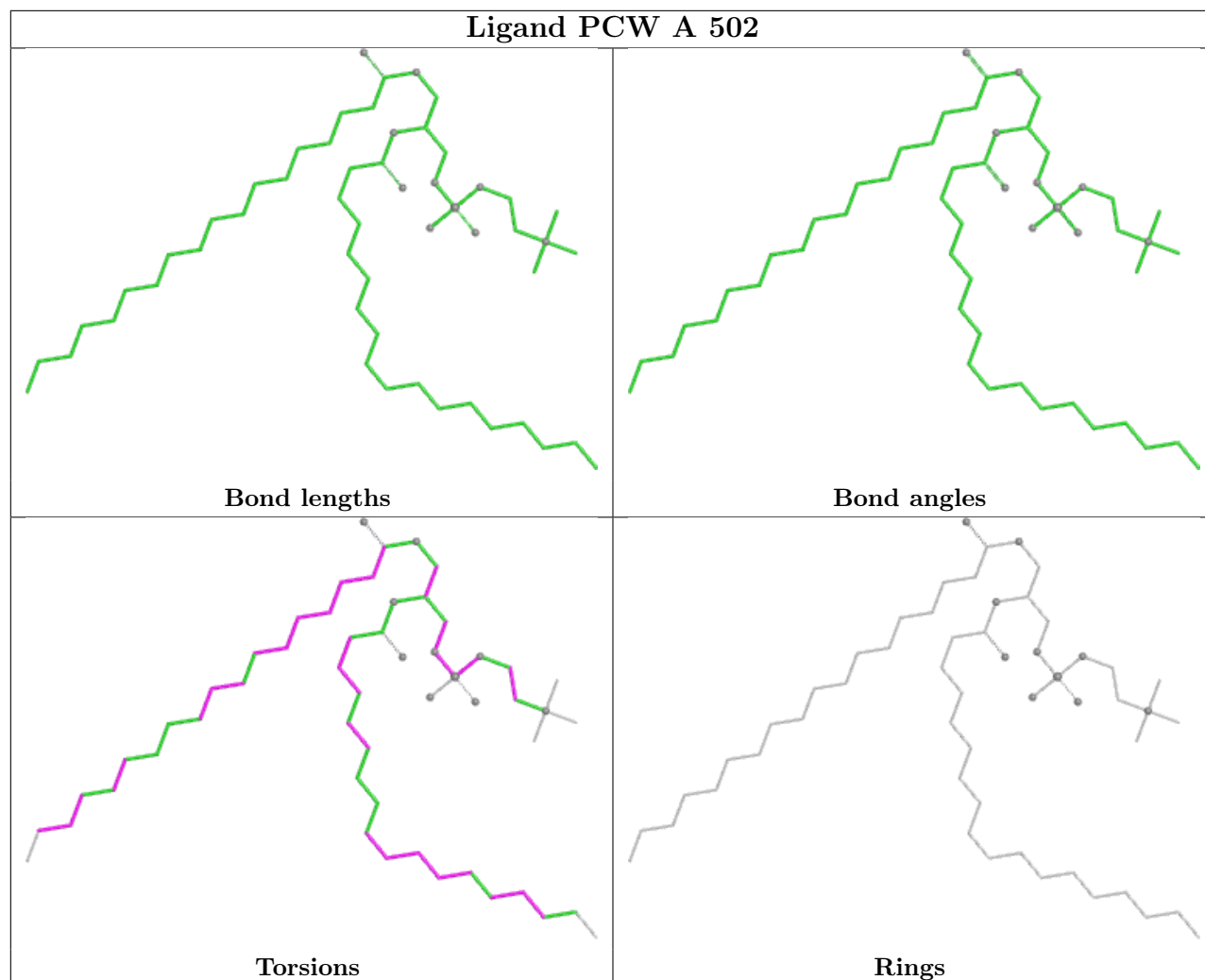
equivalents in the CSD to analyse the geometry.

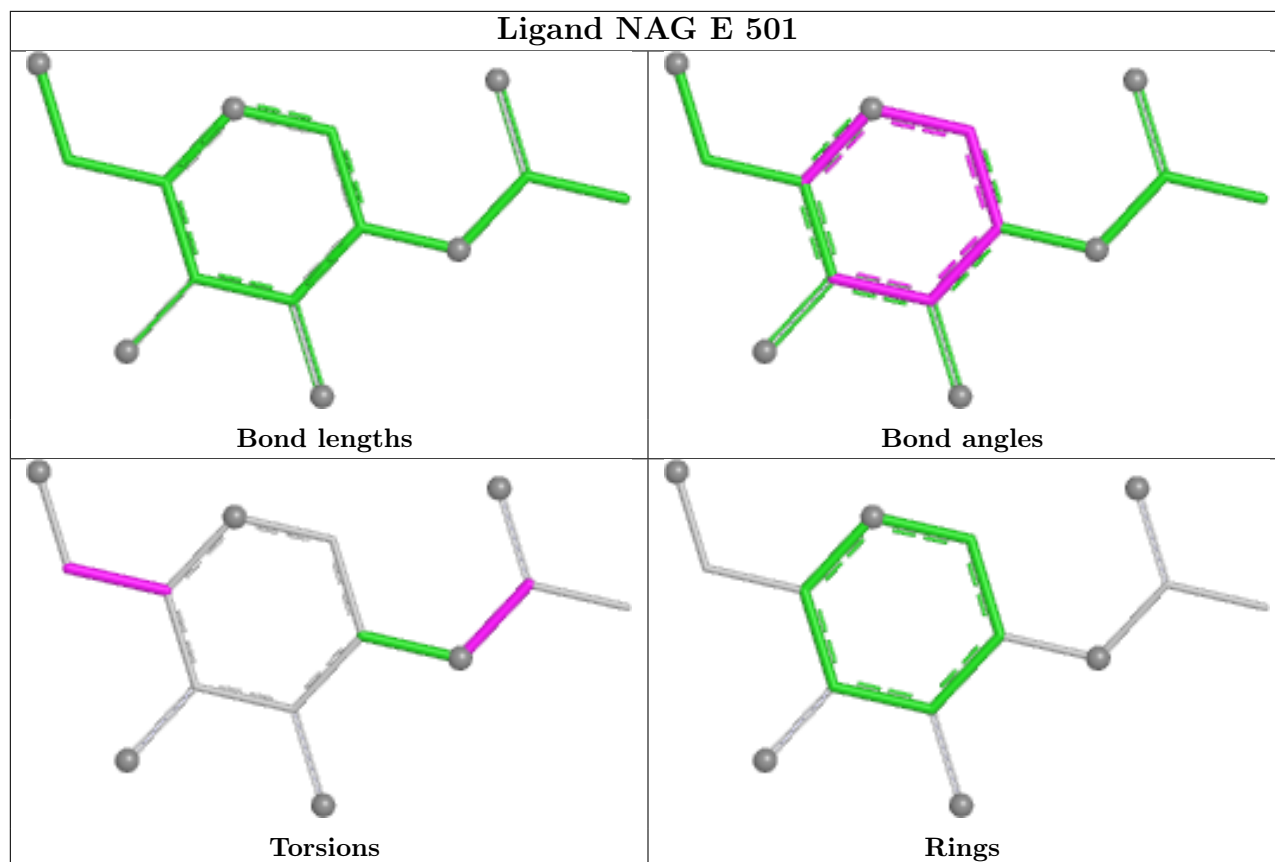


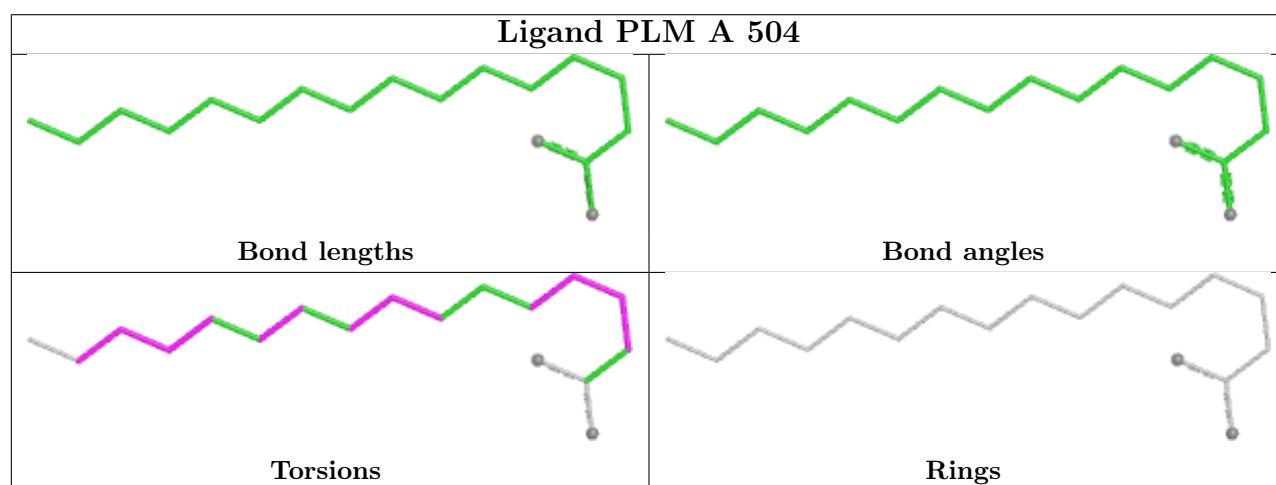
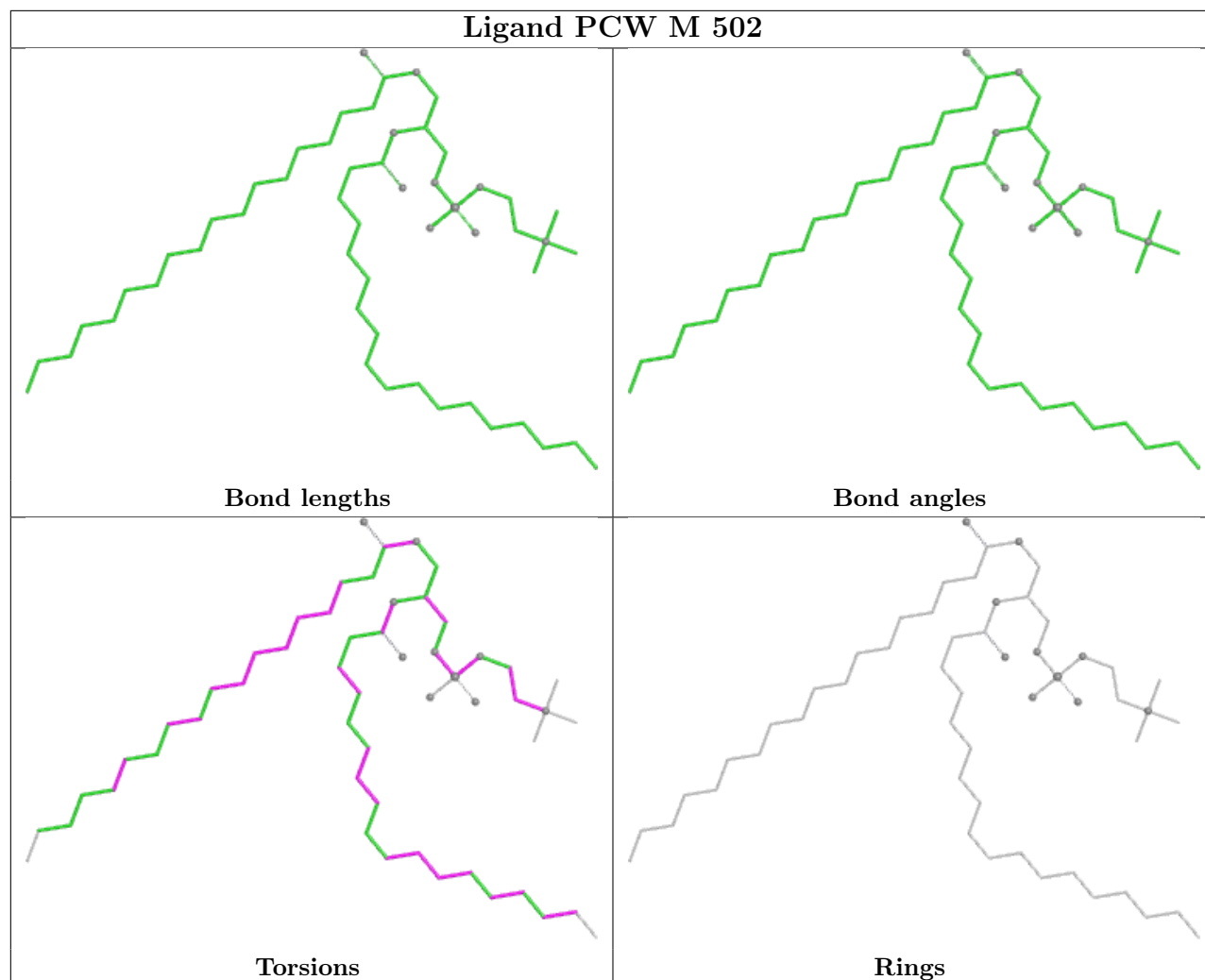


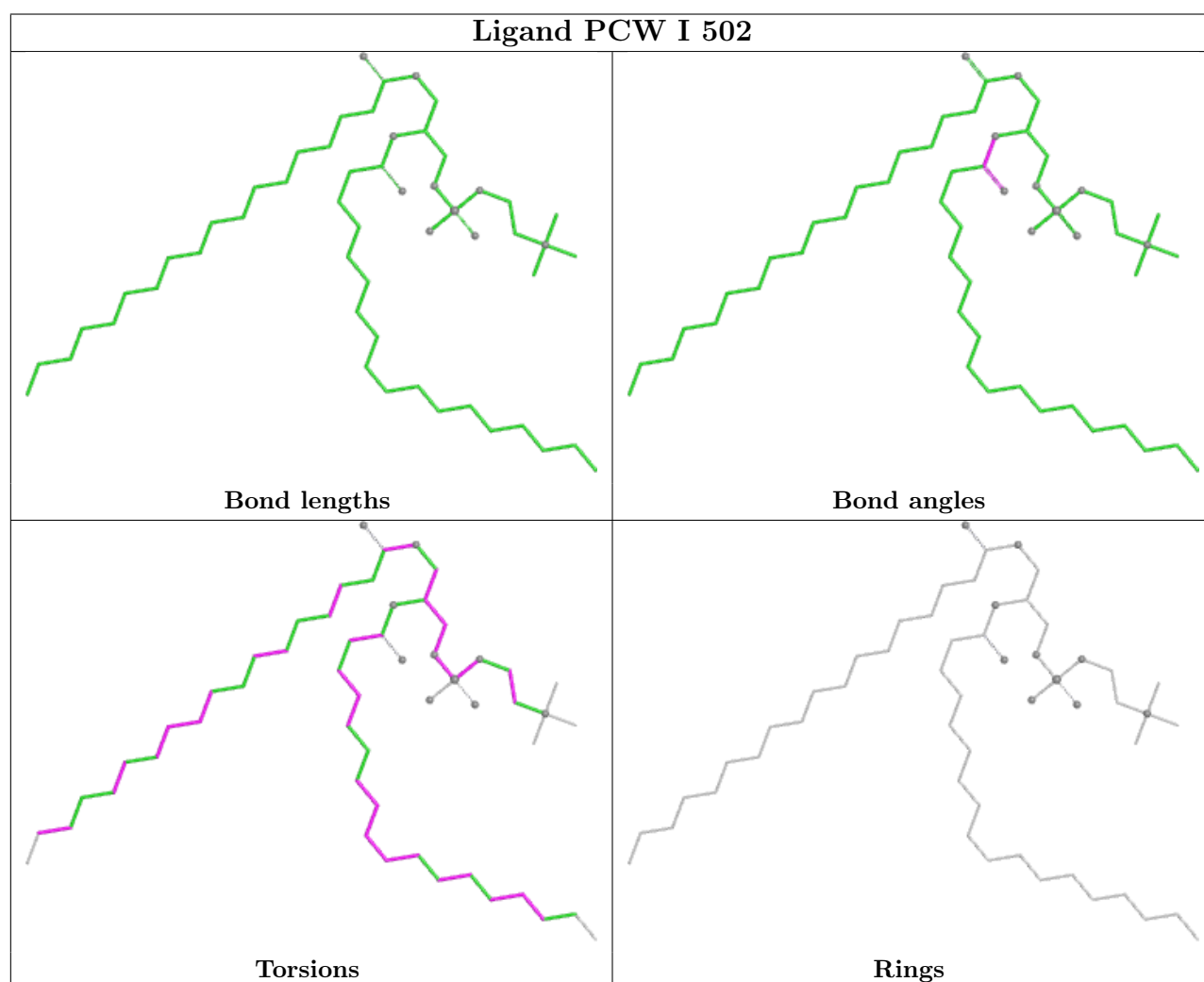
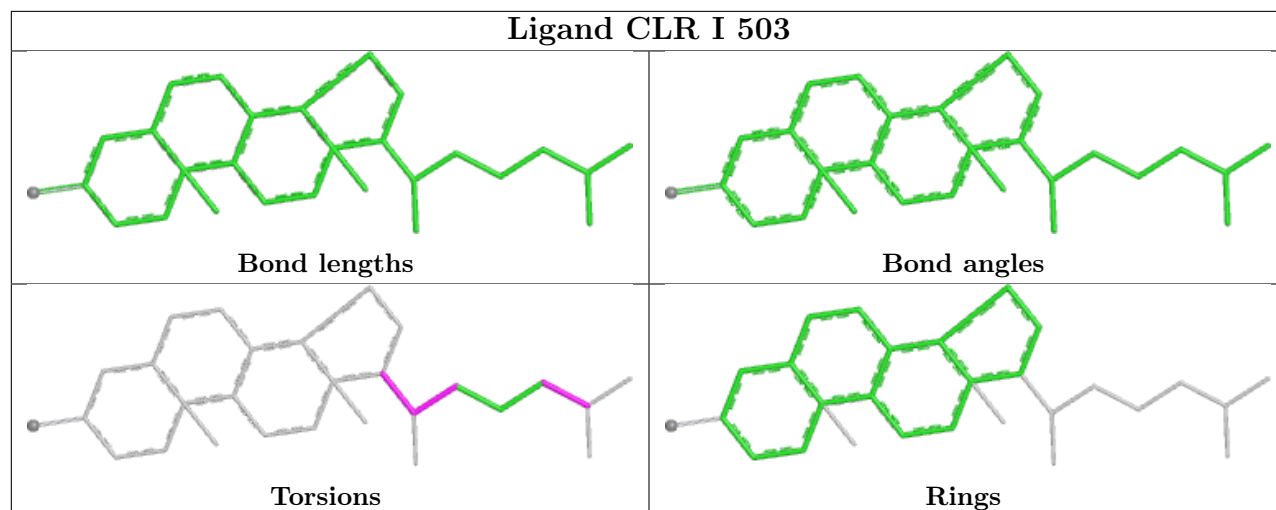


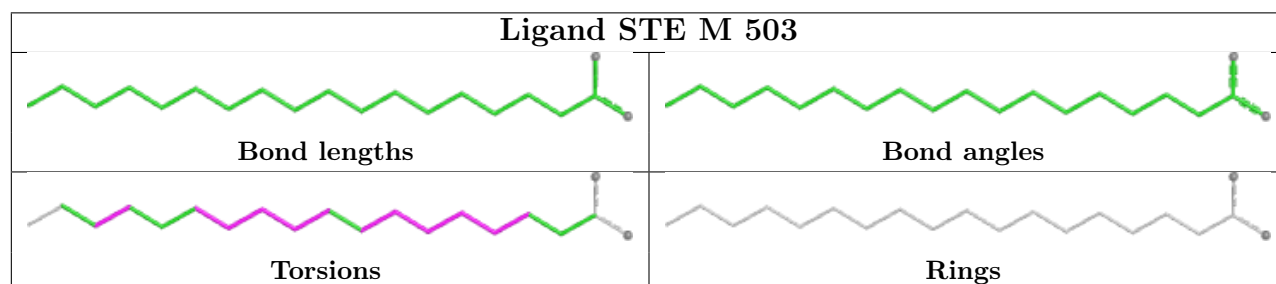
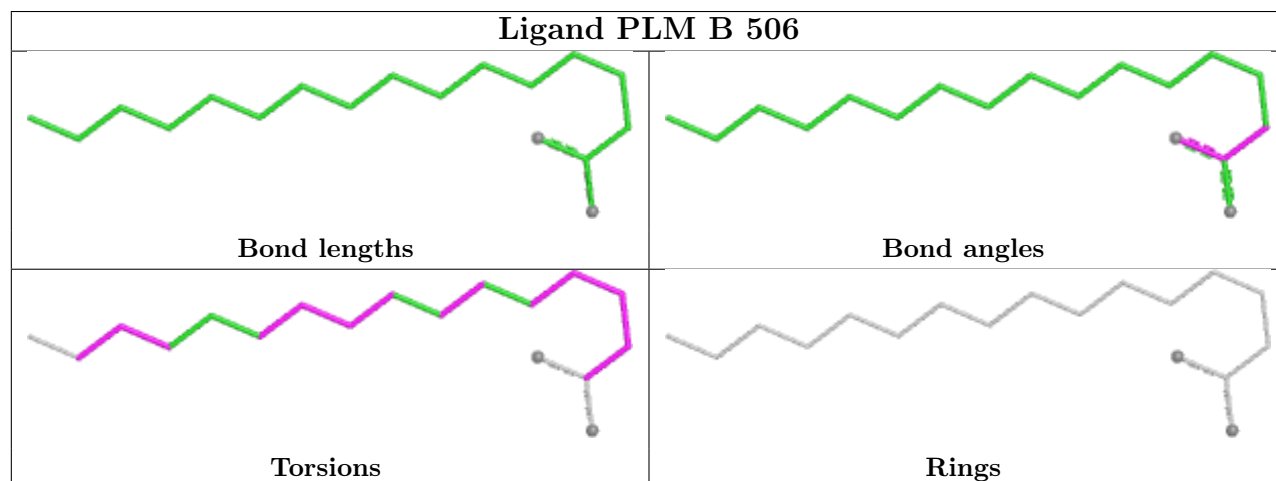
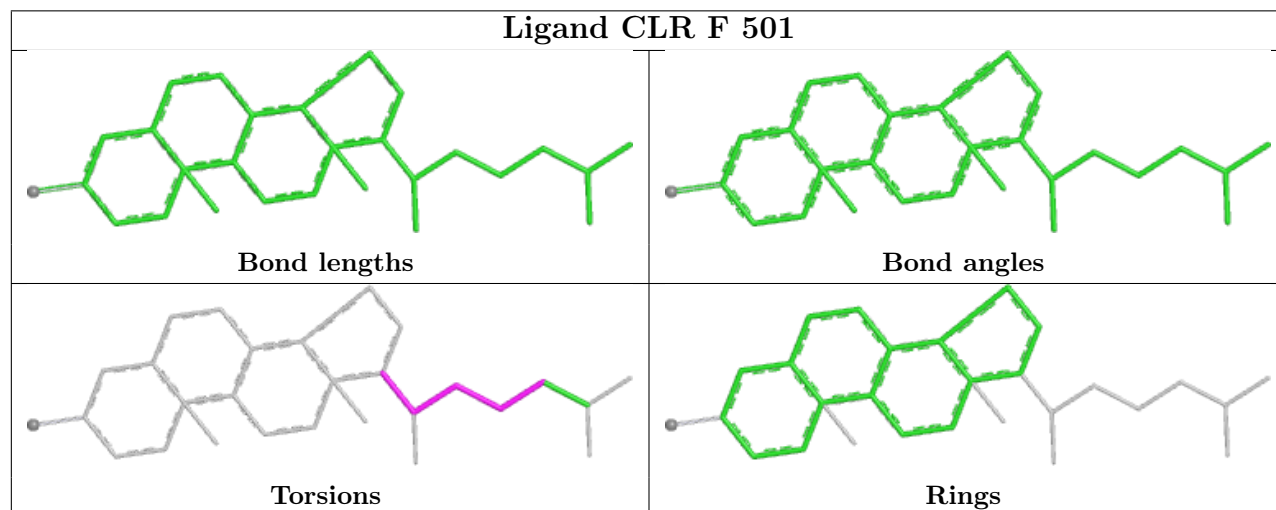
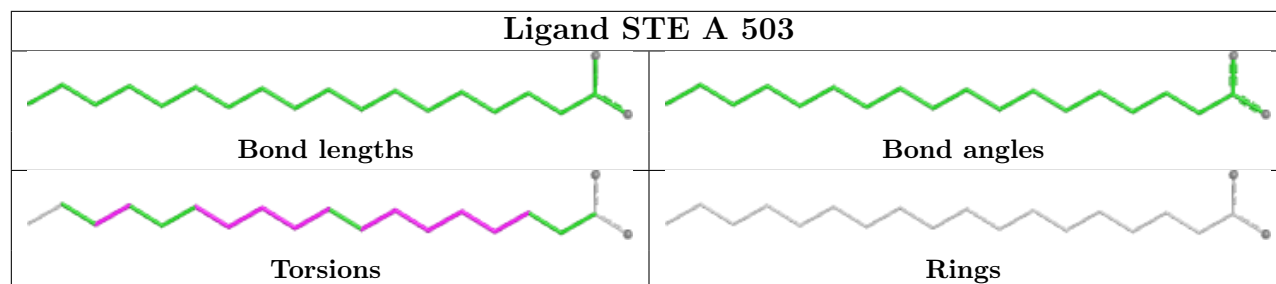


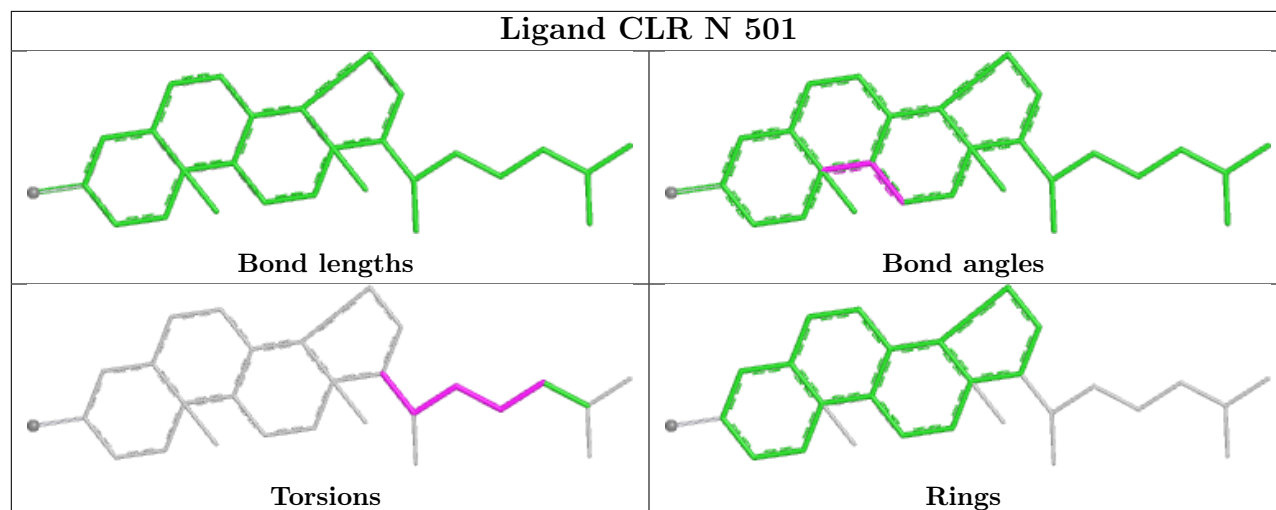
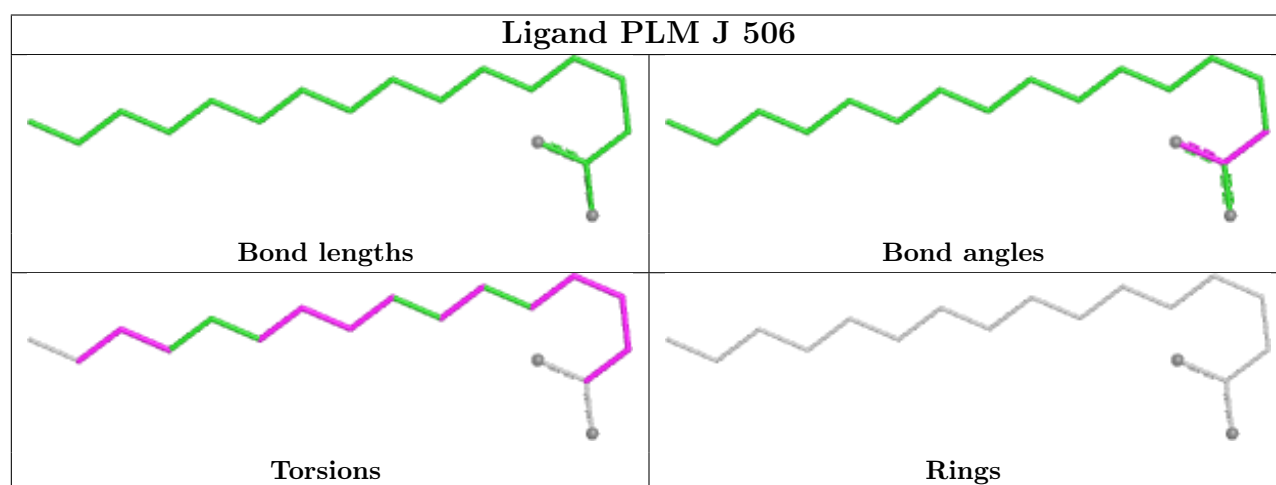
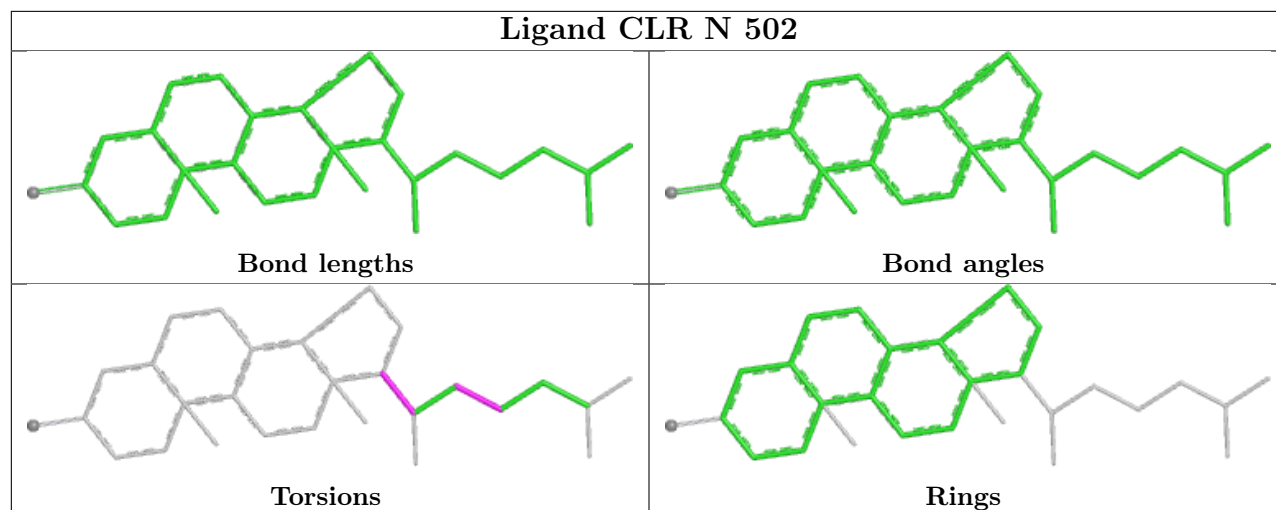


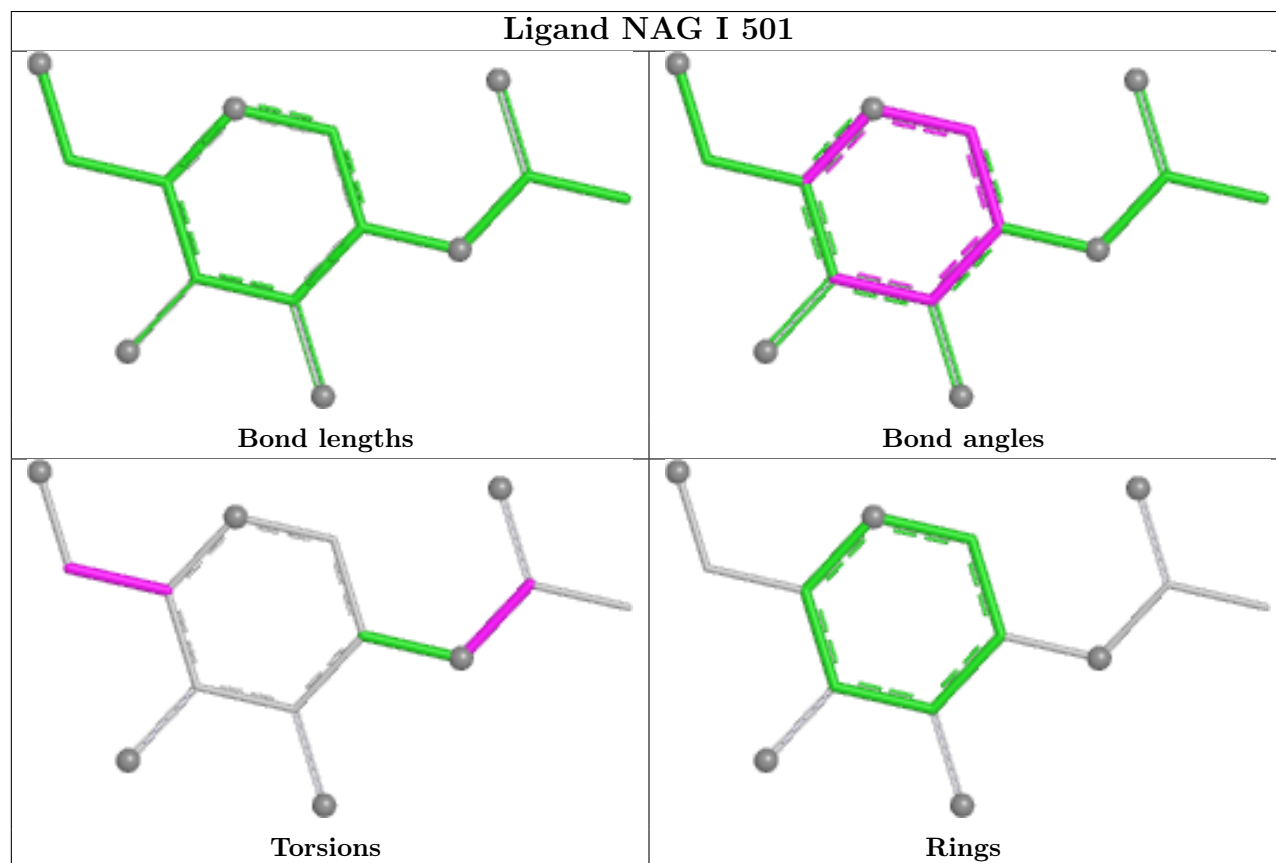
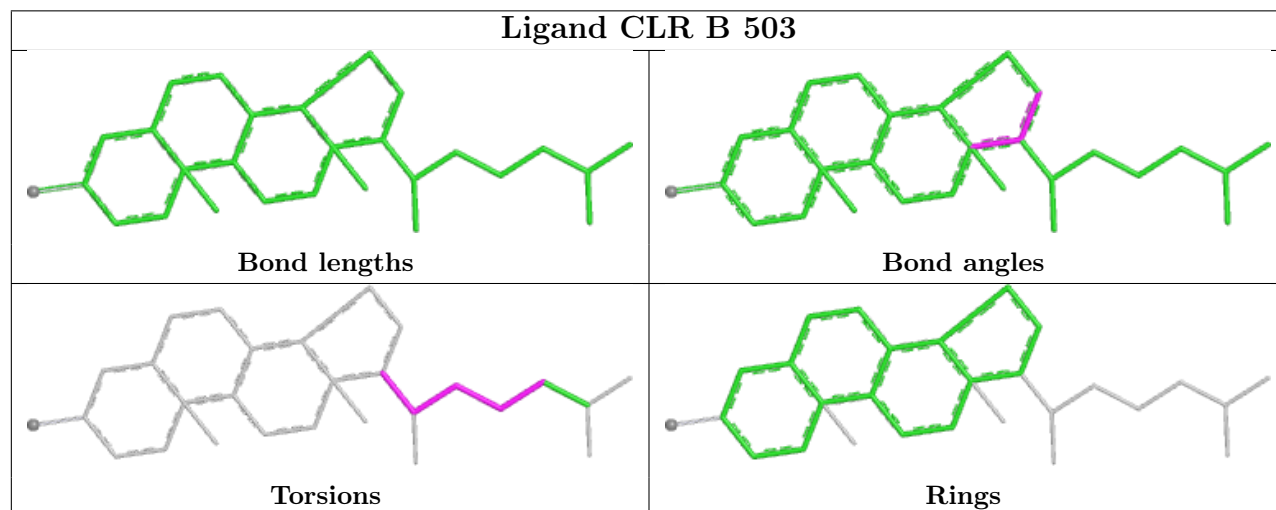
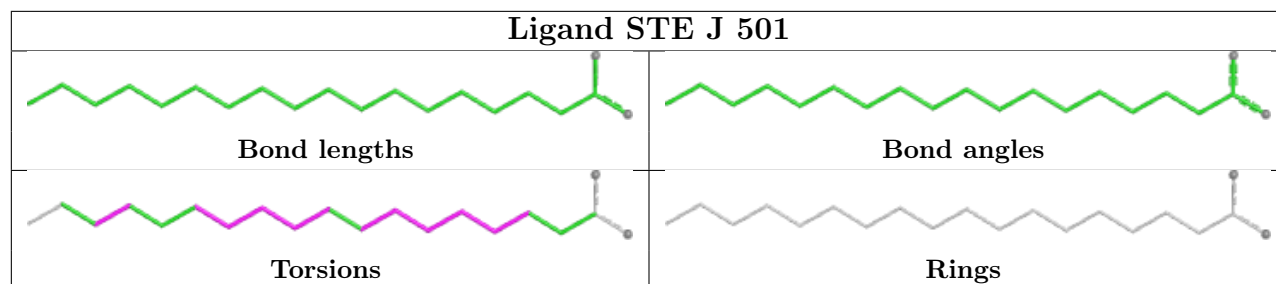


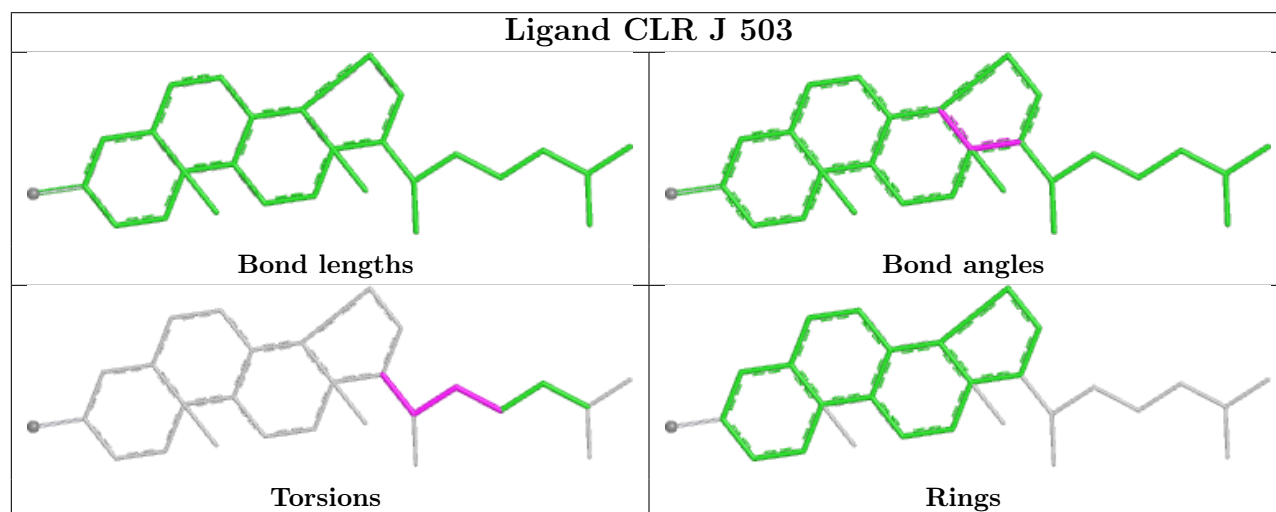
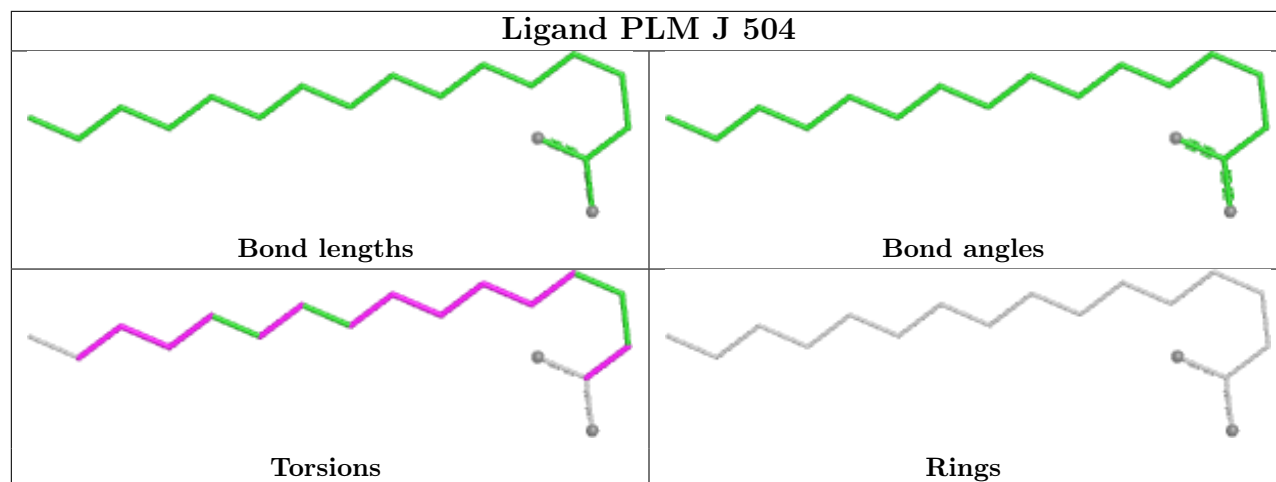


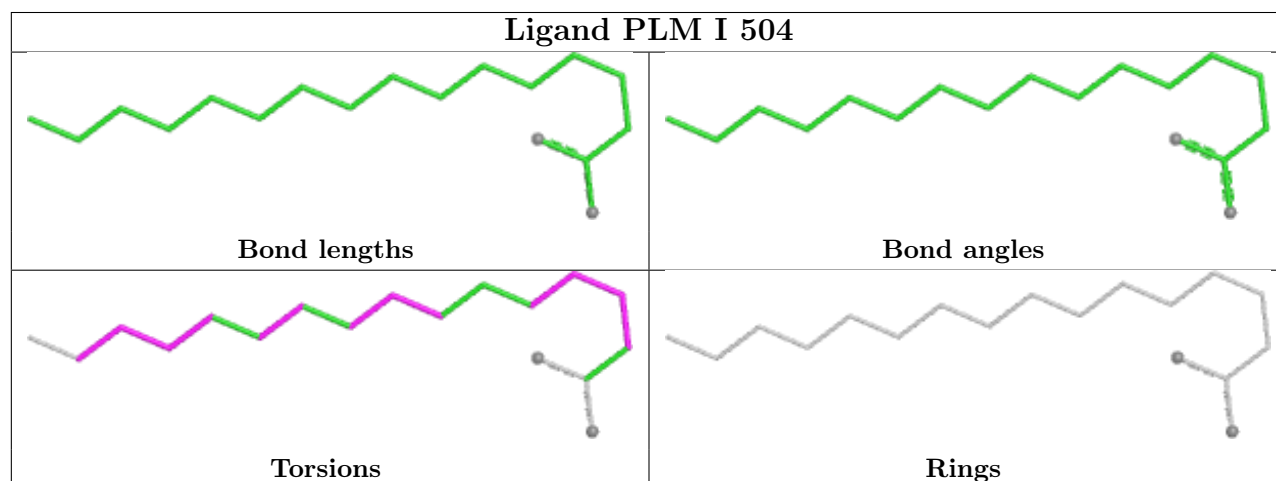
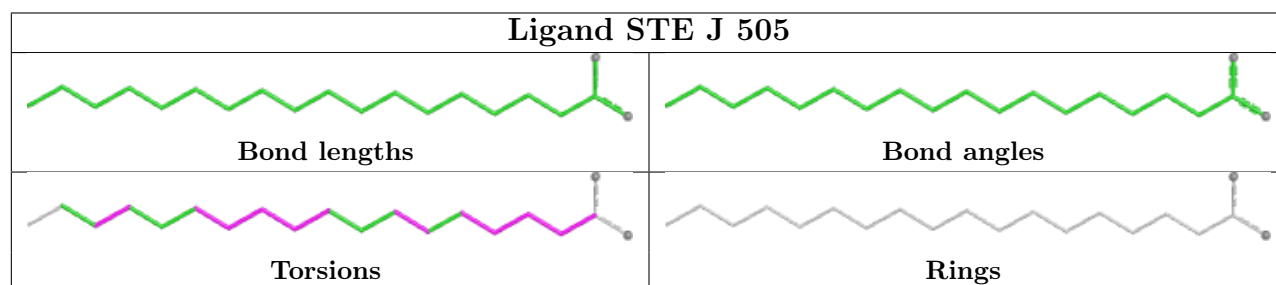
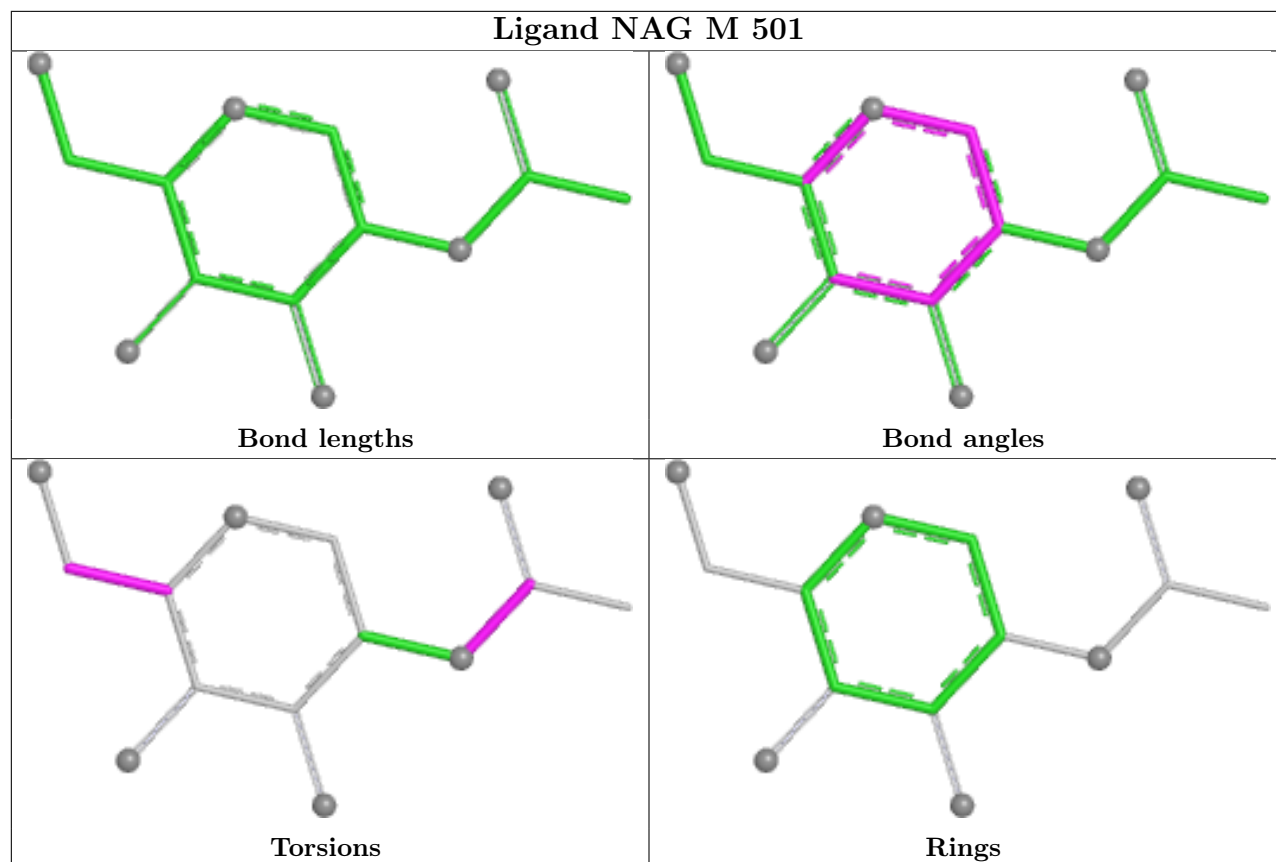


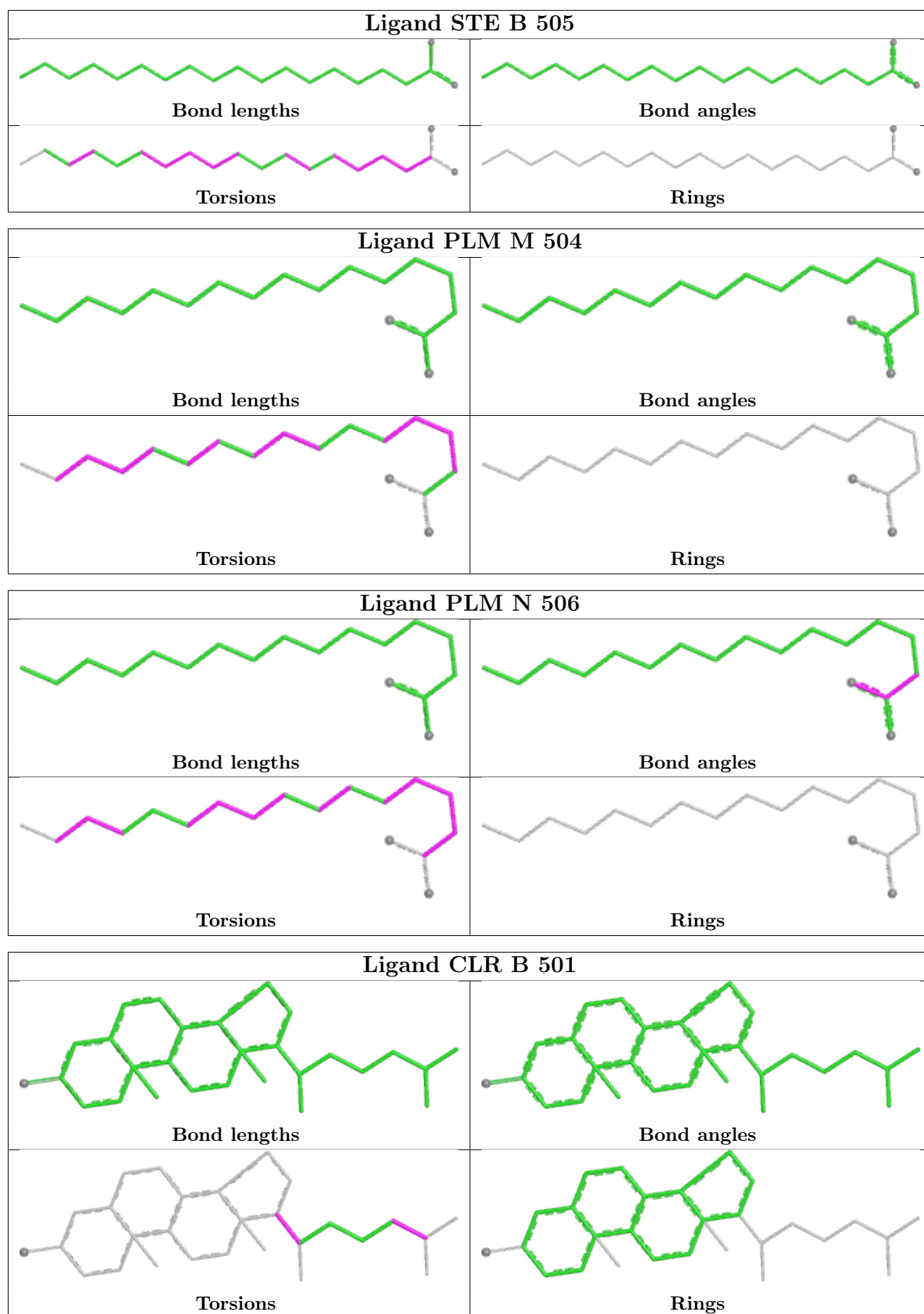


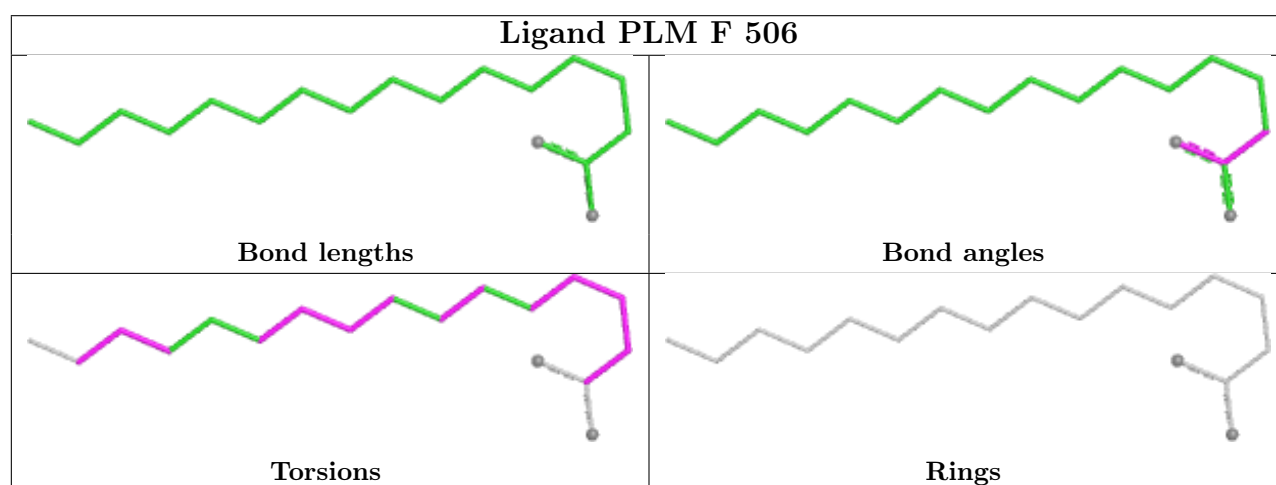
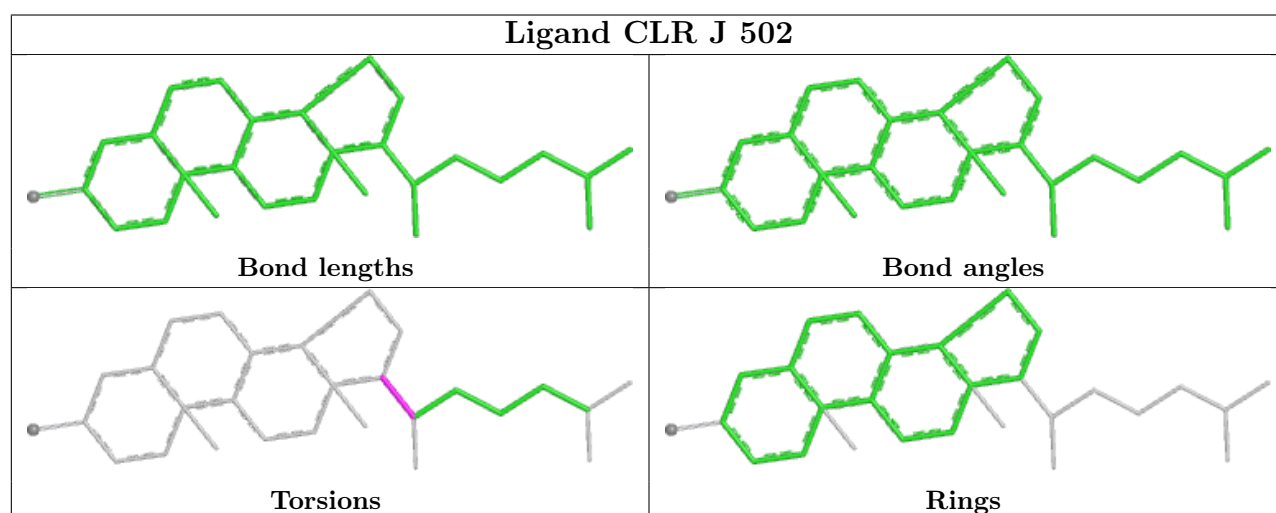
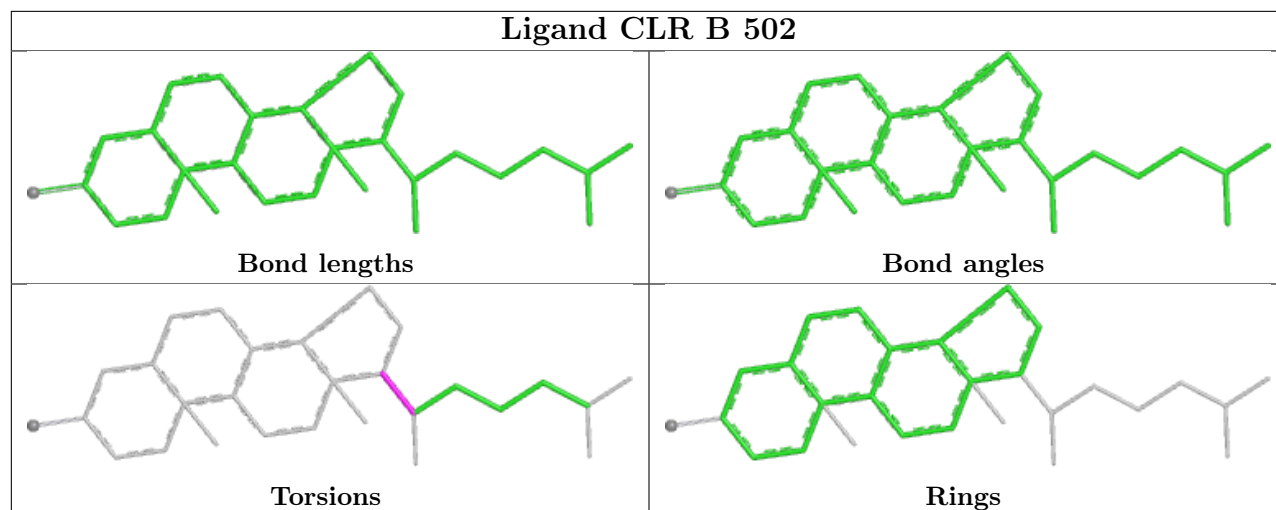


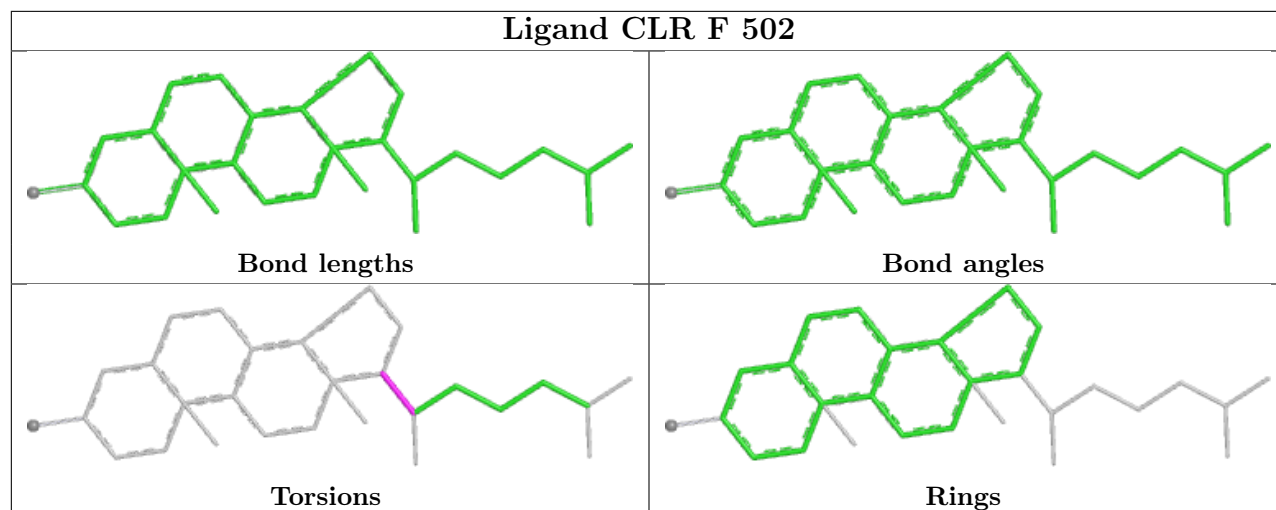












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

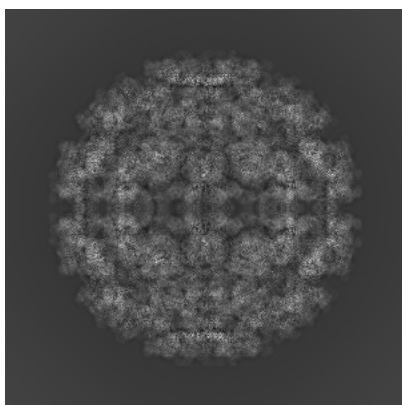
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31533. These allow visual inspection of the internal detail of the map and identification of artifacts.

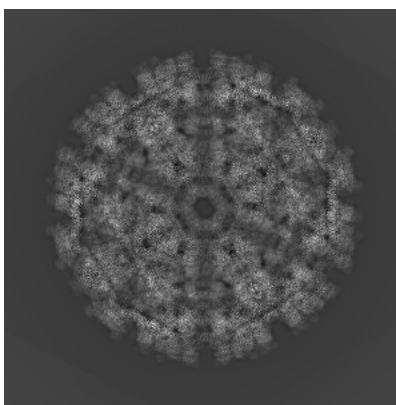
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

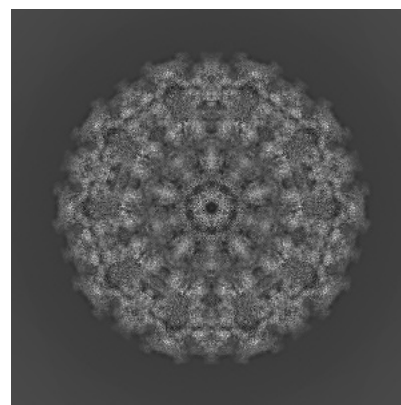
#### 6.1.1 Primary map



X



Y

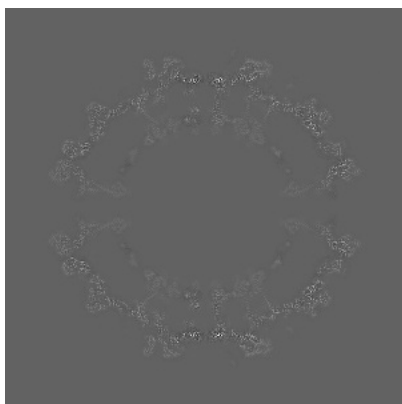


Z

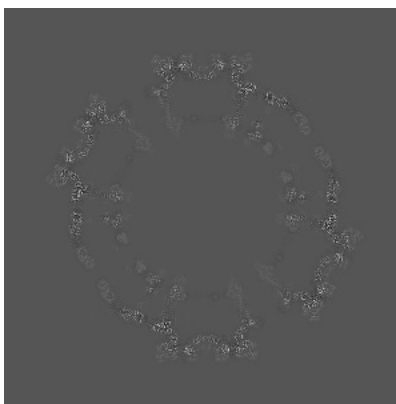
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 256



Y Index: 256

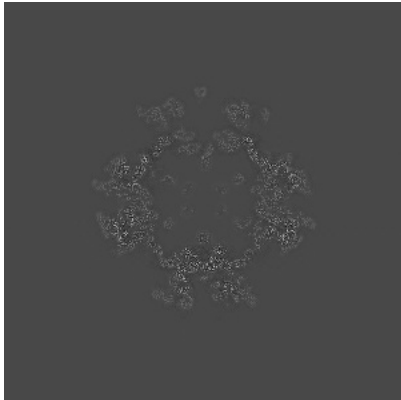


Z Index: 256

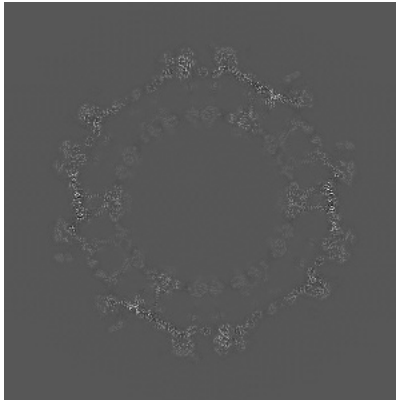
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

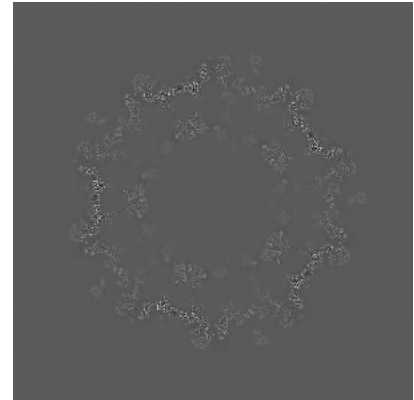
### 6.3.1 Primary map



X Index: 113



Y Index: 242

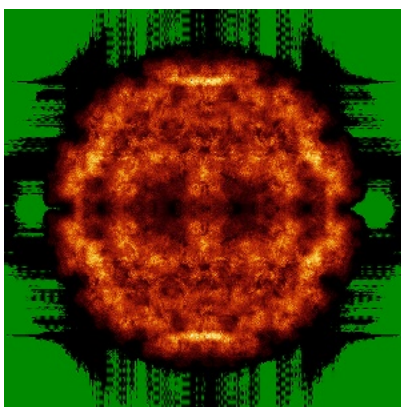


Z Index: 192

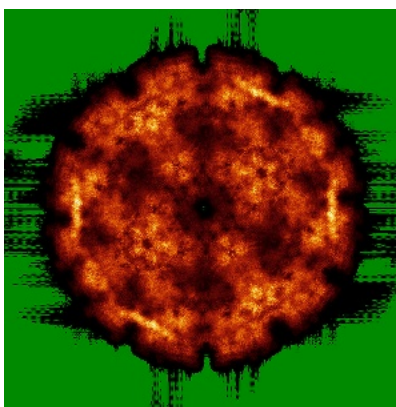
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

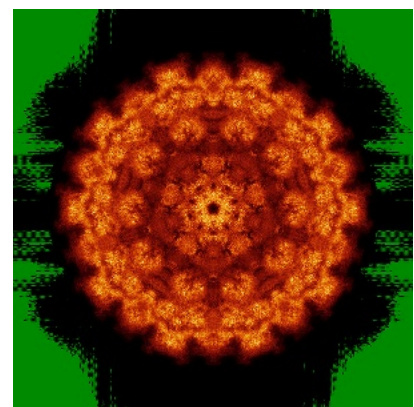
### 6.4.1 Primary map



X



Y

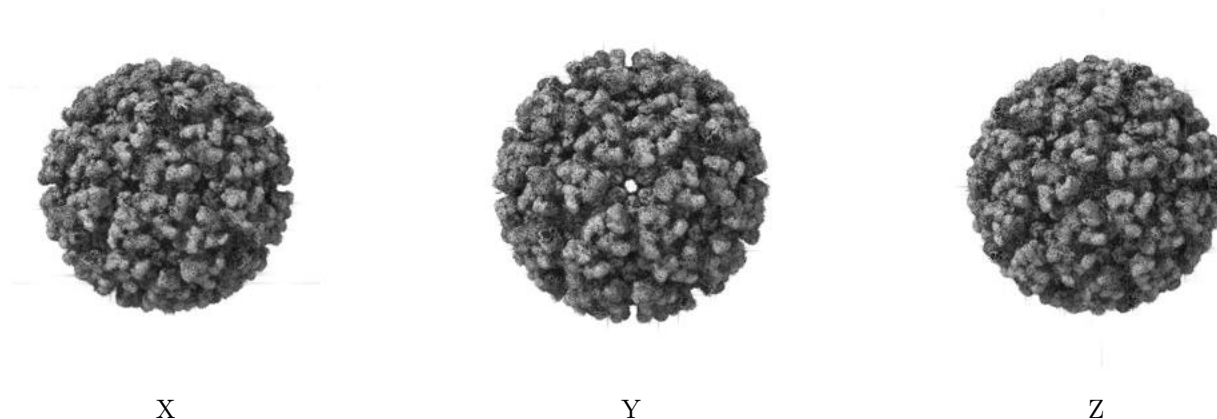


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

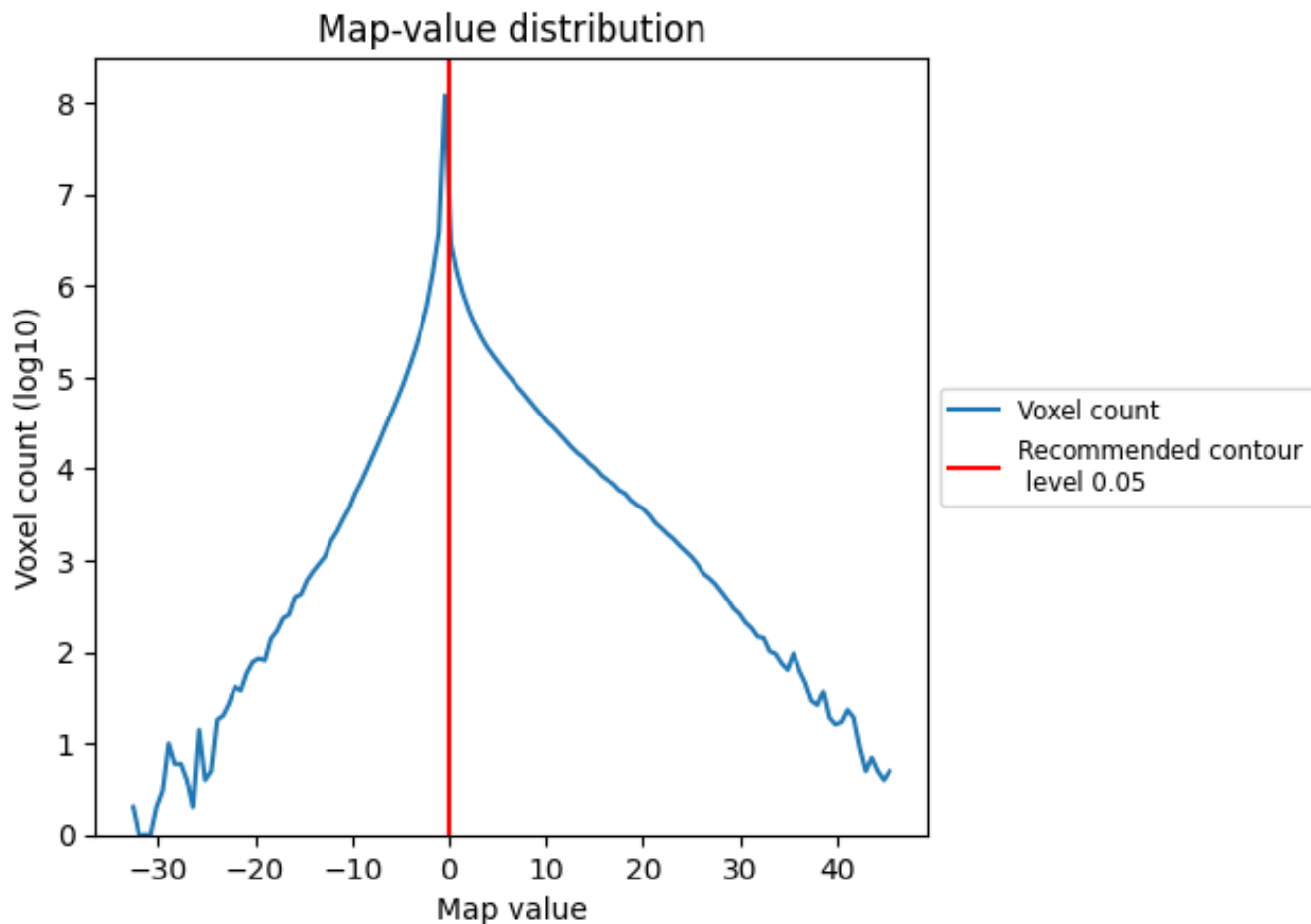
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

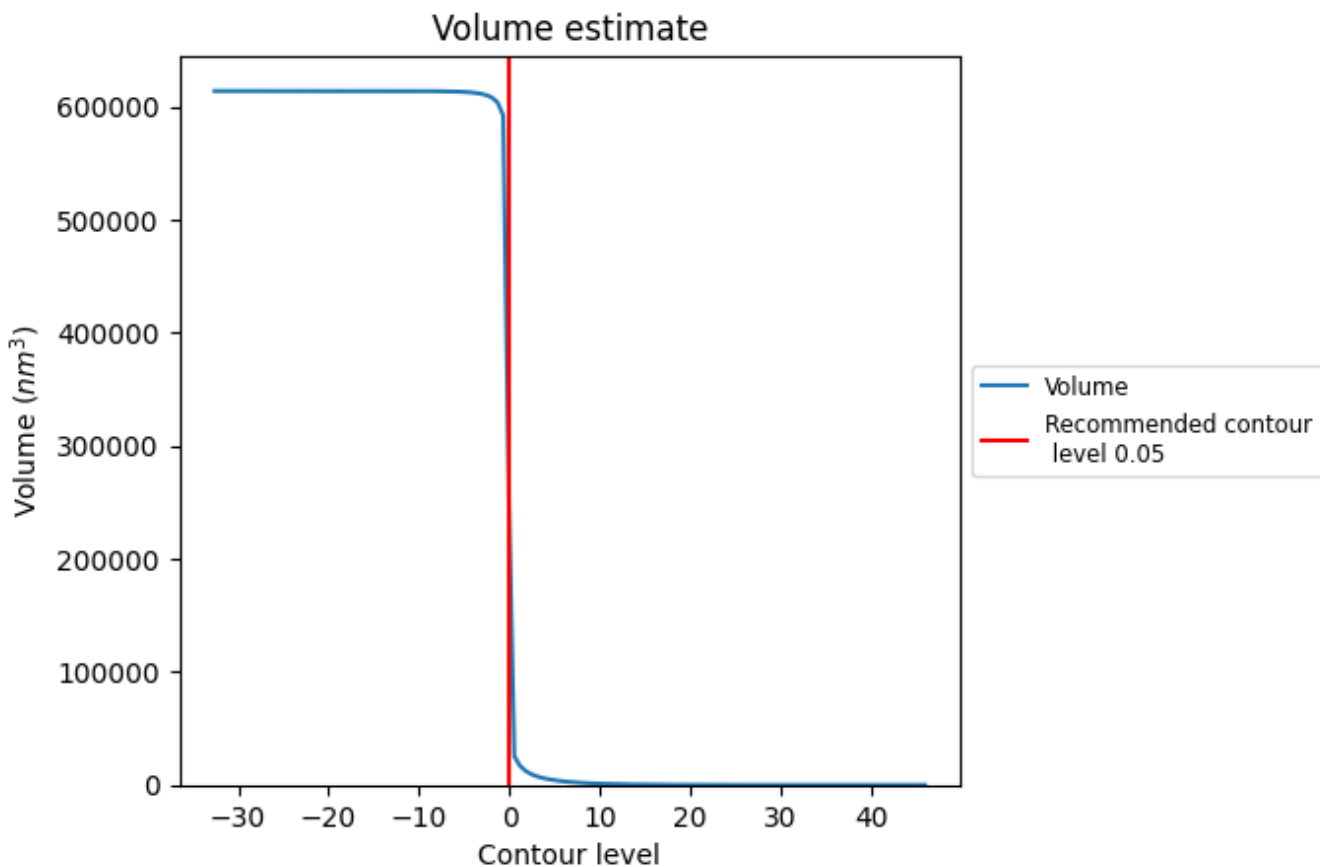
This section contains the results of statistical analysis of the map.

### 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.

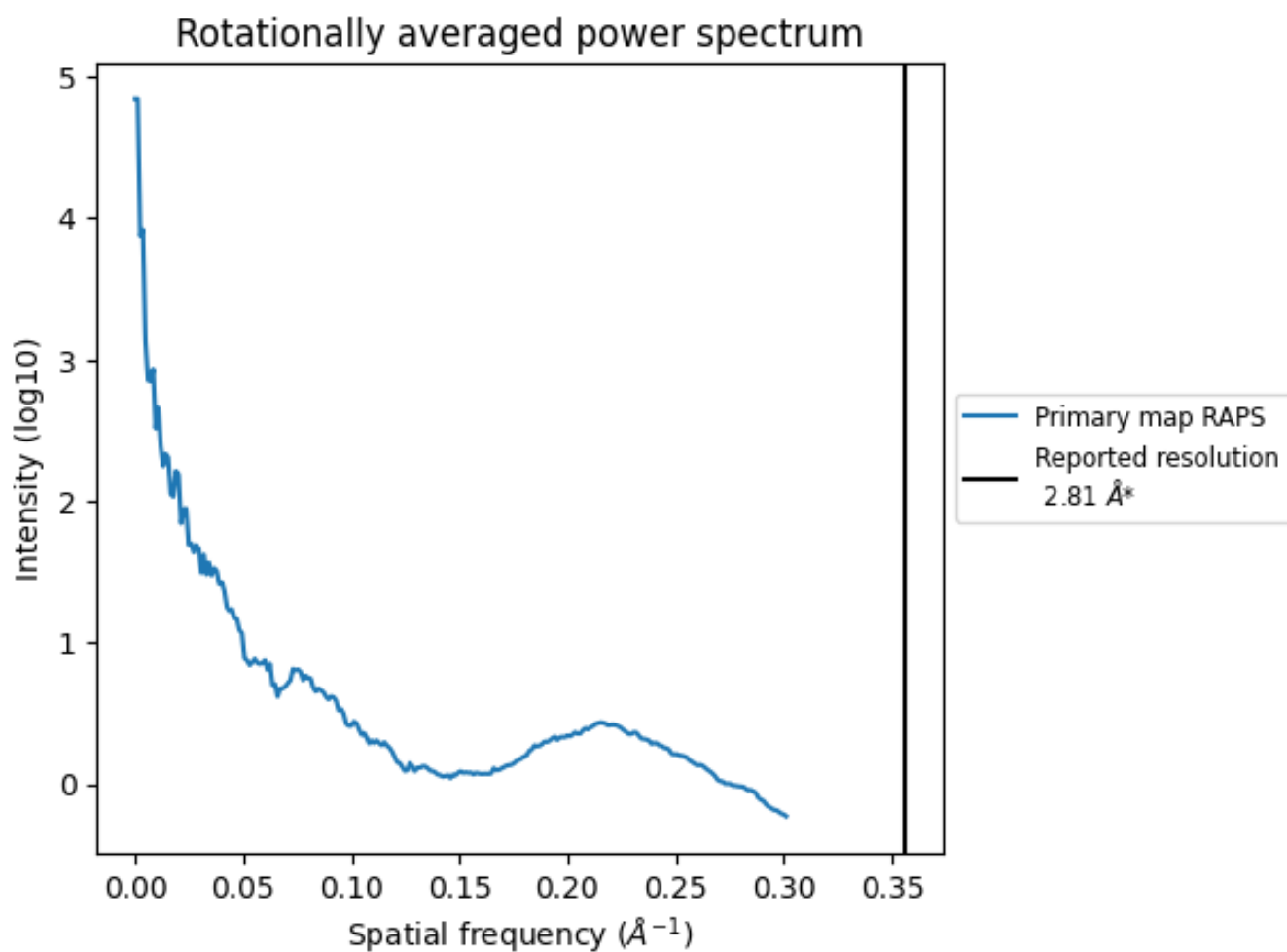
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220944  $\text{nm}^3$ ; this corresponds to an approximate mass of 199585 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 [\(i\)](#)

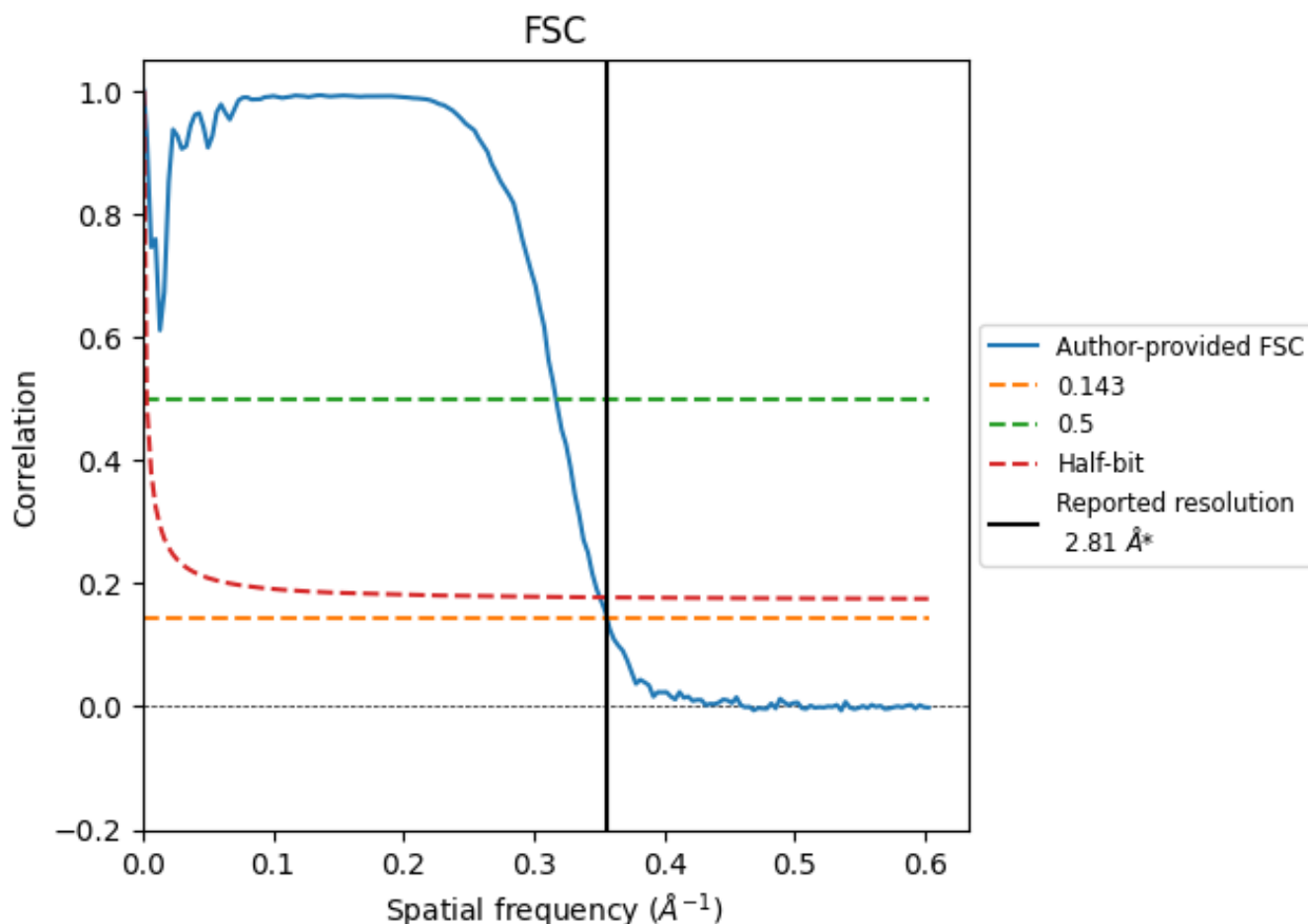


\*Reported resolution corresponds to spatial frequency of 0.356 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.356 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.16	2.85
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

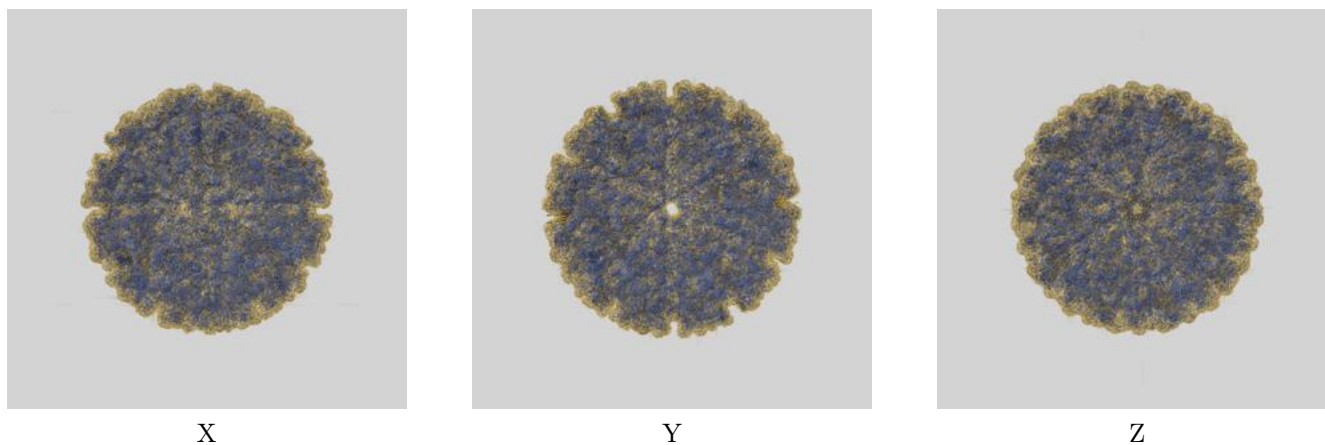
This section contains information regarding the fit between EMDB map EMD-31533 and PDB model 7FD2. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

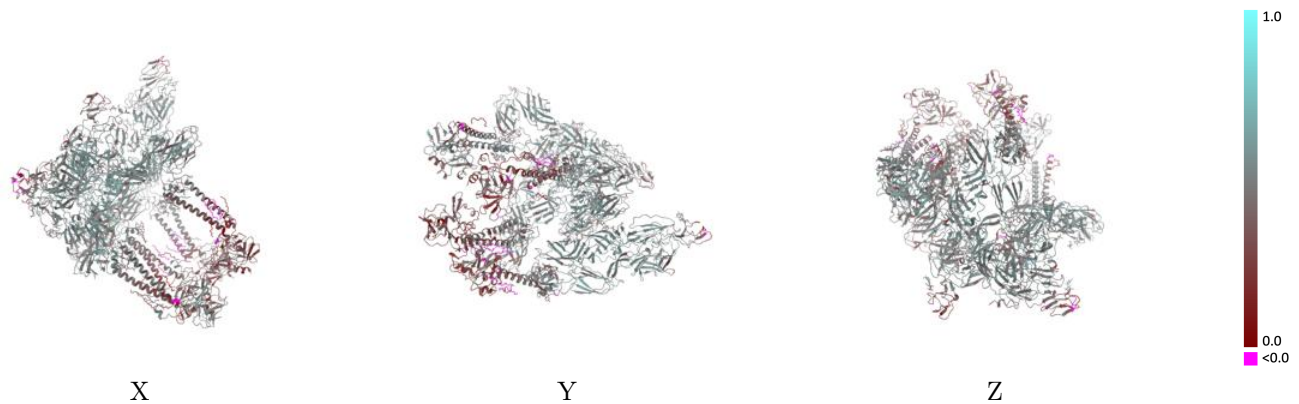


#### 9.1.2 Map-model assembly overlay [i](#)



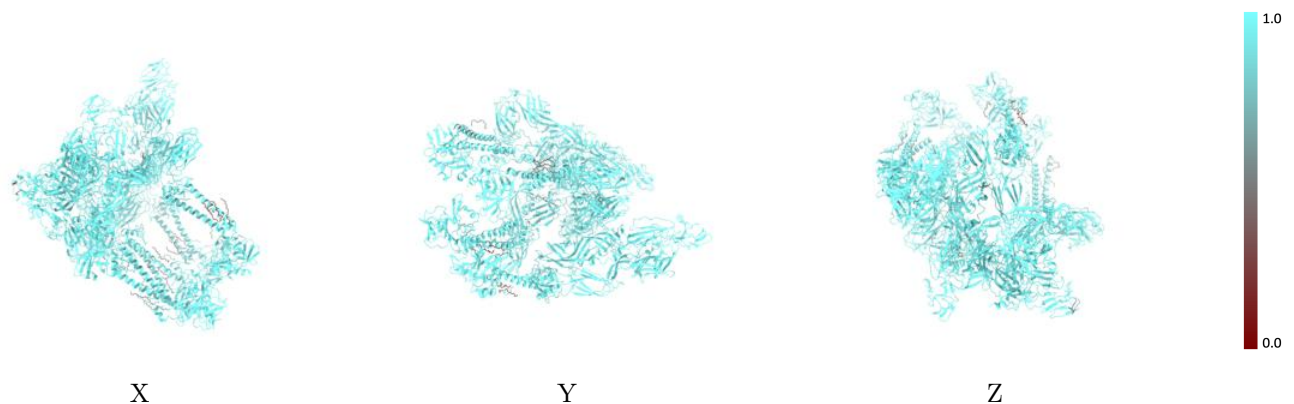
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



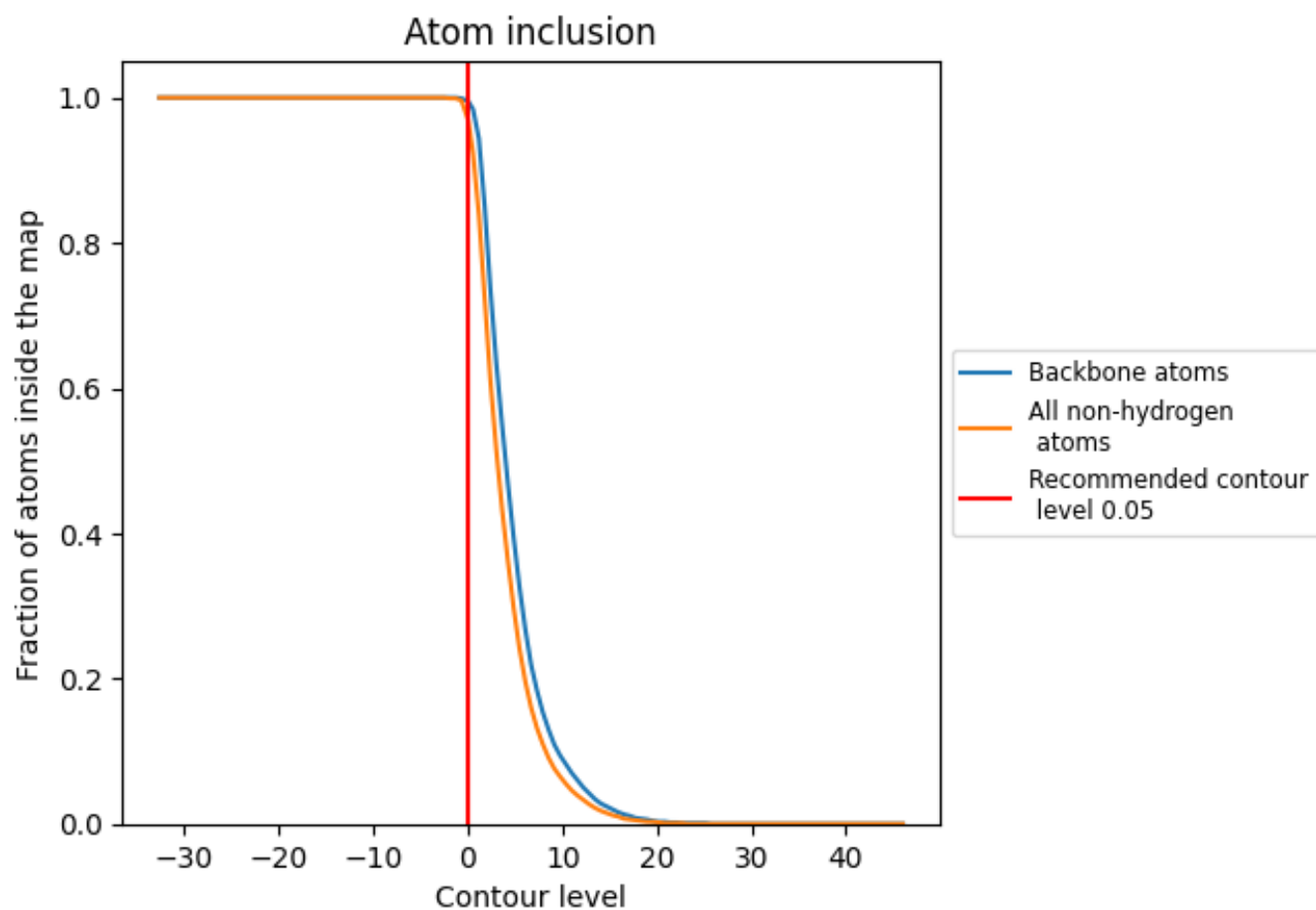
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.05).



















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.4520
A	 0.9640	 0.4850
B	 0.9830	 0.4990
C	 0.9650	 0.4350
D	 1.0000	 0.5000
E	 0.9710	 0.4970
F	 0.9640	 0.4410
G	 0.9620	 0.3020
H	 1.0000	 0.5550
I	 0.9720	 0.4560
J	 0.9600	 0.4520
K	 0.9680	 0.2980
L	 1.0000	 0.4530
M	 0.9690	 0.4900
N	 0.9700	 0.4590
O	 0.9620	 0.2880
P	 1.0000	 0.4480
Q	 1.0000	 0.5650
R	 1.0000	 0.4350
S	 1.0000	 0.4800
T	 1.0000	 0.5550
U	 1.0000	 0.4370
V	 1.0000	 0.4830
W	 1.0000	 0.5580
X	 1.0000	 0.4620

