



Full wwPDB EM Validation Report ⓘ

Oct 27, 2024 – 09:23 PM JST

PDB ID : 7FD2
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

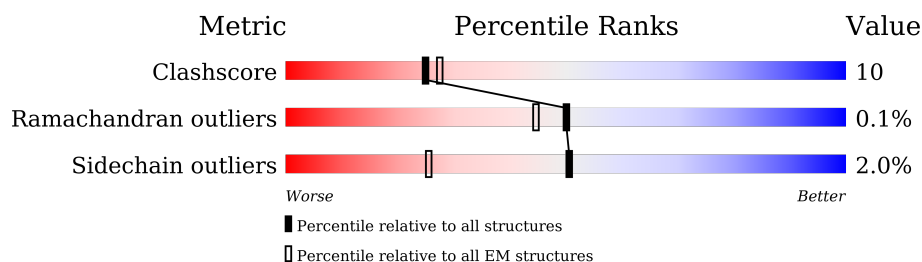
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 78% 22%
1	E	438	 79% 21%
1	I	438	 79% 21% .
1	M	438	 80% 20%
2	B	419	 78% 22%
2	F	419	 76% 24%
2	J	419	 74% 25% .
2	N	419	 79% 20% .

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Mol	Chain	Length	Quality of chain
3	C	268	
3	G	268	
3	K	268	
3	O	268	
4	D	4	
4	P	4	
4	S	4	
4	V	4	
5	H	2	
5	Q	2	
5	T	2	
5	W	2	
6	L	3	
6	R	3	
6	U	3	
6	X	3	

2 Entry composition [i](#)

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
1	A	438	Total	C	N	O	S	0	0
			3333	2101	567	640	25		
1	E	438	Total	C	N	O	S	0	0
			3328	2098	565	640	25		
1	I	438	Total	C	N	O	S	0	0
			3331	2099	567	640	25		
1	M	438	Total	C	N	O	S	0	0
			3333	2101	567	640	25		

- Molecule 2 is a protein called Envelope glycoprotein 2.

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

- Molecule 3 is a protein called capsid protein.

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

- 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
4	D	4	Total	C	N	O	0	0
			50	28	2	20		
4	P	4	Total	C	N	O	0	0
			50	28	2	20		
4	S	4	Total	C	N	O	0	0
			50	28	2	20		
4	V	4	Total	C	N	O	0	0
			50	28	2	20		

- 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
5	H	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



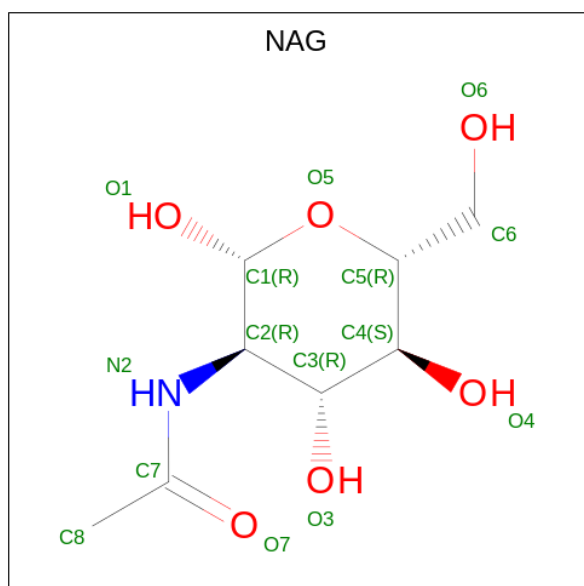
Mol	Chain	Residues	Atoms				AltConf	Trace
6	L	3	Total	C	N	O	0	0
			39	22	2	15		

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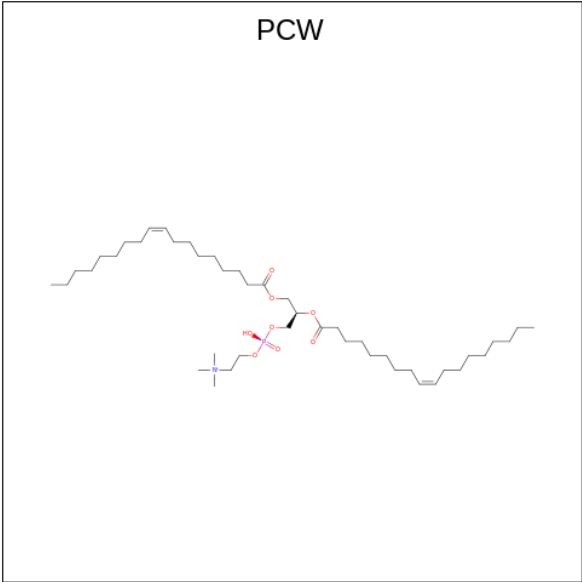
Mol	Chain	Residues	Atoms				AltConf	Trace
6	R	3	Total	C	N	O	0	0
			39	22	2	15		
6	U	3	Total	C	N	O	0	0
			39	22	2	15		
6	X	3	Total	C	N	O	0	0
			39	22	2	15		

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



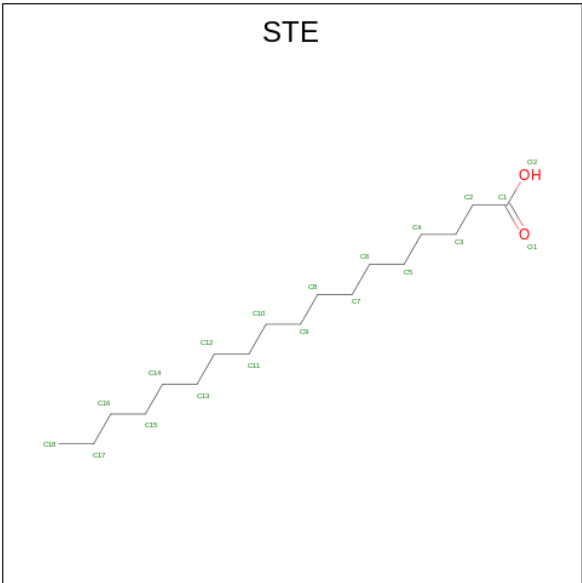
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	I	1	Total	C	N	O	0
			14	8	1	5	
7	M	1	Total	C	N	O	0
			14	8	1	5	

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



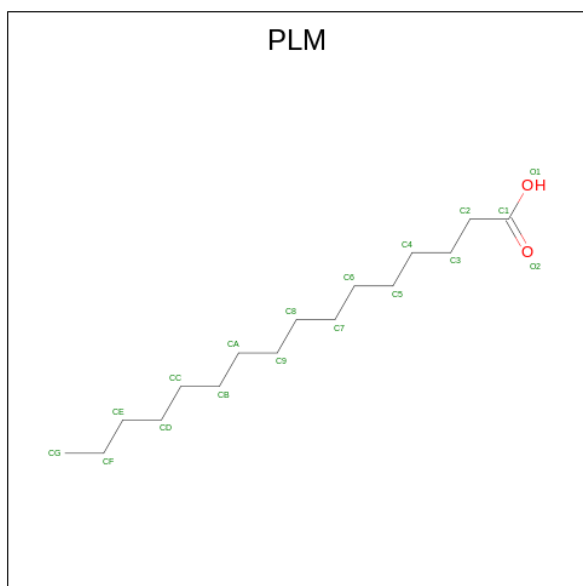
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	E	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	I	1	Total	C	N	O	P	0
			54	44	1	8	1	
8	M	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 9 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂) (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 (three-letter code: PLM) (formula: C₁₆H₃₂O₂) (labeled as "Ligand of Interest" by depositor).



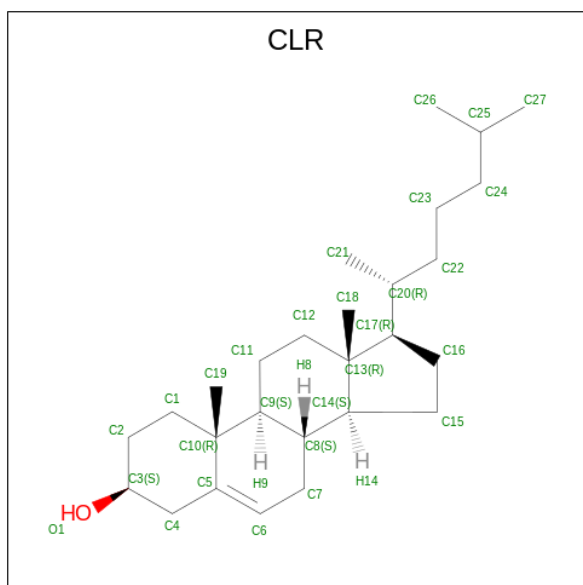
Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			18	16	2	
10	B	1	Total	C	O	0
			18	16	2	
10	B	1	Total	C	O	0
			18	16	2	

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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 (three-letter code: 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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Mol	Chain	Residues	Atoms			AltConf
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	

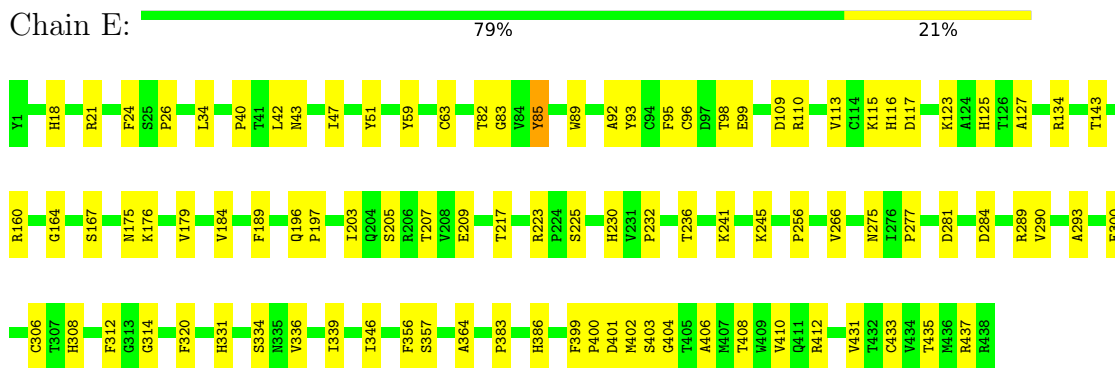
3 Residue-property plots

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.

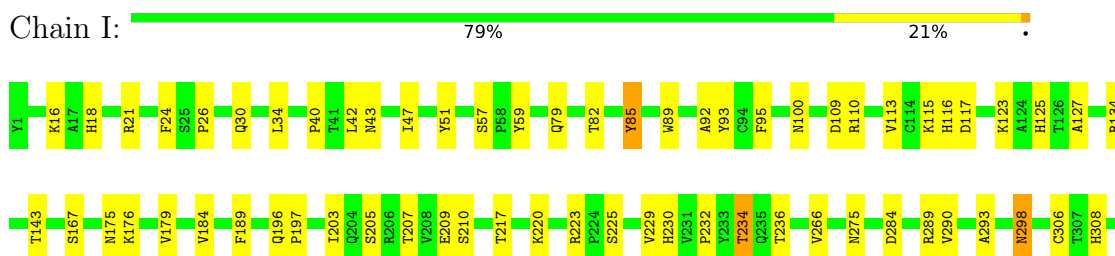
• Molecule 1: Envelope glycoprotein 1



• Molecule 1: Envelope glycoprotein 1



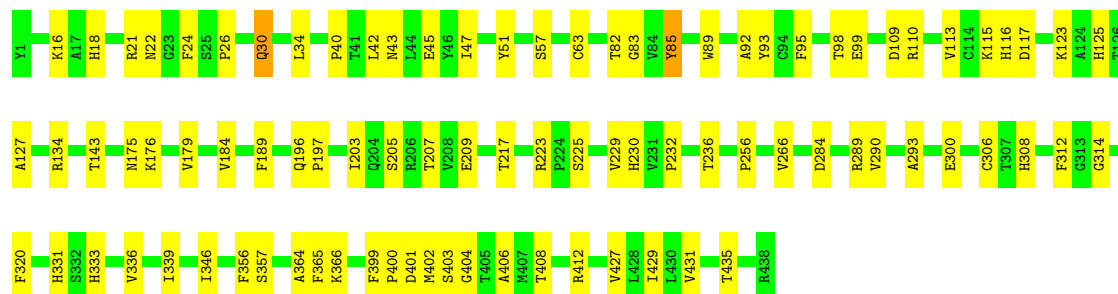
• Molecule 1: Envelope glycoprotein 1





• Molecule 1: Envelope glycoprotein 1

Chain M: 80% 20%



• Molecule 2: Envelope glycoprotein 2

Chain B: 78% 22%



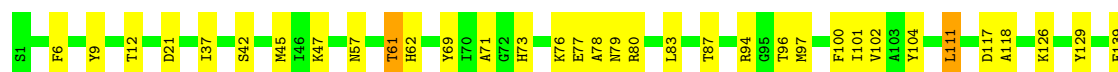
• Molecule 2: Envelope glycoprotein 2

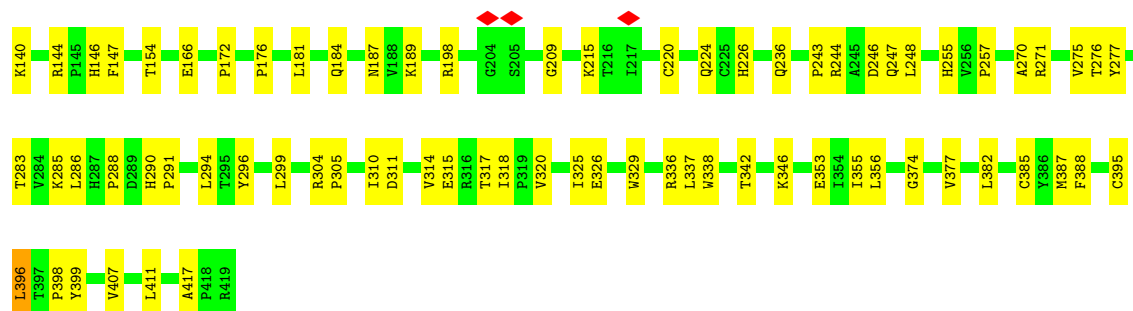
Chain F: 76% 24%



• Molecule 2: Envelope glycoprotein 2

Chain J: 74% 25%





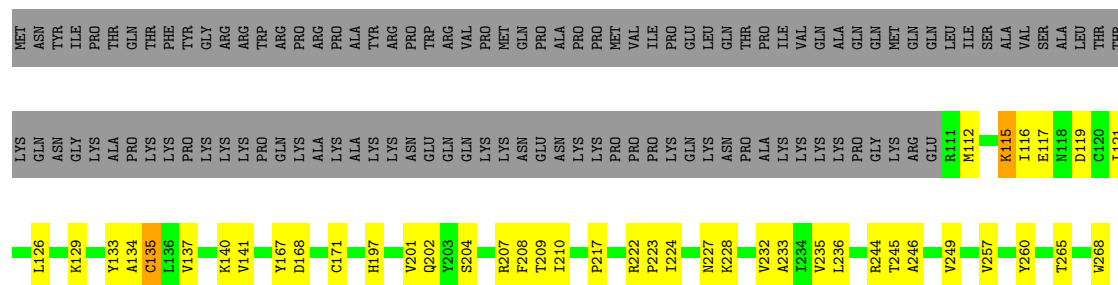
• Molecule 2: Envelope glycoprotein 2

Chain N: 79% 20% .



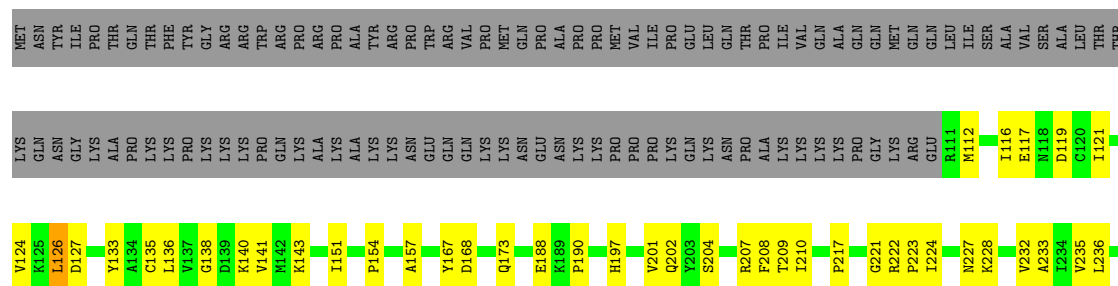
• Molecule 3: capsid protein

Chain C: 43% 15% 41%



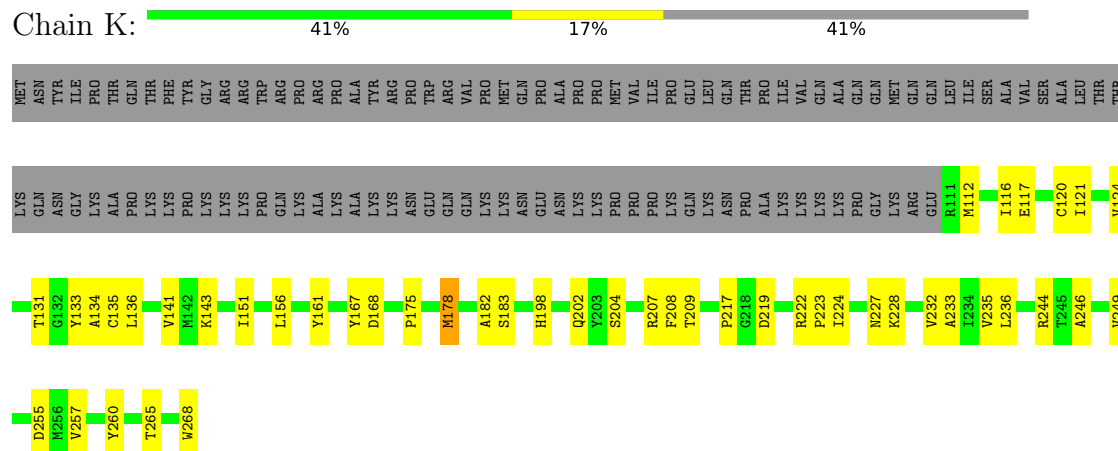
• Molecule 3: capsid protein

Chain G: 41% 18% 41%

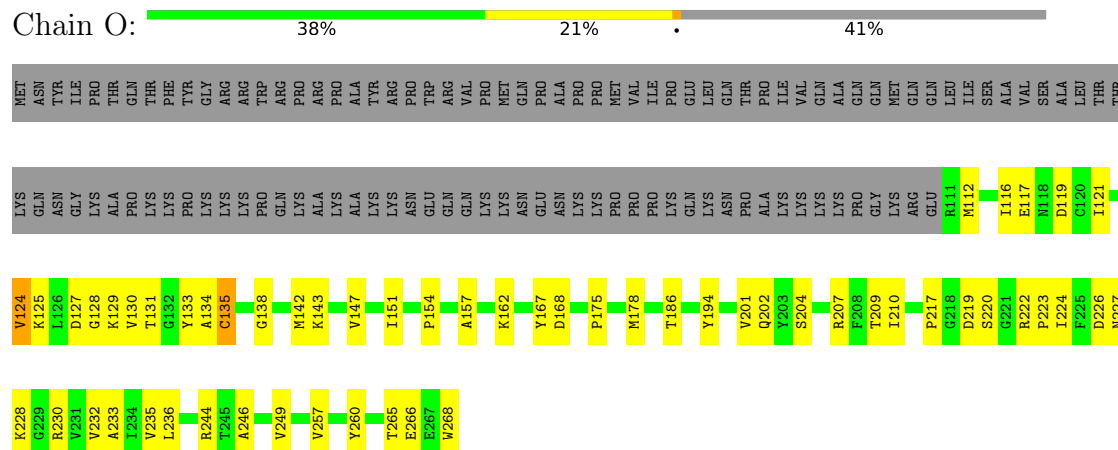




- Molecule 3: capsid protein



- Molecule 3: capsid protein



- 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



- 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

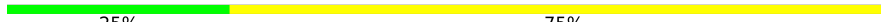


- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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:  25% 75%

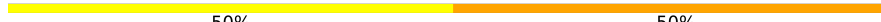


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%



- 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:  33% 67%


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 (\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 (\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: NAG, BMA, MAN, PCW, STE, CLR, PLM

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	0.38	0/3417	0.58	0/4663
1	E	0.38	0/3411	0.57	0/4655
1	I	0.38	0/3415	0.58	0/4660
1	M	0.38	0/3417	0.57	0/4663
2	B	0.35	0/3326	0.57	0/4538
2	F	0.35	0/3326	0.57	0/4538
2	J	0.46	0/3326	0.67	0/4538
2	N	0.41	0/3326	0.60	0/4538
3	C	0.47	0/1249	0.66	0/1687
3	G	0.46	0/1249	0.63	0/1687
3	K	0.46	0/1249	0.65	0/1687
3	O	0.46	0/1249	0.66	0/1687
All	All	0.40	0/31960	0.60	0/43541

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3236	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3328	0	3230	76	0
1	I	3331	0	3228	74	0
1	M	3333	0	3235	68	0
2	B	3239	0	3191	61	0
2	F	3239	0	3191	75	0
2	J	3239	0	3191	75	0
2	N	3239	0	3190	59	0
3	C	1220	0	1204	27	0
3	G	1220	0	1204	28	0
3	K	1220	0	1204	33	0
3	O	1220	0	1204	38	0
4	D	50	0	43	1	0
4	P	50	0	43	3	0
4	S	50	0	43	0	0
4	V	50	0	43	0	0
5	H	28	0	25	5	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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	671	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 10.

All (671) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:184:GLN:OE1	2:N:215:LYS:NZ	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG12	2:B:111:LEU:HD23	1.92	0.50
2:B:37:ILE:HG21	2:B:129:TYR:CE2	2.47	0.50
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
2:J:382:LEU:C	2:J:385:CYS:H	2.16	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:220:CYS:HB2	2:J:224:GLN:HB2	1.97	0.47
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
2:F:286:LEU:C	2:F:287:HIS:HD1	2.18	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
2:F:69:TYR:OH	2:F:117:ASP:OD1	2.22	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
1:E:196:GLN:HA	1:E:196:GLN:OE1	2.15	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
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
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:N:352:HIS:HB2	11:N:502:CLR:H9	1.98	0.45
1:E:95:PHE:HE2	6:R:1:NAG:HO6	1.56	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
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
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
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:OE1	1:M:22:ASN:CG	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:K:198:HIS:HE2	3:K:219:ASP:CG	2.20	0.44
2:B:326:GLU:O	2:B:326:GLU:HG3	2.18	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
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
2:N:189:LYS:HB2	2:N:215:LYS:HZ2	1.83	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:326:GLU:O	2:N:326:GLU:HG3	2.18	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
2:N:290:HIS:O	2:N:291:PRO:C	2.57	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
2:F:326:GLU:O	2:F:326:GLU:HG3	2.18	0.43
3:G:201:VAL:HG22	3:G:210:ILE:HD11	2.00	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
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:F:189:LYS:HB2	2:F:215:LYS:HZ2	1.82	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:308:GLU:CD	2:F:316:ARG:HH21	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:M:45:GLU:OE1	1:M:123:LYS:NZ	2.38	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:N:385:CYS:O	2:N:386:TYR:C	2.59	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:9:TYR:O	2:J:12:THR:OG1	2.26	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
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
2:B:308:GLU:CD	2:B:316:ARG:HH21	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

5.3.1 Protein backbone

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%)	44	71
2	N	417/419 (100%)	394 (94%)	21 (5%)	2 (0%)	25	54
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%)	22	49
All	All	4036/4500 (90%)	3872 (96%)	160 (4%)	4 (0%)	50	76

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 ⓘ

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%)	86	95
1	E	367/368 (100%)	366 (100%)	1 (0%)	91	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	367/368 (100%)	362 (99%)	5 (1%)	62	86
1	M	368/368 (100%)	365 (99%)	3 (1%)	79	93
2	B	350/350 (100%)	342 (98%)	8 (2%)	45	77
2	F	350/350 (100%)	345 (99%)	5 (1%)	62	86
2	J	350/350 (100%)	338 (97%)	12 (3%)	32	64
2	N	350/350 (100%)	344 (98%)	6 (2%)	56	83
3	C	130/228 (57%)	125 (96%)	5 (4%)	28	60
3	G	130/228 (57%)	125 (96%)	5 (4%)	28	60
3	K	130/228 (57%)	124 (95%)	6 (5%)	23	53
3	O	130/228 (57%)	121 (93%)	9 (7%)	13	35
All	All	3390/3784 (90%)	3323 (98%)	67 (2%)	50	80

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	234	THR
2	B	45	MET
2	B	61	THR
2	B	129	TYR
2	B	287	HIS
2	B	304	ARG
2	B	402	THR
2	B	406	VAL
2	B	414	LEU
3	C	115	LYS
3	C	119	ASP
3	C	135	CYS
3	C	204	SER
3	C	265	THR
1	E	85	TYR
2	F	45	MET
2	F	61	THR
2	F	129	TYR
2	F	287	HIS
2	F	304	ARG
3	G	119	ASP
3	G	126	LEU

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Mol	Chain	Res	Type
3	G	135	CYS
3	G	204	SER
3	G	265	THR
1	I	30	GLN
1	I	85	TYR
1	I	100	ASN
1	I	234	THR
1	I	298	ASN
2	J	45	MET
2	J	61	THR
2	J	62	HIS
2	J	111	LEU
2	J	129	TYR
2	J	275	VAL
2	J	276	THR
2	J	290	HIS
2	J	304	ARG
2	J	317	THR
2	J	396	LEU
2	J	411	LEU
3	K	117	GLU
3	K	131	THR
3	K	135	CYS
3	K	178	MET
3	K	204	SER
3	K	265	THR
1	M	30	GLN
1	M	82	THR
1	M	85	TYR
2	N	45	MET
2	N	61	THR
2	N	62	HIS
2	N	129	TYR
2	N	226	HIS
2	N	304	ARG
3	O	117	GLU
3	O	119	ASP
3	O	124	VAL
3	O	127	ASP
3	O	129	LYS
3	O	135	CYS
3	O	204	SER

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Mol	Chain	Res	Type
3	O	265	THR
3	O	266	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	141	ASN
1	A	302	GLN
2	B	146	HIS
2	B	226	HIS
1	E	230	HIS
1	E	302	GLN
2	F	226	HIS
1	I	79	GLN
2	J	146	HIS
2	J	226	HIS
3	K	197	HIS
1	M	22	ASN
1	M	30	GLN
1	M	79	GLN
1	M	298	ASN
2	N	226	HIS
2	N	287	HIS
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	2,4	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
4	NAG	D	2	4	14,14,15	0.66	0	17,19,21	1.16	3 (17%)
4	BMA	D	3	4	11,11,12	0.42	0	15,15,17	1.09	2 (13%)
4	MAN	D	4	4	11,11,12	0.31	0	15,15,17	0.98	1 (6%)
5	NAG	H	1	5,1	14,14,15	0.77	0	17,19,21	1.60	3 (17%)
5	NAG	H	2	5	14,14,15	0.47	0	17,19,21	1.36	2 (11%)
6	NAG	L	1	6,2	14,14,15	0.87	0	17,19,21	2.56	4 (23%)
6	NAG	L	2	6	14,14,15	0.47	0	17,19,21	1.52	2 (11%)
6	BMA	L	3	6	11,11,12	0.39	0	15,15,17	1.45	1 (6%)
4	NAG	P	1	2,4	14,14,15	0.72	0	17,19,21	1.24	1 (5%)
4	NAG	P	2	4	14,14,15	0.57	0	17,19,21	2.00	5 (29%)
4	BMA	P	3	4	11,11,12	0.31	0	15,15,17	1.21	2 (13%)
4	MAN	P	4	4	11,11,12	0.22	0	15,15,17	0.52	0
5	NAG	Q	1	5,1	14,14,15	1.51	2 (14%)	17,19,21	1.79	4 (23%)
5	NAG	Q	2	5	14,14,15	0.45	0	17,19,21	0.82	1 (5%)
6	NAG	R	1	6,2	14,14,15	0.98	1 (7%)	17,19,21	2.72	9 (52%)
6	NAG	R	2	6	14,14,15	0.46	0	17,19,21	1.64	5 (29%)
6	BMA	R	3	6	11,11,12	0.37	0	15,15,17	1.04	1 (6%)
4	NAG	S	1	2,4	14,14,15	1.93	1 (7%)	17,19,21	2.38	4 (23%)
4	NAG	S	2	4	14,14,15	0.51	0	17,19,21	1.35	1 (5%)
4	BMA	S	3	4	11,11,12	0.31	0	15,15,17	0.89	1 (6%)
4	MAN	S	4	4	11,11,12	0.22	0	15,15,17	0.88	0
5	NAG	T	1	5,1	14,14,15	0.83	0	17,19,21	2.14	5 (29%)
5	NAG	T	2	5	14,14,15	0.56	0	17,19,21	1.01	2 (11%)
6	NAG	U	1	6,2	14,14,15	1.43	1 (7%)	17,19,21	1.78	4 (23%)
6	NAG	U	2	6	14,14,15	0.56	0	17,19,21	0.90	1 (5%)
6	BMA	U	3	6	11,11,12	0.33	0	15,15,17	1.52	2 (13%)
4	NAG	V	1	2,4	14,14,15	1.30	1 (7%)	17,19,21	2.00	2 (11%)
4	NAG	V	2	4	14,14,15	0.75	0	17,19,21	1.16	2 (11%)
4	BMA	V	3	4	11,11,12	0.35	0	15,15,17	0.93	0
4	MAN	V	4	4	11,11,12	0.25	0	15,15,17	1.04	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	W	1	5,1	14,14,15	1.67	1 (7%)	17,19,21	1.63	4 (23%)
5	NAG	W	2	5	14,14,15	0.41	0	17,19,21	0.98	1 (5%)
6	NAG	X	1	6,2	14,14,15	0.95	1 (7%)	17,19,21	1.87	4 (23%)
6	NAG	X	2	6	14,14,15	0.54	0	17,19,21	1.38	2 (11%)
6	BMA	X	3	6	11,11,12	0.34	0	15,15,17	0.96	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	2,4	-	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	5,1	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
6	NAG	L	1	6,2	-	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	2,4	-	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	5,1	-	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	6,2	-	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	2,4	-	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	5,1	-	5/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
6	NAG	U	1	6,2	-	4/6/23/26	0/1/1/1
6	NAG	U	2	6	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	U	3	6	-	1/2/19/22	0/1/1/1
4	NAG	V	1	2,4	-	4/6/23/26	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	5,1	-	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	6,2	-	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	6.94	1.62	1.52
5	W	1	NAG	C1-C2	5.57	1.60	1.52
6	U	1	NAG	C1-C2	5.16	1.60	1.52
5	Q	1	NAG	C1-C2	4.45	1.59	1.52
4	V	1	NAG	C1-C2	3.74	1.57	1.52
6	R	1	NAG	C1-C2	3.10	1.57	1.52
5	Q	1	NAG	O5-C1	3.08	1.48	1.43
6	X	1	NAG	C1-C2	2.74	1.56	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	O5-C1-C2	-8.00	98.65	111.29
6	R	1	NAG	C1-O5-C5	7.32	122.11	112.19
4	S	1	NAG	C4-C3-C2	-5.81	102.50	111.02
5	T	1	NAG	O5-C1-C2	-5.66	102.35	111.29
6	X	1	NAG	O5-C1-C2	-5.65	102.36	111.29
4	V	1	NAG	O5-C1-C2	-5.27	102.96	111.29
5	Q	1	NAG	C1-O5-C5	5.26	119.33	112.19
6	L	2	NAG	O5-C1-C2	-5.11	103.22	111.29
4	P	2	NAG	C4-C3-C2	-5.07	103.59	111.02
4	S	1	NAG	O5-C1-C2	-4.87	103.60	111.29
4	S	2	NAG	O5-C1-C2	-4.65	103.94	111.29
4	S	1	NAG	C3-C4-C5	-4.63	101.98	110.24
6	L	3	BMA	C1-O5-C5	-4.26	106.42	112.19
6	U	1	NAG	C2-N2-C7	-3.94	117.29	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1	NAG	C3-C4-C5	-3.85	103.38	110.24
6	X	2	NAG	C2-N2-C7	-3.84	117.44	122.90
6	U	1	NAG	C3-C4-C5	-3.77	103.51	110.24
5	H	1	NAG	O3-C3-C2	-3.76	101.68	109.47
4	V	1	NAG	C1-O5-C5	3.65	117.14	112.19
5	W	1	NAG	O5-C1-C2	-3.63	105.56	111.29
6	L	1	NAG	C2-N2-C7	-3.63	117.74	122.90
6	U	3	BMA	C1-O5-C5	3.61	117.08	112.19
5	H	2	NAG	O5-C1-C2	-3.59	105.61	111.29
4	P	2	NAG	C2-N2-C7	-3.54	117.86	122.90
5	H	1	NAG	C3-C4-C5	-3.49	104.02	110.24
5	T	1	NAG	O5-C5-C4	-3.45	102.43	110.83
5	T	1	NAG	C1-O5-C5	3.44	116.85	112.19
6	U	1	NAG	O5-C5-C6	3.37	112.49	107.20
6	U	3	BMA	C1-C2-C3	3.36	113.80	109.67
6	R	1	NAG	C2-N2-C7	-3.33	118.16	122.90
6	R	1	NAG	O5-C5-C6	3.28	112.34	107.20
6	R	2	NAG	O5-C1-C2	-3.25	106.16	111.29
5	Q	1	NAG	O5-C1-C2	-3.23	106.19	111.29
6	R	2	NAG	C1-O5-C5	3.22	116.55	112.19
4	P	3	BMA	C1-O5-C5	3.17	116.49	112.19
6	R	1	NAG	O5-C5-C4	3.07	118.29	110.83
6	R	1	NAG	O5-C1-C2	-3.02	106.51	111.29
4	P	2	NAG	C3-C4-C5	-2.91	105.05	110.24
5	T	2	NAG	C3-C4-C5	-2.89	105.09	110.24
5	W	1	NAG	C1-O5-C5	2.82	116.01	112.19
4	P	2	NAG	C1-O5-C5	2.79	115.98	112.19
5	W	1	NAG	C3-C4-C5	-2.75	105.33	110.24
6	R	1	NAG	C1-C2-N2	2.74	115.18	110.49
6	R	2	NAG	O4-C4-C3	-2.74	104.01	110.35
6	X	1	NAG	C3-C4-C5	-2.71	105.40	110.24
5	W	1	NAG	O4-C4-C3	-2.67	104.19	110.35
4	V	2	NAG	C4-C3-C2	2.66	114.92	111.02
6	R	1	NAG	C6-C5-C4	-2.66	106.77	113.00
6	X	1	NAG	C4-C3-C2	-2.65	107.13	111.02
6	U	2	NAG	O5-C1-C2	-2.64	107.12	111.29
6	X	3	BMA	C2-C3-C4	-2.59	106.42	110.89
6	L	2	NAG	O4-C4-C3	-2.57	104.40	110.35
4	P	1	NAG	O5-C1-C2	-2.55	107.26	111.29
6	X	1	NAG	O5-C5-C6	2.54	111.19	107.20
6	L	1	NAG	O5-C5-C4	-2.52	104.69	110.83
5	Q	1	NAG	C3-C4-C5	-2.52	105.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	1	NAG	O6-C6-C5	-2.51	102.67	111.29
6	R	3	BMA	C1-C2-C3	-2.50	106.59	109.67
4	D	2	NAG	O5-C1-C2	-2.47	107.39	111.29
6	X	2	NAG	O5-C5-C4	-2.45	104.86	110.83
6	R	2	NAG	O5-C5-C6	-2.42	103.41	107.20
5	T	1	NAG	C4-C3-C2	2.33	114.44	111.02
4	P	2	NAG	O5-C5-C6	2.31	110.83	107.20
5	Q	1	NAG	O5-C5-C4	-2.31	105.21	110.83
4	S	3	BMA	C1-O5-C5	2.30	115.31	112.19
4	V	4	MAN	O5-C5-C6	2.28	110.78	107.20
4	P	3	BMA	O5-C1-C2	-2.28	107.25	110.77
4	S	1	NAG	C1-O5-C5	2.28	115.28	112.19
4	V	2	NAG	O4-C4-C3	-2.25	105.14	110.35
4	D	2	NAG	C3-C4-C5	-2.24	106.24	110.24
4	D	4	MAN	O5-C5-C6	2.20	110.66	107.20
5	T	2	NAG	O5-C5-C4	-2.19	105.49	110.83
6	R	1	NAG	O3-C3-C4	-2.16	105.35	110.35
5	Q	2	NAG	O5-C5-C6	2.12	110.53	107.20
4	D	1	NAG	O4-C4-C3	-2.10	105.49	110.35
4	D	3	BMA	C1-C2-C3	2.10	112.25	109.67
5	H	2	NAG	C2-N2-C7	-2.09	119.92	122.90
6	U	1	NAG	O5-C5-C4	-2.09	105.74	110.83
5	T	1	NAG	C1-C2-N2	-2.07	106.95	110.49
6	R	2	NAG	C1-C2-N2	2.05	114.00	110.49
5	H	1	NAG	O5-C1-C2	-2.05	108.05	111.29
5	W	2	NAG	O5-C1-C2	-2.03	108.09	111.29
4	D	3	BMA	O5-C5-C4	-2.03	105.89	110.83
4	D	2	NAG	C2-N2-C7	-2.02	120.02	122.90

There are no chirality outliers.

All (68) 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	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

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Mol	Chain	Res	Type	Atoms
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	C8-C7-N2-C2
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
4	S	1	NAG	C1-C2-N2-C7
6	L	2	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	X	1	NAG	O5-C5-C6-O6
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	R	1	NAG	O5-C5-C6-O6
6	X	1	NAG	O7-C7-N2-C2

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

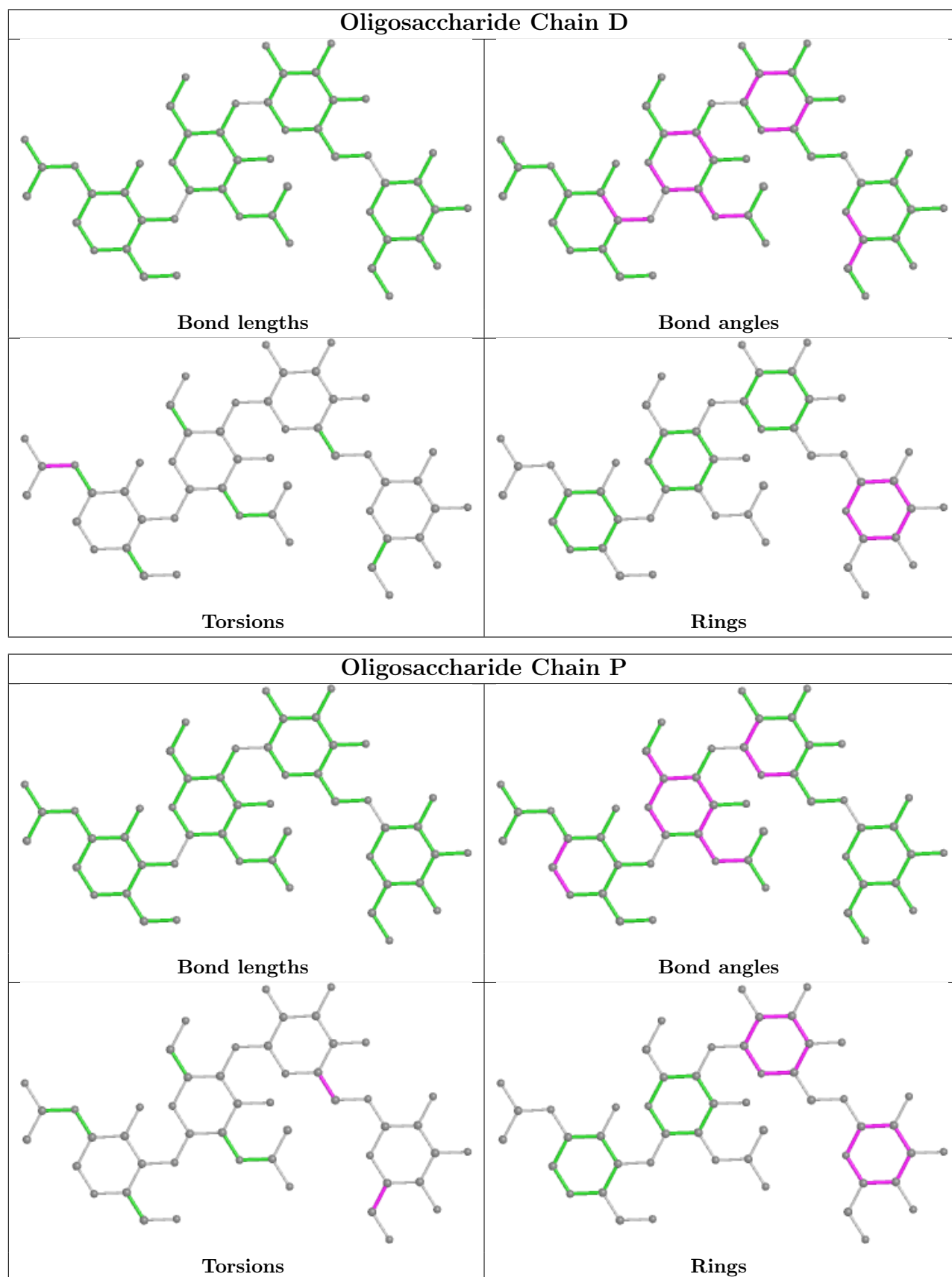
All (5) ring outliers are listed below:

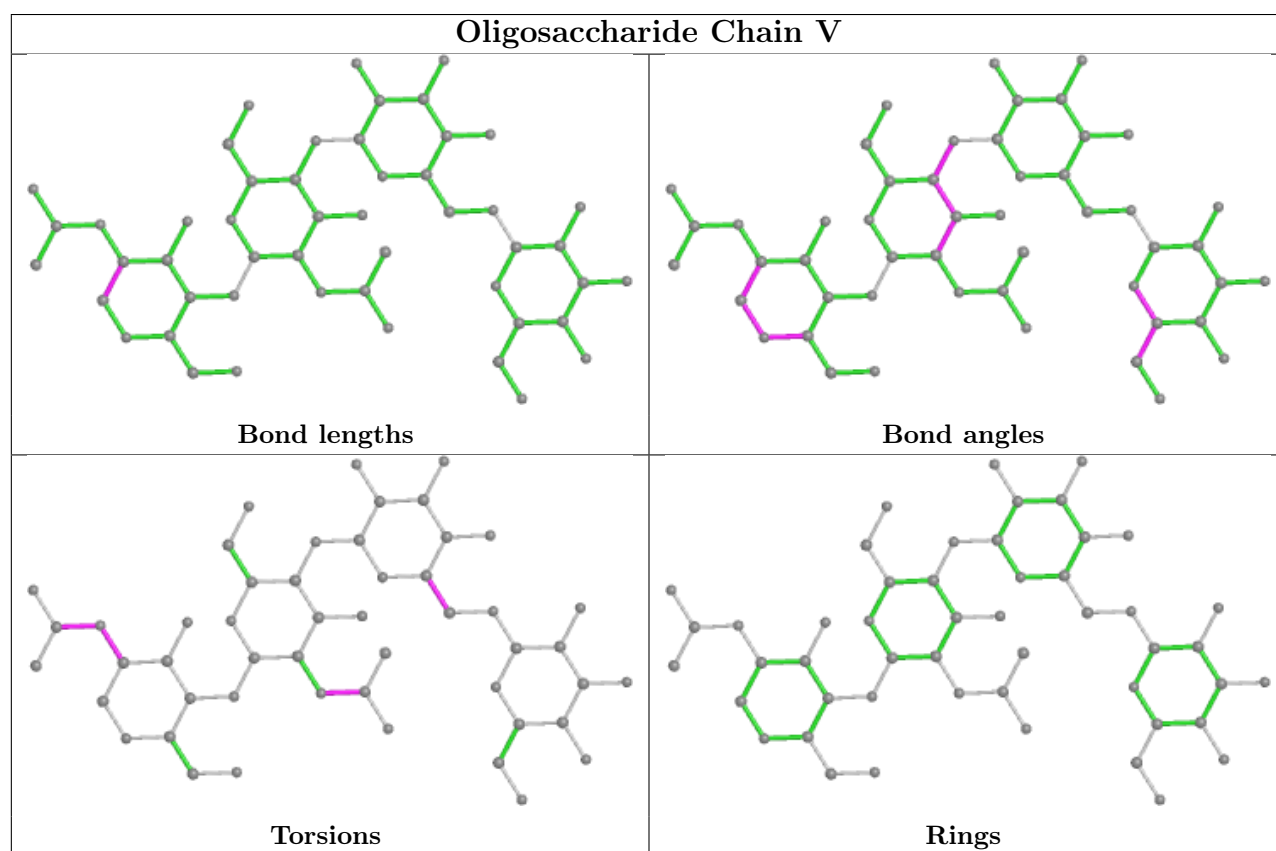
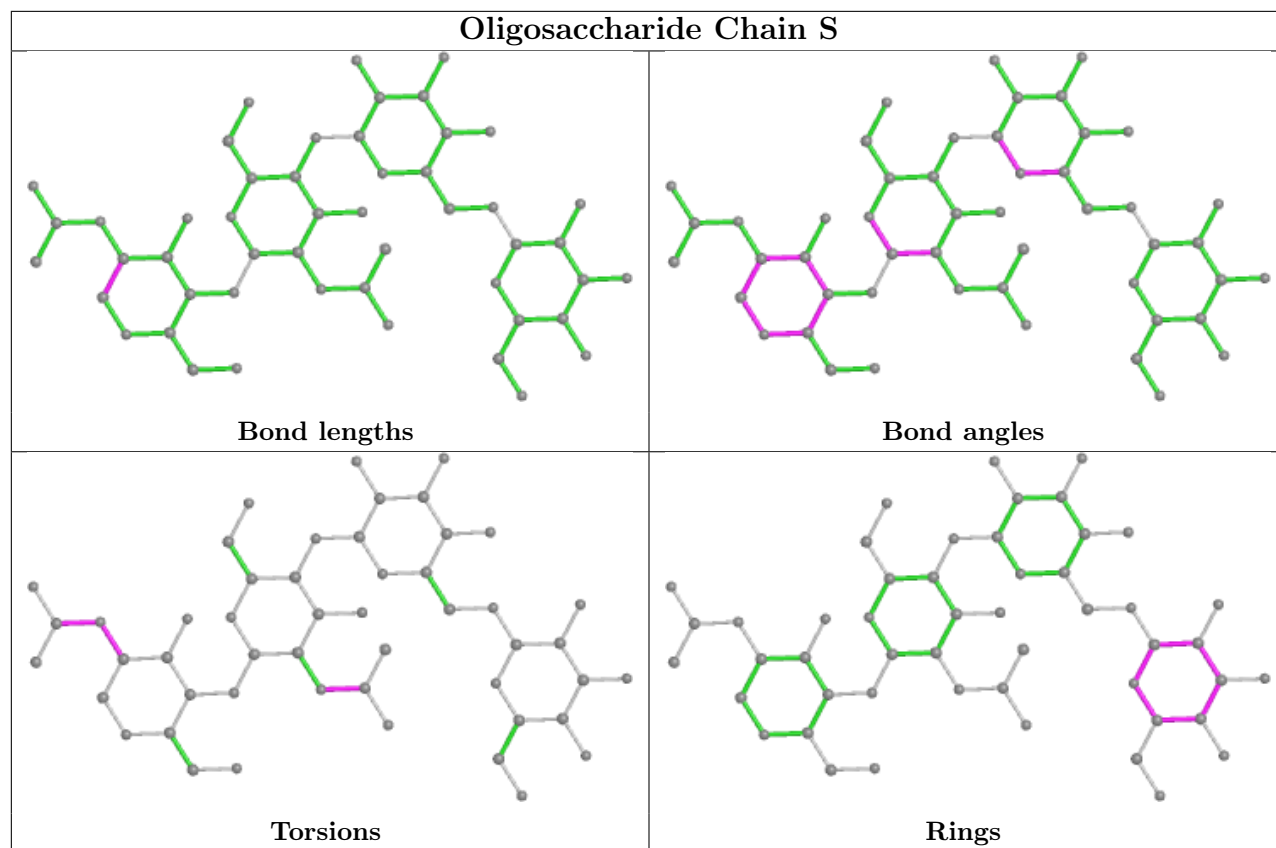
Mol	Chain	Res	Type	Atoms
4	P	4	MAN	C1-C2-C3-C4-C5-O5
4	D	4	MAN	C1-C2-C3-C4-C5-O5
4	S	4	MAN	C1-C2-C3-C4-C5-O5
6	X	3	BMA	C1-C2-C3-C4-C5-O5
4	P	3	BMA	C1-C2-C3-C4-C5-O5

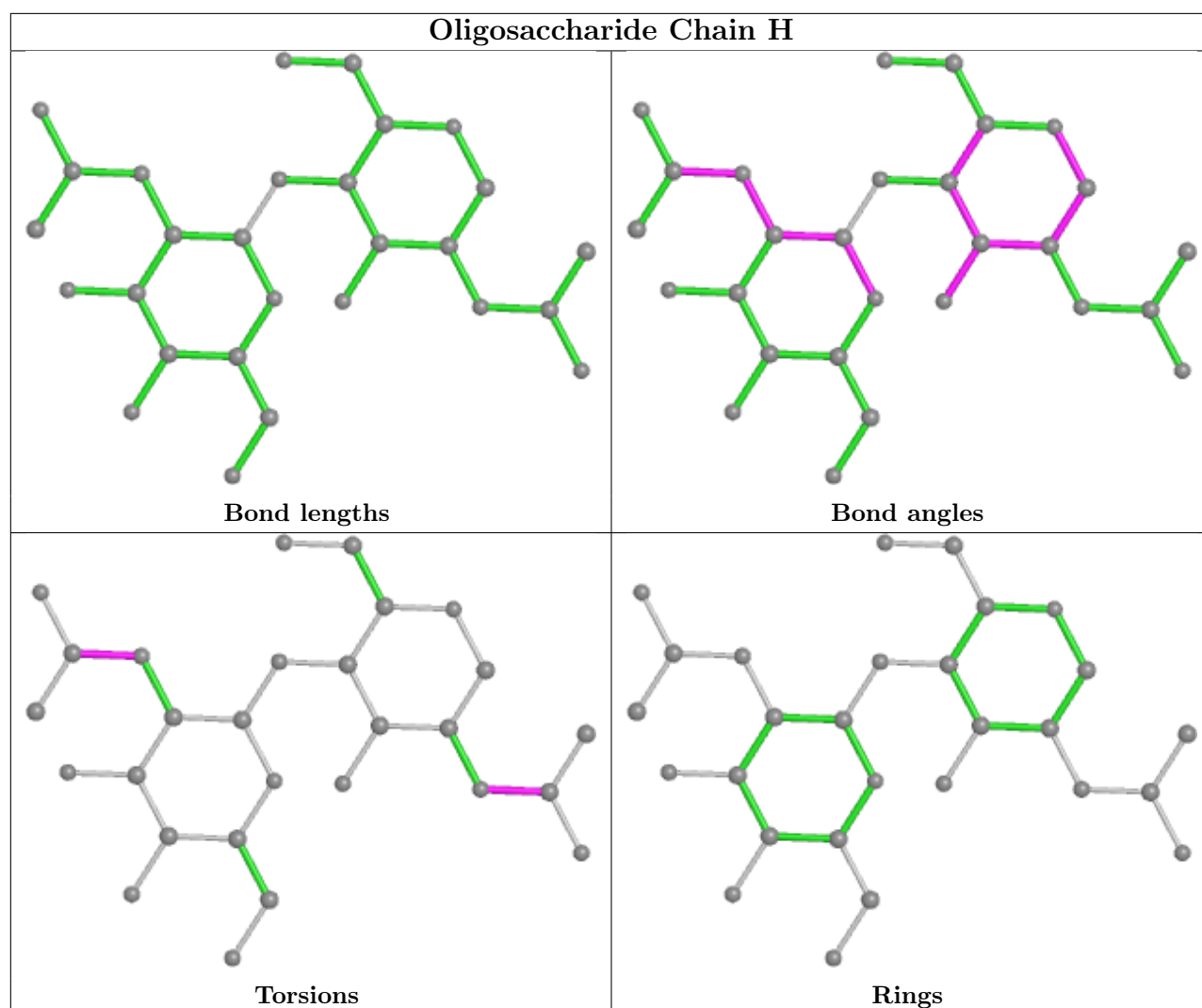
12 monomers are involved in 18 short contacts:

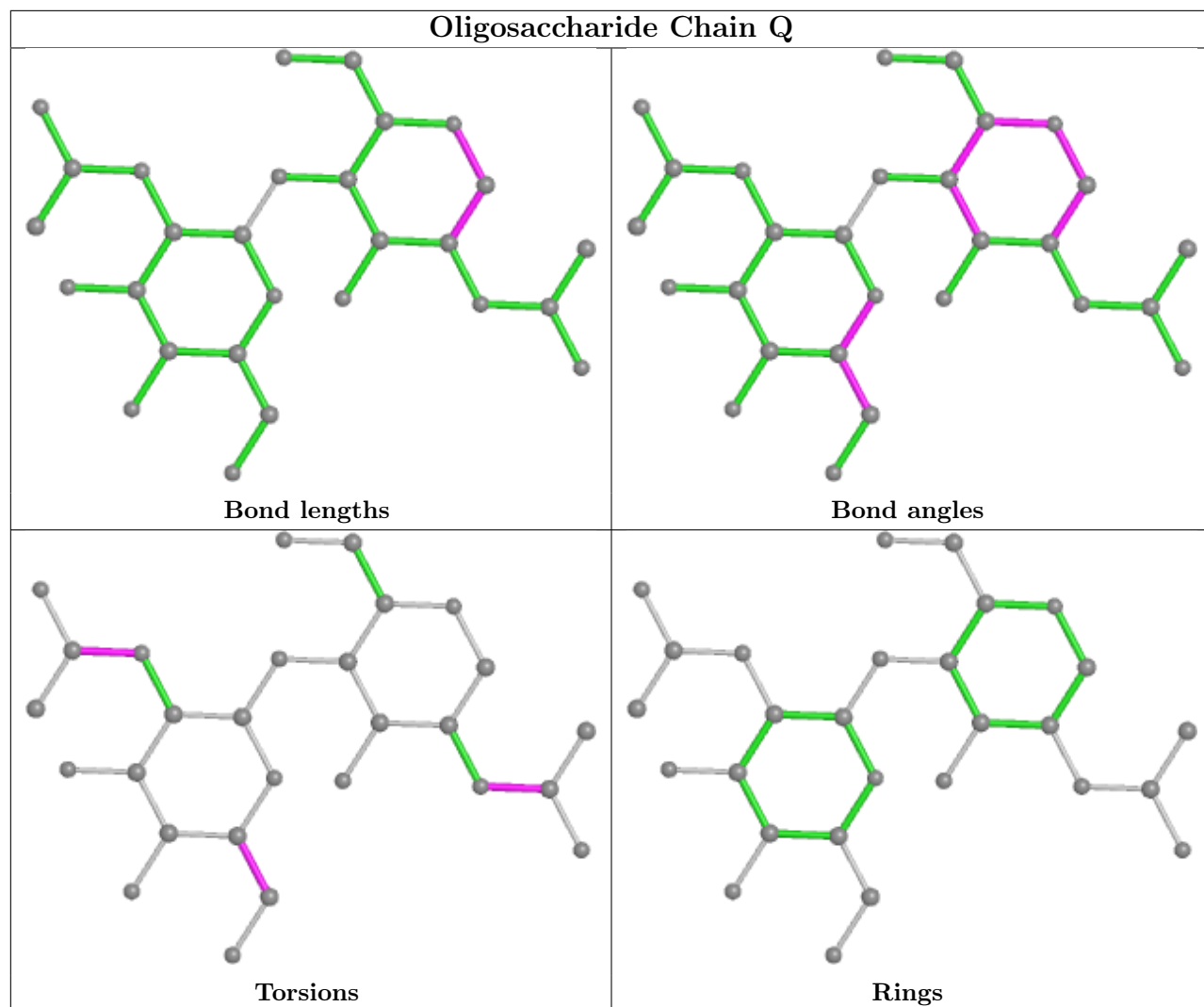
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3	BMA	1	0
6	R	2	NAG	1	0
6	U	2	NAG	1	0
5	H	1	NAG	4	0
4	D	4	MAN	1	0
4	P	1	NAG	3	0
6	L	1	NAG	1	0
6	X	1	NAG	1	0
5	H	2	NAG	1	0
5	Q	1	NAG	2	0
6	R	1	NAG	1	0
5	W	1	NAG	2	0

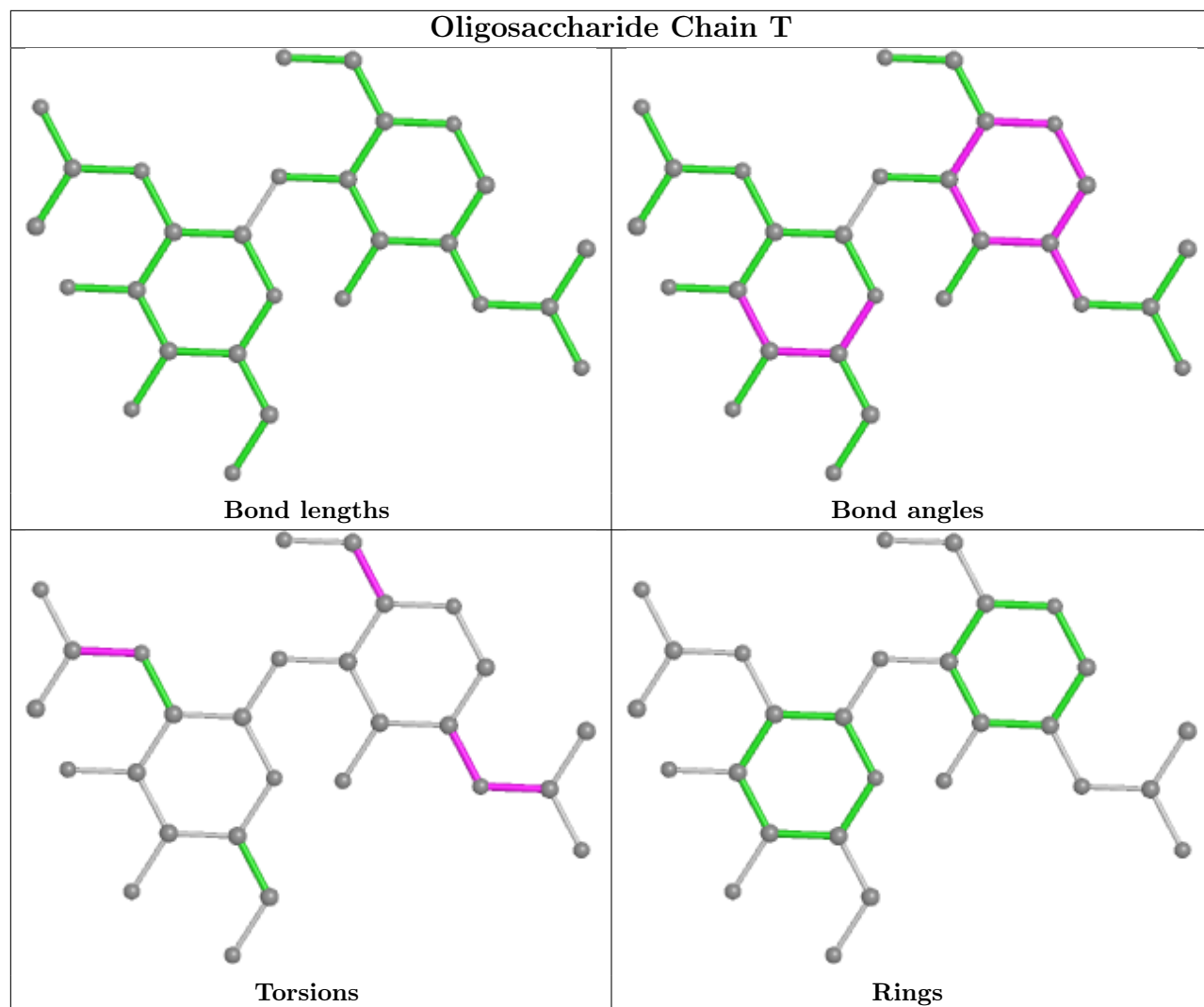
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

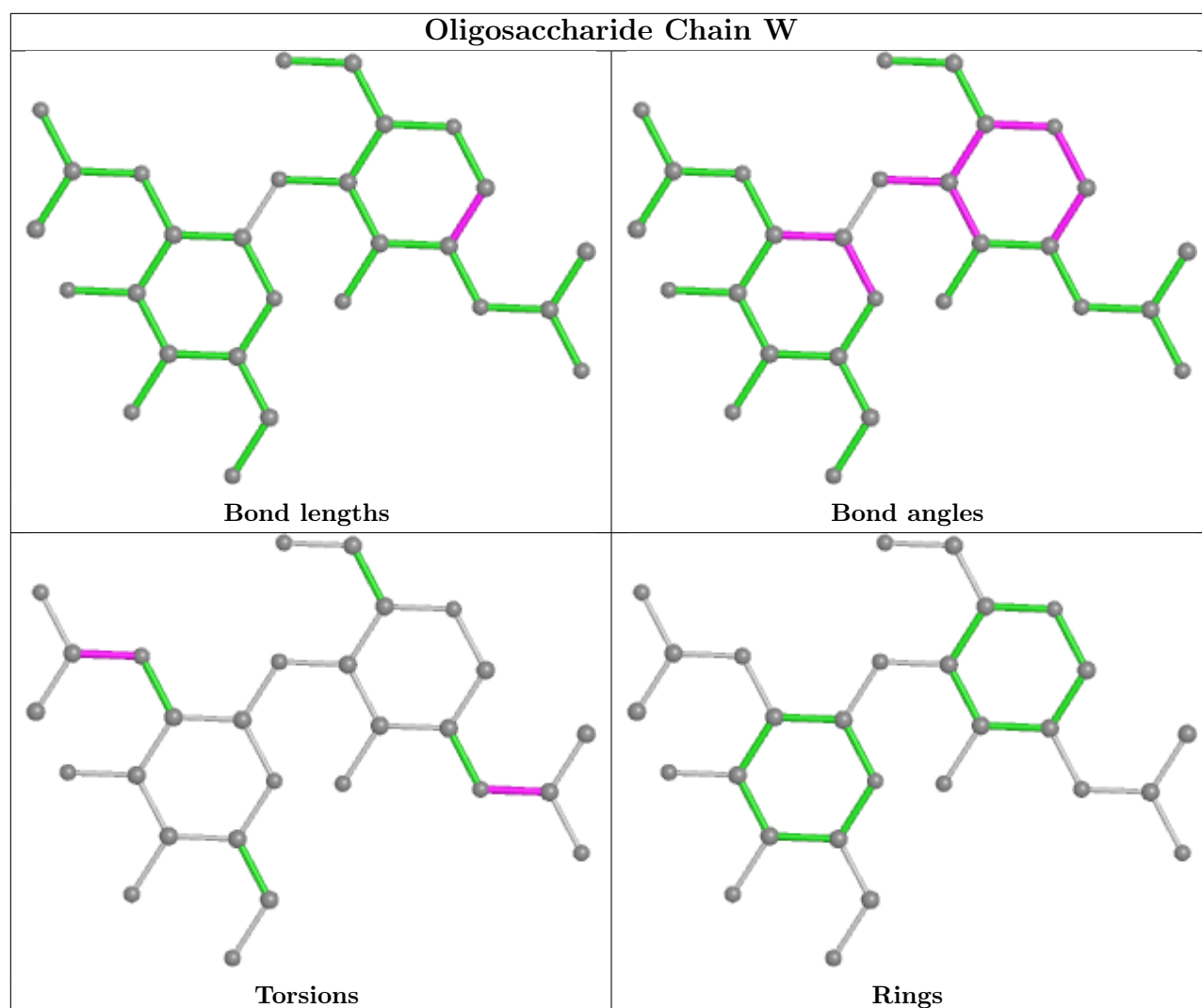


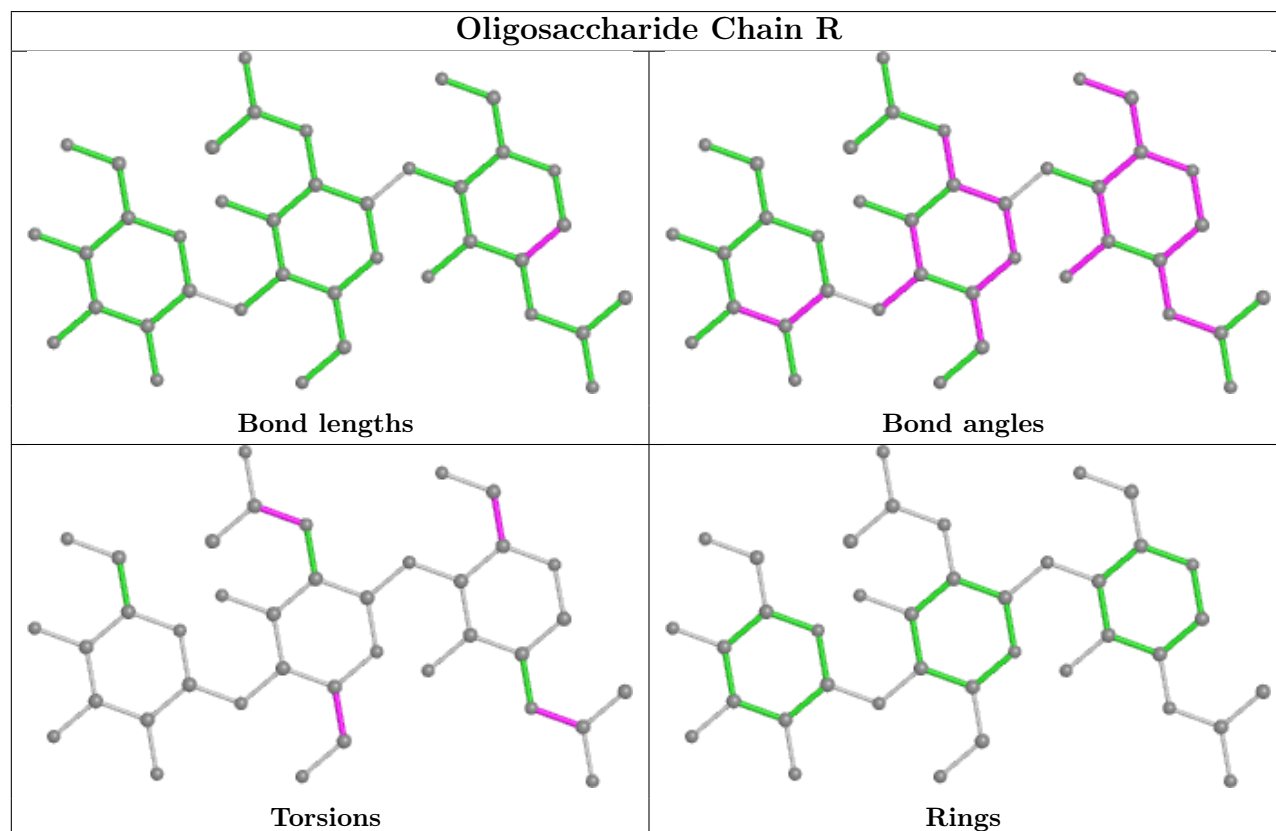
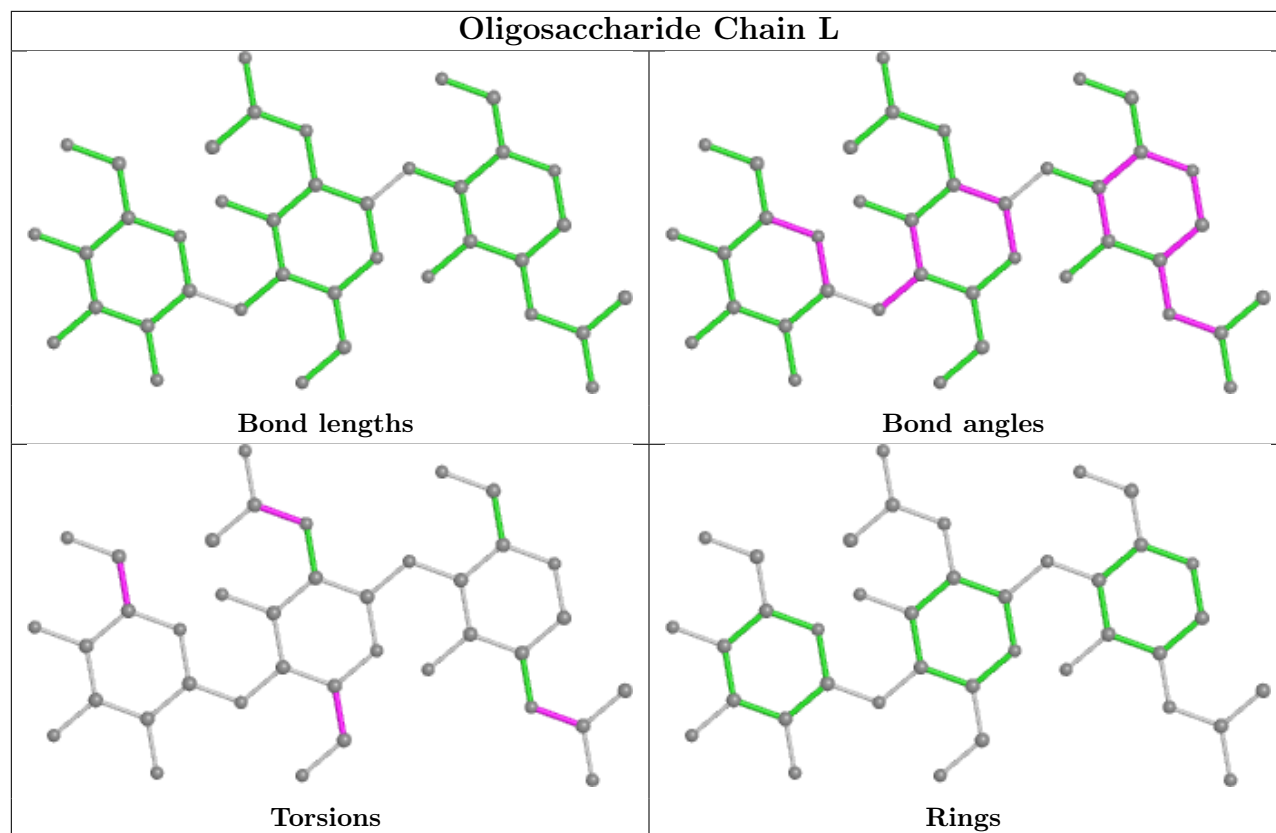


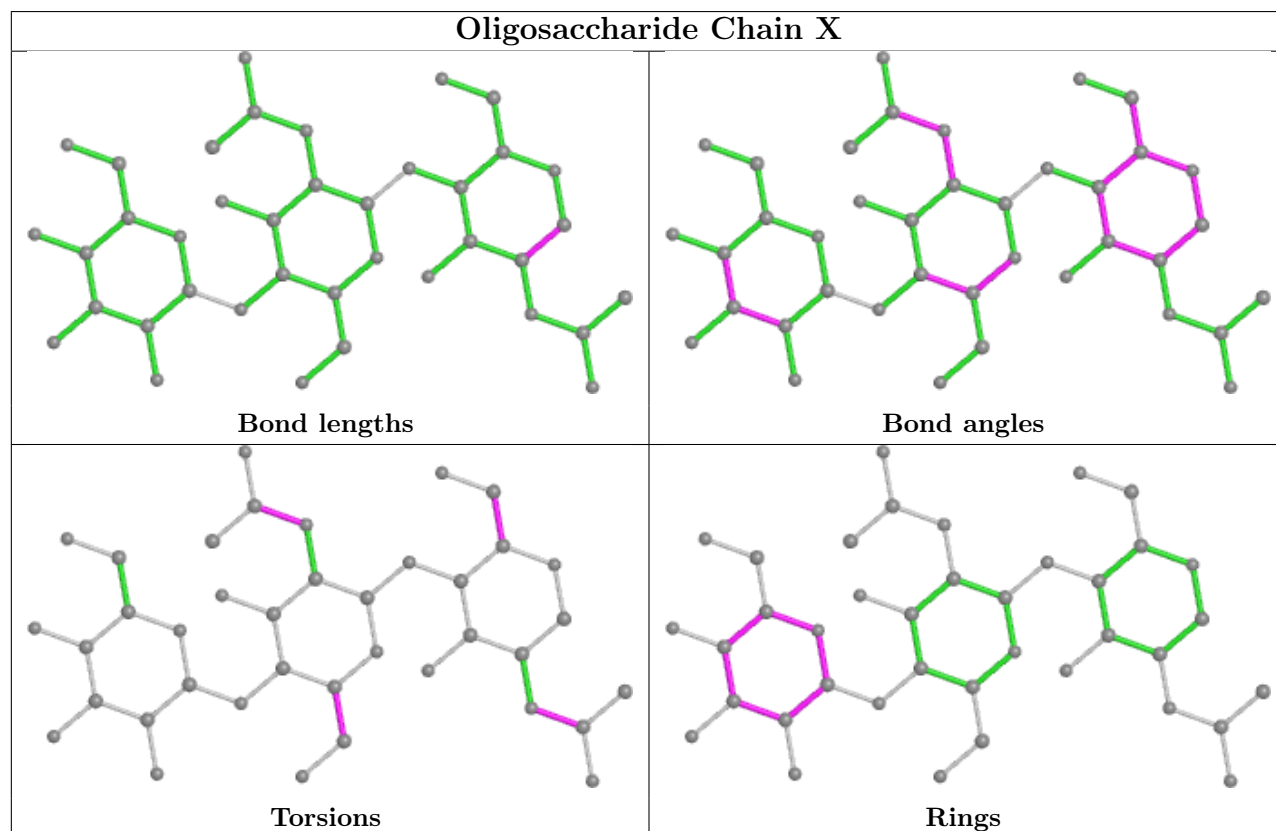
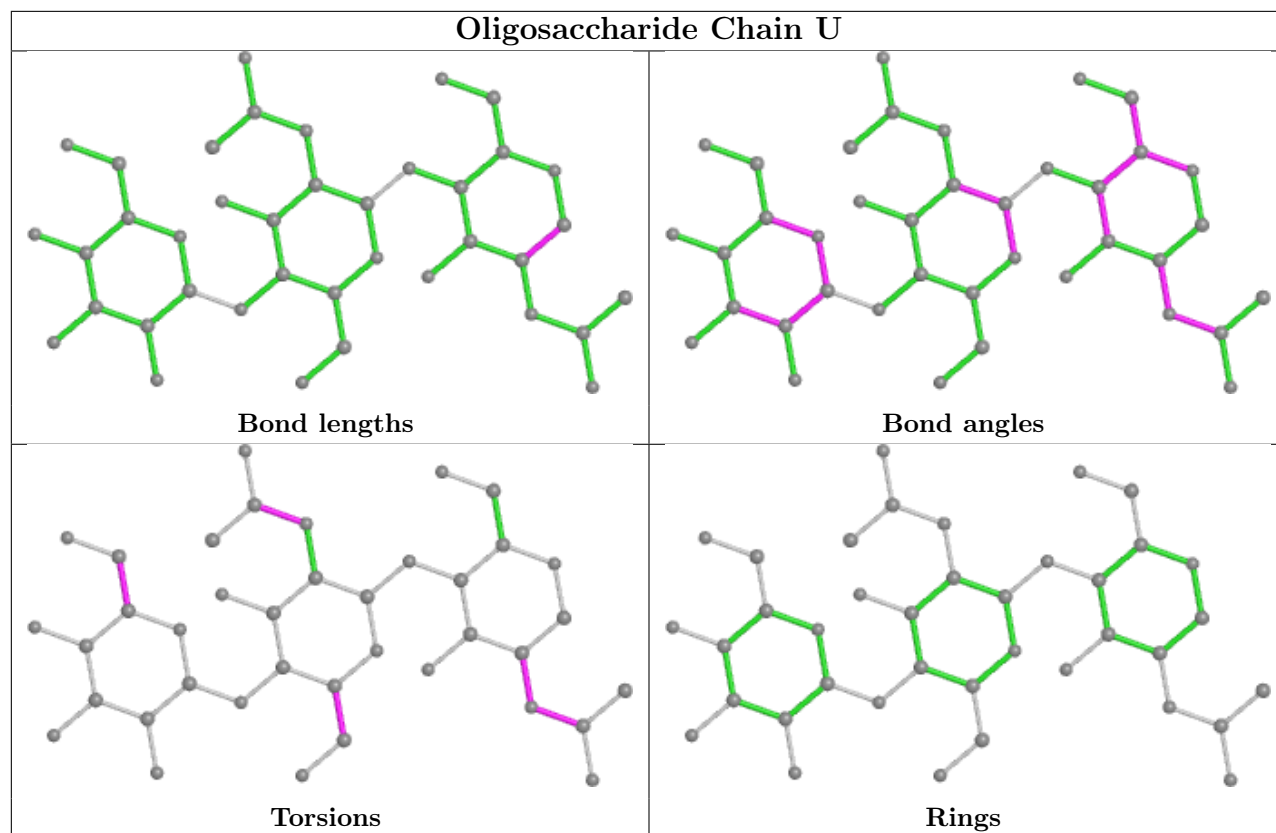












5.6 Ligand geometry

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	$\# Z > 2$
7	NAG	M	501	1	14,14,15	0.53	0	17,19,21	1.45	3 (17%)
11	CLR	F	501	-	31,31,31	0.31	0	48,48,48	0.57	0
7	NAG	A	501	1	14,14,15	0.52	0	17,19,21	1.45	3 (17%)
11	CLR	N	503	-	31,31,31	0.30	0	48,48,48	0.47	0
11	CLR	B	501	-	31,31,31	0.28	0	48,48,48	0.50	0
11	CLR	I	503	-	31,31,31	0.27	0	48,48,48	0.43	0
10	PLM	E	504	-	17,17,17	0.58	0	17,17,17	0.70	0
11	CLR	N	502	-	31,31,31	0.30	0	48,48,48	0.38	0
10	PLM	I	504	-	17,17,17	0.58	0	17,17,17	0.71	0
10	PLM	N	506	-	17,17,17	0.58	0	17,17,17	0.76	1 (5%)
9	STE	M	503	-	19,19,19	0.56	0	19,19,19	0.67	0
8	PCW	I	502	-	53,53,53	0.36	0	59,61,61	0.61	1 (1%)
11	CLR	J	503	-	31,31,31	0.28	0	48,48,48	0.68	1 (2%)
9	STE	E	503	-	19,19,19	0.55	0	19,19,19	0.67	0
7	NAG	I	501	1	14,14,15	0.52	0	17,19,21	1.44	3 (17%)
10	PLM	B	506	-	17,17,17	0.58	0	17,17,17	0.77	1 (5%)
11	CLR	B	503	-	31,31,31	0.26	0	48,48,48	0.57	1 (2%)
10	PLM	A	504	-	17,17,17	0.59	0	17,17,17	0.71	0
11	CLR	N	501	-	31,31,31	0.35	0	48,48,48	0.63	1 (2%)
9	STE	B	505	-	19,19,19	0.55	0	19,19,19	0.69	0
11	CLR	F	502	-	31,31,31	0.27	0	48,48,48	0.39	0
9	STE	J	505	-	19,19,19	0.55	0	19,19,19	0.69	0
10	PLM	N	504	-	17,17,17	0.58	0	17,17,17	0.68	0
10	PLM	F	504	-	17,17,17	0.58	0	17,17,17	0.67	0
10	PLM	F	506	-	17,17,17	0.57	0	17,17,17	0.77	1 (5%)
9	STE	A	503	-	19,19,19	0.57	0	19,19,19	0.67	0
10	PLM	M	504	-	17,17,17	0.58	0	17,17,17	0.70	0
8	PCW	E	502	-	53,53,53	0.42	0	59,61,61	0.98	4 (6%)
10	PLM	J	506	-	17,17,17	0.58	0	17,17,17	0.77	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	E	501	1	14,14,15	0.52	0	17,19,21	1.45	3 (17%)
10	PLM	J	504	-	17,17,17	0.58	0	17,17,17	0.68	0
8	PCW	M	502	-	53,53,53	0.31	0	59,61,61	0.30	0
8	PCW	A	502	-	53,53,53	0.31	0	59,61,61	0.31	0
9	STE	N	505	-	19,19,19	0.55	0	19,19,19	0.69	0
11	CLR	B	502	-	31,31,31	0.27	0	48,48,48	0.41	0
9	STE	J	501	-	19,19,19	0.56	0	19,19,19	0.67	0
11	CLR	F	503	-	31,31,31	0.27	0	48,48,48	0.44	0
9	STE	F	505	-	19,19,19	0.55	0	19,19,19	0.69	0
11	CLR	J	502	-	31,31,31	0.28	0	48,48,48	0.39	0
10	PLM	B	504	-	17,17,17	0.57	0	17,17,17	0.68	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
7	NAG	M	501	1	-	4/6/23/26	0/1/1/1
11	CLR	F	501	-	-	5/10/68/68	0/4/4/4
7	NAG	A	501	1	-	4/6/23/26	0/1/1/1
11	CLR	N	503	-	-	8/10/68/68	0/4/4/4
11	CLR	B	501	-	-	4/10/68/68	0/4/4/4
11	CLR	I	503	-	-	7/10/68/68	0/4/4/4
10	PLM	E	504	-	-	9/15/15/15	-
11	CLR	N	502	-	-	5/10/68/68	0/4/4/4
10	PLM	I	504	-	-	9/15/15/15	-
10	PLM	N	506	-	-	11/15/15/15	-
9	STE	M	503	-	-	10/17/17/17	-
8	PCW	I	502	-	-	28/57/57/57	-
11	CLR	J	503	-	-	5/10/68/68	0/4/4/4
9	STE	E	503	-	-	10/17/17/17	-
7	NAG	I	501	1	-	4/6/23/26	0/1/1/1
10	PLM	B	506	-	-	11/15/15/15	-
11	CLR	B	503	-	-	8/10/68/68	0/4/4/4
10	PLM	A	504	-	-	9/15/15/15	-
11	CLR	N	501	-	-	8/10/68/68	0/4/4/4
9	STE	B	505	-	-	11/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLR	F	502	-	-	4/10/68/68	0/4/4/4
9	STE	J	505	-	-	11/17/17/17	-
10	PLM	N	504	-	-	11/15/15/15	-
10	PLM	F	504	-	-	11/15/15/15	-
10	PLM	F	506	-	-	11/15/15/15	-
9	STE	A	503	-	-	10/17/17/17	-
10	PLM	M	504	-	-	9/15/15/15	-
8	PCW	E	502	-	-	31/57/57/57	-
10	PLM	J	506	-	-	11/15/15/15	-
7	NAG	E	501	1	-	4/6/23/26	0/1/1/1
10	PLM	J	504	-	-	11/15/15/15	-
8	PCW	M	502	-	-	31/57/57/57	-
8	PCW	A	502	-	-	27/57/57/57	-
9	STE	N	505	-	-	11/17/17/17	-
11	CLR	B	502	-	-	4/10/68/68	0/4/4/4
9	STE	J	501	-	-	10/17/17/17	-
11	CLR	F	503	-	-	4/10/68/68	0/4/4/4
9	STE	F	505	-	-	11/17/17/17	-
11	CLR	J	502	-	-	4/10/68/68	0/4/4/4
10	PLM	B	504	-	-	11/15/15/15	-

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	4.44	118.21	112.19
7	A	501	NAG	C1-O5-C5	4.44	118.21	112.19
7	M	501	NAG	C1-O5-C5	4.44	118.20	112.19
7	I	501	NAG	C1-O5-C5	4.40	118.15	112.19
8	E	502	PCW	O4P-P-O2P	-4.29	92.32	109.07
8	E	502	PCW	O2-C31-C32	3.33	118.67	111.50
8	E	502	PCW	O2-C31-O31	-2.76	117.04	123.70
11	J	503	CLR	C17-C13-C14	-2.40	97.23	100.07
8	E	502	PCW	O3P-P-O2P	2.36	118.28	109.07
8	I	502	PCW	O2-C31-O31	-2.29	118.16	123.70
7	E	501	NAG	O5-C1-C2	2.29	114.90	111.29
7	A	501	NAG	O5-C1-C2	2.28	114.89	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	501	NAG	O5-C1-C2	2.28	114.88	111.29
7	M	501	NAG	O5-C1-C2	2.27	114.87	111.29
11	B	503	CLR	C16-C17-C13	-2.26	101.12	103.84
7	A	501	NAG	C4-C3-C2	-2.10	107.94	111.02
11	N	501	CLR	C11-C9-C10	-2.09	110.33	113.08
7	I	501	NAG	C4-C3-C2	-2.05	108.01	111.02
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
10	J	506	PLM	O1-C1-C2	2.03	120.54	114.03
10	B	506	PLM	O1-C1-C2	2.03	120.54	114.03
10	F	506	PLM	O1-C1-C2	2.01	120.49	114.03
10	N	506	PLM	O1-C1-C2	2.00	120.47	114.03

There are no chirality outliers.

All (407) 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	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	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
8	M	502	PCW	C1-O3P-P-O1P
8	M	502	PCW	C4-O4P-P-O2P
11	B	502	CLR	C13-C17-C20-C21
11	B	502	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
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	C12-C13-C14-C15
7	I	501	NAG	O5-C5-C6-O6
7	M	501	NAG	O5-C5-C6-O6
8	A	502	PCW	C38-C39-C40-C41
8	E	502	PCW	C18-C19-C20-C21
7	A	501	NAG	O5-C5-C6-O6
7	E	501	NAG	O5-C5-C6-O6
11	F	501	CLR	C21-C20-C22-C23
11	B	503	CLR	C16-C17-C20-C22
11	N	502	CLR	C16-C17-C20-C22
11	N	503	CLR	C16-C17-C20-C22
11	N	501	CLR	C17-C20-C22-C23
11	N	503	CLR	C17-C20-C22-C23
8	E	502	PCW	C14-C15-C16-C17
8	I	502	PCW	C41-C42-C43-C44
11	B	503	CLR	C17-C20-C22-C23
8	I	502	PCW	C44-C45-C46-C47
8	M	502	PCW	C43-C44-C45-C46
8	A	502	PCW	C15-C16-C17-C18
7	M	501	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
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	C12-C11-O3-C3
7	A	501	NAG	C4-C5-C6-O6
7	E	501	NAG	C4-C5-C6-O6
7	I	501	NAG	C4-C5-C6-O6
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	I	502	PCW	O11-C11-O3-C3
8	A	502	PCW	C22-C23-C24-C25
8	A	502	PCW	C11-C12-C13-C14
8	A	502	PCW	C31-C32-C33-C34
8	E	502	PCW	C11-C12-C13-C14
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
8	A	502	PCW	C18-C19-C20-C21
11	N	501	CLR	C13-C17-C20-C22
8	M	502	PCW	C4-C5-N-C6
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	503	CLR	C20-C22-C23-C24
8	I	502	PCW	C38-C39-C40-C41
11	N	502	CLR	C20-C22-C23-C24
8	A	502	PCW	C4-O4P-P-O3P
8	I	502	PCW	C4-O4P-P-O3P
11	N	501	CLR	C13-C17-C20-C21
8	A	502	PCW	C32-C33-C34-C35
8	I	502	PCW	C32-C33-C34-C35
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
10	N	504	PLM	C6-C7-C8-C9
8	E	502	PCW	C23-C24-C25-C26
8	M	502	PCW	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
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	E	502	PCW	C44-C45-C46-C47
9	A	503	STE	C14-C15-C16-C17
10	A	504	PLM	C7-C8-C9-CA
10	B	504	PLM	CC-CD-CE-CF
10	E	504	PLM	C7-C8-C9-CA
10	I	504	PLM	C7-C8-C9-CA
10	J	504	PLM	CC-CD-CE-CF
10	M	504	PLM	C7-C8-C9-CA
10	N	504	PLM	CC-CD-CE-CF
8	A	502	PCW	C44-C45-C46-C47
8	E	502	PCW	C13-C14-C15-C16
8	M	502	PCW	C13-C14-C15-C16
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	F	504	PLM	CC-CD-CE-CF
9	A	503	STE	C9-C10-C11-C12
9	B	505	STE	C14-C15-C16-C17
9	E	503	STE	C9-C10-C11-C12
9	F	505	STE	C14-C15-C16-C17
9	J	501	STE	C9-C10-C11-C12
9	J	505	STE	C14-C15-C16-C17
9	M	503	STE	C9-C10-C11-C12
9	N	505	STE	C14-C15-C16-C17
10	B	504	PLM	C3-C4-C5-C6
10	F	504	PLM	C3-C4-C5-C6
10	J	504	PLM	C3-C4-C5-C6
10	N	504	PLM	C3-C4-C5-C6
10	B	506	PLM	C7-C8-C9-CA
10	E	504	PLM	C6-C7-C8-C9
10	F	506	PLM	C7-C8-C9-CA
10	M	504	PLM	C6-C7-C8-C9
10	N	506	PLM	C7-C8-C9-CA
10	A	504	PLM	C6-C7-C8-C9
10	I	504	PLM	C6-C7-C8-C9
10	J	506	PLM	C7-C8-C9-CA
10	A	504	PLM	C3-C4-C5-C6
10	E	504	PLM	C3-C4-C5-C6
10	I	504	PLM	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
10	M	504	PLM	C3-C4-C5-C6
8	I	502	PCW	C15-C16-C17-C18
8	E	502	PCW	C33-C34-C35-C36
8	M	502	PCW	C14-C15-C16-C17
8	M	502	PCW	C15-C16-C17-C18
10	A	504	PLM	CC-CD-CE-CF
10	E	504	PLM	CC-CD-CE-CF
10	I	504	PLM	CC-CD-CE-CF
10	M	504	PLM	CC-CD-CE-CF
8	E	502	PCW	C4-C5-N-C6
8	M	502	PCW	C4-C5-N-C8
8	A	502	PCW	C13-C14-C15-C16
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
11	F	501	CLR	C22-C23-C24-C25
8	I	502	PCW	C12-C13-C14-C15
9	A	503	STE	C4-C5-C6-C7
9	E	503	STE	C4-C5-C6-C7
8	I	502	PCW	C18-C19-C20-C21
9	J	501	STE	C4-C5-C6-C7
9	M	503	STE	C4-C5-C6-C7
8	E	502	PCW	C24-C25-C26-C27
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	A	502	PCW	C40-C41-C42-C43
8	I	502	PCW	C36-C37-C38-C39
8	M	502	PCW	C36-C37-C38-C39
9	A	503	STE	C3-C4-C5-C6
9	B	505	STE	C10-C11-C12-C13
9	E	503	STE	C3-C4-C5-C6
9	F	505	STE	C10-C11-C12-C13
9	J	501	STE	C3-C4-C5-C6
9	M	503	STE	C3-C4-C5-C6
9	N	505	STE	C10-C11-C12-C13
9	J	505	STE	C10-C11-C12-C13
9	M	503	STE	C10-C11-C12-C13
8	E	502	PCW	C35-C36-C37-C38
9	A	503	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	E	503	STE	C10-C11-C12-C13
9	J	501	STE	C10-C11-C12-C13
10	B	506	PLM	C5-C6-C7-C8
10	F	506	PLM	C5-C6-C7-C8
10	J	506	PLM	C5-C6-C7-C8
10	N	506	PLM	C5-C6-C7-C8
11	N	501	CLR	C16-C17-C20-C21
8	M	502	PCW	C40-C41-C42-C43
8	M	502	PCW	O31-C31-O2-C2
10	B	506	PLM	C1-C2-C3-C4
10	F	506	PLM	C1-C2-C3-C4
10	J	506	PLM	C1-C2-C3-C4
10	N	506	PLM	C1-C2-C3-C4
8	A	502	PCW	C41-C42-C43-C44
8	M	502	PCW	C35-C36-C37-C38
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	E	502	PCW	C34-C35-C36-C37
8	I	502	PCW	C33-C34-C35-C36
10	B	504	PLM	C5-C6-C7-C8
10	B	504	PLM	C7-C8-C9-CA
10	F	504	PLM	C5-C6-C7-C8
10	J	504	PLM	C5-C6-C7-C8
10	J	504	PLM	C7-C8-C9-CA
10	N	504	PLM	C5-C6-C7-C8
8	M	502	PCW	C32-C31-O2-C2
10	F	504	PLM	C7-C8-C9-CA
10	N	504	PLM	C7-C8-C9-CA
8	E	502	PCW	C40-C41-C42-C43
8	M	502	PCW	C16-C17-C18-C19
8	I	502	PCW	C22-C23-C24-C25
8	E	502	PCW	C41-C42-C43-C44
8	E	502	PCW	C4-O4P-P-O3P
8	M	502	PCW	C4-O4P-P-O3P
9	A	503	STE	C6-C7-C8-C9
9	J	501	STE	C6-C7-C8-C9
10	B	506	PLM	C9-CA-CB-CC
10	F	506	PLM	C9-CA-CB-CC
10	N	506	PLM	C9-CA-CB-CC
9	E	503	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
9	M	503	STE	C6-C7-C8-C9
10	J	506	PLM	C9-CA-CB-CC
8	M	502	PCW	O3P-C1-C2-C3
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
8	E	502	PCW	C16-C17-C18-C19
8	M	502	PCW	C12-C13-C14-C15
8	A	502	PCW	C1-C2-C3-O3
11	N	501	CLR	C16-C17-C20-C22
11	J	503	CLR	C21-C20-C22-C23
9	J	505	STE	C9-C10-C11-C12
9	B	505	STE	C9-C10-C11-C12
9	F	505	STE	C9-C10-C11-C12
9	N	505	STE	C9-C10-C11-C12
8	I	502	PCW	C20-C21-C22-C23
8	I	502	PCW	C37-C38-C39-C40
8	A	502	PCW	C25-C26-C27-C28
9	B	505	STE	C2-C3-C4-C5
9	F	505	STE	C2-C3-C4-C5
9	J	505	STE	C2-C3-C4-C5
9	N	505	STE	C2-C3-C4-C5
10	F	506	PLM	CC-CD-CE-CF
10	J	506	PLM	CC-CD-CE-CF
10	B	506	PLM	CC-CD-CE-CF
10	N	506	PLM	CC-CD-CE-CF
8	E	502	PCW	O2-C2-C3-O3
10	M	504	PLM	C2-C3-C4-C5
10	A	504	PLM	C2-C3-C4-C5
10	E	504	PLM	C2-C3-C4-C5
10	I	504	PLM	C2-C3-C4-C5
8	M	502	PCW	C45-C46-C47-C48
11	I	503	CLR	C16-C17-C20-C21
11	I	503	CLR	C21-C20-C22-C23
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
8	I	502	PCW	C25-C26-C27-C28
8	I	502	PCW	C39-C40-C41-C42

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

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Mol	Chain	Res	Type	Atoms
10	F	504	PLM	CD-CE-CF-CG
10	B	504	PLM	CD-CE-CF-CG
11	J	503	CLR	C16-C17-C20-C22
10	N	504	PLM	CD-CE-CF-CG
8	A	502	PCW	O3-C11-C12-C13
10	J	504	PLM	CD-CE-CF-CG
10	B	506	PLM	C8-C9-CA-CB
10	N	506	PLM	C8-C9-CA-CB
9	M	503	STE	C2-C3-C4-C5
10	F	506	PLM	C8-C9-CA-CB
10	J	506	PLM	C8-C9-CA-CB
9	J	501	STE	C2-C3-C4-C5
9	A	503	STE	C2-C3-C4-C5
9	E	503	STE	C2-C3-C4-C5
11	B	501	CLR	C23-C24-C25-C27
8	E	502	PCW	C2-C1-O3P-P
9	B	505	STE	C1-C2-C3-C4
9	J	505	STE	C1-C2-C3-C4
10	E	504	PLM	CB-CC-CD-CE
9	F	505	STE	C1-C2-C3-C4
10	A	504	PLM	CB-CC-CD-CE
10	M	504	PLM	CB-CC-CD-CE
10	I	504	PLM	CB-CC-CD-CE
9	N	505	STE	C1-C2-C3-C4
11	J	503	CLR	C13-C17-C20-C22
8	A	502	PCW	C34-C35-C36-C37
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	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
9	B	505	STE	O1-C1-C2-C3
10	J	506	PLM	O2-C1-C2-C3
10	N	506	PLM	O2-C1-C2-C3
9	F	505	STE	O1-C1-C2-C3
9	J	505	STE	O1-C1-C2-C3
9	N	505	STE	O1-C1-C2-C3
10	B	506	PLM	O2-C1-C2-C3
10	F	506	PLM	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
11	F	501	CLR	C20-C22-C23-C24
8	I	502	PCW	C19-C20-C21-C22
11	N	501	CLR	C20-C22-C23-C24
11	J	503	CLR	C13-C17-C20-C21
10	B	506	PLM	O1-C1-C2-C3
11	B	501	CLR	C16-C17-C20-C22
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
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	B	501	CLR	C13-C17-C20-C21
11	I	503	CLR	C23-C24-C25-C26
8	M	502	PCW	C19-C20-C21-C22
8	E	502	PCW	C19-C20-C21-C22
8	E	502	PCW	C37-C38-C39-C40
8	M	502	PCW	C17-C18-C19-C20
8	A	502	PCW	C39-C40-C41-C42
9	F	505	STE	C11-C12-C13-C14
8	I	502	PCW	C43-C44-C45-C46
9	J	505	STE	C11-C12-C13-C14
9	N	505	STE	C11-C12-C13-C14
8	E	502	PCW	C45-C46-C47-C48
9	B	505	STE	C11-C12-C13-C14
11	F	501	CLR	C17-C20-C22-C23
11	B	501	CLR	C21-C20-C22-C23
11	N	503	CLR	C23-C24-C25-C27
8	M	502	PCW	C1-O3P-P-O2P
8	I	502	PCW	O3P-C1-C2-C3
8	A	502	PCW	C24-C25-C26-C27
10	F	504	PLM	CB-CC-CD-CE
11	B	503	CLR	C20-C22-C23-C24
10	B	504	PLM	CB-CC-CD-CE
10	J	504	PLM	CB-CC-CD-CE
10	N	504	PLM	CB-CC-CD-CE
10	B	506	PLM	C2-C3-C4-C5
10	F	506	PLM	C2-C3-C4-C5
10	J	506	PLM	C2-C3-C4-C5
10	N	506	PLM	C2-C3-C4-C5
8	I	502	PCW	O2-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
8	A	502	PCW	C2-C1-O3P-P
8	I	502	PCW	O31-C31-C32-C33
8	M	502	PCW	C39-C40-C41-C42
11	F	501	CLR	C13-C17-C20-C21

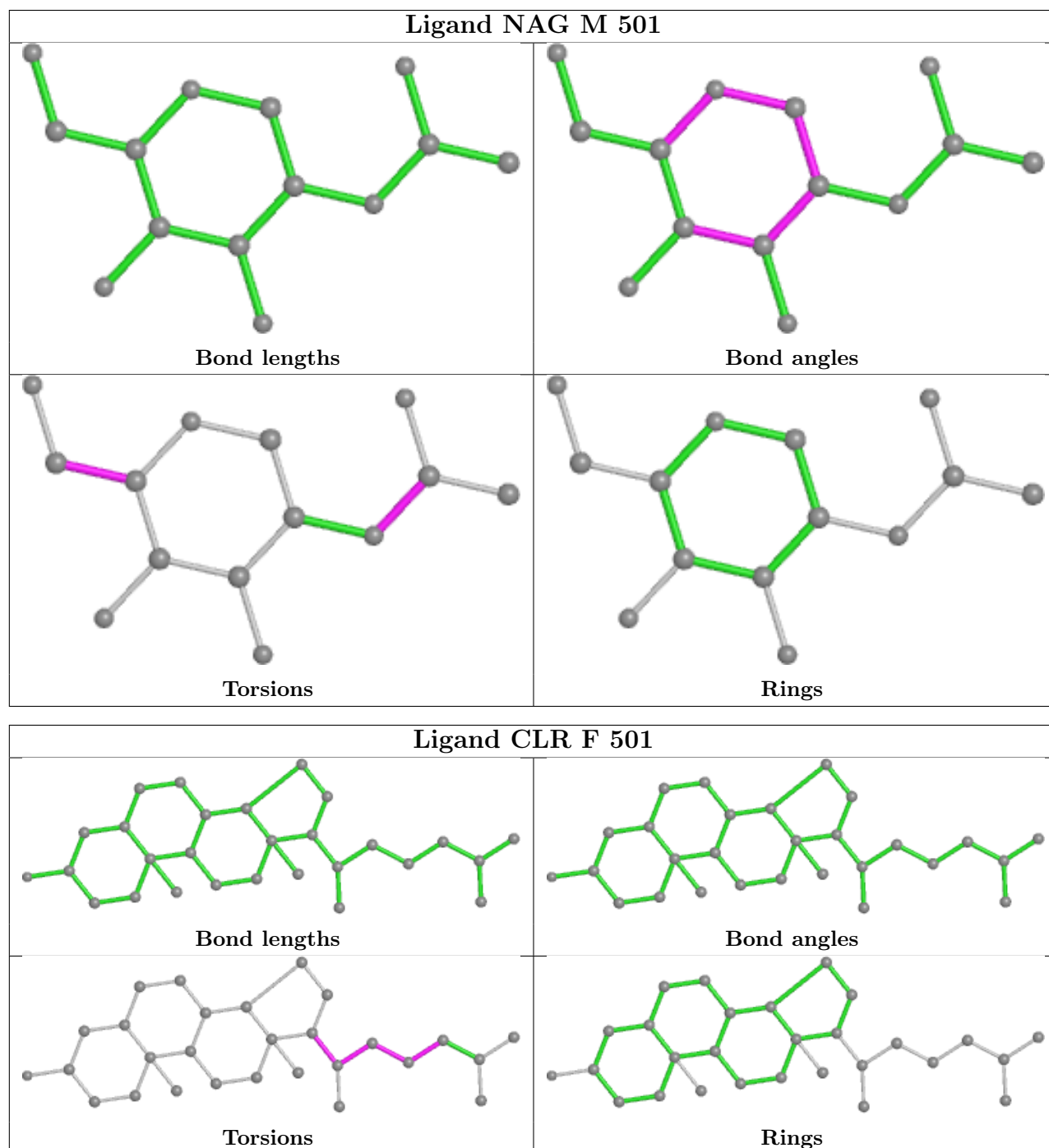
There are no ring outliers.

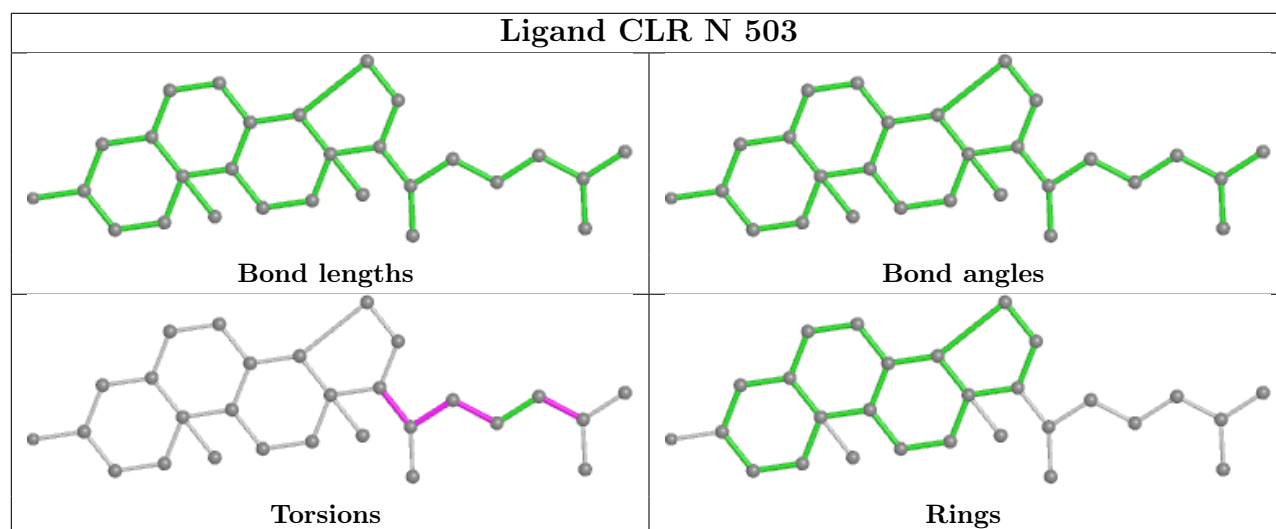
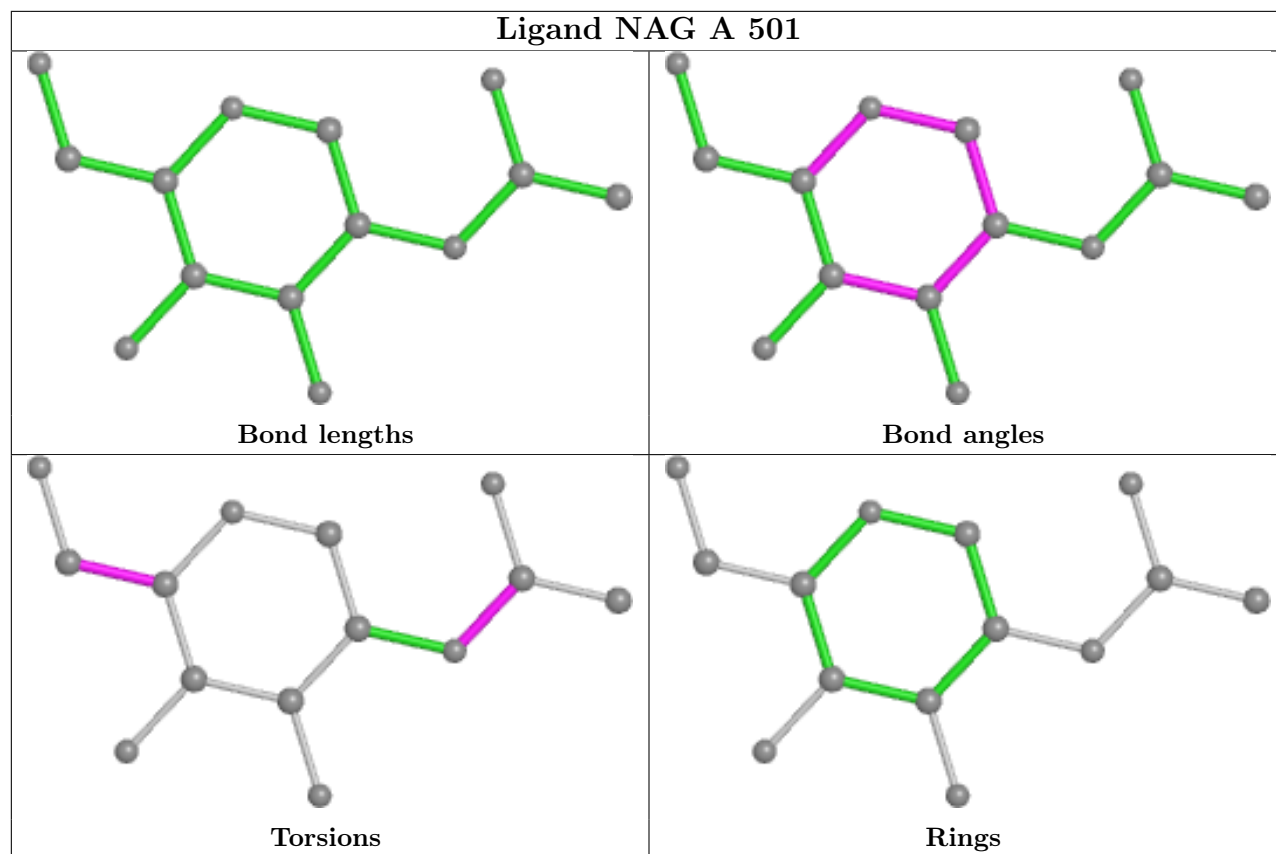
29 monomers are involved in 63 short contacts:

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

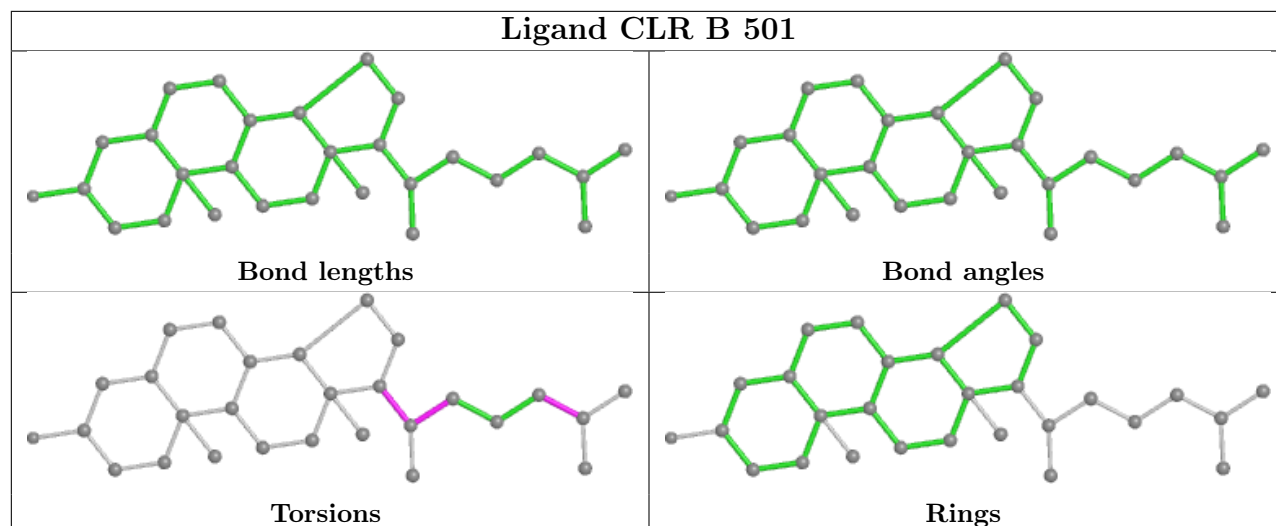
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

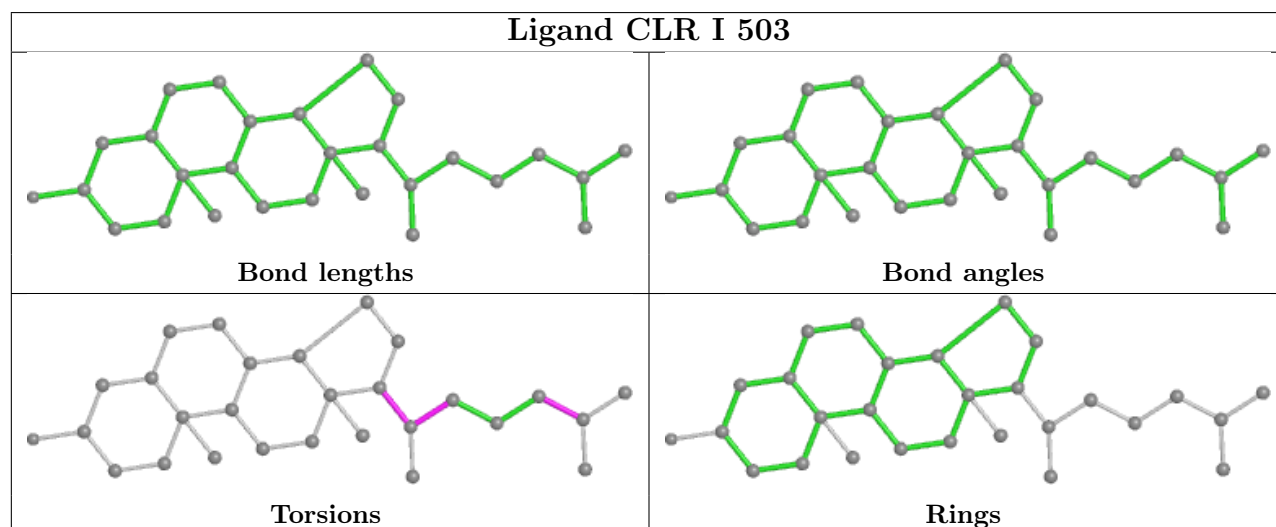




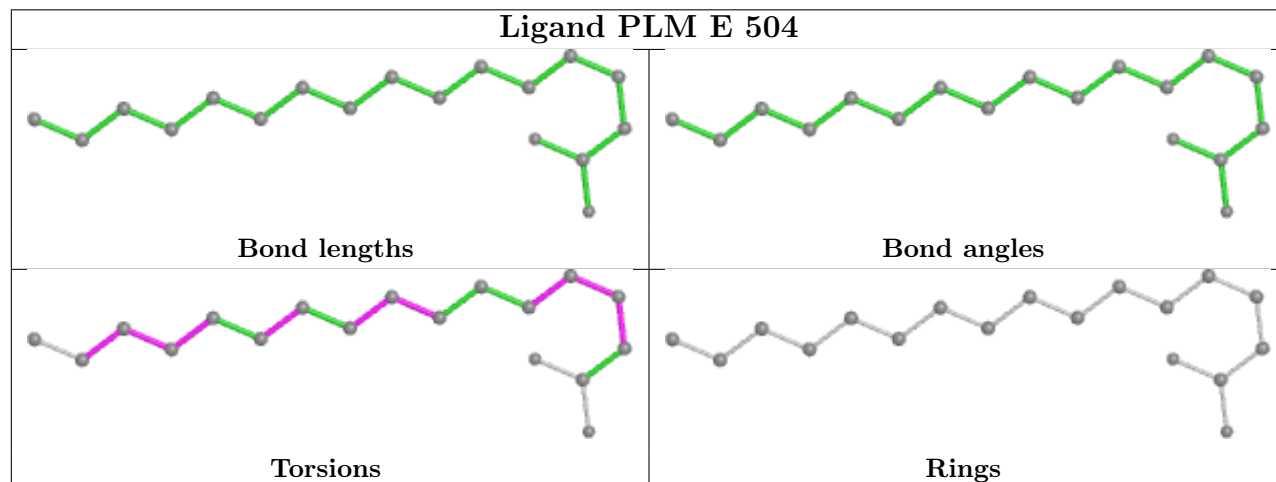
Ligand CLR B 501

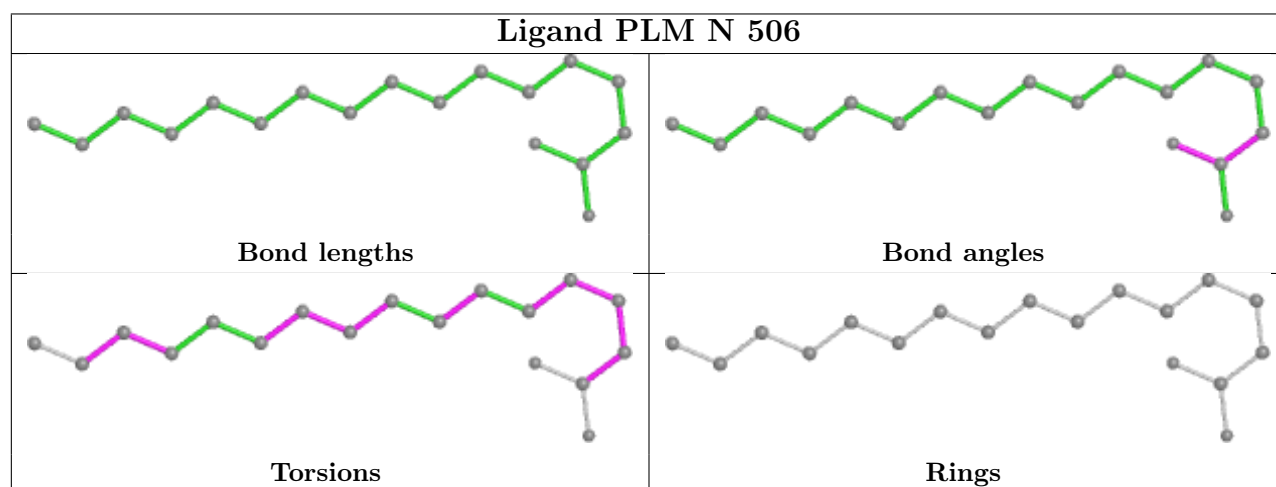
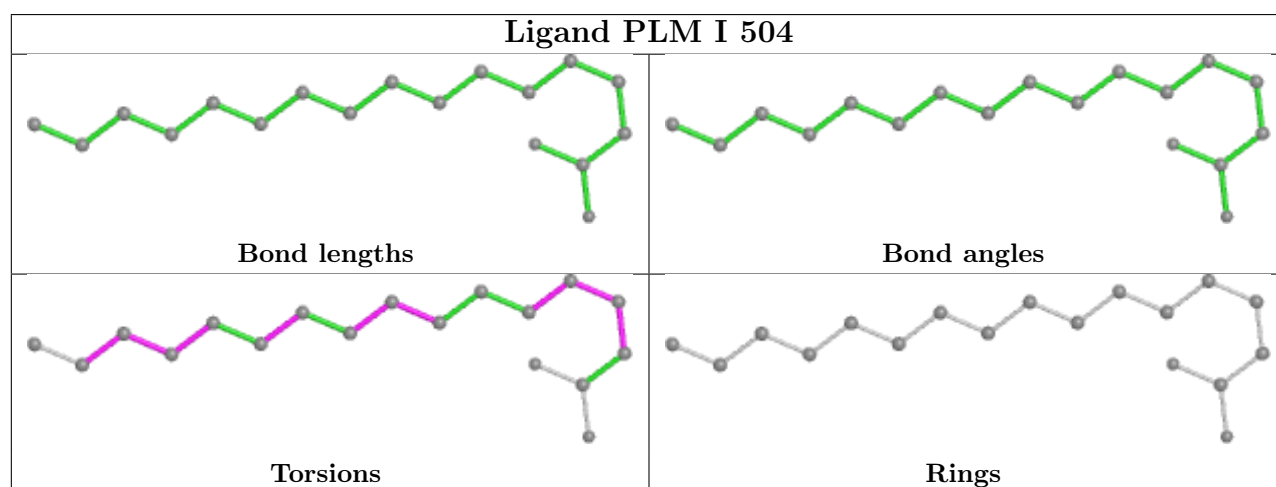
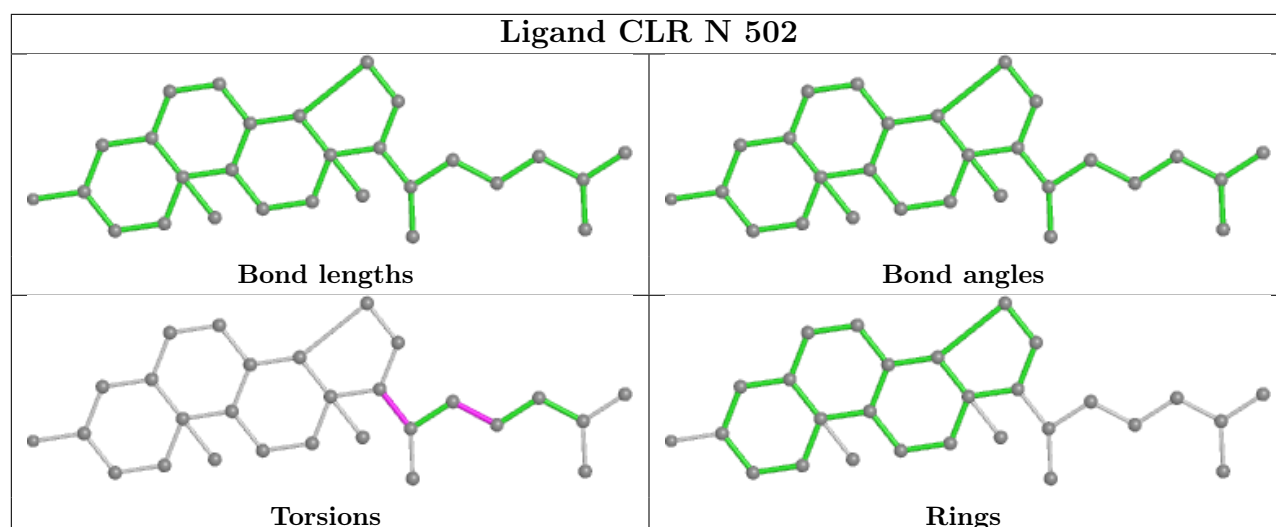


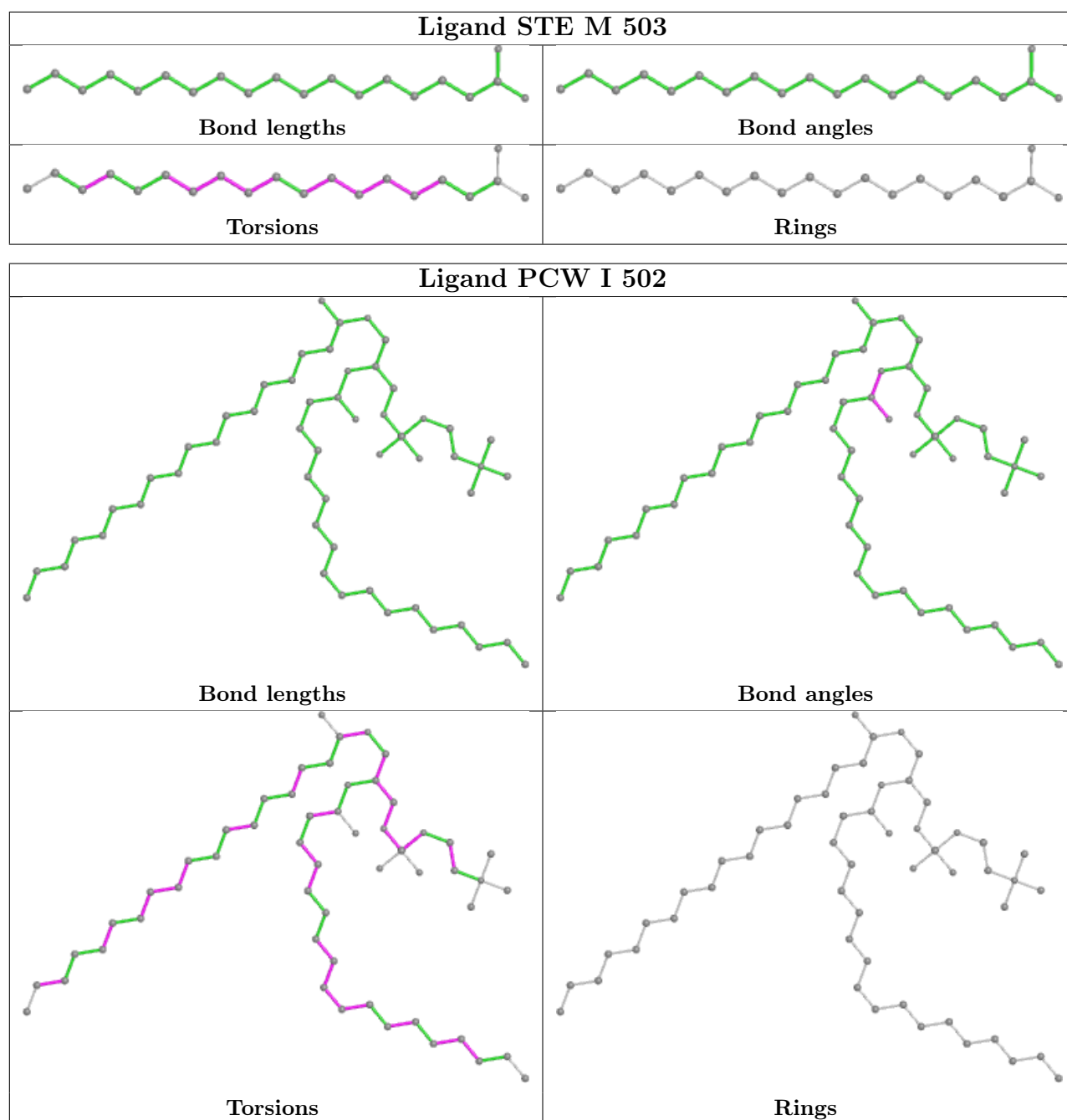
Ligand CLR I 503

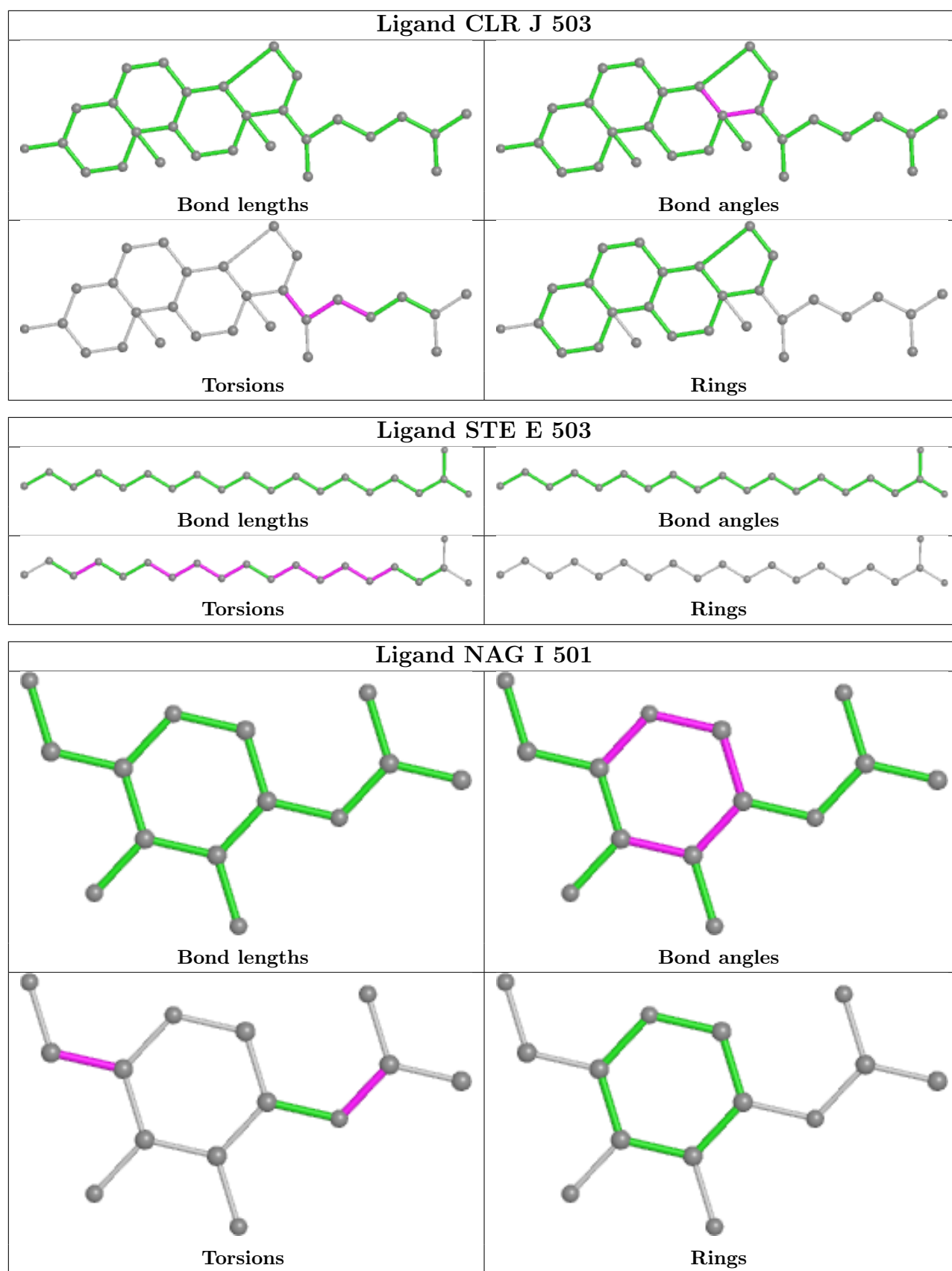


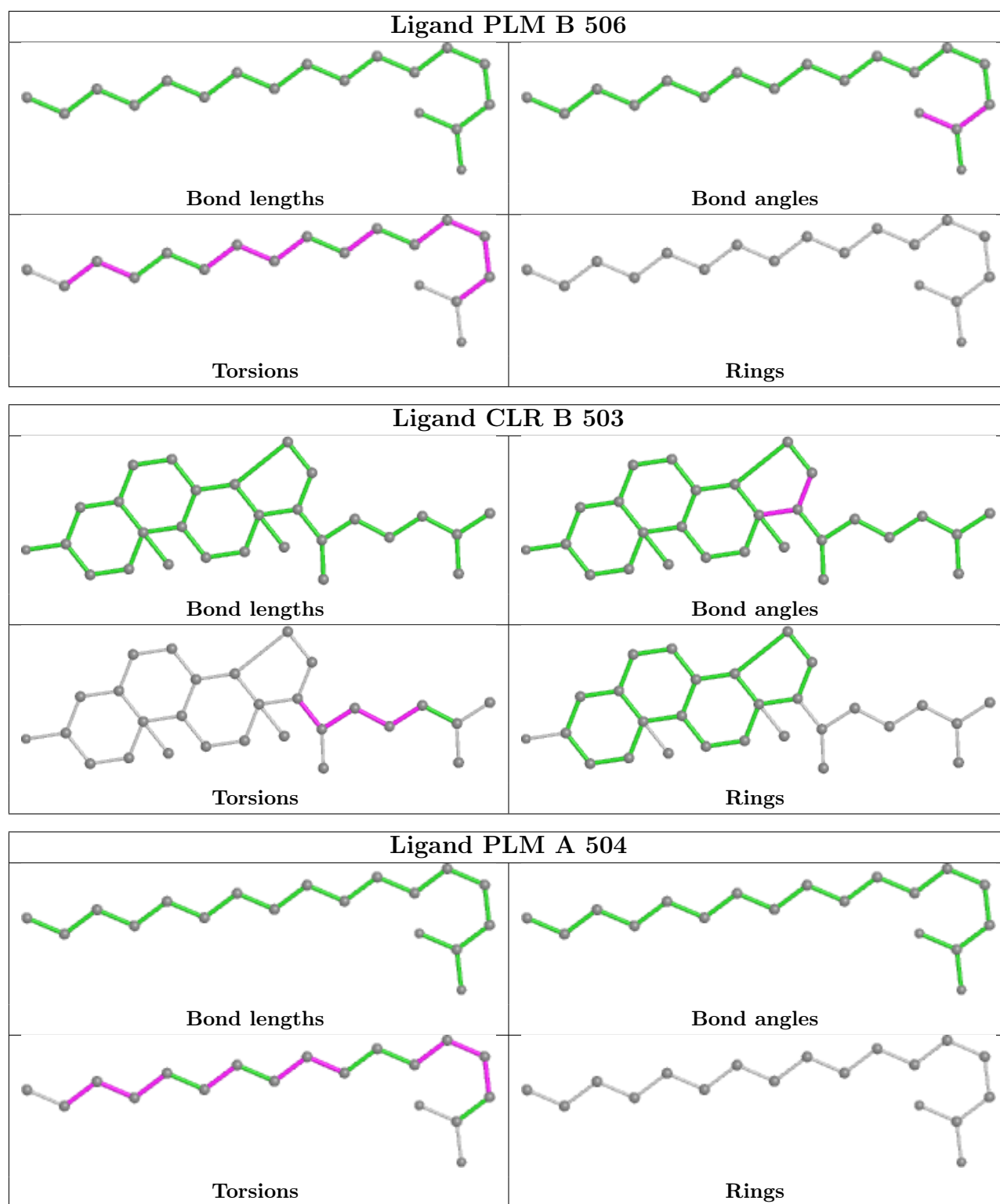
Ligand PLM E 504

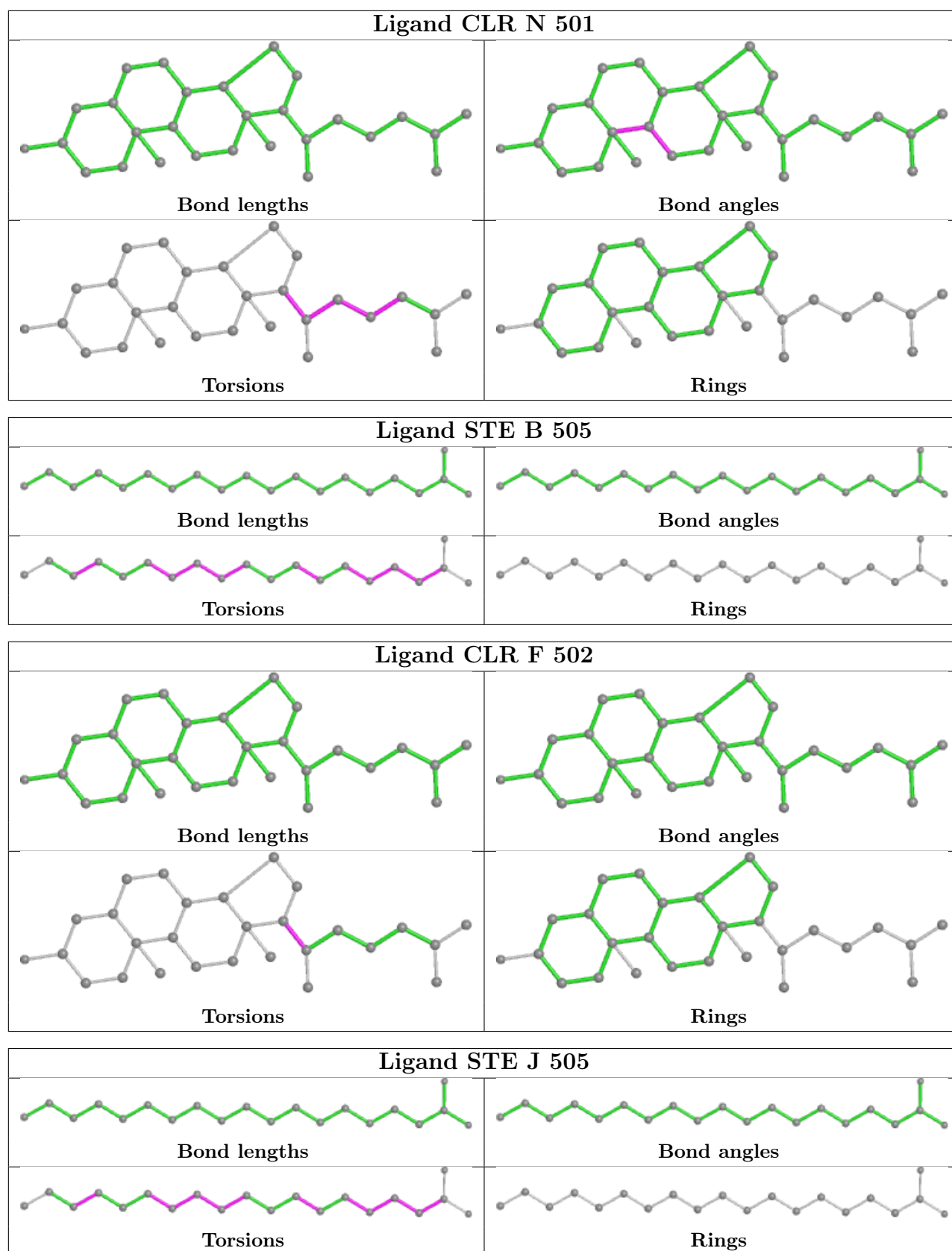


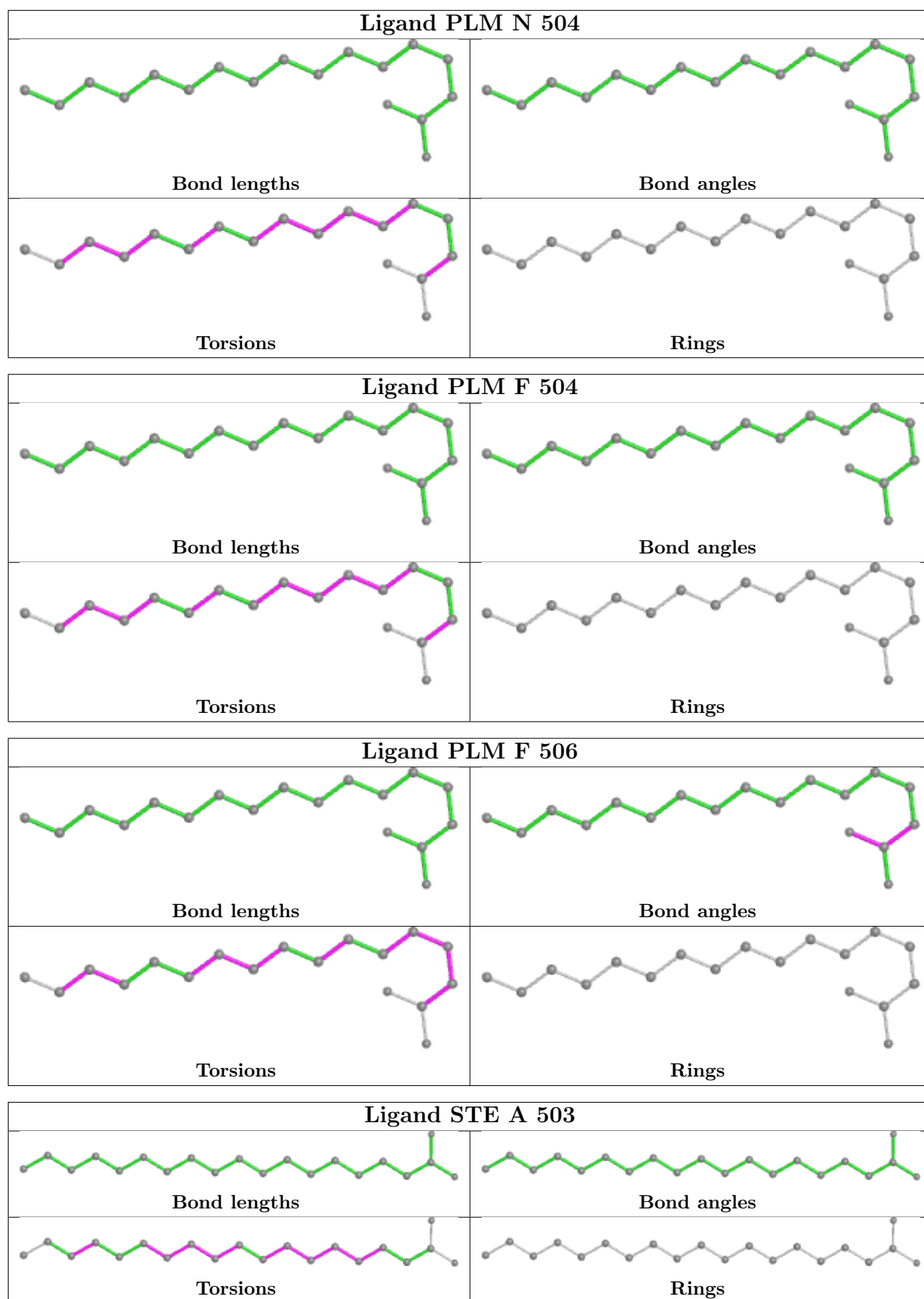


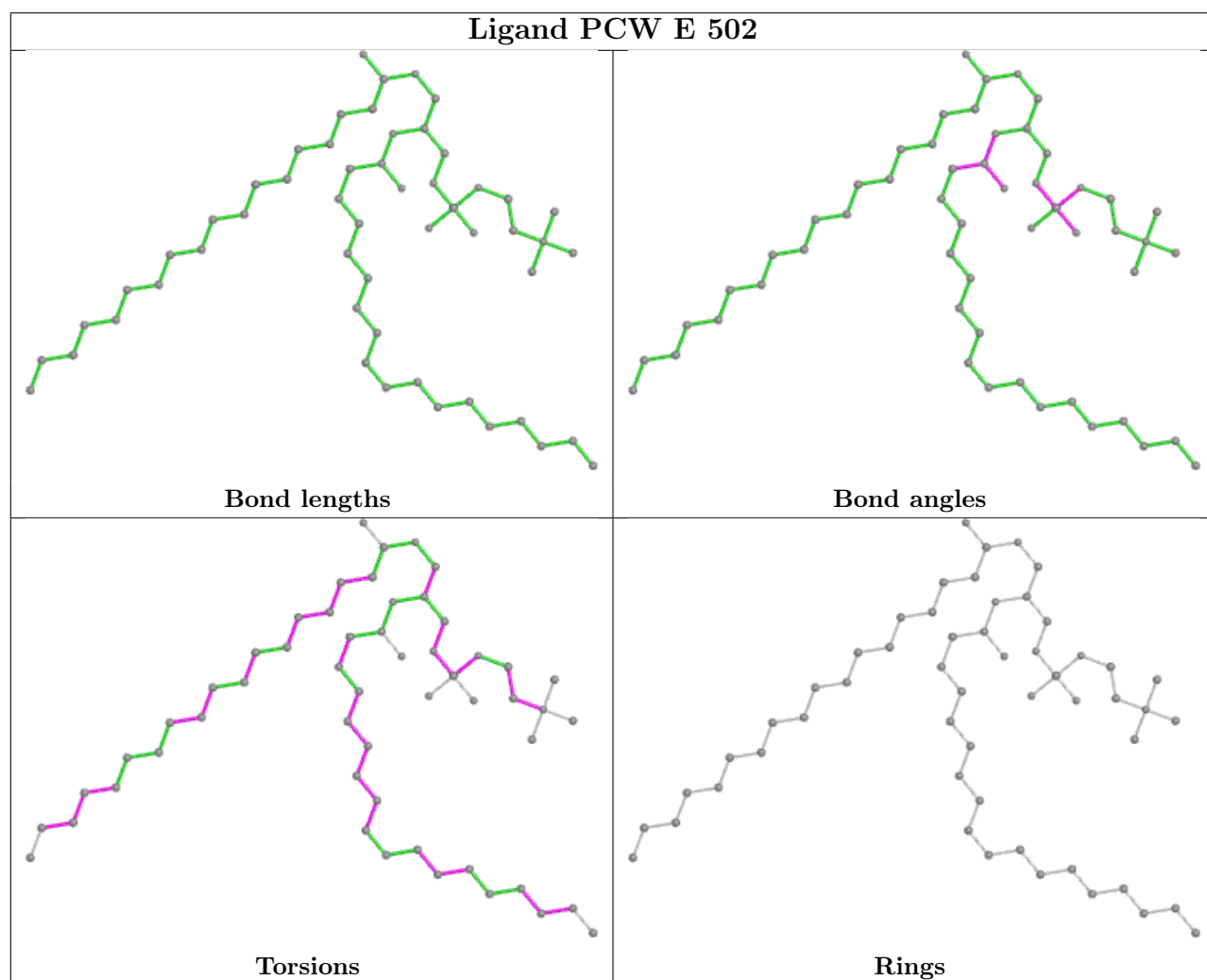
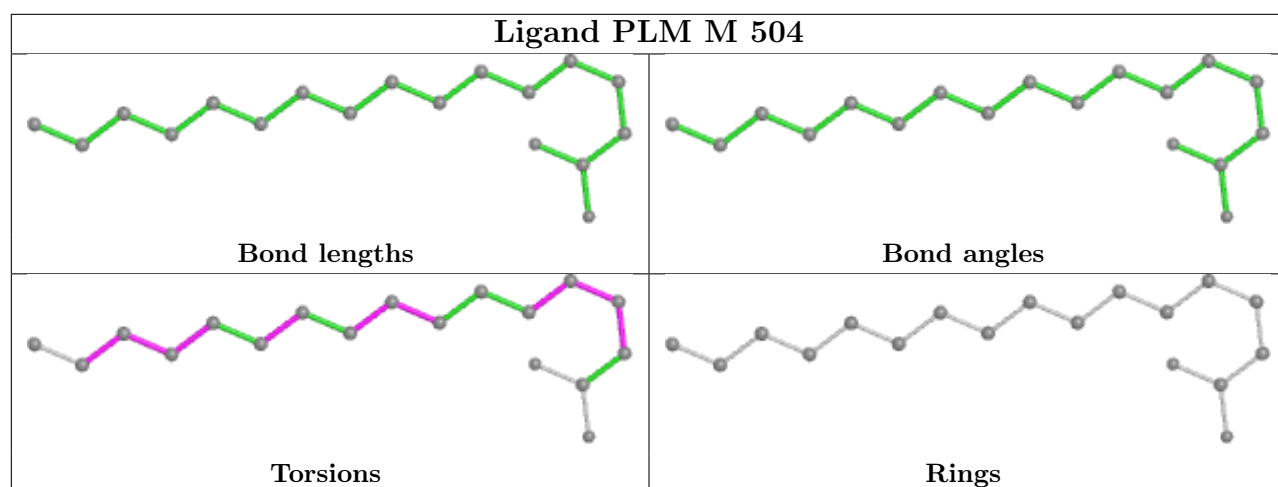


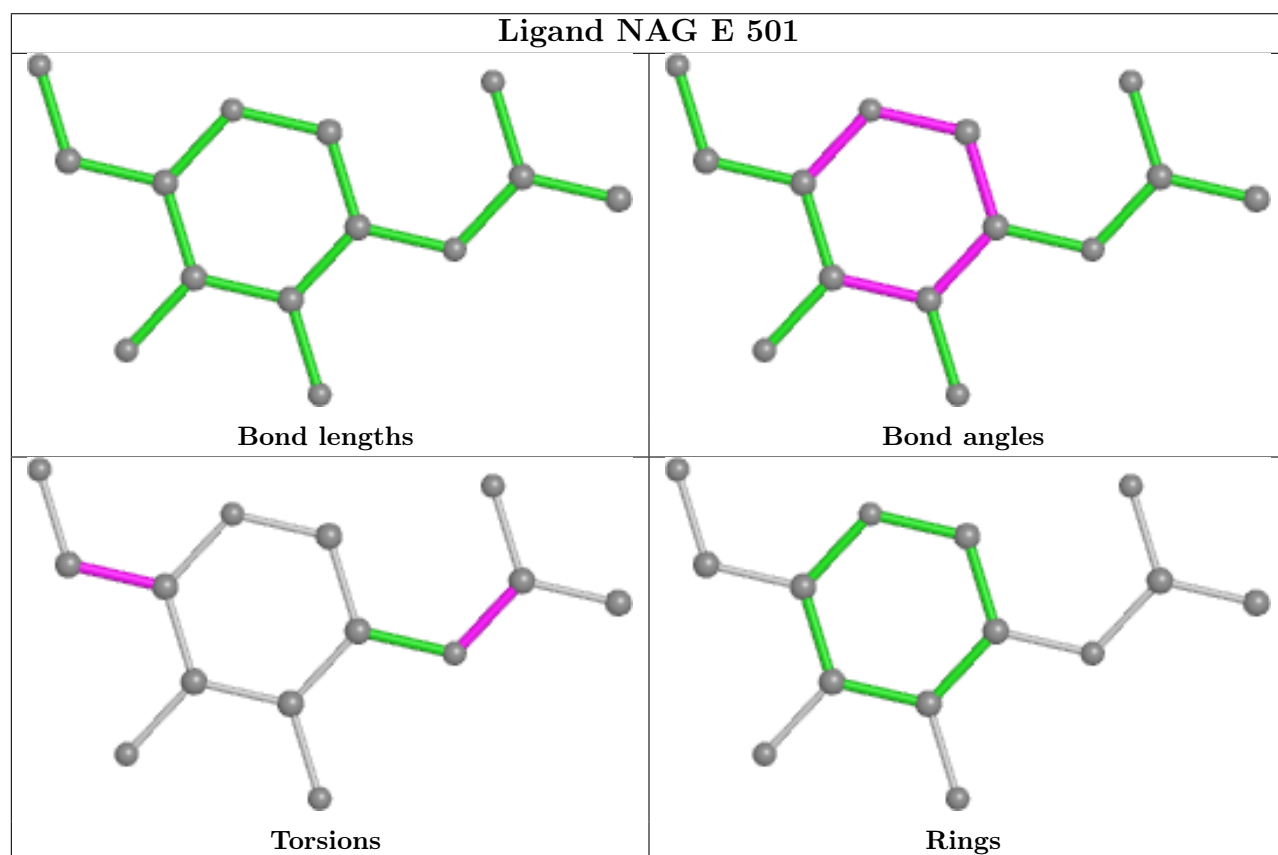
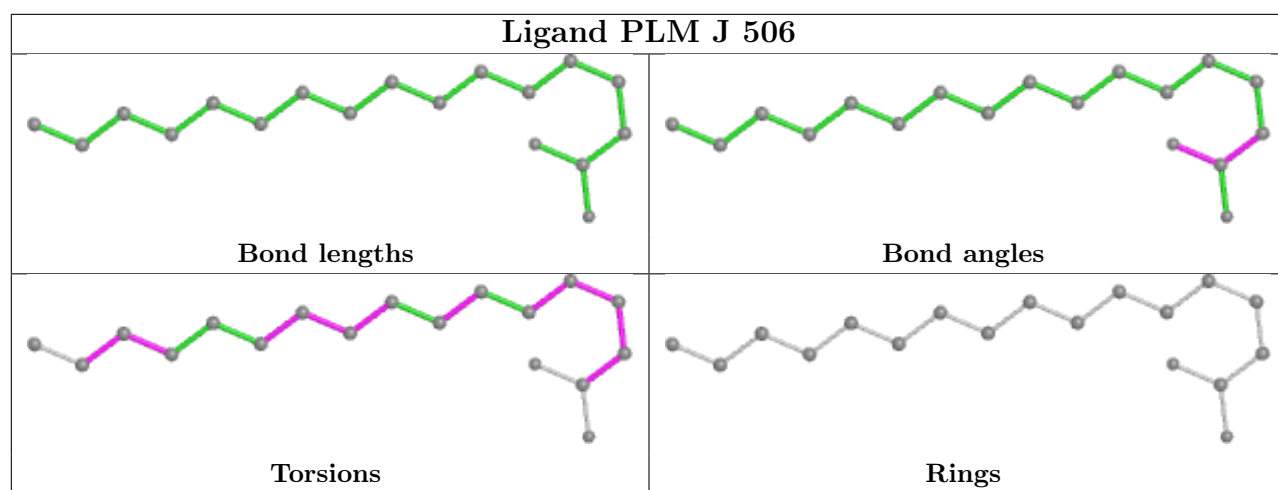


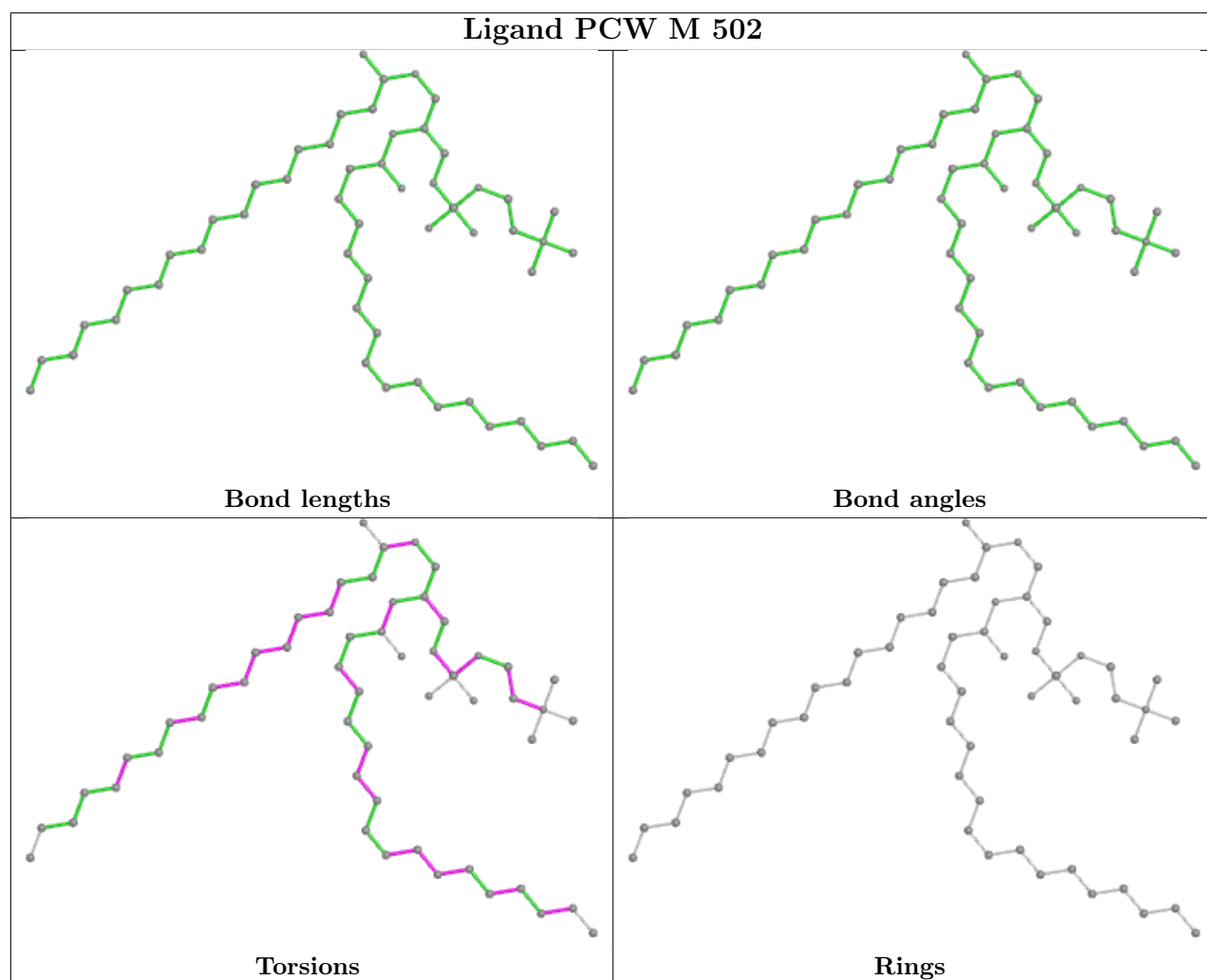
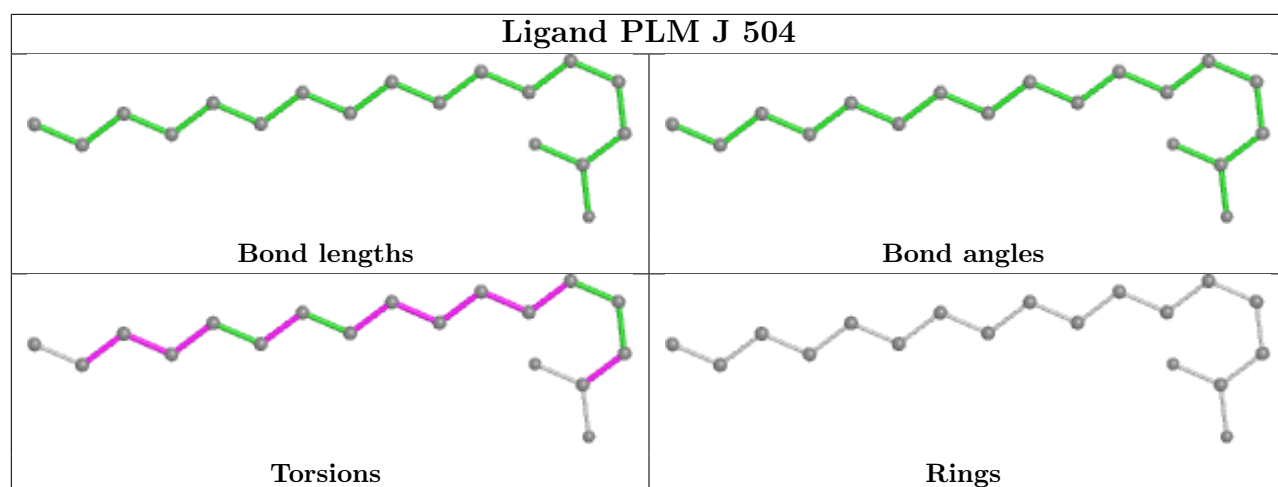


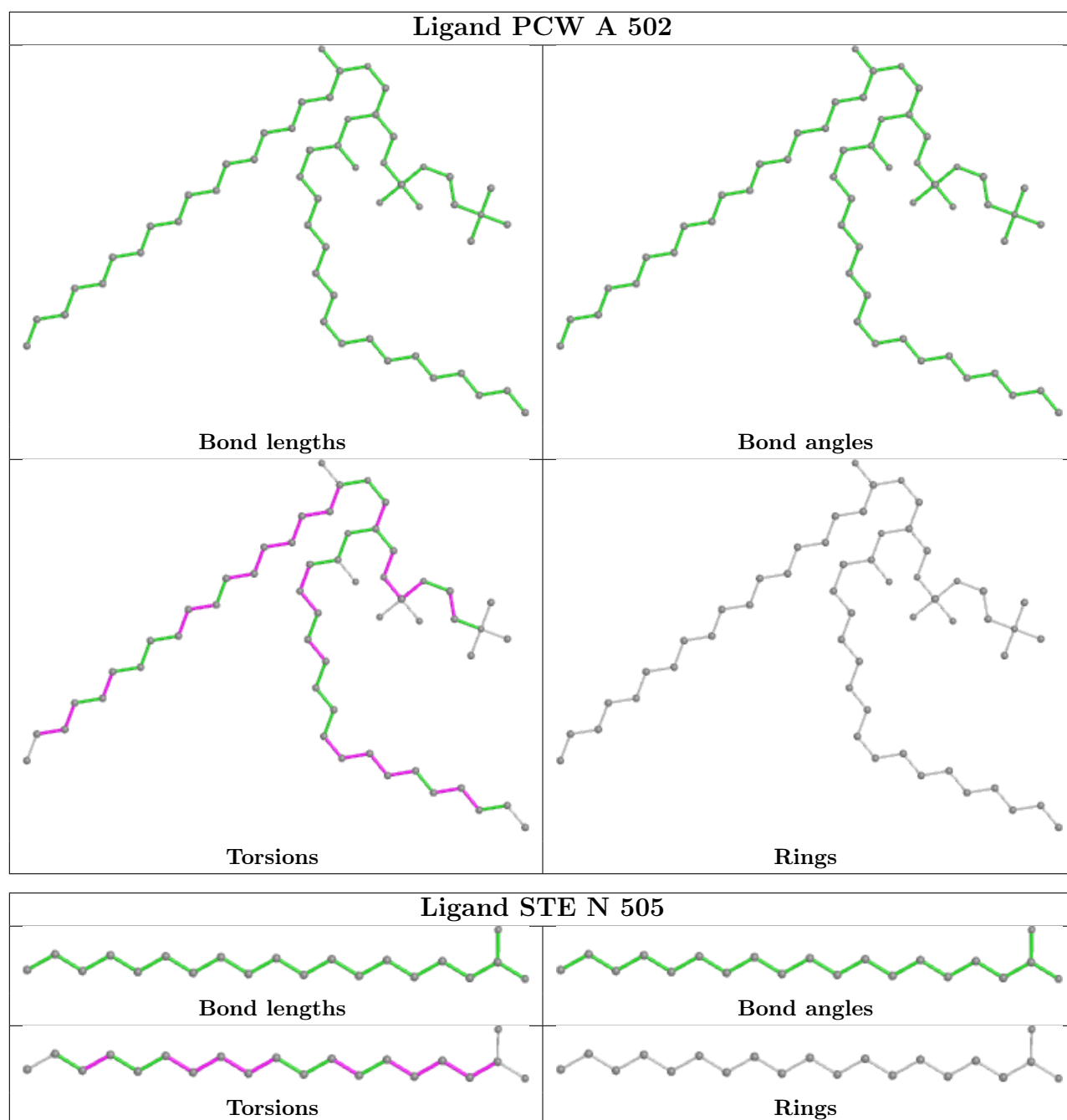


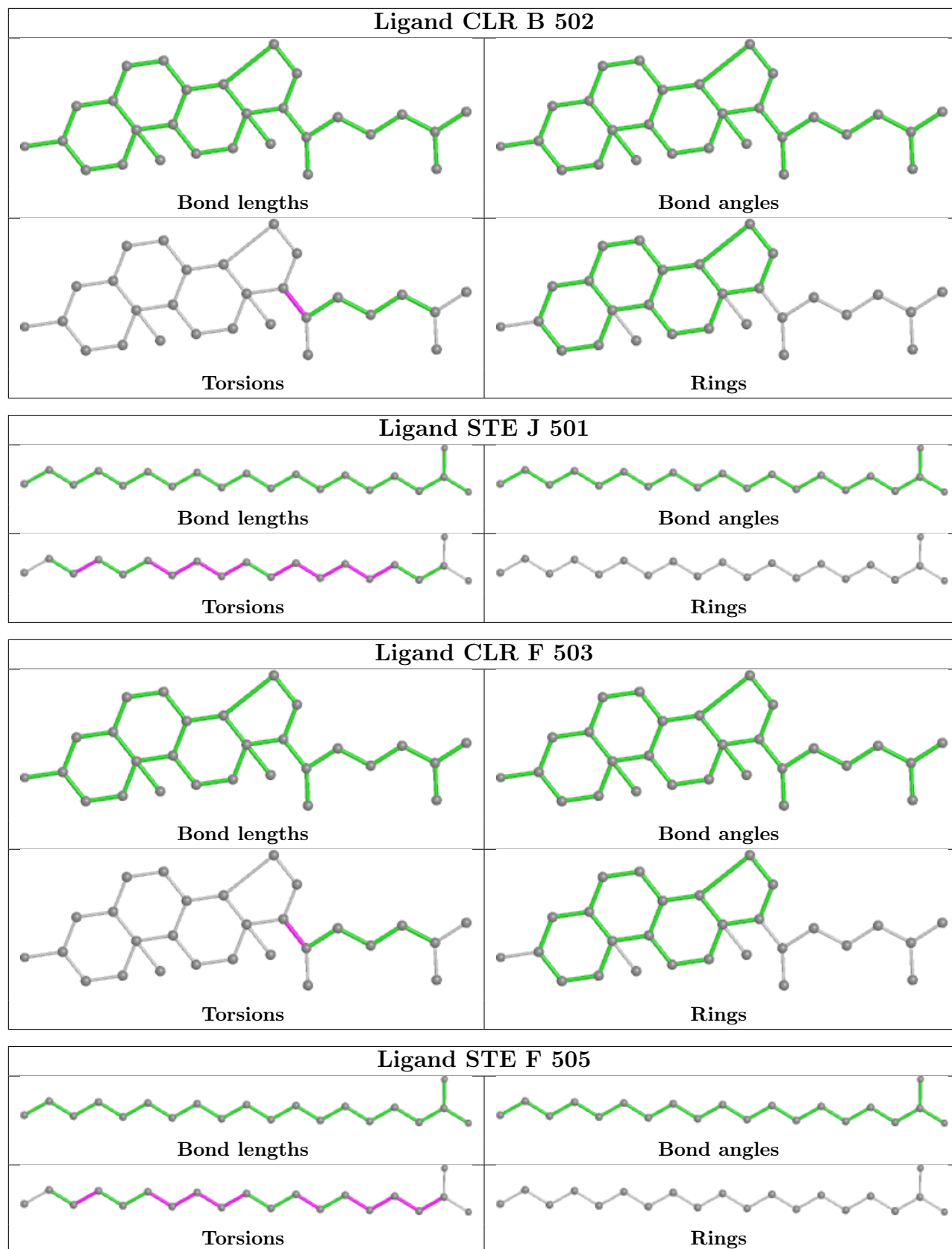


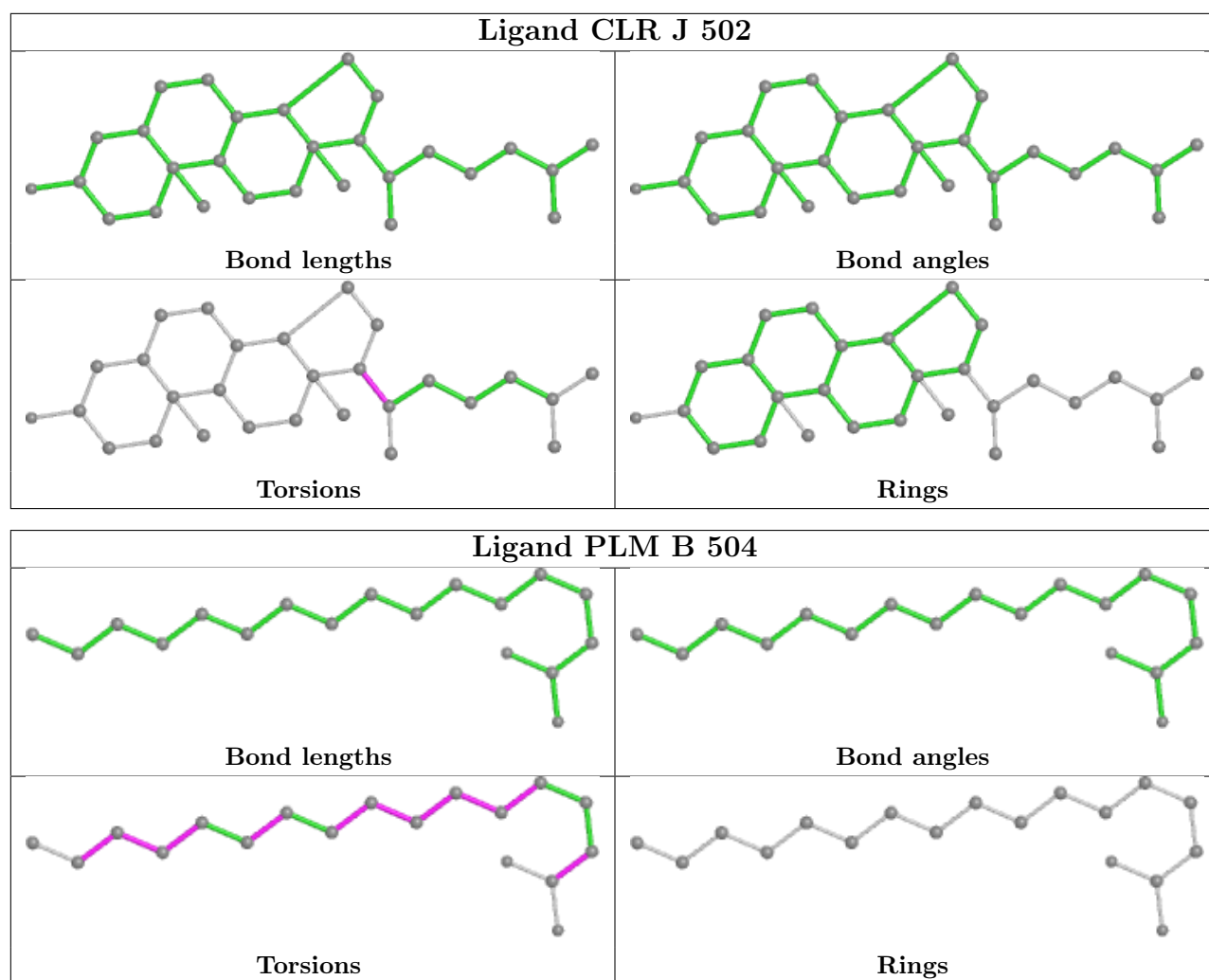












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

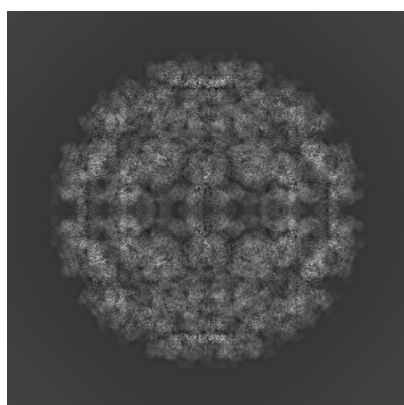
6 Map visualisation [i](#)

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.

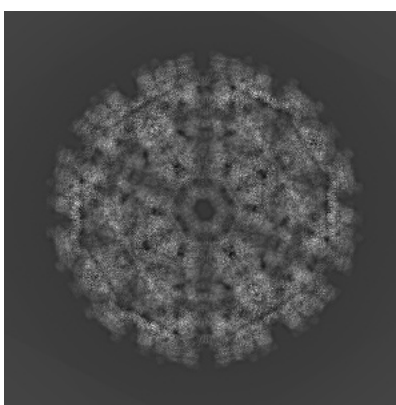
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

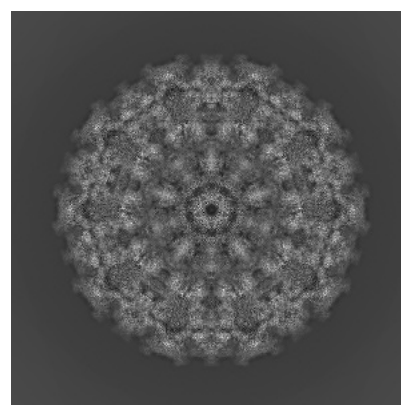
6.1.1 Primary map



X



Y



Z

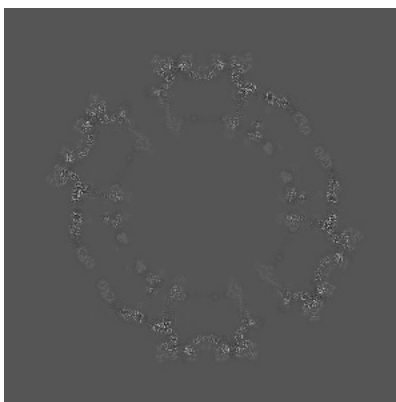
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256

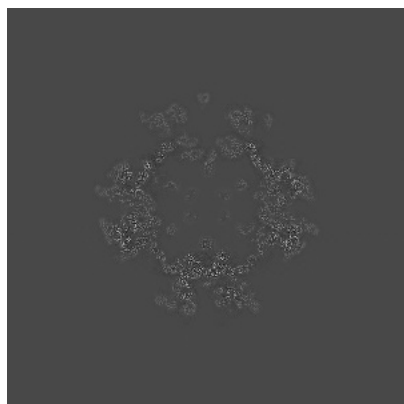


Z Index: 256

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

6.3 Largest variance slices [i](#)

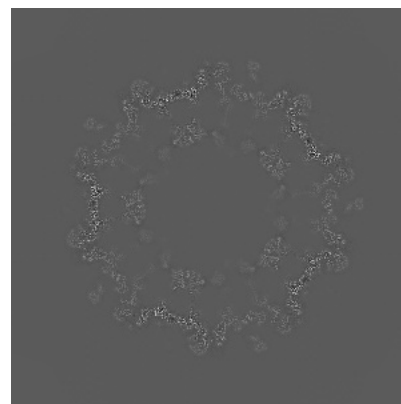
6.3.1 Primary map



X Index: 113



Y Index: 242

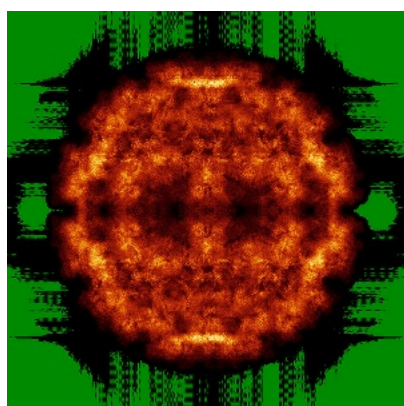


Z Index: 192

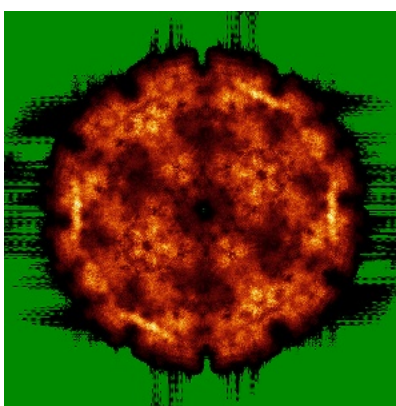
The images above show the largest variance slices of the map in three orthogonal directions.

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

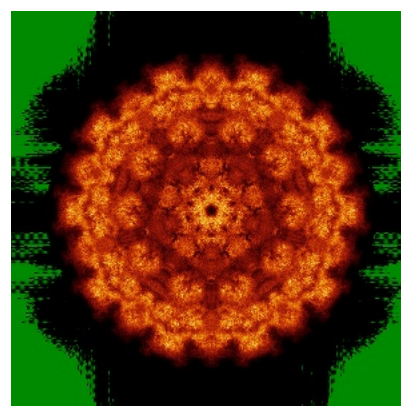
6.4.1 Primary map



X



Y

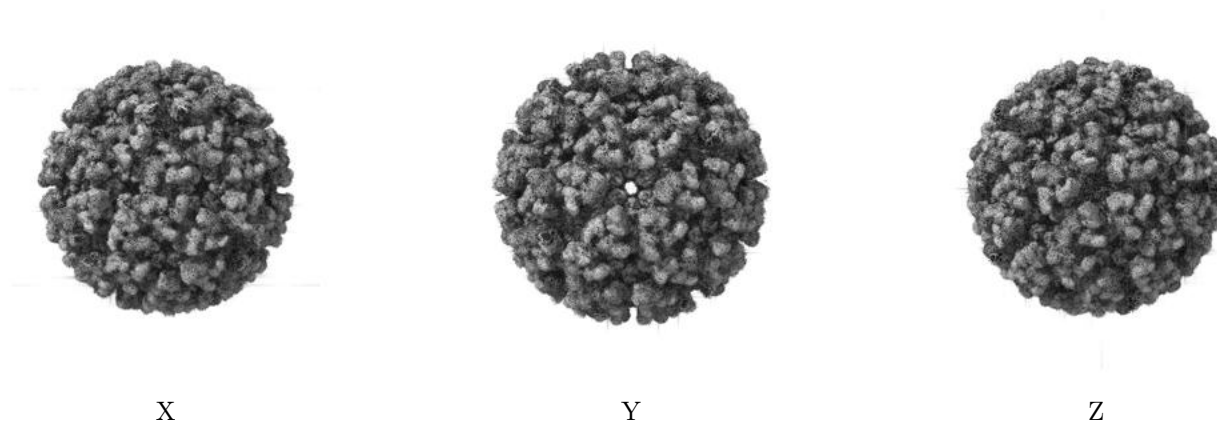


Z

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.

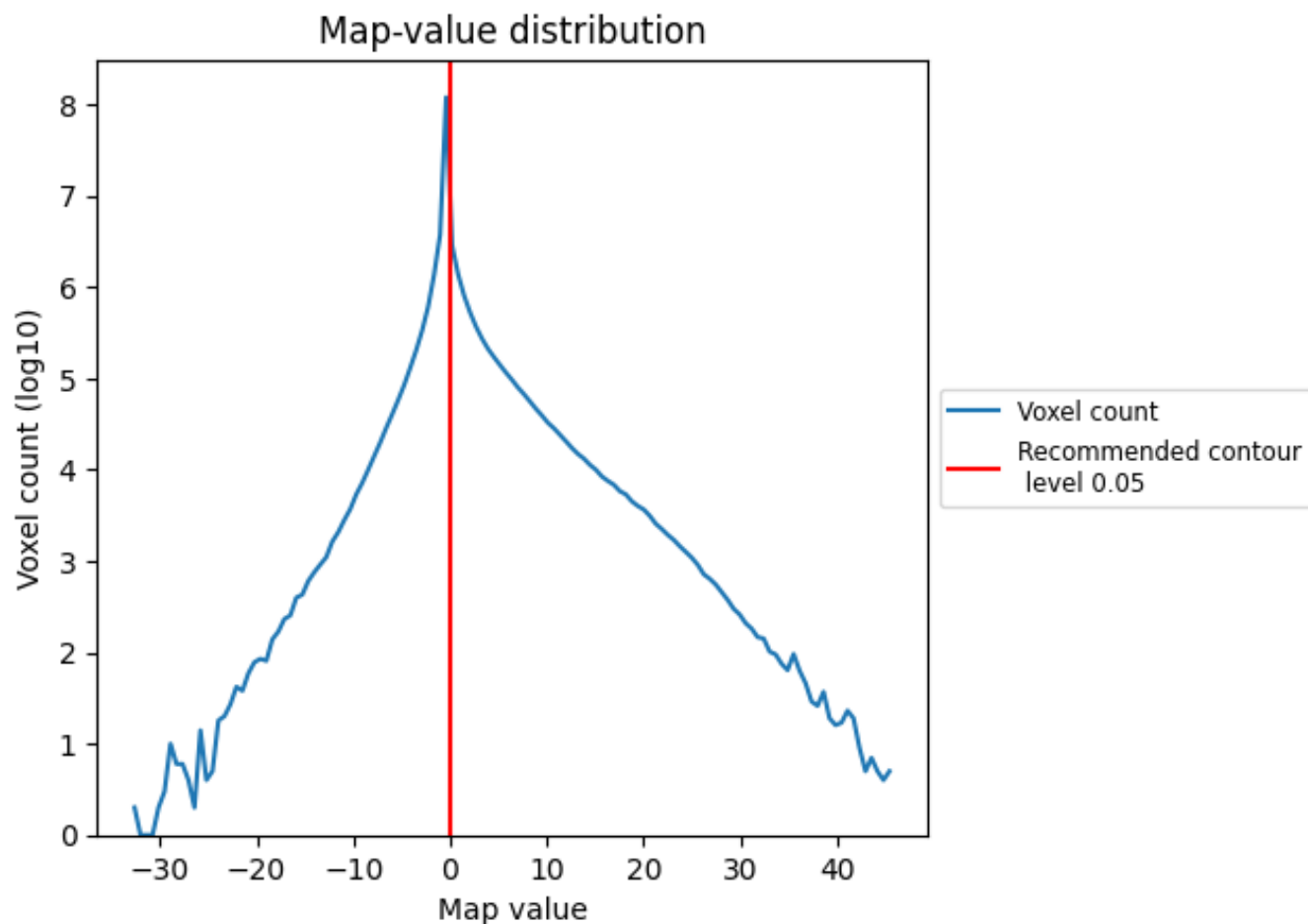
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

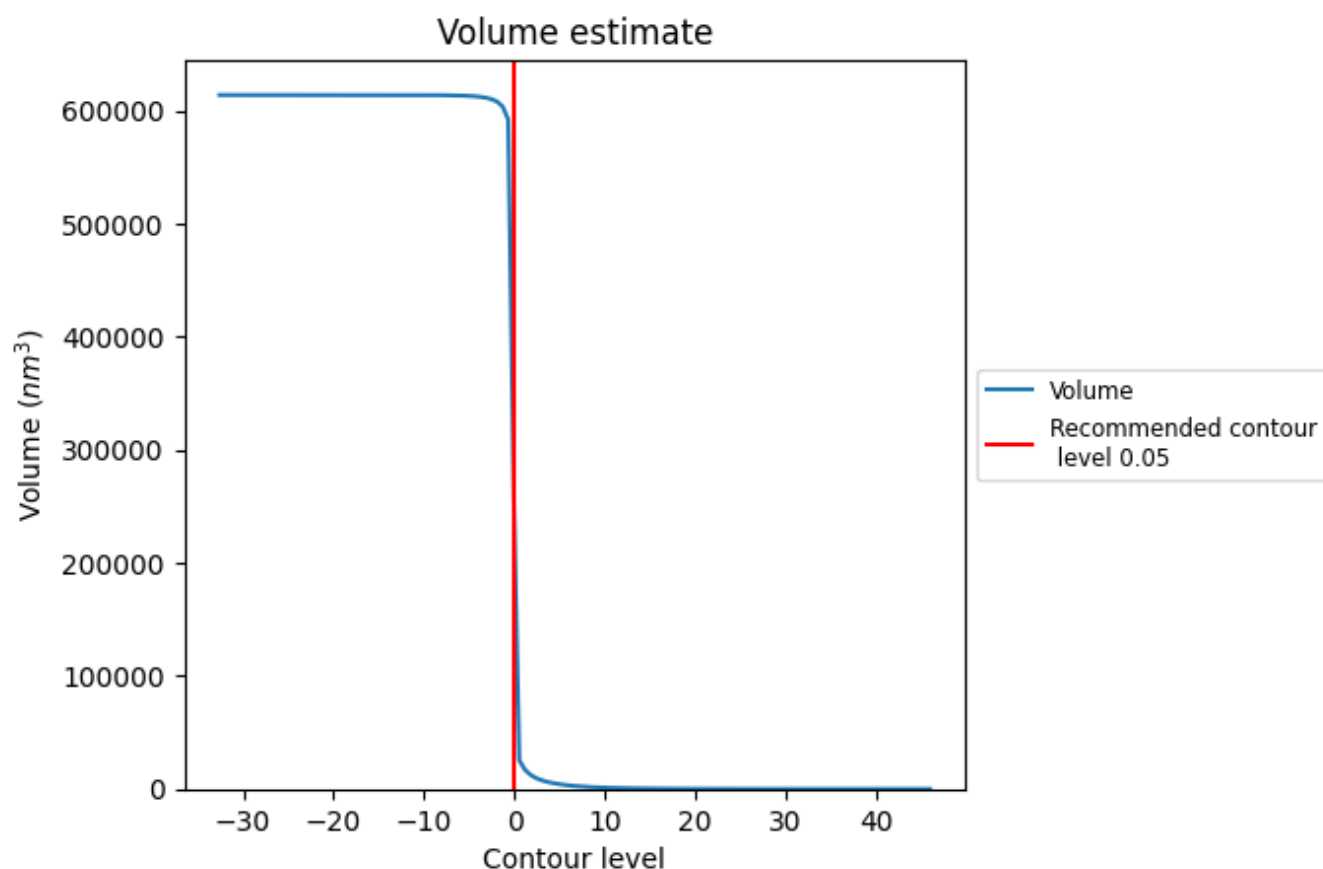
This section contains the results of statistical analysis of the map.

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.

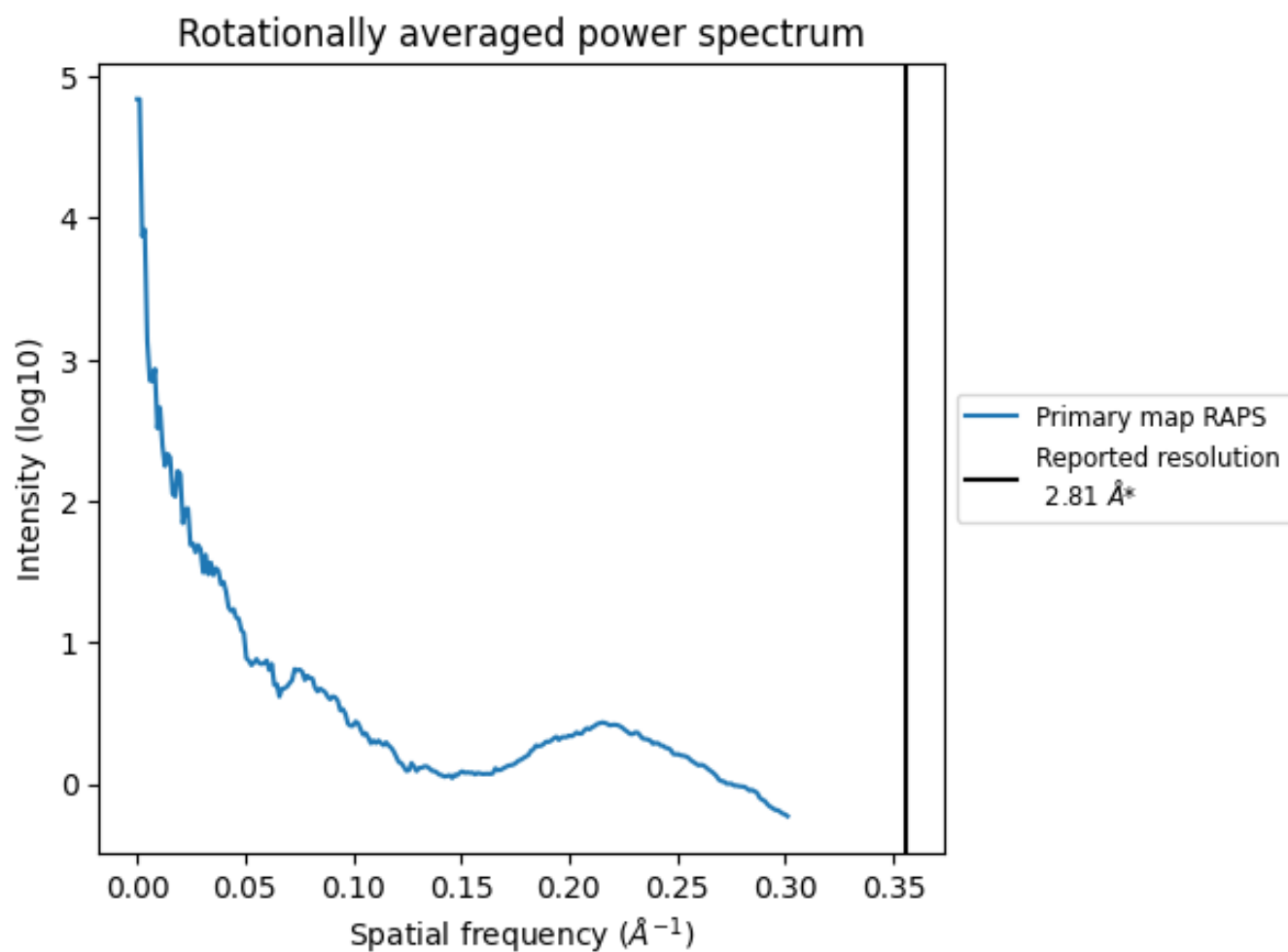
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 220944 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 ⓘ

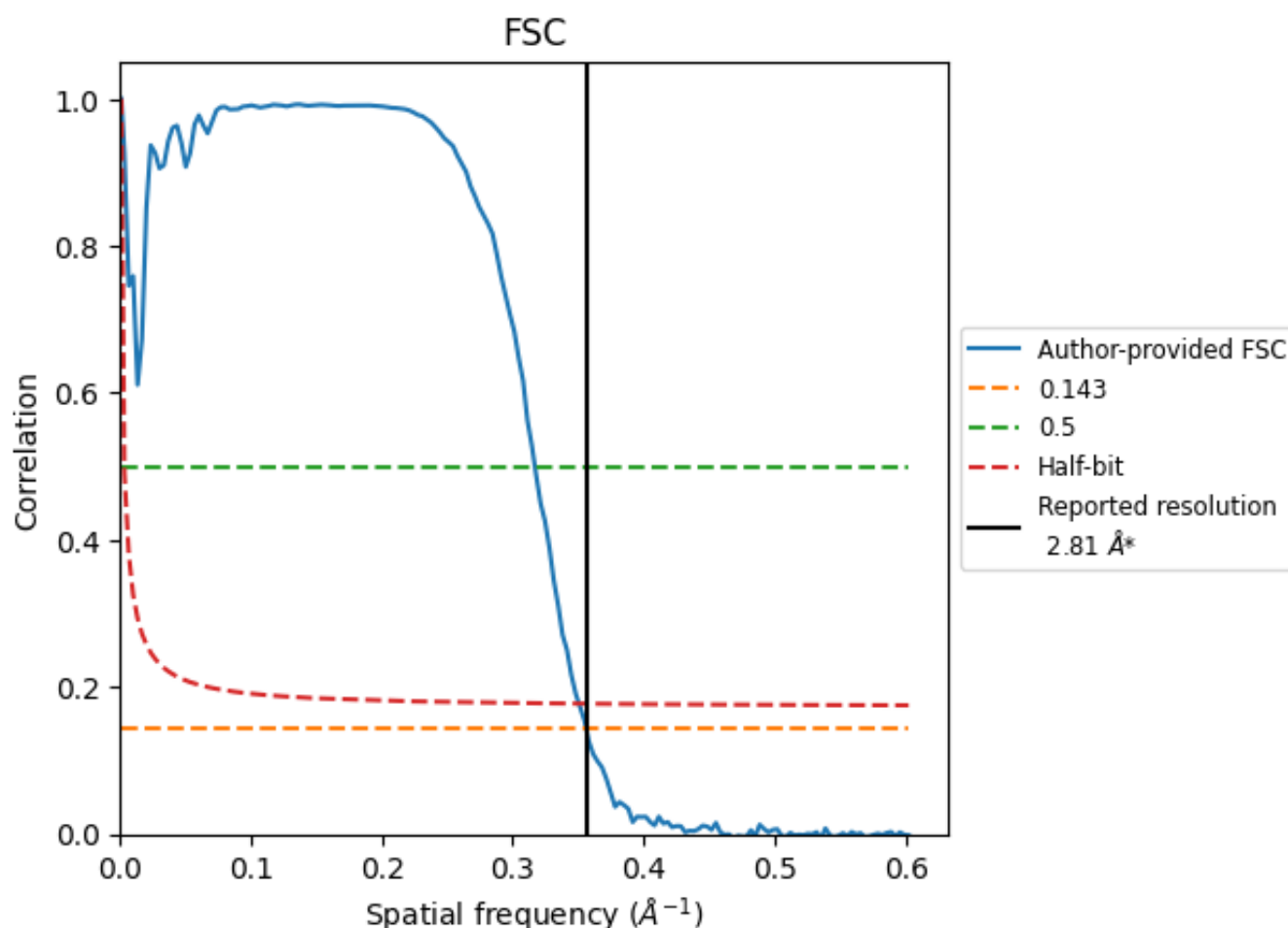


*Reported resolution corresponds to spatial frequency of 0.356 Å⁻¹

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 \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*	-	-	-

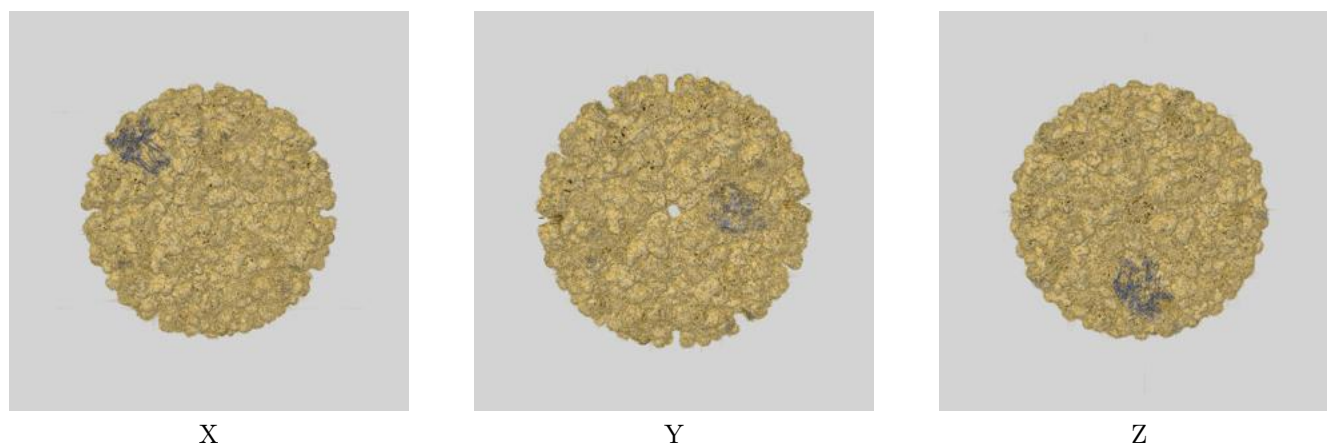
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

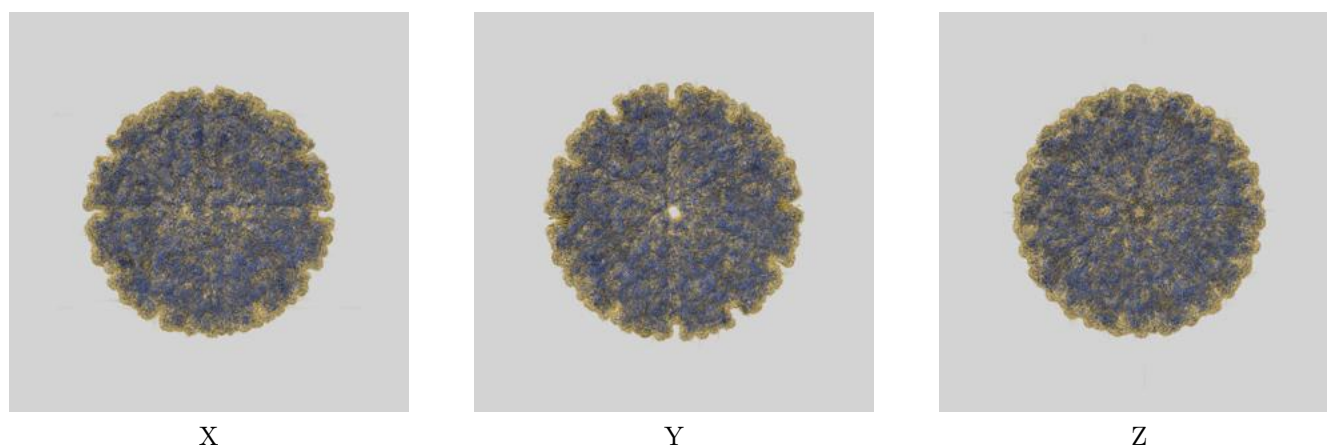
This section contains information regarding the fit between EMDB map EMD-31533 and PDB model 7FD2. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

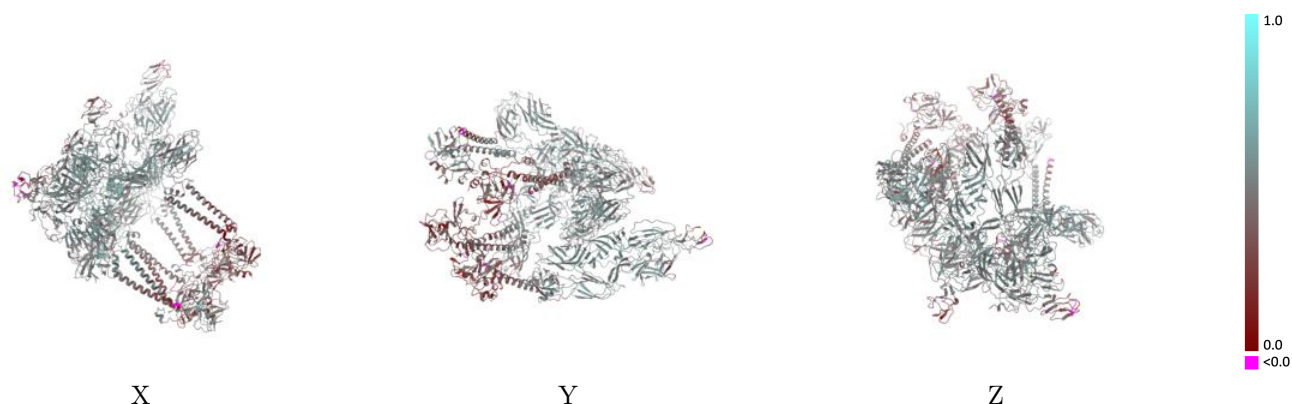


9.1.2 Map-model assembly overlay [i](#)



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](#)



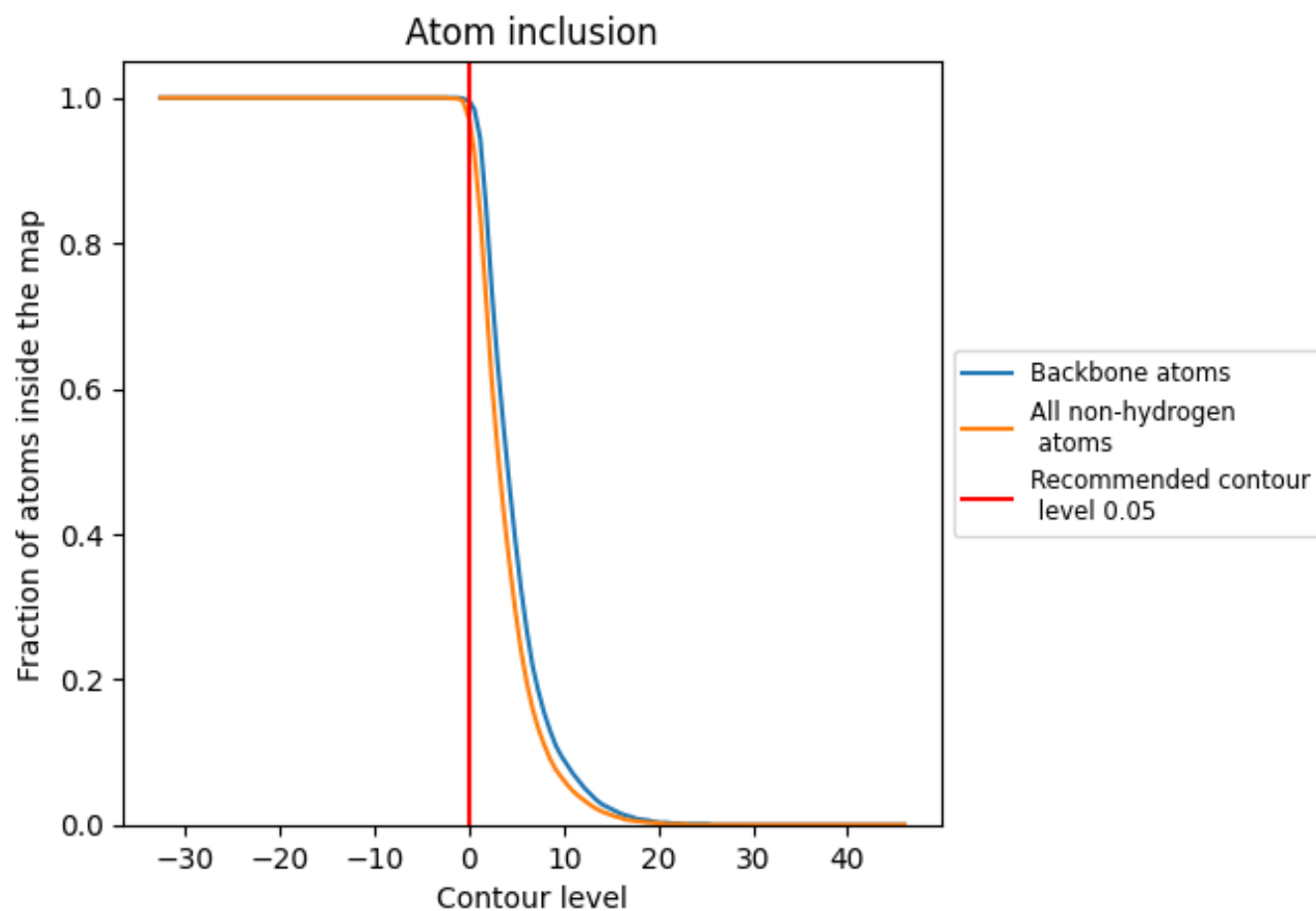
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

