



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 01:08 AM UTC

PDB ID : 8VT9 / pdb_00008vt9
EMDB ID : EMD-43520
Title : WT SthK in the presence of PIP2 and cAMP
Authors : Schmidpeter, P.A.M.; Thon, O.; Nimigean, C.M.
Deposited on : 2024-01-26
Resolution : 2.90 Å(reported)
Based on initial model : 6CJQ

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

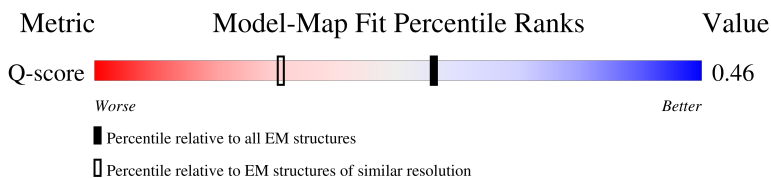
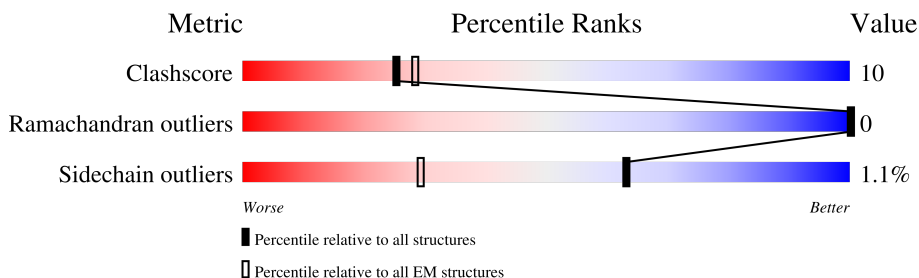
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	456	7% 70% 18% 11%
1	B	456	7% 70% 19% 11%
1	C	456	7% 71% 18% 11%
1	D	456	7% 71% 18% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14012 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 Transcriptional regulator, Crp/Fnr family.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total	C	N	O	S	0	0
			3228	2112	541	568	7		
1	B	406	Total	C	N	O	S	0	0
			3228	2112	541	568	7		
1	C	406	Total	C	N	O	S	0	0
			3228	2112	541	568	7		
1	D	406	Total	C	N	O	S	0	0
			3228	2112	541	568	7		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP G0GA88
A	-17	ALA	-	expression tag	UNP G0GA88
A	-16	LYS	-	expression tag	UNP G0GA88
A	-15	ASP	-	expression tag	UNP G0GA88
A	-14	ILE	-	expression tag	UNP G0GA88
A	-13	GLY	-	expression tag	UNP G0GA88
A	-12	ILE	-	expression tag	UNP G0GA88
A	-11	ASN	-	expression tag	UNP G0GA88
A	-10	SER	-	expression tag	UNP G0GA88
A	-9	ASP	-	expression tag	UNP G0GA88
A	-8	PRO	-	expression tag	UNP G0GA88
A	-7	ASN	-	expression tag	UNP G0GA88
A	-6	SER	-	expression tag	UNP G0GA88
A	-5	SER	-	expression tag	UNP G0GA88
A	-4	SER	-	expression tag	UNP G0GA88
A	-3	VAL	-	expression tag	UNP G0GA88
A	-2	ASP	-	expression tag	UNP G0GA88
A	-1	LYS	-	expression tag	UNP G0GA88
A	0	LEU	-	expression tag	UNP G0GA88
A	421	LEU	-	expression tag	UNP G0GA88
A	422	GLU	-	expression tag	UNP G0GA88
A	423	SER	-	expression tag	UNP G0GA88

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Chain	Residue	Modelled	Actual	Comment	Reference
A	424	SER	-	expression tag	UNP G0GA88
A	425	GLY	-	expression tag	UNP G0GA88
A	426	LEU	-	expression tag	UNP G0GA88
A	427	VAL	-	expression tag	UNP G0GA88
A	428	PRO	-	expression tag	UNP G0GA88
A	429	ARG	-	expression tag	UNP G0GA88
A	430	GLY	-	expression tag	UNP G0GA88
A	431	SER	-	expression tag	UNP G0GA88
A	432	VAL	-	expression tag	UNP G0GA88
A	433	LYS	-	expression tag	UNP G0GA88
A	434	HIS	-	expression tag	UNP G0GA88
A	435	HIS	-	expression tag	UNP G0GA88
A	436	HIS	-	expression tag	UNP G0GA88
A	437	HIS	-	expression tag	UNP G0GA88
B	-18	MET	-	initiating methionine	UNP G0GA88
B	-17	ALA	-	expression tag	UNP G0GA88
B	-16	LYS	-	expression tag	UNP G0GA88
B	-15	ASP	-	expression tag	UNP G0GA88
B	-14	ILE	-	expression tag	UNP G0GA88
B	-13	GLY	-	expression tag	UNP G0GA88
B	-12	ILE	-	expression tag	UNP G0GA88
B	-11	ASN	-	expression tag	UNP G0GA88
B	-10	SER	-	expression tag	UNP G0GA88
B	-9	ASP	-	expression tag	UNP G0GA88
B	-8	PRO	-	expression tag	UNP G0GA88
B	-7	ASN	-	expression tag	UNP G0GA88
B	-6	SER	-	expression tag	UNP G0GA88
B	-5	SER	-	expression tag	UNP G0GA88
B	-4	SER	-	expression tag	UNP G0GA88
B	-3	VAL	-	expression tag	UNP G0GA88
B	-2	ASP	-	expression tag	UNP G0GA88
B	-1	LYS	-	expression tag	UNP G0GA88
B	0	LEU	-	expression tag	UNP G0GA88
B	421	LEU	-	expression tag	UNP G0GA88
B	422	GLU	-	expression tag	UNP G0GA88
B	423	SER	-	expression tag	UNP G0GA88
B	424	SER	-	expression tag	UNP G0GA88
B	425	GLY	-	expression tag	UNP G0GA88
B	426	LEU	-	expression tag	UNP G0GA88
B	427	VAL	-	expression tag	UNP G0GA88
B	428	PRO	-	expression tag	UNP G0GA88
B	429	ARG	-	expression tag	UNP G0GA88

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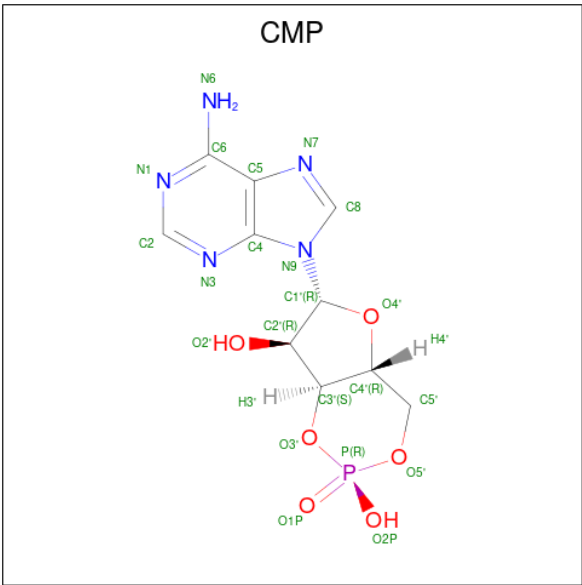
Chain	Residue	Modelled	Actual	Comment	Reference
B	430	GLY	-	expression tag	UNP G0GA88
B	431	SER	-	expression tag	UNP G0GA88
B	432	VAL	-	expression tag	UNP G0GA88
B	433	LYS	-	expression tag	UNP G0GA88
B	434	HIS	-	expression tag	UNP G0GA88
B	435	HIS	-	expression tag	UNP G0GA88
B	436	HIS	-	expression tag	UNP G0GA88
B	437	HIS	-	expression tag	UNP G0GA88
C	-18	MET	-	initiating methionine	UNP G0GA88
C	-17	ALA	-	expression tag	UNP G0GA88
C	-16	LYS	-	expression tag	UNP G0GA88
C	-15	ASP	-	expression tag	UNP G0GA88
C	-14	ILE	-	expression tag	UNP G0GA88
C	-13	GLY	-	expression tag	UNP G0GA88
C	-12	ILE	-	expression tag	UNP G0GA88
C	-11	ASN	-	expression tag	UNP G0GA88
C	-10	SER	-	expression tag	UNP G0GA88
C	-9	ASP	-	expression tag	UNP G0GA88
C	-8	PRO	-	expression tag	UNP G0GA88
C	-7	ASN	-	expression tag	UNP G0GA88
C	-6	SER	-	expression tag	UNP G0GA88
C	-5	SER	-	expression tag	UNP G0GA88
C	-4	SER	-	expression tag	UNP G0GA88
C	-3	VAL	-	expression tag	UNP G0GA88
C	-2	ASP	-	expression tag	UNP G0GA88
C	-1	LYS	-	expression tag	UNP G0GA88
C	0	LEU	-	expression tag	UNP G0GA88
C	421	LEU	-	expression tag	UNP G0GA88
C	422	GLU	-	expression tag	UNP G0GA88
C	423	SER	-	expression tag	UNP G0GA88
C	424	SER	-	expression tag	UNP G0GA88
C	425	GLY	-	expression tag	UNP G0GA88
C	426	LEU	-	expression tag	UNP G0GA88
C	427	VAL	-	expression tag	UNP G0GA88
C	428	PRO	-	expression tag	UNP G0GA88
C	429	ARG	-	expression tag	UNP G0GA88
C	430	GLY	-	expression tag	UNP G0GA88
C	431	SER	-	expression tag	UNP G0GA88
C	432	VAL	-	expression tag	UNP G0GA88
C	433	LYS	-	expression tag	UNP G0GA88
C	434	HIS	-	expression tag	UNP G0GA88
C	435	HIS	-	expression tag	UNP G0GA88

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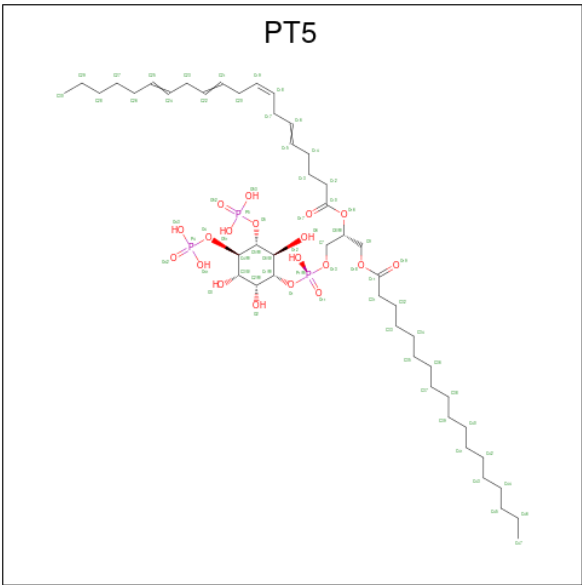
Chain	Residue	Modelled	Actual	Comment	Reference
C	436	HIS	-	expression tag	UNP G0GA88
C	437	HIS	-	expression tag	UNP G0GA88
D	-18	MET	-	initiating methionine	UNP G0GA88
D	-17	ALA	-	expression tag	UNP G0GA88
D	-16	LYS	-	expression tag	UNP G0GA88
D	-15	ASP	-	expression tag	UNP G0GA88
D	-14	ILE	-	expression tag	UNP G0GA88
D	-13	GLY	-	expression tag	UNP G0GA88
D	-12	ILE	-	expression tag	UNP G0GA88
D	-11	ASN	-	expression tag	UNP G0GA88
D	-10	SER	-	expression tag	UNP G0GA88
D	-9	ASP	-	expression tag	UNP G0GA88
D	-8	PRO	-	expression tag	UNP G0GA88
D	-7	ASN	-	expression tag	UNP G0GA88
D	-6	SER	-	expression tag	UNP G0GA88
D	-5	SER	-	expression tag	UNP G0GA88
D	-4	SER	-	expression tag	UNP G0GA88
D	-3	VAL	-	expression tag	UNP G0GA88
D	-2	ASP	-	expression tag	UNP G0GA88
D	-1	LYS	-	expression tag	UNP G0GA88
D	0	LEU	-	expression tag	UNP G0GA88
D	421	LEU	-	expression tag	UNP G0GA88
D	422	GLU	-	expression tag	UNP G0GA88
D	423	SER	-	expression tag	UNP G0GA88
D	424	SER	-	expression tag	UNP G0GA88
D	425	GLY	-	expression tag	UNP G0GA88
D	426	LEU	-	expression tag	UNP G0GA88
D	427	VAL	-	expression tag	UNP G0GA88
D	428	PRO	-	expression tag	UNP G0GA88
D	429	ARG	-	expression tag	UNP G0GA88
D	430	GLY	-	expression tag	UNP G0GA88
D	431	SER	-	expression tag	UNP G0GA88
D	432	VAL	-	expression tag	UNP G0GA88
D	433	LYS	-	expression tag	UNP G0GA88
D	434	HIS	-	expression tag	UNP G0GA88
D	435	HIS	-	expression tag	UNP G0GA88
D	436	HIS	-	expression tag	UNP G0GA88
D	437	HIS	-	expression tag	UNP G0GA88

- Molecule 2 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (CCD ID: CMP) (formula: $C_{10}H_{12}N_5O_6P$).



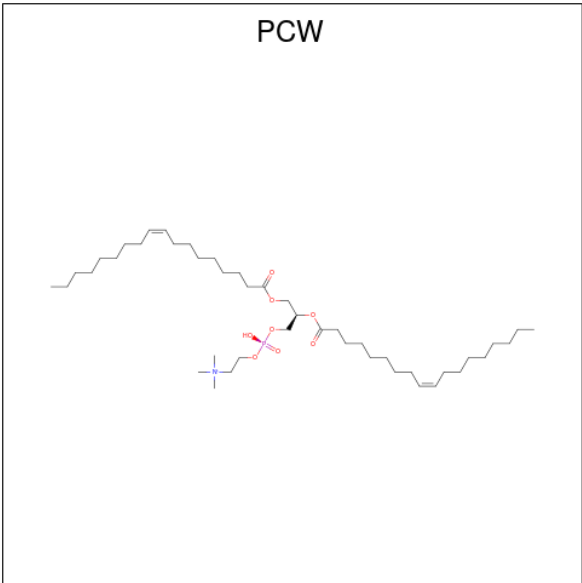
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	B	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	C	1	Total	C	N	O	P	0
			22	10	5	6	1	
2	D	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 3 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: C₄₇H₈₅O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			57	35	19	3	
3	B	1	Total	C	O	P	0
			57	35	19	3	
3	C	1	Total	C	O	P	0
			57	35	19	3	
3	D	1	Total	C	O	P	0
			57	35	19	3	

- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O P 38 29 8 1	0
4	A	1	Total C 14 14	0
4	A	1	Total C O P 34 25 8 1	0
4	A	1	Total C O P 23 16 6 1	0
4	A	1	Total C O P 36 27 8 1	0
4	A	1	Total C O 41 36 5	0
4	A	1	Total C O 10 8 2	0
4	B	1	Total C O P 38 29 8 1	0
4	B	1	Total C 14 14	0
4	B	1	Total C O P 34 25 8 1	0
4	B	1	Total C O P 23 16 6 1	0
4	B	1	Total C O P 36 27 8 1	0
4	B	1	Total C O 41 36 5	0
4	B	1	Total C O 10 8 2	0
4	C	1	Total C O P 38 29 8 1	0
4	C	1	Total C 14 14	0
4	C	1	Total C O P 34 25 8 1	0
4	C	1	Total C O P 23 16 6 1	0
4	C	1	Total C O P 36 27 8 1	0
4	C	1	Total C O 41 36 5	0
4	C	1	Total C O 10 8 2	0
4	D	1	Total C O P 38 29 8 1	0

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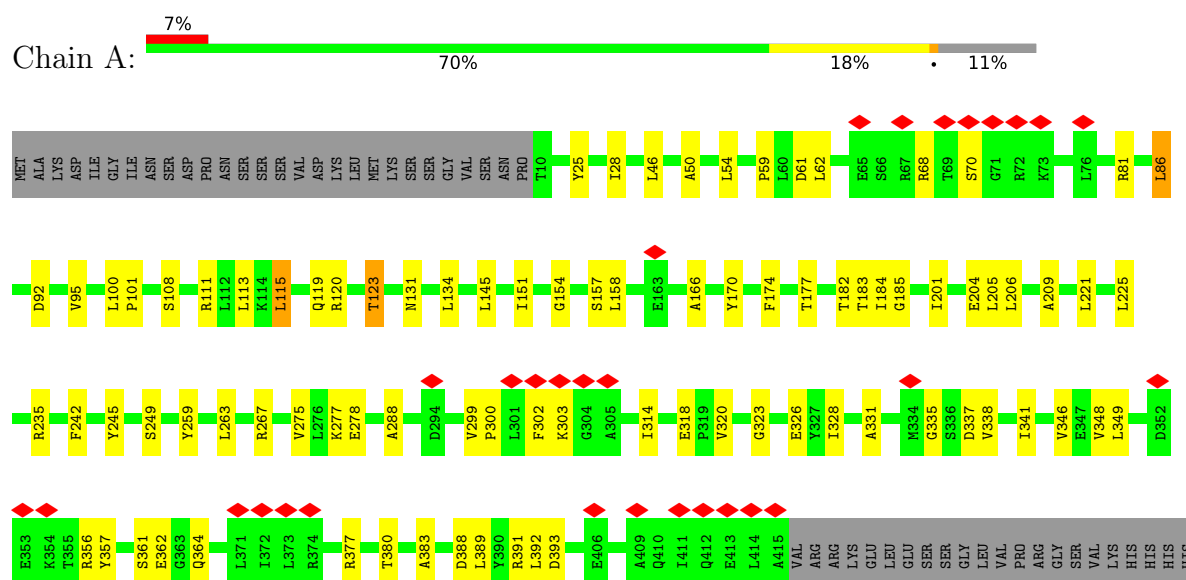
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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C			0
			14	14			
4	D	1	Total	C	O	P	0
			34	25	8	1	
4	D	1	Total	C	O	P	0
			23	16	6	1	
4	D	1	Total	C	O	P	0
			36	27	8	1	
4	D	1	Total	C	O		0
			41	36	5		
4	D	1	Total	C	O		0
			10	8	2		

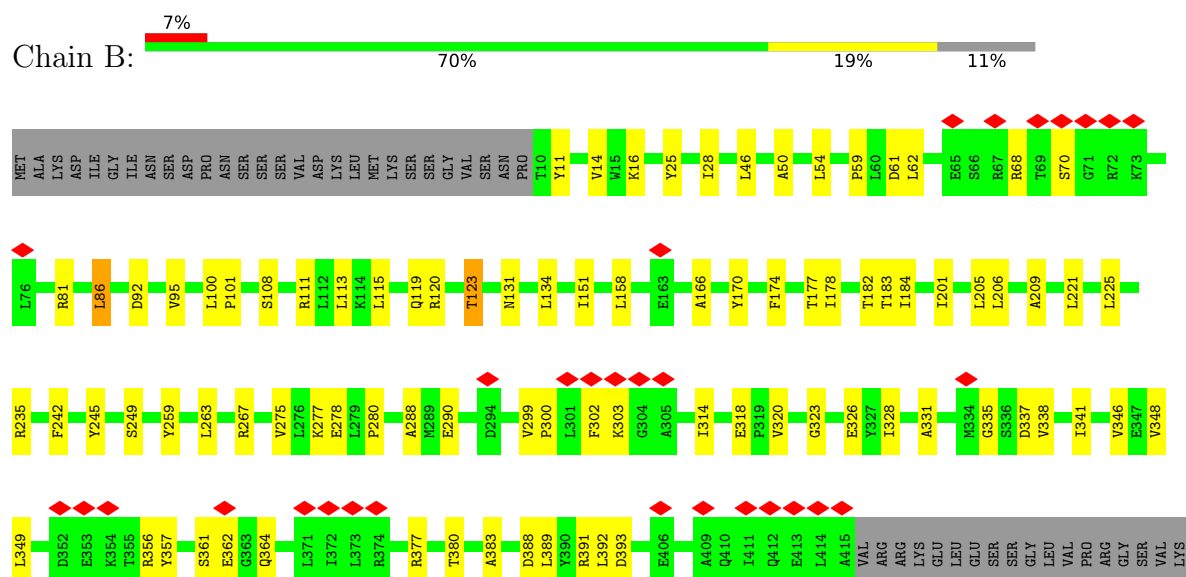
3 Residue-property plots

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: Transcriptional regulator, Crp/Fnr family



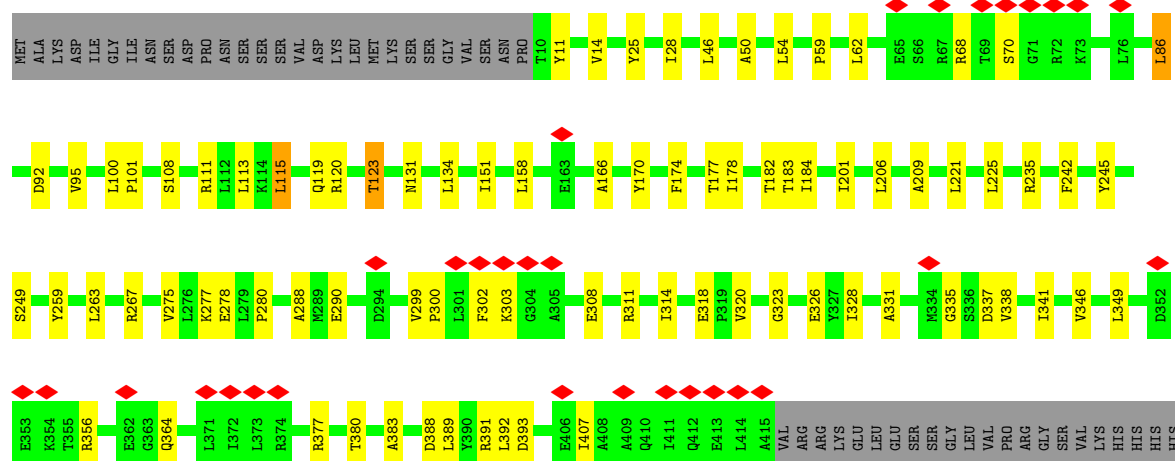
- Molecule 1: Transcriptional regulator, Crp/Fnr family



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HIS
HIS

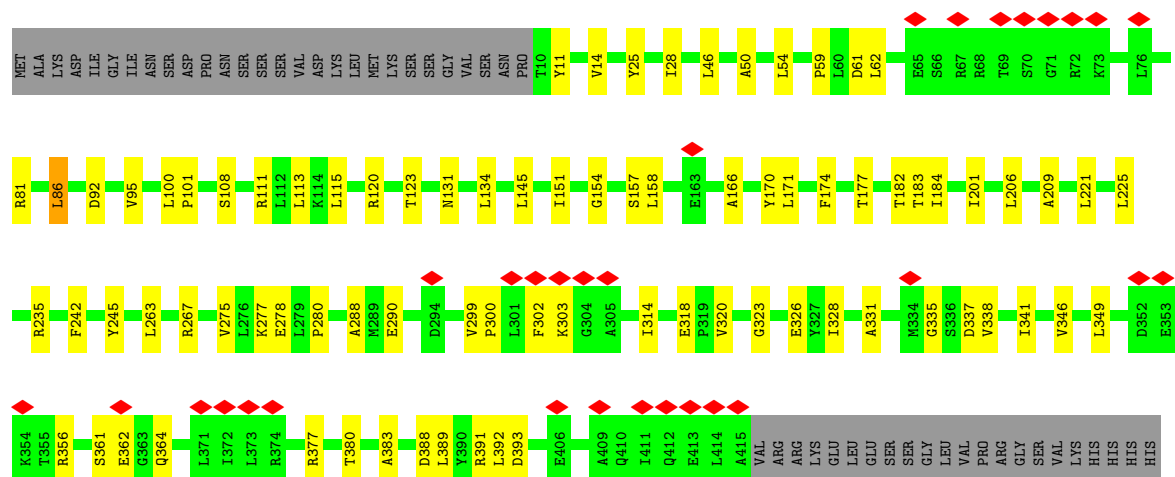
- Molecule 1: Transcriptional regulator, Crp/Fnr family

Chain C: 



- Molecule 1: Transcriptional regulator, Crp/Fnr family

Chain D: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	1059574	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.56	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	36000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.052	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0172	Depositor
Map size ($\text{\AA}$)	280.576, 280.576, 280.576	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.096, 1.096, 1.096	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: CMP, PT5, PCW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.13	0/3302	0.36	1/4499 (0.0%)
1	B	0.13	0/3302	0.36	1/4499 (0.0%)
1	C	0.13	0/3302	0.36	1/4499 (0.0%)
1	D	0.13	0/3302	0.36	1/4499 (0.0%)
All	All	0.13	0/13208	0.36	4/17996 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LYS	N-CA-C	-5.58	107.47	114.56
1	B	277	LYS	N-CA-C	-5.58	107.48	114.56
1	C	277	LYS	N-CA-C	-5.57	107.48	114.56
1	D	277	LYS	N-CA-C	-5.55	107.50	114.56

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	3228	0	3368	70	0
1	B	3228	0	3368	71	0
1	C	3228	0	3368	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3228	0	3368	69	0
2	A	22	0	11	1	0
2	B	22	0	11	1	0
2	C	22	0	11	1	0
2	D	22	0	11	1	0
3	A	57	0	51	10	0
3	B	57	0	51	9	0
3	C	57	0	51	9	0
3	D	57	0	51	9	0
4	A	196	0	241	24	0
4	B	196	0	241	24	0
4	C	196	0	241	23	0
4	D	196	0	241	23	0
All	All	14012	0	14684	297	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 (297) 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)
2:C:501:CMP:H2	2:C:501:CMP:C2	0.97	1.50
2:A:501:CMP:H2	2:A:501:CMP:C2	0.97	1.49
2:B:501:CMP:H2	2:B:501:CMP:C2	0.97	1.49
2:D:501:CMP:H2	2:D:501:CMP:C2	0.97	1.48
1:C:25:TYR:HD1	4:C:509:PCW:H152	1.43	0.83
1:D:25:TYR:HD1	4:D:509:PCW:H152	1.43	0.83
1:A:25:TYR:HD1	4:A:509:PCW:H152	1.43	0.82
1:B:25:TYR:HD1	4:B:509:PCW:H152	1.43	0.81
1:A:184:ILE:HG12	1:B:183:THR:HA	1.68	0.74
1:C:25:TYR:CD1	4:C:509:PCW:H152	2.24	0.73
3:A:502:PT5:H17	1:D:225:LEU:HD11	1.71	0.73
1:B:25:TYR:CD1	4:B:509:PCW:H152	2.24	0.73
1:D:25:TYR:CD1	4:D:509:PCW:H152	2.24	0.73
1:A:25:TYR:CD1	4:A:509:PCW:H152	2.24	0.72
3:A:502:PT5:H24	1:D:131:ASN:HB2	1.71	0.72
4:C:507:PCW:H182	4:C:507:PCW:H412	1.74	0.70
4:B:507:PCW:H182	4:B:507:PCW:H412	1.74	0.69
1:C:267:ARG:NH2	1:C:388:ASP:OD2	2.22	0.69
4:D:507:PCW:H182	4:D:507:PCW:H412	1.74	0.68
4:A:507:PCW:H182	4:A:507:PCW:H412	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:HD11	3:D:502:PT5:H17	1.76	0.68
1:B:225:LEU:HD11	3:C:502:PT5:H17	1.75	0.68
1:A:183:THR:HA	1:D:184:ILE:HG12	1.76	0.67
1:D:331:ALA:H	1:D:380:THR:HG22	1.60	0.67
1:A:331:ALA:H	1:A:380:THR:HG22	1.60	0.66
1:C:331:ALA:H	1:C:380:THR:HG22	1.60	0.66
1:A:267:ARG:NH2	1:A:388:ASP:OD2	2.22	0.66
1:B:331:ALA:H	1:B:380:THR:HG22	1.60	0.66
1:C:184:ILE:HG12	1:D:183:THR:HA	1.77	0.65
1:A:120:ARG:NE	3:A:502:PT5:H2	2.12	0.65
1:D:120:ARG:NE	3:D:502:PT5:H2	2.12	0.64
1:A:131:ASN:HB2	3:B:502:PT5:H24	1.80	0.64
1:C:120:ARG:NE	3:C:502:PT5:H2	2.12	0.64
1:B:184:ILE:HG12	1:C:183:THR:HA	1.78	0.64
1:B:338:VAL:HG12	1:B:392:LEU:HB3	1.80	0.64
1:A:338:VAL:HG12	1:A:392:LEU:HB3	1.81	0.63
1:D:338:VAL:HG12	1:D:392:LEU:HB3	1.80	0.63
1:D:267:ARG:NH2	1:D:388:ASP:OD2	2.22	0.63
1:B:120:ARG:NE	3:B:502:PT5:H2	2.12	0.63
1:A:225:LEU:HD11	3:B:502:PT5:H17	1.81	0.63
1:B:131:ASN:HB2	3:C:502:PT5:H24	1.81	0.63
1:C:338:VAL:HG12	1:C:392:LEU:HB3	1.80	0.63
1:C:131:ASN:HB2	3:D:502:PT5:H24	1.82	0.62
1:A:170:TYR:CD2	4:A:508:PCW:H362	2.35	0.62
1:B:170:TYR:CD2	4:B:508:PCW:H362	2.35	0.62
1:B:267:ARG:NH2	1:B:388:ASP:OD2	2.22	0.61
1:D:170:TYR:CD2	4:D:508:PCW:H362	2.35	0.61
1:C:170:TYR:CD2	4:C:508:PCW:H362	2.35	0.61
1:A:235:ARG:NH1	1:B:278:GLU:OE1	2.34	0.60
4:B:507:PCW:H321	4:B:507:PCW:H122	1.85	0.59
4:C:507:PCW:H122	4:C:507:PCW:H321	1.85	0.59
1:C:46:LEU:O	1:C:50:ALA:N	2.32	0.59
4:A:507:PCW:H122	4:A:507:PCW:H321	1.85	0.58
4:A:503:PCW:H342	1:D:221:LEU:HD22	1.84	0.58
4:D:507:PCW:H122	4:D:507:PCW:H321	1.85	0.58
1:D:46:LEU:O	1:D:50:ALA:N	2.32	0.56
3:A:502:PT5:H30	1:D:134:LEU:HD23	1.86	0.56
1:D:100:LEU:HD12	1:D:101:PRO:HD2	1.88	0.56
1:A:201:ILE:HD13	1:D:174:PHE:HD2	1.71	0.56
1:B:100:LEU:HD12	1:B:101:PRO:HD2	1.88	0.56
1:A:100:LEU:HD12	1:A:101:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:HD12	1:C:101:PRO:HD2	1.88	0.55
1:A:174:PHE:HA	1:A:177:THR:HG22	1.89	0.55
1:C:174:PHE:HA	1:C:177:THR:HG22	1.89	0.55
1:C:235:ARG:NH1	1:D:278:GLU:OE1	2.39	0.55
1:A:46:LEU:O	1:A:50:ALA:N	2.32	0.55
1:D:174:PHE:HA	1:D:177:THR:HG22	1.89	0.55
1:B:174:PHE:HA	1:B:177:THR:HG22	1.89	0.55
3:A:502:PT5:H30	1:D:134:LEU:CD2	2.37	0.55
1:D:337:ASP:OD1	1:D:377:ARG:NH2	2.40	0.55
1:A:337:ASP:OD1	1:A:377:ARG:NH2	2.40	0.54
1:B:46:LEU:O	1:B:50:ALA:N	2.32	0.54
1:C:337:ASP:OD1	1:C:377:ARG:NH2	2.40	0.54
1:B:337:ASP:OD1	1:B:377:ARG:NH2	2.40	0.54
1:B:242:PHE:HB3	1:C:275:VAL:HG11	1.89	0.54
3:C:502:PT5:C11	4:C:503:PCW:H321	2.38	0.54
3:D:502:PT5:C11	4:D:503:PCW:H321	2.38	0.54
1:B:209:ALA:CB	4:B:503:PCW:H171	2.38	0.54
1:A:249:SER:N	1:B:290:GLU:OE2	2.29	0.54
1:B:235:ARG:NH1	1:C:278:GLU:OE1	2.40	0.54
1:C:209:ALA:CB	4:C:503:PCW:H171	2.38	0.53
3:A:502:PT5:C11	4:A:503:PCW:H321	2.38	0.53
3:B:502:PT5:C11	4:B:503:PCW:H321	2.38	0.53
1:D:209:ALA:CB	4:D:503:PCW:H171	2.38	0.53
1:A:209:ALA:CB	4:A:503:PCW:H171	2.38	0.53
1:C:245:TYR:OH	1:D:267:ARG:NH2	2.42	0.53
1:A:182:THR:HG22	4:B:503:PCW:H461	1.91	0.53
1:B:391:ARG:NH1	1:B:393:ASP:OD2	2.41	0.53
1:C:242:PHE:HB3	1:D:275:VAL:HG11	1.90	0.53
1:A:245:TYR:OH	1:B:388:ASP:OD2	2.25	0.53
1:B:245:TYR:OH	1:C:267:ARG:NH2	2.41	0.52
3:A:502:PT5:H22	3:A:502:PT5:H51	1.91	0.52
1:B:134:LEU:CD2	3:C:502:PT5:H30	2.39	0.52
1:C:59:PRO:O	1:C:62:LEU:HB3	2.10	0.52
1:A:391:ARG:NH1	1:A:393:ASP:OD2	2.41	0.52
1:D:59:PRO:O	1:D:62:LEU:HB3	2.10	0.52
1:C:86:LEU:HD21	1:C:113:LEU:HG	1.92	0.52
1:B:86:LEU:HD21	1:B:113:LEU:HG	1.92	0.52
3:B:502:PT5:H51	3:B:502:PT5:H22	1.91	0.52
1:C:318:GLU:OE2	1:C:391:ARG:NH2	2.34	0.52
1:A:59:PRO:O	1:A:62:LEU:HB3	2.10	0.51
1:D:318:GLU:OE2	1:D:391:ARG:NH2	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:LEU:HD22	4:D:503:PCW:H342	1.92	0.51
3:C:502:PT5:H51	3:C:502:PT5:H22	1.91	0.51
1:D:391:ARG:NH1	1:D:393:ASP:OD2	2.41	0.51
1:B:221:LEU:HD22	4:C:503:PCW:H342	1.92	0.51
1:C:245:TYR:OH	1:D:388:ASP:OD2	2.29	0.51
1:C:328:ILE:HD13	1:C:389:LEU:HD21	1.92	0.51
1:B:59:PRO:O	1:B:62:LEU:HB3	2.10	0.51
1:B:245:TYR:OH	1:C:388:ASP:OD2	2.28	0.51
1:C:391:ARG:NH1	1:C:393:ASP:OD2	2.41	0.51
3:D:502:PT5:H22	3:D:502:PT5:H51	1.91	0.51
1:D:86:LEU:HD21	1:D:113:LEU:HG	1.92	0.51
1:B:328:ILE:HD13	1:B:389:LEU:HD21	1.92	0.51
1:A:242:PHE:HB3	1:B:275:VAL:HG11	1.93	0.51
1:A:328:ILE:HD13	1:A:389:LEU:HD21	1.93	0.51
1:B:288:ALA:HB1	1:B:314:ILE:HG22	1.93	0.50
1:C:134:LEU:CD2	3:D:502:PT5:H30	2.41	0.50
1:D:288:ALA:HB1	1:D:314:ILE:HG22	1.93	0.50
1:A:86:LEU:HD21	1:A:113:LEU:HG	1.92	0.50
3:A:502:PT5:H60	1:D:134:LEU:HD11	1.93	0.50
1:C:288:ALA:HB1	1:C:314:ILE:HG22	1.93	0.50
1:A:267:ARG:NH2	1:D:245:TYR:OH	2.45	0.49
1:A:299:VAL:HB	1:A:302:PHE:HB2	1.94	0.49
1:D:328:ILE:HD13	1:D:389:LEU:HD21	1.93	0.49
1:A:134:LEU:CD2	3:B:502:PT5:H30	2.42	0.49
1:A:278:GLU:OE1	1:D:235:ARG:NH1	2.45	0.49
1:A:288:ALA:HB1	1:A:314:ILE:HG22	1.93	0.49
1:B:299:VAL:HB	1:B:302:PHE:HB2	1.95	0.49
1:A:275:VAL:HG11	1:D:242:PHE:HB3	1.94	0.49
1:D:299:VAL:HB	1:D:302:PHE:HB2	1.95	0.49
1:B:134:LEU:HD23	3:C:502:PT5:H30	1.93	0.49
1:C:335:GLY:HA3	1:C:377:ARG:NE	2.29	0.48
1:C:299:VAL:HB	1:C:302:PHE:HB2	1.95	0.48
1:B:182:THR:HG22	4:C:503:PCW:H461	1.94	0.48
1:D:335:GLY:HA3	1:D:377:ARG:NE	2.28	0.48
1:D:349:LEU:HD13	1:D:356:ARG:HA	1.96	0.48
1:A:318:GLU:OE2	1:A:391:ARG:NH2	2.34	0.48
1:A:204:GLU:HG2	1:D:184:ILE:HD12	1.96	0.48
1:A:205:LEU:HD21	1:D:145:LEU:HD21	1.95	0.48
1:A:335:GLY:HA3	1:A:377:ARG:NE	2.29	0.48
1:A:349:LEU:HD13	1:A:356:ARG:HA	1.96	0.48
1:D:154:GLY:O	1:D:157:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:HD23	3:D:502:PT5:H30	1.95	0.47
1:B:28:ILE:HG21	4:B:509:PCW:H142	1.96	0.47
1:C:349:LEU:HD13	1:C:356:ARG:HA	1.96	0.47
1:A:259:TYR:CZ	1:B:280:PRO:HD3	2.49	0.47
4:A:505:PCW:H321	4:A:505:PCW:H362	1.97	0.47
1:C:28:ILE:HG21	4:C:509:PCW:H142	1.96	0.47
4:D:505:PCW:H321	4:D:505:PCW:H362	1.97	0.47
1:B:335:GLY:HA3	1:B:377:ARG:NE	2.28	0.47
4:B:505:PCW:H321	4:B:505:PCW:H362	1.97	0.47
4:C:505:PCW:H362	4:C:505:PCW:H321	1.97	0.47
1:D:28:ILE:HG21	4:D:509:PCW:H142	1.96	0.47
1:A:119:GLN:O	1:A:123:THR:OG1	2.33	0.47
1:A:245:TYR:OH	1:B:267:ARG:NH2	2.47	0.47
4:D:505:PCW:H162	4:D:506:PCW:H421	1.97	0.47
4:D:507:PCW:H321	4:D:507:PCW:C12	2.44	0.47
1:B:95:VAL:HG11	1:B:108:SER:HB2	1.98	0.46
1:B:349:LEU:HD13	1:B:356:ARG:HA	1.96	0.46
1:C:182:THR:HG22	4:D:503:PCW:H461	1.96	0.46
1:A:28:ILE:HG21	4:A:509:PCW:H142	1.96	0.46
1:A:95:VAL:HG11	1:A:108:SER:HB2	1.98	0.46
1:A:134:LEU:HD23	3:B:502:PT5:H30	1.96	0.46
4:A:507:PCW:H321	4:A:507:PCW:C12	2.44	0.46
1:D:95:VAL:HG11	1:D:108:SER:HB2	1.97	0.46
4:A:505:PCW:H162	4:A:506:PCW:H421	1.97	0.46
4:C:507:PCW:H321	4:C:507:PCW:C12	2.44	0.46
1:A:170:TYR:CD2	4:A:508:PCW:C36	2.99	0.46
1:A:221:LEU:HD22	4:B:503:PCW:H342	1.98	0.46
1:C:174:PHE:HD2	1:D:201:ILE:HD13	1.81	0.46
1:C:95:VAL:HG11	1:C:108:SER:HB2	1.98	0.46
1:C:170:TYR:CD2	4:C:508:PCW:C36	2.99	0.46
1:C:209:ALA:HB2	4:C:503:PCW:H171	1.98	0.45
1:A:154:GLY:O	1:A:157:SER:OG	2.30	0.45
1:A:166:ALA:HB1	4:A:508:PCW:H322	1.99	0.45
4:B:505:PCW:H162	4:B:506:PCW:H421	1.97	0.45
3:A:502:PT5:H30	3:A:502:PT5:H26	1.62	0.45
1:B:166:ALA:HB1	4:B:508:PCW:H322	1.99	0.45
1:C:166:ALA:HB1	4:C:508:PCW:H322	1.99	0.45
1:A:174:PHE:HD2	1:B:201:ILE:HD13	1.81	0.45
1:A:388:ASP:OD2	1:D:245:TYR:OH	2.35	0.45
4:B:507:PCW:H321	4:B:507:PCW:C12	2.44	0.45
4:C:505:PCW:H372	4:C:506:PCW:H39	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:505:PCW:H162	4:C:506:PCW:H421	1.97	0.45
1:D:166:ALA:HB1	4:D:508:PCW:H322	1.99	0.45
1:B:320:VAL:HG13	1:B:389:LEU:HD12	1.99	0.45
1:A:209:ALA:HB2	4:A:503:PCW:H171	1.98	0.44
1:B:318:GLU:OE2	1:B:391:ARG:NH2	2.34	0.44
1:D:170:TYR:CD2	4:D:508:PCW:C36	2.99	0.44
1:B:170:TYR:CD2	4:B:508:PCW:C36	2.99	0.44
1:B:209:ALA:HB2	4:B:503:PCW:H171	1.98	0.44
1:C:320:VAL:HG13	1:C:389:LEU:HD12	1.99	0.44
4:B:505:PCW:H372	4:B:506:PCW:H39	1.99	0.44
1:A:54:LEU:HD23	1:A:111:ARG:NH1	2.32	0.44
1:A:320:VAL:HG13	1:A:389:LEU:HD12	1.99	0.44
1:C:54:LEU:HD23	1:C:111:ARG:NH1	2.33	0.44
1:B:174:PHE:HD2	1:C:201:ILE:HD13	1.82	0.44
1:B:242:PHE:CB	1:C:275:VAL:HG11	2.47	0.44
4:B:508:PCW:H381	4:B:508:PCW:H411	1.80	0.44
1:D:209:ALA:HB2	4:D:503:PCW:H171	1.98	0.44
1:D:300:PRO:O	1:D:303:LYS:HG2	2.18	0.44
4:D:505:PCW:H372	4:D:506:PCW:H39	1.99	0.44
1:B:346:VAL:HG23	1:B:383:ALA:HA	1.99	0.44
1:B:361:SER:OG	1:B:362:GLU:N	2.51	0.44
1:A:300:PRO:O	1:A:303:LYS:HG2	2.18	0.44
1:D:54:LEU:HD23	1:D:111:ARG:NH1	2.32	0.44
1:C:346:VAL:HG23	1:C:383:ALA:HA	1.99	0.44
1:A:346:VAL:HG23	1:A:383:ALA:HA	1.99	0.43
1:B:54:LEU:HD23	1:B:111:ARG:NH1	2.32	0.43
1:C:242:PHE:CB	1:D:275:VAL:HG11	2.48	0.43
1:D:320:VAL:HG13	1:D:389:LEU:HD12	1.99	0.43
1:D:346:VAL:HG23	1:D:383:ALA:HA	1.99	0.43
4:D:508:PCW:H381	4:D:508:PCW:H411	1.80	0.43
4:A:505:PCW:H372	4:A:506:PCW:H39	1.99	0.43
1:B:119:GLN:O	1:B:123:THR:OG1	2.33	0.43
1:C:119:GLN:O	1:C:123:THR:OG1	2.33	0.43
1:C:300:PRO:O	1:C:303:LYS:HG2	2.18	0.43
1:B:323:GLY:O	1:B:326:GLU:HG2	2.19	0.43
1:B:300:PRO:O	1:B:303:LYS:HG2	2.18	0.43
3:B:502:PT5:H30	3:B:502:PT5:H26	1.62	0.43
1:C:178:ILE:HD13	1:C:178:ILE:HA	1.89	0.43
1:D:323:GLY:O	1:D:326:GLU:HG2	2.19	0.43
1:C:249:SER:N	1:D:290:GLU:OE2	2.34	0.43
1:A:323:GLY:O	1:A:326:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ASP:OD1	1:D:92:ASP:N	2.52	0.43
1:A:361:SER:OG	1:A:362:GLU:N	2.51	0.42
4:A:508:PCW:H40	4:A:508:PCW:H431	1.78	0.42
1:C:28:ILE:CG2	4:C:509:PCW:H142	2.49	0.42
4:A:507:PCW:H341	1:D:171:LEU:HD13	2.00	0.42
1:A:28:ILE:CG2	4:A:509:PCW:H142	2.49	0.42
1:C:323:GLY:O	1:C:326:GLU:HG2	2.19	0.42
3:D:502:PT5:H17	3:D:502:PT5:H20	1.89	0.42
1:C:115:LEU:HD13	1:C:115:LEU:HA	1.92	0.42
1:A:185:GLY:HA3	1:D:184:ILE:O	2.19	0.42
4:D:508:PCW:H40	4:D:508:PCW:H431	1.78	0.42
1:B:28:ILE:CG2	4:B:509:PCW:H142	2.49	0.42
1:A:92:ASP:N	1:A:92:ASP:OD1	2.52	0.42
1:A:158:LEU:HD21	4:A:505:PCW:H341	2.01	0.42
1:B:16:LYS:HA	1:B:16:LYS:HD3	1.88	0.42
3:C:502:PT5:H30	3:C:502:PT5:H26	1.62	0.42
1:D:28:ILE:CG2	4:D:509:PCW:H142	2.49	0.42
4:A:503:PCW:H461	1:D:182:THR:HG22	2.02	0.42
1:B:337:ASP:OD1	1:B:337:ASP:N	2.53	0.42
1:C:92:ASP:N	1:C:92:ASP:OD1	2.52	0.42
1:B:341:ILE:HD12	1:B:364:GLN:HB3	2.02	0.42
1:A:275:VAL:HG11	1:D:242:PHE:CB	2.50	0.41
1:A:337:ASP:OD1	1:A:337:ASP:N	2.53	0.41
1:D:61:ASP:OD2	1:D:81:ARG:NH1	2.45	0.41
1:B:158:LEU:HD21	4:B:505:PCW:H341	2.01	0.41
3:B:502:PT5:H17	3:B:502:PT5:H20	1.89	0.41
1:C:158:LEU:HD21	4:C:505:PCW:H341	2.01	0.41
1:D:158:LEU:HD21	4:D:505:PCW:H341	2.01	0.41
1:B:249:SER:N	1:C:290:GLU:OE2	2.34	0.41
1:D:337:ASP:OD1	1:D:337:ASP:N	2.53	0.41
1:A:115:LEU:HD13	1:A:115:LEU:HA	1.92	0.41
1:B:61:ASP:OD2	1:B:81:ARG:NH1	2.45	0.41
1:B:178:ILE:HD13	1:B:178:ILE:HA	1.90	0.41
1:C:341:ILE:HD12	1:C:364:GLN:HB3	2.02	0.41
1:A:68:ARG:C	1:A:70:SER:H	2.29	0.41
3:A:502:PT5:H17	3:A:502:PT5:H20	1.89	0.41
1:B:11:TYR:O	1:B:14:VAL:HG12	2.21	0.41
4:C:508:PCW:H431	4:C:508:PCW:H40	1.78	0.41
1:A:151:ILE:HD11	1:A:206:LEU:HD23	2.03	0.41
1:A:170:TYR:CE2	4:A:508:PCW:H381	2.56	0.41
1:A:341:ILE:HD12	1:A:364:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD21	4:B:506:PCW:H431	2.03	0.41
1:B:348:VAL:O	1:B:357:TYR:N	2.54	0.41
1:C:151:ILE:HD11	1:C:206:LEU:HD23	2.03	0.41
1:C:170:TYR:CE2	4:C:508:PCW:H381	2.56	0.41
1:D:11:TYR:O	1:D:14:VAL:HG12	2.21	0.41
1:D:361:SER:OG	1:D:362:GLU:N	2.51	0.41
4:D:507:PCW:H31	4:D:507:PCW:P	2.61	0.41
1:A:348:VAL:O	1:A:357:TYR:N	2.54	0.41
4:A:508:PCW:H381	4:A:508:PCW:H411	1.80	0.41
1:B:92:ASP:OD1	1:B:92:ASP:N	2.52	0.41
4:B:507:PCW:H31	4:B:507:PCW:P	2.61	0.41
3:C:502:PT5:H17	3:C:502:PT5:H20	1.89	0.41
1:D:170:TYR:CE2	4:D:508:PCW:H381	2.56	0.41
1:C:68:ARG:C	1:C:70:SER:H	2.29	0.40
1:C:259:TYR:CZ	1:D:280:PRO:HD3	2.57	0.40
1:B:68:ARG:C	1:B:70:SER:H	2.29	0.40
4:B:508:PCW:H431	4:B:508:PCW:H40	1.78	0.40
1:C:206:LEU:HD21	4:C:506:PCW:H431	2.03	0.40
3:D:502:PT5:H30	3:D:502:PT5:H26	1.62	0.40
1:B:259:TYR:CZ	1:C:280:PRO:HD3	2.57	0.40
1:D:151:ILE:HD11	1:D:206:LEU:HD23	2.03	0.40
4:A:507:PCW:H31	4:A:507:PCW:P	2.61	0.40
1:B:151:ILE:HD11	1:B:206:LEU:HD23	2.03	0.40
1:B:170:TYR:CE2	4:B:508:PCW:H381	2.56	0.40
1:C:11:TYR:O	1:C:14:VAL:HG12	2.21	0.40
1:C:308:GLU:HA	1:C:311:ARG:HG2	2.04	0.40
1:C:407:ILE:HD12	1:C:407:ILE:HA	1.97	0.40
4:C:507:PCW:P	4:C:507:PCW:H31	2.61	0.40
1:A:61:ASP:OD2	1:A:81:ARG:NH1	2.45	0.40
1:A:145:LEU:HD21	1:B:205:LEU:HD21	2.02	0.40
1:D:341:ILE:HD12	1:D:364:GLN:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	404/456 (89%)	389 (96%)	15 (4%)	0	100	100
1	B	404/456 (89%)	389 (96%)	15 (4%)	0	100	100
1	C	404/456 (89%)	389 (96%)	15 (4%)	0	100	100
1	D	404/456 (89%)	389 (96%)	15 (4%)	0	100	100
All	All	1616/1824 (89%)	1556 (96%)	60 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	348/393 (88%)	344 (99%)	4 (1%)	65	88
1	B	348/393 (88%)	344 (99%)	4 (1%)	65	88
1	C	348/393 (88%)	344 (99%)	4 (1%)	65	88
1	D	348/393 (88%)	344 (99%)	4 (1%)	65	88
All	All	1392/1572 (88%)	1376 (99%)	16 (1%)	63	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LEU
1	A	115	LEU
1	A	123	THR
1	A	263	LEU
1	B	86	LEU
1	B	115	LEU
1	B	123	THR
1	B	263	LEU
1	C	86	LEU
1	C	115	LEU

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Mol	Chain	Res	Type
1	C	123	THR
1	C	263	LEU
1	D	86	LEU
1	D	115	LEU
1	D	123	THR
1	D	263	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	B	164	ASN
1	C	164	ASN
1	D	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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
4	PCW	D	509	-	9,9,53	1.54	2 (22%)	9,9,61	0.99	1 (11%)
4	PCW	C	505	-	33,33,53	1.45	5 (15%)	36,38,61	1.22	3 (8%)
2	CMP	D	501	-	25,25,25	0.64	0	37,39,39	1.05	3 (8%)
4	PCW	A	506	-	22,22,53	1.47	3 (13%)	25,25,61	0.88	1 (4%)
4	PCW	B	509	-	9,9,53	1.55	2 (22%)	9,9,61	0.99	0
4	PCW	C	509	-	9,9,53	1.54	2 (22%)	9,9,61	0.99	0
4	PCW	C	507	-	35,35,53	1.39	5 (14%)	38,40,61	1.29	4 (10%)
3	PT5	A	502	-	57,57,69	1.48	8 (14%)	72,75,87	1.12	6 (8%)
3	PT5	B	502	-	57,57,69	1.48	8 (14%)	72,75,87	1.12	6 (8%)
4	PCW	D	506	-	22,22,53	1.46	3 (13%)	25,25,61	0.88	1 (4%)
4	PCW	A	504	-	13,13,53	0.88	0	12,12,61	0.49	0
4	PCW	B	505	-	33,33,53	1.44	5 (15%)	36,38,61	1.22	3 (8%)
2	CMP	B	501	-	25,25,25	0.65	0	37,39,39	1.05	2 (5%)
2	CMP	C	501	-	25,25,25	0.64	0	37,39,39	1.05	2 (5%)
4	PCW	C	503	-	37,37,53	1.38	5 (13%)	40,42,61	1.05	3 (7%)
4	PCW	C	504	-	13,13,53	0.88	0	12,12,61	0.49	0
4	PCW	C	506	-	22,22,53	1.46	3 (13%)	25,25,61	0.88	1 (4%)
4	PCW	A	509	-	9,9,53	1.55	2 (22%)	9,9,61	0.99	0
4	PCW	D	505	-	33,33,53	1.45	5 (15%)	36,38,61	1.22	3 (8%)
4	PCW	B	503	-	37,37,53	1.38	5 (13%)	40,42,61	1.05	3 (7%)
4	PCW	D	503	-	37,37,53	1.38	5 (13%)	40,42,61	1.04	3 (7%)
4	PCW	B	504	-	13,13,53	0.88	0	12,12,61	0.48	0
4	PCW	A	507	-	35,35,53	1.39	5 (14%)	38,40,61	1.29	4 (10%)
4	PCW	B	506	-	22,22,53	1.46	3 (13%)	25,25,61	0.88	1 (4%)
3	PT5	C	502	-	57,57,69	1.48	8 (14%)	72,75,87	1.12	6 (8%)
4	PCW	A	508	-	40,40,53	1.19	3 (7%)	42,42,61	1.31	4 (9%)
3	PT5	D	502	-	57,57,69	1.48	8 (14%)	72,75,87	1.12	6 (8%)
4	PCW	D	504	-	13,13,53	0.88	0	12,12,61	0.48	0
4	PCW	B	508	-	40,40,53	1.19	3 (7%)	42,42,61	1.30	4 (9%)
4	PCW	C	508	-	40,40,53	1.19	3 (7%)	42,42,61	1.30	4 (9%)
4	PCW	D	508	-	40,40,53	1.18	3 (7%)	42,42,61	1.30	4 (9%)
4	PCW	B	507	-	35,35,53	1.39	5 (14%)	38,40,61	1.29	4 (10%)
4	PCW	A	505	-	33,33,53	1.44	5 (15%)	36,38,61	1.22	3 (8%)
2	CMP	A	501	-	25,25,25	0.64	0	37,39,39	1.05	2 (5%)
4	PCW	A	503	-	37,37,53	1.38	5 (13%)	40,42,61	1.05	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PCW	D	507	-	35,35,53	1.40	5 (14%)	38,40,61	1.29	4 (10%)

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	PCW	D	509	-	-	4/7/7/57	-
4	PCW	C	505	-	-	14/35/35/57	-
2	CMP	D	501	-	-	0/4/31/31	1/4/4/4
4	PCW	A	506	-	-	14/21/21/57	-
4	PCW	B	509	-	-	4/7/7/57	-
4	PCW	C	509	-	-	4/7/7/57	-
4	PCW	C	507	-	-	15/37/37/57	-
3	PT5	A	502	-	-	29/54/78/90	0/1/1/1
3	PT5	B	502	-	-	29/54/78/90	0/1/1/1
4	PCW	D	506	-	-	14/21/21/57	-
4	PCW	A	504	-	-	6/11/11/57	-
4	PCW	B	505	-	-	14/35/35/57	-
2	CMP	B	501	-	-	0/4/31/31	1/4/4/4
2	CMP	C	501	-	-	0/4/31/31	1/4/4/4
4	PCW	C	503	-	-	20/39/39/57	-
4	PCW	C	504	-	-	6/11/11/57	-
4	PCW	C	506	-	-	14/21/21/57	-
4	PCW	A	509	-	-	4/7/7/57	-
4	PCW	D	505	-	-	14/35/35/57	-
4	PCW	B	503	-	-	20/39/39/57	-
4	PCW	D	503	-	-	20/39/39/57	-
4	PCW	B	504	-	-	6/11/11/57	-
4	PCW	A	507	-	-	15/37/37/57	-
4	PCW	B	506	-	-	14/21/21/57	-
3	PT5	C	502	-	-	29/54/78/90	0/1/1/1
4	PCW	A	508	-	-	15/42/42/57	-
3	PT5	D	502	-	-	29/54/78/90	0/1/1/1
4	PCW	D	504	-	-	6/11/11/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCW	B	508	-	-	15/42/42/57	-
4	PCW	C	508	-	-	15/42/42/57	-
4	PCW	D	508	-	-	15/42/42/57	-
4	PCW	B	507	-	-	15/37/37/57	-
4	PCW	A	505	-	-	14/35/35/57	-
2	CMP	A	501	-	-	0/4/31/31	1/4/4/4
4	PCW	A	503	-	-	20/39/39/57	-
4	PCW	D	507	-	-	15/37/37/57	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	PT5	O16-C10	4.40	1.46	1.34
3	A	502	PT5	O16-C10	4.36	1.46	1.34
3	B	502	PT5	O16-C10	4.36	1.46	1.34
3	C	502	PT5	O16-C10	4.36	1.46	1.34
3	B	502	PT5	O18-C11	4.33	1.46	1.33
3	D	502	PT5	O18-C11	4.33	1.46	1.33
3	C	502	PT5	O18-C11	4.30	1.45	1.33
3	A	502	PT5	O18-C11	4.30	1.45	1.33
3	A	502	PT5	P4-O4	3.56	1.65	1.59
4	B	509	PCW	O3-C11	3.54	1.42	1.30
4	A	509	PCW	O3-C11	3.53	1.42	1.30
4	C	509	PCW	O3-C11	3.53	1.42	1.30
4	D	509	PCW	O3-C11	3.53	1.42	1.30
3	B	502	PT5	P4-O4	3.51	1.65	1.59
3	C	502	PT5	P4-O4	3.47	1.65	1.59
3	D	502	PT5	P4-O4	3.47	1.65	1.59
4	B	505	PCW	P-O4P	3.30	1.67	1.54
4	B	507	PCW	P-O4P	3.29	1.67	1.54
4	C	506	PCW	P-O4P	3.29	1.67	1.54
4	A	505	PCW	P-O4P	3.29	1.67	1.54
4	C	505	PCW	P-O4P	3.28	1.67	1.54
4	D	505	PCW	P-O4P	3.28	1.67	1.54
4	D	506	PCW	P-O4P	3.28	1.67	1.54
4	A	507	PCW	P-O4P	3.28	1.67	1.54
4	C	507	PCW	P-O4P	3.28	1.67	1.54
4	D	507	PCW	P-O4P	3.27	1.67	1.54
4	B	506	PCW	P-O4P	3.27	1.67	1.54
4	A	506	PCW	P-O4P	3.27	1.67	1.54
4	A	503	PCW	P-O4P	3.26	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	503	PCW	P-O4P	3.26	1.66	1.54
4	A	506	PCW	O2-C31	3.25	1.42	1.33
4	B	506	PCW	O2-C31	3.25	1.42	1.33
4	D	503	PCW	P-O4P	3.24	1.66	1.54
4	C	506	PCW	O2-C31	3.24	1.42	1.33
4	D	506	PCW	O2-C31	3.23	1.42	1.33
4	C	503	PCW	P-O4P	3.22	1.66	1.54
3	A	502	PT5	C12-C10	3.15	1.59	1.50
4	D	508	PCW	O3-C11	3.15	1.42	1.33
4	A	508	PCW	O3-C11	3.15	1.42	1.33
3	B	502	PT5	C12-C10	3.14	1.59	1.50
3	C	502	PT5	C12-C10	3.14	1.59	1.50
4	B	508	PCW	O3-C11	3.13	1.42	1.33
4	C	508	PCW	O3-C11	3.13	1.42	1.33
3	D	502	PT5	C12-C10	3.12	1.59	1.50
4	A	503	PCW	O3-C11	3.08	1.42	1.33
4	B	503	PCW	O3-C11	3.08	1.42	1.33
4	D	505	PCW	O3-C11	3.08	1.42	1.33
4	D	507	PCW	O2-C2	-3.08	1.39	1.46
4	B	505	PCW	O3-C11	3.07	1.42	1.33
4	C	505	PCW	O3-C11	3.07	1.42	1.33
4	D	503	PCW	O3-C11	3.05	1.42	1.33
4	A	507	PCW	O2-C2	-3.05	1.39	1.46
4	C	503	PCW	O3-C11	3.04	1.42	1.33
4	C	507	PCW	O3-C11	3.04	1.42	1.33
4	B	507	PCW	O2-C2	-3.04	1.39	1.46
4	C	507	PCW	O2-C2	-3.03	1.39	1.46
4	A	505	PCW	O3-C11	3.03	1.42	1.33
4	C	505	PCW	O2-C31	3.03	1.42	1.34
4	A	507	PCW	O3-C11	3.03	1.42	1.33
4	B	507	PCW	O3-C11	3.03	1.42	1.33
4	D	507	PCW	O3-C11	3.03	1.42	1.33
4	D	505	PCW	O2-C31	3.01	1.42	1.34
4	A	505	PCW	O2-C31	3.00	1.42	1.34
4	A	503	PCW	O2-C2	-2.99	1.39	1.46
4	B	503	PCW	O2-C2	-2.99	1.39	1.46
4	C	503	PCW	O2-C2	-2.99	1.39	1.46
4	D	503	PCW	O2-C2	-2.99	1.39	1.46
4	B	505	PCW	O2-C31	2.98	1.42	1.34
4	A	508	PCW	O2-C31	2.96	1.42	1.34
4	C	508	PCW	O2-C2	-2.96	1.39	1.46
4	B	508	PCW	O2-C31	2.96	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	508	PCW	O2-C31	2.96	1.42	1.34
4	B	508	PCW	O2-C2	-2.96	1.39	1.46
4	A	508	PCW	O2-C2	-2.96	1.39	1.46
4	D	508	PCW	O2-C2	-2.93	1.39	1.46
4	D	508	PCW	O2-C31	2.93	1.42	1.34
3	A	502	PT5	P5-O5	2.90	1.64	1.59
3	B	502	PT5	P5-O5	2.86	1.64	1.59
4	B	507	PCW	O2-C31	2.85	1.42	1.34
4	D	507	PCW	O2-C31	2.83	1.42	1.34
3	C	502	PT5	P5-O5	2.83	1.64	1.59
3	D	502	PT5	P5-O5	2.82	1.64	1.59
4	C	507	PCW	O2-C31	2.82	1.42	1.34
4	A	507	PCW	O2-C31	2.81	1.42	1.34
4	C	503	PCW	O2-C31	2.80	1.42	1.34
4	A	503	PCW	O2-C31	2.78	1.42	1.34
4	B	503	PCW	O2-C31	2.78	1.42	1.34
4	D	503	PCW	O2-C31	2.78	1.42	1.34
4	C	505	PCW	O2-C2	-2.77	1.40	1.46
4	D	505	PCW	O2-C2	-2.77	1.40	1.46
3	A	502	PT5	P1-O1	2.74	1.67	1.59
3	D	502	PT5	P1-O1	2.73	1.67	1.59
4	A	505	PCW	O2-C2	-2.73	1.40	1.46
4	B	505	PCW	O2-C2	-2.73	1.40	1.46
3	B	502	PT5	P1-O1	2.71	1.67	1.59
3	C	502	PT5	P1-O1	2.71	1.67	1.59
4	D	506	PCW	P-O3P	2.49	1.68	1.60
4	A	506	PCW	P-O3P	2.46	1.68	1.60
4	B	506	PCW	P-O3P	2.46	1.68	1.60
4	C	506	PCW	P-O3P	2.46	1.68	1.60
3	C	502	PT5	C31-C11	2.34	1.57	1.50
3	D	502	PT5	P1-O13	2.32	1.68	1.59
3	B	502	PT5	P1-O13	2.32	1.68	1.59
3	C	502	PT5	P1-O13	2.32	1.68	1.59
4	C	505	PCW	P-O3P	2.32	1.67	1.60
3	B	502	PT5	C31-C11	2.31	1.57	1.50
3	A	502	PT5	C31-C11	2.31	1.57	1.50
4	C	503	PCW	P-O3P	2.30	1.67	1.60
3	A	502	PT5	P1-O13	2.30	1.68	1.59
3	D	502	PT5	C31-C11	2.30	1.57	1.50
4	D	503	PCW	P-O3P	2.30	1.67	1.60
4	D	507	PCW	P-O3P	2.29	1.67	1.60
4	A	505	PCW	P-O3P	2.28	1.67	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	PCW	P-O3P	2.28	1.67	1.60
4	B	503	PCW	P-O3P	2.28	1.67	1.60
4	D	505	PCW	P-O3P	2.28	1.67	1.60
4	A	507	PCW	P-O3P	2.27	1.67	1.60
4	A	503	PCW	P-O3P	2.26	1.67	1.60
4	C	507	PCW	P-O3P	2.26	1.67	1.60
4	B	507	PCW	P-O3P	2.25	1.67	1.60
4	A	509	PCW	C12-C11	2.13	1.55	1.50
4	D	509	PCW	C12-C11	2.12	1.55	1.50
4	B	509	PCW	C12-C11	2.11	1.55	1.50
4	C	509	PCW	C12-C11	2.10	1.55	1.50

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	508	PCW	C21-C20-C19	4.04	155.08	124.83
4	C	508	PCW	C21-C20-C19	4.04	155.07	124.83
4	B	508	PCW	C21-C20-C19	4.03	155.06	124.83
4	A	508	PCW	C21-C20-C19	4.03	155.04	124.83
4	A	508	PCW	C18-C19-C20	4.01	154.88	124.83
4	A	505	PCW	O2-C31-C32	4.01	120.16	111.48
4	B	508	PCW	C18-C19-C20	4.01	154.86	124.83
4	D	508	PCW	C18-C19-C20	4.01	154.85	124.83
4	C	508	PCW	C18-C19-C20	4.01	154.85	124.83
4	C	505	PCW	O2-C31-C32	4.00	120.13	111.48
4	D	505	PCW	O2-C31-C32	4.00	120.13	111.48
4	B	505	PCW	O2-C31-C32	3.99	120.12	111.48
3	D	502	PT5	O16-C10-C12	3.87	119.84	111.48
3	C	502	PT5	O16-C10-C12	3.85	119.81	111.48
3	B	502	PT5	O16-C10-C12	3.85	119.80	111.48
3	A	502	PT5	O16-C10-C12	3.84	119.80	111.48
4	A	508	PCW	O2-C31-C32	3.80	119.71	111.48
4	B	508	PCW	O2-C31-C32	3.80	119.70	111.48
4	C	508	PCW	O2-C31-C32	3.80	119.70	111.48
4	D	508	PCW	O2-C31-C32	3.79	119.67	111.48
4	B	505	PCW	C18-C19-C20	3.76	154.03	126.65
4	C	505	PCW	C18-C19-C20	3.75	154.03	126.65
4	D	505	PCW	C18-C19-C20	3.75	154.01	126.65
4	A	505	PCW	C18-C19-C20	3.75	154.01	126.65
4	B	507	PCW	C21-C20-C19	3.62	154.73	126.43
4	A	507	PCW	C21-C20-C19	3.62	154.72	126.43
4	C	507	PCW	C21-C20-C19	3.62	154.71	126.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	507	PCW	C21-C20-C19	3.61	154.69	126.43
4	A	503	PCW	O2-C31-C32	3.58	119.23	111.48
4	B	507	PCW	O2-C31-C32	3.58	119.22	111.48
4	C	503	PCW	O2-C31-C32	3.58	119.22	111.48
4	A	507	PCW	O2-C31-C32	3.57	119.20	111.48
4	D	507	PCW	O2-C31-C32	3.57	119.19	111.48
4	C	507	PCW	O2-C31-C32	3.56	119.19	111.48
3	D	502	PT5	C23-C22-C21	3.56	153.61	123.57
4	B	503	PCW	O2-C31-C32	3.56	119.18	111.48
3	A	502	PT5	C23-C22-C21	3.55	153.56	123.57
3	B	502	PT5	C23-C22-C21	3.55	153.56	123.57
3	C	502	PT5	C23-C22-C21	3.55	153.52	123.57
4	D	503	PCW	O2-C31-C32	3.55	119.16	111.48
2	B	501	CMP	O2P-P-O1P	3.46	119.19	108.56
2	D	501	CMP	O2P-P-O1P	3.45	119.16	108.56
2	A	501	CMP	O2P-P-O1P	3.45	119.15	108.56
2	C	501	CMP	O2P-P-O1P	3.44	119.14	108.56
4	A	507	PCW	C18-C19-C20	3.09	153.86	130.48
4	D	507	PCW	C18-C19-C20	3.08	153.84	130.48
4	B	507	PCW	C18-C19-C20	3.08	153.82	130.48
4	C	507	PCW	C18-C19-C20	3.08	153.81	130.48
3	A	502	PT5	O18-C11-C31	3.05	121.14	111.83
3	B	502	PT5	O18-C11-C31	3.05	121.13	111.83
3	C	502	PT5	O18-C11-C31	3.04	121.12	111.83
3	D	502	PT5	O18-C11-C31	3.04	121.10	111.83
4	C	506	PCW	O2-C31-C32	2.86	120.57	111.83
4	D	506	PCW	O2-C31-C32	2.86	120.56	111.83
4	B	506	PCW	O2-C31-C32	2.86	120.54	111.83
4	A	506	PCW	O2-C31-C32	2.85	120.52	111.83
3	A	502	PT5	P4-O4-C4	-2.75	116.08	123.43
3	D	502	PT5	P4-O4-C4	-2.74	116.11	123.43
3	B	502	PT5	P4-O4-C4	-2.74	116.12	123.43
3	C	502	PT5	P4-O4-C4	-2.74	116.13	123.43
4	C	503	PCW	O3-C11-C12	2.73	120.17	111.83
4	B	503	PCW	O3-C11-C12	2.73	120.15	111.83
4	A	503	PCW	O3-C11-C12	2.72	120.13	111.83
4	C	507	PCW	O3-C11-C12	2.72	120.13	111.83
4	D	507	PCW	O3-C11-C12	2.72	120.13	111.83
2	B	501	CMP	O5'-P-O3'	-2.72	102.06	105.70
4	D	503	PCW	O3-C11-C12	2.72	120.12	111.83
2	D	501	CMP	O5'-P-O3'	-2.71	102.07	105.70
2	A	501	CMP	O5'-P-O3'	-2.71	102.07	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	CMP	O5'-P-O3'	-2.71	102.07	105.70
4	A	508	PCW	O3-C11-C12	2.71	120.10	111.83
4	B	507	PCW	O3-C11-C12	2.71	120.09	111.83
4	B	508	PCW	O3-C11-C12	2.70	120.07	111.83
4	A	507	PCW	O3-C11-C12	2.70	120.07	111.83
4	C	508	PCW	O3-C11-C12	2.69	120.04	111.83
4	D	508	PCW	O3-C11-C12	2.68	120.01	111.83
4	A	505	PCW	O3-C11-C12	2.56	119.64	111.83
4	B	505	PCW	O3-C11-C12	2.55	119.61	111.83
4	D	505	PCW	O3-C11-C12	2.54	119.59	111.83
4	C	505	PCW	O3-C11-C12	2.54	119.58	111.83
4	C	503	PCW	C2-O2-C31	-2.51	111.78	117.80
4	A	503	PCW	C2-O2-C31	-2.51	111.79	117.80
4	B	503	PCW	C2-O2-C31	-2.51	111.79	117.80
4	D	503	PCW	C2-O2-C31	-2.51	111.79	117.80
3	D	502	PT5	C8-O16-C10	-2.23	112.47	117.80
3	A	502	PT5	C8-O16-C10	-2.22	112.48	117.80
3	B	502	PT5	C8-O16-C10	-2.21	112.51	117.80
3	C	502	PT5	C8-O16-C10	-2.19	112.55	117.80
3	C	502	PT5	P5-O5-C5	-2.09	117.86	123.43
3	D	502	PT5	P5-O5-C5	-2.08	117.88	123.43
3	A	502	PT5	P5-O5-C5	-2.08	117.88	123.43
3	B	502	PT5	P5-O5-C5	-2.08	117.88	123.43
2	D	501	CMP	O3'-C3'-C4'	-2.01	109.19	110.71
4	D	509	PCW	O3-C11-C12	2.01	120.35	114.00

There are no chirality outliers.

All (468) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	PT5	C1-O1-P1-O12
3	A	502	PT5	C1-O1-P1-O13
3	A	502	PT5	O17-C10-O16-C8
3	A	502	PT5	C12-C10-O16-C8
3	B	502	PT5	C1-O1-P1-O12
3	B	502	PT5	C1-O1-P1-O13
3	B	502	PT5	O17-C10-O16-C8
3	B	502	PT5	C12-C10-O16-C8
3	C	502	PT5	C1-O1-P1-O12
3	C	502	PT5	C1-O1-P1-O13
3	C	502	PT5	O17-C10-O16-C8
3	C	502	PT5	C12-C10-O16-C8

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Mol	Chain	Res	Type	Atoms
3	D	502	PT5	C1-O1-P1-O12
3	D	502	PT5	C1-O1-P1-O13
3	D	502	PT5	O17-C10-O16-C8
3	D	502	PT5	C12-C10-O16-C8
4	A	503	PCW	O3P-C1-C2-O2
4	A	503	PCW	C32-C31-O2-C2
4	A	503	PCW	C1-O3P-P-O1P
4	A	503	PCW	C1-O3P-P-O4P
4	A	505	PCW	C32-C31-O2-C2
4	A	505	PCW	C1-O3P-P-O1P
4	A	505	PCW	C1-O3P-P-O4P
4	A	506	PCW	O3P-C1-C2-O2
4	A	506	PCW	C1-O3P-P-O1P
4	A	506	PCW	C1-O3P-P-O4P
4	A	507	PCW	C32-C31-O2-C2
4	A	507	PCW	O31-C31-O2-C2
4	A	508	PCW	C40-C41-C42-C43
4	B	503	PCW	O3P-C1-C2-O2
4	B	503	PCW	C32-C31-O2-C2
4	B	503	PCW	C1-O3P-P-O1P
4	B	503	PCW	C1-O3P-P-O4P
4	B	505	PCW	C32-C31-O2-C2
4	B	505	PCW	C1-O3P-P-O1P
4	B	505	PCW	C1-O3P-P-O4P
4	B	506	PCW	O3P-C1-C2-O2
4	B	506	PCW	C1-O3P-P-O1P
4	B	506	PCW	C1-O3P-P-O4P
4	B	507	PCW	C32-C31-O2-C2
4	B	507	PCW	O31-C31-O2-C2
4	B	508	PCW	C40-C41-C42-C43
4	C	503	PCW	O3P-C1-C2-O2
4	C	503	PCW	C32-C31-O2-C2
4	C	503	PCW	C1-O3P-P-O1P
4	C	503	PCW	C1-O3P-P-O4P
4	C	505	PCW	C32-C31-O2-C2
4	C	505	PCW	C1-O3P-P-O1P
4	C	505	PCW	C1-O3P-P-O4P
4	C	506	PCW	O3P-C1-C2-O2
4	C	506	PCW	C1-O3P-P-O1P
4	C	506	PCW	C1-O3P-P-O4P
4	C	507	PCW	C32-C31-O2-C2
4	C	507	PCW	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
4	C	508	PCW	C40-C41-C42-C43
4	D	503	PCW	O3P-C1-C2-O2
4	D	503	PCW	C32-C31-O2-C2
4	D	503	PCW	C1-O3P-P-O1P
4	D	503	PCW	C1-O3P-P-O4P
4	D	505	PCW	C32-C31-O2-C2
4	D	505	PCW	C1-O3P-P-O1P
4	D	505	PCW	C1-O3P-P-O4P
4	D	506	PCW	O3P-C1-C2-O2
4	D	506	PCW	C1-O3P-P-O1P
4	D	506	PCW	C1-O3P-P-O4P
4	D	507	PCW	C32-C31-O2-C2
4	D	507	PCW	O31-C31-O2-C2
4	D	508	PCW	C40-C41-C42-C43
3	A	502	PT5	O19-C11-O18-C9
3	B	502	PT5	O19-C11-O18-C9
3	C	502	PT5	O19-C11-O18-C9
3	D	502	PT5	O19-C11-O18-C9
4	A	503	PCW	O11-C11-O3-C3
4	B	503	PCW	O11-C11-O3-C3
4	C	503	PCW	O11-C11-O3-C3
4	D	503	PCW	O11-C11-O3-C3
3	A	502	PT5	C31-C11-O18-C9
3	B	502	PT5	C31-C11-O18-C9
3	C	502	PT5	C31-C11-O18-C9
3	D	502	PT5	C31-C11-O18-C9
4	A	503	PCW	O31-C31-O2-C2
4	A	505	PCW	O31-C31-O2-C2
4	B	503	PCW	O31-C31-O2-C2
4	B	505	PCW	O31-C31-O2-C2
4	C	503	PCW	O31-C31-O2-C2
4	C	505	PCW	O31-C31-O2-C2
4	D	503	PCW	O31-C31-O2-C2
4	D	505	PCW	O31-C31-O2-C2
4	A	503	PCW	C12-C11-O3-C3
4	A	508	PCW	C12-C11-O3-C3
4	B	503	PCW	C12-C11-O3-C3
4	B	508	PCW	C12-C11-O3-C3
4	C	503	PCW	C12-C11-O3-C3
4	C	508	PCW	C12-C11-O3-C3
4	D	503	PCW	C12-C11-O3-C3
4	D	508	PCW	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
4	A	507	PCW	C12-C11-O3-C3
4	B	507	PCW	C12-C11-O3-C3
4	C	507	PCW	C12-C11-O3-C3
4	D	507	PCW	C12-C11-O3-C3
4	A	508	PCW	O11-C11-O3-C3
4	B	508	PCW	O11-C11-O3-C3
4	C	508	PCW	O11-C11-O3-C3
4	D	508	PCW	O11-C11-O3-C3
4	A	506	PCW	C32-C31-O2-C2
4	B	506	PCW	C32-C31-O2-C2
4	C	506	PCW	C32-C31-O2-C2
4	D	506	PCW	C32-C31-O2-C2
4	C	507	PCW	O11-C11-O3-C3
4	A	507	PCW	O11-C11-O3-C3
4	B	507	PCW	O11-C11-O3-C3
4	D	507	PCW	O11-C11-O3-C3
4	A	506	PCW	O31-C31-O2-C2
4	B	506	PCW	O31-C31-O2-C2
4	C	506	PCW	O31-C31-O2-C2
4	D	506	PCW	O31-C31-O2-C2
4	A	506	PCW	C32-C33-C34-C35
4	B	506	PCW	C32-C33-C34-C35
4	C	506	PCW	C32-C33-C34-C35
4	D	506	PCW	C32-C33-C34-C35
4	A	508	PCW	C32-C31-O2-C2
4	B	508	PCW	C32-C31-O2-C2
4	C	508	PCW	C32-C31-O2-C2
4	D	508	PCW	C32-C31-O2-C2
4	A	503	PCW	C31-C32-C33-C34
4	A	505	PCW	C31-C32-C33-C34
4	B	503	PCW	C31-C32-C33-C34
4	B	505	PCW	C31-C32-C33-C34
4	C	503	PCW	C31-C32-C33-C34
4	C	505	PCW	C31-C32-C33-C34
4	D	503	PCW	C31-C32-C33-C34
4	D	505	PCW	C31-C32-C33-C34
4	A	507	PCW	C31-C32-C33-C34
4	B	507	PCW	C31-C32-C33-C34
4	C	507	PCW	C31-C32-C33-C34
4	D	507	PCW	C31-C32-C33-C34
3	A	502	PT5	C11-C31-C32-C33
3	B	502	PT5	C11-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	C	502	PT5	C11-C31-C32-C33
3	D	502	PT5	C11-C31-C32-C33
4	A	503	PCW	C32-C33-C34-C35
4	B	503	PCW	C32-C33-C34-C35
4	C	503	PCW	C32-C33-C34-C35
4	D	503	PCW	C32-C33-C34-C35
4	A	508	PCW	O31-C31-O2-C2
4	B	508	PCW	O31-C31-O2-C2
4	C	508	PCW	O31-C31-O2-C2
4	D	508	PCW	O31-C31-O2-C2
4	A	505	PCW	C12-C11-O3-C3
4	B	505	PCW	C12-C11-O3-C3
4	C	505	PCW	C12-C11-O3-C3
4	D	505	PCW	C12-C11-O3-C3
4	A	503	PCW	C33-C34-C35-C36
4	A	507	PCW	C35-C36-C37-C38
4	B	503	PCW	C33-C34-C35-C36
4	B	507	PCW	C35-C36-C37-C38
4	C	503	PCW	C33-C34-C35-C36
4	C	507	PCW	C35-C36-C37-C38
4	D	503	PCW	C33-C34-C35-C36
4	D	507	PCW	C35-C36-C37-C38
4	A	507	PCW	C11-C12-C13-C14
4	B	507	PCW	C11-C12-C13-C14
4	C	507	PCW	C11-C12-C13-C14
4	D	507	PCW	C11-C12-C13-C14
4	A	503	PCW	C34-C35-C36-C37
4	B	503	PCW	C34-C35-C36-C37
4	C	503	PCW	C34-C35-C36-C37
4	D	503	PCW	C34-C35-C36-C37
4	A	508	PCW	C33-C34-C35-C36
4	D	508	PCW	C33-C34-C35-C36
4	A	505	PCW	O11-C11-O3-C3
4	B	505	PCW	O11-C11-O3-C3
4	C	505	PCW	O11-C11-O3-C3
4	D	505	PCW	O11-C11-O3-C3
4	A	504	PCW	C21-C22-C23-C24
4	B	504	PCW	C21-C22-C23-C24
4	B	508	PCW	C33-C34-C35-C36
4	C	504	PCW	C21-C22-C23-C24
4	C	508	PCW	C33-C34-C35-C36
4	A	505	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	B	505	PCW	C35-C36-C37-C38
4	C	505	PCW	C35-C36-C37-C38
4	D	504	PCW	C21-C22-C23-C24
4	D	505	PCW	C35-C36-C37-C38
4	A	509	PCW	C13-C14-C15-C16
4	D	509	PCW	C13-C14-C15-C16
4	B	509	PCW	C13-C14-C15-C16
4	C	509	PCW	C13-C14-C15-C16
4	C	506	PCW	C31-C32-C33-C34
4	A	506	PCW	C31-C32-C33-C34
4	B	506	PCW	C31-C32-C33-C34
4	D	506	PCW	C31-C32-C33-C34
4	B	506	PCW	C34-C35-C36-C37
4	D	506	PCW	C34-C35-C36-C37
4	A	506	PCW	C34-C35-C36-C37
4	C	506	PCW	C34-C35-C36-C37
4	C	504	PCW	C24-C25-C26-C27
4	D	504	PCW	C24-C25-C26-C27
4	A	504	PCW	C24-C25-C26-C27
4	B	504	PCW	C24-C25-C26-C27
4	A	507	PCW	C13-C14-C15-C16
4	B	507	PCW	C13-C14-C15-C16
4	C	507	PCW	C13-C14-C15-C16
4	D	507	PCW	C13-C14-C15-C16
4	C	508	PCW	C20-C21-C22-C23
3	A	502	PT5	C7-C8-C9-O18
3	B	502	PT5	C7-C8-C9-O18
3	C	502	PT5	C7-C8-C9-O18
3	D	502	PT5	C7-C8-C9-O18
4	A	507	PCW	C1-C2-C3-O3
4	B	507	PCW	C1-C2-C3-O3
4	C	507	PCW	C1-C2-C3-O3
4	D	507	PCW	C1-C2-C3-O3
3	A	502	PT5	C12-C13-C14-C15
3	B	502	PT5	C12-C13-C14-C15
3	C	502	PT5	C12-C13-C14-C15
3	D	502	PT5	C12-C13-C14-C15
4	A	507	PCW	C16-C17-C18-C19
4	A	508	PCW	C20-C21-C22-C23
4	B	507	PCW	C16-C17-C18-C19
4	B	508	PCW	C20-C21-C22-C23
4	C	507	PCW	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
4	D	507	PCW	C16-C17-C18-C19
4	D	508	PCW	C20-C21-C22-C23
4	C	508	PCW	C35-C36-C37-C38
4	D	508	PCW	C35-C36-C37-C38
4	A	508	PCW	C35-C36-C37-C38
4	B	508	PCW	C35-C36-C37-C38
4	A	503	PCW	C1-O3P-P-O2P
4	A	505	PCW	C1-O3P-P-O2P
4	A	506	PCW	C1-O3P-P-O2P
4	B	503	PCW	C1-O3P-P-O2P
4	B	505	PCW	C1-O3P-P-O2P
4	B	506	PCW	C1-O3P-P-O2P
4	C	503	PCW	C1-O3P-P-O2P
4	C	505	PCW	C1-O3P-P-O2P
4	C	506	PCW	C1-O3P-P-O2P
4	D	503	PCW	C1-O3P-P-O2P
4	D	505	PCW	C1-O3P-P-O2P
4	D	506	PCW	C1-O3P-P-O2P
4	A	504	PCW	C20-C21-C22-C23
4	B	504	PCW	C20-C21-C22-C23
4	C	504	PCW	C20-C21-C22-C23
4	D	504	PCW	C20-C21-C22-C23
4	A	503	PCW	C12-C13-C14-C15
4	C	503	PCW	C12-C13-C14-C15
4	D	503	PCW	C12-C13-C14-C15
4	B	503	PCW	C12-C13-C14-C15
4	C	507	PCW	C33-C34-C35-C36
4	A	507	PCW	C33-C34-C35-C36
4	B	507	PCW	C33-C34-C35-C36
4	D	507	PCW	C33-C34-C35-C36
4	B	508	PCW	C23-C24-C25-C26
4	A	508	PCW	C23-C24-C25-C26
4	C	508	PCW	C23-C24-C25-C26
4	D	508	PCW	C23-C24-C25-C26
4	B	503	PCW	C42-C43-C44-C45
4	D	503	PCW	C42-C43-C44-C45
4	A	503	PCW	C42-C43-C44-C45
4	C	503	PCW	C42-C43-C44-C45
4	A	503	PCW	O3P-C1-C2-C3
4	B	503	PCW	O3P-C1-C2-C3
4	C	503	PCW	O3P-C1-C2-C3
4	D	503	PCW	O3P-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	B	508	PCW	C22-C23-C24-C25
4	D	508	PCW	C22-C23-C24-C25
4	C	508	PCW	C22-C23-C24-C25
4	A	508	PCW	C22-C23-C24-C25
4	A	506	PCW	C36-C37-C38-C39
4	B	506	PCW	C36-C37-C38-C39
4	C	506	PCW	C36-C37-C38-C39
4	D	506	PCW	C36-C37-C38-C39
4	A	507	PCW	O2-C2-C3-O3
4	B	507	PCW	O2-C2-C3-O3
4	C	507	PCW	O2-C2-C3-O3
4	D	507	PCW	O2-C2-C3-O3
3	A	502	PT5	C16-C17-C18-C19
3	A	502	PT5	C19-C20-C21-C22
3	A	502	PT5	C21-C22-C23-C24
3	B	502	PT5	C16-C17-C18-C19
3	B	502	PT5	C19-C20-C21-C22
3	B	502	PT5	C21-C22-C23-C24
3	C	502	PT5	C16-C17-C18-C19
3	C	502	PT5	C19-C20-C21-C22
3	C	502	PT5	C21-C22-C23-C24
3	D	502	PT5	C16-C17-C18-C19
3	D	502	PT5	C19-C20-C21-C22
3	D	502	PT5	C21-C22-C23-C24
4	A	509	PCW	C15-C16-C17-C18
4	B	509	PCW	C15-C16-C17-C18
4	D	509	PCW	C15-C16-C17-C18
4	A	503	PCW	C35-C36-C37-C38
4	C	503	PCW	C35-C36-C37-C38
4	C	509	PCW	C15-C16-C17-C18
4	B	503	PCW	C35-C36-C37-C38
4	D	503	PCW	C35-C36-C37-C38
3	A	502	PT5	C37-C38-C39-C40
3	B	502	PT5	C37-C38-C39-C40
3	C	502	PT5	C37-C38-C39-C40
3	D	502	PT5	C37-C38-C39-C40
3	A	502	PT5	O13-C7-C8-C9
3	B	502	PT5	O13-C7-C8-C9
3	C	502	PT5	O13-C7-C8-C9
3	D	502	PT5	O13-C7-C8-C9
4	D	508	PCW	C12-C13-C14-C15
4	B	508	PCW	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
4	C	508	PCW	C12-C13-C14-C15
4	A	508	PCW	C12-C13-C14-C15
3	A	502	PT5	O13-C7-C8-O16
3	B	502	PT5	O13-C7-C8-O16
3	C	502	PT5	O13-C7-C8-O16
3	D	502	PT5	O13-C7-C8-O16
4	A	503	PCW	C1-C2-C3-O3
4	B	503	PCW	C1-C2-C3-O3
4	C	503	PCW	C1-C2-C3-O3
4	D	503	PCW	C1-C2-C3-O3
4	B	506	PCW	C35-C36-C37-C38
4	C	506	PCW	C35-C36-C37-C38
4	D	506	PCW	C35-C36-C37-C38
4	A	506	PCW	C35-C36-C37-C38
4	B	509	PCW	C12-C13-C14-C15
4	C	509	PCW	C12-C13-C14-C15
4	D	509	PCW	C12-C13-C14-C15
4	A	509	PCW	C12-C13-C14-C15
3	A	502	PT5	C1-O1-P1-O11
3	B	502	PT5	C1-O1-P1-O11
3	C	502	PT5	C1-O1-P1-O11
3	D	502	PT5	C1-O1-P1-O11
4	A	506	PCW	C40-C41-C42-C43
4	B	506	PCW	C40-C41-C42-C43
4	C	506	PCW	C40-C41-C42-C43
4	D	506	PCW	C40-C41-C42-C43
4	D	503	PCW	C39-C40-C41-C42
4	B	504	PCW	C14-C15-C16-C17
4	C	504	PCW	C14-C15-C16-C17
4	D	504	PCW	C14-C15-C16-C17
4	A	503	PCW	O2-C2-C3-O3
4	B	503	PCW	O2-C2-C3-O3
4	C	503	PCW	O2-C2-C3-O3
4	D	503	PCW	O2-C2-C3-O3
4	A	504	PCW	C14-C15-C16-C17
4	A	503	PCW	C39-C40-C41-C42
4	B	503	PCW	C39-C40-C41-C42
4	C	503	PCW	C39-C40-C41-C42
3	A	502	PT5	C7-O13-P1-O12
3	A	502	PT5	C7-O13-P1-O11
3	A	502	PT5	C7-O13-P1-O1
3	B	502	PT5	C7-O13-P1-O12

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Mol	Chain	Res	Type	Atoms
3	B	502	PT5	C7-O13-P1-O11
3	B	502	PT5	C7-O13-P1-O1
3	C	502	PT5	C7-O13-P1-O12
3	C	502	PT5	C7-O13-P1-O11
3	C	502	PT5	C7-O13-P1-O1
3	D	502	PT5	C7-O13-P1-O12
3	D	502	PT5	C7-O13-P1-O11
3	D	502	PT5	C7-O13-P1-O1
4	C	508	PCW	C19-C20-C21-C22
4	A	503	PCW	C43-C44-C45-C46
4	B	503	PCW	C43-C44-C45-C46
4	C	503	PCW	C43-C44-C45-C46
4	D	503	PCW	C43-C44-C45-C46
4	A	505	PCW	C3-C2-O2-C31
4	A	508	PCW	C3-C2-O2-C31
4	B	505	PCW	C3-C2-O2-C31
4	B	508	PCW	C3-C2-O2-C31
4	C	505	PCW	C3-C2-O2-C31
4	C	508	PCW	C3-C2-O2-C31
4	D	505	PCW	C3-C2-O2-C31
4	D	508	PCW	C3-C2-O2-C31
4	A	508	PCW	C19-C20-C21-C22
4	B	508	PCW	C19-C20-C21-C22
4	D	508	PCW	C19-C20-C21-C22
4	A	505	PCW	O3P-C1-C2-O2
4	B	505	PCW	O3P-C1-C2-O2
4	C	505	PCW	O3P-C1-C2-O2
4	D	505	PCW	O3P-C1-C2-O2
3	A	502	PT5	C36-C37-C38-C39
3	B	502	PT5	C36-C37-C38-C39
3	C	502	PT5	C36-C37-C38-C39
3	D	502	PT5	C36-C37-C38-C39
3	A	502	PT5	O16-C8-C9-O18
3	B	502	PT5	O16-C8-C9-O18
3	C	502	PT5	O16-C8-C9-O18
3	D	502	PT5	O16-C8-C9-O18
4	B	505	PCW	C12-C13-C14-C15
4	D	505	PCW	C12-C13-C14-C15
4	A	505	PCW	C12-C13-C14-C15
4	C	505	PCW	C12-C13-C14-C15
4	C	506	PCW	C33-C34-C35-C36
4	D	506	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	A	506	PCW	C33-C34-C35-C36
4	B	506	PCW	C33-C34-C35-C36
4	B	509	PCW	C14-C15-C16-C17
4	C	509	PCW	C14-C15-C16-C17
4	D	509	PCW	C14-C15-C16-C17
4	A	509	PCW	C14-C15-C16-C17
3	A	502	PT5	C35-C36-C37-C38
3	B	502	PT5	C35-C36-C37-C38
3	C	502	PT5	C35-C36-C37-C38
3	D	502	PT5	C35-C36-C37-C38
4	A	507	PCW	C2-C1-O3P-P
4	B	507	PCW	C2-C1-O3P-P
4	C	507	PCW	C2-C1-O3P-P
4	D	507	PCW	C2-C1-O3P-P
3	A	502	PT5	C4-O4-P4-O42
3	B	502	PT5	C4-O4-P4-O42
3	C	502	PT5	C4-O4-P4-O42
3	D	502	PT5	C4-O4-P4-O42
3	A	502	PT5	C34-C35-C36-C37
3	C	502	PT5	C34-C35-C36-C37
3	D	502	PT5	C34-C35-C36-C37
3	B	502	PT5	C34-C35-C36-C37
4	A	504	PCW	C23-C24-C25-C26
4	C	504	PCW	C23-C24-C25-C26
4	D	504	PCW	C23-C24-C25-C26
4	B	504	PCW	C23-C24-C25-C26
3	A	502	PT5	C22-C23-C24-C25
3	B	502	PT5	C22-C23-C24-C25
3	C	502	PT5	C22-C23-C24-C25
3	D	502	PT5	C22-C23-C24-C25
4	B	504	PCW	C19-C20-C21-C22
4	C	504	PCW	C19-C20-C21-C22
4	D	504	PCW	C19-C20-C21-C22
3	A	502	PT5	C33-C34-C35-C36
3	C	502	PT5	C33-C34-C35-C36
3	B	502	PT5	C33-C34-C35-C36
3	D	502	PT5	C33-C34-C35-C36
4	A	504	PCW	C19-C20-C21-C22
4	C	505	PCW	C33-C34-C35-C36
4	D	505	PCW	C33-C34-C35-C36
4	B	505	PCW	C33-C34-C35-C36
4	A	505	PCW	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
4	A	507	PCW	C39-C40-C41-C42
4	B	507	PCW	C39-C40-C41-C42
4	C	507	PCW	C39-C40-C41-C42
4	D	507	PCW	C39-C40-C41-C42
4	C	507	PCW	C15-C16-C17-C18
4	A	507	PCW	C15-C16-C17-C18
4	B	507	PCW	C15-C16-C17-C18
4	D	507	PCW	C15-C16-C17-C18
3	A	502	PT5	C4-O4-P4-O41
3	B	502	PT5	C4-O4-P4-O41
3	C	502	PT5	C4-O4-P4-O41
3	D	502	PT5	C4-O4-P4-O41
4	D	505	PCW	C32-C33-C34-C35
4	C	505	PCW	C32-C33-C34-C35
3	B	502	PT5	C8-C7-O13-P1
4	A	505	PCW	C32-C33-C34-C35
4	B	505	PCW	C32-C33-C34-C35
4	A	508	PCW	O3-C11-C12-C13
4	B	508	PCW	O3-C11-C12-C13
4	C	508	PCW	O3-C11-C12-C13
4	D	508	PCW	O3-C11-C12-C13
3	A	502	PT5	C8-C7-O13-P1
3	C	502	PT5	C8-C7-O13-P1
3	D	502	PT5	C8-C7-O13-P1
4	A	508	PCW	O11-C11-C12-C13
4	D	508	PCW	O11-C11-C12-C13
4	C	506	PCW	C41-C42-C43-C44
4	D	506	PCW	C41-C42-C43-C44
4	B	506	PCW	C41-C42-C43-C44
4	C	508	PCW	O11-C11-C12-C13
4	A	506	PCW	C41-C42-C43-C44
4	B	508	PCW	O11-C11-C12-C13
3	A	502	PT5	O18-C11-C31-C32
3	B	502	PT5	O18-C11-C31-C32
3	C	502	PT5	O18-C11-C31-C32
3	D	502	PT5	O18-C11-C31-C32

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	CMP	C3'-C4'-C5'-O3'-O5'-P
2	D	501	CMP	C3'-C4'-C5'-O3'-O5'-P

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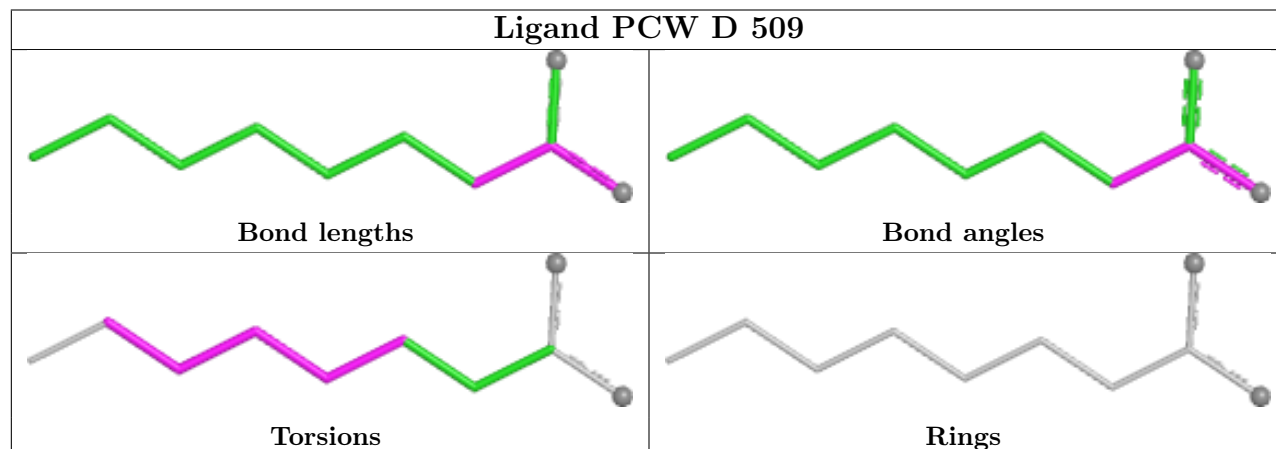
Mol	Chain	Res	Type	Atoms
2	A	501	CMP	C3'-C4'-C5'-O3'-O5'-P
2	B	501	CMP	C3'-C4'-C5'-O3'-O5'-P

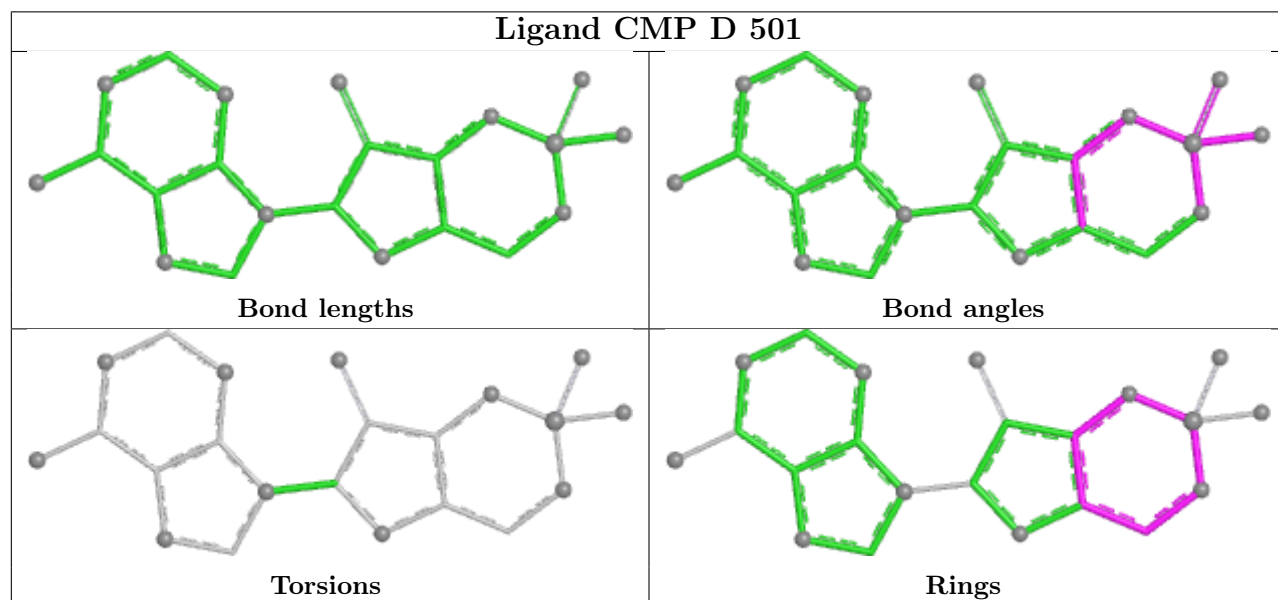
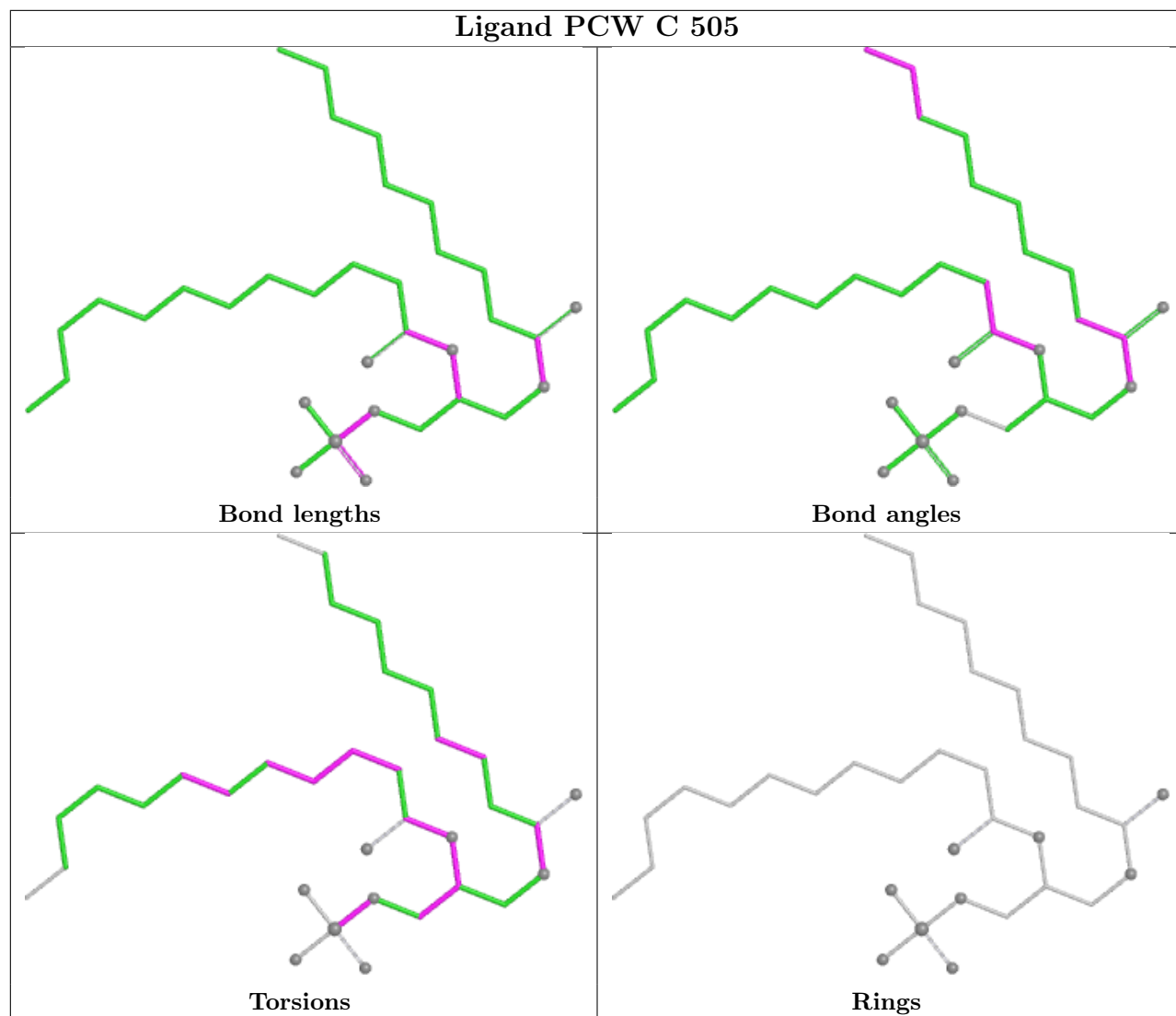
32 monomers are involved in 131 short contacts:

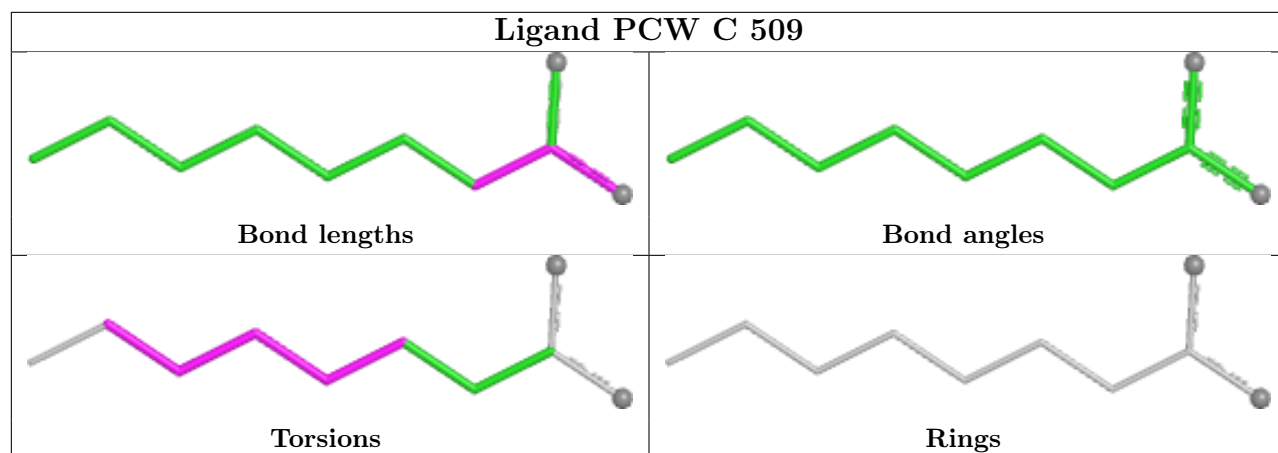
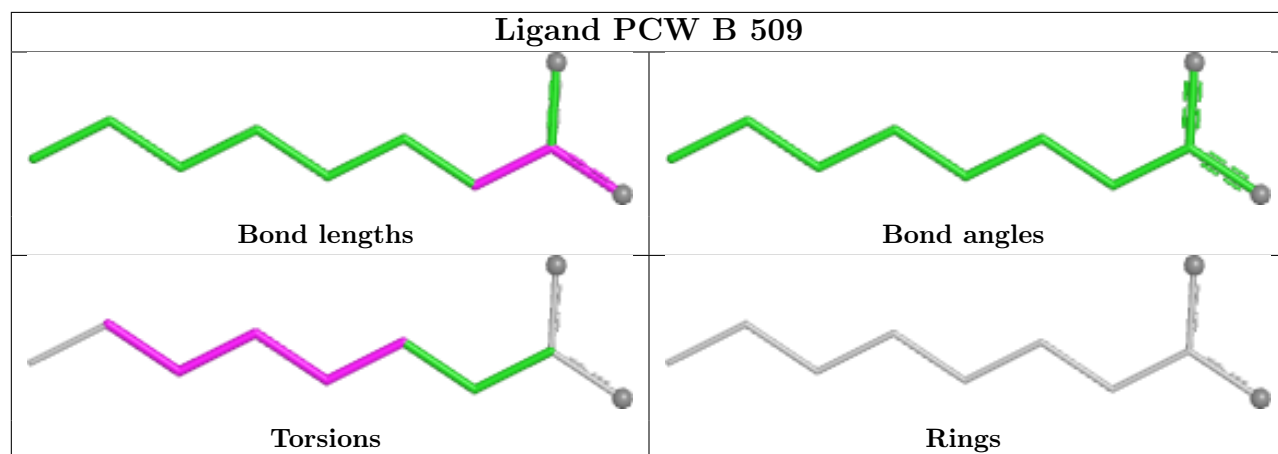
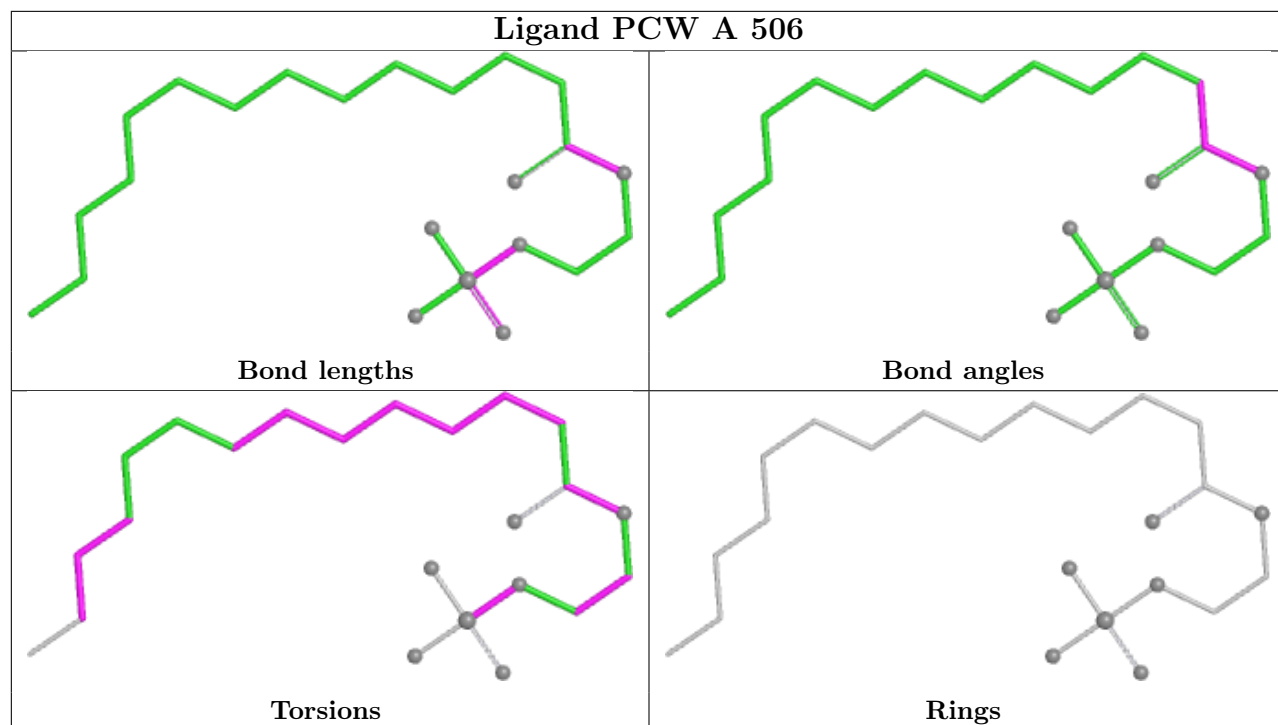
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	509	PCW	4	0
4	C	505	PCW	4	0
2	D	501	CMP	1	0
4	A	506	PCW	2	0
4	B	509	PCW	4	0
4	C	509	PCW	4	0
4	C	507	PCW	4	0
3	A	502	PT5	10	0
3	B	502	PT5	9	0
4	D	506	PCW	2	0
4	B	505	PCW	4	0
2	B	501	CMP	1	0
2	C	501	CMP	1	0
4	C	503	PCW	5	0
4	C	506	PCW	3	0
4	A	509	PCW	4	0
4	D	505	PCW	4	0
4	B	503	PCW	5	0
4	D	503	PCW	5	0
4	A	507	PCW	5	0
4	B	506	PCW	3	0
3	C	502	PT5	9	0
4	A	508	PCW	6	0
3	D	502	PT5	9	0
4	B	508	PCW	6	0
4	C	508	PCW	5	0
4	D	508	PCW	6	0
4	B	507	PCW	4	0
4	A	505	PCW	4	0
2	A	501	CMP	1	0
4	A	503	PCW	5	0
4	D	507	PCW	4	0

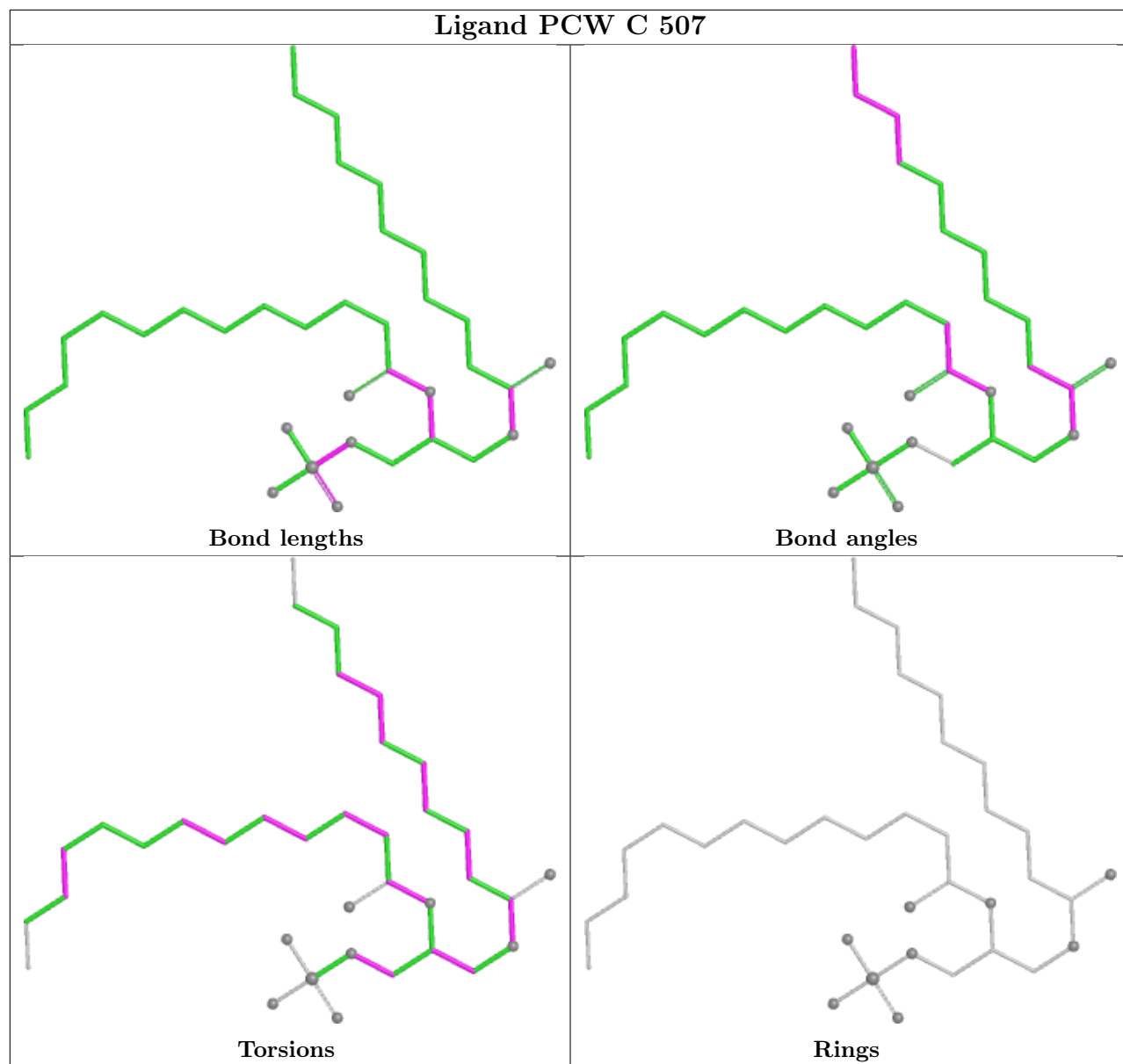
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

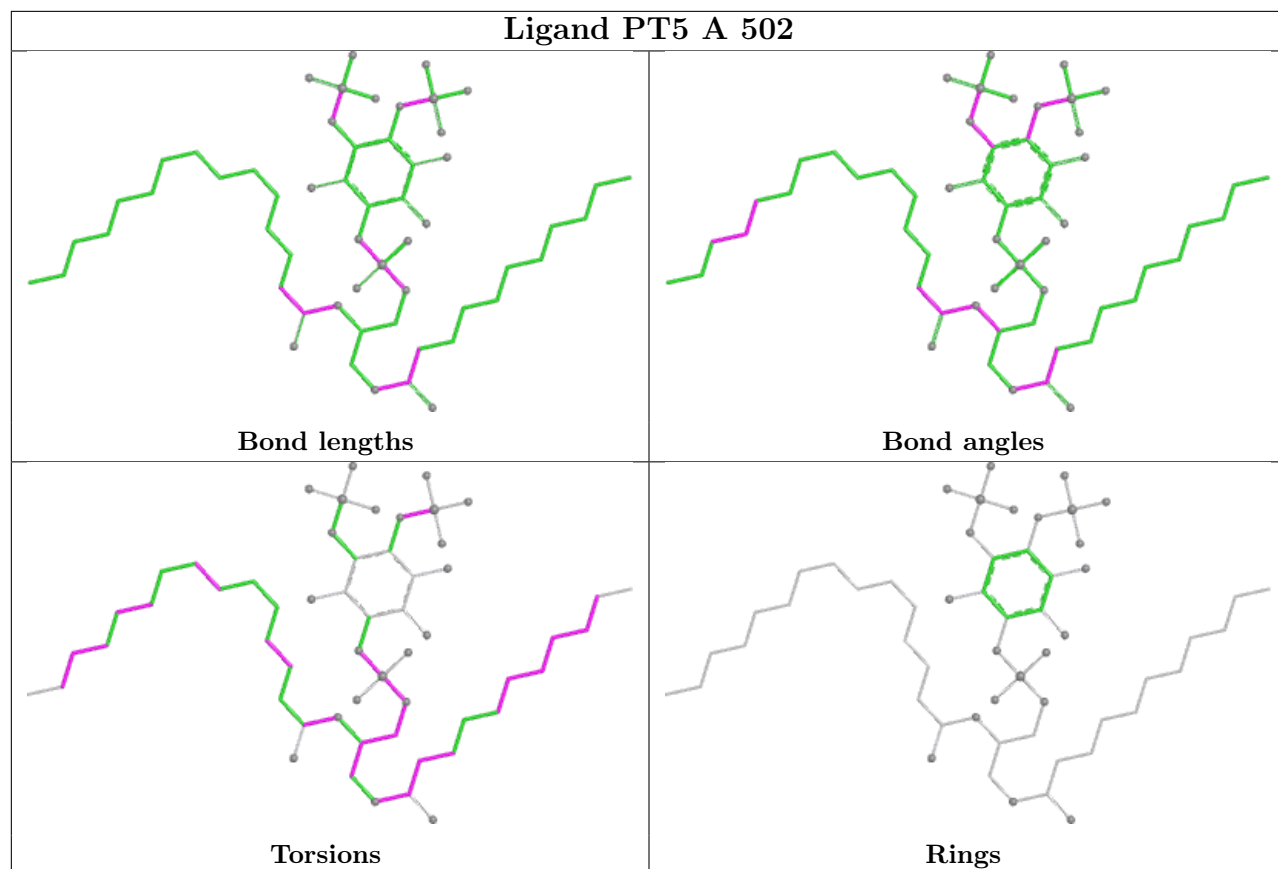




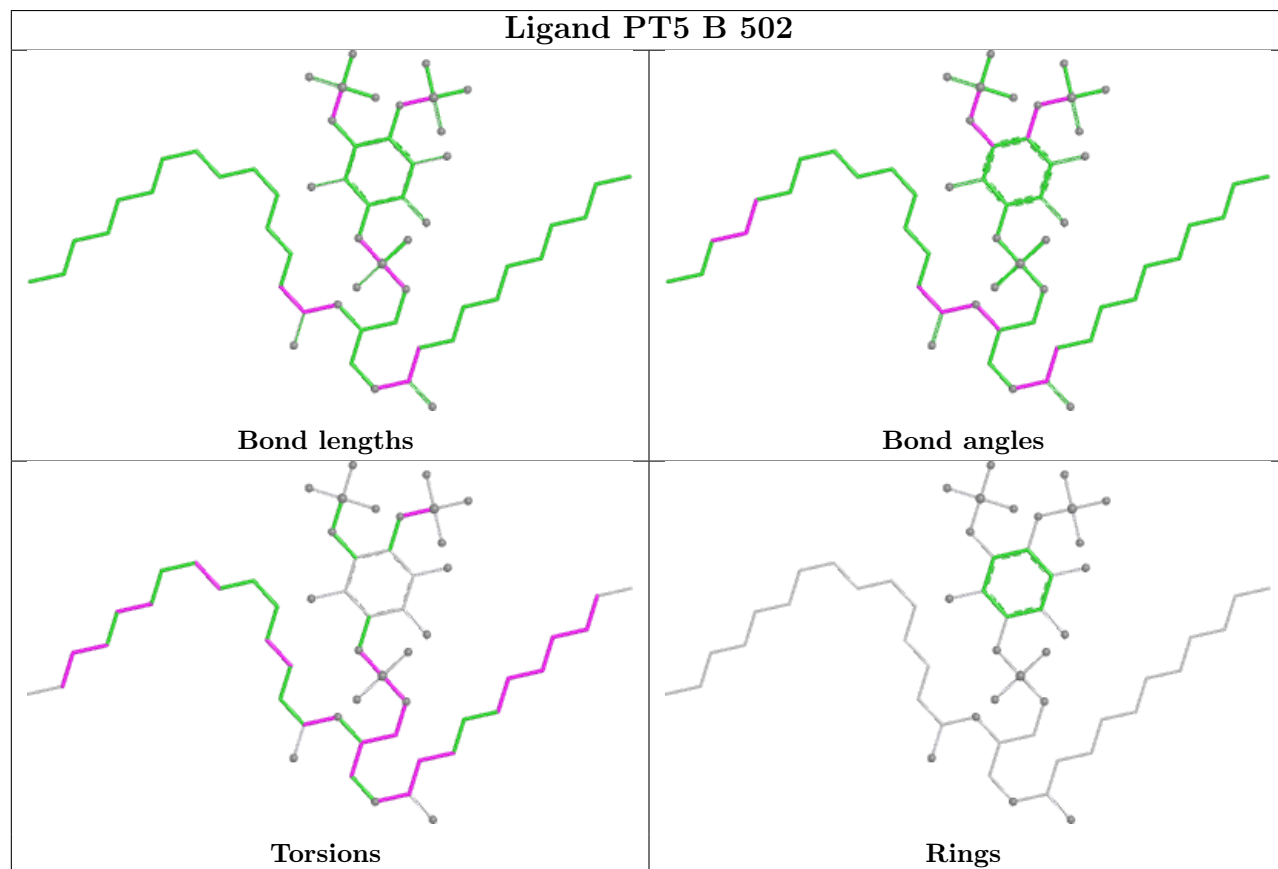


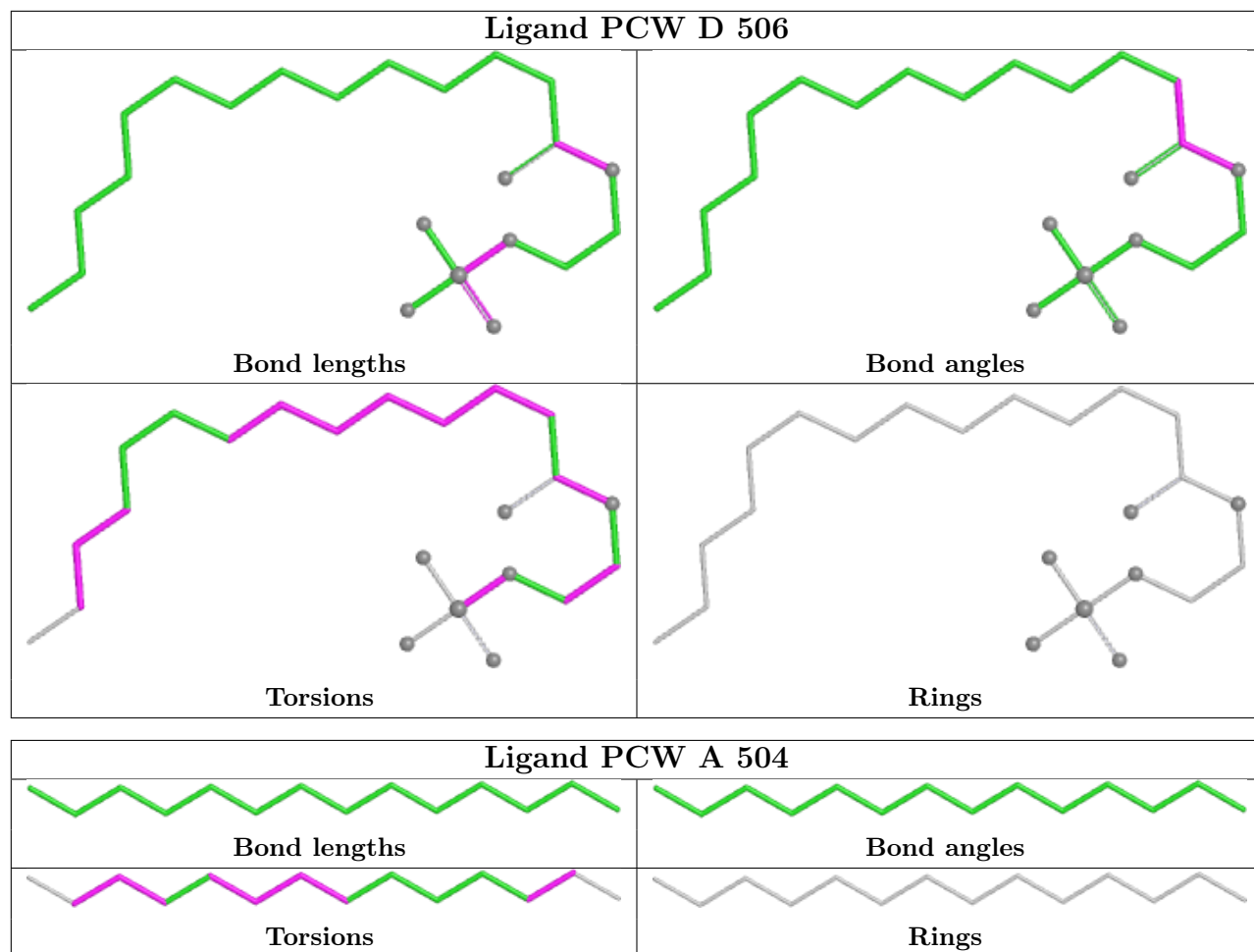


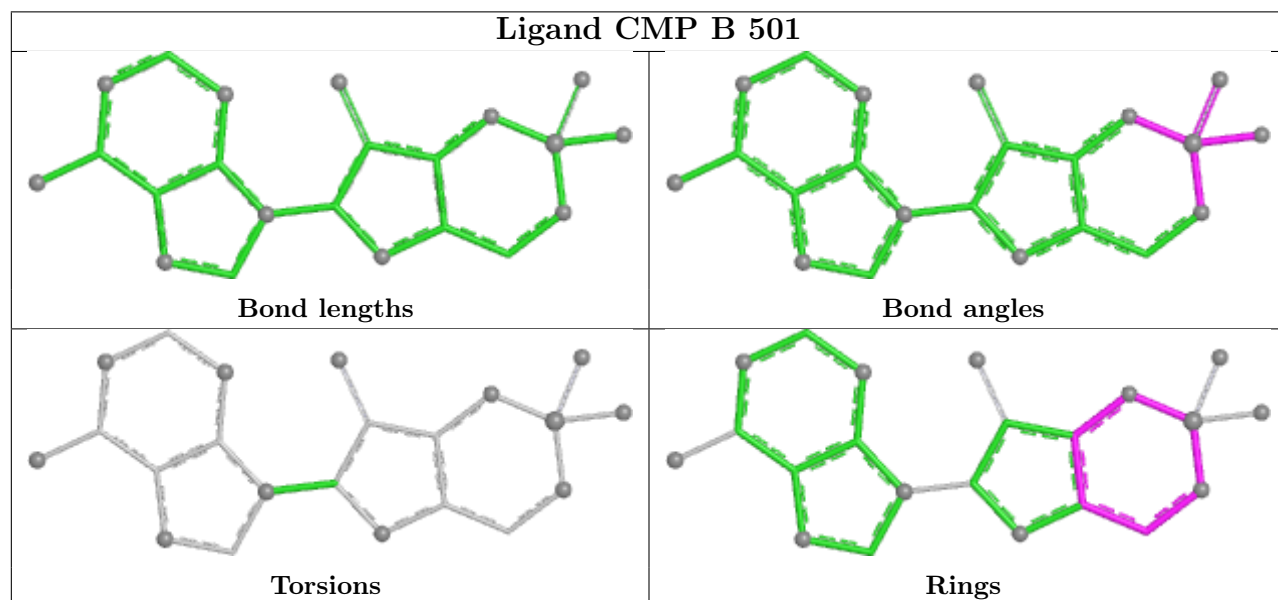
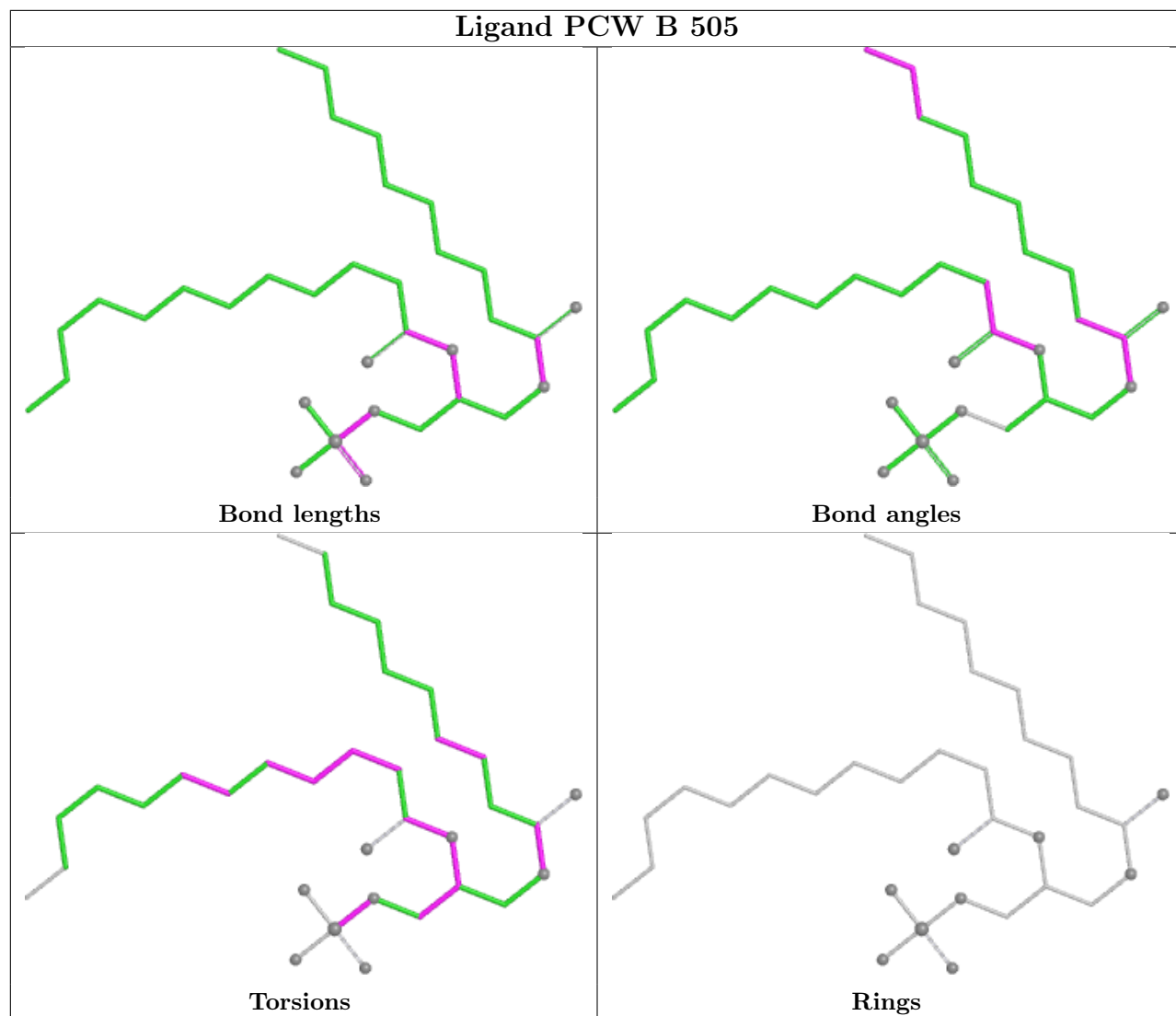
Ligand PT5 A 502

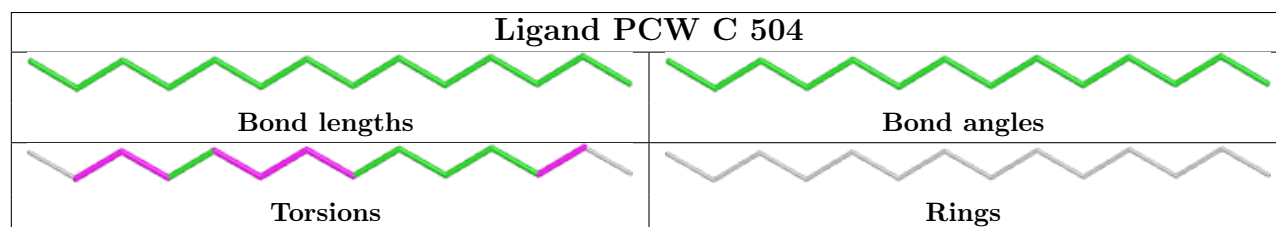
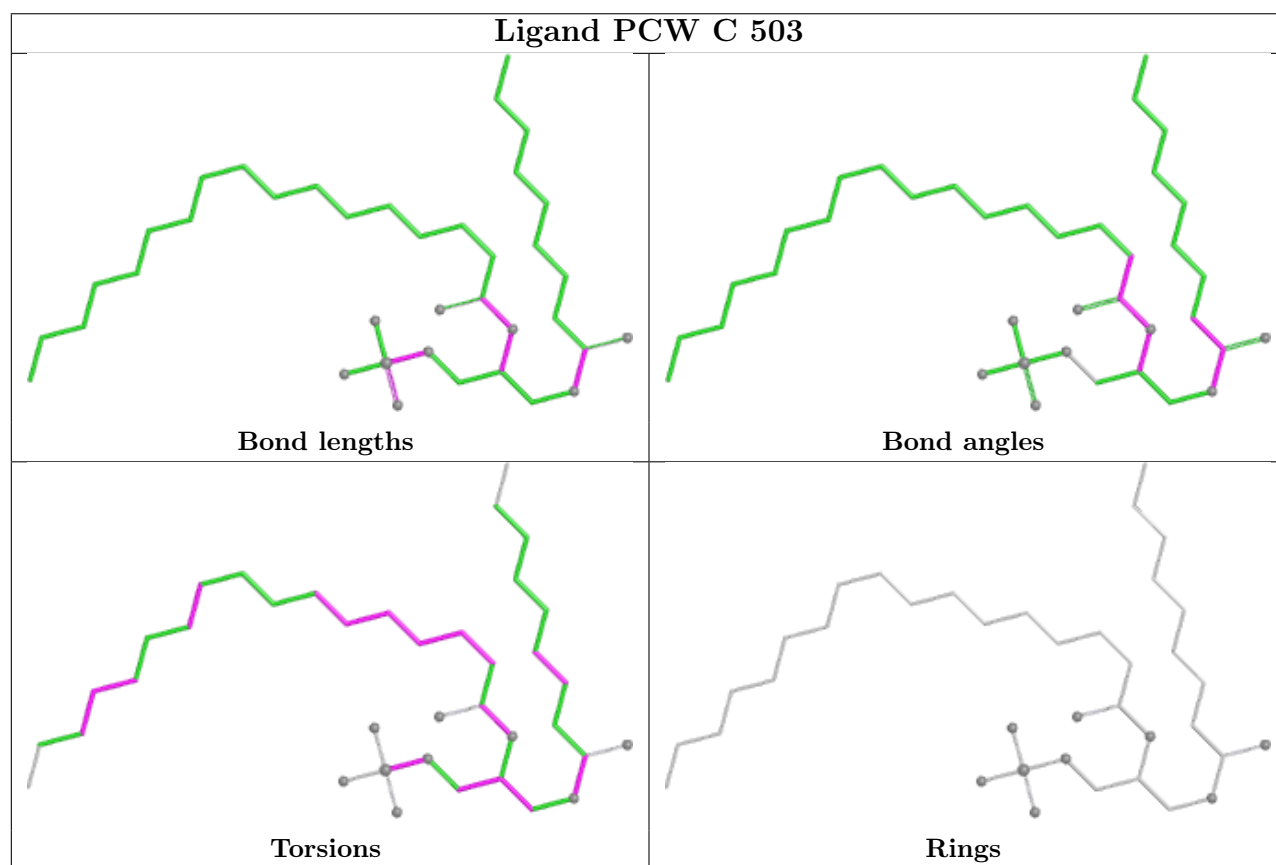
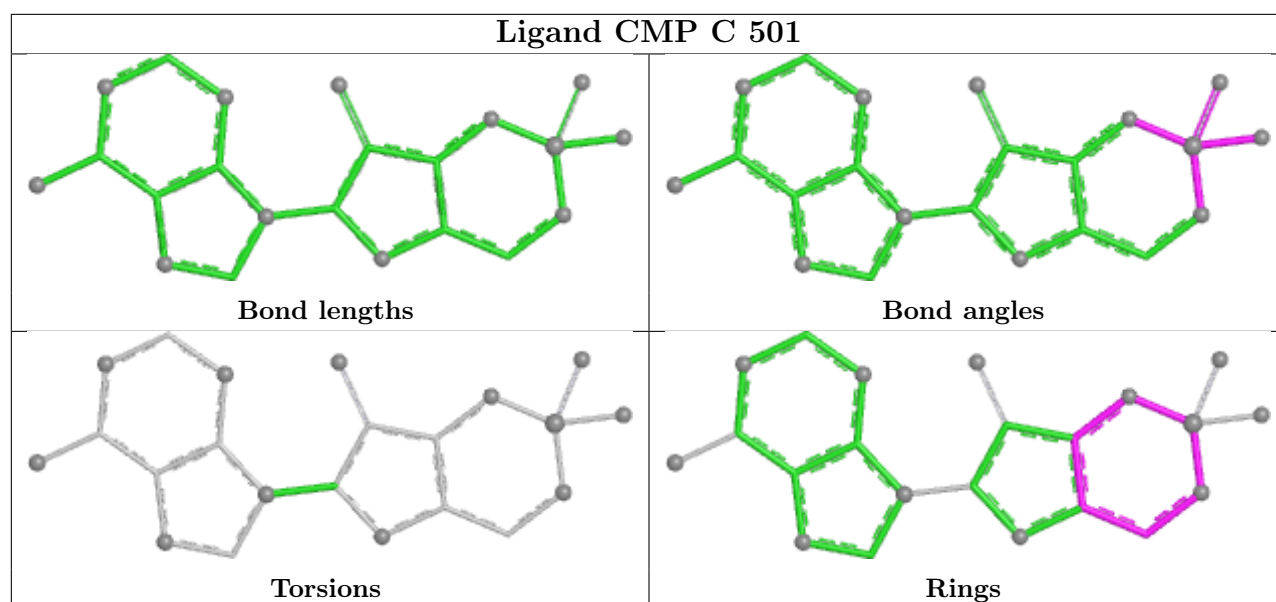


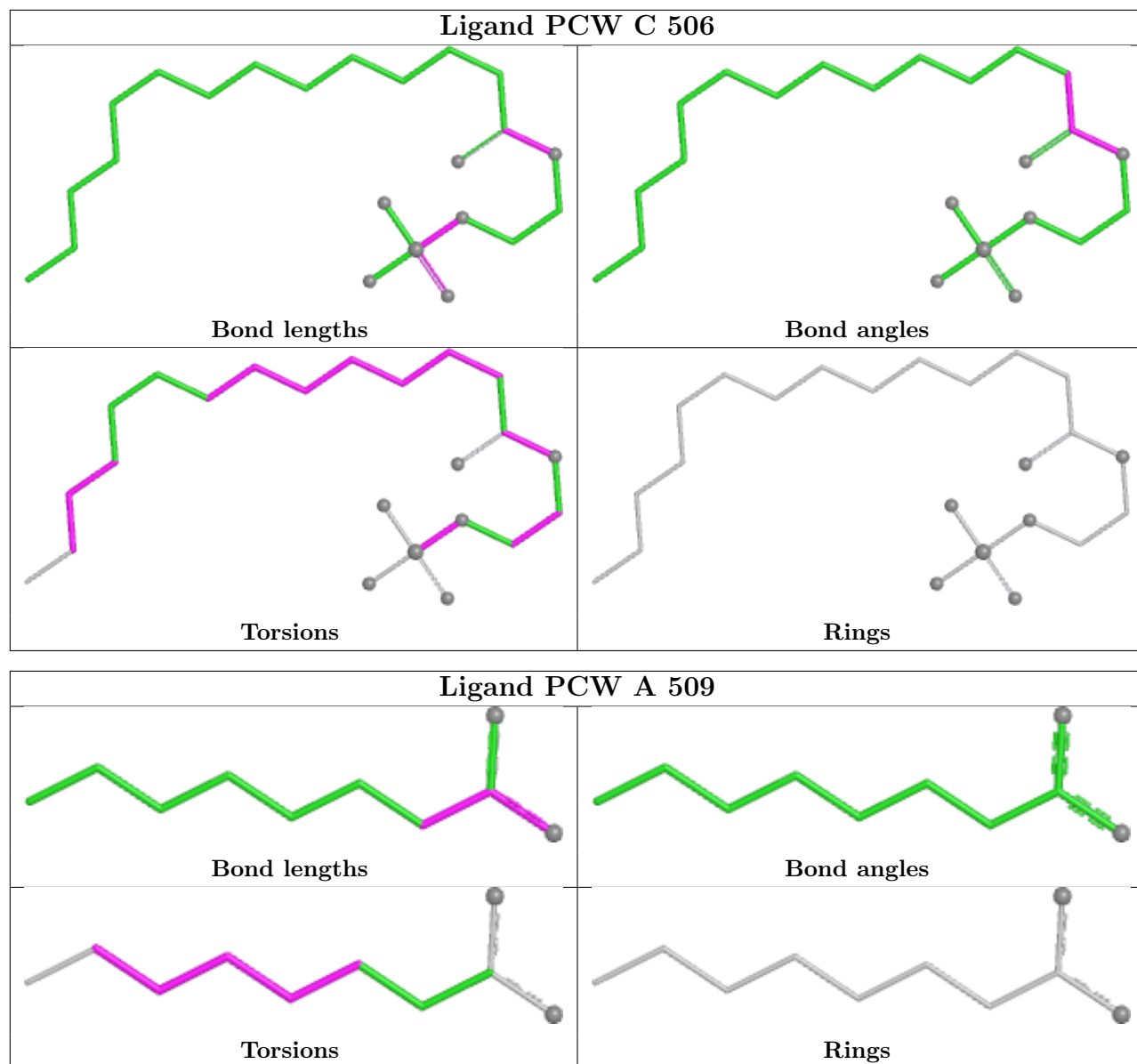
Ligand PT5 B 502

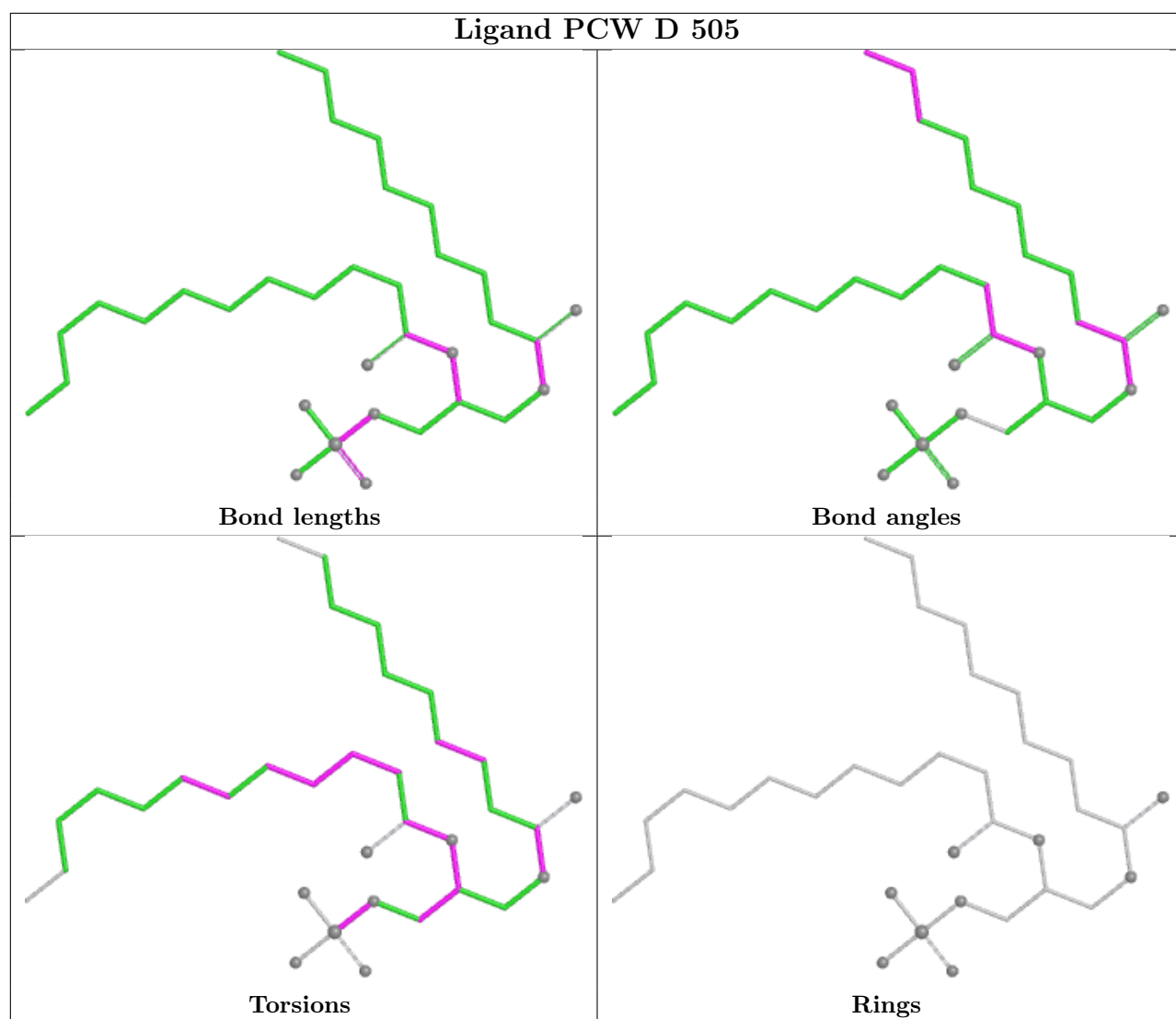


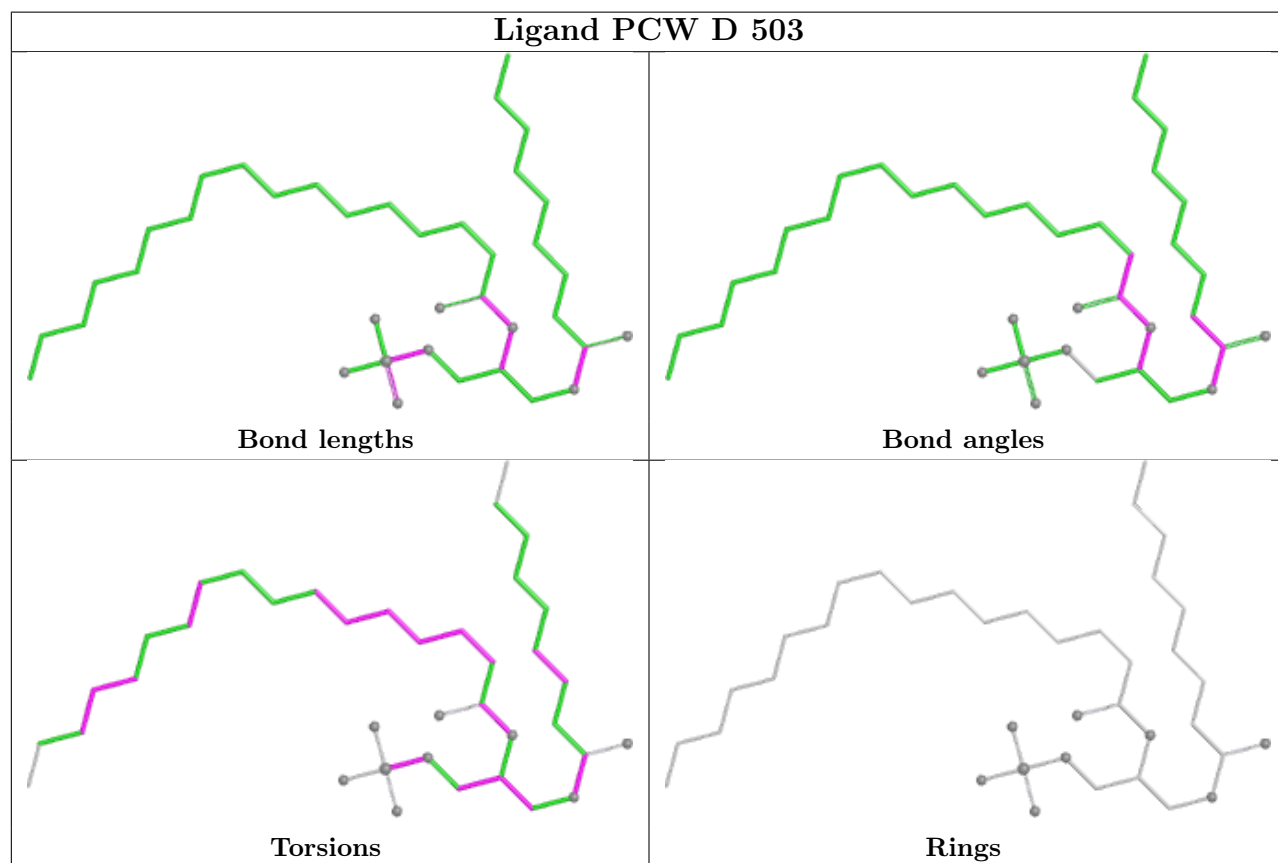
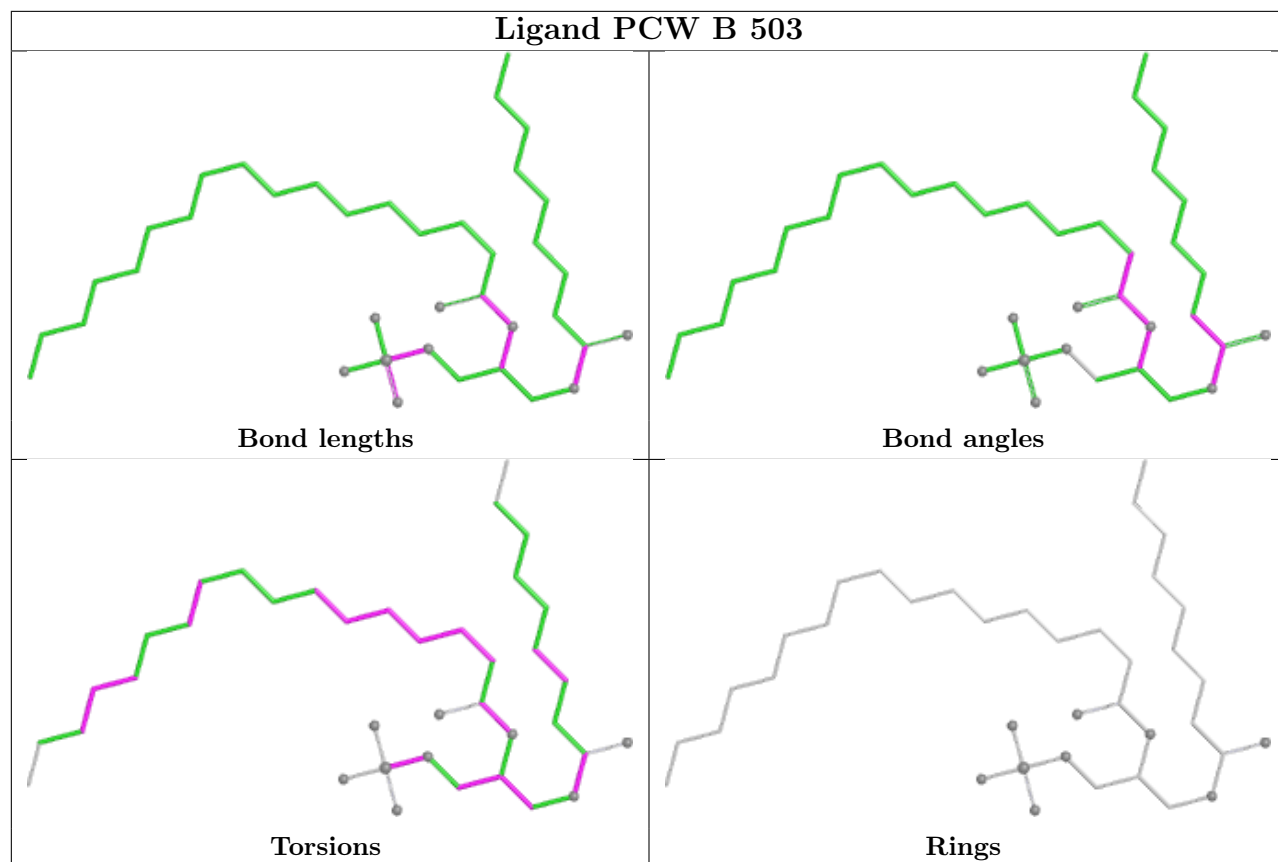


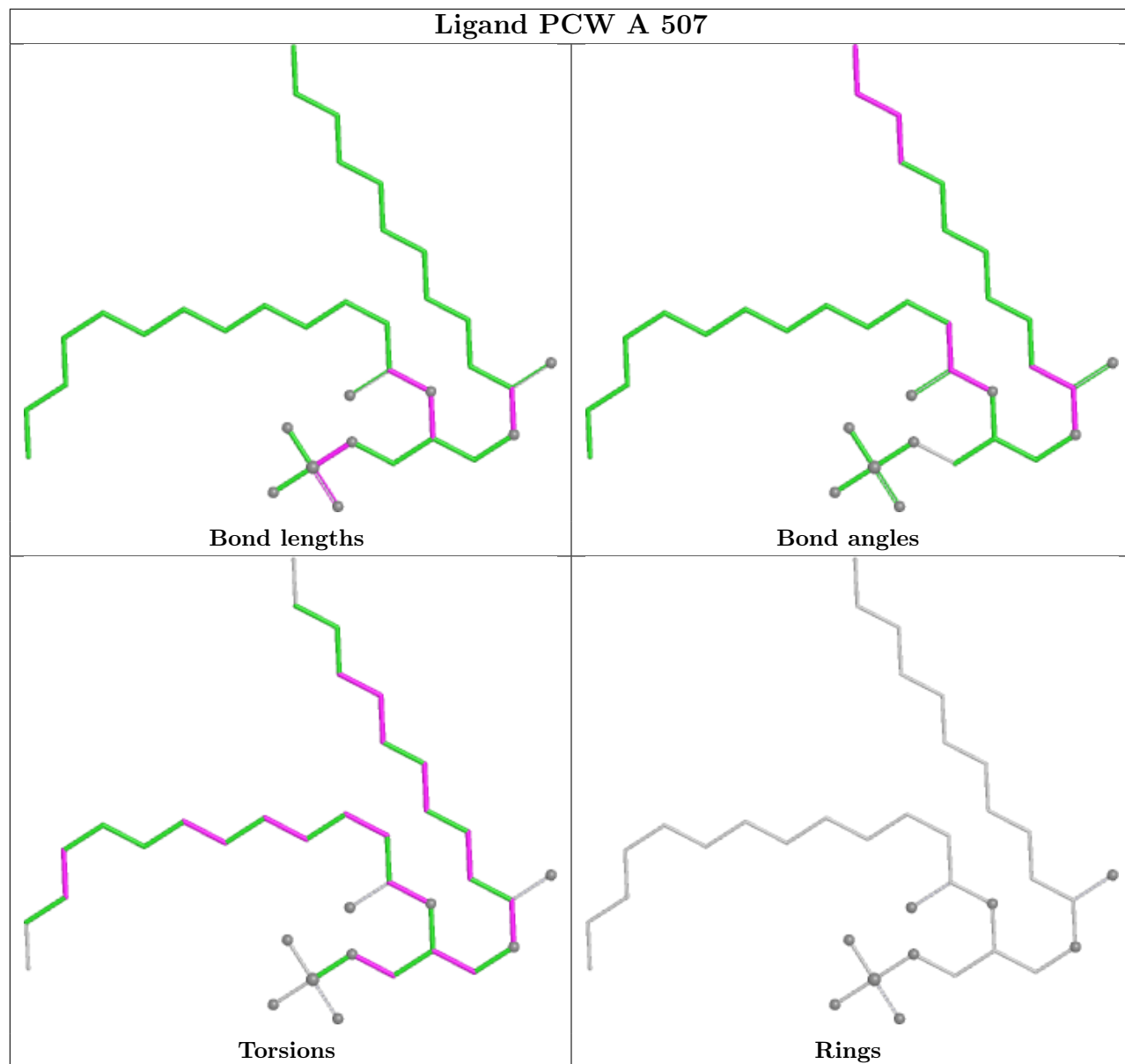
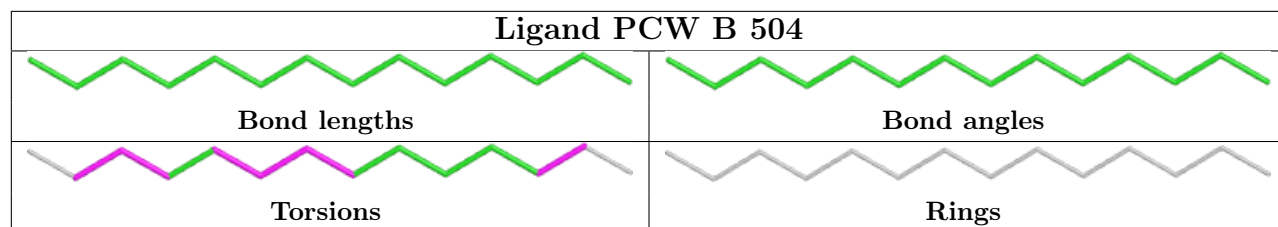


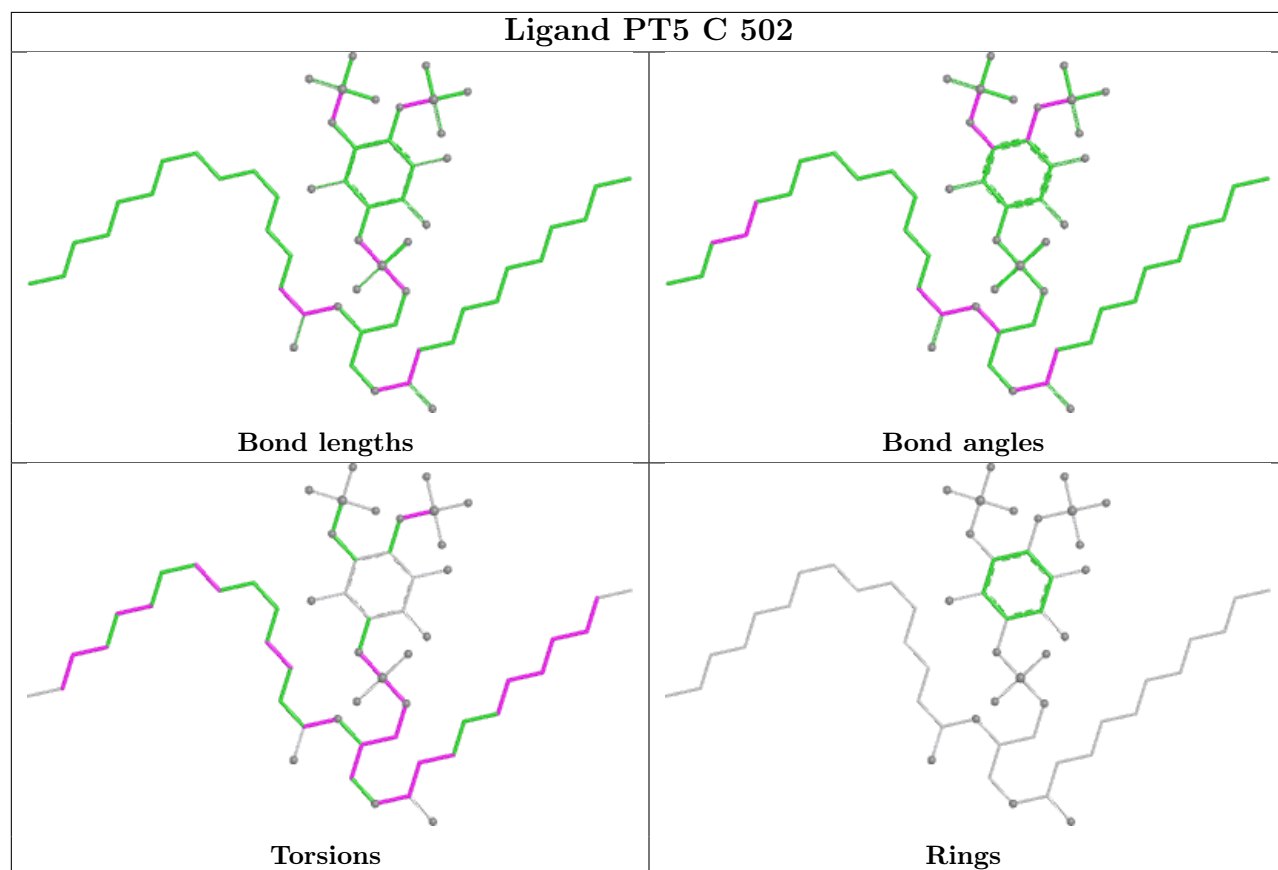
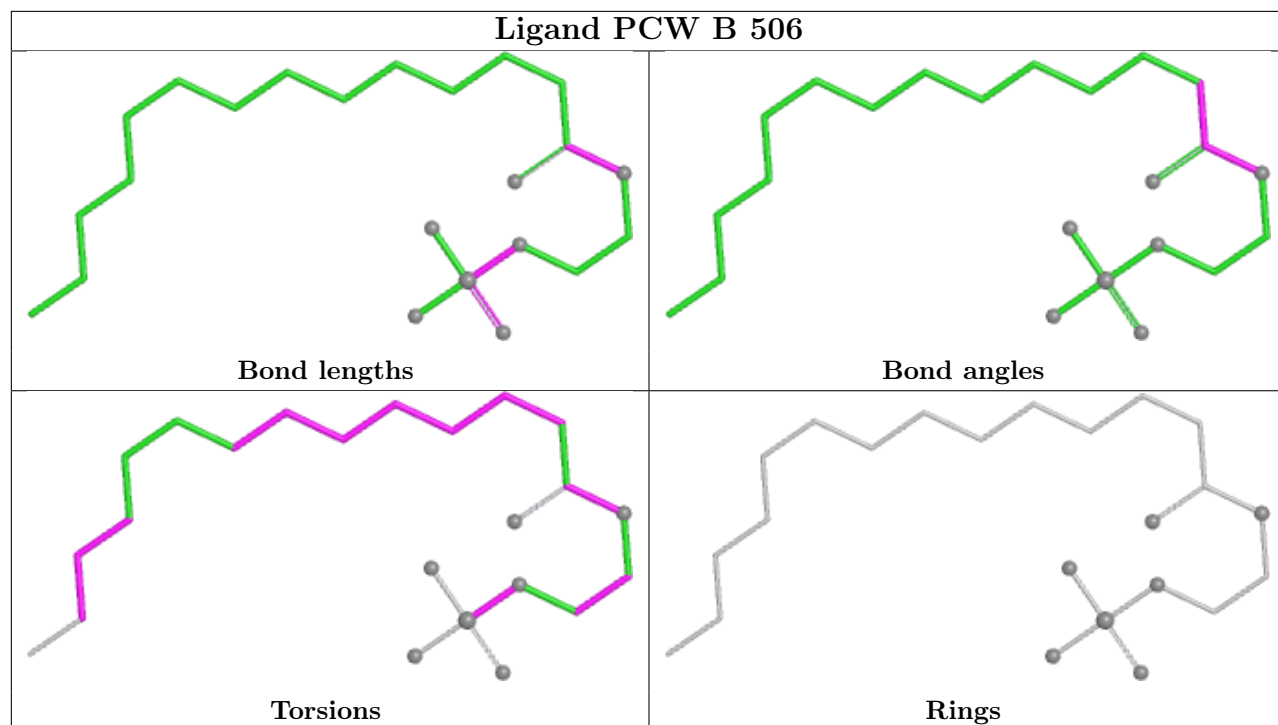


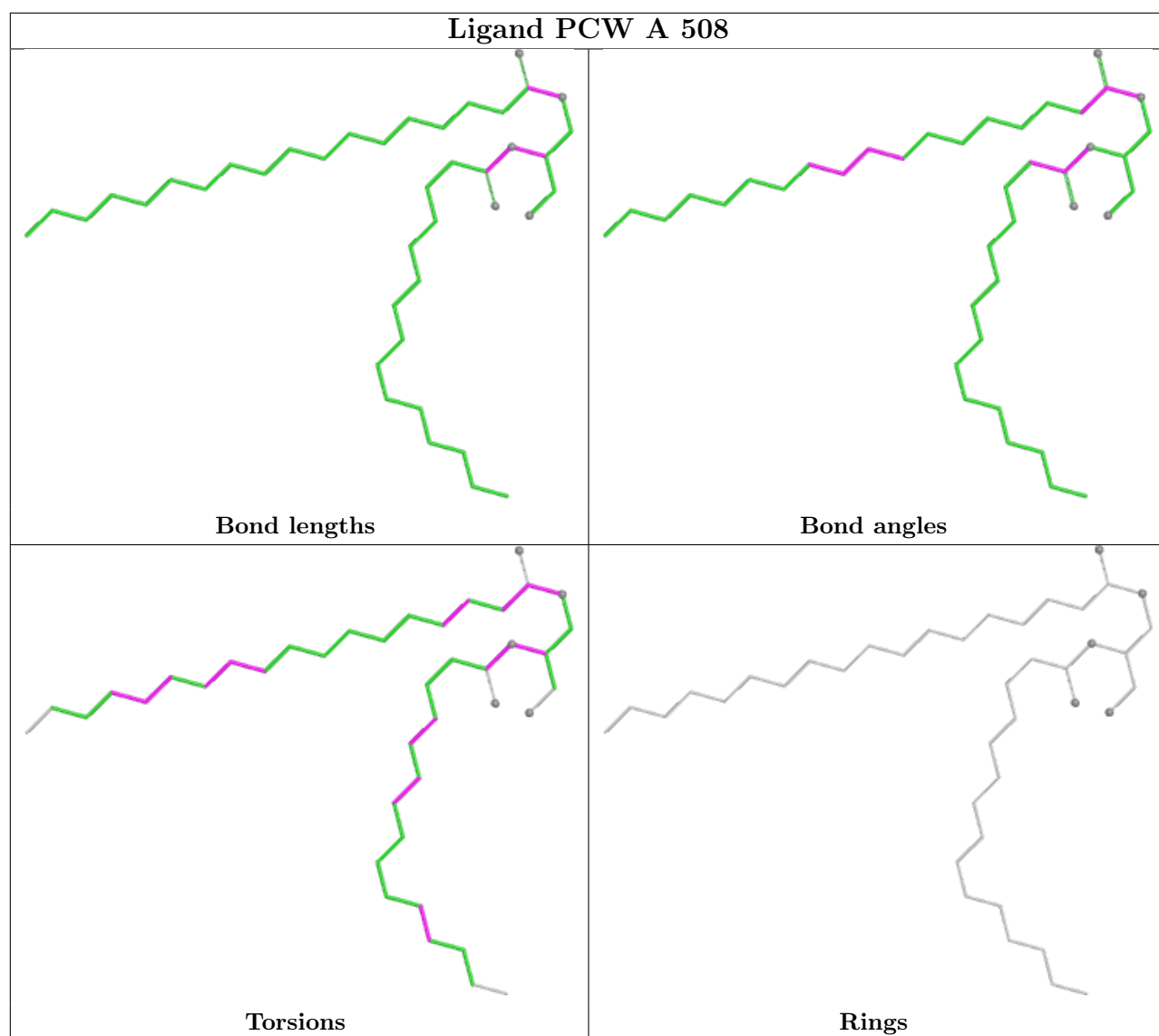


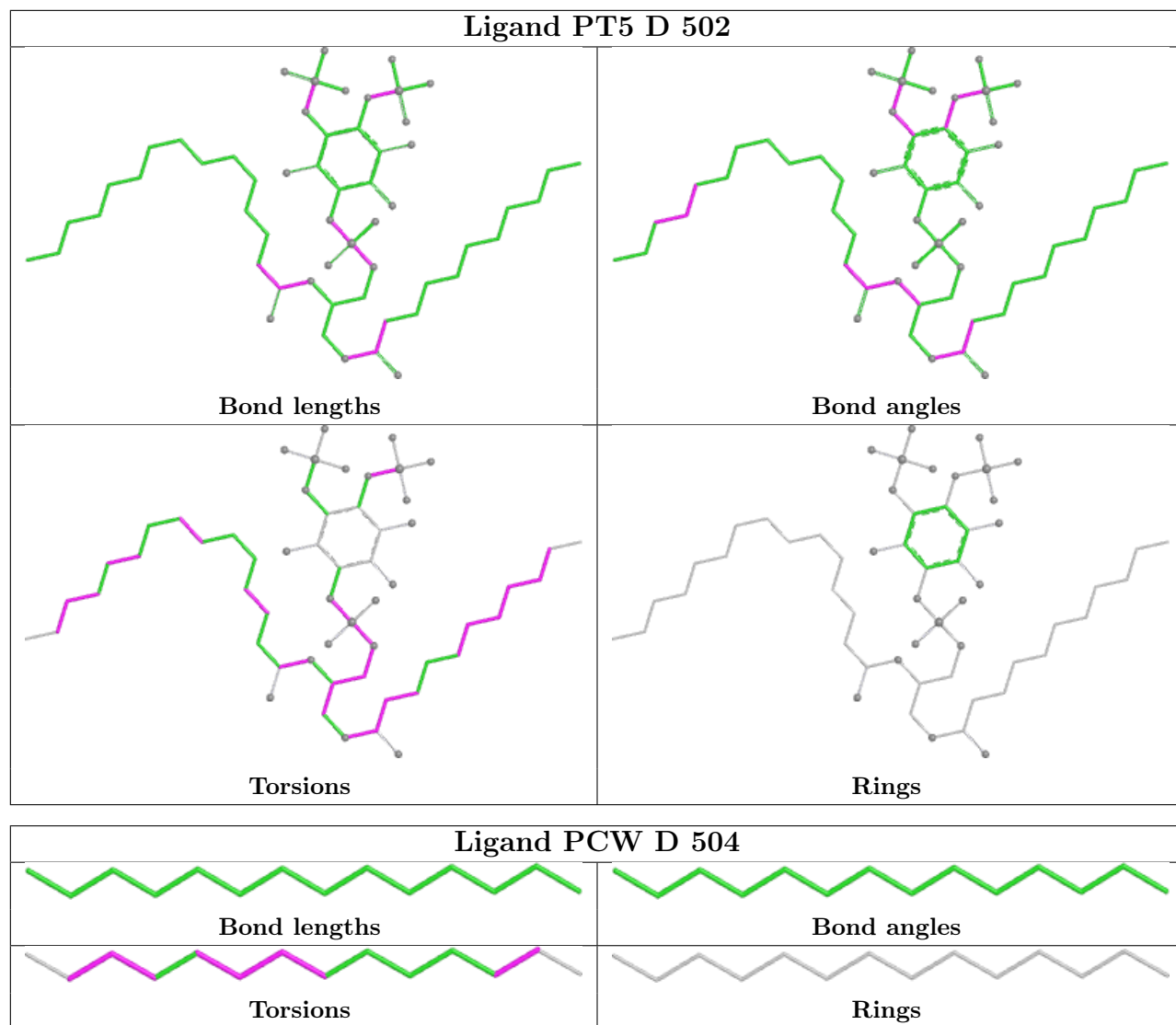


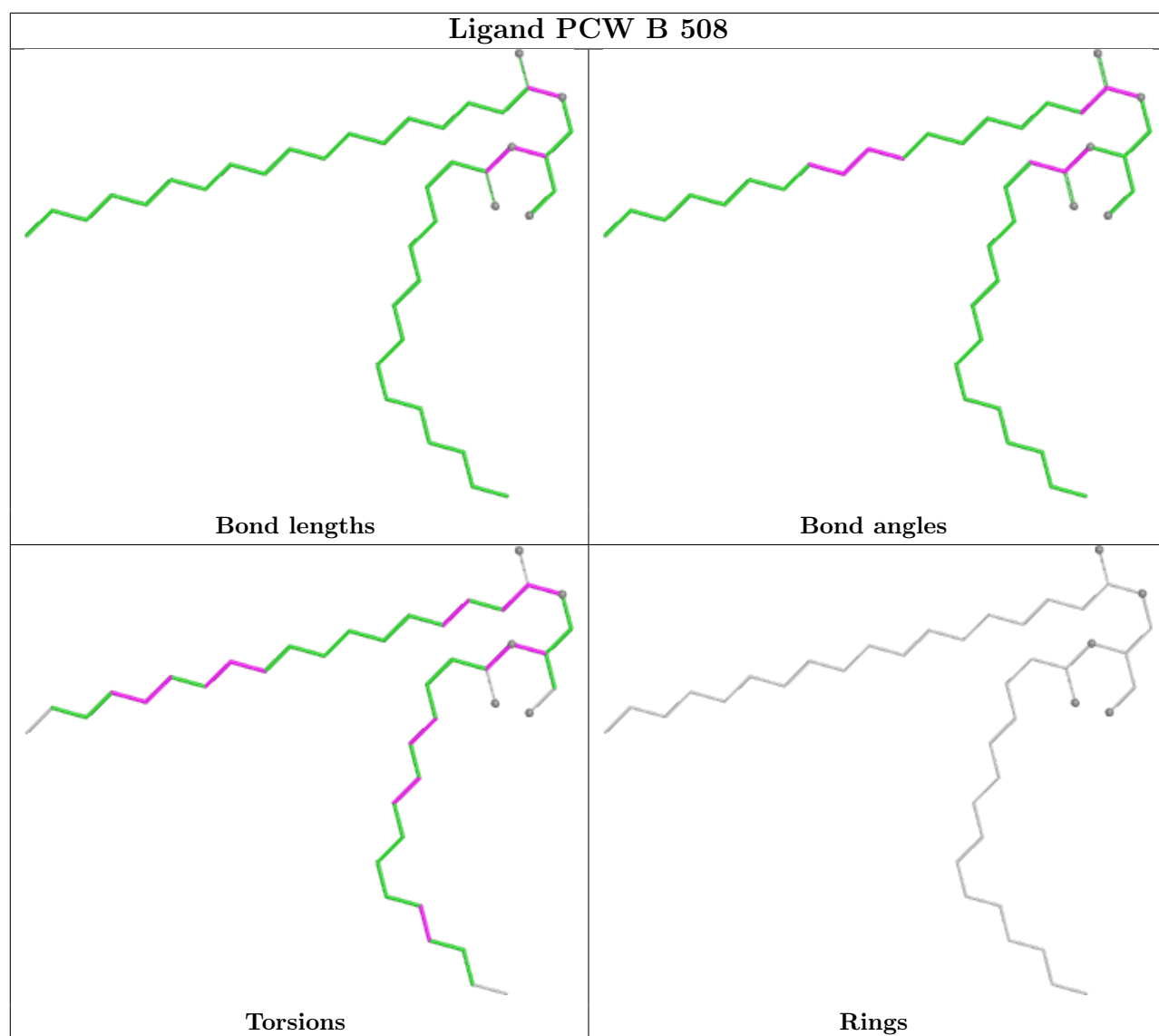


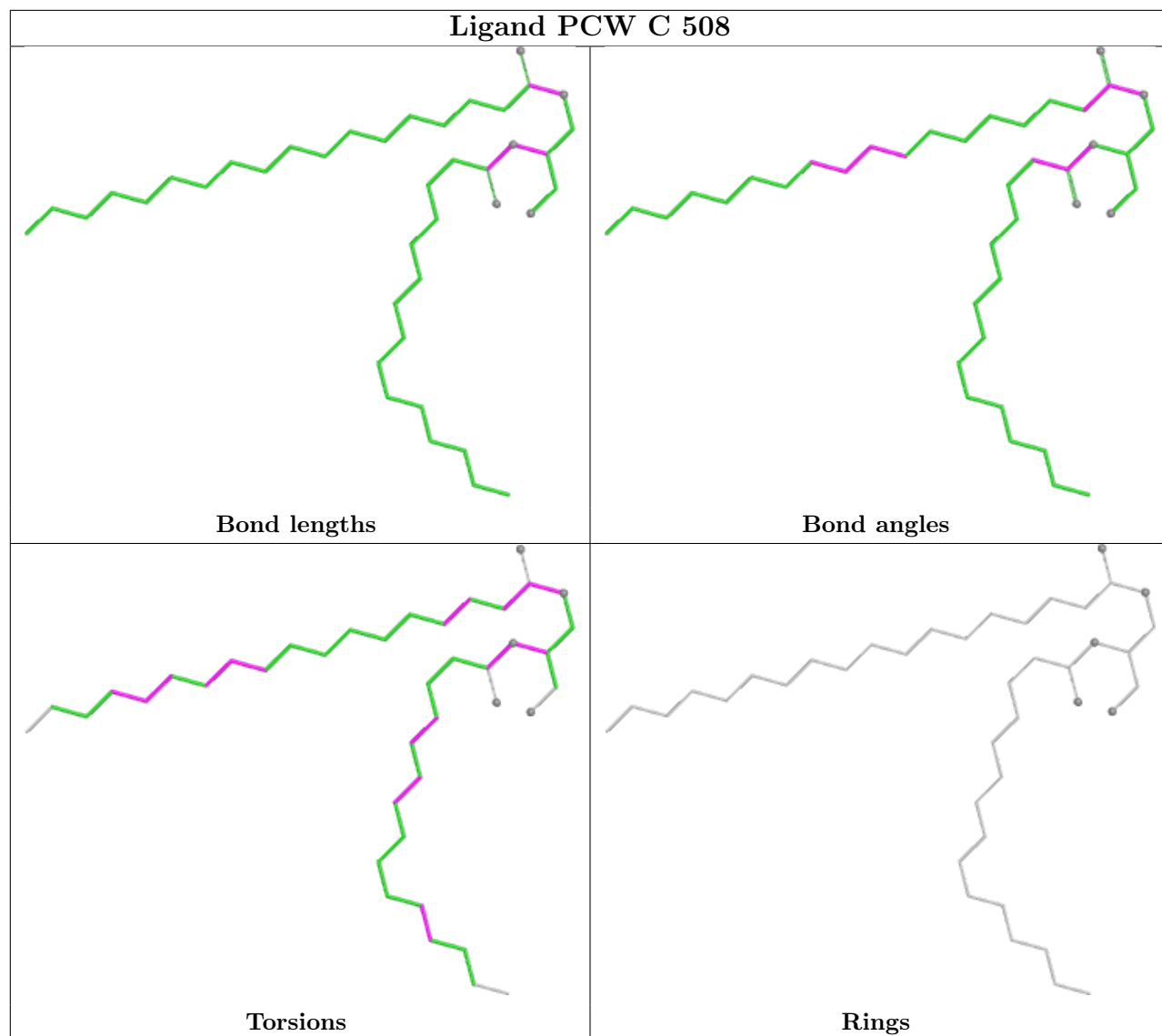


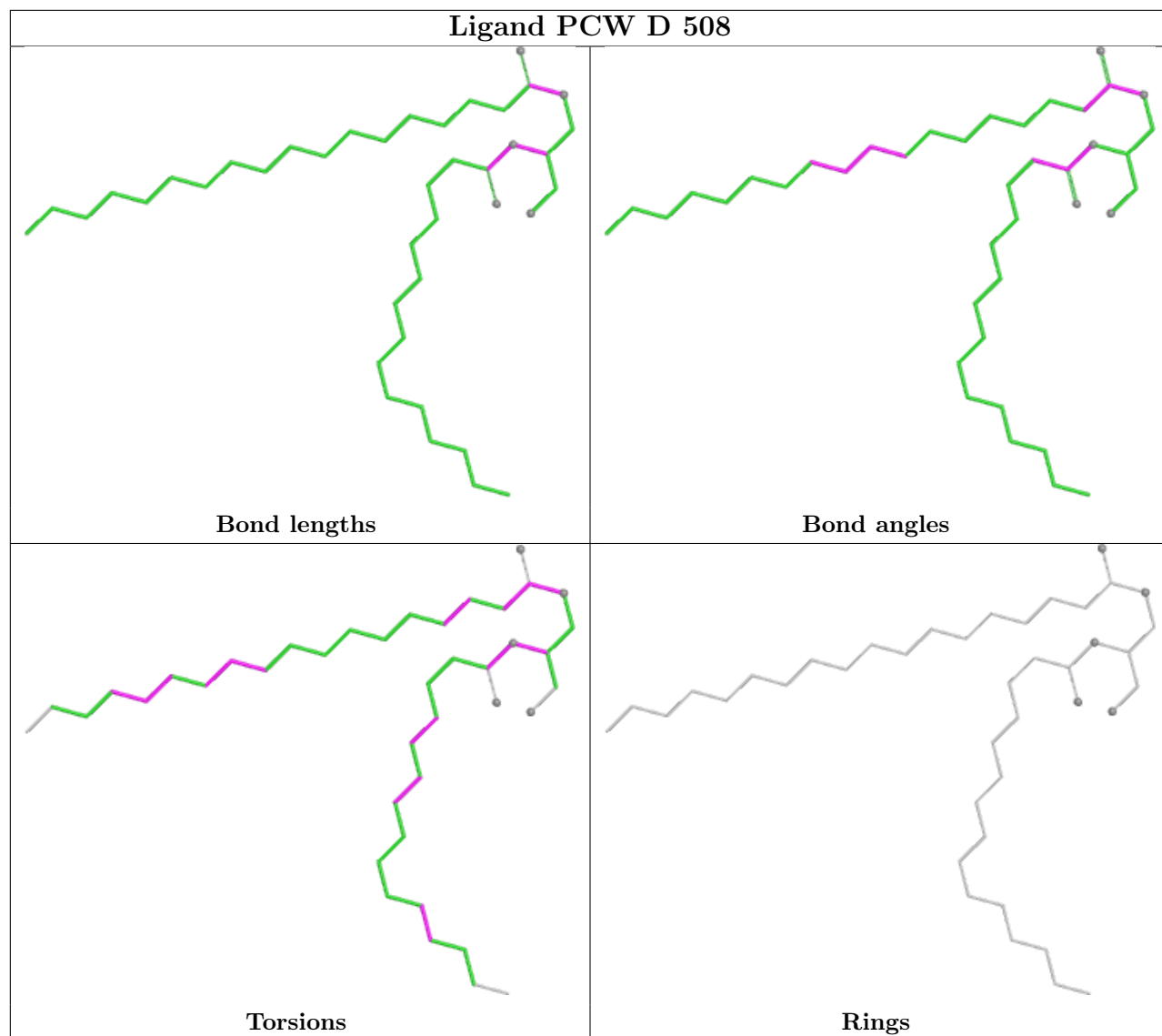


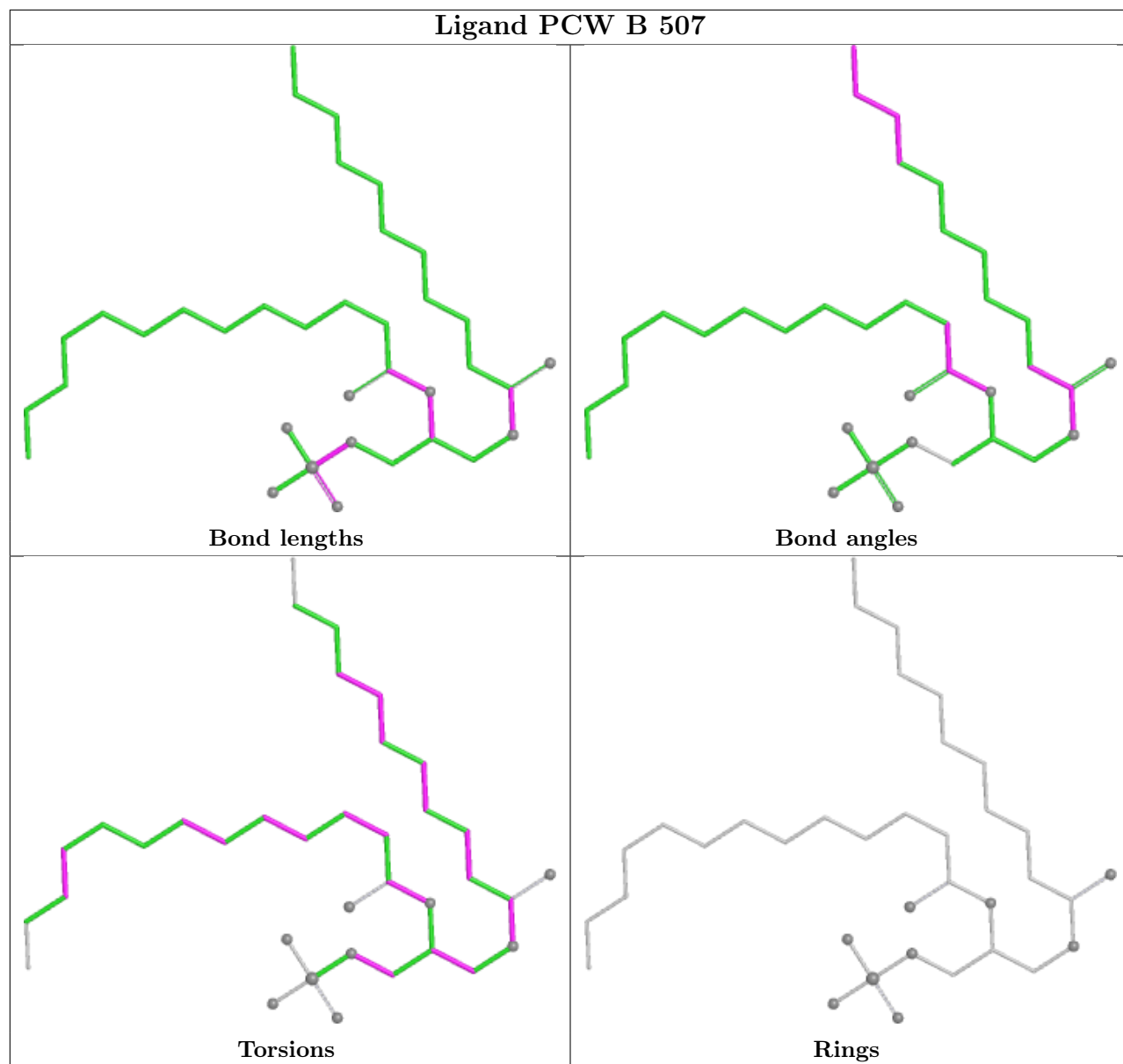


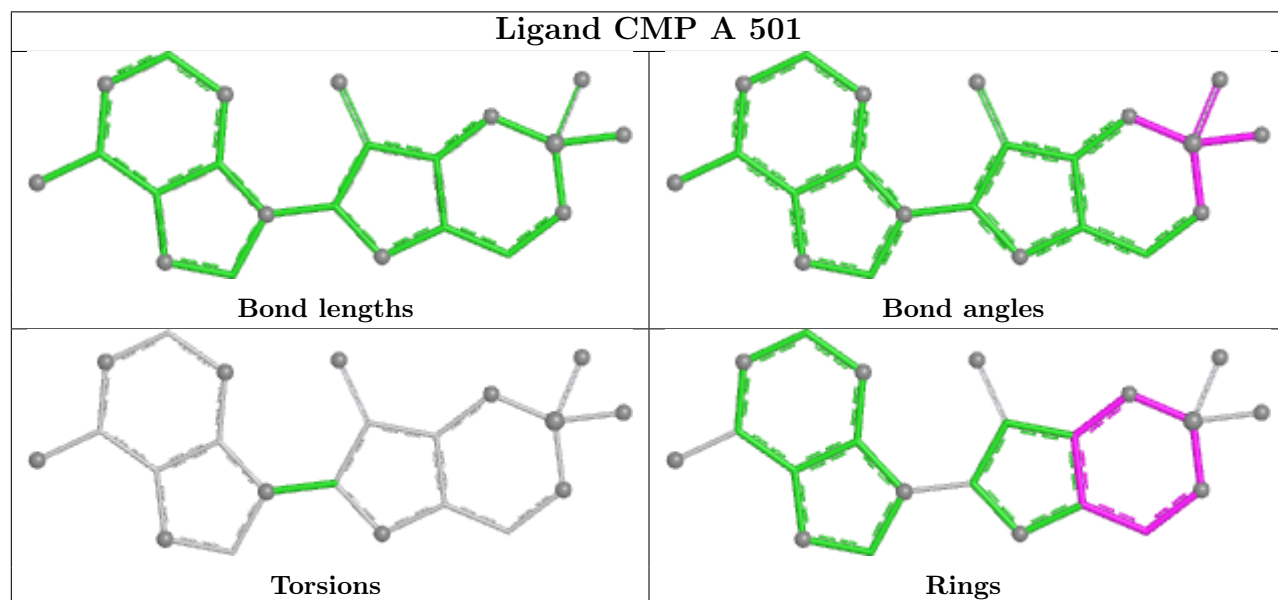
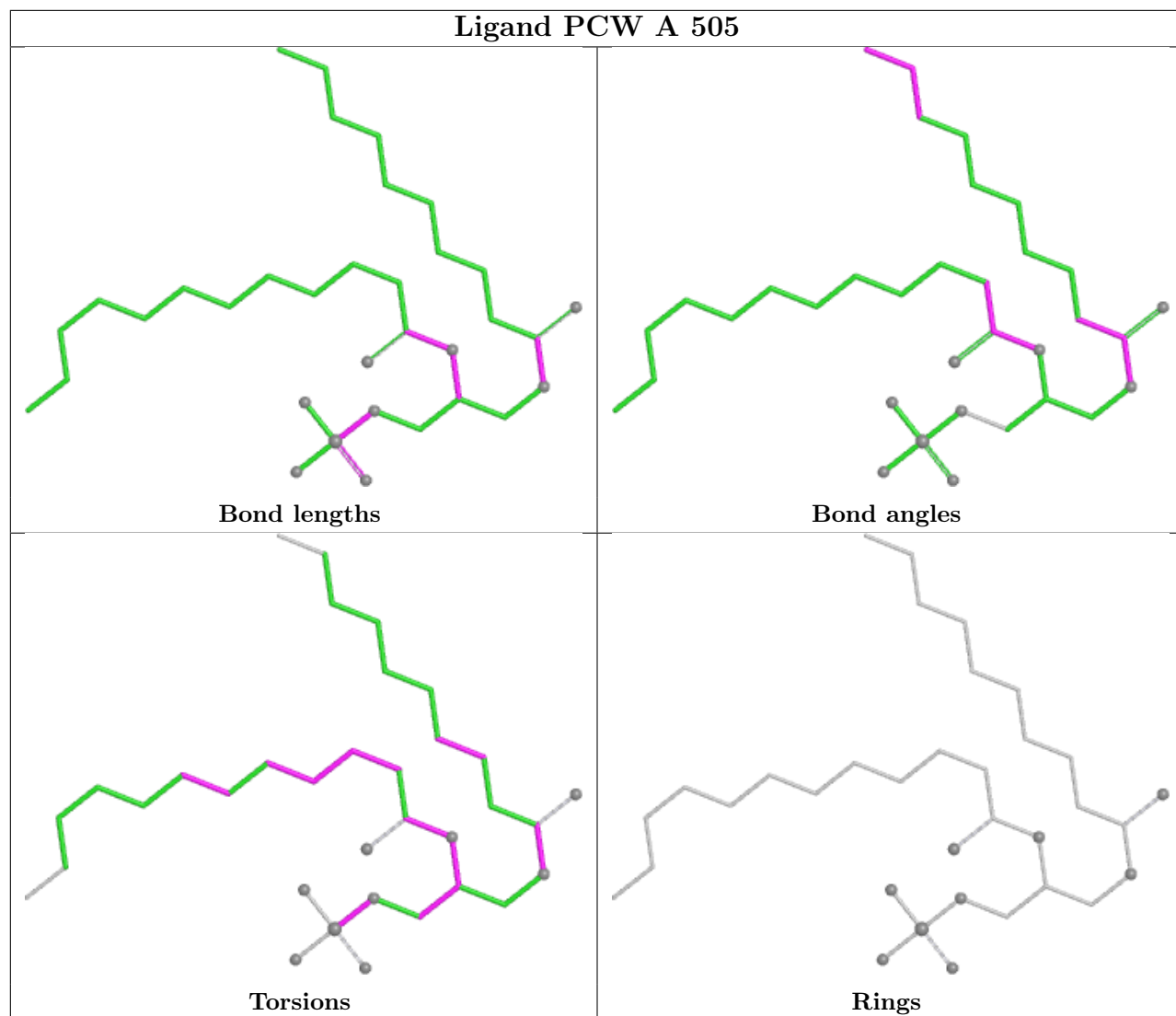


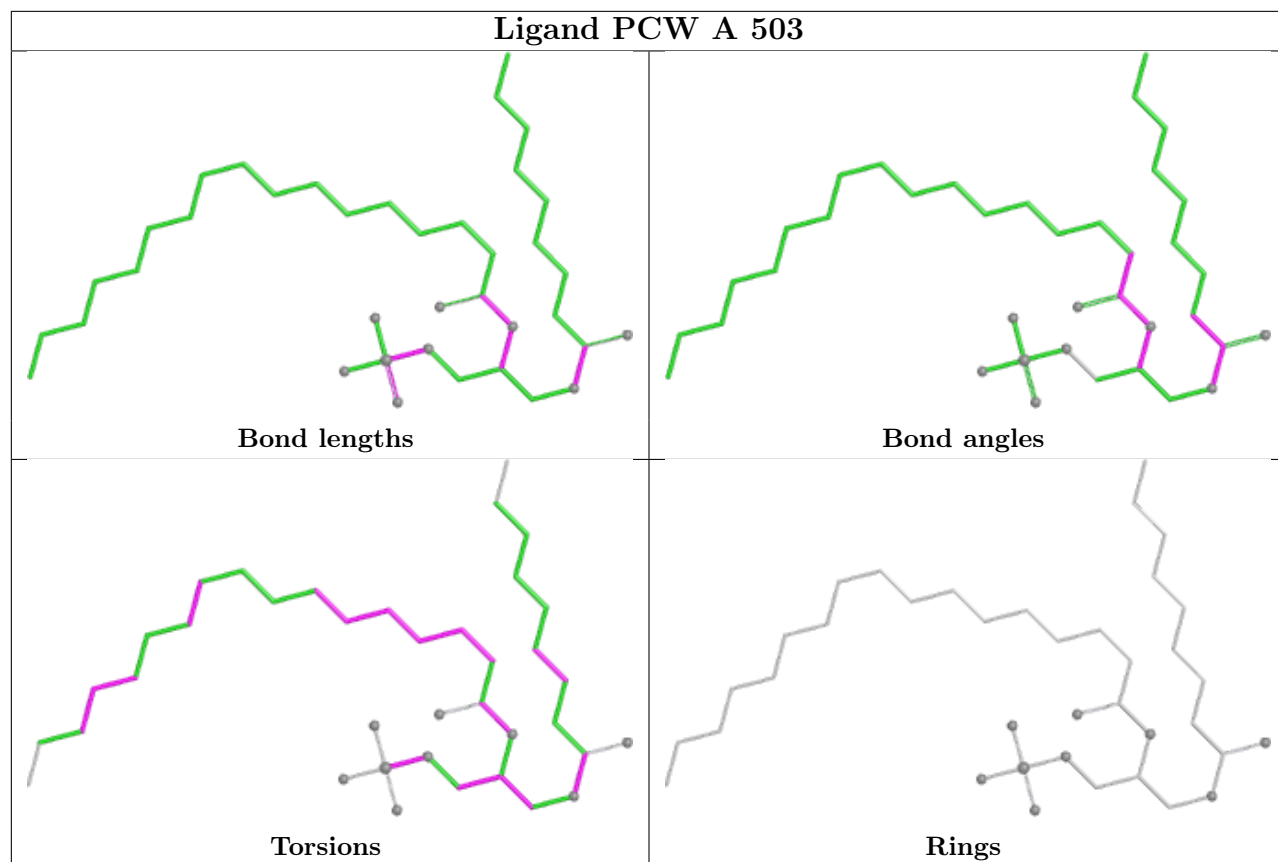


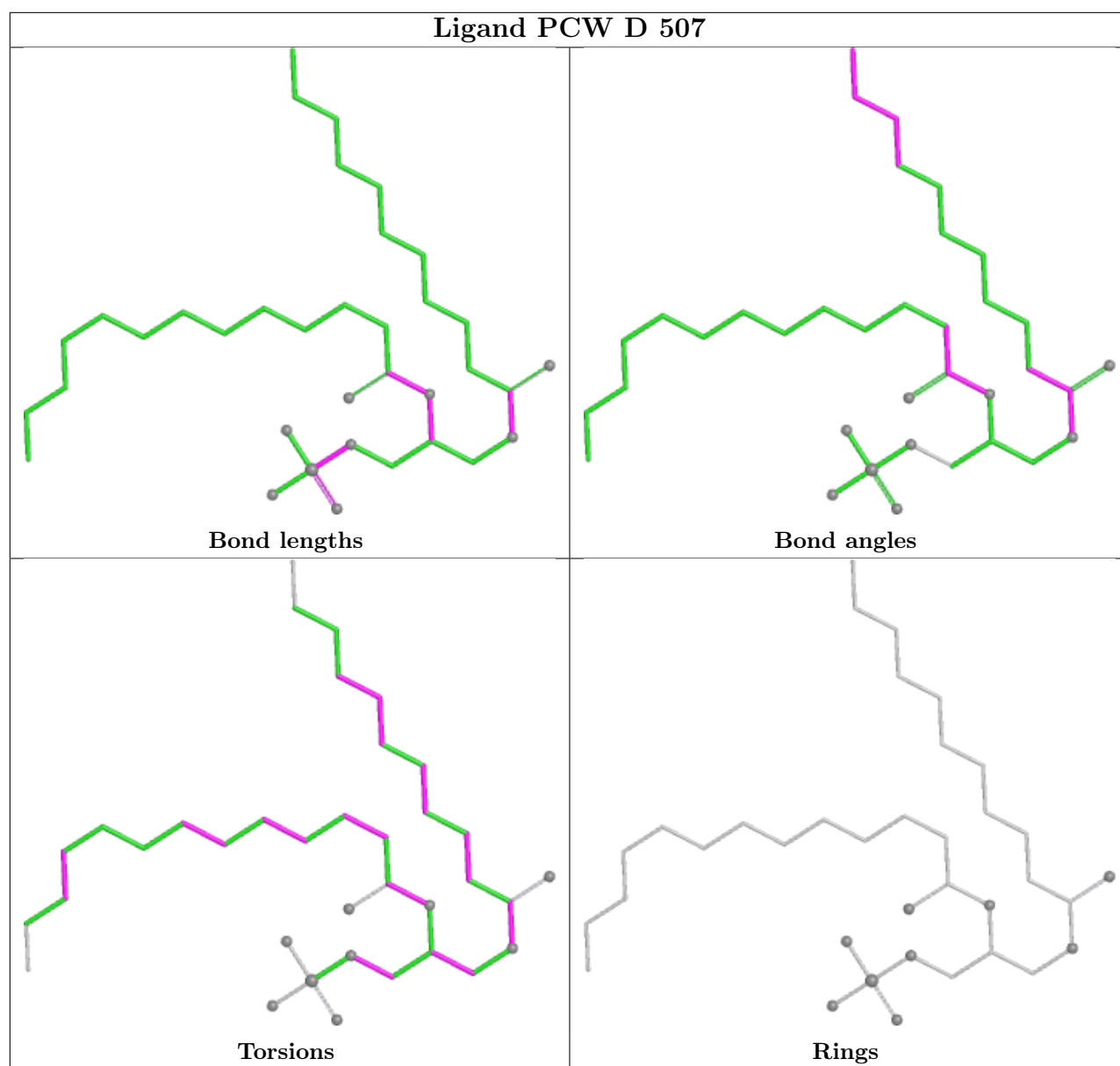












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

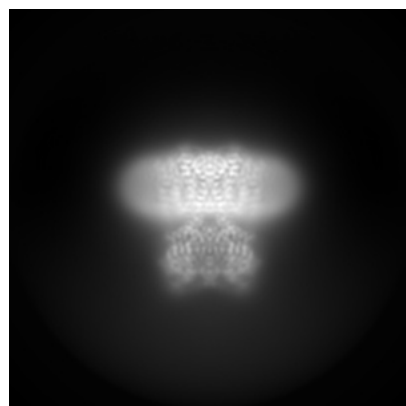
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43520. These allow visual inspection of the internal detail of the map and identification of artifacts.

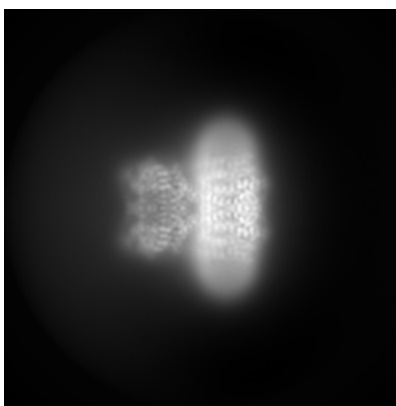
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

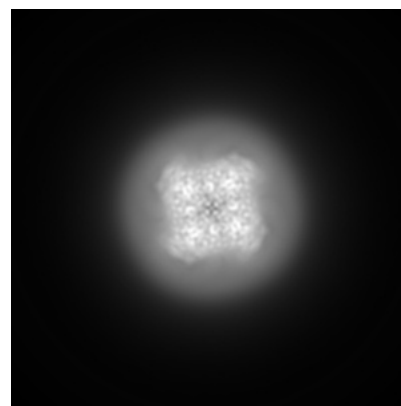
6.1.1 Primary map



X

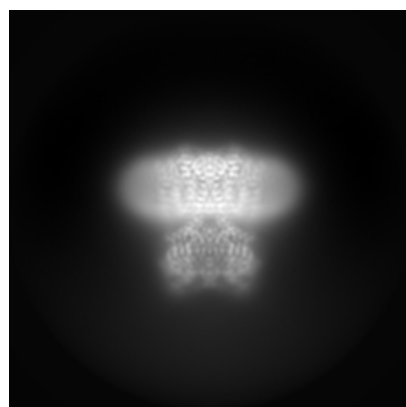


Y

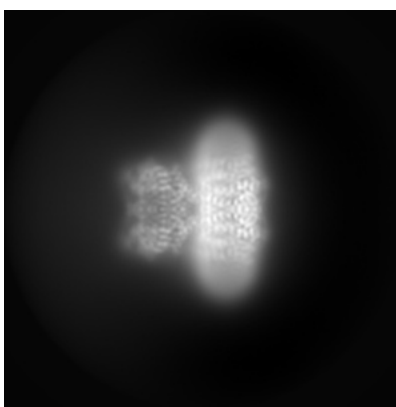


Z

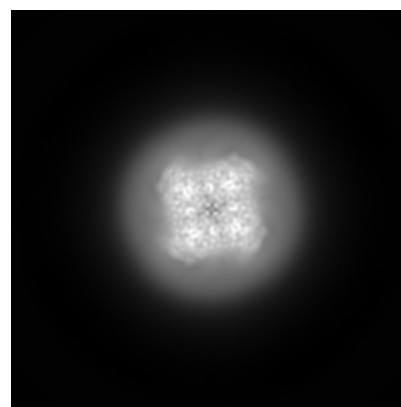
6.1.2 Raw map



X



Y

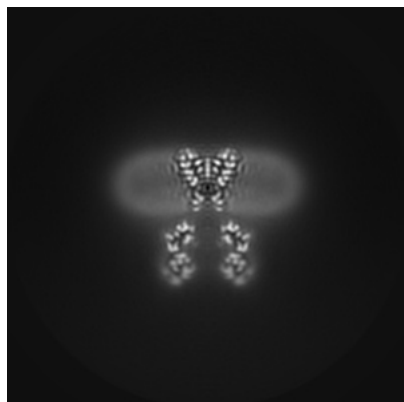


Z

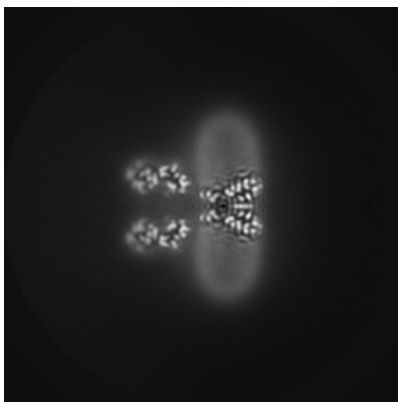
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

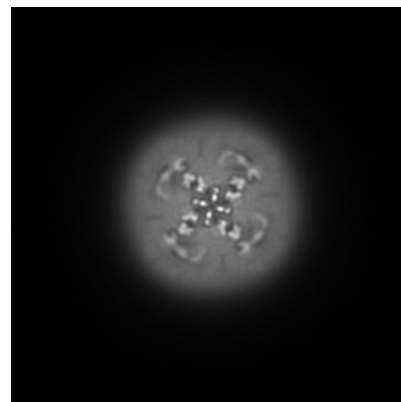
6.2.1 Primary map



X Index: 128

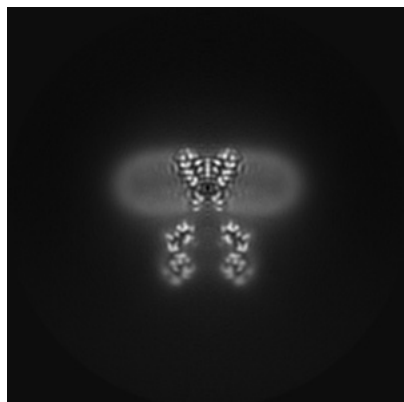


Y Index: 128

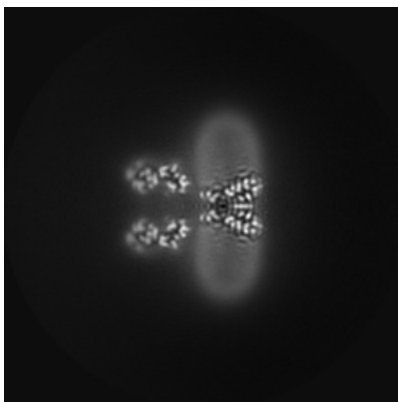


Z Index: 128

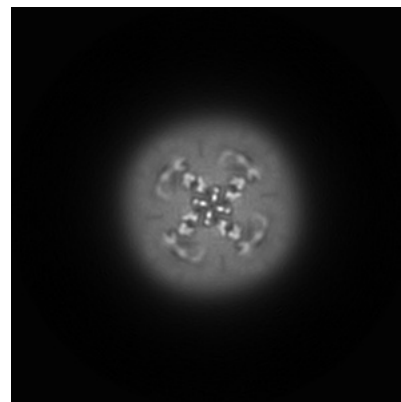
6.2.2 Raw map



X Index: 128



Y Index: 128

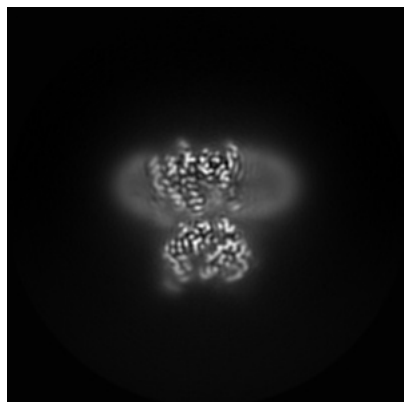


Z Index: 128

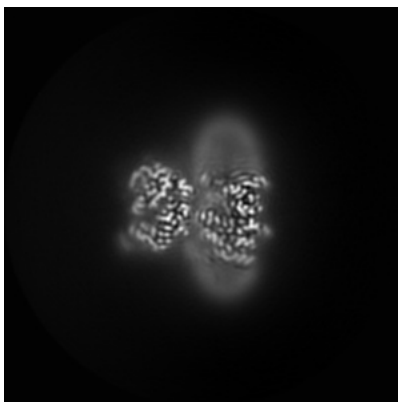
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

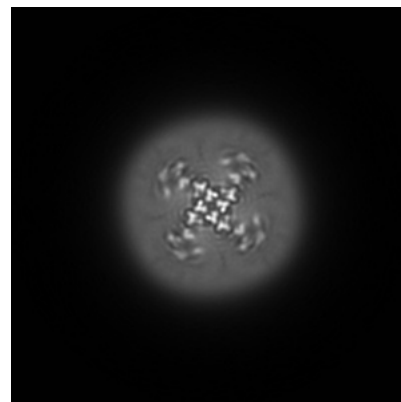
6.3.1 Primary map



X Index: 114

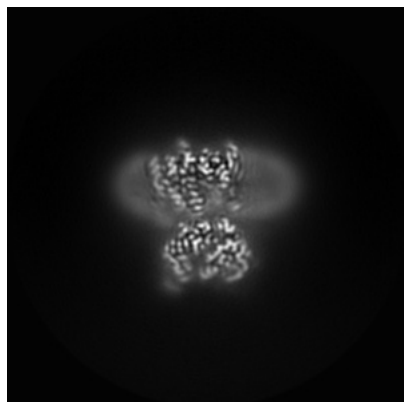


Y Index: 142

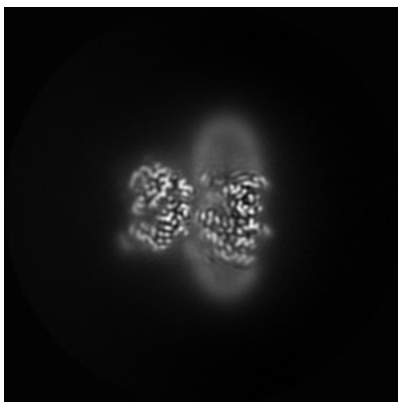


Z Index: 131

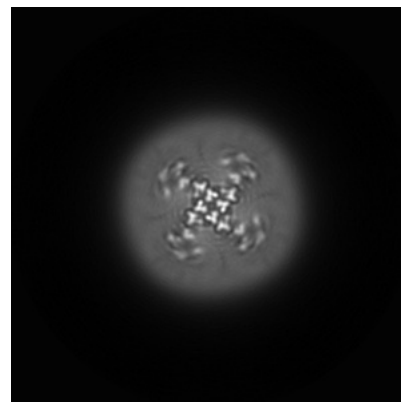
6.3.2 Raw map



X Index: 114



Y Index: 142

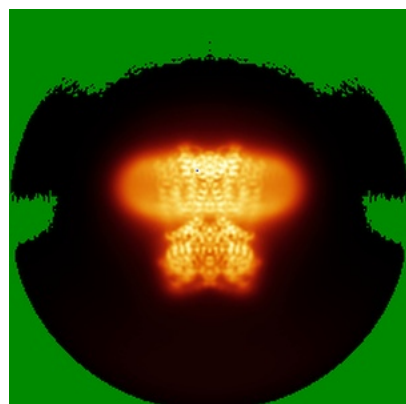


Z Index: 131

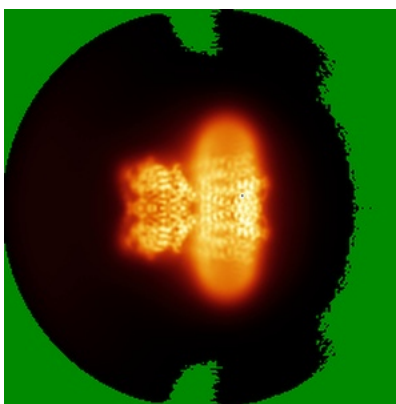
The images above show the largest variance slices of the map in three orthogonal directions.

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

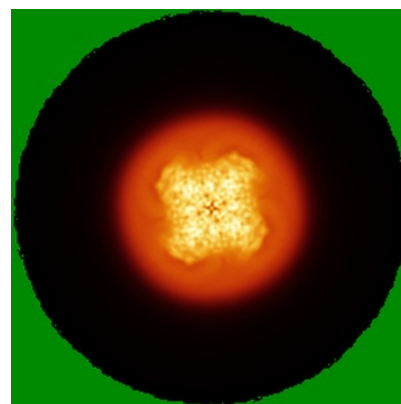
6.4.1 Primary map



X

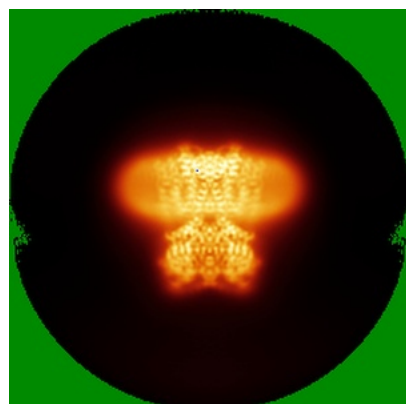


Y

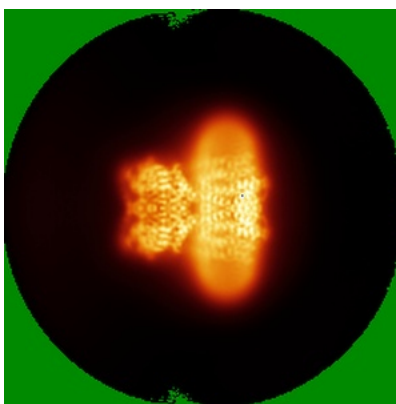


Z

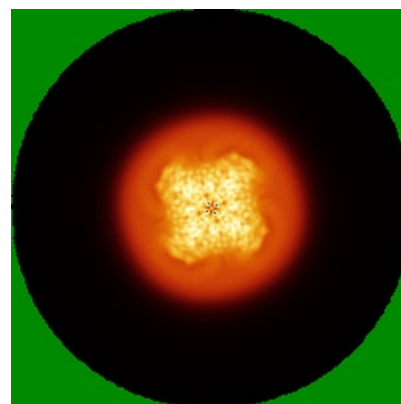
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

This section was not generated.

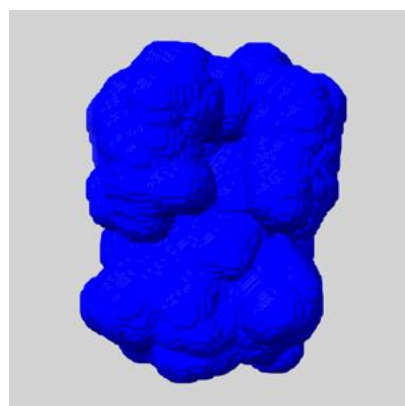
6.6 Mask visualisation [i](#)

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

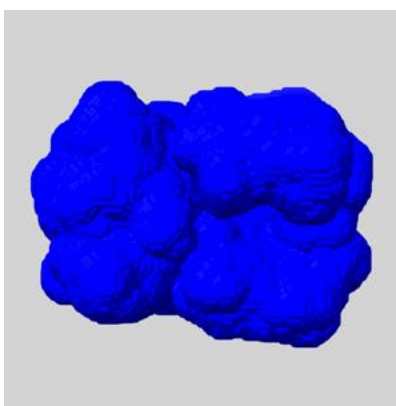
A mask typically either:

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

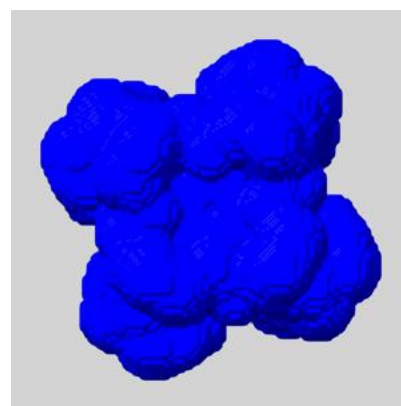
6.6.1 emd_43520_msk_1.map [i](#)



X



Y

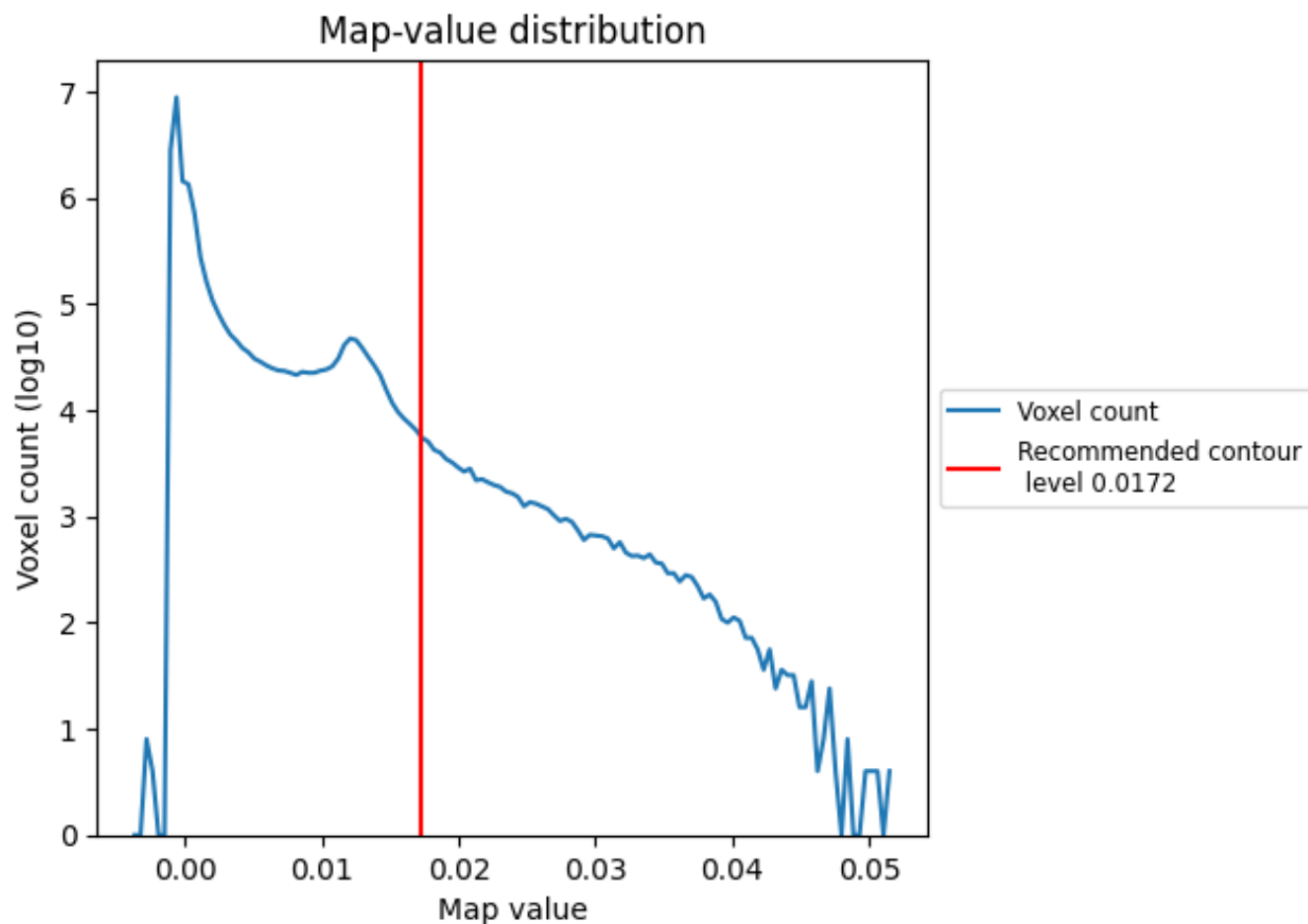


Z

7 Map analysis [i](#)

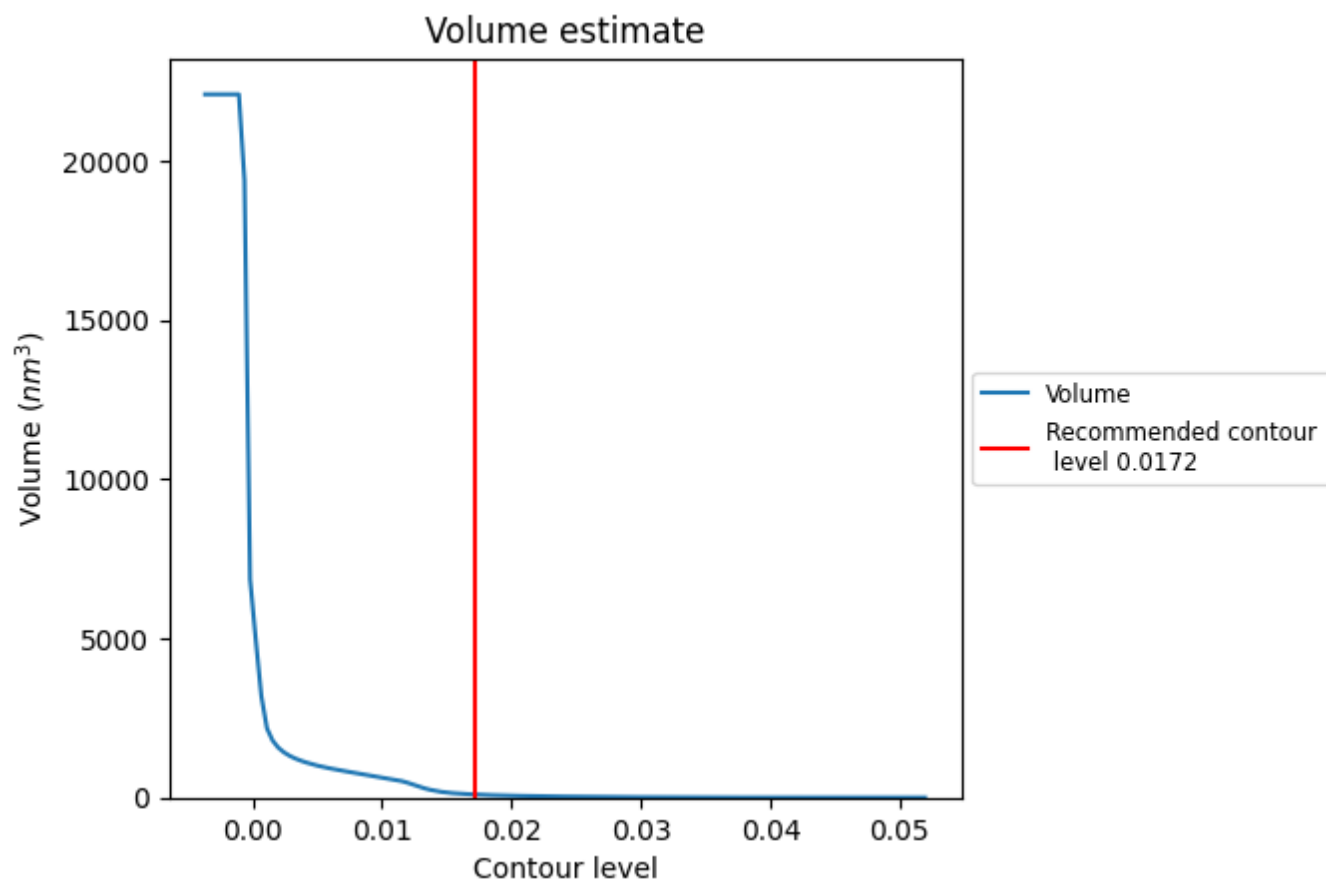
This section contains the results of statistical analysis of the map.

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.

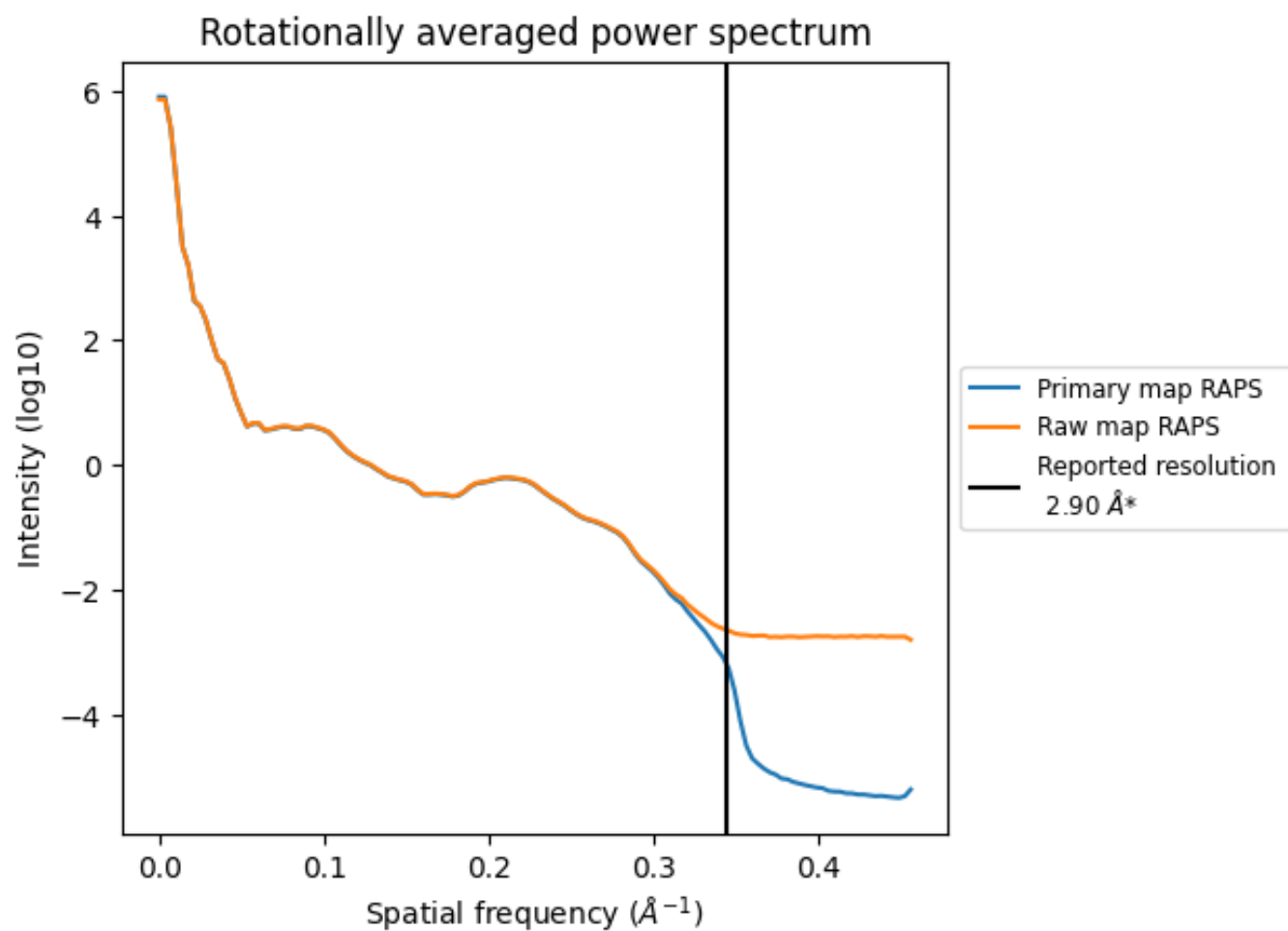
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm^3 ; this corresponds to an approximate mass of 86 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 ⓘ

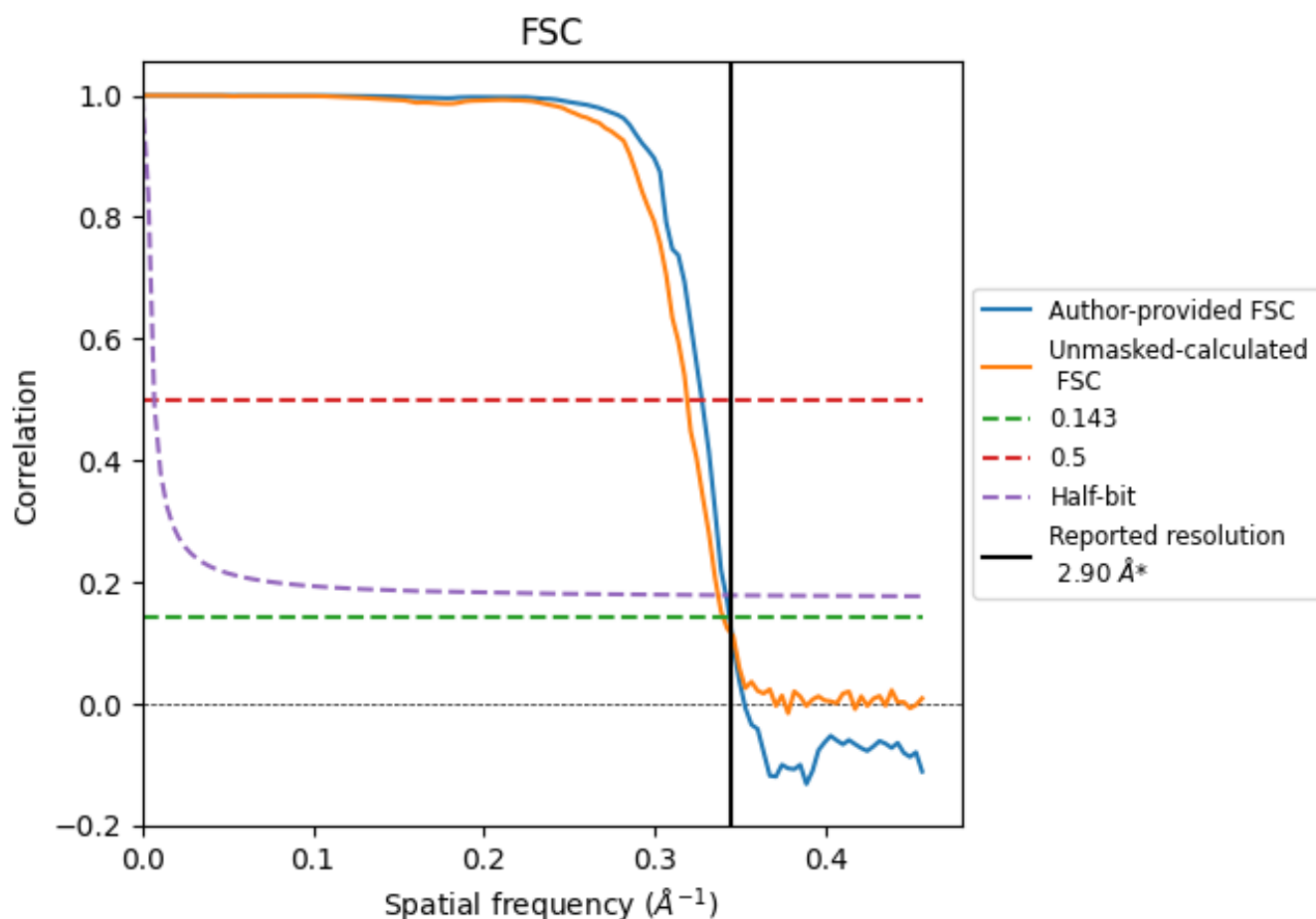


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

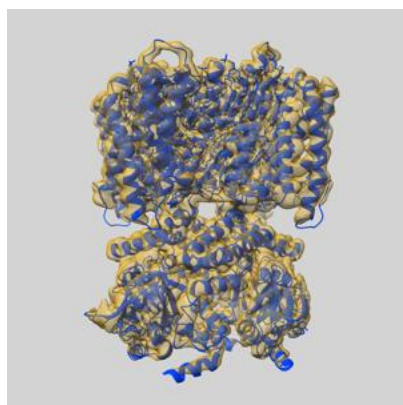
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.91	3.06	2.93
Unmasked-calculated*	2.94	3.14	2.97

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

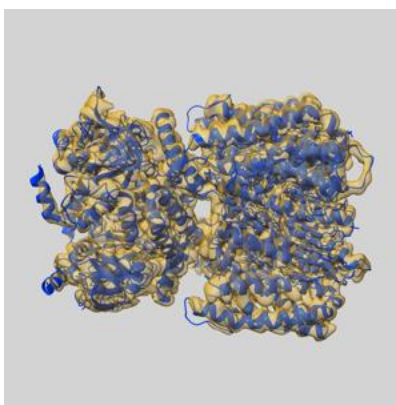
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43520 and PDB model 8VT9. Per-residue inclusion information can be found in section 3 on page 11.

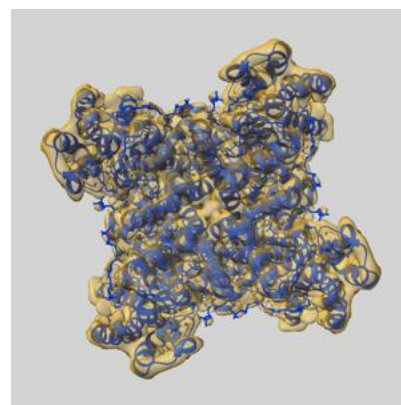
9.1 Map-model overlay [i](#)



X



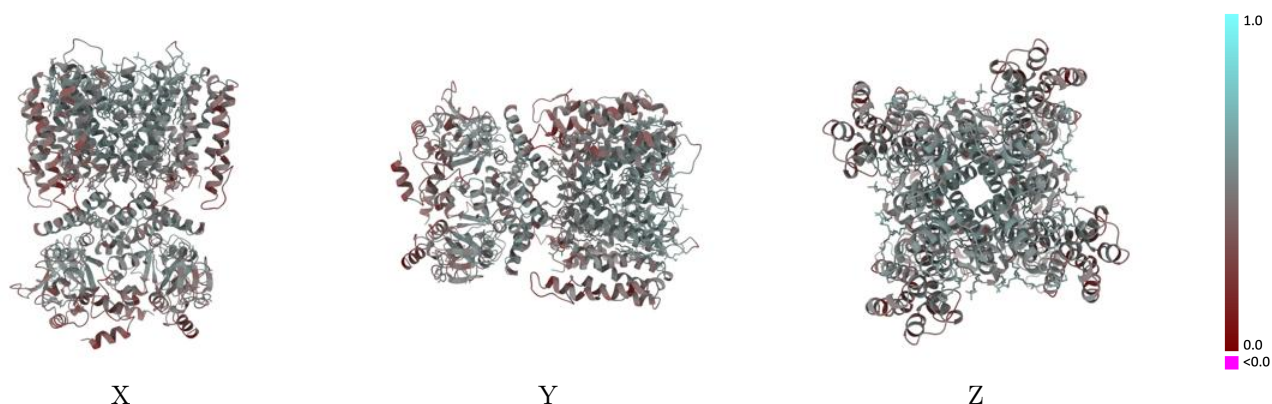
Y



Z

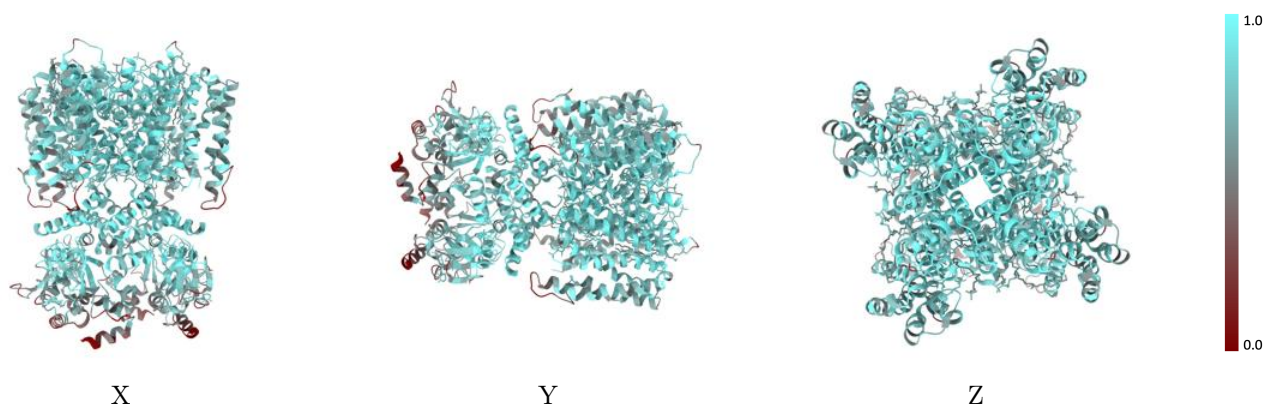
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



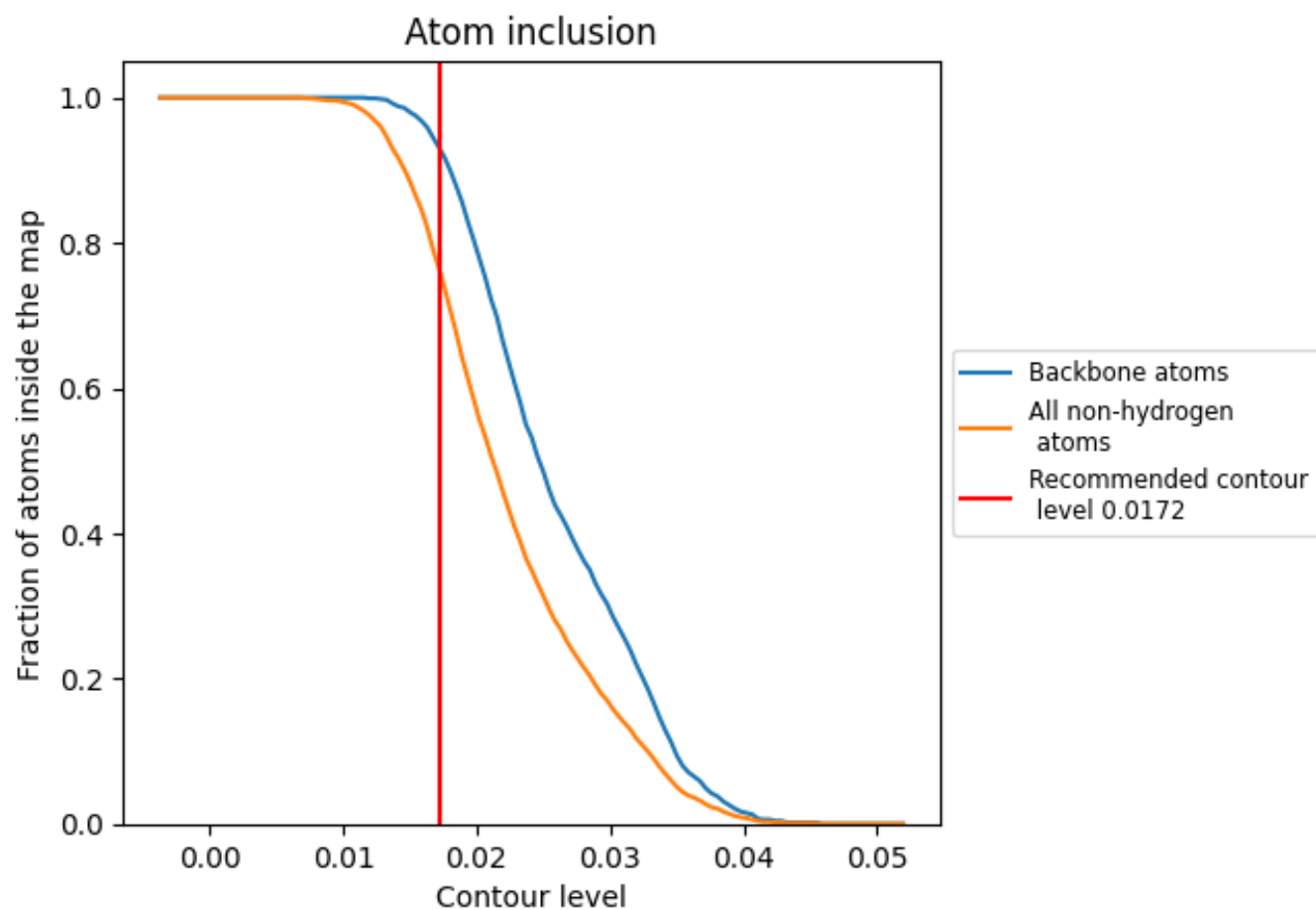
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0172).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 76% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7640	0.4600
A	0.7630	0.4600
B	0.7650	0.4590
C	0.7640	0.4590
D	0.7630	0.4590

