



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:13 PM EDT

PDB ID : 5KLB / pdb_00005klb
Title : Crystal structure of the CavAb voltage-gated calcium channel(wild-type, 2.7Å)
Authors : Tang, L.; Gamal EL-Din, T.M.; Swanson, T.M.; Pryde, D.C.; Scheuer, T.;
Zheng, N.; Catterall, W.A.
Deposited on : 2016-06-23
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

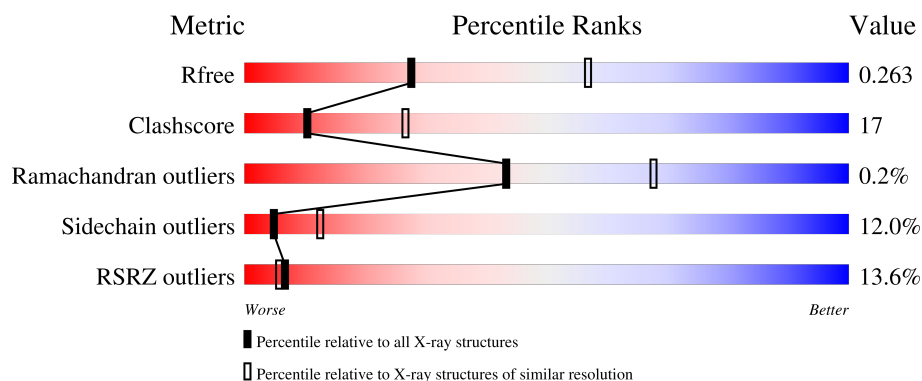
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	
1	D	285	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CPS	A	1304	-	X	X	-
4	CPS	A	1305	-	-	X	-
4	CPS	A	1306	-	X	-	-
4	CPS	B	1307	-	X	-	-
4	CPS	B	1308	-	X	X	-
4	CPS	D	1308	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Ion transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	B	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	C	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			
1	D	267	Total	C	N	O	S	0	0	0
			2195	1472	337	375	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	MET	-	initiating methionine	UNP A8EVM5
A	984	ASP	-	expression tag	UNP A8EVM5
A	985	TYR	-	expression tag	UNP A8EVM5
A	986	LYS	-	expression tag	UNP A8EVM5
A	987	ASP	-	expression tag	UNP A8EVM5
A	988	ASP	-	expression tag	UNP A8EVM5
A	989	ASP	-	expression tag	UNP A8EVM5
A	990	ASP	-	expression tag	UNP A8EVM5
A	991	LYS	-	expression tag	UNP A8EVM5
A	992	GLY	-	expression tag	UNP A8EVM5
A	993	SER	-	expression tag	UNP A8EVM5
A	994	LEU	-	expression tag	UNP A8EVM5
A	995	VAL	-	expression tag	UNP A8EVM5
A	996	PRO	-	expression tag	UNP A8EVM5
A	997	ARG	-	expression tag	UNP A8EVM5
A	998	GLY	-	expression tag	UNP A8EVM5
A	999	SER	-	expression tag	UNP A8EVM5
A	1000	HIS	-	expression tag	UNP A8EVM5
A	1177	ASP	GLU	conflict	UNP A8EVM5
A	1178	ASP	SER	conflict	UNP A8EVM5
A	1181	ASN	MET	conflict	UNP A8EVM5

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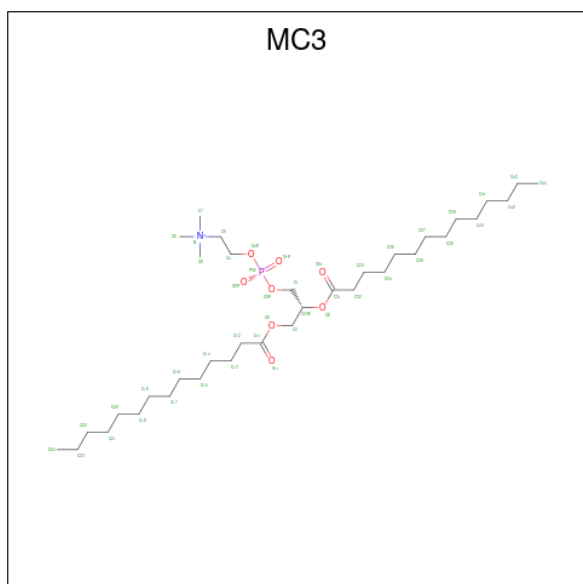
Chain	Residue	Modelled	Actual	Comment	Reference
B	983	MET	-	initiating methionine	UNP A8EVM5
B	984	ASP	-	expression tag	UNP A8EVM5
B	985	TYR	-	expression tag	UNP A8EVM5
B	986	LYS	-	expression tag	UNP A8EVM5
B	987	ASP	-	expression tag	UNP A8EVM5
B	988	ASP	-	expression tag	UNP A8EVM5
B	989	ASP	-	expression tag	UNP A8EVM5
B	990	ASP	-	expression tag	UNP A8EVM5
B	991	LYS	-	expression tag	UNP A8EVM5
B	992	GLY	-	expression tag	UNP A8EVM5
B	993	SER	-	expression tag	UNP A8EVM5
B	994	LEU	-	expression tag	UNP A8EVM5
B	995	VAL	-	expression tag	UNP A8EVM5
B	996	PRO	-	expression tag	UNP A8EVM5
B	997	ARG	-	expression tag	UNP A8EVM5
B	998	GLY	-	expression tag	UNP A8EVM5
B	999	SER	-	expression tag	UNP A8EVM5
B	1000	HIS	-	expression tag	UNP A8EVM5
B	1177	ASP	GLU	conflict	UNP A8EVM5
B	1178	ASP	SER	conflict	UNP A8EVM5
B	1181	ASN	MET	conflict	UNP A8EVM5
C	983	MET	-	initiating methionine	UNP A8EVM5
C	984	ASP	-	expression tag	UNP A8EVM5
C	985	TYR	-	expression tag	UNP A8EVM5
C	986	LYS	-	expression tag	UNP A8EVM5
C	987	ASP	-	expression tag	UNP A8EVM5
C	988	ASP	-	expression tag	UNP A8EVM5
C	989	ASP	-	expression tag	UNP A8EVM5
C	990	ASP	-	expression tag	UNP A8EVM5
C	991	LYS	-	expression tag	UNP A8EVM5
C	992	GLY	-	expression tag	UNP A8EVM5
C	993	SER	-	expression tag	UNP A8EVM5
C	994	LEU	-	expression tag	UNP A8EVM5
C	995	VAL	-	expression tag	UNP A8EVM5
C	996	PRO	-	expression tag	UNP A8EVM5
C	997	ARG	-	expression tag	UNP A8EVM5
C	998	GLY	-	expression tag	UNP A8EVM5
C	999	SER	-	expression tag	UNP A8EVM5
C	1000	HIS	-	expression tag	UNP A8EVM5
C	1177	ASP	GLU	conflict	UNP A8EVM5
C	1178	ASP	SER	conflict	UNP A8EVM5
C	1181	ASN	MET	conflict	UNP A8EVM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	983	MET	-	initiating methionine	UNP A8EVM5
D	984	ASP	-	expression tag	UNP A8EVM5
D	985	TYR	-	expression tag	UNP A8EVM5
D	986	LYS	-	expression tag	UNP A8EVM5
D	987	ASP	-	expression tag	UNP A8EVM5
D	988	ASP	-	expression tag	UNP A8EVM5
D	989	ASP	-	expression tag	UNP A8EVM5
D	990	ASP	-	expression tag	UNP A8EVM5
D	991	LYS	-	expression tag	UNP A8EVM5
D	992	GLY	-	expression tag	UNP A8EVM5
D	993	SER	-	expression tag	UNP A8EVM5
D	994	LEU	-	expression tag	UNP A8EVM5
D	995	VAL	-	expression tag	UNP A8EVM5
D	996	PRO	-	expression tag	UNP A8EVM5
D	997	ARG	-	expression tag	UNP A8EVM5
D	998	GLY	-	expression tag	UNP A8EVM5
D	999	SER	-	expression tag	UNP A8EVM5
D	1000	HIS	-	expression tag	UNP A8EVM5
D	1177	ASP	GLU	conflict	UNP A8EVM5
D	1178	ASP	SER	conflict	UNP A8EVM5
D	1181	ASN	MET	conflict	UNP A8EVM5

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).

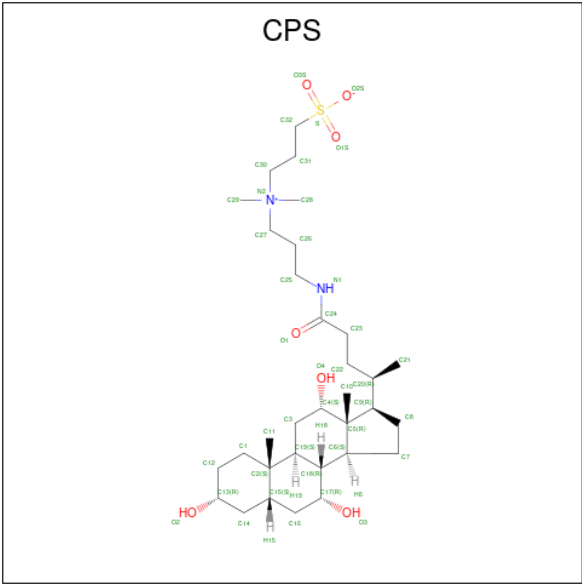


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 21 13 7 1	0	0
2	A	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C O P 21 13 7 1	0	0
2	B	1	Total C O P 41 32 8 1	0	0
2	B	1	Total C N O P 41 31 1 8 1	0	0
2	B	1	Total C N O P 46 36 1 8 1	0	0
2	B	1	Total C 8 8	0	0
2	C	1	Total C O P 21 13 7 1	0	0
2	C	1	Total C O P 41 32 8 1	0	0
2	C	1	Total C N O P 40 30 1 8 1	0	0
2	C	1	Total C N O P 46 36 1 8 1	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C O P 21 13 7 1	0	0
2	D	1	Total C O P 41 32 8 1	0	0
2	D	1	Total C N O P 43 33 1 8 1	0	0
2	D	1	Total C N O P 42 32 1 8 1	0	0
2	D	1	Total C N O P 46 36 1 8 1	0	0
2	D	1	Total C 8 8	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (CCD ID: CPS) (formula: C₃₂H₅₈N₂O₇S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 42 32 2 7 1	0	0
4	A	1	Total C N O S 42 32 2 7 1	0	0
4	A	1	Total C N O S 42 32 2 7 1	0	0
4	B	1	Total C N O S 42 32 2 7 1	0	0
4	B	1	Total C N O S 42 32 2 7 1	0	0
4	D	1	Total C N O S 42 32 2 7 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	6	Total 6	O 6	0	0
5	C	3	Total 3	O 3	0	0
5	D	5	Total 5	O 5	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.90Å 125.70Å 191.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.70 29.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.93-2.70) 91.7 (29.93-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.68Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.219 , 0.260 0.225 , 0.263	Depositor DCC
R_{free} test set	3791 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9684	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MC3, CPS

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	0.75	0/2248	0.98	6/3053 (0.2%)
1	B	0.74	1/2248 (0.0%)	0.97	4/3053 (0.1%)
1	C	0.75	1/2248 (0.0%)	0.94	3/3053 (0.1%)
1	D	0.77	2/2248 (0.1%)	0.97	6/3053 (0.2%)
All	All	0.75	4/8992 (0.0%)	0.97	19/12212 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1180	SER	CA-C	8.38	1.60	1.53
1	D	1180	SER	CA-C	7.95	1.61	1.53
1	B	1180	SER	CA-C	6.42	1.59	1.53
1	D	1184	VAL	CA-CB	6.38	1.63	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	VAL	CA-C-N	7.65	128.12	119.93
1	A	1089	VAL	C-N-CA	7.65	128.12	119.93
1	A	1247	ILE	N-CA-C	-6.55	107.48	113.71
1	A	1002	TYR	N-CA-C	-6.40	103.43	111.11
1	C	1248	ILE	N-CA-C	-6.24	105.54	113.22
1	D	1238	SER	N-CA-C	-6.03	106.53	114.31
1	D	1089	VAL	CA-C-N	6.01	127.36	119.84
1	D	1089	VAL	C-N-CA	6.01	127.36	119.84
1	C	1153	GLY	N-CA-C	5.70	121.05	114.16
1	C	1258	LYS	N-CA-C	-5.66	105.48	112.38
1	D	1266	LYS	CA-C-N	5.54	131.68	121.70
1	D	1266	LYS	C-N-CA	5.54	131.68	121.70
1	B	1264	SER	N-CA-C	-5.53	101.29	109.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1084	VAL	N-CA-C	-5.22	106.60	111.45
1	B	1155	ARG	CA-C-N	-5.21	117.12	122.85
1	B	1155	ARG	C-N-CA	-5.21	117.12	122.85
1	B	1002	TYR	N-CA-C	5.15	117.30	111.02
1	A	1266	LYS	N-CA-C	5.05	121.56	110.80
1	A	1068	ARG	CB-CA-C	-5.05	110.74	116.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2195	0	2274	59	0
1	B	2195	0	2274	62	0
1	C	2195	0	2274	56	0
1	D	2195	0	2274	54	0
2	A	67	0	91	4	0
2	B	157	0	218	12	0
2	C	207	0	291	23	0
2	D	201	0	283	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	126	0	135	67	0
4	B	84	0	89	38	0
4	D	42	0	45	22	0
5	A	3	0	0	0	0
5	B	6	0	0	0	0
5	C	3	0	0	0	0
5	D	5	0	0	1	0
All	All	9684	0	10248	339	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 17.

All (339) 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)
4:A:1305:CPS:O3	4:A:1305:CPS:C17	1.69	1.39
4:D:1308:CPS:O3	4:D:1308:CPS:C17	1.70	1.39
4:A:1306:CPS:C17	4:A:1306:CPS:O3	1.70	1.39
4:B:1307:CPS:C17	4:B:1307:CPS:O3	1.69	1.38
4:A:1304:CPS:C4	4:A:1304:CPS:C10	2.02	1.37
4:A:1306:CPS:C13	4:A:1306:CPS:O2	1.73	1.36
4:A:1304:CPS:C17	4:A:1304:CPS:O3	1.71	1.36
4:A:1305:CPS:O2	4:A:1305:CPS:C13	1.73	1.36
4:B:1307:CPS:O2	4:B:1307:CPS:C13	1.73	1.36
4:B:1308:CPS:O3	4:B:1308:CPS:C17	1.71	1.35
4:D:1308:CPS:C4	4:D:1308:CPS:C10	2.05	1.34
4:D:1308:CPS:C13	4:D:1308:CPS:O2	1.73	1.34
4:A:1305:CPS:C4	4:A:1305:CPS:C10	2.06	1.34
4:A:1306:CPS:O4	4:A:1306:CPS:C4	1.76	1.33
4:B:1308:CPS:C13	4:B:1308:CPS:O2	1.75	1.33
4:A:1304:CPS:C13	4:A:1304:CPS:O2	1.74	1.32
4:A:1305:CPS:C4	4:A:1305:CPS:C9	2.05	1.32
4:D:1308:CPS:C4	4:D:1308:CPS:C9	2.08	1.32
4:A:1305:CPS:C4	4:A:1305:CPS:O4	1.77	1.31
4:D:1308:CPS:C4	4:D:1308:CPS:O4	1.78	1.31
4:A:1304:CPS:C4	4:A:1304:CPS:O4	1.77	1.31
4:B:1308:CPS:C4	4:B:1308:CPS:C9	2.08	1.31
4:B:1308:CPS:C4	4:B:1308:CPS:O4	1.78	1.30
4:A:1304:CPS:C4	4:A:1304:CPS:C9	2.08	1.30
4:B:1307:CPS:O4	4:B:1307:CPS:C4	1.78	1.30
4:B:1308:CPS:C4	4:B:1308:CPS:C10	2.08	1.29
4:D:1308:CPS:C5	4:D:1308:CPS:C3	2.13	1.16
4:D:1308:CPS:C4	4:D:1308:CPS:C6	2.09	1.14
4:A:1305:CPS:C5	4:A:1305:CPS:C3	2.13	1.13
4:A:1304:CPS:C5	4:A:1304:CPS:C3	2.11	1.10
4:A:1304:CPS:C4	4:A:1304:CPS:C6	2.12	1.09
4:B:1308:CPS:C5	4:B:1308:CPS:C3	2.14	1.08
4:B:1308:CPS:C4	4:B:1308:CPS:C6	2.05	1.08
4:A:1305:CPS:C4	4:A:1305:CPS:C6	2.10	1.05
1:B:1221:MET:HE2	1:D:1221:MET:HB3	1.46	0.95
4:D:1308:CPS:C4	4:D:1308:CPS:C5	0.94	0.94
4:A:1304:CPS:C4	4:A:1304:CPS:C5	0.93	0.93
4:A:1305:CPS:C4	4:A:1305:CPS:C5	0.93	0.92
4:B:1308:CPS:C4	4:B:1308:CPS:C5	0.93	0.92
4:B:1308:CPS:O4	4:B:1308:CPS:C5	2.22	0.88
4:A:1306:CPS:O4	4:A:1306:CPS:C5	2.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1305:CPS:O4	4:A:1305:CPS:C5	2.25	0.83
1:A:1257:LEU:HD21	1:C:1257:LEU:HD21	1.61	0.82
1:B:1162:THR:HG22	1:B:1165:GLU:H	1.44	0.82
4:B:1307:CPS:O2	4:B:1307:CPS:C14	2.25	0.81
1:D:1162:THR:HG22	1:D:1165:GLU:H	1.45	0.81
4:A:1304:CPS:O4	4:A:1304:CPS:C5	2.26	0.81
4:A:1305:CPS:O2	4:A:1305:CPS:C14	2.27	0.80
4:D:1308:CPS:O4	4:D:1308:CPS:C5	2.29	0.80
4:B:1307:CPS:O4	4:B:1307:CPS:C5	2.27	0.78
1:A:1038:MET:HE1	1:A:1045:THR:HG21	1.66	0.78
4:B:1308:CPS:C10	4:B:1308:CPS:C3	2.60	0.77
2:C:1304:MC3:H381	2:C:1304:MC3:H161	1.67	0.76
1:A:1122:ALA:HB1	4:A:1305:CPS:H25A	1.69	0.75
1:B:1265:LEU:HD12	1:B:1265:LEU:O	1.86	0.74
4:A:1306:CPS:O2	4:A:1306:CPS:C14	2.29	0.74
1:A:1127:ILE:HA	1:A:1130:MET:HE2	1.69	0.74
1:C:1247:ILE:HA	1:C:1250:LEU:HB2	1.72	0.71
1:A:1162:THR:HG22	1:A:1165:GLU:H	1.55	0.70
4:D:1308:CPS:C10	4:D:1308:CPS:C3	2.63	0.70
4:A:1304:CPS:O2	4:A:1304:CPS:C14	2.31	0.70
1:B:1254:ILE:HG12	1:D:1254:ILE:HD13	1.75	0.69
1:C:1162:THR:HG22	1:C:1165:GLU:H	1.57	0.69
2:C:1302:MC3:H121	2:C:1302:MC3:H342	1.74	0.68
1:A:1163:LEU:HB2	1:D:1033:THR:HG21	1.74	0.68
1:C:1206:THR:HG21	2:C:1306:MC3:H332	1.76	0.67
1:B:1038:MET:HE2	1:B:1038:MET:HA	1.75	0.67
1:A:1025:ASN:OD1	1:A:1105:ARG:NH1	2.26	0.67
1:A:1026:GLY:HA3	2:C:1307:MC3:H231	1.77	0.67
1:A:1073:LYS:NZ	4:A:1304:CPS:H3	2.09	0.67
4:D:1308:CPS:H10A	4:D:1308:CPS:H3A	1.76	0.66
4:D:1308:CPS:O2	4:D:1308:CPS:C12	2.44	0.65
1:B:1030:GLY:O	1:B:1033:THR:HB	1.97	0.65
4:B:1308:CPS:C3	4:B:1308:CPS:H10A	2.27	0.64
1:C:1252:GLU:HA	1:C:1255:VAL:HB	1.79	0.64
1:C:1127:ILE:HA	1:C:1130:MET:HE2	1.79	0.64
1:A:1070:SER:HG	4:A:1304:CPS:HO4	1.43	0.64
1:C:1026:GLY:HA3	2:C:1302:MC3:H231	1.79	0.64
4:B:1308:CPS:H10A	4:B:1308:CPS:H3A	1.79	0.63
1:D:1003:LEU:O	1:D:1007:ASN:ND2	2.30	0.63
4:D:1308:CPS:O2	4:D:1308:CPS:C14	2.31	0.63
1:D:1265:LEU:O	1:D:1267:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:GLU:HA	1:A:1038:MET:HE3	1.80	0.63
4:A:1305:CPS:O3	4:A:1305:CPS:C18	2.37	0.63
1:B:1132:SER:HB2	1:C:1119:ILE:HD11	1.80	0.63
4:A:1306:CPS:O4	4:A:1306:CPS:C3	2.47	0.62
4:B:1308:CPS:H10B	4:B:1308:CPS:H21A	1.82	0.62
2:B:1303:MC3:H182	2:B:1303:MC3:H402	1.81	0.62
1:D:1259:GLU:HA	1:D:1262:LYS:HB2	1.80	0.61
1:A:1070:SER:OG	4:A:1304:CPS:O4	2.13	0.61
1:B:1254:ILE:HD12	1:C:1250:LEU:HD22	1.83	0.61
1:D:1251:ARG:O	1:D:1255:VAL:HG13	2.01	0.61
4:A:1305:CPS:O4	4:A:1305:CPS:H9	2.01	0.61
1:C:1202:ILE:O	1:C:1206:THR:HG22	2.00	0.60
4:A:1304:CPS:C10	4:A:1304:CPS:C3	2.68	0.60
1:B:1129:GLY:HA3	4:B:1307:CPS:O3	2.00	0.60
1:C:1037:PHE:HE1	1:C:1045:THR:HG21	1.64	0.60
1:D:1171:PHE:HB2	2:D:1304:MC3:H142	1.83	0.60
1:D:1091:THR:HA	1:D:1102:ARG:HH22	1.66	0.60
4:D:1308:CPS:O3	4:D:1308:CPS:C16	2.48	0.60
4:B:1308:CPS:O3	4:B:1308:CPS:C18	2.39	0.60
1:A:1254:ILE:HD13	1:D:1253:GLU:HG2	1.83	0.59
1:D:1177:ASP:OD1	5:D:1401:HOH:O	2.17	0.59
4:D:1308:CPS:O2S	4:D:1308:CPS:H30	2.03	0.59
1:B:1001:MET:N	4:B:1308:CPS:H29B	2.17	0.59
1:A:1003:LEU:HA	1:A:1006:THR:HB	1.85	0.59
1:A:1257:LEU:HD11	1:C:1257:LEU:HD11	1.84	0.59
4:A:1304:CPS:H10A	4:A:1304:CPS:H3A	1.85	0.58
1:C:1057:THR:O	1:C:1061:ILE:HG12	2.03	0.58
1:C:1258:LYS:HD2	1:C:1258:LYS:O	2.03	0.58
4:D:1308:CPS:C3	4:D:1308:CPS:H10A	2.31	0.58
4:A:1306:CPS:O3	4:A:1306:CPS:C16	2.49	0.58
1:A:1050:GLN:O	1:A:1053:ILE:HG22	2.05	0.57
1:C:1080:ASP:OD1	1:C:1111:THR:HG21	2.05	0.57
1:B:1076:TRP:CH2	2:B:1302:MC3:H121	2.41	0.56
1:B:1033:THR:HG21	1:D:1163:LEU:HB2	1.88	0.56
1:A:1221:MET:HE1	1:C:1218:VAL:HA	1.88	0.56
1:A:1137:MET:HE1	1:A:1205:VAL:HG22	1.88	0.56
4:A:1305:CPS:C4	4:A:1305:CPS:H9	2.29	0.56
1:A:1130:MET:HE3	1:A:1134:ILE:HD11	1.88	0.56
2:B:1304:MC3:H122	1:C:1167:PHE:HB3	1.88	0.56
4:B:1308:CPS:O4	4:B:1308:CPS:C6	2.54	0.55
4:A:1305:CPS:C9	4:A:1305:CPS:O4	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1306:CPS:O2S	4:A:1306:CPS:H29B	2.07	0.55
1:D:1195:TRP:CD1	1:D:1195:TRP:H	2.24	0.55
1:D:1255:VAL:O	1:D:1258:LYS:HG2	2.07	0.55
1:A:1253:GLU:HB3	1:C:1254:ILE:HG21	1.87	0.55
4:A:1306:CPS:C17	4:A:1306:CPS:HO3	2.13	0.55
1:B:1206:THR:HG21	2:C:1305:MC3:H332	1.89	0.55
4:A:1304:CPS:C3	4:A:1304:CPS:H10A	2.37	0.54
1:B:1162:THR:HG22	1:B:1165:GLU:N	2.19	0.54
1:D:1030:GLY:O	1:D:1033:THR:HB	2.08	0.54
1:C:1080:ASP:OD1	1:C:1108:ARG:NE	2.39	0.54
1:B:1239:HIS:HB3	1:D:1240:GLU:HG2	1.90	0.54
4:B:1307:CPS:O3	4:B:1307:CPS:C16	2.52	0.54
2:C:1302:MC3:H352	2:D:1305:MC3:O31	2.07	0.54
4:A:1305:CPS:O2	4:A:1305:CPS:C12	2.50	0.54
1:B:1004:ARG:NH1	4:B:1308:CPS:O1S	2.41	0.53
1:A:1252:GLU:HA	1:A:1255:VAL:HG12	1.89	0.53
4:D:1308:CPS:O4	4:D:1308:CPS:C3	2.54	0.53
1:B:1032:GLU:HA	1:B:1038:MET:HE3	1.90	0.53
4:D:1308:CPS:C10	4:D:1308:CPS:H3A	2.36	0.53
4:B:1308:CPS:C10	4:B:1308:CPS:H3A	2.34	0.53
1:A:1195:TRP:H	1:A:1195:TRP:CD1	2.27	0.52
1:B:1035:LYS:HG3	1:B:1036:THR:N	2.24	0.52
1:A:1076:TRP:CD2	1:A:1117:ARG:HD2	2.44	0.52
1:B:1002:TYR:HD2	1:B:1003:LEU:HD23	1.74	0.52
1:A:1001:MET:HA	1:A:1004:ARG:HD3	1.92	0.52
1:B:1101:LEU:O	1:B:1104:LEU:HB2	2.10	0.52
1:D:1060:ILE:O	1:D:1064:ILE:HG13	2.09	0.52
1:B:1264:SER:O	1:B:1265:LEU:HB3	2.09	0.52
2:B:1305:MC3:H182	2:B:1305:MC3:H402	1.91	0.52
2:C:1303:MC3:H321	2:D:1303:MC3:H352	1.92	0.51
1:B:1091:THR:HG23	1:B:1102:ARG:HH21	1.74	0.51
1:B:1056:PHE:O	1:B:1060:ILE:HG12	2.10	0.51
1:A:1040:SER:HB3	1:A:1041:PHE:CD2	2.45	0.51
1:D:1117:ARG:O	1:D:1121:SER:HB2	2.11	0.51
4:B:1308:CPS:O2	4:B:1308:CPS:C14	2.36	0.51
1:B:1254:ILE:CG1	1:D:1254:ILE:HD13	2.39	0.51
1:B:1227:LYS:O	1:B:1231:HIS:ND1	2.44	0.51
1:D:1025:ASN:OD1	1:D:1105:ARG:HD2	2.11	0.51
4:D:1308:CPS:C4	4:D:1308:CPS:H9	2.30	0.51
2:B:1304:MC3:H321	2:B:1304:MC3:H121	1.93	0.51
1:D:1217:ILE:HG22	1:D:1221:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:GLY:O	1:A:1046:THR:OG1	2.29	0.50
1:B:1163:LEU:HD12	2:C:1302:MC3:H351	1.93	0.50
1:B:1175:THR:HG22	2:B:1306:MC3:H161	1.93	0.50
1:D:1074:ASP:OD2	1:D:1077:SER:OG	2.22	0.50
4:A:1305:CPS:O3	1:C:1129:GLY:HA3	2.12	0.50
1:B:1079:PHE:CD1	2:B:1302:MC3:H162	2.47	0.50
1:B:1227:LYS:HE2	1:B:1231:HIS:CE1	2.46	0.50
1:D:1115:GLN:OE1	1:D:1115:GLN:N	2.40	0.50
1:A:1073:LYS:HZ3	4:A:1304:CPS:H3	1.74	0.50
1:B:1143:ILE:HD11	1:C:1106:LEU:HB2	1.92	0.50
1:C:1087:SER:OG	1:C:1105:ARG:NH1	2.45	0.50
1:C:1050:GLN:HA	1:C:1053:ILE:HG22	1.94	0.50
1:C:1217:ILE:O	1:C:1221:MET:HG2	2.12	0.50
1:D:1075:PRO:HB2	2:D:1302:MC3:H121	1.93	0.50
1:C:1098:LEU:HD23	1:C:1101:LEU:HD23	1.94	0.49
1:D:1043:VAL:HA	1:D:1046:THR:HG22	1.94	0.49
1:B:1018:ILE:HD13	1:B:1108:ARG:HH21	1.76	0.49
1:C:1076:TRP:CZ2	1:C:1117:ARG:HG2	2.47	0.49
1:A:1150:GLN:OE1	1:D:1100:VAL:HG22	2.12	0.49
1:A:1221:MET:SD	1:D:1221:MET:SD	3.11	0.49
4:A:1304:CPS:HO4	4:A:1304:CPS:H9	1.77	0.49
1:A:1080:ASP:OD1	1:A:1111:THR:HG21	2.12	0.49
1:A:1106:LEU:HB3	2:C:1307:MC3:H241	1.95	0.49
2:A:1303:MC3:H362	1:D:1097:ILE:HD12	1.94	0.49
1:B:1267:ASN:N	1:B:1267:ASN:OD1	2.45	0.49
4:A:1305:CPS:O3	4:A:1305:CPS:C16	2.52	0.49
1:B:1240:GLU:HA	1:B:1243:ILE:HG12	1.94	0.49
1:A:1262:LYS:HD2	1:A:1265:LEU:HB2	1.95	0.49
1:B:1113:VAL:O	1:B:1116:MET:HB2	2.13	0.49
1:C:1195:TRP:H	1:C:1195:TRP:CD1	2.30	0.49
4:A:1304:CPS:C17	4:A:1304:CPS:HO3	2.14	0.48
1:C:1056:PHE:O	1:C:1060:ILE:HG12	2.12	0.48
1:A:1174:MET:HE2	1:A:1205:VAL:HG13	1.96	0.48
4:B:1308:CPS:H272	4:B:1308:CPS:O1	2.13	0.48
2:D:1306:MC3:H381	2:D:1306:MC3:H161	1.94	0.48
1:A:1155:ARG:HH21	2:A:1303:MC3:H61	1.78	0.48
1:A:1076:TRP:CZ2	2:A:1301:MC3:H2	2.48	0.48
1:A:1129:GLY:HA3	4:A:1306:CPS:O3	2.14	0.48
4:A:1306:CPS:O2	4:A:1306:CPS:C12	2.54	0.48
1:A:1244:ASN:O	1:A:1248:ILE:HG13	2.13	0.48
4:B:1307:CPS:C17	4:B:1307:CPS:HO3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:VAL:HG21	1:A:1098:LEU:HD13	1.96	0.47
1:C:1106:LEU:HB3	2:C:1302:MC3:H241	1.97	0.47
1:A:1079:PHE:O	1:A:1083:VAL:HB	2.15	0.47
1:C:1023:VAL:O	1:C:1027:ILE:HG13	2.14	0.47
1:C:1035:LYS:HD3	1:C:1035:LYS:HA	1.71	0.47
1:D:1080:ASP:OD2	1:D:1111:THR:HG21	2.15	0.47
1:B:1195:TRP:NE1	2:B:1304:MC3:H42	2.30	0.47
2:B:1304:MC3:O2P	1:C:1164:GLY:HA3	2.15	0.47
1:A:1172:GLN:OE1	1:C:1185:ARG:NH1	2.48	0.46
4:A:1305:CPS:H31	4:A:1305:CPS:H28	1.44	0.46
4:B:1308:CPS:C17	4:B:1308:CPS:HO3	2.14	0.46
1:C:1195:TRP:CZ2	2:C:1303:MC3:H12	2.51	0.46
1:B:1100:VAL:HG22	1:D:1150:GLN:OE1	2.15	0.46
1:C:1097:ILE:HG13	1:C:1101:LEU:HD22	1.96	0.46
4:A:1304:CPS:C13	4:A:1304:CPS:HO2	2.17	0.46
1:D:1188:MET:HA	1:D:1191:TYR:O	2.15	0.46
1:A:1076:TRP:CZ2	1:A:1117:ARG:HG3	2.51	0.46
1:B:1009:VAL:HA	1:B:1014:PHE:CD2	2.50	0.46
4:B:1308:CPS:O3	4:B:1308:CPS:C6	2.62	0.46
1:C:1071:PHE:CE2	1:C:1077:SER:HB3	2.51	0.46
4:D:1308:CPS:H23	4:D:1308:CPS:H21	1.78	0.46
1:D:1036:THR:O	1:D:1039:GLN:HG2	2.16	0.46
1:D:1115:GLN:O	1:D:1119:ILE:HG12	2.16	0.46
1:A:1035:LYS:HD2	1:A:1035:LYS:HA	1.75	0.46
1:C:1050:GLN:O	1:C:1053:ILE:HG22	2.16	0.46
1:C:1174:MET:HE3	2:C:1305:MC3:H321	1.98	0.46
1:D:1018:ILE:O	1:D:1022:ILE:HG13	2.16	0.45
1:A:1071:PHE:CE1	1:A:1077:SER:HB3	2.52	0.45
4:A:1305:CPS:C10	4:A:1305:CPS:C3	2.78	0.45
1:B:1256:GLU:O	1:B:1260:LEU:HB2	2.17	0.45
4:A:1305:CPS:C17	4:A:1305:CPS:HO3	2.12	0.45
4:A:1306:CPS:H29	4:A:1306:CPS:H31A	1.67	0.45
1:B:1266:LYS:HB3	1:B:1266:LYS:HE3	1.76	0.45
4:B:1308:CPS:N1	4:B:1308:CPS:H21B	2.31	0.45
1:C:1195:TRP:CH2	2:C:1303:MC3:H12	2.51	0.45
1:B:1232:ILE:HD13	1:D:1232:ILE:HG21	1.99	0.45
4:B:1307:CPS:C13	4:B:1307:CPS:HO2	2.16	0.45
4:B:1308:CPS:O4	4:B:1308:CPS:C3	2.58	0.45
1:A:1058:ILE:HA	1:A:1061:ILE:HD12	1.97	0.45
1:A:1222:ALA:O	1:A:1226:GLN:HG2	2.16	0.45
4:A:1304:CPS:O2	4:A:1304:CPS:C12	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:ASP:O	1:B:1178:ASP:C	2.59	0.45
1:D:1113:VAL:HA	1:D:1114:PRO:HD3	1.76	0.45
4:B:1308:CPS:C9	4:B:1308:CPS:O4	2.65	0.45
1:A:1038:MET:HA	1:A:1038:MET:HE2	1.98	0.45
4:A:1305:CPS:H21	4:A:1305:CPS:H23	1.60	0.45
1:B:1250:LEU:HD13	1:C:1250:LEU:HD13	1.99	0.44
1:C:1078:LEU:HD23	1:C:1078:LEU:HA	1.74	0.44
1:A:1170:LEU:HD12	1:A:1170:LEU:HA	1.86	0.44
4:A:1304:CPS:O4	4:A:1304:CPS:H9	2.18	0.44
1:D:1167:PHE:CE2	2:D:1304:MC3:H341	2.53	0.44
2:D:1306:MC3:H41	2:D:1306:MC3:H83	1.66	0.44
2:D:1306:MC3:H141	2:D:1306:MC3:H362	1.99	0.44
4:A:1304:CPS:O4	4:A:1304:CPS:C9	2.66	0.44
1:B:1195:TRP:CZ3	2:B:1304:MC3:H32	2.53	0.44
4:B:1307:CPS:H11B	4:B:1307:CPS:H3A	1.76	0.44
1:C:1108:ARG:O	1:C:1111:THR:HG22	2.17	0.44
1:A:1037:PHE:HD1	1:A:1038:MET:HE2	1.83	0.44
1:B:1261:ILE:HD12	1:B:1261:ILE:HA	1.82	0.44
1:C:1090:PRO:O	1:C:1092:SER:N	2.49	0.44
4:D:1308:CPS:C17	4:D:1308:CPS:HO3	2.13	0.44
1:A:1221:MET:SD	1:C:1221:MET:HG3	2.58	0.44
4:A:1306:CPS:O4	4:A:1306:CPS:H9	2.18	0.44
1:B:1089:VAL:HA	1:B:1090:PRO:HD3	1.89	0.44
2:C:1303:MC3:H41	2:C:1303:MC3:H73	1.53	0.44
4:A:1305:CPS:H29B	4:A:1305:CPS:H261	1.73	0.43
2:C:1303:MC3:H332	2:D:1303:MC3:H372	2.00	0.43
1:D:1256:GLU:HG3	1:D:1257:LEU:N	2.33	0.43
1:B:1195:TRP:CD1	1:B:1195:TRP:H	2.35	0.43
1:C:1049:ASN:OD1	1:C:1105:ARG:NH2	2.51	0.43
1:C:1069:ILE:HD12	1:C:1069:ILE:HA	1.83	0.43
4:A:1306:CPS:O4	4:A:1306:CPS:C6	2.66	0.43
1:B:1003:LEU:O	1:B:1007:ASN:N	2.46	0.43
1:B:1250:LEU:O	1:B:1254:ILE:HG13	2.19	0.43
1:A:1053:ILE:HD12	1:A:1053:ILE:HA	1.79	0.43
4:A:1305:CPS:O3	4:A:1305:CPS:C6	2.67	0.43
1:B:1221:MET:HG2	1:D:1221:MET:HE3	2.01	0.43
1:C:1250:LEU:HD23	1:C:1250:LEU:HA	1.81	0.43
1:D:1255:VAL:HA	1:D:1258:LYS:HD2	2.01	0.43
4:D:1308:CPS:O3	4:D:1308:CPS:C18	2.43	0.43
1:C:1257:LEU:HD13	1:C:1261:ILE:HD12	2.00	0.43
1:B:1080:ASP:OD2	1:B:1108:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1307:CPS:H29	4:B:1307:CPS:H31A	1.82	0.43
1:D:1101:LEU:HD22	1:D:1104:LEU:HD11	2.00	0.43
1:C:1076:TRP:CH2	1:C:1117:ARG:HG2	2.54	0.42
1:D:1028:THR:O	1:D:1032:GLU:HG3	2.19	0.42
1:D:1162:THR:HG22	1:D:1165:GLU:N	2.24	0.42
1:B:1255:VAL:HG12	1:B:1258:LYS:HZ3	1.84	0.42
4:B:1307:CPS:O4	4:B:1307:CPS:H9	2.19	0.42
1:B:1168:TYR:OH	1:D:1184:VAL:HG22	2.20	0.42
1:D:1193:TYR:HA	1:D:1195:TRP:NE1	2.35	0.42
1:A:1097:ILE:HG13	1:A:1101:LEU:CD2	2.50	0.42
1:B:1130:MET:HE1	1:B:1216:ILE:HD11	2.00	0.42
1:B:1101:LEU:HD23	1:B:1101:LEU:HA	1.79	0.42
2:C:1304:MC3:H72	2:C:1304:MC3:H42	1.81	0.42
1:A:1252:GLU:O	1:A:1256:GLU:HB2	2.20	0.42
1:B:1254:ILE:C	1:B:1256:GLU:H	2.27	0.42
4:A:1305:CPS:C13	4:A:1305:CPS:HO2	2.16	0.41
1:B:1143:ILE:O	1:B:1147:MET:HG3	2.20	0.41
1:B:1234:ASP:HA	1:B:1237:GLN:HB3	2.01	0.41
2:B:1305:MC3:H351	2:B:1305:MC3:H322	1.57	0.41
1:D:1059:GLU:OE1	1:D:1108:ARG:NH2	2.53	0.41
1:A:1260:LEU:HA	1:A:1263:THR:OG1	2.20	0.41
1:A:1053:ILE:O	1:A:1057:THR:OG1	2.34	0.41
1:B:1195:TRP:CE3	2:B:1304:MC3:H32	2.55	0.41
1:D:1005:ILE:O	1:D:1008:ILE:HG23	2.20	0.41
1:A:1250:LEU:HD23	1:A:1250:LEU:HA	1.87	0.41
4:A:1306:CPS:H11B	4:A:1306:CPS:H3A	1.85	0.41
1:C:1101:LEU:HD12	1:C:1101:LEU:HA	1.89	0.41
1:D:1060:ILE:HD13	1:D:1060:ILE:HA	1.93	0.41
1:B:1265:LEU:O	1:B:1265:LEU:CD1	2.64	0.41
2:A:1303:MC3:H131	2:A:1303:MC3:O31	2.21	0.41
4:A:1304:CPS:H8A	4:A:1304:CPS:H10	1.58	0.41
1:B:1095:PHE:HD2	1:B:1095:PHE:HA	1.77	0.41
4:B:1307:CPS:O4	4:B:1307:CPS:C9	2.69	0.41
1:C:1163:LEU:HD22	2:C:1307:MC3:H122	2.02	0.41
1:A:1201:PHE:O	1:A:1205:VAL:HB	2.20	0.41
4:A:1304:CPS:O3	4:A:1304:CPS:C18	2.46	0.41
1:B:1143:ILE:CD1	1:C:1106:LEU:HB2	2.50	0.41
1:C:1175:THR:HG22	2:C:1305:MC3:H342	2.02	0.41
1:D:1004:ARG:O	1:D:1008:ILE:HG22	2.21	0.41
1:D:1224:LEU:HD23	1:D:1224:LEU:HA	1.84	0.41
1:C:1144:PHE:HZ	2:C:1304:MC3:H202	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1303:MC3:H181	2:C:1303:MC3:H392	2.04	0.40
4:A:1304:CPS:H261	4:A:1304:CPS:H28A	1.53	0.40
1:D:1069:ILE:HD12	1:D:1069:ILE:HA	1.78	0.40
1:A:1160:PHE:CZ	1:A:1169:THR:HG21	2.56	0.40
1:B:1064:ILE:O	1:B:1068:ARG:N	2.44	0.40
1:C:1163:LEU:CD2	2:C:1307:MC3:H122	2.52	0.40
1:D:1080:ASP:CG	1:D:1111:THR:HG21	2.47	0.40
1:A:1167:PHE:HB3	2:C:1303:MC3:H121	2.03	0.40
1:A:1221:MET:CE	1:C:1221:MET:HG3	2.52	0.40
4:A:1306:CPS:O3	4:A:1306:CPS:C18	2.43	0.40
1:D:1078:LEU:HD12	1:D:1078:LEU:HA	1.96	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 X-ray entries followed by that with respect to entries of similar resolution.

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	265/285 (93%)	251 (95%)	14 (5%)	0	100	100
1	B	265/285 (93%)	254 (96%)	10 (4%)	1 (0%)	30	54
1	C	265/285 (93%)	254 (96%)	11 (4%)	0	100	100
1	D	265/285 (93%)	252 (95%)	12 (4%)	1 (0%)	30	54
All	All	1060/1140 (93%)	1011 (95%)	47 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1266	LYS
1	B	1255	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	248/264 (94%)	214 (86%)	34 (14%)	3	9
1	B	248/264 (94%)	224 (90%)	24 (10%)	8	20
1	C	248/264 (94%)	221 (89%)	27 (11%)	6	16
1	D	248/264 (94%)	214 (86%)	34 (14%)	3	9
All	All	992/1056 (94%)	873 (88%)	119 (12%)	5	12

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1002	TYR
1	A	1021	LEU
1	A	1024	LEU
1	A	1028	THR
1	A	1036	THR
1	A	1040	SER
1	A	1045	THR
1	A	1046	THR
1	A	1053	ILE
1	A	1059	GLU
1	A	1069	ILE
1	A	1078	LEU
1	A	1083	VAL
1	A	1095	PHE
1	A	1101	LEU
1	A	1111	THR
1	A	1121	SER
1	A	1155	ARG
1	A	1162	THR
1	A	1170	LEU
1	A	1205	VAL
1	A	1221	MET
1	A	1223	ILE
1	A	1228	GLU

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Mol	Chain	Res	Type
1	A	1233	ILE
1	A	1238	SER
1	A	1239	HIS
1	A	1240	GLU
1	A	1244	ASN
1	A	1247	ILE
1	A	1251	ARG
1	A	1256	GLU
1	A	1261	ILE
1	A	1263	THR
1	B	1009	VAL
1	B	1024	LEU
1	B	1033	THR
1	B	1054	THR
1	B	1058	ILE
1	B	1068	ARG
1	B	1091	THR
1	B	1095	PHE
1	B	1098	LEU
1	B	1104	LEU
1	B	1115	GLN
1	B	1116	MET
1	B	1162	THR
1	B	1163	LEU
1	B	1187	LEU
1	B	1199	ILE
1	B	1221	MET
1	B	1233	ILE
1	B	1250	LEU
1	B	1256	GLU
1	B	1257	LEU
1	B	1260	LEU
1	B	1265	LEU
1	B	1267	ASN
1	C	1024	LEU
1	C	1035	LYS
1	C	1043	VAL
1	C	1049	ASN
1	C	1050	GLN
1	C	1069	ILE
1	C	1083	VAL
1	C	1086	ILE

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Mol	Chain	Res	Type
1	C	1089	VAL
1	C	1101	LEU
1	C	1111	THR
1	C	1155	ARG
1	C	1162	THR
1	C	1185	ARG
1	C	1187	LEU
1	C	1205	VAL
1	C	1221	MET
1	C	1224	LEU
1	C	1229	GLU
1	C	1230	GLN
1	C	1232	ILE
1	C	1235	GLU
1	C	1236	VAL
1	C	1246	GLU
1	C	1252	GLU
1	C	1253	GLU
1	C	1255	VAL
1	D	1008	ILE
1	D	1009	VAL
1	D	1010	GLU
1	D	1028	THR
1	D	1033	THR
1	D	1034	SER
1	D	1049	ASN
1	D	1051	ILE
1	D	1069	ILE
1	D	1078	LEU
1	D	1091	THR
1	D	1095	PHE
1	D	1097	ILE
1	D	1109	LEU
1	D	1117	ARG
1	D	1121	SER
1	D	1155	ARG
1	D	1162	THR
1	D	1167	PHE
1	D	1176	LEU
1	D	1184	VAL
1	D	1187	LEU
1	D	1189	GLU

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Mol	Chain	Res	Type
1	D	1233	ILE
1	D	1240	GLU
1	D	1252	GLU
1	D	1253	GLU
1	D	1254	ILE
1	D	1255	VAL
1	D	1256	GLU
1	D	1260	LEU
1	D	1265	LEU
1	D	1266	LYS
1	D	1267	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1211	ASN
1	B	1007	ASN
1	B	1239	HIS
1	C	1067	HIS
1	C	1242	ASN
1	D	1231	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	MC3	B	1304	-	40,40,45	1.79	6 (15%)	46,48,53	1.85	5 (10%)
2	MC3	D	1307	-	7,7,45	0.78	0	6,6,53	0.21	0
2	MC3	C	1307	-	40,40,45	1.76	6 (15%)	43,45,53	1.66	5 (11%)
4	CPS	A	1306	-	45,45,45	11.55	29 (64%)	70,70,70	3.54	41 (58%)
2	MC3	D	1304	-	42,42,45	1.72	5 (11%)	48,50,53	1.76	6 (12%)
2	MC3	B	1306	-	7,7,45	0.75	0	6,6,53	0.23	0
2	MC3	D	1306	-	45,45,45	1.67	7 (15%)	51,53,53	1.59	6 (11%)
2	MC3	C	1304	-	45,45,45	1.74	8 (17%)	51,53,53	1.69	6 (11%)
2	MC3	C	1306	-	8,8,45	0.68	0	7,7,53	0.43	0
4	CPS	A	1304	-	45,45,45	11.61	30 (66%)	70,70,70	3.58	42 (60%)
2	MC3	C	1301	-	20,20,45	1.82	4 (20%)	22,24,53	1.65	2 (9%)
2	MC3	B	1305	-	45,45,45	1.65	6 (13%)	51,53,53	1.64	5 (9%)
4	CPS	B	1308	-	45,45,45	11.53	30 (66%)	70,70,70	3.65	40 (57%)
4	CPS	D	1308	-	45,45,45	11.57	31 (68%)	70,70,70	3.83	43 (61%)
2	MC3	C	1302	-	40,40,45	1.75	6 (15%)	43,45,53	1.65	5 (11%)
2	MC3	C	1303	-	39,39,45	1.67	5 (12%)	45,47,53	1.79	7 (15%)
2	MC3	D	1303	-	40,40,45	1.80	6 (15%)	43,45,53	1.57	4 (9%)
2	MC3	D	1305	-	41,41,45	1.69	4 (9%)	47,49,53	1.83	6 (12%)
2	MC3	C	1305	-	8,8,45	0.79	0	7,7,53	0.37	0
4	CPS	B	1307	-	45,45,45	11.61	29 (64%)	70,70,70	3.58	44 (62%)
2	MC3	A	1301	-	20,20,45	1.87	4 (20%)	22,24,53	1.44	2 (9%)
2	MC3	A	1303	-	45,45,45	1.58	6 (13%)	51,53,53	1.74	6 (11%)
2	MC3	D	1302	-	20,20,45	1.83	4 (20%)	22,24,53	1.69	3 (13%)
2	MC3	B	1302	-	20,20,45	1.82	4 (20%)	22,24,53	2.02	4 (18%)
2	MC3	B	1303	-	40,40,45	1.73	6 (15%)	43,45,53	1.64	4 (9%)
4	CPS	A	1305	-	45,45,45	11.66	31 (68%)	70,70,70	3.48	40 (57%)

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
2	MC3	B	1304	-	-	22/44/44/49	-
2	MC3	D	1307	-	-	3/5/5/49	-
2	MC3	C	1307	-	-	24/44/44/49	-
4	CPS	A	1306	-	-	14/25/90/90	0/4/4/4
2	MC3	D	1304	-	-	19/46/46/49	-
2	MC3	B	1306	-	-	1/5/5/49	-
2	MC3	D	1306	-	-	19/49/49/49	-
2	MC3	C	1304	-	-	21/49/49/49	-
2	MC3	C	1306	-	-	1/6/6/49	-
4	CPS	A	1304	-	-	14/25/90/90	0/4/4/4
2	MC3	C	1301	-	-	8/22/22/49	-
2	MC3	B	1305	-	-	28/49/49/49	-
4	CPS	B	1308	-	-	18/25/90/90	0/4/4/4
4	CPS	D	1308	-	-	16/25/90/90	0/4/4/4
2	MC3	C	1302	-	-	18/44/44/49	-
2	MC3	C	1303	-	-	18/43/43/49	-
2	MC3	D	1303	-	-	18/44/44/49	-
2	MC3	D	1305	-	-	20/45/45/49	-
2	MC3	C	1305	-	-	4/6/6/49	-
4	CPS	B	1307	-	-	11/25/90/90	0/4/4/4
2	MC3	A	1301	-	-	10/22/22/49	-
2	MC3	A	1303	-	-	22/49/49/49	-
2	MC3	D	1302	-	-	10/22/22/49	-
2	MC3	B	1302	-	-	10/22/22/49	-
2	MC3	B	1303	-	-	23/44/44/49	-
4	CPS	A	1305	-	-	2/25/90/90	0/4/4/4

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1304	CPS	C5-C4	-39.97	0.93	1.54
4	B	1308	CPS	C5-C4	-39.92	0.93	1.54
4	A	1305	CPS	C5-C4	-39.89	0.93	1.54
4	D	1308	CPS	C5-C4	-39.43	0.94	1.54
4	A	1306	CPS	C5-C4	-39.19	0.94	1.54
4	B	1307	CPS	C5-C4	-39.09	0.94	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1307	CPS	C14-C13	-28.47	1.02	1.52
4	B	1308	CPS	C14-C13	-28.18	1.02	1.52
4	A	1306	CPS	C14-C13	-27.99	1.02	1.52
4	A	1305	CPS	C14-C13	-27.95	1.02	1.52
4	D	1308	CPS	C14-C13	-27.86	1.03	1.52
4	A	1304	CPS	C14-C13	-27.58	1.03	1.52
4	B	1307	CPS	C16-C15	-24.96	1.14	1.53
4	B	1308	CPS	C16-C15	-24.04	1.15	1.53
4	A	1305	CPS	C16-C15	-24.01	1.15	1.53
4	A	1304	CPS	C16-C15	-23.99	1.15	1.53
4	A	1306	CPS	C16-C15	-23.74	1.15	1.53
4	D	1308	CPS	C16-C15	-23.44	1.16	1.53
4	D	1308	CPS	O4-C4	21.24	1.78	1.43
4	D	1308	CPS	C1-C2	-21.22	1.17	1.54
4	A	1305	CPS	C18-C17	-21.19	1.15	1.53
4	A	1306	CPS	C1-C2	-21.19	1.17	1.54
4	B	1308	CPS	O4-C4	21.08	1.78	1.43
4	B	1307	CPS	O4-C4	21.05	1.78	1.43
4	A	1304	CPS	C1-C2	-20.86	1.17	1.54
4	B	1308	CPS	C18-C17	-20.76	1.16	1.53
4	A	1305	CPS	O4-C4	20.68	1.77	1.43
4	A	1305	CPS	C1-C2	-20.66	1.18	1.54
4	B	1307	CPS	C18-C17	-20.63	1.16	1.53
4	A	1306	CPS	C18-C17	-20.58	1.16	1.53
4	D	1308	CPS	C18-C17	-20.47	1.16	1.53
4	B	1308	CPS	C1-C2	-20.47	1.18	1.54
4	A	1304	CPS	O4-C4	20.42	1.77	1.43
4	A	1306	CPS	O4-C4	20.36	1.76	1.43
4	B	1307	CPS	C1-C2	-20.30	1.18	1.54
4	B	1307	CPS	C2-C15	-20.29	1.23	1.55
4	A	1304	CPS	C18-C17	-20.26	1.16	1.53
4	D	1308	CPS	C2-C15	-20.11	1.24	1.55
4	A	1306	CPS	C2-C15	-19.88	1.24	1.55
4	A	1305	CPS	C2-C15	-19.85	1.24	1.55
4	A	1304	CPS	C2-C15	-19.84	1.24	1.55
4	B	1308	CPS	C2-C15	-18.85	1.26	1.55
4	B	1307	CPS	C18-C19	-17.08	1.21	1.53
4	A	1305	CPS	C18-C19	-17.07	1.21	1.53
4	A	1304	CPS	C18-C19	-16.88	1.21	1.53
4	D	1308	CPS	C18-C19	-16.72	1.21	1.53
4	A	1306	CPS	C18-C19	-16.59	1.22	1.53
4	B	1308	CPS	C18-C19	-16.26	1.22	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1304	CPS	O3-C17	13.42	1.71	1.43
4	B	1308	CPS	O3-C17	13.24	1.71	1.43
4	A	1306	CPS	C18-C6	-13.18	1.28	1.53
4	A	1304	CPS	C18-C6	-13.13	1.28	1.53
4	B	1307	CPS	C18-C6	-12.85	1.29	1.53
4	A	1306	CPS	O3-C17	12.82	1.70	1.43
4	D	1308	CPS	O3-C17	12.74	1.70	1.43
4	B	1307	CPS	O3-C17	12.66	1.69	1.43
4	A	1305	CPS	C32-S	-12.63	1.59	1.77
4	A	1305	CPS	O3-C17	12.45	1.69	1.43
4	A	1305	CPS	C18-C6	-12.40	1.30	1.53
4	D	1308	CPS	C18-C6	-12.23	1.30	1.53
4	B	1308	CPS	C18-C6	-12.17	1.30	1.53
4	A	1306	CPS	C32-S	-12.10	1.60	1.77
4	A	1304	CPS	C32-S	-11.24	1.61	1.77
4	B	1307	CPS	C32-S	-11.19	1.61	1.77
4	B	1308	CPS	O2-C13	11.01	1.75	1.43
4	A	1304	CPS	O2-C13	10.86	1.74	1.43
4	A	1305	CPS	C3-C19	-10.63	1.36	1.53
4	A	1305	CPS	O2-C13	10.50	1.73	1.43
4	A	1306	CPS	O2-C13	10.44	1.73	1.43
4	B	1307	CPS	O2-C13	10.43	1.73	1.43
4	D	1308	CPS	O2-C13	10.42	1.73	1.43
4	D	1308	CPS	C32-S	-10.03	1.63	1.77
4	D	1308	CPS	C3-C19	-9.99	1.37	1.53
4	A	1304	CPS	C5-C9	-9.98	1.38	1.55
4	B	1307	CPS	C3-C19	-9.79	1.37	1.53
4	A	1304	CPS	C3-C19	-9.60	1.38	1.53
4	B	1308	CPS	C32-S	-9.60	1.64	1.77
4	A	1306	CPS	C3-C19	-9.46	1.38	1.53
4	B	1307	CPS	C5-C9	-9.30	1.39	1.55
4	A	1305	CPS	C5-C9	-9.20	1.40	1.55
4	D	1308	CPS	C5-C9	-9.19	1.40	1.55
4	B	1308	CPS	C3-C19	-9.06	1.39	1.53
4	A	1306	CPS	C5-C9	-9.05	1.40	1.55
4	B	1308	CPS	C5-C9	-8.33	1.41	1.55
4	B	1307	CPS	C2-C19	-7.99	1.42	1.56
4	D	1308	CPS	C24-N1	7.93	1.52	1.33
4	A	1305	CPS	O1S-S	7.88	1.67	1.45
4	A	1304	CPS	C2-C19	-7.86	1.42	1.56
4	A	1306	CPS	C2-C19	-7.80	1.42	1.56
4	A	1305	CPS	C24-N1	7.80	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1308	CPS	O1S-S	7.78	1.67	1.45
4	D	1308	CPS	C2-C19	-7.73	1.42	1.56
4	D	1308	CPS	O1S-S	7.73	1.66	1.45
4	B	1308	CPS	O3S-S	7.63	1.66	1.45
4	A	1304	CPS	O1S-S	7.62	1.66	1.45
4	A	1304	CPS	O3S-S	7.60	1.66	1.45
4	B	1307	CPS	O3S-S	7.60	1.66	1.45
4	A	1306	CPS	C24-N1	7.60	1.51	1.33
4	D	1308	CPS	O3S-S	7.55	1.66	1.45
4	A	1306	CPS	O1S-S	7.53	1.66	1.45
4	B	1307	CPS	O1S-S	7.45	1.66	1.45
4	A	1305	CPS	C2-C19	-7.44	1.43	1.56
4	B	1308	CPS	C2-C19	-7.33	1.43	1.56
4	A	1305	CPS	O3S-S	7.19	1.65	1.45
4	B	1307	CPS	C24-N1	7.15	1.50	1.33
4	B	1308	CPS	C24-N1	7.12	1.50	1.33
4	A	1306	CPS	O3S-S	7.11	1.65	1.45
4	A	1304	CPS	C24-N1	6.51	1.48	1.33
2	D	1304	MC3	O31-C31	6.23	1.41	1.22
2	D	1303	MC3	O11-C11	6.15	1.40	1.22
2	C	1302	MC3	O11-C11	6.14	1.40	1.22
2	A	1301	MC3	O11-C11	6.13	1.40	1.22
2	D	1305	MC3	O31-C31	6.13	1.40	1.22
2	D	1306	MC3	O11-C11	6.08	1.40	1.22
2	B	1305	MC3	O11-C11	6.07	1.40	1.22
2	C	1304	MC3	O11-C11	6.06	1.40	1.22
2	C	1307	MC3	O11-C11	6.05	1.40	1.22
2	C	1303	MC3	O31-C31	6.03	1.40	1.22
2	C	1301	MC3	O11-C11	6.01	1.40	1.22
2	B	1302	MC3	O11-C11	5.96	1.40	1.22
2	C	1304	MC3	O31-C31	5.95	1.40	1.22
2	B	1303	MC3	O31-C31	5.93	1.40	1.22
2	D	1306	MC3	O31-C31	5.93	1.40	1.22
2	C	1307	MC3	O31-C31	5.91	1.40	1.22
4	B	1308	CPS	C14-C15	5.90	1.63	1.53
2	D	1302	MC3	O11-C11	5.90	1.40	1.22
2	B	1304	MC3	O31-C31	5.90	1.40	1.22
4	A	1304	CPS	C14-C15	5.89	1.63	1.53
2	A	1303	MC3	O11-C11	5.87	1.40	1.22
2	D	1305	MC3	O11-C11	5.78	1.39	1.22
2	B	1303	MC3	O11-C11	5.74	1.39	1.22
2	B	1304	MC3	O11-C11	5.69	1.39	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1305	MC3	O31-C31	5.66	1.39	1.22
2	A	1303	MC3	O31-C31	5.66	1.39	1.22
2	D	1303	MC3	O31-C31	5.65	1.39	1.22
2	D	1304	MC3	O11-C11	5.64	1.39	1.22
4	D	1308	CPS	C14-C15	5.62	1.62	1.53
4	B	1308	CPS	C8-C9	5.50	1.65	1.54
2	C	1302	MC3	O31-C31	5.45	1.38	1.22
2	C	1303	MC3	O11-C11	5.38	1.38	1.22
4	A	1304	CPS	C8-C9	5.27	1.65	1.54
4	A	1305	CPS	C8-C9	5.26	1.65	1.54
4	A	1306	CPS	C14-C15	5.23	1.62	1.53
4	A	1305	CPS	C14-C15	5.20	1.62	1.53
4	D	1308	CPS	C8-C9	4.94	1.64	1.54
4	D	1308	CPS	C20-C9	4.92	1.62	1.54
4	D	1308	CPS	C1-C12	-4.82	1.43	1.53
4	A	1305	CPS	C1-C12	-4.79	1.43	1.53
4	A	1306	CPS	C1-C12	-4.77	1.43	1.53
4	B	1307	CPS	C14-C15	4.70	1.61	1.53
4	B	1307	CPS	C8-C9	4.67	1.63	1.54
4	A	1306	CPS	C8-C9	4.62	1.63	1.54
4	A	1305	CPS	C20-C9	4.54	1.62	1.54
4	B	1308	CPS	C20-C9	4.52	1.62	1.54
4	B	1307	CPS	C20-C9	4.44	1.62	1.54
4	D	1308	CPS	C23-C24	4.42	1.60	1.51
4	A	1306	CPS	C20-C9	4.39	1.61	1.54
4	A	1306	CPS	C23-C24	4.33	1.60	1.51
4	A	1304	CPS	C1-C12	-4.27	1.44	1.53
4	B	1308	CPS	C1-C12	-4.15	1.45	1.53
4	B	1307	CPS	C1-C12	-4.01	1.45	1.53
4	B	1308	CPS	C10-C5	3.93	1.60	1.54
4	B	1308	CPS	C11-C2	3.80	1.60	1.54
2	B	1304	MC3	O2-C2	-3.80	1.37	1.46
4	B	1307	CPS	C23-C24	3.68	1.58	1.51
4	A	1306	CPS	C10-C5	3.64	1.60	1.54
4	A	1305	CPS	C11-C2	3.55	1.60	1.54
4	A	1305	CPS	C23-C24	3.53	1.58	1.51
4	A	1304	CPS	C10-C5	3.51	1.59	1.54
4	A	1304	CPS	C20-C9	3.51	1.60	1.54
2	D	1304	MC3	O2-C2	-3.45	1.38	1.46
4	B	1308	CPS	C23-C24	3.44	1.58	1.51
4	A	1304	CPS	C11-C2	3.41	1.59	1.54
4	A	1305	CPS	C10-C5	3.30	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1308	CPS	C8-C7	-3.24	1.45	1.54
4	B	1307	CPS	C16-C17	-3.22	1.46	1.52
4	B	1307	CPS	C11-C2	3.20	1.59	1.54
4	A	1304	CPS	C8-C7	-3.19	1.45	1.54
4	B	1307	CPS	C10-C5	3.18	1.59	1.54
4	A	1304	CPS	C23-C24	3.18	1.57	1.51
2	D	1305	MC3	O2-C2	-3.18	1.39	1.46
2	C	1302	MC3	O3-C11	3.12	1.42	1.33
4	D	1308	CPS	C10-C5	3.11	1.59	1.54
4	A	1306	CPS	C8-C7	-2.97	1.45	1.54
2	A	1301	MC3	O3-C11	2.96	1.42	1.33
2	D	1303	MC3	O3-C11	2.95	1.41	1.33
4	D	1308	CPS	C11-C2	2.92	1.59	1.54
2	C	1304	MC3	O2-C2	-2.90	1.39	1.46
2	C	1307	MC3	O2-C2	-2.89	1.39	1.46
2	C	1303	MC3	O2-C2	-2.89	1.39	1.46
4	A	1306	CPS	C11-C2	2.89	1.59	1.54
2	B	1305	MC3	O2-C2	-2.89	1.39	1.46
4	B	1308	CPS	C16-C17	-2.84	1.47	1.52
2	D	1304	MC3	O2-C31	2.84	1.42	1.34
4	B	1307	CPS	C8-C7	-2.83	1.46	1.54
2	A	1301	MC3	P-O4P	2.82	1.68	1.58
4	A	1306	CPS	C12-C13	-2.82	1.45	1.51
2	D	1302	MC3	O3-C11	2.81	1.41	1.33
4	D	1308	CPS	C12-C13	-2.78	1.45	1.51
4	A	1306	CPS	C16-C17	-2.78	1.47	1.52
2	B	1302	MC3	P-O4P	2.74	1.67	1.58
2	D	1306	MC3	O2-C2	-2.72	1.40	1.46
2	C	1302	MC3	O2-C2	-2.71	1.40	1.46
2	B	1303	MC3	O2-C2	-2.71	1.40	1.46
4	A	1305	CPS	C12-C13	-2.70	1.45	1.51
4	A	1306	CPS	C22-C23	2.69	1.61	1.52
2	D	1303	MC3	P-O4P	2.69	1.67	1.58
2	C	1301	MC3	O3-C11	2.68	1.41	1.33
4	A	1304	CPS	C7-C6	2.67	1.59	1.54
2	B	1304	MC3	O3-C11	2.63	1.41	1.33
4	D	1308	CPS	C16-C17	-2.62	1.47	1.52
2	C	1304	MC3	O3-C11	2.62	1.41	1.33
2	C	1303	MC3	O3-C11	2.62	1.41	1.33
2	C	1304	MC3	O2-C31	2.61	1.41	1.34
2	D	1303	MC3	O2-C31	2.60	1.41	1.34
2	B	1303	MC3	O3-C11	2.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1308	CPS	C7-C6	2.58	1.59	1.54
4	D	1308	CPS	C22-C23	2.57	1.60	1.52
4	A	1305	CPS	C16-C17	-2.57	1.47	1.52
4	A	1305	CPS	C7-C6	2.54	1.59	1.54
4	D	1308	CPS	C8-C7	-2.50	1.47	1.54
4	A	1304	CPS	C16-C17	-2.49	1.48	1.52
2	D	1305	MC3	O2-C31	2.48	1.41	1.34
2	B	1302	MC3	O3-C11	2.47	1.40	1.33
2	C	1307	MC3	O3-C11	2.46	1.40	1.33
4	B	1308	CPS	C22-C23	2.45	1.60	1.52
4	A	1304	CPS	C22-C23	2.45	1.60	1.52
2	D	1302	MC3	P-O4P	2.41	1.66	1.58
2	A	1303	MC3	O2-C31	2.41	1.41	1.34
2	C	1301	MC3	P-O4P	2.40	1.66	1.58
2	C	1302	MC3	P-O4P	2.40	1.66	1.58
2	D	1306	MC3	O2-C31	2.40	1.41	1.34
4	A	1305	CPS	C8-C7	-2.40	1.47	1.54
2	B	1303	MC3	P-O4P	2.38	1.66	1.58
4	B	1308	CPS	C12-C13	-2.37	1.46	1.51
2	C	1302	MC3	O2-C31	2.36	1.41	1.34
4	B	1307	CPS	C22-C23	2.36	1.60	1.52
2	D	1303	MC3	O2-C2	-2.35	1.41	1.46
2	D	1306	MC3	O3-C11	2.34	1.40	1.33
2	B	1303	MC3	O2-C31	2.33	1.40	1.34
2	C	1303	MC3	O2-C31	2.32	1.40	1.34
2	C	1307	MC3	O2-C31	2.31	1.40	1.34
2	C	1307	MC3	P-O4P	2.31	1.66	1.58
2	B	1305	MC3	O3-C11	2.29	1.40	1.33
4	D	1308	CPS	C25-N1	2.27	1.51	1.46
4	A	1304	CPS	C12-C13	-2.27	1.46	1.51
4	A	1305	CPS	C22-C23	2.25	1.59	1.52
2	D	1304	MC3	O3-C11	2.20	1.39	1.33
2	B	1305	MC3	O2-C31	2.20	1.40	1.34
2	A	1303	MC3	O2-C2	-2.19	1.41	1.46
2	B	1305	MC3	P-O4P	2.18	1.67	1.59
2	D	1306	MC3	O3-C3	-2.14	1.40	1.45
4	B	1307	CPS	C12-C13	-2.11	1.46	1.51
2	A	1303	MC3	P-O3P	2.10	1.67	1.59
2	C	1301	MC3	P-O3P	2.09	1.67	1.59
4	A	1305	CPS	C25-N1	2.07	1.50	1.46
2	B	1304	MC3	C5-C4	2.07	1.57	1.51
2	C	1304	MC3	P-O4P	2.05	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1302	MC3	P-O3P	2.05	1.67	1.59
2	A	1301	MC3	P-O3P	2.04	1.67	1.59
2	B	1302	MC3	P-O3P	2.04	1.67	1.59
4	D	1308	CPS	C31-C32	2.04	1.58	1.52
2	C	1304	MC3	C12-C11	2.02	1.56	1.50
2	B	1304	MC3	O2-C31	2.01	1.40	1.34
2	C	1304	MC3	O3-C3	-2.01	1.40	1.45
2	D	1306	MC3	P-O4P	2.00	1.67	1.59
2	A	1303	MC3	P-O4P	2.00	1.67	1.59

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1304	CPS	C9-C5-C4	10.34	126.97	117.67
4	B	1307	CPS	O1S-S-C32	-10.17	91.36	106.73
4	B	1307	CPS	C9-C5-C4	9.26	126.00	117.67
4	B	1307	CPS	O3S-S-C32	8.91	120.20	106.73
4	A	1305	CPS	C3-C4-C5	8.86	120.27	111.26
4	B	1308	CPS	C31-C32-S	8.66	126.51	113.25
4	D	1308	CPS	O3S-S-C32	8.17	119.07	106.73
4	A	1306	CPS	C9-C5-C4	8.13	124.98	117.67
4	D	1308	CPS	C9-C5-C4	7.99	124.86	117.67
4	A	1306	CPS	C25-N1-C24	7.82	137.38	122.82
2	B	1304	MC3	O2-C31-O31	-7.79	105.49	123.70
4	B	1308	CPS	C5-C9-C20	7.77	128.89	119.48
4	B	1308	CPS	C8-C9-C20	-7.58	100.71	112.18
4	D	1308	CPS	C27-C26-C25	7.41	125.45	110.95
2	B	1302	MC3	O3-C11-O11	-7.31	105.34	123.63
2	D	1305	MC3	O3-C11-O11	-7.28	105.43	123.63
4	B	1308	CPS	C3-C4-C5	7.25	118.64	111.26
4	A	1305	CPS	C1-C2-C15	7.23	118.12	107.75
4	D	1308	CPS	C1-C2-C15	7.22	118.11	107.75
2	C	1302	MC3	O2-C31-O31	-7.14	107.01	123.70
4	A	1304	CPS	C6-C5-C4	7.07	113.88	107.42
4	A	1306	CPS	C1-C2-C15	7.06	117.88	107.75
2	B	1304	MC3	O3-C11-O11	-7.05	106.00	123.63
2	A	1303	MC3	O2-C31-O31	-7.01	107.31	123.70
4	D	1308	CPS	C31-C32-S	6.89	123.81	113.25
4	B	1308	CPS	C9-C5-C4	6.85	123.83	117.67
2	C	1304	MC3	O3-C11-O11	-6.79	106.64	123.63
4	A	1306	CPS	C3-C4-C5	6.67	118.05	111.26
4	A	1304	CPS	O3S-S-C32	6.63	116.75	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	CPS	C11-C2-C1	-6.56	97.87	108.31
4	B	1308	CPS	C11-C2-C19	-6.53	102.40	111.18
2	B	1305	MC3	O2-C31-O31	-6.52	108.47	123.70
4	D	1308	CPS	C11-C2-C1	-6.51	97.95	108.31
2	A	1303	MC3	O3-C11-O11	-6.49	107.39	123.63
4	A	1305	CPS	O2S-S-O3S	6.41	127.44	111.40
4	A	1304	CPS	C10-C5-C9	-6.41	101.17	111.20
2	C	1301	MC3	O3-C11-O11	-6.40	107.63	123.63
4	A	1305	CPS	C6-C5-C4	6.38	113.24	107.42
2	C	1307	MC3	O2-C31-O31	-6.28	109.02	123.70
4	A	1304	CPS	C11-C2-C1	-6.28	98.33	108.31
4	D	1308	CPS	C3-C4-C5	6.25	117.62	111.26
2	B	1303	MC3	O2-C31-O31	-6.25	109.10	123.70
2	C	1307	MC3	O3-C11-O11	-6.18	108.16	123.63
2	B	1305	MC3	O3-C11-O11	-6.15	108.25	123.63
2	D	1302	MC3	O3-C11-O11	-6.11	108.35	123.63
2	D	1304	MC3	O3-C11-O11	-6.00	108.61	123.63
4	A	1305	CPS	C9-C5-C6	6.00	106.13	100.11
4	A	1304	CPS	C10-C5-C4	-5.98	103.07	109.06
4	B	1308	CPS	O3S-S-C32	5.97	115.75	106.73
4	A	1306	CPS	C16-C15-C2	5.95	119.00	112.66
4	A	1306	CPS	O3S-S-C32	5.94	115.71	106.73
2	C	1303	MC3	O2-C31-O31	-5.94	109.82	123.70
4	A	1305	CPS	C10-C5-C9	-5.94	101.90	111.20
4	B	1307	CPS	C3-C4-C5	5.93	117.30	111.26
4	B	1308	CPS	C1-C2-C15	5.92	116.25	107.75
2	B	1303	MC3	O3-C11-O11	-5.90	108.88	123.63
4	A	1305	CPS	O1S-S-C32	-5.87	97.85	106.73
2	D	1303	MC3	O2-C31-O31	-5.84	110.05	123.70
4	A	1306	CPS	O4-C4-C3	-5.83	97.26	109.12
4	D	1308	CPS	C2-C19-C18	5.83	118.33	111.84
4	B	1307	CPS	C1-C2-C15	5.83	116.11	107.75
4	B	1308	CPS	C25-N1-C24	5.80	133.62	122.82
4	B	1307	CPS	C6-C5-C4	5.78	112.70	107.42
4	B	1308	CPS	C16-C15-C2	5.78	118.81	112.66
4	D	1308	CPS	C12-C1-C2	5.71	122.38	112.74
2	C	1304	MC3	O2-C31-O31	-5.69	110.40	123.70
2	D	1306	MC3	O2-C31-O31	-5.69	110.41	123.70
2	D	1305	MC3	O2-C31-O31	-5.62	110.56	123.70
2	D	1304	MC3	O2-C31-O31	-5.61	110.59	123.70
4	A	1306	CPS	O2S-S-O3S	5.60	125.42	111.40
4	A	1305	CPS	C9-C5-C4	5.60	122.71	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1308	CPS	C16-C17-C18	5.60	117.61	111.50
4	B	1308	CPS	C19-C18-C6	5.55	117.50	109.75
4	A	1304	CPS	C23-C22-C20	5.46	124.67	114.46
4	B	1307	CPS	C19-C18-C17	5.43	118.69	111.86
4	A	1304	CPS	C3-C4-C5	5.40	116.76	111.26
2	C	1303	MC3	O11-C11-C12	-5.40	102.65	123.78
4	A	1304	CPS	C1-C2-C15	5.39	115.48	107.75
4	B	1307	CPS	C10-C5-C9	-5.38	102.78	111.20
4	A	1305	CPS	O3S-S-C32	5.38	114.85	106.73
4	D	1308	CPS	C10-C5-C9	-5.31	102.88	111.20
4	A	1304	CPS	O2S-S-O1S	-5.30	98.13	111.40
4	A	1304	CPS	C19-C18-C17	5.30	118.53	111.86
4	A	1305	CPS	C2-C19-C18	5.25	117.69	111.84
4	A	1305	CPS	C14-C13-C12	5.24	117.01	110.62
4	D	1308	CPS	C14-C13-C12	5.23	117.00	110.62
4	D	1308	CPS	O1S-S-C32	-5.22	98.85	106.73
4	A	1304	CPS	O2S-S-O3S	5.21	124.43	111.40
4	A	1305	CPS	C16-C17-C18	5.21	117.19	111.50
4	B	1308	CPS	C10-C5-C6	-5.19	103.07	111.20
2	D	1303	MC3	O3-C11-O11	-5.19	110.64	123.63
4	D	1308	CPS	O1S-S-O3S	-5.18	96.99	113.82
2	C	1303	MC3	O3-C11-O11	-5.15	110.76	123.63
4	A	1306	CPS	C11-C2-C15	-5.10	101.91	110.44
4	B	1308	CPS	C27-C26-C25	-5.10	100.99	110.95
4	A	1306	CPS	C11-C2-C1	-5.07	100.24	108.31
4	B	1307	CPS	C16-C15-C2	5.06	118.04	112.66
2	D	1306	MC3	O3-C11-O11	-5.05	110.99	123.63
4	A	1304	CPS	C31-C32-S	5.01	120.93	113.25
4	A	1306	CPS	C6-C5-C4	4.96	111.95	107.42
4	A	1305	CPS	C21-C20-C22	-4.92	102.72	110.34
4	A	1306	CPS	C19-C2-C15	4.90	115.32	108.51
4	D	1308	CPS	C9-C5-C6	4.89	105.02	100.11
4	A	1306	CPS	C10-C5-C6	-4.88	103.56	111.20
4	A	1304	CPS	C12-C1-C2	4.88	120.97	112.74
4	D	1308	CPS	C6-C18-C17	4.85	118.29	111.85
4	D	1308	CPS	C19-C2-C15	4.85	115.25	108.51
4	A	1306	CPS	O1S-S-O3S	-4.80	98.20	113.82
4	A	1306	CPS	C10-C5-C9	-4.80	103.69	111.20
4	A	1305	CPS	C12-C1-C2	4.79	120.82	112.74
4	B	1308	CPS	C16-C17-C18	4.78	116.72	111.50
4	A	1305	CPS	C7-C6-C18	4.78	124.91	118.36
4	A	1306	CPS	C16-C17-C18	4.74	116.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1305	CPS	C1-C12-C13	4.70	116.71	110.48
4	B	1307	CPS	C12-C1-C2	4.67	120.62	112.74
4	D	1308	CPS	C26-C27-N2	4.67	124.84	115.35
4	B	1308	CPS	O1S-S-O3S	-4.66	98.67	113.82
4	A	1305	CPS	O1S-S-O3S	-4.66	98.67	113.82
4	B	1308	CPS	O2S-S-O1S	-4.66	99.75	111.40
2	A	1301	MC3	O3-C11-O11	-4.65	111.98	123.63
4	B	1307	CPS	C11-C2-C15	-4.64	102.68	110.44
4	B	1307	CPS	C19-C2-C15	4.62	114.93	108.51
4	A	1305	CPS	C16-C15-C2	4.59	117.54	112.66
4	A	1306	CPS	C19-C18-C17	4.57	117.61	111.86
4	A	1304	CPS	C1-C12-C13	4.57	116.53	110.48
4	B	1307	CPS	C25-N1-C24	4.53	131.26	122.82
2	A	1301	MC3	O11-C11-C12	-4.51	106.14	123.78
4	A	1304	CPS	C14-C13-C12	4.51	116.12	110.62
4	B	1308	CPS	C19-C2-C15	4.49	114.75	108.51
4	A	1306	CPS	C12-C1-C2	4.46	120.27	112.74
4	A	1304	CPS	C16-C15-C2	4.44	117.39	112.66
4	A	1306	CPS	C31-C32-S	4.42	120.02	113.25
2	D	1304	MC3	C8-N-C6	4.41	120.56	108.98
4	B	1308	CPS	C19-C18-C17	4.41	117.41	111.86
4	D	1308	CPS	O4-C4-C3	-4.39	100.18	109.12
2	B	1303	MC3	O11-C11-C12	-4.39	106.59	123.78
2	B	1305	MC3	O31-C31-C32	-4.39	106.61	123.78
2	D	1304	MC3	O31-C31-C32	-4.38	106.64	123.78
4	B	1308	CPS	C9-C5-C6	4.37	104.50	100.11
4	D	1308	CPS	C1-C12-C13	4.37	116.27	110.48
4	D	1308	CPS	C16-C15-C2	4.35	117.28	112.66
2	D	1306	MC3	C8-N-C6	4.30	120.26	108.98
4	B	1307	CPS	C21-C20-C22	-4.29	103.71	110.34
4	D	1308	CPS	C11-C2-C15	-4.28	103.28	110.44
4	A	1304	CPS	C6-C18-C17	4.27	117.52	111.85
4	A	1305	CPS	C10-C5-C6	-4.27	104.52	111.20
4	B	1307	CPS	C6-C18-C17	4.26	117.51	111.85
2	C	1304	MC3	C3-C2-C1	-4.26	101.85	111.78
4	B	1307	CPS	C19-C18-C6	4.25	115.69	109.75
2	C	1302	MC3	O11-C11-C12	-4.23	107.22	123.78
4	B	1307	CPS	C16-C17-C18	4.22	116.11	111.50
4	D	1308	CPS	C21-C20-C22	-4.22	103.81	110.34
4	B	1307	CPS	C10-C5-C6	-4.20	104.62	111.20
4	A	1306	CPS	C26-C25-N1	4.18	123.93	112.20
4	D	1308	CPS	C19-C18-C17	4.17	117.11	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1308	CPS	C29-N2-C30	-4.16	98.17	109.49
4	B	1308	CPS	C21-C20-C9	4.15	119.12	112.88
2	D	1306	MC3	O31-C31-C32	-4.14	107.59	123.78
4	B	1307	CPS	C16-C15-C14	-4.14	106.50	111.23
2	C	1302	MC3	O3-C11-O11	-4.12	113.33	123.63
4	A	1306	CPS	C21-C20-C22	-4.11	103.98	110.34
4	A	1304	CPS	O1S-S-O3S	-4.11	100.46	113.82
4	B	1307	CPS	O2S-S-O1S	-4.10	101.15	111.40
4	A	1304	CPS	C8-C9-C20	-4.09	105.98	112.18
4	B	1308	CPS	C12-C1-C2	4.08	119.63	112.74
4	A	1304	CPS	C16-C17-C18	4.08	115.95	111.50
4	D	1308	CPS	C22-C23-C24	4.06	122.11	113.06
2	A	1303	MC3	C8-N-C6	4.04	119.60	108.98
2	C	1304	MC3	O31-C31-C32	-4.04	107.98	123.78
4	D	1308	CPS	C7-C6-C18	4.03	123.89	118.36
4	A	1306	CPS	C2-C19-C18	4.02	116.32	111.84
4	D	1308	CPS	C6-C5-C4	4.01	111.08	107.42
4	A	1306	CPS	C14-C13-C12	4.01	115.51	110.62
4	A	1306	CPS	O2S-S-O1S	-3.99	101.42	111.40
4	A	1304	CPS	C25-N1-C24	-3.99	115.40	122.82
4	B	1307	CPS	C11-C2-C1	-3.99	101.97	108.31
2	D	1305	MC3	O11-C11-C12	-3.96	108.28	123.78
4	A	1305	CPS	C11-C2-C15	-3.95	103.84	110.44
4	D	1308	CPS	O2-C13-C12	-3.94	99.87	110.17
4	B	1307	CPS	C2-C19-C18	3.92	116.21	111.84
4	A	1306	CPS	C28-N2-C30	-3.90	98.89	109.49
4	A	1306	CPS	C5-C9-C20	3.85	124.15	119.48
4	A	1304	CPS	C22-C23-C24	3.85	121.65	113.06
4	B	1307	CPS	C22-C20-C9	3.85	118.31	110.33
2	D	1305	MC3	O31-C31-C32	-3.85	108.74	123.78
2	D	1306	MC3	O11-C11-C12	-3.82	108.82	123.78
2	D	1304	MC3	O11-C11-C12	-3.82	108.84	123.78
4	A	1305	CPS	C6-C18-C17	3.81	116.91	111.85
2	B	1302	MC3	O11-C11-C12	-3.81	108.87	123.78
4	A	1304	CPS	C19-C2-C15	3.81	113.81	108.51
4	B	1307	CPS	C31-C32-S	3.81	119.08	113.25
4	A	1304	CPS	C19-C18-C6	3.79	115.05	109.75
4	A	1304	CPS	C23-C24-N1	3.79	123.25	116.34
4	D	1308	CPS	C25-N1-C24	3.75	129.81	122.82
4	A	1305	CPS	C19-C2-C15	3.75	113.72	108.51
4	B	1308	CPS	C31-C30-N2	3.74	122.94	115.35
4	D	1308	CPS	O2S-S-O1S	-3.73	102.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1308	CPS	C10-C5-C6	-3.73	105.36	111.20
4	A	1305	CPS	C31-C30-N2	-3.71	107.80	115.35
4	B	1308	CPS	O2S-S-O3S	3.70	120.67	111.40
2	D	1303	MC3	O11-C11-C12	-3.69	109.33	123.78
4	A	1306	CPS	O1S-S-C32	-3.67	101.19	106.73
4	A	1304	CPS	O1-C24-N1	-3.66	115.85	123.03
4	D	1308	CPS	C22-C20-C9	3.64	117.88	110.33
4	B	1308	CPS	C21-C20-C22	-3.62	104.74	110.34
4	A	1304	CPS	O1S-S-C32	-3.62	101.27	106.73
2	A	1303	MC3	O31-C31-C32	-3.61	109.67	123.78
4	B	1308	CPS	C16-C15-C14	-3.60	107.11	111.23
4	D	1308	CPS	O2S-S-O3S	3.57	120.33	111.40
4	D	1308	CPS	O2S-S-C32	3.56	112.96	106.00
4	D	1308	CPS	C15-C16-C17	3.53	118.60	114.40
2	D	1302	MC3	O11-C11-C12	-3.53	109.98	123.78
2	C	1303	MC3	O31-C31-C32	-3.53	109.99	123.78
2	B	1305	MC3	C8-N-C6	3.51	118.20	108.98
4	B	1308	CPS	O2S-S-C32	3.49	112.84	106.00
2	C	1302	MC3	O31-C31-C32	-3.48	110.18	123.78
2	C	1307	MC3	O31-C31-C32	-3.45	110.28	123.78
2	C	1307	MC3	O11-C11-C12	-3.45	110.29	123.78
2	B	1304	MC3	O11-C11-C12	-3.45	110.30	123.78
4	A	1306	CPS	C1-C12-C13	3.42	115.01	110.48
4	B	1308	CPS	C28-N2-C27	-3.41	100.22	109.49
4	A	1306	CPS	C6-C18-C17	3.40	116.36	111.85
4	B	1307	CPS	O2S-S-C32	3.39	112.64	106.00
2	D	1305	MC3	C8-N-C6	3.37	117.84	108.98
4	B	1307	CPS	C1-C12-C13	3.33	114.89	110.48
4	A	1304	CPS	C2-C19-C18	3.32	115.54	111.84
4	B	1308	CPS	O4-C4-C3	-3.32	102.37	109.12
4	B	1307	CPS	O2S-S-O3S	3.31	119.69	111.40
4	B	1308	CPS	C8-C9-C5	3.31	106.75	103.54
4	B	1307	CPS	O3-C17-C18	3.28	117.05	109.52
4	A	1305	CPS	C23-C24-N1	3.28	122.32	116.34
2	D	1303	MC3	O31-C31-C32	-3.26	111.02	123.78
4	B	1308	CPS	C6-C18-C17	3.21	116.12	111.85
2	C	1301	MC3	O11-C11-C12	-3.19	111.29	123.78
2	C	1303	MC3	C8-N-C6	3.19	117.34	108.98
4	B	1308	CPS	O4-C4-C5	-3.18	105.65	111.02
4	D	1308	CPS	C10-C5-C4	-3.15	105.90	109.06
2	B	1302	MC3	C3-C2-C1	-3.13	103.63	112.65
4	B	1307	CPS	C14-C13-C12	3.13	114.44	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1304	MC3	C8-N-C6	3.11	117.14	108.98
2	B	1305	MC3	O11-C11-C12	-3.08	111.75	123.78
2	A	1303	MC3	O11-C11-C12	-3.05	111.86	123.78
4	A	1306	CPS	C15-C16-C17	3.04	118.01	114.40
4	B	1308	CPS	C11-C2-C15	-3.03	105.37	110.44
4	A	1306	CPS	C22-C20-C9	3.02	116.58	110.33
4	A	1306	CPS	C26-C27-N2	-3.00	109.24	115.35
2	C	1304	MC3	O11-C11-C12	-2.98	112.12	123.78
4	B	1307	CPS	O1-C24-N1	-2.98	117.18	123.03
2	B	1304	MC3	O31-C31-C32	-2.97	112.17	123.78
4	B	1307	CPS	O4-C4-C3	-2.92	103.17	109.12
4	B	1307	CPS	C26-C27-N2	-2.91	109.42	115.35
4	A	1305	CPS	C15-C14-C13	2.91	117.09	112.71
4	A	1304	CPS	C11-C2-C19	-2.90	107.27	111.18
4	B	1307	CPS	O1S-S-O3S	-2.89	104.44	113.82
2	B	1303	MC3	O31-C31-C32	-2.86	112.58	123.78
4	D	1308	CPS	O3-C17-C16	-2.85	102.76	109.86
4	B	1308	CPS	C14-C15-C2	2.85	115.70	112.66
4	A	1304	CPS	O3-C17-C18	2.84	116.03	109.52
2	C	1303	MC3	C2-O2-C31	-2.83	111.03	117.80
4	B	1308	CPS	C29-N2-C30	2.82	117.16	109.49
4	B	1307	CPS	C5-C9-C20	2.76	122.83	119.48
4	A	1305	CPS	O2S-S-O1S	-2.76	104.49	111.40
4	A	1306	CPS	C21-C20-C9	-2.73	108.78	112.88
4	A	1305	CPS	C29-N2-C28	2.73	120.35	108.91
4	B	1308	CPS	C2-C19-C18	2.71	114.86	111.84
4	A	1306	CPS	C19-C18-C6	2.70	113.53	109.75
4	A	1305	CPS	C10-C5-C4	-2.70	106.35	109.06
4	D	1308	CPS	C15-C14-C13	2.70	116.78	112.71
4	B	1307	CPS	C23-C24-N1	2.70	121.26	116.34
4	A	1305	CPS	C26-C27-N2	-2.68	109.89	115.35
4	A	1305	CPS	C28-N2-C30	-2.68	102.20	109.49
4	D	1308	CPS	C19-C18-C6	2.67	113.48	109.75
4	B	1308	CPS	C1-C12-C13	2.66	114.01	110.48
4	A	1306	CPS	O3-C17-C16	-2.64	103.29	109.86
4	A	1304	CPS	C31-C30-N2	-2.64	109.98	115.35
4	A	1305	CPS	O1-C24-C23	-2.62	117.27	122.02
4	D	1308	CPS	C5-C9-C20	2.62	122.66	119.48
2	D	1302	MC3	C3-C2-C1	-2.61	105.14	112.65
4	D	1308	CPS	O3-C17-C18	2.61	115.50	109.52
4	A	1304	CPS	C15-C14-C13	2.59	116.62	112.71
4	A	1305	CPS	O2-C13-C12	-2.59	103.40	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1305	MC3	C2-O2-C31	-2.55	111.69	117.80
4	A	1305	CPS	C19-C18-C17	2.55	115.07	111.86
4	B	1307	CPS	C15-C16-C17	2.55	117.43	114.40
4	A	1304	CPS	C5-C9-C20	2.54	122.57	119.48
4	A	1304	CPS	C30-C31-C32	2.54	116.41	109.43
4	A	1306	CPS	C23-C22-C20	2.51	119.16	114.46
4	B	1307	CPS	C29-N2-C28	2.51	119.44	108.91
4	A	1306	CPS	O3-C17-C18	2.45	115.14	109.52
4	A	1305	CPS	C19-C18-C6	2.45	113.16	109.75
4	A	1304	CPS	C8-C9-C5	-2.42	101.19	103.54
4	A	1304	CPS	C15-C16-C17	2.40	117.26	114.40
4	A	1305	CPS	C26-C25-N1	2.38	118.87	112.20
4	B	1307	CPS	C10-C5-C4	-2.37	106.69	109.06
4	D	1308	CPS	C29-N2-C28	2.35	118.76	108.91
4	A	1304	CPS	C16-C15-C14	-2.35	108.54	111.23
4	B	1308	CPS	O2-C13-C14	2.35	114.51	109.84
4	B	1307	CPS	C11-C2-C19	-2.31	108.07	111.18
4	B	1308	CPS	C29-N2-C28	2.28	118.48	108.91
4	B	1307	CPS	C22-C23-C24	2.28	118.15	113.06
4	B	1307	CPS	C28-N2-C30	-2.27	103.31	109.49
4	B	1307	CPS	C7-C6-C18	2.27	121.47	118.36
2	D	1304	MC3	C3-C2-C1	-2.26	106.51	111.78
4	A	1306	CPS	C22-C23-C24	2.26	118.10	113.06
4	B	1308	CPS	C7-C6-C18	2.24	121.44	118.36
4	A	1304	CPS	C7-C6-C5	2.23	105.70	103.54
4	A	1306	CPS	O4-C4-C5	-2.22	107.27	111.02
4	A	1305	CPS	C16-C15-C14	-2.20	108.71	111.23
4	A	1306	CPS	C9-C5-C6	2.19	102.31	100.11
4	A	1305	CPS	C15-C16-C17	2.19	117.00	114.40
2	B	1304	MC3	C2-O2-C31	-2.17	112.59	117.80
2	B	1302	MC3	O3-C3-C2	2.17	116.06	105.85
4	A	1305	CPS	C3-C19-C2	-2.17	111.50	113.70
4	A	1306	CPS	C7-C6-C18	2.15	121.31	118.36
4	B	1307	CPS	C27-C26-C25	2.12	115.10	110.95
4	B	1308	CPS	C10-C5-C9	-2.12	107.88	111.20
2	C	1307	MC3	C2-O2-C31	-2.11	112.75	117.80
2	C	1303	MC3	C4-C5-N	-2.10	109.08	115.82
4	A	1305	CPS	C21-C20-C9	2.09	116.02	112.88
4	A	1304	CPS	O2S-S-C32	2.04	110.00	106.00
4	B	1307	CPS	C5-C6-C18	2.04	117.31	114.72
2	A	1303	MC3	C3-C2-C1	-2.04	107.04	111.78
4	A	1304	CPS	C11-C2-C15	-2.03	107.04	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1302	MC3	O3-C3-C2	2.03	114.24	108.40
2	D	1306	MC3	O3-C11-C12	-2.01	105.71	111.83
4	A	1304	CPS	C28-N2-C27	-2.01	104.03	109.49

There are no chirality outliers.

All (374) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	MC3	O2-C2-C3-O3
2	A	1301	MC3	C1-O3P-P-O1P
2	A	1301	MC3	C1-O3P-P-O4P
2	A	1303	MC3	O3P-C1-C2-O2
2	A	1303	MC3	O4P-C4-C5-N
2	A	1303	MC3	C4-O4P-P-O3P
2	B	1302	MC3	C1-C2-C3-O3
2	B	1302	MC3	O2-C2-C3-O3
2	B	1303	MC3	O2-C2-C3-O3
2	B	1304	MC3	O2-C2-C3-O3
2	B	1304	MC3	C32-C31-O2-C2
2	B	1304	MC3	O31-C31-O2-C2
2	B	1304	MC3	C1-O3P-P-O2P
2	B	1304	MC3	C1-O3P-P-O4P
2	B	1305	MC3	O4P-C4-C5-N
2	B	1305	MC3	C5-C4-O4P-P
2	B	1305	MC3	O31-C31-O2-C2
2	B	1305	MC3	C1-O3P-P-O1P
2	B	1305	MC3	C1-O3P-P-O2P
2	B	1305	MC3	C1-O3P-P-O4P
2	B	1305	MC3	C4-O4P-P-O2P
2	B	1305	MC3	C4-O4P-P-O3P
2	C	1301	MC3	C1-O3P-P-O1P
2	C	1301	MC3	C1-O3P-P-O4P
2	C	1301	MC3	C4-O4P-P-O2P
2	C	1303	MC3	C4-O4P-P-O2P
2	C	1303	MC3	C4-O4P-P-O3P
2	C	1304	MC3	O31-C31-O2-C2
2	C	1304	MC3	C1-O3P-P-O1P
2	C	1304	MC3	C1-O3P-P-O2P
2	C	1304	MC3	C1-O3P-P-O4P
2	C	1304	MC3	C4-O4P-P-O1P
2	C	1304	MC3	C4-O4P-P-O2P
2	C	1304	MC3	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	C	1307	MC3	C1-O3P-P-O1P
2	C	1307	MC3	C1-O3P-P-O2P
2	C	1307	MC3	C4-O4P-P-O1P
2	C	1307	MC3	C4-O4P-P-O2P
2	D	1302	MC3	C1-C2-C3-O3
2	D	1302	MC3	O2-C2-C3-O3
2	D	1302	MC3	C1-O3P-P-O1P
2	D	1302	MC3	C1-O3P-P-O4P
2	D	1304	MC3	C32-C31-O2-C2
2	D	1304	MC3	O31-C31-O2-C2
2	D	1304	MC3	C1-O3P-P-O1P
2	D	1304	MC3	C1-O3P-P-O2P
2	D	1304	MC3	C1-O3P-P-O4P
2	D	1305	MC3	C32-C31-O2-C2
2	D	1305	MC3	O31-C31-O2-C2
2	D	1305	MC3	C4-O4P-P-O3P
4	A	1304	CPS	C20-C22-C23-C24
4	A	1304	CPS	C30-C31-C32-S
4	A	1306	CPS	C20-C22-C23-C24
4	A	1306	CPS	N2-C30-C31-C32
4	B	1307	CPS	C30-C31-C32-S
4	B	1308	CPS	C21-C20-C9-C5
4	B	1308	CPS	C22-C20-C9-C8
4	B	1308	CPS	N2-C30-C31-C32
4	D	1308	CPS	C25-C26-C27-N2
4	D	1308	CPS	C30-C31-C32-S
2	A	1301	MC3	O11-C11-O3-C3
2	B	1302	MC3	O11-C11-O3-C3
2	C	1301	MC3	O11-C11-O3-C3
4	A	1306	CPS	C26-C25-N1-C24
2	C	1303	MC3	O31-C31-O2-C2
2	D	1303	MC3	O31-C31-O2-C2
4	B	1308	CPS	C21-C20-C22-C23
4	B	1308	CPS	C21-C20-C9-C8
4	B	1308	CPS	C22-C20-C9-C5
4	B	1307	CPS	C23-C24-N1-C25
4	A	1304	CPS	C26-C27-N2-C29
4	A	1306	CPS	C31-C30-N2-C28
4	A	1306	CPS	C31-C30-N2-C29
4	B	1308	CPS	C26-C27-N2-C28
4	B	1308	CPS	C31-C30-N2-C28
4	D	1308	CPS	C26-C27-N2-C29

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Mol	Chain	Res	Type	Atoms
4	D	1308	CPS	C31-C30-N2-C29
2	B	1304	MC3	O11-C11-O3-C3
2	C	1302	MC3	O11-C11-O3-C3
2	D	1304	MC3	O11-C11-O3-C3
2	C	1302	MC3	O31-C31-O2-C2
2	D	1306	MC3	O31-C31-O2-C2
4	D	1308	CPS	C20-C22-C23-C24
2	C	1304	MC3	C12-C11-O3-C3
4	B	1308	CPS	C26-C25-N1-C24
2	C	1307	MC3	C31-C32-C33-C34
4	B	1308	CPS	C9-C20-C22-C23
2	D	1303	MC3	O11-C11-O3-C3
2	D	1305	MC3	O11-C11-O3-C3
2	D	1302	MC3	C12-C11-O3-C3
4	B	1307	CPS	O1-C24-N1-C25
4	A	1304	CPS	C26-C27-N2-C28
4	B	1308	CPS	C26-C27-N2-C29
4	D	1308	CPS	C26-C27-N2-C28
4	D	1308	CPS	C31-C30-N2-C28
4	A	1304	CPS	C31-C32-S-O2S
4	A	1304	CPS	C26-C27-N2-C30
4	A	1304	CPS	C31-C30-N2-C27
4	A	1306	CPS	C31-C30-N2-C27
4	D	1308	CPS	C31-C30-N2-C27
2	C	1301	MC3	C12-C11-O3-C3
2	B	1304	MC3	C4-C5-N-C6
2	B	1305	MC3	C4-C5-N-C7
2	D	1305	MC3	C4-C5-N-C7
2	C	1303	MC3	O11-C11-O3-C3
4	A	1306	CPS	N1-C25-C26-C27
4	B	1307	CPS	C22-C20-C9-C5
2	C	1303	MC3	C35-C36-C37-C38
2	B	1305	MC3	C4-C5-N-C6
2	D	1305	MC3	C4-C5-N-C6
2	A	1303	MC3	C31-C32-C33-C34
2	C	1303	MC3	C11-C12-C13-C14
4	A	1306	CPS	C22-C20-C9-C5
4	D	1308	CPS	C22-C20-C9-C5
2	C	1307	MC3	C11-C12-C13-C14
2	D	1305	MC3	C11-C12-C13-C14
2	C	1307	MC3	O11-C11-O3-C3
2	D	1306	MC3	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
4	B	1307	CPS	C21-C20-C9-C8
4	B	1307	CPS	C21-C20-C9-C5
4	B	1308	CPS	C22-C23-C24-O1
2	A	1303	MC3	O11-C11-O3-C3
4	B	1307	CPS	C31-C32-S-O2S
4	D	1308	CPS	C31-C32-S-O2S
4	A	1306	CPS	C21-C20-C9-C5
4	B	1308	CPS	C26-C27-N2-C30
2	B	1305	MC3	C32-C33-C34-C35
2	C	1303	MC3	C31-C32-C33-C34
2	A	1303	MC3	O31-C31-O2-C2
2	B	1303	MC3	O31-C31-O2-C2
2	C	1307	MC3	O31-C31-O2-C2
4	B	1308	CPS	C22-C23-C24-N1
2	A	1303	MC3	C4-C5-N-C7
2	B	1305	MC3	C4-C5-N-C8
2	D	1305	MC3	C4-C5-N-C8
4	A	1305	CPS	C21-C20-C22-C23
4	A	1306	CPS	C21-C20-C9-C8
4	D	1308	CPS	C21-C20-C9-C8
4	D	1308	CPS	C21-C20-C9-C5
2	B	1302	MC3	C11-C12-C13-C14
2	B	1302	MC3	C4-O4P-P-O1P
2	B	1303	MC3	O11-C11-O3-C3
2	B	1305	MC3	C32-C31-O2-C2
2	A	1303	MC3	C4-C5-N-C6
2	D	1306	MC3	C34-C35-C36-C37
2	B	1304	MC3	C17-C18-C19-C20
2	D	1304	MC3	C36-C37-C38-C39
2	C	1307	MC3	C16-C17-C18-C19
2	C	1304	MC3	C20-C21-C22-C23
2	A	1303	MC3	C35-C36-C37-C38
4	A	1304	CPS	C31-C30-N2-C28
4	A	1304	CPS	C31-C30-N2-C29
4	A	1306	CPS	C31-C32-S-O2S
2	C	1301	MC3	C14-C15-C16-C17
2	A	1301	MC3	C11-C12-C13-C14
2	D	1302	MC3	C11-C12-C13-C14
2	B	1304	MC3	C33-C34-C35-C36
2	C	1307	MC3	C20-C21-C22-C23
2	D	1305	MC3	C37-C38-C39-C40
2	D	1305	MC3	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	D	1307	MC3	C12-C13-C14-C15
2	A	1303	MC3	C4-C5-N-C8
2	B	1303	MC3	C17-C18-C19-C20
2	B	1302	MC3	C12-C11-O3-C3
2	A	1303	MC3	C18-C19-C20-C21
2	A	1303	MC3	C37-C38-C39-C40
2	B	1303	MC3	C15-C16-C17-C18
2	C	1307	MC3	C38-C39-C40-C41
2	D	1306	MC3	O11-C11-O3-C3
2	D	1304	MC3	C32-C33-C34-C35
2	D	1303	MC3	C38-C39-C40-C41
2	D	1306	MC3	C16-C17-C18-C19
2	B	1303	MC3	C20-C21-C22-C23
2	B	1305	MC3	C16-C17-C18-C19
4	B	1307	CPS	N1-C25-C26-C27
2	B	1304	MC3	C4-C5-N-C7
2	D	1303	MC3	C17-C18-C19-C20
2	C	1303	MC3	C32-C31-O2-C2
2	D	1305	MC3	C15-C16-C17-C18
2	D	1305	MC3	C16-C17-C18-C19
4	D	1308	CPS	C26-C27-N2-C30
2	D	1303	MC3	C33-C34-C35-C36
2	C	1305	MC3	C32-C33-C34-C35
2	B	1305	MC3	C14-C15-C16-C17
2	C	1302	MC3	C15-C16-C17-C18
2	C	1302	MC3	C33-C34-C35-C36
2	D	1306	MC3	C33-C34-C35-C36
2	C	1301	MC3	C13-C14-C15-C16
2	D	1306	MC3	C31-C32-C33-C34
2	C	1307	MC3	C13-C14-C15-C16
2	C	1303	MC3	C12-C13-C14-C15
2	A	1301	MC3	C12-C11-O3-C3
4	A	1305	CPS	C30-C31-C32-S
2	B	1303	MC3	C1-C2-C3-O3
2	C	1307	MC3	C1-C2-C3-O3
2	D	1305	MC3	C1-C2-C3-O3
2	B	1305	MC3	C33-C34-C35-C36
2	D	1305	MC3	C32-C33-C34-C35
2	B	1305	MC3	C39-C40-C41-C42
2	B	1304	MC3	C4-C5-N-C8
2	B	1303	MC3	C34-C35-C36-C37
4	A	1306	CPS	C22-C20-C9-C8

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Mol	Chain	Res	Type	Atoms
2	B	1303	MC3	C14-C15-C16-C17
2	D	1304	MC3	C17-C18-C19-C20
2	B	1304	MC3	C16-C17-C18-C19
2	D	1302	MC3	C15-C16-C17-C18
4	A	1304	CPS	C31-C32-S-O3S
4	A	1304	CPS	C31-C32-S-O1S
4	B	1307	CPS	C31-C32-S-O3S
4	B	1307	CPS	C31-C32-S-O1S
4	B	1308	CPS	C31-C32-S-O3S
2	B	1302	MC3	C15-C16-C17-C18
2	D	1305	MC3	C34-C35-C36-C37
2	C	1301	MC3	C15-C16-C17-C18
2	C	1304	MC3	C21-C22-C23-C24
4	D	1308	CPS	C22-C20-C9-C8
2	C	1305	MC3	C31-C32-C33-C34
2	B	1303	MC3	C39-C40-C41-C42
2	B	1303	MC3	C35-C36-C37-C38
2	C	1303	MC3	C37-C38-C39-C40
2	B	1305	MC3	C35-C36-C37-C38
2	D	1307	MC3	C15-C16-C17-C18
2	C	1304	MC3	C15-C16-C17-C18
2	B	1306	MC3	C15-C16-C17-C18
2	C	1302	MC3	C37-C38-C39-C40
2	A	1301	MC3	C16-C17-C18-C19
2	D	1303	MC3	C13-C14-C15-C16
2	C	1304	MC3	C41-C42-C43-C44
2	A	1303	MC3	C17-C18-C19-C20
2	A	1303	MC3	C2-C1-O3P-P
2	C	1305	MC3	C33-C34-C35-C36
2	D	1303	MC3	C16-C17-C18-C19
2	C	1302	MC3	C39-C40-C41-C42
2	D	1302	MC3	C13-C14-C15-C16
2	D	1304	MC3	C21-C22-C23-C24
4	A	1304	CPS	C25-C26-C27-N2
2	C	1302	MC3	C12-C11-O3-C3
2	A	1303	MC3	C20-C21-C22-C23
2	D	1303	MC3	C37-C38-C39-C40
2	D	1306	MC3	C20-C21-C22-C23
2	D	1304	MC3	C37-C38-C39-C40
2	D	1303	MC3	C18-C19-C20-C21
2	A	1303	MC3	C38-C39-C40-C41
2	D	1303	MC3	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1302	MC3	C16-C17-C18-C19
2	C	1307	MC3	C37-C38-C39-C40
2	C	1305	MC3	C36-C37-C38-C39
2	B	1303	MC3	C19-C20-C21-C22
2	B	1303	MC3	C38-C39-C40-C41
2	C	1302	MC3	O2-C2-C3-O3
2	A	1303	MC3	C40-C41-C42-C43
2	B	1303	MC3	C33-C34-C35-C36
2	A	1301	MC3	C1-C2-C3-O3
2	C	1302	MC3	C31-C32-C33-C34
2	C	1307	MC3	C36-C37-C38-C39
2	C	1303	MC3	C18-C19-C20-C21
2	D	1304	MC3	C19-C20-C21-C22
2	B	1305	MC3	O11-C11-O3-C3
2	D	1303	MC3	C4-O4P-P-O1P
2	A	1303	MC3	C3-C2-O2-C31
2	C	1302	MC3	C19-C20-C21-C22
4	B	1307	CPS	C22-C20-C9-C8
2	B	1303	MC3	C21-C22-C23-C24
2	B	1304	MC3	C1-C2-C3-O3
2	B	1305	MC3	C38-C39-C40-C41
2	C	1307	MC3	O2-C2-C3-O3
2	D	1305	MC3	O2-C2-C3-O3
2	D	1304	MC3	C12-C13-C14-C15
2	D	1304	MC3	C38-C39-C40-C41
2	B	1303	MC3	C13-C14-C15-C16
2	B	1305	MC3	C36-C37-C38-C39
2	A	1303	MC3	O3P-C1-C2-C3
2	C	1307	MC3	C32-C33-C34-C35
2	D	1304	MC3	C12-C11-O3-C3
2	D	1303	MC3	C40-C41-C42-C43
4	B	1308	CPS	C31-C30-N2-C27
4	A	1306	CPS	C22-C23-C24-O1
2	A	1301	MC3	C1-O3P-P-O2P
2	A	1303	MC3	C4-O4P-P-O1P
2	B	1302	MC3	C1-O3P-P-O1P
2	B	1303	MC3	C1-O3P-P-O1P
2	B	1303	MC3	C1-O3P-P-O2P
2	B	1303	MC3	C1-O3P-P-O4P
2	B	1304	MC3	C1-O3P-P-O1P
2	B	1304	MC3	C4-O4P-P-O1P
2	B	1304	MC3	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	B	1304	MC3	C4-O4P-P-O3P
2	C	1302	MC3	C1-O3P-P-O1P
2	C	1302	MC3	C1-O3P-P-O2P
2	C	1302	MC3	C1-O3P-P-O4P
2	C	1303	MC3	C4-O4P-P-O1P
2	C	1307	MC3	C1-O3P-P-O4P
2	D	1305	MC3	C4-O4P-P-O1P
2	C	1302	MC3	C17-C18-C19-C20
4	B	1308	CPS	C31-C30-N2-C29
4	A	1304	CPS	C22-C20-C9-C5
2	B	1304	MC3	C12-C13-C14-C15
2	D	1303	MC3	C3-C2-O2-C31
2	C	1304	MC3	C36-C37-C38-C39
2	B	1303	MC3	C31-C32-C33-C34
2	D	1303	MC3	O3P-C1-C2-C3
2	D	1306	MC3	O3P-C1-C2-O2
2	D	1306	MC3	C13-C14-C15-C16
2	D	1306	MC3	C14-C15-C16-C17
2	C	1303	MC3	O2-C2-C3-O3
2	B	1305	MC3	O3-C11-C12-C13
2	C	1307	MC3	C21-C22-C23-C24
2	B	1302	MC3	C4-O4P-P-O2P
2	C	1302	MC3	C38-C39-C40-C41
2	C	1302	MC3	C1-C2-C3-O3
2	D	1306	MC3	C32-C33-C34-C35
2	C	1304	MC3	C16-C17-C18-C19
2	B	1304	MC3	C12-C11-O3-C3
4	B	1308	CPS	N1-C25-C26-C27
2	B	1305	MC3	C12-C11-O3-C3
2	D	1305	MC3	C17-C18-C19-C20
2	C	1304	MC3	O2-C2-C3-O3
2	B	1305	MC3	C17-C18-C19-C20
2	C	1302	MC3	C40-C41-C42-C43
2	D	1304	MC3	C4-C5-N-C6
2	C	1303	MC3	C38-C39-C40-C41
4	A	1306	CPS	C22-C23-C24-N1
2	D	1303	MC3	C20-C21-C22-C23
2	A	1303	MC3	C12-C13-C14-C15
2	D	1306	MC3	C4-C5-N-C6
2	C	1304	MC3	O11-C11-C12-C13
2	D	1302	MC3	C14-C15-C16-C17
4	A	1304	CPS	C21-C20-C9-C5

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Mol	Chain	Res	Type	Atoms
2	D	1304	MC3	O2-C2-C3-O3
2	B	1303	MC3	C12-C13-C14-C15
2	B	1305	MC3	C34-C35-C36-C37
2	D	1303	MC3	C15-C16-C17-C18
2	B	1304	MC3	C14-C15-C16-C17
2	D	1305	MC3	C19-C20-C21-C22
2	D	1306	MC3	C2-C1-O3P-P
2	C	1303	MC3	C1-C2-C3-O3
2	C	1304	MC3	C1-C2-C3-O3
2	D	1304	MC3	C1-C2-C3-O3
2	B	1304	MC3	C32-C33-C34-C35
2	D	1306	MC3	O3-C11-C12-C13
2	B	1305	MC3	C18-C19-C20-C21
2	D	1306	MC3	O3P-C1-C2-C3
2	C	1306	MC3	C32-C33-C34-C35
2	C	1304	MC3	C40-C41-C42-C43
2	C	1307	MC3	C18-C19-C20-C21
2	D	1306	MC3	C21-C22-C23-C24
2	B	1304	MC3	C35-C36-C37-C38
4	D	1308	CPS	N1-C25-C26-C27
2	C	1307	MC3	C4-O4P-P-O3P
2	C	1304	MC3	C37-C38-C39-C40
2	D	1305	MC3	C13-C14-C15-C16
2	B	1303	MC3	O2-C31-C32-C33
2	C	1303	MC3	C34-C35-C36-C37
2	B	1305	MC3	O2-C31-C32-C33
2	D	1307	MC3	C11-C12-C13-C14
2	C	1307	MC3	C35-C36-C37-C38
2	D	1303	MC3	C35-C36-C37-C38
2	B	1305	MC3	C15-C16-C17-C18
2	A	1301	MC3	C14-C15-C16-C17
2	D	1306	MC3	C4-C5-N-C7
4	D	1308	CPS	C22-C23-C24-O1
2	B	1303	MC3	C41-C42-C43-C44
2	C	1303	MC3	C33-C34-C35-C36
2	C	1304	MC3	C35-C36-C37-C38
2	A	1303	MC3	O3-C11-C12-C13
2	C	1302	MC3	O31-C31-C32-C33
2	C	1307	MC3	O31-C31-C32-C33
2	C	1303	MC3	O11-C11-C12-C13
2	D	1302	MC3	O11-C11-C12-C13
2	D	1303	MC3	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
2	D	1304	MC3	C34-C35-C36-C37
2	C	1304	MC3	O31-C31-C32-C33
2	C	1307	MC3	C39-C40-C41-C42
2	D	1306	MC3	C15-C16-C17-C18

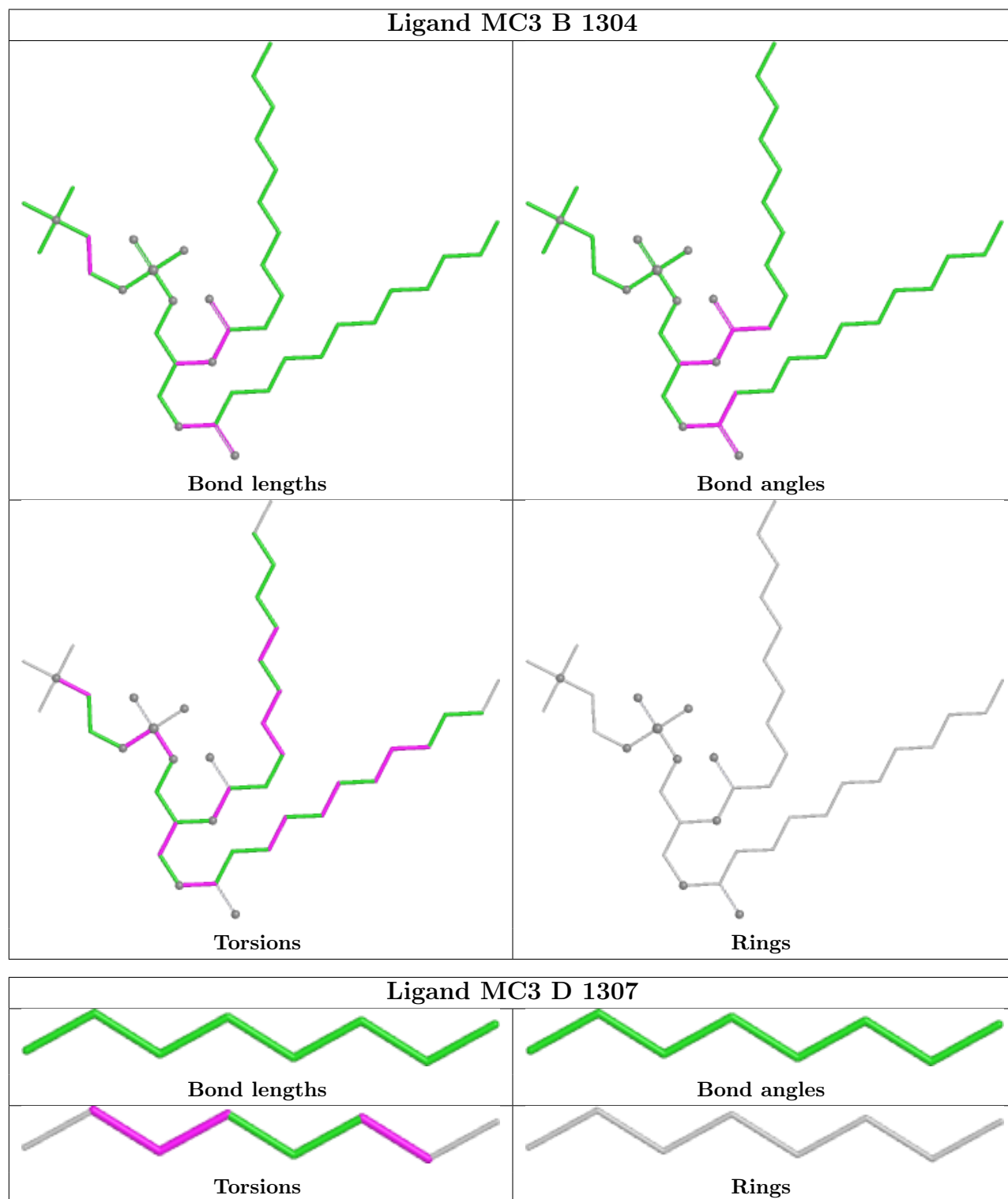
There are no ring outliers.

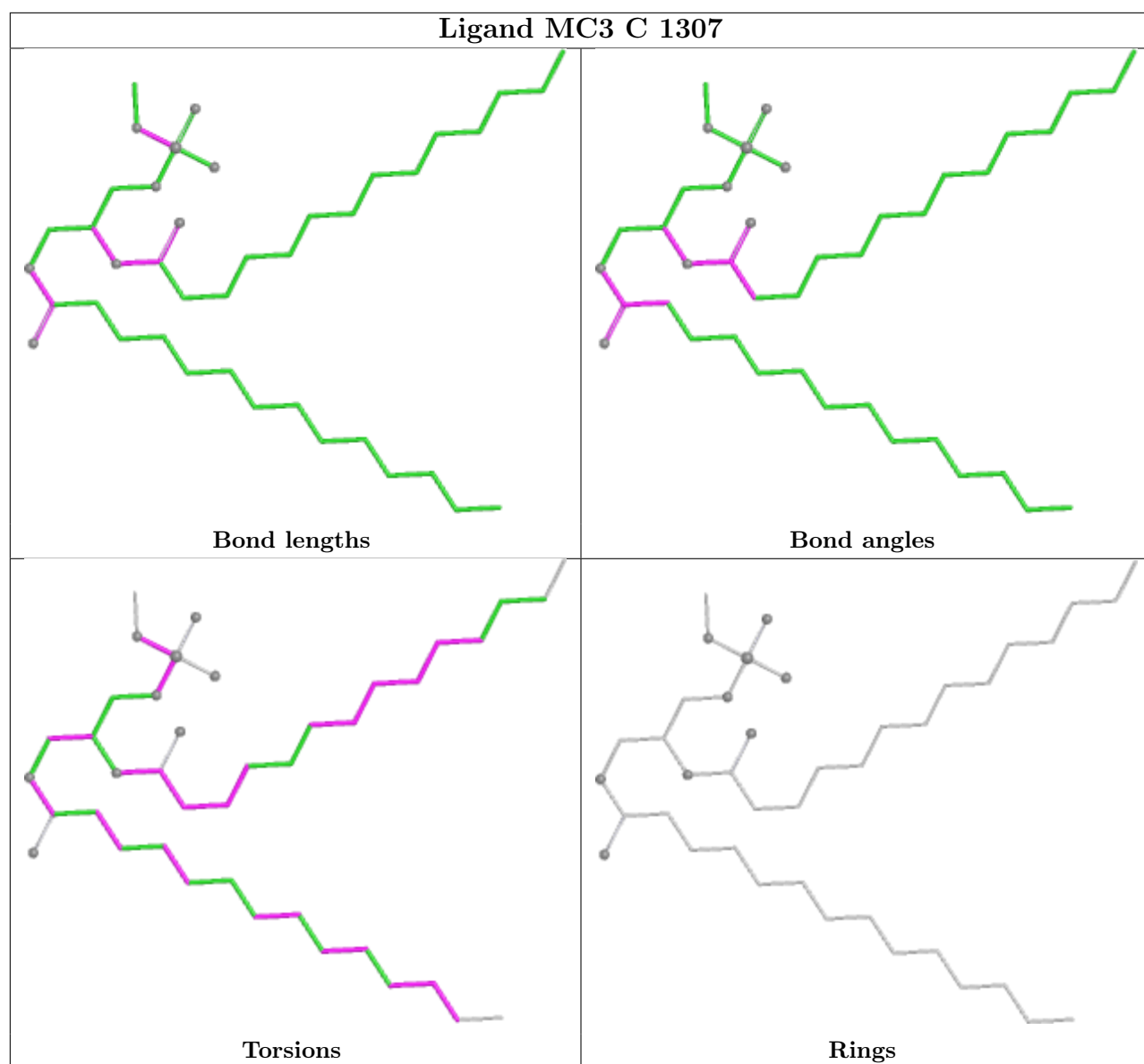
24 monomers are involved in 172 short contacts:

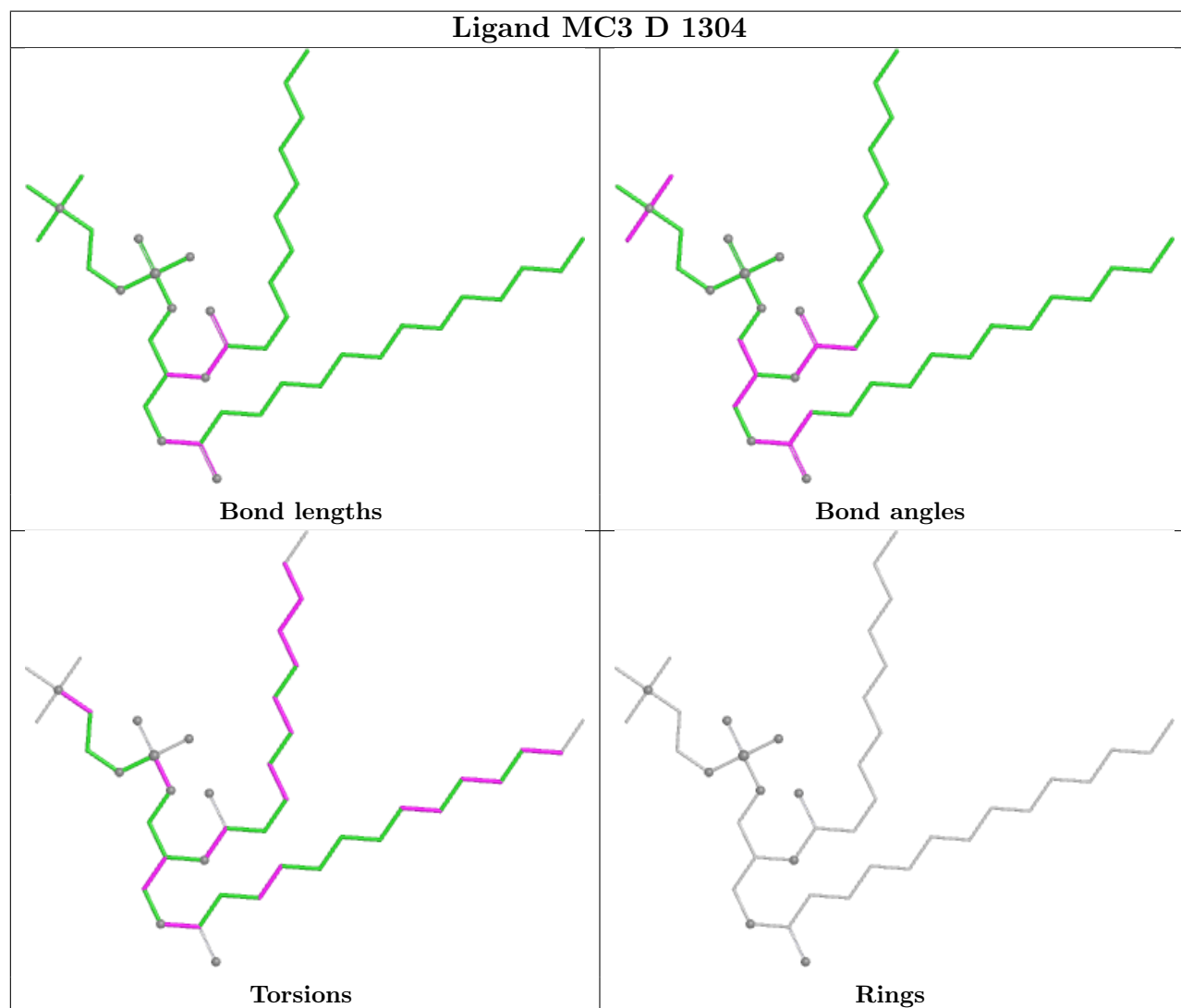
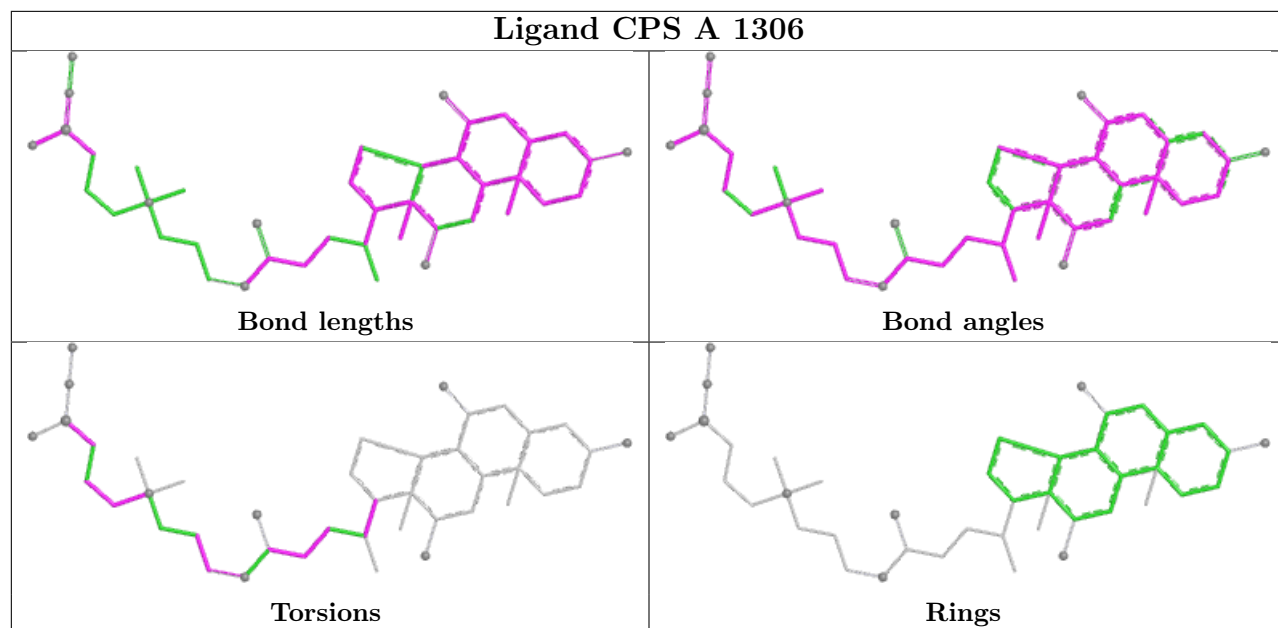
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1304	MC3	6	0
2	C	1307	MC3	4	0
4	A	1306	CPS	16	0
2	D	1304	MC3	2	0
2	B	1306	MC3	1	0
2	D	1306	MC3	3	0
2	C	1304	MC3	3	0
2	C	1306	MC3	1	0
4	A	1304	CPS	26	0
2	B	1305	MC3	2	0
4	B	1308	CPS	25	0
4	D	1308	CPS	22	0
2	C	1302	MC3	5	0
2	C	1303	MC3	7	0
2	D	1303	MC3	2	0
2	D	1305	MC3	1	0
2	C	1305	MC3	3	0
4	B	1307	CPS	13	0
2	A	1301	MC3	1	0
2	A	1303	MC3	3	0
2	D	1302	MC3	1	0
2	B	1302	MC3	2	0
2	B	1303	MC3	1	0
4	A	1305	CPS	25	0

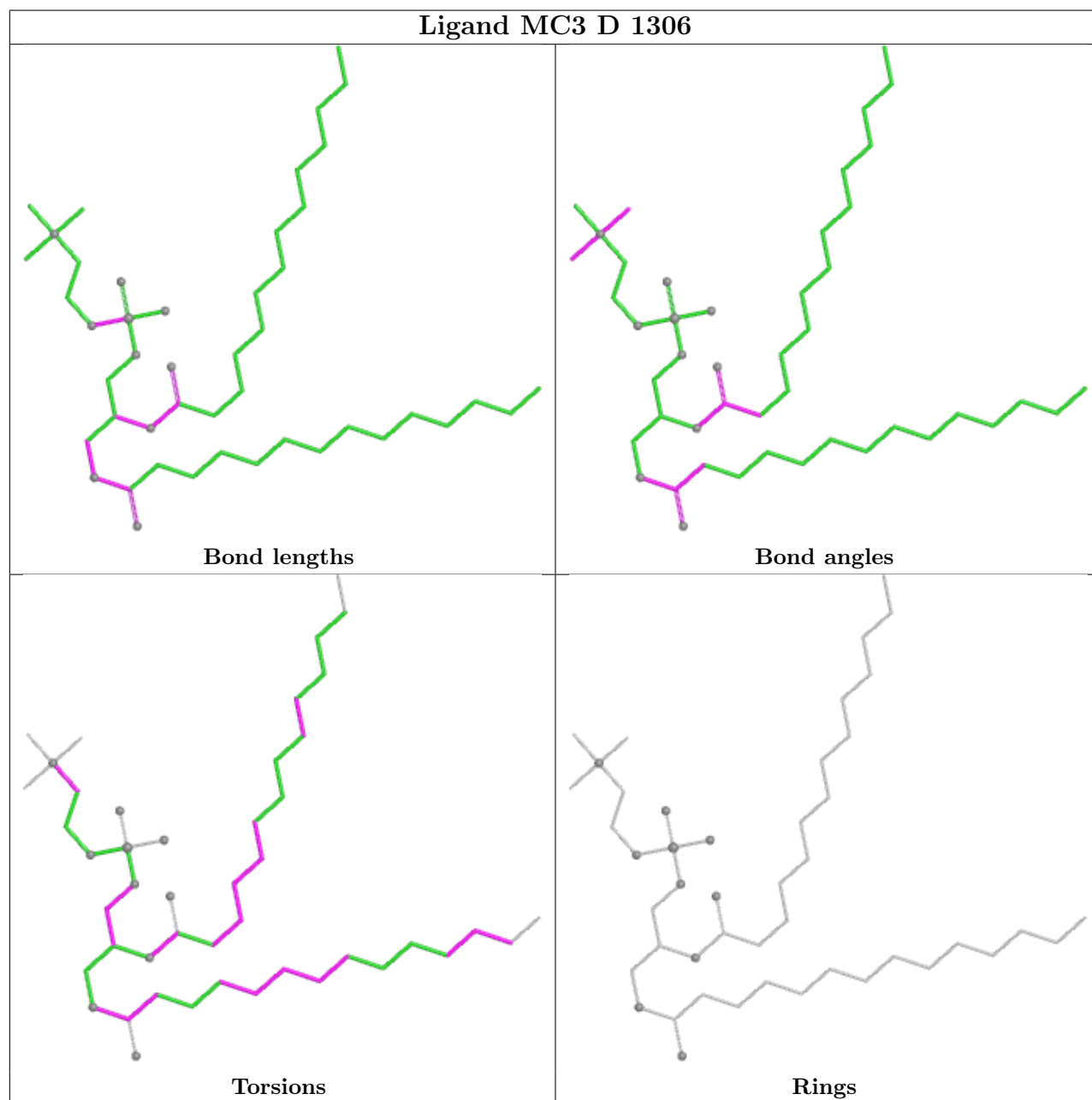
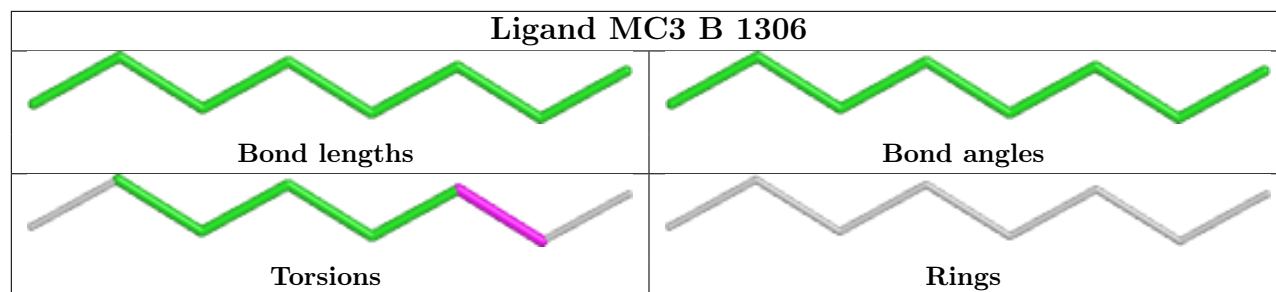
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

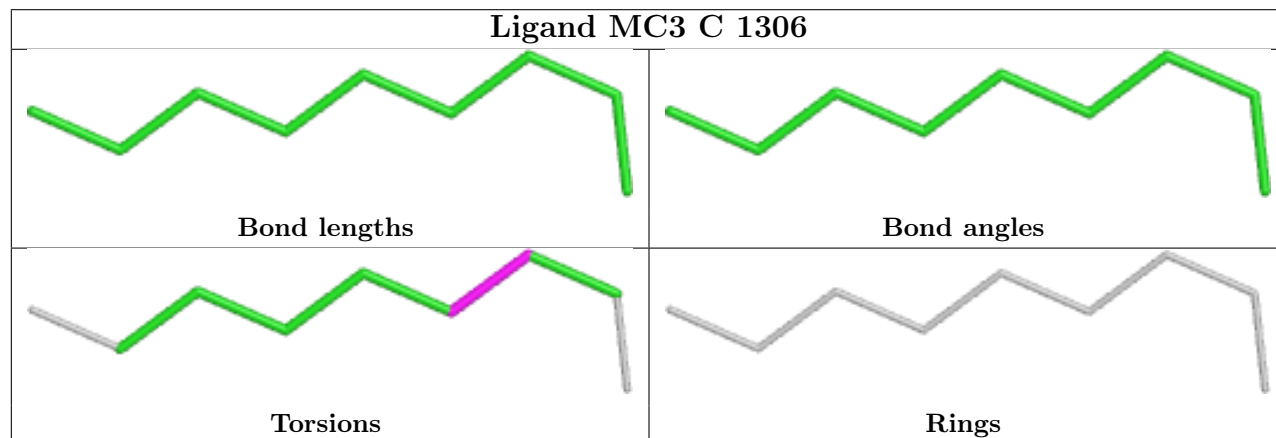
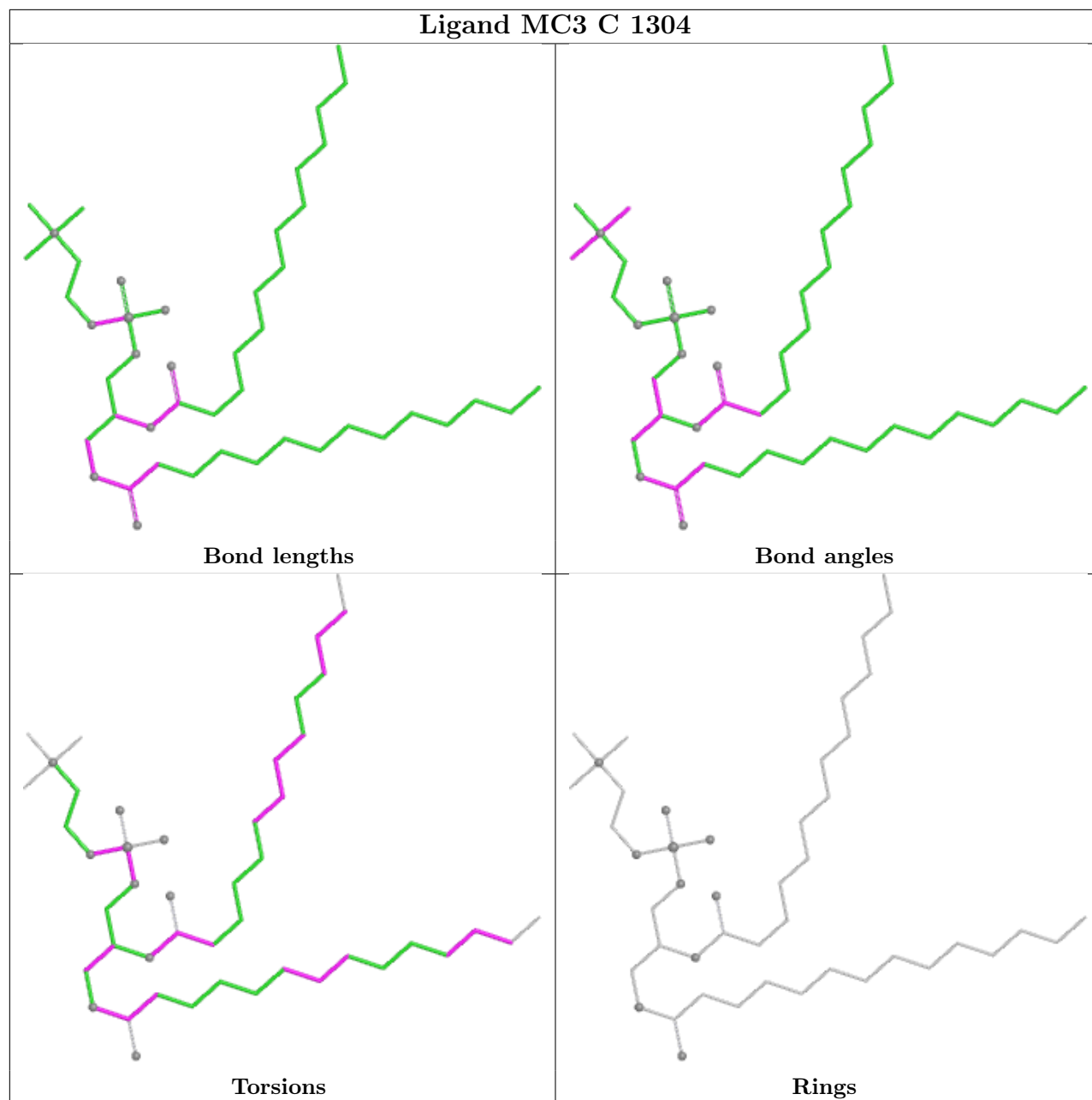
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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



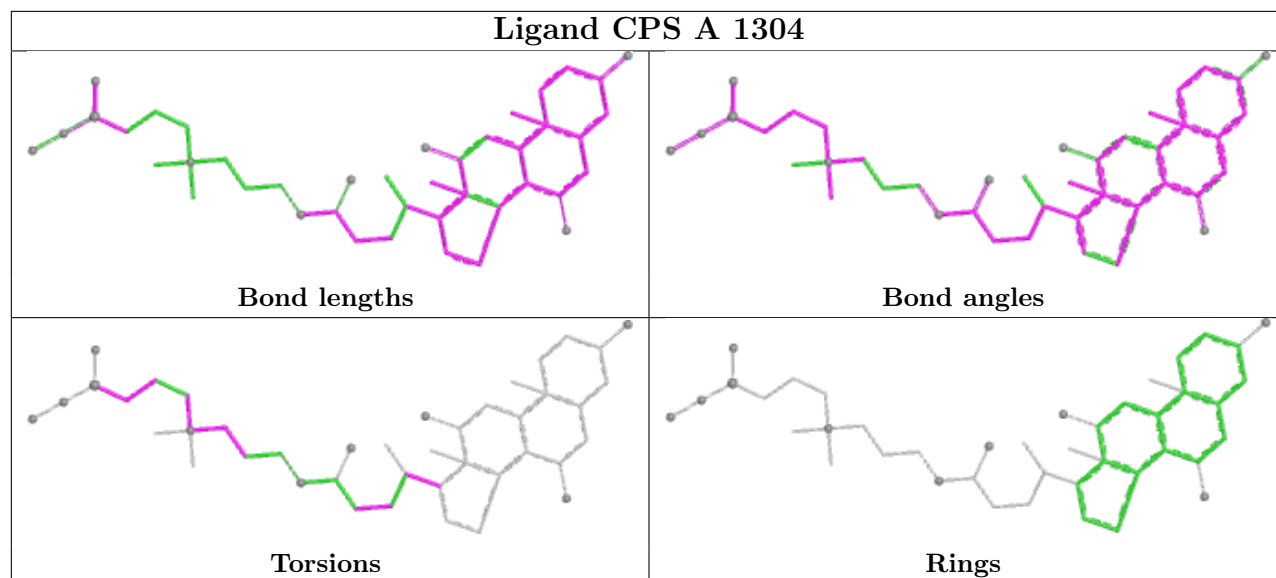




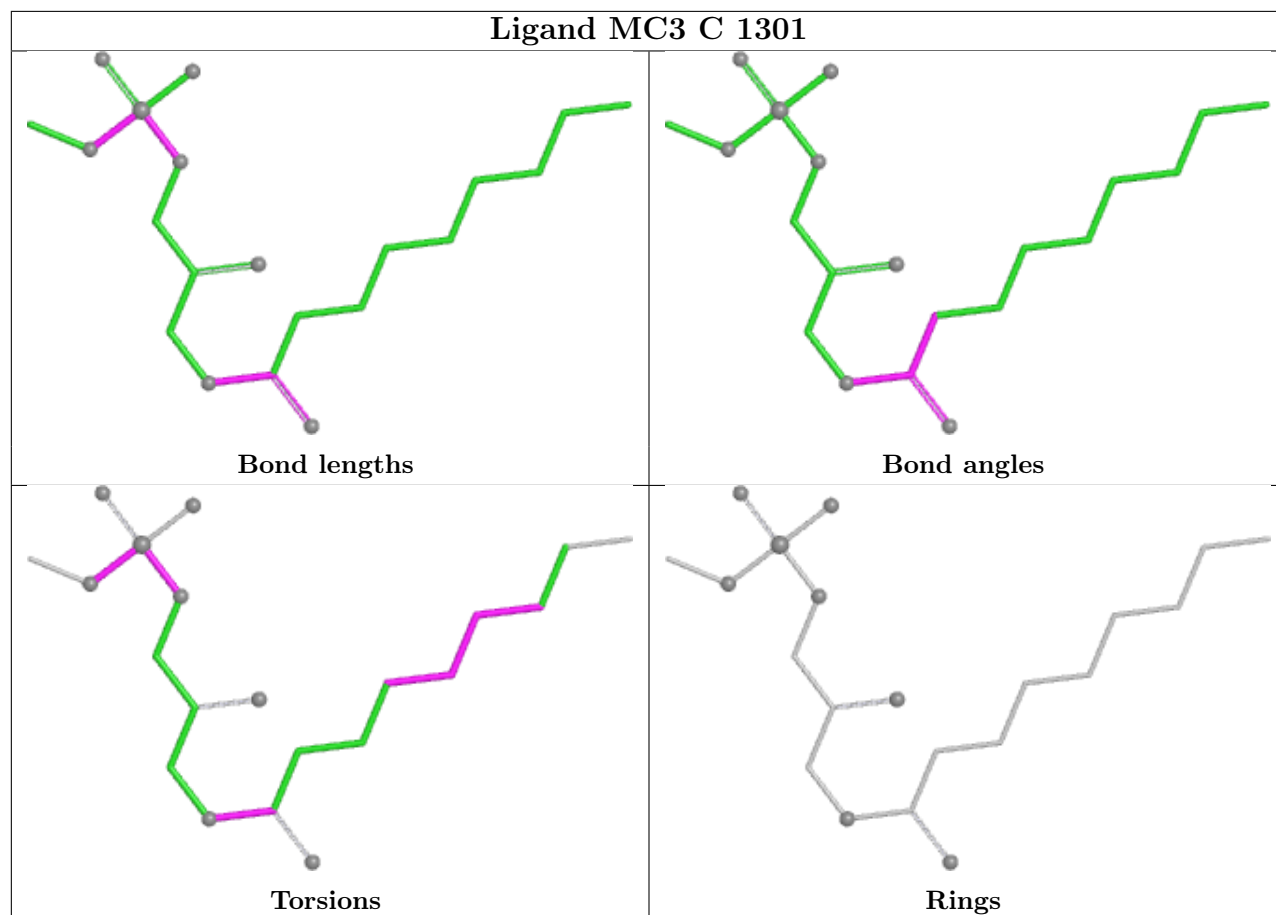


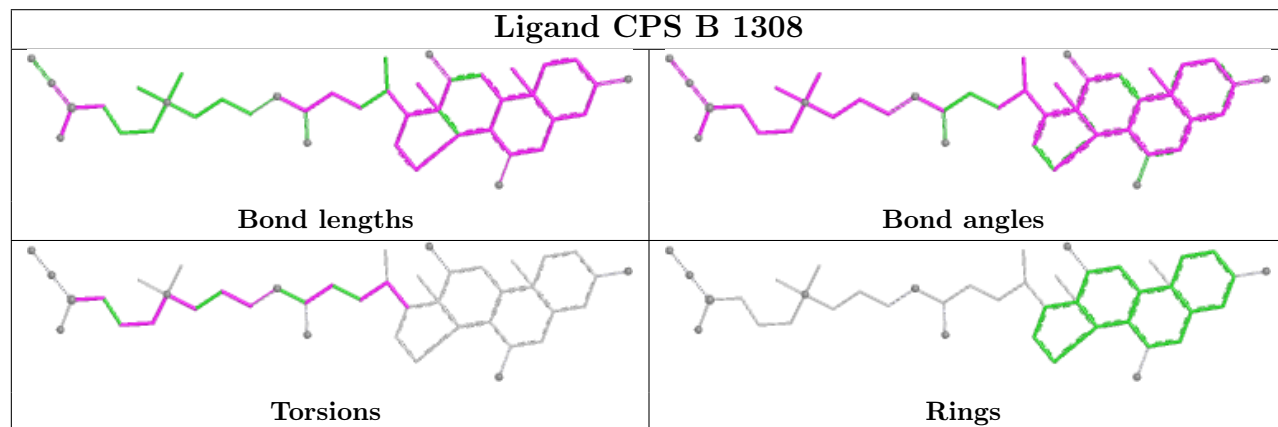
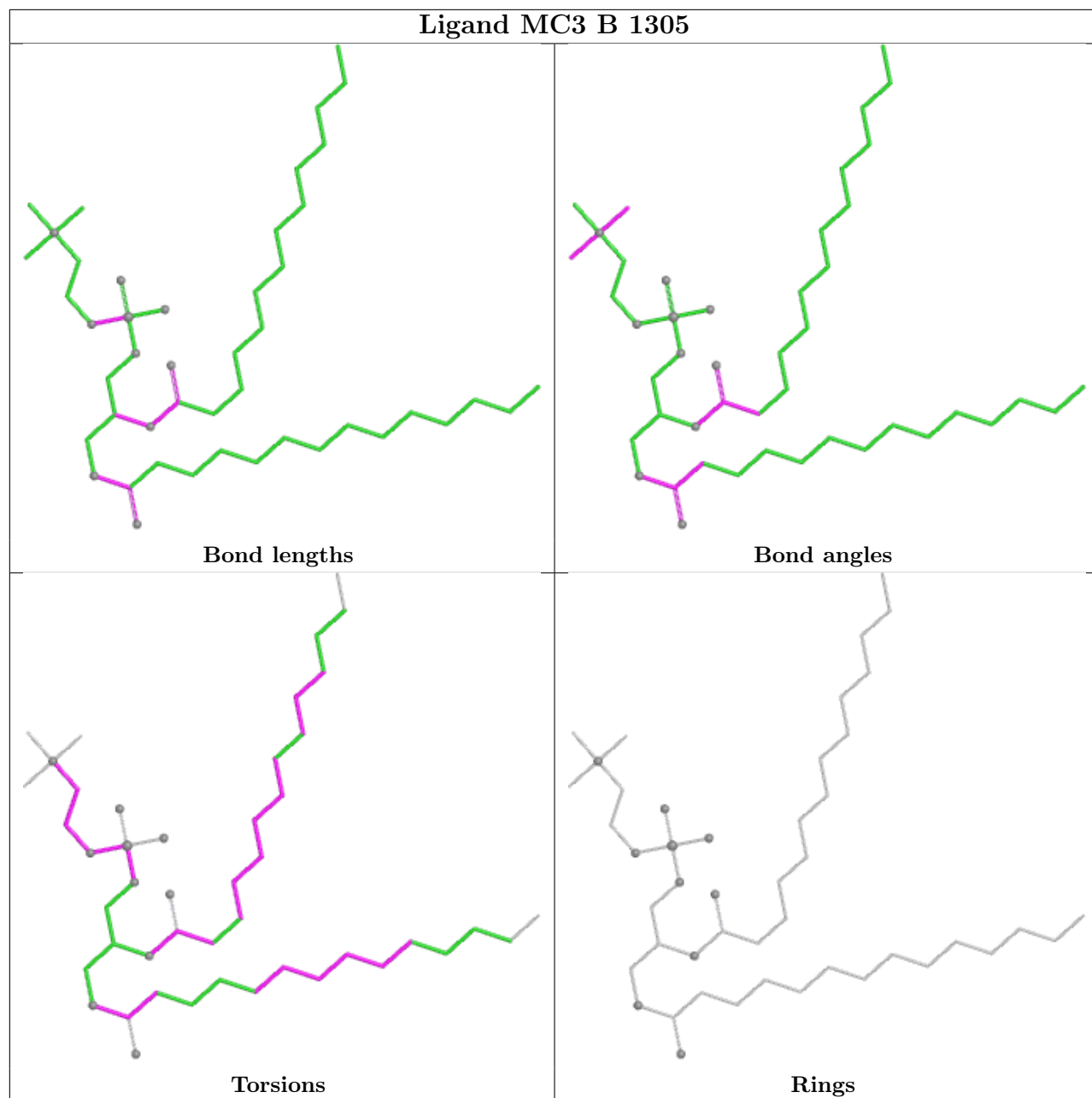


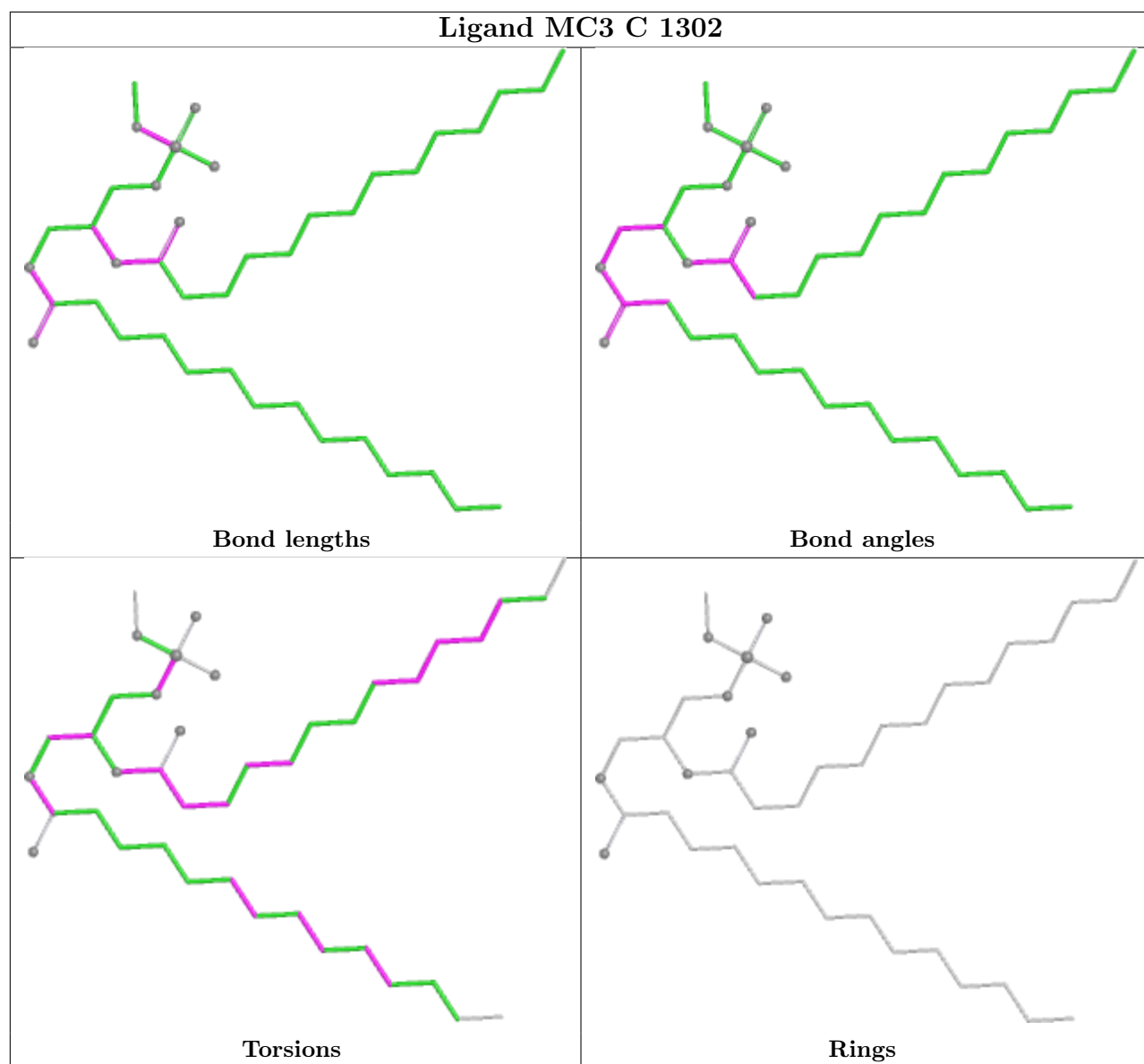
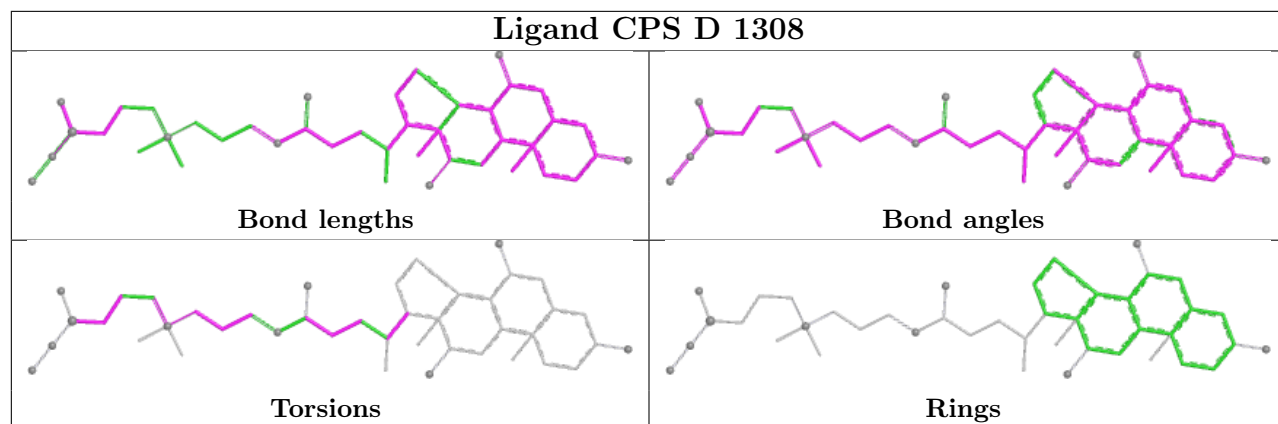
Ligand CPS A 1304

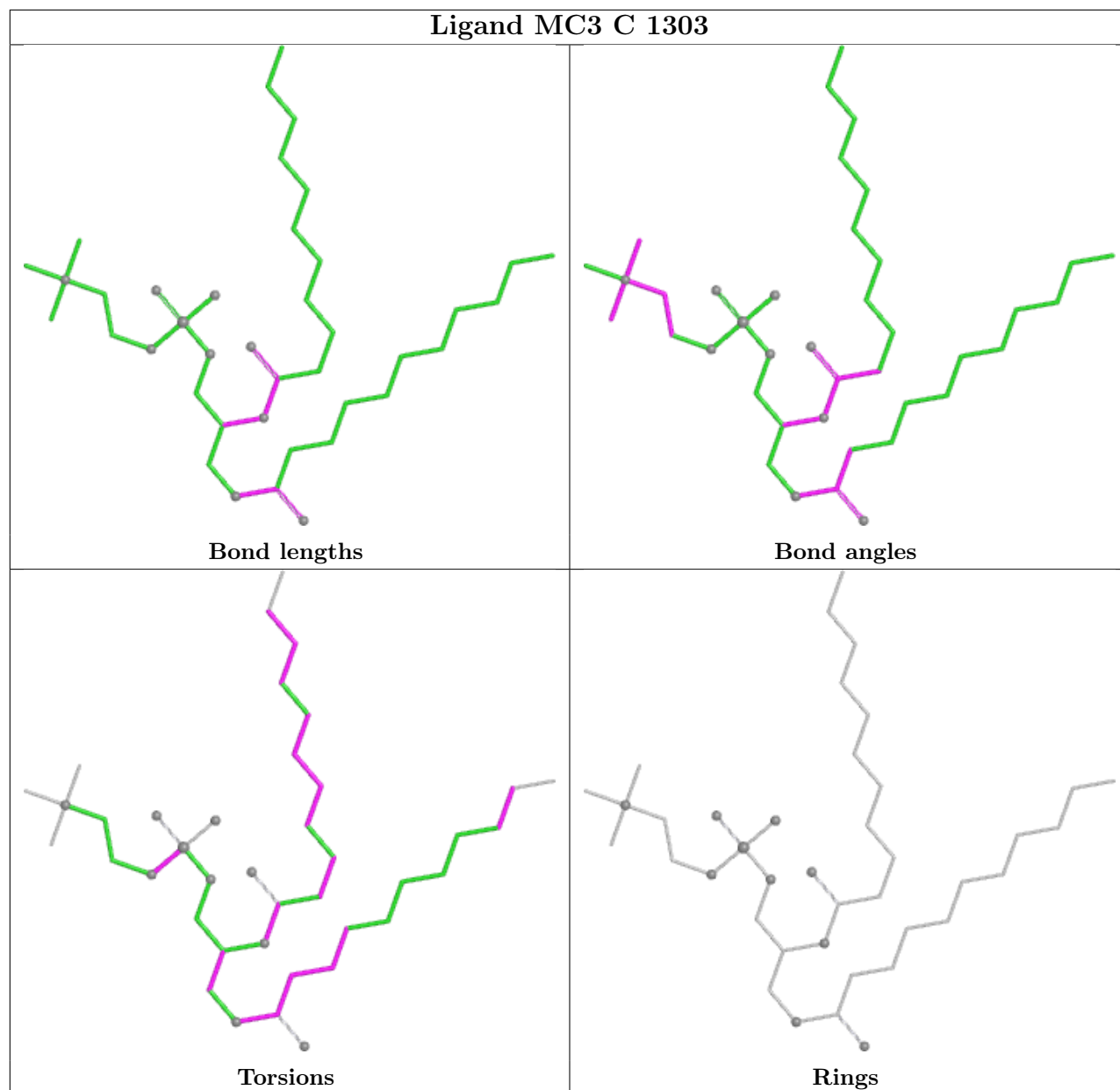


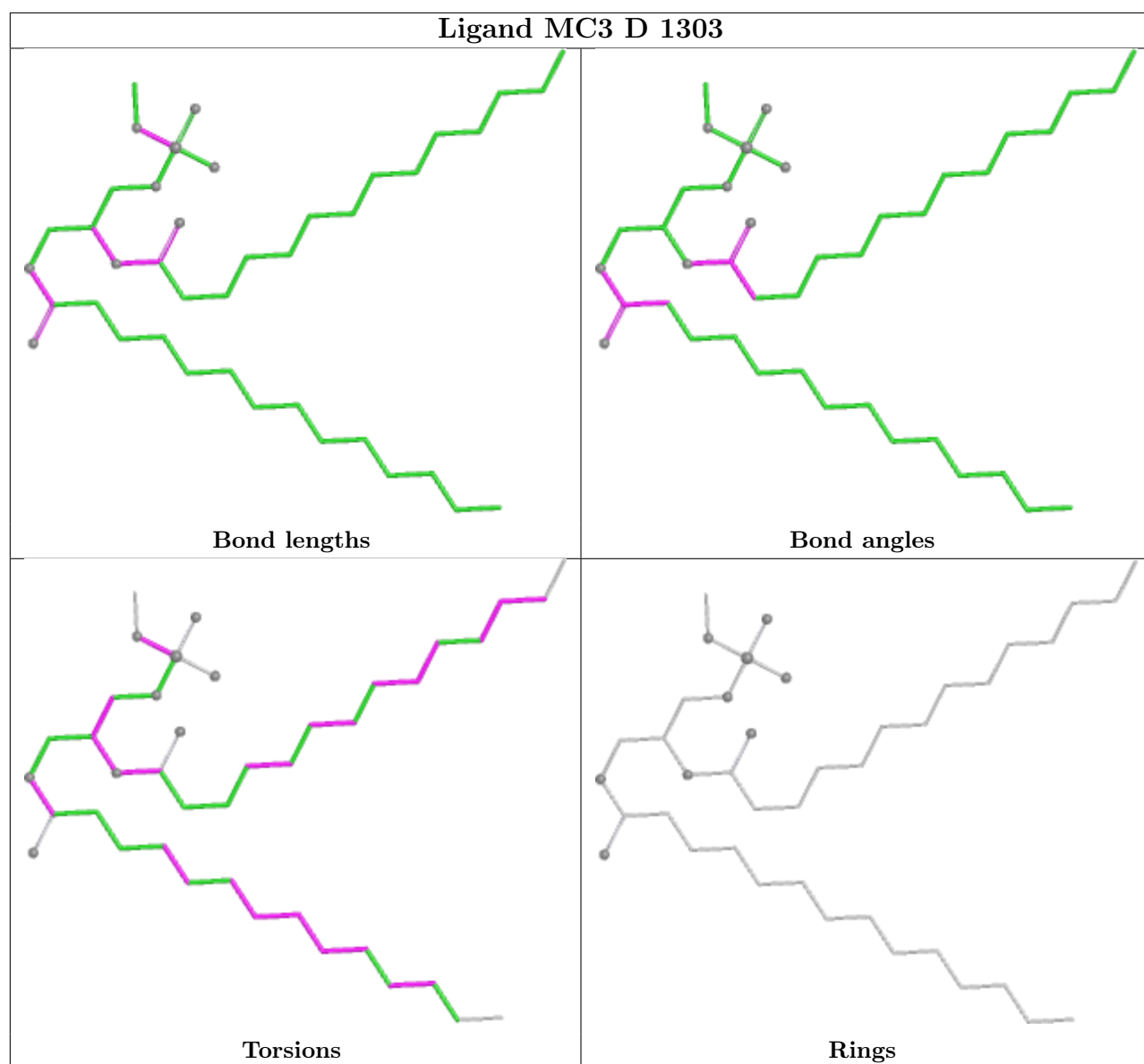
Ligand MC3 C 1301

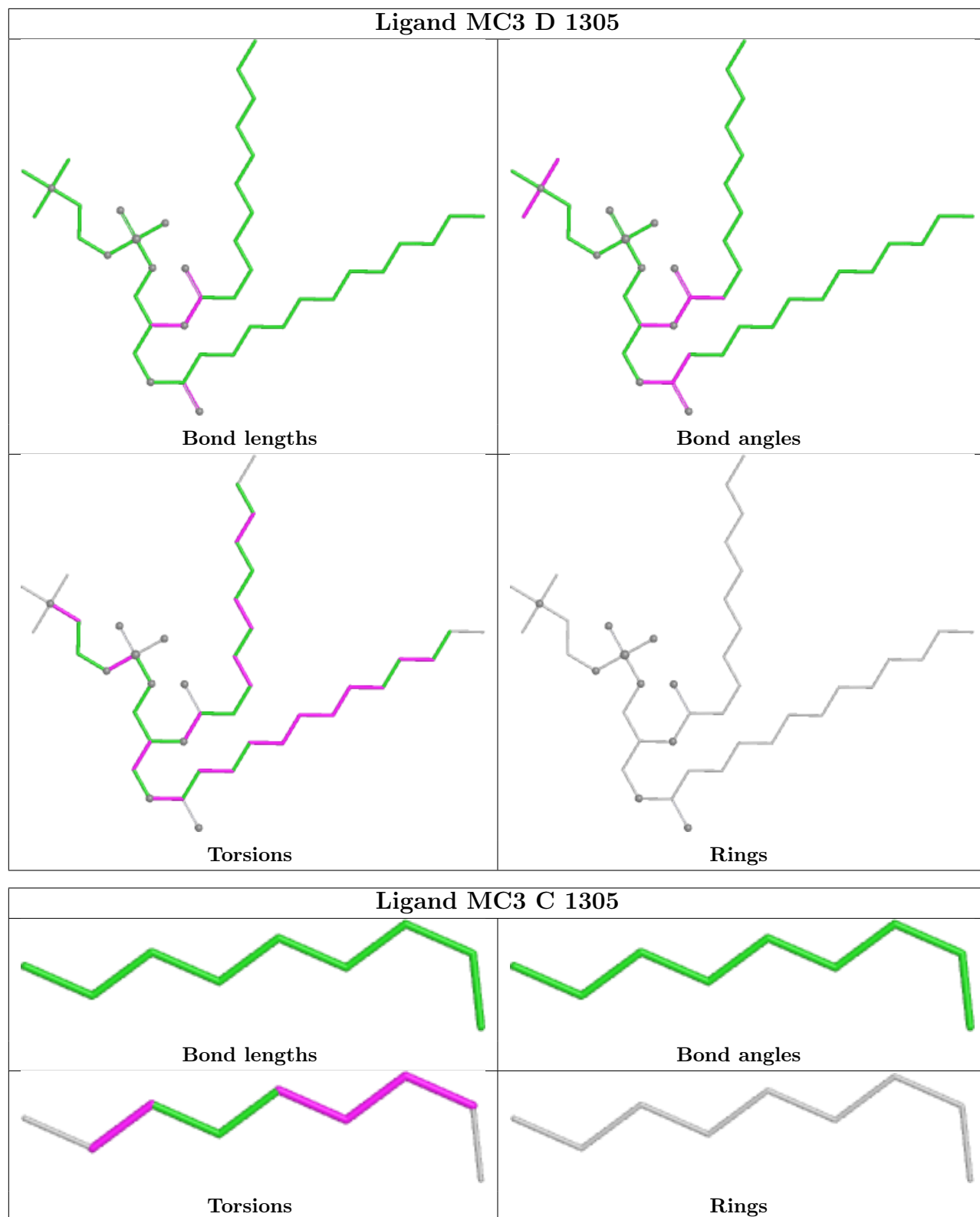


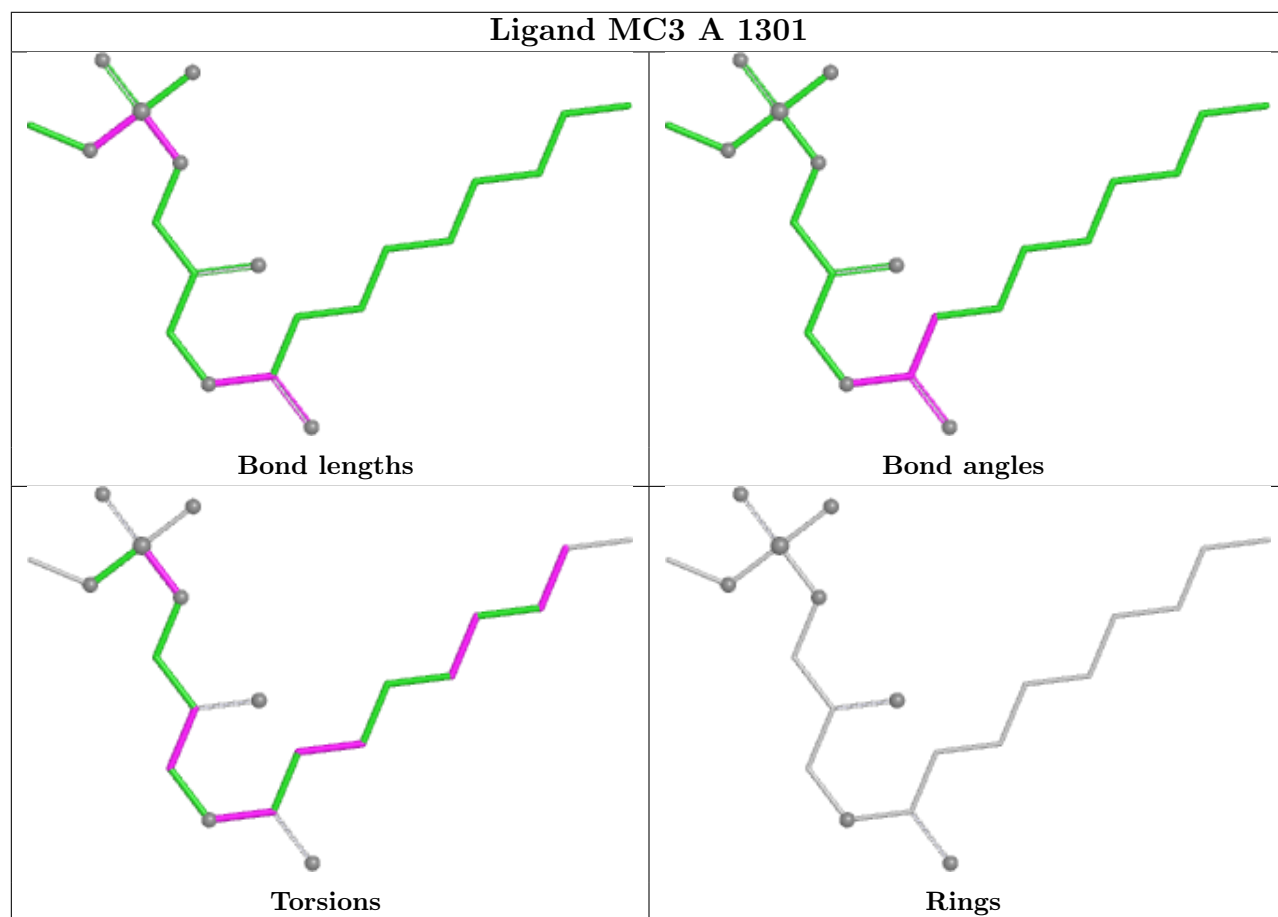
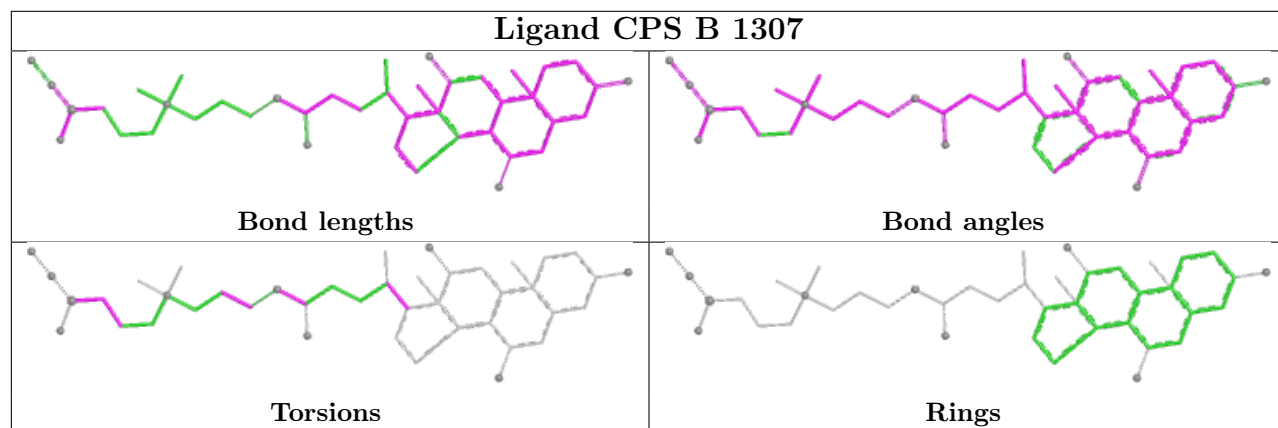


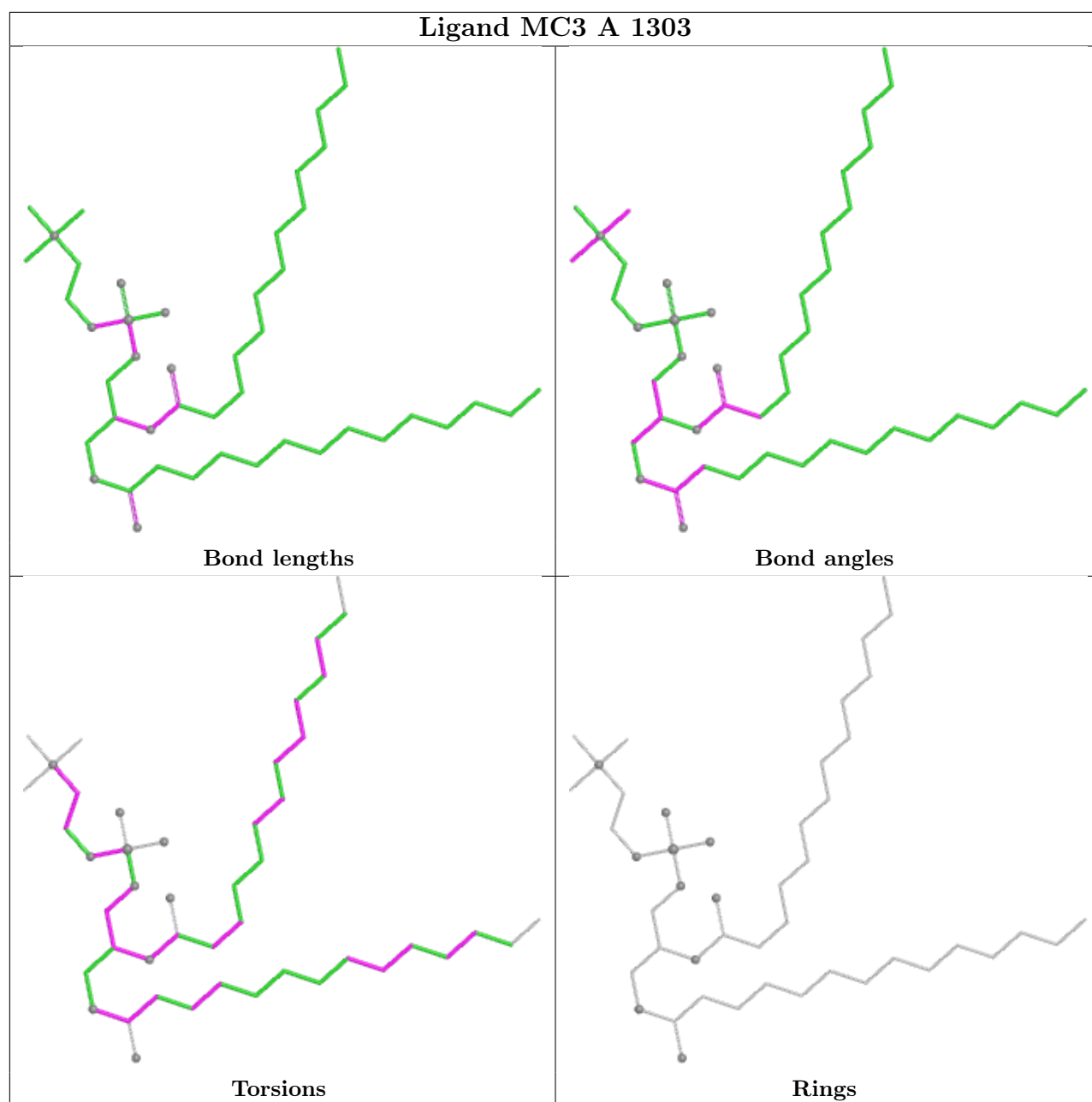


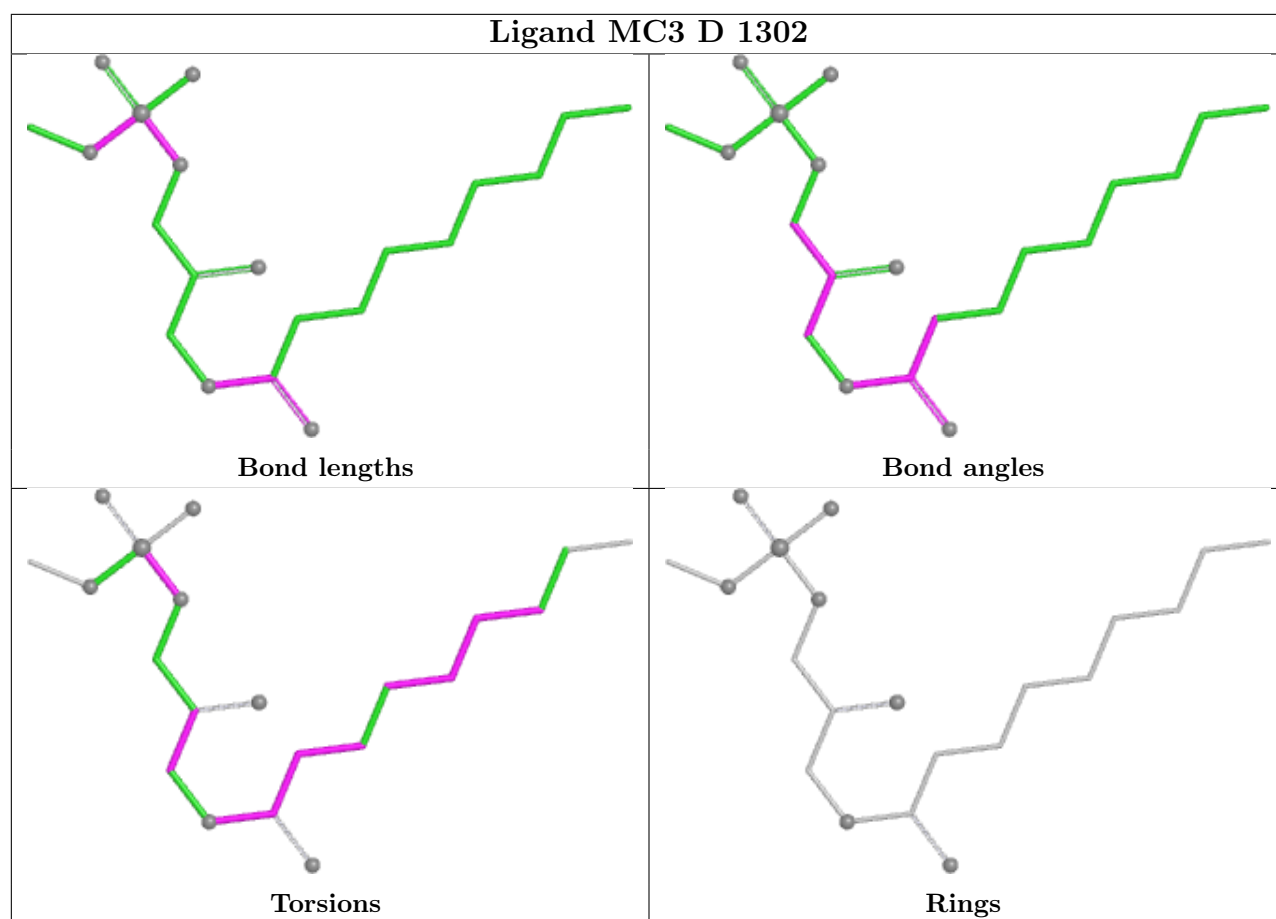


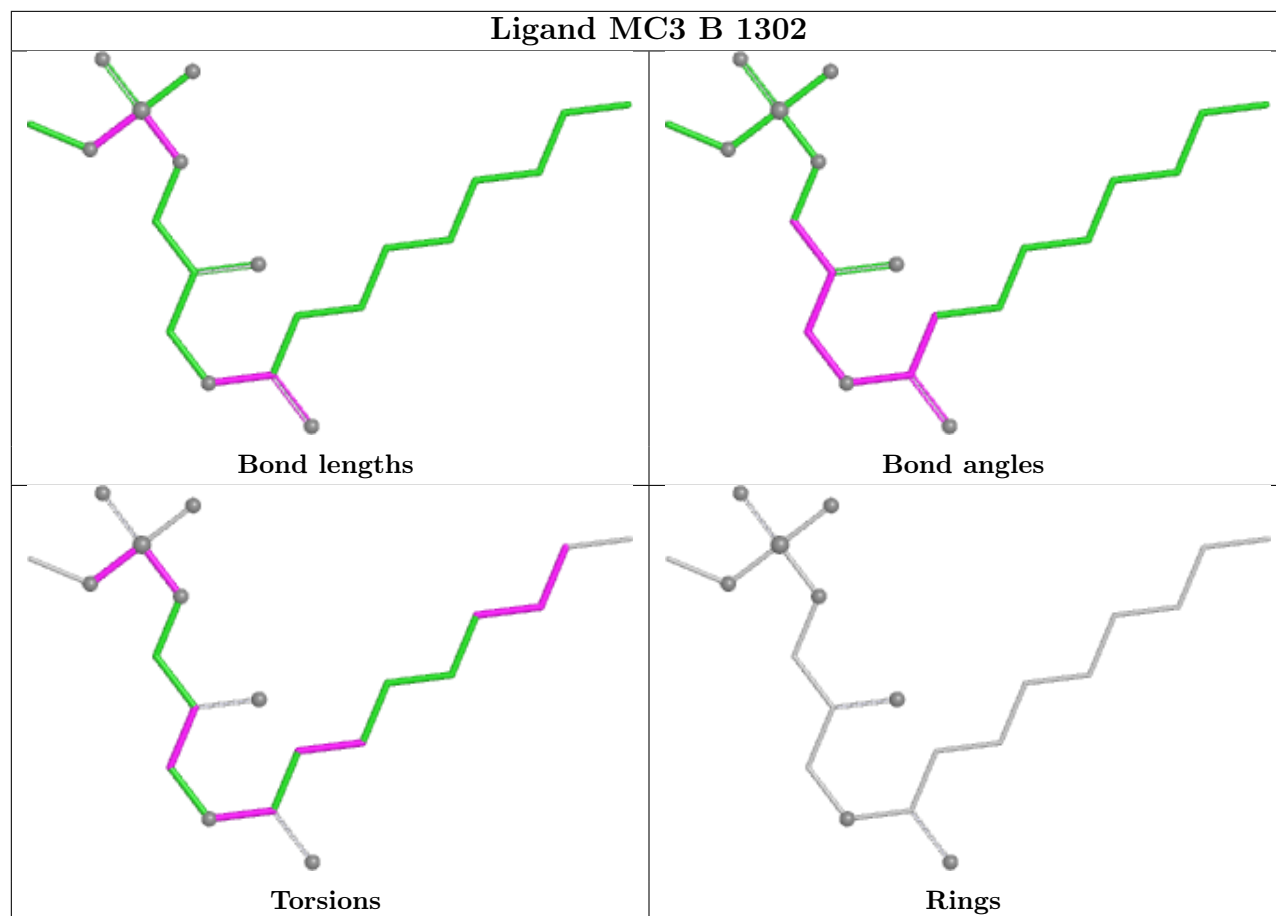


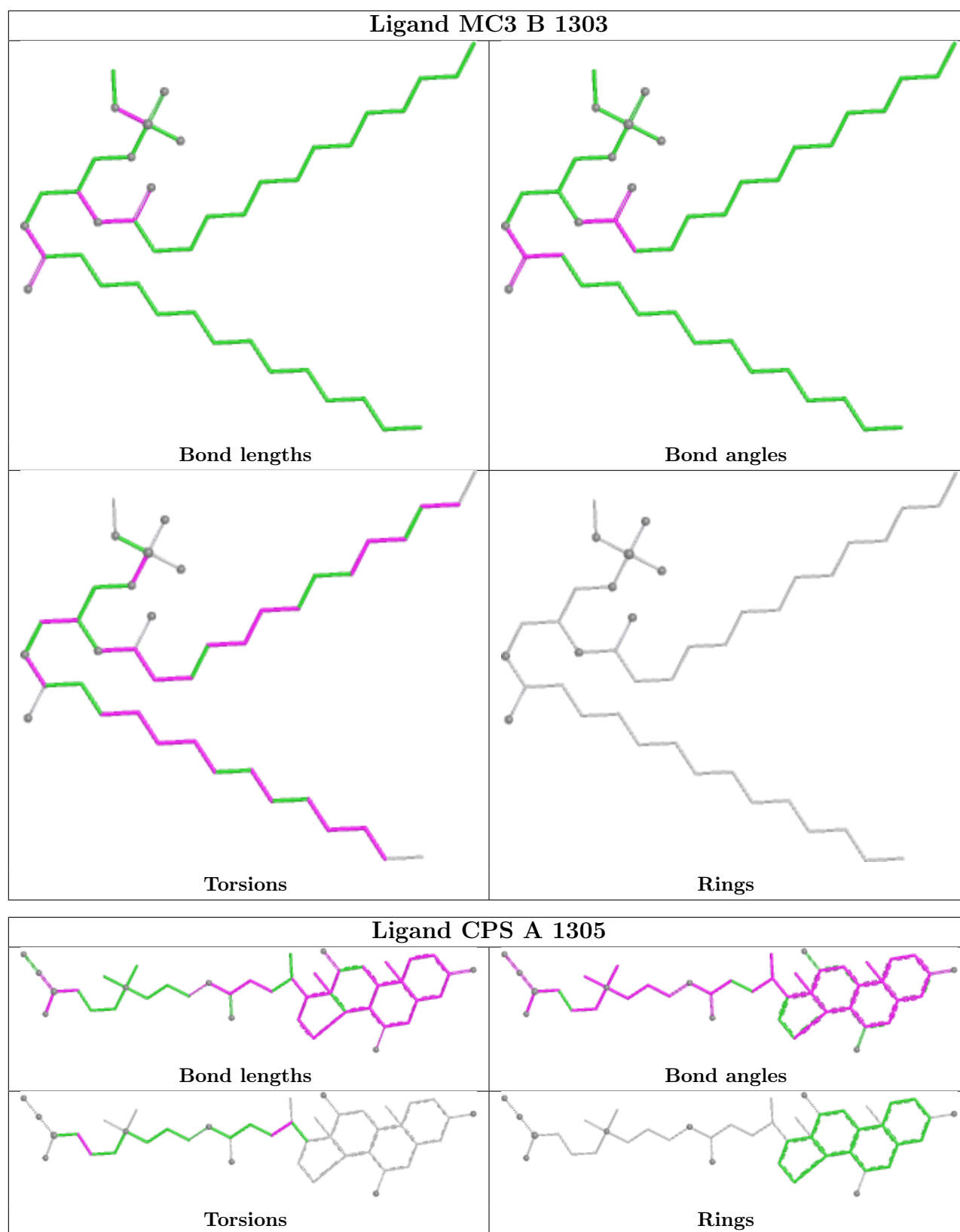












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/285 (93%)	0.75	37 (13%) 6 5	33, 73, 160, 168	0
1	B	267/285 (93%)	0.73	40 (14%) 5 4	35, 69, 162, 181	0
1	C	267/285 (93%)	0.74	37 (13%) 6 5	35, 70, 180, 206	0
1	D	267/285 (93%)	0.65	31 (11%) 9 8	35, 70, 151, 164	0
All	All	1068/1140 (93%)	0.72	145 (13%) 7 6	33, 71, 161, 206	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1260	LEU	7.4
1	B	1265	LEU	7.1
1	D	1260	LEU	6.9
1	D	1261	ILE	6.6
1	B	1261	ILE	6.5
1	D	1265	LEU	6.5
1	C	1265	LEU	6.4
1	D	1095	PHE	6.1
1	C	1248	ILE	6.0
1	A	1248	ILE	6.0
1	C	1257	LEU	5.9
1	C	1261	ILE	5.7
1	B	1257	LEU	5.5
1	D	1257	LEU	5.2
1	A	1257	LEU	4.9
1	C	1250	LEU	4.9
1	A	1258	LYS	4.9
1	D	1255	VAL	4.9
1	D	1258	LYS	4.9
1	C	1258	LYS	4.8
1	A	1254	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	1260	LEU	4.7
1	A	1260	LEU	4.7
1	D	1254	ILE	4.7
1	A	1001	MET	4.6
1	B	1263	THR	4.6
1	B	1248	ILE	4.6
1	A	1261	ILE	4.4
1	C	1247	ILE	4.3
1	A	1002	TYR	4.3
1	C	1262	LYS	4.3
1	A	1267	ASN	4.2
1	D	1264	SER	4.2
1	A	1250	LEU	4.2
1	B	1065	TYR	4.2
1	A	1255	VAL	4.0
1	D	1091	THR	4.0
1	D	1262	LYS	4.0
1	A	1221	MET	4.0
1	B	1255	VAL	3.9
1	C	1256	GLU	3.8
1	C	1255	VAL	3.8
1	A	1247	ILE	3.7
1	A	1095	PHE	3.7
1	B	1001	MET	3.7
1	D	1251	ARG	3.7
1	B	1266	LYS	3.6
1	C	1254	ILE	3.6
1	C	1094	GLY	3.5
1	D	1250	LEU	3.5
1	B	1221	MET	3.4
1	B	1195	TRP	3.4
1	A	1262	LYS	3.3
1	D	1094	GLY	3.3
1	B	1162	THR	3.3
1	C	1251	ARG	3.2
1	A	1249	LYS	3.2
1	C	1233	ILE	3.2
1	D	1065	TYR	3.2
1	B	1254	ILE	3.2
1	D	1044	TYR	3.2
1	D	1020	TYR	3.1
1	B	1267	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1242	ASN	3.1
1	B	1258	LYS	3.1
1	A	1263	THR	3.0
1	C	1221	MET	3.0
1	B	1092	SER	3.0
1	A	1246	GLU	3.0
1	D	1244	ASN	3.0
1	B	1247	ILE	3.0
1	C	1259	GLU	3.0
1	C	1238	SER	2.9
1	B	1250	LEU	2.9
1	C	1243	ILE	2.9
1	B	1095	PHE	2.9
1	C	1115	GLN	2.9
1	B	1090	PRO	2.8
1	B	1040	SER	2.8
1	D	1243	ILE	2.8
1	C	1263	THR	2.8
1	B	1262	LYS	2.8
1	B	1225	ASN	2.8
1	C	1010	GLU	2.8
1	C	1096	GLU	2.8
1	D	1240	GLU	2.8
1	D	1035	LYS	2.7
1	D	1246	GLU	2.7
1	B	1003	LEU	2.7
1	A	1245	ASN	2.7
1	D	1263	THR	2.7
1	C	1266	LYS	2.7
1	C	1249	LYS	2.6
1	C	1095	PHE	2.6
1	A	1265	LEU	2.6
1	B	1002	TYR	2.6
1	B	1259	GLU	2.5
1	C	1264	SER	2.5
1	B	1043	VAL	2.5
1	D	1013	PHE	2.5
1	D	1082	PHE	2.5
1	B	1264	SER	2.4
1	C	1030	GLY	2.4
1	A	1266	LYS	2.4
1	A	1251	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1011	SER	2.4
1	A	1100	VAL	2.4
1	D	1043	VAL	2.4
1	C	1041	PHE	2.4
1	C	1267	ASN	2.4
1	D	1267	ASN	2.4
1	D	1238	SER	2.4
1	A	1234	ASP	2.4
1	D	1226	GLN	2.4
1	B	1089	VAL	2.4
1	B	1094	GLY	2.3
1	A	1094	GLY	2.3
1	B	1044	TYR	2.3
1	B	1007	ASN	2.3
1	A	1092	SER	2.2
1	B	1013	PHE	2.2
1	C	1091	THR	2.2
1	A	1007	ASN	2.2
1	D	1115	GLN	2.2
1	B	1088	LEU	2.2
1	A	1061	ILE	2.2
1	C	1195	TRP	2.1
1	C	1118	LYS	2.1
1	A	1003	LEU	2.1
1	A	1232	ILE	2.1
1	B	1037	PHE	2.1
1	C	1253	GLU	2.1
1	B	1068	ARG	2.1
1	A	1244	ASN	2.1
1	C	1244	ASN	2.1
1	A	1005	ILE	2.1
1	A	1069	ILE	2.1
1	B	1041	PHE	2.1
1	B	1243	ILE	2.1
1	D	1249	LYS	2.0
1	A	1236	VAL	2.0
1	C	1044	TYR	2.0
1	A	1054	THR	2.0
1	A	1090	PRO	2.0
1	A	1162	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CPS	A	1304	42/42	0.57	0.26	83,108,131,133	2
4	CPS	B	1308	42/42	0.66	0.27	90,108,122,124	2
4	CPS	A	1305	42/42	0.73	0.22	60,78,87,91	1
4	CPS	D	1308	42/42	0.75	0.19	53,71,78,86	2
2	MC3	C	1301	21/46	0.76	0.21	64,81,101,115	0
2	MC3	C	1305	9/46	0.78	0.25	42,48,60,60	0
2	MC3	B	1306	8/46	0.80	0.22	43,47,54,60	0
3	CA	B	1301	1/1	0.80	0.58	103,103,103,103	0
2	MC3	D	1302	21/46	0.82	0.18	57,80,121,128	0
4	CPS	A	1306	42/42	0.82	0.20	54,77,81,83	2
2	MC3	A	1301	21/46	0.83	0.16	54,79,94,104	0
4	CPS	B	1307	42/42	0.83	0.17	55,72,79,81	1
2	MC3	C	1306	9/46	0.84	0.17	44,50,54,55	0
2	MC3	B	1302	21/46	0.86	0.15	56,78,93,104	0
2	MC3	C	1302	41/46	0.88	0.16	50,66,89,93	0
2	MC3	C	1304	46/46	0.88	0.16	51,71,83,90	0
2	MC3	A	1303	46/46	0.88	0.17	52,69,84,93	0
2	MC3	D	1307	8/46	0.89	0.15	42,49,51,54	0
2	MC3	D	1303	41/46	0.89	0.15	53,67,92,103	0
2	MC3	B	1305	46/46	0.90	0.15	51,70,88,99	0
3	CA	D	1301	1/1	0.90	0.17	70,70,70,70	0
2	MC3	D	1306	46/46	0.90	0.14	54,68,77,82	0
2	MC3	B	1303	41/46	0.90	0.15	58,68,93,98	0
2	MC3	C	1307	41/46	0.92	0.14	58,71,88,96	0
2	MC3	B	1304	41/46	0.93	0.13	46,60,75,77	0
2	MC3	D	1305	42/46	0.93	0.14	45,60,73,77	0
2	MC3	C	1303	40/46	0.94	0.13	49,59,72,78	0

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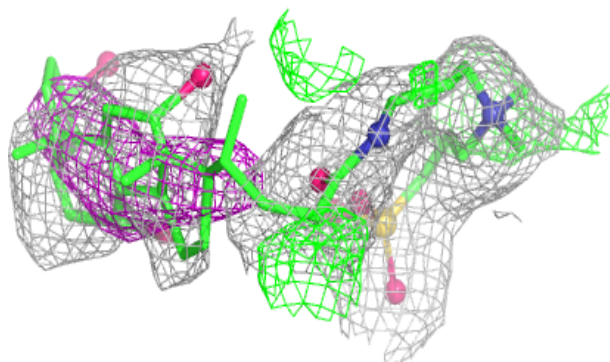
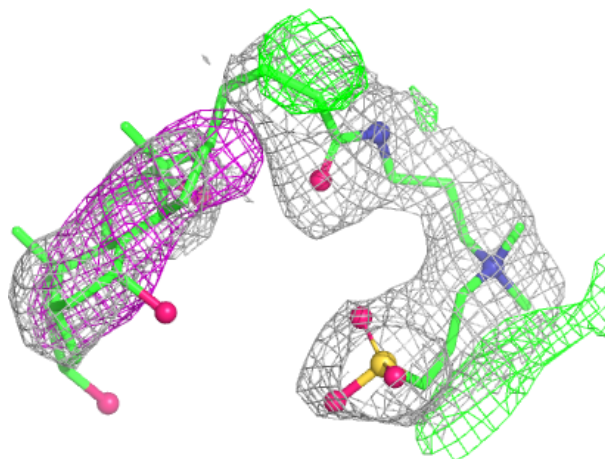
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MC3	D	1304	43/46	0.96	0.10	44,56,70,77	0
3	CA	A	1302	1/1	0.98	0.19	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

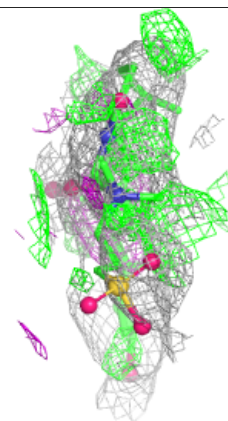
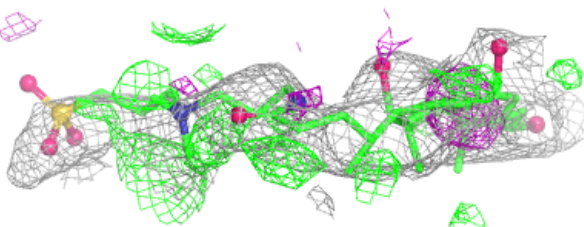
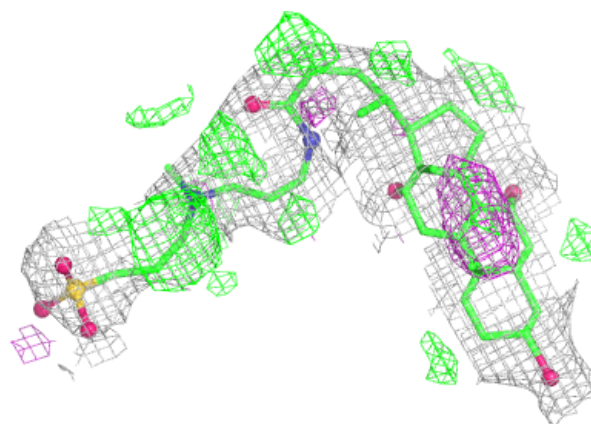
Electron density around CPS A 1304:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

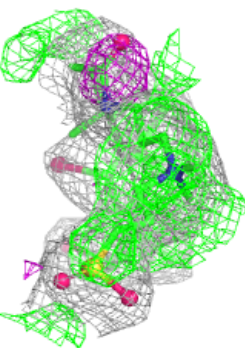
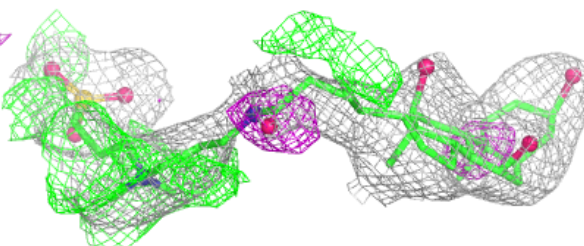
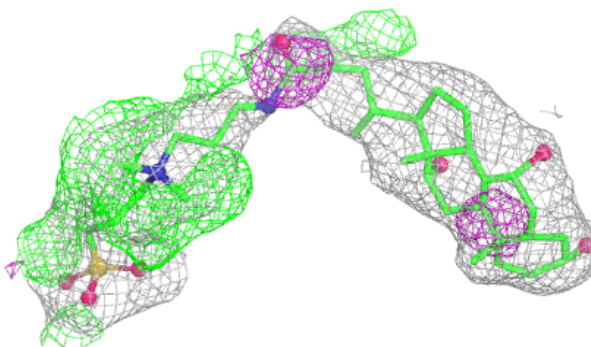


Electron density around CPS B 1308:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

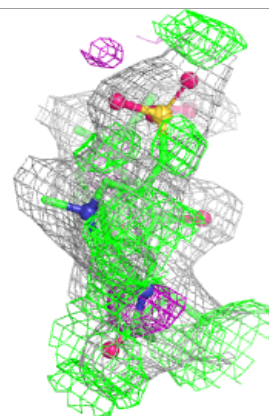
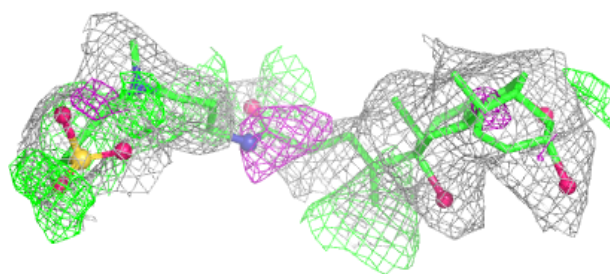
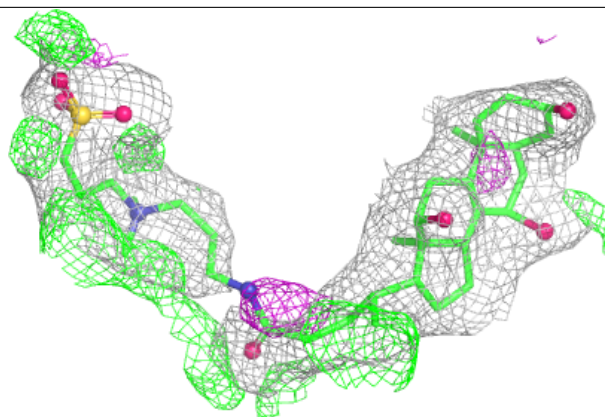
**Electron density around CPS A 1305:**

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and green (positive)

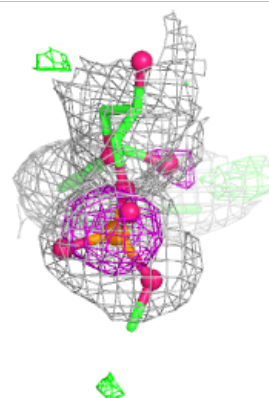
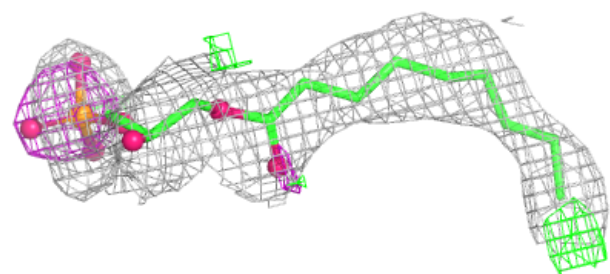
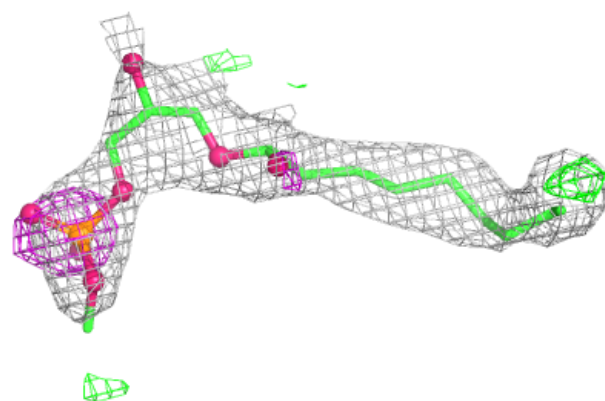


Electron density around CPS D 1308:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

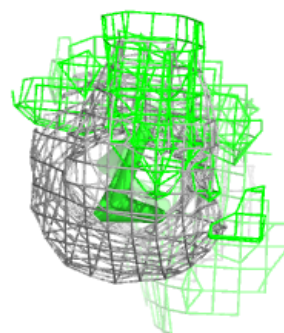
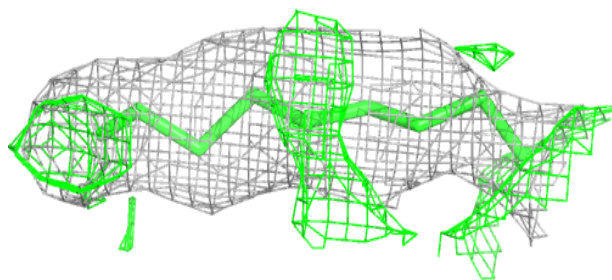
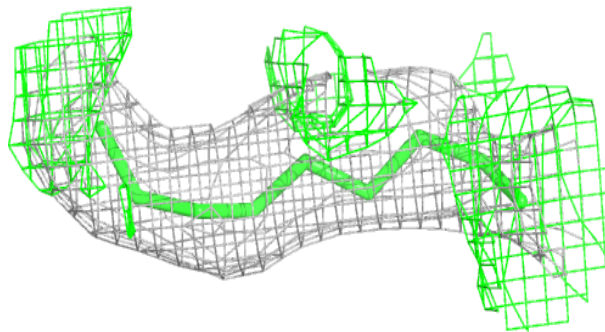
**Electron density around MC3 C 1301:**

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and green (positive)

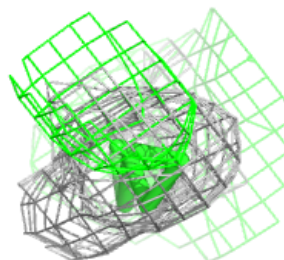
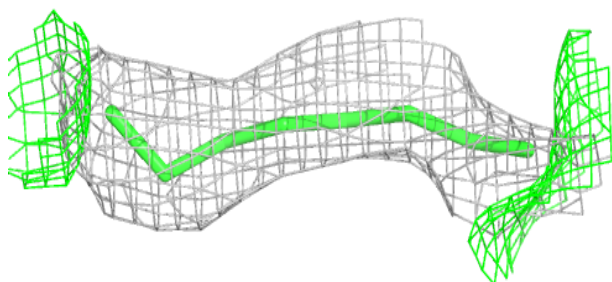
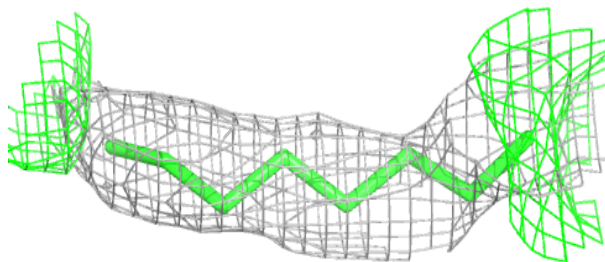


Electron density around MC3 C 1305:

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and green (positive)

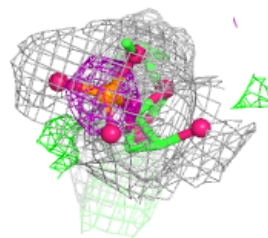
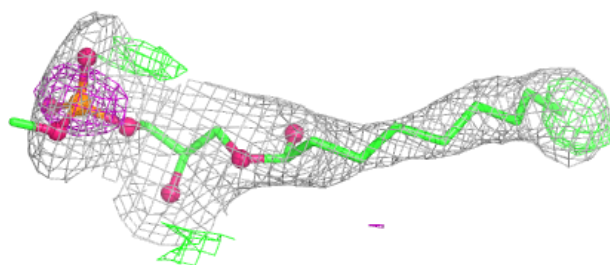
**Electron density around MC3 B 1306:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

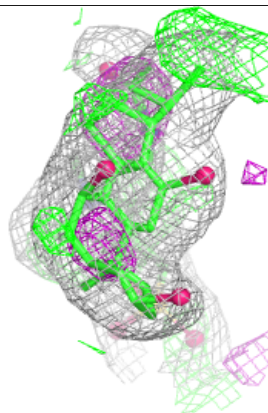
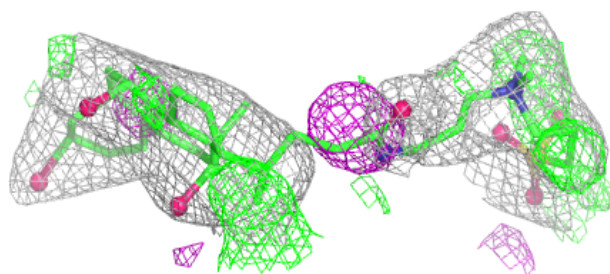
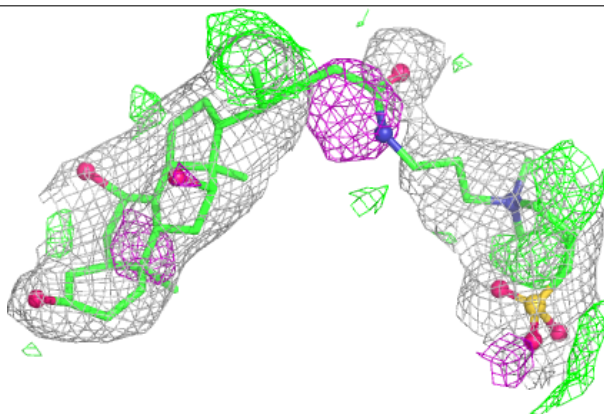


Electron density around MC3 D 1302:

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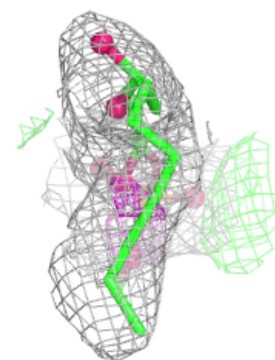
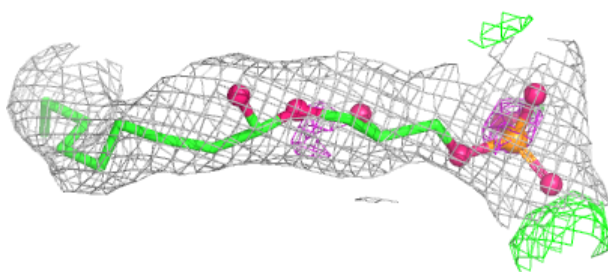
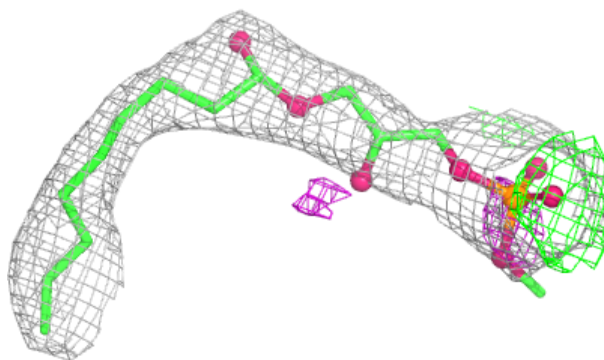
**Electron density around CPS A 1306:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

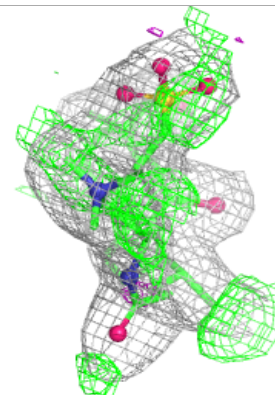
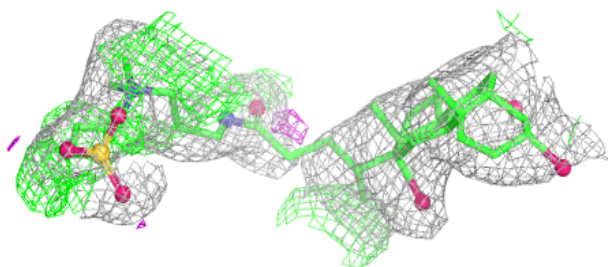
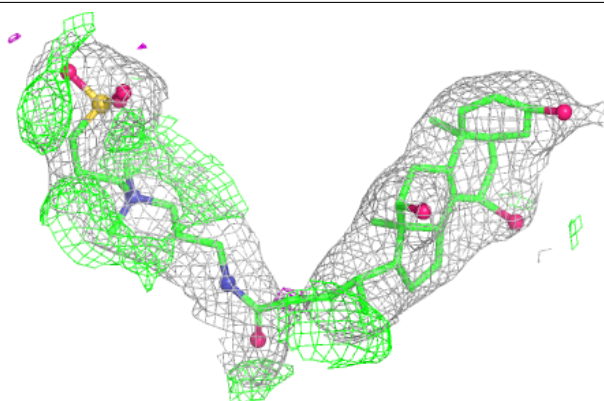


Electron density around MC3 A 1301:

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and green (positive)

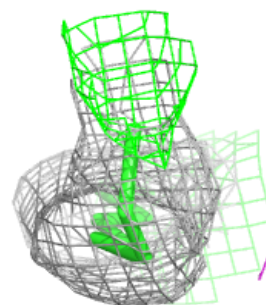
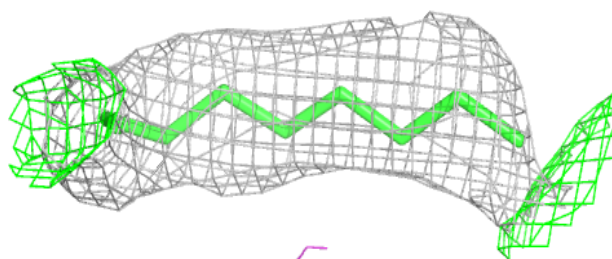
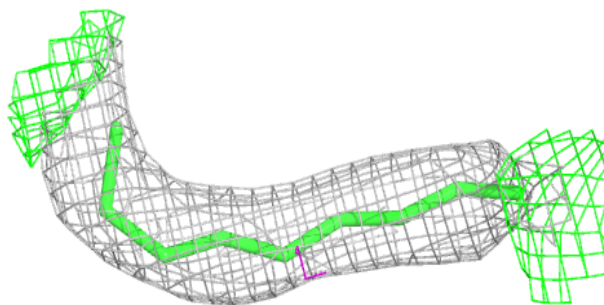
**Electron density around CPS B 1307:**

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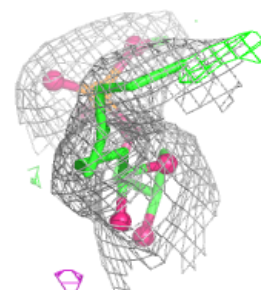
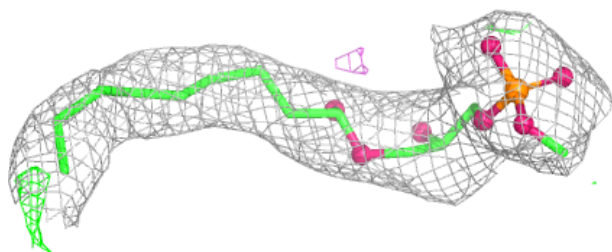


Electron density around MC3 C 1306:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

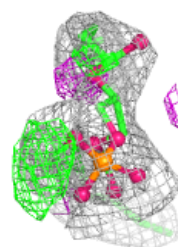
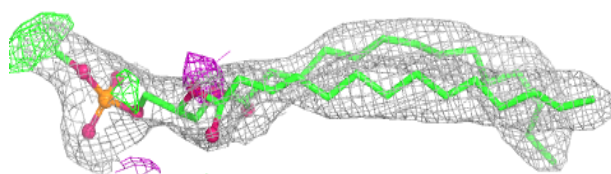
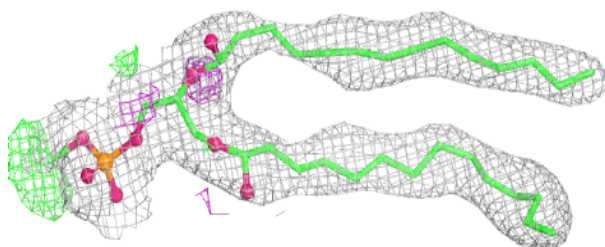
**Electron density around MC3 B 1302:**

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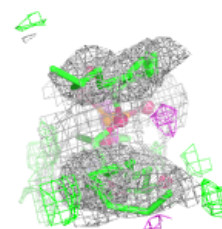
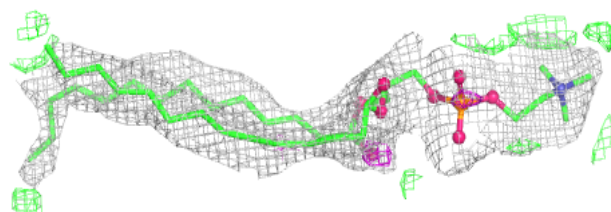
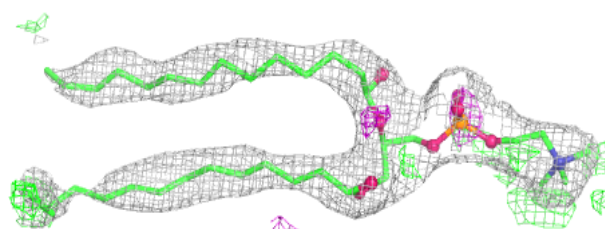


Electron density around MC3 C 1302:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

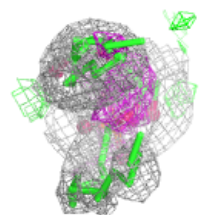
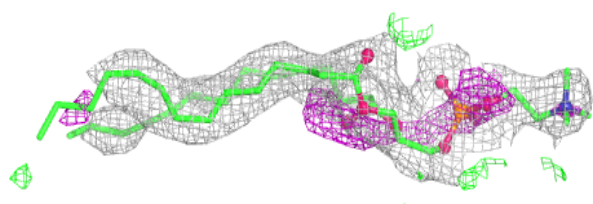
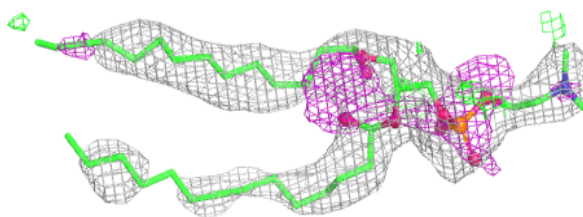
**Electron density around MC3 C 1304:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

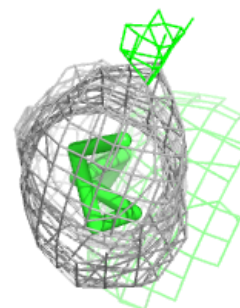
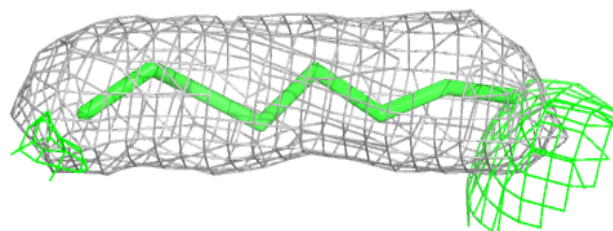
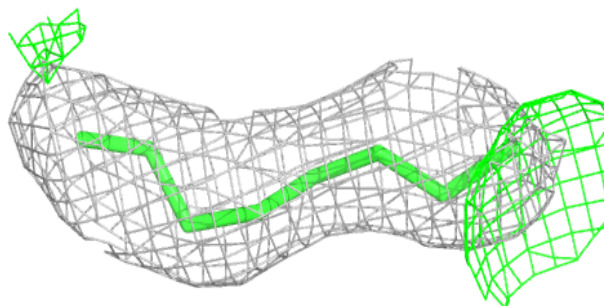


Electron density around MC3 A 1303:

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and green (positive)

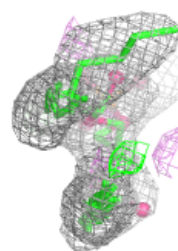
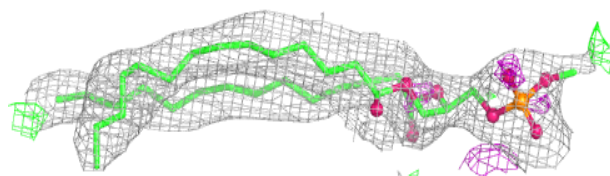
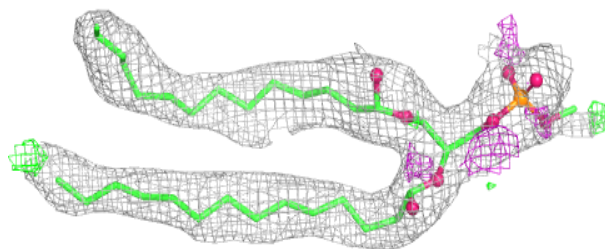
**Electron density around MC3 D 1307:**

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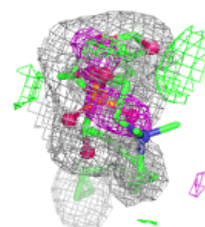
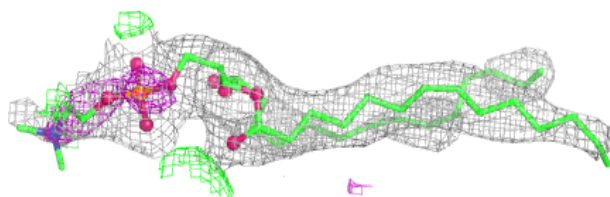
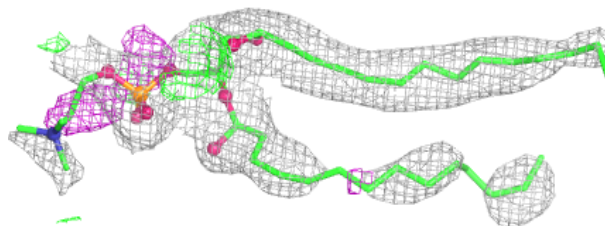


Electron density around MC3 D 1303:

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and green (positive)

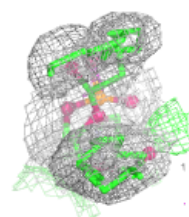
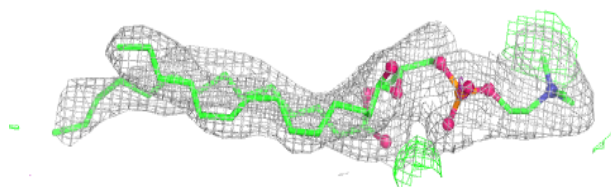
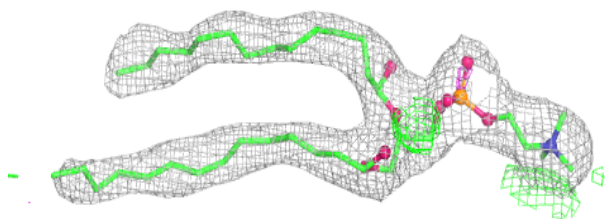
**Electron density around MC3 B 1305:**

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and green (positive)

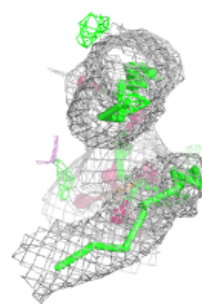
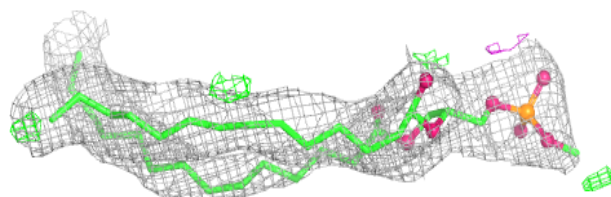
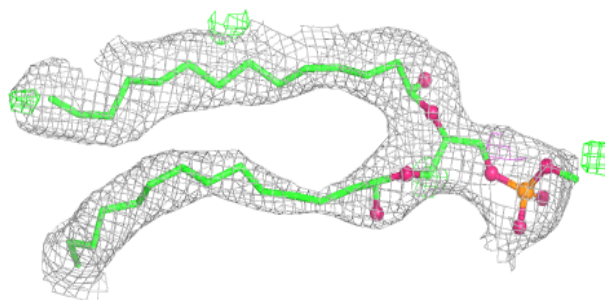


Electron density around MC3 D 1306:

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and green (positive)

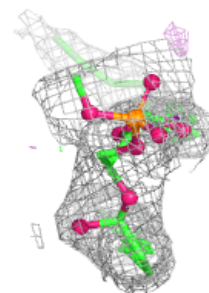
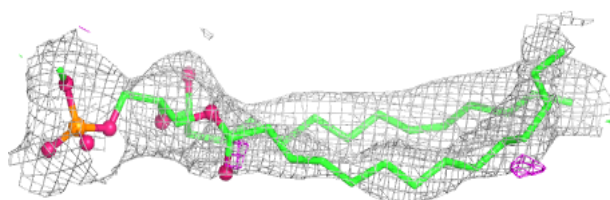
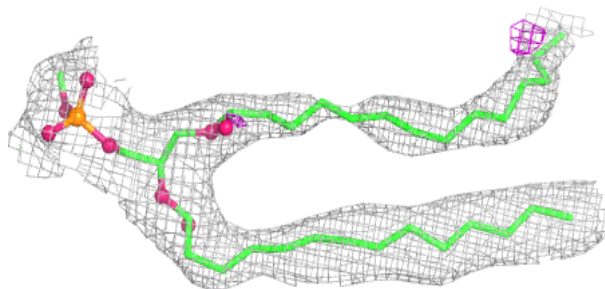
**Electron density around MC3 B 1303:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

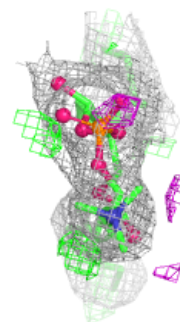
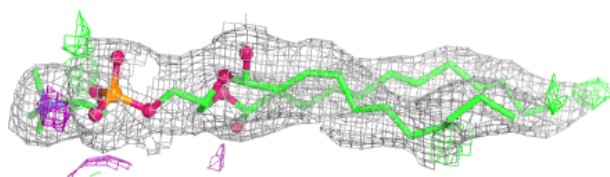
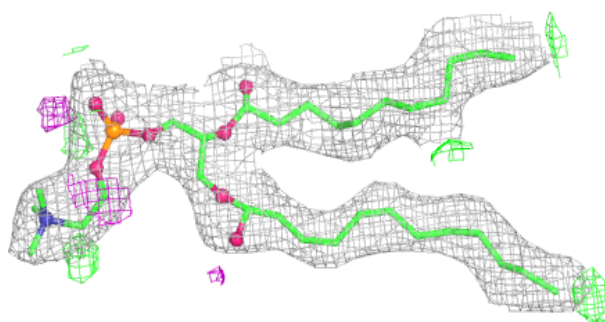


Electron density around MC3 C 1307:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

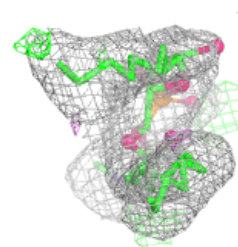
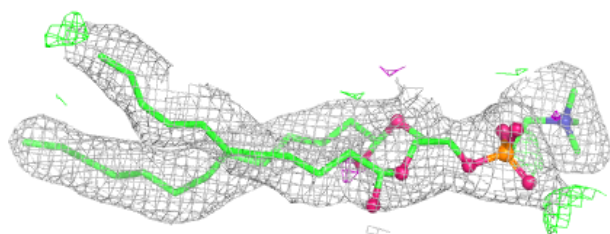
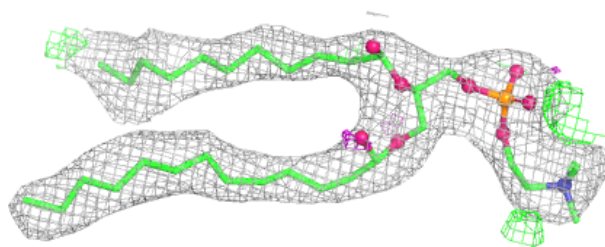
**Electron density around MC3 B 1304:**

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and green (positive)

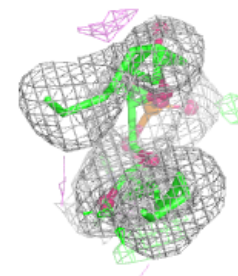
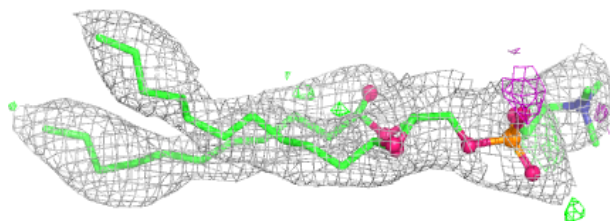
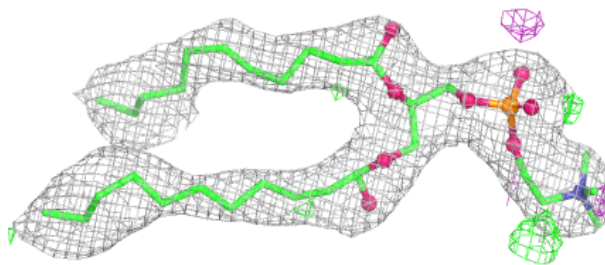


Electron density around MC3 D 1305:

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and green (positive)

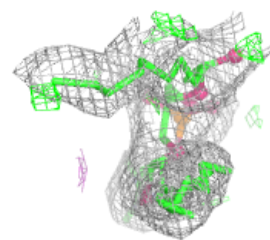
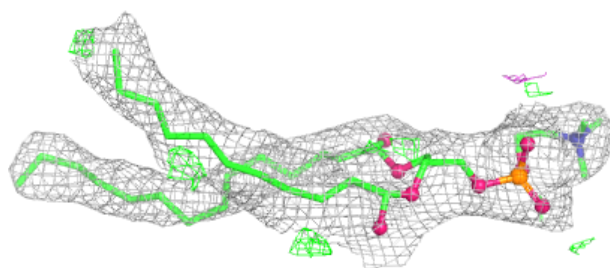
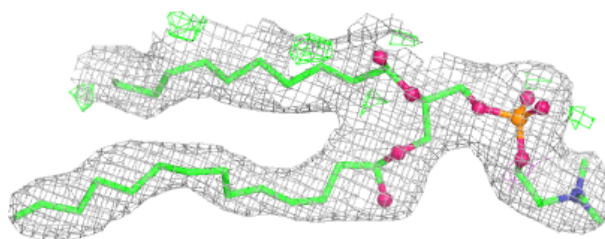
**Electron density around MC3 C 1303:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MC3 D 1304:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.