



Full wwPDB EM Validation Report ⓘ

May 14, 2026 – 02:09 pm BST

PDB ID : 7ZP9 / pdb_00007zp9
EMDB ID : EMD-14851
Title : KtrAB complex - KtrA8 ring with a KtrB dimer on each side
Authors : Vonck, J.; Stautz, J.
Deposited on : 2022-04-27
Resolution : 2.82 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

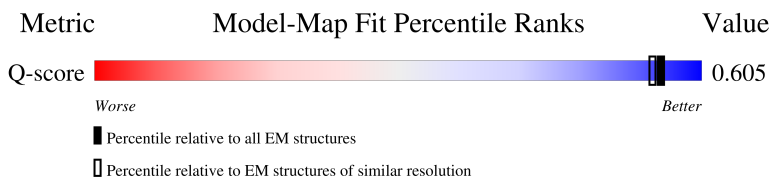
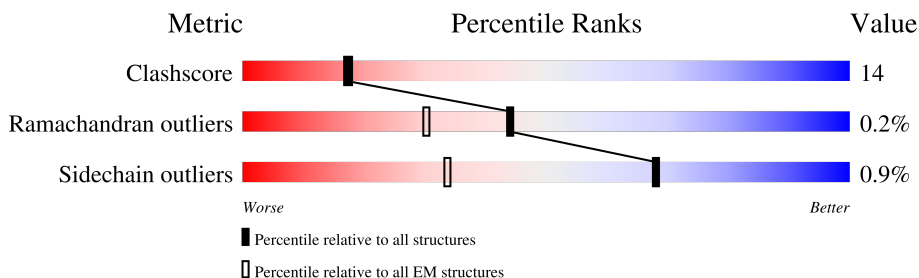
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 Å.

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



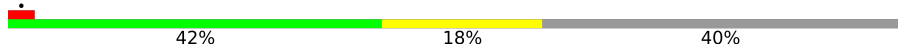
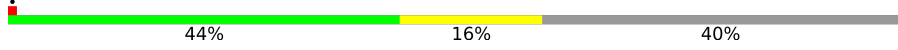
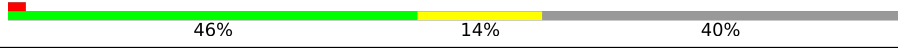
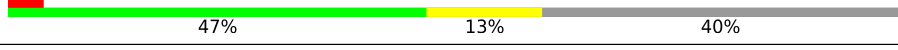
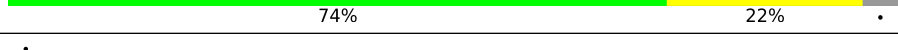
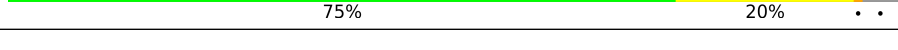
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11795 (2.32 - 3.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	220	
1	B	220	
1	D	220	
1	E	220	

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Mol	Chain	Length	Quality of chain
1	F	220	
1	H	220	
1	J	220	
1	L	220	
2	C	455	
2	G	455	
2	I	455	
2	M	455	

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
5	LMT	C	504	-	-	X	-
5	LMT	I	503	-	-	X	-
5	LMT	M	508	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 22339 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	132	Total	C	N	O	S	0	0
			983	621	176	179	7		
1	D	132	Total	C	N	O	S	0	0
			956	612	168	169	7		
1	E	132	Total	C	N	O	S	0	0
			939	597	168	167	7		
1	F	132	Total	C	N	O	S	0	0
			963	614	173	169	7		
1	A	132	Total	C	N	O	S	0	0
			956	609	170	170	7		
1	B	132	Total	C	N	O	S	0	0
			971	616	175	173	7		
1	J	132	Total	C	N	O	S	0	0
			934	600	167	160	7		
1	L	132	Total	C	N	O	S	0	0
			948	607	169	165	7		

- Molecule 2 is a protein called Ktr system potassium uptake protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	436	Total	C	N	O	S	1	0
			3288	2183	524	560	21		
2	M	437	Total	C	N	O	S	0	0
			3286	2178	523	564	21		
2	C	436	Total	C	N	O	S	1	0
			3295	2191	524	559	21		
2	G	437	Total	C	N	O	S	0	0
			3289	2181	520	567	21		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

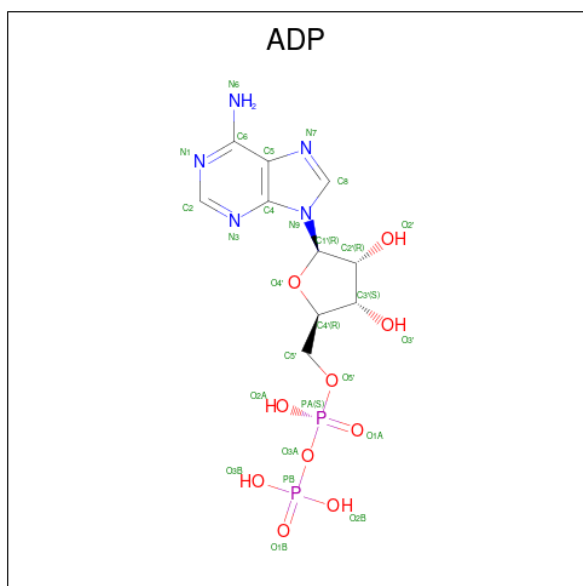
Mol	Chain	Residues	Atoms		AltConf
3	H	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	J	1	Total	Mg	0
			1	1	
3	L	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



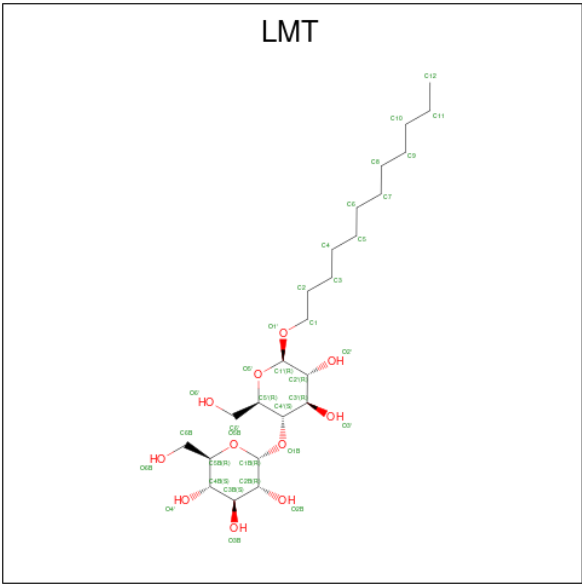
Mol	Chain	Residues	Atoms					AltConf
4	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 5 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	I	1	Total	C	O	0
			35	24	11	
5	A	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	M	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	
5	C	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	
5	G	1	Total	C	O	0
			35	24	11	

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
6	I	1	Total	K	0
			1	1	
6	M	1	Total	K	0
			1	1	
6	C	1	Total	K	0
			1	1	
6	G	1	Total	K	0
			1	1	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	H	1	Total	O	0
			1	1	
7	D	1	Total	O	0
			1	1	
7	E	1	Total	O	0
			1	1	
7	F	1	Total	O	0
			1	1	
7	I	13	Total	O	0
			13	13	

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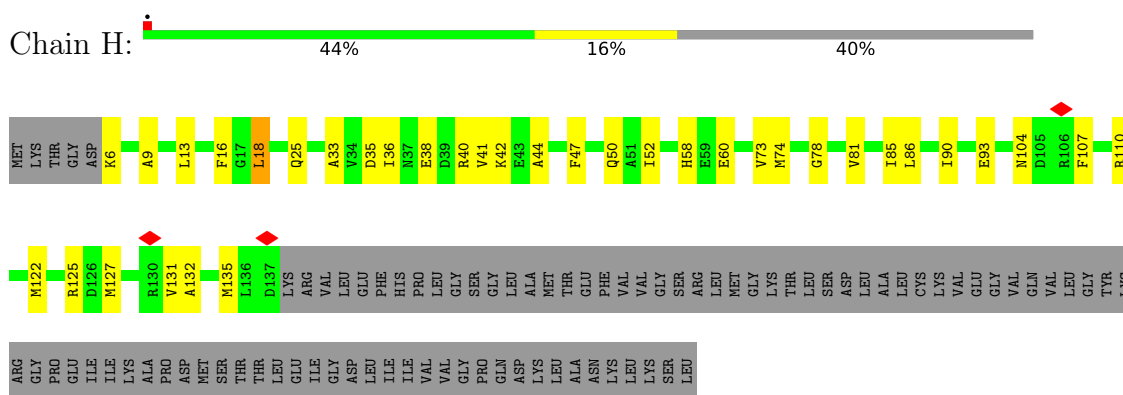
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Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total 1	O 1	0
7	B	3	Total 3	O 3	0
7	J	7	Total 7	O 7	0
7	L	1	Total 1	O 1	0
7	M	14	Total 14	O 14	0

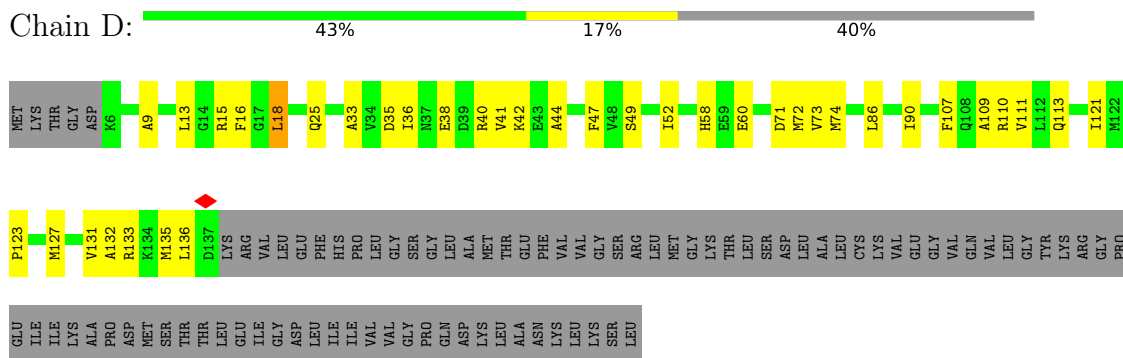
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

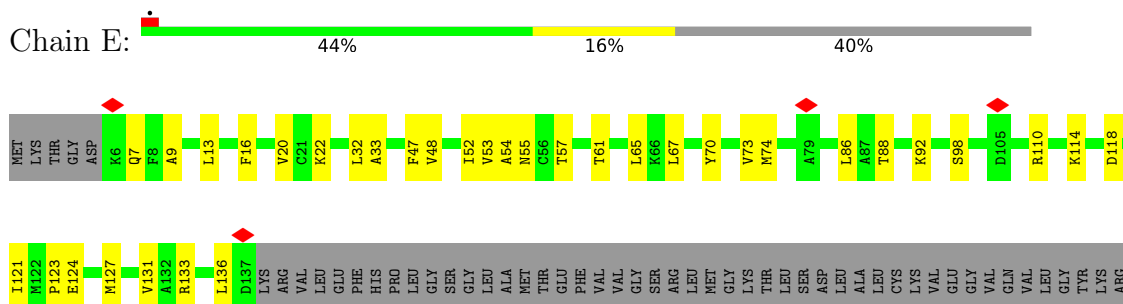
- Molecule 1: Ktr system potassium uptake protein A



- Molecule 1: Ktr system potassium uptake protein A

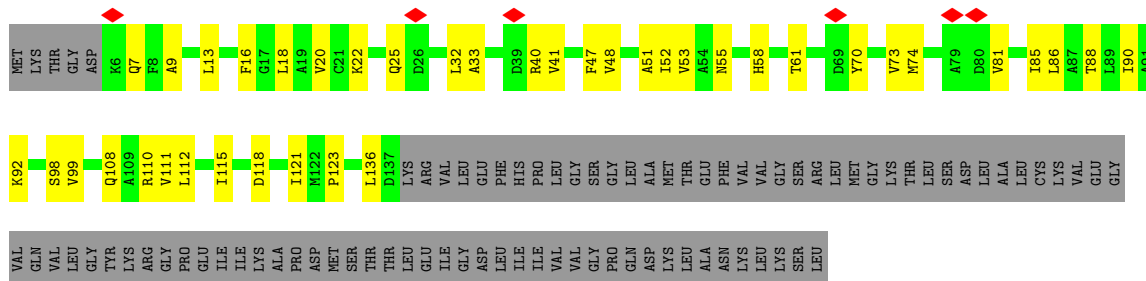
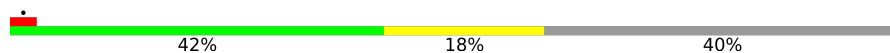


- Molecule 1: Ktr system potassium uptake protein A



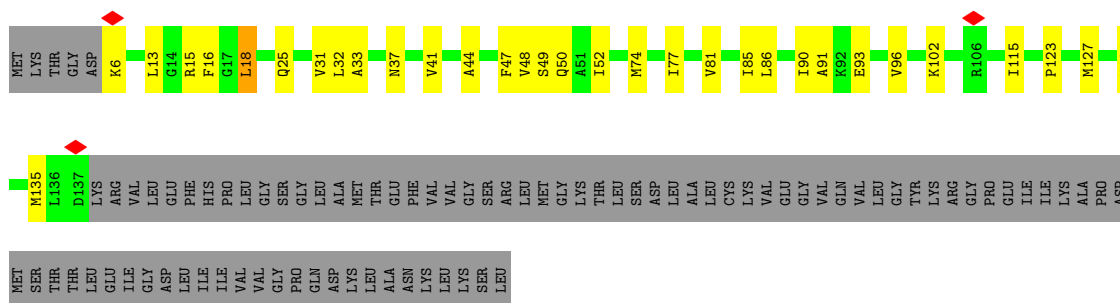
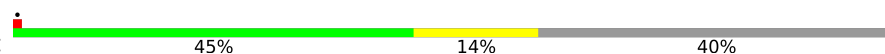
- Molecule 1: Ktr system potassium uptake protein A

Chain F:



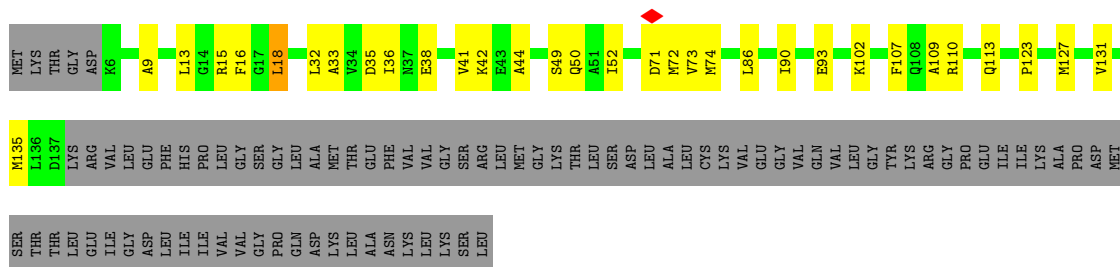
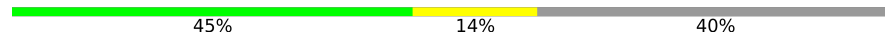
- Molecule 1: Ktr system potassium uptake protein A

Chain A:



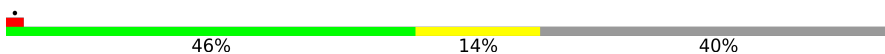
- Molecule 1: Ktr system potassium uptake protein A

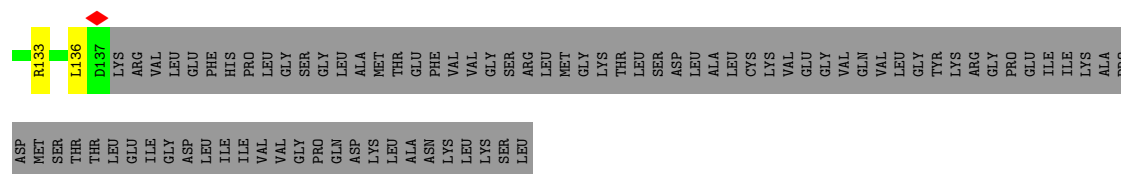
Chain B:



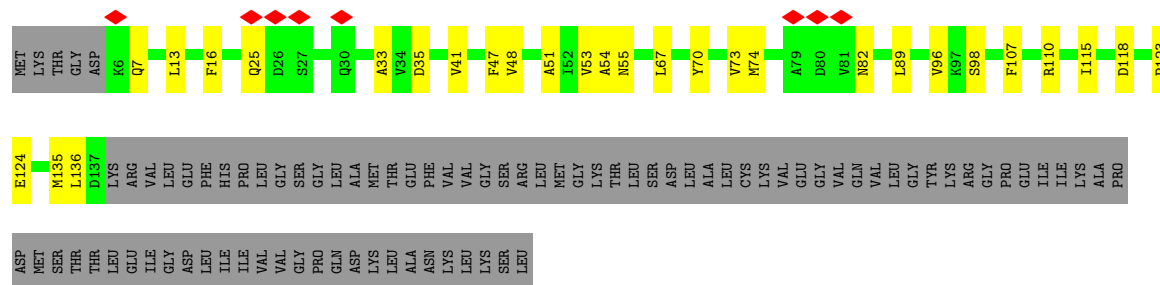
- Molecule 1: Ktr system potassium uptake protein A

Chain J:

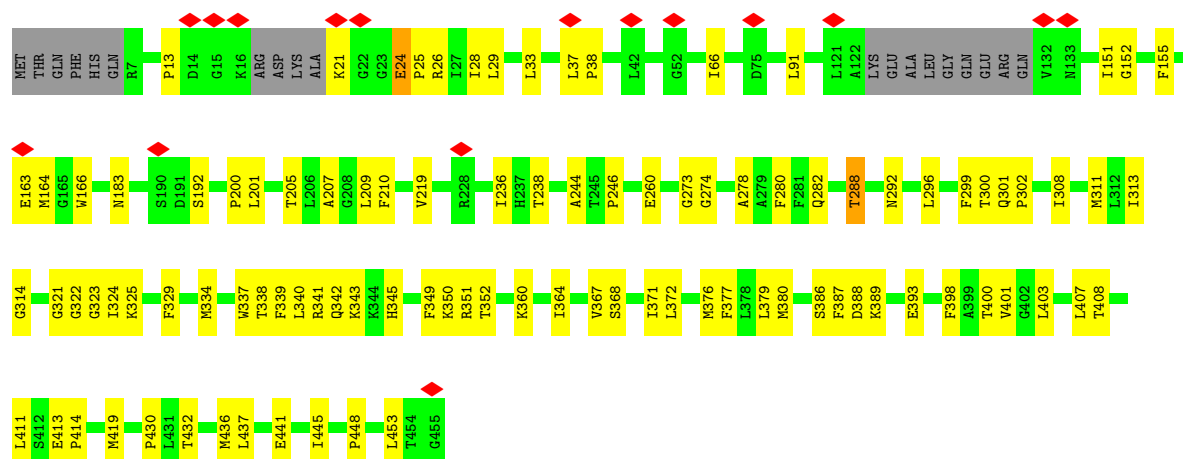




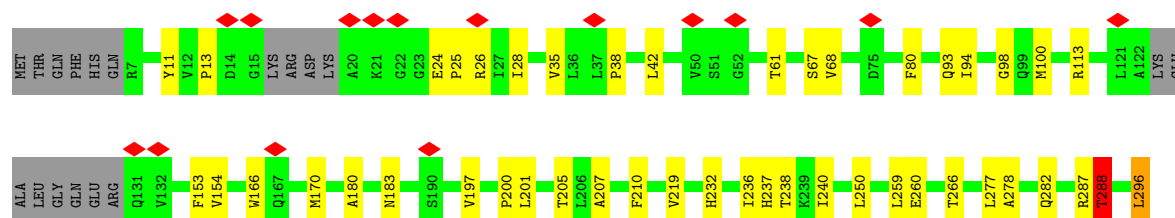
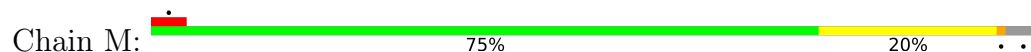
• Molecule 1: Ktr system potassium uptake protein A

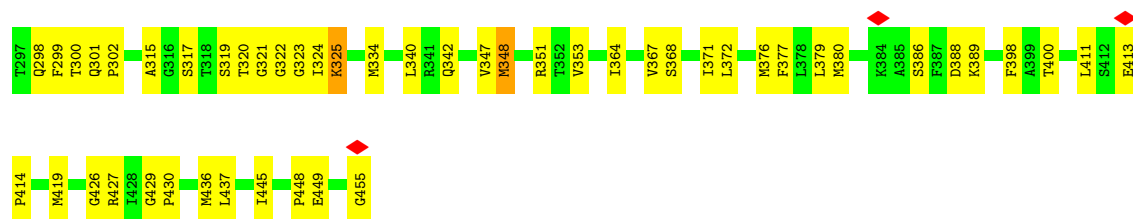


• Molecule 2: Ktr system potassium uptake protein B



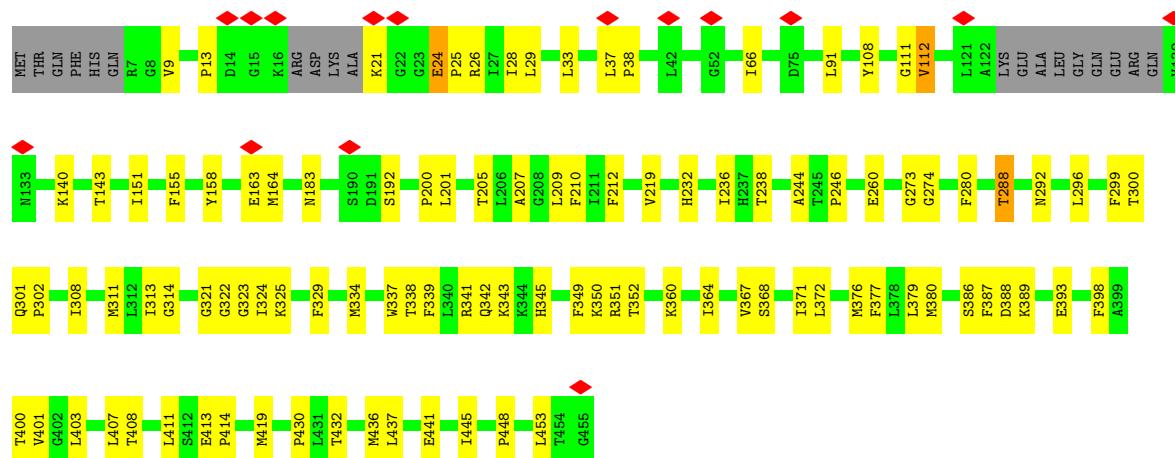
• Molecule 2: Ktr system potassium uptake protein B





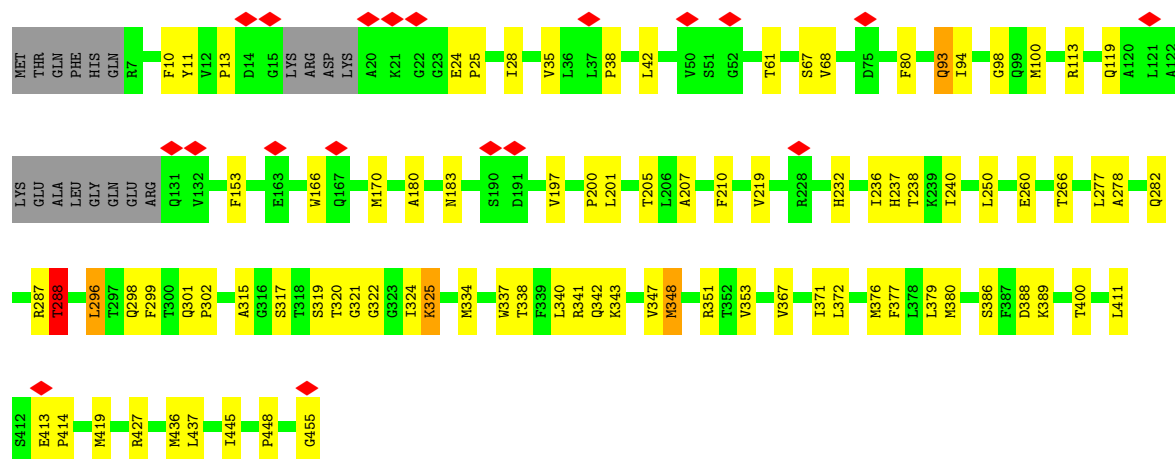
• Molecule 2: Ktr system potassium uptake protein B

Chain C: 73% 22%



• Molecule 2: Ktr system potassium uptake protein B

Chain G: 76% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	73965	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60168	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.050	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	299.16, 299.16, 299.16	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83100003, 0.83100003, 0.83100003	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ADP, LMT

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	0.31	0/965	0.46	0/1303
1	B	0.34	0/980	0.50	0/1322
1	D	0.34	0/965	0.49	0/1303
1	E	0.29	0/947	0.41	0/1282
1	F	0.34	0/972	0.57	0/1311
1	H	0.25	0/990	0.42	0/1334
1	J	0.13	0/943	0.30	0/1275
1	L	0.12	0/954	0.27	0/1289
2	C	0.42	1/3375 (0.0%)	0.57	1/4587 (0.0%)
2	G	0.35	0/3366	0.54	0/4581
2	I	0.36	0/3368	0.54	0/4581
2	M	0.36	0/3361	0.54	0/4570
All	All	0.34	1/21186 (0.0%)	0.51	1/28738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	111	GLY	C-N	9.88	1.46	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	112	VAL	CA-C-O	5.35	126.52	120.85

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	956	0	970	25	0
1	B	971	0	993	28	0
1	D	956	0	970	33	0
1	E	939	0	936	32	0
1	F	963	0	989	38	0
1	H	983	0	1006	30	0
1	J	934	0	941	25	0
1	L	948	0	961	34	0
2	C	3295	0	3409	117	0
2	G	3289	0	3382	83	0
2	I	3288	0	3396	109	0
2	M	3286	0	3397	138	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
4	H	27	0	12	1	0
4	J	27	0	12	1	0
4	L	27	0	12	1	0
5	A	35	0	45	0	0
5	C	350	0	452	53	0
5	G	280	0	362	16	0
5	I	350	0	453	54	0
5	M	245	0	317	72	0
6	C	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	1	0	0	0	0
7	B	3	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	I	13	0	0	0	0
7	J	7	0	0	0	0
7	L	1	0	0	0	0
7	M	14	0	0	1	0
All	All	22339	0	23075	623	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 14.

All (623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:430:PRO:HG3	5:M:508:LMT:C8	1.51	1.41
2:M:430:PRO:HG3	5:M:508:LMT:C7	1.53	1.36
2:M:398:PHE:CE2	5:M:508:LMT:C9	2.30	1.15
2:M:430:PRO:HG3	5:M:508:LMT:H81	1.23	1.14
2:M:26:ARG:HA	5:M:508:LMT:H6'2	1.28	1.14
2:M:398:PHE:CE2	5:M:508:LMT:H92	1.88	1.09
2:M:430:PRO:CG	5:M:508:LMT:H81	1.81	1.08
2:C:26:ARG:HA	5:C:504:LMT:H6'2	1.34	1.08
2:M:430:PRO:HG3	5:M:508:LMT:H71	1.34	1.07
1:L:89:LEU:HD21	1:L:115:ILE:HD12	1.33	1.04
2:I:26:ARG:HA	5:I:503:LMT:H6'2	1.34	1.04
2:M:323:GLY:HA2	5:M:508:LMT:H123	1.42	1.02
1:E:47:PHE:CD2	1:E:47:PHE:CZ	2.39	1.01
2:M:398:PHE:CZ	5:M:508:LMT:H92	1.99	0.98
2:M:430:PRO:CG	5:M:508:LMT:H71	1.93	0.97
2:M:430:PRO:CG	5:M:508:LMT:C7	2.42	0.96
2:M:398:PHE:HE2	5:M:508:LMT:C9	1.75	0.96
2:M:323:GLY:C	5:M:508:LMT:H111	1.93	0.94
2:M:430:PRO:CG	5:M:508:LMT:C8	2.39	0.93
2:M:324:ILE:HG22	5:M:508:LMT:H82	1.50	0.93
2:M:398:PHE:HE2	5:M:508:LMT:H91	1.36	0.90
2:M:430:PRO:HD3	5:M:508:LMT:H62	1.58	0.85
1:L:89:LEU:CD2	1:L:115:ILE:HG23	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:323:GLY:H	5:C:504:LMT:H123	1.42	0.84
2:I:323:GLY:H	5:I:503:LMT:H123	1.42	0.83
1:H:50:GLN:CG	1:H:50:GLN:NE2	2.42	0.83
1:L:82:ASN:CB	1:L:82:ASN:ND2	2.42	0.83
2:I:334:MET:HE2	2:I:334:MET:HA	1.61	0.82
2:C:334:MET:HE2	2:C:334:MET:HA	1.61	0.82
1:J:82:ASN:ND2	1:L:107:PHE:HB3	1.95	0.82
1:B:41:VAL:HG12	2:C:448:PRO:HG3	1.62	0.81
2:I:342:GLN:NE2	5:M:508:LMT:O3B	2.13	0.81
2:C:430:PRO:HG3	5:C:504:LMT:H81	1.63	0.81
1:L:89:LEU:HD23	1:L:115:ILE:HG23	1.61	0.81
2:M:25:PRO:HB2	5:M:508:LMT:H4B	1.61	0.81
1:H:18:LEU:HD11	1:H:44:ALA:HB2	1.64	0.80
2:I:430:PRO:HG3	5:I:503:LMT:H81	1.63	0.80
2:C:430:PRO:HG3	5:C:504:LMT:C8	2.12	0.80
2:I:430:PRO:HG3	5:I:503:LMT:C8	2.12	0.79
2:C:398:PHE:CE2	5:C:504:LMT:H92	2.19	0.78
2:M:364:ILE:HG23	5:M:508:LMT:H72	1.65	0.78
1:D:18:LEU:HD11	1:D:44:ALA:HB2	1.65	0.78
2:I:398:PHE:CE2	5:I:503:LMT:H92	2.19	0.78
1:E:114:LYS:HE3	1:F:90:ILE:HD13	1.67	0.77
2:M:323:GLY:HA2	5:M:508:LMT:C12	2.14	0.77
2:M:320:THR:O	2:M:427:ARG:NH2	2.19	0.76
2:C:21:LYS:HB3	2:C:441:GLU:HG2	1.68	0.76
2:I:21:LYS:HB3	2:I:441:GLU:HG2	1.68	0.75
2:C:379:LEU:HD11	2:C:419:MET:HE3	1.69	0.75
2:G:320:THR:O	2:G:427:ARG:NH2	2.19	0.75
2:M:430:PRO:CB	5:M:508:LMT:H71	2.16	0.75
2:I:379:LEU:HD11	2:I:419:MET:HE3	1.69	0.74
1:D:41:VAL:HG12	2:G:448:PRO:HG3	1.69	0.74
1:D:127:MET:HG2	1:E:127:MET:HG2	1.70	0.73
5:C:504:LMT:O3B	2:G:342:GLN:NE2	2.21	0.73
5:I:503:LMT:O3B	2:M:342:GLN:NE2	2.21	0.73
2:C:393:GLU:HG3	2:C:407:LEU:HB3	1.70	0.73
2:M:26:ARG:CA	5:M:508:LMT:H6'2	2.15	0.73
2:M:426:GLY:O	5:M:508:LMT:C12	2.36	0.73
2:C:311:MET:HG2	2:C:401:VAL:HG21	1.71	0.72
2:I:430:PRO:HG3	5:I:503:LMT:C7	2.20	0.72
2:M:430:PRO:CG	5:M:508:LMT:H102	2.19	0.72
2:I:209:LEU:HD23	5:I:505:LMT:H111	1.71	0.72
2:I:311:MET:HG2	2:I:401:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:393:GLU:HG3	2:I:407:LEU:HB3	1.70	0.72
2:C:209:LEU:HD23	5:C:505:LMT:H111	1.71	0.71
2:M:398:PHE:CE2	5:M:508:LMT:H91	2.13	0.71
2:C:288:THR:HG21	2:C:321:GLY:HA2	1.73	0.71
2:M:100:MET:HE3	2:M:319:SER:HA	1.73	0.71
2:C:430:PRO:HG3	5:C:504:LMT:C7	2.20	0.70
1:H:50:GLN:NE2	1:H:50:GLN:OE1	2.24	0.70
1:F:41:VAL:HG12	2:C:13:PRO:HG3	1.73	0.70
2:M:436:MET:HE1	5:M:508:LMT:H4'	1.74	0.70
1:H:50:GLN:CG	1:H:50:GLN:OE1	2.39	0.69
2:I:288:THR:HG21	2:I:321:GLY:HA2	1.73	0.69
1:L:82:ASN:CB	1:L:82:ASN:OD1	2.40	0.69
2:M:278:ALA:O	2:M:282:GLN:NE2	2.25	0.69
1:L:82:ASN:ND2	1:L:82:ASN:OD1	2.24	0.69
2:G:278:ALA:O	2:G:282:GLN:NE2	2.25	0.69
2:M:430:PRO:CD	5:M:508:LMT:H62	2.22	0.69
2:G:100:MET:HE3	2:G:319:SER:HA	1.73	0.69
2:G:379:LEU:HD11	2:G:419:MET:HE3	1.74	0.68
2:M:398:PHE:CE2	5:M:508:LMT:C10	2.77	0.68
2:M:379:LEU:HD11	2:M:419:MET:HE3	1.74	0.68
1:B:18:LEU:HD11	1:B:44:ALA:HB2	1.74	0.68
2:I:350:LYS:HE2	5:I:508:LMT:H3B	1.76	0.68
2:I:436:MET:HB3	2:M:342:GLN:HG2	1.77	0.67
2:M:436:MET:CE	5:M:508:LMT:H4'	2.23	0.67
2:C:350:LYS:HE2	5:C:509:LMT:H3B	1.75	0.67
1:H:41:VAL:HG12	2:M:448:PRO:HG3	1.76	0.67
2:C:108:TYR:O	2:C:112:VAL:HG23	1.94	0.67
2:M:411:LEU:HD21	2:M:419:MET:HG3	1.77	0.67
2:C:436:MET:HB3	2:G:342:GLN:HG2	1.77	0.67
2:G:411:LEU:HD21	2:G:419:MET:HG3	1.77	0.67
2:I:372:LEU:O	2:I:376:MET:HG3	1.95	0.67
2:C:398:PHE:HE2	5:C:504:LMT:H92	1.60	0.67
2:G:236:ILE:HD11	2:G:348:MET:HB2	1.77	0.67
1:D:127:MET:HG3	1:E:123:PRO:HA	1.75	0.67
2:I:183:ASN:HB3	2:I:288:THR:HG22	1.78	0.66
1:A:102:LYS:HD2	1:A:123:PRO:HG2	1.76	0.66
2:M:371:ILE:HD11	5:M:508:LMT:H22	1.77	0.66
2:G:24:GLU:N	2:G:25:PRO:HD2	2.10	0.66
2:M:236:ILE:HD11	2:M:348:MET:HB2	1.77	0.66
2:M:24:GLU:N	2:M:25:PRO:HD2	2.10	0.66
2:C:200:PRO:CG	5:C:506:LMT:H3'	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:372:LEU:O	2:C:376:MET:HG3	1.95	0.66
1:F:22:LYS:HE2	1:F:47:PHE:CE2	2.30	0.66
2:I:200:PRO:CG	5:I:506:LMT:H3'	2.26	0.66
2:C:183:ASN:HB3	2:C:288:THR:HG22	1.78	0.66
2:C:432:THR:HG22	2:C:436:MET:HE3	1.77	0.65
2:M:317:SER:HA	2:M:325:LYS:HG2	1.78	0.65
2:I:364:ILE:HG23	5:I:503:LMT:H72	1.78	0.65
2:G:183:ASN:HB3	2:G:288:THR:HG23	1.78	0.65
2:M:183:ASN:HB3	2:M:288:THR:HG23	1.78	0.65
2:M:430:PRO:CD	5:M:508:LMT:H102	2.27	0.65
2:I:398:PHE:HE2	5:I:503:LMT:H92	1.60	0.65
1:H:110:ARG:NE	1:B:93:GLU:OE2	2.29	0.65
5:I:510:LMT:H32	5:M:508:LMT:H3'	1.77	0.65
5:C:504:LMT:H3'	5:G:508:LMT:H32	1.77	0.65
1:L:89:LEU:HD21	1:L:115:ILE:HG23	1.79	0.64
2:I:432:THR:HG22	2:I:436:MET:HE3	1.77	0.64
5:I:503:LMT:H3'	5:I:511:LMT:H32	1.77	0.64
1:J:40:ARG:NH2	4:J:301:ADP:O1B	2.25	0.64
2:M:426:GLY:O	5:M:508:LMT:H121	1.96	0.64
2:G:321:GLY:HA2	2:G:427:ARG:HH12	1.63	0.64
1:E:114:LYS:HE3	1:F:90:ILE:CD1	2.27	0.64
2:C:364:ILE:HG23	5:C:504:LMT:H72	1.78	0.64
2:M:348:MET:HA	5:M:505:LMT:H3'	1.80	0.64
2:C:200:PRO:HG2	5:C:506:LMT:H3'	1.79	0.63
2:I:340:LEU:HD22	5:M:508:LMT:O2'	1.98	0.63
2:M:321:GLY:HA2	2:M:427:ARG:HH12	1.63	0.63
2:G:317:SER:HA	2:G:325:LYS:HG2	1.78	0.63
2:M:25:PRO:HB2	5:M:508:LMT:C4B	2.29	0.63
2:G:348:MET:HA	5:G:507:LMT:H3'	1.80	0.63
1:D:110:ARG:NE	1:A:93:GLU:OE2	2.31	0.63
1:E:74:MET:HE1	1:E:121:ILE:HD13	1.81	0.62
2:I:200:PRO:HG2	5:I:506:LMT:H3'	1.79	0.62
2:M:430:PRO:HG2	5:M:508:LMT:H81	1.76	0.62
2:M:288:THR:HG21	2:M:321:GLY:HA3	1.82	0.61
2:M:426:GLY:O	5:M:508:LMT:H122	2.00	0.61
2:I:219:VAL:HG13	2:I:238:THR:HG23	1.83	0.61
1:D:38:GLU:HG2	1:D:42:LYS:HE2	1.82	0.60
2:G:288:THR:HG21	2:G:321:GLY:HA3	1.82	0.60
2:C:26:ARG:CA	5:C:504:LMT:H6'2	2.21	0.60
1:D:13:LEU:HD22	1:D:18:LEU:HD13	1.84	0.60
1:A:127:MET:HG2	1:L:123:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HA	4:A:1002:ADP:H5'2	1.84	0.60
1:L:53:VAL:HG23	2:G:13:PRO:HD3	1.84	0.60
2:C:219:VAL:HG13	2:C:238:THR:HG23	1.83	0.60
2:C:338:THR:HG23	2:C:343:LYS:HB2	1.83	0.60
1:H:38:GLU:HG2	1:H:42:LYS:HE3	1.83	0.60
2:I:338:THR:HG23	2:I:343:LYS:HB2	1.83	0.59
2:G:296:LEU:H	2:G:296:LEU:HD22	1.67	0.59
2:G:348:MET:HG3	2:G:353:VAL:CG2	2.32	0.59
1:L:55:ASN:ND2	2:G:119:GLN:OE1	2.33	0.59
2:M:348:MET:HG3	2:M:353:VAL:CG2	2.32	0.59
2:M:296:LEU:HD22	2:M:296:LEU:H	1.67	0.59
1:A:16:PHE:HE2	1:A:74:MET:HE2	1.68	0.59
2:M:154:VAL:HG12	5:M:507:LMT:H92	1.82	0.59
2:M:398:PHE:CE2	5:M:508:LMT:H101	2.37	0.59
2:I:26:ARG:CA	5:I:503:LMT:H6'2	2.21	0.59
2:M:430:PRO:CA	5:M:508:LMT:H71	2.32	0.59
1:H:93:GLU:OE2	1:B:110:ARG:NE	2.35	0.59
2:I:386:SER:OG	2:I:388:ASP:OD1	2.21	0.59
2:I:430:PRO:HG3	5:I:503:LMT:H71	1.85	0.59
2:C:386:SER:OG	2:C:388:ASP:OD1	2.21	0.59
1:F:86:LEU:O	1:F:90:ILE:HG12	2.03	0.58
5:C:504:LMT:O2'	2:G:340:LEU:HD22	2.04	0.58
1:J:53:VAL:HG23	2:M:13:PRO:HD3	1.85	0.58
1:H:78:GLY:O	1:H:104:ASN:ND2	2.36	0.58
1:B:127:MET:HG2	1:J:123:PRO:HA	1.84	0.58
5:I:503:LMT:O2'	2:M:340:LEU:HD22	2.04	0.58
1:F:85:ILE:HD13	1:F:111:VAL:HG11	1.86	0.57
2:I:436:MET:HE1	5:I:503:LMT:H4'	1.86	0.57
1:B:9:ALA:HB3	1:B:73:VAL:HG22	1.86	0.57
2:C:201:LEU:HD12	5:C:505:LMT:O2'	2.04	0.57
1:B:41:VAL:CG1	2:C:448:PRO:HG3	2.34	0.57
1:L:89:LEU:HD23	1:L:115:ILE:CG2	2.32	0.57
2:M:398:PHE:HZ	5:M:508:LMT:H61	1.68	0.57
2:C:37:LEU:N	2:C:38:PRO:HD2	2.20	0.57
1:E:53:VAL:HG23	2:I:13:PRO:HD3	1.86	0.57
1:J:82:ASN:HD21	1:L:107:PHE:HB3	1.65	0.57
2:C:430:PRO:HG3	5:C:504:LMT:H71	1.85	0.57
1:B:16:PHE:HE2	1:B:74:MET:HE2	1.69	0.56
2:G:372:LEU:O	2:G:376:MET:HG3	2.05	0.56
2:C:9:VAL:CG1	2:C:112:VAL:HG13	2.35	0.56
2:C:398:PHE:CE2	5:C:504:LMT:C9	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:LYS:NZ	1:F:136:LEU:O	2.37	0.56
2:I:288:THR:HG21	2:I:321:GLY:CA	2.36	0.56
5:I:510:LMT:H81	2:M:371:ILE:HG23	1.86	0.56
1:D:9:ALA:HB3	1:D:73:VAL:HG22	1.88	0.56
2:I:37:LEU:N	2:I:38:PRO:HD2	2.20	0.56
2:G:324:ILE:O	2:G:325:LYS:HB2	2.05	0.56
2:I:448:PRO:HG3	1:A:41:VAL:HG12	1.87	0.56
1:H:50:GLN:NE2	1:H:50:GLN:CB	2.69	0.56
2:G:315:ALA:H	2:G:322:GLY:HA2	1.71	0.56
2:I:201:LEU:HD12	5:I:505:LMT:O2'	2.04	0.56
2:C:436:MET:HE1	5:C:504:LMT:H4'	1.86	0.56
5:C:511:LMT:H81	2:G:371:ILE:HG23	1.86	0.56
2:I:398:PHE:CE2	5:I:503:LMT:C9	2.89	0.55
2:M:372:LEU:O	2:M:376:MET:HG3	2.05	0.55
2:C:288:THR:HG21	2:C:321:GLY:CA	2.36	0.55
1:E:32:LEU:HD11	1:E:52:ILE:HD12	1.87	0.55
1:F:74:MET:HE1	1:F:121:ILE:HD13	1.88	0.55
2:I:323:GLY:C	5:I:503:LMT:H111	2.31	0.55
2:C:244:ALA:HB2	5:C:509:LMT:H22	1.87	0.55
2:M:315:ALA:H	2:M:322:GLY:HA2	1.71	0.55
2:M:324:ILE:O	2:M:325:LYS:HB2	2.05	0.55
1:E:88:THR:O	1:E:92:LYS:HG2	2.06	0.55
1:F:40:ARG:NH1	4:F:301:ADP:O3'	2.39	0.55
2:M:348:MET:CB	5:M:505:LMT:O2'	2.55	0.55
1:D:131:VAL:O	1:D:135:MET:HG3	2.07	0.55
1:D:35:ASP:OD1	1:D:36:ILE:N	2.39	0.55
2:C:323:GLY:C	5:C:504:LMT:H111	2.31	0.55
2:I:244:ALA:HB2	5:I:508:LMT:H22	1.88	0.55
2:I:246:PRO:HG3	5:I:509:LMT:H112	1.89	0.55
2:I:411:LEU:HD11	2:I:419:MET:HG3	1.88	0.55
2:M:323:GLY:O	5:M:508:LMT:H111	2.07	0.55
2:C:411:LEU:HD11	2:C:419:MET:HG3	1.88	0.55
2:M:429:GLY:HA3	5:M:508:LMT:H42	1.89	0.55
1:B:52:ILE:HG23	2:C:445:ILE:HG23	1.88	0.55
2:M:323:GLY:HA2	5:M:508:LMT:C11	2.37	0.55
2:G:348:MET:HB3	5:G:507:LMT:O2'	2.07	0.54
2:M:348:MET:HB3	5:M:505:LMT:O2'	2.07	0.54
1:J:57:THR:HG22	1:L:110:ARG:HH12	1.72	0.54
1:A:31:VAL:HG13	1:A:48:VAL:HG13	1.89	0.54
1:E:16:PHE:HE2	1:E:74:MET:HE2	1.73	0.54
2:G:348:MET:CB	5:G:507:LMT:O2'	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:323:GLY:N	5:I:503:LMT:H123	2.19	0.54
1:F:53:VAL:HG23	2:C:13:PRO:HD3	1.90	0.53
1:F:88:THR:O	1:F:92:LYS:HG2	2.07	0.53
2:M:236:ILE:HD12	2:M:351:ARG:HB2	1.90	0.53
1:D:52:ILE:HG23	2:G:445:ILE:HG23	1.89	0.53
1:F:112:LEU:HD23	1:F:115:ILE:HD11	1.90	0.53
1:J:16:PHE:HE2	1:J:74:MET:HE2	1.73	0.53
2:C:430:PRO:HG3	5:C:504:LMT:H102	1.90	0.53
2:I:371:ILE:HD11	5:I:503:LMT:H22	1.91	0.53
1:A:18:LEU:HD11	1:A:44:ALA:HB2	1.91	0.53
2:G:338:THR:HG23	2:G:343:LYS:HB2	1.90	0.53
2:G:388:ASP:OD1	2:G:389:LYS:N	2.42	0.53
1:B:35:ASP:OD1	1:B:36:ILE:N	2.42	0.53
2:M:364:ILE:HG23	5:M:508:LMT:C7	2.37	0.53
2:C:246:PRO:HG3	5:C:510:LMT:H112	1.89	0.53
1:E:57:THR:HG22	1:F:110:ARG:HH22	1.74	0.53
2:M:430:PRO:HG3	5:M:508:LMT:C6	2.36	0.53
1:E:67:LEU:HA	1:E:70:TYR:HD2	1.73	0.53
2:M:388:ASP:OD1	2:M:389:LYS:N	2.42	0.53
2:M:430:PRO:HD3	5:M:508:LMT:H102	1.90	0.53
2:I:166:TRP:CD1	5:I:504:LMT:H6E	2.43	0.53
2:C:323:GLY:N	5:C:504:LMT:H123	2.19	0.53
2:C:430:PRO:HB2	2:G:455:GLY:OXT	2.09	0.52
2:G:386:SER:OG	2:G:388:ASP:OD1	2.25	0.52
1:B:13:LEU:HD22	1:B:18:LEU:HD13	1.91	0.52
1:A:13:LEU:HD11	1:A:33:ALA:HB1	1.91	0.52
1:H:131:VAL:O	1:H:135:MET:HG3	2.09	0.52
2:G:236:ILE:HD12	2:G:351:ARG:HB2	1.90	0.52
2:I:430:PRO:HB2	2:M:455:GLY:OXT	2.09	0.52
1:J:67:LEU:HA	1:J:70:TYR:HD2	1.74	0.52
1:L:25:GLN:HG3	1:L:47:PHE:O	2.09	0.52
1:F:55:ASN:OD1	4:F:301:ADP:N6	2.43	0.52
2:I:345:HIS:HB3	2:I:352:THR:HG23	1.92	0.52
2:I:432:THR:O	2:I:436:MET:HG3	2.10	0.52
1:H:40:ARG:NH2	4:H:1002:ADP:O1B	2.43	0.51
1:H:42:LYS:HE2	2:M:449:GLU:HB2	1.92	0.51
2:I:236:ILE:HD12	2:I:351[A]:ARG:HB2	1.92	0.51
2:I:400:THR:HG22	2:I:400:THR:O	2.11	0.51
2:C:432:THR:O	2:C:436:MET:HG3	2.10	0.51
1:A:32:LEU:HD13	1:A:50:GLN:HG3	1.92	0.51
2:C:400:THR:HG22	2:C:400:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:334:MET:HE2	5:G:507:LMT:H2'	1.93	0.51
2:I:430:PRO:HG3	5:I:503:LMT:H102	1.90	0.51
2:C:371:ILE:HD11	5:C:504:LMT:H22	1.91	0.51
1:E:7:GLN:HG2	1:E:70:TYR:CD1	2.46	0.51
1:F:16:PHE:HE2	1:F:74:MET:HE2	1.76	0.51
1:L:7:GLN:HG2	1:L:70:TYR:CD1	2.46	0.51
2:M:436:MET:HE1	5:M:508:LMT:C4'	2.40	0.51
2:C:236:ILE:HD12	2:C:351[A]:ARG:HB2	1.92	0.51
2:C:236:ILE:HD12	2:C:351[B]:ARG:HB2	1.93	0.51
1:B:15:ARG:CZ	1:J:124:GLU:HG3	2.41	0.51
1:L:55:ASN:OD1	4:L:301:ADP:N6	2.44	0.51
2:C:200:PRO:HG3	5:C:506:LMT:H3'	1.93	0.51
2:C:337:TRP:NE1	2:C:341:ARG:HH11	2.09	0.51
2:I:278:ALA:O	2:I:282:GLN:HG2	2.11	0.50
1:F:7:GLN:HG2	1:F:70:TYR:CD1	2.46	0.50
1:F:33:ALA:HB2	1:F:48:VAL:HG11	1.93	0.50
1:B:38:GLU:HG2	1:B:42:LYS:HE2	1.93	0.50
2:C:360:LYS:HA	2:C:437:LEU:HD13	1.93	0.50
1:F:18:LEU:HG	1:F:22:LYS:HE3	1.92	0.50
2:C:345:HIS:HB3	2:C:352:THR:HG23	1.92	0.50
2:G:200:PRO:HG2	5:G:504:LMT:H3'	1.93	0.50
2:I:337:TRP:NE1	2:I:341:ARG:HH11	2.09	0.50
1:J:33:ALA:HB2	1:J:48:VAL:HG11	1.92	0.50
2:M:11:TYR:CZ	2:M:113:ARG:HG2	2.47	0.50
2:C:430:PRO:CB	5:C:504:LMT:H71	2.42	0.50
1:J:7:GLN:HG2	1:J:70:TYR:CD1	2.46	0.50
2:M:200:PRO:HG2	5:M:503:LMT:H3'	1.93	0.50
1:F:16:PHE:O	1:F:20:VAL:HG23	2.12	0.50
2:I:201:LEU:HB2	5:I:505:LMT:O2'	2.11	0.50
2:I:273:GLY:C	5:I:506:LMT:H6E	2.37	0.50
2:M:334:MET:HE2	5:M:505:LMT:H2'	1.93	0.50
2:C:9:VAL:HG13	2:C:112:VAL:HG13	1.94	0.50
2:C:371:ILE:HG23	5:G:508:LMT:H81	1.94	0.50
2:C:201:LEU:HB2	5:C:505:LMT:O2'	2.11	0.50
1:E:33:ALA:HB2	1:E:48:VAL:HG11	1.94	0.49
2:I:360:LYS:HA	2:I:437:LEU:HD13	1.93	0.49
2:I:371:ILE:HG23	5:I:511:LMT:H81	1.94	0.49
2:C:209:LEU:HD21	5:C:505:LMT:H122	1.94	0.49
2:I:236:ILE:HD12	2:I:351[B]:ARG:HB2	1.93	0.49
1:D:18:LEU:HD11	1:D:44:ALA:CB	2.39	0.49
1:D:16:PHE:HE2	1:D:74:MET:HE2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:183:ASN:OD1	2:M:288:THR:HG22	2.13	0.49
2:I:430:PRO:CB	5:I:503:LMT:H71	2.42	0.49
2:C:334:MET:HA	2:C:334:MET:CE	2.40	0.49
2:G:11:TYR:CZ	2:G:113:ARG:HG2	2.47	0.49
1:E:16:PHE:CE2	1:E:74:MET:HE2	2.48	0.49
1:A:6:LYS:NZ	1:L:136:LEU:O	2.45	0.49
2:M:288:THR:HG23	7:M:610:HOH:O	2.12	0.49
2:I:398:PHE:O	5:I:503:LMT:H121	2.13	0.49
1:A:15:ARG:CZ	1:L:124:GLU:HG3	2.43	0.49
1:B:52:ILE:CG2	2:C:445:ILE:HG23	2.42	0.49
2:C:430:PRO:HB2	2:G:455:GLY:C	2.38	0.49
1:F:16:PHE:CE2	1:F:74:MET:HE2	2.47	0.48
2:I:155:PHE:CD2	5:I:505:LMT:H51	2.48	0.48
1:J:110:ARG:O	1:J:114:LYS:HG3	2.13	0.48
2:C:314:GLY:HA3	2:C:323:GLY:HA3	1.96	0.48
2:C:273:GLY:C	5:C:506:LMT:H6E	2.37	0.48
2:C:398:PHE:O	5:C:504:LMT:H121	2.13	0.48
1:F:92:LYS:CD	1:F:99:VAL:HG21	2.43	0.48
2:I:388:ASP:OD1	2:I:389:LYS:N	2.47	0.48
1:A:131:VAL:O	1:A:135:MET:HG3	2.14	0.48
1:H:16:PHE:HE2	1:H:74:MET:HE2	1.78	0.48
2:I:209:LEU:HD21	5:I:505:LMT:H122	1.94	0.48
2:I:314:GLY:HA3	2:I:323:GLY:HA3	1.96	0.48
1:L:33:ALA:HB2	1:L:48:VAL:HG11	1.95	0.48
2:M:348:MET:SD	5:M:505:LMT:O2'	2.71	0.48
2:G:348:MET:HA	5:G:507:LMT:O2'	2.14	0.48
1:H:127:MET:HG2	1:F:123:PRO:HA	1.95	0.48
2:C:324:ILE:HD11	2:C:329:PHE:HB2	1.96	0.48
2:C:430:PRO:CG	5:C:504:LMT:H102	2.44	0.48
2:I:324:ILE:HD11	2:I:329:PHE:HB2	1.96	0.48
1:F:92:LYS:HD3	1:F:99:VAL:CG2	2.44	0.48
1:L:13:LEU:HG	1:L:35:ASP:HB2	1.95	0.48
2:C:155:PHE:CD2	5:C:505:LMT:H51	2.48	0.48
2:C:388:ASP:OD1	2:C:389:LYS:N	2.47	0.48
2:G:183:ASN:OD1	2:G:288:THR:HG22	2.13	0.47
2:I:430:PRO:HB2	2:M:455:GLY:C	2.38	0.47
2:I:430:PRO:CG	5:I:503:LMT:H102	2.44	0.47
2:M:348:MET:HA	5:M:505:LMT:O2'	2.14	0.47
1:F:41:VAL:CG1	2:C:13:PRO:HG3	2.42	0.47
2:I:200:PRO:HG3	5:I:506:LMT:H3'	1.93	0.47
1:A:25:GLN:HG2	1:A:47:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:323:GLY:CA	5:M:508:LMT:H111	2.44	0.47
1:H:25:GLN:HG2	1:H:47:PHE:O	2.15	0.47
2:C:430:PRO:CG	5:C:504:LMT:H71	2.44	0.47
2:G:153:PHE:HZ	2:G:170:MET:HE3	1.79	0.47
2:M:367:VAL:O	2:M:371:ILE:HG13	2.15	0.47
2:C:260:GLU:OE2	2:C:300:THR:OG1	2.31	0.47
1:F:112:LEU:HA	1:F:115:ILE:HG12	1.96	0.47
2:I:430:PRO:CG	5:I:503:LMT:H71	2.44	0.47
1:L:16:PHE:HE2	1:L:74:MET:HE2	1.79	0.47
2:M:153:PHE:HZ	2:M:170:MET:HE3	1.79	0.47
2:M:324:ILE:HG22	5:M:508:LMT:C8	2.34	0.47
2:G:348:MET:SD	5:G:507:LMT:O2'	2.71	0.47
2:I:436:MET:CE	5:I:503:LMT:H4'	2.45	0.47
2:M:166:TRP:O	2:M:170:MET:HG2	2.15	0.47
1:E:65:LEU:O	1:E:67:LEU:N	2.48	0.47
2:M:296:LEU:HD22	2:M:296:LEU:N	2.29	0.47
1:J:9:ALA:HB3	1:J:73:VAL:HG22	1.97	0.46
1:J:82:ASN:HD22	1:L:107:PHE:HB3	1.75	0.46
2:C:29:LEU:HD13	5:C:504:LMT:O6'	2.15	0.46
2:C:308:ILE:HA	2:C:311:MET:HE2	1.97	0.46
1:D:49:SER:O	2:C:232:HIS:NE2	2.40	0.46
2:I:308:ILE:HA	2:I:311:MET:HE2	1.97	0.46
2:C:158:TYR:HA	5:C:503:LMT:H32	1.97	0.46
2:C:274:GLY:N	5:C:506:LMT:H6E	2.30	0.46
1:D:16:PHE:CZ	1:E:131:VAL:HG21	2.50	0.46
2:I:29:LEU:HD13	5:I:503:LMT:O6'	2.15	0.46
2:G:367:VAL:O	2:G:371:ILE:HG13	2.15	0.46
1:H:58:HIS:CE1	1:H:60:GLU:HB2	2.50	0.46
1:E:9:ALA:HB3	1:E:73:VAL:HG22	1.98	0.46
1:B:71:ASP:OD1	1:B:72:MET:N	2.49	0.46
1:J:16:PHE:CE2	1:J:74:MET:HE2	2.50	0.46
1:D:121:ILE:HG12	1:E:131:VAL:HG11	1.97	0.46
2:I:274:GLY:N	5:I:506:LMT:H6E	2.30	0.46
1:A:49:SER:O	2:M:232:HIS:NE2	2.41	0.46
2:C:436:MET:CE	5:C:504:LMT:H4'	2.45	0.46
1:D:123:PRO:HA	1:E:127:MET:HG3	1.98	0.46
2:M:219:VAL:HG13	2:M:238:THR:HG23	1.98	0.46
2:I:380:MET:HB3	2:M:302:PRO:HG3	1.97	0.46
2:M:386:SER:OG	2:M:388:ASP:OD1	2.25	0.46
2:C:151:ILE:CG2	5:C:505:LMT:H121	2.46	0.46
2:G:166:TRP:O	2:G:170:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:296:LEU:HD22	2:G:296:LEU:N	2.29	0.46
1:L:89:LEU:CD2	1:L:115:ILE:CG2	2.87	0.46
1:D:15:ARG:NH1	1:E:124:GLU:HG3	2.31	0.46
2:I:24:GLU:O	2:I:28:ILE:HG13	2.16	0.46
2:I:413:GLU:HB2	2:I:414:PRO:HD3	1.98	0.46
2:C:212:PHE:CZ	5:C:508:LMT:H81	2.50	0.46
2:C:342:GLN:HG2	2:G:436:MET:HB3	1.98	0.46
1:E:16:PHE:O	1:E:20:VAL:HG23	2.16	0.45
1:B:49:SER:O	2:G:232:HIS:NE2	2.38	0.45
2:G:240:ILE:HD11	2:G:348:MET:HE2	1.97	0.45
1:H:9:ALA:HB3	1:H:73:VAL:HG22	1.98	0.45
1:H:81:VAL:O	1:H:85:ILE:HD12	2.17	0.45
2:I:302:PRO:HG3	2:M:380:MET:HB3	1.98	0.45
1:J:36:ILE:HD13	1:J:55:ASN:HB2	1.99	0.45
2:M:400:THR:HG22	2:M:400:THR:O	2.17	0.45
2:G:400:THR:O	2:G:400:THR:HG22	2.17	0.45
1:D:40:ARG:NH1	4:D:1001:ADP:O3'	2.49	0.45
1:A:91:ALA:O	1:A:96:VAL:HG22	2.17	0.45
2:C:380:MET:HB3	2:G:302:PRO:HG3	1.98	0.45
2:G:94:ILE:O	2:G:98:GLY:HA3	2.16	0.45
2:G:205:THR:HA	5:G:503:LMT:H81	1.99	0.45
1:E:110:ARG:CZ	1:F:86:LEU:HD21	2.46	0.45
1:F:92:LYS:HD3	1:F:99:VAL:HG21	1.99	0.45
2:I:342:GLN:HG2	2:M:436:MET:HB3	1.98	0.45
1:B:13:LEU:HD21	1:B:33:ALA:HB1	1.98	0.45
2:C:24:GLU:O	2:C:28:ILE:HG13	2.16	0.45
5:C:508:LMT:H22	5:C:508:LMT:H52	1.56	0.45
1:D:13:LEU:HD21	1:D:33:ALA:HB1	1.98	0.45
2:I:151:ILE:CG2	5:I:505:LMT:H121	2.46	0.45
2:C:430:PRO:CG	5:C:504:LMT:H81	2.41	0.45
2:G:219:VAL:HG13	2:G:238:THR:HG23	1.98	0.45
2:M:240:ILE:HD11	2:M:348:MET:HE2	1.97	0.45
2:M:205:THR:HA	5:M:502:LMT:H81	1.99	0.45
1:D:111:VAL:HG13	1:A:115:ILE:HD11	1.99	0.45
1:J:14:GLY:HA2	1:J:40:ARG:NH1	2.32	0.45
1:L:13:LEU:HD11	1:L:33:ALA:HB1	1.99	0.45
2:M:67:SER:O	2:M:68:VAL:HG22	2.17	0.45
2:C:280:PHE:CD1	5:C:506:LMT:H81	2.52	0.45
2:C:302:PRO:HG3	2:G:380:MET:HB3	1.98	0.45
2:C:413:GLU:HB2	2:C:414:PRO:HD3	1.98	0.45
1:H:13:LEU:HD22	1:H:18:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:334:MET:HA	2:I:334:MET:CE	2.40	0.45
2:M:207:ALA:HA	2:M:210:PHE:CZ	2.52	0.45
2:M:430:PRO:CG	5:M:508:LMT:C10	2.93	0.45
2:G:413:GLU:HB3	2:G:414:PRO:HD3	1.99	0.45
1:E:55:ASN:OD1	4:E:301:ADP:N6	2.49	0.44
2:M:323:GLY:CA	5:M:508:LMT:C11	2.95	0.44
2:C:324:ILE:HG22	5:C:504:LMT:H82	1.99	0.44
2:I:207:ALA:HA	2:I:210:PHE:CZ	2.52	0.44
2:M:413:GLU:HB3	2:M:414:PRO:HD3	1.99	0.44
2:G:301:GLN:HB2	2:G:302:PRO:HD3	1.99	0.44
2:M:94:ILE:O	2:M:98:GLY:HA3	2.16	0.44
2:M:301:GLN:HB2	2:M:302:PRO:HD3	1.99	0.44
2:G:207:ALA:HA	2:G:210:PHE:CZ	2.52	0.44
1:E:22:LYS:HE2	1:E:47:PHE:CZ	2.52	0.44
1:E:98:SER:HA	1:E:118:ASP:OD2	2.18	0.44
1:F:98:SER:HA	1:F:118:ASP:OD2	2.17	0.44
1:F:25:GLN:HG2	1:F:47:PHE:O	2.18	0.44
2:I:260:GLU:OE2	2:I:300:THR:OG1	2.31	0.44
1:D:58:HIS:CE1	1:D:60:GLU:HB2	2.52	0.44
1:B:35:ASP:OD1	4:B:1001:ADP:O2'	2.34	0.44
2:I:324:ILE:HG22	5:I:503:LMT:H82	1.99	0.44
1:J:57:THR:HG21	1:L:107:PHE:HE1	1.83	0.44
2:C:207:ALA:HA	2:C:210:PHE:CZ	2.52	0.44
2:C:377:PHE:HE2	5:G:509:LMT:H72	1.82	0.44
2:G:67:SER:O	2:G:68:VAL:HG22	2.17	0.44
2:I:280:PHE:CD1	5:I:506:LMT:H81	2.52	0.44
1:J:41:VAL:HG21	1:J:53:VAL:HG22	1.99	0.44
1:L:98:SER:HA	1:L:118:ASP:OD2	2.18	0.44
2:G:24:GLU:O	2:G:28:ILE:HG13	2.18	0.44
1:H:35:ASP:OD1	1:H:36:ILE:N	2.51	0.44
1:F:22:LYS:HE2	1:F:47:PHE:CZ	2.52	0.43
1:A:81:VAL:O	1:A:85:ILE:HG12	2.18	0.43
2:G:38:PRO:O	2:G:42:LEU:HG	2.18	0.43
1:D:133:ARG:HA	1:D:136:LEU:HD12	2.00	0.43
1:E:13:LEU:HD11	1:E:33:ALA:HB1	2.00	0.43
2:I:66:ILE:HD11	2:I:91:LEU:HD22	2.00	0.43
2:I:377:PHE:HE2	5:M:506:LMT:H72	1.82	0.43
2:I:380:MET:HE3	2:I:387:PHE:HA	2.00	0.43
1:B:131:VAL:O	1:B:135:MET:HG3	2.18	0.43
2:M:24:GLU:N	2:M:25:PRO:CD	2.81	0.43
2:M:38:PRO:O	2:M:42:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:200:PRO:CG	5:M:503:LMT:H3'	2.48	0.43
2:M:430:PRO:HG2	5:M:508:LMT:H102	1.98	0.43
2:G:180:ALA:O	2:G:210:PHE:HB3	2.18	0.43
1:H:52:ILE:HG23	2:M:445:ILE:HG23	2.00	0.43
2:C:296:LEU:HD21	2:C:403:LEU:HD13	2.01	0.43
2:C:380:MET:HE3	2:C:387:PHE:HA	2.00	0.43
5:C:501:LMT:H72	2:G:377:PHE:HE2	1.84	0.43
2:M:180:ALA:O	2:M:210:PHE:HB3	2.18	0.43
2:C:360:LYS:HG2	2:C:437:LEU:HD13	2.00	0.43
2:G:35:VAL:HG11	2:G:94:ILE:HG21	2.01	0.43
2:G:200:PRO:CG	5:G:504:LMT:H3'	2.48	0.43
1:E:57:THR:HG23	1:E:86:LEU:HD23	1.99	0.43
2:I:360:LYS:HG2	2:I:437:LEU:HD13	2.00	0.43
2:C:368:SER:OG	5:C:504:LMT:C7	2.67	0.43
2:C:380:MET:CE	2:G:301:GLN:HB3	2.49	0.43
1:F:32:LEU:HD11	1:F:52:ILE:HD12	2.00	0.43
1:L:41:VAL:HG13	1:L:51:ALA:HB1	2.01	0.43
2:M:24:GLU:O	2:M:28:ILE:HG13	2.18	0.43
2:G:197:VAL:O	2:G:277:LEU:HD23	2.19	0.43
2:I:339:PHE:CG	2:M:437:LEU:HD21	2.54	0.43
2:I:364:ILE:HG23	5:I:503:LMT:C7	2.48	0.43
2:M:197:VAL:O	2:M:277:LEU:HD23	2.19	0.43
2:C:24:GLU:N	2:C:25:PRO:CD	2.82	0.43
1:E:54:ALA:HB1	1:E:61:THR:HG21	2.01	0.43
2:I:368:SER:OG	5:I:503:LMT:C7	2.67	0.43
5:I:501:LMT:H72	2:M:377:PHE:HE2	1.84	0.43
5:I:504:LMT:H3'	5:I:504:LMT:H1B	1.67	0.43
1:J:50:GLN:NE2	1:J:52:ILE:HD11	2.34	0.43
1:F:58:HIS:HB3	1:F:61:THR:HB	2.00	0.42
2:I:24:GLU:N	2:I:25:PRO:CD	2.82	0.42
1:B:18:LEU:HD12	1:B:18:LEU:HA	1.69	0.42
2:C:367:VAL:O	2:C:371:ILE:HG13	2.18	0.42
2:G:337:TRP:CD1	2:G:341:ARG:HH12	2.36	0.42
1:D:127:MET:HG2	1:E:127:MET:CG	2.45	0.42
2:M:35:VAL:HG11	2:M:94:ILE:HG21	2.01	0.42
2:M:153:PHE:CZ	2:M:170:MET:HE3	2.54	0.42
2:M:260:GLU:OE1	2:M:300:THR:OG1	2.33	0.42
2:M:288:THR:CG2	2:M:321:GLY:HA3	2.49	0.42
2:G:153:PHE:CZ	2:G:170:MET:HE3	2.54	0.42
1:L:41:VAL:HG21	1:L:53:VAL:HG22	2.01	0.42
5:G:506:LMT:H22	5:G:506:LMT:H52	1.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:LEU:HD12	1:H:18:LEU:HA	1.70	0.42
2:I:296:LEU:HD21	2:I:403:LEU:HD13	2.01	0.42
2:I:380:MET:CE	2:M:301:GLN:HB3	2.49	0.42
2:I:445:ILE:HG23	1:A:52:ILE:HG23	2.00	0.42
1:J:65:LEU:O	1:J:67:LEU:N	2.52	0.42
2:M:398:PHE:O	5:M:508:LMT:H121	2.19	0.42
2:I:367:VAL:O	2:I:371:ILE:HG13	2.18	0.42
2:C:66:ILE:HD11	2:C:91:LEU:HD22	2.00	0.42
1:E:133:ARG:HA	1:E:136:LEU:HD12	2.01	0.42
1:F:9:ALA:HB3	1:F:73:VAL:HG22	2.02	0.42
5:I:503:LMT:H92	5:I:503:LMT:H61	1.75	0.42
1:L:54:ALA:HB2	2:G:10:PHE:HB3	2.02	0.42
2:G:61:THR:HG21	2:G:80:PHE:HZ	1.85	0.42
2:G:347:VAL:C	2:G:348:MET:HG2	2.44	0.42
5:G:502:LMT:H3'	5:G:502:LMT:H1B	1.67	0.42
2:I:37:LEU:HD13	2:I:37:LEU:HA	1.91	0.42
2:I:453:LEU:HB2	2:M:237:HIS:CD2	2.55	0.42
1:A:86:LEU:O	1:A:90:ILE:HG12	2.20	0.42
2:M:287:ARG:HG3	2:M:287:ARG:HH11	1.85	0.42
2:G:348:MET:HB3	2:G:348:MET:HE3	1.82	0.42
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.69	0.42
2:I:349:PHE:HA	5:I:508:LMT:H2B	2.02	0.42
1:A:37:ASN:O	1:A:41:VAL:HG23	2.20	0.42
1:B:16:PHE:CD2	1:B:102:LYS:HD3	2.55	0.42
2:M:348:MET:HG3	2:M:353:VAL:HG23	2.01	0.42
1:J:88:THR:O	1:J:92:LYS:HG2	2.19	0.42
2:M:398:PHE:CZ	5:M:508:LMT:C9	2.78	0.42
5:M:508:LMT:H92	5:M:508:LMT:H61	1.75	0.42
2:C:9:VAL:HG12	2:C:112:VAL:HG13	2.01	0.42
2:C:339:PHE:CG	2:G:437:LEU:HD21	2.54	0.42
2:C:453:LEU:HB2	2:G:237:HIS:CD2	2.55	0.42
1:H:90:ILE:HD11	1:B:107:PHE:CE1	2.55	0.42
1:D:13:LEU:HD11	1:D:33:ALA:HB1	2.02	0.42
1:F:13:LEU:HD11	1:F:33:ALA:HB1	2.01	0.42
2:I:205:THR:HA	5:I:505:LMT:H81	2.01	0.42
2:G:250:LEU:HD12	5:G:504:LMT:H121	2.02	0.42
2:G:287:ARG:HG3	2:G:287:ARG:HH11	1.85	0.42
1:H:86:LEU:O	1:H:90:ILE:HG12	2.20	0.41
1:F:41:VAL:HG13	1:F:51:ALA:HB1	2.02	0.41
2:I:192:SER:O	2:I:292:ASN:O	2.38	0.41
2:I:368:SER:OG	5:I:503:LMT:H72	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:67:LEU:HA	1:L:70:TYR:HD2	1.85	0.41
2:C:205:THR:HA	5:C:505:LMT:H81	2.01	0.41
2:G:348:MET:HG3	2:G:353:VAL:HG23	2.01	0.41
1:B:86:LEU:O	1:B:90:ILE:HG12	2.20	0.41
2:C:349:PHE:HA	5:C:509:LMT:H2B	2.03	0.41
1:H:13:LEU:HD21	1:H:33:ALA:HB1	2.02	0.41
1:D:52:ILE:CG2	2:G:445:ILE:HG23	2.48	0.41
2:I:441:GLU:HG3	2:M:342:GLN:O	2.21	0.41
1:L:41:VAL:HG12	2:G:13:PRO:HG3	2.01	0.41
2:G:201:LEU:C	2:G:201:LEU:HD23	2.45	0.41
1:D:132:ALA:HA	1:D:135:MET:HE2	2.01	0.41
2:M:347:VAL:C	2:M:348:MET:HG2	2.44	0.41
5:C:504:LMT:H92	5:C:504:LMT:H61	1.75	0.41
1:B:32:LEU:HD13	1:B:50:GLN:HG3	2.02	0.41
2:C:325:LYS:HG2	2:G:455:GLY:OXT	2.20	0.41
1:H:122:MET:SD	1:H:125:ARG:NH2	2.93	0.41
1:F:81:VAL:HG13	1:F:108:GLN:HG3	2.02	0.41
1:A:74:MET:HB2	1:L:135:MET:HE1	2.03	0.41
2:C:368:SER:OG	5:C:504:LMT:H72	2.20	0.41
2:G:93:GLN:HE21	2:G:93:GLN:HB2	1.57	0.41
1:D:86:LEU:O	1:D:90:ILE:HG12	2.21	0.41
2:I:325:LYS:HG2	2:M:455:GLY:OXT	2.20	0.41
2:C:441:GLU:HG3	2:G:342:GLN:O	2.21	0.41
1:D:109:ALA:O	1:D:113:GLN:HG3	2.21	0.41
2:M:250:LEU:HD12	5:M:503:LMT:H121	2.02	0.41
2:C:288:THR:HG21	2:C:322:GLY:N	2.36	0.41
2:I:29:LEU:HG	2:I:33:LEU:HD23	2.03	0.41
2:I:288:THR:HG21	2:I:322:GLY:N	2.36	0.41
2:I:313:ILE:HA	2:I:324:ILE:HG12	2.03	0.41
2:I:408:THR:HA	2:I:411:LEU:HG	2.02	0.41
1:B:52:ILE:HG21	2:C:445:ILE:HD12	2.03	0.41
1:J:37:ASN:O	1:J:41:VAL:HG23	2.20	0.41
1:L:73:VAL:HG12	1:L:96:VAL:HG11	2.03	0.41
2:M:61:THR:HG21	2:M:80:PHE:HZ	1.85	0.41
2:M:183:ASN:HB3	2:M:288:THR:CG2	2.48	0.41
2:C:192:SER:O	2:C:292:ASN:O	2.38	0.41
2:C:364:ILE:HG23	5:C:504:LMT:C7	2.48	0.41
1:D:71:ASP:OD1	1:D:72:MET:N	2.54	0.41
2:C:140:LYS:HA	2:C:143:THR:HG22	2.03	0.41
2:C:313:ILE:HA	2:C:324:ILE:HG12	2.03	0.41
2:G:334:MET:HG3	5:G:507:LMT:H2'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:PHE:CE1	1:A:90:ILE:HD11	2.56	0.40
2:I:301:GLN:N	2:I:302:PRO:CD	2.85	0.40
1:J:112:LEU:HA	1:J:115:ILE:HG12	2.03	0.40
2:M:201:LEU:HD23	2:M:201:LEU:C	2.45	0.40
2:M:260:GLU:OE2	2:M:266:THR:HG21	2.22	0.40
2:I:152:GLY:HA3	2:I:209:LEU:HD11	2.03	0.40
1:A:123:PRO:O	1:A:127:MET:HB2	2.21	0.40
1:J:133:ARG:HA	1:J:136:LEU:HD12	2.04	0.40
2:C:33:LEU:HD13	2:C:33:LEU:HA	1.92	0.40
1:H:132:ALA:HB2	1:F:20:VAL:HA	2.03	0.40
2:M:25:PRO:O	5:M:508:LMT:O6B	2.28	0.40
1:H:107:PHE:CE1	1:B:90:ILE:HD11	2.56	0.40
2:I:163:GLU:HG3	2:I:164:MET:HG3	2.03	0.40
5:I:507:LMT:H42	5:I:507:LMT:H12	1.88	0.40
1:A:25:GLN:OE1	1:A:31:VAL:HG12	2.21	0.40
1:B:109:ALA:O	1:B:113:GLN:HG3	2.21	0.40
2:M:259:LEU:HD22	2:M:302:PRO:HB2	2.03	0.40
2:C:408:THR:HA	2:C:411:LEU:HG	2.02	0.40
2:G:260:GLU:OE2	2:G:266:THR:HG21	2.22	0.40
1:D:25:GLN:HG2	1:D:47:PHE:O	2.21	0.40
1:E:86:LEU:HD21	1:F:110:ARG:CZ	2.51	0.40
1:B:123:PRO:O	1:B:127:MET:HB2	2.20	0.40
2:M:368:SER:OG	5:M:508:LMT:C7	2.70	0.40
2:M:398:PHE:CZ	5:M:508:LMT:H61	2.53	0.40
2:C:163:GLU:HG3	2:C:164:MET:HG3	2.03	0.40
2:C:301:GLN:N	2:C:302:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/220 (59%)	125 (96%)	5 (4%)	0	100	100
1	B	130/220 (59%)	128 (98%)	2 (2%)	0	100	100
1	D	130/220 (59%)	128 (98%)	2 (2%)	0	100	100
1	E	130/220 (59%)	126 (97%)	4 (3%)	0	100	100
1	F	130/220 (59%)	126 (97%)	4 (3%)	0	100	100
1	H	130/220 (59%)	128 (98%)	2 (2%)	0	100	100
1	J	130/220 (59%)	126 (97%)	4 (3%)	0	100	100
1	L	130/220 (59%)	126 (97%)	4 (3%)	0	100	100
2	C	431/455 (95%)	422 (98%)	8 (2%)	1 (0%)	43	71
2	G	431/455 (95%)	420 (97%)	9 (2%)	2 (0%)	24	53
2	I	431/455 (95%)	422 (98%)	8 (2%)	1 (0%)	43	71
2	M	431/455 (95%)	420 (97%)	9 (2%)	2 (0%)	24	53
All	All	2764/3580 (77%)	2697 (98%)	61 (2%)	6 (0%)	44	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	288	THR
2	C	288	THR
2	M	288	THR
2	M	325	LYS
2	G	288	THR
2	G	325	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/179 (51%)	91 (99%)	1 (1%)	65	86
1	B	95/179 (53%)	94 (99%)	1 (1%)	65	86
1	D	90/179 (50%)	89 (99%)	1 (1%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/179 (49%)	88 (100%)	0	100	100
1	F	93/179 (52%)	93 (100%)	0	100	100
1	H	98/179 (55%)	97 (99%)	1 (1%)	68	88
1	J	84/179 (47%)	84 (100%)	0	100	100
1	L	88/179 (49%)	88 (100%)	0	100	100
2	C	344/374 (92%)	342 (99%)	2 (1%)	78	92
2	G	347/374 (93%)	341 (98%)	6 (2%)	53	81
2	I	346/374 (92%)	344 (99%)	2 (1%)	78	92
2	M	347/374 (93%)	341 (98%)	6 (2%)	53	81
All	All	2112/2928 (72%)	2092 (99%)	20 (1%)	68	89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	18	LEU
1	D	18	LEU
2	I	24	GLU
2	I	299	PHE
1	A	18	LEU
1	B	18	LEU
2	M	93	GLN
2	M	288	THR
2	M	296	LEU
2	M	298	GLN
2	M	299	PHE
2	M	348	MET
2	C	24	GLU
2	C	299	PHE
2	G	93	GLN
2	G	288	THR
2	G	296	LEU
2	G	298	GLN
2	G	299	PHE
2	G	348	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	50	GLN
2	I	237	HIS
2	I	262	HIS
2	I	342	GLN
2	I	345	HIS
1	J	50	GLN
1	J	108	GLN
2	M	93	GLN
2	M	99	GLN
2	M	235	HIS
2	M	301	GLN
2	M	342	GLN
2	M	345	HIS
2	C	237	HIS
2	C	262	HIS
2	G	93	GLN
2	G	99	GLN
2	G	301	GLN
2	G	342	GLN
2	G	345	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 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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
5	LMT	C	505	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	2 (4%)
5	LMT	C	504	-	36,36,36	0.38	0	47,47,47	0.95	2 (4%)
4	ADP	L	301	3	27,29,29	1.32	4 (14%)	42,45,45	1.97	10 (23%)
5	LMT	C	507	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	1 (2%)
5	LMT	I	507	-	36,36,36	1.17	6 (16%)	47,47,47	0.97	1 (2%)
5	LMT	C	501	-	36,36,36	1.17	6 (16%)	47,47,47	0.99	2 (4%)
4	ADP	A	1002	3	27,29,29	0.42	0	42,45,45	0.49	0
5	LMT	M	504	-	36,36,36	1.17	6 (16%)	47,47,47	0.96	1 (2%)
5	LMT	M	507	-	36,36,36	1.19	5 (13%)	47,47,47	0.99	1 (2%)
5	LMT	G	505	-	36,36,36	1.17	6 (16%)	47,47,47	0.97	1 (2%)
5	LMT	G	502	-	36,36,36	1.17	6 (16%)	47,47,47	1.10	2 (4%)
4	ADP	E	301	3	27,29,29	1.33	4 (14%)	42,45,45	1.97	11 (26%)
4	ADP	D	1001	3	27,29,29	1.34	4 (14%)	42,45,45	1.98	11 (26%)
5	LMT	C	508	-	36,36,36	1.13	5 (13%)	47,47,47	1.05	3 (6%)
5	LMT	I	505	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	2 (4%)
5	LMT	C	510	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
5	LMT	G	503	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	2 (4%)
5	LMT	G	507	-	36,36,36	1.15	7 (19%)	47,47,47	1.10	5 (10%)
5	LMT	G	506	-	36,36,36	1.14	5 (13%)	47,47,47	1.05	3 (6%)
5	LMT	M	505	-	36,36,36	1.15	7 (19%)	47,47,47	1.10	5 (10%)
5	LMT	G	504	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	2 (4%)
5	LMT	M	508	-	36,36,36	0.38	0	47,47,47	0.95	2 (4%)
5	LMT	I	504	-	36,36,36	1.17	6 (16%)	47,47,47	1.10	2 (4%)
5	LMT	C	511	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)
5	LMT	I	501	-	36,36,36	1.17	6 (16%)	47,47,47	0.99	2 (4%)
5	LMT	A	1003	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
5	LMT	C	506	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	2 (4%)
5	LMT	C	509	-	36,36,36	0.19	0	47,47,47	0.43	0
4	ADP	J	301	3	27,29,29	0.49	0	42,45,45	0.47	0
5	LMT	I	506	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	2 (4%)
4	ADP	H	1002	3	27,29,29	1.35	4 (14%)	42,45,45	1.98	11 (26%)
5	LMT	G	508	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LMT	I	510	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)
5	LMT	I	508	-	36,36,36	0.18	0	47,47,47	0.43	0
5	LMT	C	503	-	36,36,36	1.19	5 (13%)	47,47,47	0.99	1 (2%)
5	LMT	I	503	-	36,36,36	0.38	0	47,47,47	0.95	2 (4%)
5	LMT	M	506	-	36,36,36	1.17	6 (16%)	47,47,47	0.99	2 (4%)
5	LMT	G	509	-	36,36,36	1.17	6 (16%)	47,47,47	0.99	2 (4%)
5	LMT	I	509	-	36,36,36	1.17	5 (13%)	47,47,47	0.98	2 (4%)
4	ADP	F	301	3	27,29,29	1.33	4 (14%)	42,45,45	1.95	10 (23%)
5	LMT	M	503	-	36,36,36	1.16	5 (13%)	47,47,47	1.02	2 (4%)
4	ADP	B	1001	3	27,29,29	1.33	4 (14%)	42,45,45	1.96	11 (26%)
5	LMT	M	502	-	36,36,36	1.15	5 (13%)	47,47,47	0.95	2 (4%)
5	LMT	I	511	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	C	505	-	-	3/21/61/61	0/2/2/2
5	LMT	C	504	-	-	6/21/61/61	0/2/2/2
4	ADP	L	301	3	-	3/16/32/32	0/3/3/3
5	LMT	C	507	-	-	10/21/61/61	0/2/2/2
5	LMT	I	507	-	-	10/21/61/61	0/2/2/2
5	LMT	C	501	-	-	5/21/61/61	0/2/2/2
4	ADP	A	1002	3	-	4/16/32/32	0/3/3/3
5	LMT	M	504	-	-	10/21/61/61	0/2/2/2
5	LMT	M	507	-	-	5/21/61/61	0/2/2/2
5	LMT	G	505	-	-	10/21/61/61	0/2/2/2
5	LMT	G	502	-	-	6/21/61/61	0/2/2/2
4	ADP	E	301	3	-	4/16/32/32	0/3/3/3
4	ADP	D	1001	3	-	1/16/32/32	0/3/3/3
5	LMT	C	508	-	-	13/21/61/61	0/2/2/2
5	LMT	I	505	-	-	3/21/61/61	0/2/2/2
5	LMT	C	510	-	-	7/21/61/61	0/2/2/2
5	LMT	G	503	-	-	3/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LMT	G	507	-	-	9/21/61/61	0/2/2/2
5	LMT	G	506	-	-	13/21/61/61	0/2/2/2
5	LMT	M	505	-	-	9/21/61/61	0/2/2/2
5	LMT	G	504	-	-	5/21/61/61	0/2/2/2
5	LMT	M	508	-	-	6/21/61/61	0/2/2/2
5	LMT	I	504	-	-	6/21/61/61	0/2/2/2
5	LMT	C	511	-	-	9/21/61/61	0/2/2/2
5	LMT	I	501	-	-	5/21/61/61	0/2/2/2
5	LMT	A	1003	-	-	7/21/61/61	0/2/2/2
5	LMT	C	506	-	-	5/21/61/61	0/2/2/2
5	LMT	C	509	-	-	7/21/61/61	0/2/2/2
4	ADP	J	301	3	-	4/16/32/32	0/3/3/3
5	LMT	I	506	-	-	5/21/61/61	0/2/2/2
4	ADP	H	1002	3	-	1/16/32/32	0/3/3/3
5	LMT	G	508	-	-	9/21/61/61	0/2/2/2
5	LMT	I	510	-	-	9/21/61/61	0/2/2/2
5	LMT	I	508	-	-	7/21/61/61	0/2/2/2
5	LMT	C	503	-	-	5/21/61/61	0/2/2/2
5	LMT	I	503	-	-	6/21/61/61	0/2/2/2
5	LMT	M	506	-	-	5/21/61/61	0/2/2/2
5	LMT	G	509	-	-	5/21/61/61	0/2/2/2
5	LMT	I	509	-	-	7/21/61/61	0/2/2/2
4	ADP	F	301	3	-	3/16/32/32	0/3/3/3
5	LMT	M	503	-	-	5/21/61/61	0/2/2/2
4	ADP	B	1001	3	-	4/16/32/32	0/3/3/3
5	LMT	M	502	-	-	3/21/61/61	0/2/2/2
5	LMT	I	511	-	-	9/21/61/61	0/2/2/2

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1001	ADP	C5-C4	4.42	1.47	1.39
4	H	1002	ADP	C5-C4	4.40	1.47	1.39
4	B	1001	ADP	C5-C4	4.35	1.47	1.39
4	E	301	ADP	C5-C4	4.33	1.47	1.39
4	L	301	ADP	C5-C4	4.31	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	ADP	C5-C4	4.30	1.47	1.39
5	I	505	LMT	O3'-C3'	-2.69	1.36	1.43
5	M	502	LMT	O3'-C3'	-2.69	1.36	1.43
5	C	505	LMT	O3'-C3'	-2.69	1.36	1.43
5	G	503	LMT	O3'-C3'	-2.69	1.36	1.43
5	I	509	LMT	O3'-C3'	-2.67	1.36	1.43
5	A	1003	LMT	O3'-C3'	-2.67	1.36	1.43
5	C	510	LMT	O3'-C3'	-2.67	1.36	1.43
4	H	1002	ADP	C5-C6	2.66	1.48	1.41
5	I	501	LMT	O3'-C3'	-2.66	1.36	1.43
5	M	506	LMT	O3'-C3'	-2.66	1.36	1.43
5	M	507	LMT	O3'-C3'	-2.66	1.36	1.43
5	C	501	LMT	O3'-C3'	-2.66	1.36	1.43
5	C	503	LMT	O3'-C3'	-2.66	1.36	1.43
5	G	509	LMT	O3'-C3'	-2.66	1.36	1.43
5	G	506	LMT	O3'-C3'	-2.64	1.36	1.43
4	B	1001	ADP	C5-C6	2.64	1.48	1.41
4	E	301	ADP	C5-C6	2.63	1.48	1.41
5	C	508	LMT	O3'-C3'	-2.63	1.36	1.43
5	I	506	LMT	O3'-C3'	-2.63	1.36	1.43
5	M	503	LMT	O3'-C3'	-2.63	1.36	1.43
5	C	506	LMT	O3'-C3'	-2.63	1.36	1.43
5	G	504	LMT	O3'-C3'	-2.63	1.36	1.43
5	I	507	LMT	O3'-C3'	-2.63	1.36	1.43
5	M	504	LMT	O3'-C3'	-2.63	1.36	1.43
5	C	507	LMT	O3'-C3'	-2.63	1.36	1.43
5	G	505	LMT	O3'-C3'	-2.63	1.36	1.43
5	I	510	LMT	O3'-C3'	-2.62	1.36	1.43
5	I	511	LMT	O3'-C3'	-2.62	1.36	1.43
5	C	511	LMT	O3'-C3'	-2.62	1.36	1.43
5	G	508	LMT	O3'-C3'	-2.62	1.36	1.43
4	D	1001	ADP	C5-C6	2.61	1.48	1.41
4	F	301	ADP	C5-C6	2.61	1.48	1.41
4	L	301	ADP	C5-C6	2.57	1.48	1.41
5	I	504	LMT	O3'-C3'	-2.56	1.37	1.43
5	G	502	LMT	O3'-C3'	-2.56	1.37	1.43
5	I	505	LMT	O2'-C2'	-2.51	1.37	1.43
5	M	502	LMT	O2'-C2'	-2.51	1.37	1.43
5	C	505	LMT	O2'-C2'	-2.51	1.37	1.43
5	G	503	LMT	O2'-C2'	-2.51	1.37	1.43
5	I	510	LMT	O2'-C2'	-2.50	1.37	1.43
5	I	511	LMT	O2'-C2'	-2.50	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	511	LMT	O2'-C2'	-2.50	1.37	1.43
5	G	508	LMT	O2'-C2'	-2.50	1.37	1.43
5	M	505	LMT	O3'-C3'	-2.49	1.37	1.43
5	G	507	LMT	O3'-C3'	-2.48	1.37	1.43
5	M	507	LMT	O2B-C2B	-2.44	1.37	1.43
5	C	503	LMT	O2B-C2B	-2.44	1.37	1.43
4	D	1001	ADP	C8-N7	2.41	1.36	1.31
5	I	505	LMT	O3B-C3B	-2.40	1.37	1.43
5	M	502	LMT	O3B-C3B	-2.40	1.37	1.43
5	C	505	LMT	O3B-C3B	-2.40	1.37	1.43
5	G	503	LMT	O3B-C3B	-2.40	1.37	1.43
5	I	507	LMT	O2'-C2'	-2.38	1.37	1.43
5	M	504	LMT	O2'-C2'	-2.38	1.37	1.43
5	C	507	LMT	O2'-C2'	-2.38	1.37	1.43
5	G	505	LMT	O2'-C2'	-2.38	1.37	1.43
4	H	1002	ADP	C8-N7	2.38	1.36	1.31
5	I	509	LMT	O2B-C2B	-2.36	1.37	1.43
5	A	1003	LMT	O2B-C2B	-2.36	1.37	1.43
5	C	510	LMT	O2B-C2B	-2.36	1.37	1.43
5	I	509	LMT	O3B-C3B	-2.36	1.37	1.43
5	A	1003	LMT	O3B-C3B	-2.36	1.37	1.43
5	C	510	LMT	O3B-C3B	-2.36	1.37	1.43
5	I	507	LMT	O2B-C2B	-2.35	1.37	1.43
5	M	504	LMT	O2B-C2B	-2.35	1.37	1.43
5	C	507	LMT	O2B-C2B	-2.35	1.37	1.43
5	G	505	LMT	O2B-C2B	-2.35	1.37	1.43
4	B	1001	ADP	C8-N7	2.34	1.36	1.31
5	I	510	LMT	O2B-C2B	-2.34	1.37	1.43
5	I	511	LMT	O2B-C2B	-2.34	1.37	1.43
5	C	511	LMT	O2B-C2B	-2.34	1.37	1.43
5	G	508	LMT	O2B-C2B	-2.34	1.37	1.43
5	I	506	LMT	O2B-C2B	-2.33	1.37	1.43
5	M	503	LMT	O2B-C2B	-2.33	1.37	1.43
5	C	506	LMT	O2B-C2B	-2.33	1.37	1.43
5	G	504	LMT	O2B-C2B	-2.33	1.37	1.43
5	I	501	LMT	O2'-C2'	-2.33	1.37	1.43
5	M	506	LMT	O2'-C2'	-2.33	1.37	1.43
5	C	501	LMT	O2'-C2'	-2.33	1.37	1.43
5	G	509	LMT	O2'-C2'	-2.33	1.37	1.43
5	I	501	LMT	O2B-C2B	-2.33	1.37	1.43
5	M	506	LMT	O2B-C2B	-2.33	1.37	1.43
5	C	501	LMT	O2B-C2B	-2.33	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	509	LMT	O2B-C2B	-2.33	1.37	1.43
5	I	510	LMT	O3B-C3B	-2.32	1.37	1.43
5	I	511	LMT	O3B-C3B	-2.32	1.37	1.43
5	C	511	LMT	O3B-C3B	-2.32	1.37	1.43
5	G	508	LMT	O3B-C3B	-2.32	1.37	1.43
5	C	508	LMT	O2B-C2B	-2.32	1.37	1.43
5	G	506	LMT	O2B-C2B	-2.32	1.37	1.43
4	E	301	ADP	C8-N7	2.32	1.36	1.31
4	F	301	ADP	C8-N7	2.32	1.36	1.31
5	C	508	LMT	O3B-C3B	-2.32	1.37	1.43
5	G	506	LMT	O3B-C3B	-2.32	1.37	1.43
5	I	501	LMT	O3B-C3B	-2.31	1.37	1.43
5	I	506	LMT	O3B-C3B	-2.31	1.37	1.43
5	M	503	LMT	O3B-C3B	-2.31	1.37	1.43
5	M	506	LMT	O3B-C3B	-2.31	1.37	1.43
5	C	501	LMT	O3B-C3B	-2.31	1.37	1.43
5	C	506	LMT	O3B-C3B	-2.31	1.37	1.43
5	G	504	LMT	O3B-C3B	-2.31	1.37	1.43
5	G	509	LMT	O3B-C3B	-2.31	1.37	1.43
5	I	504	LMT	O3B-C3B	-2.31	1.37	1.43
5	G	502	LMT	O3B-C3B	-2.31	1.37	1.43
5	M	505	LMT	O2B-C2B	-2.30	1.37	1.43
5	G	507	LMT	O2B-C2B	-2.30	1.37	1.43
5	I	504	LMT	O2B-C2B	-2.30	1.37	1.43
5	G	502	LMT	O2B-C2B	-2.30	1.37	1.43
5	I	505	LMT	O2B-C2B	-2.30	1.37	1.43
5	M	502	LMT	O2B-C2B	-2.30	1.37	1.43
5	C	505	LMT	O2B-C2B	-2.30	1.37	1.43
5	G	503	LMT	O2B-C2B	-2.30	1.37	1.43
5	M	507	LMT	O2'-C2'	-2.29	1.37	1.43
5	C	503	LMT	O2'-C2'	-2.29	1.37	1.43
5	I	507	LMT	O3B-C3B	-2.28	1.37	1.43
5	M	504	LMT	O3B-C3B	-2.28	1.37	1.43
5	C	507	LMT	O3B-C3B	-2.28	1.37	1.43
5	G	505	LMT	O3B-C3B	-2.28	1.37	1.43
4	L	301	ADP	C8-N7	2.27	1.35	1.31
5	I	506	LMT	O2'-C2'	-2.25	1.37	1.43
5	M	503	LMT	O2'-C2'	-2.25	1.37	1.43
5	C	506	LMT	O2'-C2'	-2.25	1.37	1.43
5	G	504	LMT	O2'-C2'	-2.25	1.37	1.43
5	I	509	LMT	O2'-C2'	-2.24	1.37	1.43
5	A	1003	LMT	O2'-C2'	-2.24	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	510	LMT	O2'-C2'	-2.24	1.37	1.43
4	H	1002	ADP	C5-N7	-2.23	1.34	1.39
5	C	508	LMT	O2'-C2'	-2.23	1.37	1.43
5	G	506	LMT	O2'-C2'	-2.23	1.37	1.43
4	F	301	ADP	C5-N7	-2.21	1.34	1.39
5	M	505	LMT	O3B-C3B	-2.21	1.37	1.43
5	G	507	LMT	O3B-C3B	-2.21	1.37	1.43
5	I	504	LMT	O2'-C2'	-2.21	1.37	1.43
5	G	502	LMT	O2'-C2'	-2.21	1.37	1.43
4	B	1001	ADP	C5-N7	-2.20	1.34	1.39
4	E	301	ADP	C5-N7	-2.20	1.34	1.39
4	L	301	ADP	C5-N7	-2.19	1.34	1.39
4	D	1001	ADP	C5-N7	-2.18	1.34	1.39
5	G	506	LMT	O4'-C4B	-2.18	1.37	1.43
5	I	501	LMT	O4'-C4B	-2.17	1.37	1.43
5	M	506	LMT	O4'-C4B	-2.17	1.37	1.43
5	C	501	LMT	O4'-C4B	-2.17	1.37	1.43
5	G	509	LMT	O4'-C4B	-2.17	1.37	1.43
5	C	508	LMT	O4'-C4B	-2.15	1.37	1.43
5	M	507	LMT	O3B-C3B	-2.15	1.37	1.43
5	C	503	LMT	O3B-C3B	-2.15	1.37	1.43
5	M	505	LMT	C3'-C2'	2.14	1.57	1.52
5	G	507	LMT	C3'-C2'	2.14	1.57	1.52
5	I	509	LMT	O4'-C4B	-2.13	1.38	1.43
5	A	1003	LMT	O4'-C4B	-2.13	1.38	1.43
5	C	510	LMT	O4'-C4B	-2.13	1.38	1.43
5	I	506	LMT	O4'-C4B	-2.12	1.38	1.43
5	M	503	LMT	O4'-C4B	-2.12	1.38	1.43
5	C	506	LMT	O4'-C4B	-2.12	1.38	1.43
5	G	504	LMT	O4'-C4B	-2.12	1.38	1.43
5	I	510	LMT	O4'-C4B	-2.10	1.38	1.43
5	G	508	LMT	O4'-C4B	-2.10	1.38	1.43
5	I	511	LMT	O4'-C4B	-2.10	1.38	1.43
5	C	511	LMT	O4'-C4B	-2.10	1.38	1.43
5	I	504	LMT	O5'-C5'	-2.07	1.39	1.44
5	G	502	LMT	O5'-C5'	-2.07	1.39	1.44
5	I	507	LMT	O1'-C1'	-2.06	1.36	1.40
5	M	504	LMT	O1'-C1'	-2.06	1.36	1.40
5	C	507	LMT	O1'-C1'	-2.06	1.36	1.40
5	G	505	LMT	O1'-C1'	-2.06	1.36	1.40
5	M	505	LMT	O5'-C5'	-2.05	1.39	1.44
5	G	507	LMT	O5'-C5'	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	507	LMT	O4'-C4B	-2.05	1.38	1.43
5	M	504	LMT	O4'-C4B	-2.05	1.38	1.43
5	C	507	LMT	O4'-C4B	-2.05	1.38	1.43
5	G	505	LMT	O4'-C4B	-2.05	1.38	1.43
5	I	505	LMT	O4'-C4B	-2.05	1.38	1.43
5	M	502	LMT	O4'-C4B	-2.05	1.38	1.43
5	C	505	LMT	O4'-C4B	-2.05	1.38	1.43
5	G	503	LMT	O4'-C4B	-2.05	1.38	1.43
5	M	505	LMT	O1'-C1'	-2.04	1.36	1.40
5	G	507	LMT	O1'-C1'	-2.04	1.36	1.40
5	I	504	LMT	O4'-C4B	-2.04	1.38	1.43
5	G	502	LMT	O4'-C4B	-2.04	1.38	1.43
5	M	505	LMT	O4'-C4B	-2.03	1.38	1.43
5	G	507	LMT	O4'-C4B	-2.03	1.38	1.43
5	I	501	LMT	O1'-C1'	-2.01	1.36	1.40
5	M	506	LMT	O1'-C1'	-2.01	1.36	1.40
5	C	501	LMT	O1'-C1'	-2.01	1.36	1.40
5	G	509	LMT	O1'-C1'	-2.01	1.36	1.40
5	M	507	LMT	O4'-C4B	-2.00	1.38	1.43
5	C	503	LMT	O4'-C4B	-2.00	1.38	1.43

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1002	ADP	C5-C4-N3	-6.14	118.75	126.75
4	D	1001	ADP	C5-C4-N3	-6.13	118.75	126.75
4	E	301	ADP	C5-C4-N3	-6.07	118.83	126.75
4	B	1001	ADP	C5-C4-N3	-6.06	118.84	126.75
4	L	301	ADP	C5-C4-N3	-5.95	118.98	126.75
4	F	301	ADP	C5-C4-N3	-5.93	119.02	126.75
4	H	1002	ADP	N3-C4-N9	4.75	134.90	127.08
4	D	1001	ADP	N3-C4-N9	4.73	134.88	127.08
4	L	301	ADP	N3-C4-N9	4.73	134.88	127.08
4	B	1001	ADP	N3-C4-N9	4.72	134.86	127.08
4	E	301	ADP	N3-C4-N9	4.70	134.83	127.08
4	F	301	ADP	N3-C4-N9	4.69	134.81	127.08
4	H	1002	ADP	C2-N3-C4	3.93	121.03	111.75
4	D	1001	ADP	C2-N3-C4	3.89	120.95	111.75
4	B	1001	ADP	C2-N3-C4	3.87	120.89	111.75
4	E	301	ADP	C2-N3-C4	3.82	120.77	111.75
4	F	301	ADP	C2-N3-C4	3.80	120.72	111.75
4	L	301	ADP	C2-N3-C4	3.79	120.70	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	301	ADP	PA-O3A-PB	-3.63	120.36	132.83
4	D	1001	ADP	PA-O3A-PB	-3.55	120.64	132.83
4	H	1002	ADP	PA-O3A-PB	-3.38	121.22	132.83
4	F	301	ADP	PA-O3A-PB	-3.38	121.24	132.83
4	E	301	ADP	C4-C5-N7	-3.33	106.56	110.62
4	D	1001	ADP	C4-C5-N7	-3.31	106.59	110.62
4	H	1002	ADP	C4-C5-N7	-3.28	106.62	110.62
4	B	1001	ADP	C4-C5-N7	-3.26	106.65	110.62
4	H	1002	ADP	N3-C2-N1	-3.25	123.52	128.60
4	F	301	ADP	C4-C5-N7	-3.24	106.67	110.62
4	L	301	ADP	C4-C5-N7	-3.24	106.67	110.62
4	B	1001	ADP	N3-C2-N1	-3.23	123.56	128.60
4	L	301	ADP	PA-O3A-PB	-3.22	121.78	132.83
4	D	1001	ADP	N3-C2-N1	-3.20	123.61	128.60
4	F	301	ADP	N3-C2-N1	-3.16	123.66	128.60
4	L	301	ADP	N3-C2-N1	-3.14	123.69	128.60
4	E	301	ADP	N3-C2-N1	-3.13	123.71	128.60
5	I	503	LMT	C1B-O1B-C4'	-3.00	110.55	117.96
5	M	508	LMT	C1B-O1B-C4'	-3.00	110.55	117.96
5	C	504	LMT	C1B-O1B-C4'	-3.00	110.55	117.96
5	I	506	LMT	C1'-O5'-C5'	-2.97	107.86	113.69
5	M	503	LMT	C1'-O5'-C5'	-2.97	107.86	113.69
5	C	506	LMT	C1'-O5'-C5'	-2.97	107.86	113.69
5	G	504	LMT	C1'-O5'-C5'	-2.97	107.86	113.69
4	B	1001	ADP	PA-O3A-PB	-2.95	122.72	132.83
4	L	301	ADP	C4-N9-C8	2.88	108.85	105.73
4	F	301	ADP	C4-N9-C8	2.87	108.84	105.73
5	I	507	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
5	M	504	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
5	C	507	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
5	G	505	LMT	C1'-O5'-C5'	-2.86	108.07	113.69
4	E	301	ADP	C5-N7-C8	2.81	107.50	103.51
4	F	301	ADP	C5-N7-C8	2.79	107.47	103.51
5	I	504	LMT	C1'-O5'-C5'	-2.78	108.23	113.69
5	G	502	LMT	C1'-O5'-C5'	-2.78	108.23	113.69
4	L	301	ADP	C5-N7-C8	2.77	107.44	103.51
4	H	1002	ADP	C5-N7-C8	2.75	107.42	103.51
4	B	1001	ADP	C5-N7-C8	2.74	107.40	103.51
4	D	1001	ADP	C5-N7-C8	2.74	107.39	103.51
4	H	1002	ADP	O4'-C1'-N9	2.72	113.42	108.06
5	M	507	LMT	C1'-O5'-C5'	-2.68	108.43	113.69
5	C	503	LMT	C1'-O5'-C5'	-2.68	108.43	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	501	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
5	M	506	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
5	C	501	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
5	G	509	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
5	I	509	LMT	C3'-C4'-C5'	-2.64	104.87	110.93
5	A	1003	LMT	C3'-C4'-C5'	-2.64	104.87	110.93
5	C	510	LMT	C3'-C4'-C5'	-2.64	104.87	110.93
4	E	301	ADP	C4-N9-C8	2.64	108.59	105.73
4	B	1001	ADP	C4-N9-C8	2.62	108.57	105.73
5	M	505	LMT	C3'-C4'-C5'	-2.60	104.95	110.93
5	G	507	LMT	C3'-C4'-C5'	-2.60	104.95	110.93
4	D	1001	ADP	O4'-C1'-N9	2.58	113.15	108.06
4	D	1001	ADP	C4-N9-C8	2.58	108.53	105.73
5	G	506	LMT	C1'-O5'-C5'	-2.56	108.66	113.69
5	C	508	LMT	C1'-O5'-C5'	-2.56	108.67	113.69
4	H	1002	ADP	C4-N9-C8	2.55	108.49	105.73
4	B	1001	ADP	O4'-C1'-N9	2.51	113.01	108.06
5	I	501	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
5	M	506	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
5	C	501	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
5	G	509	LMT	C3'-C4'-C5'	-2.50	105.20	110.93
5	I	509	LMT	C1'-O5'-C5'	-2.50	108.78	113.69
5	A	1003	LMT	C1'-O5'-C5'	-2.50	108.78	113.69
5	C	510	LMT	C1'-O5'-C5'	-2.50	108.78	113.69
5	M	505	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
5	G	507	LMT	C1'-O5'-C5'	-2.49	108.81	113.69
5	M	505	LMT	C2'-C3'-C4'	2.47	115.32	109.68
5	G	507	LMT	C2'-C3'-C4'	2.47	115.32	109.68
5	C	508	LMT	O5B-C5B-C4B	2.42	114.08	109.69
5	G	506	LMT	O5B-C5B-C4B	2.42	114.08	109.69
5	I	510	LMT	O5'-C5'-C6'	2.41	112.44	106.44
5	I	511	LMT	O5'-C5'-C6'	2.41	112.44	106.44
5	C	511	LMT	O5'-C5'-C6'	2.41	112.44	106.44
5	G	508	LMT	O5'-C5'-C6'	2.41	112.44	106.44
5	M	505	LMT	O5'-C1'-O1'	-2.39	104.32	109.97
5	G	507	LMT	O5'-C1'-O1'	-2.39	104.32	109.97
4	H	1002	ADP	C6-C5-N7	2.30	136.31	132.02
4	D	1001	ADP	C6-C5-N7	2.28	136.28	132.02
5	M	505	LMT	O5B-C5B-C4B	2.27	113.82	109.69
5	G	507	LMT	O5B-C5B-C4B	2.27	113.82	109.69
4	F	301	ADP	C6-C5-N7	2.26	136.23	132.02
4	B	1001	ADP	C6-C5-N7	2.26	136.23	132.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	301	ADP	C6-C5-N7	2.25	136.21	132.02
5	I	510	LMT	O1'-C1'-C2'	2.24	111.81	108.30
5	I	511	LMT	O1'-C1'-C2'	2.24	111.81	108.30
5	C	511	LMT	O1'-C1'-C2'	2.24	111.81	108.30
5	G	508	LMT	O1'-C1'-C2'	2.24	111.81	108.30
4	F	301	ADP	N9-C8-N7	-2.24	110.85	113.91
4	E	301	ADP	C6-C5-N7	2.23	136.18	132.02
4	E	301	ADP	O4'-C1'-N9	2.23	112.46	108.06
5	I	505	LMT	C1'-O5'-C5'	-2.23	109.31	113.69
5	M	502	LMT	C1'-O5'-C5'	-2.23	109.31	113.69
5	C	505	LMT	C1'-O5'-C5'	-2.23	109.31	113.69
5	G	503	LMT	C1'-O5'-C5'	-2.23	109.31	113.69
4	L	301	ADP	N9-C8-N7	-2.21	110.89	113.91
5	I	510	LMT	O5'-C5'-C4'	2.19	114.36	109.75
5	I	511	LMT	O5'-C5'-C4'	2.19	114.36	109.75
5	C	511	LMT	O5'-C5'-C4'	2.19	114.36	109.75
5	G	508	LMT	O5'-C5'-C4'	2.19	114.36	109.75
5	I	504	LMT	C3'-C4'-C5'	-2.14	106.02	110.93
5	G	502	LMT	C3'-C4'-C5'	-2.14	106.02	110.93
4	E	301	ADP	N9-C8-N7	-2.12	111.01	113.91
4	B	1001	ADP	N9-C8-N7	-2.07	111.08	113.91
5	I	503	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
5	M	508	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
5	C	504	LMT	C3'-C4'-C5'	-2.07	106.19	110.93
5	I	506	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
5	M	503	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
5	C	506	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
5	G	504	LMT	C3'-C4'-C5'	-2.05	106.22	110.93
4	H	1002	ADP	N9-C8-N7	-2.05	111.11	113.91
4	D	1001	ADP	N9-C8-N7	-2.04	111.12	113.91
5	I	505	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
5	M	502	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
5	C	505	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
5	G	503	LMT	C3'-C4'-C5'	-2.04	106.25	110.93
5	C	508	LMT	O5B-C5B-C6B	2.01	111.42	106.44
5	G	506	LMT	O5B-C5B-C6B	2.01	111.42	106.44

There are no chirality outliers.

All (271) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	301	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	A	1002	ADP	C5'-O5'-PA-O2A
4	A	1002	ADP	C5'-O5'-PA-O3A
4	B	1001	ADP	C5'-O5'-PA-O2A
4	B	1001	ADP	C5'-O5'-PA-O3A
4	J	301	ADP	C5'-O5'-PA-O3A
4	L	301	ADP	C5'-O5'-PA-O2A
4	L	301	ADP	C5'-O5'-PA-O3A
5	I	503	LMT	C2'-C1'-O1'-C1
5	I	503	LMT	O5'-C1'-O1'-C1
5	I	503	LMT	C2-C1-O1'-C1'
5	I	504	LMT	C2'-C1'-O1'-C1
5	I	504	LMT	O5'-C1'-O1'-C1
5	I	506	LMT	C2-C1-O1'-C1'
5	I	510	LMT	O5'-C1'-O1'-C1
5	I	510	LMT	C2-C1-O1'-C1'
5	I	511	LMT	O5'-C1'-O1'-C1
5	I	511	LMT	C2-C1-O1'-C1'
5	M	503	LMT	C2-C1-O1'-C1'
5	M	507	LMT	C2'-C1'-O1'-C1
5	M	507	LMT	O5'-C1'-O1'-C1
5	M	508	LMT	C2'-C1'-O1'-C1
5	M	508	LMT	O5'-C1'-O1'-C1
5	M	508	LMT	C2-C1-O1'-C1'
5	C	503	LMT	C2'-C1'-O1'-C1
5	C	503	LMT	O5'-C1'-O1'-C1
5	C	504	LMT	C2'-C1'-O1'-C1
5	C	504	LMT	O5'-C1'-O1'-C1
5	C	504	LMT	C2-C1-O1'-C1'
5	C	506	LMT	C2-C1-O1'-C1'
5	C	511	LMT	O5'-C1'-O1'-C1
5	C	511	LMT	C2-C1-O1'-C1'
5	G	502	LMT	C2'-C1'-O1'-C1
5	G	502	LMT	O5'-C1'-O1'-C1
5	G	504	LMT	C2-C1-O1'-C1'
5	G	508	LMT	O5'-C1'-O1'-C1
5	G	508	LMT	C2-C1-O1'-C1'
5	I	504	LMT	C3'-C4'-O1B-C1B
5	G	502	LMT	C3'-C4'-O1B-C1B
5	M	505	LMT	O5B-C1B-O1B-C4'
5	G	507	LMT	O5B-C1B-O1B-C4'
5	I	504	LMT	O5B-C5B-C6B-O6B
5	G	502	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
5	C	508	LMT	O5B-C5B-C6B-O6B
5	G	506	LMT	O5B-C5B-C6B-O6B
5	I	503	LMT	C6-C7-C8-C9
5	M	508	LMT	C6-C7-C8-C9
5	C	504	LMT	C6-C7-C8-C9
5	I	505	LMT	C4'-C5'-C6'-O6'
5	M	502	LMT	C4'-C5'-C6'-O6'
5	C	505	LMT	C4'-C5'-C6'-O6'
5	G	503	LMT	C4'-C5'-C6'-O6'
4	B	1001	ADP	O4'-C4'-C5'-O5'
4	J	301	ADP	O4'-C4'-C5'-O5'
4	J	301	ADP	C3'-C4'-C5'-O5'
4	L	301	ADP	O4'-C4'-C5'-O5'
5	M	505	LMT	O5'-C5'-C6'-O6'
5	G	507	LMT	O5'-C5'-C6'-O6'
5	I	510	LMT	O5'-C5'-C6'-O6'
5	I	511	LMT	O5'-C5'-C6'-O6'
5	C	511	LMT	O5'-C5'-C6'-O6'
5	G	508	LMT	O5'-C5'-C6'-O6'
5	I	504	LMT	C4B-C5B-C6B-O6B
5	G	502	LMT	C4B-C5B-C6B-O6B
5	I	506	LMT	C4B-C5B-C6B-O6B
5	M	503	LMT	C4B-C5B-C6B-O6B
5	C	506	LMT	C4B-C5B-C6B-O6B
5	G	504	LMT	C4B-C5B-C6B-O6B
5	I	505	LMT	O5'-C5'-C6'-O6'
5	M	502	LMT	O5'-C5'-C6'-O6'
5	C	505	LMT	O5'-C5'-C6'-O6'
5	G	503	LMT	O5'-C5'-C6'-O6'
5	M	507	LMT	C2B-C1B-O1B-C4'
5	C	503	LMT	C2B-C1B-O1B-C4'
5	M	507	LMT	O5B-C1B-O1B-C4'
5	C	503	LMT	O5B-C1B-O1B-C4'
5	I	510	LMT	C4'-C5'-C6'-O6'
5	I	511	LMT	C4'-C5'-C6'-O6'
5	C	508	LMT	C4B-C5B-C6B-O6B
5	C	511	LMT	C4'-C5'-C6'-O6'
5	G	506	LMT	C4B-C5B-C6B-O6B
5	G	508	LMT	C4'-C5'-C6'-O6'
5	M	504	LMT	C4B-C5B-C6B-O6B
5	C	507	LMT	C4B-C5B-C6B-O6B
5	C	508	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
5	G	506	LMT	C2B-C1B-O1B-C4'
5	I	507	LMT	C4B-C5B-C6B-O6B
5	M	505	LMT	C4'-C5'-C6'-O6'
5	G	505	LMT	C4B-C5B-C6B-O6B
5	G	507	LMT	C4'-C5'-C6'-O6'
5	C	508	LMT	O5B-C1B-O1B-C4'
5	G	506	LMT	O5B-C1B-O1B-C4'
5	I	501	LMT	C4B-C5B-C6B-O6B
5	M	506	LMT	C4B-C5B-C6B-O6B
5	C	501	LMT	C4B-C5B-C6B-O6B
5	G	509	LMT	C4B-C5B-C6B-O6B
5	C	508	LMT	O5'-C5'-C6'-O6'
5	G	506	LMT	O5'-C5'-C6'-O6'
4	E	301	ADP	O4'-C4'-C5'-O5'
4	E	301	ADP	C3'-C4'-C5'-O5'
5	C	508	LMT	O5'-C1'-O1'-C1
5	G	506	LMT	O5'-C1'-O1'-C1
5	I	507	LMT	O1'-C1-C2-C3
5	M	504	LMT	O1'-C1-C2-C3
5	C	507	LMT	O1'-C1-C2-C3
5	G	505	LMT	O1'-C1-C2-C3
5	I	506	LMT	O5B-C5B-C6B-O6B
5	M	503	LMT	O5B-C5B-C6B-O6B
5	C	506	LMT	O5B-C5B-C6B-O6B
5	G	504	LMT	O5B-C5B-C6B-O6B
5	I	509	LMT	C6-C7-C8-C9
5	A	1003	LMT	C6-C7-C8-C9
5	C	510	LMT	C6-C7-C8-C9
5	I	509	LMT	C4'-C5'-C6'-O6'
5	A	1003	LMT	C4'-C5'-C6'-O6'
5	C	510	LMT	C4'-C5'-C6'-O6'
5	C	508	LMT	C2'-C1'-O1'-C1
5	G	506	LMT	C2'-C1'-O1'-C1
5	I	508	LMT	C5'-C4'-O1B-C1B
5	C	509	LMT	C5'-C4'-O1B-C1B
5	I	507	LMT	C2-C1-O1'-C1'
5	M	504	LMT	C2-C1-O1'-C1'
5	C	507	LMT	C2-C1-O1'-C1'
5	C	508	LMT	C2-C1-O1'-C1'
5	G	505	LMT	C2-C1-O1'-C1'
5	G	506	LMT	C2-C1-O1'-C1'
4	B	1001	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	I	504	LMT	C1-C2-C3-C4
5	G	502	LMT	C1-C2-C3-C4
5	I	510	LMT	C11-C10-C9-C8
5	I	511	LMT	C11-C10-C9-C8
5	C	511	LMT	C11-C10-C9-C8
5	G	508	LMT	C11-C10-C9-C8
5	I	508	LMT	C3'-C4'-O1B-C1B
5	C	509	LMT	C3'-C4'-O1B-C1B
5	I	503	LMT	C7-C8-C9-C10
5	I	505	LMT	C11-C10-C9-C8
5	M	502	LMT	C11-C10-C9-C8
5	M	508	LMT	C7-C8-C9-C10
5	C	504	LMT	C7-C8-C9-C10
5	C	505	LMT	C11-C10-C9-C8
5	G	503	LMT	C11-C10-C9-C8
5	I	509	LMT	C4B-C5B-C6B-O6B
5	A	1003	LMT	C4B-C5B-C6B-O6B
5	C	510	LMT	C4B-C5B-C6B-O6B
5	I	507	LMT	O5'-C1'-O1'-C1
5	M	504	LMT	O5'-C1'-O1'-C1
5	C	507	LMT	O5'-C1'-O1'-C1
5	G	505	LMT	O5'-C1'-O1'-C1
5	I	510	LMT	C2'-C1'-O1'-C1
5	I	511	LMT	C2'-C1'-O1'-C1
5	C	511	LMT	C2'-C1'-O1'-C1
5	G	508	LMT	C2'-C1'-O1'-C1
5	I	508	LMT	O5B-C5B-C6B-O6B
5	C	509	LMT	O5B-C5B-C6B-O6B
5	I	508	LMT	O5'-C5'-C6'-O6'
5	I	510	LMT	O5B-C5B-C6B-O6B
5	I	511	LMT	O5B-C5B-C6B-O6B
5	C	509	LMT	O5'-C5'-C6'-O6'
5	C	511	LMT	O5B-C5B-C6B-O6B
5	G	508	LMT	O5B-C5B-C6B-O6B
5	M	505	LMT	C5'-C4'-O1B-C1B
5	G	507	LMT	C5'-C4'-O1B-C1B
5	M	505	LMT	O5B-C5B-C6B-O6B
5	G	507	LMT	O5B-C5B-C6B-O6B
5	M	507	LMT	O5B-C5B-C6B-O6B
5	C	503	LMT	O5B-C5B-C6B-O6B
5	I	507	LMT	C4-C5-C6-C7
5	M	504	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
5	C	507	LMT	C4-C5-C6-C7
5	G	505	LMT	C4-C5-C6-C7
5	I	507	LMT	O5B-C5B-C6B-O6B
5	G	505	LMT	O5B-C5B-C6B-O6B
5	I	507	LMT	C2'-C1'-O1'-C1
5	M	504	LMT	C2'-C1'-O1'-C1
5	C	507	LMT	C2'-C1'-O1'-C1
5	G	505	LMT	C2'-C1'-O1'-C1
5	M	504	LMT	O5B-C5B-C6B-O6B
5	C	507	LMT	O5B-C5B-C6B-O6B
5	I	501	LMT	O5B-C5B-C6B-O6B
5	M	506	LMT	O5B-C5B-C6B-O6B
5	C	501	LMT	O5B-C5B-C6B-O6B
5	G	509	LMT	O5B-C5B-C6B-O6B
5	I	509	LMT	O5'-C1'-O1'-C1
5	A	1003	LMT	O5'-C1'-O1'-C1
5	C	510	LMT	O5'-C1'-O1'-C1
5	I	509	LMT	C2-C1-O1'-C1'
5	A	1003	LMT	C2-C1-O1'-C1'
5	C	510	LMT	C2-C1-O1'-C1'
5	C	508	LMT	C5-C6-C7-C8
5	G	506	LMT	C5-C6-C7-C8
5	C	509	LMT	O5B-C1B-O1B-C4'
5	C	508	LMT	C11-C10-C9-C8
5	G	506	LMT	C11-C10-C9-C8
5	I	508	LMT	O5B-C1B-O1B-C4'
5	I	507	LMT	C7-C8-C9-C10
5	M	504	LMT	C7-C8-C9-C10
5	C	507	LMT	C7-C8-C9-C10
5	G	505	LMT	C7-C8-C9-C10
5	C	508	LMT	C6-C7-C8-C9
5	G	506	LMT	C6-C7-C8-C9
5	I	501	LMT	O5'-C1'-O1'-C1
5	M	506	LMT	O5'-C1'-O1'-C1
5	C	501	LMT	O5'-C1'-O1'-C1
5	G	509	LMT	O5'-C1'-O1'-C1
5	M	505	LMT	C11-C10-C9-C8
5	G	507	LMT	C11-C10-C9-C8
5	I	507	LMT	C6-C7-C8-C9
5	M	504	LMT	C6-C7-C8-C9
5	C	507	LMT	C6-C7-C8-C9
5	G	505	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
4	E	301	ADP	PB-O3A-PA-O1A
5	I	506	LMT	O1'-C1-C2-C3
5	M	503	LMT	O1'-C1-C2-C3
5	C	506	LMT	O1'-C1-C2-C3
5	G	504	LMT	O1'-C1-C2-C3
4	A	1002	ADP	C2'-C1'-N9-C8
5	I	509	LMT	O5'-C5'-C6'-O6'
5	A	1003	LMT	O5'-C5'-C6'-O6'
5	C	510	LMT	O5'-C5'-C6'-O6'
4	J	301	ADP	C5'-O5'-PA-O2A
5	I	507	LMT	C1-C2-C3-C4
5	M	504	LMT	C1-C2-C3-C4
5	C	507	LMT	C1-C2-C3-C4
5	G	505	LMT	C1-C2-C3-C4
5	I	503	LMT	C11-C10-C9-C8
5	M	508	LMT	C11-C10-C9-C8
5	C	504	LMT	C11-C10-C9-C8
5	G	506	LMT	C4-C5-C6-C7
5	C	508	LMT	C4-C5-C6-C7
5	M	505	LMT	C3'-C4'-O1B-C1B
5	G	507	LMT	C3'-C4'-O1B-C1B
5	M	505	LMT	C3-C4-C5-C6
5	G	507	LMT	C3-C4-C5-C6
5	I	508	LMT	C2B-C1B-O1B-C4'
5	M	505	LMT	C7-C8-C9-C10
5	G	507	LMT	C7-C8-C9-C10
5	C	508	LMT	C1-C2-C3-C4
5	G	506	LMT	C1-C2-C3-C4
5	I	501	LMT	C2'-C1'-O1'-C1
5	M	506	LMT	C2'-C1'-O1'-C1
5	C	501	LMT	C2'-C1'-O1'-C1
5	G	509	LMT	C2'-C1'-O1'-C1
5	I	510	LMT	C7-C8-C9-C10
5	I	511	LMT	C7-C8-C9-C10
5	C	511	LMT	C7-C8-C9-C10
5	G	508	LMT	C7-C8-C9-C10
5	C	509	LMT	C2B-C1B-O1B-C4'
4	H	1002	ADP	PB-O3A-PA-O2A
5	I	501	LMT	C3-C4-C5-C6
5	M	506	LMT	C3-C4-C5-C6
5	C	501	LMT	C3-C4-C5-C6
5	G	509	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
5	I	509	LMT	O5B-C5B-C6B-O6B
5	A	1003	LMT	O5B-C5B-C6B-O6B
5	C	510	LMT	O5B-C5B-C6B-O6B
5	I	508	LMT	C5-C6-C7-C8
5	C	509	LMT	C5-C6-C7-C8
4	F	301	ADP	O4'-C4'-C5'-O5'
4	A	1002	ADP	O4'-C4'-C5'-O5'
5	I	510	LMT	C4-C5-C6-C7
5	I	511	LMT	C4-C5-C6-C7
5	C	511	LMT	C4-C5-C6-C7
5	G	508	LMT	C4-C5-C6-C7
4	F	301	ADP	C5'-O5'-PA-O3A
4	E	301	ADP	PB-O3A-PA-O2A
4	D	1001	ADP	C5'-O5'-PA-O1A
5	I	506	LMT	C5'-C4'-O1B-C1B
5	M	503	LMT	C5'-C4'-O1B-C1B
5	C	506	LMT	C5'-C4'-O1B-C1B
5	G	504	LMT	C5'-C4'-O1B-C1B

There are no ring outliers.

40 monomers are involved in 202 short contacts:

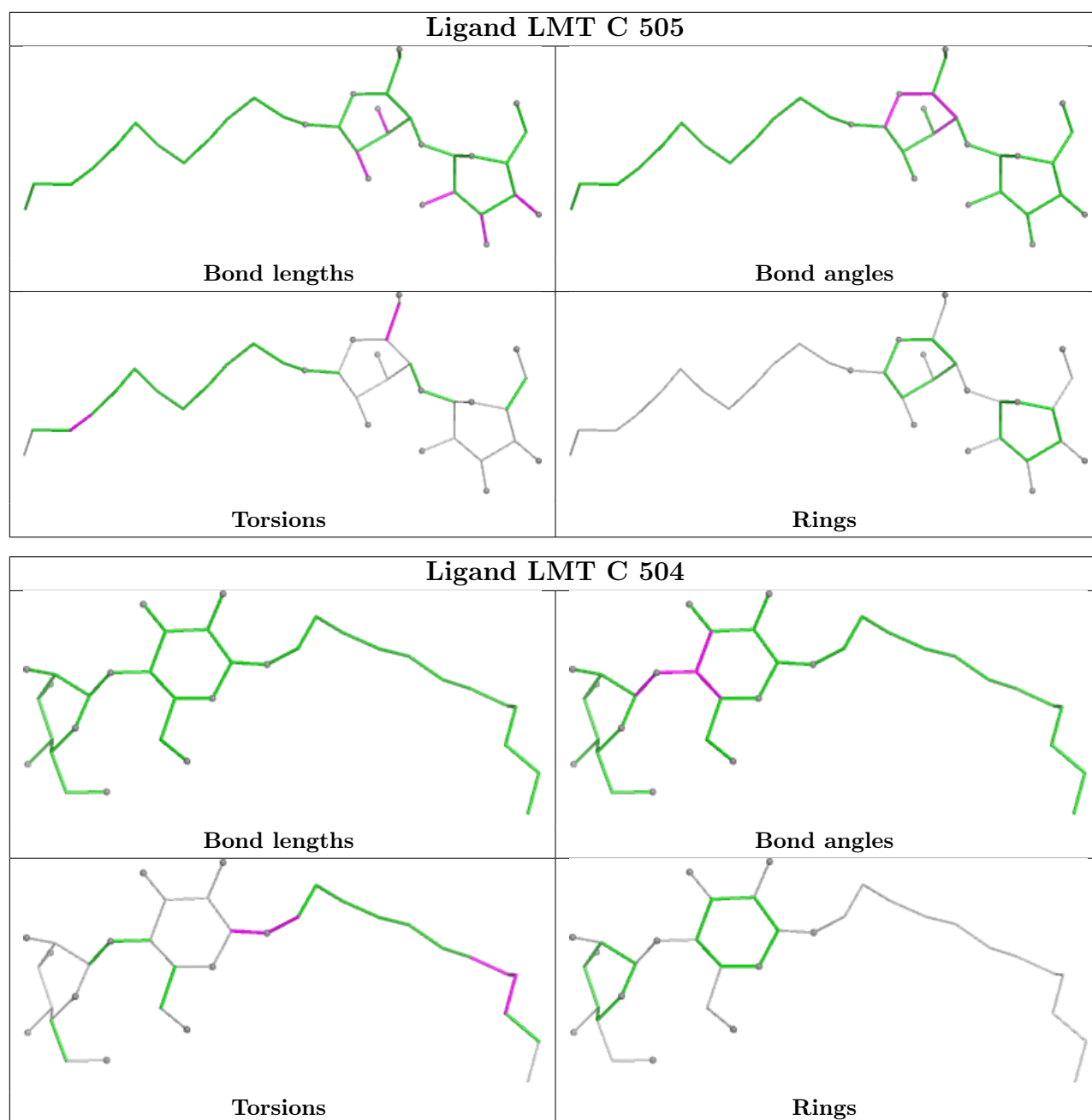
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	LMT	7	0
5	C	504	LMT	31	0
4	L	301	ADP	1	0
5	I	507	LMT	1	0
5	C	501	LMT	1	0
4	A	1002	ADP	1	0
5	M	507	LMT	1	0
5	G	502	LMT	1	0
4	E	301	ADP	1	0
4	D	1001	ADP	1	0
5	C	508	LMT	2	0
5	I	505	LMT	7	0
5	C	510	LMT	1	0
5	G	503	LMT	1	0
5	G	507	LMT	7	0
5	G	506	LMT	1	0
5	M	505	LMT	6	0
5	G	504	LMT	3	0
5	M	508	LMT	60	0

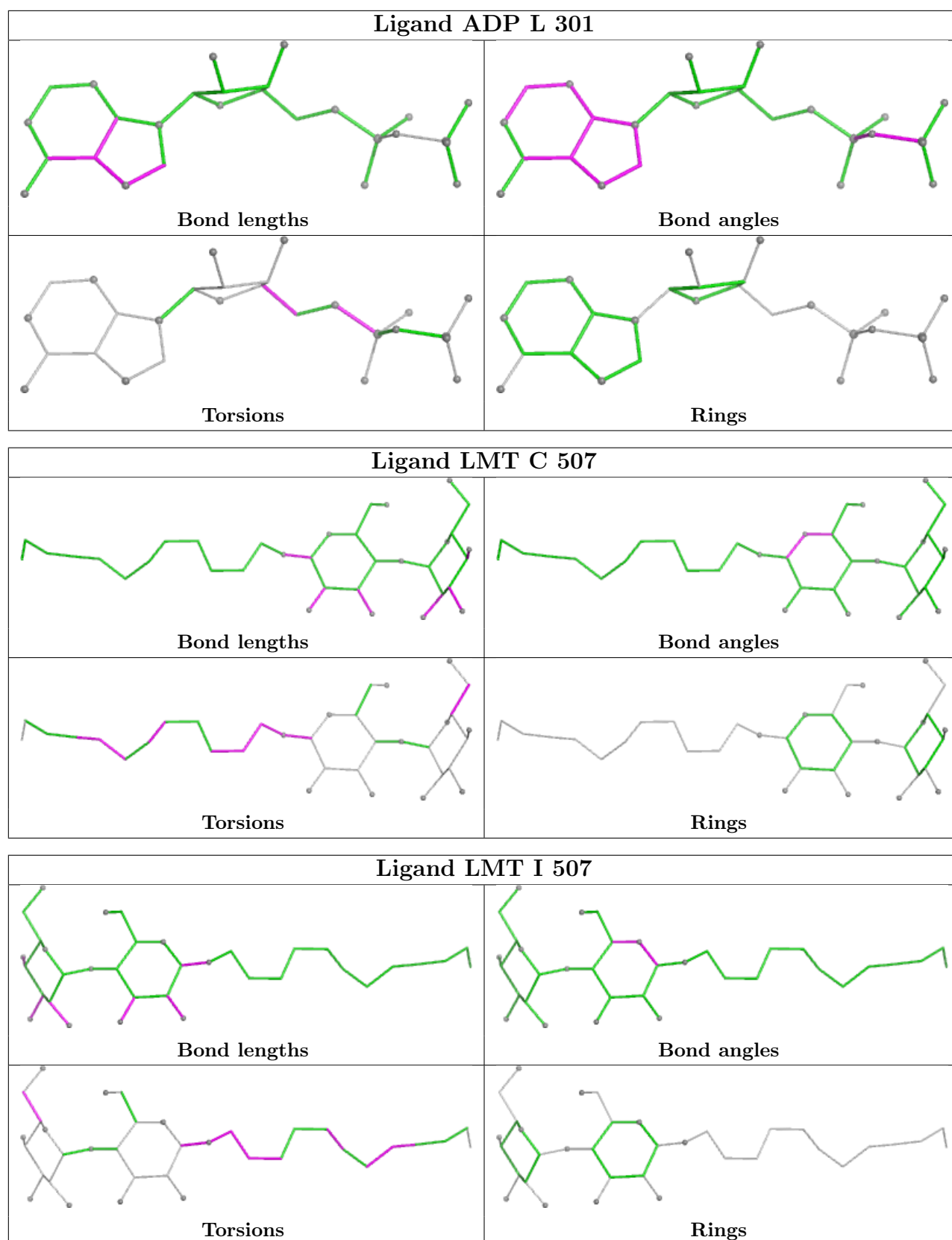
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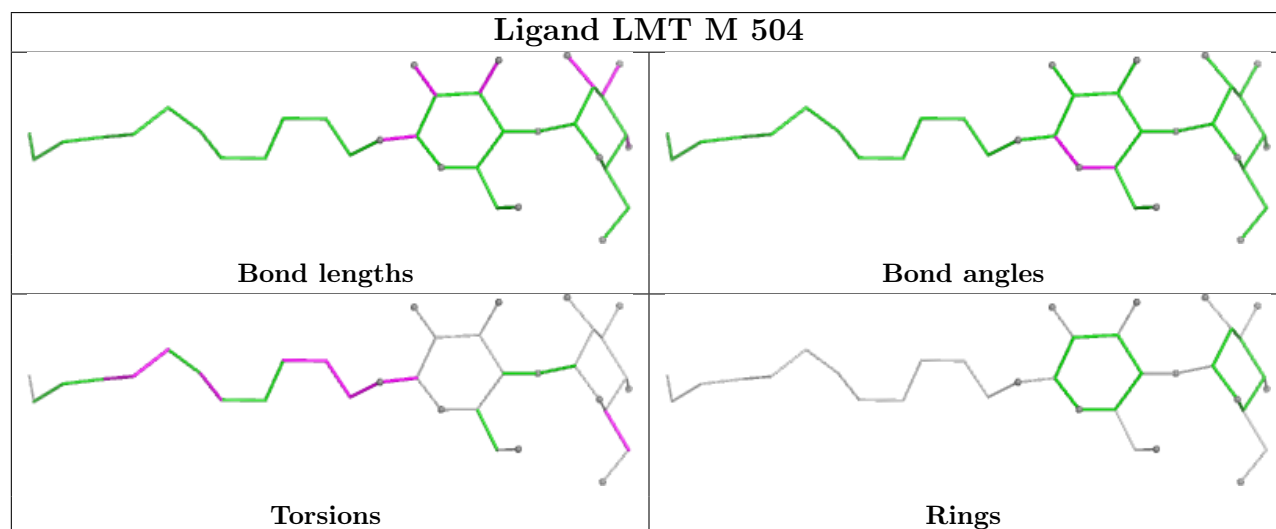
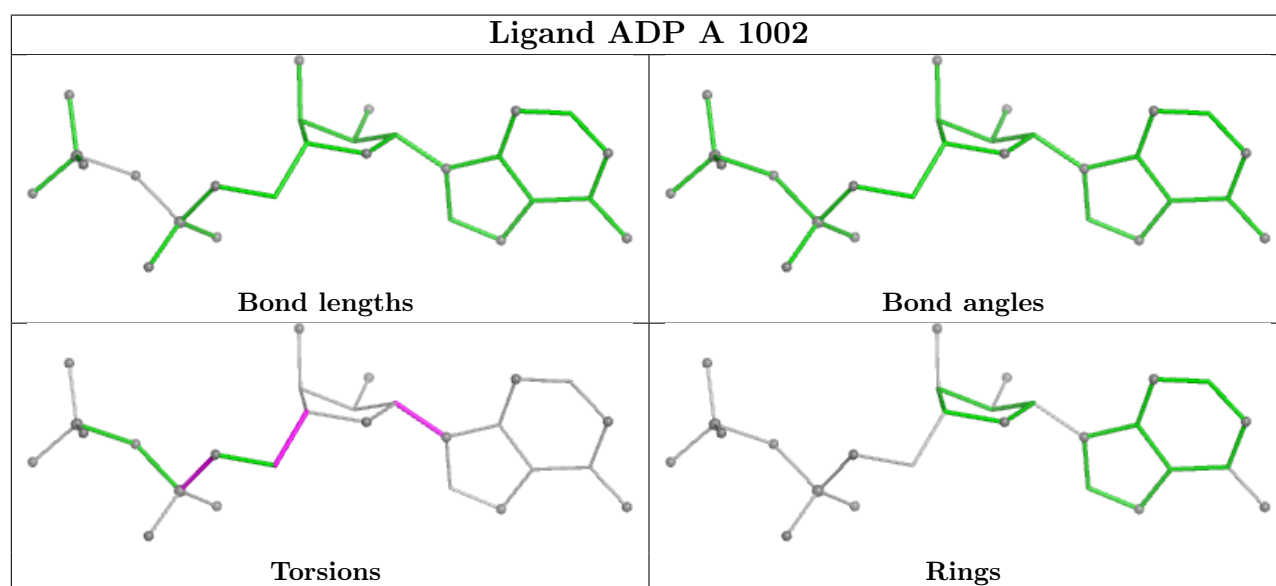
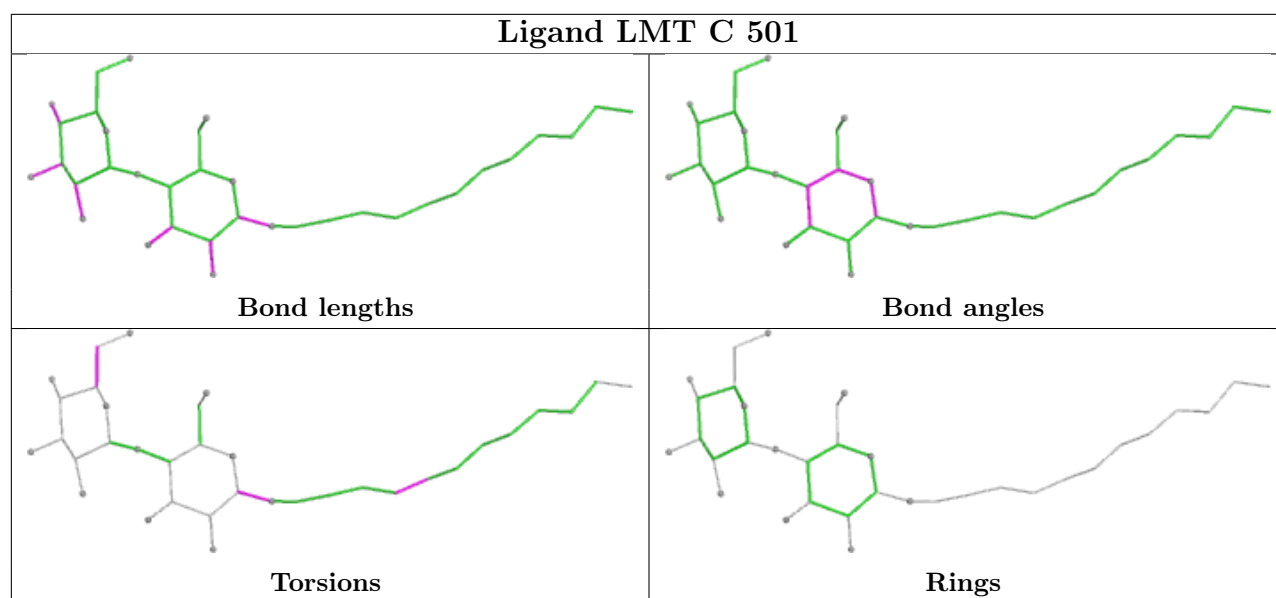
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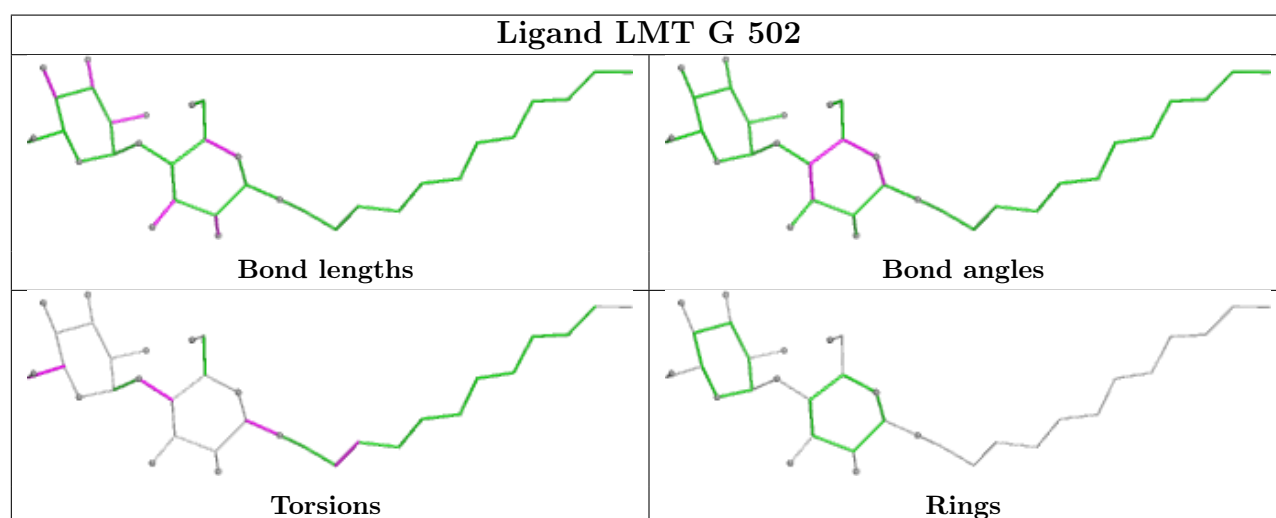
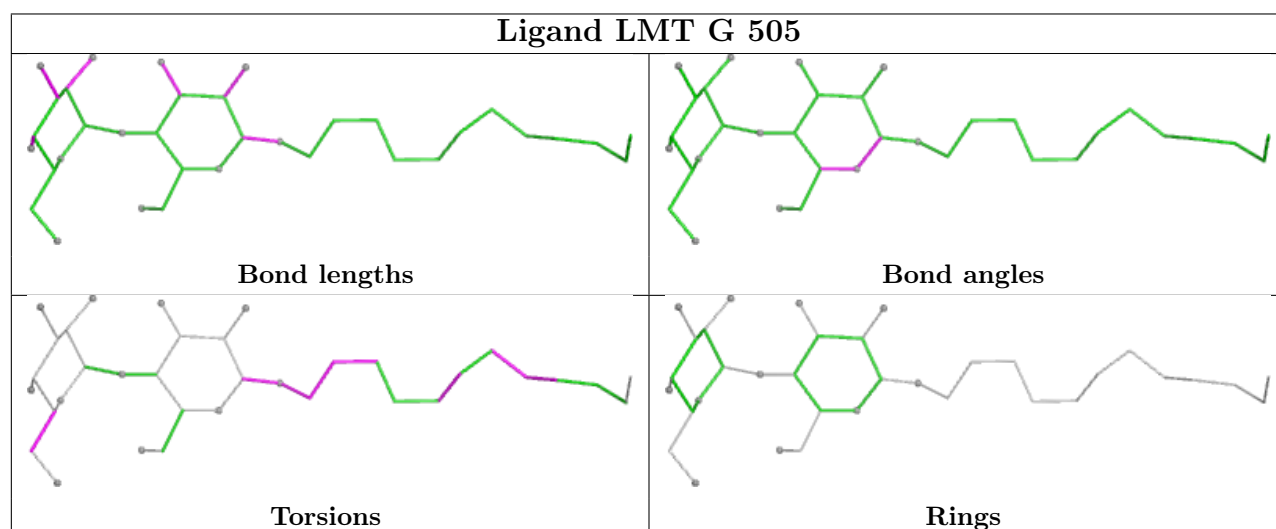
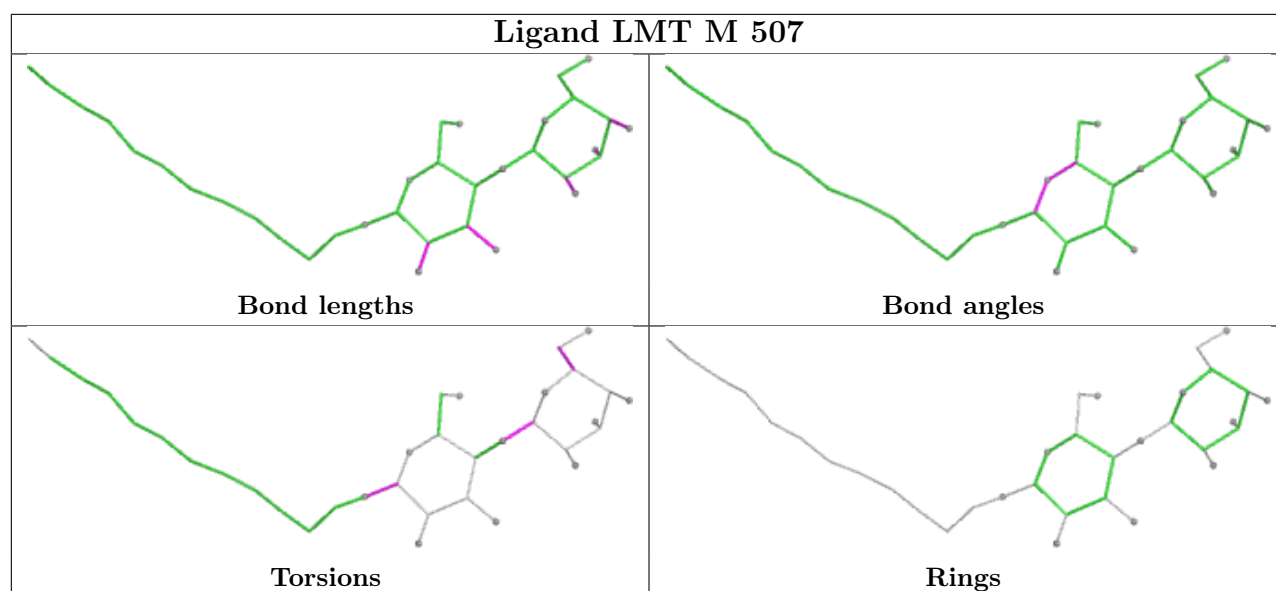
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	504	LMT	2	0
5	C	511	LMT	1	0
5	I	501	LMT	1	0
5	C	506	LMT	6	0
5	C	509	LMT	3	0
4	J	301	ADP	1	0
5	I	506	LMT	6	0
4	H	1002	ADP	1	0
5	G	508	LMT	2	0
5	I	510	LMT	2	0
5	I	508	LMT	3	0
5	C	503	LMT	1	0
5	I	503	LMT	30	0
5	M	506	LMT	1	0
5	G	509	LMT	1	0
5	I	509	LMT	1	0
4	F	301	ADP	2	0
5	M	503	LMT	3	0
4	B	1001	ADP	1	0
5	M	502	LMT	1	0
5	I	511	LMT	2	0

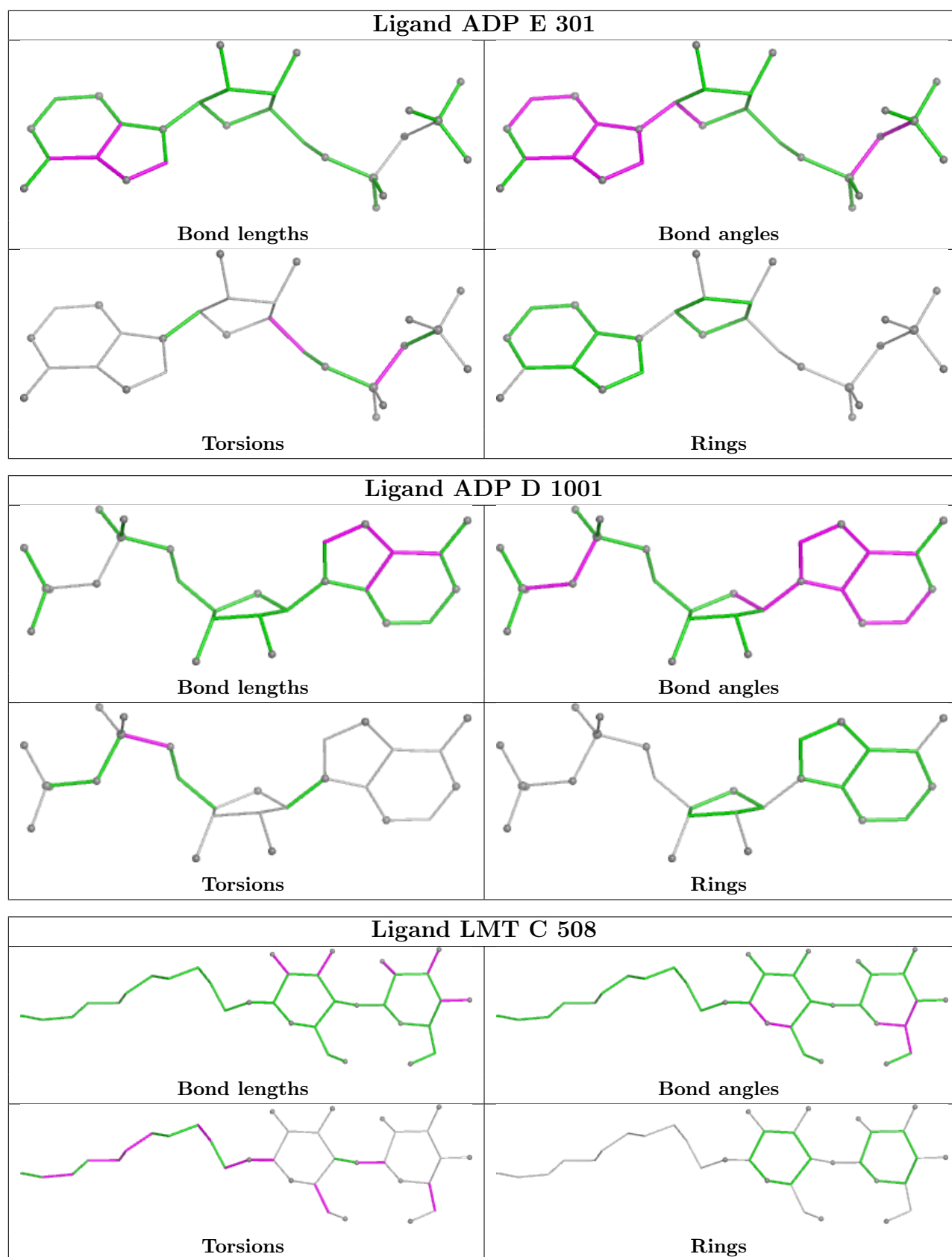
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

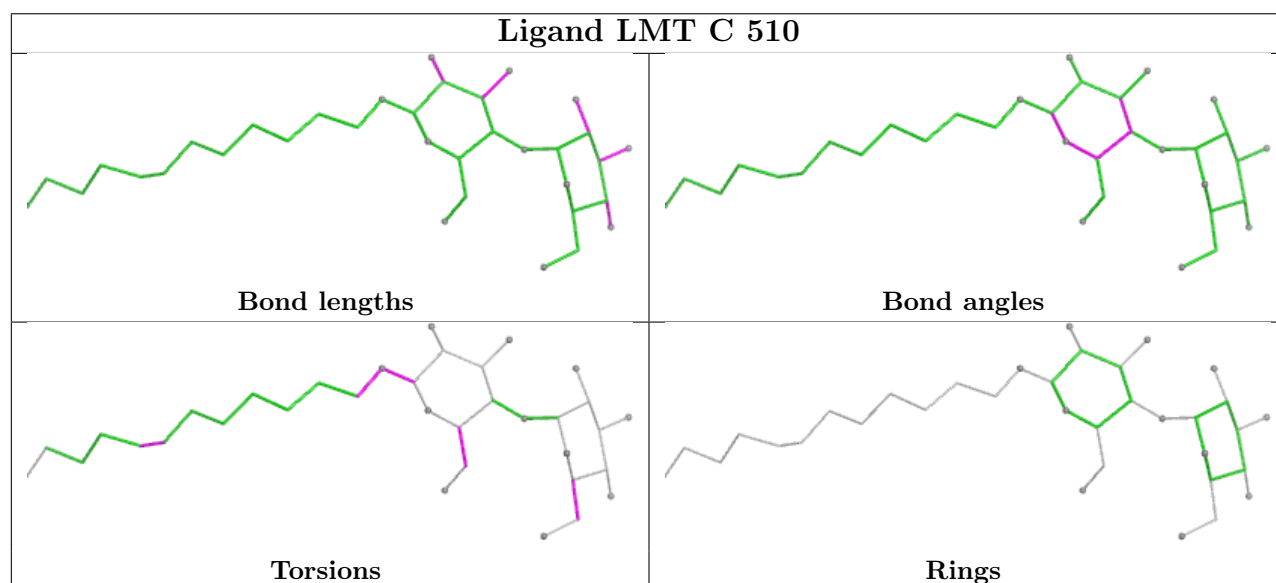
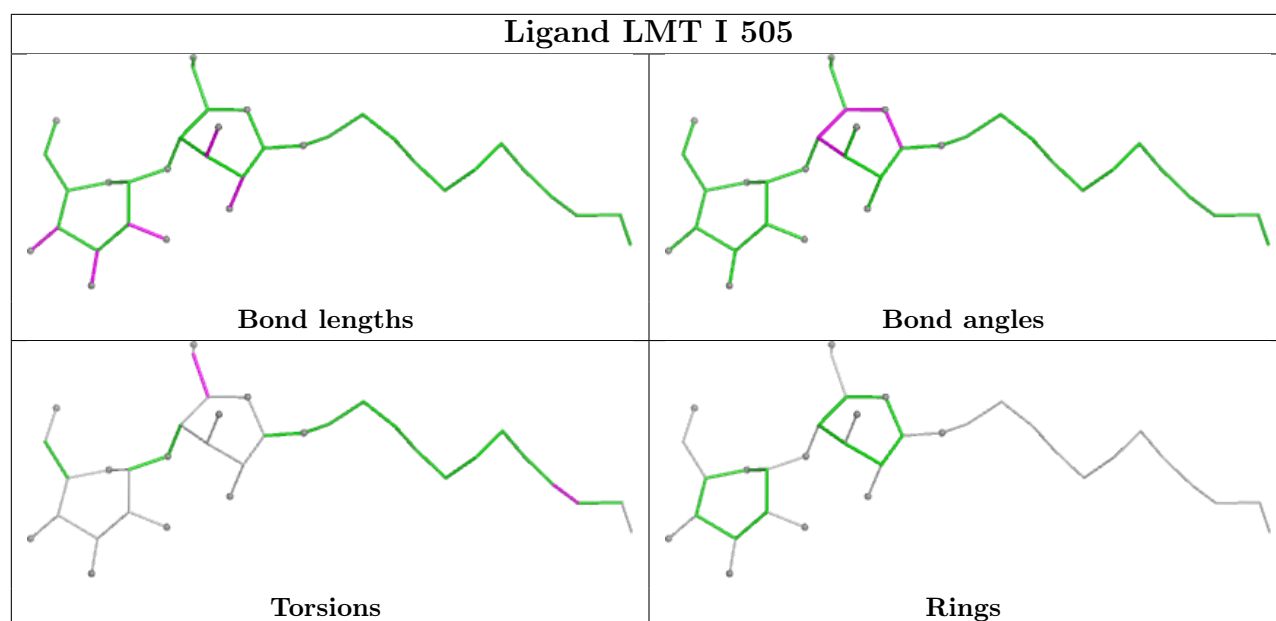


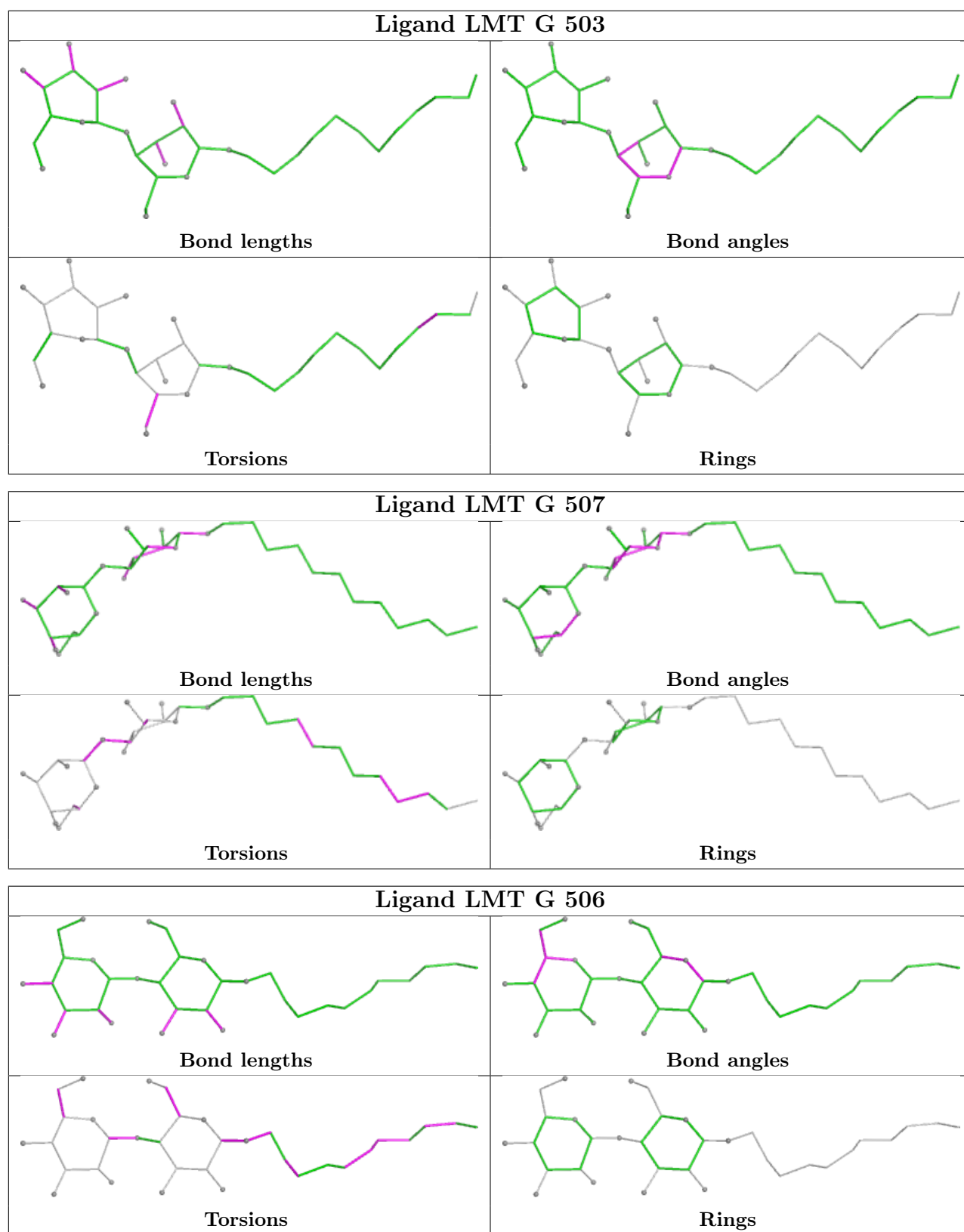


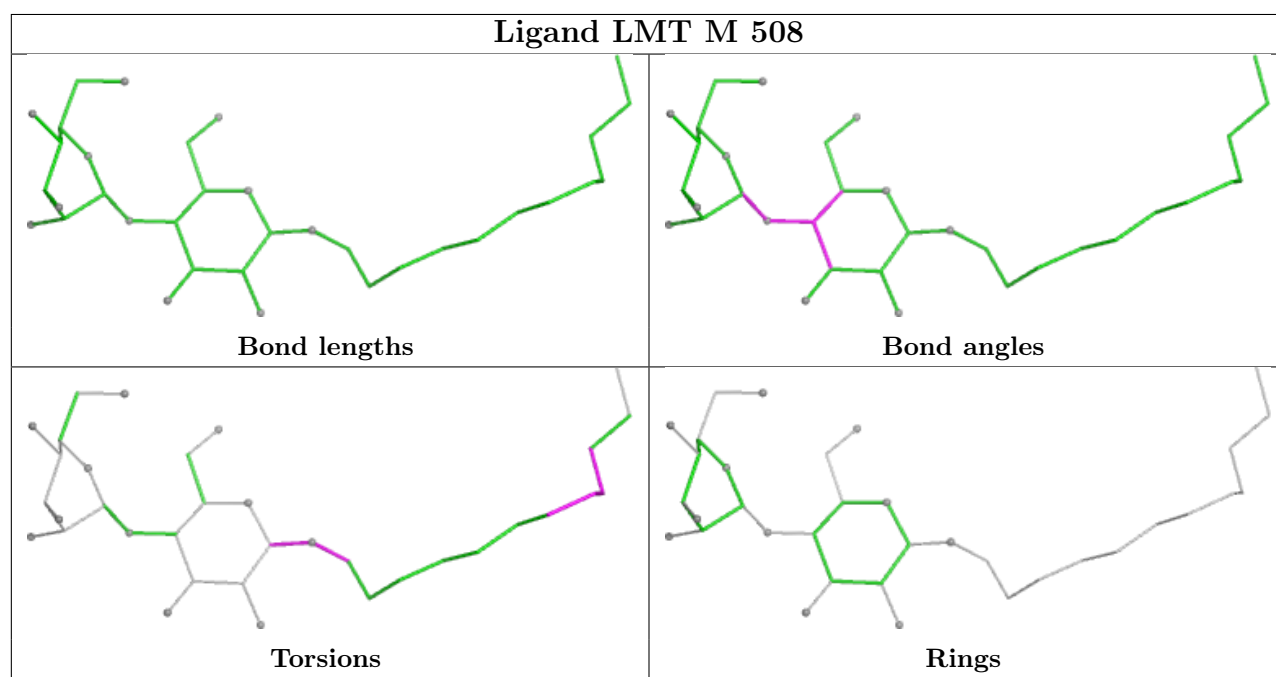
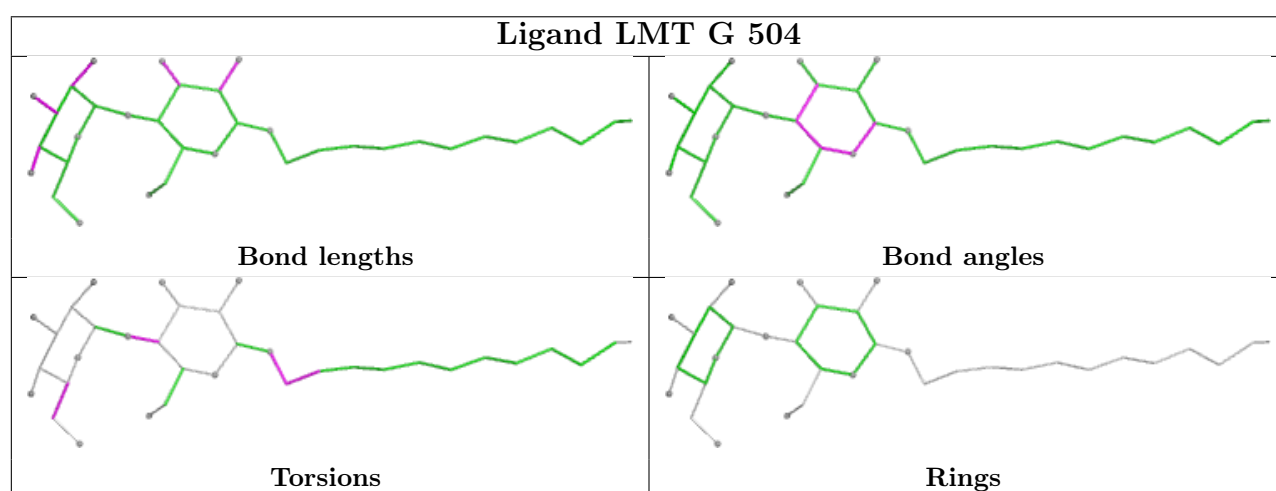
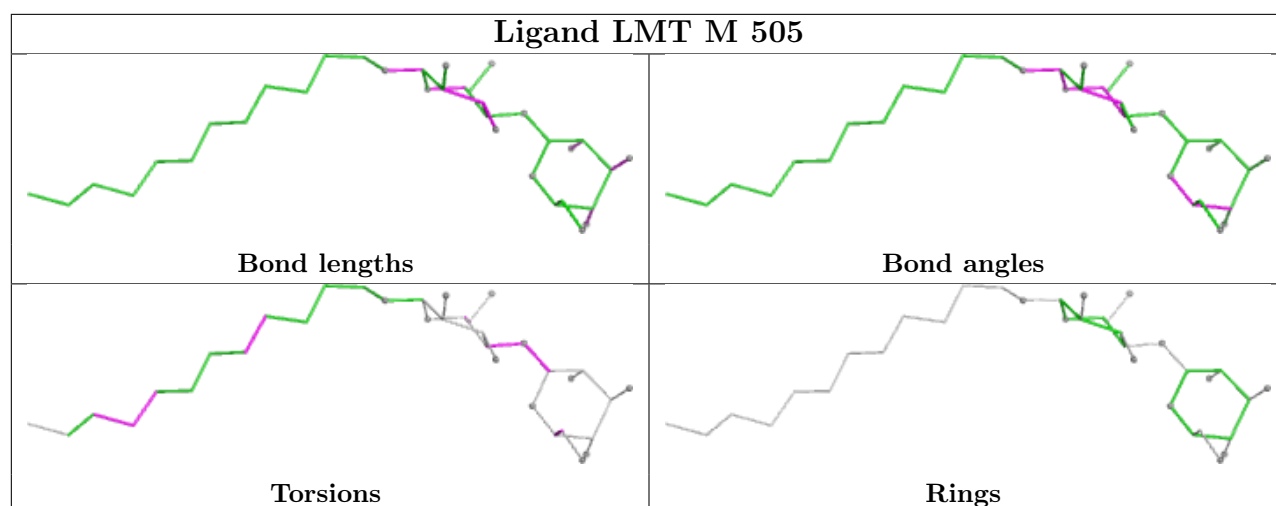


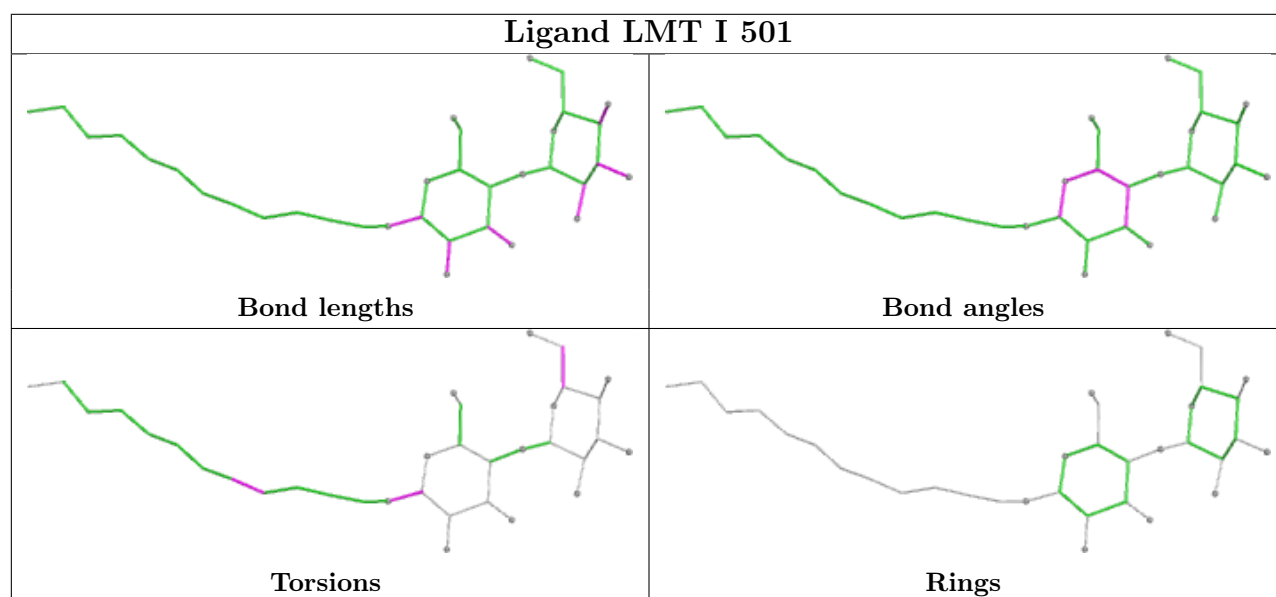
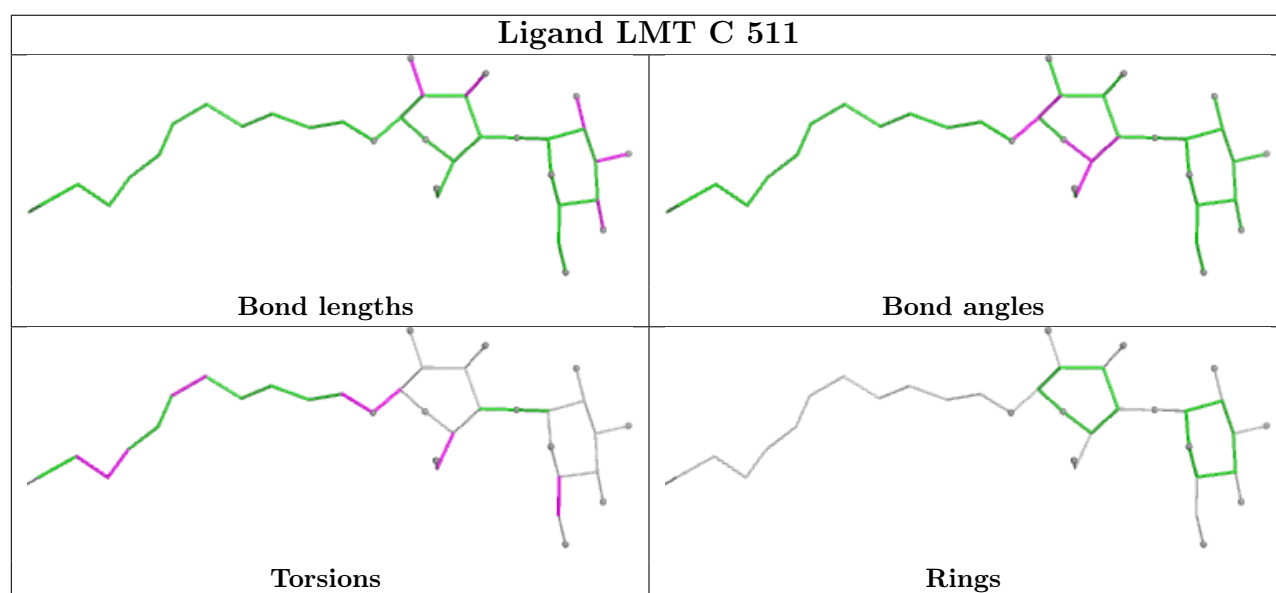
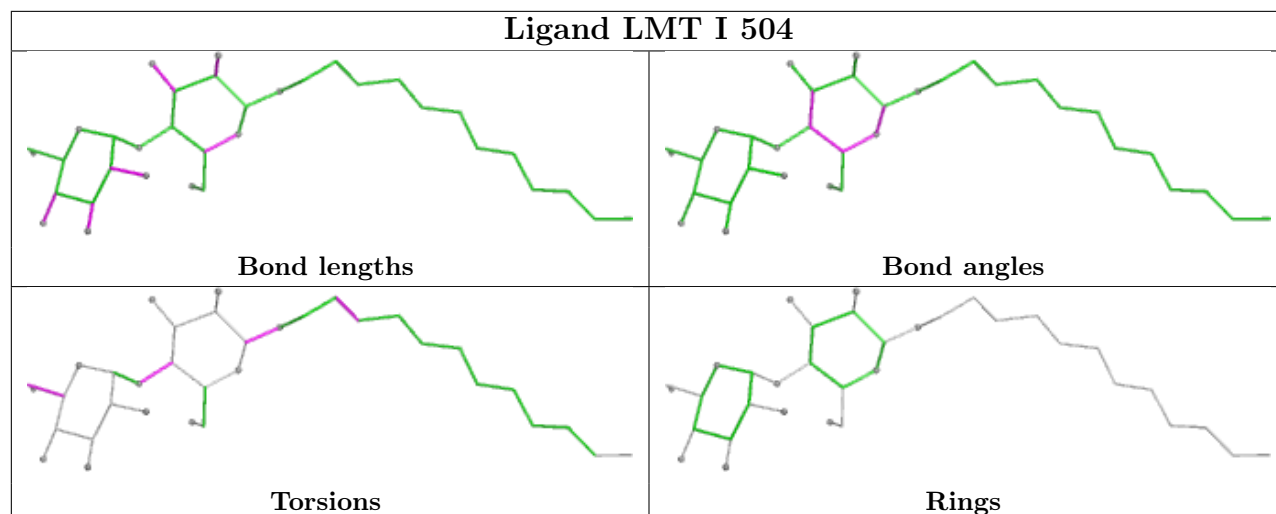


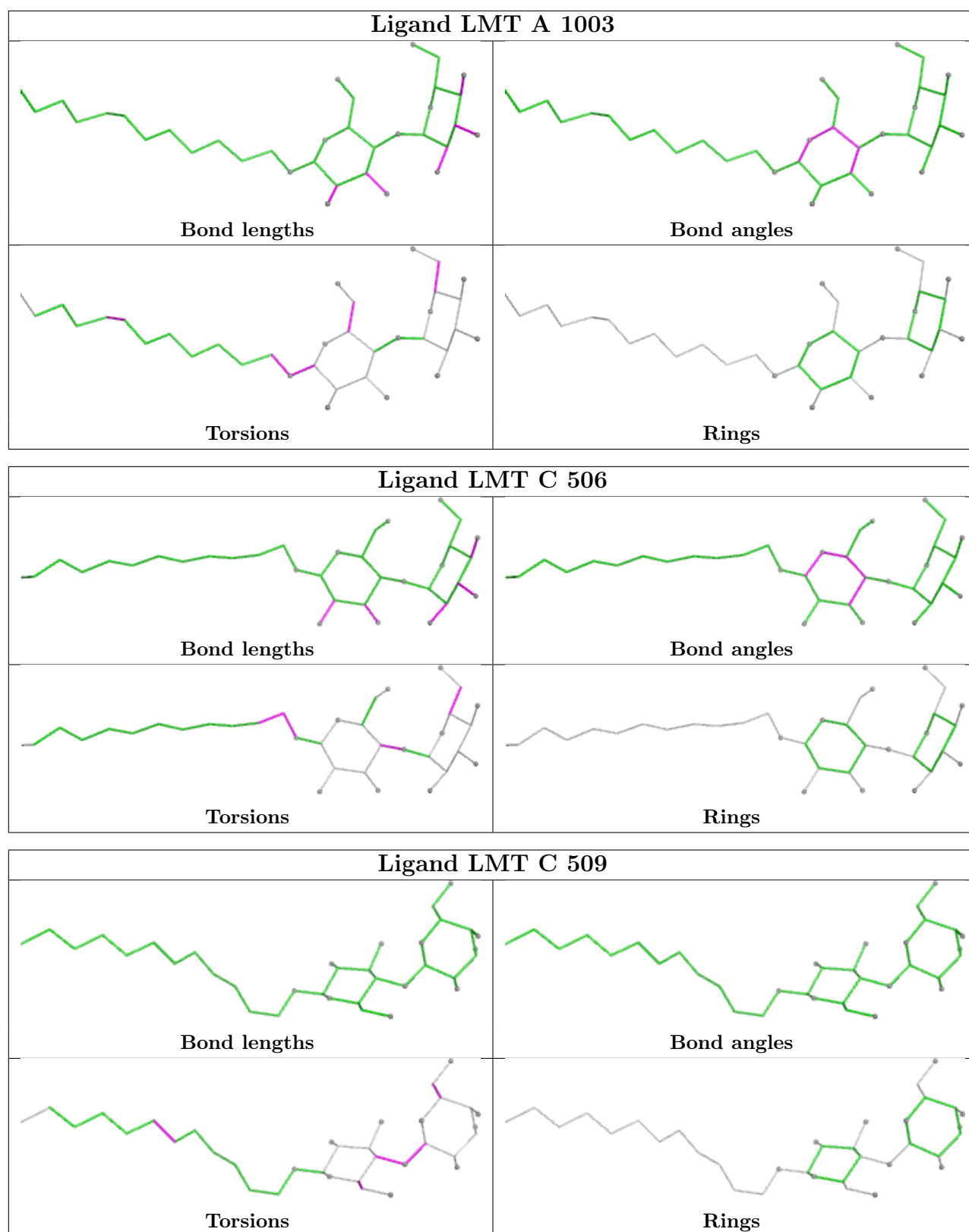




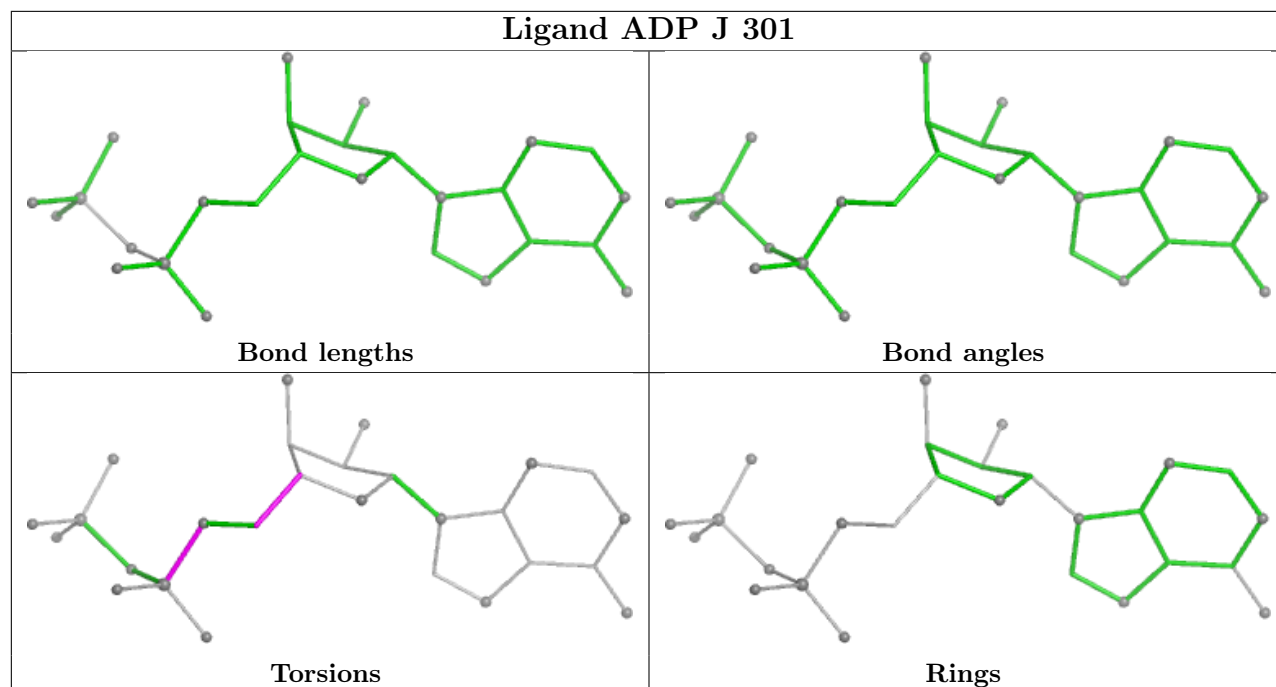




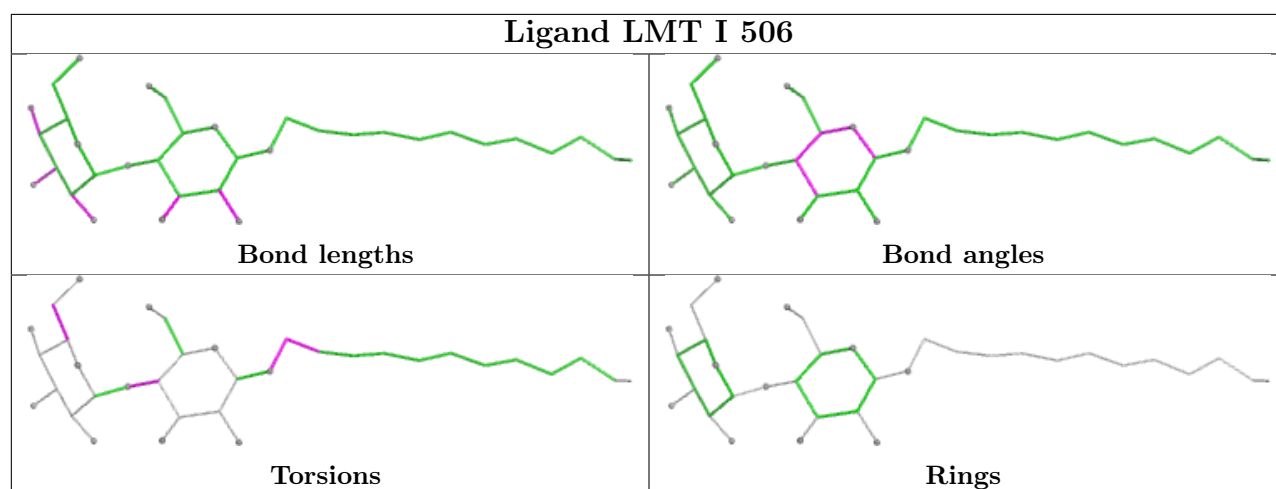




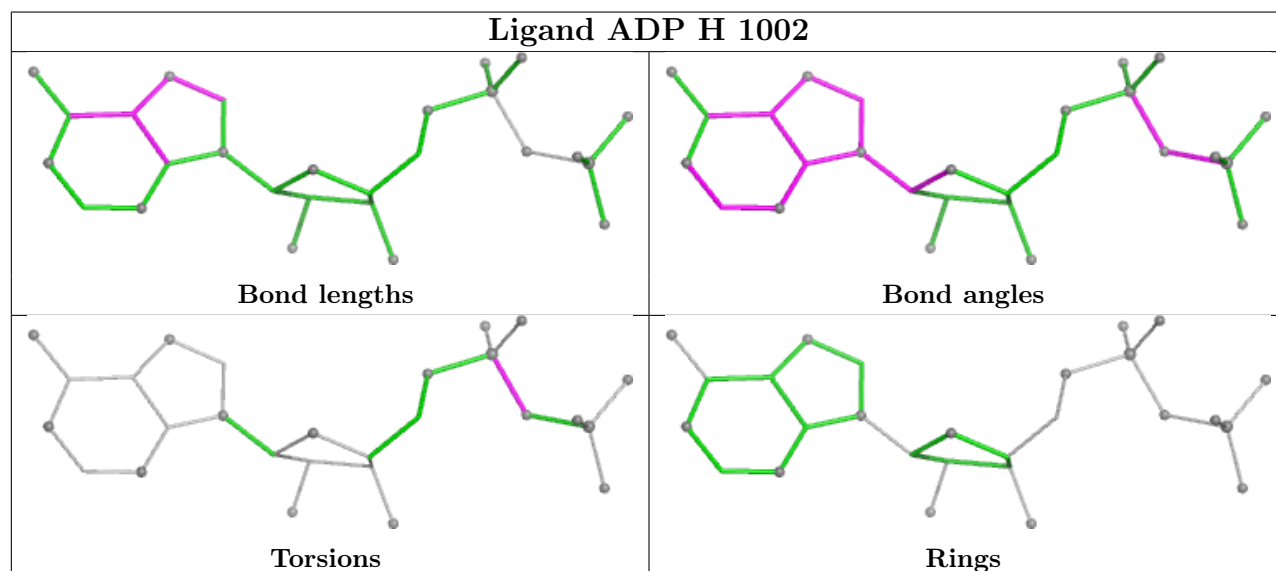
Ligand ADP J 301

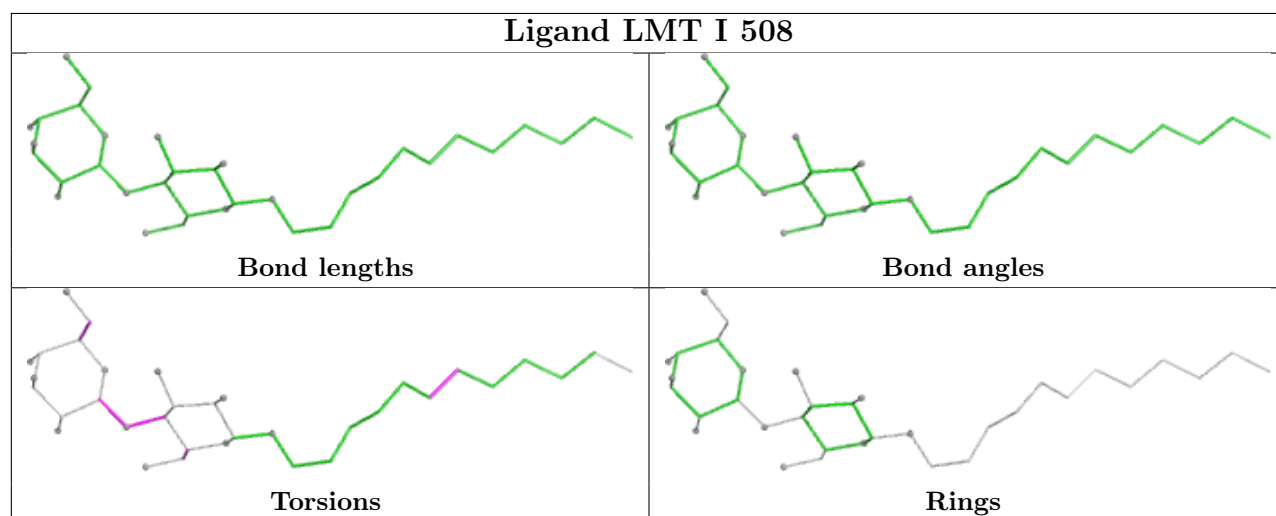
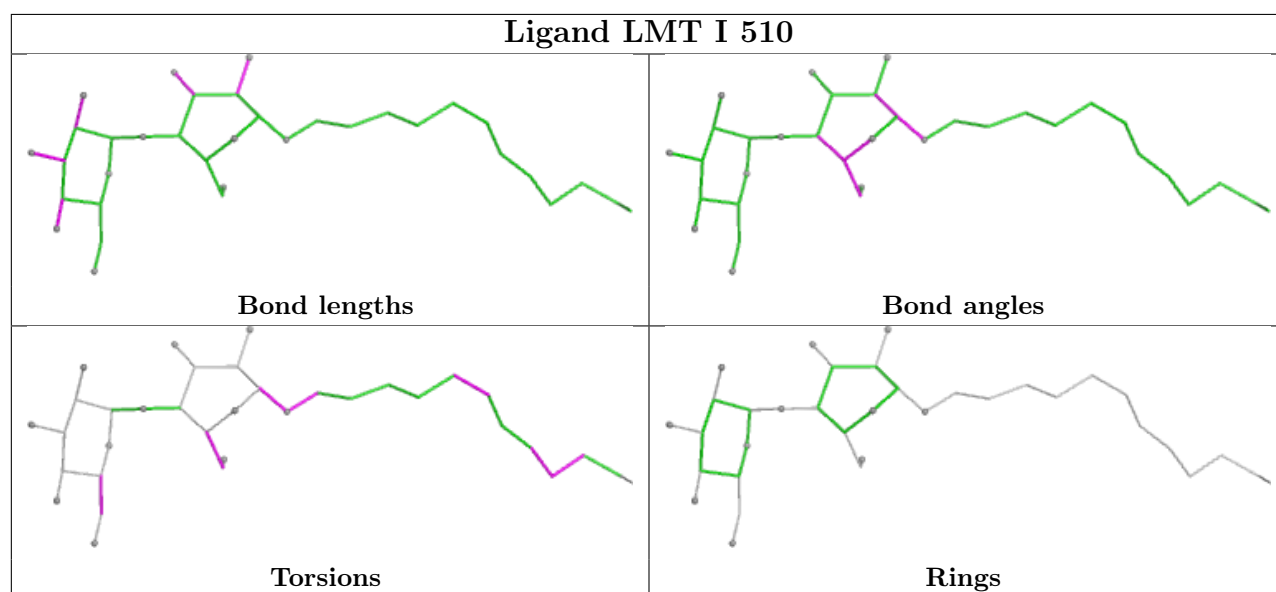
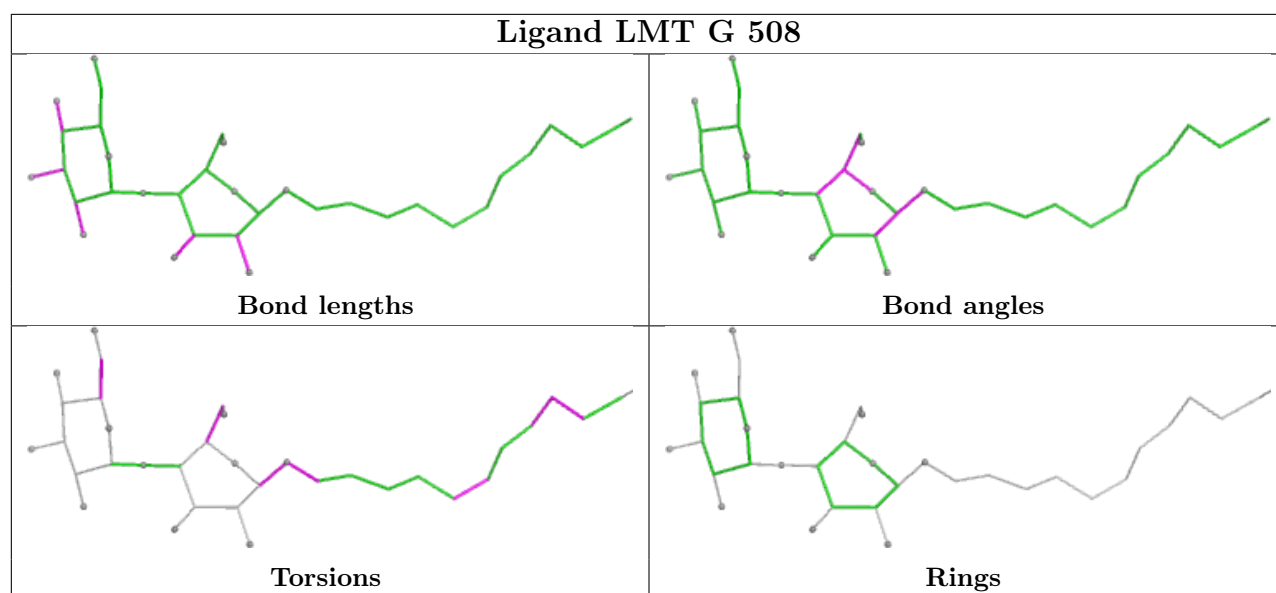


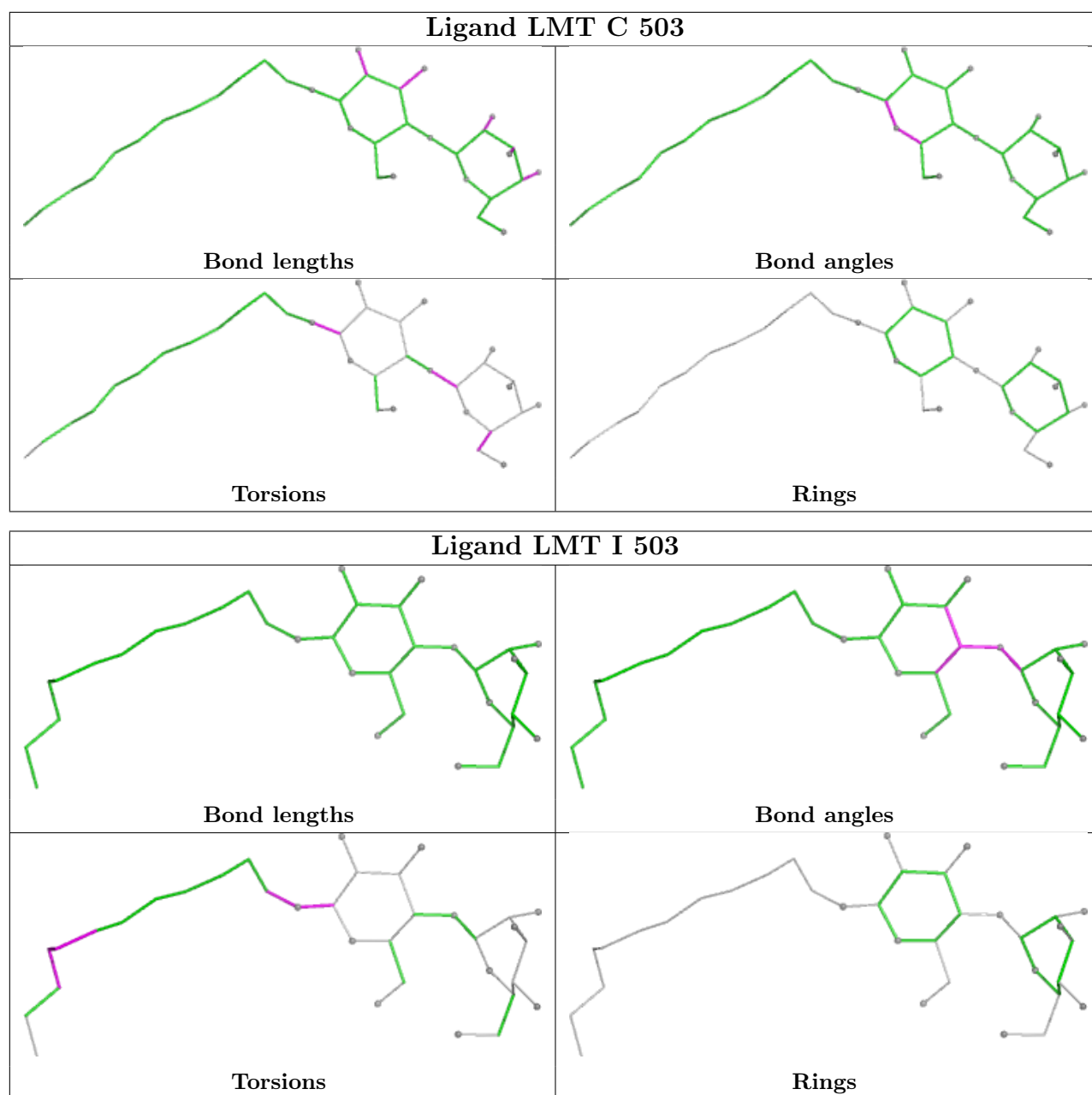
Ligand LMT I 506

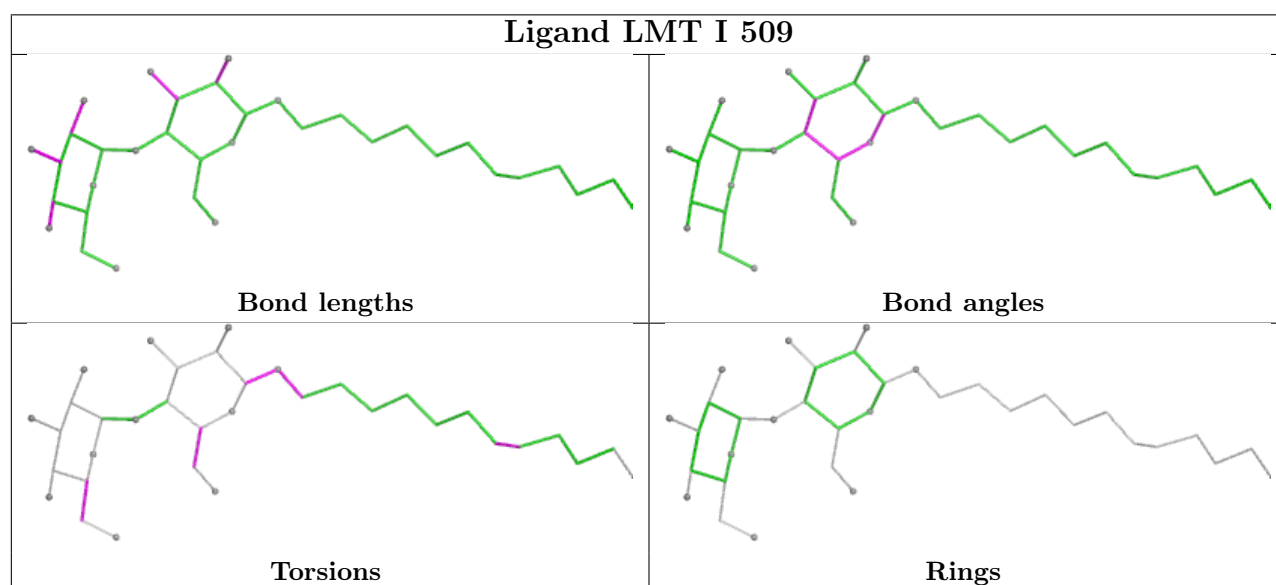
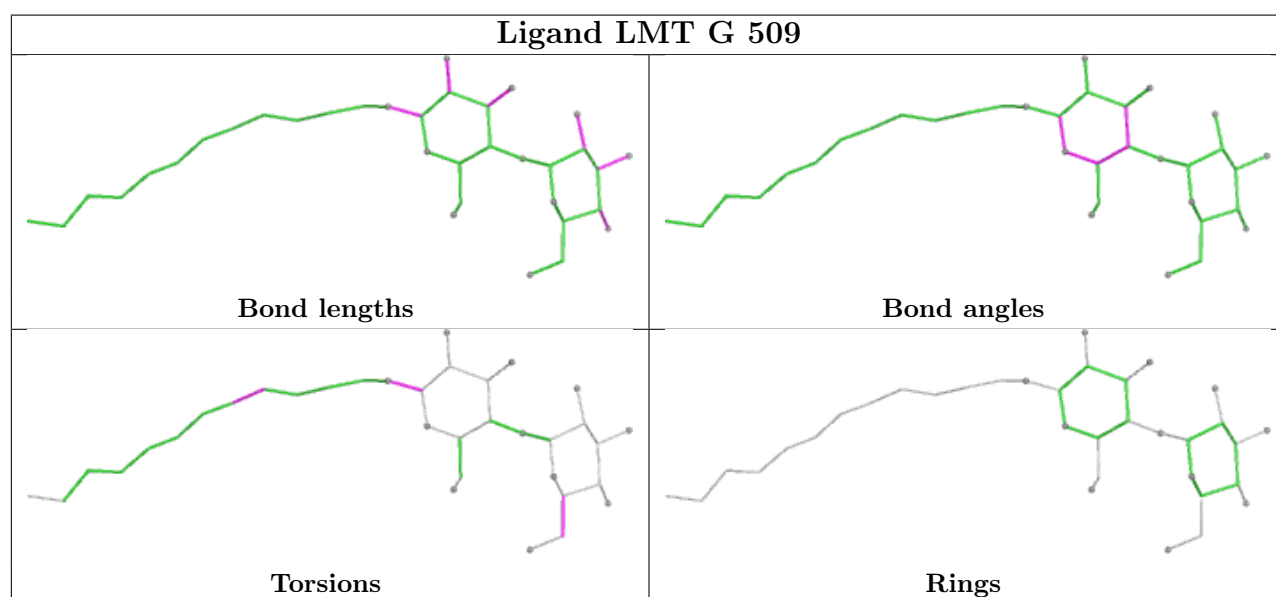
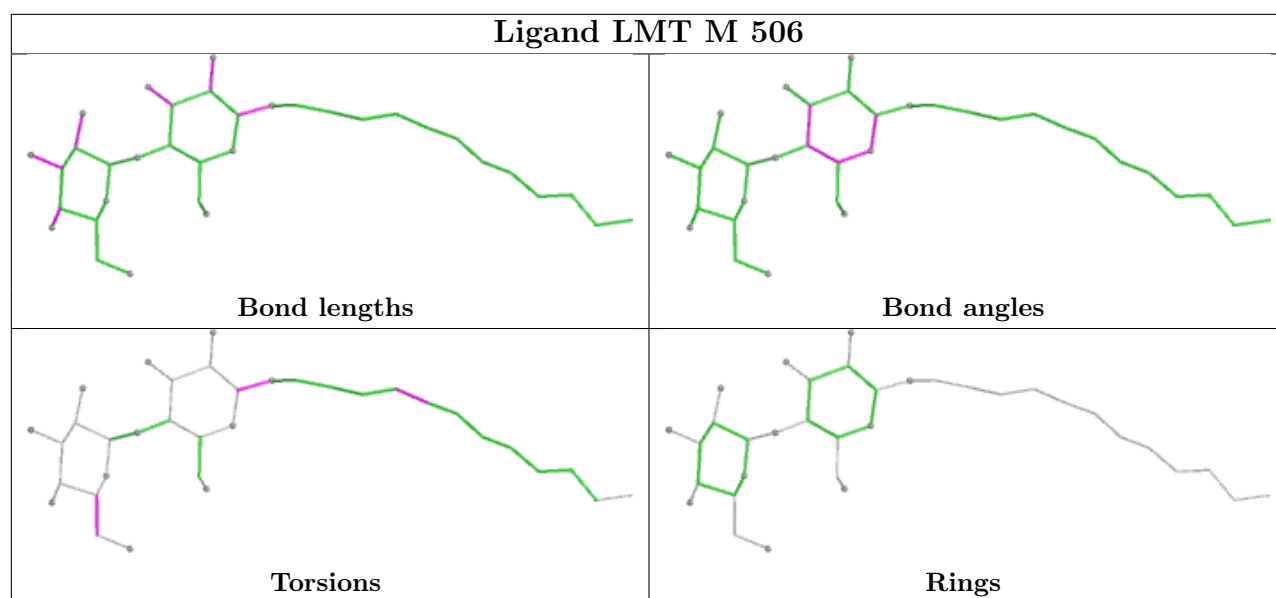


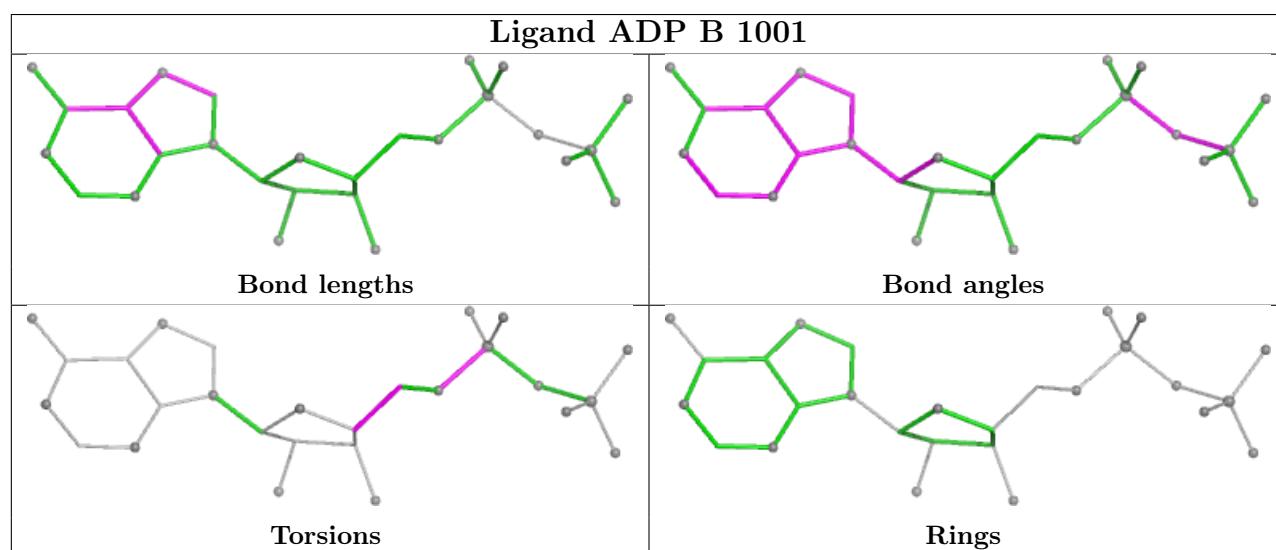
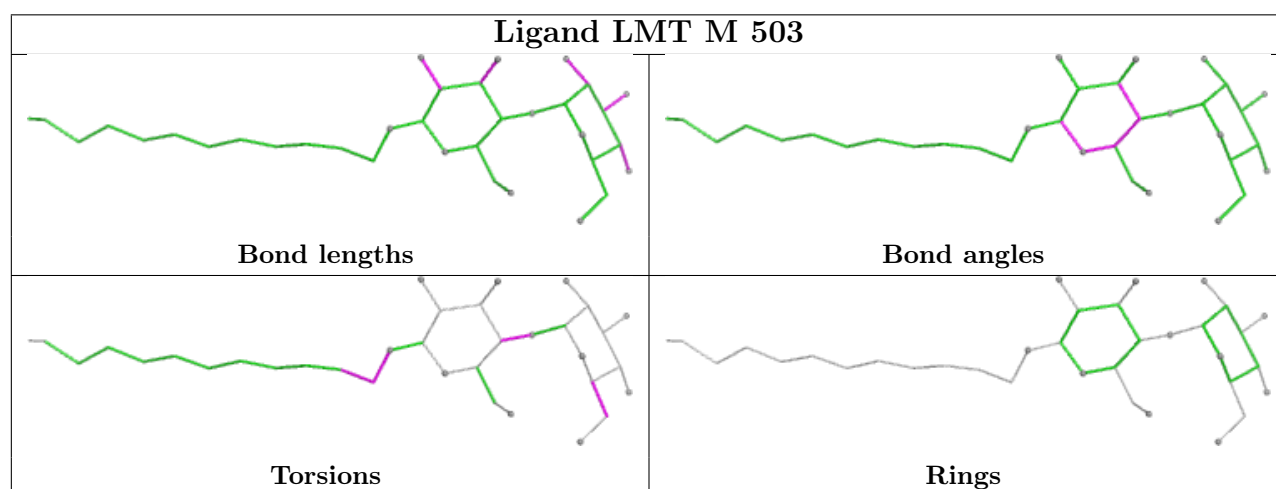
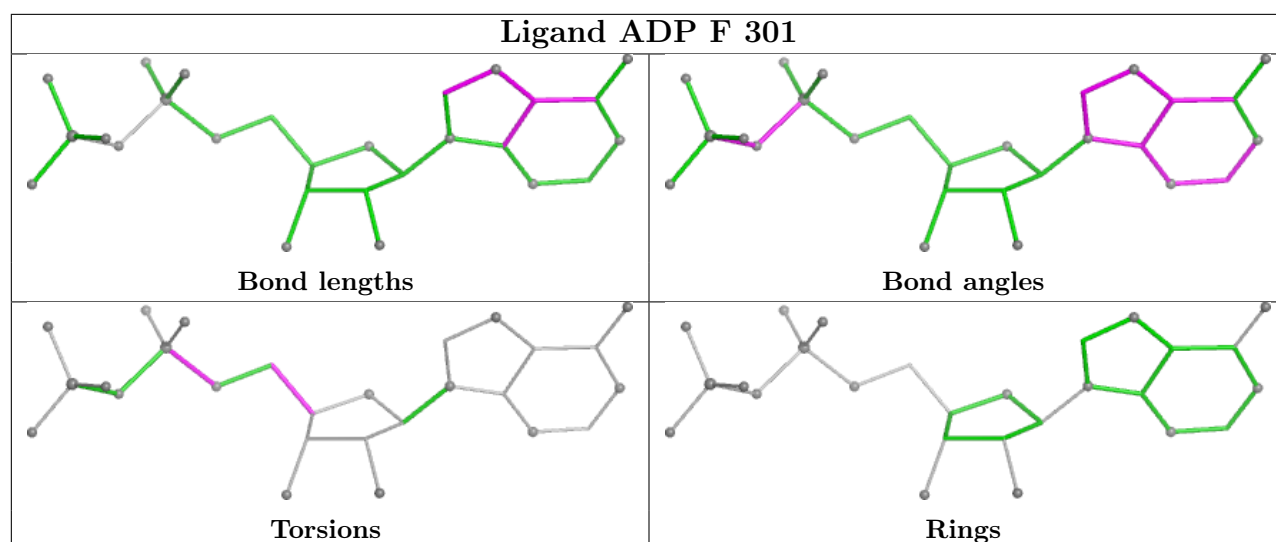
Ligand ADP H 1002

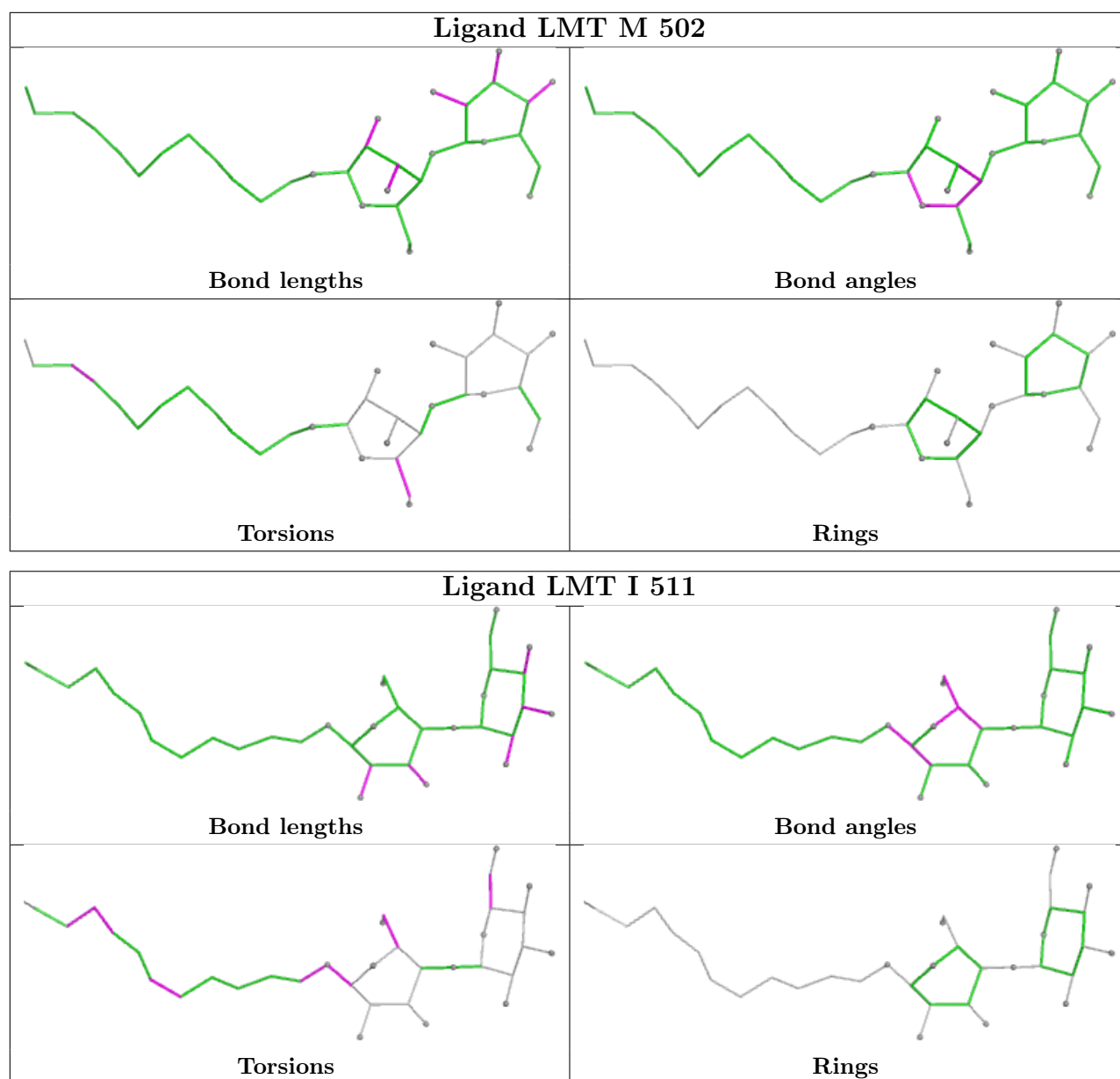












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

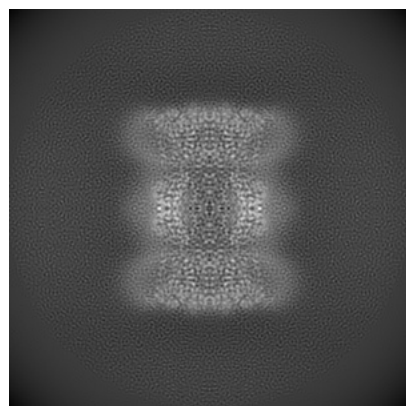
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14851. These allow visual inspection of the internal detail of the map and identification of artifacts.

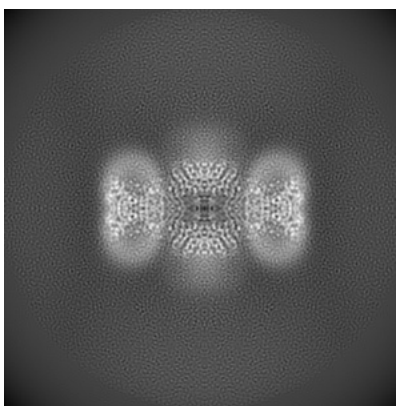
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

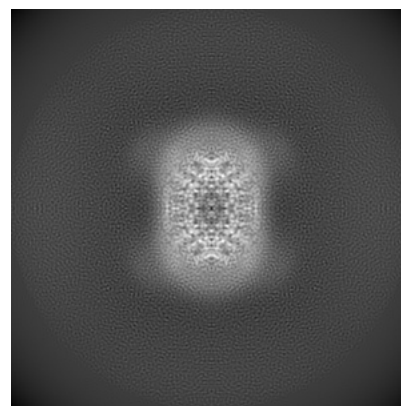
6.1.1 Primary map



X

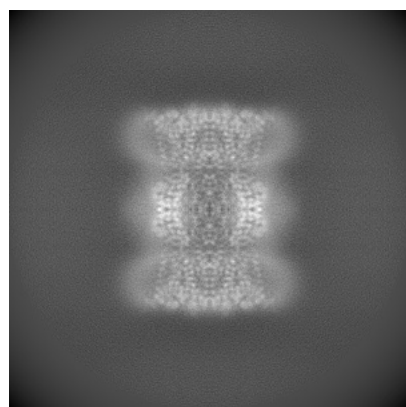


Y

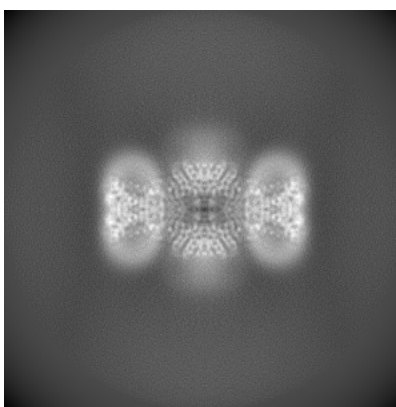


Z

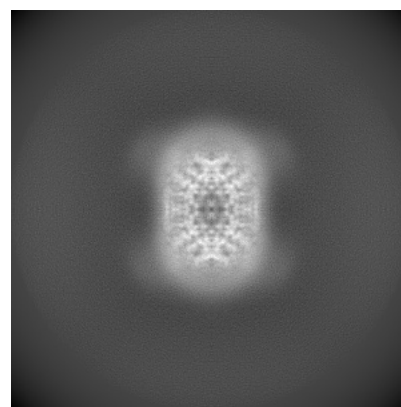
6.1.2 Raw map



X



Y

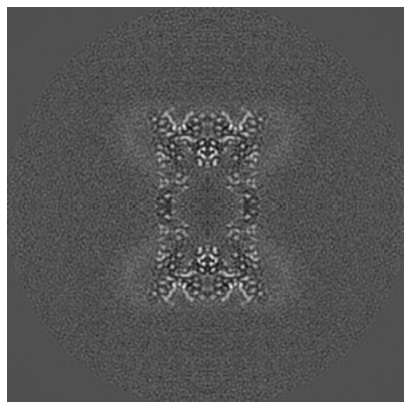


Z

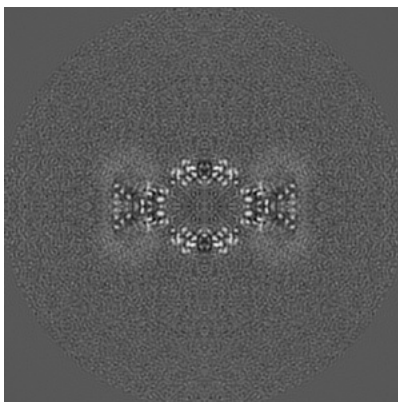
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

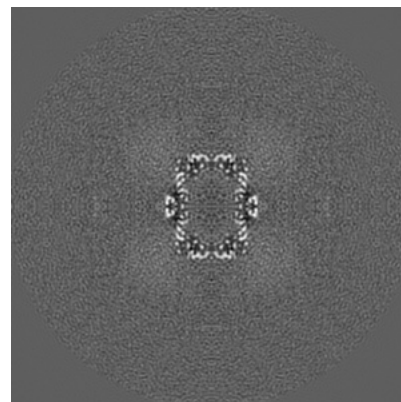
6.2.1 Primary map



X Index: 180

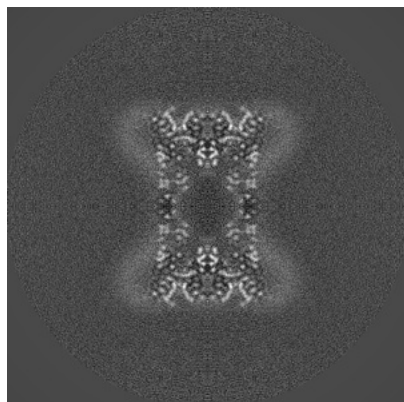


Y Index: 180

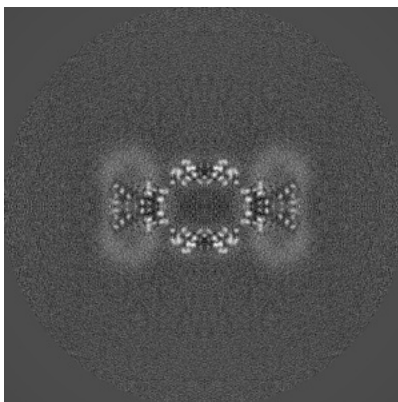


Z Index: 180

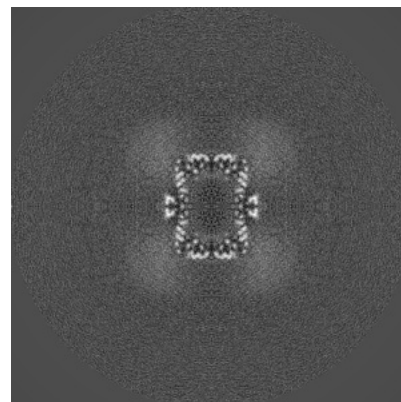
6.2.2 Raw map



X Index: 180



Y Index: 180

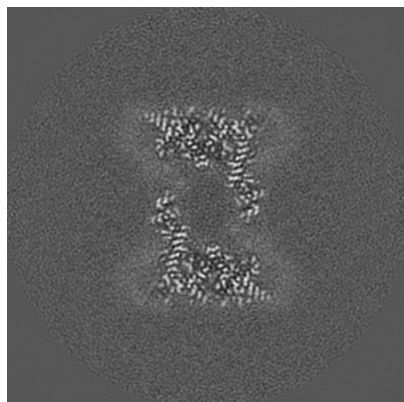


Z Index: 180

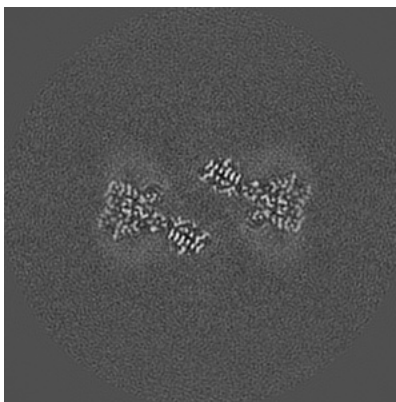
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

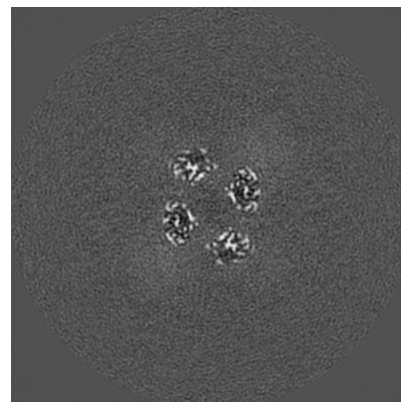
6.3.1 Primary map



X Index: 185

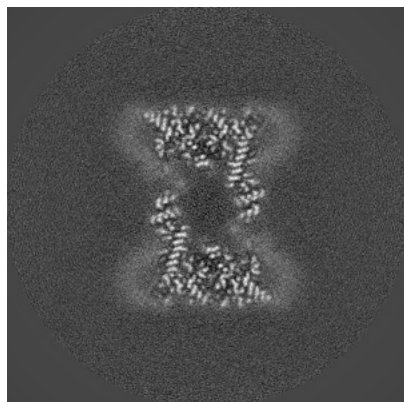


Y Index: 165

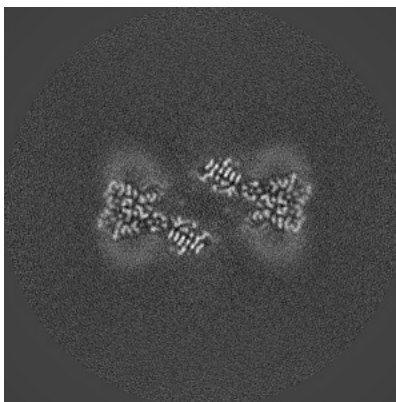


Z Index: 166

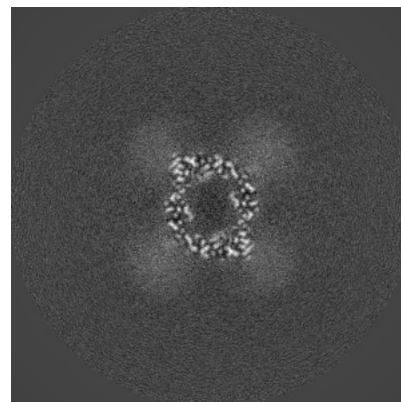
6.3.2 Raw map



X Index: 185



Y Index: 165

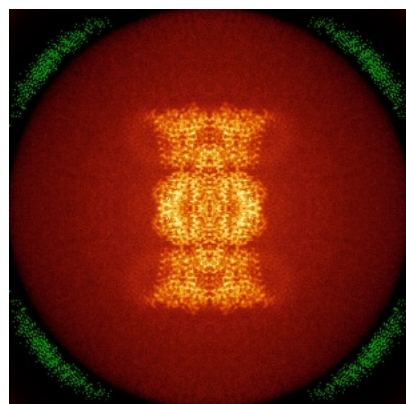


Z Index: 176

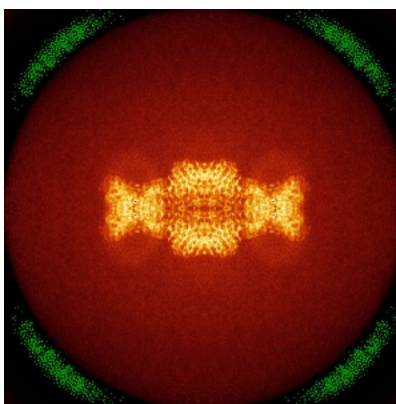
The images above show the largest variance slices of the map in three orthogonal directions.

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

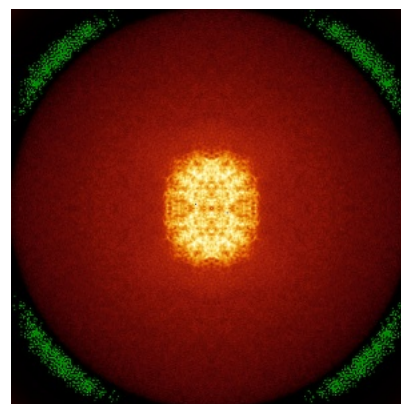
6.4.1 Primary map



X

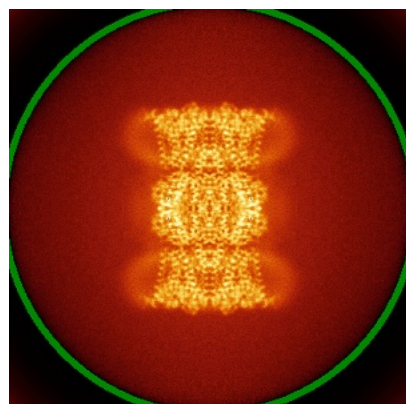


Y

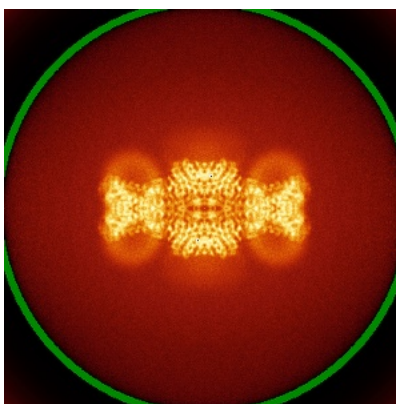


Z

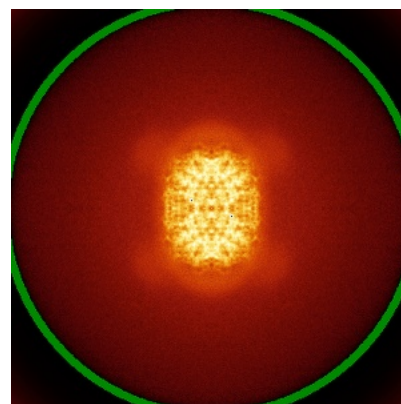
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



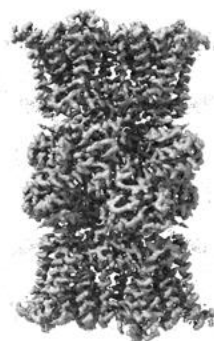
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

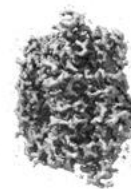
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

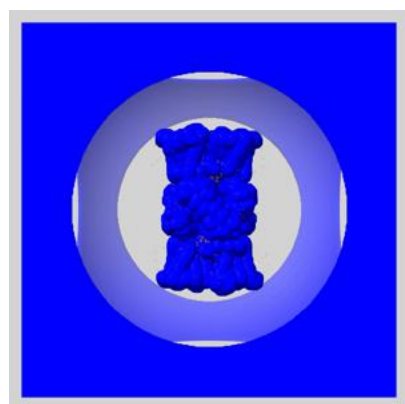
6.6 Mask visualisation [i](#)

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

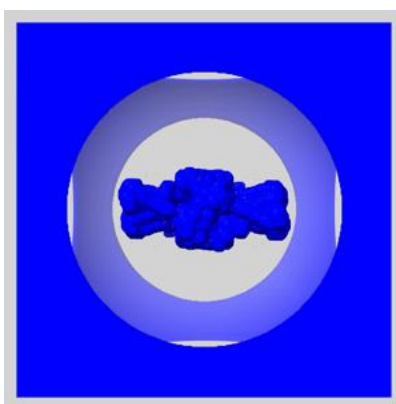
A mask typically either:

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

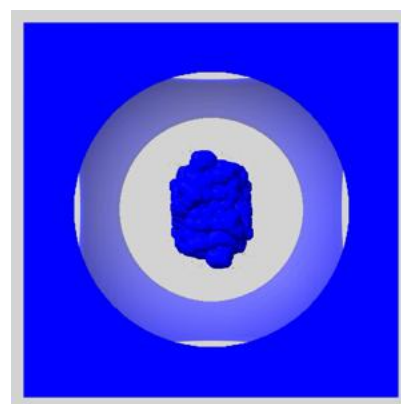
6.6.1 emd_14851_msk_1.map [i](#)



X



Y

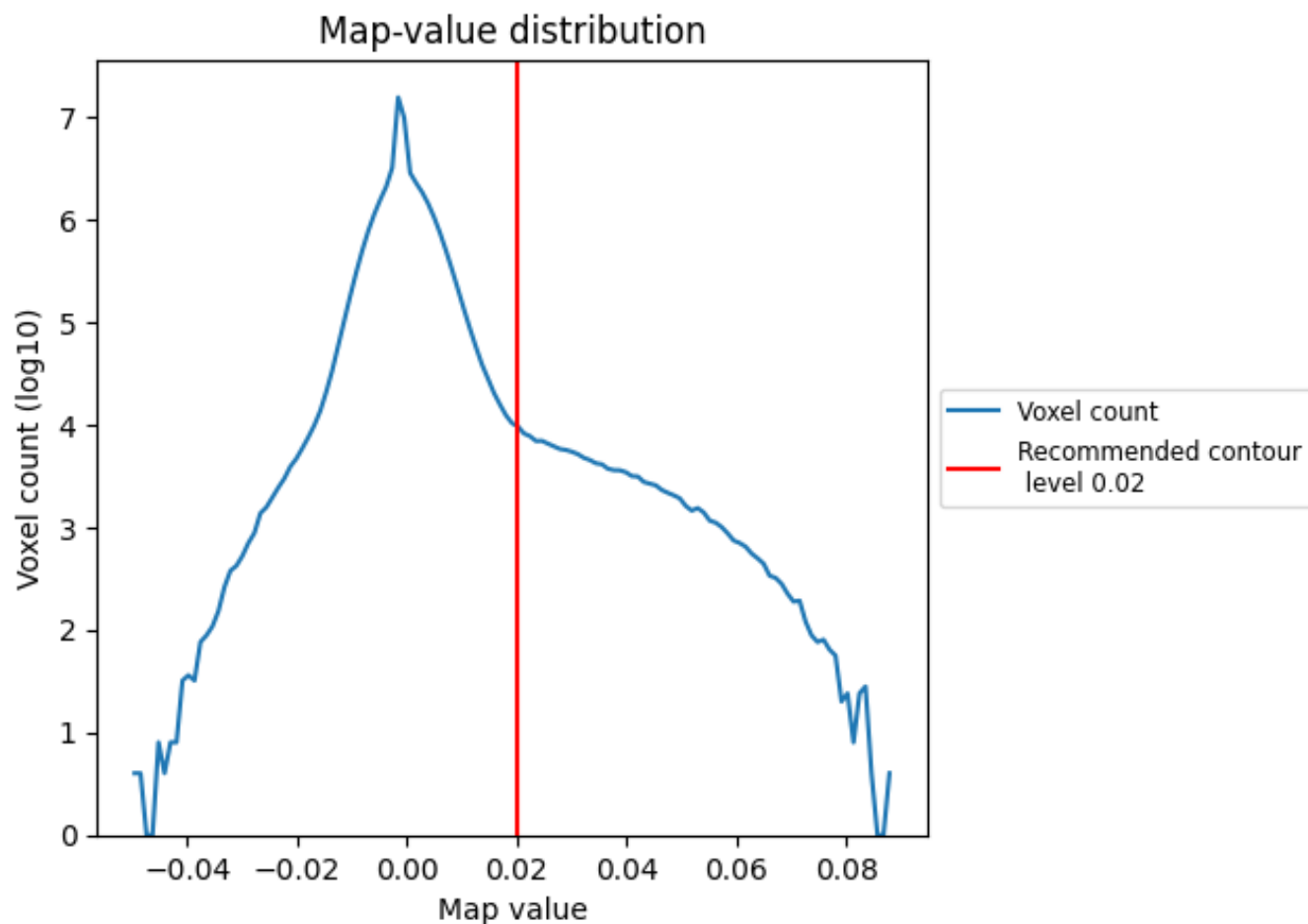


Z

7 Map analysis [i](#)

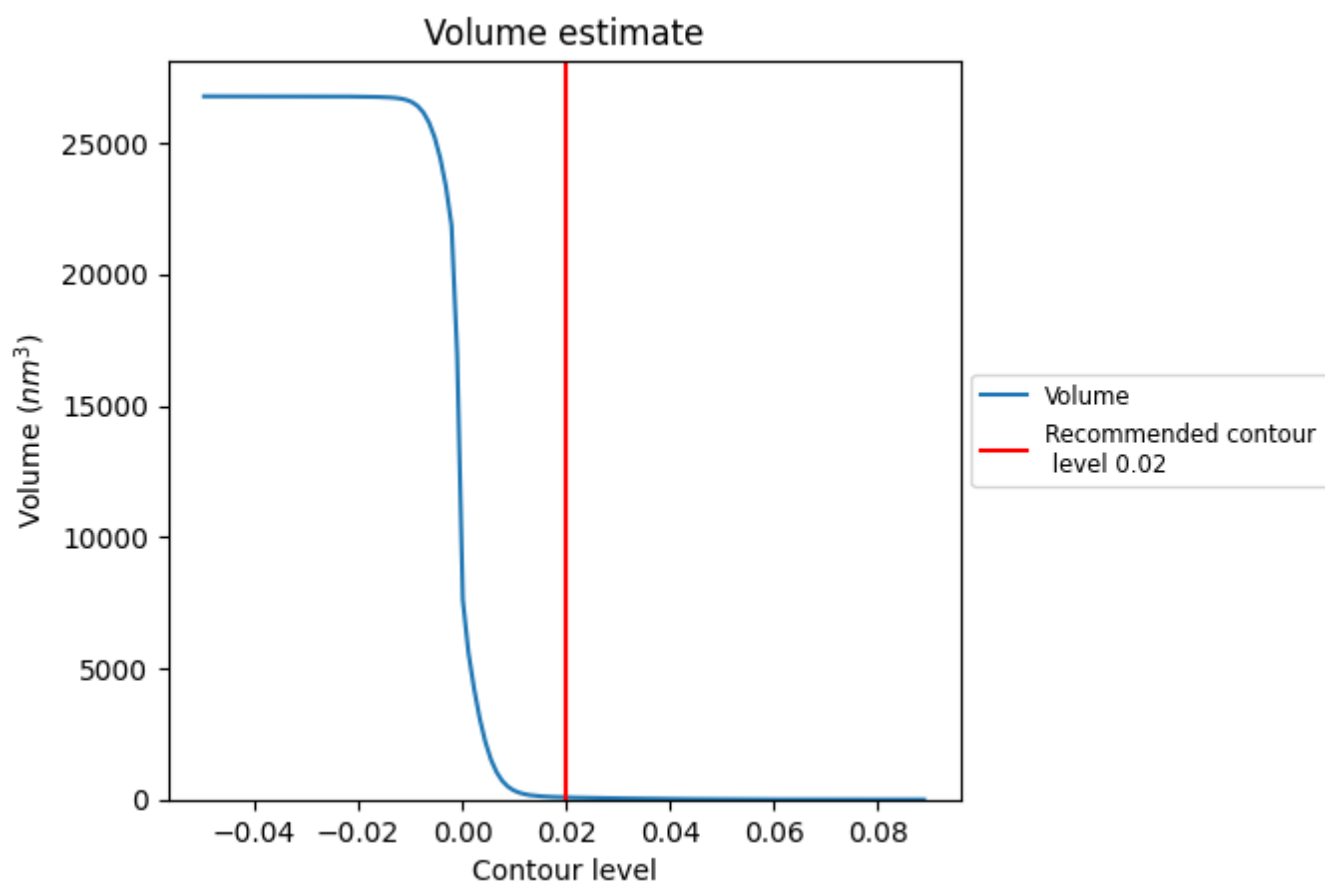
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

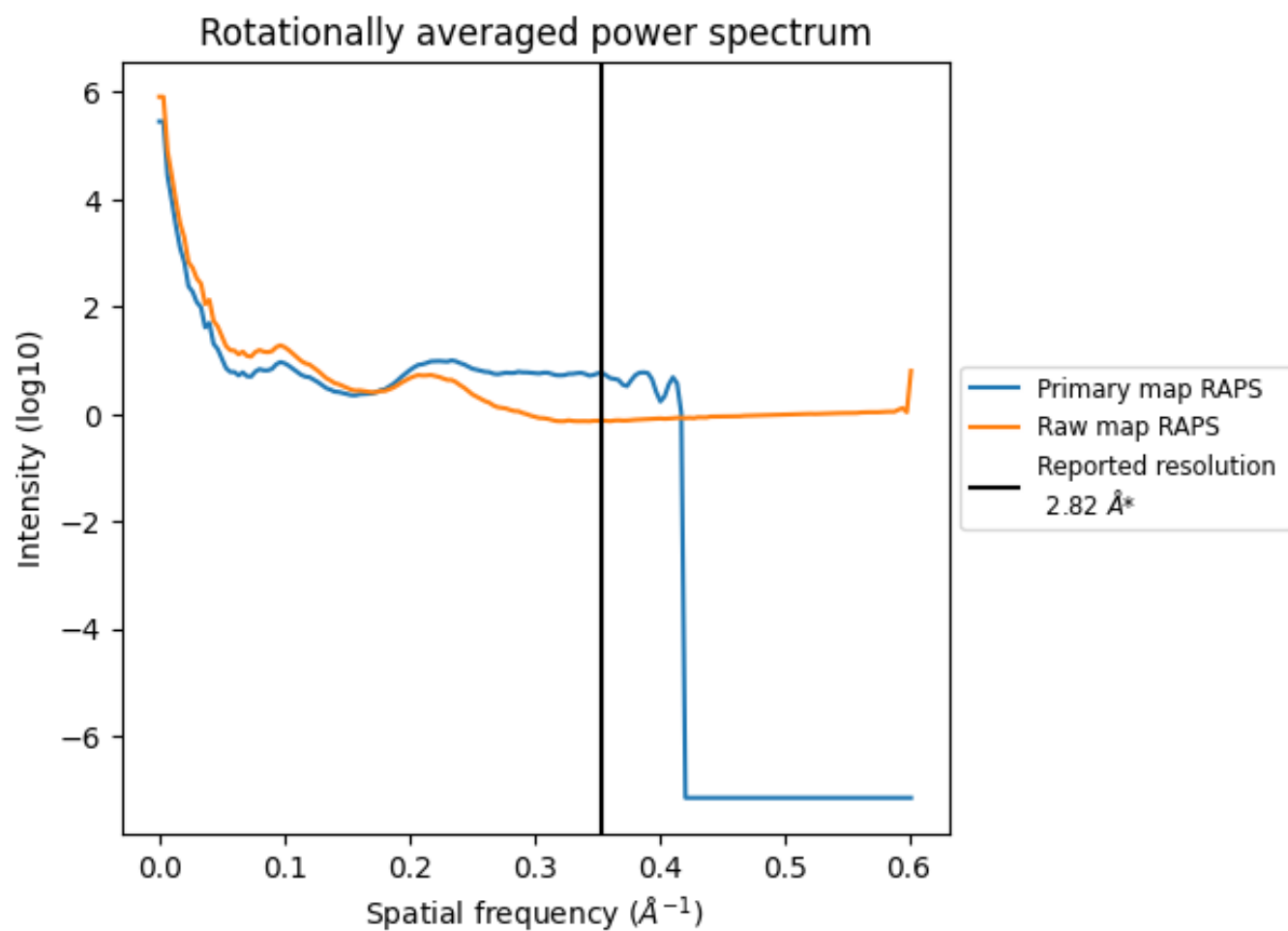
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

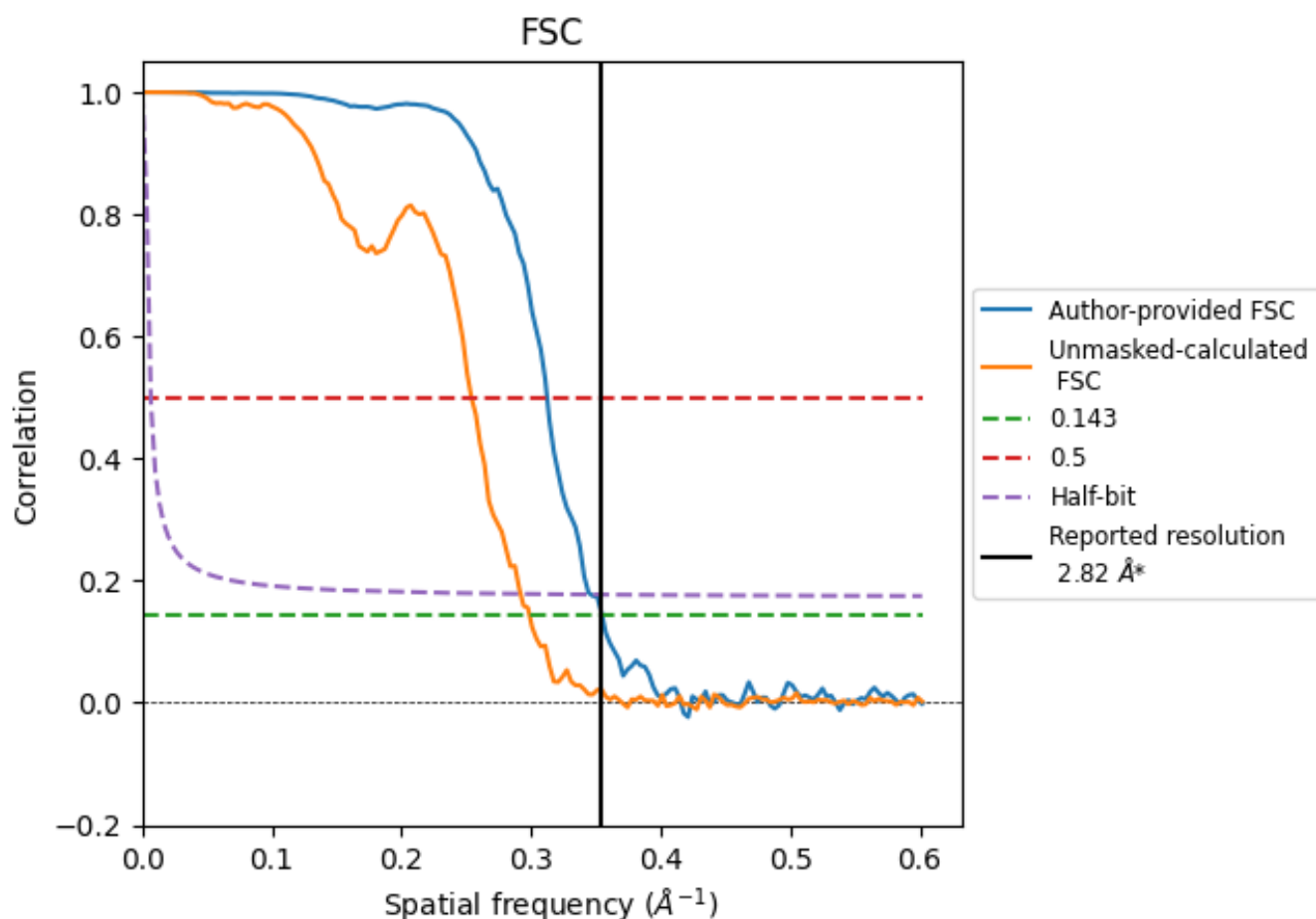


*Reported resolution corresponds to spatial frequency of 0.355 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.355 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

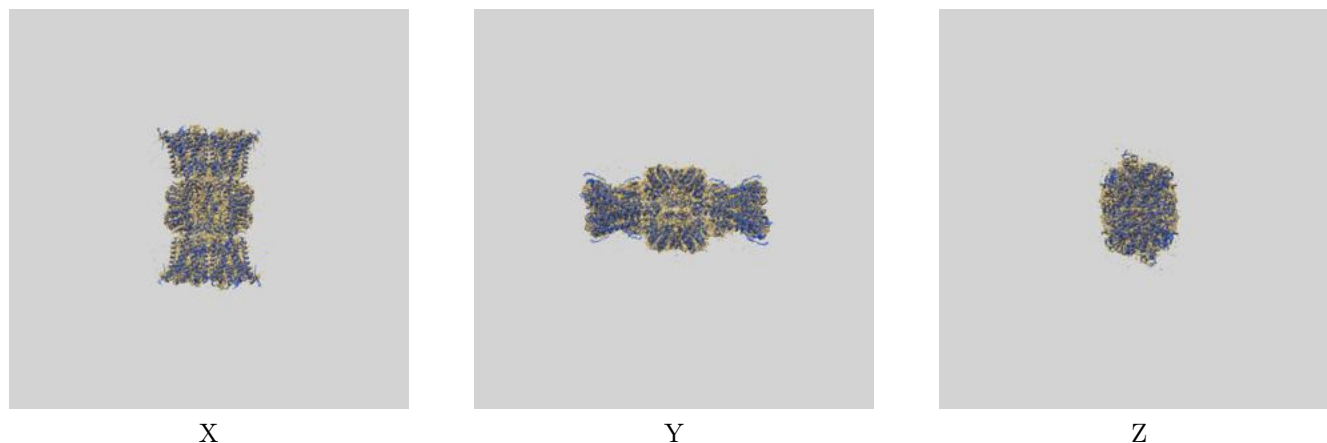
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.82	-	-
Author-provided FSC curve	2.82	3.20	2.89
Unmasked-calculated*	3.35	3.94	3.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.35 differs from the reported value 2.82 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14851 and PDB model 7ZP9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



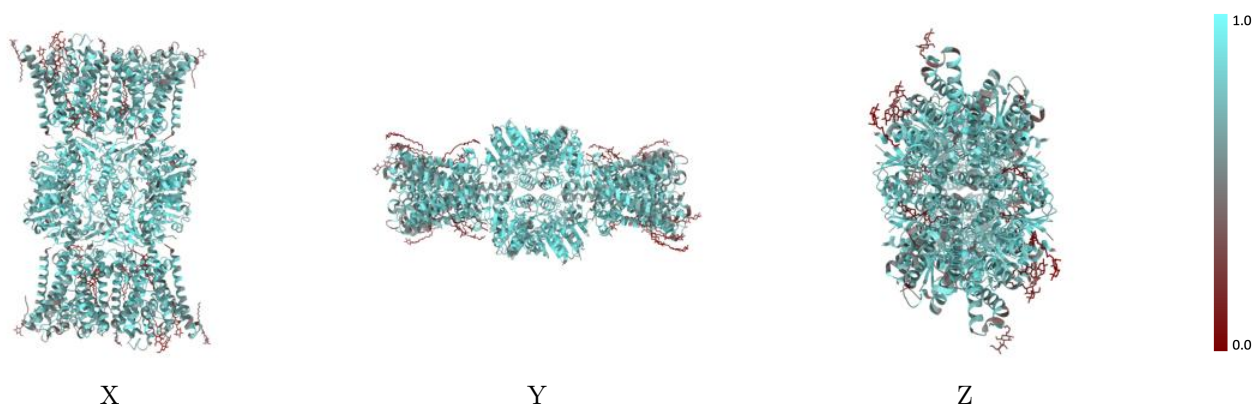
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



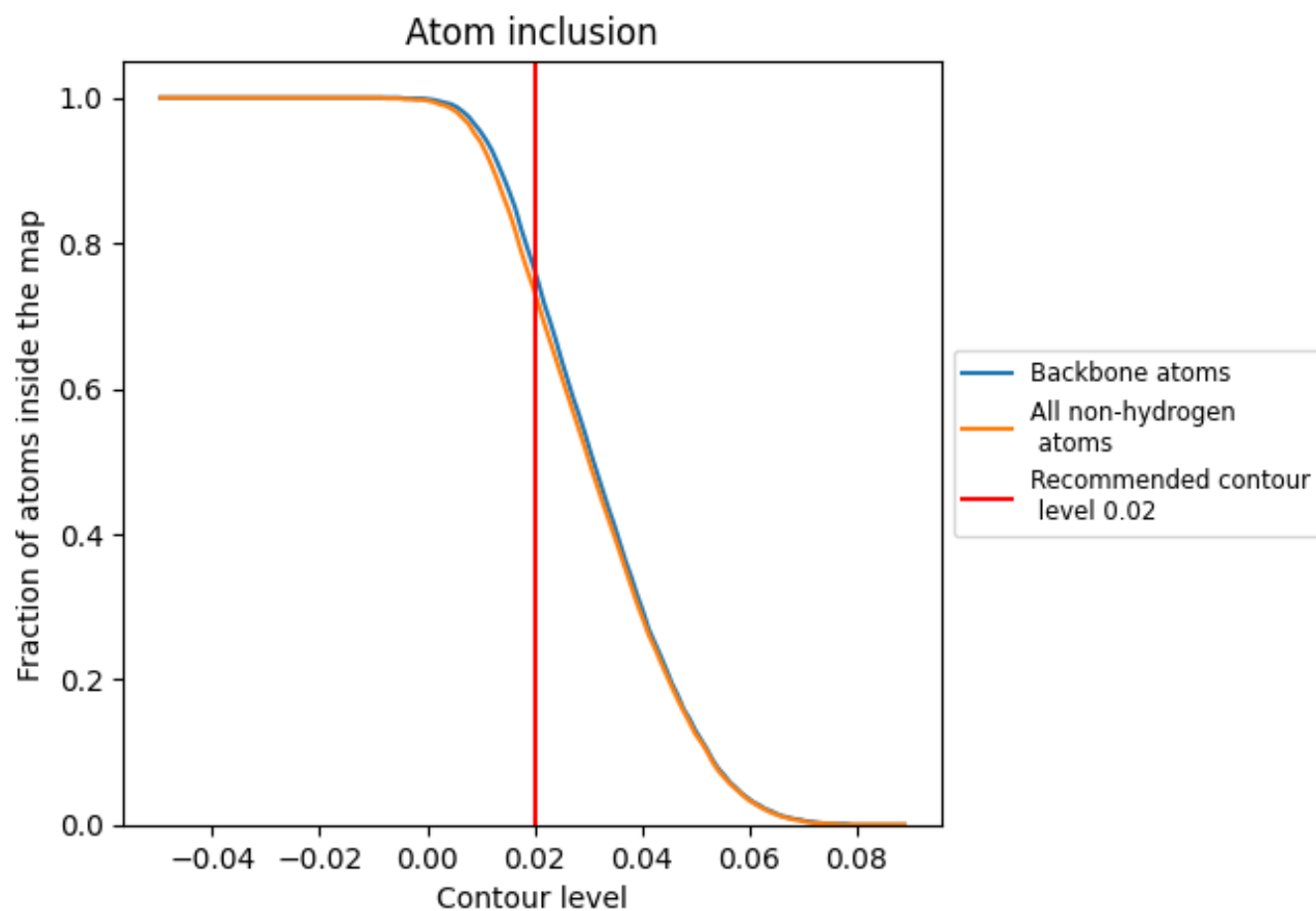
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.6050
A	0.8060	0.6270
B	0.8290	0.6270
C	0.6890	0.5920
D	0.8510	0.6300
E	0.7940	0.6200
F	0.7810	0.6120
G	0.7050	0.5970
H	0.8200	0.6220
I	0.6910	0.5940
J	0.8040	0.6250
L	0.7900	0.6220
M	0.7130	0.5990

1.0

0.0

<0.0