Full wwPDB EM Validation Report ⓘ

Dec 17, 2023 – 04:15 pm GMT

PDB ID	:	7OJF
EMDB ID	:	EMD-12949
Title	:	CRYO-EM STRUCTURE OF SLYB13-BAMA FROM ESCHERICHIA COLI
Authors	:	Nguyen, V.S.; Remaut, H.
Deposited on	:	2021-05-14
Resolution	:	3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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:

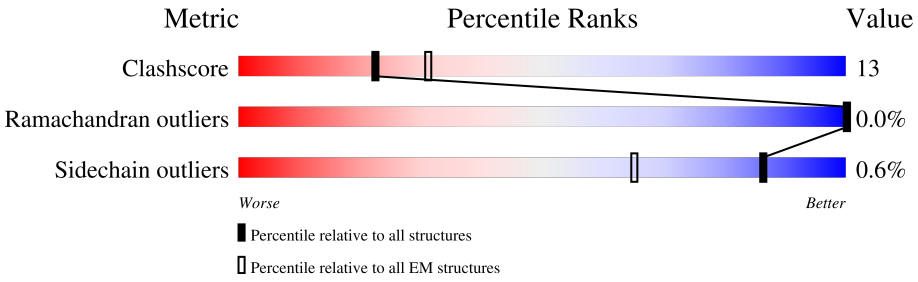
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	155	72% 17% 11%
1	B	155	69% 19% • 11%
1	C	155	71% 17% • 11%
1	D	155	73% 15% • 11%
1	E	155	74% 15% • 11%
1	F	155	68% 21% 11%
1	G	155	68% 21% 11%
1	H	155	69% 19% • 11%
1	I	155	68% 21% 11%

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Mol	Chain	Length	Quality of chain
1	J	155	77% 12% 11%
1	K	155	75% 14% 11%
1	L	155	67% 22% 11%
1	M	155	65% 25% 11%
2	N	810	40% 24% 35%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19318 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.

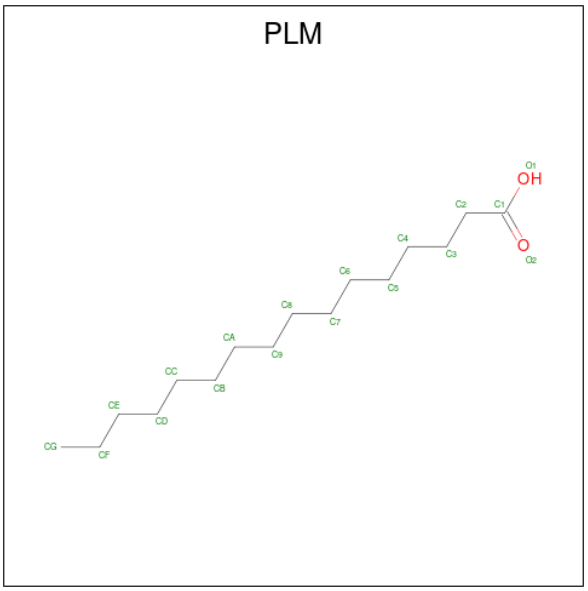
- Molecule 1 is a protein called Outer membrane lipoprotein slyB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	B	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	C	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	D	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	E	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	F	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	G	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	H	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	I	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	J	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	K	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	L	138	Total	C	N	O	S	0	0
			967	584	181	199	3		
1	M	138	Total	C	N	O	S	0	0
			967	584	181	199	3		

- Molecule 2 is a protein called Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	525	Total	C	N	O	S	0	0
			4139	2614	691	820	14		

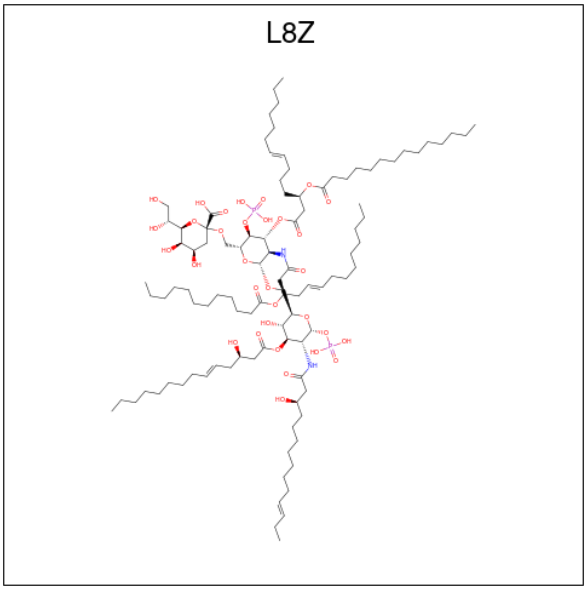
- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 17 16 1	0
3	B	1	Total C O 17 16 1	0
3	C	1	Total C O 17 16 1	0
3	D	1	Total C O 17 16 1	0
3	E	1	Total C O 17 16 1	0
3	F	1	Total C O 17 16 1	0
3	G	1	Total C O 17 16 1	0
3	H	1	Total C O 17 16 1	0
3	I	1	Total C O 17 16 1	0
3	J	1	Total C O 17 16 1	0
3	K	1	Total C O 17 16 1	0
3	L	1	Total C O 17 16 1	0
3	M	1	Total C O 17 16 1	0

- Molecule 4 is (2 {R},4 {R},5 {R},6 {R})-6-[(1 {R})-1,2-bis(oxidanyl)ethyl]-2-[[(2 {R},3 {S}

,4 {R},5 {R},6 {R})-5-[[({E},3 {R})-3-dodecanoyloxytetradec-5-enoyl]amino]-6-[[(2 {R},3 {S},4 {R},5 {R},6 {R})-3-oxidanyl-5-[[({E},3 {R})-3-oxidanyltetradec-11-enoyl]amino]-4-[({E},3 {R})-3-oxidanyltetradec-5-enoyl]oxy-6-phosphonooxy-oxan-2-yl]methoxy]-3-phosphonooxy-4-[({E},3 {R})-3-tetradecanoyloxytetradec-7-enoyl]oxy-oxan-2-yl]methoxy]-4,5-bis(oxidanyl)oxane-2-carboxylic acid (three-letter code: L8Z) (formula: $C_{102}H_{182}N_2O_{32}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	B	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	C	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	D	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	E	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	F	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	G	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	H	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	I	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	J	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	K	1	Total	C	N	O	P	0
			138	102	2	32	2	

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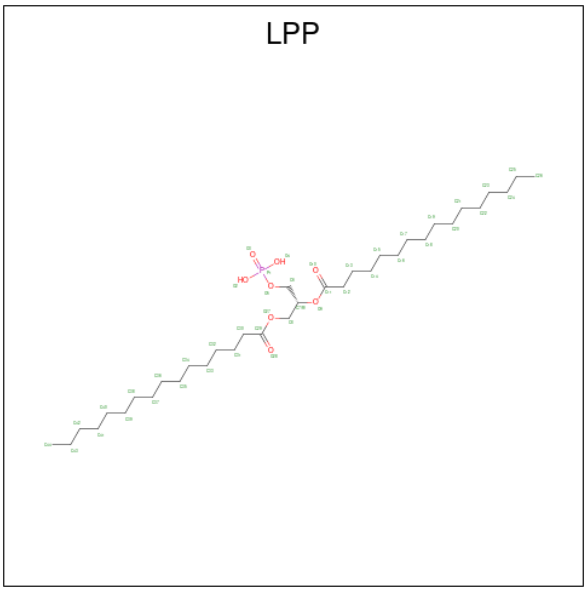
Mol	Chain	Residues	Atoms					AltConf
4	L	1	Total	C	N	O	P	0
			138	102	2	32	2	
4	M	1	Total	C	N	O	P	0
			138	102	2	32	2	

- Molecule 5 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (three-letter code: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			44	35	8	1	
5	B	1	Total	C	O	P	0
			44	35	8	1	
5	C	1	Total	C	O	P	0
			44	35	8	1	
5	D	1	Total	C	O	P	0
			44	35	8	1	
5	F	1	Total	C	O	P	0
			44	35	8	1	
5	G	1	Total	C	O	P	0
			44	35	8	1	
5	H	1	Total	C	O	P	0
			44	35	8	1	
5	I	1	Total	C	O	P	0
			44	35	8	1	
5	J	1	Total	C	O	P	0
			44	35	8	1	

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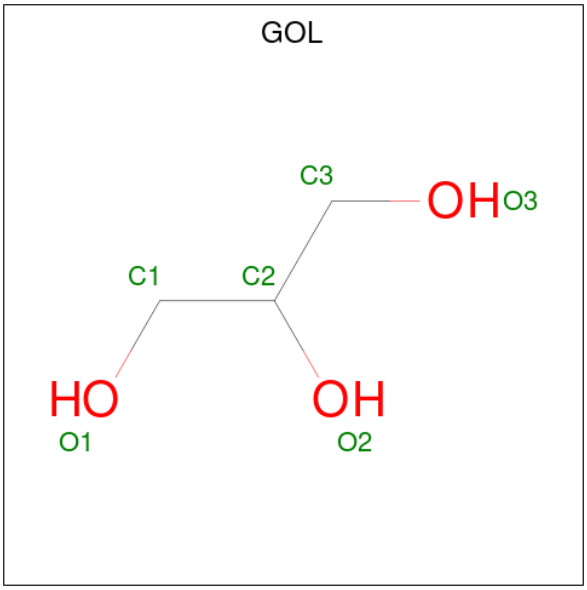
Mol	Chain	Residues	Atoms	AltConf
5	K	1	Total C O P 44 35 8 1	0
5	L	1	Total C O P 44 35 8 1	0
5	M	1	Total C O P 44 35 8 1	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C O 5 3 2	0
6	C	1	Total C O 5 3 2	0
6	D	1	Total C O 5 3 2	0
6	D	1	Total C O 5 3 2	0
6	E	1	Total C O 5 3 2	0
6	F	1	Total C O 5 3 2	0
6	H	1	Total C O 5 3 2	0
6	H	1	Total C O 5 3 2	0

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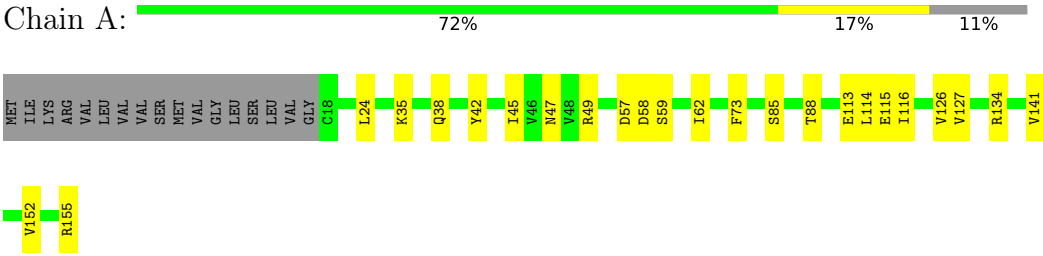
Mol	Chain	Residues	Atoms	AltConf
6	J	1	Total C O 5 3 2	0
6	J	1	Total C O 5 3 2	0
6	K	1	Total C O 5 3 2	0
6	M	1	Total C O 5 3 2	0
6	M	1	Total C O 5 3 2	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

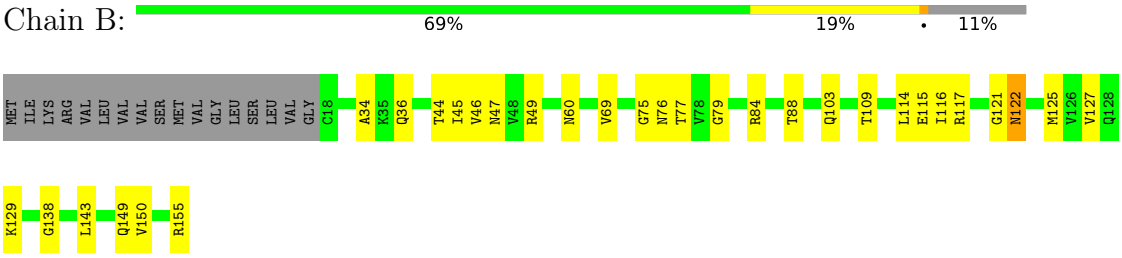
• Molecule 1: Outer membrane lipoprotein slyB

Chain A:



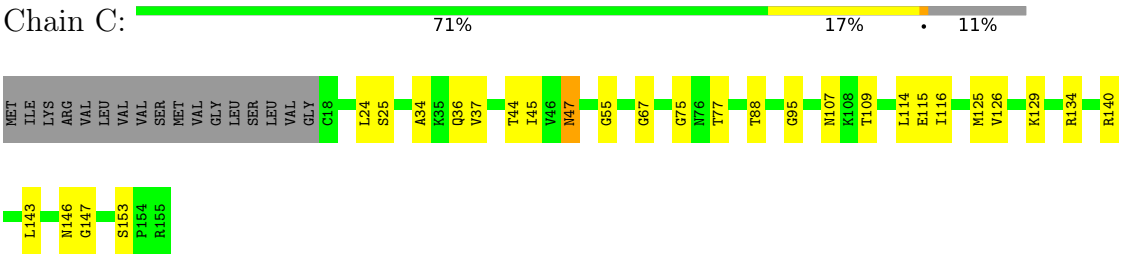
• Molecule 1: Outer membrane lipoprotein slyB

Chain B:



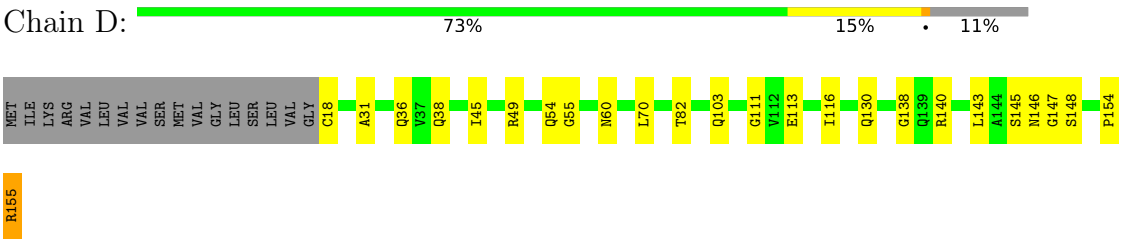
• Molecule 1: Outer membrane lipoprotein slyB

Chain C:



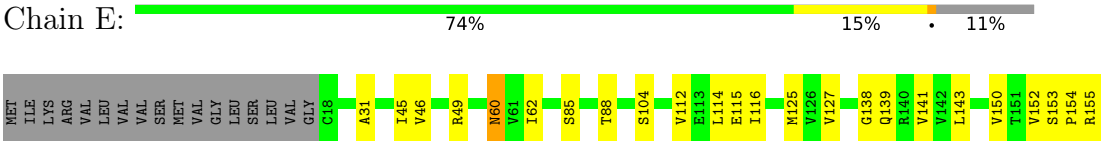
• Molecule 1: Outer membrane lipoprotein slyB

Chain D:



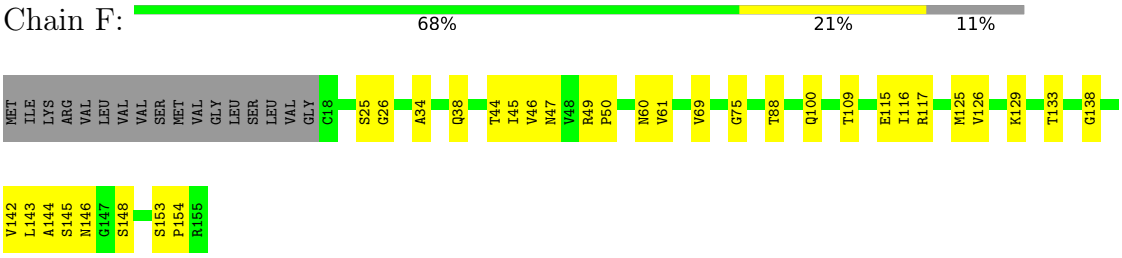
• Molecule 1: Outer membrane lipoprotein slyB

Chain E:



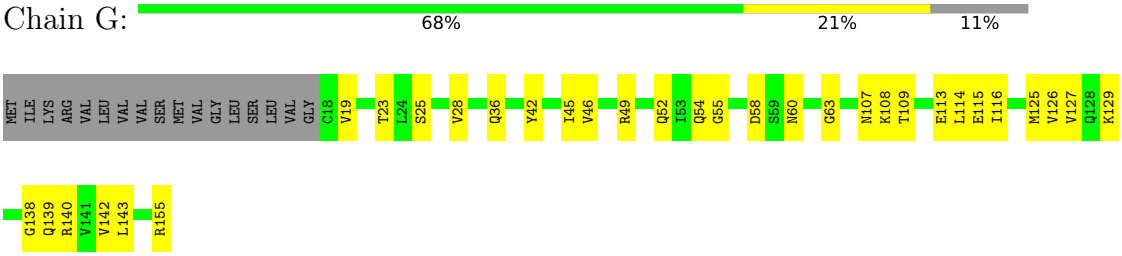
• Molecule 1: Outer membrane lipoprotein slyB

Chain F:



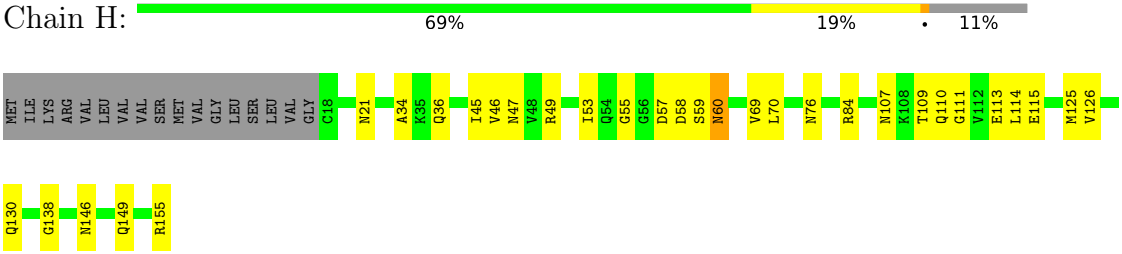
• Molecule 1: Outer membrane lipoprotein slyB

Chain G:



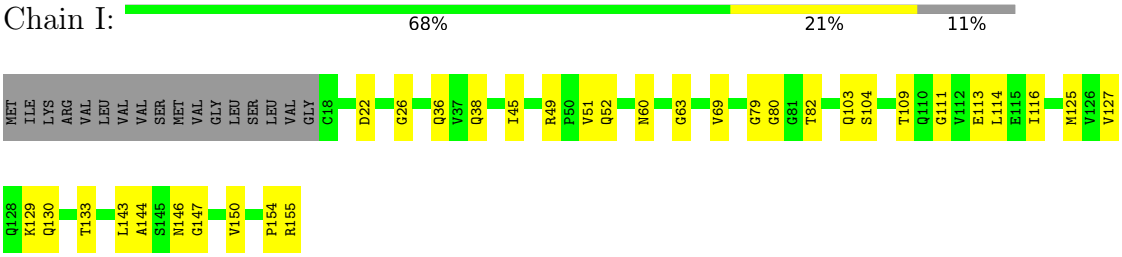
• Molecule 1: Outer membrane lipoprotein slyB

Chain H:



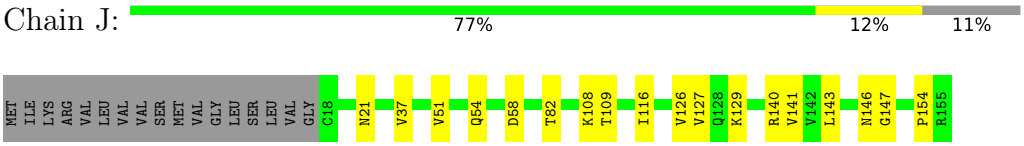
• Molecule 1: Outer membrane lipoprotein slyB

Chain I:



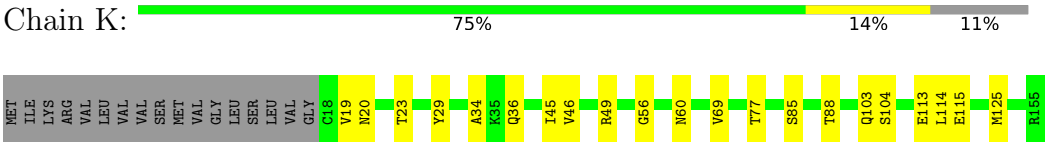
• Molecule 1: Outer membrane lipoprotein slyB

Chain J:



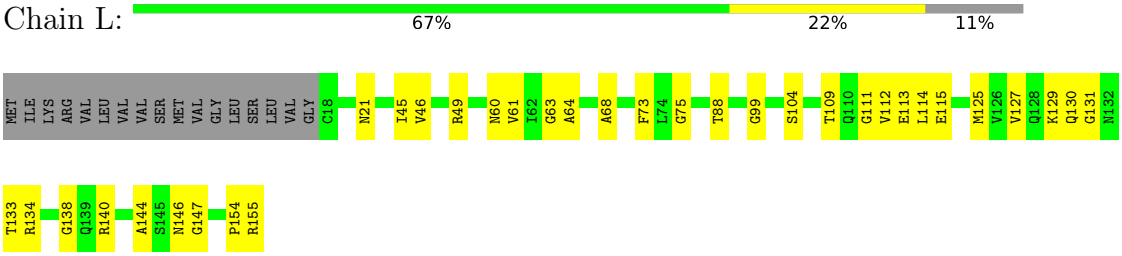
• Molecule 1: Outer membrane lipoprotein slyB

Chain K:



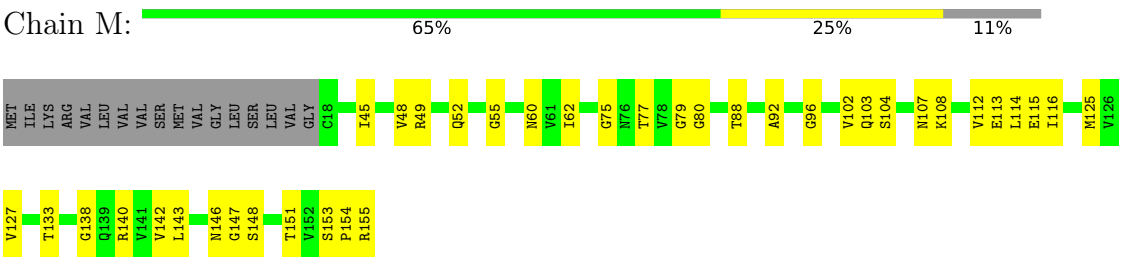
• Molecule 1: Outer membrane lipoprotein slyB

Chain L:



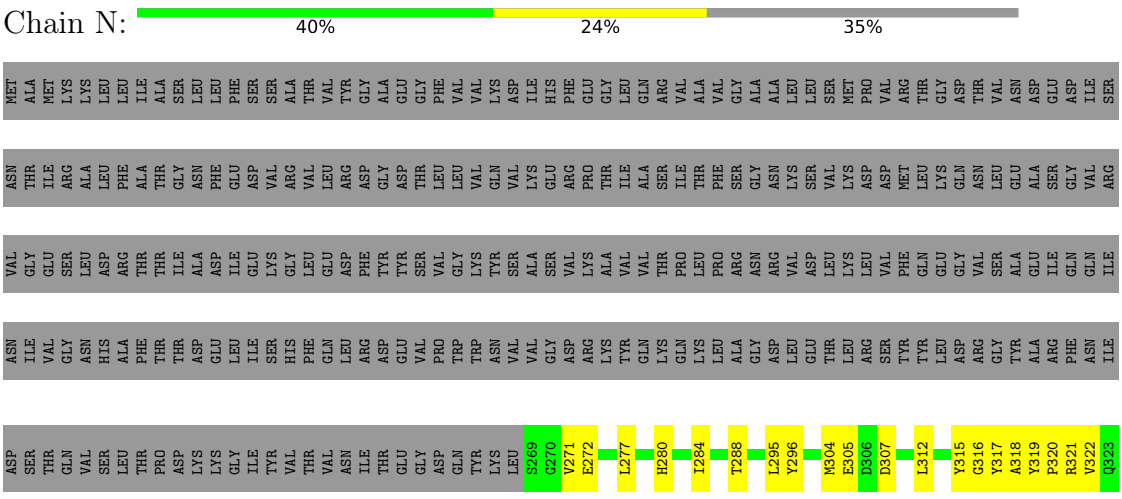
• Molecule 1: Outer membrane lipoprotein slyB

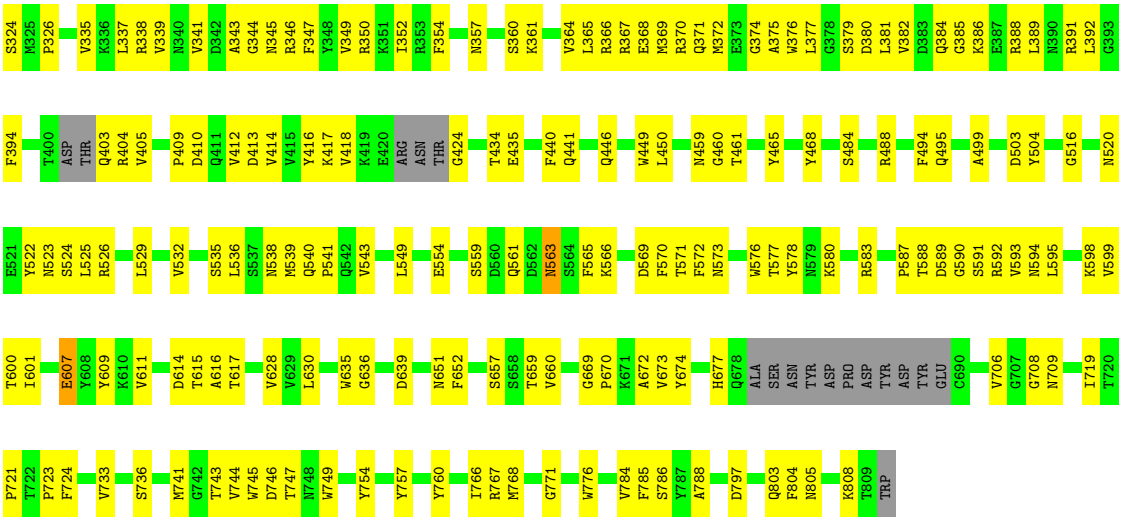
Chain M:



• Molecule 2: Outer membrane protein assembly factor BamA

Chain N:




S324 M325 P326 V335 K336 L337 R338 V339 N340 V341 D342 A343 G344 N345 R346 F347 Y348 V349 R350 K351 I352 R353 F354 N357 S360 K361 V364 L365 R366 R367 E368 M369 R370 Q371 M372 E373 G374 A375 W376 L377 G378 S379 D380 L381 V382 D383 Q384 G385 K386 E387 R388 L389 N390 R391 L392 G393
F394 T400 ASP THR Q403 R404 V405 P409 D410 Q411 V412 D413 V414 V415 Y416 K417 V418 K419 E420 ARG ASN THR G424 T434 E435 F440 Q441 Q446 W449 L450 M459 G460 T461 Y465 Y468 S484 R488 F494 Q495 A499 D503 Y504 G516 N520
E521 Y522 N523 S524 L525 R526 L529 V532 S535 L536 S537 N538 M539 Q540 P541 Q542 V543 L549 E554 S559 D560 Q561 D562 N563 S564 F565 K566 D569 F570 T571 F572 N573 W576 T577 Y578 N579 K580 R583 P587 T588 D589 G590 S591 R592 V593 N594 L595 K598 V599
T600 I601 E607 Y608 Y609 K610 V611 D614 T615 A616 T617 V628 V629 L630 W635 G636 D639 N651 F652 S657 S658 T659 V660 G669 P670 K671 A672 V673 Y674 H677 Q678 ALA SER ASN TYR ASP PRO ASP TYR ASP TYR GLU G690 V706 G707 G708 N709 I719 T720
P721 T722 P723 F724 V733 S736 M741 G742 T743 V744 W745 D746 T747 N748 W749 Y754 Y757 Y760 I766 R767 M768 G771 W776 V784 F785 S786 Y787 A788 D797 Q803 F804 N805 K808 T809 TRP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, GOL, L8Z, PLM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.43	0/973	0.56	0/1317
1	B	0.46	0/973	0.58	0/1317
1	C	0.45	0/973	0.57	0/1317
1	D	0.45	0/973	0.55	0/1317
1	E	0.49	1/973 (0.1%)	0.58	0/1317
1	F	0.46	0/973	0.63	0/1317
1	G	0.45	0/973	0.58	0/1317
1	H	0.45	0/973	0.56	0/1317
1	I	0.46	0/973	0.57	0/1317
1	J	0.45	0/973	0.57	0/1317
1	K	0.47	0/973	0.57	0/1317
1	L	0.44	0/973	0.57	0/1317
1	M	0.44	0/973	0.58	0/1317
2	N	0.37	0/4243	0.57	0/5751
All	All	0.44	1/16892 (0.0%)	0.57	0/22872

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	VAL	C-N	-5.18	1.22	1.34

There are no bond angle outliers.

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	967	0	963	20	0
1	B	967	0	963	26	0
1	C	967	0	963	23	0
1	D	967	0	963	21	0
1	E	967	0	963	20	0
1	F	967	0	963	24	0
1	G	967	0	963	25	0
1	H	967	0	963	33	0
1	I	967	0	963	30	0
1	J	967	0	963	15	0
1	K	967	0	963	18	0
1	L	967	0	963	28	0
1	M	967	0	963	32	0
2	N	4139	0	3882	161	0
3	A	17	0	31	1	0
3	B	17	0	31	0	0
3	C	17	0	31	2	0
3	D	17	0	31	2	0
3	E	17	0	31	0	0
3	F	17	0	31	0	0
3	G	17	0	31	1	0
3	H	17	0	31	1	0
3	I	17	0	31	2	0
3	J	17	0	31	0	0
3	K	17	0	31	1	0
3	L	17	0	31	1	0
3	M	17	0	31	2	0
4	A	138	0	0	1	0
4	B	138	0	0	1	0
4	C	138	0	0	2	0
4	D	138	0	0	2	0
4	E	138	0	0	3	0
4	F	138	0	0	1	0
4	G	138	0	0	2	0
4	H	138	0	0	2	0
4	I	138	0	0	3	0
4	J	138	0	0	2	0
4	K	138	0	0	2	0
4	L	138	0	0	4	0
4	M	138	0	0	3	0
5	A	44	0	67	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	44	0	67	3	0
5	C	44	0	67	3	0
5	D	44	0	67	0	0
5	F	44	0	67	2	0
5	G	44	0	67	1	0
5	H	44	0	67	5	0
5	I	44	0	67	1	0
5	J	44	0	67	1	0
5	K	44	0	67	2	0
5	L	44	0	67	3	0
5	M	44	0	67	3	0
6	A	5	0	4	0	0
6	C	5	0	5	0	0
6	D	10	0	10	1	0
6	E	5	0	5	0	0
6	F	5	0	5	0	0
6	H	10	0	10	0	0
6	J	10	0	10	0	0
6	K	5	0	5	0	0
6	M	10	0	10	0	0
All	All	19318	0	17672	466	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 13.

All (466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:202:L8Z:C1G	4:L:202:L8Z:C2E	1.75	1.60
1:H:59:SER:C	1:H:60:ASN:HD22	1.62	1.02
2:N:312:LEU:HB3	2:N:320:PRO:HB3	1.56	0.84
2:N:594:ASN:HB3	2:N:614:ASP:HB3	1.60	0.81
2:N:357:ASN:HD22	2:N:360:SER:HB3	1.46	0.81
2:N:784:VAL:HG12	2:N:805:ASN:HB3	1.62	0.80
1:A:45:ILE:HD11	1:A:114:LEU:HD22	1.62	0.79
2:N:404:ARG:HA	2:N:412:VAL:HG22	1.70	0.74
2:N:743:THR:HG21	2:N:766:ILE:HD13	1.68	0.74
2:N:571:THR:HA	2:N:600:THR:HA	1.67	0.73
2:N:592:ARG:HB3	2:N:616:ALA:HB3	1.70	0.73
4:G:202:L8Z:O8	4:G:202:L8Z:O62	2.04	0.73
1:E:116:ILE:HD12	1:E:143:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:384:GLN:O	2:N:388:ARG:NH2	2.23	0.72
2:N:628:VAL:HB	2:N:719:ILE:HB	1.72	0.71
1:H:59:SER:C	1:H:60:ASN:ND2	2.42	0.71
1:H:76:ASN:HD21	5:H:204:LPP:H132	1.56	0.70
1:D:60:ASN:ND2	1:D:103:GLN:OE1	2.25	0.70
1:M:49:ARG:NE	1:M:113:GLU:OE2	2.24	0.70
1:L:49:ARG:NH2	1:M:153:SER:OG	2.24	0.70
2:N:614:ASP:OD1	2:N:615:THR:N	2.24	0.70
2:N:271:VAL:HG12	2:N:272:GLU:H	1.57	0.69
1:M:103:GLN:HG3	3:M:202:PLM:H32	1.74	0.69
2:N:719:ILE:HG13	2:N:736:SER:HB2	1.73	0.69
4:L:202:L8Z:C1G	4:L:202:L8Z:C3D	2.70	0.69
1:M:45:ILE:HD11	1:M:114:LEU:HD22	1.75	0.69
1:E:45:ILE:HG23	1:E:138:GLY:H	1.57	0.69
1:B:121:GLY:O	1:B:122:ASN:ND2	2.19	0.69
2:N:523:ASN:HD22	2:N:576:TRP:HE1	1.41	0.69
2:N:540:GLN:OE1	2:N:677:HIS:NE2	2.26	0.69
1:F:109:THR:HG21	1:F:129:LYS:HE2	1.74	0.69
1:I:109:THR:HG21	1:I:129:LYS:HD2	1.73	0.69
2:N:540:GLN:OE1	2:N:561:GLN:NE2	2.26	0.68
2:N:771:GLY:HA3	2:N:788:ALA:HA	1.75	0.68
1:C:125:MET:SD	1:D:38:GLN:NE2	2.66	0.68
4:E:1002:L8Z:O11	4:E:1002:L8Z:O23	2.11	0.68
1:H:49:ARG:HD3	1:I:155:ARG:HH12	1.58	0.68
2:N:322:VAL:HG13	2:N:341:VAL:HG22	1.76	0.68
1:H:47:ASN:HD21	1:I:155:ARG:HE	1.42	0.68
2:N:272:GLU:HB3	2:N:338:ARG:HA	1.75	0.68
1:A:49:ARG:NE	1:A:113:GLU:OE2	2.25	0.68
2:N:339:VAL:HG12	2:N:341:VAL:HG23	1.76	0.68
1:G:45:ILE:HD11	1:G:114:LEU:HD22	1.75	0.67
1:I:60:ASN:ND2	1:I:103:GLN:OE1	2.27	0.67
1:B:121:GLY:C	1:B:122:ASN:HD22	1.97	0.67
1:M:92:ALA:O	1:M:96:GLY:N	2.26	0.67
1:E:125:MET:HE1	1:F:144:ALA:HB2	1.76	0.66
1:H:47:ASN:ND2	1:I:155:ARG:HE	1.93	0.66
1:L:115:GLU:OE1	1:L:125:MET:HB3	1.95	0.66
4:H:203:L8Z:O8	4:H:203:L8Z:O62	2.12	0.66
2:N:484:SER:N	2:N:516:GLY:O	2.27	0.66
1:I:116:ILE:HD12	1:I:143:LEU:HD11	1.75	0.66
2:N:529:LEU:HD22	2:N:570:PHE:HZ	1.61	0.66
1:A:57:ASP:OD1	1:A:58:ASP:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:ASN:ND2	1:L:109:THR:OG1	2.30	0.65
1:B:45:ILE:HG23	1:B:138:GLY:H	1.61	0.65
2:N:319:TYR:HD1	2:N:379:SER:HG	1.44	0.65
2:N:767:ARG:NE	2:N:797:ASP:OD2	2.29	0.65
1:G:63:GLY:HA2	3:G:201:PLM:H52	1.77	0.65
1:L:45:ILE:HD11	1:L:114:LEU:HD22	1.79	0.65
1:B:149:GLN:OE1	1:C:36:GLN:NE2	2.31	0.64
1:D:116:ILE:HD12	1:D:143:LEU:HD11	1.79	0.64
2:N:543:VAL:HG12	2:N:673:VAL:HB	1.79	0.64
4:C:203:L8Z:O62	4:C:203:L8Z:O8	2.12	0.64
1:D:18:CYS:SG	6:D:202:GOL:H12	2.37	0.64
5:M:205:LPP:H121	5:M:205:LPP:H322	1.78	0.64
2:N:652:PHE:N	2:N:708:GLY:O	2.24	0.64
2:N:468:TYR:OH	2:N:488:ARG:NH2	2.31	0.64
2:N:503:ASP:HB3	2:N:540:GLN:HB2	1.79	0.64
2:N:600:THR:HG21	2:N:607:GLU:HA	1.79	0.64
1:H:60:ASN:ND2	1:H:60:ASN:N	2.45	0.64
2:N:540:GLN:HG2	2:N:674:TYR:HE2	1.62	0.63
1:C:47:ASN:HB3	1:C:115:GLU:HB3	1.80	0.63
1:F:133:THR:HG21	1:F:154:PRO:HG3	1.79	0.63
2:N:349:VAL:HG22	2:N:377:LEU:HD13	1.79	0.63
2:N:288:THR:HG22	2:N:307:ASP:HB2	1.80	0.63
1:I:133:THR:HG21	1:I:154:PRO:HG3	1.80	0.63
1:C:109:THR:HG21	1:C:129:LYS:HD2	1.80	0.62
1:D:38:GLN:HB2	1:D:145:SER:O	1.99	0.62
2:N:589:ASP:OD1	2:N:590:GLY:N	2.31	0.62
1:A:42:TYR:OH	1:A:155:ARG:NH2	2.33	0.62
1:B:60:ASN:HD22	1:B:103:GLN:CD	2.02	0.62
2:N:441:GLN:HE22	2:N:808:LYS:HB3	1.65	0.62
1:L:63:GLY:HA2	3:L:201:PLM:H52	1.81	0.61
1:F:46:VAL:O	1:F:115:GLU:HB2	1.99	0.61
1:B:60:ASN:HD22	1:B:103:GLN:NE2	1.99	0.61
1:E:45:ILE:HD11	1:E:114:LEU:HD22	1.83	0.61
2:N:573:ASN:HB3	2:N:598:LYS:HG3	1.83	0.61
4:M:204:L8Z:O8	4:M:204:L8Z:O62	2.19	0.61
1:H:49:ARG:NE	1:H:113:GLU:OE2	2.24	0.60
2:N:277:LEU:HD22	2:N:280:HIS:HB2	1.83	0.60
2:N:536:LEU:HD12	2:N:565:PHE:HD2	1.66	0.60
4:A:202:L8Z:O62	4:A:202:L8Z:O8	2.18	0.60
4:K:202:L8Z:N2	4:K:202:L8Z:O12	2.34	0.60
2:N:377:LEU:HD23	2:N:412:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:403:GLN:O	2:N:413:ASP:N	2.27	0.60
2:N:659:THR:HG22	2:N:660:VAL:HG23	1.84	0.60
4:J:203:L8Z:O52	4:J:203:L8Z:O7	2.13	0.60
2:N:361:LYS:HG3	2:N:364:VAL:H	1.67	0.60
2:N:563:ASN:O	2:N:563:ASN:ND2	2.31	0.60
1:B:116:ILE:HD12	1:B:143:LEU:HD11	1.83	0.59
2:N:318:ALA:N	2:N:345:ASN:O	2.33	0.59
1:E:141:VAL:HG12	1:E:154:PRO:HA	1.83	0.59
1:H:70:LEU:HD22	3:H:201:PLM:HB1	1.85	0.59
1:L:131:GLY:O	1:L:134:ARG:NH2	2.36	0.59
2:N:347:PHE:HB3	2:N:412:VAL:HG21	1.85	0.59
1:E:60:ASN:OD1	1:E:104:SER:OG	2.21	0.58
4:C:203:L8Z:O3	4:C:203:L8Z:O12	2.20	0.58
1:D:49:ARG:NH2	1:E:153:SER:OG	2.36	0.58
1:J:146:ASN:OD1	1:J:147:GLY:N	2.32	0.58
1:A:134:ARG:HB2	1:A:134:ARG:NH1	2.18	0.58
2:N:583:ARG:NH2	2:N:588:THR:OG1	2.37	0.58
1:K:46:VAL:O	1:K:115:GLU:HB2	2.04	0.58
2:N:733:VAL:HG13	2:N:776:TRP:HB3	1.84	0.58
1:E:127:VAL:HG13	1:F:34:ALA:HA	1.85	0.58
5:G:203:LPP:H232	5:G:203:LPP:H422	1.86	0.58
1:M:115:GLU:OE1	1:M:125:MET:HB3	2.02	0.58
1:J:54:GLN:OE1	1:J:108:LYS:NZ	2.32	0.57
1:L:73:PHE:CE1	5:L:203:LPP:H151	2.39	0.57
1:B:45:ILE:HD11	1:B:114:LEU:HD13	1.86	0.57
1:D:154:PRO:O	1:D:155:ARG:HB3	2.04	0.57
1:H:45:ILE:HD11	1:H:114:LEU:HD22	1.87	0.57
1:D:111:GLY:HA2	1:D:130:GLN:H	1.68	0.57
1:G:142:VAL:HG21	1:G:155:ARG:HE	1.69	0.57
1:H:146:ASN:HB3	1:H:149:GLN:HB2	1.87	0.57
1:L:109:THR:HG21	1:L:129:LYS:HD2	1.86	0.57
1:E:49:ARG:NH2	1:F:153:SER:OG	2.38	0.56
1:G:45:ILE:HG23	1:G:138:GLY:H	1.70	0.56
1:H:60:ASN:HD22	1:H:60:ASN:N	1.99	0.56
1:L:46:VAL:O	1:L:115:GLU:HB2	2.05	0.56
1:I:113:GLU:HA	1:I:127:VAL:HA	1.87	0.56
2:N:410:ASP:OD1	2:N:410:ASP:N	2.38	0.56
4:D:203:L8Z:O8	4:D:203:L8Z:O62	2.24	0.56
2:N:570:PHE:CD2	2:N:601:ILE:HG12	2.40	0.56
1:I:45:ILE:HD11	1:I:114:LEU:HD22	1.87	0.56
2:N:540:GLN:HG2	2:N:674:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:417:LYS:HD3	2:N:418:VAL:N	2.20	0.56
4:H:203:L8Z:O21	4:H:203:L8Z:N2	2.39	0.56
1:B:75:GLY:HA3	1:B:88:THR:HA	1.87	0.55
1:J:116:ILE:HD12	1:J:143:LEU:HD11	1.86	0.55
2:N:535:SER:HB2	2:N:566:LYS:HE2	1.88	0.55
2:N:326:PRO:HD3	2:N:337:LEU:HD12	1.88	0.55
1:I:60:ASN:ND2	1:I:104:SER:OG	2.39	0.55
2:N:357:ASN:ND2	2:N:360:SER:HB3	2.18	0.55
1:C:75:GLY:HA3	1:C:88:THR:HA	1.87	0.55
1:D:147:GLY:O	1:D:148:SER:OG	2.24	0.55
2:N:350:ARG:HH11	2:N:405:VAL:HG22	1.72	0.55
5:B:203:LPP:H252	5:B:203:LPP:H442	1.89	0.55
1:J:127:VAL:HG13	1:K:34:ALA:HA	1.88	0.55
1:K:69:VAL:HG12	5:K:203:LPP:H202	1.88	0.55
2:N:543:VAL:HG21	2:N:754:TYR:OH	2.07	0.55
4:L:202:L8Z:C1G	4:L:202:L8Z:C67	2.85	0.55
1:A:35:LYS:HD2	1:M:151:THR:HG22	1.89	0.54
2:N:369:MET:SD	2:N:371:GLN:N	2.79	0.54
2:N:754:TYR:HB3	2:N:757:TYR:HD2	1.71	0.54
4:E:1002:L8Z:O8	4:E:1002:L8Z:O62	2.23	0.54
2:N:554:GLU:HG3	2:N:565:PHE:CE1	2.42	0.54
1:I:80:GLY:N	4:I:202:L8Z:O22	2.40	0.54
2:N:434:THR:HG21	2:N:804:PHE:H	1.72	0.54
2:N:549:LEU:HB3	2:N:554:GLU:O	2.07	0.54
1:F:116:ILE:HD12	1:F:143:LEU:HD11	1.90	0.54
1:M:45:ILE:HG23	1:M:138:GLY:H	1.72	0.54
2:N:520:ASN:HD22	2:N:523:ASN:CG	2.11	0.54
1:C:116:ILE:HD12	1:C:143:LEU:HD11	1.89	0.54
1:I:82:THR:OG1	4:I:202:L8Z:O25	2.24	0.54
1:M:102:VAL:HG11	3:M:202:PLM:H81	1.87	0.54
1:A:38:GLN:HG2	1:A:146:ASN:OD1	2.07	0.54
5:C:204:LPP:H382	5:C:204:LPP:H191	1.90	0.54
1:G:42:TYR:HD2	1:G:140:ARG:HH21	1.54	0.54
2:N:611:VAL:O	2:N:636:GLY:HA2	2.07	0.54
1:E:46:VAL:O	1:E:115:GLU:HB2	2.08	0.54
2:N:347:PHE:O	2:N:377:LEU:N	2.32	0.53
2:N:271:VAL:HG12	2:N:272:GLU:N	2.23	0.53
2:N:272:GLU:OE1	2:N:338:ARG:HG2	2.09	0.53
1:M:48:VAL:HA	1:M:113:GLU:O	2.08	0.53
2:N:368:GLU:HB2	2:N:389:LEU:HD23	1.90	0.53
1:J:21:ASN:ND2	1:J:109:THR:OG1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:522:TYR:O	2:N:578:TYR:HA	2.09	0.53
2:N:524:SER:OG	2:N:525:LEU:N	2.40	0.53
1:B:77:THR:HG22	1:B:77:THR:O	2.09	0.53
2:N:316:GLY:HA2	2:N:376:TRP:CD1	2.44	0.53
2:N:271:VAL:HG11	2:N:284:ILE:HG21	1.90	0.53
1:A:73:PHE:HE1	5:A:203:LPP:H131	1.74	0.53
1:H:49:ARG:NH2	1:I:26:GLY:O	2.34	0.52
1:A:57:ASP:OD2	1:A:59:SER:OG	2.26	0.52
4:G:202:L8Z:O11	4:G:202:L8Z:O23	2.27	0.52
2:N:617:THR:O	2:N:630:LEU:HA	2.10	0.52
2:N:484:SER:O	2:N:516:GLY:N	2.43	0.52
1:G:49:ARG:NE	1:G:113:GLU:OE1	2.43	0.52
1:M:142:VAL:HG21	1:M:155:ARG:CZ	2.40	0.52
2:N:749:TRP:CD1	2:N:760:TYR:HB2	2.44	0.52
1:F:148:SER:OG	2:N:374:GLY:O	2.27	0.52
1:L:75:GLY:HA3	1:L:88:THR:HA	1.92	0.52
2:N:746:ASP:HB3	2:N:749:TRP:HB2	1.92	0.52
1:I:63:GLY:HA2	3:I:201:PLM:H52	1.92	0.52
2:N:434:THR:CG2	2:N:804:PHE:H	2.23	0.52
1:L:45:ILE:HG23	1:L:138:GLY:H	1.74	0.51
2:N:435:GLU:OE1	2:N:657:SER:OG	2.22	0.51
2:N:536:LEU:HD12	2:N:565:PHE:CD2	2.46	0.51
1:L:49:ARG:NE	1:L:113:GLU:OE2	2.44	0.51
1:B:115:GLU:HA	1:B:125:MET:HA	1.93	0.51
1:J:126:VAL:HG23	1:K:36:GLN:O	2.11	0.51
2:N:757:TYR:HB3	2:N:760:TYR:HE1	1.75	0.51
1:H:49:ARG:HD3	1:I:155:ARG:NH1	2.25	0.51
2:N:525:LEU:HD23	2:N:526:ARG:N	2.26	0.51
2:N:350:ARG:HB3	2:N:413:ASP:OD1	2.11	0.51
1:C:55:GLY:O	1:C:107:ASN:ND2	2.34	0.51
1:K:60:ASN:ND2	1:K:104:SER:OG	2.35	0.51
1:D:82:THR:OG1	4:D:203:L8Z:O25	2.29	0.51
1:B:79:GLY:N	4:B:202:L8Z:O2	2.37	0.51
2:N:315:TYR:HB3	2:N:317:TYR:HD1	1.74	0.51
1:H:76:ASN:ND2	5:H:204:LPP:H132	2.23	0.50
1:L:133:THR:HG21	1:L:154:PRO:HG3	1.93	0.50
1:G:109:THR:HG21	1:G:129:LYS:HE2	1.94	0.50
1:M:80:GLY:N	4:M:204:L8Z:O22	2.44	0.50
1:M:77:THR:O	1:M:77:THR:HG22	2.12	0.50
4:K:202:L8Z:O62	4:K:202:L8Z:O8	2.30	0.50
2:N:296:TYR:CD1	2:N:335:VAL:HG11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:651:ASN:HB3	2:N:708:GLY:O	2.12	0.50
1:A:24:LEU:HD13	1:B:34:ALA:HB3	1.93	0.50
1:D:55:GLY:HA2	1:E:31:ALA:HB2	1.93	0.50
1:B:49:ARG:NH2	1:C:153:SER:OG	2.45	0.50
1:F:47:ASN:OD1	1:G:155:ARG:NH1	2.45	0.50
1:I:146:ASN:OD1	1:I:147:GLY:N	2.36	0.50
1:G:116:ILE:HD12	1:G:143:LEU:HD11	1.93	0.50
2:N:559:SER:HB2	2:N:677:HIS:HA	1.94	0.50
1:H:69:VAL:HG12	5:H:204:LPP:H202	1.94	0.50
2:N:743:THR:HB	2:N:745:TRP:HZ3	1.76	0.50
1:B:116:ILE:CD1	1:B:143:LEU:HD11	2.41	0.49
1:L:46:VAL:HG23	1:L:115:GLU:HB2	1.93	0.49
2:N:577:THR:HG22	2:N:578:TYR:N	2.26	0.49
1:B:150:VAL:HG21	1:C:37:VAL:HG23	1.94	0.49
1:F:75:GLY:HA3	1:F:88:THR:HA	1.93	0.49
2:N:404:ARG:HD3	2:N:409:PRO:HA	1.94	0.49
1:D:45:ILE:HG23	1:D:138:GLY:H	1.77	0.49
2:N:554:GLU:HG3	2:N:565:PHE:CD1	2.48	0.49
1:M:146:ASN:OD1	1:M:147:GLY:N	2.42	0.49
1:E:116:ILE:HD11	1:E:143:LEU:HD21	1.94	0.49
1:M:60:ASN:ND2	1:M:104:SER:OG	2.46	0.49
2:N:535:SER:HA	2:N:566:LYS:HD3	1.95	0.49
1:F:38:GLN:HB3	1:F:145:SER:O	2.13	0.49
1:H:46:VAL:O	1:H:115:GLU:HB2	2.13	0.49
1:L:115:GLU:OE2	1:M:155:ARG:NH2	2.44	0.48
2:N:305:GLU:OE2	2:N:324:SER:OG	2.24	0.48
2:N:540:GLN:OE1	2:N:677:HIS:CE1	2.66	0.48
1:H:21:ASN:HD22	1:H:55:GLY:HA3	1.78	0.48
5:H:204:LPP:H331	5:H:204:LPP:H301	1.47	0.48
1:M:60:ASN:ND2	1:M:103:GLN:OE1	2.44	0.48
2:N:388:ARG:HG2	2:N:391:ARG:NH2	2.29	0.48
1:D:49:ARG:NE	1:D:113:GLU:OE1	2.47	0.48
1:G:54:GLN:HG3	1:G:55:GLY:H	1.78	0.48
2:N:539:MET:O	2:N:541:PRO:HD3	2.14	0.48
2:N:786:SER:OG	2:N:803:GLN:O	2.20	0.48
1:M:75:GLY:HA3	1:M:88:THR:HA	1.95	0.48
2:N:434:THR:HG21	2:N:803:GLN:HA	1.96	0.47
2:N:549:LEU:HD12	2:N:554:GLU:HB2	1.96	0.47
2:N:741:MET:HG3	2:N:768:MET:HG3	1.96	0.47
1:C:24:LEU:C	1:C:129:LYS:HB3	2.35	0.47
1:B:69:VAL:HG22	5:B:203:LPP:H202	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:130:GLN:CD	1:L:134:ARG:HH21	2.18	0.47
2:N:529:LEU:HD22	2:N:570:PHE:CZ	2.45	0.47
2:N:721:PRO:O	2:N:723:PRO:HD3	2.15	0.47
1:A:126:VAL:HG23	1:B:36:GLN:O	2.15	0.47
1:G:127:VAL:HG13	1:H:34:ALA:HA	1.97	0.47
2:N:354:PHE:CE1	2:N:416:TYR:HB2	2.50	0.47
1:A:47:ASN:HB3	1:A:115:GLU:OE1	2.15	0.47
1:J:58:ASP:OD1	1:K:20:ASN:HB3	2.14	0.47
1:K:77:THR:O	1:K:77:THR:HG22	2.15	0.47
5:M:205:LPP:H322	5:M:205:LPP:C12	2.45	0.47
2:N:580:LYS:HB3	2:N:591:SER:H	1.79	0.47
2:N:593:VAL:HG12	2:N:594:ASN:N	2.30	0.47
5:L:203:LPP:H301	5:L:203:LPP:H331	1.53	0.47
5:A:203:LPP:H331	5:A:203:LPP:H301	1.68	0.46
1:H:55:GLY:O	1:H:107:ASN:ND2	2.37	0.46
1:B:46:VAL:HG23	1:B:115:GLU:HG2	1.97	0.46
2:N:583:ARG:O	2:N:587:PRO:HB3	2.15	0.46
1:F:145:SER:OG	1:F:146:ASN:N	2.49	0.46
2:N:386:LYS:HB3	2:N:386:LYS:HE2	1.77	0.46
1:I:79:GLY:N	4:I:202:L8Z:O2	2.46	0.46
2:N:367:ARG:O	2:N:370:ARG:NH1	2.48	0.46
1:G:52:GLN:OE1	1:G:108:LYS:NZ	2.43	0.46
2:N:571:THR:HG22	2:N:598:LYS:HG2	1.96	0.46
1:H:115:GLU:OE1	1:H:115:GLU:HA	2.14	0.46
2:N:312:LEU:O	2:N:317:TYR:HB2	2.16	0.46
2:N:609:TYR:CE1	2:N:639:ASP:HB3	2.50	0.46
5:F:203:LPP:H331	5:F:203:LPP:H301	1.48	0.46
1:L:73:PHE:CD1	5:L:203:LPP:H151	2.51	0.46
1:F:109:THR:HG21	1:F:129:LYS:CE	2.43	0.46
1:M:79:GLY:N	4:M:204:L8Z:O2	2.48	0.46
1:A:127:VAL:HG13	1:B:34:ALA:HA	1.98	0.46
1:C:126:VAL:HG23	1:D:36:GLN:O	2.15	0.46
5:C:204:LPP:H301	5:C:204:LPP:H331	1.62	0.46
1:M:114:LEU:O	1:M:125:MET:HA	2.15	0.46
2:N:768:MET:SD	2:N:768:MET:N	2.89	0.46
1:A:62:ILE:HG22	3:A:201:PLM:H42	1.97	0.45
1:F:115:GLU:OE2	1:F:125:MET:HB3	2.16	0.45
1:K:19:VAL:HG21	1:K:56:GLY:HA3	1.99	0.45
2:N:366:ARG:NH1	2:N:372:MET:HA	2.31	0.45
1:C:55:GLY:HA2	1:D:31:ALA:HB2	1.99	0.45
1:D:111:GLY:HA2	1:D:130:GLN:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:357:ASN:HB3	2:N:418:VAL:HG21	1.98	0.45
1:L:61:VAL:HG23	2:N:724:PHE:CE2	2.51	0.45
2:N:317:TYR:HD2	2:N:344:GLY:C	2.20	0.45
1:D:103:GLN:HG3	3:D:201:PLM:H22	1.98	0.45
1:F:60:ASN:HB2	1:F:100:GLN:HG2	1.98	0.45
2:N:320:PRO:HD2	2:N:380:ASP:HB2	1.97	0.45
2:N:349:VAL:HG23	2:N:375:ALA:O	2.16	0.45
1:K:103:GLN:HG3	3:K:201:PLM:H32	1.99	0.45
1:G:25:SER:HA	1:G:129:LYS:HB3	1.97	0.45
1:I:111:GLY:HA2	1:I:130:GLN:H	1.81	0.45
2:N:388:ARG:HG2	2:N:391:ARG:CZ	2.46	0.45
1:C:146:ASN:OD1	1:C:147:GLY:N	2.42	0.45
2:N:754:TYR:HB3	2:N:757:TYR:CD2	2.51	0.45
1:B:127:VAL:HG13	1:C:34:ALA:HA	1.98	0.45
1:L:154:PRO:O	1:L:155:ARG:HB2	2.17	0.45
1:M:133:THR:HG21	1:M:154:PRO:HG3	1.99	0.45
1:M:146:ASN:O	1:M:148:SER:N	2.51	0.45
2:N:733:VAL:HG22	2:N:776:TRP:CB	2.47	0.45
1:F:25:SER:OG	1:F:26:GLY:N	2.50	0.44
1:F:116:ILE:HD12	1:F:143:LEU:HD21	1.98	0.44
1:H:47:ASN:ND2	1:I:155:ARG:NE	2.64	0.44
1:J:51:VAL:HG11	1:K:29:TYR:CD1	2.52	0.44
1:C:114:LEU:O	1:C:125:MET:HA	2.17	0.44
1:E:112:VAL:O	1:E:127:VAL:HG23	2.17	0.44
1:F:69:VAL:HG22	5:F:203:LPP:H202	2.00	0.44
4:F:202:L8Z:O2	4:F:202:L8Z:O3	2.34	0.44
1:K:60:ASN:ND2	1:K:103:GLN:OE1	2.51	0.44
1:M:113:GLU:HA	1:M:127:VAL:HG12	2.00	0.44
2:N:570:PHE:HD2	2:N:601:ILE:HG12	1.80	0.44
2:N:459:ASN:OD1	2:N:460:GLY:N	2.49	0.44
2:N:532:VAL:CG1	2:N:569:ASP:HB2	2.47	0.44
2:N:440:PHE:O	2:N:461:THR:HA	2.18	0.44
1:B:109:THR:HG21	1:B:129:LYS:HE2	1.99	0.44
1:J:82:THR:OG1	4:J:203:L8Z:O25	2.34	0.44
2:N:316:GLY:O	2:N:346:ARG:HA	2.17	0.44
1:C:44:THR:HG22	1:C:45:ILE:H	1.83	0.44
1:J:127:VAL:CG1	1:K:34:ALA:HA	2.47	0.44
5:B:203:LPP:H301	5:B:203:LPP:H331	1.58	0.44
1:I:114:LEU:O	1:I:125:MET:HA	2.17	0.44
1:K:45:ILE:HD11	1:K:114:LEU:HD22	1.99	0.44
2:N:322:VAL:HG22	2:N:341:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HG13	1:A:116:ILE:HG22	1.99	0.44
1:A:134:ARG:HB2	1:A:134:ARG:CZ	2.48	0.44
1:C:140:ARG:HE	1:C:140:ARG:HB3	1.65	0.43
2:N:315:TYR:HB3	2:N:317:TYR:CD1	2.52	0.43
2:N:296:TYR:HD1	2:N:335:VAL:HG11	1.82	0.43
2:N:572:PHE:N	2:N:599:VAL:O	2.51	0.43
1:C:95:GLY:HA2	3:C:201:PLM:HD2	2.00	0.43
1:G:116:ILE:HD11	1:G:143:LEU:HD21	2.00	0.43
1:J:141:VAL:HG12	1:J:154:PRO:HA	2.00	0.43
2:N:424:GLY:N	2:N:446:GLN:OE1	2.51	0.43
1:A:141:VAL:HB	1:A:152:VAL:HG13	2.00	0.43
1:C:134:ARG:HB3	1:C:134:ARG:CZ	2.48	0.43
1:L:111:GLY:HA2	1:L:130:GLN:H	1.82	0.43
2:N:465:TYR:HB3	2:N:499:ALA:HB2	1.99	0.43
1:B:47:ASN:HB3	1:B:115:GLU:OE2	2.18	0.43
1:F:44:THR:O	1:F:117:ARG:N	2.42	0.43
1:K:49:ARG:NE	1:K:113:GLU:OE1	2.51	0.43
2:N:592:ARG:O	2:N:616:ALA:N	2.51	0.43
2:N:369:MET:HA	2:N:385:GLY:CA	2.48	0.43
2:N:532:VAL:HG13	2:N:569:ASP:HB2	2.01	0.43
1:L:60:ASN:OD1	1:L:104:SER:OG	2.36	0.43
5:C:204:LPP:H382	5:C:204:LPP:C19	2.48	0.43
2:N:709:ASN:ND2	2:N:747:THR:OG1	2.35	0.43
1:A:85:SER:HA	1:A:88:THR:HG22	2.01	0.43
1:B:44:THR:O	1:B:117:ARG:N	2.48	0.43
1:E:62:ILE:HD13	1:E:62:ILE:HA	1.83	0.43
5:J:204:LPP:H301	5:J:204:LPP:H331	1.51	0.43
1:L:111:GLY:HA2	1:L:130:GLN:N	2.33	0.43
5:K:203:LPP:H301	5:K:203:LPP:H331	1.69	0.43
1:C:77:THR:O	1:C:77:THR:HG22	2.19	0.42
1:D:146:ASN:OD1	1:D:147:GLY:N	2.44	0.42
1:E:60:ASN:N	1:E:60:ASN:ND2	2.68	0.42
1:I:103:GLN:HG3	3:I:201:PLM:H32	2.01	0.42
1:M:52:GLN:OE1	1:M:108:LYS:HE3	2.19	0.42
1:M:142:VAL:HG11	1:M:155:ARG:NH1	2.33	0.42
1:C:67:GLY:HA2	3:C:201:PLM:H92	2.02	0.42
1:K:125:MET:SD	1:L:144:ALA:HB2	2.59	0.42
2:N:377:LEU:HD11	2:N:382:VAL:HG21	2.01	0.42
1:G:19:VAL:HB	1:G:107:ASN:HD21	1.84	0.42
1:H:109:THR:HG22	1:H:110:GLN:O	2.19	0.42
1:H:125:MET:SD	1:I:144:ALA:HB2	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:THR:HG21	1:J:129:LYS:HE2	2.01	0.42
2:N:312:LEU:HD21	2:N:343:ALA:HA	2.00	0.42
2:N:381:LEU:HA	2:N:381:LEU:HD23	1.76	0.42
1:F:142:VAL:HG23	1:F:142:VAL:O	2.19	0.42
1:G:126:VAL:HG23	1:H:36:GLN:O	2.19	0.42
1:J:140:ARG:HE	1:J:140:ARG:HB3	1.67	0.42
2:N:352:ILE:HA	2:N:414:VAL:O	2.20	0.42
1:B:150:VAL:HG21	1:C:37:VAL:CG2	2.50	0.42
4:E:1002:L8Z:O21	4:E:1002:L8Z:N2	2.53	0.42
1:G:139:GLN:HG2	1:G:140:ARG:H	1.84	0.42
1:L:146:ASN:OD1	1:L:147:GLY:N	2.50	0.42
1:M:116:ILE:HD12	1:M:143:LEU:HD12	2.02	0.42
2:N:272:GLU:O	2:N:339:VAL:HB	2.20	0.42
2:N:670:PRO:HB3	2:N:760:TYR:CD2	2.55	0.42
2:N:733:VAL:HG22	2:N:776:TRP:HB2	2.01	0.42
2:N:743:THR:HB	2:N:745:TRP:CZ3	2.54	0.42
2:N:504:TYR:HA	2:N:538:ASN:O	2.20	0.42
2:N:672:ALA:HB2	2:N:706:VAL:HG11	2.01	0.42
1:L:64:ALA:O	1:L:68:ALA:N	2.52	0.42
2:N:635:TRP:CD1	2:N:636:GLY:N	2.88	0.42
1:E:85:SER:HA	1:E:88:THR:HG22	2.01	0.42
1:G:58:ASP:O	1:G:60:ASN:ND2	2.53	0.42
1:H:84:ARG:NH1	5:H:204:LPP:O28	2.39	0.42
1:H:125:MET:O	1:I:38:GLN:HB2	2.20	0.42
2:N:576:TRP:CG	2:N:577:THR:N	2.87	0.42
2:N:577:THR:HG22	2:N:578:TYR:H	1.85	0.42
1:G:46:VAL:O	1:G:115:GLU:HB3	2.20	0.42
1:B:76:ASN:O	1:B:84:ARG:NH1	2.53	0.41
1:D:54:GLN:HG3	1:D:55:GLY:H	1.85	0.41
1:G:114:LEU:O	1:G:125:MET:HA	2.19	0.41
1:K:115:GLU:OE2	1:K:125:MET:HB3	2.19	0.41
5:M:205:LPP:H202	5:M:205:LPP:H171	1.87	0.41
1:H:45:ILE:HG23	1:H:138:GLY:H	1.85	0.41
1:H:57:ASP:OD2	2:N:450:LEU:HD11	2.20	0.41
1:M:115:GLU:CD	1:M:125:MET:HB3	2.41	0.41
1:E:143:LEU:HD23	1:E:150:VAL:HG11	2.01	0.41
1:G:140:ARG:HE	1:G:140:ARG:HB3	1.65	0.41
1:L:140:ARG:HE	1:L:140:ARG:HB3	1.73	0.41
1:M:140:ARG:HE	1:M:140:ARG:HB3	1.70	0.41
1:L:112:VAL:O	1:L:127:VAL:HG23	2.19	0.41
1:M:55:GLY:O	1:M:107:ASN:ND2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:HD22	3:D:201:PLM:HD1	2.02	0.41
1:F:49:ARG:HA	1:F:50:PRO:HD3	1.92	0.41
2:N:271:VAL:HG22	2:N:304:MET:HE1	2.01	0.41
2:N:743:THR:HG21	2:N:766:ILE:CD1	2.47	0.41
1:F:45:ILE:HG23	1:F:138:GLY:H	1.85	0.41
1:H:111:GLY:HA2	1:H:130:GLN:H	1.86	0.41
1:H:126:VAL:HG23	1:I:36:GLN:O	2.20	0.41
2:N:563:ASN:HD22	2:N:563:ASN:C	2.14	0.41
2:N:669:GLY:HA2	2:N:744:VAL:HG23	2.02	0.41
1:E:139:GLN:OE1	1:E:155:ARG:NH1	2.53	0.41
1:I:69:VAL:HG12	5:I:203:LPP:H202	2.03	0.41
1:M:62:ILE:HG12	2:N:724:PHE:HD1	1.86	0.41
1:C:25:SER:OG	1:C:129:LYS:HG2	2.21	0.41
1:D:140:ARG:HE	1:D:140:ARG:HB3	1.66	0.41
1:J:54:GLN:HG3	1:K:23:THR:HG22	2.01	0.41
2:N:322:VAL:HG13	2:N:341:VAL:CG2	2.48	0.41
2:N:361:LYS:O	2:N:365:LEU:HB2	2.20	0.41
2:N:494:PHE:CG	2:N:495:GLN:N	2.89	0.41
2:N:784:VAL:O	2:N:785:PHE:HD1	2.04	0.41
1:E:60:ASN:N	1:E:60:ASN:HD22	2.19	0.41
1:G:23:THR:HA	1:G:28:VAL:HG21	2.03	0.41
1:H:58:ASP:O	1:H:60:ASN:ND2	2.54	0.41
1:I:22:ASP:HA	1:I:129:LYS:NZ	2.36	0.41
1:F:126:VAL:HG23	1:G:36:GLN:O	2.21	0.40
1:G:23:THR:HA	1:G:28:VAL:CG2	2.51	0.40
1:I:49:ARG:HG2	1:I:113:GLU:OE2	2.21	0.40
1:A:116:ILE:HD12	1:A:143:LEU:HD11	2.04	0.40
1:G:109:THR:HG21	1:G:129:LYS:CE	2.51	0.40
1:H:53:ILE:CD1	1:H:111:GLY:HA3	2.50	0.40
1:I:51:VAL:HG12	1:I:52:GLN:O	2.21	0.40
1:M:142:VAL:HG11	1:M:155:ARG:HH12	1.87	0.40
1:I:150:VAL:HG21	1:J:37:VAL:HG23	2.02	0.40
4:L:202:L8Z:O1	4:L:202:L8Z:O22	2.39	0.40
1:M:112:VAL:O	1:M:127:VAL:HA	2.21	0.40
2:N:449:TRP:CE3	2:N:449:TRP:HA	2.57	0.40
1:A:57:ASP:CG	1:A:59:SER:H	2.23	0.40
1:E:127:VAL:CG1	1:F:34:ALA:HA	2.51	0.40
1:K:85:SER:HA	1:K:88:THR:HG22	2.04	0.40
1:L:63:GLY:O	1:L:99:GLY:HA3	2.21	0.40
2:N:392:LEU:HD22	2:N:394:PHE:HB3	2.02	0.40
1:I:113:GLU:HB3	1:I:127:VAL:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:295:LEU:HG	2:N:296:TYR:H	1.87	0.40
2:N:594:ASN:OD1	2:N:595:LEU:N	2.54	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	136/155 (88%)	123 (90%)	13 (10%)	0	100	100
1	B	136/155 (88%)	125 (92%)	11 (8%)	0	100	100
1	C	136/155 (88%)	127 (93%)	9 (7%)	0	100	100
1	D	136/155 (88%)	127 (93%)	9 (7%)	0	100	100
1	E	136/155 (88%)	123 (90%)	13 (10%)	0	100	100
1	F	136/155 (88%)	122 (90%)	13 (10%)	1 (1%)	22	60
1	G	136/155 (88%)	125 (92%)	11 (8%)	0	100	100
1	H	136/155 (88%)	128 (94%)	8 (6%)	0	100	100
1	I	136/155 (88%)	126 (93%)	10 (7%)	0	100	100
1	J	136/155 (88%)	121 (89%)	15 (11%)	0	100	100
1	K	136/155 (88%)	124 (91%)	12 (9%)	0	100	100
1	L	136/155 (88%)	124 (91%)	12 (9%)	0	100	100
1	M	136/155 (88%)	122 (90%)	14 (10%)	0	100	100
2	N	517/810 (64%)	445 (86%)	72 (14%)	0	100	100
All	All	2285/2825 (81%)	2062 (90%)	222 (10%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	61	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	102/117 (87%)	102 (100%)	0	100 100
1	B	102/117 (87%)	100 (98%)	2 (2%)	55 74
1	C	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	D	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	E	102/117 (87%)	101 (99%)	1 (1%)	76 86
1	F	102/117 (87%)	102 (100%)	0	100 100
1	G	102/117 (87%)	102 (100%)	0	100 100
1	H	102/117 (87%)	100 (98%)	2 (2%)	55 74
1	I	102/117 (87%)	102 (100%)	0	100 100
1	J	102/117 (87%)	102 (100%)	0	100 100
1	K	102/117 (87%)	102 (100%)	0	100 100
1	L	102/117 (87%)	102 (100%)	0	100 100
1	M	102/117 (87%)	102 (100%)	0	100 100
2	N	441/688 (64%)	438 (99%)	3 (1%)	84 90
All	All	1767/2209 (80%)	1757 (99%)	10 (1%)	86 91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	ASN
1	B	155	ARG
1	C	47	ASN
1	D	155	ARG
1	E	60	ASN
1	H	60	ASN
1	H	155	ARG

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Mol	Chain	Res	Type
2	N	321	ARG
2	N	563	ASN
2	N	607	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	B	60	ASN
1	B	122	ASN
1	E	60	ASN
1	G	60	ASN
1	H	47	ASN
1	H	100	GLN
1	I	60	ASN
1	J	21	ASN
1	K	60	ASN
1	L	21	ASN
1	M	60	ASN
2	N	520	ASN
2	N	523	ASN
2	N	561	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PLM	M	202	1	16,16,17	0.59	0	15,15,17	0.41	0
4	L8Z	I	202	-	138,140,140	1.96	27 (19%)	162,176,176	2.09	30 (18%)
6	GOL	H	202	-	3,4,5	0.92	0	1,4,5	0.63	0
4	L8Z	G	202	-	138,140,140	1.93	28 (20%)	162,176,176	2.29	35 (21%)
5	LPP	B	203	-	43,43,43	1.61	3 (6%)	47,48,48	1.00	5 (10%)
3	PLM	D	201	1	16,16,17	0.50	0	15,15,17	0.39	0
4	L8Z	C	203	-	138,140,140	1.94	26 (18%)	162,176,176	2.22	30 (18%)
6	GOL	M	201	-	3,4,5	1.08	0	1,4,5	0.82	0
5	LPP	H	204	-	43,43,43	1.63	3 (6%)	47,48,48	0.96	4 (8%)
6	GOL	H	205	-	3,4,5	0.63	0	1,4,5	0.28	0
6	GOL	D	205	-	3,4,5	0.97	0	1,4,5	0.45	0
5	LPP	G	203	-	43,43,43	1.64	3 (6%)	47,48,48	1.05	5 (10%)
6	GOL	K	204	-	3,4,5	0.86	0	1,4,5	0.33	0
4	L8Z	E	1002	-	138,140,140	1.93	27 (19%)	162,176,176	2.19	33 (20%)
3	PLM	A	201	1	16,16,17	0.58	0	15,15,17	0.43	0
3	PLM	L	201	1	16,16,17	0.53	0	15,15,17	0.45	0
4	L8Z	M	204	-	138,140,140	1.90	26 (18%)	162,176,176	2.13	27 (16%)
3	PLM	K	201	1	16,16,17	0.57	0	15,15,17	0.41	0
4	L8Z	K	202	-	138,140,140	1.93	27 (19%)	162,176,176	2.44	32 (19%)
6	GOL	J	205	-	3,4,5	1.02	0	1,4,5	0.80	0
4	L8Z	L	202	-	138,140,140	1.99	27 (19%)	162,176,176	2.14	33 (20%)
5	LPP	K	203	-	43,43,43	1.61	3 (6%)	47,48,48	0.92	4 (8%)
3	PLM	G	201	1	16,16,17	0.45	0	15,15,17	0.43	0
4	L8Z	A	202	-	138,140,140	1.97	26 (18%)	162,176,176	2.12	34 (20%)
3	PLM	B	201	1	16,16,17	0.47	0	15,15,17	0.39	0
5	LPP	J	204	-	43,43,43	1.66	3 (6%)	47,48,48	0.97	4 (8%)
6	GOL	J	202	-	3,4,5	0.95	0	1,4,5	0.99	0
6	GOL	D	202	-	3,4,5	1.02	0	1,4,5	0.62	0
4	L8Z	J	203	-	138,140,140	1.89	25 (18%)	162,176,176	2.20	31 (19%)
3	PLM	E	1001	1	16,16,17	0.48	0	15,15,17	0.43	0
5	LPP	A	203	-	43,43,43	1.61	4 (9%)	47,48,48	1.05	5 (10%)
6	GOL	A	204	-	3,4,5	1.05	0	1,4,5	0.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PLM	J	201	1	16,16,17	0.51	0	15,15,17	0.40	0
5	LPP	I	203	-	43,43,43	1.66	3 (6%)	47,48,48	0.96	4 (8%)
3	PLM	F	201	1	16,16,17	0.63	0	15,15,17	0.42	0
5	LPP	C	204	-	43,43,43	1.59	3 (6%)	47,48,48	1.05	4 (8%)
5	LPP	L	203	-	43,43,43	1.58	4 (9%)	47,48,48	1.01	5 (10%)
6	GOL	E	1003	-	3,4,5	1.05	0	1,4,5	1.43	0
6	GOL	M	203	-	3,4,5	1.09	0	1,4,5	0.76	0
5	LPP	D	204	-	43,43,43	1.67	3 (6%)	47,48,48	0.91	4 (8%)
6	GOL	F	204	-	3,4,5	0.65	0	1,4,5	0.33	0
4	L8Z	D	203	-	138,140,140	1.91	24 (17%)	162,176,176	2.20	30 (18%)
4	L8Z	F	202	-	138,140,140	2.00	33 (23%)	162,176,176	2.24	30 (18%)
6	GOL	C	202	-	3,4,5	0.80	0	1,4,5	0.30	0
3	PLM	I	201	1	16,16,17	0.56	0	15,15,17	0.42	0
3	PLM	C	201	1	16,16,17	0.57	0	15,15,17	0.39	0
4	L8Z	H	203	-	138,140,140	1.94	28 (20%)	162,176,176	2.16	31 (19%)
5	LPP	F	203	-	43,43,43	1.58	3 (6%)	47,48,48	0.97	4 (8%)
5	LPP	M	205	-	43,43,43	1.74	3 (6%)	47,48,48	1.00	3 (6%)
3	PLM	H	201	1	16,16,17	0.56	0	15,15,17	0.48	0
4	L8Z	B	202	-	138,140,140	1.98	30 (21%)	162,176,176	2.03	28 (17%)

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
3	PLM	M	202	1	-	4/13/14/15	-
4	L8Z	I	202	-	-	68/140/199/199	0/3/3/3
6	GOL	H	202	-	-	0/2/2/4	-
4	L8Z	G	202	-	-	66/140/199/199	0/3/3/3
5	LPP	B	203	-	-	22/45/45/45	-
3	PLM	D	201	1	-	4/13/14/15	-
4	L8Z	C	203	-	-	60/140/199/199	0/3/3/3
6	GOL	M	201	-	-	2/2/2/4	-
5	LPP	H	204	-	-	19/45/45/45	-
6	GOL	H	205	-	-	2/2/2/4	-
6	GOL	D	205	-	-	2/2/2/4	-
5	LPP	G	203	-	-	20/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	K	204	-	-	1/2/2/4	-
4	L8Z	E	1002	-	-	62/140/199/199	0/3/3/3
3	PLM	A	201	1	-	7/13/14/15	-
3	PLM	L	201	1	-	4/13/14/15	-
4	L8Z	M	204	-	-	60/140/199/199	0/3/3/3
3	PLM	K	201	1	-	3/13/14/15	-
4	L8Z	K	202	-	-	53/140/199/199	0/3/3/3
6	GOL	J	205	-	-	0/2/2/4	-
4	L8Z	L	202	-	-	59/140/199/199	0/3/3/3
5	LPP	K	203	-	-	15/45/45/45	-
3	PLM	G	201	1	-	4/13/14/15	-
4	L8Z	A	202	-	-	65/140/199/199	0/3/3/3
3	PLM	B	201	1	-	4/13/14/15	-
5	LPP	J	204	-	-	18/45/45/45	-
6	GOL	J	202	-	-	0/2/2/4	-
6	GOL	D	202	-	-	0/2/2/4	-
4	L8Z	J	203	-	-	50/140/199/199	0/3/3/3
3	PLM	E	1001	1	-	5/13/14/15	-
5	LPP	A	203	-	-	22/45/45/45	-
6	GOL	A	204	-	-	2/2/2/4	-
3	PLM	J	201	1	-	4/13/14/15	-
5	LPP	I	203	-	-	21/45/45/45	-
3	PLM	F	201	1	-	5/13/14/15	-
5	LPP	C	204	-	-	23/45/45/45	-
5	LPP	L	203	-	-	21/45/45/45	-
6	GOL	E	1003	-	-	2/2/2/4	-
6	GOL	M	203	-	-	0/2/2/4	-
5	LPP	D	204	-	-	20/45/45/45	-
6	GOL	F	204	-	-	2/2/2/4	-
4	L8Z	D	203	-	-	49/140/199/199	0/3/3/3
4	L8Z	F	202	-	-	52/140/199/199	0/3/3/3
6	GOL	C	202	-	-	2/2/2/4	-
3	PLM	I	201	1	-	2/13/14/15	-
3	PLM	C	201	1	-	4/13/14/15	-
4	L8Z	H	203	-	-	55/140/199/199	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	LPP	F	203	-	-	23/45/45/45	-
5	LPP	M	205	-	-	19/45/45/45	-
3	PLM	H	201	1	-	3/13/14/15	-
4	L8Z	B	202	-	-	55/140/199/199	0/3/3/3

All (392) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	205	LPP	P1-O5	8.53	1.87	1.60
5	I	203	LPP	P1-O5	8.50	1.87	1.60
5	H	204	LPP	P1-O5	8.35	1.87	1.60
5	J	204	LPP	P1-O5	8.30	1.87	1.60
5	K	203	LPP	P1-O5	8.18	1.86	1.60
5	D	204	LPP	P1-O5	8.17	1.86	1.60
4	L	202	L8Z	C2E-C1G	8.14	1.75	1.54
5	B	203	LPP	P1-O5	8.04	1.86	1.60
5	C	204	LPP	P1-O5	8.01	1.86	1.60
5	G	203	LPP	P1-O5	8.00	1.86	1.60
5	F	203	LPP	P1-O5	7.81	1.85	1.60
5	A	203	LPP	P1-O5	7.73	1.85	1.60
5	L	203	LPP	P1-O5	7.51	1.84	1.60
4	C	203	L8Z	C2E-C1G	7.30	1.73	1.54
4	A	202	L8Z	C2E-C1G	7.18	1.73	1.54
4	G	202	L8Z	O22-C1A	7.15	1.37	1.23
4	C	203	L8Z	O22-C1A	7.15	1.37	1.23
4	M	204	L8Z	O22-C1A	7.15	1.37	1.23
4	I	202	L8Z	O22-C1A	7.13	1.37	1.23
4	B	202	L8Z	C2E-C1G	7.06	1.73	1.54
4	A	202	L8Z	O22-C1A	6.98	1.37	1.23
4	H	203	L8Z	O2-C1	6.97	1.37	1.23
4	B	202	L8Z	O2-C1	6.94	1.37	1.23
4	L	202	L8Z	O22-C1A	6.92	1.37	1.23
4	D	203	L8Z	O2-C1	6.89	1.37	1.23
4	D	203	L8Z	O22-C1A	6.86	1.37	1.23
4	J	203	L8Z	C2E-C1G	6.83	1.72	1.54
4	C	203	L8Z	O2-C1	6.83	1.37	1.23
4	G	202	L8Z	O2-C1	6.82	1.37	1.23
4	E	1002	L8Z	O22-C1A	6.81	1.37	1.23
4	A	202	L8Z	O2-C1	6.79	1.37	1.23
4	J	203	L8Z	O22-C1A	6.79	1.37	1.23
4	K	202	L8Z	C2E-C1G	6.76	1.72	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	L8Z	O22-C1A	6.76	1.37	1.23
4	K	202	L8Z	O2-C1	6.75	1.37	1.23
4	H	203	L8Z	O22-C1A	6.73	1.36	1.23
4	E	1002	L8Z	O2-C1	6.73	1.36	1.23
4	M	204	L8Z	O2-C1	6.69	1.36	1.23
4	I	202	L8Z	O2-C1	6.66	1.36	1.23
4	F	202	L8Z	O22-C1A	6.63	1.36	1.23
4	L	202	L8Z	O2-C1	6.61	1.36	1.23
4	K	202	L8Z	O22-C1A	6.60	1.36	1.23
4	J	203	L8Z	O2-C1	6.56	1.36	1.23
4	F	202	L8Z	O2-C1	6.50	1.36	1.23
4	F	202	L8Z	C2E-C1G	6.46	1.71	1.54
4	C	203	L8Z	O1-C1B	5.75	1.39	1.22
4	K	202	L8Z	O1-C1B	5.71	1.39	1.22
4	L	202	L8Z	O1-C1B	5.57	1.39	1.22
4	H	203	L8Z	O1-C1B	5.52	1.38	1.22
4	B	202	L8Z	O1-C1B	5.52	1.38	1.22
4	D	203	L8Z	C2E-C1G	5.51	1.69	1.54
4	E	1002	L8Z	O1-C1B	5.47	1.38	1.22
4	D	203	L8Z	O1-C1B	5.45	1.38	1.22
4	I	202	L8Z	C2E-C1G	5.44	1.68	1.54
4	M	204	L8Z	O1-C1B	5.43	1.38	1.22
4	I	202	L8Z	O1-C1B	5.39	1.38	1.22
4	G	202	L8Z	O1-C1B	5.29	1.38	1.22
4	F	202	L8Z	O1-C1B	5.29	1.38	1.22
4	J	203	L8Z	O1-C1B	5.26	1.38	1.22
5	J	204	LPP	C6-C7	5.14	1.66	1.50
4	A	202	L8Z	O1-C1B	5.14	1.37	1.22
4	L	202	L8Z	O23-C1C	5.11	1.37	1.22
4	H	203	L8Z	O21-C15	5.04	1.37	1.22
4	D	203	L8Z	O21-C15	5.04	1.37	1.22
4	G	202	L8Z	O23-C1C	5.01	1.37	1.22
4	M	204	L8Z	O21-C15	5.00	1.37	1.22
4	A	202	L8Z	O21-C15	4.97	1.37	1.22
5	D	204	LPP	C6-C7	4.97	1.65	1.50
5	A	203	LPP	C6-C7	4.97	1.65	1.50
5	M	205	LPP	C6-C7	4.96	1.65	1.50
4	E	1002	L8Z	O23-C1C	4.94	1.37	1.22
4	B	202	L8Z	O21-C15	4.92	1.37	1.22
4	F	202	L8Z	C61-C51	4.92	1.60	1.31
4	I	202	L8Z	O23-C1C	4.92	1.37	1.22
4	E	1002	L8Z	O21-C15	4.91	1.37	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	203	L8Z	O23-C1C	4.91	1.37	1.22
4	E	1002	L8Z	C2E-C1G	4.88	1.67	1.54
4	K	202	L8Z	O36-C3B	-4.84	1.37	1.44
4	B	202	L8Z	O23-C1C	4.84	1.36	1.22
4	L	202	L8Z	O21-C15	4.83	1.36	1.22
4	C	203	L8Z	O23-C1C	4.81	1.36	1.22
5	L	203	LPP	C6-C7	4.80	1.65	1.50
4	K	202	L8Z	O21-C15	4.80	1.36	1.22
4	I	202	L8Z	C76-C68	4.79	1.62	1.52
4	F	202	L8Z	O23-C1C	4.78	1.36	1.22
4	K	202	L8Z	O23-C1C	4.77	1.36	1.22
4	D	203	L8Z	O23-C1C	4.75	1.36	1.22
4	A	202	L8Z	O23-C1C	4.75	1.36	1.22
4	G	202	L8Z	C2E-C1G	4.74	1.67	1.54
4	G	202	L8Z	O21-C15	4.71	1.36	1.22
4	C	203	L8Z	O21-C15	4.71	1.36	1.22
4	J	203	L8Z	O23-C1C	4.69	1.36	1.22
4	I	202	L8Z	O21-C15	4.68	1.36	1.22
5	G	203	LPP	C6-C7	4.68	1.65	1.50
4	I	202	L8Z	C41-C31	4.66	1.59	1.53
5	I	203	LPP	C6-C7	4.63	1.64	1.50
4	M	204	L8Z	O23-C1C	4.63	1.36	1.22
4	J	203	L8Z	O21-C15	4.60	1.36	1.22
4	H	203	L8Z	C76-C68	4.58	1.62	1.52
4	M	204	L8Z	O32-C32	-4.56	1.35	1.46
4	H	203	L8Z	C61-C51	4.55	1.58	1.31
4	K	202	L8Z	C61-C51	4.55	1.58	1.31
4	G	202	L8Z	O33-C35	-4.54	1.35	1.46
5	F	203	LPP	C6-C7	4.54	1.64	1.50
4	B	202	L8Z	C62-C52	4.53	1.58	1.31
4	D	203	L8Z	O32-C32	-4.51	1.35	1.46
4	J	203	L8Z	O33-C35	-4.51	1.35	1.46
4	L	202	L8Z	C12-C11	4.51	1.57	1.31
5	K	203	LPP	C6-C7	4.49	1.64	1.50
4	F	202	L8Z	O21-C15	4.48	1.35	1.22
4	E	1002	L8Z	C61-C51	4.47	1.57	1.31
4	G	202	L8Z	O36-C3B	-4.46	1.38	1.44
4	B	202	L8Z	C84-C74	4.43	1.57	1.31
4	I	202	L8Z	C61-C51	4.41	1.57	1.31
4	B	202	L8Z	C61-C51	4.40	1.57	1.31
5	H	204	LPP	C6-C7	4.39	1.64	1.50
4	J	203	L8Z	C62-C52	4.39	1.57	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	202	L8Z	O33-C35	-4.38	1.35	1.46
4	L	202	L8Z	O33-C35	-4.38	1.35	1.46
4	C	203	L8Z	C12-C11	4.38	1.57	1.31
4	M	204	L8Z	C61-C51	4.37	1.57	1.31
4	D	203	L8Z	C62-C52	4.35	1.57	1.31
4	F	202	L8Z	C62-C52	4.34	1.56	1.31
4	A	202	L8Z	C62-C52	4.33	1.56	1.31
4	D	203	L8Z	C84-C74	4.33	1.56	1.31
4	D	203	L8Z	C61-C51	4.31	1.56	1.31
4	A	202	L8Z	C12-C11	4.29	1.56	1.31
4	A	202	L8Z	C61-C51	4.29	1.56	1.31
4	K	202	L8Z	C12-C11	4.29	1.56	1.31
4	I	202	L8Z	C84-C74	4.29	1.56	1.31
4	G	202	L8Z	C12-C11	4.28	1.56	1.31
4	E	1002	L8Z	C84-C74	4.28	1.56	1.31
4	L	202	L8Z	C61-C51	4.27	1.56	1.31
4	G	202	L8Z	C61-C51	4.27	1.56	1.31
4	J	203	L8Z	C61-C51	4.26	1.56	1.31
4	J	203	L8Z	C12-C11	4.25	1.56	1.31
4	J	203	L8Z	C84-C74	4.22	1.56	1.31
4	B	202	L8Z	O36-C3B	-4.22	1.38	1.44
4	E	1002	L8Z	O32-C32	-4.22	1.36	1.46
4	M	204	L8Z	C84-C74	4.20	1.56	1.31
4	G	202	L8Z	C62-C52	4.20	1.56	1.31
4	A	202	L8Z	O33-C35	-4.20	1.36	1.46
4	E	1002	L8Z	C12-C11	4.20	1.56	1.31
4	E	1002	L8Z	C62-C52	4.19	1.56	1.31
4	G	202	L8Z	O32-C32	-4.19	1.36	1.46
5	B	203	LPP	C6-C7	4.19	1.63	1.50
4	D	203	L8Z	C12-C11	4.18	1.56	1.31
4	H	203	L8Z	C12-C11	4.18	1.56	1.31
4	H	203	L8Z	O33-C35	-4.18	1.36	1.46
4	K	202	L8Z	C62-C52	4.15	1.55	1.31
4	M	204	L8Z	C62-C52	4.15	1.55	1.31
4	A	202	L8Z	C84-C74	4.15	1.55	1.31
4	M	204	L8Z	O33-C35	-4.14	1.36	1.46
4	H	203	L8Z	C41-C31	4.13	1.58	1.53
4	F	202	L8Z	C12-C11	4.12	1.55	1.31
4	C	203	L8Z	O32-C32	-4.12	1.36	1.46
4	C	203	L8Z	C61-C51	4.12	1.55	1.31
4	M	204	L8Z	C12-C11	4.11	1.55	1.31
4	B	202	L8Z	C12-C11	4.11	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	202	L8Z	C84-C74	4.10	1.55	1.31
5	C	204	LPP	C6-C7	4.09	1.63	1.50
4	H	203	L8Z	C62-C52	4.08	1.55	1.31
4	C	203	L8Z	C76-C68	4.07	1.61	1.52
4	L	202	L8Z	C84-C74	4.07	1.55	1.31
4	J	203	L8Z	O32-C32	-4.05	1.36	1.46
4	F	202	L8Z	O32-C32	-4.04	1.36	1.46
4	H	203	L8Z	C84-C74	4.03	1.55	1.31
4	B	202	L8Z	O32-C32	-4.01	1.36	1.46
4	C	203	L8Z	C62-C52	4.00	1.55	1.31
4	E	1002	L8Z	O33-C35	-3.97	1.36	1.46
4	I	202	L8Z	O32-C32	-3.97	1.36	1.46
4	A	202	L8Z	O32-C32	-3.96	1.36	1.46
4	L	202	L8Z	O36-C3B	-3.95	1.38	1.44
4	L	202	L8Z	C62-C52	3.94	1.54	1.31
4	I	202	L8Z	C12-C11	3.93	1.54	1.31
4	M	204	L8Z	C76-C68	3.93	1.61	1.52
4	K	202	L8Z	C84-C74	3.91	1.54	1.31
4	E	1002	L8Z	C76-C68	3.89	1.61	1.52
4	G	202	L8Z	C84-C74	3.86	1.54	1.31
4	H	203	L8Z	O32-C32	-3.86	1.36	1.46
4	F	202	L8Z	C41-C31	3.86	1.58	1.53
4	C	203	L8Z	C84-C74	3.85	1.54	1.31
4	K	202	L8Z	O33-C35	-3.85	1.37	1.46
4	D	203	L8Z	C41-C31	3.84	1.58	1.53
4	I	202	L8Z	O36-C3B	-3.84	1.39	1.44
4	I	202	L8Z	C62-C52	3.83	1.54	1.31
4	D	203	L8Z	O33-C35	-3.83	1.37	1.46
4	M	204	L8Z	O7-C76	-3.83	1.35	1.43
4	F	202	L8Z	O33-C35	-3.81	1.37	1.46
4	H	203	L8Z	C2E-C1G	3.75	1.64	1.54
4	L	202	L8Z	O7-C76	-3.73	1.35	1.43
4	K	202	L8Z	O32-C32	-3.72	1.37	1.46
4	E	1002	L8Z	O7-C76	-3.72	1.35	1.43
4	M	204	L8Z	C2E-C1G	3.70	1.64	1.54
4	L	202	L8Z	C3D-C2E	3.67	1.57	1.52
4	G	202	L8Z	C76-C68	3.66	1.60	1.52
4	A	202	L8Z	C76-C68	3.65	1.60	1.52
4	B	202	L8Z	C76-C68	3.64	1.60	1.52
4	K	202	L8Z	O7-C76	-3.63	1.35	1.43
4	F	202	L8Z	C76-C68	3.61	1.60	1.52
4	E	1002	L8Z	O36-C3B	-3.60	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	203	L8Z	O7-C76	-3.60	1.35	1.43
4	F	202	L8Z	C3D-C2E	3.56	1.57	1.52
4	C	203	L8Z	O7-C76	-3.53	1.35	1.43
4	B	202	L8Z	O33-C35	-3.48	1.37	1.46
4	H	203	L8Z	O7-C76	-3.47	1.36	1.43
4	C	203	L8Z	O33-C35	-3.47	1.37	1.46
4	I	202	L8Z	C3C-C2D	-3.46	1.47	1.53
4	M	204	L8Z	C4C-C58	3.42	1.57	1.52
4	A	202	L8Z	O36-C3B	-3.40	1.39	1.44
4	C	203	L8Z	C3D-C2E	3.40	1.56	1.52
4	G	202	L8Z	O7-C76	-3.39	1.36	1.43
4	M	204	L8Z	C41-C31	3.36	1.57	1.53
4	B	202	L8Z	O7-C76	-3.35	1.36	1.43
4	G	202	L8Z	O51-C1F	3.33	1.50	1.41
4	J	203	L8Z	O7-C76	-3.30	1.36	1.43
5	C	204	LPP	O5-C6	-3.30	1.32	1.44
4	J	203	L8Z	O51-C1F	3.26	1.50	1.41
4	L	202	L8Z	O51-C1F	3.24	1.50	1.41
4	F	202	L8Z	O7-C76	-3.24	1.36	1.43
4	C	203	L8Z	O36-C3B	-3.23	1.39	1.44
4	K	202	L8Z	O1B-C1G	-3.21	1.18	1.30
4	F	202	L8Z	O1B-C1G	-3.21	1.18	1.30
4	M	204	L8Z	O1B-C1G	-3.21	1.18	1.30
4	E	1002	L8Z	O1B-C1G	-3.20	1.18	1.30
4	G	202	L8Z	O1B-C1G	-3.20	1.18	1.30
4	D	203	L8Z	O1B-C1G	-3.18	1.18	1.30
5	L	203	LPP	O5-C6	-3.18	1.32	1.44
4	L	202	L8Z	C76-C68	3.18	1.59	1.52
4	I	202	L8Z	O1B-C1G	-3.18	1.18	1.30
4	B	202	L8Z	O1B-C1G	-3.18	1.18	1.30
4	J	203	L8Z	O1B-C1G	-3.18	1.18	1.30
4	H	203	L8Z	O1B-C1G	-3.18	1.18	1.30
4	C	203	L8Z	O1B-C1G	-3.17	1.18	1.30
4	A	202	L8Z	O1B-C1G	-3.17	1.18	1.30
4	L	202	L8Z	O1B-C1G	-3.17	1.18	1.30
5	B	203	LPP	O5-C6	-3.16	1.32	1.44
4	J	203	L8Z	C76-C68	3.16	1.59	1.52
4	F	202	L8Z	O51-C1F	3.15	1.49	1.41
4	H	203	L8Z	C58-C68	3.13	1.60	1.52
5	G	203	LPP	O5-C6	-3.13	1.32	1.44
4	H	203	L8Z	O36-C3B	-3.09	1.40	1.44
4	I	202	L8Z	O51-C1F	3.08	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	203	L8Z	O51-C1F	3.07	1.49	1.41
4	E	1002	L8Z	O51-C1F	3.06	1.49	1.41
4	A	202	L8Z	O51-C1F	3.06	1.49	1.41
5	F	203	LPP	O5-C6	-3.05	1.33	1.44
4	E	1002	L8Z	C58-C68	3.05	1.60	1.52
5	H	204	LPP	O5-C6	-3.03	1.33	1.44
5	A	203	LPP	O5-C6	-3.03	1.33	1.44
5	M	205	LPP	O5-C6	-3.03	1.33	1.44
5	I	203	LPP	O5-C6	-3.03	1.33	1.44
4	L	202	L8Z	O32-C32	-3.01	1.39	1.46
4	I	202	L8Z	O7-C76	-3.00	1.37	1.43
4	M	204	L8Z	O51-C1F	3.00	1.49	1.41
5	K	203	LPP	O5-C6	-3.00	1.33	1.44
4	K	202	L8Z	O51-C1F	2.98	1.49	1.41
4	A	202	L8Z	O7-C76	-2.98	1.37	1.43
5	D	204	LPP	O5-C6	-2.97	1.33	1.44
4	G	202	L8Z	C41-C31	2.91	1.57	1.53
4	E	1002	L8Z	C2D-N21	2.91	1.50	1.45
4	F	202	L8Z	C3D-C4C	2.90	1.57	1.53
4	G	202	L8Z	C86-C76	2.90	1.60	1.52
5	J	204	LPP	O5-C6	-2.88	1.33	1.44
4	F	202	L8Z	C41-C51	2.88	1.59	1.50
4	C	203	L8Z	O51-C1F	2.87	1.49	1.41
4	B	202	L8Z	C41-C31	2.85	1.57	1.53
4	I	202	L8Z	C86-C76	2.83	1.59	1.52
4	A	202	L8Z	C86-C76	2.81	1.59	1.52
4	D	203	L8Z	O51-C1F	2.80	1.49	1.41
4	B	202	L8Z	C58-C68	2.80	1.59	1.52
4	L	202	L8Z	C3C-C2D	-2.79	1.48	1.53
4	B	202	L8Z	O51-C1F	2.79	1.48	1.41
4	G	202	L8Z	C2D-N21	2.77	1.50	1.45
4	M	204	L8Z	C58-C68	2.75	1.59	1.52
4	F	202	L8Z	O5-C56	-2.74	1.37	1.44
4	A	202	L8Z	C3C-C2D	-2.74	1.48	1.53
4	E	1002	L8Z	C41-C31	2.72	1.56	1.53
4	F	202	L8Z	C2D-N21	2.69	1.50	1.45
4	H	203	L8Z	C86-C76	2.69	1.59	1.52
4	H	203	L8Z	C41-C51	2.69	1.58	1.50
4	J	203	L8Z	C3C-C2D	-2.68	1.48	1.53
4	A	202	L8Z	C2D-N21	2.68	1.50	1.45
4	E	1002	L8Z	C41-C51	2.67	1.58	1.50
4	M	204	L8Z	O36-C3B	-2.66	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	L8Z	C3C-C2D	-2.66	1.48	1.53
4	H	203	L8Z	C2D-N21	2.65	1.50	1.45
4	A	202	L8Z	C42-C52	2.64	1.58	1.50
4	I	202	L8Z	C41-C51	2.62	1.58	1.50
4	E	1002	L8Z	C4C-C58	2.61	1.56	1.52
4	C	203	L8Z	C2D-N21	2.60	1.50	1.45
4	F	202	L8Z	C22-C1A	2.59	1.57	1.51
4	F	202	L8Z	C3C-C2D	-2.57	1.48	1.53
4	K	202	L8Z	C41-C51	2.57	1.58	1.50
4	F	202	L8Z	C86-C76	2.57	1.59	1.52
4	F	202	L8Z	O31-C31	-2.57	1.35	1.43
4	G	202	L8Z	C58-C68	2.54	1.59	1.52
4	B	202	L8Z	C2D-N21	2.54	1.49	1.45
4	D	203	L8Z	C86-C76	2.51	1.59	1.52
4	F	202	L8Z	O36-C3B	-2.51	1.41	1.44
4	C	203	L8Z	O62-C68	-2.50	1.40	1.44
4	K	202	L8Z	C3C-C2D	-2.50	1.48	1.53
4	F	202	L8Z	O3-C3	-2.50	1.35	1.43
4	H	203	L8Z	O62-C68	-2.49	1.40	1.44
4	B	202	L8Z	C41-C51	2.48	1.57	1.50
4	A	202	L8Z	O62-C68	-2.47	1.40	1.44
4	K	202	L8Z	C76-C68	2.47	1.58	1.52
4	D	203	L8Z	C3C-C2D	-2.45	1.49	1.53
4	B	202	L8Z	C86-C76	2.45	1.58	1.52
4	M	204	L8Z	C3C-C2D	-2.44	1.49	1.53
4	K	202	L8Z	C86-C76	2.43	1.58	1.52
4	B	202	L8Z	C42-C52	2.42	1.57	1.50
4	D	203	L8Z	C2D-N21	2.41	1.49	1.45
4	L	202	L8Z	O62-C68	-2.39	1.40	1.44
4	E	1002	L8Z	C3C-C2D	-2.38	1.49	1.53
4	M	204	L8Z	C41-C51	2.38	1.57	1.50
4	F	202	L8Z	O5-C1E	-2.36	1.35	1.41
4	C	203	L8Z	C3C-C2D	-2.35	1.49	1.53
4	D	203	L8Z	C76-C68	2.34	1.57	1.52
4	L	202	L8Z	O31-C31	-2.33	1.36	1.43
4	I	202	L8Z	C2D-N21	2.33	1.49	1.45
4	G	202	L8Z	C41-C51	2.32	1.57	1.50
4	C	203	L8Z	O31-C31	-2.32	1.36	1.43
4	B	202	L8Z	O33-C1D	2.31	1.40	1.34
4	I	202	L8Z	O52-C58	-2.30	1.37	1.43
4	C	203	L8Z	O33-C1D	2.29	1.40	1.34
4	A	202	L8Z	O3-C3	-2.28	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	202	L8Z	C2D-N21	2.28	1.49	1.45
4	B	202	L8Z	O3-C3	-2.28	1.36	1.43
4	E	1002	L8Z	O31-C31	-2.28	1.36	1.43
4	K	202	L8Z	O3-C3	-2.27	1.36	1.43
4	D	203	L8Z	O3-C3	-2.27	1.36	1.43
4	K	202	L8Z	O52-C58	-2.26	1.37	1.43
4	L	202	L8Z	C2D-N21	2.25	1.49	1.45
4	A	202	L8Z	C41-C31	2.25	1.56	1.53
4	F	202	L8Z	C58-C68	2.24	1.58	1.52
4	L	202	L8Z	O32-C1B	2.24	1.40	1.34
4	H	203	L8Z	O31-C31	-2.23	1.36	1.43
4	J	203	L8Z	O31-C31	-2.22	1.36	1.43
4	F	202	L8Z	O33-C1D	2.22	1.40	1.34
4	B	202	L8Z	O31-C31	-2.22	1.36	1.43
4	K	202	L8Z	C41-C31	2.22	1.56	1.53
4	M	204	L8Z	C66-C56	2.22	1.58	1.51
4	H	203	L8Z	C21-C15	2.22	1.55	1.50
4	A	202	L8Z	C41-C51	2.21	1.57	1.50
4	H	203	L8Z	C4C-C58	2.21	1.55	1.52
4	L	202	L8Z	C41-C31	2.20	1.56	1.53
4	G	202	L8Z	C4C-C58	2.20	1.55	1.52
4	J	203	L8Z	C2D-N21	2.19	1.49	1.45
4	K	202	L8Z	C22-C32	2.19	1.56	1.51
4	J	203	L8Z	O3-C3	-2.19	1.36	1.43
4	L	202	L8Z	O3-C3	-2.19	1.36	1.43
4	M	204	L8Z	C2D-N21	2.19	1.49	1.45
4	I	202	L8Z	O42-C4C	-2.19	1.38	1.43
4	J	203	L8Z	C86-C76	2.19	1.58	1.52
4	M	204	L8Z	O3-C3	-2.17	1.36	1.43
4	G	202	L8Z	C66-C56	2.17	1.58	1.51
4	G	202	L8Z	C3C-C2D	-2.17	1.49	1.53
4	B	202	L8Z	O52-C58	-2.16	1.37	1.43
4	K	202	L8Z	O31-C31	-2.16	1.36	1.43
4	J	203	L8Z	O52-C58	-2.15	1.37	1.43
4	K	202	L8Z	O42-C4C	-2.14	1.38	1.43
4	E	1002	L8Z	O32-C1B	2.13	1.40	1.34
5	A	203	LPP	C8-C7	2.12	1.57	1.50
4	E	1002	L8Z	O3-C3	-2.11	1.37	1.43
4	I	202	L8Z	O32-C1B	2.11	1.40	1.34
4	F	202	L8Z	O32-C1B	2.11	1.40	1.34
4	L	202	L8Z	C41-C51	2.11	1.56	1.50
4	M	204	L8Z	O31-C31	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	203	LPP	C8-C7	2.10	1.57	1.50
4	J	203	L8Z	C1E-C2C	2.10	1.56	1.53
4	E	1002	L8Z	O33-C1D	2.10	1.40	1.34
4	I	202	L8Z	C58-C68	2.10	1.58	1.52
4	A	202	L8Z	O31-C31	-2.10	1.37	1.43
4	D	203	L8Z	O5-C56	-2.10	1.39	1.44
4	G	202	L8Z	O32-C1B	2.08	1.40	1.34
4	G	202	L8Z	O3-C3	-2.07	1.37	1.43
4	B	202	L8Z	O42-C4C	-2.06	1.39	1.43
4	C	203	L8Z	C66-C56	2.06	1.58	1.51
4	C	203	L8Z	O3-C3	-2.06	1.37	1.43
4	G	202	L8Z	O31-C31	-2.06	1.37	1.43
4	C	203	L8Z	O32-C1B	2.05	1.40	1.34
4	D	203	L8Z	C41-C51	2.05	1.56	1.50
4	L	202	L8Z	O33-C1D	2.04	1.40	1.34
4	H	203	L8Z	O37-C1C	2.04	1.40	1.34
4	H	203	L8Z	O3-C3	-2.04	1.37	1.43
4	B	202	L8Z	O62-C68	-2.04	1.40	1.44
4	I	202	L8Z	O3-C3	-2.03	1.37	1.43
4	J	203	L8Z	O62-C68	-2.03	1.40	1.44
4	D	203	L8Z	O52-C58	-2.03	1.38	1.43
4	J	203	L8Z	C42-C52	2.02	1.56	1.50
4	F	202	L8Z	C4C-C58	2.01	1.55	1.52

All (455) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	202	L8Z	O61-C2E-O62	-12.79	74.56	110.07
4	K	202	L8Z	O61-C2E-C3D	11.00	135.72	107.31
4	G	202	L8Z	O61-C2E-O62	-10.17	81.84	110.07
4	F	202	L8Z	C22-C1A-N21	9.22	128.41	116.33
4	L	202	L8Z	O61-C2E-O62	-8.98	85.15	110.07
4	D	203	L8Z	C22-C1A-N21	8.29	127.19	116.33
4	G	202	L8Z	C22-C1A-N21	8.10	126.94	116.33
4	F	202	L8Z	O36-C15-C21	8.09	126.33	111.46
4	C	203	L8Z	C22-C1A-N21	7.92	126.71	116.33
4	D	203	L8Z	O37-C1C-C2A	7.92	126.01	111.46
4	H	203	L8Z	C2-C1-N2	7.79	126.53	116.33
4	E	1002	L8Z	C22-C1A-N21	7.73	126.45	116.33
4	F	202	L8Z	O37-C1C-C2A	7.56	125.36	111.46
4	E	1002	L8Z	O37-C1C-C2A	7.56	125.36	111.46
4	H	203	L8Z	O37-C1C-C2A	7.55	125.34	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	202	L8Z	C22-C1A-N21	7.47	126.12	116.33
4	I	202	L8Z	C22-C1A-N21	7.46	126.10	116.33
4	C	203	L8Z	O61-C2E-O62	-7.34	89.68	110.07
4	J	203	L8Z	C3B-O36-C15	7.32	129.72	117.53
4	M	204	L8Z	O37-C1C-C2A	7.31	124.90	111.46
4	M	204	L8Z	C22-C1A-N21	7.26	125.85	116.33
4	M	204	L8Z	O36-C15-C21	7.24	124.76	111.46
4	J	203	L8Z	C2-C1-N2	7.24	125.81	116.33
4	E	1002	L8Z	C2-C1-N2	7.20	125.76	116.33
4	G	202	L8Z	O37-C1C-C2A	7.19	124.67	111.46
4	H	203	L8Z	O2-C1-C2	-7.15	111.03	121.50
4	E	1002	L8Z	O32-C1B-C28	7.14	126.88	111.50
4	M	204	L8Z	C2-C1-N2	7.14	125.68	116.33
4	C	203	L8Z	O36-C15-C21	7.11	124.53	111.46
4	G	202	L8Z	C2-C1-N2	7.11	125.64	116.33
4	K	202	L8Z	C1E-O5-C56	7.09	127.61	113.69
4	C	203	L8Z	O37-C1C-C2A	7.05	124.41	111.46
4	D	203	L8Z	O22-C1A-C22	-6.99	111.26	121.50
4	H	203	L8Z	C22-C1A-N21	6.98	125.48	116.33
4	L	202	L8Z	C22-C1A-N21	6.96	125.44	116.33
4	J	203	L8Z	O32-C1B-C28	6.89	126.35	111.50
4	B	202	L8Z	O22-C1A-C22	-6.87	111.43	121.50
4	K	202	L8Z	C2-C1-N2	6.84	125.29	116.33
4	A	202	L8Z	O37-C1C-C2A	6.79	123.94	111.46
4	D	203	L8Z	O2-C1-C2	-6.72	111.65	121.50
4	A	202	L8Z	O36-C15-C21	6.69	123.76	111.46
4	F	202	L8Z	O32-C1B-C28	6.66	125.86	111.50
4	B	202	L8Z	O37-C1C-C2A	6.64	123.66	111.46
4	D	203	L8Z	C2-C1-N2	6.62	125.00	116.33
4	I	202	L8Z	O32-C1B-C28	6.58	125.69	111.50
4	E	1002	L8Z	O22-C1A-C22	-6.56	111.88	121.50
4	J	203	L8Z	C22-C1A-N21	6.54	124.89	116.33
4	H	203	L8Z	O22-C1A-C22	-6.51	111.96	121.50
4	B	202	L8Z	O2-C1-C2	-6.49	112.00	121.50
4	G	202	L8Z	O2-C1-C2	-6.48	112.00	121.50
4	C	203	L8Z	O22-C1A-C22	-6.47	112.01	121.50
4	I	202	L8Z	O37-C1C-C2A	6.45	123.32	111.46
4	M	204	L8Z	O2-C1-C2	-6.44	112.07	121.50
4	B	202	L8Z	C22-C1A-N21	6.41	124.73	116.33
4	C	203	L8Z	C1E-O5-C56	6.41	126.27	113.69
4	K	202	L8Z	O37-C1C-C2A	6.39	123.20	111.46
4	H	203	L8Z	O32-C1B-C28	6.37	125.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	203	L8Z	O37-C1C-C2A	6.37	123.17	111.46
4	L	202	L8Z	O36-C15-C21	6.34	123.11	111.46
4	E	1002	L8Z	C1E-O5-C56	6.32	126.09	113.69
4	J	203	L8Z	O22-C1A-C22	-6.30	112.27	121.50
4	B	202	L8Z	O32-C1B-C28	6.29	125.07	111.50
4	A	202	L8Z	C2-C1-N2	6.29	124.57	116.33
4	K	202	L8Z	O32-C1B-C28	6.28	125.05	111.50
4	E	1002	L8Z	O2-C1-C2	-6.28	112.29	121.50
4	M	204	L8Z	C2D-N21-C1A	-6.28	113.65	122.90
4	G	202	L8Z	O22-C1A-C22	-6.27	112.31	121.50
4	D	203	L8Z	O32-C1B-C28	6.26	124.99	111.50
4	F	202	L8Z	O21-C15-C21	-6.22	110.98	124.73
4	J	203	L8Z	O2-C1-C2	-6.22	112.39	121.50
4	C	203	L8Z	O2-C1-C2	-6.20	112.42	121.50
4	E	1002	L8Z	O36-C15-C21	6.19	122.84	111.46
4	A	202	L8Z	O22-C1A-C22	-6.16	112.47	121.50
4	F	202	L8Z	C2D-N21-C1A	-6.15	113.83	122.90
4	C	203	L8Z	C2-C1-N2	6.15	124.39	116.33
4	M	204	L8Z	O32-C1B-C28	6.15	124.76	111.50
4	A	202	L8Z	O61-C2E-O62	-6.15	93.00	110.07
4	F	202	L8Z	O22-C1A-C22	-6.15	112.50	121.50
4	A	202	L8Z	O32-C1B-C28	6.14	124.73	111.50
4	C	203	L8Z	O32-C1B-C28	6.10	124.64	111.50
4	K	202	L8Z	O22-C1A-C22	-6.10	112.57	121.50
4	A	202	L8Z	O2-C1-C2	-6.09	112.57	121.50
4	H	203	L8Z	C1E-O5-C56	6.09	125.65	113.69
4	K	202	L8Z	O2-C1-C2	-6.06	112.61	121.50
4	H	203	L8Z	O36-C15-C21	6.06	122.59	111.46
4	F	202	L8Z	O2-C1-C2	-6.04	112.66	121.50
4	G	202	L8Z	O32-C1B-C28	6.03	124.49	111.50
4	D	203	L8Z	O5-C1E-O14	-6.01	103.51	111.36
4	M	204	L8Z	O21-C15-C21	-6.00	111.47	124.73
4	F	202	L8Z	C2-C1-N2	5.97	124.15	116.33
4	I	202	L8Z	C1E-O5-C56	5.96	125.38	113.69
4	B	202	L8Z	C2-C1-N2	5.90	124.05	116.33
4	I	202	L8Z	O2-C1-C2	-5.88	112.88	121.50
4	L	202	L8Z	O22-C1A-C22	-5.88	112.88	121.50
4	M	204	L8Z	O22-C1A-C22	-5.85	112.93	121.50
4	E	1002	L8Z	C2C-N2-C1	-5.81	114.33	122.90
4	D	203	L8Z	C3B-O36-C15	5.80	127.19	117.53
4	I	202	L8Z	O22-C1A-C22	-5.77	113.05	121.50
4	L	202	L8Z	C1E-O5-C56	5.71	124.90	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	202	L8Z	O23-C1C-C2A	-5.67	112.21	124.73
4	D	203	L8Z	O36-C15-C21	5.67	121.88	111.46
4	K	202	L8Z	C22-C1A-N21	5.67	123.75	116.33
4	L	202	L8Z	O2-C1-C2	-5.66	113.20	121.50
4	J	203	L8Z	C2C-N2-C1	-5.66	114.57	122.90
4	H	203	L8Z	O23-C1C-C2A	-5.65	112.25	124.73
4	L	202	L8Z	C2-C1-N2	5.62	123.69	116.33
4	A	202	L8Z	C1E-O5-C56	5.62	124.71	113.69
4	F	202	L8Z	O23-C1C-C2A	-5.59	112.38	124.73
4	I	202	L8Z	C2D-N21-C1A	-5.58	114.67	122.90
4	M	204	L8Z	O23-C1C-C2A	-5.53	112.52	124.73
4	D	203	L8Z	O21-C15-C21	-5.53	112.52	124.73
4	I	202	L8Z	C2-C1-N2	5.41	123.42	116.33
4	D	203	L8Z	O23-C1C-C2A	-5.39	112.81	124.73
4	L	202	L8Z	O32-C1B-C28	5.39	123.11	111.50
4	G	202	L8Z	O5-C1E-O14	-5.37	104.35	111.36
4	L	202	L8Z	O21-C15-C21	-5.35	112.90	124.73
4	J	203	L8Z	O21-C15-C21	-5.34	112.94	124.73
4	C	203	L8Z	O21-C15-C21	-5.33	112.96	124.73
4	B	202	L8Z	O36-C15-C21	5.29	121.18	111.46
4	J	203	L8Z	C1E-O5-C56	5.29	124.06	113.69
4	I	202	L8Z	O36-C15-C21	5.29	121.17	111.46
4	M	204	L8Z	C1E-O5-C56	5.26	124.00	113.69
4	I	202	L8Z	O23-C1C-C2A	-5.25	113.14	124.73
4	J	203	L8Z	O36-C15-C21	5.25	121.10	111.46
4	J	203	L8Z	O23-C1C-C2A	-5.23	113.18	124.73
4	G	202	L8Z	O36-C15-C21	5.23	121.06	111.46
4	D	203	L8Z	O33-C1D-C2B	5.23	122.76	111.50
4	A	202	L8Z	O21-C15-C21	-5.21	113.23	124.73
4	A	202	L8Z	O5-C1E-O14	-5.19	104.58	111.36
4	K	202	L8Z	O23-C1C-C2A	-5.17	113.30	124.73
4	L	202	L8Z	O37-C1C-C2A	5.17	120.96	111.46
4	B	202	L8Z	O5-C1E-O14	-5.11	104.69	111.36
4	E	1002	L8Z	O21-C15-C21	-5.08	113.51	124.73
4	A	202	L8Z	O23-C1C-C2A	-5.07	113.53	124.73
4	J	203	L8Z	O36-C3B-C2C	5.07	117.39	107.91
4	D	203	L8Z	C2C-N2-C1	-5.05	115.46	122.90
4	F	202	L8Z	O61-C2E-O62	-5.03	96.11	110.07
4	E	1002	L8Z	O23-C1C-C2A	-5.02	113.63	124.73
4	G	202	L8Z	O23-C1C-C2A	-4.96	113.77	124.73
4	E	1002	L8Z	O4-C4A-C3B	-4.96	96.80	109.94
4	G	202	L8Z	C2D-N21-C1A	-4.95	115.60	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	202	L8Z	O4-C4A-C3B	-4.94	96.86	109.94
4	C	203	L8Z	O23-C1C-C2A	-4.91	113.88	124.73
4	C	203	L8Z	C2D-N21-C1A	-4.91	115.67	122.90
4	F	202	L8Z	O4-C4A-C3B	-4.87	97.05	109.94
4	I	202	L8Z	O21-C15-C21	-4.85	114.01	124.73
4	L	202	L8Z	O5-C1E-O14	-4.85	105.03	111.36
4	D	203	L8Z	C2D-N21-C1A	-4.85	115.76	122.90
4	H	203	L8Z	C2C-N2-C1	-4.84	115.77	122.90
4	B	202	L8Z	C1E-O5-C56	4.83	123.17	113.69
4	I	202	L8Z	O4-C4A-C3B	-4.82	97.17	109.94
4	E	1002	L8Z	O36-C3B-C4A	-4.81	96.73	107.70
4	H	203	L8Z	O5-C1E-O14	-4.69	105.23	111.36
4	L	202	L8Z	O23-C1C-C2A	-4.69	114.36	124.73
4	C	203	L8Z	O33-C1D-C2B	4.66	121.54	111.50
4	G	202	L8Z	C1E-O5-C56	4.64	122.81	113.69
4	F	202	L8Z	O5-C1E-O14	-4.64	105.29	111.36
4	C	203	L8Z	O4-C4A-C3B	-4.62	97.70	109.94
4	B	202	L8Z	O21-C15-C21	-4.62	114.53	124.73
4	K	202	L8Z	O33-C1D-C2B	4.62	121.45	111.50
4	L	202	L8Z	C2D-N21-C1A	-4.59	116.13	122.90
4	B	202	L8Z	O4-C4A-C3B	-4.59	97.78	109.94
4	I	202	L8Z	O36-C3B-C4A	-4.58	97.26	107.70
4	M	204	L8Z	O33-C1D-C2B	4.58	121.38	111.50
4	B	202	L8Z	O61-C2E-O62	-4.58	97.35	110.07
4	F	202	L8Z	C2E-C3D-C4C	4.58	119.91	110.66
4	H	203	L8Z	O1A-C1G-C2E	-4.56	109.03	123.70
4	G	202	L8Z	C2C-N2-C1	-4.50	116.27	122.90
4	J	203	L8Z	C66-O6-C1F	4.48	122.50	113.74
4	B	202	L8Z	O33-C1D-C2B	4.48	121.15	111.50
4	H	203	L8Z	O21-C15-C21	-4.47	114.85	124.73
4	M	204	L8Z	O4-C4A-C3B	-4.40	98.29	109.94
4	G	202	L8Z	O4-C4A-C3B	-4.38	98.33	109.94
4	B	202	L8Z	O36-C3B-C4A	-4.37	97.74	107.70
4	E	1002	L8Z	O33-C1D-C2B	4.36	120.91	111.50
4	H	203	L8Z	O33-C1D-C2B	4.35	120.87	111.50
4	F	202	L8Z	O33-C1D-C2B	4.34	120.86	111.50
4	L	202	L8Z	O32-C32-C22	4.34	115.19	106.65
4	K	202	L8Z	O4-C4A-C3B	-4.33	98.48	109.94
4	K	202	L8Z	C31-C21-C15	4.30	122.12	112.81
4	K	202	L8Z	O36-C15-C21	4.30	119.35	111.46
4	D	203	L8Z	C1F-O51-C57	-4.29	105.26	113.69
4	J	203	L8Z	O5-C1E-O14	-4.29	105.76	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	204	L8Z	O5-C1E-O14	-4.26	105.80	111.36
4	L	202	L8Z	C32-O32-C1B	4.24	128.24	117.79
4	A	202	L8Z	O4-C4A-C3B	-4.21	98.78	109.94
4	K	202	L8Z	C2C-N2-C1	-4.21	116.70	122.90
4	C	203	L8Z	C66-O6-C1F	4.18	121.91	113.74
4	M	204	L8Z	O1A-C1G-C2E	-4.18	110.25	123.70
4	K	202	L8Z	C3D-C4C-C58	-4.16	106.77	110.84
4	G	202	L8Z	O21-C15-C21	-4.15	115.56	124.73
4	K	202	L8Z	O21-C15-C21	-4.09	115.70	124.73
4	K	202	L8Z	O36-C3B-C4A	-4.08	98.39	107.70
4	G	202	L8Z	C31-C21-C15	4.08	121.65	112.81
4	H	203	L8Z	O4-C4A-C3B	-4.07	99.15	109.94
4	H	203	L8Z	O36-C3B-C4A	-4.04	98.50	107.70
4	A	202	L8Z	O33-C1D-C2B	4.03	120.19	111.50
4	I	202	L8Z	O37-C3C-C4B	4.00	116.24	108.25
4	G	202	L8Z	O61-C2E-C3D	3.99	117.61	107.31
4	E	1002	L8Z	C3B-O36-C15	3.95	124.11	117.53
4	F	202	L8Z	C1E-O5-C56	3.92	121.39	113.69
4	G	202	L8Z	O36-C3B-C4A	-3.92	98.76	107.70
4	I	202	L8Z	O1A-C1G-C2E	-3.88	111.23	123.70
4	E	1002	L8Z	O1A-C1G-C2E	-3.86	111.26	123.70
4	H	203	L8Z	C1F-C2D-N21	-3.86	104.36	111.00
4	A	202	L8Z	C2D-N21-C1A	-3.85	117.23	122.90
4	J	203	L8Z	O33-C1D-C2B	3.85	119.80	111.50
4	K	202	L8Z	O5-C1E-O14	-3.84	106.35	111.36
4	G	202	L8Z	O33-C1D-C2B	3.83	119.77	111.50
4	L	202	L8Z	C2E-C3D-C4C	3.81	118.37	110.66
4	I	202	L8Z	O33-C1D-C2B	3.80	119.68	111.50
4	L	202	L8Z	O1-C1B-C28	-3.79	108.94	123.73
4	J	203	L8Z	O1A-C1G-C2E	-3.78	111.52	123.70
5	J	204	LPP	C7-O9-C11	3.76	127.05	117.79
4	C	203	L8Z	C2C-N2-C1	-3.76	117.36	122.90
4	D	203	L8Z	C1E-O5-C56	3.75	121.05	113.69
4	M	204	L8Z	C2C-N2-C1	-3.74	117.39	122.90
4	L	202	L8Z	C3C-O37-C1C	3.74	123.76	117.53
4	J	203	L8Z	C2D-N21-C1A	-3.74	117.39	122.90
4	G	202	L8Z	O1A-C1G-C2E	-3.72	111.72	123.70
4	L	202	L8Z	C1E-C2C-C3B	-3.72	103.06	109.88
4	M	204	L8Z	C66-O6-C1F	3.71	120.99	113.74
4	A	202	L8Z	C66-O6-C1F	3.71	120.99	113.74
4	E	1002	L8Z	C2D-N21-C1A	-3.71	117.43	122.90
5	G	203	LPP	C7-O9-C11	3.70	126.90	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	202	L8Z	O1A-C1G-C2E	-3.70	111.80	123.70
4	D	203	L8Z	O1A-C1G-C2E	-3.68	111.86	123.70
4	C	203	L8Z	C1F-O51-C57	-3.65	106.52	113.69
4	H	203	L8Z	C3B-O36-C15	3.65	123.60	117.53
4	D	203	L8Z	C76-C68-C58	-3.63	108.01	114.03
4	E	1002	L8Z	O1-C1B-C28	-3.63	109.58	123.73
5	C	204	LPP	C7-O9-C11	3.62	126.70	117.79
4	H	203	L8Z	O1-C1B-C28	-3.61	109.64	123.73
5	A	203	LPP	C7-O9-C11	3.61	126.68	117.79
4	K	202	L8Z	O1-C1B-C28	-3.59	109.73	123.73
4	G	202	L8Z	O1-C1B-C28	-3.56	109.86	123.73
4	J	203	L8Z	C31-C21-C15	3.55	120.51	112.81
4	I	202	L8Z	O1-C1B-C28	-3.55	109.87	123.73
4	A	202	L8Z	O1A-C1G-C2E	-3.55	112.27	123.70
4	F	202	L8Z	O1-C1B-C28	-3.53	109.97	123.73
4	I	202	L8Z	C2C-N2-C1	-3.53	117.70	122.90
4	B	202	L8Z	O1A-C1G-C2E	-3.51	112.40	123.70
4	F	202	L8Z	O1A-C1G-C2E	-3.51	112.42	123.70
4	J	203	L8Z	O1-C1B-C28	-3.50	110.07	123.73
4	C	203	L8Z	O1A-C1G-C2E	-3.50	112.43	123.70
4	J	203	L8Z	O5-C56-C66	3.49	113.70	106.67
4	B	202	L8Z	C1F-O51-C57	-3.48	106.86	113.69
4	C	203	L8Z	C2E-C3D-C4C	3.47	117.67	110.66
4	I	202	L8Z	O51-C57-C4B	3.47	117.06	109.75
4	F	202	L8Z	C3D-C4C-C58	3.46	114.23	110.84
4	J	203	L8Z	O61-C2E-O62	-3.46	100.48	110.07
4	H	203	L8Z	C2D-N21-C1A	-3.45	117.81	122.90
4	E	1002	L8Z	C1E-C2C-N2	-3.45	105.06	111.00
4	C	203	L8Z	O5-C1E-O14	-3.45	106.86	111.36
4	I	202	L8Z	O5-C1E-O14	-3.44	106.87	111.36
4	M	204	L8Z	C1E-C2C-C3B	-3.43	103.60	109.88
4	K	202	L8Z	O14-C1E-C2C	3.42	114.60	108.40
4	J	203	L8Z	O4-C4A-C3B	-3.42	100.89	109.94
4	A	202	L8Z	O1-C1B-C28	-3.41	110.43	123.73
4	G	202	L8Z	C66-O6-C1F	3.40	120.39	113.74
4	L	202	L8Z	O1A-C1G-C2E	-3.40	112.75	123.70
4	M	204	L8Z	O1-C1B-C28	-3.40	110.48	123.73
4	B	202	L8Z	O1-C1B-C28	-3.39	110.50	123.73
4	F	202	L8Z	C2C-N2-C1	-3.39	117.90	122.90
4	G	202	L8Z	O62-C68-C58	3.38	113.32	108.52
4	I	202	L8Z	C3B-O36-C15	3.38	123.16	117.53
4	I	202	L8Z	C66-C56-C4A	-3.38	105.04	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	203	L8Z	O1-C1B-C28	-3.36	110.64	123.73
4	D	203	L8Z	O1-C1B-C28	-3.32	110.78	123.73
5	I	203	LPP	C7-O9-C11	3.29	125.90	117.79
4	K	202	L8Z	C3B-O36-C15	3.29	123.00	117.53
5	A	203	LPP	O2-P1-O5	-3.26	98.06	106.73
4	F	202	L8Z	C3B-C4A-C56	3.25	116.59	109.66
4	I	202	L8Z	C3C-O37-C1C	3.24	122.92	117.53
4	C	203	L8Z	O36-C3B-C4A	-3.23	100.34	107.70
4	I	202	L8Z	C66-O6-C1F	3.18	119.94	113.74
4	B	202	L8Z	C1F-C2D-N21	-3.16	105.56	111.00
4	E	1002	L8Z	O62-C68-C58	3.10	112.93	108.52
4	E	1002	L8Z	O5-C1E-O14	-3.05	107.38	111.36
5	B	203	LPP	O2-P1-O5	-3.03	98.67	106.73
4	G	202	L8Z	C76-C68-C58	-3.03	109.01	114.03
4	F	202	L8Z	O14-C1E-C2C	3.01	113.85	108.40
4	C	203	L8Z	O37-C3C-C2D	3.00	113.52	107.91
4	D	203	L8Z	O4-C4A-C3B	-2.99	102.01	109.94
5	B	203	LPP	C7-O9-C11	2.98	125.13	117.79
5	C	204	LPP	O2-P1-O5	-2.98	98.81	106.73
4	M	204	L8Z	C3D-C2E-C1G	-2.97	104.36	111.19
5	M	205	LPP	C7-O9-C11	2.97	125.10	117.79
5	G	203	LPP	O2-P1-O5	-2.96	98.85	106.73
5	K	203	LPP	C7-O9-C11	2.96	125.07	117.79
4	J	203	L8Z	C1E-C2C-C3B	-2.95	104.46	109.88
4	D	203	L8Z	C1F-C2D-N21	-2.95	105.92	111.00
4	A	202	L8Z	O36-C3B-C4A	-2.95	100.99	107.70
4	J	203	L8Z	C1F-O51-C57	-2.94	107.92	113.69
4	F	202	L8Z	C76-C68-C58	-2.91	109.20	114.03
5	F	203	LPP	O2-P1-O5	-2.91	98.99	106.73
4	C	203	L8Z	C41-C51-C61	-2.90	115.64	126.40
4	G	202	L8Z	O37-C3C-C2D	2.89	113.31	107.91
4	E	1002	L8Z	C1F-C2D-N21	-2.87	106.06	111.00
4	H	203	L8Z	C31-C21-C15	2.86	119.01	112.81
4	L	202	L8Z	O33-C1D-C2B	2.86	117.67	111.50
4	D	203	L8Z	O14-C1E-C2C	2.86	113.57	108.40
4	F	202	L8Z	C42-C52-C62	-2.85	115.82	126.40
4	I	202	L8Z	C42-C52-C62	-2.85	115.82	126.40
4	C	203	L8Z	C3C-C2D-N21	2.84	115.64	110.91
4	K	202	L8Z	C42-C52-C62	-2.83	115.89	126.40
4	A	202	L8Z	C76-C68-C58	-2.80	109.38	114.03
5	L	203	LPP	O9-C7-C8	2.79	118.50	108.40
4	C	203	L8Z	C42-C52-C62	-2.78	116.10	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	202	L8Z	C4B-C3C-C2D	2.77	115.72	110.57
5	L	203	LPP	O2-P1-O5	-2.76	99.38	106.73
5	I	203	LPP	O2-P1-O5	-2.75	99.40	106.73
4	G	202	L8Z	C41-C51-C61	-2.75	116.19	126.40
4	I	202	L8Z	C41-C51-C61	-2.75	116.20	126.40
4	J	203	L8Z	C41-C51-C61	-2.75	116.21	126.40
4	E	1002	L8Z	C3C-C2D-N21	2.72	115.43	110.91
5	C	204	LPP	O4-P1-O5	-2.72	99.50	106.73
4	A	202	L8Z	C66-C56-C4A	-2.71	106.44	112.09
4	L	202	L8Z	C41-C51-C61	-2.70	116.36	126.40
5	C	204	LPP	O4-P1-O2	2.70	117.96	107.64
4	A	202	L8Z	C3B-C4A-C56	2.69	115.40	109.66
4	B	202	L8Z	C3B-O36-C15	2.69	122.01	117.53
4	H	203	L8Z	C42-C52-C62	-2.69	116.40	126.40
5	H	204	LPP	C7-O9-C11	2.69	124.41	117.79
4	C	203	L8Z	O14-C1E-C2C	2.68	113.26	108.40
4	G	202	L8Z	C2E-O62-C68	2.68	120.44	114.20
4	E	1002	L8Z	O61-C2E-O62	-2.68	102.63	110.07
4	L	202	L8Z	O37-C3C-C4B	2.67	113.60	108.25
4	L	202	L8Z	O36-C3B-C4A	-2.67	101.63	107.70
4	I	202	L8Z	O52-C58-C4C	-2.65	104.91	109.99
4	H	203	L8Z	C3B-C2C-N2	2.65	115.32	110.91
4	M	204	L8Z	C41-C51-C61	-2.65	116.56	126.40
4	B	202	L8Z	C66-O6-C1F	2.64	118.90	113.74
4	J	203	L8Z	C66-C56-C4A	-2.64	106.59	112.09
5	D	204	LPP	C7-O9-C11	2.61	124.21	117.79
4	G	202	L8Z	O5-C56-C66	2.60	111.92	106.67
4	B	202	L8Z	C41-C51-C61	-2.60	116.74	126.40
5	I	203	LPP	O5-P1-O3	-2.60	99.18	106.47
4	H	203	L8Z	O36-C3B-C2C	2.60	112.78	107.91
4	A	202	L8Z	O14-C1E-C2C	2.59	113.09	108.40
4	E	1002	L8Z	C42-C52-C62	-2.59	116.79	126.40
4	L	202	L8Z	O61-C2E-C3D	2.57	113.96	107.31
4	M	204	L8Z	O37-C3C-C2D	2.57	112.72	107.91
4	M	204	L8Z	C42-C52-C62	-2.57	116.86	126.40
4	A	202	L8Z	O5-C1E-C2C	-2.57	105.56	110.58
4	G	202	L8Z	C3B-O36-C15	2.56	121.79	117.53
4	C	203	L8Z	O42-C4C-C58	-2.55	105.03	110.14
4	B	202	L8Z	C1E-C2C-C3B	-2.54	105.22	109.88
4	H	203	L8Z	C1F-O51-C57	-2.54	108.70	113.69
4	K	202	L8Z	C2D-N21-C1A	-2.54	119.16	122.90
5	G	203	LPP	O9-C7-C8	2.54	117.58	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	202	L8Z	C66-C56-C4A	-2.53	106.80	112.09
4	L	202	L8Z	C42-C52-C62	-2.52	117.03	126.40
5	M	205	LPP	O4-P1-O2	2.52	117.26	107.64
4	B	202	L8Z	C3D-C4C-C58	-2.52	108.37	110.84
5	L	203	LPP	O5-P1-O3	-2.51	99.42	106.47
5	L	203	LPP	O4-P1-O2	2.50	117.19	107.64
4	I	202	L8Z	C3D-C4C-C58	-2.50	108.39	110.84
5	A	203	LPP	O4-P1-O2	2.50	117.18	107.64
4	M	204	L8Z	C3C-C2D-N21	2.49	115.05	110.91
4	E	1002	L8Z	C41-C51-C61	-2.49	117.17	126.40
4	L	202	L8Z	C66-O6-C1F	2.49	118.59	113.74
4	C	203	L8Z	C1F-C2D-N21	-2.48	106.73	111.00
5	A	203	LPP	O9-C7-C8	2.48	117.38	108.40
5	H	204	LPP	O2-P1-O5	-2.48	100.14	106.73
5	F	203	LPP	O4-P1-O2	2.47	117.08	107.64
4	E	1002	L8Z	O32-C32-C22	2.47	111.50	106.65
4	D	203	L8Z	O5-C56-C66	2.47	111.64	106.67
4	D	203	L8Z	O62-C68-C58	2.46	112.02	108.52
4	M	204	L8Z	C1F-C2D-N21	-2.45	106.79	111.00
4	H	203	L8Z	C1E-C2C-C3B	-2.44	105.40	109.88
4	A	202	L8Z	C41-C51-C61	-2.44	117.35	126.40
5	F	203	LPP	C7-O9-C11	2.43	123.78	117.79
4	A	202	L8Z	O32-C32-C22	2.43	111.42	106.65
4	G	202	L8Z	O51-C57-C67	2.42	111.56	106.67
4	A	202	L8Z	C2C-N2-C1	-2.42	119.34	122.90
4	H	203	L8Z	C41-C51-C61	-2.41	117.45	126.40
4	A	202	L8Z	C3A-C2B-C1D	-2.41	104.86	113.62
5	H	204	LPP	O4-P1-O2	2.40	116.80	107.64
4	J	203	L8Z	C42-C52-C62	-2.40	117.50	126.40
4	B	202	L8Z	C42-C52-C62	-2.39	117.51	126.40
5	B	203	LPP	O4-P1-O2	2.39	116.78	107.64
4	A	202	L8Z	C1E-C2C-C3B	-2.39	105.50	109.88
4	H	203	L8Z	O14-C1E-C2C	2.39	112.72	108.40
4	K	202	L8Z	O36-C3B-C2C	-2.38	103.46	107.91
4	J	203	L8Z	O14-C1E-C2C	2.38	112.71	108.40
5	D	204	LPP	O2-P1-O5	-2.35	100.47	106.73
5	J	204	LPP	O2-P1-O5	-2.35	100.48	106.73
4	D	203	L8Z	C41-C51-C61	-2.35	117.68	126.40
5	G	203	LPP	O4-P1-O2	2.35	116.61	107.64
4	M	204	L8Z	O33-C35-C2A	2.34	111.26	106.65
5	H	204	LPP	O5-P1-O3	-2.34	99.91	106.47
4	G	202	L8Z	C42-C52-C62	-2.34	117.72	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	202	L8Z	C41-C51-C61	-2.32	117.78	126.40
4	E	1002	L8Z	O37-C3C-C2D	2.32	112.25	107.91
5	K	203	LPP	O5-P1-O3	-2.32	99.98	106.47
4	L	202	L8Z	O14-C1E-C2C	2.31	112.59	108.40
5	F	203	LPP	O9-C7-C8	2.31	116.76	108.40
5	M	205	LPP	O2-P1-O5	-2.30	100.61	106.73
5	B	203	LPP	O9-C7-C8	2.30	116.74	108.40
4	G	202	L8Z	C1F-C2D-N21	-2.30	107.05	111.00
5	J	204	LPP	O4-P1-O2	2.30	116.42	107.64
4	F	202	L8Z	O22-C1A-N21	-2.30	119.08	122.95
4	J	203	L8Z	O36-C3B-C4A	-2.29	102.49	107.70
4	F	202	L8Z	C3C-C2D-N21	2.28	114.70	110.91
4	I	202	L8Z	O42-C4C-C58	-2.28	105.57	110.14
4	L	202	L8Z	C3A-C2B-C1D	-2.27	105.36	113.62
4	K	202	L8Z	C1F-O51-C57	-2.27	109.23	113.69
4	B	202	L8Z	C2D-N21-C1A	-2.27	119.56	122.90
4	G	202	L8Z	O61-C67-C57	2.25	112.64	107.68
5	K	203	LPP	O4-P1-O2	2.25	116.23	107.64
4	D	203	L8Z	C3B-C4A-C56	-2.24	104.90	109.66
4	D	203	L8Z	C3D-C2E-C1G	-2.23	106.05	111.19
5	K	203	LPP	O2-P1-O5	-2.23	100.80	106.73
4	A	202	L8Z	O37-C3C-C4B	2.23	112.71	108.25
5	I	203	LPP	O4-P1-O2	2.22	116.13	107.64
4	F	202	L8Z	C1F-C2D-N21	-2.22	107.18	111.00
4	D	203	L8Z	C42-C52-C62	-2.20	118.22	126.40
4	L	202	L8Z	C76-C68-C58	-2.20	110.38	114.03
4	E	1002	L8Z	C3B-C2C-N2	2.19	114.55	110.91
5	D	204	LPP	O4-P1-O2	2.16	115.89	107.64
4	K	202	L8Z	C3B-C4A-C56	2.16	114.26	109.66
4	A	202	L8Z	O5-C56-C4A	2.15	113.60	109.69
4	A	202	L8Z	C42-C52-C62	-2.15	118.42	126.40
4	D	203	L8Z	O33-C1D-O11	-2.14	118.53	123.70
4	C	203	L8Z	C1F-C2D-C3C	-2.14	105.95	109.88
4	M	204	L8Z	C1F-O51-C57	-2.14	109.49	113.69
4	I	202	L8Z	O14-C1E-C2C	2.13	112.26	108.40
4	K	202	L8Z	C66-O6-C1F	2.13	117.89	113.74
4	F	202	L8Z	C41-C51-C61	-2.12	118.51	126.40
4	L	202	L8Z	O62-C2E-C3D	2.12	114.29	111.24
4	E	1002	L8Z	C76-C68-C58	-2.11	110.53	114.03
4	L	202	L8Z	O5-C56-C66	2.11	110.92	106.67
4	H	203	L8Z	C31-C41-C51	2.11	119.61	113.84
5	D	204	LPP	O5-P1-O3	-2.10	100.58	106.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1002	L8Z	O8-C86-C76	-2.10	106.49	111.07
4	E	1002	L8Z	C3D-C2E-C1G	-2.10	106.37	111.19
4	H	203	L8Z	C33-C28-C1B	-2.10	106.00	113.62
5	G	203	LPP	O5-P1-O3	-2.10	100.60	106.47
4	A	202	L8Z	O51-C57-C4B	2.09	114.17	109.75
4	G	202	L8Z	C3C-C2D-N21	2.09	114.39	110.91
4	D	203	L8Z	C3A-C2B-C1D	-2.09	106.03	113.62
5	J	204	LPP	O5-P1-O3	-2.08	100.63	106.47
4	E	1002	L8Z	C1F-O51-C57	-2.07	109.62	113.69
4	F	202	L8Z	O36-C3B-C2C	-2.07	104.03	107.91
4	J	203	L8Z	C1F-C2D-N21	-2.07	107.45	111.00
4	B	202	L8Z	O52-C58-C4C	-2.06	106.06	109.99
4	F	202	L8Z	O62-C2E-C3D	2.05	114.19	111.24
5	B	203	LPP	O5-P1-O3	-2.04	100.74	106.47
4	G	202	L8Z	O33-C35-C2A	2.04	110.66	106.65
4	H	203	L8Z	O37-C3C-C2D	2.04	111.72	107.91
4	A	202	L8Z	O5-C56-C66	2.03	110.76	106.67
4	K	202	L8Z	C76-C68-C58	-2.01	110.70	114.03
5	L	203	LPP	C7-O9-C11	2.01	122.74	117.79
5	A	203	LPP	O5-P1-O3	-2.00	100.86	106.47

There are no chirality outliers.

All (1065) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1001	PLM	C1-C2-C3-C4
3	I	201	PLM	C1-C2-C3-C4
3	J	201	PLM	C1-C2-C3-C4
4	A	202	L8Z	C1A-C22-C32-C42
4	A	202	L8Z	C1A-C22-C32-O32
4	A	202	L8Z	O32-C32-C42-C52
4	A	202	L8Z	C1C-C2A-C35-C44
4	A	202	L8Z	C1C-C2A-C35-O33
4	A	202	L8Z	O33-C35-C44-C54
4	A	202	L8Z	C2D-C1F-O6-C66
4	A	202	L8Z	C1G-C2E-O61-C67
4	A	202	L8Z	C3D-C2E-O61-C67
4	A	202	L8Z	O62-C2E-O61-C67
4	A	202	L8Z	O1B-C1G-C2E-O61
4	B	202	L8Z	C1-C2-C3-C4
4	B	202	L8Z	C11-C12-C13-C14
4	B	202	L8Z	C15-C21-C31-C41

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Mol	Chain	Res	Type	Atoms
4	B	202	L8Z	C15-C21-C31-O31
4	B	202	L8Z	C1A-C22-C32-C42
4	B	202	L8Z	C1A-C22-C32-O32
4	B	202	L8Z	C22-C32-C42-C52
4	B	202	L8Z	C2A-C35-C44-C54
4	B	202	L8Z	O33-C35-C44-C54
4	B	202	L8Z	C1G-C2E-O61-C67
4	B	202	L8Z	C3D-C2E-O61-C67
4	B	202	L8Z	O62-C2E-O61-C67
4	B	202	L8Z	O1B-C1G-C2E-O61
4	B	202	L8Z	C58-C68-C76-O7
4	B	202	L8Z	C58-C68-C76-C86
4	B	202	L8Z	O62-C68-C76-O7
4	B	202	L8Z	O62-C68-C76-C86
4	C	203	L8Z	C10-C11-C12-C13
4	C	203	L8Z	O22-C1A-C22-C32
4	C	203	L8Z	C1A-C22-C32-C42
4	C	203	L8Z	C1A-C22-C32-O32
4	C	203	L8Z	O32-C32-C42-C52
4	C	203	L8Z	C1C-C2A-C35-C44
4	C	203	L8Z	C1C-C2A-C35-O33
4	C	203	L8Z	C2D-C1F-O6-C66
4	C	203	L8Z	O51-C1F-O6-C66
4	C	203	L8Z	C1G-C2E-O61-C67
4	C	203	L8Z	C3D-C2E-O61-C67
4	C	203	L8Z	O62-C2E-O61-C67
4	C	203	L8Z	O1B-C1G-C2E-O61
4	C	203	L8Z	C58-C68-C76-O7
4	C	203	L8Z	C58-C68-C76-C86
4	C	203	L8Z	O62-C68-C76-O7
4	C	203	L8Z	O62-C68-C76-C86
4	D	203	L8Z	C1-C2-C3-C4
4	D	203	L8Z	C1-C2-C3-O3
4	D	203	L8Z	C15-C21-C31-C41
4	D	203	L8Z	C15-C21-C31-O31
4	D	203	L8Z	O22-C1A-C22-C32
4	D	203	L8Z	N21-C1A-C22-C32
4	D	203	L8Z	C1A-C22-C32-C42
4	D	203	L8Z	C1A-C22-C32-O32
4	D	203	L8Z	O32-C32-C42-C52
4	D	203	L8Z	C1C-C2A-C35-C44
4	D	203	L8Z	C1C-C2A-C35-O33

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Mol	Chain	Res	Type	Atoms
4	D	203	L8Z	O5-C1E-O14-P
4	D	203	L8Z	C2C-C3B-O36-C15
4	D	203	L8Z	C68-C76-C86-O8
4	E	1002	L8Z	C2-C3-C4-C5
4	E	1002	L8Z	C15-C21-C31-C41
4	E	1002	L8Z	C15-C21-C31-O31
4	E	1002	L8Z	C1A-C22-C32-O32
4	E	1002	L8Z	O32-C32-C42-C52
4	E	1002	L8Z	C1C-C2A-C35-C44
4	E	1002	L8Z	C1C-C2A-C35-O33
4	E	1002	L8Z	O33-C35-C44-C54
4	E	1002	L8Z	C1E-O14-P-O24
4	E	1002	L8Z	O51-C1F-O6-C66
4	E	1002	L8Z	C1G-C2E-O61-C67
4	E	1002	L8Z	C3D-C2E-O61-C67
4	E	1002	L8Z	O62-C2E-O61-C67
4	E	1002	L8Z	O1B-C1G-C2E-O61
4	E	1002	L8Z	C58-C68-C76-O7
4	E	1002	L8Z	C58-C68-C76-C86
4	E	1002	L8Z	O62-C68-C76-O7
4	E	1002	L8Z	O62-C68-C76-C86
4	F	202	L8Z	C1-C2-C3-C4
4	F	202	L8Z	C11-C12-C13-C14
4	F	202	L8Z	C1A-C22-C32-C42
4	F	202	L8Z	C1A-C22-C32-O32
4	F	202	L8Z	O32-C32-C42-C52
4	F	202	L8Z	O51-C1F-O6-C66
4	F	202	L8Z	C1G-C2E-O61-C67
4	F	202	L8Z	C3D-C2E-O61-C67
4	F	202	L8Z	O62-C2E-O61-C67
4	F	202	L8Z	O1B-C1G-C2E-O61
4	G	202	L8Z	C2-C3-C4-C5
4	G	202	L8Z	O3-C3-C4-C5
4	G	202	L8Z	C15-C21-C31-C41
4	G	202	L8Z	C15-C21-C31-O31
4	G	202	L8Z	C21-C31-C41-C51
4	G	202	L8Z	O31-C31-C41-C51
4	G	202	L8Z	C1A-C22-C32-C42
4	G	202	L8Z	C1A-C22-C32-O32
4	G	202	L8Z	C1C-C2A-C35-O33
4	G	202	L8Z	C2A-C35-C44-C54
4	G	202	L8Z	O33-C35-C44-C54

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Mol	Chain	Res	Type	Atoms
4	G	202	L8Z	O5-C1E-O14-P
4	G	202	L8Z	O1A-C1G-C2E-C3D
4	G	202	L8Z	O1B-C1G-C2E-O61
4	G	202	L8Z	O1B-C1G-C2E-C3D
4	G	202	L8Z	O1B-C1G-C2E-O62
4	G	202	L8Z	C58-C68-C76-O7
4	G	202	L8Z	C58-C68-C76-C86
4	G	202	L8Z	O62-C68-C76-O7
4	G	202	L8Z	O62-C68-C76-C86
4	G	202	L8Z	C68-C76-C86-O8
4	H	203	L8Z	C15-C21-C31-C41
4	H	203	L8Z	C15-C21-C31-O31
4	H	203	L8Z	C21-C31-C41-C51
4	H	203	L8Z	O31-C31-C41-C51
4	H	203	L8Z	C1A-C22-C32-C42
4	H	203	L8Z	C1A-C22-C32-O32
4	H	203	L8Z	C1C-C2A-C35-C44
4	H	203	L8Z	C1C-C2A-C35-O33
4	H	203	L8Z	C1E-O14-P-O12
4	H	203	L8Z	C1E-O14-P-O24
4	H	203	L8Z	C1G-C2E-O61-C67
4	H	203	L8Z	C3D-C2E-O61-C67
4	H	203	L8Z	O62-C2E-O61-C67
4	H	203	L8Z	O1B-C1G-C2E-O61
4	H	203	L8Z	O62-C68-C76-O7
4	I	202	L8Z	C11-C12-C13-C14
4	I	202	L8Z	C1A-C22-C32-C42
4	I	202	L8Z	C1A-C22-C32-O32
4	I	202	L8Z	C1C-C2A-C35-O33
4	I	202	L8Z	O33-C35-C44-C54
4	I	202	L8Z	O5-C1E-O14-P
4	I	202	L8Z	C4A-C56-C66-O6
4	I	202	L8Z	C2D-C1F-O6-C66
4	I	202	L8Z	O51-C1F-O6-C66
4	I	202	L8Z	C1G-C2E-O61-C67
4	I	202	L8Z	C3D-C2E-O61-C67
4	I	202	L8Z	O62-C2E-O61-C67
4	I	202	L8Z	O1B-C1G-C2E-O61
4	I	202	L8Z	C58-C68-C76-O7
4	I	202	L8Z	C58-C68-C76-C86
4	I	202	L8Z	O62-C68-C76-O7
4	I	202	L8Z	O62-C68-C76-C86

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Mol	Chain	Res	Type	Atoms
4	J	203	L8Z	C15-C21-C31-C41
4	J	203	L8Z	C15-C21-C31-O31
4	J	203	L8Z	C1A-C22-C32-C42
4	J	203	L8Z	C1A-C22-C32-O32
4	J	203	L8Z	C1C-C2A-C35-O33
4	J	203	L8Z	O33-C35-C44-C54
4	J	203	L8Z	C2C-C3B-O36-C15
4	J	203	L8Z	C4A-C56-C66-O6
4	J	203	L8Z	C2D-C1F-O6-C66
4	J	203	L8Z	O51-C1F-O6-C66
4	J	203	L8Z	C1G-C2E-O61-C67
4	J	203	L8Z	C3D-C2E-O61-C67
4	J	203	L8Z	O62-C2E-O61-C67
4	J	203	L8Z	O1B-C1G-C2E-O61
4	J	203	L8Z	C58-C68-C76-O7
4	J	203	L8Z	C58-C68-C76-C86
4	J	203	L8Z	O62-C68-C76-O7
4	J	203	L8Z	O62-C68-C76-C86
4	K	202	L8Z	C10-C11-C12-C13
4	K	202	L8Z	C1C-C2A-C35-C44
4	K	202	L8Z	C1C-C2A-C35-O33
4	K	202	L8Z	O33-C35-C44-C54
4	K	202	L8Z	O5-C1E-O14-P
4	K	202	L8Z	C4A-C56-C66-O6
4	K	202	L8Z	O51-C1F-O6-C66
4	K	202	L8Z	C57-C67-O61-C2E
4	K	202	L8Z	C3D-C2E-O61-C67
4	K	202	L8Z	O62-C2E-O61-C67
4	K	202	L8Z	O1B-C1G-C2E-O61
4	L	202	L8Z	O2-C1-C2-C3
4	L	202	L8Z	N2-C1-C2-C3
4	L	202	L8Z	C2-C3-C4-C5
4	L	202	L8Z	C15-C21-C31-C41
4	L	202	L8Z	C15-C21-C31-O31
4	L	202	L8Z	C1A-C22-C32-O32
4	L	202	L8Z	O32-C32-C42-C52
4	L	202	L8Z	C22-C32-O32-C1B
4	L	202	L8Z	C1C-C2A-C35-O33
4	L	202	L8Z	O33-C35-C44-C54
4	L	202	L8Z	O5-C1E-O14-P
4	L	202	L8Z	C4A-C56-C66-O6
4	L	202	L8Z	C57-C67-O61-C2E

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Mol	Chain	Res	Type	Atoms
4	L	202	L8Z	C1G-C2E-O61-C67
4	L	202	L8Z	C3D-C2E-O61-C67
4	L	202	L8Z	O62-C2E-O61-C67
4	L	202	L8Z	O1B-C1G-C2E-O61
4	L	202	L8Z	C58-C68-C76-O7
4	L	202	L8Z	C58-C68-C76-C86
4	L	202	L8Z	O62-C68-C76-O7
4	L	202	L8Z	O62-C68-C76-C86
4	M	204	L8Z	C2-C3-C4-C5
4	M	204	L8Z	C3-C4-C5-C6
4	M	204	L8Z	C21-C31-C41-C51
4	M	204	L8Z	O22-C1A-C22-C32
4	M	204	L8Z	N21-C1A-C22-C32
4	M	204	L8Z	C1A-C22-C32-O32
4	M	204	L8Z	O32-C32-C42-C52
4	M	204	L8Z	C1C-C2A-C35-C44
4	M	204	L8Z	C1C-C2A-C35-O33
4	M	204	L8Z	O33-C35-C44-C54
4	M	204	L8Z	O5-C1E-O14-P
4	M	204	L8Z	C2D-C1F-O6-C66
4	M	204	L8Z	O51-C1F-O6-C66
4	M	204	L8Z	C1G-C2E-O61-C67
4	M	204	L8Z	C3D-C2E-O61-C67
4	M	204	L8Z	O62-C2E-O61-C67
4	M	204	L8Z	O1B-C1G-C2E-O61
4	M	204	L8Z	O62-C68-C76-O7
4	M	204	L8Z	C68-C76-C86-O8
5	B	203	LPP	O9-C7-C8-O27
5	C	204	LPP	C6-O5-P1-O3
5	C	204	LPP	C6-O5-P1-O4
5	D	204	LPP	C6-O5-P1-O2
5	D	204	LPP	C6-O5-P1-O4
5	G	203	LPP	C6-O5-P1-O3
5	G	203	LPP	C6-O5-P1-O4
5	H	204	LPP	C6-O5-P1-O2
5	H	204	LPP	C6-O5-P1-O4
5	I	203	LPP	C6-O5-P1-O4
5	J	204	LPP	C6-O5-P1-O2
5	J	204	LPP	C6-O5-P1-O4
5	L	203	LPP	C6-O5-P1-O3
5	L	203	LPP	C6-O5-P1-O4
5	M	205	LPP	C6-O5-P1-O2

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Mol	Chain	Res	Type	Atoms
5	M	205	LPP	C6-O5-P1-O3
5	M	205	LPP	C6-O5-P1-O4
6	A	204	GOL	O1-C1-C2-O2
6	A	204	GOL	O1-C1-C2-C3
6	D	205	GOL	O1-C1-C2-O2
6	D	205	GOL	O1-C1-C2-C3
6	E	1003	GOL	O1-C1-C2-O2
6	F	204	GOL	O1-C1-C2-O2
6	F	204	GOL	O1-C1-C2-C3
6	H	205	GOL	O1-C1-C2-O2
6	H	205	GOL	O1-C1-C2-C3
6	M	201	GOL	O1-C1-C2-O2
4	F	202	L8Z	O51-C57-C67-O61
4	E	1002	L8Z	C4A-C56-C66-O6
4	G	202	L8Z	C4A-C56-C66-O6
4	G	202	L8Z	O51-C57-C67-O61
4	I	202	L8Z	O51-C57-C67-O61
4	J	203	L8Z	O51-C57-C67-O61
4	M	204	L8Z	O51-C57-C67-O61
4	J	203	L8Z	O5-C56-C66-O6
5	B	203	LPP	C30-C31-C32-C33
4	A	202	L8Z	C41-C51-C61-C71
4	F	202	L8Z	C64-C74-C84-C94
4	C	203	L8Z	O51-C57-C67-O61
4	A	202	L8Z	C4A-C56-C66-O6
4	D	203	L8Z	O7-C76-C86-O8
4	G	202	L8Z	O7-C76-C86-O8
4	M	204	L8Z	O7-C76-C86-O8
4	K	202	L8Z	C72-C82-C92-C23
5	J	204	LPP	C30-C31-C32-C33
4	H	203	L8Z	C68-C76-C86-O8
4	L	202	L8Z	C68-C76-C86-O8
4	H	203	L8Z	O51-C57-C67-O61
4	A	202	L8Z	C23-C24-C25-C26
4	L	202	L8Z	C92-C23-C24-C25
4	A	202	L8Z	C4-C5-C6-C7
4	G	202	L8Z	C72-C82-C92-C23
5	D	204	LPP	C30-C31-C32-C33
5	L	203	LPP	C30-C31-C32-C33
4	A	202	L8Z	C7-C8-C9-C10
4	B	202	L8Z	C6-C7-C8-C9
4	C	203	L8Z	C75-C85-C95-C46

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Mol	Chain	Res	Type	Atoms
4	M	204	L8Z	C94-C36-C37-C38
5	F	203	LPP	C30-C31-C32-C33
5	H	204	LPP	C30-C31-C32-C33
4	I	202	L8Z	O5-C56-C66-O6
4	G	202	L8Z	C4B-C57-C67-O61
5	A	203	LPP	C30-C31-C32-C33
4	L	202	L8Z	O5-C56-C66-O6
4	H	203	L8Z	C4A-C56-C66-O6
4	C	203	L8Z	C3A-C45-C55-C65
4	E	1002	L8Z	C5-C6-C7-C8
4	B	202	L8Z	O51-C1F-O6-C66
5	K	203	LPP	C30-C31-C32-C33
4	B	202	L8Z	C4A-C56-C66-O6
4	C	203	L8Z	C4A-C56-C66-O6
4	L	202	L8Z	O7-C76-C86-O8
5	C	204	LPP	C17-C18-C19-C20
4	C	203	L8Z	C5-C6-C7-C8
5	D	204	LPP	C17-C18-C19-C20
4	F	202	L8Z	C1D-C2B-C3A-C45
4	A	202	L8Z	O51-C57-C67-O61
4	J	203	L8Z	C72-C82-C92-C23
4	A	202	L8Z	C1D-C2B-C3A-C45
5	A	203	LPP	C11-C12-C13-C14
5	K	203	LPP	C29-C30-C31-C32
4	E	1002	L8Z	O5-C56-C66-O6
4	E	1002	L8Z	C4A-C3B-O36-C15
4	C	203	L8Z	C91-C16-C17-C18
4	D	203	L8Z	C41-C51-C61-C71
4	M	204	L8Z	C10-C11-C12-C13
4	G	202	L8Z	O5-C56-C66-O6
4	K	202	L8Z	O5-C56-C66-O6
4	L	202	L8Z	C11-C10-C9-C8
4	E	1002	L8Z	C1B-C28-C33-C43
4	M	204	L8Z	C1B-C28-C33-C43
5	A	203	LPP	C29-C30-C31-C32
5	B	203	LPP	C29-C30-C31-C32
5	I	203	LPP	C11-C12-C13-C14
5	L	203	LPP	C29-C30-C31-C32
3	C	201	PLM	C3-C4-C5-C6
4	H	203	L8Z	O3-C3-C4-C5
4	L	202	L8Z	O3-C3-C4-C5
4	M	204	L8Z	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	L	202	L8Z	C71-C81-C91-C16
5	C	204	LPP	C30-C31-C32-C33
5	B	203	LPP	C11-C12-C13-C14
4	D	203	L8Z	C75-C85-C95-C46
4	A	202	L8Z	O51-C1F-O6-C66
5	I	203	LPP	C29-C30-C31-C32
4	A	202	L8Z	C62-C72-C82-C92
4	B	202	L8Z	C62-C72-C82-C92
4	F	202	L8Z	C11-C10-C9-C8
4	A	202	L8Z	C10-C11-C12-C13
4	A	202	L8Z	C42-C52-C62-C72
4	B	202	L8Z	C10-C11-C12-C13
4	K	202	L8Z	C41-C51-C61-C71
4	J	203	L8Z	C4B-C57-C67-O61
4	I	202	L8Z	C3A-C45-C55-C65
5	G	203	LPP	C29-C30-C31-C32
4	A	202	L8Z	C2A-C35-C44-C54
4	I	202	L8Z	C2A-C35-C44-C54
4	K	202	L8Z	C2A-C35-C44-C54
4	A	202	L8Z	O5-C56-C66-O6
4	C	203	L8Z	C1D-C2B-C3A-C45
5	J	204	LPP	C11-C12-C13-C14
4	B	202	L8Z	C94-C36-C37-C38
4	K	202	L8Z	C71-C81-C91-C16
4	F	202	L8Z	O33-C35-C44-C54
4	H	203	L8Z	C4A-C3B-O36-C15
4	C	203	L8Z	C37-C36-C94-C84
4	E	1002	L8Z	C37-C36-C94-C84
4	K	202	L8Z	C5-C6-C7-C8
5	C	204	LPP	C31-C32-C33-C34
4	A	202	L8Z	C68-C76-C86-O8
4	C	203	L8Z	C68-C76-C86-O8
4	C	203	L8Z	C36-C37-C38-C39
4	E	1002	L8Z	C30-C29-C93-C83
4	K	202	L8Z	C55-C65-C75-C85
5	A	203	LPP	C19-C20-C21-C22
5	B	203	LPP	C14-C15-C16-C17
5	B	203	LPP	C32-C33-C34-C35
5	C	204	LPP	C18-C19-C20-C21
3	E	1001	PLM	C3-C4-C5-C6
3	F	201	PLM	C8-C9-CA-CB
4	B	202	L8Z	C91-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
4	C	203	L8Z	C2B-C3A-C45-C55
4	D	203	L8Z	C17-C16-C91-C81
4	E	1002	L8Z	C2B-C3A-C45-C55
4	F	202	L8Z	C72-C82-C92-C23
4	H	203	L8Z	C7-C8-C9-C10
4	H	203	L8Z	C17-C16-C91-C81
4	J	203	L8Z	C17-C16-C91-C81
4	M	204	L8Z	C63-C73-C83-C93
3	D	201	PLM	C6-C7-C8-C9
3	J	201	PLM	C3-C4-C5-C6
4	B	202	L8Z	C36-C37-C38-C39
5	B	203	LPP	C19-C20-C21-C22
4	H	203	L8Z	C64-C74-C84-C94
3	B	201	PLM	C5-C6-C7-C8
4	A	202	L8Z	C6-C7-C8-C9
4	A	202	L8Z	C71-C81-C91-C16
4	A	202	L8Z	C94-C36-C37-C38
4	D	203	L8Z	C91-C16-C17-C18
4	E	1002	L8Z	C4-C5-C6-C7
4	F	202	L8Z	C94-C36-C37-C38
5	L	203	LPP	C39-C40-C41-C42
4	B	202	L8Z	C65-C75-C85-C95
4	G	202	L8Z	C17-C16-C91-C81
4	I	202	L8Z	C5-C6-C7-C8
4	M	204	L8Z	C24-C23-C92-C82
5	F	203	LPP	C17-C18-C19-C20
5	L	203	LPP	C19-C20-C21-C22
4	K	202	L8Z	C1B-C28-C33-C43
4	H	203	L8Z	C28-C33-C43-C53
4	M	204	L8Z	C33-C43-C53-C63
5	D	204	LPP	C14-C15-C16-C17
5	K	203	LPP	C19-C20-C21-C22
4	C	203	L8Z	C57-C67-O61-C2E
4	I	202	L8Z	C57-C67-O61-C2E
4	M	204	L8Z	C57-C67-O61-C2E
4	C	203	L8Z	C17-C16-C91-C81
4	D	203	L8Z	C94-C36-C37-C38
4	E	1002	L8Z	C24-C23-C92-C82
4	I	202	L8Z	C91-C16-C17-C18
4	J	203	L8Z	C91-C16-C17-C18
4	M	204	L8Z	C55-C65-C75-C85
5	H	204	LPP	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
5	K	203	LPP	C17-C18-C19-C20
4	C	203	L8Z	O5-C56-C66-O6
5	H	204	LPP	C11-C12-C13-C14
3	A	201	PLM	C6-C7-C8-C9
3	C	201	PLM	C7-C8-C9-CA
4	E	1002	L8Z	C92-C23-C24-C25
4	J	203	L8Z	C24-C23-C92-C82
5	I	203	LPP	C21-C22-C23-C24
5	M	205	LPP	C14-C15-C16-C17
3	D	201	PLM	C2-C3-C4-C5
4	D	203	L8Z	C55-C65-C75-C85
4	H	203	L8Z	C75-C85-C95-C46
4	L	202	L8Z	C16-C17-C18-C19
5	L	203	LPP	C15-C16-C17-C18
4	A	202	L8Z	C17-C16-C91-C81
4	B	202	L8Z	C71-C81-C91-C16
4	L	202	L8Z	C23-C24-C25-C26
4	A	202	L8Z	C11-C10-C9-C8
4	H	203	L8Z	C37-C36-C94-C84
4	I	202	L8Z	C61-C71-C81-C91
5	D	204	LPP	C11-C12-C13-C14
5	M	205	LPP	C29-C30-C31-C32
4	D	203	L8Z	C23-C24-C25-C26
4	E	1002	L8Z	C7-C8-C9-C10
4	E	1002	L8Z	C72-C82-C92-C23
4	F	202	L8Z	C36-C37-C38-C39
4	I	202	L8Z	C16-C17-C18-C19
4	J	203	L8Z	C4-C5-C6-C7
4	L	202	L8Z	C63-C73-C83-C93
5	C	204	LPP	C15-C16-C17-C18
5	F	203	LPP	C19-C20-C21-C22
5	I	203	LPP	C39-C40-C41-C42
4	L	202	L8Z	O51-C57-C67-O61
3	E	1001	PLM	C7-C8-C9-CA
4	H	203	L8Z	C5-C6-C7-C8
4	I	202	L8Z	C4-C5-C6-C7
4	G	202	L8Z	C94-C36-C37-C38
4	M	204	L8Z	C5-C6-C7-C8
5	B	203	LPP	C15-C16-C17-C18
5	I	203	LPP	C31-C32-C33-C34
5	C	204	LPP	C11-C12-C13-C14
4	E	1002	L8Z	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
4	F	202	L8Z	C5-C6-C7-C8
4	M	204	L8Z	C53-C63-C73-C83
4	I	202	L8Z	C45-C55-C65-C75
5	J	204	LPP	C19-C20-C21-C22
5	D	204	LPP	C31-C32-C33-C34
5	I	203	LPP	C18-C19-C20-C21
4	D	203	L8Z	C28-C33-C43-C53
4	E	1002	L8Z	C75-C85-C95-C46
5	M	205	LPP	C17-C18-C19-C20
4	C	203	L8Z	C64-C74-C84-C94
4	G	202	L8Z	C10-C11-C12-C13
4	J	203	L8Z	C41-C51-C61-C71
4	K	202	L8Z	C42-C52-C62-C72
4	K	202	L8Z	C64-C74-C84-C94
4	D	203	L8Z	C24-C23-C92-C82
4	L	202	L8Z	C91-C16-C17-C18
5	M	205	LPP	C39-C40-C41-C42
4	A	202	L8Z	C22-C32-O32-C1B
3	A	201	PLM	C5-C6-C7-C8
4	G	202	L8Z	C30-C29-C93-C83
4	H	203	L8Z	C72-C82-C92-C23
4	K	202	L8Z	C94-C36-C37-C38
5	B	203	LPP	C17-C18-C19-C20
5	D	204	LPP	C19-C20-C21-C22
4	D	203	L8Z	C61-C71-C81-C91
4	H	203	L8Z	C2C-C3B-O36-C15
4	A	202	L8Z	C5-C6-C7-C8
4	L	202	L8Z	C28-C33-C43-C53
4	M	204	L8Z	C4B-C57-C67-O61
4	D	203	L8Z	O3-C3-C4-C5
4	A	202	L8Z	C65-C75-C85-C95
4	E	1002	L8Z	C16-C17-C18-C19
5	G	203	LPP	C19-C20-C21-C22
5	F	203	LPP	C29-C30-C31-C32
4	K	202	L8Z	C92-C23-C24-C25
5	L	203	LPP	C21-C22-C23-C24
4	C	203	L8Z	C53-C63-C73-C83
4	C	203	L8Z	C16-C17-C18-C19
5	J	204	LPP	C31-C32-C33-C34
5	M	205	LPP	C19-C20-C21-C22
4	A	202	L8Z	C37-C38-C39-C40
4	J	203	L8Z	C94-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	C	203	L8Z	C92-C23-C24-C25
5	K	203	LPP	C35-C36-C37-C38
5	K	203	LPP	C39-C40-C41-C42
4	B	202	L8Z	C1D-C2B-C3A-C45
4	F	202	L8Z	C23-C24-C25-C26
4	C	203	L8Z	C11-C12-C13-C14
4	M	204	L8Z	C11-C12-C13-C14
4	A	202	L8Z	C36-C37-C38-C39
4	B	202	L8Z	C4-C5-C6-C7
4	B	202	L8Z	C75-C85-C95-C46
4	E	1002	L8Z	C10-C11-C12-C13
4	E	1002	L8Z	C41-C51-C61-C71
4	G	202	L8Z	C42-C52-C62-C72
4	L	202	L8Z	C41-C51-C61-C71
4	E	1002	L8Z	C53-C63-C73-C83
4	K	202	L8Z	C24-C25-C26-C27
4	A	202	L8Z	C61-C71-C81-C91
4	J	203	L8Z	C11-C10-C9-C8
4	L	202	L8Z	C4B-C3C-O37-C1C
5	H	204	LPP	C29-C30-C31-C32
4	K	202	L8Z	C47-C46-C95-C85
5	I	203	LPP	C15-C16-C17-C18
4	H	203	L8Z	O7-C76-C86-O8
3	F	201	PLM	C3-C4-C5-C6
3	G	201	PLM	C7-C8-C9-CA
4	D	203	L8Z	C16-C17-C18-C19
4	F	202	L8Z	C91-C16-C17-C18
5	C	204	LPP	C39-C40-C41-C42
5	D	204	LPP	C15-C16-C17-C18
4	K	202	L8Z	C24-C23-C92-C82
4	L	202	L8Z	C3A-C45-C55-C65
3	L	201	PLM	C4-C5-C6-C7
4	H	203	L8Z	C92-C23-C24-C25
5	C	204	LPP	C32-C33-C34-C35
5	F	203	LPP	C20-C21-C22-C23
3	G	201	PLM	C6-C7-C8-C9
4	G	202	L8Z	C53-C63-C73-C83
5	H	204	LPP	C15-C16-C17-C18
4	F	202	L8Z	C52-C62-C72-C82
4	A	202	L8Z	C92-C23-C24-C25
5	F	203	LPP	C39-C40-C41-C42
4	F	202	L8Z	C4B-C57-C67-O61

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Mol	Chain	Res	Type	Atoms
4	I	202	L8Z	C1D-C2B-C3A-C45
5	C	204	LPP	C37-C38-C39-C40
5	G	203	LPP	O9-C7-C8-O27
5	L	203	LPP	O9-C7-C8-O27
5	M	205	LPP	O9-C7-C8-O27
4	D	203	L8Z	C72-C82-C92-C23
4	H	203	L8Z	C3A-C45-C55-C65
5	G	203	LPP	C39-C40-C41-C42
4	D	203	L8Z	C11-C10-C9-C8
4	F	202	L8Z	C37-C36-C94-C84
4	I	202	L8Z	C37-C36-C94-C84
4	J	203	L8Z	C37-C36-C94-C84
4	K	202	L8Z	C11-C10-C9-C8
4	K	202	L8Z	C62-C72-C82-C92
4	K	202	L8Z	C37-C36-C94-C84
3	F	201	PLM	C6-C7-C8-C9
4	F	202	L8Z	C92-C23-C24-C25
4	J	203	L8Z	C33-C43-C53-C63
4	J	203	L8Z	C43-C53-C63-C73
3	I	201	PLM	C3-C4-C5-C6
4	I	202	L8Z	C10-C11-C12-C13
4	A	202	L8Z	C42-C32-O32-C1B
3	A	201	PLM	CA-CB-CC-CD
4	J	203	L8Z	C37-C38-C39-C40
4	B	202	L8Z	C92-C23-C24-C25
4	B	202	L8Z	C23-C24-C25-C26
5	B	203	LPP	O5-C6-C7-C8
4	D	203	L8Z	C6-C7-C8-C9
4	G	202	L8Z	C43-C53-C63-C73
3	M	202	PLM	C9-CA-CB-CC
4	E	1002	L8Z	C33-C43-C53-C63
4	L	202	L8Z	C2A-C35-C44-C54
4	F	202	L8Z	C7-C8-C9-C10
4	G	202	L8Z	C73-C83-C93-C29
5	B	203	LPP	C13-C14-C15-C16
4	I	202	L8Z	C94-C36-C37-C38
5	H	204	LPP	C31-C32-C33-C34
4	G	202	L8Z	O22-C1A-C22-C32
4	H	203	L8Z	C71-C81-C91-C16
4	A	202	L8Z	C9-C10-C11-C12
5	B	203	LPP	C18-C19-C20-C21
4	D	203	L8Z	C63-C73-C83-C93

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Mol	Chain	Res	Type	Atoms
4	C	203	L8Z	N21-C1A-C22-C32
5	A	203	LPP	C6-C7-C8-O27
5	D	204	LPP	C6-C7-C8-O27
5	F	203	LPP	C6-C7-C8-O27
5	G	203	LPP	C6-C7-C8-O27
5	G	203	LPP	C17-C18-C19-C20
5	I	203	LPP	C6-C7-C8-O27
5	M	205	LPP	C6-C7-C8-O27
4	L	202	L8Z	C10-C11-C12-C13
4	K	202	L8Z	C17-C16-C91-C81
5	H	204	LPP	C21-C22-C23-C24
4	E	1002	L8Z	O51-C57-C67-O61
4	A	202	L8Z	O31-C31-C41-C51
4	B	202	L8Z	O31-C31-C41-C51
4	M	204	L8Z	O31-C31-C41-C51
4	B	202	L8Z	C37-C38-C39-C40
4	F	202	L8Z	C16-C17-C18-C19
4	G	202	L8Z	C5-C6-C7-C8
4	I	202	L8Z	C71-C81-C91-C16
4	M	204	L8Z	C92-C23-C24-C25
5	L	203	LPP	C14-C15-C16-C17
4	B	202	L8Z	C44-C54-C64-C74
4	D	203	L8Z	C62-C72-C82-C92
4	G	202	L8Z	C37-C36-C94-C84
4	H	203	L8Z	C61-C71-C81-C91
4	L	202	L8Z	C61-C71-C81-C91
4	L	202	L8Z	C44-C54-C64-C74
5	J	204	LPP	C29-C30-C31-C32
5	D	204	LPP	C18-C19-C20-C21
4	A	202	L8Z	C46-C47-C48-C49
4	C	203	L8Z	C24-C23-C92-C82
4	I	202	L8Z	C4B-C3C-O37-C1C
4	I	202	L8Z	C1B-C28-C33-C43
4	M	204	L8Z	C37-C38-C39-C40
5	H	204	LPP	C12-C13-C14-C15
4	M	204	L8Z	C65-C75-C85-C95
5	A	203	LPP	C14-C15-C16-C17
5	D	204	LPP	C6-O5-P1-O3
5	F	203	LPP	C6-O5-P1-O3
5	H	204	LPP	C6-O5-P1-O3
5	I	203	LPP	C6-O5-P1-O3
5	J	204	LPP	C6-O5-P1-O3

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Mol	Chain	Res	Type	Atoms
3	D	201	PLM	C4-C5-C6-C7
5	G	203	LPP	C34-C35-C36-C37
5	M	205	LPP	O5-C6-C7-O9
4	H	203	L8Z	C10-C11-C12-C13
3	L	201	PLM	CD-CE-CF-CG
4	K	202	L8Z	C33-C43-C53-C63
4	L	202	L8Z	C72-C82-C92-C23
4	J	203	L8Z	C73-C83-C93-C29
4	E	1002	L8Z	C62-C72-C82-C92
5	A	203	LPP	O9-C7-C8-O27
5	D	204	LPP	O9-C7-C8-O27
5	F	203	LPP	O9-C7-C8-O27
5	I	203	LPP	O9-C7-C8-O27
5	G	203	LPP	C15-C16-C17-C18
4	E	1002	L8Z	C57-C67-O61-C2E
4	F	202	L8Z	C57-C67-O61-C2E
4	G	202	L8Z	C57-C67-O61-C2E
4	J	203	L8Z	C57-C67-O61-C2E
4	I	202	L8Z	C4B-C57-C67-O61
4	K	202	L8Z	C91-C16-C17-C18
4	L	202	L8Z	C1A-C22-C32-C42
4	M	204	L8Z	C1A-C22-C32-C42
3	F	201	PLM	C7-C8-C9-CA
5	K	203	LPP	C33-C34-C35-C36
3	B	201	PLM	C3-C4-C5-C6
4	C	203	L8Z	C93-C29-C30-C34
4	H	203	L8Z	O5-C56-C66-O6
4	E	1002	L8Z	C65-C75-C85-C95
4	K	202	L8Z	C73-C83-C93-C29
4	K	202	L8Z	C37-C38-C39-C40
4	D	203	L8Z	C10-C11-C12-C13
4	F	202	L8Z	C10-C11-C12-C13
4	J	203	L8Z	C10-C11-C12-C13
5	B	203	LPP	C33-C34-C35-C36
4	F	202	L8Z	C31-C41-C51-C61
4	I	202	L8Z	C31-C41-C51-C61
4	L	202	L8Z	C31-C41-C51-C61
4	H	203	L8Z	C1D-C2B-C3A-C45
4	G	202	L8Z	C71-C81-C91-C16
4	I	202	L8Z	C92-C23-C24-C25
4	C	203	L8Z	O7-C76-C86-O8
4	H	203	L8Z	C94-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
4	C	203	L8Z	C71-C81-C91-C16
4	C	203	L8Z	C30-C29-C93-C83
3	M	202	PLM	C2-C3-C4-C5
4	M	204	L8Z	C17-C16-C91-C81
4	D	203	L8Z	C92-C23-C24-C25
4	C	203	L8Z	C94-C36-C37-C38
5	F	203	LPP	C14-C15-C16-C17
4	B	202	L8Z	O5-C56-C66-O6
4	L	202	L8Z	C17-C16-C91-C81
5	B	203	LPP	C6-C7-C8-O27
5	L	203	LPP	C6-C7-C8-O27
4	B	202	L8Z	C42-C52-C62-C72
4	H	203	L8Z	C42-C52-C62-C72
4	F	202	L8Z	C17-C16-C91-C81
4	G	202	L8Z	C24-C25-C26-C27
4	G	202	L8Z	C28-C33-C43-C53
4	I	202	L8Z	C47-C46-C95-C85
5	J	204	LPP	C39-C40-C41-C42
5	B	203	LPP	C31-C32-C33-C34
5	M	205	LPP	C15-C16-C17-C18
4	G	202	L8Z	C9-C10-C11-C12
4	J	203	L8Z	C16-C17-C18-C19
4	J	203	L8Z	C23-C24-C25-C26
5	D	204	LPP	C13-C14-C15-C16
4	H	203	L8Z	C91-C16-C17-C18
5	C	204	LPP	C14-C15-C16-C17
5	D	204	LPP	C16-C17-C18-C19
5	A	203	LPP	O5-C6-C7-O9
5	J	204	LPP	O5-C6-C7-O9
5	C	204	LPP	C13-C14-C15-C16
4	G	202	L8Z	C11-C10-C9-C8
4	G	202	L8Z	C62-C72-C82-C92
4	L	202	L8Z	C2D-C3C-O37-C1C
4	H	203	L8Z	C36-C37-C38-C39
4	A	202	L8Z	O3-C3-C4-C5
4	J	203	L8Z	O3-C3-C4-C5
4	J	203	L8Z	C2A-C35-C44-C54
4	A	202	L8Z	C47-C48-C49-C50
5	B	203	LPP	C41-C42-C43-C44
5	C	204	LPP	O9-C7-C8-O27
4	G	202	L8Z	C3A-C45-C55-C65
5	H	204	LPP	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
4	E	1002	L8Z	C36-C37-C38-C39
4	G	202	L8Z	C2B-C3A-C45-C55
3	A	201	PLM	CB-CC-CD-CE
3	D	201	PLM	C7-C8-C9-CA
4	I	202	L8Z	C72-C82-C92-C23
5	F	203	LPP	C15-C16-C17-C18
5	F	203	LPP	C7-C6-O5-P1
5	M	205	LPP	C7-C6-O5-P1
4	L	202	L8Z	C4-C5-C6-C7
5	I	203	LPP	C13-C14-C15-C16
5	L	203	LPP	C32-C33-C34-C35
5	A	203	LPP	C12-C13-C14-C15
4	H	203	L8Z	O62-C68-C76-C86
4	M	204	L8Z	O62-C68-C76-C86
3	J	201	PLM	C7-C8-C9-CA
4	E	1002	L8Z	C17-C16-C91-C81
4	D	203	L8Z	C11-C12-C13-C14
4	J	203	L8Z	C11-C12-C13-C14
4	K	202	L8Z	C11-C12-C13-C14
4	L	202	L8Z	C11-C12-C13-C14
5	C	204	LPP	O5-C6-C7-C8
5	J	204	LPP	O5-C6-C7-C8
4	B	202	L8Z	C11-C10-C9-C8
5	L	203	LPP	C31-C32-C33-C34
4	D	203	L8Z	C3-C4-C5-C6
4	F	202	L8Z	C3-C4-C5-C6
4	C	203	L8Z	C43-C53-C63-C73
4	H	203	L8Z	C2-C3-C4-C5
4	J	203	L8Z	C4B-O41-P1-O25
5	I	203	LPP	C6-O5-P1-O2
4	F	202	L8Z	C53-C63-C73-C83
4	I	202	L8Z	C17-C16-C91-C81
3	H	201	PLM	CD-CE-CF-CG
5	F	203	LPP	C18-C19-C20-C21
5	H	204	LPP	C16-C17-C18-C19
5	J	204	LPP	C6-C7-O9-C11
4	G	202	L8Z	C63-C73-C83-C93
5	A	203	LPP	C41-C42-C43-C44
4	E	1002	L8Z	C2C-C3B-O36-C15
4	I	202	L8Z	C2D-C3C-O37-C1C
4	B	202	L8Z	C17-C16-C91-C81
4	G	202	L8Z	C31-C41-C51-C61

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Mol	Chain	Res	Type	Atoms
4	J	203	L8Z	C61-C71-C81-C91
4	C	203	L8Z	C15-C21-C31-C41
4	C	203	L8Z	O1A-C1G-C2E-O61
4	E	1002	L8Z	O1A-C1G-C2E-O61
4	F	202	L8Z	O1A-C1G-C2E-O61
4	J	203	L8Z	O1A-C1G-C2E-O61
4	L	202	L8Z	O1A-C1G-C2E-O61
5	C	204	LPP	C6-C7-C8-O27
5	G	203	LPP	C7-C6-O5-P1
5	L	203	LPP	C7-C6-O5-P1
5	D	204	LPP	O5-C6-C7-O9
5	F	203	LPP	O5-C6-C7-O9
5	I	203	LPP	O5-C6-C7-O9
5	G	203	LPP	C14-C15-C16-C17
4	A	202	L8Z	C1-C2-C3-O3
4	B	202	L8Z	C1-C2-C3-O3
4	F	202	L8Z	C1-C2-C3-O3
4	M	204	L8Z	C1-C2-C3-O3
6	C	202	GOL	O1-C1-C2-C3
6	E	1003	GOL	O1-C1-C2-C3
6	M	201	GOL	O1-C1-C2-C3
5	C	204	LPP	C21-C22-C23-C24
4	G	202	L8Z	C17-C18-C19-C20
4	H	203	L8Z	C16-C17-C18-C19
4	E	1002	L8Z	C91-C16-C17-C18
5	A	203	LPP	C32-C33-C34-C35
4	L	202	L8Z	C62-C72-C82-C92
4	D	203	L8Z	C47-C46-C95-C85
4	M	204	L8Z	C28-C33-C43-C53
5	A	203	LPP	C13-C14-C15-C16
4	K	202	L8Z	C7-C8-C9-C10
5	I	203	LPP	C41-C42-C43-C44
4	G	202	L8Z	C1C-C2A-C35-C44
4	I	202	L8Z	C1C-C2A-C35-C44
4	J	203	L8Z	C1C-C2A-C35-C44
4	L	202	L8Z	C1C-C2A-C35-C44
4	F	202	L8Z	O3-C3-C4-C5
4	F	202	L8Z	C35-C44-C54-C64
4	H	203	L8Z	C35-C44-C54-C64
4	I	202	L8Z	C3-C4-C5-C6
4	K	202	L8Z	O32-C32-C42-C52
4	M	204	L8Z	O5-C56-C66-O6

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Mol	Chain	Res	Type	Atoms
4	C	203	L8Z	C45-C55-C65-C75
4	E	1002	L8Z	C1-C2-C3-C4
5	J	204	LPP	C15-C16-C17-C18
4	G	202	L8Z	O51-C1F-O6-C66
5	A	203	LPP	O5-C6-C7-C8
5	D	204	LPP	O5-C6-C7-C8
5	F	203	LPP	O5-C6-C7-C8
5	G	203	LPP	O5-C6-C7-C8
5	I	203	LPP	O5-C6-C7-C8
5	M	205	LPP	O5-C6-C7-C8
3	G	201	PLM	C5-C6-C7-C8
3	M	202	PLM	CA-CB-CC-CD
5	G	203	LPP	C30-C31-C32-C33
3	A	201	PLM	C7-C8-C9-CA
4	J	203	L8Z	C45-C55-C65-C75
4	C	203	L8Z	C41-C51-C61-C71
4	M	204	L8Z	C30-C29-C93-C83
4	G	202	L8Z	O62-C2E-O61-C67
4	G	202	L8Z	C16-C17-C18-C19
4	I	202	L8Z	C6-C7-C8-C9
4	I	202	L8Z	C73-C83-C93-C29
4	B	202	L8Z	C5-C6-C7-C8
5	L	203	LPP	C38-C39-C40-C41
4	A	202	L8Z	C21-C31-C41-C51
4	A	202	L8Z	C22-C32-C42-C52
4	B	202	L8Z	C21-C31-C41-C51
4	C	203	L8Z	C22-C32-C42-C52
4	D	203	L8Z	C22-C32-C42-C52
4	E	1002	L8Z	C22-C32-C42-C52
4	F	202	L8Z	C22-C32-C42-C52
4	K	202	L8Z	C21-C31-C41-C51
4	K	202	L8Z	C22-C32-C42-C52
4	M	204	L8Z	C22-C32-C42-C52
5	B	203	LPP	O5-C6-C7-O9
5	C	204	LPP	O5-C6-C7-O9
5	G	203	LPP	O5-C6-C7-O9
4	B	202	L8Z	C30-C29-C93-C83
5	J	204	LPP	C14-C15-C16-C17
4	I	202	L8Z	C43-C53-C63-C73
5	B	203	LPP	C16-C17-C18-C19
4	B	202	L8Z	C2B-C3A-C45-C55
4	F	202	L8Z	C75-C85-C95-C46

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Mol	Chain	Res	Type	Atoms
5	F	203	LPP	C35-C36-C37-C38
5	K	203	LPP	C37-C38-C39-C40
3	B	201	PLM	C1-C2-C3-C4
3	K	201	PLM	C1-C2-C3-C4
3	L	201	PLM	C1-C2-C3-C4
4	G	202	L8Z	N21-C1A-C22-C32
4	C	203	L8Z	C73-C83-C93-C29
4	J	203	L8Z	C64-C74-C84-C94
4	A	202	L8Z	C24-C25-C26-C27
5	H	204	LPP	C13-C14-C15-C16
3	A	201	PLM	C2-C3-C4-C5
3	H	201	PLM	CA-CB-CC-CD
4	I	202	L8Z	C23-C24-C25-C26
5	A	203	LPP	C16-C17-C18-C19
4	I	202	L8Z	C53-C63-C73-C83
3	C	201	PLM	C6-C7-C8-C9
5	D	204	LPP	C32-C33-C34-C35
4	M	204	L8Z	C31-C41-C51-C61
4	L	202	L8Z	C52-C62-C72-C82
4	K	202	L8Z	C36-C37-C38-C39
5	M	205	LPP	C11-C12-C13-C14
4	K	202	L8Z	C2B-C3A-C45-C55
4	D	203	L8Z	C65-C75-C85-C95
5	J	204	LPP	C38-C39-C40-C41
4	I	202	L8Z	C24-C25-C26-C27
4	A	202	L8Z	C91-C16-C17-C18
5	F	203	LPP	C31-C32-C33-C34
5	F	203	LPP	C8-C7-O9-C11
5	K	203	LPP	C8-C7-O9-C11
5	M	205	LPP	C8-C7-O9-C11
4	G	202	L8Z	C92-C23-C24-C25
5	L	203	LPP	C18-C19-C20-C21
4	K	202	L8Z	O23-C1C-C2A-C35
5	A	203	LPP	C6-O5-P1-O3
5	J	204	LPP	C22-C23-C24-C25
4	L	202	L8Z	C93-C29-C30-C34
3	B	201	PLM	C7-C8-C9-CA
4	G	202	L8Z	C6-C7-C8-C9
4	M	204	L8Z	C36-C37-C38-C39
4	I	202	L8Z	C55-C65-C75-C85
4	A	202	L8Z	C11-C12-C13-C14
4	H	203	L8Z	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	A	202	L8Z	C3B-C2C-N2-C1
4	M	204	L8Z	C3A-C45-C55-C65
4	A	202	L8Z	O5-C1E-O14-P
4	C	203	L8Z	O5-C1E-O14-P
4	E	1002	L8Z	C1A-C22-C32-C42
4	F	202	L8Z	O5-C1E-O14-P
4	F	202	L8Z	C3A-C45-C55-C65
4	A	202	L8Z	O23-C1C-C2A-C35
3	G	201	PLM	C3-C4-C5-C6
4	H	203	L8Z	C24-C25-C26-C27
5	C	204	LPP	C7-C6-O5-P1
4	J	203	L8Z	C52-C62-C72-C82
4	I	202	L8Z	O7-C76-C86-O8
5	G	203	LPP	C11-C12-C13-C14
4	E	1002	L8Z	C61-C71-C81-C91
4	F	202	L8Z	C61-C71-C81-C91
4	A	202	L8Z	C64-C74-C84-C94
4	K	202	L8Z	C4-C5-C6-C7
4	E	1002	L8Z	C93-C29-C30-C34
4	I	202	L8Z	C30-C29-C93-C83
4	E	1002	L8Z	C51-C61-C71-C81
3	A	201	PLM	C4-C5-C6-C7
5	A	203	LPP	C39-C40-C41-C42
4	I	202	L8Z	C46-C47-C48-C49
4	A	202	L8Z	O37-C1C-C2A-C35
4	C	203	L8Z	C37-C38-C39-C40
4	B	202	L8Z	C53-C63-C73-C83
4	H	203	L8Z	C23-C24-C25-C26
5	A	203	LPP	C15-C16-C17-C18
3	L	201	PLM	C6-C7-C8-C9
4	E	1002	L8Z	C24-C25-C26-C27
6	C	202	GOL	O1-C1-C2-O2
4	B	202	L8Z	C3-C4-C5-C6
4	L	202	L8Z	C3-C4-C5-C6
5	K	203	LPP	C12-C13-C14-C15
3	K	201	PLM	C3-C4-C5-C6
4	M	204	L8Z	C73-C83-C93-C29
5	A	203	LPP	O27-C29-C30-C31
4	A	202	L8Z	C30-C29-C93-C83
4	D	203	L8Z	C36-C37-C38-C39
4	D	203	L8Z	C1E-O14-P-O12
3	K	201	PLM	CB-CC-CD-CE

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Mol	Chain	Res	Type	Atoms
4	M	204	L8Z	C44-C54-C64-C74
3	F	201	PLM	CC-CD-CE-CF
4	K	202	L8Z	C17-C18-C19-C20
4	E	1002	L8Z	C3-C4-C5-C6
4	F	202	L8Z	C4-C5-C6-C7
4	K	202	L8Z	C1G-C2E-O61-C67
5	M	205	LPP	C18-C19-C20-C21
4	B	202	L8Z	C3A-C45-C55-C65
4	B	202	L8Z	C37-C36-C94-C84
5	A	203	LPP	C6-C7-O9-C11
5	C	204	LPP	C6-C7-O9-C11
5	D	204	LPP	C8-C7-O9-C11
5	G	203	LPP	C6-C7-O9-C11
5	H	204	LPP	C8-C7-O9-C11
5	I	203	LPP	C6-C7-O9-C11
5	L	203	LPP	C8-C7-O9-C11
4	H	203	L8Z	C33-C43-C53-C63
4	H	203	L8Z	C3-C4-C5-C6
4	D	203	L8Z	C2-C3-C4-C5
5	I	203	LPP	C34-C35-C36-C37
5	J	204	LPP	C20-C21-C22-C23
4	K	202	L8Z	O37-C1C-C2A-C35
5	D	204	LPP	C41-C42-C43-C44
4	F	202	L8Z	C37-C38-C39-C40
4	L	202	L8Z	C94-C36-C37-C38
4	M	204	L8Z	C43-C53-C63-C73
4	B	202	L8Z	C73-C83-C93-C29
4	I	202	L8Z	C32-C42-C52-C62
4	A	202	L8Z	O22-C1A-C22-C32
4	I	202	L8Z	O2-C1-C2-C3
4	I	202	L8Z	O22-C1A-C22-C32
4	L	202	L8Z	C5-C6-C7-C8
3	H	201	PLM	C6-C7-C8-C9
4	A	202	L8Z	O7-C76-C86-O8
5	K	203	LPP	C16-C17-C18-C19
5	K	203	LPP	C20-C21-C22-C23
4	D	203	L8Z	C42-C52-C62-C72
4	F	202	L8Z	C41-C51-C61-C71
4	M	204	L8Z	C64-C74-C84-C94
4	E	1002	L8Z	C63-C73-C83-C93
4	F	202	L8Z	O31-C31-C41-C51
4	I	202	L8Z	O31-C31-C41-C51

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Mol	Chain	Res	Type	Atoms
4	J	203	L8Z	O31-C31-C41-C51
3	C	201	PLM	C8-C9-CA-CB
4	B	202	L8Z	C9-C10-C11-C12
4	K	202	L8Z	C15-C21-C31-O31
4	L	202	L8Z	C1E-C2C-N2-C1
5	M	205	LPP	O27-C29-C30-C31
5	A	203	LPP	C31-C32-C33-C34
4	G	202	L8Z	C74-C84-C94-C36
3	J	201	PLM	C6-C7-C8-C9
4	H	203	L8Z	C45-C55-C65-C75
4	M	204	L8Z	C45-C55-C65-C75
4	G	202	L8Z	C61-C71-C81-C91
3	M	202	PLM	CB-CC-CD-CE
4	K	202	L8Z	C74-C84-C94-C36
4	A	202	L8Z	C2-C3-C4-C5
4	C	203	L8Z	C4B-O41-P1-O25
4	I	202	L8Z	C4B-O41-P1-O25
5	C	204	LPP	C6-O5-P1-O2
5	F	203	LPP	C6-O5-P1-O4
5	G	203	LPP	C6-O5-P1-O2
5	L	203	LPP	C6-O5-P1-O2
4	M	204	L8Z	O32-C1B-C28-C33
4	M	204	L8Z	C24-C25-C26-C27
4	D	203	L8Z	C33-C43-C53-C63
4	D	203	L8Z	C35-C44-C54-C64
4	G	202	L8Z	C35-C44-C54-C64
5	K	203	LPP	C13-C14-C15-C16
5	B	203	LPP	C6-C7-O9-C11
5	B	203	LPP	C8-C7-O9-C11
5	H	204	LPP	C6-C7-O9-C11
4	D	203	L8Z	C24-C25-C26-C27
4	F	202	L8Z	C24-C23-C92-C82
4	G	202	L8Z	C23-C24-C25-C26
4	B	202	L8Z	O32-C1B-C28-C33
4	G	202	L8Z	O33-C1D-C2B-C3A
4	I	202	L8Z	O33-C1D-C2B-C3A
5	L	203	LPP	O27-C29-C30-C31
4	A	202	L8Z	C2B-C3A-C45-C55
3	E	1001	PLM	C4-C5-C6-C7
4	D	203	L8Z	C17-C18-C19-C20
4	I	202	L8Z	C15-C21-C31-C41
4	K	202	L8Z	O1A-C1G-C2E-O61

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Mol	Chain	Res	Type	Atoms
4	H	203	L8Z	C3B-C2C-N2-C1
3	E	1001	PLM	C6-C7-C8-C9
5	K	203	LPP	C18-C19-C20-C21
4	E	1002	L8Z	C3A-C45-C55-C65
4	A	202	L8Z	C3-C4-C5-C6
4	E	1002	L8Z	C1-C2-C3-O3
6	K	204	GOL	O1-C1-C2-C3
5	I	203	LPP	O27-C29-C30-C31
4	D	203	L8Z	C5-C6-C7-C8
5	H	204	LPP	C20-C21-C22-C23
5	J	204	LPP	O9-C7-C8-O27
4	C	203	L8Z	C9-C10-C11-C12
4	J	203	L8Z	C3-C4-C5-C6
5	B	203	LPP	C20-C21-C22-C23
4	A	202	L8Z	C57-C67-O61-C2E
4	B	202	L8Z	C57-C67-O61-C2E
4	C	203	L8Z	C1E-O14-P-O34
4	C	203	L8Z	C4B-O41-P1-O13
4	C	203	L8Z	C4B-O41-P1-O35
4	D	203	L8Z	C1E-O14-P-O34
4	E	1002	L8Z	O1B-C1G-C2E-O62
4	F	202	L8Z	C4B-O41-P1-O35
4	G	202	L8Z	C1E-O14-P-O24
4	I	202	L8Z	C1E-O14-P-O24
4	I	202	L8Z	C4B-O41-P1-O13
4	I	202	L8Z	C4B-O41-P1-O35
4	K	202	L8Z	C4B-O41-P1-O13
5	G	203	LPP	C33-C34-C35-C36
4	G	202	L8Z	C55-C65-C75-C85
5	C	204	LPP	C16-C17-C18-C19
4	M	204	L8Z	O1-C1B-C28-C33
4	E	1002	L8Z	C95-C46-C47-C48
4	A	202	L8Z	O33-C1D-C2B-C3A
5	C	204	LPP	O27-C29-C30-C31
4	H	203	L8Z	C6-C7-C8-C9
4	M	204	L8Z	C72-C82-C92-C23
5	L	203	LPP	C13-C14-C15-C16
5	F	203	LPP	O27-C29-C30-C31
4	G	202	L8Z	C1D-C2B-C3A-C45
5	F	203	LPP	C34-C35-C36-C37
4	A	202	L8Z	C63-C73-C83-C93
5	H	204	LPP	C22-C23-C24-C25

Continued on next page...

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Mol	Chain	Res	Type	Atoms
4	E	1002	L8Z	C71-C81-C91-C16
5	A	203	LPP	C33-C34-C35-C36
4	G	202	L8Z	O11-C1D-C2B-C3A
5	L	203	LPP	O28-C29-C30-C31
4	H	203	L8Z	C2B-C3A-C45-C55
4	C	203	L8Z	C54-C64-C74-C84
5	A	203	LPP	C20-C21-C22-C23
5	K	203	LPP	C15-C16-C17-C18
4	I	202	L8Z	O11-C1D-C2B-C3A
4	H	203	L8Z	C65-C75-C85-C95
5	H	204	LPP	O27-C29-C30-C31
5	I	203	LPP	O28-C29-C30-C31
4	L	202	L8Z	C73-C83-C93-C29
4	B	202	L8Z	O1-C1B-C28-C33
4	I	202	L8Z	C28-C33-C43-C53
5	F	203	LPP	C38-C39-C40-C41
5	G	203	LPP	C8-C7-O9-C11
4	A	202	L8Z	O11-C1D-C2B-C3A
5	F	203	LPP	O28-C29-C30-C31
5	B	203	LPP	C22-C23-C24-C25
4	K	202	L8Z	O32-C1B-C28-C33
4	L	202	L8Z	C55-C65-C75-C85
5	M	205	LPP	C32-C33-C34-C35
4	M	204	L8Z	C7-C8-C9-C10
5	I	203	LPP	C19-C20-C21-C22
4	F	202	L8Z	O22-C1A-C22-C32
4	I	202	L8Z	C21-C31-C41-C51
4	B	202	L8Z	O33-C1D-C2B-C3A
4	A	202	L8Z	C51-C61-C71-C81
4	F	202	L8Z	C54-C64-C74-C84
4	C	203	L8Z	O3-C3-C4-C5
4	B	202	L8Z	C1E-O14-P-O12
4	C	203	L8Z	C1E-O14-P-O12
4	I	202	L8Z	C1E-O14-P-O12
4	F	202	L8Z	O32-C1B-C28-C33
4	M	204	L8Z	O33-C1D-C2B-C3A
4	E	1002	L8Z	C17-C18-C19-C20
4	F	202	L8Z	C95-C46-C47-C48
4	K	202	L8Z	C9-C10-C11-C12
4	K	202	L8Z	O1-C1B-C28-C33

There are no ring outliers.

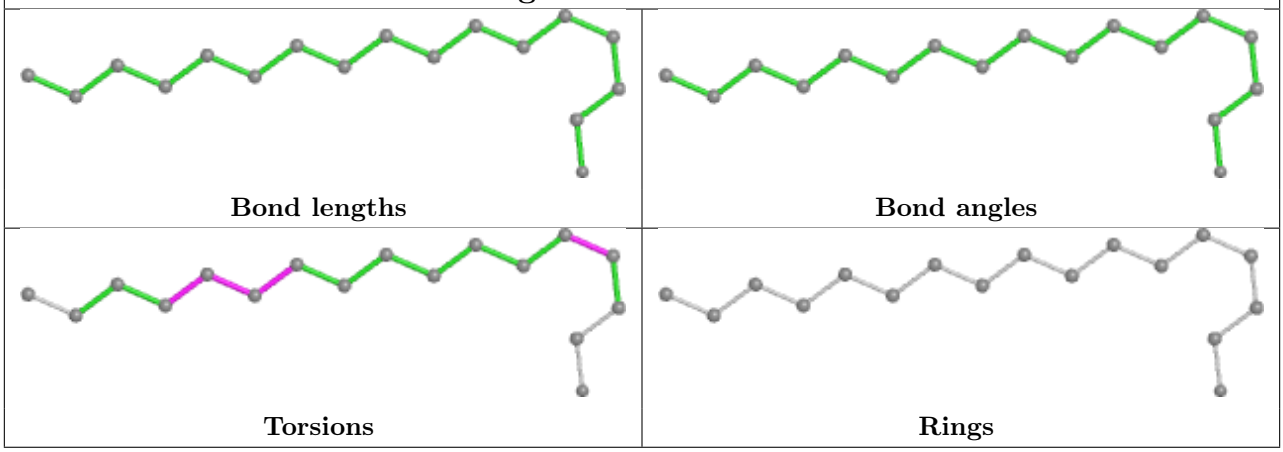
34 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	202	PLM	2	0
4	I	202	L8Z	3	0
4	G	202	L8Z	2	0
5	B	203	LPP	3	0
3	D	201	PLM	2	0
4	C	203	L8Z	2	0
5	H	204	LPP	5	0
5	G	203	LPP	1	0
4	E	1002	L8Z	3	0
3	A	201	PLM	1	0
3	L	201	PLM	1	0
4	M	204	L8Z	3	0
3	K	201	PLM	1	0
4	K	202	L8Z	2	0
4	L	202	L8Z	4	0
5	K	203	LPP	2	0
3	G	201	PLM	1	0
4	A	202	L8Z	1	0
5	J	204	LPP	1	0
6	D	202	GOL	1	0
4	J	203	L8Z	2	0
5	A	203	LPP	2	0
5	I	203	LPP	1	0
5	C	204	LPP	3	0
5	L	203	LPP	3	0
4	D	203	L8Z	2	0
4	F	202	L8Z	1	0
3	I	201	PLM	2	0
3	C	201	PLM	2	0
4	H	203	L8Z	2	0
5	F	203	LPP	2	0
5	M	205	LPP	3	0
3	H	201	PLM	1	0
4	B	202	L8Z	1	0

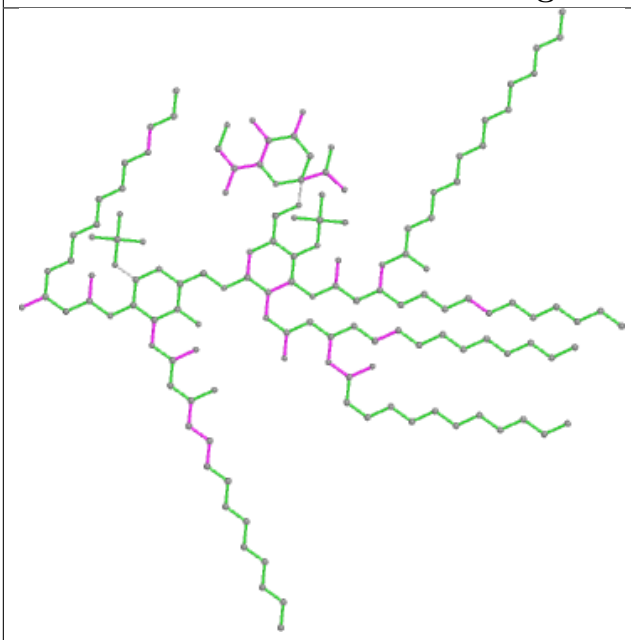
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

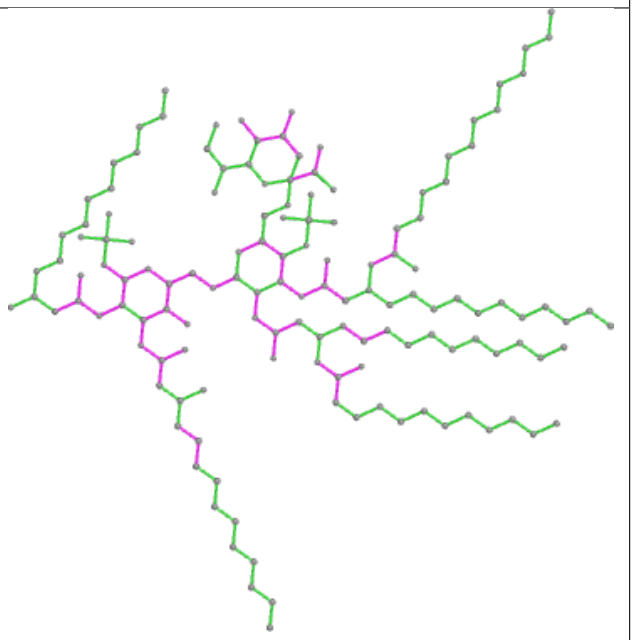
Ligand PLM M 202



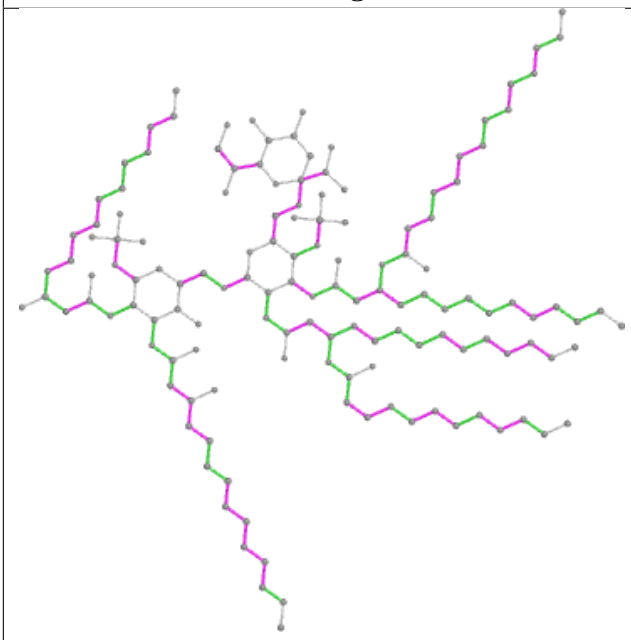
Ligand L8Z I 202



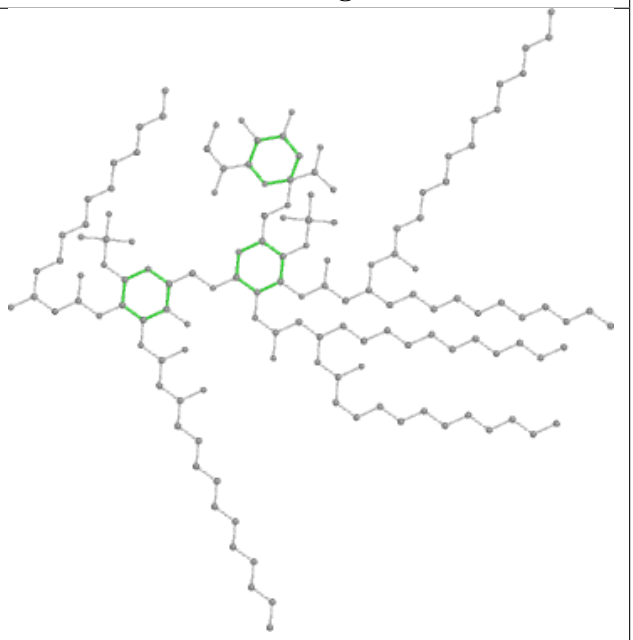
Bond lengths



Bond angles

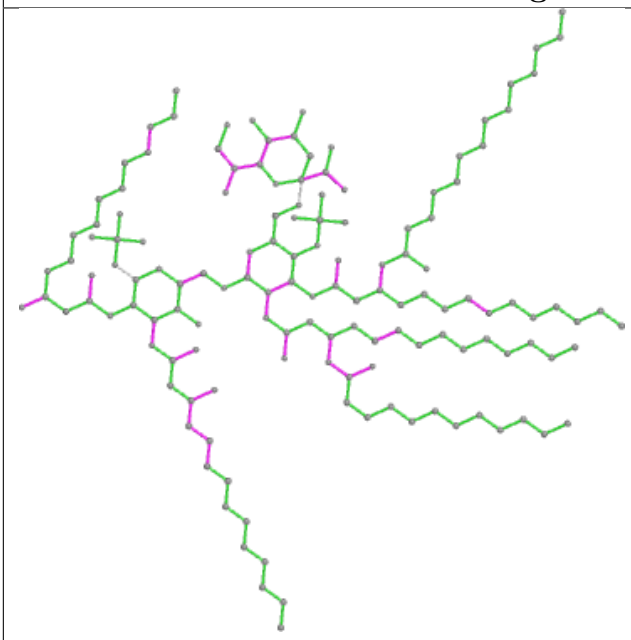


Torsions

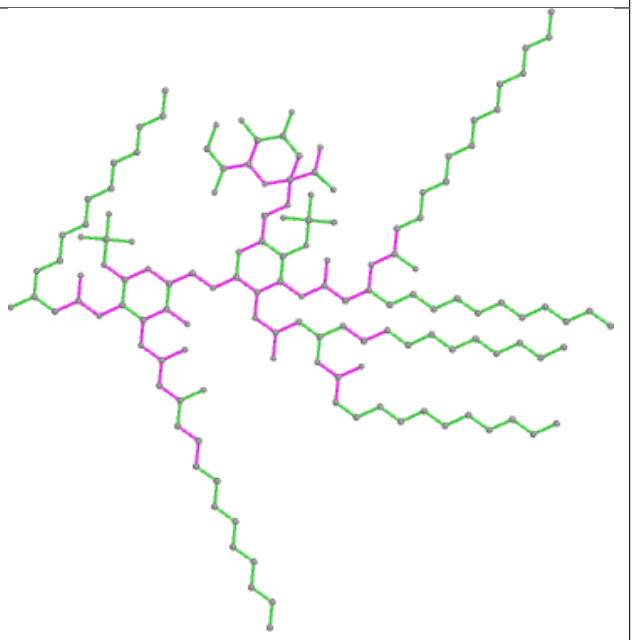


Rings

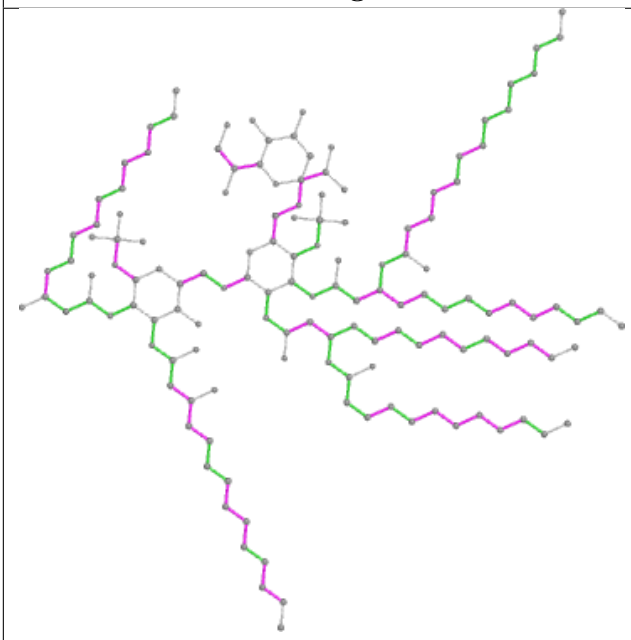
Ligand L8Z G 202



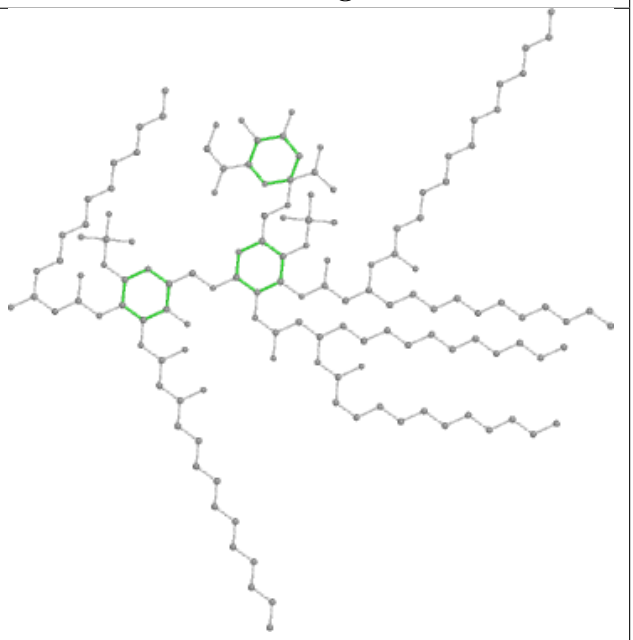
Bond lengths



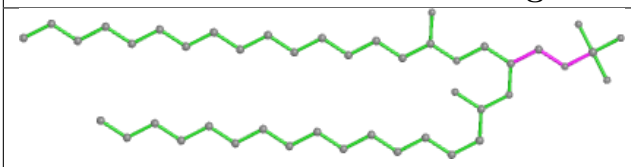
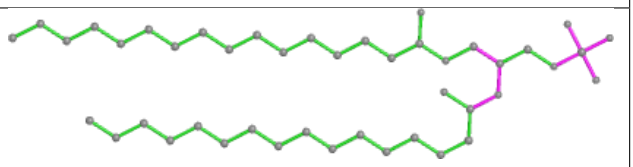
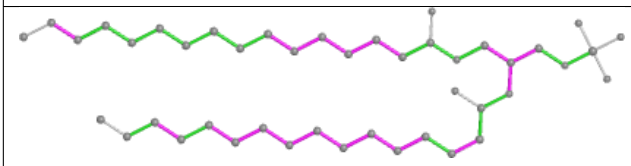
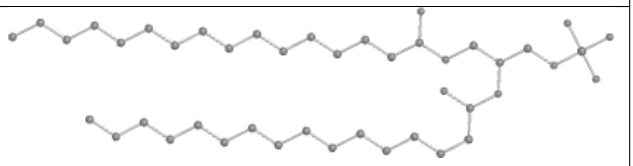
Bond angles

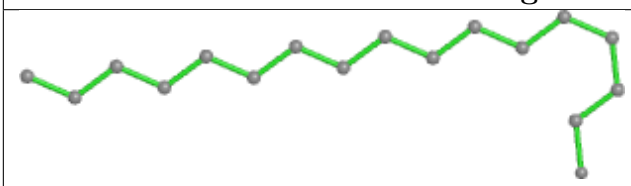
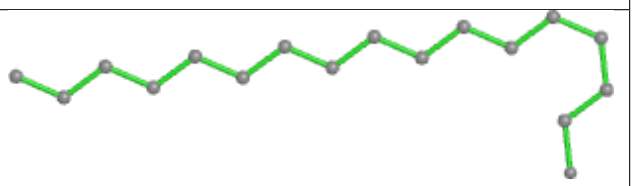
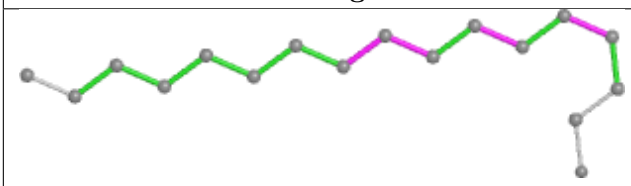
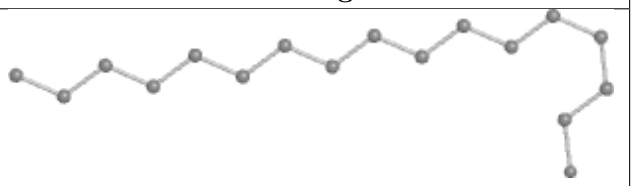


Torsions

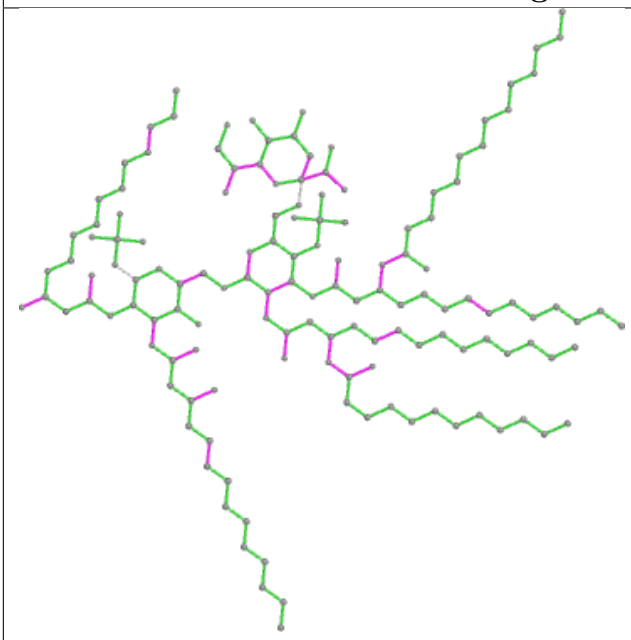


Rings

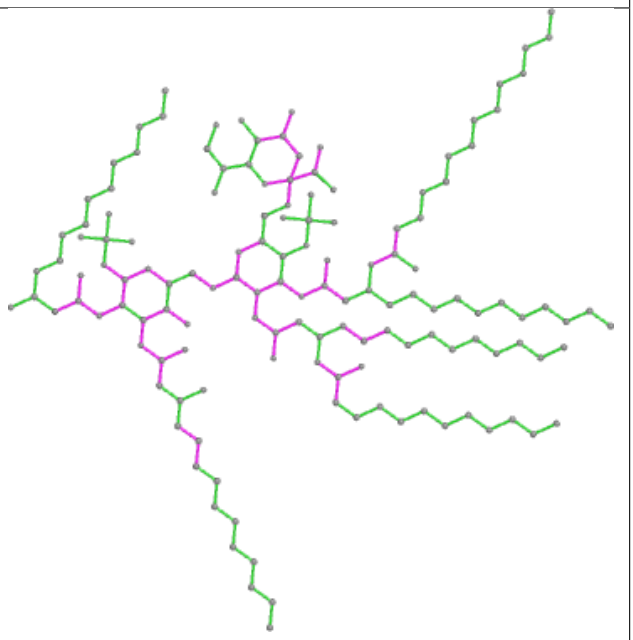
Ligand LPP B 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM D 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

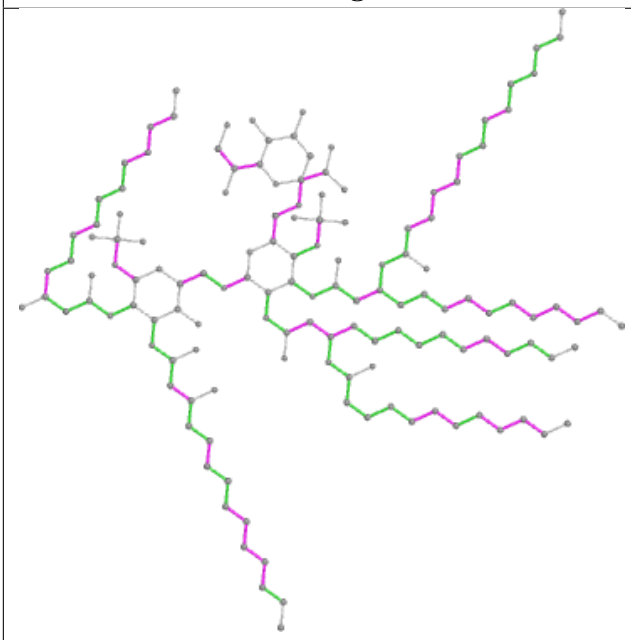
Ligand L8Z C 203



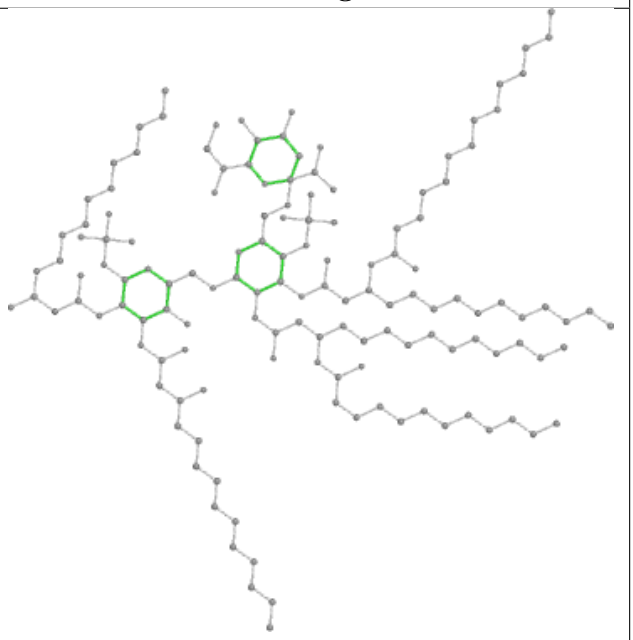
Bond lengths



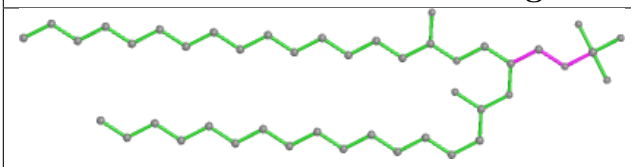
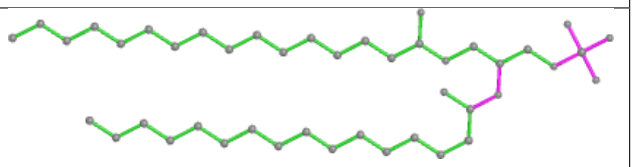
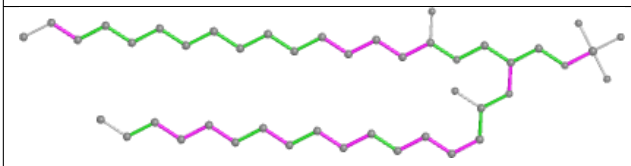
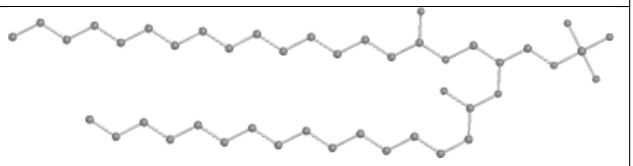
Bond angles

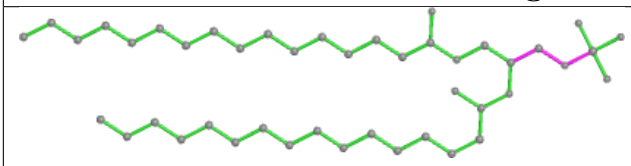
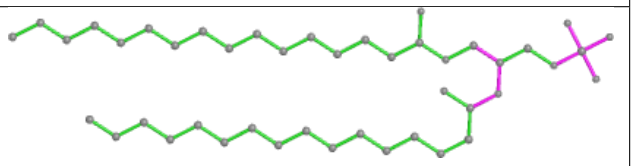
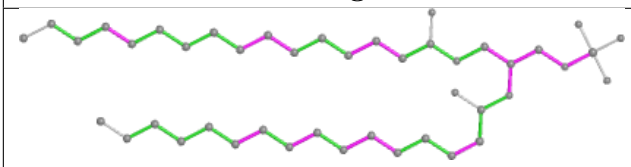
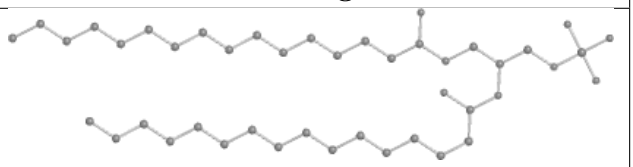


Torsions

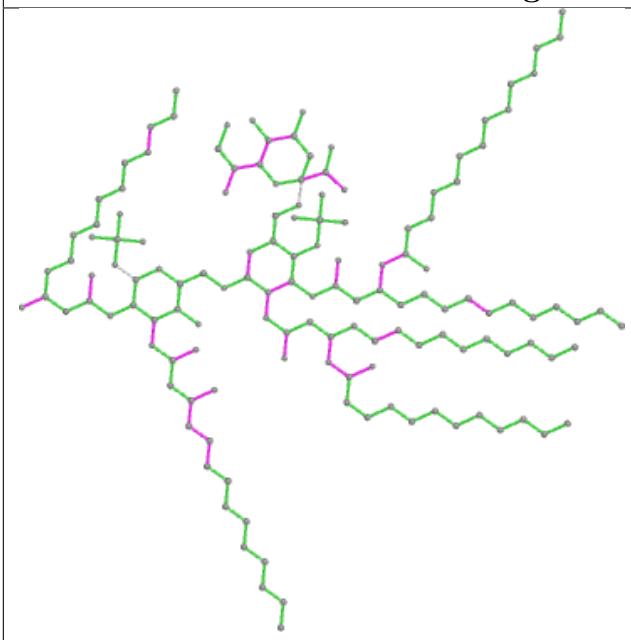


Rings

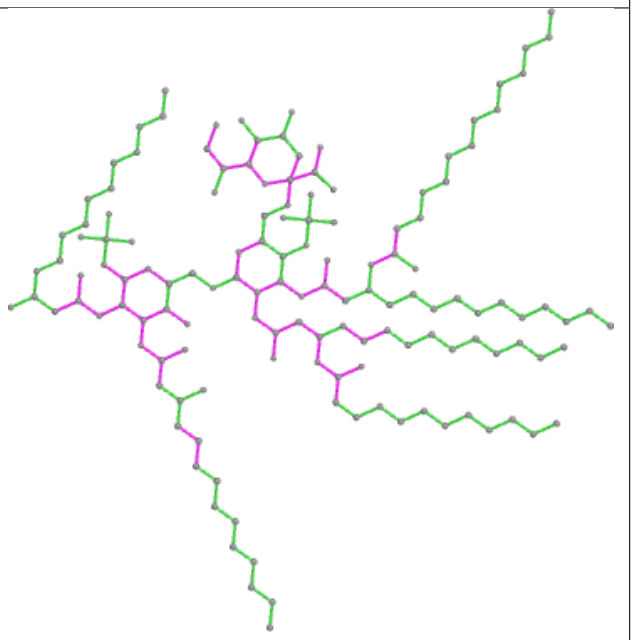
Ligand LPP H 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPP G 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

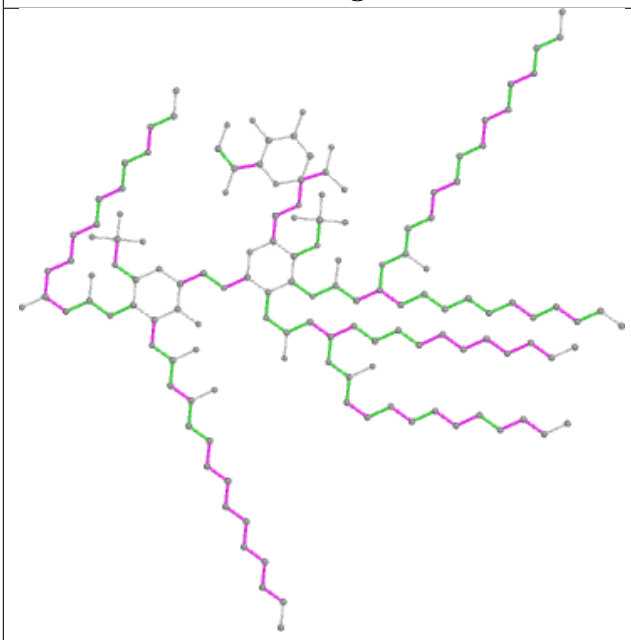
Ligand L8Z E 1002



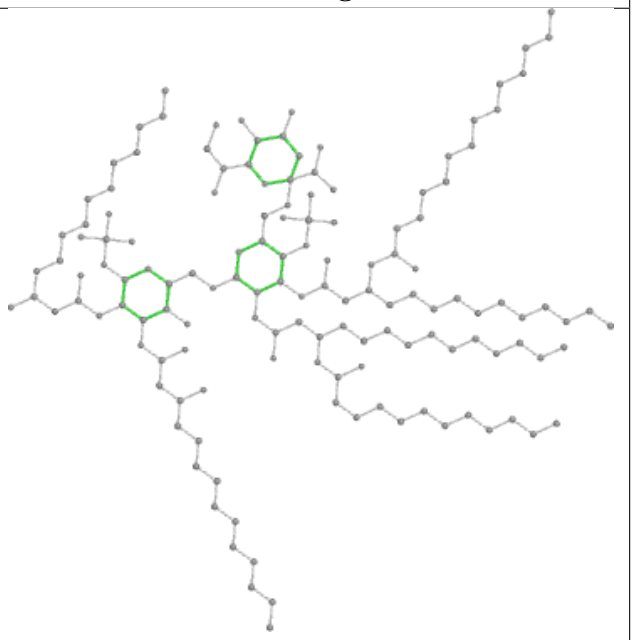
Bond lengths



Bond angles

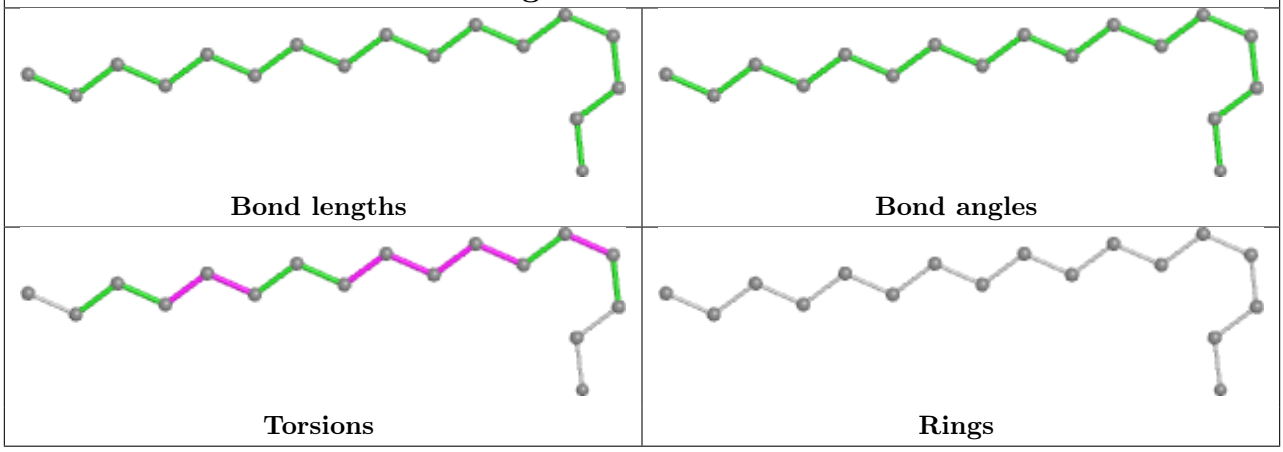


Torsions

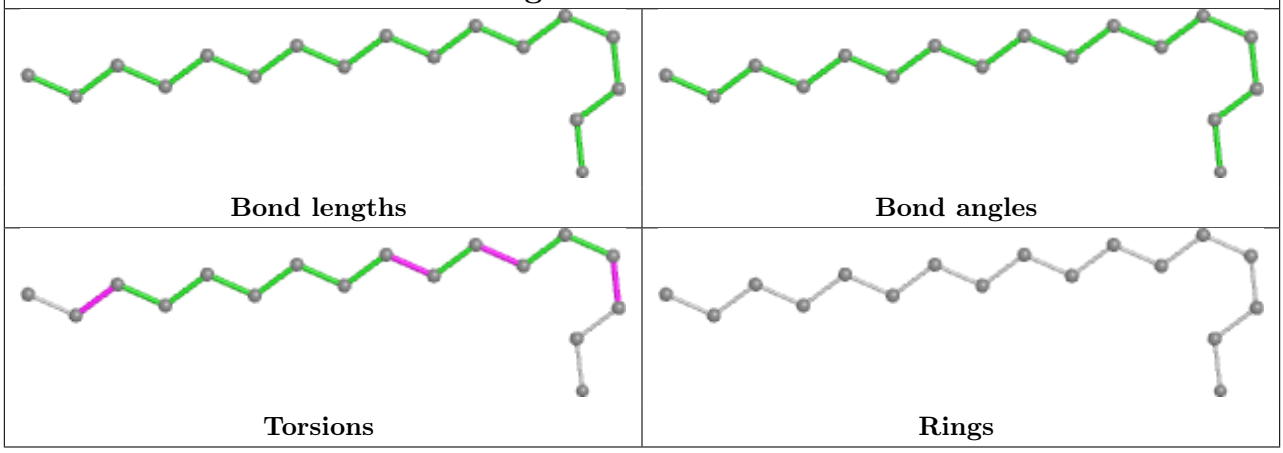


Rings

Ligand PLM A 201



Ligand PLM L 201



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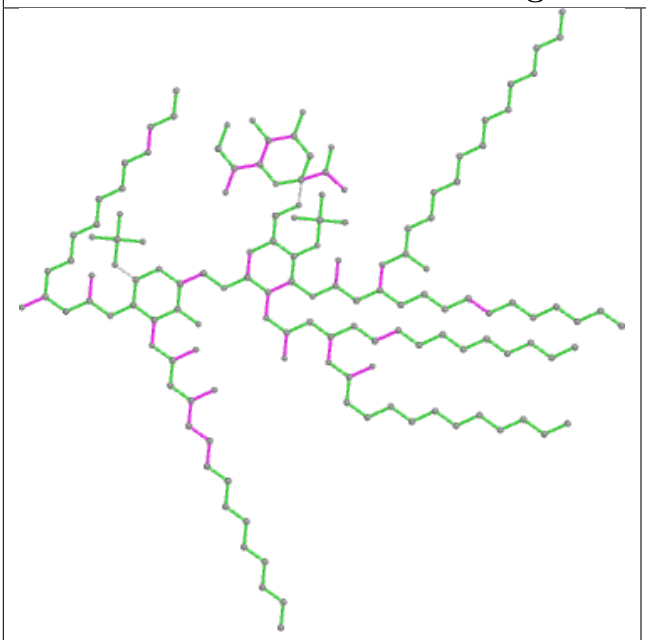
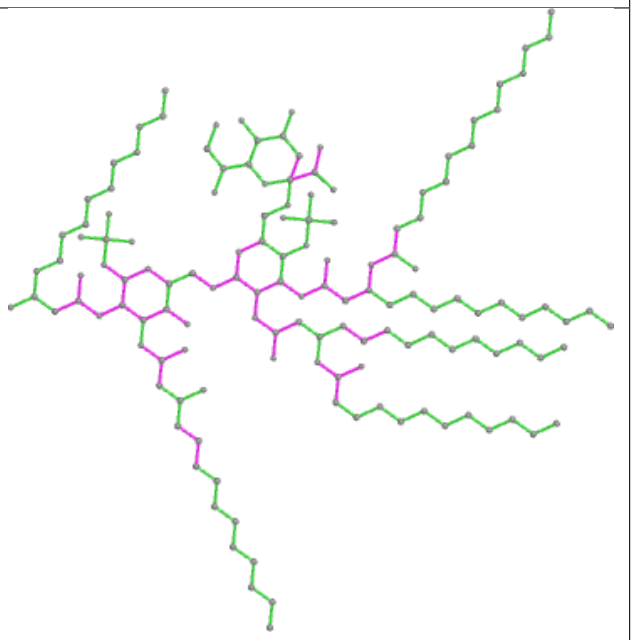
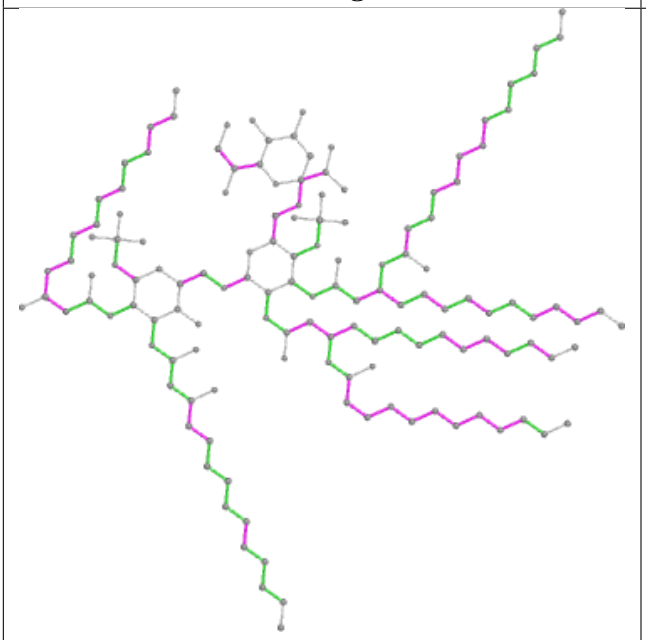


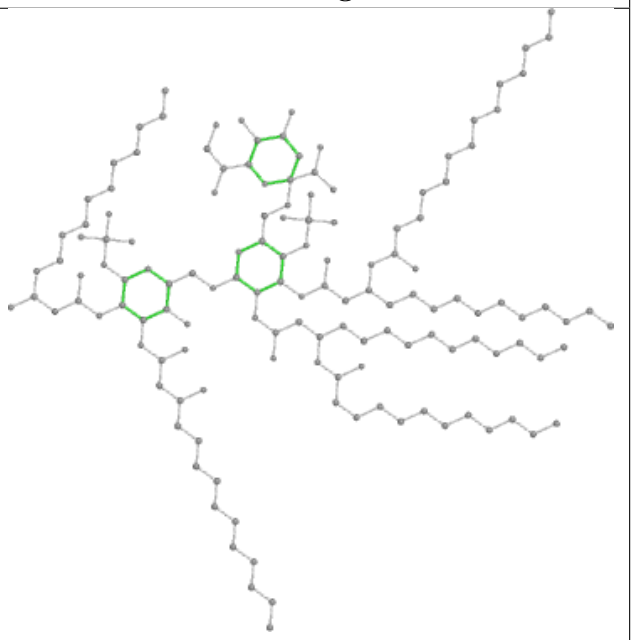
Bond lengths



Bond angles

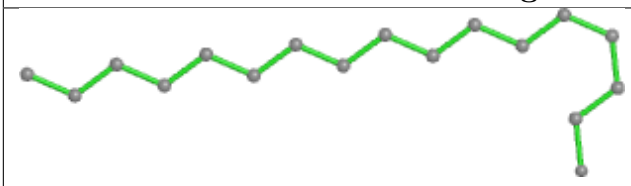


Torsions

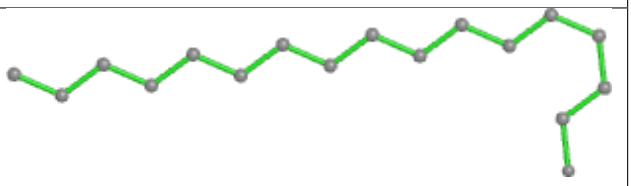


Rings

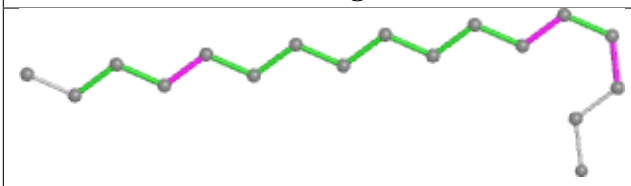
Ligand PLM K 201



Bond lengths



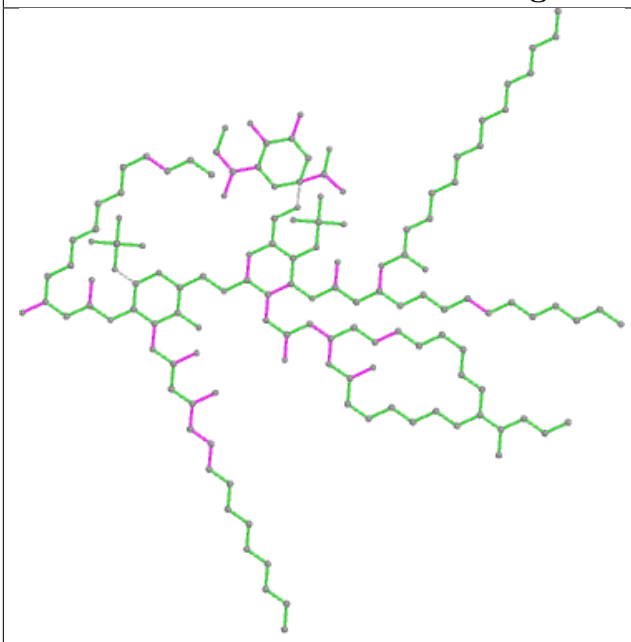
Bond angles



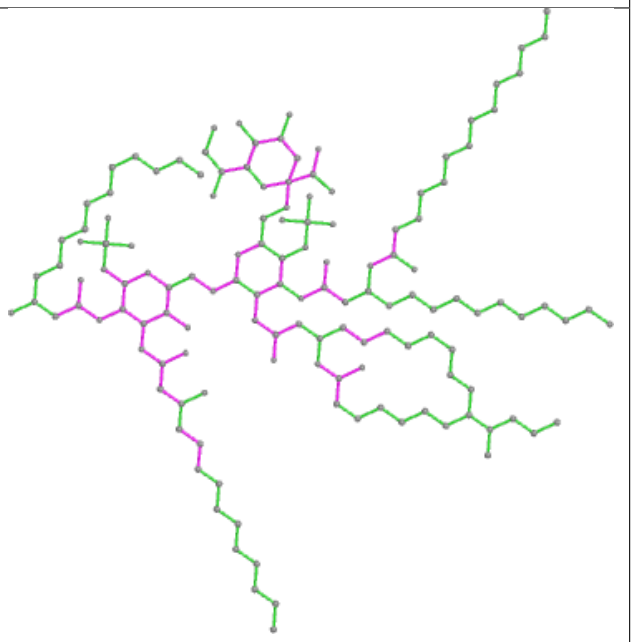
Torsions

Rings

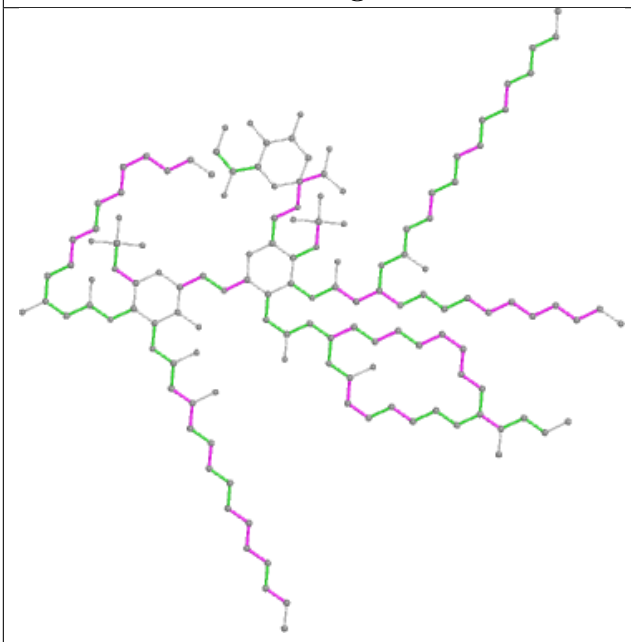
Ligand L8Z K 202



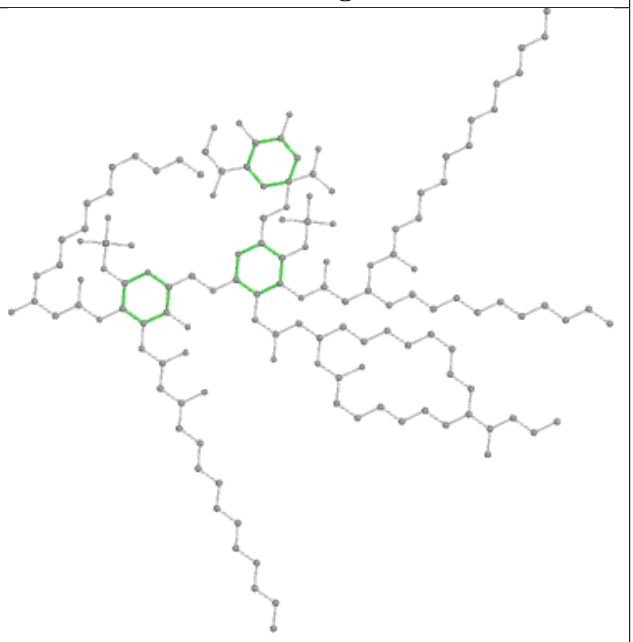
Bond lengths



Bond angles

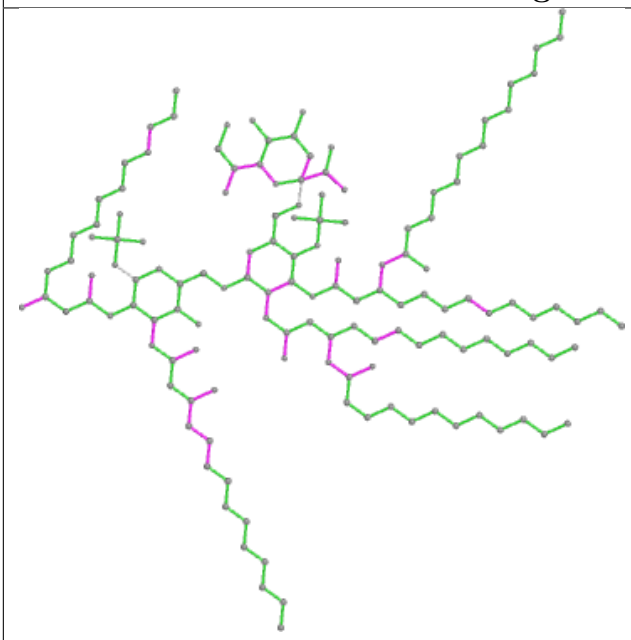


Torsions



Rings

Ligand L8Z L 202



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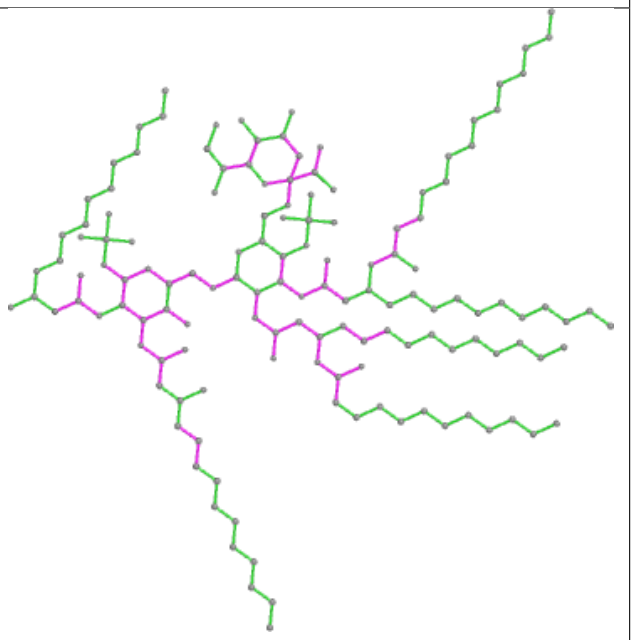
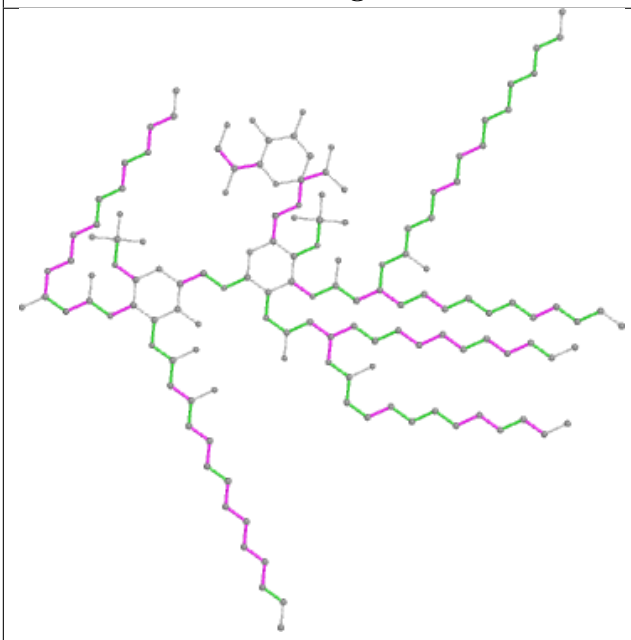


Bond angles



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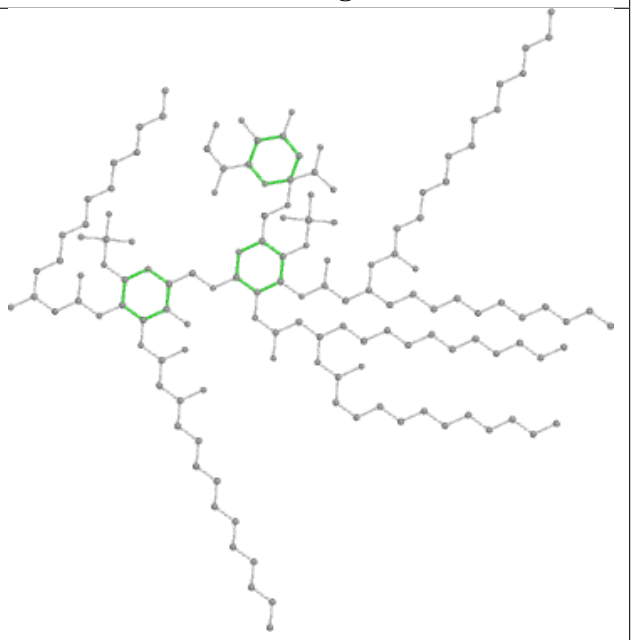
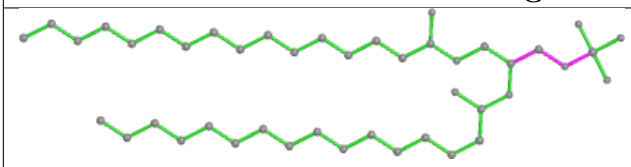


Rings

Ligand LPP K 203



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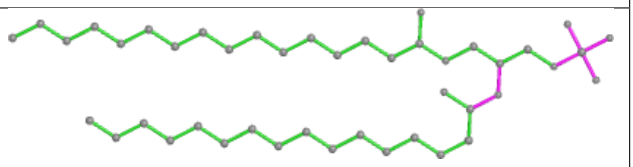

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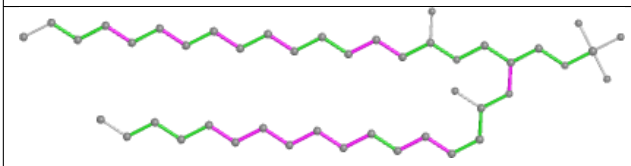

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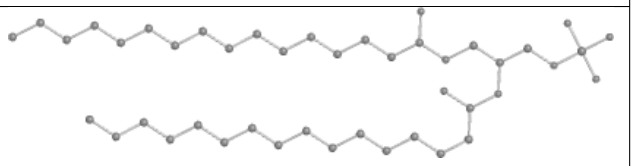
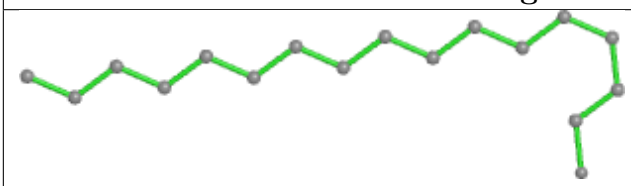


Rings

Ligand PLM G 201



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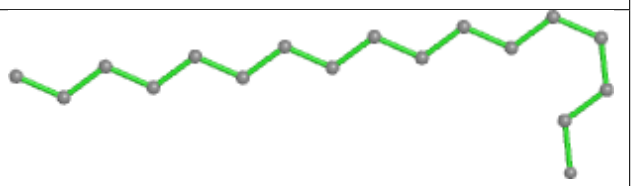
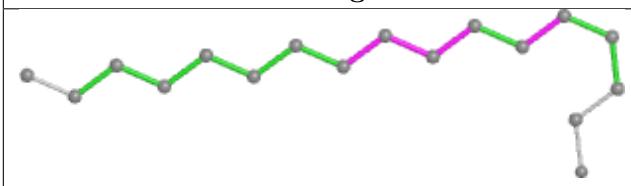


Bond angles



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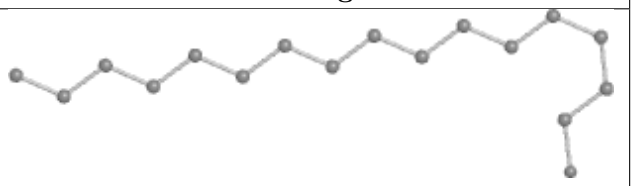
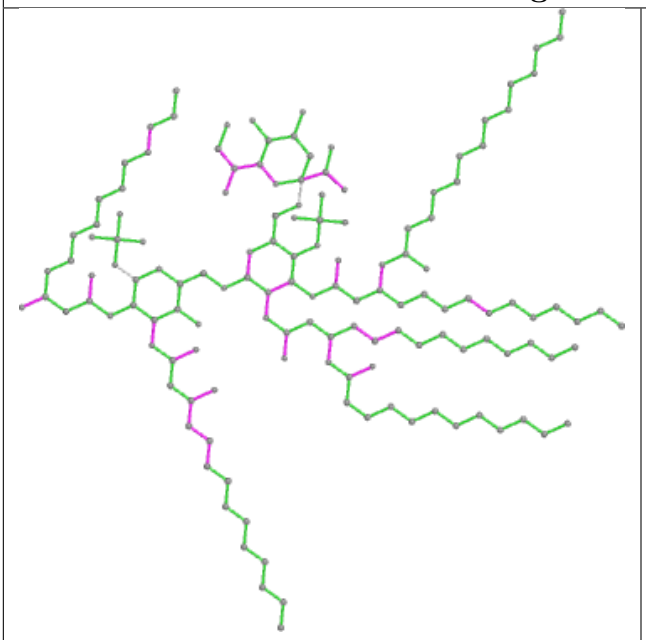


Rings

Ligand L8Z A 202



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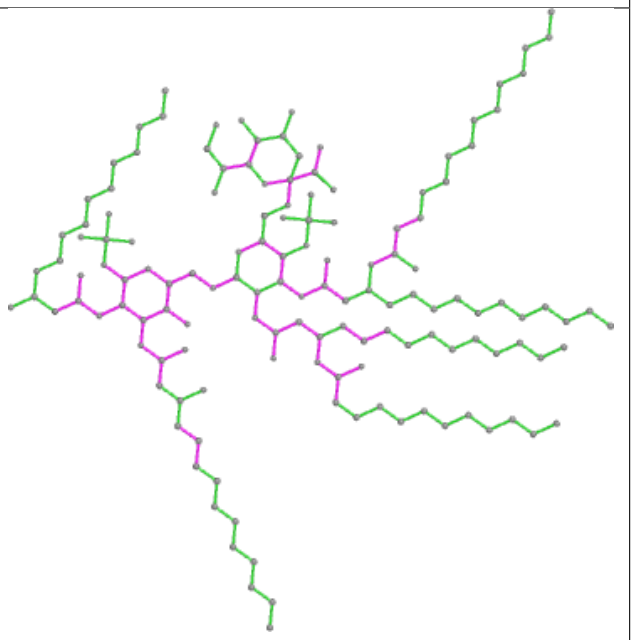

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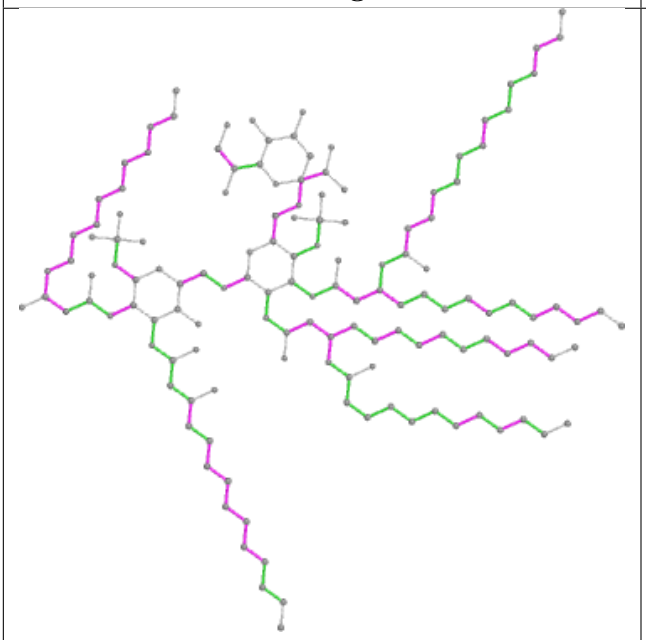

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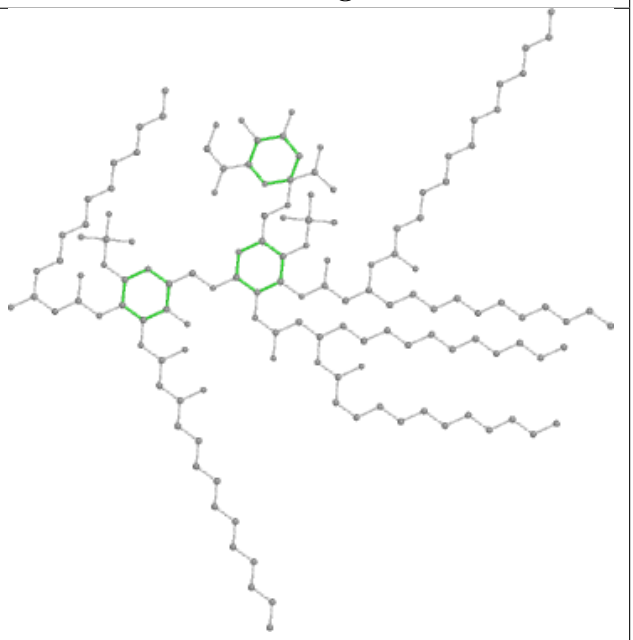
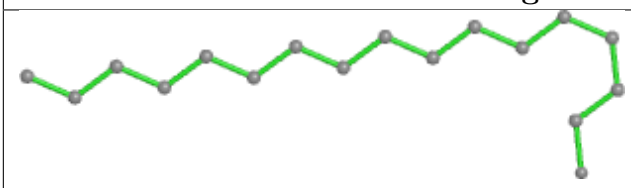


Rings

Ligand PLM B 201



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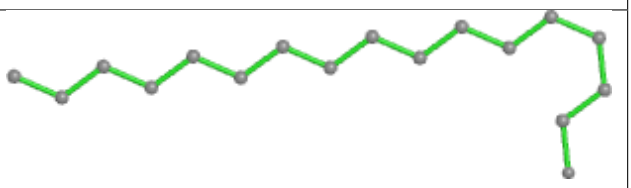
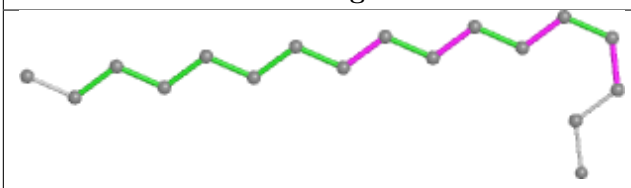


Bond angles



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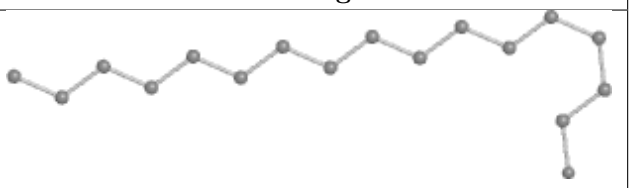
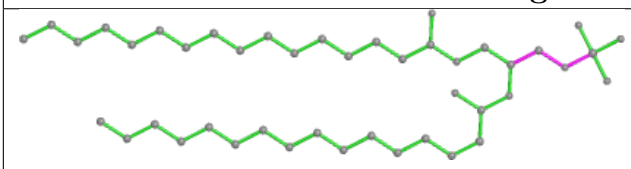


Rings

Ligand LPP J 204



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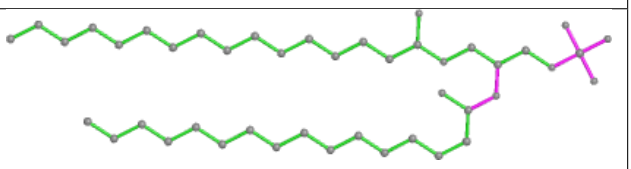
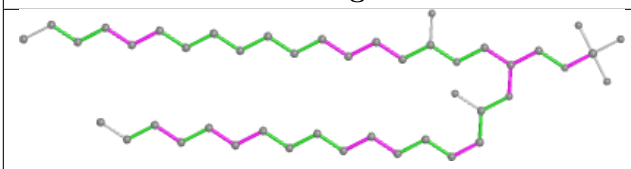


Bond angles



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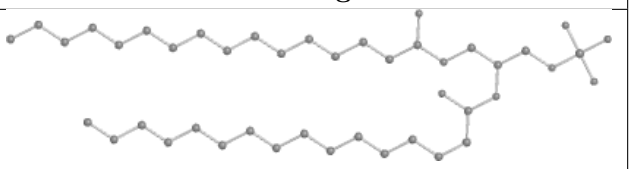
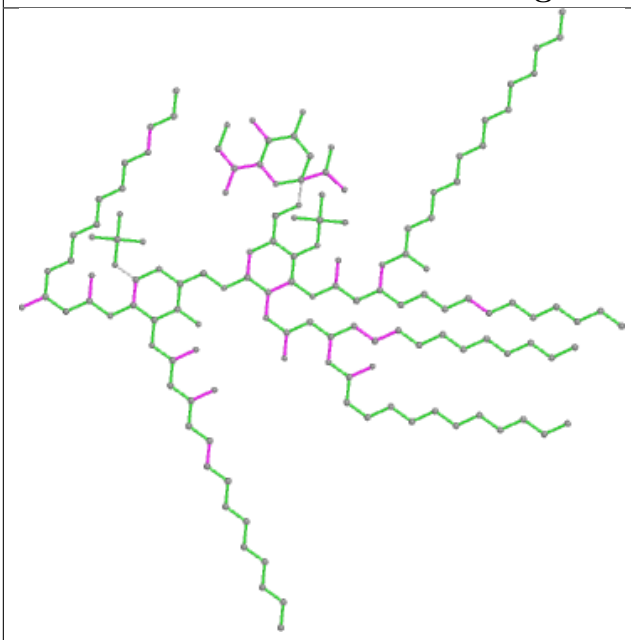


Rings

Ligand L8Z J 203



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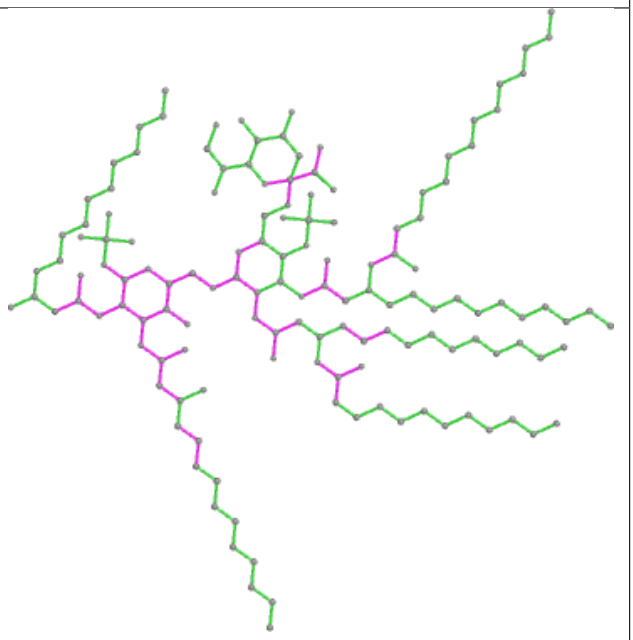

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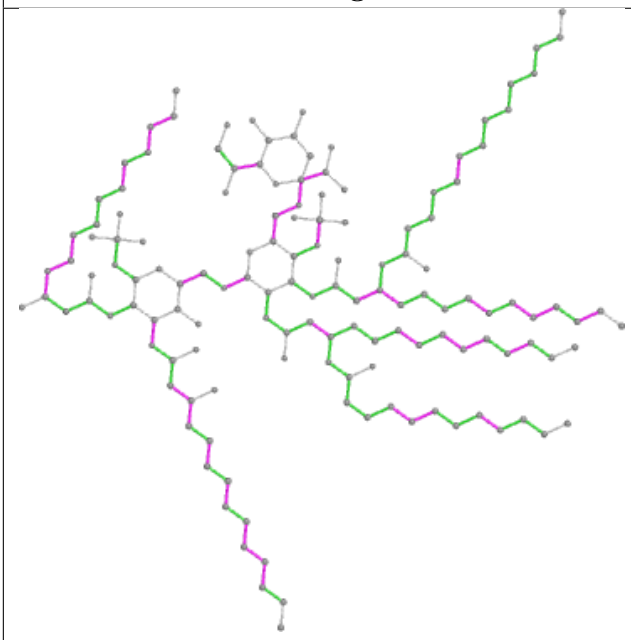

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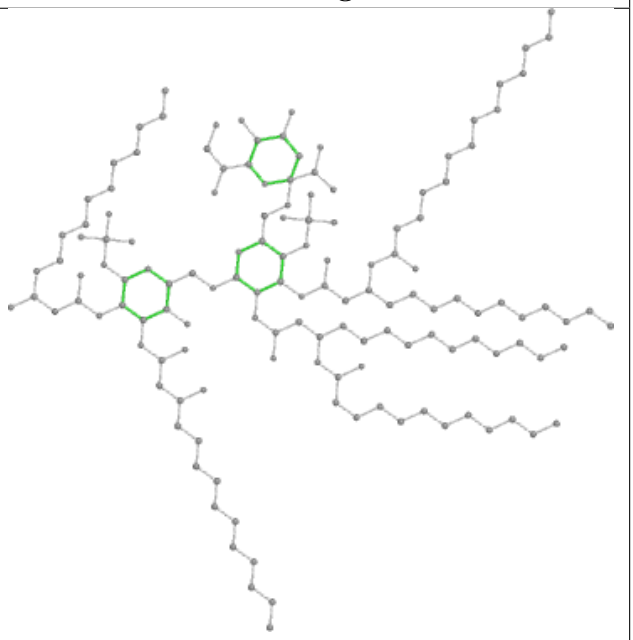
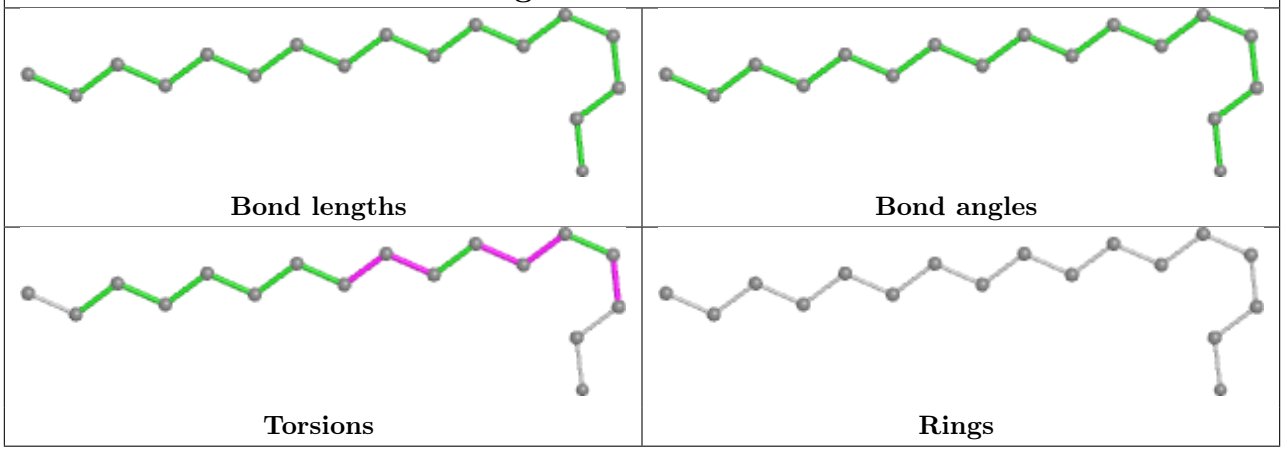
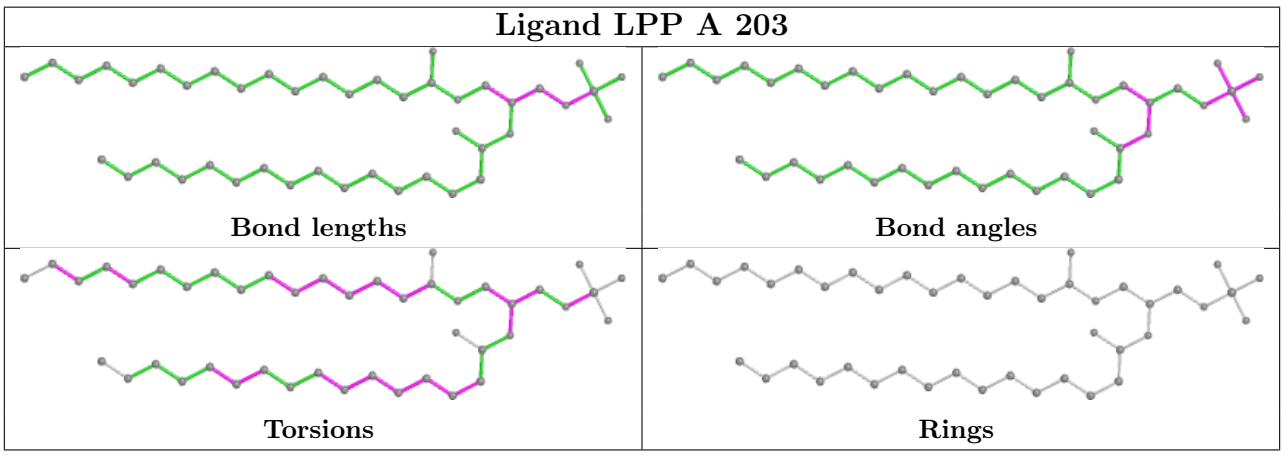


Rings

Ligand PLM E 1001



Ligand LPP A 203



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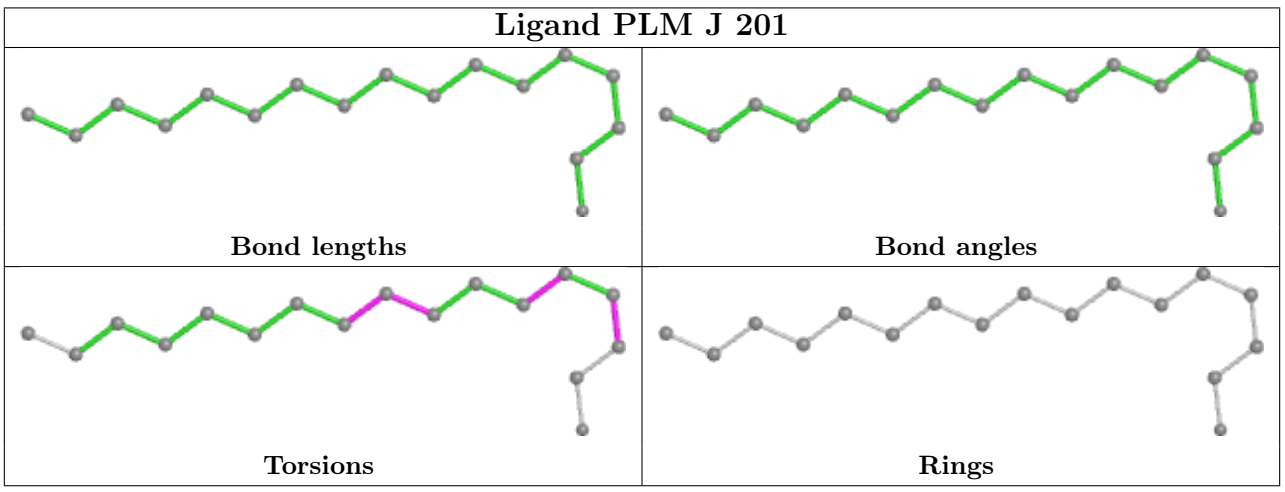

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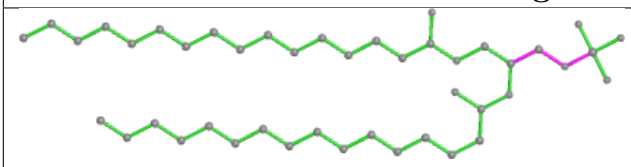
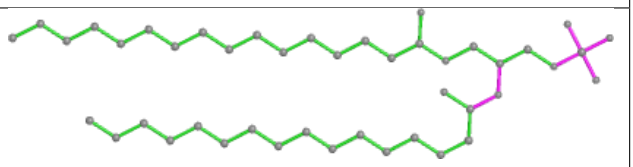
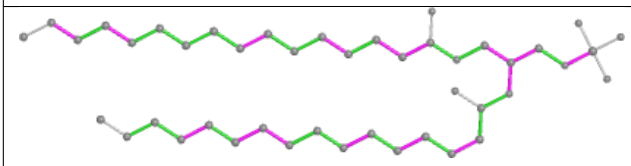


Bond lengths



Bond angles



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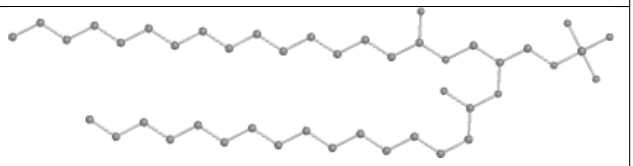
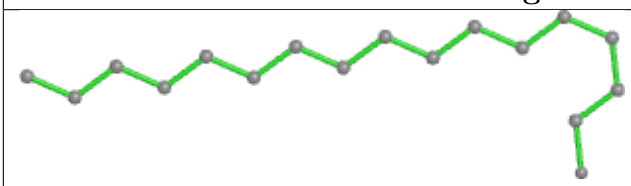


Rings

Ligand PLM F 201



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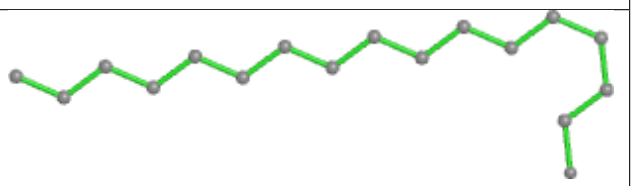
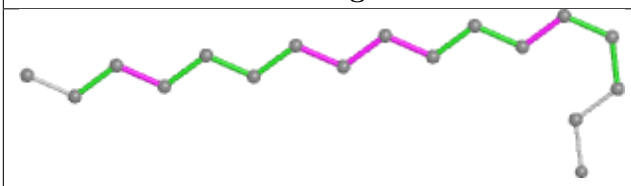


Bond angles



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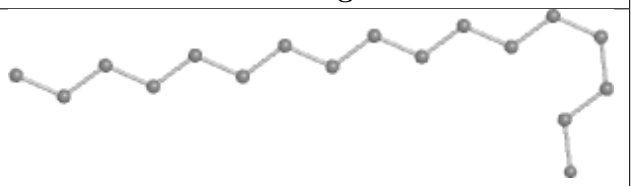
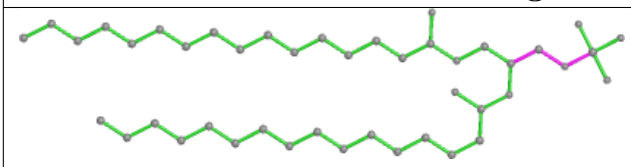


Rings

Ligand LPP C 204



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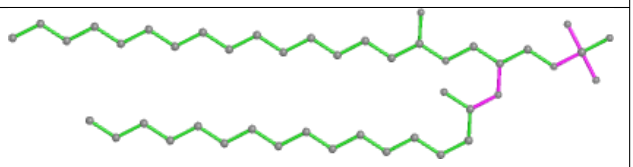
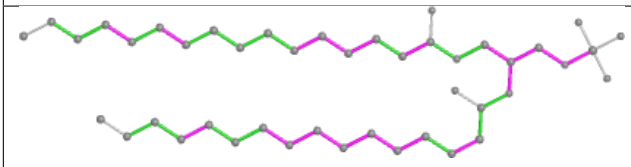


Bond angles



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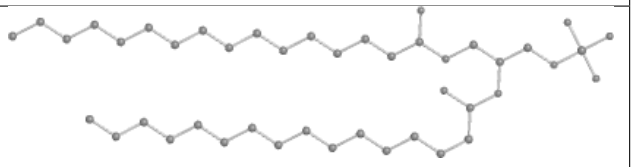
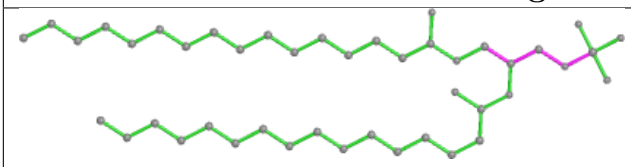
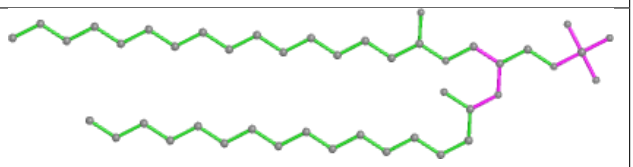
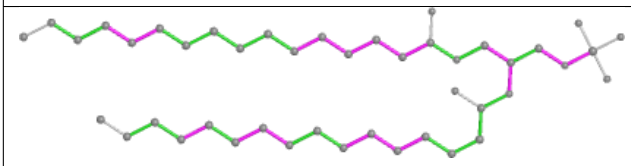
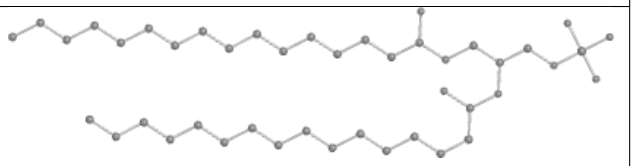
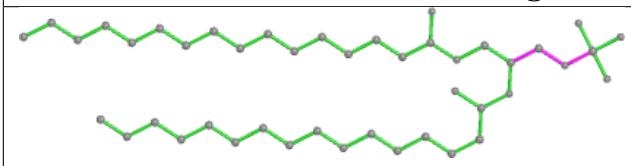
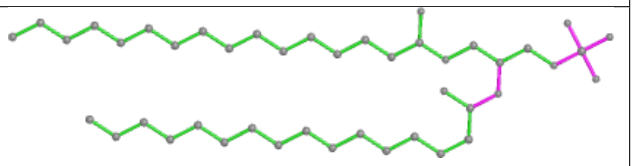
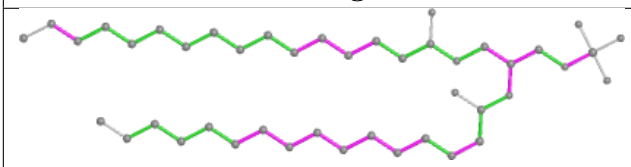
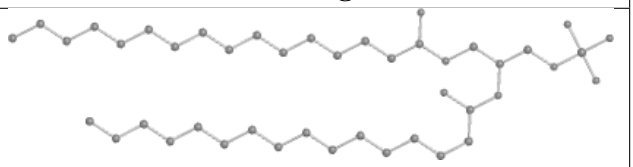
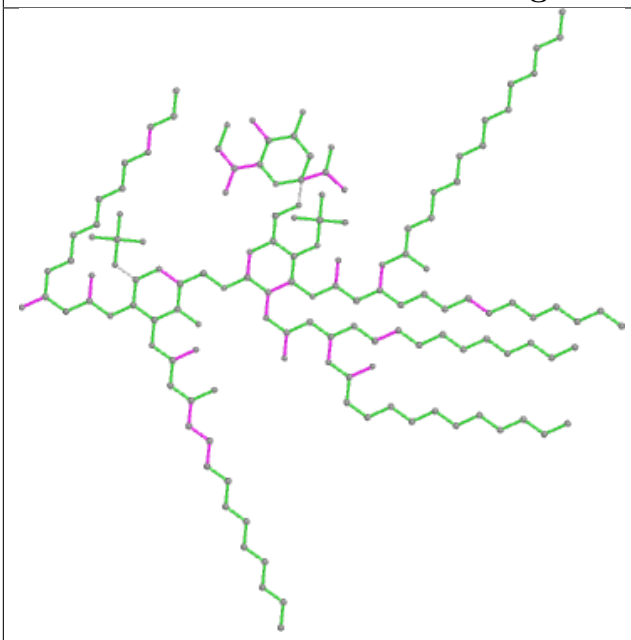


Rings

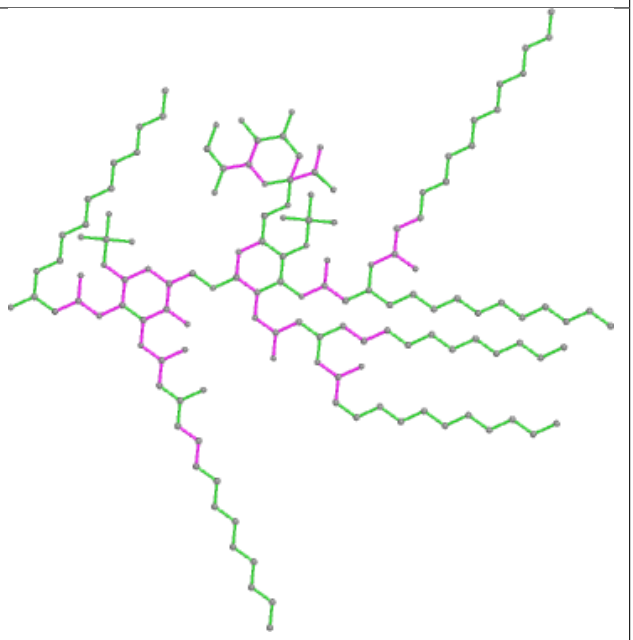
Ligand LPP L 203	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LPP D 204	
 Bond lengths	 Bond angles
 Torsions	 Rings

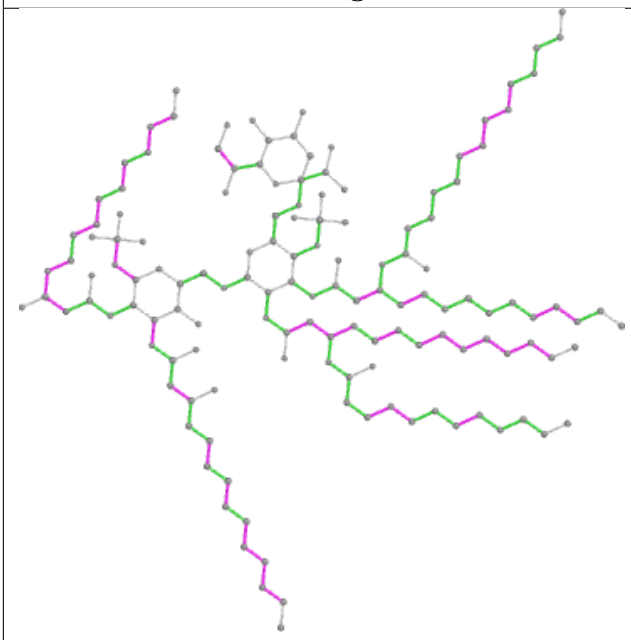
Ligand L8Z D 203



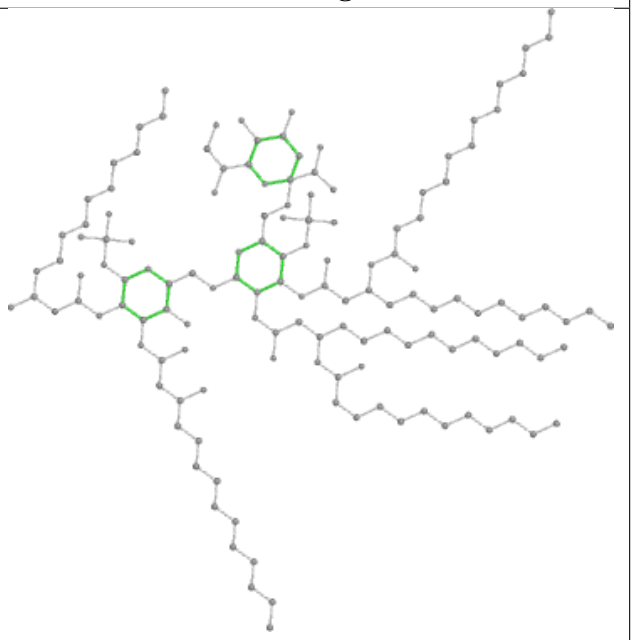
Bond lengths



Bond angles

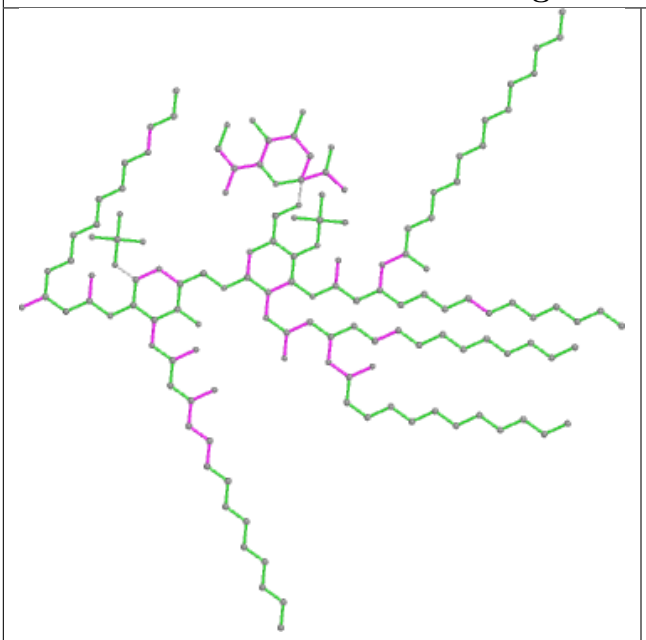


Torsions

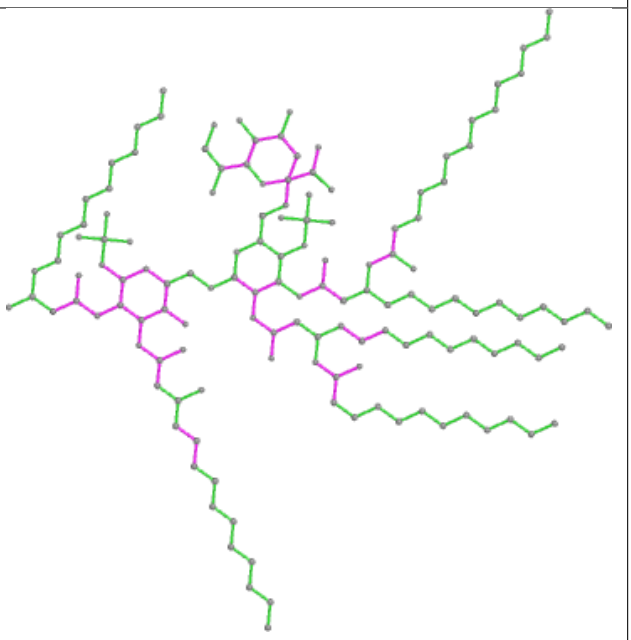


Rings

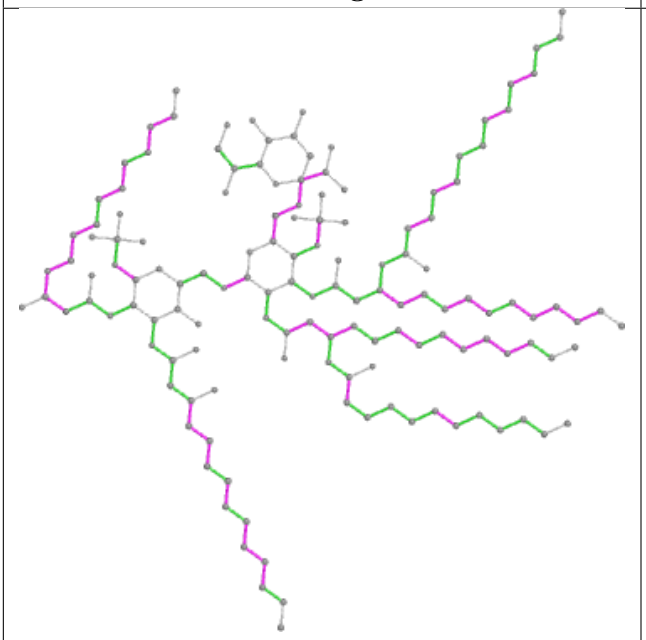
Ligand L8Z F 202



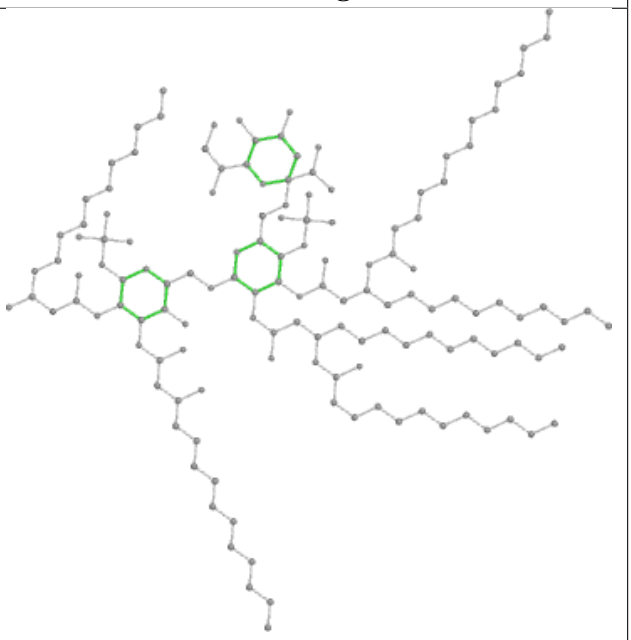
Bond lengths



Bond angles

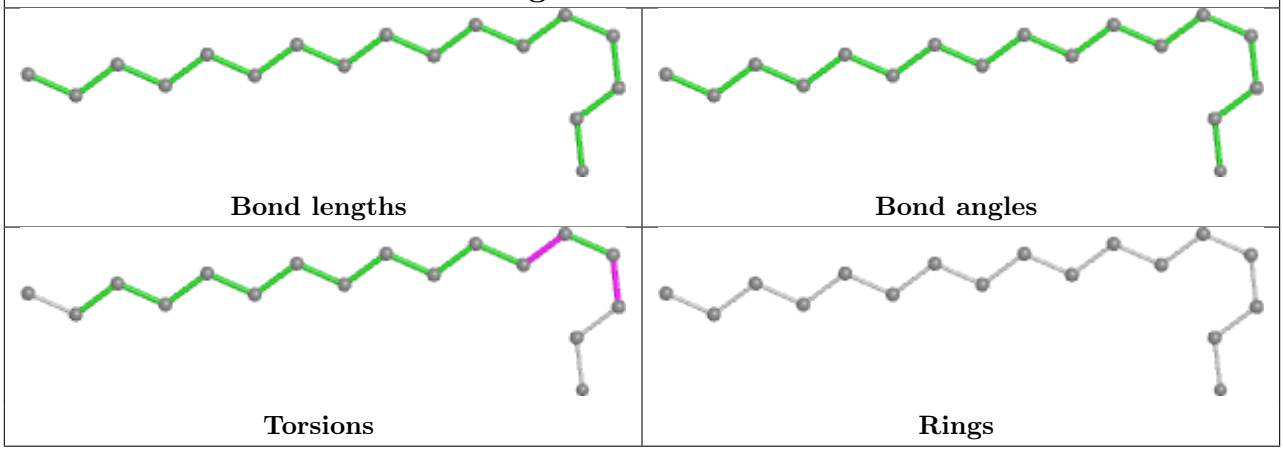


Torsions

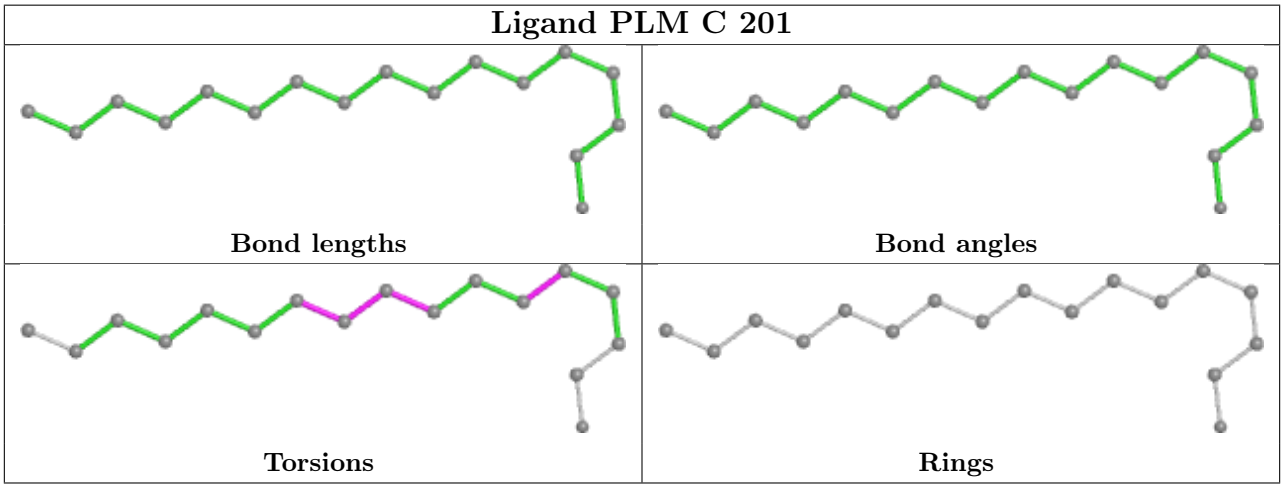


Rings

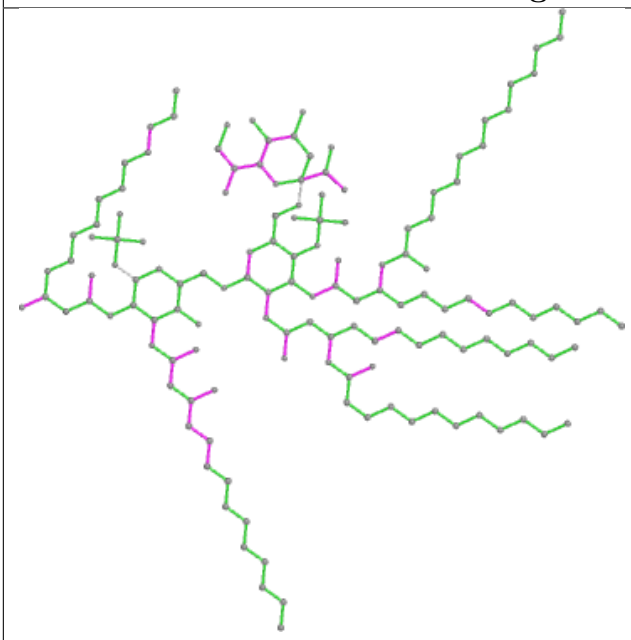
Ligand PLM I 201



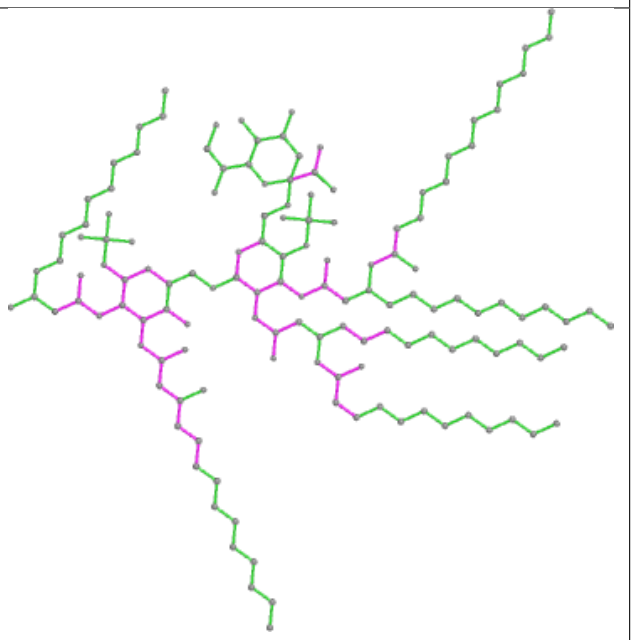
Ligand PLM C 201



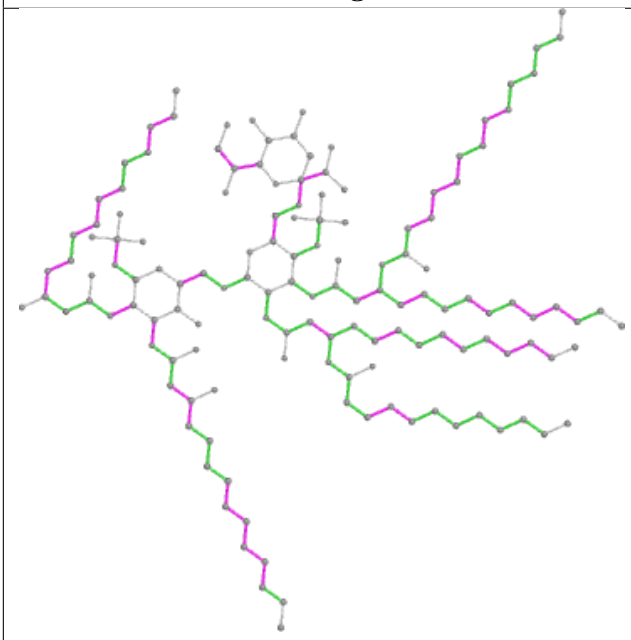
Ligand L8Z H 203



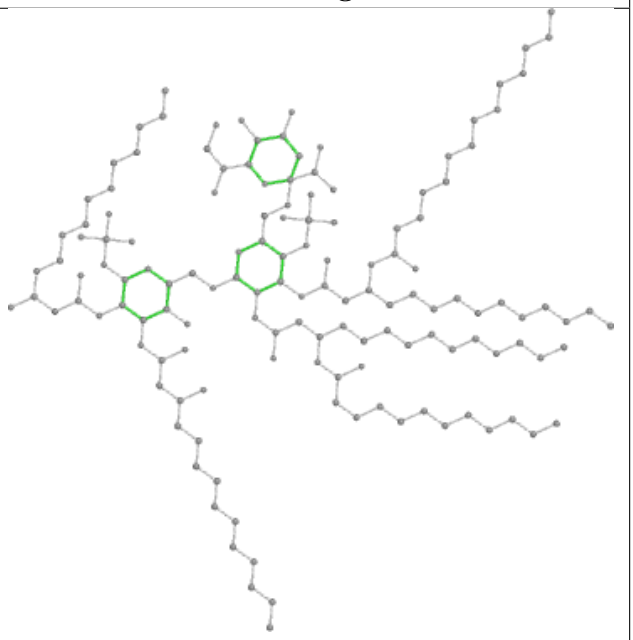
Bond lengths



Bond angles

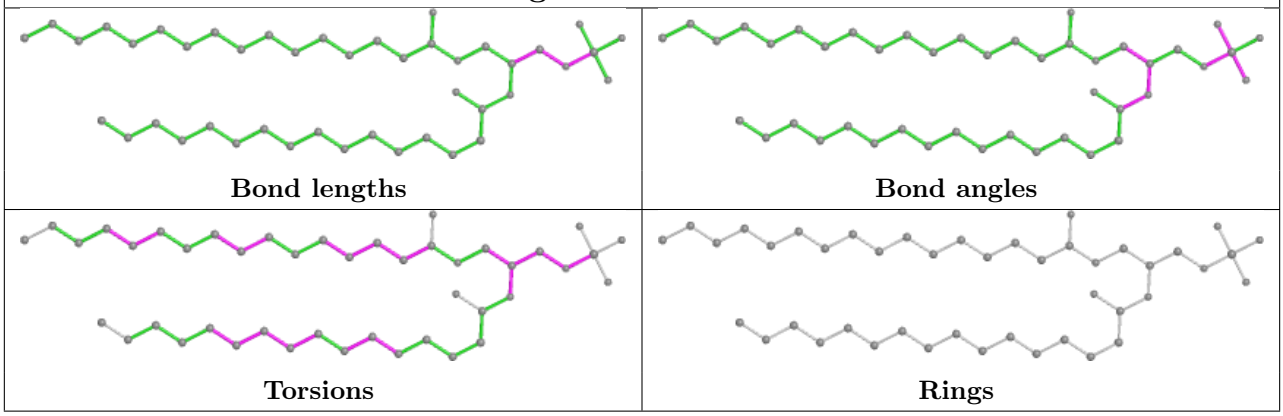


Torsions

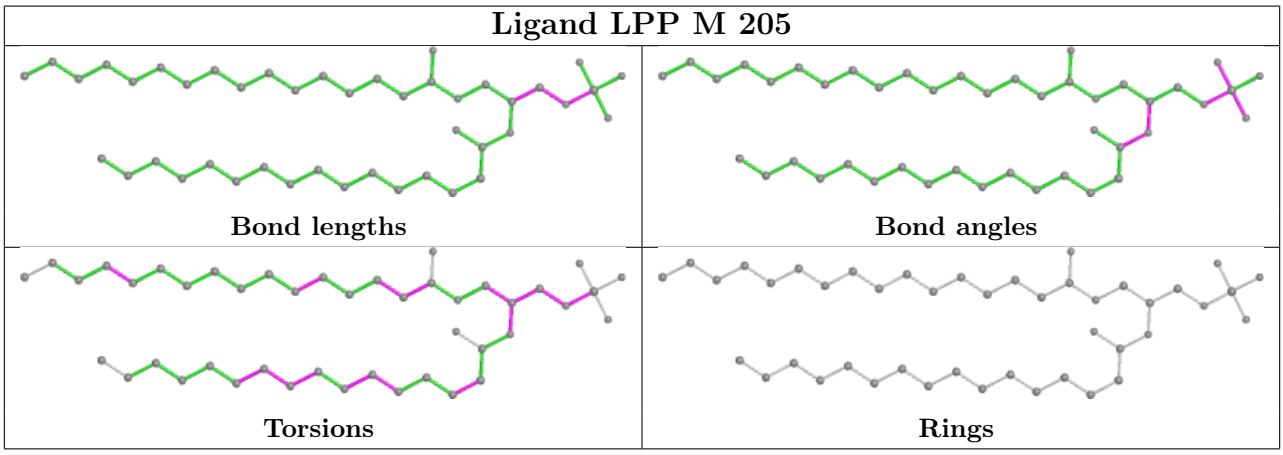


Rings

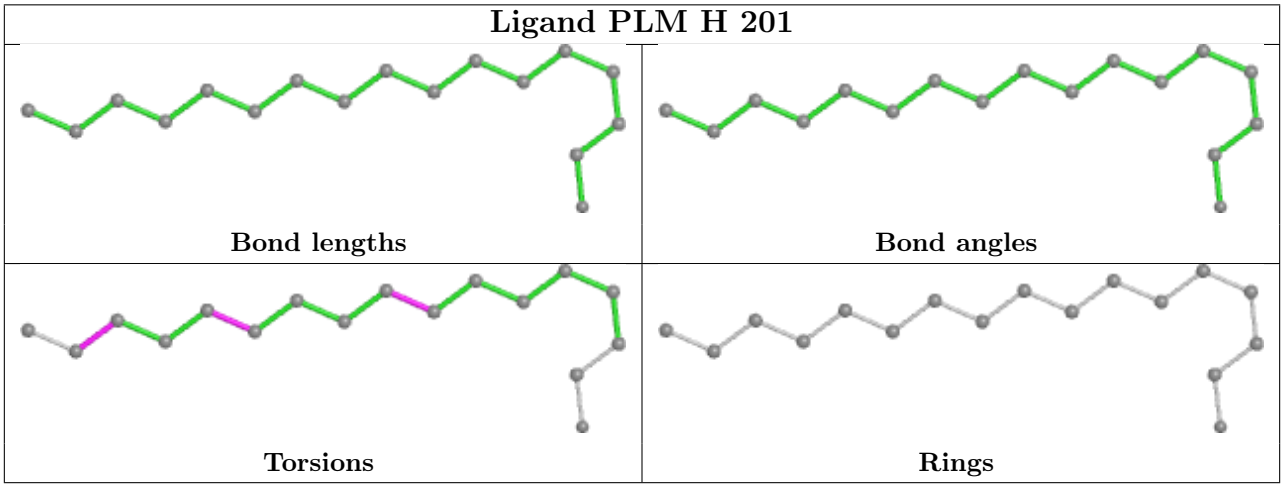
Ligand LPP F 203



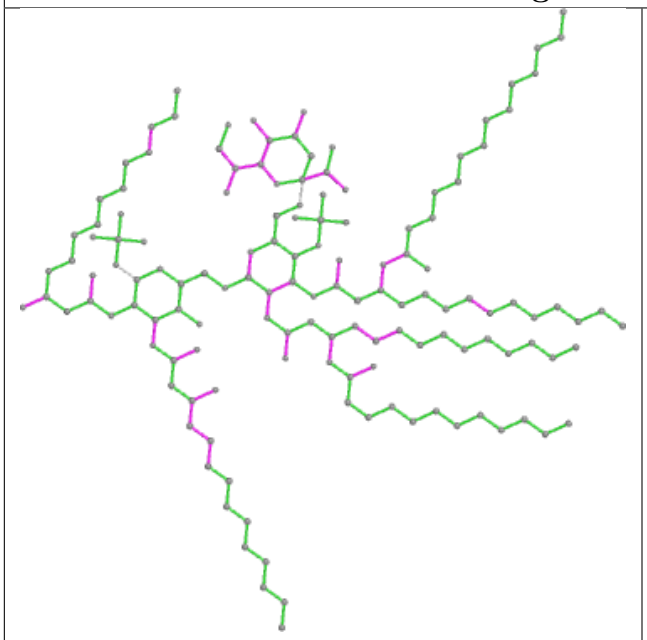
Ligand LPP M 205



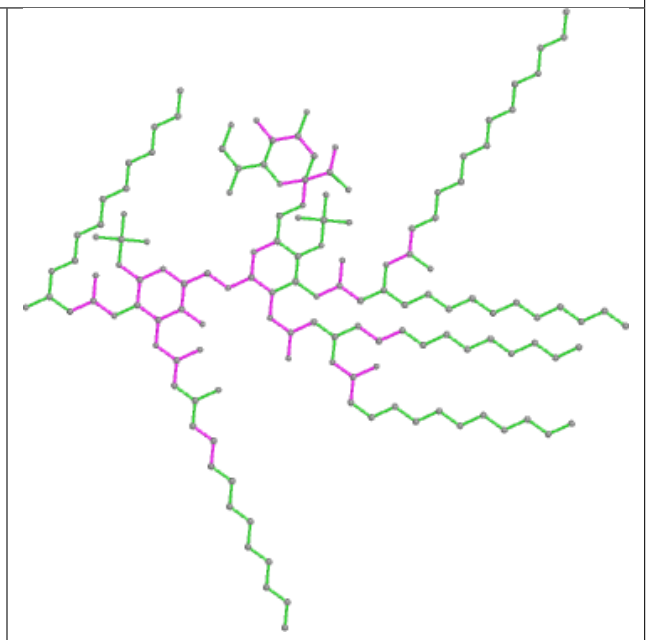
Ligand PLM H 201



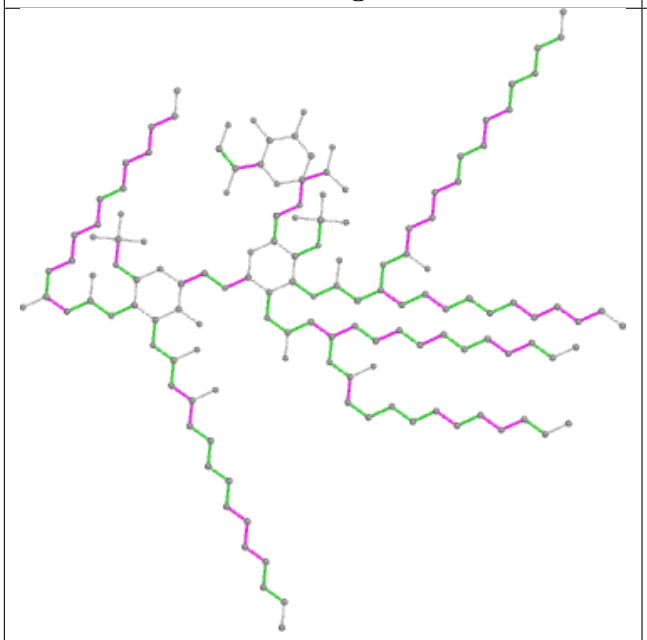
Ligand L8Z B 202



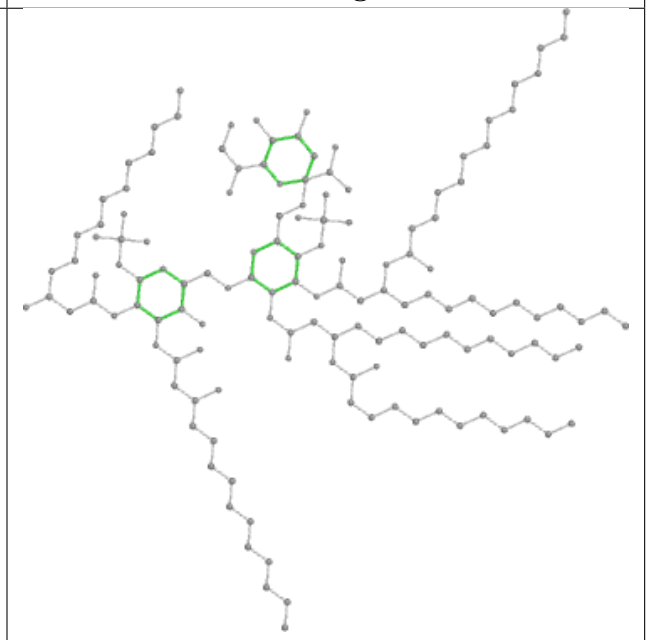
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.