



Full wwPDB EM Validation Report ⓘ

May 3, 2026 – 12:53 AM JST

PDB ID : 9VL3 / pdb_00009vl3
EMDB ID : EMD-65153
Title : Cryo-EM structure of human lipid phosphate phosphatase 1 complexed with PO4 in nanodiscs
Authors : Yang, M.; Qian, H.W.
Deposited on : 2025-06-24
Resolution : 2.82 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

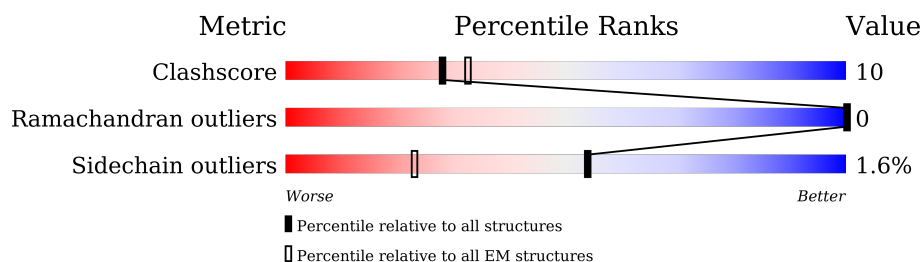
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	284	 67% 21% 11%
1	B	284	 69% 20% 11%
1	C	284	 69% 19% 11%
1	D	284	 69% 20% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8692 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.

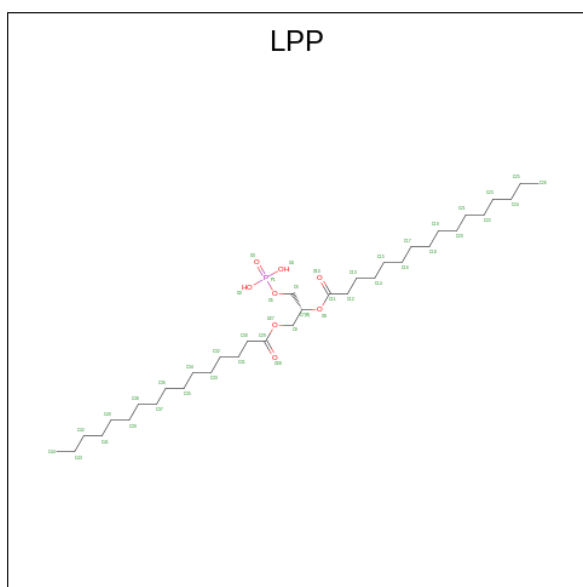
- Molecule 1 is a protein called Phospholipid phosphatase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	B	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	C	252	Total 2003	C 1312	N 329	O 352	S 10	0	0
1	D	252	Total 2003	C 1312	N 329	O 352	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

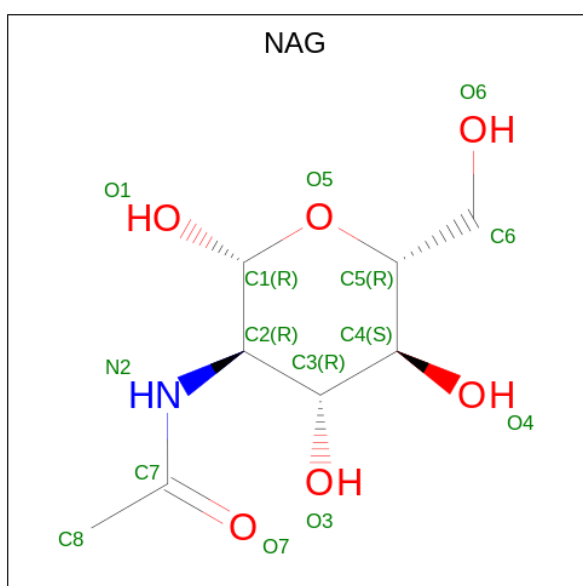
Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	HIS	engineered mutation	UNP O14494
B	223	ALA	HIS	engineered mutation	UNP O14494
C	223	ALA	HIS	engineered mutation	UNP O14494
D	223	ALA	HIS	engineered mutation	UNP O14494

- Molecule 2 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: C₃₅H₆₉O₈P) (labeled as "Ligand of Interest" by depositor).



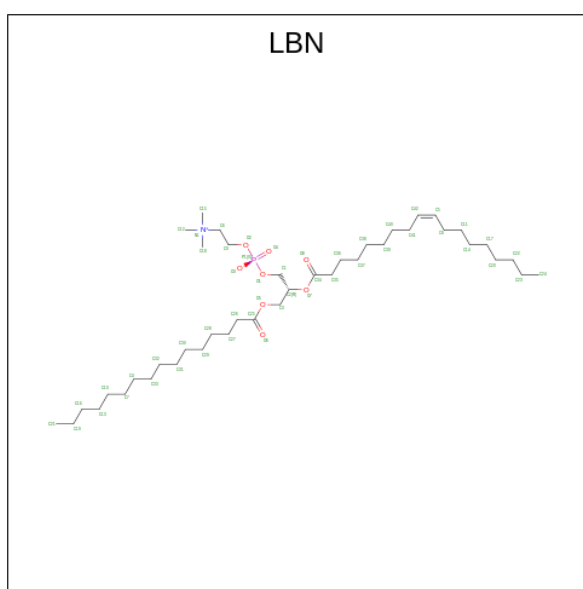
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			44	35	8	1	
2	B	1	Total	C	O	P	0
			44	35	8	1	
2	C	1	Total	C	O	P	0
			44	35	8	1	
2	D	1	Total	C	O	P	0
			44	35	8	1	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



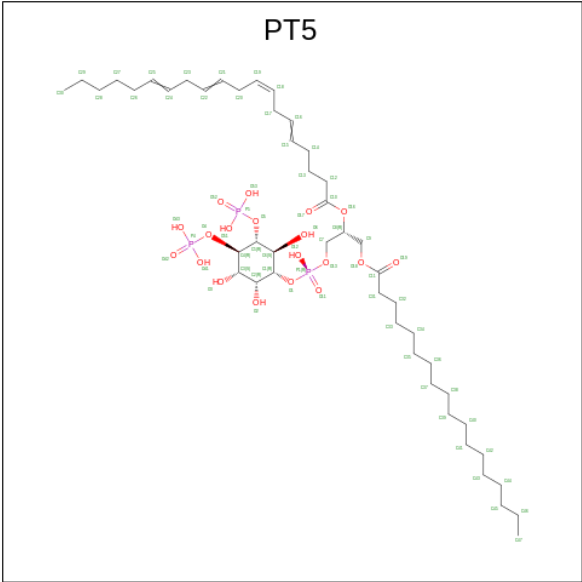
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (CCD ID: LBN) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



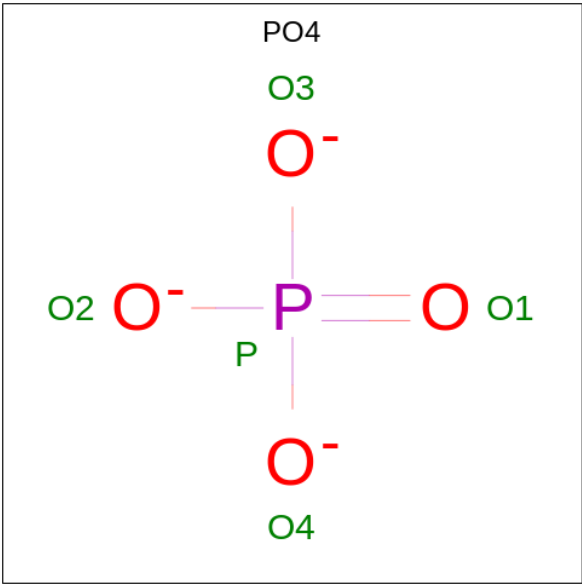
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			45	36	8	1	
4	B	1	Total	C	O	P	0
			45	36	8	1	
4	C	1	Total	C	O	P	0
			45	36	8	1	
4	D	1	Total	C	O	P	0
			45	36	8	1	

- Molecule 5 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (CCD ID: PT5) (formula: $C_{47}H_{85}O_{19}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			62	40	19	3	
5	B	1	Total	C	O	P	0
			62	40	19	3	
5	C	1	Total	C	O	P	0
			62	40	19	3	
5	D	1	Total	C	O	P	0
			62	40	19	3	

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

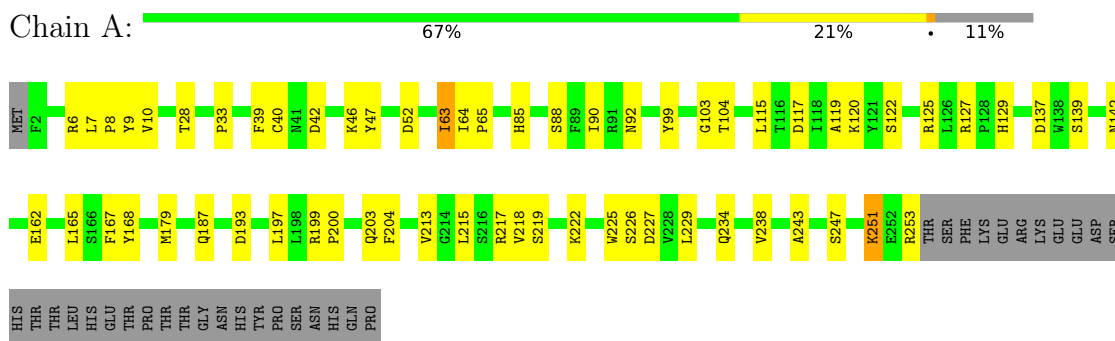


Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	O	P	0
			5	4	1	
6	B	1	Total	O	P	0
			5	4	1	
6	C	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

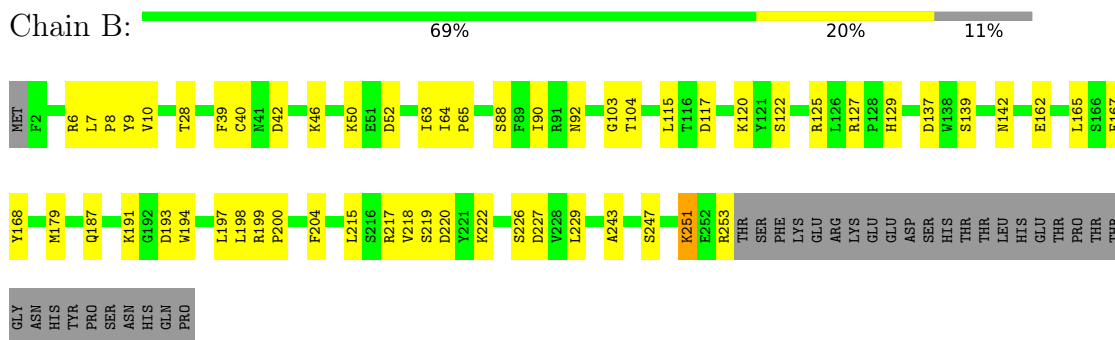
3 Residue-property plots [i](#)

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.

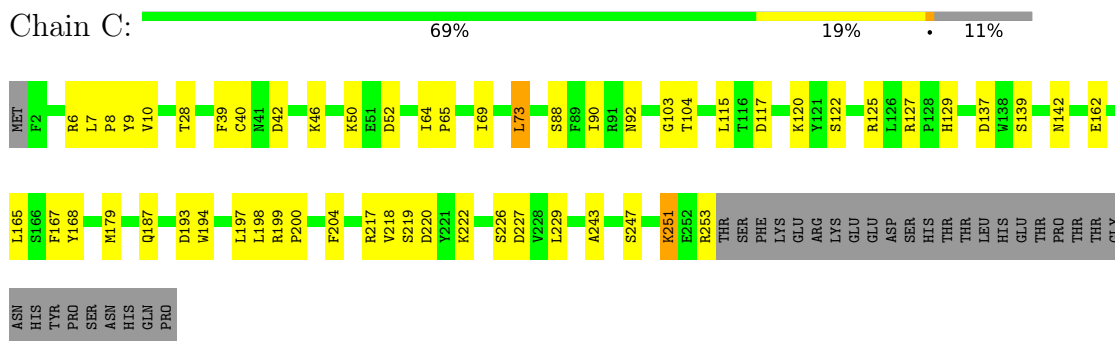
- Molecule 1: Phospholipid phosphatase 1



- Molecule 1: Phospholipid phosphatase 1

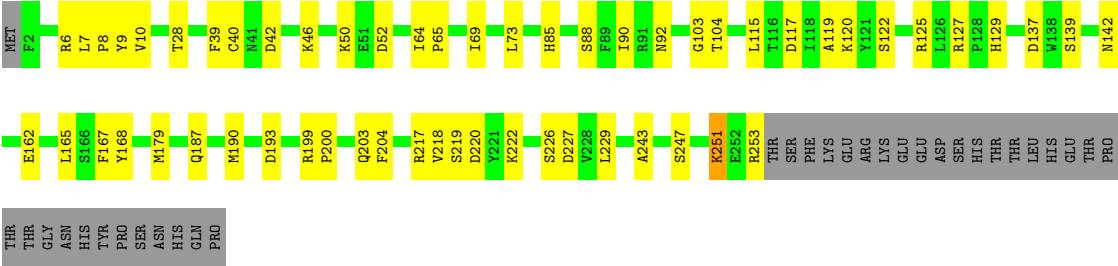


- Molecule 1: Phospholipid phosphatase 1



- Molecule 1: Phospholipid phosphatase 1

Chain D: 69% 20% 11%



THR
THR
GLY
ASN
HIS
TYR
PRO
SER
ASN
HIS
GLN
PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LPP, NAG, PO4, LBN, PT5

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	0.15	0/2054	0.36	0/2789
1	B	0.12	0/2054	0.33	0/2789
1	C	0.12	0/2054	0.33	0/2789
1	D	0.12	0/2054	0.33	0/2789
All	All	0.13	0/8216	0.34	0/11156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2003	0	2015	49	0
1	B	2003	0	2015	43	0
1	C	2003	0	2015	41	0
1	D	2003	0	2015	44	0
2	A	44	0	67	6	0
2	B	44	0	67	5	0
2	C	44	0	67	5	0
2	D	44	0	67	8	0
3	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	14	0	13	0	0
3	D	14	0	13	0	0
4	A	45	0	0	0	0
4	B	45	0	0	0	0
4	C	45	0	0	0	0
4	D	45	0	0	0	0
5	A	62	0	65	3	0
5	B	62	0	65	4	0
5	C	62	0	65	2	0
5	D	62	0	65	2	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
All	All	8692	0	8640	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:NZ	1:B:168:TYR:O	2.16	0.78
1:C:104:THR:HG21	1:C:247:SER:HB3	1.65	0.78
1:A:120:LYS:NZ	1:A:168:TYR:O	2.17	0.78
1:D:104:THR:HG21	1:D:247:SER:HB3	1.65	0.78
1:C:120:LYS:NZ	1:C:168:TYR:O	2.16	0.78
1:D:120:LYS:NZ	1:D:168:TYR:O	2.16	0.77
1:B:104:THR:HG21	1:B:247:SER:HB3	1.65	0.76
1:A:104:THR:HG21	1:A:247:SER:HB3	1.67	0.75
1:A:193:ASP:OD2	1:D:6:ARG:NH2	2.20	0.71
1:A:125:ARG:NH1	1:A:227:ASP:OD1	2.26	0.68
1:A:218:VAL:HG11	2:D:301:LPP:H302	1.74	0.68
1:B:6:ARG:NH2	1:C:193:ASP:OD1	2.22	0.68
1:B:125:ARG:NH1	1:B:227:ASP:OD1	2.29	0.66
1:D:125:ARG:NH1	1:D:227:ASP:OD1	2.29	0.66
1:C:125:ARG:NH1	1:C:227:ASP:OD1	2.29	0.65
1:C:6:ARG:NH2	1:D:193:ASP:OD1	2.21	0.65
1:C:127:ARG:NH1	1:C:162:GLU:O	2.29	0.64
1:A:127:ARG:NH1	1:A:162:GLU:O	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:NH1	1:B:162:GLU:O	2.29	0.63
1:A:6:ARG:NH2	1:B:193:ASP:OD1	2.22	0.63
1:A:229:LEU:HD22	2:D:301:LPP:H192	1.81	0.61
1:A:40:CYS:O	1:A:46:LYS:NZ	2.34	0.61
1:D:127:ARG:NH1	1:D:162:GLU:O	2.29	0.61
2:C:301:LPP:H192	1:D:229:LEU:HD22	1.83	0.60
2:A:301:LPP:H192	1:B:229:LEU:HD22	1.82	0.60
2:B:301:LPP:H192	1:C:229:LEU:HD22	1.83	0.60
1:A:187:GLN:HA	1:A:199:ARG:HD2	1.84	0.59
1:B:40:CYS:O	1:B:46:LYS:NZ	2.35	0.59
1:D:40:CYS:O	1:D:46:LYS:NZ	2.35	0.59
1:D:190:MET:HB2	1:D:199:ARG:HD3	1.85	0.59
1:A:122:SER:O	1:B:219:SER:OG	2.20	0.59
1:C:40:CYS:O	1:C:46:LYS:NZ	2.35	0.58
1:D:187:GLN:HA	1:D:199:ARG:HD2	1.85	0.58
1:D:127:ARG:HD3	1:D:129:HIS:CE1	2.40	0.57
2:B:301:LPP:H261	2:B:301:LPP:H411	1.88	0.56
2:D:301:LPP:H411	2:D:301:LPP:H261	1.88	0.56
1:A:137:ASP:OD1	1:A:139:SER:OG	2.23	0.56
1:C:127:ARG:HD3	1:C:129:HIS:CE1	2.40	0.56
2:C:301:LPP:H411	2:C:301:LPP:H261	1.88	0.56
1:B:127:ARG:HD3	1:B:129:HIS:CE1	2.40	0.56
1:B:137:ASP:OD1	1:B:139:SER:OG	2.23	0.56
1:A:127:ARG:HD3	1:A:129:HIS:CE1	2.41	0.56
2:A:301:LPP:H411	2:A:301:LPP:H261	1.88	0.55
1:B:187:GLN:HA	1:B:199:ARG:HD2	1.88	0.55
1:C:187:GLN:HA	1:C:199:ARG:HD2	1.89	0.55
2:A:301:LPP:H302	1:B:218:VAL:HG11	1.89	0.54
2:B:301:LPP:H302	1:C:218:VAL:HG11	1.88	0.54
1:C:115:LEU:HG	1:D:204:PHE:HE1	1.73	0.54
1:A:204:PHE:HE1	1:D:115:LEU:HG	1.72	0.54
2:C:301:LPP:H302	1:D:218:VAL:HG11	1.88	0.53
1:D:10:VAL:HG11	5:D:304:PT5:H27	1.90	0.53
1:B:115:LEU:HG	1:C:204:PHE:HE1	1.72	0.53
1:C:10:VAL:HG11	5:C:304:PT5:H27	1.90	0.53
1:D:137:ASP:OD1	1:D:139:SER:OG	2.27	0.53
1:C:137:ASP:OD1	1:C:139:SER:OG	2.27	0.53
1:A:115:LEU:HG	1:B:204:PHE:HE1	1.73	0.52
1:B:243:ALA:O	1:B:247:SER:OG	2.28	0.52
1:D:39:PHE:HB2	1:D:42:ASP:HB2	1.92	0.52
1:B:10:VAL:HG11	5:B:304:PT5:H27	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:ALA:O	1:D:247:SER:OG	2.27	0.52
1:A:10:VAL:HG11	5:A:304:PT5:H27	1.91	0.52
1:A:64:ILE:HB	1:A:65:PRO:HD3	1.91	0.52
1:A:28:THR:OG1	1:A:117:ASP:OD2	2.27	0.51
1:B:28:THR:OG1	1:B:117:ASP:OD2	2.25	0.51
1:C:28:THR:OG1	1:C:117:ASP:OD2	2.25	0.51
1:A:39:PHE:HB2	1:A:42:ASP:HB2	1.92	0.51
2:A:301:LPP:H241	1:B:229:LEU:HD11	1.92	0.51
1:C:39:PHE:HB2	1:C:42:ASP:HB2	1.92	0.51
1:C:243:ALA:O	1:C:247:SER:OG	2.28	0.51
1:A:199:ARG:HB3	1:A:200:PRO:HD3	1.92	0.51
1:A:52:ASP:OD1	1:A:217:ARG:NH1	2.43	0.51
1:D:69:ILE:O	1:D:73:LEU:HD23	2.10	0.51
1:B:122:SER:O	1:C:219:SER:OG	2.26	0.51
1:B:64:ILE:HB	1:B:65:PRO:HD3	1.93	0.50
1:B:39:PHE:HB2	1:B:42:ASP:HB2	1.92	0.50
1:C:64:ILE:HB	1:C:65:PRO:HD3	1.93	0.50
1:B:199:ARG:HB3	1:B:200:PRO:HD3	1.93	0.50
1:C:69:ILE:O	1:C:73:LEU:HD23	2.12	0.49
1:D:64:ILE:HB	1:D:65:PRO:HD3	1.93	0.49
1:A:6:ARG:HA	1:A:9:TYR:HD2	1.78	0.49
1:B:179:MET:HA	1:B:179:MET:HE2	1.94	0.49
1:C:199:ARG:HB3	1:C:200:PRO:HD3	1.93	0.49
1:B:167:PHE:HA	1:B:168:TYR:HA	1.63	0.49
1:C:179:MET:HA	1:C:179:MET:HE2	1.94	0.49
1:D:199:ARG:HB3	1:D:200:PRO:HD3	1.94	0.48
2:C:301:LPP:H241	1:D:229:LEU:HD11	1.95	0.48
1:D:179:MET:HA	1:D:179:MET:HE2	1.94	0.48
1:D:28:THR:OG1	1:D:117:ASP:OD2	2.25	0.48
2:B:301:LPP:H241	1:C:229:LEU:HD11	1.96	0.48
1:A:63:ILE:HG12	1:A:179:MET:HE3	1.95	0.48
1:A:103:GLY:HA2	5:A:304:PT5:H69	1.96	0.48
1:B:251:LYS:HE2	1:B:253:ARG:HH11	1.79	0.48
1:C:122:SER:O	1:D:219:SER:OG	2.26	0.47
1:C:251:LYS:HE2	1:C:253:ARG:HH11	1.79	0.47
1:D:85:HIS:O	1:D:253:ARG:NE	2.40	0.47
1:D:251:LYS:HE2	1:D:253:ARG:HH11	1.79	0.47
1:B:52:ASP:OD1	1:B:217:ARG:NH1	2.44	0.47
1:A:213:VAL:O	1:A:217:ARG:HG2	2.13	0.47
1:A:243:ALA:O	1:A:247:SER:OG	2.33	0.47
1:B:115:LEU:HG	1:C:204:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HG	1:D:204:PHE:CE1	2.50	0.47
1:A:215:LEU:HD13	1:D:119:ALA:HA	1.97	0.46
1:D:226:SER:HB2	2:D:301:LPP:H172	1.97	0.46
1:A:229:LEU:HD11	2:D:301:LPP:H241	1.98	0.46
1:A:63:ILE:CG1	1:A:179:MET:HE3	2.46	0.46
1:C:129:HIS:CE1	1:C:222:LYS:HD3	2.51	0.46
1:C:226:SER:HB2	2:C:301:LPP:H172	1.98	0.46
1:A:204:PHE:CE1	1:D:115:LEU:HG	2.51	0.46
1:B:226:SER:HB2	2:B:301:LPP:H172	1.98	0.46
1:D:129:HIS:CE1	1:D:222:LYS:HD3	2.51	0.45
1:A:226:SER:HB2	2:A:301:LPP:H172	1.99	0.45
1:A:251:LYS:HE2	1:A:253:ARG:HH11	1.82	0.45
1:B:129:HIS:CE1	1:B:222:LYS:HD3	2.51	0.45
1:A:234:GLN:HE21	1:A:238:VAL:HG21	1.81	0.45
1:D:103:GLY:HA2	5:D:304:PT5:H69	1.99	0.45
1:C:103:GLY:HA2	5:C:304:PT5:H69	1.99	0.45
1:A:129:HIS:CE1	1:A:222:LYS:HD3	2.52	0.45
1:A:90:ILE:HG23	1:A:92:ASN:H	1.82	0.45
1:A:219:SER:OG	1:D:122:SER:O	2.30	0.45
1:A:115:LEU:HG	1:B:204:PHE:CE1	2.51	0.44
1:B:103:GLY:HA2	5:B:304:PT5:H69	1.99	0.44
1:D:167:PHE:HA	1:D:168:TYR:HA	1.65	0.44
5:B:304:PT5:H28	5:B:304:PT5:H25	1.85	0.44
1:A:187:GLN:HB2	1:A:203:GLN:NE2	2.32	0.44
1:D:52:ASP:OD1	1:D:217:ARG:NH1	2.44	0.44
1:B:50:LYS:HE2	1:B:220:ASP:HA	1.99	0.43
1:D:120:LYS:HB3	1:D:165:LEU:HD22	2.00	0.43
1:D:6:ARG:HE	1:D:6:ARG:HB3	1.59	0.43
1:C:90:ILE:HG23	1:C:92:ASN:H	1.83	0.43
1:C:52:ASP:OD1	1:C:217:ARG:NH1	2.44	0.43
1:C:7:LEU:N	1:C:8:PRO:HD2	2.34	0.43
1:A:197:LEU:C	1:A:200:PRO:HD2	2.44	0.43
1:B:90:ILE:HG23	1:B:92:ASN:H	1.83	0.43
1:C:120:LYS:HB3	1:C:165:LEU:HD22	2.01	0.43
1:D:50:LYS:HE2	1:D:220:ASP:HA	2.00	0.43
1:D:90:ILE:HG23	1:D:92:ASN:H	1.84	0.43
1:D:190:MET:O	1:D:199:ARG:NH1	2.52	0.42
1:A:47:TYR:OH	2:D:301:LPP:O2	2.31	0.42
1:B:194:TRP:HZ3	1:B:198:LEU:HD23	1.84	0.42
1:C:167:PHE:HA	1:C:168:TYR:HA	1.65	0.42
1:A:167:PHE:HA	1:A:168:TYR:HA	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:C	1:C:200:PRO:HD2	2.44	0.42
1:A:7:LEU:N	1:A:8:PRO:HD2	2.34	0.42
1:A:85:HIS:O	1:A:253:ARG:NE	2.41	0.42
1:D:7:LEU:N	1:D:8:PRO:HD2	2.34	0.42
2:A:301:LPP:H402	2:A:301:LPP:H372	1.92	0.42
1:A:225:TRP:HB2	2:D:301:LPP:H311	2.02	0.42
1:B:7:LEU:N	1:B:8:PRO:HD2	2.34	0.42
1:C:50:LYS:HE2	1:C:220:ASP:HA	2.00	0.42
1:A:33:PRO:HG3	1:A:165:LEU:HD21	2.01	0.42
1:B:191:LYS:HE3	1:B:191:LYS:HB2	1.89	0.42
1:A:99:TYR:CG	5:A:304:PT5:H23	2.55	0.42
1:B:120:LYS:HB3	1:B:165:LEU:HD22	2.02	0.42
1:C:194:TRP:HZ3	1:C:198:LEU:HD23	1.85	0.41
1:A:119:ALA:HA	1:B:215:LEU:HD13	2.02	0.41
1:D:6:ARG:HA	1:D:9:TYR:HD2	1.85	0.41
1:A:127:ARG:NH2	6:A:305:PO4:O3	2.53	0.41
1:B:6:ARG:HA	1:B:9:TYR:HD2	1.85	0.41
1:B:197:LEU:C	1:B:200:PRO:HD2	2.44	0.41
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.94	0.41
1:C:6:ARG:HA	1:C:9:TYR:HD2	1.86	0.41
1:C:6:ARG:HE	1:C:6:ARG:HB3	1.60	0.41
2:D:301:LPP:H402	2:D:301:LPP:H372	1.91	0.41
1:B:63:ILE:HG12	1:B:179:MET:HE3	2.03	0.40
1:B:251:LYS:NZ	5:B:304:PT5:O41	2.55	0.40
1:D:187:GLN:HB2	1:D:203:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	250/284 (88%)	245 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
1	C	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
1	D	250/284 (88%)	245 (98%)	5 (2%)	0	100	100
All	All	1000/1136 (88%)	980 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/247 (87%)	212 (98%)	4 (2%)	50	79
1	B	216/247 (87%)	213 (99%)	3 (1%)	59	84
1	C	216/247 (87%)	212 (98%)	4 (2%)	50	79
1	D	216/247 (87%)	213 (99%)	3 (1%)	59	84
All	All	864/988 (87%)	850 (98%)	14 (2%)	54	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	88	SER
1	A	142	ASN
1	A	251	LYS
1	B	88	SER
1	B	142	ASN
1	B	251	LYS
1	C	73	LEU
1	C	88	SER
1	C	142	ASN
1	C	251	LYS
1	D	88	SER
1	D	142	ASN

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Mol	Chain	Res	Type
1	D	251	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	NAG	B	302	1	14,14,15	0.45	0	17,19,21	0.98	2 (11%)
5	PT5	B	304	-	62,62,69	0.88	2 (3%)	76,80,87	0.98	2 (2%)
6	PO4	B	305	-	4,4,4	0.96	0	6,6,6	0.41	0
6	PO4	D	305	-	4,4,4	0.95	0	6,6,6	0.41	0
6	PO4	A	305	-	4,4,4	0.97	0	6,6,6	0.41	0
6	PO4	C	305	-	4,4,4	0.98	0	6,6,6	0.42	0
2	LPP	A	301	-	43,43,43	0.90	4 (9%)	47,48,48	1.10	2 (4%)
2	LPP	D	301	-	43,43,43	0.90	4 (9%)	47,48,48	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LPP	B	301	-	43,43,43	0.91	4 (9%)	47,48,48	1.10	2 (4%)
4	LBN	B	303	-	44,44,51	1.27	7 (15%)	48,49,59	1.17	3 (6%)
3	NAG	C	302	1	14,14,15	0.46	0	17,19,21	0.98	2 (11%)
3	NAG	A	302	1	14,14,15	0.46	0	17,19,21	0.98	2 (11%)
5	PT5	A	304	-	62,62,69	0.88	2 (3%)	76,80,87	0.98	2 (2%)
4	LBN	A	303	-	44,44,51	1.27	7 (15%)	48,49,59	1.17	3 (6%)
3	NAG	D	302	1	14,14,15	0.47	0	17,19,21	0.97	2 (11%)
4	LBN	C	303	-	44,44,51	1.27	7 (15%)	48,49,59	1.17	3 (6%)
5	PT5	D	304	-	62,62,69	0.88	2 (3%)	76,80,87	0.98	2 (2%)
4	LBN	D	303	-	44,44,51	1.27	7 (15%)	48,49,59	1.17	3 (6%)
5	PT5	C	304	-	62,62,69	0.88	2 (3%)	76,80,87	0.98	2 (2%)
2	LPP	C	301	-	43,43,43	0.90	4 (9%)	47,48,48	1.10	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LBN	D	303	-	-	24/46/46/55	-
2	LPP	B	301	-	-	20/45/45/45	-
3	NAG	B	302	1	-	2/6/23/26	0/1/1/1
4	LBN	B	303	-	-	24/46/46/55	-
3	NAG	C	302	1	-	2/6/23/26	0/1/1/1
3	NAG	A	302	1	-	2/6/23/26	0/1/1/1
5	PT5	A	304	-	-	15/59/83/90	0/1/1/1
4	LBN	A	303	-	-	24/46/46/55	-
3	NAG	D	302	1	-	2/6/23/26	0/1/1/1
4	LBN	C	303	-	-	24/46/46/55	-
5	PT5	B	304	-	-	15/59/83/90	0/1/1/1
2	LPP	C	301	-	-	20/45/45/45	-
5	PT5	C	304	-	-	15/59/83/90	0/1/1/1
2	LPP	A	301	-	-	20/45/45/45	-
5	PT5	D	304	-	-	15/59/83/90	0/1/1/1
2	LPP	D	301	-	-	20/45/45/45	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	304	PT5	O18-C11	4.23	1.45	1.33
5	B	304	PT5	O18-C11	4.23	1.45	1.33
5	C	304	PT5	O18-C11	4.23	1.45	1.33
5	D	304	PT5	O18-C11	4.23	1.45	1.33
5	D	304	PT5	O16-C10	4.18	1.46	1.34
5	A	304	PT5	O16-C10	4.18	1.46	1.34
5	B	304	PT5	O16-C10	4.18	1.46	1.34
5	C	304	PT5	O16-C10	4.18	1.46	1.34
4	D	303	LBN	C42-C5	3.70	1.53	1.31
4	B	303	LBN	C42-C5	3.68	1.53	1.31
4	C	303	LBN	C42-C5	3.68	1.53	1.31
4	A	303	LBN	C42-C5	3.68	1.53	1.31
4	A	303	LBN	C33-C4	-3.53	1.31	1.51
4	C	303	LBN	C33-C4	-3.52	1.31	1.51
4	D	303	LBN	C33-C4	-3.52	1.31	1.51
4	B	303	LBN	C33-C4	-3.52	1.31	1.51
4	B	303	LBN	C41-C42	-3.20	1.32	1.50
4	A	303	LBN	C41-C42	-3.19	1.32	1.50
4	C	303	LBN	C41-C42	-3.19	1.32	1.50
4	D	303	LBN	C41-C42	-3.19	1.32	1.50
2	C	301	LPP	O9-C7	-2.68	1.39	1.46
2	B	301	LPP	O9-C7	-2.67	1.39	1.46
2	D	301	LPP	O9-C7	-2.67	1.39	1.46
2	A	301	LPP	O9-C7	-2.64	1.40	1.46
4	B	303	LBN	O7-C2	-2.62	1.40	1.46
4	C	303	LBN	O7-C2	-2.62	1.40	1.46
4	D	303	LBN	O7-C2	-2.62	1.40	1.46
4	A	303	LBN	O7-C2	-2.61	1.40	1.46
2	A	301	LPP	O27-C29	2.50	1.40	1.33
2	B	301	LPP	O27-C29	2.50	1.40	1.33
2	D	301	LPP	O27-C29	2.49	1.40	1.33
2	C	301	LPP	O27-C29	2.47	1.40	1.33
4	B	303	LBN	O5-C25	2.42	1.40	1.33
4	A	303	LBN	O5-C25	2.40	1.40	1.33
4	D	303	LBN	O5-C25	2.39	1.40	1.33
4	C	303	LBN	O5-C25	2.37	1.40	1.33
4	A	303	LBN	O5-C3	-2.17	1.40	1.45
4	B	303	LBN	O5-C3	-2.15	1.40	1.45
4	C	303	LBN	O5-C3	-2.15	1.40	1.45
2	C	301	LPP	O9-C11	2.13	1.40	1.34
4	D	303	LBN	O5-C3	-2.12	1.40	1.45
2	D	301	LPP	O9-C11	2.10	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	LPP	O9-C11	2.10	1.40	1.34
2	A	301	LPP	O9-C11	2.10	1.40	1.34
4	B	303	LBN	O7-C34	2.10	1.40	1.34
4	C	303	LBN	O7-C34	2.08	1.40	1.34
2	D	301	LPP	O27-C8	-2.08	1.40	1.45
4	A	303	LBN	O7-C34	2.08	1.40	1.34
4	D	303	LBN	O7-C34	2.07	1.40	1.34
2	B	301	LPP	O27-C8	-2.07	1.40	1.45
2	A	301	LPP	O27-C8	-2.04	1.40	1.45
2	C	301	LPP	O27-C8	-2.04	1.40	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	304	PT5	O16-C10-C12	4.32	120.80	111.50
5	A	304	PT5	O16-C10-C12	4.31	120.78	111.50
5	C	304	PT5	O16-C10-C12	4.30	120.76	111.50
5	D	304	PT5	O16-C10-C12	4.29	120.74	111.50
4	A	303	LBN	O7-C34-C35	3.88	119.86	111.50
4	D	303	LBN	O7-C34-C35	3.87	119.83	111.50
4	B	303	LBN	O7-C34-C35	3.86	119.82	111.50
4	C	303	LBN	O7-C34-C35	3.84	119.78	111.50
2	B	301	LPP	O9-C11-C12	3.79	119.68	111.50
2	C	301	LPP	O9-C11-C12	3.77	119.63	111.50
2	D	301	LPP	O9-C11-C12	3.77	119.63	111.50
2	A	301	LPP	O9-C11-C12	3.76	119.61	111.50
3	C	302	NAG	C1-O5-C5	2.78	115.96	112.19
3	B	302	NAG	C1-O5-C5	2.77	115.94	112.19
3	A	302	NAG	C1-O5-C5	2.75	115.92	112.19
3	D	302	NAG	C1-O5-C5	2.74	115.91	112.19
5	D	304	PT5	O18-C11-C31	2.56	119.95	111.91
5	C	304	PT5	O18-C11-C31	2.56	119.95	111.91
5	B	304	PT5	O18-C11-C31	2.56	119.94	111.91
5	A	304	PT5	O18-C11-C31	2.56	119.94	111.91
4	C	303	LBN	O5-C25-C26	2.50	119.75	111.91
4	D	303	LBN	O5-C25-C26	2.49	119.74	111.91
4	B	303	LBN	O5-C25-C26	2.49	119.73	111.91
4	A	303	LBN	O5-C25-C26	2.49	119.71	111.91
2	D	301	LPP	O27-C29-C30	2.43	119.54	111.91
2	C	301	LPP	O27-C29-C30	2.39	119.41	111.91
2	B	301	LPP	O27-C29-C30	2.39	119.40	111.91
2	A	301	LPP	O27-C29-C30	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	NAG	C3-C4-C5	2.28	114.30	110.24
3	B	302	NAG	C3-C4-C5	2.26	114.27	110.24
3	C	302	NAG	C3-C4-C5	2.25	114.25	110.24
3	D	302	NAG	C3-C4-C5	2.24	114.24	110.24
4	D	303	LBN	C8-C5-C42	-2.02	109.21	124.73
4	C	303	LBN	C8-C5-C42	-2.02	109.22	124.73
4	A	303	LBN	C8-C5-C42	-2.02	109.24	124.73
4	B	303	LBN	C8-C5-C42	-2.02	109.26	124.73

There are no chirality outliers.

All (244) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	LPP	C6-O5-P1-O2
2	A	301	LPP	C6-O5-P1-O4
2	B	301	LPP	C6-O5-P1-O2
2	B	301	LPP	C6-O5-P1-O4
2	C	301	LPP	C6-O5-P1-O2
2	C	301	LPP	C6-O5-P1-O4
2	D	301	LPP	C6-O5-P1-O2
2	D	301	LPP	C6-O5-P1-O4
5	A	304	PT5	C1-O1-P1-O12
5	A	304	PT5	C12-C10-O16-C8
5	B	304	PT5	C1-O1-P1-O12
5	B	304	PT5	C12-C10-O16-C8
5	C	304	PT5	C1-O1-P1-O12
5	C	304	PT5	C12-C10-O16-C8
5	D	304	PT5	C1-O1-P1-O12
5	D	304	PT5	C12-C10-O16-C8
5	A	304	PT5	O17-C10-O16-C8
5	B	304	PT5	O17-C10-O16-C8
5	C	304	PT5	O17-C10-O16-C8
5	D	304	PT5	O17-C10-O16-C8
3	A	302	NAG	O5-C5-C6-O6
3	B	302	NAG	O5-C5-C6-O6
3	C	302	NAG	O5-C5-C6-O6
3	D	302	NAG	O5-C5-C6-O6
3	B	302	NAG	C4-C5-C6-O6
3	D	302	NAG	C4-C5-C6-O6
3	A	302	NAG	C4-C5-C6-O6
3	C	302	NAG	C4-C5-C6-O6
4	B	303	LBN	C26-C25-O5-C3

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Mol	Chain	Res	Type	Atoms
4	C	303	LBN	C26-C25-O5-C3
4	D	303	LBN	C26-C25-O5-C3
4	A	303	LBN	C26-C25-O5-C3
4	A	303	LBN	C41-C42-C5-C8
4	B	303	LBN	C41-C42-C5-C8
4	C	303	LBN	C41-C42-C5-C8
4	D	303	LBN	C41-C42-C5-C8
4	A	303	LBN	O6-C25-O5-C3
4	B	303	LBN	O6-C25-O5-C3
4	C	303	LBN	O6-C25-O5-C3
4	D	303	LBN	O6-C25-O5-C3
5	A	304	PT5	C7-O13-P1-O1
5	B	304	PT5	C7-O13-P1-O1
5	C	304	PT5	C7-O13-P1-O1
5	D	304	PT5	C7-O13-P1-O1
2	B	301	LPP	C34-C35-C36-C37
2	C	301	LPP	C34-C35-C36-C37
5	A	304	PT5	C38-C39-C40-C41
5	B	304	PT5	C38-C39-C40-C41
5	C	304	PT5	C38-C39-C40-C41
2	A	301	LPP	C34-C35-C36-C37
4	A	303	LBN	C38-C39-C40-C41
5	D	304	PT5	C38-C39-C40-C41
5	A	304	PT5	C7-C8-O16-C10
5	B	304	PT5	C7-C8-O16-C10
5	C	304	PT5	C7-C8-O16-C10
5	D	304	PT5	C7-C8-O16-C10
2	D	301	LPP	C34-C35-C36-C37
4	C	303	LBN	C38-C39-C40-C41
4	D	303	LBN	C38-C39-C40-C41
2	B	301	LPP	C39-C40-C41-C42
2	C	301	LPP	C39-C40-C41-C42
2	D	301	LPP	C39-C40-C41-C42
4	B	303	LBN	C38-C39-C40-C41
2	A	301	LPP	C39-C40-C41-C42
4	B	303	LBN	C31-C32-C33-C4
4	C	303	LBN	C31-C32-C33-C4
4	D	303	LBN	C31-C32-C33-C4
5	B	304	PT5	C40-C41-C42-C43
5	C	304	PT5	C40-C41-C42-C43
5	D	304	PT5	C40-C41-C42-C43
5	A	304	PT5	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
4	A	303	LBN	C31-C32-C33-C4
5	C	304	PT5	C34-C35-C36-C37
5	D	304	PT5	C34-C35-C36-C37
5	A	304	PT5	C34-C35-C36-C37
5	B	304	PT5	C34-C35-C36-C37
2	D	301	LPP	C12-C11-O9-C7
2	D	301	LPP	C36-C37-C38-C39
4	B	303	LBN	C33-C4-C7-C10
2	A	301	LPP	C36-C37-C38-C39
4	A	303	LBN	C33-C4-C7-C10
4	C	303	LBN	C33-C4-C7-C10
4	D	303	LBN	C33-C4-C7-C10
2	A	301	LPP	C12-C11-O9-C7
2	B	301	LPP	C12-C11-O9-C7
4	A	303	LBN	C35-C34-O7-C2
4	B	303	LBN	C35-C34-O7-C2
4	C	303	LBN	C35-C34-O7-C2
4	D	303	LBN	C35-C34-O7-C2
2	B	301	LPP	C36-C37-C38-C39
2	C	301	LPP	C36-C37-C38-C39
2	C	301	LPP	C12-C11-O9-C7
4	A	303	LBN	C27-C28-C29-C30
4	B	303	LBN	C27-C28-C29-C30
4	C	303	LBN	C27-C28-C29-C30
4	D	303	LBN	C27-C28-C29-C30
2	A	301	LPP	O10-C11-O9-C7
2	B	301	LPP	O10-C11-O9-C7
2	C	301	LPP	O10-C11-O9-C7
4	A	303	LBN	O8-C34-O7-C2
4	A	303	LBN	C1-C2-C3-O5
4	B	303	LBN	C1-C2-C3-O5
4	C	303	LBN	C1-C2-C3-O5
4	D	303	LBN	C1-C2-C3-O5
5	B	304	PT5	C33-C34-C35-C36
5	A	304	PT5	C1-O1-P1-O13
5	B	304	PT5	C1-O1-P1-O13
5	C	304	PT5	C1-O1-P1-O13
5	D	304	PT5	C1-O1-P1-O13
4	A	303	LBN	C39-C40-C41-C42
4	B	303	LBN	C39-C40-C41-C42
4	C	303	LBN	C39-C40-C41-C42
4	D	303	LBN	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
5	A	304	PT5	C33-C34-C35-C36
5	C	304	PT5	C33-C34-C35-C36
5	D	304	PT5	C33-C34-C35-C36
4	D	303	LBN	O8-C34-O7-C2
2	A	301	LPP	C6-O5-P1-O3
2	B	301	LPP	C6-O5-P1-O3
2	C	301	LPP	C6-O5-P1-O3
2	D	301	LPP	C6-O5-P1-O3
4	B	303	LBN	C8-C11-C14-C17
4	C	303	LBN	C8-C11-C14-C17
4	D	303	LBN	C8-C11-C14-C17
4	A	303	LBN	C8-C11-C14-C17
2	D	301	LPP	O10-C11-O9-C7
4	B	303	LBN	O8-C34-O7-C2
4	C	303	LBN	O8-C34-O7-C2
4	A	303	LBN	C7-C10-C13-C16
4	B	303	LBN	C7-C10-C13-C16
4	C	303	LBN	C7-C10-C13-C16
4	D	303	LBN	C7-C10-C13-C16
4	A	303	LBN	C14-C17-C20-C22
5	A	304	PT5	C1-O1-P1-O11
5	B	304	PT5	C1-O1-P1-O11
5	C	304	PT5	C1-O1-P1-O11
5	D	304	PT5	C1-O1-P1-O11
5	A	304	PT5	C15-C16-C17-C18
5	B	304	PT5	C15-C16-C17-C18
5	C	304	PT5	C15-C16-C17-C18
5	D	304	PT5	C15-C16-C17-C18
4	A	303	LBN	C29-C30-C31-C32
4	A	303	LBN	C28-C29-C30-C31
4	C	303	LBN	C14-C17-C20-C22
4	B	303	LBN	C14-C17-C20-C22
4	D	303	LBN	C14-C17-C20-C22
4	B	303	LBN	C28-C29-C30-C31
4	C	303	LBN	C28-C29-C30-C31
4	D	303	LBN	C28-C29-C30-C31
2	D	301	LPP	C17-C18-C19-C20
2	C	301	LPP	C40-C41-C42-C43
2	D	301	LPP	C40-C41-C42-C43
2	A	301	LPP	C40-C41-C42-C43
2	B	301	LPP	C40-C41-C42-C43
2	A	301	LPP	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
2	B	301	LPP	C17-C18-C19-C20
2	C	301	LPP	C17-C18-C19-C20
4	D	303	LBN	C29-C30-C31-C32
4	A	303	LBN	C30-C31-C32-C33
4	C	303	LBN	C29-C30-C31-C32
4	B	303	LBN	C29-C30-C31-C32
4	C	303	LBN	C30-C31-C32-C33
4	D	303	LBN	C30-C31-C32-C33
4	B	303	LBN	C30-C31-C32-C33
4	C	303	LBN	C14-C11-C8-C5
4	D	303	LBN	C14-C11-C8-C5
4	B	303	LBN	O1-C1-C2-O7
4	C	303	LBN	O1-C1-C2-O7
4	D	303	LBN	O1-C1-C2-O7
4	A	303	LBN	O7-C2-C3-O5
2	D	301	LPP	C19-C20-C21-C22
2	A	301	LPP	C19-C20-C21-C22
4	B	303	LBN	C14-C11-C8-C5
2	B	301	LPP	C19-C20-C21-C22
2	D	301	LPP	C30-C29-O27-C8
2	C	301	LPP	C19-C20-C21-C22
5	A	304	PT5	C7-O13-P1-O11
5	B	304	PT5	C7-O13-P1-O11
5	C	304	PT5	C7-O13-P1-O11
5	D	304	PT5	C7-O13-P1-O11
2	A	301	LPP	O5-C6-C7-C8
2	B	301	LPP	O5-C6-C7-C8
2	C	301	LPP	O5-C6-C7-C8
4	A	303	LBN	C14-C11-C8-C5
2	D	301	LPP	O28-C29-O27-C8
4	A	303	LBN	C36-C37-C38-C39
4	B	303	LBN	O7-C2-C3-O5
4	C	303	LBN	O7-C2-C3-O5
4	D	303	LBN	O7-C2-C3-O5
4	D	303	LBN	C36-C37-C38-C39
2	D	301	LPP	C21-C22-C23-C24
4	B	303	LBN	C36-C37-C38-C39
4	C	303	LBN	C36-C37-C38-C39
2	B	301	LPP	C21-C22-C23-C24
2	C	301	LPP	C21-C22-C23-C24
4	A	303	LBN	C40-C41-C42-C5
4	B	303	LBN	C40-C41-C42-C5

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Mol	Chain	Res	Type	Atoms
4	C	303	LBN	C40-C41-C42-C5
4	D	303	LBN	C40-C41-C42-C5
2	D	301	LPP	O5-C6-C7-C8
2	A	301	LPP	C21-C22-C23-C24
2	D	301	LPP	C32-C33-C34-C35
2	A	301	LPP	C32-C33-C34-C35
2	C	301	LPP	C32-C33-C34-C35
4	B	303	LBN	O1-C1-C2-C3
4	C	303	LBN	O1-C1-C2-C3
4	D	303	LBN	O1-C1-C2-C3
2	B	301	LPP	C32-C33-C34-C35
2	D	301	LPP	C35-C36-C37-C38
2	A	301	LPP	O5-C6-C7-O9
4	A	303	LBN	O1-C1-C2-O7
2	B	301	LPP	C35-C36-C37-C38
2	C	301	LPP	C35-C36-C37-C38
4	A	303	LBN	C42-C5-C8-C11
4	C	303	LBN	C42-C5-C8-C11
4	D	303	LBN	C42-C5-C8-C11
2	A	301	LPP	C35-C36-C37-C38
2	B	301	LPP	O5-C6-C7-O9
2	C	301	LPP	O5-C6-C7-O9
2	D	301	LPP	O5-C6-C7-O9
4	A	303	LBN	O1-C1-C2-C3
2	B	301	LPP	O28-C29-O27-C8
4	B	303	LBN	C42-C5-C8-C11
2	C	301	LPP	O28-C29-O27-C8
2	B	301	LPP	C30-C29-O27-C8
2	C	301	LPP	C30-C29-O27-C8
2	A	301	LPP	O28-C29-O27-C8
2	A	301	LPP	O9-C11-C12-C13
2	B	301	LPP	O9-C11-C12-C13
2	C	301	LPP	O9-C11-C12-C13
5	A	304	PT5	O16-C10-C12-C13
2	D	301	LPP	O9-C11-C12-C13
2	A	301	LPP	C30-C29-O27-C8
5	B	304	PT5	O16-C10-C12-C13
5	C	304	PT5	O16-C10-C12-C13
5	D	304	PT5	O16-C10-C12-C13
2	D	301	LPP	O10-C11-C12-C13
2	A	301	LPP	O10-C11-C12-C13
2	B	301	LPP	O10-C11-C12-C13

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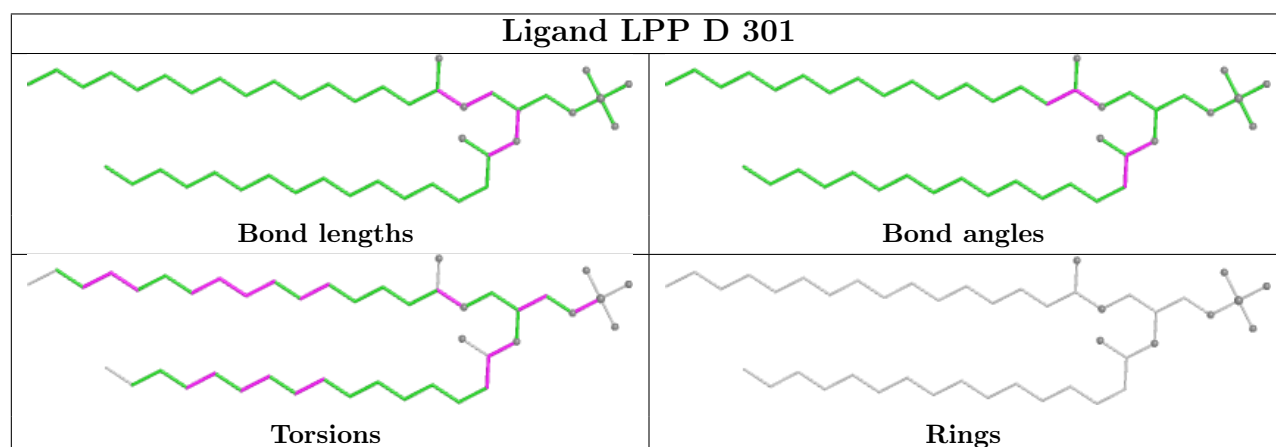
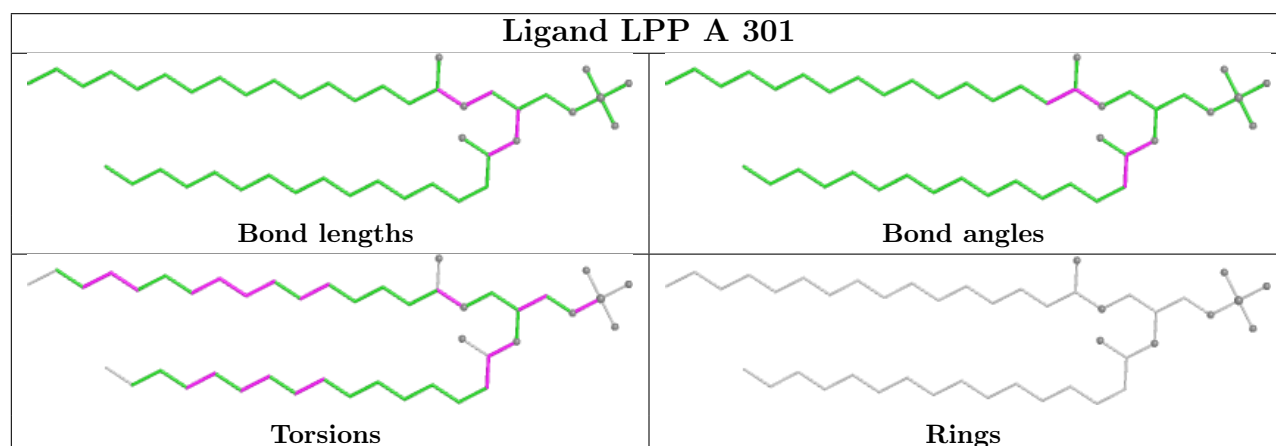
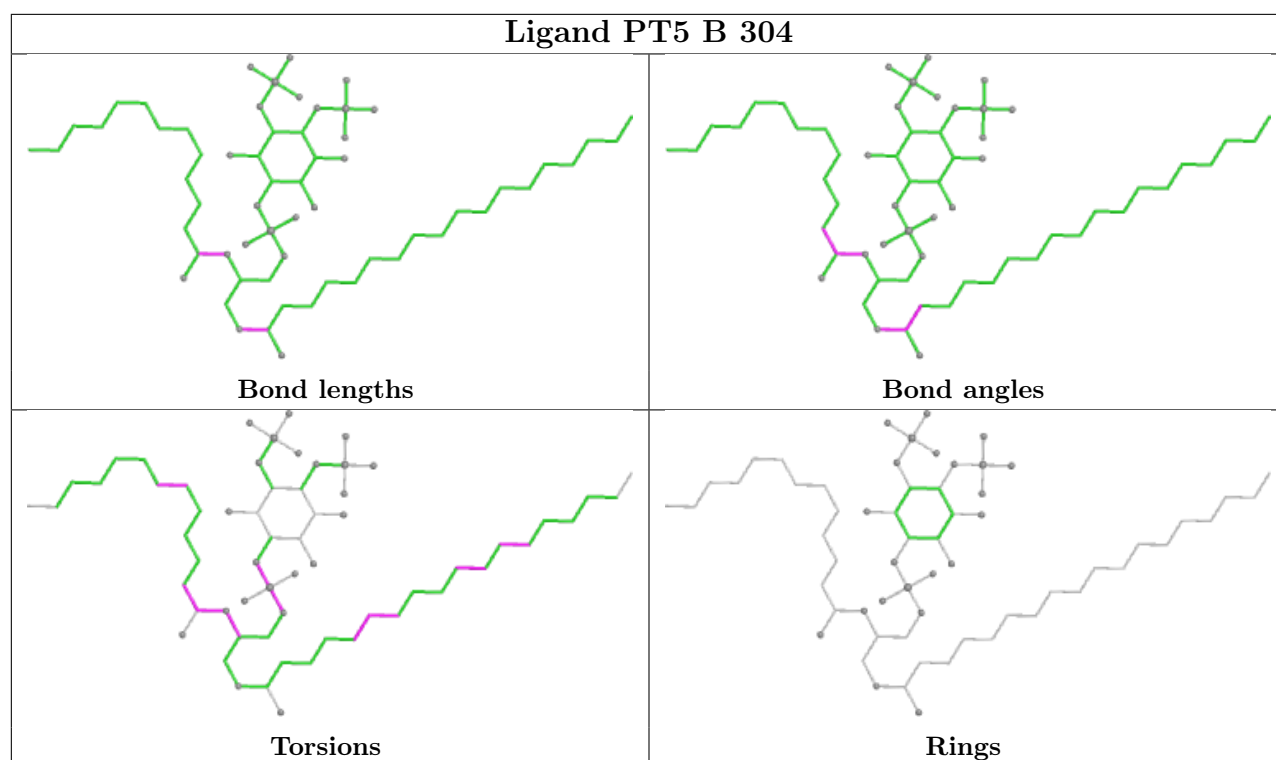
Mol	Chain	Res	Type	Atoms
2	C	301	LPP	O10-C11-C12-C13
5	A	304	PT5	O17-C10-C12-C13
5	B	304	PT5	O17-C10-C12-C13
5	D	304	PT5	O17-C10-C12-C13
5	C	304	PT5	O17-C10-C12-C13

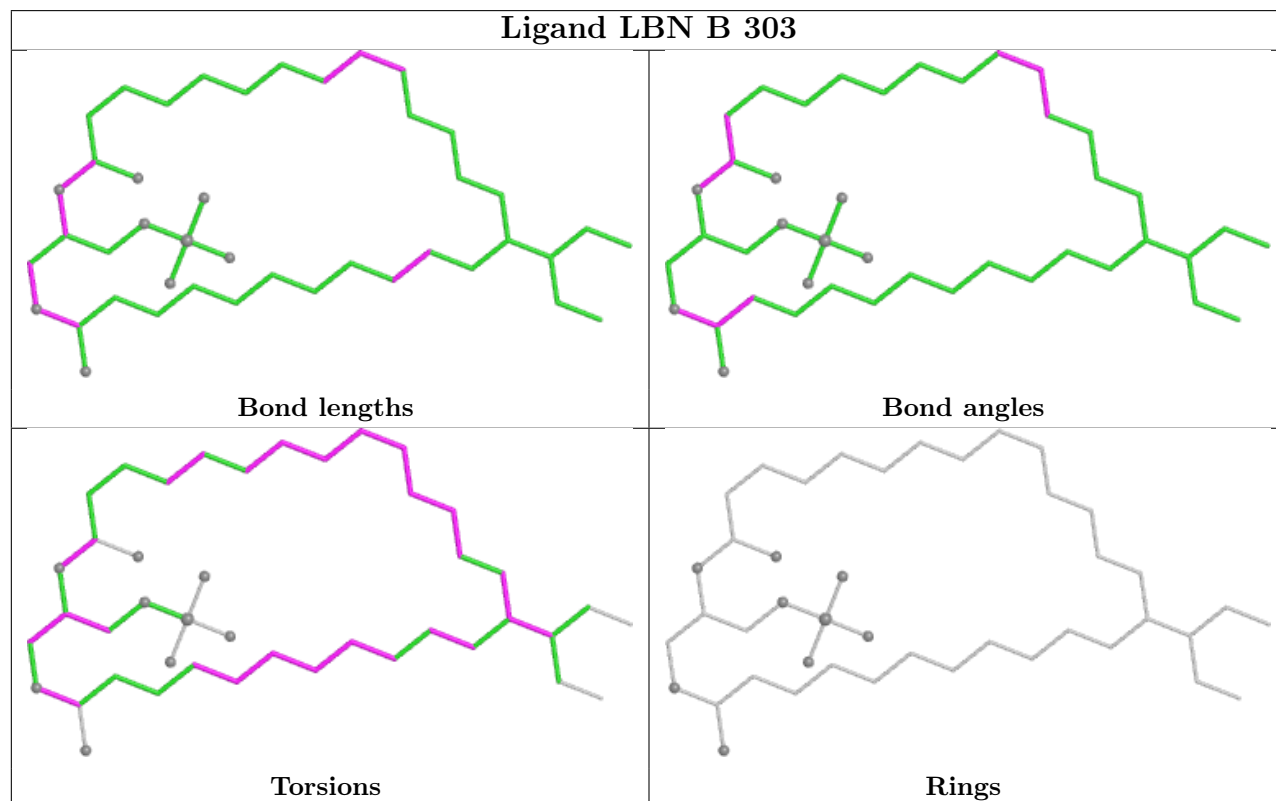
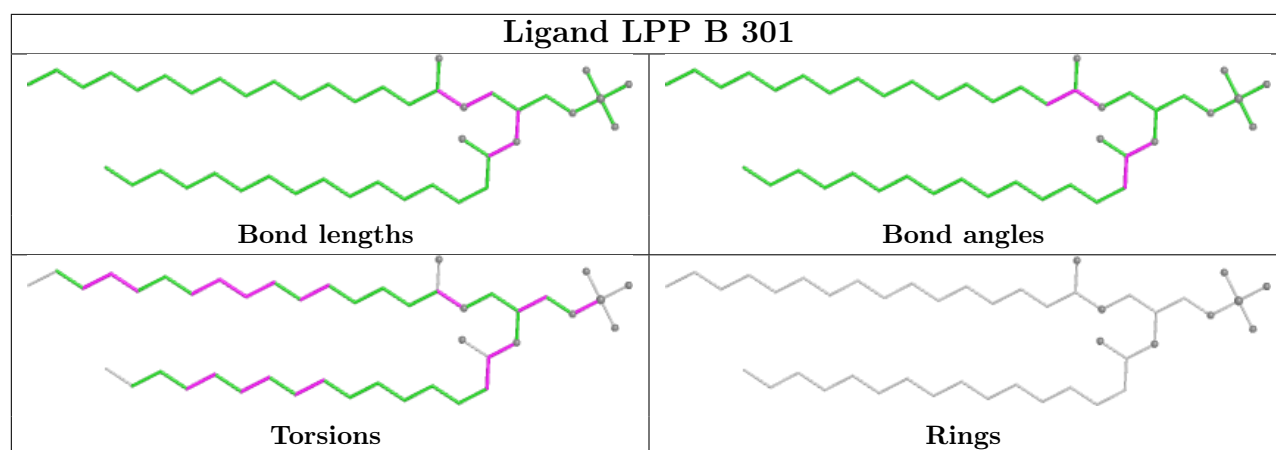
There are no ring outliers.

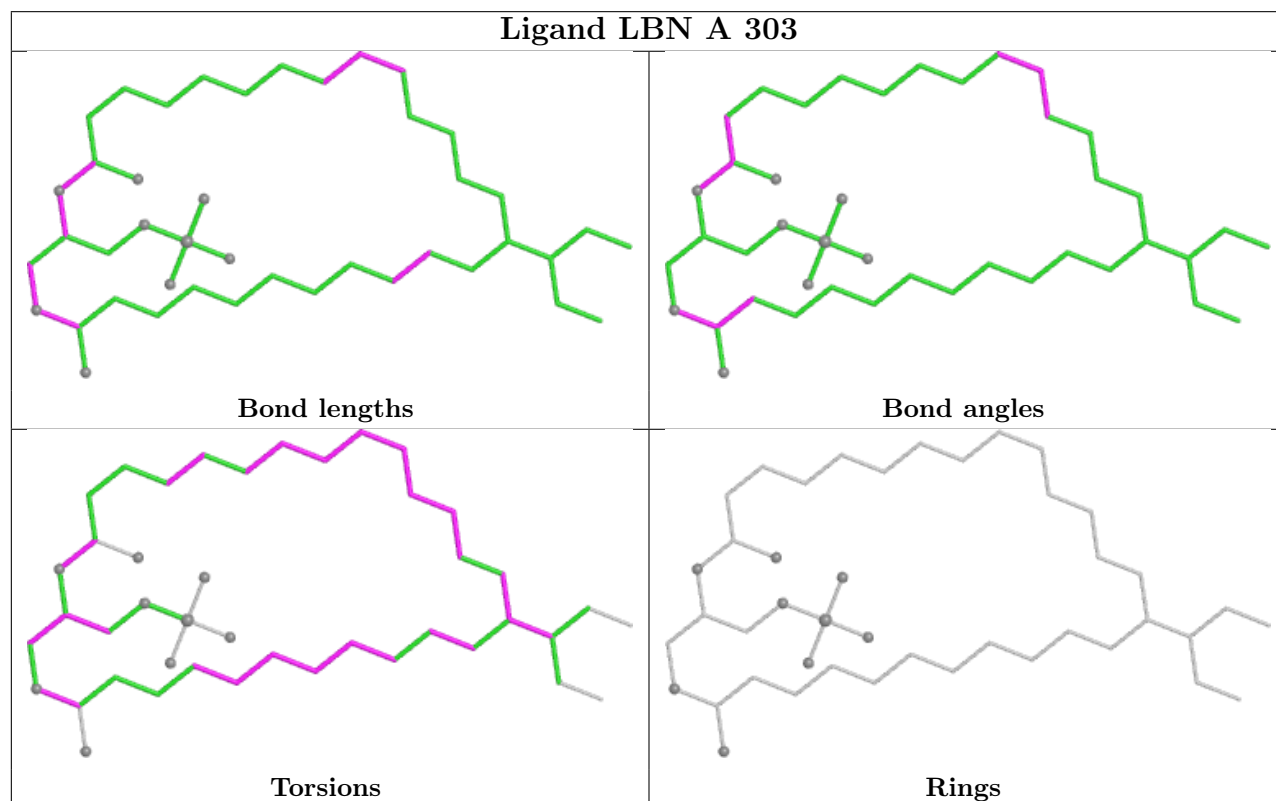
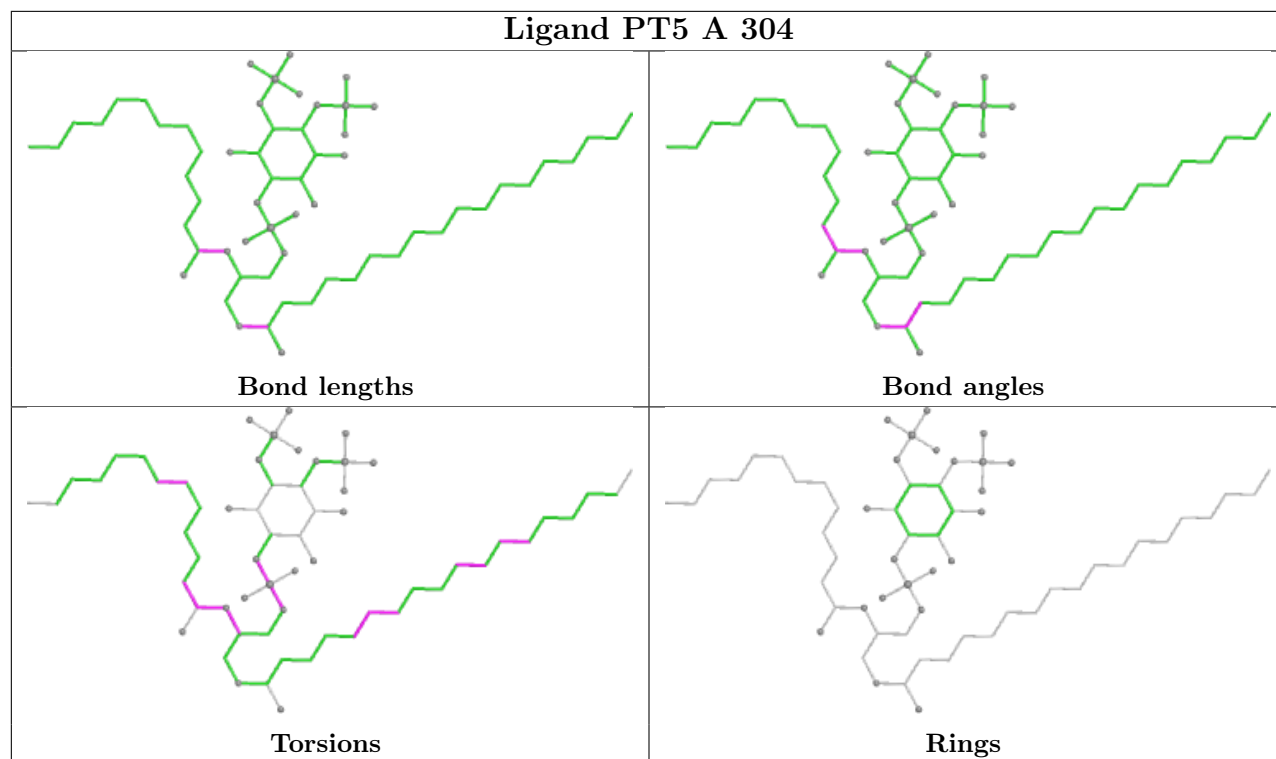
9 monomers are involved in 36 short contacts:

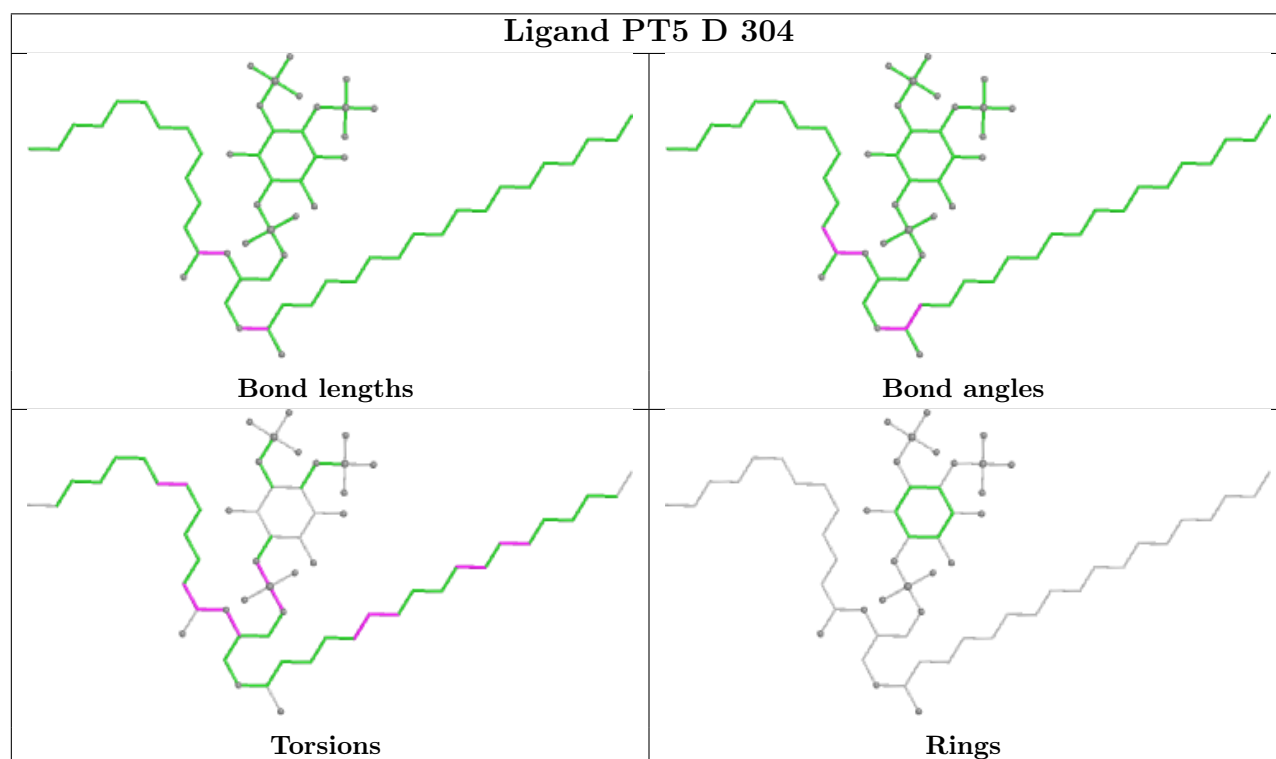
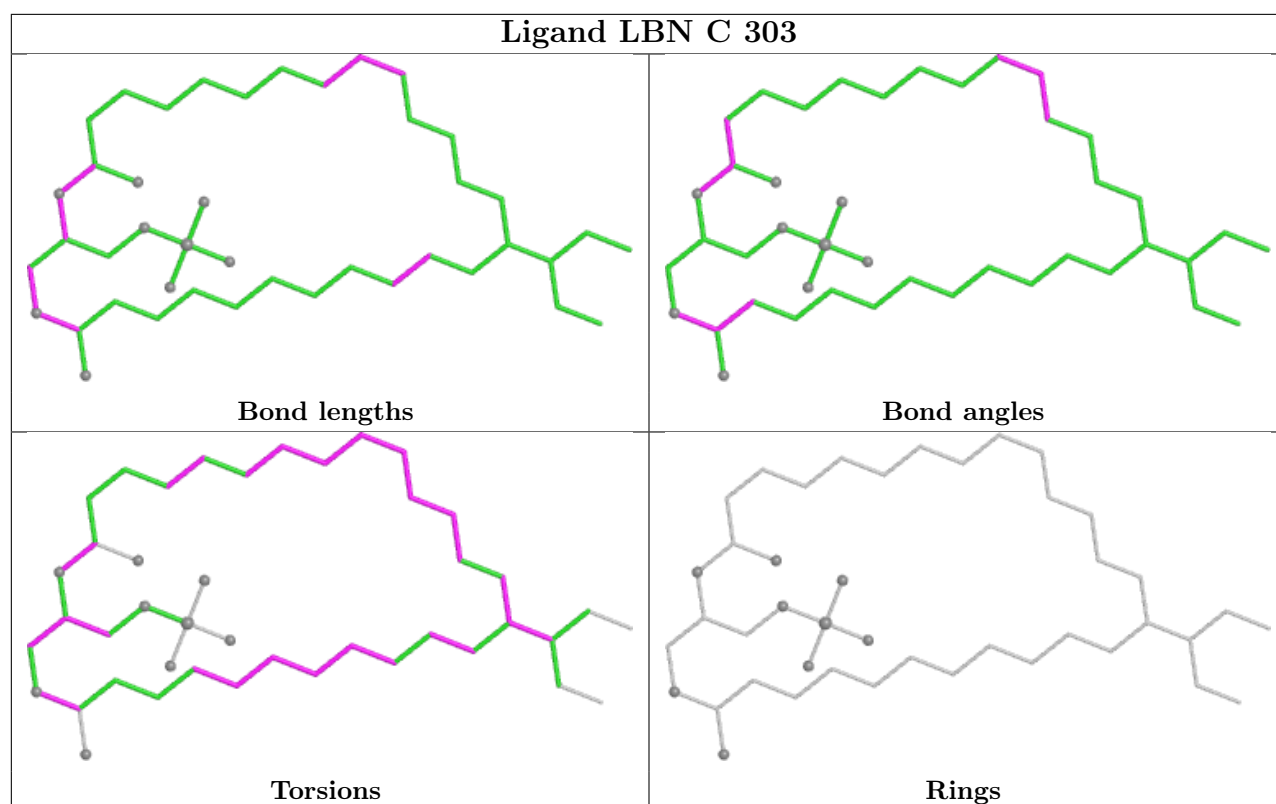
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	PT5	4	0
6	A	305	PO4	1	0
2	A	301	LPP	6	0
2	D	301	LPP	8	0
2	B	301	LPP	5	0
5	A	304	PT5	3	0
5	D	304	PT5	2	0
5	C	304	PT5	2	0
2	C	301	LPP	5	0

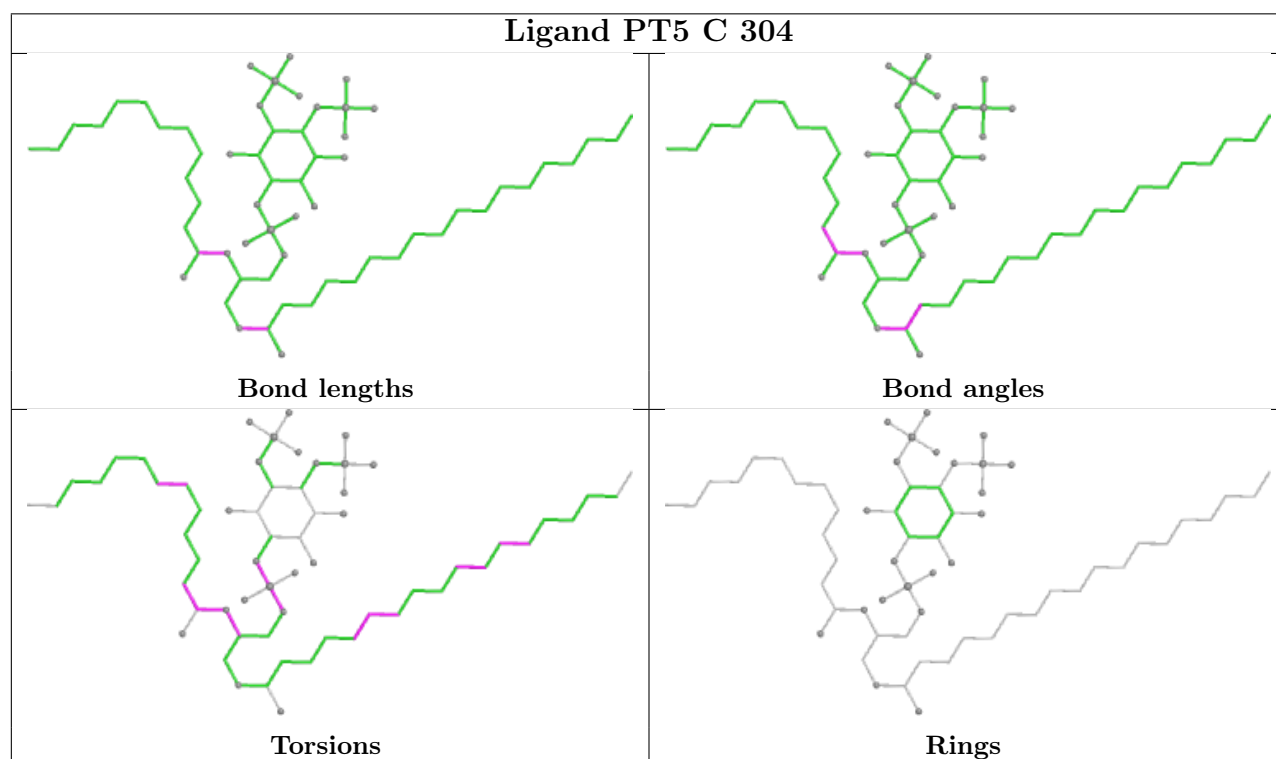
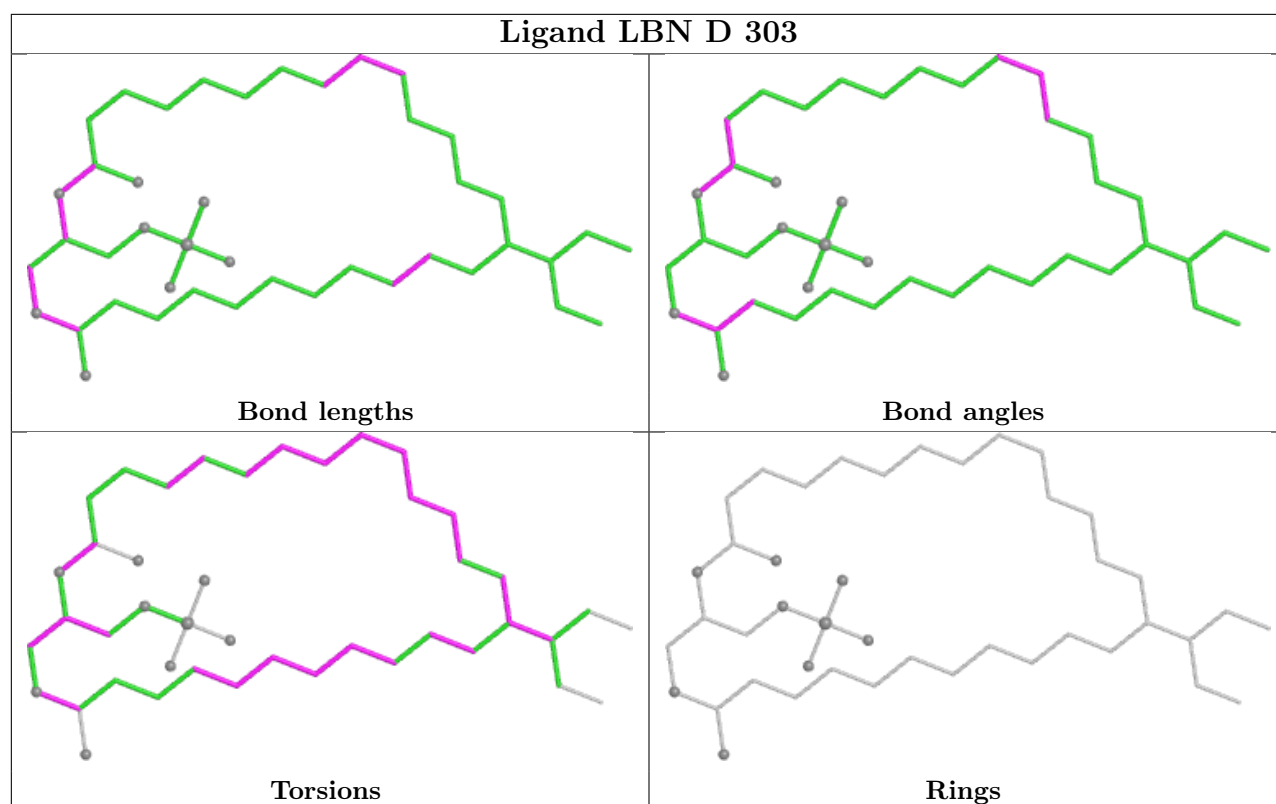
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

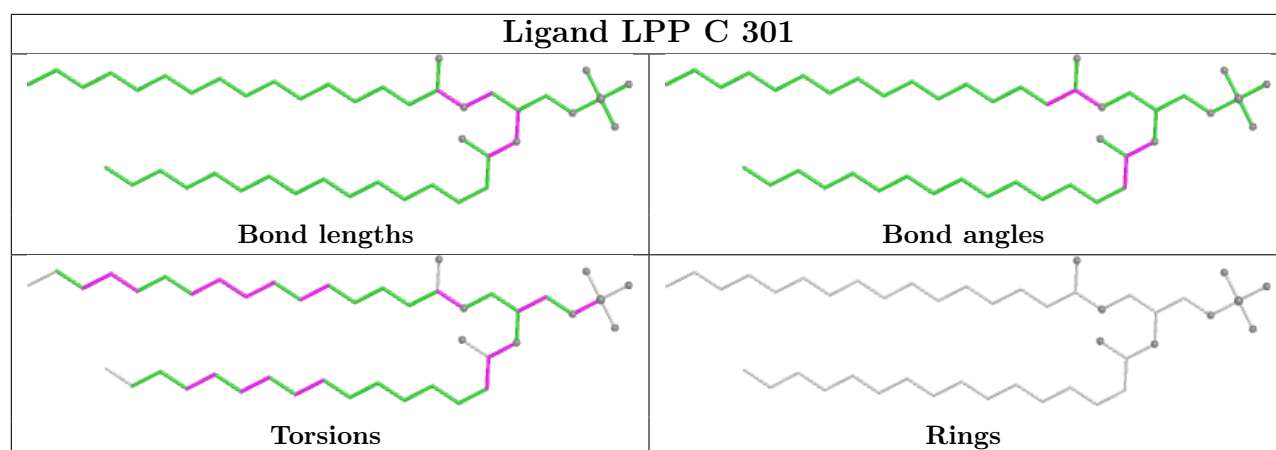












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.