



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 16, 2019 – 12:46 PM EDT

PDB ID : 6PW5
EMDB ID: : EMD-20499
Title : Cryo-EM Structure of Thermo-Sensitive TRP Channel TRP1 from the Alga
Chlamydomonas reinhardtii in Nanodiscs
Authors : McGoldrick, L.L.; Singh, A.K.; Sobolevsky, A.I.
Deposited on : 2019-07-22
Resolution : 3.45 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

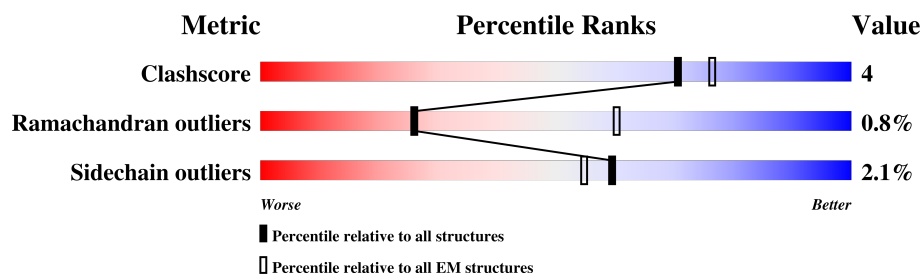
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.45 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	901	72% 9% • 19%
1	B	901	75% 11% • 13%
1	C	901	72% 9% • 19%
1	D	901	74% 11% • 13%

2 Entry composition i

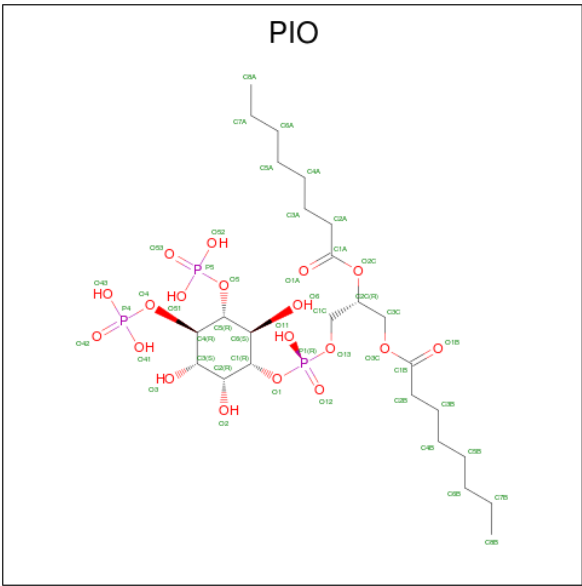
There are 4 unique types of molecules in this entry. The entry contains 24740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRP-like ion channel.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	734	Total 5858	3794	977	1040	47	0	0
1	B	782	Total 6197	3992	1039	1118	48	0	0
1	C	734	Total 5858	3794	977	1040	47	0	0
1	D	782	Total 6197	3992	1039	1118	48	0	0

- Molecule 2 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C₂₅H₄₉O₁₉P₃).



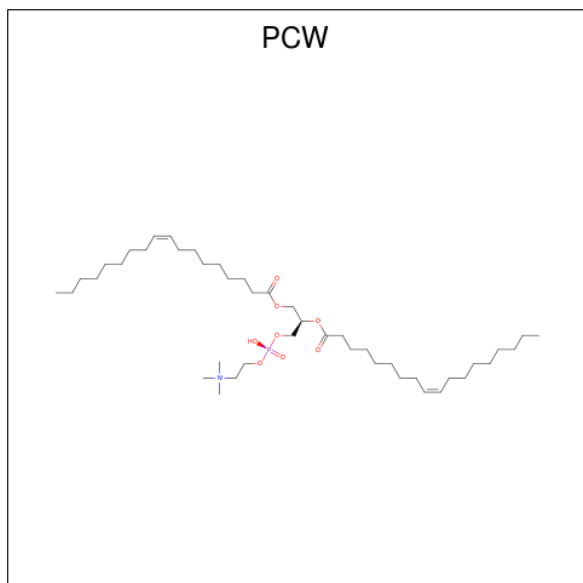
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
2	A	1	Total 47	25	19	3	0
2	B	1	Total 47	25	19	3	0

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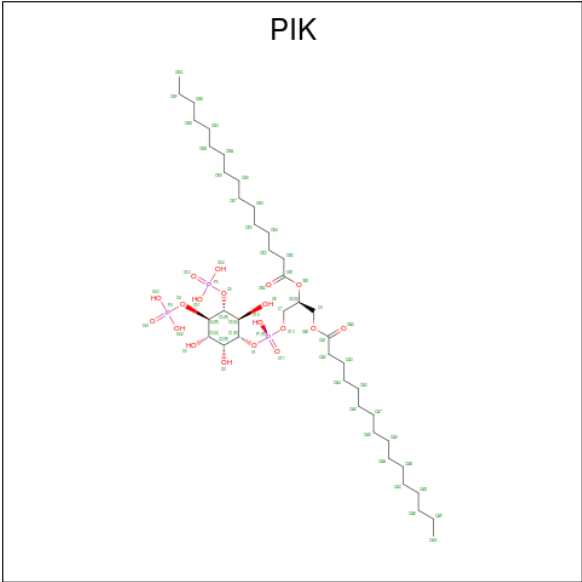
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	O	P	0
			47	25	19	3	
2	D	1	Total	C	O	P	0
			47	25	19	3	

- Molecule 3 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
3	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
3	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
3	D	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 4 is (2S)-3-{[(R)-hydroxy{[(1R,2R,3S,4R,5R,6S)-2,3,6-trihydroxy-4,5-bis(phosphonoxy)cyclohexyl]oxy}phosphoryl]oxy}propane-1,2-diyl dihexadecanoate (three-letter code: PIK) (formula: $C_{41}H_{81}O_{19}P_3$).

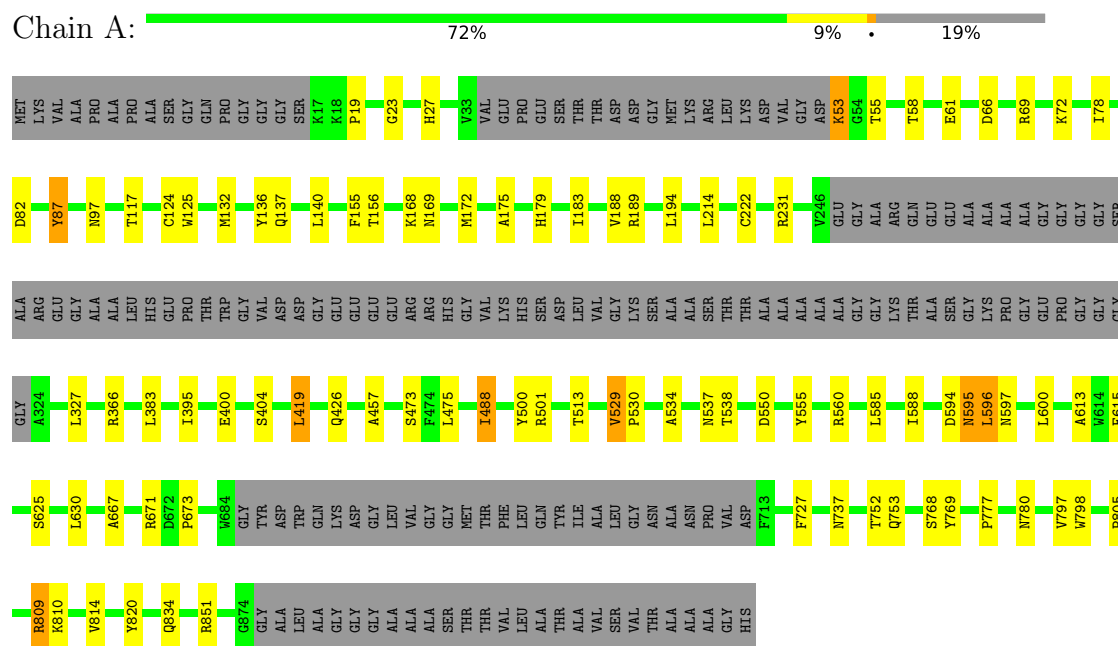


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	O	P	0
			63	41	19	3	
4	B	1	Total	C	O	P	0
			63	41	19	3	
4	C	1	Total	C	O	P	0
			63	41	19	3	
4	D	1	Total	C	O	P	0
			63	41	19	3	

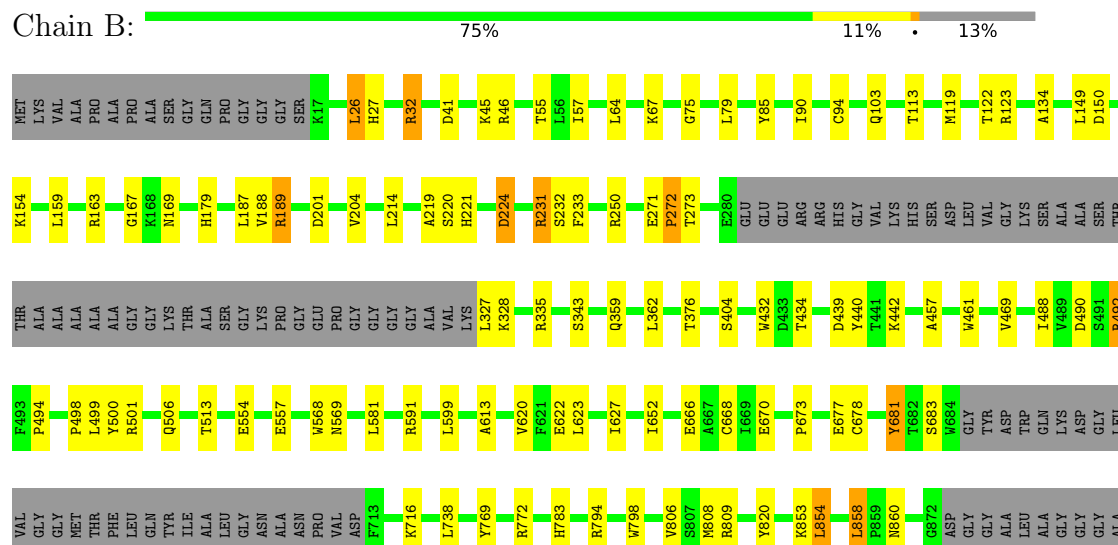
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: TRP-like ion channel



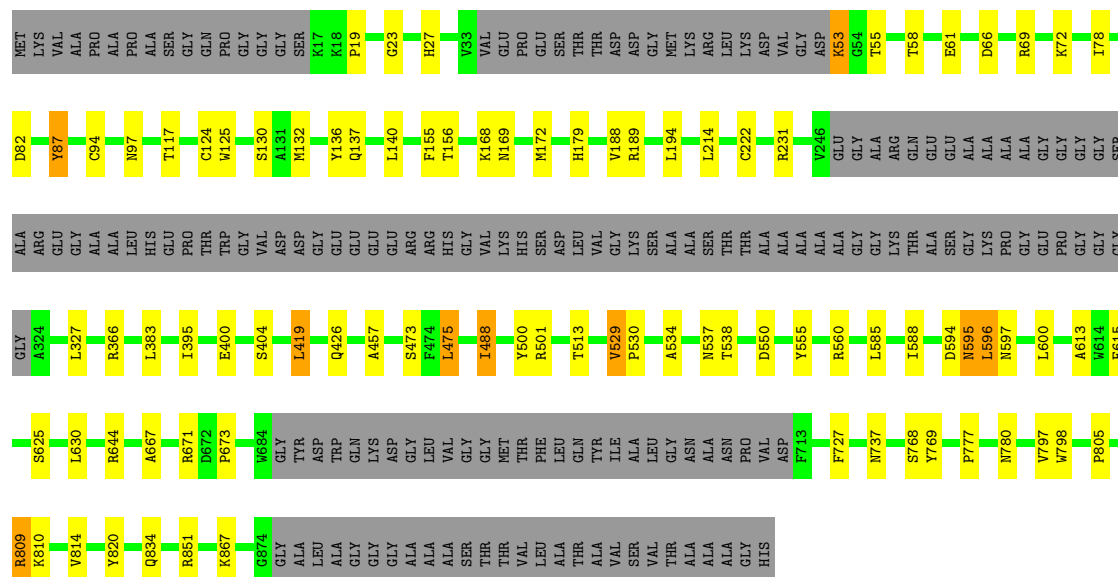
- Molecule 1: TRP-like ion channel



ALA
ALA
SER
THR
THR
VAL
LEU
ALA
THR
ALA
VAL
SER
VAL
THR
ALA
ALA
ALA
GLY
HIS

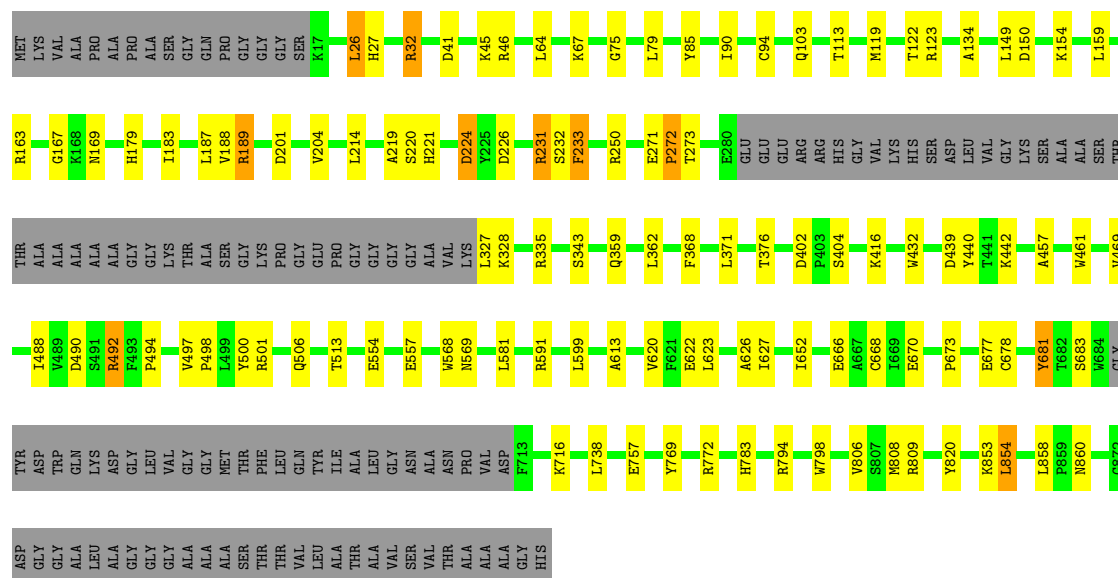
- Molecule 1: TRP-like ion channel

Chain C:  72% 9% 19%



- Molecule 1: TRP-like ion channel

Chain D:  74% 11% 13%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	255973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: PIK, PCW, PIO

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.57	0/5991	0.70	6/8133 (0.1%)
1	B	0.57	0/6336	0.74	6/8601 (0.1%)
1	C	0.57	0/5991	0.70	6/8133 (0.1%)
1	D	0.57	0/6336	0.74	5/8601 (0.1%)
All	All	0.57	0/24654	0.72	23/33468 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	7
1	C	0	3
1	D	0	7
All	All	0	20

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	LEU	CA-CB-CG	8.34	134.48	115.30
1	D	159	LEU	CA-CB-CG	8.33	134.47	115.30
1	D	623	LEU	CB-CG-CD2	-7.06	99.00	111.00
1	B	623	LEU	CB-CG-CD2	-7.05	99.02	111.00
1	C	419	LEU	CA-CB-CG	6.80	130.94	115.30
1	A	419	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	222	CYS	CA-CB-SG	6.25	125.25	114.00
1	C	222	CYS	CA-CB-SG	6.24	125.23	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	596	LEU	CA-CB-CG	6.02	129.14	115.30
1	A	596	LEU	CA-CB-CG	6.00	129.09	115.30
1	A	140	LEU	CB-CG-CD2	-5.33	101.93	111.00
1	C	140	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	B	738	LEU	CA-CB-CG	5.28	127.45	115.30
1	B	79	LEU	CA-CB-CG	5.24	127.36	115.30
1	D	79	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	738	LEU	CA-CB-CG	5.17	127.20	115.30
1	C	327	LEU	CA-CB-CG	5.15	127.14	115.30
1	D	627	ILE	CG1-CB-CG2	-5.15	100.07	111.40
1	A	327	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	627	ILE	CG1-CB-CG2	-5.12	100.15	111.40
1	C	194	LEU	CA-CB-CG	5.07	126.96	115.30
1	A	194	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	858	LEU	CB-CG-CD2	-5.04	102.44	111.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	488	ILE	Peptide
1	A	797	VAL	Peptide
1	A	820	TYR	Peptide
1	B	122	THR	Peptide
1	B	231	ARG	Peptide
1	B	271	GLU	Peptide
1	B	272	PRO	Peptide
1	B	681	TYR	Peptide
1	B	683	SER	Peptide
1	B	75	GLY	Peptide
1	C	488	ILE	Peptide
1	C	797	VAL	Peptide
1	C	820	TYR	Peptide
1	D	122	THR	Peptide
1	D	231	ARG	Peptide
1	D	271	GLU	Peptide
1	D	272	PRO	Peptide
1	D	681	TYR	Peptide
1	D	683	SER	Peptide
1	D	75	GLY	Peptide

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	5858	0	5916	51	0
1	B	6197	0	6215	54	0
1	C	5858	0	5916	54	0
1	D	6197	0	6215	60	0
2	A	47	0	44	2	0
2	B	47	0	44	2	0
2	C	47	0	44	1	0
2	D	47	0	44	2	0
3	A	54	0	82	2	0
3	B	41	0	53	3	0
3	C	54	0	82	2	0
3	D	41	0	53	3	0
4	A	63	0	77	1	0
4	B	63	0	75	1	0
4	C	63	0	77	0	0
4	D	63	0	75	1	0
All	All	24740	0	25012	196	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 4.

All (196) 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:C:53:LYS:N	1:C:58:THR:HG1	1.58	1.02
1:A:53:LYS:N	1:A:58:THR:HG1	1.58	1.00
1:A:625:SER:H	2:A:1001:PIO:H2	1.65	0.62
1:B:440:TYR:HE2	3:B:1002:PCW:H32	1.65	0.61
1:B:27:HIS:HA	1:C:404:SER:HA	1.83	0.61
1:D:469:VAL:HG13	1:D:783:HIS:HB3	1.81	0.61
1:C:501:ARG:NH2	1:C:769:TYR:O	2.33	0.61
1:A:404:SER:HA	1:D:27:HIS:HA	1.83	0.60
1:D:440:TYR:HE2	3:D:1002:PCW:H32	1.65	0.60
1:B:469:VAL:HG13	1:B:783:HIS:HB3	1.82	0.60
1:A:501:ARG:NH2	1:A:769:TYR:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:625:SER:H	2:C:1001:PIO:H2	1.66	0.60
1:C:550:ASP:OD1	1:C:809:ARG:NH1	2.35	0.60
1:D:501:ARG:NH2	1:D:772:ARG:O	2.35	0.59
1:A:529:VAL:HG23	1:A:530:PRO:HD3	1.84	0.59
1:D:568:TRP:NE1	1:D:622:GLU:OE2	2.35	0.59
1:B:568:TRP:NE1	1:B:622:GLU:OE2	2.35	0.59
1:B:201:ASP:HB3	1:B:204:VAL:HG22	1.84	0.59
1:A:550:ASP:OD1	1:A:809:ARG:NH1	2.35	0.58
1:B:219:ALA:O	1:B:221:HIS:ND1	2.36	0.58
1:B:501:ARG:NH2	1:B:772:ARG:O	2.35	0.58
1:D:201:ASP:HB3	1:D:204:VAL:HG22	1.84	0.58
1:D:219:ALA:O	1:D:221:HIS:ND1	2.36	0.58
1:C:529:VAL:HG23	1:C:530:PRO:HD3	1.84	0.58
1:D:45:LYS:HG3	1:D:46:ARG:HG3	1.85	0.57
1:B:45:LYS:HG3	1:B:46:ARG:HG3	1.85	0.57
1:B:442:LYS:HZ1	2:B:1001:PIO:H3	1.69	0.57
1:C:61:GLU:OE2	1:D:492:ARG:NH2	2.38	0.56
1:A:72:LYS:HE2	1:A:78:ILE:HD12	1.87	0.56
1:C:72:LYS:HE2	1:C:78:ILE:HD12	1.87	0.56
1:B:26:LEU:HD12	1:C:404:SER:HB2	1.88	0.56
1:A:66:ASP:OD1	1:A:69:ARG:NH2	2.39	0.56
1:A:61:GLU:OE2	1:B:492:ARG:NH2	2.39	0.56
1:C:169:ASN:H	1:C:172:MET:HB2	1.72	0.55
1:D:64:LEU:HD13	1:D:67:LYS:HD2	1.88	0.55
1:B:64:LEU:HD13	1:B:67:LYS:HD2	1.88	0.55
1:A:404:SER:HB2	1:D:26:LEU:HD12	1.88	0.55
1:C:500:TYR:HB3	3:C:1002:PCW:H19	1.88	0.55
1:A:169:ASN:H	1:A:172:MET:HB2	1.72	0.55
1:C:19:PRO:HB2	1:C:23:GLY:HA3	1.89	0.55
1:A:500:TYR:HB3	3:A:1002:PCW:H19	1.88	0.55
1:A:19:PRO:HB2	1:A:23:GLY:HA3	1.89	0.54
1:B:32:ARG:NH2	1:C:400:GLU:OE2	2.41	0.54
1:C:66:ASP:OD1	1:C:69:ARG:NH2	2.39	0.54
1:D:442:LYS:HZ1	2:D:1001:PIO:H3	1.71	0.54
1:A:400:GLU:OE2	1:D:32:ARG:NH2	2.41	0.54
1:D:204:VAL:HG12	1:D:343:SER:HB3	1.90	0.54
1:B:204:VAL:HG12	1:B:343:SER:HB3	1.90	0.54
1:D:806:VAL:HG22	1:D:808:MET:H	1.73	0.54
1:C:23:GLY:HA2	1:C:27:HIS:HD2	1.74	0.53
1:C:457:ALA:HB1	3:C:1002:PCW:H211	1.89	0.53
1:A:457:ALA:HB1	3:A:1002:PCW:H211	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:VAL:HG22	1:B:808:MET:H	1.73	0.53
1:B:501:ARG:NH1	1:B:769:TYR:O	2.42	0.52
1:D:490:ASP:OD2	1:D:492:ARG:NE	2.40	0.52
1:B:490:ASP:OD2	1:B:492:ARG:NE	2.39	0.52
1:B:90:ILE:HG13	1:B:119:MET:HG2	1.91	0.52
1:D:501:ARG:NH1	1:D:769:TYR:O	2.42	0.52
1:A:23:GLY:HA2	1:A:27:HIS:HD2	1.74	0.52
1:A:168:LYS:NZ	1:B:439:ASP:OD2	2.43	0.52
1:A:851:ARG:HE	1:D:860:ASN:HD21	1.58	0.52
1:D:163:ARG:NH1	1:D:167:GLY:O	2.43	0.52
1:A:555:TYR:OH	1:A:560:ARG:NE	2.41	0.52
1:D:90:ILE:HG13	1:D:119:MET:HG2	1.91	0.52
1:B:513:THR:HG22	1:B:613:ALA:HB1	1.93	0.51
1:C:168:LYS:NZ	1:D:439:ASP:OD2	2.43	0.51
1:B:860:ASN:HD21	1:C:851:ARG:HE	1.58	0.51
1:D:513:THR:HG22	1:D:613:ALA:HB1	1.93	0.51
1:B:163:ARG:NH1	1:B:167:GLY:O	2.43	0.51
1:D:670:GLU:HB3	1:D:677:GLU:HB2	1.93	0.51
1:C:777:PRO:HA	1:C:780:ASN:HB2	1.93	0.51
1:C:534:ALA:HB3	1:C:537:ASN:H	1.76	0.51
1:A:534:ALA:HB3	1:A:537:ASN:H	1.76	0.50
1:B:670:GLU:HB3	1:B:677:GLU:HB2	1.93	0.50
1:C:534:ALA:H	1:C:538:THR:HG23	1.77	0.50
1:B:187:LEU:HD11	1:B:362:LEU:HD23	1.93	0.50
1:A:777:PRO:HA	1:A:780:ASN:HB2	1.93	0.50
1:C:555:TYR:OH	1:C:560:ARG:NE	2.41	0.50
1:C:513:THR:HG22	1:C:613:ALA:HB1	1.94	0.50
1:A:132:MET:O	1:A:136:TYR:N	2.39	0.49
1:A:534:ALA:H	1:A:538:THR:HG23	1.77	0.49
1:D:187:LEU:HD11	1:D:362:LEU:HD23	1.93	0.49
1:A:595:ASN:HD22	1:A:596:LEU:H	1.61	0.49
1:C:366:ARG:NH1	2:D:1001:PIO:O43	2.46	0.49
1:A:366:ARG:NH1	2:B:1001:PIO:O43	2.46	0.49
1:C:595:ASN:HD22	1:C:596:LEU:H	1.61	0.49
1:A:513:THR:HG22	1:A:613:ALA:HB1	1.94	0.48
1:B:666:GLU:HG2	1:B:681:TYR:H	1.78	0.48
1:A:55:THR:HG23	1:A:58:THR:H	1.79	0.48
1:C:117:THR:HG22	1:C:155:PHE:HD1	1.79	0.48
1:C:132:MET:O	1:C:136:TYR:N	2.39	0.48
1:D:666:GLU:HG2	1:D:681:TYR:H	1.78	0.48
1:A:188:VAL:HG21	1:A:214:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:HG22	1:A:155:PHE:HD1	1.79	0.47
1:B:668:CYS:HA	1:B:678:CYS:HA	1.97	0.47
1:B:506:GLN:HE21	1:B:620:VAL:HG12	1.80	0.47
1:D:103:GLN:NE2	1:D:224:ASP:OD1	2.48	0.47
1:C:27:HIS:HA	1:D:404:SER:HA	1.97	0.47
1:C:55:THR:HG23	1:C:58:THR:H	1.79	0.47
1:A:426:GLN:HE21	1:D:179:HIS:HD2	1.63	0.47
1:D:188:VAL:HG21	1:D:214:LEU:HD12	1.97	0.47
1:B:103:GLN:NE2	1:B:224:ASP:OD1	2.48	0.46
1:A:667:ALA:HB3	1:B:599:LEU:HD21	1.98	0.46
1:A:395:ILE:HG22	1:A:834:GLN:HG3	1.97	0.46
1:B:188:VAL:HG21	1:B:214:LEU:HD12	1.97	0.46
1:C:82:ASP:N	1:C:82:ASP:OD1	2.49	0.46
1:C:667:ALA:HB3	1:D:599:LEU:HD21	1.98	0.46
1:A:124:CYS:SG	1:A:125:TRP:N	2.89	0.46
1:B:652:ILE:HA	1:C:615:PHE:HE1	1.81	0.46
1:B:179:HIS:HD2	1:C:426:GLN:HE21	1.63	0.46
1:A:27:HIS:HA	1:B:404:SER:HA	1.97	0.46
1:A:615:PHE:HE1	1:D:652:ILE:HA	1.81	0.46
1:D:668:CYS:HA	1:D:678:CYS:HA	1.97	0.46
1:C:188:VAL:HG21	1:C:214:LEU:HD22	1.96	0.46
1:C:124:CYS:SG	1:C:125:TRP:N	2.89	0.45
1:A:727:PHE:HZ	4:B:1003:PIK:H26	1.82	0.45
1:B:494:PRO:HB3	1:B:500:TYR:HD2	1.82	0.45
1:D:150:ASP:OD2	1:D:189:ARG:NH2	2.49	0.45
1:D:506:GLN:HE21	1:D:620:VAL:HG12	1.80	0.45
1:A:82:ASP:OD1	1:A:82:ASP:N	2.49	0.45
1:B:150:ASP:OD2	1:B:189:ARG:NH2	2.50	0.45
1:C:395:ILE:HG22	1:C:834:GLN:HG3	1.97	0.45
1:C:117:THR:HG21	1:C:156:THR:HG22	1.99	0.45
1:C:23:GLY:HA2	1:C:27:HIS:CD2	2.52	0.45
1:C:727:PHE:HZ	4:D:1003:PIK:H26	1.82	0.45
1:D:149:LEU:HD22	1:D:154:LYS:HG3	1.98	0.45
1:D:359:GLN:NE2	1:D:376:THR:OG1	2.50	0.45
1:A:117:THR:HG21	1:A:156:THR:HG22	1.99	0.44
1:A:596:LEU:HD13	1:A:597:ASN:H	1.82	0.44
1:C:53:LYS:N	1:C:58:THR:OG1	2.36	0.44
1:B:149:LEU:HD22	1:B:154:LYS:HG3	1.98	0.44
1:D:327:LEU:HD12	1:D:328:LYS:HG2	1.98	0.44
1:D:494:PRO:HB3	1:D:500:TYR:HD2	1.82	0.44
1:B:327:LEU:HD12	1:B:328:LYS:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:GLN:NE2	1:B:376:THR:OG1	2.50	0.44
1:A:53:LYS:N	1:A:58:THR:OG1	2.36	0.44
1:B:794:ARG:HA	1:B:798:TRP:HE3	1.83	0.44
1:C:137:GLN:HA	1:C:179:HIS:CE1	2.53	0.44
1:C:585:LEU:HD13	1:C:588:ILE:HD11	2.00	0.44
1:C:596:LEU:HD13	1:C:597:ASN:H	1.82	0.44
1:A:137:GLN:HA	1:A:179:HIS:CE1	2.53	0.43
1:B:457:ALA:O	1:B:461:TRP:N	2.50	0.43
1:B:716:LYS:HB2	1:C:600:LEU:HD12	2.00	0.43
1:B:46:ARG:HD2	1:C:488:ILE:HG22	2.01	0.43
1:B:335:ARG:HH12	1:B:853:LYS:HB2	1.84	0.43
1:D:335:ARG:HH12	1:D:853:LYS:HB2	1.83	0.43
1:B:854:LEU:HD22	1:D:858:LEU:HD21	2.00	0.43
1:B:94:CYS:HB2	1:B:134:ALA:HB2	2.01	0.43
1:D:416:LYS:NZ	1:D:757:GLU:OE2	2.39	0.43
1:A:585:LEU:HD13	1:A:588:ILE:HD11	2.00	0.43
4:A:1003:PIK:H53	4:A:1003:PIK:H59	1.79	0.43
1:C:475:LEU:HA	1:C:475:LEU:HD22	1.86	0.43
1:A:600:LEU:HD12	1:D:716:LYS:HB2	2.00	0.43
1:D:794:ARG:HA	1:D:798:TRP:HE3	1.84	0.43
1:D:233:PHE:HA	1:D:233:PHE:HD1	1.70	0.43
1:A:23:GLY:HA2	1:A:27:HIS:CD2	2.52	0.42
1:C:87:TYR:HE2	3:D:1002:PCW:H63	1.84	0.42
1:A:87:TYR:HE2	3:B:1002:PCW:H63	1.84	0.42
1:B:554:GLU:OE2	1:B:569:ASN:ND2	2.52	0.42
1:B:55:THR:OG1	1:B:55:THR:O	2.37	0.42
1:C:594:ASP:OD1	1:C:594:ASP:N	2.51	0.42
1:D:554:GLU:OE2	1:D:569:ASN:ND2	2.52	0.42
1:A:488:ILE:HG22	1:D:46:ARG:HD2	2.01	0.42
3:B:1002:PCW:H381	3:B:1002:PCW:H412	1.88	0.42
1:B:432:TRP:CD1	1:B:498:PRO:HB2	2.55	0.42
1:D:94:CYS:HB2	1:D:134:ALA:HB2	2.01	0.42
1:D:41:ASP:N	1:D:41:ASP:OD1	2.53	0.42
1:D:490:ASP:OD1	1:D:490:ASP:N	2.50	0.42
1:D:402:ASP:OD1	1:D:402:ASP:N	2.51	0.41
1:D:432:TRP:CD1	1:D:498:PRO:HB2	2.55	0.41
1:D:457:ALA:O	1:D:461:TRP:N	2.50	0.41
1:A:752:THR:HG23	1:A:753:GLN:HG2	2.02	0.41
1:B:41:ASP:OD1	1:B:41:ASP:N	2.53	0.41
1:C:473:SER:HA	1:C:805:PRO:HG2	2.03	0.41
1:D:163:ARG:HD3	1:D:169:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:LEU:HD21	1:D:854:LEU:HD22	2.02	0.41
1:A:175:ALA:HA	1:A:183:ILE:HD11	2.03	0.41
1:C:768:SER:OG	1:C:810:LYS:NZ	2.54	0.41
1:B:432:TRP:CH2	1:B:499:LEU:HD13	2.56	0.41
1:B:55:THR:HG23	1:B:57:ILE:HG22	2.03	0.41
1:B:163:ARG:HD3	1:B:169:ASN:HB3	2.02	0.41
1:C:809:ARG:HG3	1:C:809:ARG:H	1.68	0.41
1:C:867:LYS:HB3	1:C:867:LYS:HE2	1.87	0.41
1:A:473:SER:HA	1:A:805:PRO:HG2	2.02	0.41
1:A:594:ASP:N	1:A:594:ASP:OD1	2.51	0.40
1:C:94:CYS:SG	1:C:130:SER:OG	2.68	0.40
3:D:1002:PCW:H41	3:D:1002:PCW:H73	1.91	0.40
1:D:183:ILE:HD13	1:D:183:ILE:HG21	1.92	0.40
1:D:557:GLU:OE2	1:D:809:ARG:N	2.54	0.40
1:C:644:ARG:HD2	1:D:626:ALA:O	2.21	0.40
1:D:368:PHE:HD1	1:D:371:LEU:HD12	1.87	0.40
1:D:497:VAL:HA	1:D:498:PRO:HD3	1.89	0.40
2:A:1001:PIO:H5A	2:A:1001:PIO:H2AA	1.91	0.40
1:A:768:SER:OG	1:A:810:LYS:NZ	2.54	0.40
1:B:557:GLU:OE2	1:B:809:ARG:N	2.54	0.40
1:D:226:ASP:N	1:D:226:ASP:OD1	2.53	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	726/901 (81%)	645 (89%)	79 (11%)	2 (0%)	43	78
1	B	776/901 (86%)	671 (86%)	95 (12%)	10 (1%)	13	51
1	C	726/901 (81%)	644 (89%)	80 (11%)	2 (0%)	43	78
1	D	776/901 (86%)	672 (87%)	95 (12%)	9 (1%)	14	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3004/3604 (83%)	2632 (88%)	349 (12%)	23 (1%)	26	62

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	THR
1	D	273	THR
1	B	220	SER
1	B	488	ILE
1	D	220	SER
1	D	488	ILE
1	A	673	PRO
1	B	123	ARG
1	B	673	PRO
1	C	673	PRO
1	D	123	ARG
1	D	673	PRO
1	A	798	TRP
1	B	113	THR
1	C	798	TRP
1	D	113	THR
1	B	224	ASP
1	B	232	SER
1	D	224	ASP
1	D	232	SER
1	B	434	THR
1	B	272	PRO
1	D	272	PRO

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	638/740 (86%)	623 (98%)	15 (2%)	52	79
1	B	669/740 (90%)	657 (98%)	12 (2%)	62	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	638/740 (86%)	623 (98%)	15 (2%)	52	79
1	D	669/740 (90%)	657 (98%)	12 (2%)	62	84
All	All	2614/2960 (88%)	2560 (98%)	54 (2%)	59	81

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	87	TYR
1	A	97	ASN
1	A	189	ARG
1	A	231	ARG
1	A	383	LEU
1	A	419	LEU
1	A	475	LEU
1	A	529	VAL
1	A	595	ASN
1	A	630	LEU
1	A	671	ARG
1	A	737	ASN
1	A	809	ARG
1	A	814	VAL
1	B	26	LEU
1	B	32	ARG
1	B	85	TYR
1	B	189	ARG
1	B	231	ARG
1	B	233	PHE
1	B	250	ARG
1	B	492	ARG
1	B	581	LEU
1	B	591	ARG
1	B	820	TYR
1	B	854	LEU
1	C	53	LYS
1	C	87	TYR
1	C	97	ASN
1	C	189	ARG
1	C	231	ARG
1	C	383	LEU
1	C	419	LEU

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Mol	Chain	Res	Type
1	C	475	LEU
1	C	529	VAL
1	C	595	ASN
1	C	630	LEU
1	C	671	ARG
1	C	737	ASN
1	C	809	ARG
1	C	814	VAL
1	D	26	LEU
1	D	32	ARG
1	D	85	TYR
1	D	189	ARG
1	D	231	ARG
1	D	233	PHE
1	D	250	ARG
1	D	492	ARG
1	D	581	LEU
1	D	591	ARG
1	D	820	TYR
1	D	854	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	86	HIS
1	A	97	ASN
1	A	177	GLN
1	A	179	HIS
1	A	595	ASN
1	B	177	GLN
1	B	179	HIS
1	B	359	GLN
1	B	479	GLN
1	B	506	GLN
1	B	676	ASN
1	B	843	ASN
1	B	860	ASN
1	C	27	HIS
1	C	86	HIS
1	C	97	ASN
1	C	177	GLN

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Mol	Chain	Res	Type
1	C	179	HIS
1	C	595	ASN
1	D	177	GLN
1	D	179	HIS
1	D	359	GLN
1	D	479	GLN
1	D	506	GLN
1	D	676	ASN
1	D	860	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
2	PIO	A	1001	-	47,47,47	1.18	6 (12%)	61,65,65	1.17	6 (9%)
3	PCW	A	1002	-	53,53,53	0.98	5 (9%)	59,61,61	1.20	6 (10%)
4	PIK	A	1003	-	63,63,63	1.03	5 (7%)	77,81,81	0.98	4 (5%)
2	PIO	B	1001	-	47,47,47	1.19	5 (10%)	61,65,65	1.07	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PCW	B	1002	-	40,40,53	1.15	5 (12%)	46,48,61	1.03	2 (4%)
4	PIK	B	1003	-	63,63,63	1.06	6 (9%)	77,81,81	1.00	2 (2%)
2	PIO	C	1001	-	47,47,47	1.18	6 (12%)	61,65,65	1.17	6 (9%)
3	PCW	C	1002	-	53,53,53	0.99	5 (9%)	59,61,61	1.19	6 (10%)
4	PIK	C	1003	-	63,63,63	1.04	5 (7%)	77,81,81	0.99	5 (6%)
2	PIO	D	1001	-	47,47,47	1.19	5 (10%)	61,65,65	1.07	3 (4%)
3	PCW	D	1002	-	40,40,53	1.15	5 (12%)	46,48,61	1.03	2 (4%)
4	PIK	D	1003	-	63,63,63	1.06	6 (9%)	77,81,81	1.00	2 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PIO	A	1001	-	-	16/44/68/68	0/1/1/1
3	PCW	A	1002	-	-	27/57/57/57	-
4	PIK	A	1003	-	-	21/60/84/84	0/1/1/1
2	PIO	B	1001	-	-	18/44/68/68	0/1/1/1
3	PCW	B	1002	-	-	20/44/44/57	-
4	PIK	B	1003	-	-	27/60/84/84	0/1/1/1
2	PIO	C	1001	-	-	16/44/68/68	0/1/1/1
3	PCW	C	1002	-	-	27/57/57/57	-
4	PIK	C	1003	-	-	23/60/84/84	0/1/1/1
2	PIO	D	1001	-	-	18/44/68/68	0/1/1/1
3	PCW	D	1002	-	-	20/44/44/57	-
4	PIK	D	1003	-	-	27/60/84/84	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	PIO	P4-O4	3.40	1.65	1.59
2	B	1001	PIO	P4-O4	3.40	1.65	1.59
4	B	1003	PIK	P4-O4	3.29	1.65	1.59
4	A	1003	PIK	P5-O5	3.24	1.65	1.59
4	D	1003	PIK	P4-O4	3.23	1.65	1.59
4	C	1003	PIK	P5-O5	3.22	1.65	1.59
4	D	1003	PIK	P5-O5	3.16	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	PIK	P5-O5	3.14	1.65	1.59
2	C	1001	PIO	P4-O4	3.07	1.65	1.59
2	A	1001	PIO	P4-O4	3.04	1.65	1.59
2	B	1001	PIO	P5-O5	2.96	1.64	1.59
4	C	1003	PIK	P4-O4	2.95	1.64	1.59
2	D	1001	PIO	P5-O5	2.92	1.64	1.59
4	A	1003	PIK	P4-O4	2.91	1.64	1.59
2	C	1001	PIO	P5-O5	2.83	1.64	1.59
2	A	1001	PIO	P5-O5	2.81	1.64	1.59
3	D	1002	PCW	O2-C2	-2.79	1.39	1.46
3	B	1002	PCW	O2-C2	-2.78	1.39	1.46
4	D	1003	PIK	OB1-C8	-2.58	1.40	1.46
4	B	1003	PIK	OB1-C8	-2.57	1.40	1.46
2	C	1001	PIO	O3C-C3C	-2.51	1.39	1.45
2	A	1001	PIO	O3C-C3C	-2.51	1.39	1.45
2	B	1001	PIO	O2C-C2C	-2.48	1.40	1.46
2	D	1001	PIO	O2C-C2C	-2.47	1.40	1.46
4	C	1003	PIK	OB1-C8	-2.45	1.40	1.46
4	A	1003	PIK	OB1-C8	-2.44	1.40	1.46
4	C	1003	PIK	OA1-CA1	2.43	1.40	1.33
2	C	1001	PIO	O2C-C1A	2.43	1.41	1.34
4	A	1003	PIK	OA1-CA1	2.42	1.40	1.33
4	B	1003	PIK	P1-O1	2.42	1.66	1.60
2	A	1001	PIO	O2C-C1A	2.39	1.41	1.34
4	D	1003	PIK	OA1-CA1	2.39	1.40	1.33
4	B	1003	PIK	OA1-CA1	2.39	1.40	1.33
4	D	1003	PIK	P1-O1	2.39	1.66	1.60
3	A	1002	PCW	O3-C3	-2.36	1.39	1.45
2	D	1001	PIO	O3C-C3C	-2.36	1.39	1.45
2	B	1001	PIO	O3C-C3C	-2.36	1.39	1.45
3	B	1002	PCW	O3-C11	2.35	1.40	1.33
3	C	1002	PCW	O3-C3	-2.35	1.39	1.45
4	C	1003	PIK	OB1-CB1	2.32	1.40	1.34
4	A	1003	PIK	OB1-CB1	2.32	1.40	1.34
2	A	1001	PIO	O2C-C2C	-2.32	1.40	1.46
2	C	1001	PIO	O2C-C2C	-2.32	1.40	1.46
3	D	1002	PCW	O3-C11	2.31	1.40	1.33
3	C	1002	PCW	C6-N	-2.26	1.43	1.50
2	D	1001	PIO	O2C-C1A	2.25	1.40	1.34
3	A	1002	PCW	C6-N	-2.24	1.43	1.50
2	B	1001	PIO	O2C-C1A	2.21	1.40	1.34
3	D	1002	PCW	O3-C3	-2.20	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	PCW	C6-N	-2.19	1.43	1.50
3	B	1002	PCW	O3-C3	-2.19	1.40	1.45
2	A	1001	PIO	O3C-C1B	2.16	1.39	1.33
2	C	1001	PIO	O3C-C1B	2.16	1.39	1.33
3	B	1002	PCW	C6-N	-2.16	1.43	1.50
3	C	1002	PCW	O3-C11	2.15	1.39	1.33
3	A	1002	PCW	O3-C11	2.14	1.39	1.33
3	C	1002	PCW	C5-N	-2.11	1.44	1.51
3	B	1002	PCW	C5-N	-2.09	1.44	1.51
3	A	1002	PCW	O2-C31	2.08	1.40	1.34
3	D	1002	PCW	C5-N	-2.08	1.44	1.51
3	A	1002	PCW	C5-N	-2.07	1.44	1.51
3	C	1002	PCW	O2-C31	2.07	1.40	1.34
4	D	1003	PIK	OB1-CB1	2.04	1.40	1.34
4	B	1003	PIK	OB1-CB1	2.04	1.40	1.34

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	PIO	O2C-C1A-C2A	4.82	122.03	111.51
2	D	1001	PIO	O2C-C1A-C2A	4.82	122.03	111.51
2	A	1001	PIO	O2C-C1A-C2A	4.06	120.38	111.51
2	C	1001	PIO	O2C-C1A-C2A	4.06	120.37	111.51
3	D	1002	PCW	O2-C31-C32	3.98	120.19	111.51
3	B	1002	PCW	O2-C31-C32	3.98	120.19	111.51
4	D	1003	PIK	OB1-CB1-CB2	3.80	119.81	111.51
4	B	1003	PIK	OB1-CB1-CB2	3.79	119.78	111.51
4	C	1003	PIK	OB1-CB1-CB2	3.34	118.80	111.51
4	A	1003	PIK	OB1-CB1-CB2	3.33	118.77	111.51
3	A	1002	PCW	O3-C3-C2	3.26	117.95	108.43
3	C	1002	PCW	O3-C3-C2	3.25	117.92	108.43
3	A	1002	PCW	O2-C31-C32	3.12	118.33	111.51
3	C	1002	PCW	O2-C31-C32	3.10	118.28	111.51
2	C	1001	PIO	O3C-C1B-C2B	3.06	121.76	111.93
3	C	1002	PCW	C2-O2-C31	3.06	125.44	117.82
2	A	1001	PIO	C3-C2-C1	3.06	116.66	109.67
2	A	1001	PIO	O3C-C1B-C2B	3.05	121.74	111.93
3	A	1002	PCW	C2-O2-C31	3.05	125.43	117.82
2	C	1001	PIO	C3-C2-C1	3.04	116.63	109.67
2	C	1001	PIO	C2-C3-C4	3.03	116.60	109.67
2	A	1001	PIO	C2-C3-C4	3.02	116.57	109.67
4	D	1003	PIK	OA1-CA1-CA2	2.89	121.22	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	PIK	OA1-CA1-CA2	2.88	121.16	111.93
3	C	1002	PCW	C33-C32-C31	-2.74	103.73	113.62
3	A	1002	PCW	C33-C32-C31	-2.74	103.73	113.62
4	C	1003	PIK	OA1-CA1-CA2	2.68	120.53	111.93
4	A	1003	PIK	OA1-CA1-CA2	2.67	120.49	111.93
2	B	1001	PIO	O3C-C1B-C2B	2.63	120.39	111.93
2	D	1001	PIO	O3C-C1B-C2B	2.61	120.31	111.93
3	B	1002	PCW	O3-C11-C12	2.57	120.17	111.93
3	D	1002	PCW	O3-C11-C12	2.56	120.16	111.93
3	C	1002	PCW	O3-C11-C12	2.50	119.94	111.93
3	A	1002	PCW	O3-C11-C12	2.48	119.89	111.93
4	A	1003	PIK	O1-C1-C6	2.46	114.40	108.66
4	A	1003	PIK	C9-C8-C7	-2.40	106.06	111.79
4	C	1003	PIK	C9-C8-C7	-2.34	106.21	111.79
3	A	1002	PCW	O2-C2-C3	2.33	116.82	108.40
3	C	1002	PCW	O2-C2-C3	2.32	116.80	108.40
4	C	1003	PIK	O1-C1-C6	2.24	113.87	108.66
2	D	1001	PIO	O2C-C1A-O1A	-2.09	118.57	123.71
2	B	1001	PIO	O2C-C1A-O1A	-2.08	118.60	123.71
4	C	1003	PIK	C6-C1-C2	2.07	113.84	110.85
2	C	1001	PIO	C6-C1-C2	2.06	113.82	110.85
2	A	1001	PIO	C6-C1-C2	2.05	113.81	110.85
2	A	1001	PIO	C3C-C2C-C1C	-2.03	106.94	111.79
2	C	1001	PIO	C3C-C2C-C1C	-2.03	106.95	111.79

There are no chirality outliers.

All (260) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	PCW	C1-O3P-P-O2P
3	A	1002	PCW	C1-O3P-P-O4P
4	C	1003	PIK	C6-C1-O1-P1
4	C	1003	PIK	CA2-CA1-OA1-C9
2	D	1001	PIO	C2-C1-O1-P1
2	D	1001	PIO	C6-C1-O1-P1
2	D	1001	PIO	O1A-C1A-O2C-C2C
2	D	1001	PIO	C2A-C1A-O2C-C2C
4	A	1003	PIK	C6-C1-O1-P1
4	A	1003	PIK	CA2-CA1-OA1-C9
4	D	1003	PIK	C7-O13-P1-O12
4	D	1003	PIK	C8-C7-O13-P1
2	A	1001	PIO	C1-O1-P1-O13

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Mol	Chain	Res	Type	Atoms
2	A	1001	PIO	C1C-O13-P1-O1
2	A	1001	PIO	C1C-O13-P1-O11
2	A	1001	PIO	C1C-O13-P1-O12
2	A	1001	PIO	C4-O4-P4-O42
2	A	1001	PIO	C2A-C1A-O2C-C2C
3	B	1002	PCW	C40-C41-C42-C43
3	B	1002	PCW	C4-O4P-P-O1P
3	B	1002	PCW	C4-O4P-P-O2P
3	B	1002	PCW	C4-O4P-P-O3P
4	B	1003	PIK	C7-O13-P1-O12
4	B	1003	PIK	C8-C7-O13-P1
3	C	1002	PCW	C1-O3P-P-O2P
3	C	1002	PCW	C1-O3P-P-O4P
3	D	1002	PCW	C40-C41-C42-C43
3	D	1002	PCW	C4-O4P-P-O1P
3	D	1002	PCW	C4-O4P-P-O2P
3	D	1002	PCW	C4-O4P-P-O3P
2	C	1001	PIO	C1-O1-P1-O13
2	C	1001	PIO	C1C-O13-P1-O1
2	C	1001	PIO	C1C-O13-P1-O11
2	C	1001	PIO	C1C-O13-P1-O12
2	C	1001	PIO	C4-O4-P4-O42
2	C	1001	PIO	C2A-C1A-O2C-C2C
2	B	1001	PIO	C2-C1-O1-P1
2	B	1001	PIO	C6-C1-O1-P1
2	B	1001	PIO	O1A-C1A-O2C-C2C
2	B	1001	PIO	C2A-C1A-O2C-C2C
4	C	1003	PIK	OA2-CA1-OA1-C9
4	A	1003	PIK	OA2-CA1-OA1-C9
3	B	1002	PCW	C12-C11-O3-C3
3	D	1002	PCW	C12-C11-O3-C3
2	A	1001	PIO	O1A-C1A-O2C-C2C
2	C	1001	PIO	O1A-C1A-O2C-C2C
3	B	1002	PCW	O11-C11-O3-C3
3	D	1002	PCW	O11-C11-O3-C3
2	A	1001	PIO	C2C-C1C-O13-P1
2	C	1001	PIO	C2C-C1C-O13-P1
2	D	1001	PIO	C2B-C1B-O3C-C3C
2	B	1001	PIO	C2B-C1B-O3C-C3C
2	D	1001	PIO	O1B-C1B-O3C-C3C
2	B	1001	PIO	O1B-C1B-O3C-C3C
4	D	1003	PIK	CA2-CA1-OA1-C9

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Mol	Chain	Res	Type	Atoms
4	B	1003	PIK	CA2-CA1-OA1-C9
4	C	1003	PIK	CB1-CB2-CB3-CB4
3	A	1002	PCW	C11-C12-C13-C14
2	D	1001	PIO	C1A-C2A-C3A-C4A
4	A	1003	PIK	CB1-CB2-CB3-CB4
3	C	1002	PCW	C11-C12-C13-C14
2	B	1001	PIO	C1A-C2A-C3A-C4A
2	A	1001	PIO	C1B-C2B-C3B-C4B
2	C	1001	PIO	C1B-C2B-C3B-C4B
4	D	1003	PIK	CB1-CB2-CB3-CB4
4	B	1003	PIK	CB1-CB2-CB3-CB4
3	A	1002	PCW	C4-O4P-P-O3P
2	D	1001	PIO	C1C-O13-P1-O1
4	D	1003	PIK	C7-O13-P1-O1
3	B	1002	PCW	C1-O3P-P-O4P
4	B	1003	PIK	C7-O13-P1-O1
3	C	1002	PCW	C4-O4P-P-O3P
3	D	1002	PCW	C1-O3P-P-O4P
2	B	1001	PIO	C1C-O13-P1-O1
4	D	1003	PIK	OA2-CA1-OA1-C9
4	B	1003	PIK	OA2-CA1-OA1-C9
3	A	1002	PCW	C12-C13-C14-C15
3	C	1002	PCW	C12-C13-C14-C15
4	C	1003	PIK	CB6-CB7-CB8-CB9
2	A	1001	PIO	C2B-C1B-O3C-C3C
2	C	1001	PIO	C2B-C1B-O3C-C3C
4	B	1003	PIK	CB2-CB3-CB4-CB5
3	D	1002	PCW	C12-C13-C14-C15
4	A	1003	PIK	CB6-CB7-CB8-CB9
4	D	1003	PIK	CB2-CB3-CB4-CB5
3	B	1002	PCW	C12-C13-C14-C15
3	A	1002	PCW	C33-C34-C35-C36
3	C	1002	PCW	C33-C34-C35-C36
4	B	1003	PIK	CB6-CB7-CB8-CB9
4	D	1003	PIK	CB6-CB7-CB8-CB9
4	A	1003	PIK	CA5-CA6-CA7-CA8
3	D	1002	PCW	C32-C33-C34-C35
4	D	1003	PIK	CA2-CA3-CA4-CA5
4	D	1003	PIK	CA5-CA6-CA7-CA8
3	B	1002	PCW	C32-C33-C34-C35
4	B	1003	PIK	CA2-CA3-CA4-CA5
4	B	1003	PIK	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
4	D	1003	PIK	CB8-CB9-CBA-CBB
4	B	1003	PIK	CB8-CB9-CBA-CBB
3	A	1002	PCW	C32-C33-C34-C35
3	B	1002	PCW	C13-C14-C15-C16
3	C	1002	PCW	C32-C33-C34-C35
3	D	1002	PCW	C13-C14-C15-C16
2	C	1001	PIO	C3B-C4B-C5B-C6B
2	A	1001	PIO	C3B-C4B-C5B-C6B
4	C	1003	PIK	CB7-CB8-CB9-CBA
3	A	1002	PCW	C34-C35-C36-C37
4	C	1003	PIK	CA5-CA6-CA7-CA8
3	C	1002	PCW	C34-C35-C36-C37
4	D	1003	PIK	CB3-CB4-CB5-CB6
4	B	1003	PIK	CB3-CB4-CB5-CB6
4	A	1003	PIK	OB2-CB1-OB1-C8
4	C	1003	PIK	CB2-CB1-OB1-C8
4	A	1003	PIK	CB2-CB1-OB1-C8
3	A	1002	PCW	O4P-C4-C5-N
3	B	1002	PCW	O4P-C4-C5-N
3	C	1002	PCW	O4P-C4-C5-N
3	D	1002	PCW	O4P-C4-C5-N
4	C	1003	PIK	CB4-CB5-CB6-CB7
3	A	1002	PCW	C31-C32-C33-C34
3	C	1002	PCW	C31-C32-C33-C34
4	C	1003	PIK	OB2-CB1-OB1-C8
2	A	1001	PIO	O1B-C1B-O3C-C3C
2	C	1001	PIO	O1B-C1B-O3C-C3C
3	A	1002	PCW	C12-C11-O3-C3
3	C	1002	PCW	C12-C11-O3-C3
4	D	1003	PIK	CA1-CA2-CA3-CA4
4	B	1003	PIK	CA1-CA2-CA3-CA4
3	B	1002	PCW	C31-C32-C33-C34
3	D	1002	PCW	C31-C32-C33-C34
3	B	1002	PCW	O3P-C1-C2-O2
3	D	1002	PCW	O3P-C1-C2-O2
4	A	1003	PIK	CB4-CB5-CB6-CB7
4	D	1003	PIK	CBA-CBB-CBC-CBD
4	B	1003	PIK	CBA-CBB-CBC-CBD
2	D	1001	PIO	C3A-C4A-C5A-C6A
2	B	1001	PIO	C3A-C4A-C5A-C6A
3	A	1002	PCW	O11-C11-O3-C3
3	C	1002	PCW	O11-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
4	A	1003	PIK	CB5-CB6-CB7-CB8
2	B	1001	PIO	C3B-C4B-C5B-C6B
2	D	1001	PIO	C3B-C4B-C5B-C6B
4	A	1003	PIK	CA1-CA2-CA3-CA4
4	D	1003	PIK	CBB-CBC-CBD-CBE
4	B	1003	PIK	CBB-CBC-CBD-CBE
4	B	1003	PIK	CA4-CA5-CA6-CA7
4	D	1003	PIK	CA4-CA5-CA6-CA7
3	D	1002	PCW	C34-C35-C36-C37
4	A	1003	PIK	CB7-CB8-CB9-CBA
3	B	1002	PCW	C34-C35-C36-C37
3	A	1002	PCW	C20-C21-C22-C23
3	C	1002	PCW	C20-C21-C22-C23
4	C	1003	PIK	CB5-CB6-CB7-CB8
4	D	1003	PIK	CBC-CBD-CBE-CBF
4	B	1003	PIK	CBC-CBD-CBE-CBF
3	B	1002	PCW	C33-C34-C35-C36
3	B	1002	PCW	C35-C36-C37-C38
4	C	1003	PIK	O13-C7-C8-C9
4	A	1003	PIK	O13-C7-C8-C9
4	D	1003	PIK	O13-C7-C8-C9
3	B	1002	PCW	O3P-C1-C2-C3
3	D	1002	PCW	O3P-C1-C2-C3
3	D	1002	PCW	C33-C34-C35-C36
3	D	1002	PCW	C35-C36-C37-C38
3	A	1002	PCW	C1-C2-C3-O3
3	C	1002	PCW	C1-C2-C3-O3
3	A	1002	PCW	C36-C37-C38-C39
3	C	1002	PCW	C36-C37-C38-C39
2	A	1001	PIO	C1-O1-P1-O12
2	C	1001	PIO	C1-O1-P1-O12
4	C	1003	PIK	CA1-CA2-CA3-CA4
3	A	1002	PCW	O2-C2-C3-O3
3	C	1002	PCW	O2-C2-C3-O3
3	A	1002	PCW	C23-C24-C25-C26
3	C	1002	PCW	C23-C24-C25-C26
4	B	1003	PIK	O13-C7-C8-C9
4	C	1003	PIK	O13-C7-C8-OB1
4	A	1003	PIK	O13-C7-C8-OB1
4	A	1003	PIK	CA7-CA8-CA9-CAA
3	A	1002	PCW	C4-O4P-P-O1P
3	A	1002	PCW	C4-O4P-P-O2P

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Mol	Chain	Res	Type	Atoms
2	D	1001	PIO	C1C-O13-P1-O12
4	D	1003	PIK	C7-O13-P1-O11
3	B	1002	PCW	C1-O3P-P-O2P
4	B	1003	PIK	C7-O13-P1-O11
3	C	1002	PCW	C4-O4P-P-O1P
3	C	1002	PCW	C4-O4P-P-O2P
3	D	1002	PCW	C1-O3P-P-O2P
2	B	1001	PIO	C1C-O13-P1-O12
4	D	1003	PIK	CA8-CA9-CAA-CAB
4	B	1003	PIK	CA8-CA9-CAA-CAB
4	B	1003	PIK	CAB-CAC-CAD-CAE
4	D	1003	PIK	CAB-CAC-CAD-CAE
4	D	1003	PIK	OA1-CA1-CA2-CA3
4	B	1003	PIK	OA1-CA1-CA2-CA3
4	D	1003	PIK	O13-C7-C8-OB1
4	B	1003	PIK	O13-C7-C8-OB1
4	C	1003	PIK	CAB-CAC-CAD-CAE
4	A	1003	PIK	CB8-CB9-CBA-CBB
4	C	1003	PIK	CA9-CAA-CAB-CAC
4	A	1003	PIK	CA3-CA4-CA5-CA6
4	C	1003	PIK	CBB-CBC-CBD-CBE
4	C	1003	PIK	CB8-CB9-CBA-CBB
4	D	1003	PIK	C2-C1-O1-P1
4	B	1003	PIK	C2-C1-O1-P1
4	C	1003	PIK	CBA-CBB-CBC-CBD
3	A	1002	PCW	C44-C45-C46-C47
3	C	1002	PCW	C44-C45-C46-C47
2	D	1001	PIO	C1B-C2B-C3B-C4B
3	C	1002	PCW	C43-C44-C45-C46
3	A	1002	PCW	C43-C44-C45-C46
2	B	1001	PIO	C1B-C2B-C3B-C4B
4	A	1003	PIK	CBA-CBB-CBC-CBD
4	C	1003	PIK	CA3-CA4-CA5-CA6
3	A	1002	PCW	C14-C15-C16-C17
3	C	1002	PCW	C14-C15-C16-C17
4	A	1003	PIK	CB9-CBA-CBB-CBC
2	B	1001	PIO	C4B-C5B-C6B-C7B
2	D	1001	PIO	C4B-C5B-C6B-C7B
3	A	1002	PCW	O2-C31-C32-C33
3	C	1002	PCW	O2-C31-C32-C33
2	A	1001	PIO	O2C-C1A-C2A-C3A
2	C	1001	PIO	O2C-C1A-C2A-C3A

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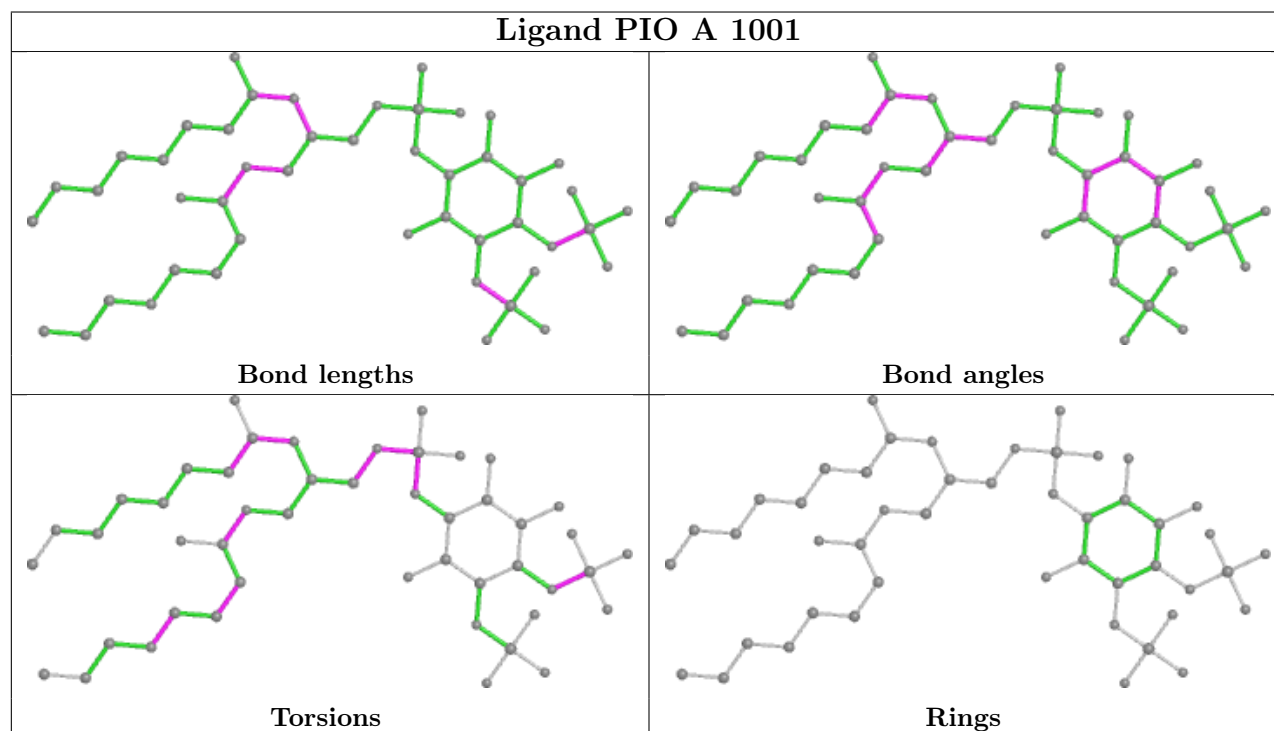
Mol	Chain	Res	Type	Atoms
3	C	1002	PCW	C16-C17-C18-C19
2	D	1001	PIO	O2C-C1A-C2A-C3A
2	B	1001	PIO	O2C-C1A-C2A-C3A
3	B	1002	PCW	O31-C31-O2-C2
3	D	1002	PCW	O31-C31-O2-C2
3	A	1002	PCW	C16-C17-C18-C19
3	A	1002	PCW	C39-C40-C41-C42
3	C	1002	PCW	C39-C40-C41-C42
4	C	1003	PIK	CBC-CBD-CBE-CBF
2	B	1001	PIO	O3C-C1B-C2B-C3B
2	D	1001	PIO	C5-O5-P5-O52
4	D	1003	PIK	C4-O4-P4-O43
2	A	1001	PIO	C4-O4-P4-O43
4	B	1003	PIK	C4-O4-P4-O43
2	C	1001	PIO	C4-O4-P4-O43
2	B	1001	PIO	C5-O5-P5-O52
4	C	1003	PIK	CA7-CA8-CA9-CAA
2	D	1001	PIO	O3C-C1B-C2B-C3B
2	D	1001	PIO	O1A-C1A-C2A-C3A
2	B	1001	PIO	O1A-C1A-C2A-C3A
3	A	1002	PCW	O31-C31-C32-C33
3	C	1002	PCW	O31-C31-C32-C33
3	B	1002	PCW	C15-C16-C17-C18
3	D	1002	PCW	C15-C16-C17-C18
4	A	1003	PIK	CBC-CBD-CBE-CBF
2	A	1001	PIO	O1A-C1A-C2A-C3A
2	C	1001	PIO	O1A-C1A-C2A-C3A
4	C	1003	PIK	OA1-CA1-CA2-CA3
3	A	1002	PCW	C22-C23-C24-C25
4	B	1003	PIK	CA3-CA4-CA5-CA6
4	D	1003	PIK	CA3-CA4-CA5-CA6
2	D	1001	PIO	C2C-C1C-O13-P1
2	B	1001	PIO	C2C-C1C-O13-P1
3	C	1002	PCW	C22-C23-C24-C25
4	A	1003	PIK	OA1-CA1-CA2-CA3
4	D	1003	PIK	OB1-CB1-CB2-CB3
4	B	1003	PIK	OB1-CB1-CB2-CB3

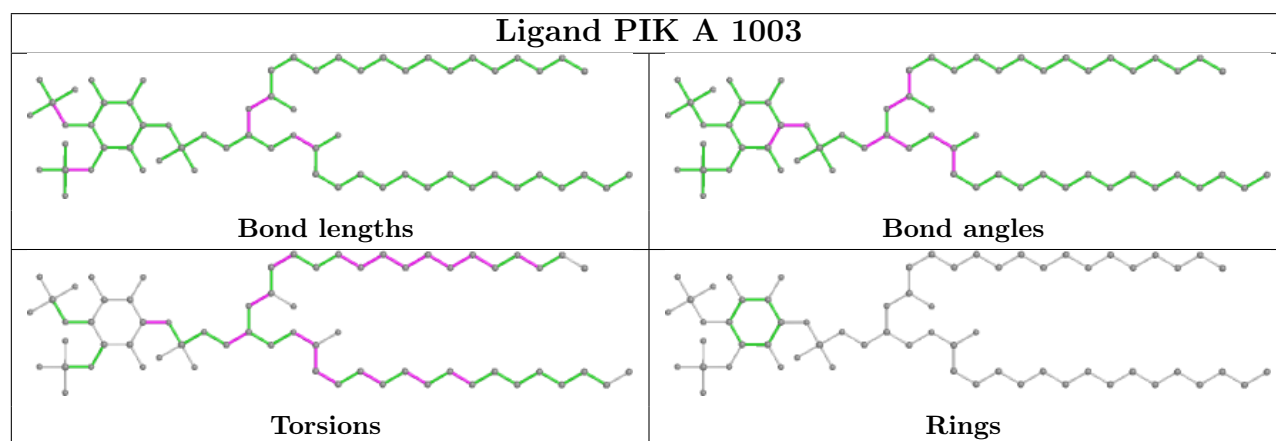
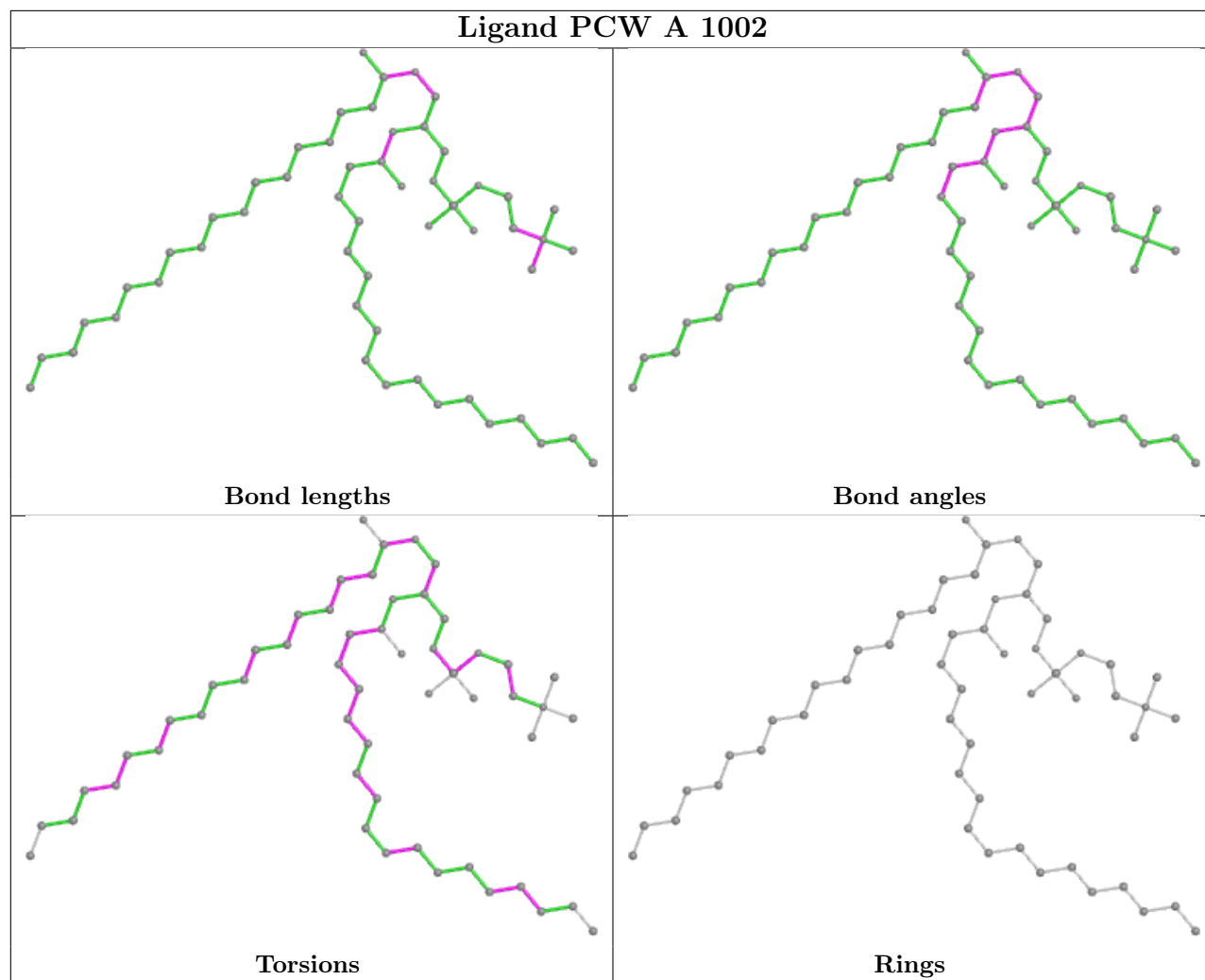
There are no ring outliers.

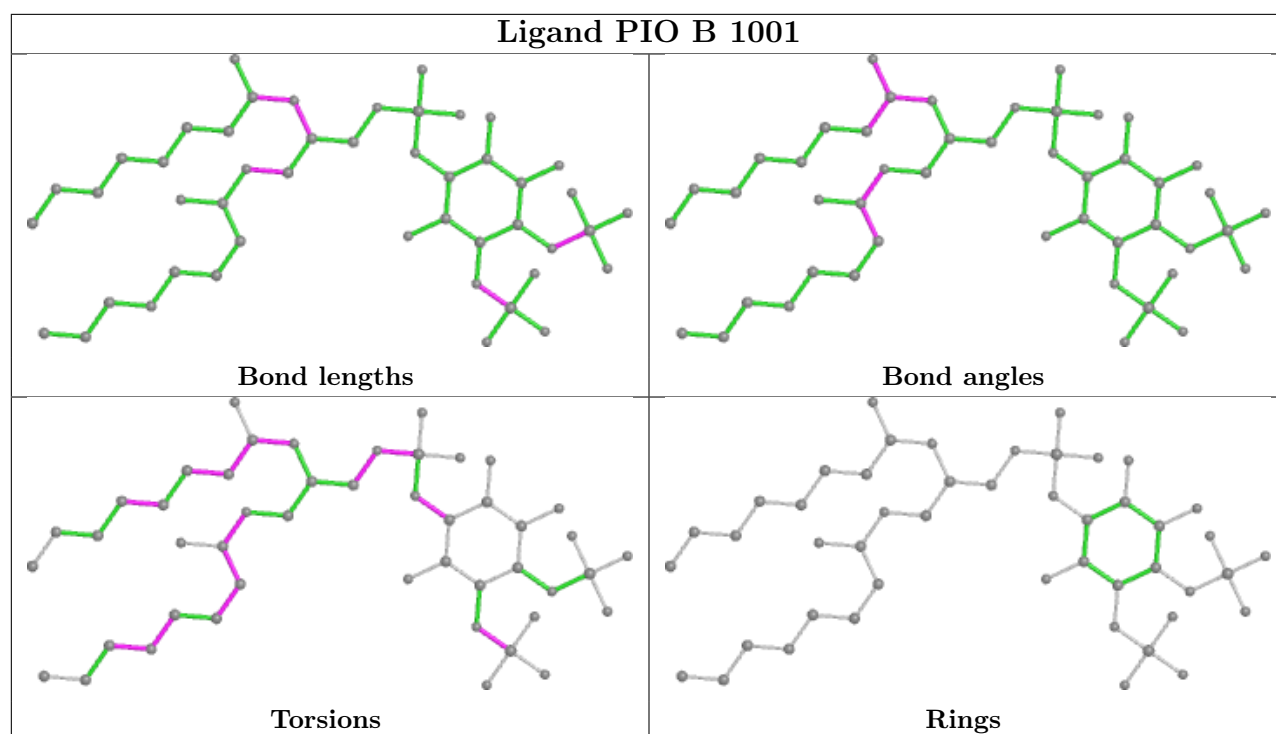
11 monomers are involved in 20 short contacts:

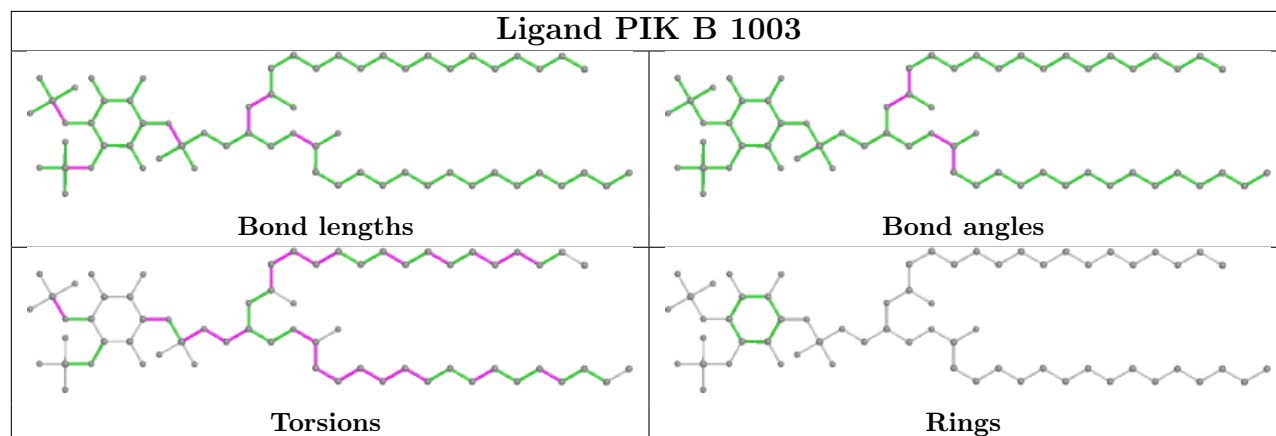
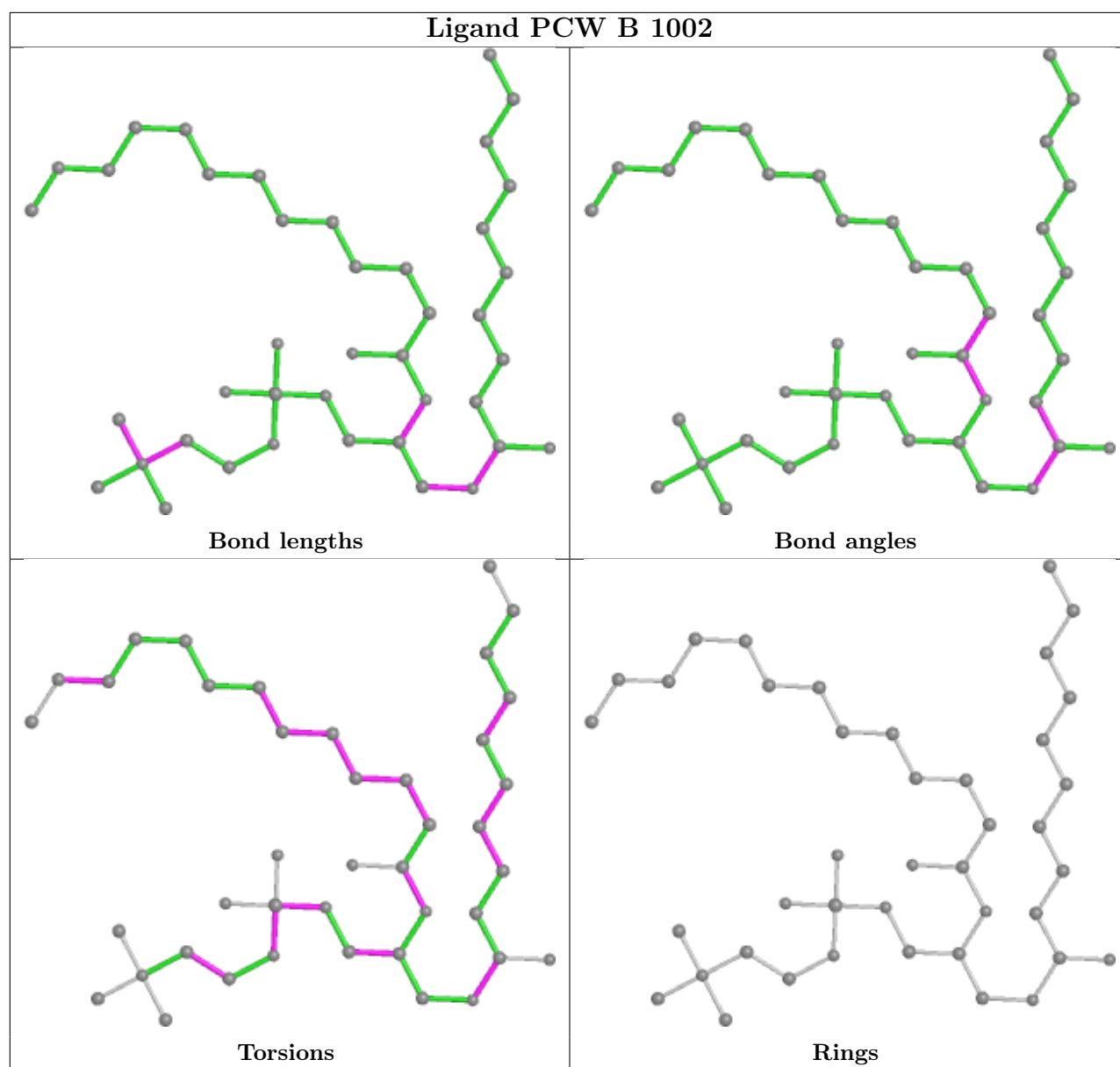
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	PIO	2	0
3	A	1002	PCW	2	0
4	A	1003	PIK	1	0
2	B	1001	PIO	2	0
3	B	1002	PCW	3	0
4	B	1003	PIK	1	0
2	C	1001	PIO	1	0
3	C	1002	PCW	2	0
2	D	1001	PIO	2	0
3	D	1002	PCW	3	0
4	D	1003	PIK	1	0

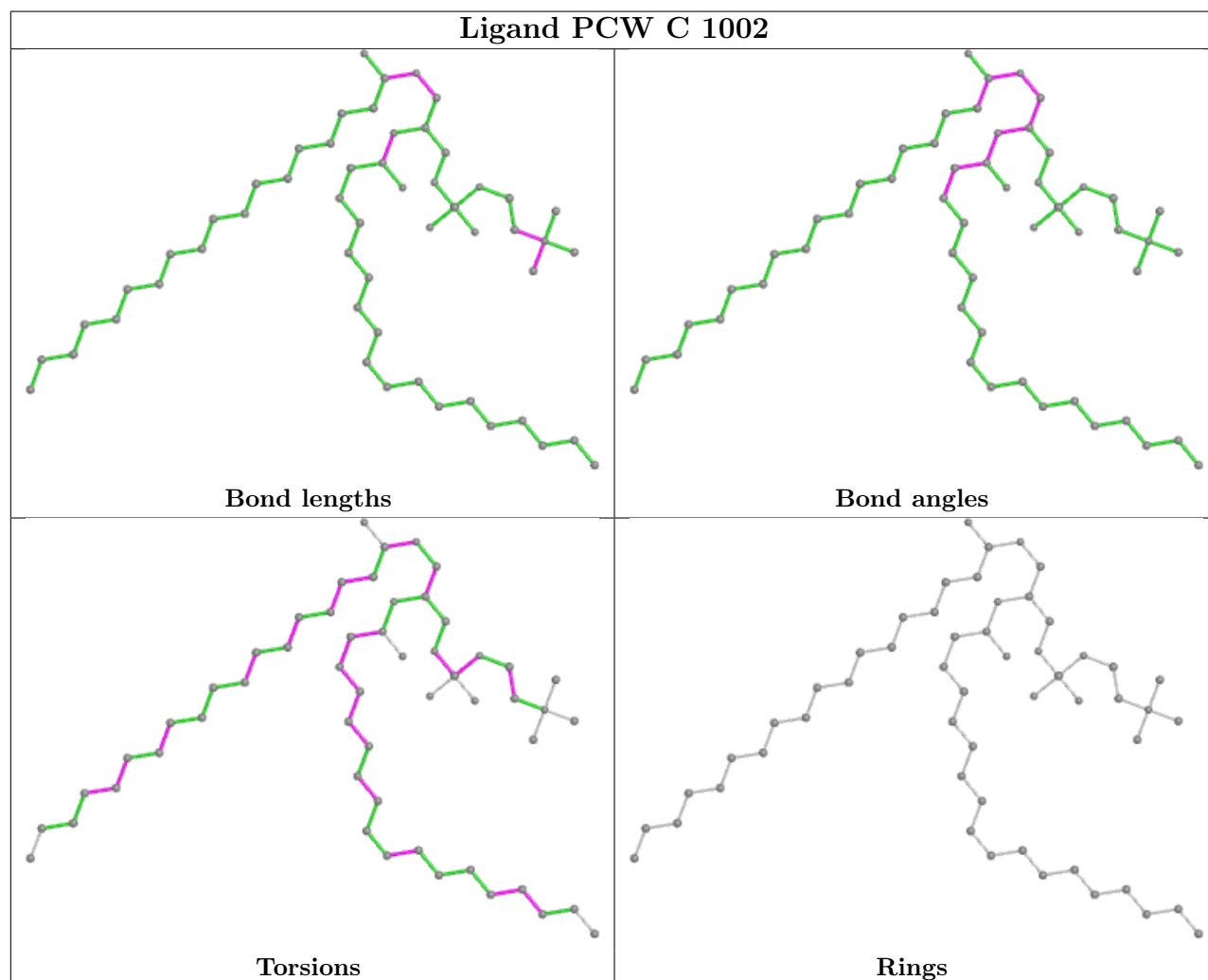
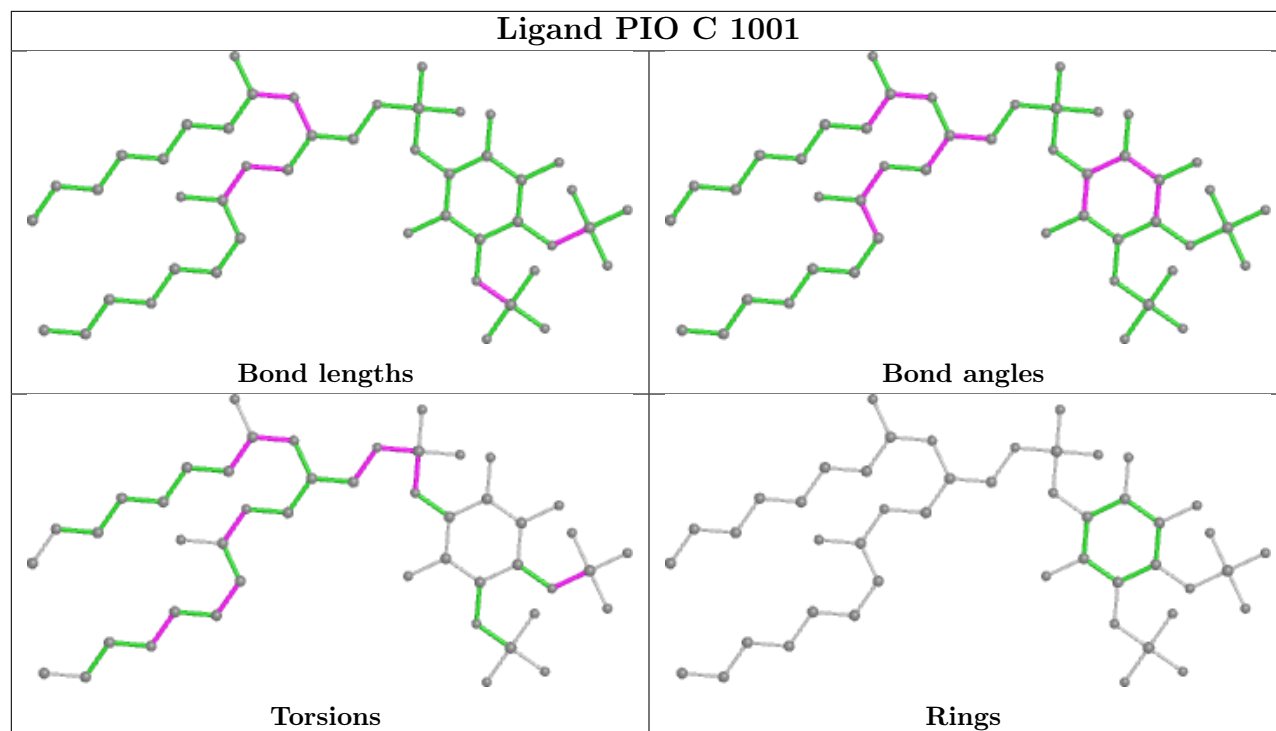
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

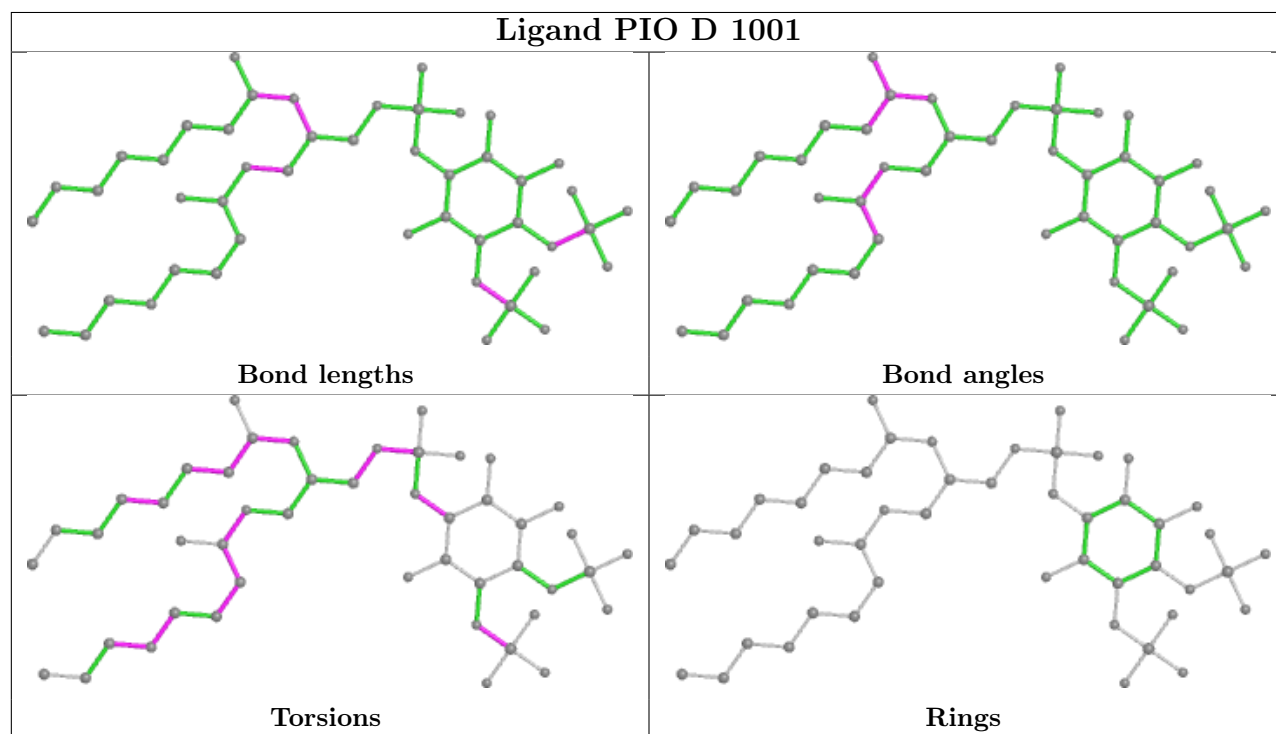
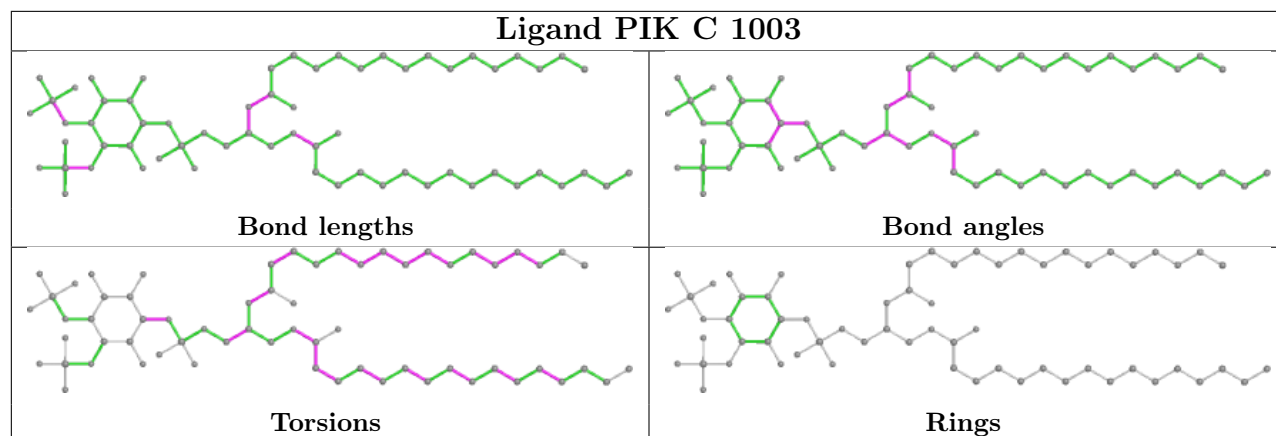


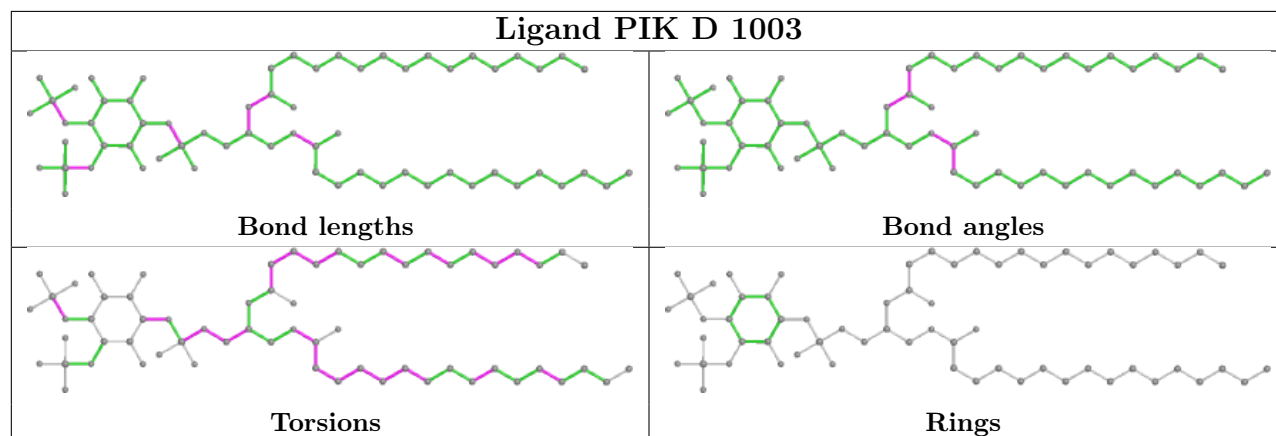
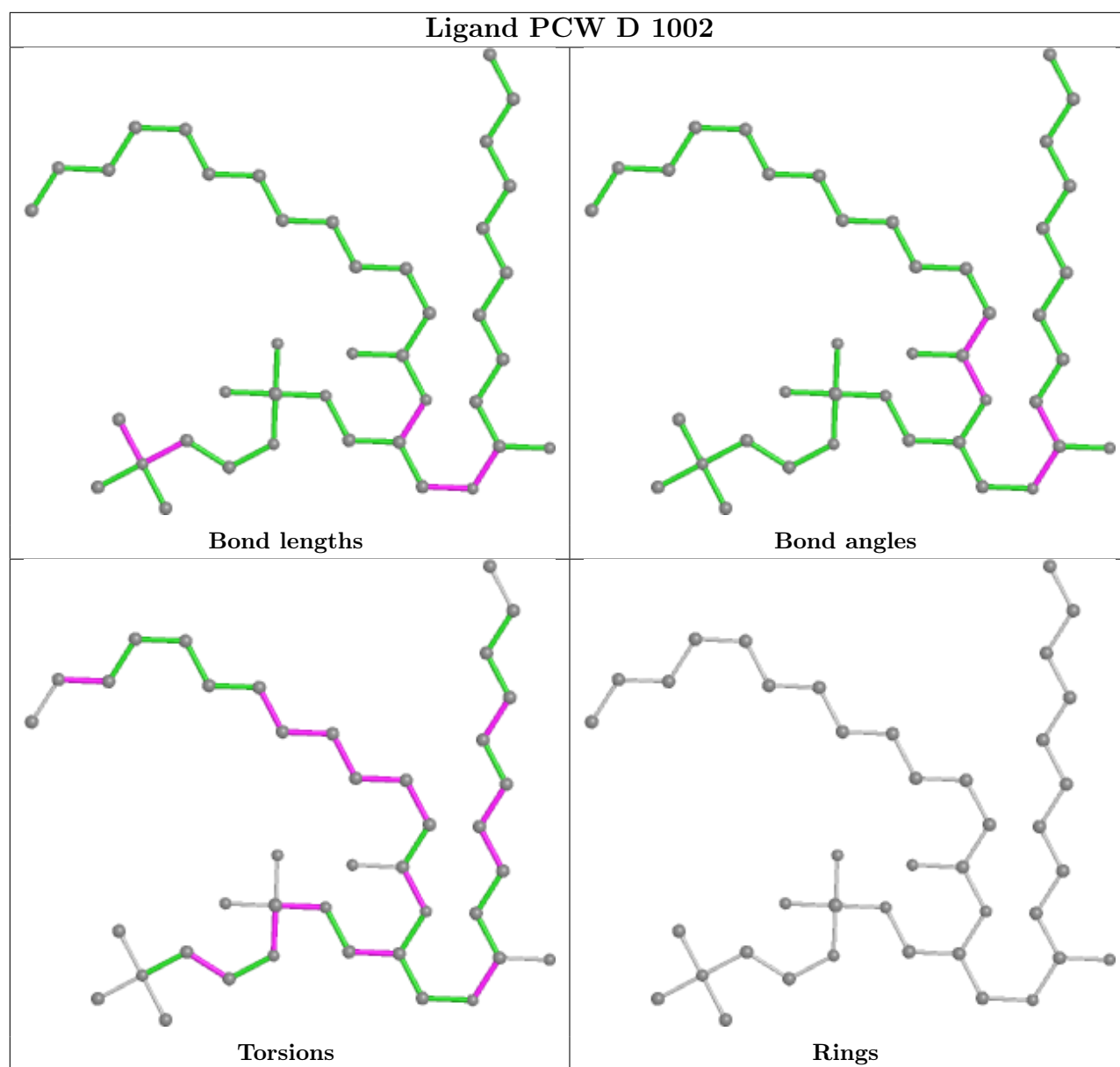












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.