



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:58 AM UTC

PDB ID : 1LIA / pdb_00001lia
Title : CRYSTAL STRUCTURE OF R-PHYCOERYTHRIN FROM POLYSIPHONIA AT 2.8 Å RESOLUTION
Authors : Liang, D.C.; Jiang, T.; Chang, W.R.
Deposited on : 1996-01-29
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

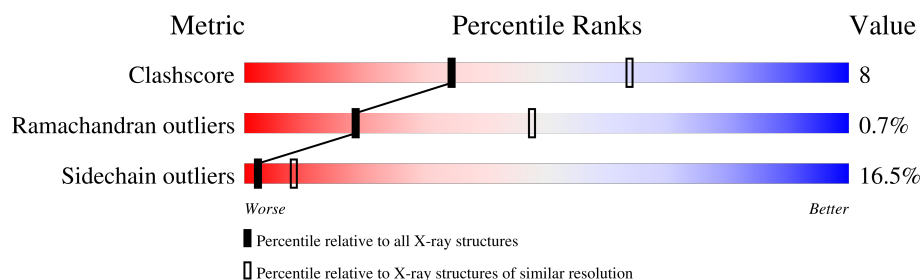
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	164	
1	K	164	
2	B	177	
2	L	177	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYC	B	176	X	-	-	-
3	CYC	K	175	X	-	-	-
3	CYC	L	177	X	-	-	-
4	PUB	B	177	X	-	-	-
4	PUB	L	175	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called R-PHYCOERYTHRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1252	779	220	246	7			
1	K	164	Total	C	N	O	S	0	0	0
			1252	779	220	246	7			

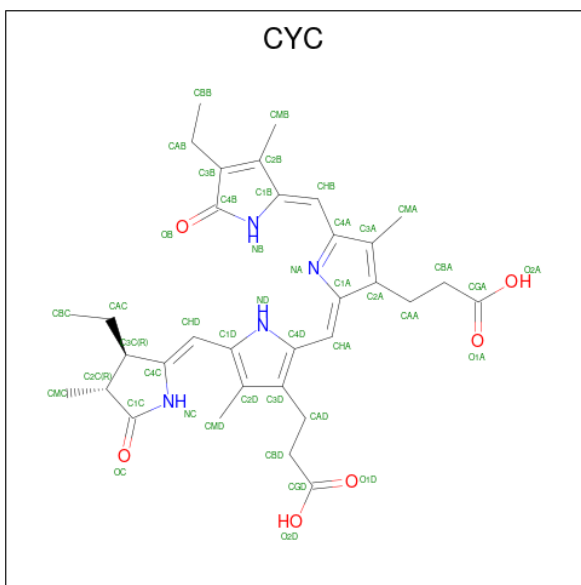
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ASN	LEU	conflict	UNP Q01921
K	66	ASN	LEU	conflict	UNP Q01921

- Molecule 2 is a protein called R-PHYCOERYTHRIN.

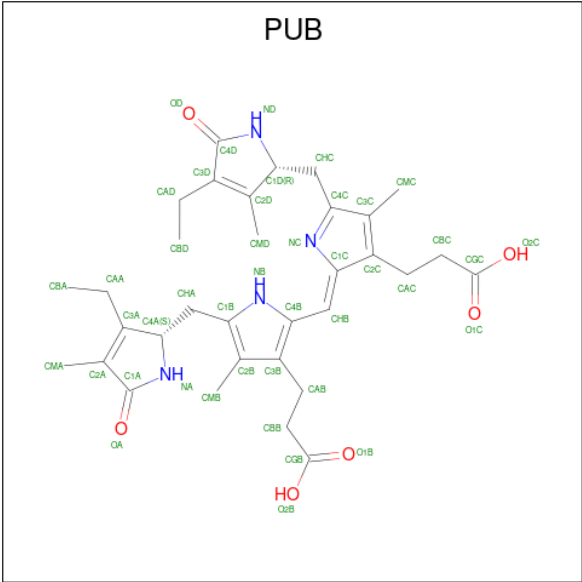
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1304	805	226	261	12			
2	L	177	Total	C	N	O	S	0	0	0
			1304	805	226	261	12			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 43	C 33	N 4	O 6	0	0
3	A	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	B	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 4 is PHYCOUROBILIN (CCD ID: PUB) (formula: $C_{33}H_{42}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			43	33	4	6		
4	L	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	22	Total	O	0	0
			22	22		
5	K	39	Total	O	0	0
			39	39		
5	L	32	Total	O	0	0
			32	32		

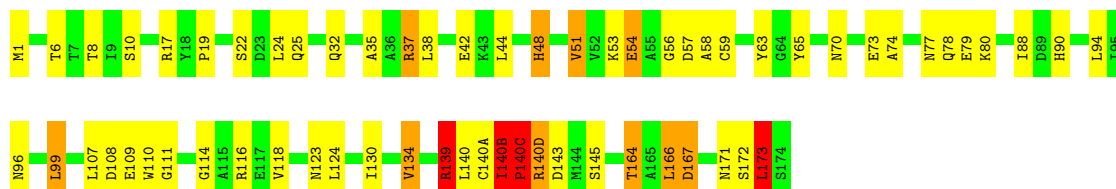
3 Residue-property plots

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

Note EDS was not executed.

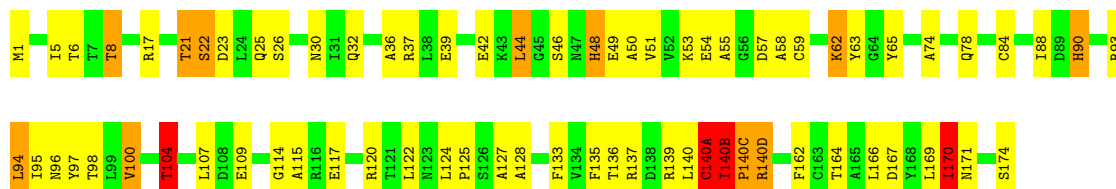
• Molecule 1: R-PHYCOERYTHRIN

Chain A: 



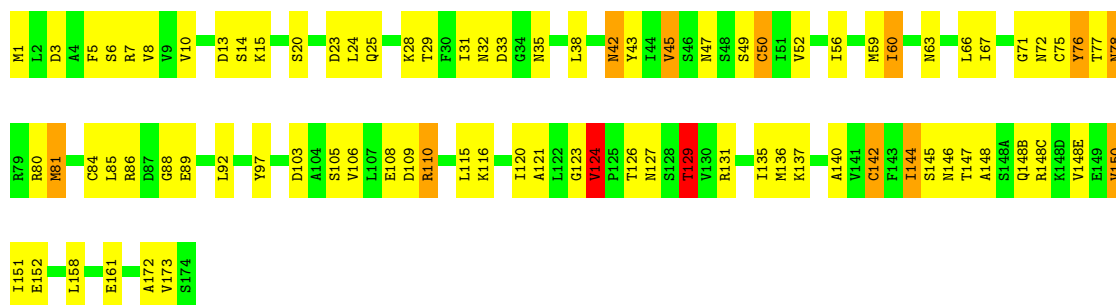
• Molecule 1: R-PHYCOERYTHRIN

Chain K: 



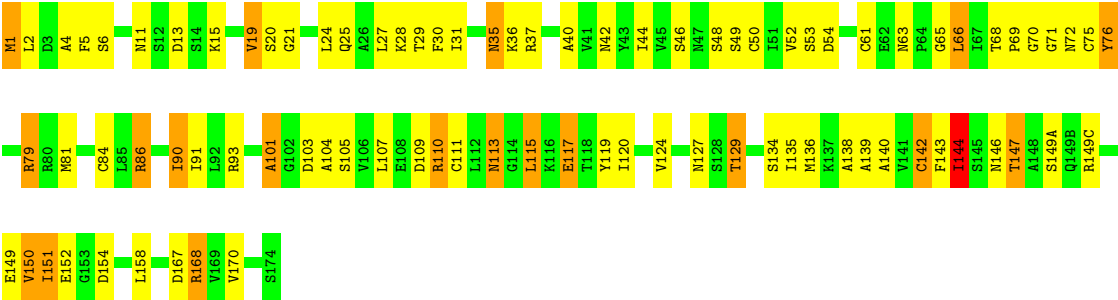
• Molecule 2: R-PHYCOERYTHRIN

Chain B: 



• Molecule 2: R-PHYCOERYTHRIN

Chain L: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	189.80 Å 189.80 Å 60.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.0 (10.00-2.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , 0.182	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5676	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PUB, CYC

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	1.15	3/1273 (0.2%)	2.07	43/1722 (2.5%)
1	K	1.28	7/1273 (0.5%)	2.23	49/1722 (2.8%)
2	B	1.25	8/1316 (0.6%)	2.22	53/1782 (3.0%)
2	L	1.32	4/1316 (0.3%)	2.26	63/1782 (3.5%)
All	All	1.25	22/5178 (0.4%)	2.20	208/7008 (3.0%)

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	4
1	K	0	2
2	B	0	1
2	L	0	1
All	All	0	8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123	GLY	C-N	11.73	1.46	1.33
1	K	51	VAL	C-N	9.13	1.46	1.34
1	K	94	LEU	C-N	8.54	1.44	1.33
2	L	1	MET	C-N	-7.68	1.22	1.33
2	B	88	GLY	C-N	-7.02	1.24	1.33
2	B	148(B)	GLN	C-N	6.49	1.49	1.34
1	A	90	HIS	CD2-NE2	-6.30	1.30	1.37
2	B	77	THR	C-N	-6.26	1.25	1.33
1	K	90	HIS	CD2-NE2	-6.24	1.30	1.37
1	K	170	ILE	CA-CB	6.00	1.62	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	48	HIS	CD2-NE2	-5.77	1.31	1.37
2	L	52	VAL	CA-CB	5.71	1.62	1.54
2	B	146	ASN	C-N	-5.65	1.26	1.33
2	B	120	ILE	CA-CB	5.52	1.60	1.54
1	A	48	HIS	CD2-NE2	-5.46	1.31	1.37
1	K	98	THR	CA-CB	5.44	1.61	1.53
2	L	139	ALA	C-N	5.41	1.41	1.33
2	B	76	TYR	C-N	-5.38	1.26	1.33
1	A	173	LEU	C-N	5.29	1.40	1.33
2	L	151	ILE	CA-CB	5.15	1.60	1.54
1	K	36	ALA	C-N	5.07	1.40	1.33
2	B	131	ARG	C-N	5.00	1.40	1.33

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	136	THR	CA-C-N	13.38	138.64	120.44
1	K	136	THR	C-N-CA	13.38	138.64	120.44
2	B	88	GLY	CA-C-N	13.03	137.74	120.28
2	B	88	GLY	C-N-CA	13.03	137.74	120.28
2	L	76	TYR	CA-C-N	11.09	142.72	121.54
2	L	76	TYR	C-N-CA	11.09	142.72	121.54
2	B	47	ASN	OD1-CG-ND2	-10.87	111.73	122.60
2	B	76	TYR	CA-C-N	10.76	142.09	121.54
2	B	76	TYR	C-N-CA	10.76	142.09	121.54
1	A	96	ASN	CA-CB-CG	10.31	122.91	112.60
2	L	109	ASP	CA-CB-CG	10.16	122.76	112.60
1	K	171	ASN	OD1-CG-ND2	-10.05	112.55	122.60
2	L	54	ASP	CA-CB-CG	9.94	122.54	112.60
2	B	109	ASP	CA-CB-CG	9.63	122.23	112.60
2	L	29	THR	CA-C-O	-9.37	110.62	120.55
1	A	108	ASP	CA-CB-CG	9.29	121.89	112.60
1	K	96	ASN	CA-CB-CG	9.27	121.87	112.60
2	B	45	VAL	N-CA-CB	-9.19	98.98	110.47
2	L	35	ASN	OD1-CG-ND2	-9.18	113.42	122.60
2	L	127	ASN	CA-CB-CG	9.08	121.68	112.60
1	A	57	ASP	CA-CB-CG	8.73	121.33	112.60
2	B	121	ALA	N-CA-C	8.70	120.76	111.28
1	K	96	ASN	CB-CG-ND2	8.63	129.35	116.40
1	K	96	ASN	OD1-CG-ND2	-8.01	114.59	122.60
1	A	74	ALA	N-CA-C	8.01	122.72	113.19
2	B	3	ASP	CA-CB-CG	7.99	120.59	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	148(E)	VAL	N-CA-CB	-7.93	103.30	112.34
2	L	101	ALA	N-CA-C	7.83	120.91	111.82
2	B	78	ASN	CA-CB-CG	7.81	120.41	112.60
2	L	76	TYR	O-C-N	-7.75	113.87	123.01
1	K	117	GLU	CB-CG-CD	7.72	125.73	112.60
2	L	151	ILE	O-C-N	7.72	131.02	122.61
2	B	127	ASN	CA-CB-CG	7.66	120.26	112.60
1	K	25	GLN	OE1-CD-NE2	-7.53	115.07	122.60
2	L	135	ILE	CA-C-N	7.45	130.13	120.44
2	L	135	ILE	C-N-CA	7.45	130.13	120.44
1	K	90	HIS	CB-CG-CD2	-7.41	121.56	131.20
2	B	60	ILE	N-CA-CB	-7.40	101.09	110.57
1	K	30	ASN	OD1-CG-ND2	-7.38	115.22	122.60
2	L	4	ALA	N-CA-C	7.36	120.17	111.71
1	K	51	VAL	CA-C-O	-7.33	113.33	120.95
2	B	115	LEU	CA-C-O	-7.24	113.22	120.82
2	L	90	ILE	CA-CB-CG1	7.21	122.66	110.40
1	A	96	ASN	OD1-CG-ND2	-7.21	115.39	122.60
2	L	90	ILE	CA-CB-CG2	-7.20	98.26	110.50
2	L	143	PHE	N-CA-C	-7.19	103.48	111.82
2	B	150	VAL	CB-CA-C	-7.11	100.66	110.90
1	A	25	GLN	N-CA-C	-7.08	103.64	111.36
1	K	8	THR	N-CA-CB	-7.03	99.75	110.16
2	B	63	ASN	CA-CB-CG	7.00	119.60	112.60
1	K	127	ALA	N-CA-C	6.99	119.75	111.71
2	L	25	GLN	OE1-CD-NE2	-6.94	115.66	122.60
2	B	63	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	L	150	VAL	CB-CA-C	-6.84	98.47	110.71
2	L	79	ARG	NE-CZ-NH2	-6.83	113.05	119.20
1	A	78	GLN	CA-C-O	-6.81	113.20	120.42
2	L	11	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	A	140(D)	ARG	N-CA-C	6.79	119.25	111.11
1	A	167	ASP	CA-CB-CG	6.78	119.38	112.60
2	L	35	ASN	CB-CG-ND2	6.77	126.56	116.40
2	B	25	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	K	36	ALA	CA-C-N	-6.74	110.72	120.29
1	K	36	ALA	C-N-CA	-6.74	110.72	120.29
1	A	143	ASP	CA-CB-CG	6.71	119.31	112.60
1	K	115	ALA	CA-C-N	6.71	129.57	120.38
1	K	115	ALA	C-N-CA	6.71	129.57	120.38
1	A	111	GLY	CA-C-N	-6.69	114.46	122.35
1	A	111	GLY	C-N-CA	-6.69	114.46	122.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	61	CYS	O-C-N	6.67	129.02	122.09
2	B	123	GLY	CA-C-N	-6.65	109.83	122.13
2	B	123	GLY	C-N-CA	-6.65	109.83	122.13
2	L	63	ASN	CA-CB-CG	6.64	119.24	112.60
1	A	90	HIS	CB-CG-CD2	-6.64	122.57	131.20
1	K	171	ASN	CB-CG-ND2	6.60	126.30	116.40
2	L	144	ILE	O-C-N	-6.60	113.02	122.12
2	L	70	GLY	CA-C-N	6.55	126.33	120.10
2	L	70	GLY	C-N-CA	6.55	126.33	120.10
2	L	42	ASN	CA-C-O	-6.51	114.00	120.70
1	K	140(B)	ILE	CA-CB-CG2	-6.43	99.58	110.50
1	A	6	THR	N-CA-C	6.40	118.34	111.36
2	B	8	VAL	CA-C-O	-6.39	114.07	120.85
2	B	161	GLU	CA-CB-CG	6.36	126.82	114.10
1	K	140(B)	ILE	N-CA-C	6.36	122.61	108.88
2	L	149(A)	SER	N-CA-C	6.35	119.19	111.82
1	K	21	THR	OG1-CB-CG2	6.30	121.91	109.30
1	K	140(B)	ILE	CB-CA-C	-6.30	99.89	111.36
2	B	135	ILE	N-CA-C	-6.25	104.66	110.53
1	A	80	LYS	N-CA-C	6.22	117.72	111.07
2	L	113	ASN	CA-CB-CG	-6.15	106.45	112.60
2	B	20	SER	CA-C-N	6.15	126.91	120.03
2	B	20	SER	C-N-CA	6.15	126.91	120.03
2	L	154	ASP	N-CA-C	6.14	118.74	108.73
1	A	110	TRP	CG-CD2-CE3	6.12	140.02	133.90
1	K	140(A)	CYS	N-CA-CB	-6.11	100.92	110.87
1	A	24	LEU	CA-C-N	6.10	128.96	120.29
1	A	24	LEU	C-N-CA	6.10	128.96	120.29
2	L	149(C)	ARG	CG-CD-NE	6.07	125.36	112.00
2	L	53	SER	CA-C-O	-6.07	114.63	121.00
2	B	136	MET	CA-C-N	6.03	128.61	120.65
2	B	136	MET	C-N-CA	6.03	128.61	120.65
1	A	171	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	109	GLU	N-CA-C	5.97	119.04	111.69
1	K	114	GLY	CA-C-O	-5.97	112.88	119.27
2	B	47	ASN	CB-CG-ND2	5.97	125.36	116.40
2	L	147	THR	N-CA-CB	-5.94	101.41	111.27
1	K	48	HIS	CA-CB-CG	5.93	119.73	113.80
2	L	110	ARG	N-CA-C	5.90	119.45	112.72
1	A	53	LYS	O-C-N	5.89	128.40	122.03
2	L	103	ASP	CA-CB-CG	5.89	118.49	112.60
1	K	78	GLN	OE1-CD-NE2	-5.89	116.71	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	104	THR	N-CA-CB	-5.88	101.98	110.56
2	B	5	PHE	CA-CB-CG	5.83	119.62	113.80
1	K	17	ARG	N-CA-C	5.82	119.21	109.95
2	B	45	VAL	N-CA-C	5.82	117.25	110.62
1	A	123	ASN	N-CA-C	5.82	119.27	111.24
2	B	131	ARG	O-C-N	-5.81	114.44	122.46
1	K	74	ALA	N-CA-C	5.76	123.07	110.80
1	K	21	THR	N-CA-C	5.75	118.00	111.11
1	A	90	HIS	CB-CG-ND1	5.74	131.31	122.70
2	B	1	MET	CA-C-N	5.74	131.67	121.75
2	B	1	MET	C-N-CA	5.74	131.67	121.75
1	A	143	ASP	N-CA-C	-5.73	104.48	112.45
1	A	48	HIS	CA-CB-CG	5.72	119.52	113.80
2	B	77	THR	O-C-N	5.71	130.19	122.59
1	A	166	LEU	N-CA-C	5.71	118.44	111.82
2	L	168	ARG	CA-CB-CG	5.70	125.51	114.10
1	K	46	SER	N-CA-C	5.70	119.41	112.23
2	L	146	ASN	CA-CB-CG	5.69	118.29	112.60
2	L	134	SER	CA-CB-OG	5.69	122.47	111.10
1	K	57	ASP	CA-CB-CG	5.68	118.28	112.60
2	L	66	LEU	N-CA-CB	-5.68	101.47	110.28
2	L	149	GLU	CA-C-N	5.67	130.98	122.58
2	L	149	GLU	C-N-CA	5.67	130.98	122.58
1	A	77	ASN	CA-CB-CG	5.67	118.27	112.60
2	B	13	ASP	CA-CB-CG	-5.67	106.94	112.60
2	B	15	LYS	N-CA-CB	-5.66	101.77	110.44
2	L	15	LYS	CA-C-N	5.66	130.40	122.36
2	L	15	LYS	C-N-CA	5.66	130.40	122.36
2	B	50	CYS	CA-CB-SG	5.66	127.41	114.40
2	B	75	CYS	N-CA-C	-5.65	105.59	112.88
1	A	48	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	171	ASN	CB-CG-ND2	5.61	124.81	116.40
2	L	151	ILE	N-CA-C	-5.59	102.37	109.58
2	L	6	SER	CA-CB-OG	5.58	122.25	111.10
2	B	76	TYR	O-C-N	-5.57	116.70	123.16
1	K	88	ILE	CA-C-O	-5.55	114.47	120.47
1	A	35	ALA	N-CA-C	5.55	117.01	111.07
2	L	158	LEU	N-CA-CB	-5.55	101.75	110.30
1	A	54	GLU	O-C-N	5.54	127.85	122.09
2	B	14	SER	CA-C-O	5.50	126.30	119.97
1	A	114	GLY	O-C-N	-5.49	115.42	122.39
1	A	118	VAL	O-C-N	-5.46	116.58	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	N-CA-C	5.45	117.92	111.33
1	K	136	THR	O-C-N	-5.45	116.35	122.12
2	L	5	PHE	CA-C-N	5.45	127.58	120.28
2	L	5	PHE	C-N-CA	5.45	127.58	120.28
1	A	171	ASN	CA-CB-CG	-5.44	107.16	112.60
2	B	81	MET	CG-SD-CE	5.44	112.87	100.90
1	K	107	LEU	O-C-N	5.43	127.66	122.07
1	K	125	PRO	N-CA-C	5.40	120.56	111.32
2	B	172	ALA	CA-C-N	-5.40	114.65	122.69
2	B	172	ALA	C-N-CA	-5.40	114.65	122.69
1	K	90	HIS	CB-CG-ND1	5.39	130.79	122.70
2	L	81	MET	CG-SD-CE	-5.38	89.06	100.90
2	L	30	PHE	CA-C-O	-5.36	115.19	120.82
2	B	42	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	K	49	GLU	CB-CG-CD	5.30	121.61	112.60
1	K	100	VAL	N-CA-C	5.30	115.50	110.42
1	K	174	SER	N-CA-CB	-5.29	101.51	110.50
2	B	105	SER	N-CA-C	5.28	117.78	111.71
2	L	142	CYS	CA-C-O	-5.28	113.13	119.15
1	K	50	ALA	O-C-N	5.28	127.51	122.07
1	K	93	ARG	N-CA-C	-5.26	105.62	111.36
1	A	172	SER	N-CA-C	5.25	117.91	111.82
2	B	129	THR	N-CA-CB	-5.23	102.43	110.12
2	B	110	ARG	CB-CG-CD	5.22	123.31	111.30
2	B	85	LEU	N-CA-C	-5.21	105.49	111.07
1	A	164	THR	N-CA-CB	-5.21	102.77	110.53
1	A	70	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	96	ASN	CB-CG-ND2	5.20	124.20	116.40
2	L	104	ALA	N-CA-C	5.20	119.25	113.01
1	A	134	VAL	N-CA-C	-5.19	105.65	110.53
2	B	67	ILE	N-CA-C	5.18	117.16	111.77
2	B	137	LYS	CA-CB-CG	5.17	124.44	114.10
2	B	60	ILE	CB-CA-C	5.17	118.79	112.02
1	A	6	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	10	SER	N-CA-C	5.16	116.90	111.28
2	L	37	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	58	ALA	N-CA-C	5.15	116.89	111.28
2	L	105	SER	N-CA-C	5.15	116.89	111.28
2	L	91	ILE	N-CA-C	-5.15	105.48	110.42
1	K	124	LEU	N-CA-C	-5.13	99.20	108.85
2	L	75	CYS	N-CA-C	-5.13	106.61	112.92
2	B	71	GLY	N-CA-C	-5.12	104.57	111.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	138	ALA	O-C-N	5.12	127.55	122.12
1	K	55	ALA	N-CA-C	5.11	116.93	111.36
2	B	32	ASN	N-CA-C	5.10	116.83	111.28
1	K	133	PHE	CA-CB-CG	5.08	118.88	113.80
1	K	23	ASP	CA-CB-CG	5.08	117.67	112.60
2	L	93	ARG	CB-CA-C	-5.08	102.69	110.81
2	L	63	ASN	CA-C-N	5.07	125.14	119.87
2	L	63	ASN	C-N-CA	5.07	125.14	119.87
2	L	48	SER	CA-C-O	-5.06	115.06	120.42
1	K	58	ALA	N-CA-C	5.05	117.17	111.11
1	K	62	LYS	CA-CB-CG	5.02	124.14	114.10
2	L	86	ARG	CG-CD-NE	-5.01	100.97	112.00
2	L	28	LYS	N-CA-C	-5.01	105.82	111.28
1	K	170	ILE	CB-CG1-CD1	5.01	124.32	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	140(B)	ILE	Peptide
1	A	173	LEU	Mainchain
1	A	37	ARG	Sidechain
2	B	124	VAL	Mainchain
1	K	140(B)	ILE	Peptide
1	K	37	ARG	Mainchain
2	L	79	ARG	Sidechain

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	1252	0	1224	15	0
1	K	1252	0	1224	20	0
2	B	1304	0	1310	26	0
2	L	1304	0	1310	24	0
3	A	86	0	76	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	86	0	76	9	0
3	K	86	0	76	1	0
3	L	86	0	76	9	0
4	B	43	0	34	1	0
4	L	43	0	38	1	0
5	A	41	0	0	1	0
5	B	22	0	0	2	0
5	K	39	0	0	2	0
5	L	32	0	0	0	0
All	All	5676	0	5444	83	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 8.

All (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:35:ASN:HD22	3:L:176:CYC:HB	1.11	0.92
2:B:35:ASN:HD22	3:B:176:CYC:HB	1.25	0.85
2:B:142:CYS:SG	4:B:177:PUB:HMB1	2.26	0.75
1:A:140(C):PRO:HD2	5:A:206:HOH:O	1.90	0.70
3:B:175:CYC:HMD2	3:B:175:CYC:HC	1.56	0.69
1:K:140(A):CYS:SG	1:K:140(D):ARG:HB2	2.31	0.69
1:K:170:ILE:HG21	5:K:210:HOH:O	1.92	0.68
2:L:140:ALA:O	2:L:144:ILE:HG23	1.95	0.66
2:L:72:ASN:HD21	2:L:124:VAL:HG22	1.62	0.64
1:K:162:PHE:O	1:K:166:LEU:HD23	1.98	0.64
1:A:63:TYR:HB3	1:A:65:TYR:CE1	2.34	0.63
2:L:65:GLY:O	2:L:68:THR:HG22	2.01	0.60
2:B:7:ARG:HD3	2:B:103:ASP:OD1	2.01	0.60
2:L:72:ASN:HD22	3:L:177:CYC:HC	1.51	0.59
2:L:35:ASN:ND2	3:L:176:CYC:HB	1.93	0.58
2:L:84:CYS:HB2	3:L:177:CYC:C4C	2.34	0.56
1:A:44:LEU:O	1:A:48:HIS:HB3	2.07	0.55
2:B:49:SER:HA	5:B:192:HOH:O	2.08	0.53
2:B:72:ASN:ND2	2:B:124:VAL:HB	2.23	0.53
2:L:72:ASN:ND2	3:L:177:CYC:HMD2	2.23	0.53
1:K:140(A):CYS:SG	1:K:140(D):ARG:CB	2.96	0.52
2:B:35:ASN:HB3	3:B:176:CYC:NA	2.26	0.51
2:B:72:ASN:HD22	3:B:175:CYC:HC	1.58	0.51
1:K:84:CYS:HB2	3:K:175:CYC:C4C	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:177:CYC:HHA	3:L:177:CYC:CGA	2.41	0.50
1:A:139:ARG:NH1	3:A:141:CYC:C1A	2.75	0.50
3:B:176:CYC:HAB1	5:B:190:HOH:O	2.12	0.49
1:A:17:ARG:HH22	1:K:104:THR:HG21	1.78	0.49
1:K:97:TYR:OH	2:L:13:ASP:HA	2.13	0.49
1:K:164:THR:HA	1:K:167:ASP:HB2	1.95	0.48
2:B:52:VAL:O	2:B:56:ILE:HD13	2.13	0.48
1:A:32:GLN:HG3	1:K:32:GLN:HG3	1.95	0.48
3:A:141:CYC:HMD2	3:A:141:CYC:HC	1.78	0.48
2:L:167:ASP:HA	2:L:170:VAL:HG22	1.95	0.48
1:A:54:GLU:OE1	1:A:139:ARG:HD2	2.14	0.48
2:B:59:MET:HE2	2:B:60:ILE:HG13	1.95	0.47
2:B:72:ASN:ND2	3:B:175:CYC:HMD2	2.29	0.47
2:B:76:TYR:O	2:B:80:ARG:HD2	2.15	0.47
2:B:126:THR:HA	2:B:129:THR:HB	1.95	0.47
2:L:117:GLU:H	2:L:117:GLU:CD	2.22	0.47
1:A:130:ILE:O	1:A:134:VAL:HG23	2.14	0.47
2:B:84:CYS:HB2	3:B:175:CYC:C4C	2.45	0.47
1:K:22:SER:HB2	5:K:197:HOH:O	2.14	0.47
1:K:100:VAL:HG21	2:L:19:VAL:CG1	2.45	0.47
3:A:175:CYC:HMD2	3:A:175:CYC:HC	1.80	0.46
2:B:140:ALA:O	2:B:144:ILE:HG23	2.16	0.46
2:L:40:ALA:O	2:L:44:ILE:HG12	2.15	0.46
1:K:100:VAL:HG21	2:L:19:VAL:HG13	1.98	0.45
3:L:177:CYC:HC	3:L:177:CYC:HMD2	1.81	0.45
1:K:63:TYR:HB3	1:K:65:TYR:CE1	2.51	0.45
2:L:119:TYR:HE2	2:L:129:THR:HG21	1.82	0.45
3:B:175:CYC:HHA	3:B:175:CYC:O2A	2.17	0.45
2:B:6:SER:O	2:B:10:VAL:HG23	2.16	0.45
1:A:42:GLU:HG2	2:B:24:LEU:HD13	1.98	0.45
2:L:115:LEU:HD21	3:L:177:CYC:HMB3	1.98	0.45
2:B:148:ALA:HB3	2:B:148(C):ARG:O	2.17	0.44
1:A:164:THR:HA	1:A:167:ASP:HB2	2.00	0.44
1:K:5:ILE:HG21	2:L:101:ALA:HA	1.99	0.44
2:B:86:ARG:HH12	3:B:175:CYC:HB	1.66	0.43
2:B:106:VAL:O	2:B:110:ARG:HB2	2.18	0.43
2:L:68:THR:OG1	2:L:69:PRO:HD2	2.18	0.43
2:L:19:VAL:HG22	2:L:24:LEU:HD13	2.01	0.43
2:L:72:ASN:ND2	3:L:177:CYC:HC	2.15	0.43
1:A:56:GLY:HA2	1:A:88:ILE:HD13	2.01	0.43
2:B:28:LYS:HA	2:B:31:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PRO:HD3	2:B:97:TYR:CE1	2.54	0.42
2:B:24:LEU:O	2:B:28:LYS:HG2	2.20	0.42
1:A:37:ARG:HD2	1:A:99:LEU:O	2.20	0.42
1:K:90:HIS:O	1:K:94:LEU:HG	2.19	0.42
1:A:63:TYR:HB3	1:A:65:TYR:HE1	1.84	0.41
2:L:71:GLY:O	2:L:76:TYR:HB3	2.20	0.41
1:K:1:MET:O	1:K:6:THR:HG21	2.21	0.41
1:K:59:CYS:SG	1:K:128:ALA:HB1	2.60	0.41
1:A:51:VAL:HG12	3:A:141:CYC:HMA1	2.03	0.41
2:B:116:LYS:HB2	2:B:173:VAL:HA	2.02	0.41
2:B:43:TYR:HD2	2:B:144:ILE:HA	1.85	0.41
2:L:107:LEU:O	2:L:111:CYS:HB3	2.20	0.41
2:L:142:CYS:SG	4:L:175:PUB:HMB1	2.61	0.41
2:B:42:ASN:OD1	1:K:164:THR:HG21	2.21	0.41
1:K:54:GLU:HB3	1:K:135:PHE:HE2	1.84	0.41
2:L:1:MET:HE2	2:L:1:MET:HB3	1.98	0.40
1:K:44:LEU:O	1:K:48:HIS:HB3	2.21	0.40
2:B:86:ARG:O	2:B:89:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	156 (96%)	4 (2%)	2 (1%)	10	34
1	K	162/164 (99%)	155 (96%)	5 (3%)	2 (1%)	10	34
2	B	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
2	L	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	21	51
All	All	674/682 (99%)	653 (97%)	16 (2%)	5 (1%)	18	47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	140(C)	PRO
2	L	21	GLY
1	K	140(B)	ILE
1	A	140(C)	PRO
1	A	140(B)	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	129/129 (100%)	108 (84%)	21 (16%)	2	8
1	K	129/129 (100%)	106 (82%)	23 (18%)	2	6
2	B	144/144 (100%)	123 (85%)	21 (15%)	3	11
2	L	144/144 (100%)	119 (83%)	25 (17%)	2	7
All	All	546/546 (100%)	456 (84%)	90 (16%)	2	8

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	THR
1	A	22	SER
1	A	38	LEU
1	A	51	VAL
1	A	59	CYS
1	A	73	GLU
1	A	79	GLU
1	A	94	LEU
1	A	99	LEU
1	A	107	LEU
1	A	124	LEU
1	A	139	ARG
1	A	140	LEU
1	A	140(A)	CYS
1	A	140(B)	ILE
1	A	140(C)	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140(D)	ARG
1	A	145	SER
1	A	166	LEU
1	A	173	LEU
2	B	23	ASP
2	B	29	THR
2	B	33	ASP
2	B	38	LEU
2	B	45	VAL
2	B	50	CYS
2	B	66	LEU
2	B	78	ASN
2	B	81	MET
2	B	92	LEU
2	B	108	GLU
2	B	124	VAL
2	B	129	THR
2	B	142	CYS
2	B	144	ILE
2	B	145	SER
2	B	147	THR
2	B	150	VAL
2	B	151	ILE
2	B	152	GLU
2	B	158	LEU
1	K	8	THR
1	K	21	THR
1	K	22	SER
1	K	26	SER
1	K	39	GLU
1	K	42	GLU
1	K	44	LEU
1	K	53	LYS
1	K	62	LYS
1	K	95	ILE
1	K	104	THR
1	K	109	GLU
1	K	120	ARG
1	K	122	LEU
1	K	137	ARG
1	K	139	ARG
1	K	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	140(A)	CYS
1	K	140(B)	ILE
1	K	140(C)	PRO
1	K	140(D)	ARG
1	K	169	LEU
1	K	170	ILE
2	L	2	LEU
2	L	19	VAL
2	L	20	SER
2	L	27	LEU
2	L	31	ILE
2	L	36	LYS
2	L	46	SER
2	L	49	SER
2	L	50	CYS
2	L	66	LEU
2	L	86	ARG
2	L	90	ILE
2	L	110	ARG
2	L	113	ASN
2	L	115	LEU
2	L	117	GLU
2	L	120	ILE
2	L	129	THR
2	L	136	MET
2	L	144	ILE
2	L	147	THR
2	L	150	VAL
2	L	151	ILE
2	L	152	GLU
2	L	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	78	GLN
1	A	171	ASN
2	B	11	ASN
2	B	32	ASN
2	B	35	ASN
2	B	63	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	72	ASN
2	B	148(B)	GLN
1	K	78	GLN
2	L	25	GLN
2	L	35	ASN
2	L	47	ASN
2	L	63	ASN
2	L	72	ASN
2	L	149(B)	GLN

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](#)

10 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	CYC	K	175	1	46,46,46	2.71	11 (23%)	63,67,67	2.40	29 (46%)
4	PUB	L	175	2	45,46,46	2.66	17 (37%)	45,67,67	3.14	16 (35%)
3	CYC	K	141	1	46,46,46	2.64	13 (28%)	63,67,67	2.40	27 (42%)
3	CYC	L	176	2	46,46,46	2.46	13 (28%)	63,67,67	2.28	24 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CYC	L	177	2	46,46,46	2.83	11 (23%)	63,67,67	2.49	25 (39%)
4	PUB	B	177	2	45,46,46	2.90	19 (42%)	45,67,67	3.25	13 (28%)
3	CYC	B	175	2	46,46,46	2.81	17 (36%)	63,67,67	2.46	20 (31%)
3	CYC	A	175	1	46,46,46	2.79	14 (30%)	63,67,67	2.21	22 (34%)
3	CYC	B	176	2	46,46,46	2.67	15 (32%)	63,67,67	2.33	20 (31%)
3	CYC	A	141	1	46,46,46	2.65	14 (30%)	63,67,67	2.31	23 (36%)

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	CYC	K	175	1	1/1/14/19	14/26/74/74	0/4/4/4
3	CYC	B	176	2	1/1/14/19	13/26/74/74	0/4/4/4
3	CYC	K	141	1	-	12/26/74/74	0/4/4/4
3	CYC	L	176	2	-	14/26/74/74	0/4/4/4
3	CYC	L	177	2	1/1/14/19	15/26/74/74	0/4/4/4
4	PUB	B	177	2	2/2/14/17	13/26/74/74	0/4/4/4
3	CYC	B	175	2	-	11/26/74/74	0/4/4/4
3	CYC	A	175	1	-	13/26/74/74	0/4/4/4
4	PUB	L	175	2	1/1/14/17	14/26/74/74	0/4/4/4
3	CYC	A	141	1	-	13/26/74/74	0/4/4/4

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	177	CYC	C2C-C1C	-14.45	1.39	1.52
3	B	175	CYC	C2C-C1C	-13.41	1.40	1.52
3	A	175	CYC	C2C-C1C	-13.36	1.40	1.52
3	K	175	CYC	C2C-C1C	-13.12	1.40	1.52
3	K	141	CYC	C2C-C1C	-12.52	1.40	1.52
3	A	141	CYC	C2C-C1C	-11.71	1.41	1.52
3	B	176	CYC	C2C-C1C	-11.07	1.42	1.52
3	L	176	CYC	C2C-C1C	-10.26	1.42	1.52
4	B	177	PUB	CBA-CAA	-8.74	1.14	1.51
4	L	175	PUB	CHA-C1B	-7.73	1.40	1.50
4	B	177	PUB	C3A-C2A	6.93	1.44	1.33
4	L	175	PUB	C3A-C2A	5.73	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	175	PUB	CHA-C4A	-5.62	1.42	1.53
3	B	175	CYC	CHD-C4C	5.38	1.45	1.36
4	L	175	PUB	CHC-C1D	-5.15	1.43	1.53
3	B	175	CYC	O2D-CGD	5.05	1.47	1.30
4	B	177	PUB	CHA-C1B	-5.01	1.44	1.50
3	B	176	CYC	C4B-C3B	-5.00	1.39	1.48
3	K	141	CYC	CHD-C4C	4.84	1.44	1.36
4	B	177	PUB	O2C-CGC	4.82	1.46	1.30
3	L	177	CYC	CHD-C4C	4.78	1.44	1.36
3	A	141	CYC	O2A-CGA	4.75	1.46	1.30
3	K	175	CYC	CHD-C4C	4.65	1.44	1.36
3	A	175	CYC	CHD-C4C	4.59	1.44	1.36
4	L	175	PUB	CHC-C4C	-4.57	1.43	1.50
3	B	176	CYC	O2A-CGA	4.53	1.45	1.30
4	B	177	PUB	CHC-C4C	-4.51	1.43	1.50
3	L	177	CYC	O2D-CGD	4.51	1.45	1.30
3	A	175	CYC	O2A-CGA	4.50	1.45	1.30
3	K	175	CYC	CAC-C3C	4.50	1.62	1.54
4	B	177	PUB	CHC-C1D	-4.50	1.44	1.53
3	L	177	CYC	O2A-CGA	4.45	1.45	1.30
4	B	177	PUB	O2B-CGB	4.41	1.45	1.30
3	K	141	CYC	O2D-CGD	4.38	1.45	1.30
3	A	141	CYC	CHD-C4C	4.38	1.43	1.36
3	L	176	CYC	O2A-CGA	4.36	1.45	1.30
3	L	176	CYC	O2D-CGD	4.34	1.45	1.30
4	B	177	PUB	C4D-C3D	-4.33	1.40	1.48
3	A	175	CYC	O2D-CGD	4.29	1.45	1.30
4	B	177	PUB	CHA-C4A	-4.26	1.44	1.53
3	B	176	CYC	C1C-NC	-4.21	1.32	1.37
3	A	141	CYC	C4B-C3B	-4.19	1.40	1.48
3	L	176	CYC	CHD-C4C	4.14	1.43	1.36
4	L	175	PUB	O2C-CGC	4.14	1.44	1.30
3	B	176	CYC	O2D-CGD	4.06	1.44	1.30
3	B	175	CYC	C4C-NC	4.03	1.45	1.37
3	K	141	CYC	C4C-NC	4.02	1.45	1.37
3	K	175	CYC	O2D-CGD	4.02	1.44	1.30
3	L	176	CYC	C4B-C3B	-4.00	1.40	1.48
3	B	176	CYC	C3B-C2B	3.88	1.45	1.36
3	A	141	CYC	O2D-CGD	3.87	1.43	1.30
3	K	141	CYC	CAC-C3C	3.84	1.61	1.54
3	K	175	CYC	C4C-NC	3.83	1.44	1.37
4	B	177	PUB	C2C-C3C	3.81	1.45	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	175	CYC	C2A-C3A	3.74	1.44	1.36
4	L	175	PUB	C4D-C3D	-3.74	1.41	1.48
3	K	141	CYC	O2A-CGA	3.71	1.43	1.30
3	B	176	CYC	C2A-C3A	3.70	1.44	1.36
3	L	176	CYC	C2A-C3A	3.67	1.44	1.36
3	A	141	CYC	C1B-NB	3.57	1.43	1.37
4	L	175	PUB	C4C-NC	3.56	1.41	1.35
3	A	175	CYC	C4B-C3B	-3.52	1.41	1.48
4	L	175	PUB	C4A-C3A	-3.48	1.40	1.51
4	L	175	PUB	O2B-CGB	3.46	1.42	1.30
3	B	175	CYC	O2A-CGA	3.45	1.42	1.30
3	A	141	CYC	C4C-NC	3.44	1.44	1.37
3	B	176	CYC	CHD-C4C	3.42	1.42	1.36
4	B	177	PUB	C1B-C2B	3.39	1.42	1.38
3	K	175	CYC	C2A-C3A	3.36	1.44	1.36
3	L	177	CYC	C4C-NC	3.30	1.43	1.37
3	A	175	CYC	CAC-C3C	3.30	1.60	1.54
4	B	177	PUB	C4C-NC	3.30	1.41	1.35
3	L	176	CYC	C1A-C2A	-3.25	1.40	1.45
3	K	175	CYC	O2A-CGA	3.23	1.41	1.30
4	L	175	PUB	C2C-C3C	3.22	1.43	1.36
3	L	177	CYC	C1B-NB	3.19	1.43	1.37
3	B	175	CYC	C2A-C3A	3.19	1.43	1.36
3	L	177	CYC	C2A-C3A	3.14	1.43	1.36
3	A	175	CYC	C3B-C2B	3.12	1.43	1.36
3	A	141	CYC	C3B-C2B	3.09	1.43	1.36
3	A	175	CYC	C4C-NC	3.04	1.43	1.37
3	A	141	CYC	CHB-C1B	3.02	1.45	1.37
3	L	176	CYC	C3B-C2B	3.02	1.43	1.36
3	A	141	CYC	C4D-ND	2.99	1.42	1.37
3	B	175	CYC	C3B-C2B	2.99	1.43	1.36
3	B	176	CYC	C4C-NC	2.96	1.43	1.37
4	B	177	PUB	C4A-C3A	-2.95	1.41	1.51
3	K	141	CYC	C2A-C3A	2.95	1.43	1.36
4	B	177	PUB	C4B-NB	2.95	1.42	1.37
4	B	177	PUB	C1B-NB	2.93	1.43	1.37
4	B	177	PUB	C1A-C2A	-2.93	1.41	1.48
3	K	175	CYC	C3B-C2B	2.93	1.43	1.36
3	L	176	CYC	C4C-NC	2.86	1.42	1.37
3	K	141	CYC	C1B-NB	2.81	1.42	1.37
4	L	175	PUB	C4A-NA	-2.81	1.41	1.45
3	B	176	CYC	C4D-ND	2.76	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	141	CYC	C3B-C2B	2.75	1.42	1.36
4	L	175	PUB	C1D-C2D	-2.74	1.42	1.50
3	A	141	CYC	C2A-C3A	2.68	1.42	1.36
3	B	175	CYC	CAC-C3C	2.67	1.59	1.54
3	B	176	CYC	C4B-NB	-2.56	1.32	1.38
4	L	175	PUB	C4B-NB	2.56	1.42	1.37
3	B	176	CYC	CHB-C1B	2.53	1.43	1.37
4	L	175	PUB	C1A-C2A	-2.51	1.42	1.48
3	L	176	CYC	C4B-NB	-2.43	1.32	1.38
3	A	141	CYC	C1D-ND	2.43	1.42	1.37
3	B	176	CYC	C4A-NA	2.37	1.42	1.36
3	L	177	CYC	C3B-C2B	2.35	1.41	1.36
3	A	175	CYC	C4A-NA	2.35	1.42	1.36
4	L	175	PUB	C3B-C2B	2.35	1.45	1.38
3	B	175	CYC	C1D-ND	2.34	1.41	1.37
3	B	176	CYC	C1D-ND	2.34	1.41	1.37
3	L	177	CYC	C4B-C3B	-2.29	1.44	1.48
3	B	175	CYC	C1C-NC	-2.26	1.34	1.37
3	B	175	CYC	C3C-C4C	2.25	1.55	1.50
4	B	177	PUB	C3B-C2B	2.23	1.44	1.38
3	A	175	CYC	C1B-NB	2.20	1.41	1.37
4	B	177	PUB	C1D-C2D	-2.20	1.43	1.50
3	K	141	CYC	C4D-ND	2.19	1.41	1.37
3	B	175	CYC	C1B-NB	2.18	1.41	1.37
3	A	175	CYC	C1C-NC	-2.17	1.34	1.37
3	B	175	CYC	C4D-ND	2.17	1.41	1.37
3	L	176	CYC	C3D-C2D	2.15	1.44	1.38
3	A	141	CYC	C1A-C2A	-2.15	1.42	1.45
3	L	176	CYC	C1D-ND	2.14	1.41	1.37
3	A	175	CYC	CHD-C1D	2.14	1.45	1.40
3	B	175	CYC	CHA-C1A	2.13	1.42	1.38
3	L	177	CYC	CHB-C1B	2.13	1.43	1.37
3	B	175	CYC	C4B-C3B	-2.13	1.44	1.48
3	B	176	CYC	CHB-C4A	2.13	1.45	1.40
3	A	175	CYC	C4B-NB	-2.11	1.33	1.38
4	B	177	PUB	C1C-C2C	-2.10	1.42	1.45
3	B	175	CYC	C4B-NB	-2.09	1.33	1.38
3	K	141	CYC	C4B-NB	-2.09	1.33	1.38
3	K	141	CYC	C4A-NA	2.08	1.41	1.36
3	L	177	CYC	CMC-C2C	-2.06	1.48	1.53
3	K	175	CYC	C1B-NB	2.06	1.41	1.37
3	L	176	CYC	C4A-NA	2.06	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	175	CYC	C4D-ND	2.05	1.41	1.37
3	B	175	CYC	C1B-C2B	-2.05	1.41	1.45
3	K	175	CYC	C1D-ND	2.02	1.41	1.37
3	A	141	CYC	C4A-NA	2.02	1.41	1.36
4	L	175	PUB	C1B-C2B	2.02	1.40	1.38
3	K	141	CYC	C1A-C2A	-2.00	1.42	1.45

All (219) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	177	PUB	CHA-C4A-NA	10.85	127.06	113.73
4	L	175	PUB	CHA-C4A-NA	9.51	125.42	113.73
4	B	177	PUB	CHC-C1D-ND	8.66	124.37	113.73
3	B	175	CYC	C1B-C2B-C3B	-8.61	99.01	107.86
4	L	175	PUB	CHC-C1D-ND	8.49	124.16	113.73
4	B	177	PUB	C4A-CHA-C1B	8.11	126.98	113.32
4	B	177	PUB	CAD-C3D-C4D	-7.74	109.40	121.37
3	L	177	CYC	C1B-C2B-C3B	-7.45	100.21	107.86
4	L	175	PUB	C4A-CHA-C1B	7.42	125.81	113.32
3	B	176	CYC	CMC-C2C-C1C	7.19	127.90	112.40
3	K	175	CYC	CMC-C2C-C1C	7.18	127.89	112.40
4	L	175	PUB	C4A-NA-C1A	-7.16	102.41	113.42
3	L	176	CYC	CMC-C2C-C1C	6.75	126.96	112.40
3	B	175	CYC	C1B-NB-C4B	-6.66	102.48	110.66
3	A	141	CYC	CBC-CAC-C3C	-6.65	99.31	113.41
3	A	141	CYC	CMC-C2C-C1C	6.31	126.00	112.40
4	B	177	PUB	C1D-CHC-C4C	6.00	127.78	113.74
3	A	175	CYC	CMC-C2C-C1C	5.91	125.14	112.40
3	L	177	CYC	CAB-C3B-C4B	5.87	130.45	121.37
3	B	176	CYC	OC-C1C-NC	-5.75	118.15	124.93
3	L	177	CYC	CMC-C2C-C1C	5.70	124.68	112.40
3	L	177	CYC	CMB-C2B-C1B	5.66	131.04	124.16
3	K	141	CYC	C1B-C2B-C3B	-5.52	102.19	107.86
3	B	175	CYC	CMB-C2B-C1B	5.48	130.82	124.16
3	K	141	CYC	CMC-C2C-C1C	5.37	123.97	112.40
3	K	175	CYC	C1D-CHD-C4C	5.37	136.92	127.76
3	L	176	CYC	CMB-C2B-C1B	5.32	130.63	124.16
4	L	175	PUB	C1D-ND-C4D	-5.28	105.30	113.42
3	B	176	CYC	CBB-CAB-C3B	5.27	126.71	112.42
3	B	175	CYC	CMC-C2C-C1C	5.25	123.72	112.40
3	A	175	CYC	C1B-C2B-C3B	-5.25	102.46	107.86
3	K	175	CYC	C1B-C2B-C3B	-5.21	102.50	107.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	141	CYC	C1C-NC-C4C	-5.21	106.87	113.41
3	L	177	CYC	C1B-NB-C4B	-5.19	104.29	110.66
3	B	176	CYC	OC-C1C-C2C	5.07	130.21	126.17
3	A	175	CYC	C1D-CHD-C4C	4.98	136.27	127.76
3	K	141	CYC	C1B-NB-C4B	-4.89	104.66	110.66
4	L	175	PUB	C1D-CHC-C4C	4.83	125.05	113.74
3	K	141	CYC	C2C-C1C-NC	4.71	112.20	108.29
4	B	177	PUB	C1D-ND-C4D	-4.64	106.29	113.42
3	B	175	CYC	CAB-C3B-C4B	4.62	128.52	121.37
3	L	177	CYC	CAC-C3C-C4C	4.49	124.20	112.67
3	K	141	CYC	CBC-CAC-C3C	-4.46	103.94	113.41
3	B	176	CYC	C1B-NB-C4B	-4.46	105.19	110.66
3	A	141	CYC	C1B-C2B-C3B	-4.43	103.31	107.86
3	A	175	CYC	C3B-C4B-NB	4.42	110.29	106.77
4	L	175	PUB	CAD-C3D-C4D	-4.41	114.55	121.37
3	K	141	CYC	CAB-C3B-C4B	4.39	128.16	121.37
3	B	175	CYC	OB-C4B-C3B	4.39	132.65	128.03
3	B	176	CYC	C1B-C2B-C3B	-4.31	103.44	107.86
3	K	175	CYC	CHD-C4C-NC	4.30	131.00	125.63
3	B	175	CYC	C2C-C1C-NC	4.14	111.73	108.29
3	K	141	CYC	OC-C1C-C2C	-4.11	122.90	126.17
3	L	176	CYC	CHA-C4D-C3D	-4.05	118.52	127.22
3	B	176	CYC	C2C-C1C-NC	4.01	111.63	108.29
3	K	175	CYC	C1C-NC-C4C	-3.98	108.41	113.41
3	B	176	CYC	CBC-CAC-C3C	-3.97	104.98	113.41
3	A	175	CYC	CAC-C3C-C4C	3.93	122.76	112.67
3	A	175	CYC	C1C-NC-C4C	-3.92	108.49	113.41
3	A	141	CYC	C1D-CHD-C4C	3.91	134.45	127.76
3	B	175	CYC	C1D-CHD-C4C	3.91	134.44	127.76
3	L	176	CYC	CBC-CAC-C3C	-3.89	105.17	113.41
3	K	141	CYC	CHD-C4C-NC	3.87	130.46	125.63
3	K	175	CYC	CAB-C3B-C4B	3.85	127.33	121.37
3	B	175	CYC	O2D-CGD-CBD	3.85	126.17	114.00
4	B	177	PUB	O2B-CGB-CBB	3.71	125.74	114.00
4	L	175	PUB	OD-C4D-C3D	3.71	131.93	128.03
3	A	175	CYC	CBC-CAC-C3C	-3.71	105.54	113.41
3	A	141	CYC	CHD-C4C-NC	3.71	130.26	125.63
3	L	176	CYC	C1B-C2B-C3B	-3.70	104.06	107.86
3	L	176	CYC	CAB-C3B-C4B	3.68	127.06	121.37
3	L	176	CYC	C1D-CHD-C4C	3.63	133.96	127.76
3	K	141	CYC	C4D-ND-C1D	-3.59	103.48	109.78
4	B	177	PUB	CBA-CAA-C3A	-3.59	107.47	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	175	CYC	CMB-C2B-C1B	3.57	128.50	124.16
3	L	176	CYC	CBB-CAB-C3B	3.54	122.01	112.42
3	A	141	CYC	C3C-C4C-NC	-3.52	103.41	107.94
3	K	175	CYC	C1B-NB-C4B	-3.48	106.40	110.66
3	L	176	CYC	C1A-C2A-C3A	-3.47	102.97	106.73
3	K	141	CYC	OB-C4B-C3B	3.47	131.68	128.03
3	K	141	CYC	C1C-NC-C4C	-3.45	109.08	113.41
3	L	177	CYC	O2D-CGD-CBD	3.44	124.86	114.00
3	L	177	CYC	C1D-CHD-C4C	3.41	133.58	127.76
4	L	175	PUB	C4B-NB-C1B	-3.35	103.64	109.60
3	K	141	CYC	CBB-CAB-C3B	3.33	121.45	112.42
3	K	175	CYC	CMB-C2B-C1B	3.33	128.21	124.16
3	A	141	CYC	OC-C1C-C2C	3.33	128.82	126.17
3	A	175	CYC	C1B-NB-C4B	-3.30	106.61	110.66
3	A	175	CYC	O2A-CGA-O1A	-3.28	114.90	123.33
3	K	175	CYC	CMC-C2C-C3C	3.26	126.57	113.98
3	L	176	CYC	CHB-C4A-NA	-3.25	117.94	124.95
3	B	176	CYC	CAB-C3B-C2B	3.24	133.52	127.56
3	B	176	CYC	CBA-CAA-C2A	3.24	121.50	112.53
3	A	175	CYC	O2A-CGA-CBA	3.21	124.14	114.00
3	B	175	CYC	CMC-C2C-C3C	3.20	126.37	113.98
3	L	177	CYC	CHD-C1D-ND	-3.15	118.17	125.29
3	L	176	CYC	C1B-NB-C4B	-3.14	106.81	110.66
3	L	176	CYC	CHB-C4A-C3A	3.13	132.91	124.87
3	L	177	CYC	OB-C4B-C3B	3.12	131.31	128.03
4	B	177	PUB	C4A-NA-C1A	-3.10	108.66	113.42
3	K	141	CYC	CMB-C2B-C1B	3.09	127.92	124.16
4	L	175	PUB	CMA-C2A-C1A	3.09	127.67	121.21
4	L	175	PUB	O2C-CGC-CBC	3.07	123.71	114.00
3	L	177	CYC	C3D-C4D-ND	3.05	111.39	107.57
4	B	177	PUB	O2B-CGB-O1B	-3.04	115.51	123.33
3	L	177	CYC	CHB-C4A-NA	-3.04	118.39	124.95
3	K	175	CYC	O2A-CGA-CBA	3.03	123.58	114.00
3	K	175	CYC	CBB-CAB-C3B	3.03	120.63	112.42
3	A	141	CYC	O2D-CGD-CBD	3.01	123.50	114.00
3	A	141	CYC	C4D-ND-C1D	-3.01	104.50	109.78
3	L	177	CYC	O2D-CGD-O1D	-2.99	115.65	123.33
3	B	176	CYC	CMB-C2B-C1B	2.98	127.79	124.16
3	K	175	CYC	O2A-CGA-O1A	-2.97	115.69	123.33
3	A	175	CYC	CMC-C2C-C3C	2.96	125.41	113.98
3	L	177	CYC	CBB-CAB-C3B	2.95	120.43	112.42
3	K	141	CYC	C2B-C1B-NB	2.95	111.27	106.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	141	CYC	C1B-CHB-C4A	-2.95	120.82	128.06
3	K	175	CYC	OB-C4B-C3B	2.95	131.13	128.03
3	A	175	CYC	CMD-C2D-C1D	2.95	129.90	125.62
3	A	141	CYC	C1A-NA-C4A	-2.94	101.13	106.52
4	B	177	PUB	C4B-NB-C1B	-2.89	104.45	109.60
3	L	177	CYC	CHA-C4D-C3D	-2.89	121.01	127.22
3	A	175	CYC	O2D-CGD-CBD	2.88	123.09	114.00
3	A	141	CYC	CHD-C1D-ND	-2.85	118.84	125.29
3	L	176	CYC	CHD-C1D-ND	-2.85	118.86	125.29
3	A	141	CYC	CBB-CAB-C3B	2.84	120.11	112.42
3	A	141	CYC	O2A-CGA-CBA	2.81	122.88	114.00
3	K	175	CYC	CHD-C1D-ND	-2.79	118.99	125.29
3	L	177	CYC	O2A-CGA-CBA	2.78	122.80	114.00
3	L	176	CYC	C3D-C4D-ND	2.78	111.06	107.57
3	L	177	CYC	O2A-CGA-O1A	-2.78	116.19	123.33
3	K	175	CYC	CAD-CBD-CGD	-2.77	106.33	113.67
3	L	177	CYC	CMC-C2C-C3C	2.76	124.67	113.98
3	A	141	CYC	C3D-C4D-ND	2.76	111.03	107.57
3	L	176	CYC	C1A-NA-C4A	-2.75	101.47	106.52
3	B	175	CYC	CAC-C3C-C4C	2.75	119.72	112.67
3	B	176	CYC	O2A-CGA-CBA	2.72	122.60	114.00
3	A	175	CYC	CHD-C1D-ND	-2.68	119.22	125.29
3	B	175	CYC	O1D-CGD-CBD	-2.66	114.65	123.09
3	B	175	CYC	CHB-C4A-NA	-2.66	119.21	124.95
4	B	177	PUB	CHA-C1B-NB	2.66	124.66	121.10
3	B	176	CYC	CHD-C1D-ND	-2.65	119.30	125.29
3	L	176	CYC	CMA-C3A-C4A	2.64	129.20	125.10
3	K	141	CYC	O2D-CGD-CBD	2.63	122.32	114.00
3	K	141	CYC	O2A-CGA-CBA	2.62	122.29	114.00
4	L	175	PUB	CBA-CAA-C3A	-2.60	108.96	112.93
4	B	177	PUB	O2C-CGC-CBC	2.60	122.21	114.00
3	K	141	CYC	C4A-C3A-C2A	-2.59	103.54	106.48
3	K	141	CYC	CMC-C2C-C3C	2.57	123.92	113.98
3	K	175	CYC	CMA-C3A-C4A	2.57	129.09	125.10
3	L	177	CYC	CBC-CAC-C3C	-2.56	107.97	113.41
3	K	175	CYC	CHB-C4A-NA	-2.53	119.48	124.95
3	K	141	CYC	O2A-CGA-O1A	-2.53	116.83	123.33
3	A	141	CYC	CAA-C2A-C1A	2.53	129.45	125.02
3	A	141	CYC	CMA-C3A-C4A	2.51	129.00	125.10
3	A	141	CYC	CHA-C4D-C3D	-2.50	121.85	127.22
3	A	175	CYC	CBB-CAB-C3B	2.49	119.17	112.42
3	L	176	CYC	C2C-C1C-NC	2.47	110.35	108.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	175	CYC	C3B-C4B-NB	2.47	108.73	106.77
3	L	177	CYC	CHD-C4C-NC	2.46	128.71	125.63
3	A	141	CYC	CMD-C2D-C1D	2.46	129.19	125.62
3	A	175	CYC	CHD-C1D-C2D	2.45	133.53	127.53
3	B	176	CYC	CHB-C1B-C2B	2.45	131.85	126.97
3	L	176	CYC	C4D-ND-C1D	-2.44	105.50	109.78
3	B	176	CYC	CMC-C2C-C3C	2.44	123.41	113.98
4	L	175	PUB	CAC-C2C-C1C	2.44	129.30	125.02
3	K	175	CYC	OC-C1C-C2C	-2.43	124.24	126.17
3	B	176	CYC	C4D-ND-C1D	-2.43	105.52	109.78
3	K	141	CYC	C1A-NA-C4A	-2.42	102.08	106.52
3	K	141	CYC	CHB-C4A-NA	-2.40	119.77	124.95
3	K	175	CYC	C2A-C1A-NA	-2.40	106.65	110.04
3	K	141	CYC	CHA-C4D-C3D	-2.39	122.08	127.22
3	K	175	CYC	C4A-C3A-C2A	-2.38	103.77	106.48
3	L	177	CYC	C4D-ND-C1D	-2.38	105.61	109.78
3	K	175	CYC	C4D-ND-C1D	-2.38	105.61	109.78
4	L	175	PUB	CAC-C2C-C3C	-2.37	123.44	127.87
3	L	176	CYC	OC-C1C-NC	-2.35	122.16	124.93
3	A	175	CYC	O1D-CGD-CBD	-2.35	115.65	123.09
3	B	176	CYC	CHD-C4C-NC	-2.34	122.71	125.63
3	L	176	CYC	OB-C4B-C3B	2.34	130.49	128.03
3	A	141	CYC	CMB-C2B-C1B	2.32	126.98	124.16
3	B	176	CYC	O2A-CGA-O1A	-2.32	117.37	123.33
3	A	175	CYC	C4D-ND-C1D	-2.30	105.75	109.78
3	A	175	CYC	CHB-C4A-NA	-2.29	120.01	124.95
3	A	175	CYC	CAA-CBA-CGA	2.28	119.72	113.67
3	L	176	CYC	CHA-C4D-ND	2.27	130.41	125.29
4	L	175	PUB	O2B-CGB-CBB	2.25	121.12	114.00
3	B	175	CYC	C2A-C1A-NA	-2.25	106.86	110.04
3	K	141	CYC	C3D-C4D-ND	2.24	110.38	107.57
3	A	141	CYC	CMC-C2C-C3C	2.22	122.58	113.98
3	L	177	CYC	CAB-C3B-C2B	-2.22	123.48	127.56
3	L	177	CYC	CBD-CAD-C3D	2.22	118.66	112.53
3	B	176	CYC	C1C-NC-C4C	-2.21	110.63	113.41
3	B	175	CYC	CMD-C2D-C1D	2.21	128.83	125.62
3	K	175	CYC	CAC-C3C-C4C	2.20	118.32	112.67
3	L	177	CYC	CMD-C2D-C1D	2.19	128.81	125.62
3	B	175	CYC	C1C-NC-C4C	-2.18	110.67	113.41
3	K	141	CYC	OB-C4B-NB	-2.18	119.97	125.08
3	K	175	CYC	C2B-C1B-NB	2.17	110.13	106.97
3	K	175	CYC	CHA-C4D-C3D	-2.17	122.56	127.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	175	CYC	C3C-C4C-NC	-2.15	105.17	107.94
3	A	141	CYC	C2C-C1C-NC	-2.15	106.50	108.29
3	K	175	CYC	C1D-C2D-C3D	-2.14	105.08	107.76
3	K	175	CYC	OB-C4B-NB	-2.11	120.13	125.08
3	B	175	CYC	O2A-CGA-O1A	-2.11	117.91	123.33
3	L	176	CYC	C2A-C1A-NA	-2.11	107.06	110.04
3	A	141	CYC	O2A-CGA-O1A	-2.10	117.93	123.33
3	K	175	CYC	C1A-NA-C4A	-2.07	102.71	106.52
3	K	141	CYC	CHD-C1D-ND	-2.07	120.61	125.29
4	L	175	PUB	O1C-CGC-CBC	-2.07	116.52	123.09
3	L	176	CYC	O2A-CGA-CBA	2.07	120.54	114.00
3	K	175	CYC	O2D-CGD-CBD	2.06	120.50	114.00
3	B	176	CYC	C2D-C1D-ND	2.05	110.22	107.43
3	L	176	CYC	CMC-C2C-C3C	2.04	121.88	113.98
3	K	141	CYC	CAB-C3B-C2B	-2.04	123.81	127.56
3	B	175	CYC	O2A-CGA-CBA	2.03	120.43	114.00
3	B	175	CYC	CBC-CAC-C3C	-2.03	109.11	113.41
3	B	175	CYC	OB-C4B-NB	-2.02	120.33	125.08
3	L	177	CYC	OB-C4B-NB	-2.00	120.39	125.08

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	176	CYC	C2C
3	K	175	CYC	C2C
3	L	177	CYC	C2C
4	B	177	PUB	C1D
4	B	177	PUB	C4A
4	L	175	PUB	C1D

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	175	CYC	NA-C4A-CHB-C1B
3	A	175	CYC	C3A-C4A-CHB-C1B
3	A	175	CYC	C4C-C3C-CAC-CBC
3	A	175	CYC	C3C-C4C-CHD-C1D
3	A	141	CYC	NA-C4A-CHB-C1B
3	A	141	CYC	C3A-C4A-CHB-C1B
3	A	141	CYC	C4C-C3C-CAC-CBC
3	A	141	CYC	C3C-C4C-CHD-C1D
3	A	141	CYC	ND-C1D-CHD-C4C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	175	CYC	NA-C4A-CHB-C1B
3	B	175	CYC	C3A-C4A-CHB-C1B
3	B	175	CYC	C2C-C3C-CAC-CBC
3	B	175	CYC	C4C-C3C-CAC-CBC
3	B	176	CYC	C3A-C2A-CAA-CBA
3	B	176	CYC	NA-C4A-CHB-C1B
3	B	176	CYC	C3A-C4A-CHB-C1B
3	B	176	CYC	C4B-C3B-CAB-CBB
3	K	175	CYC	NA-C4A-CHB-C1B
3	K	175	CYC	C3A-C4A-CHB-C1B
3	K	175	CYC	C2C-C3C-CAC-CBC
3	K	175	CYC	C4C-C3C-CAC-CBC
3	K	175	CYC	C3C-C4C-CHD-C1D
3	K	141	CYC	NA-C4A-CHB-C1B
3	K	141	CYC	C3A-C4A-CHB-C1B
3	K	141	CYC	C2C-C3C-CAC-CBC
3	K	141	CYC	C4C-C3C-CAC-CBC
3	L	176	CYC	NA-C4A-CHB-C1B
3	L	176	CYC	C3A-C4A-CHB-C1B
3	L	176	CYC	C2C-C3C-CAC-CBC
3	L	176	CYC	C4C-C3C-CAC-CBC
3	L	177	CYC	NA-C4A-CHB-C1B
3	L	177	CYC	C3A-C4A-CHB-C1B
3	L	177	CYC	C2B-C3B-CAB-CBB
3	L	177	CYC	C4C-C3C-CAC-CBC
4	B	177	PUB	C3C-C4C-CHC-C1D
4	B	177	PUB	ND-C1D-CHC-C4C
4	B	177	PUB	C4D-C3D-CAD-CBD
4	B	177	PUB	NA-C4A-CHA-C1B
4	B	177	PUB	C2B-C1B-CHA-C4A
4	L	175	PUB	NC-C4C-CHC-C1D
4	L	175	PUB	ND-C1D-CHC-C4C
4	L	175	PUB	NA-C4A-CHA-C1B
3	K	175	CYC	C2B-C3B-CAB-CBB
3	K	141	CYC	C2B-C3B-CAB-CBB
3	L	176	CYC	C2B-C3B-CAB-CBB
4	B	177	PUB	C2D-C3D-CAD-CBD
3	A	175	CYC	ND-C1D-CHD-C4C
3	K	175	CYC	ND-C1D-CHD-C4C
3	K	141	CYC	ND-C1D-CHD-C4C
3	A	141	CYC	C2D-C1D-CHD-C4C
3	K	175	CYC	C2D-C1D-CHD-C4C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	141	CYC	C2D-C1D-CHD-C4C
3	B	176	CYC	C1A-C2A-CAA-CBA
3	A	175	CYC	C2B-C3B-CAB-CBB
3	K	175	CYC	C3D-CAD-CBD-CGD
3	B	175	CYC	ND-C1D-CHD-C4C
3	L	177	CYC	ND-C1D-CHD-C4C
3	A	175	CYC	C2D-C1D-CHD-C4C
3	B	175	CYC	C2D-C1D-CHD-C4C
3	B	176	CYC	C2D-C1D-CHD-C4C
3	L	176	CYC	C2D-C1D-CHD-C4C
3	L	177	CYC	C2D-C1D-CHD-C4C
3	B	176	CYC	ND-C1D-CHD-C4C
3	L	176	CYC	ND-C1D-CHD-C4C
3	K	175	CYC	C4B-C3B-CAB-CBB
3	K	141	CYC	C4B-C3B-CAB-CBB
3	L	177	CYC	C4B-C3B-CAB-CBB
3	L	177	CYC	C2B-C1B-CHB-C4A
4	L	175	PUB	NB-C4B-CHB-C1C
3	L	176	CYC	C2A-CAA-CBA-CGA
3	L	177	CYC	C2A-C1A-CHA-C4D
3	A	141	CYC	C4B-C3B-CAB-CBB
3	L	176	CYC	C4B-C3B-CAB-CBB
3	A	175	CYC	C2C-C3C-CAC-CBC
3	A	141	CYC	C2C-C3C-CAC-CBC
3	L	177	CYC	C2C-C3C-CAC-CBC
3	B	176	CYC	C2B-C3B-CAB-CBB
3	B	175	CYC	C2A-CAA-CBA-CGA
4	L	175	PUB	C3A-C4A-CHA-C1B
4	B	177	PUB	NB-C1B-CHA-C4A
3	B	176	CYC	C4C-C3C-CAC-CBC
4	L	175	PUB	C3B-C4B-CHB-C1C
4	B	177	PUB	C3B-CAB-CBB-CGB
4	B	177	PUB	NB-C4B-CHB-C1C
3	A	141	CYC	C2B-C3B-CAB-CBB
4	B	177	PUB	C4A-C3A-CAA-CBA
3	L	177	CYC	NA-C1A-CHA-C4D
3	L	176	CYC	CAA-CBA-CGA-O2A
3	B	175	CYC	CAA-CBA-CGA-O2A
3	A	175	CYC	C3D-CAD-CBD-CGD
3	B	176	CYC	CAD-CBD-CGD-O1D
3	K	141	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	CAB-CBB-CGB-O2B

Continued on next page...

Continued from previous page...

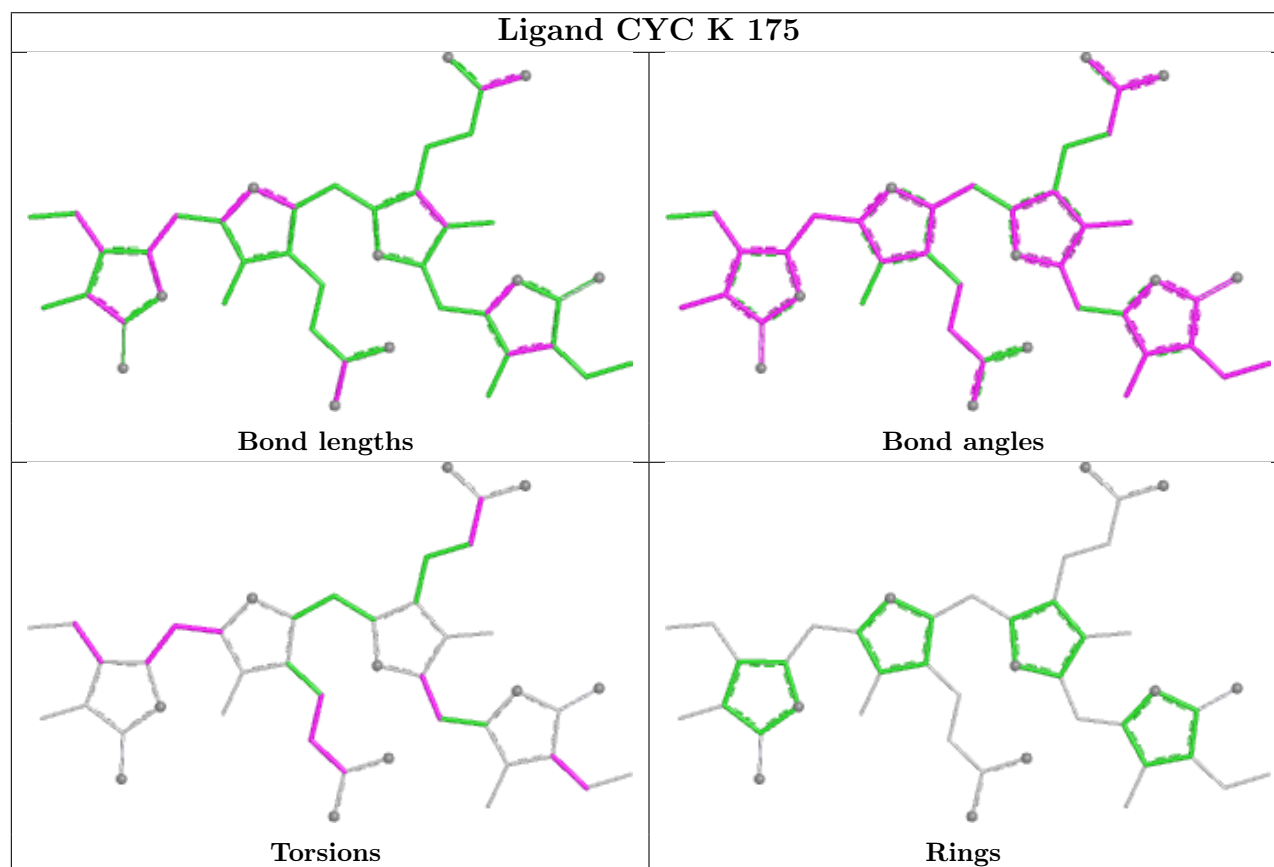
Mol	Chain	Res	Type	Atoms
4	L	175	PUB	C4A-C3A-CAA-CBA
3	B	175	CYC	CAD-CBD-CGD-O2D
3	B	175	CYC	CAA-CBA-CGA-O1A
3	L	176	CYC	CAD-CBD-CGD-O2D
3	B	176	CYC	CAA-CBA-CGA-O1A
3	B	176	CYC	CAD-CBD-CGD-O2D
3	K	175	CYC	CAA-CBA-CGA-O2A
3	L	177	CYC	CAA-CBA-CGA-O2A
3	L	177	CYC	CAD-CBD-CGD-O1D
3	A	175	CYC	CAD-CBD-CGD-O1D
3	A	141	CYC	CAA-CBA-CGA-O2A
3	A	141	CYC	CAD-CBD-CGD-O1D
4	L	175	PUB	CAB-CBB-CGB-O1B
3	B	175	CYC	CAD-CBD-CGD-O1D
3	K	141	CYC	CAA-CBA-CGA-O1A
3	L	176	CYC	CAD-CBD-CGD-O1D
3	A	175	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	CAC-CBC-CGC-O2C
3	B	176	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	NB-C1B-CHA-C4A
3	K	141	CYC	CAD-CBD-CGD-O1D
4	L	175	PUB	CAC-CBC-CGC-O1C
3	K	175	CYC	CAA-CBA-CGA-O1A
3	L	176	CYC	CAA-CBA-CGA-O1A
3	A	175	CYC	CAD-CBD-CGD-O2D
3	A	141	CYC	CAA-CBA-CGA-O1A
3	K	141	CYC	CAD-CBD-CGD-O2D
3	L	177	CYC	CAA-CBA-CGA-O1A
3	K	175	CYC	CAD-CBD-CGD-O1D
3	A	141	CYC	CAD-CBD-CGD-O2D
3	A	175	CYC	CAA-CBA-CGA-O1A
4	B	177	PUB	C3B-C4B-CHB-C1C
4	L	175	PUB	C2B-C1B-CHA-C4A
3	L	177	CYC	CAD-CBD-CGD-O2D
4	L	175	PUB	C2D-C3D-CAD-CBD
4	B	177	PUB	CAC-CBC-CGC-O1C
4	B	177	PUB	CAC-CBC-CGC-O2C
3	L	176	CYC	C3C-C4C-CHD-C1D
3	K	175	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

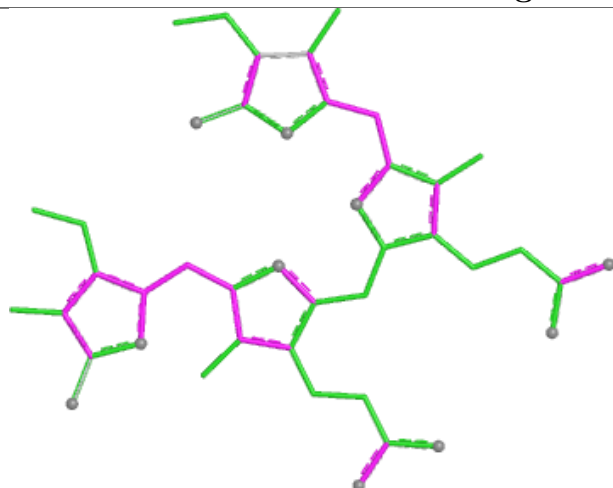
9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	175	CYC	1	0
4	L	175	PUB	1	0
3	L	176	CYC	2	0
3	L	177	CYC	7	0
4	B	177	PUB	1	0
3	B	175	CYC	6	0
3	A	175	CYC	1	0
3	B	176	CYC	3	0
3	A	141	CYC	3	0

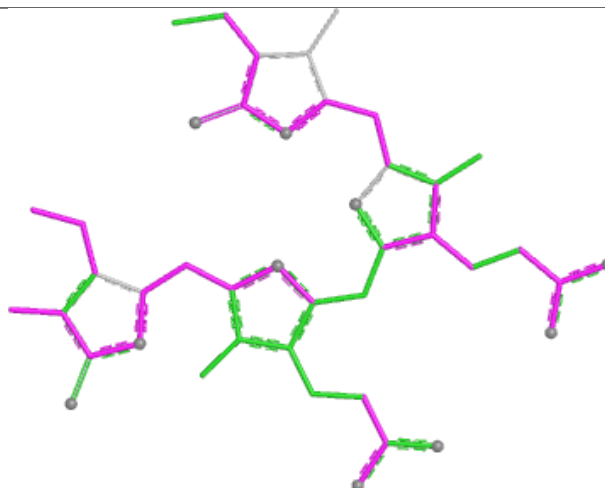
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



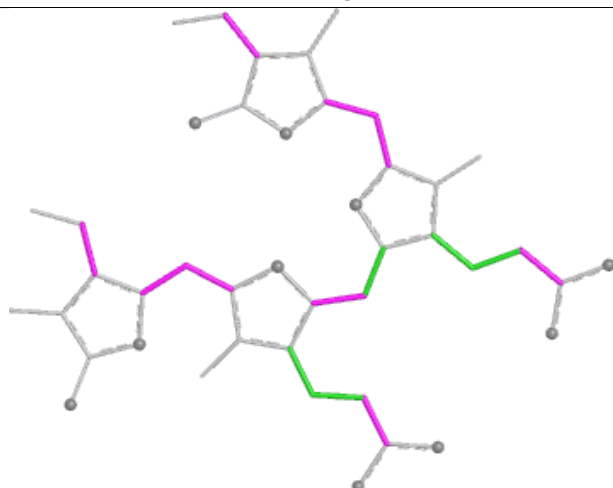
Ligand PUB L 175



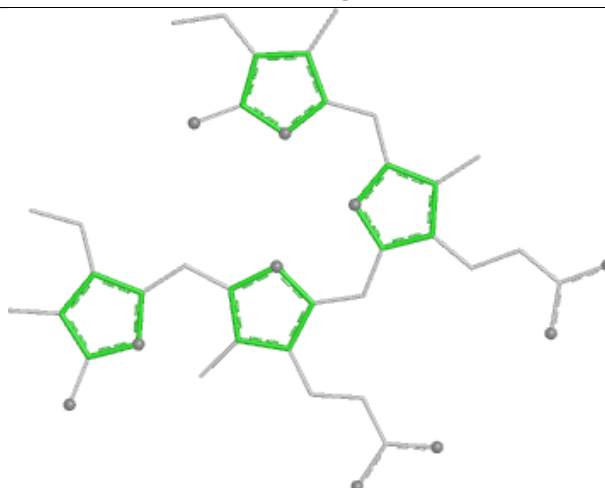
Bond lengths



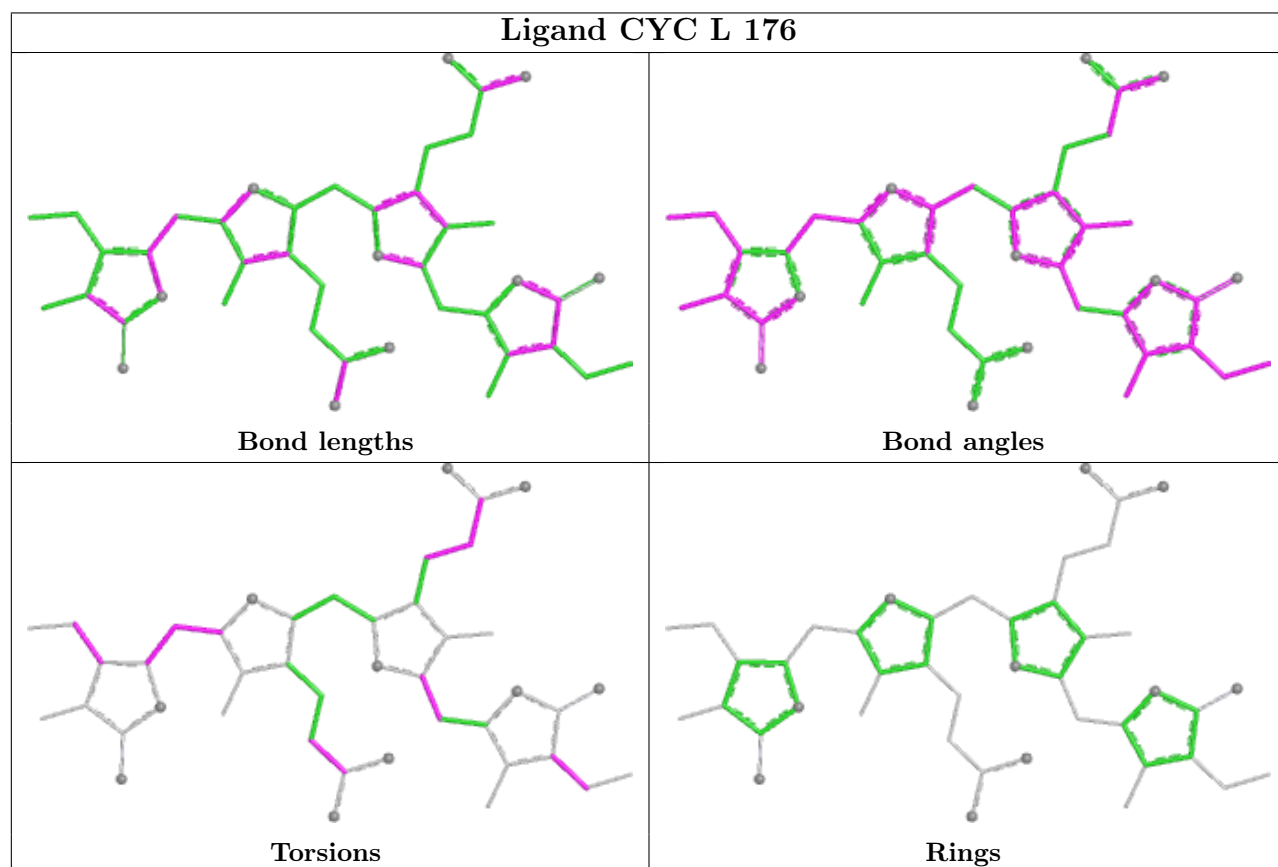
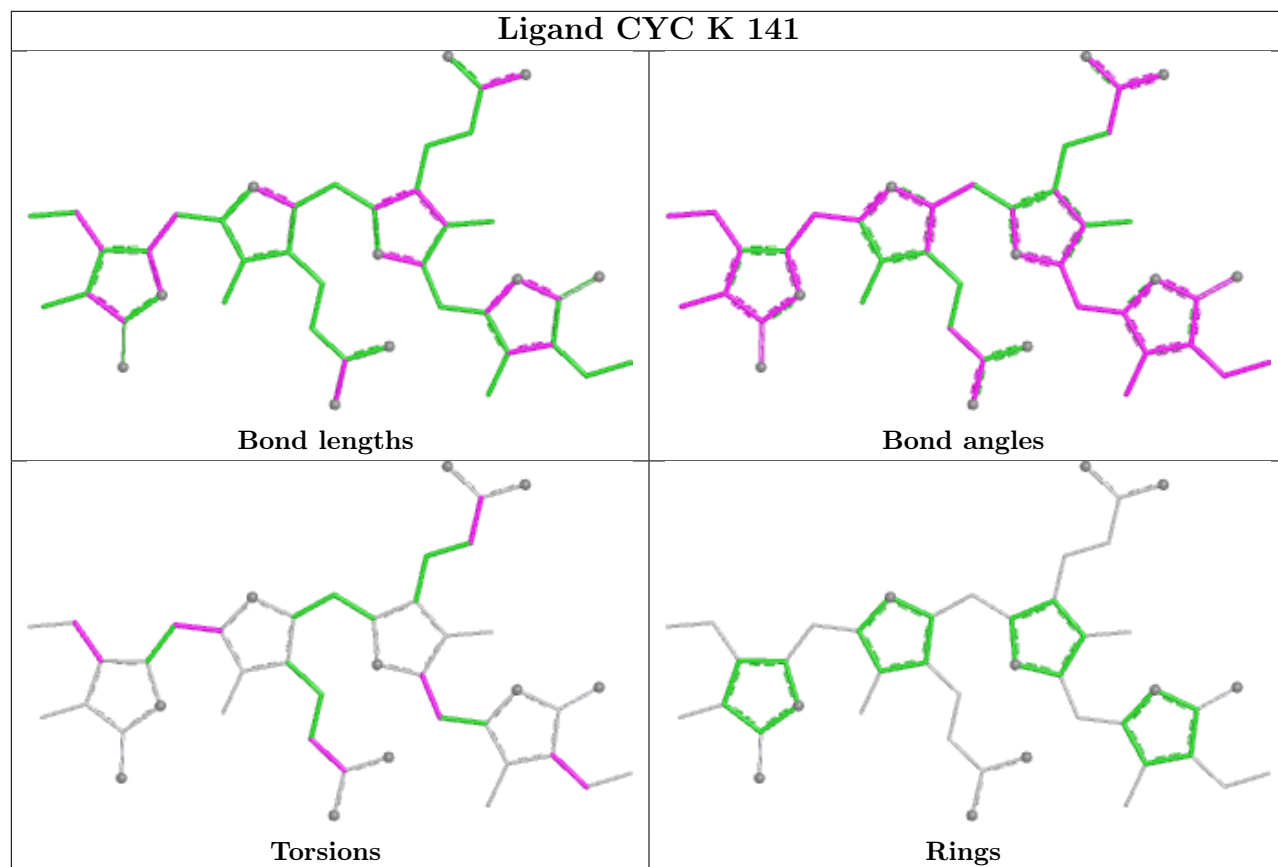
Bond angles

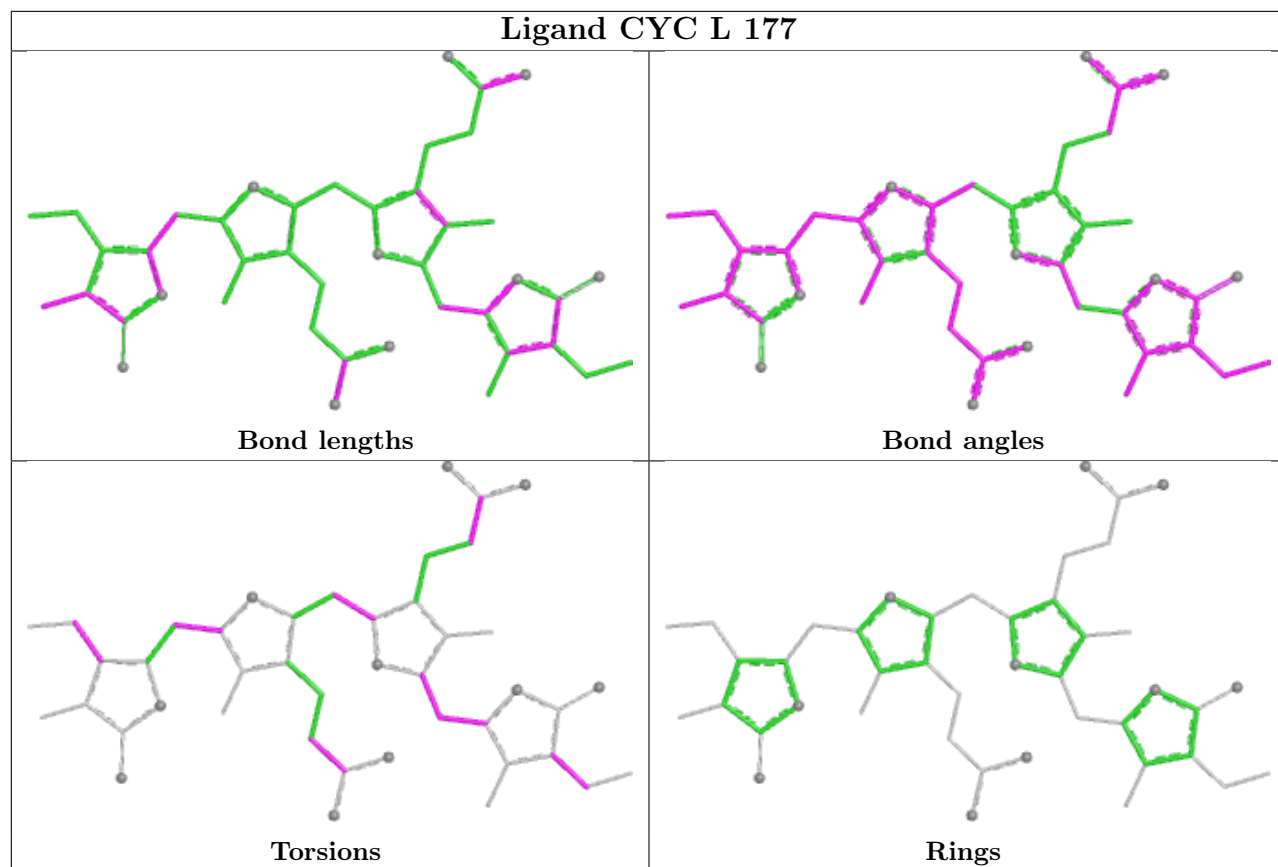


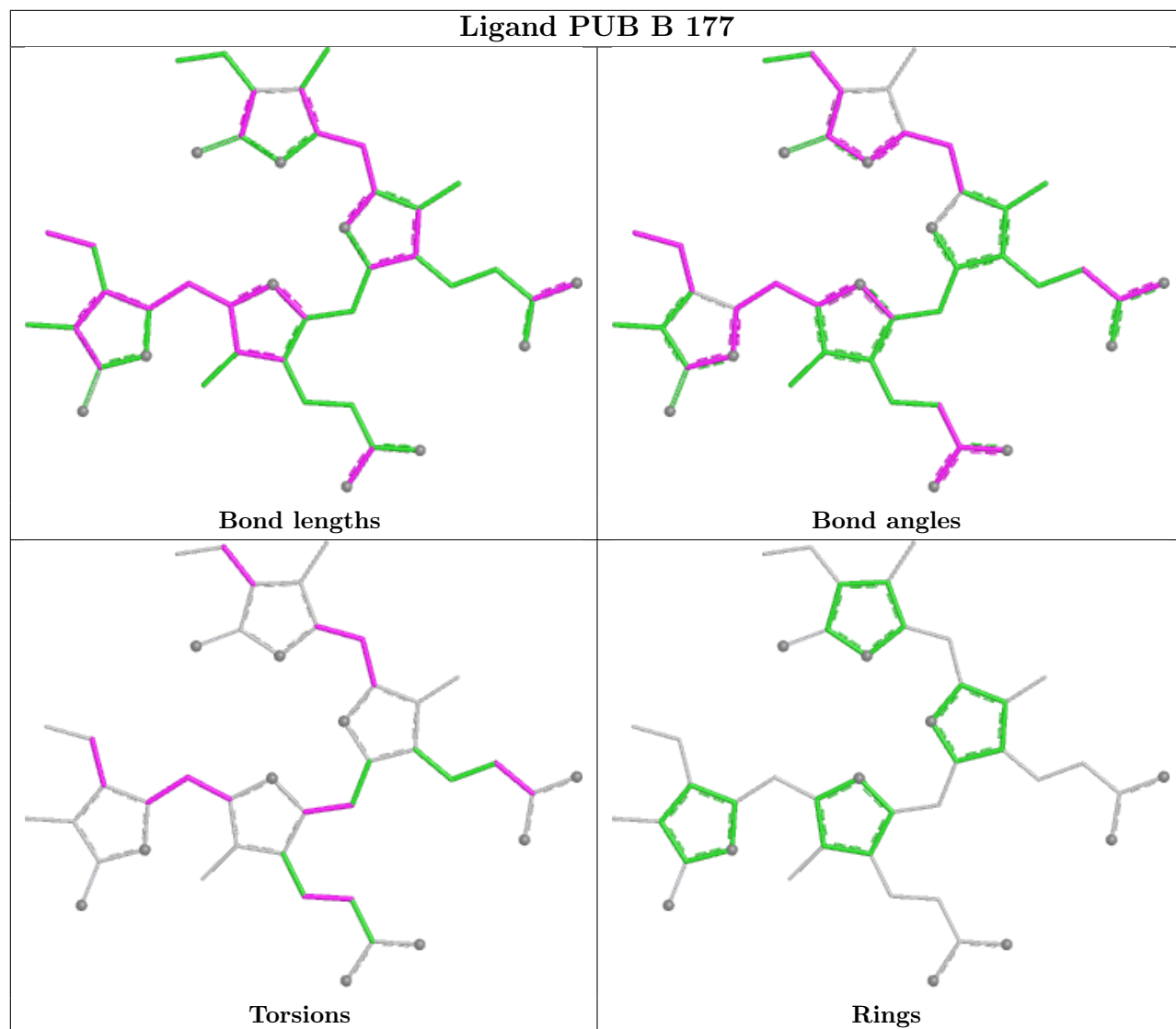
Torsions



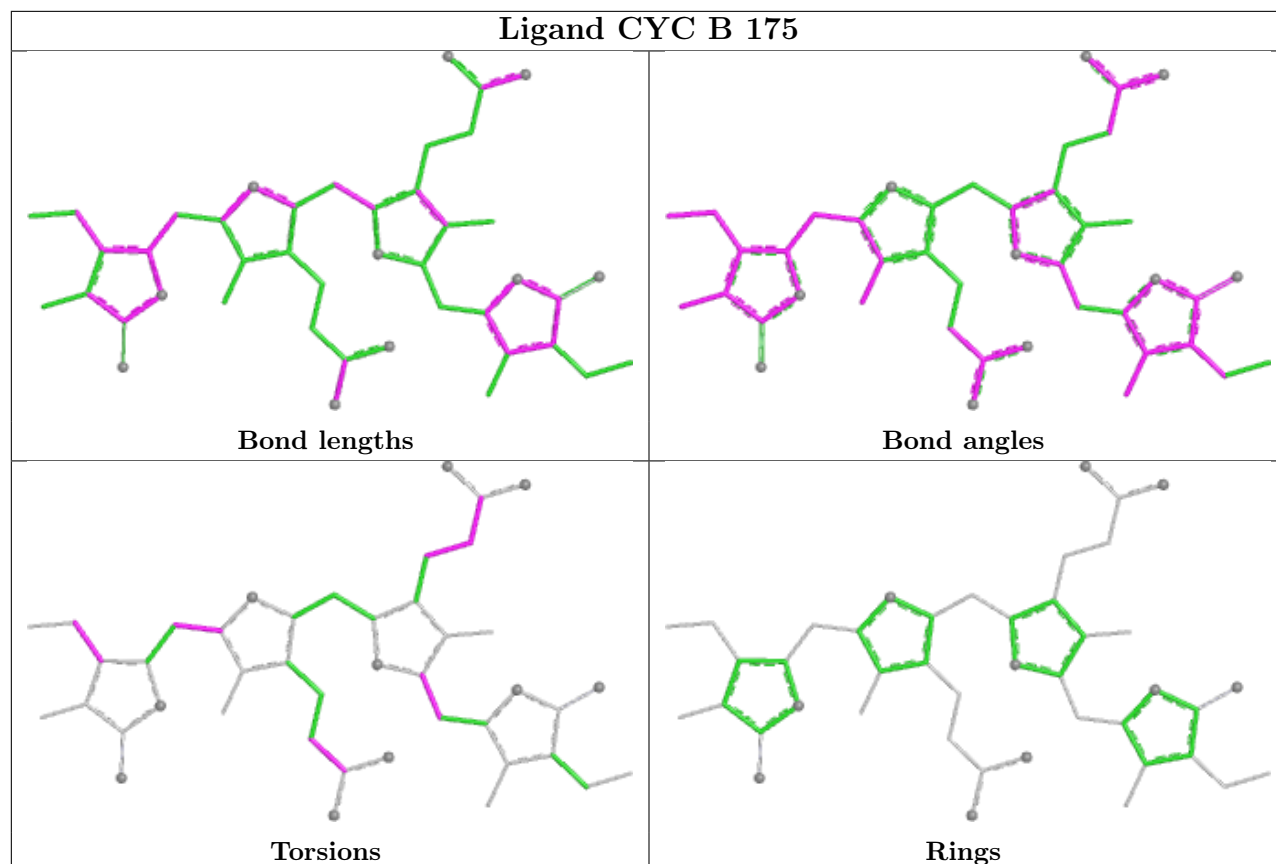
Rings



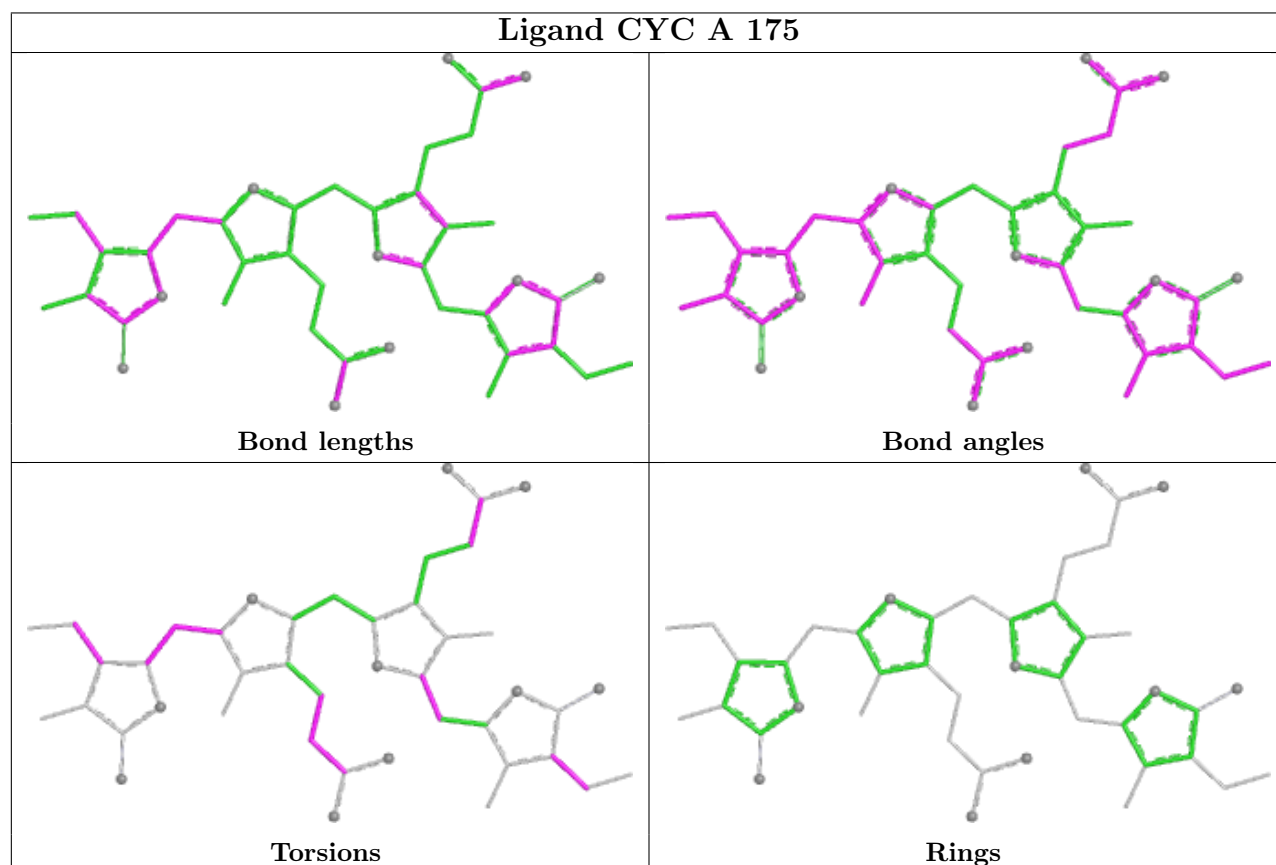


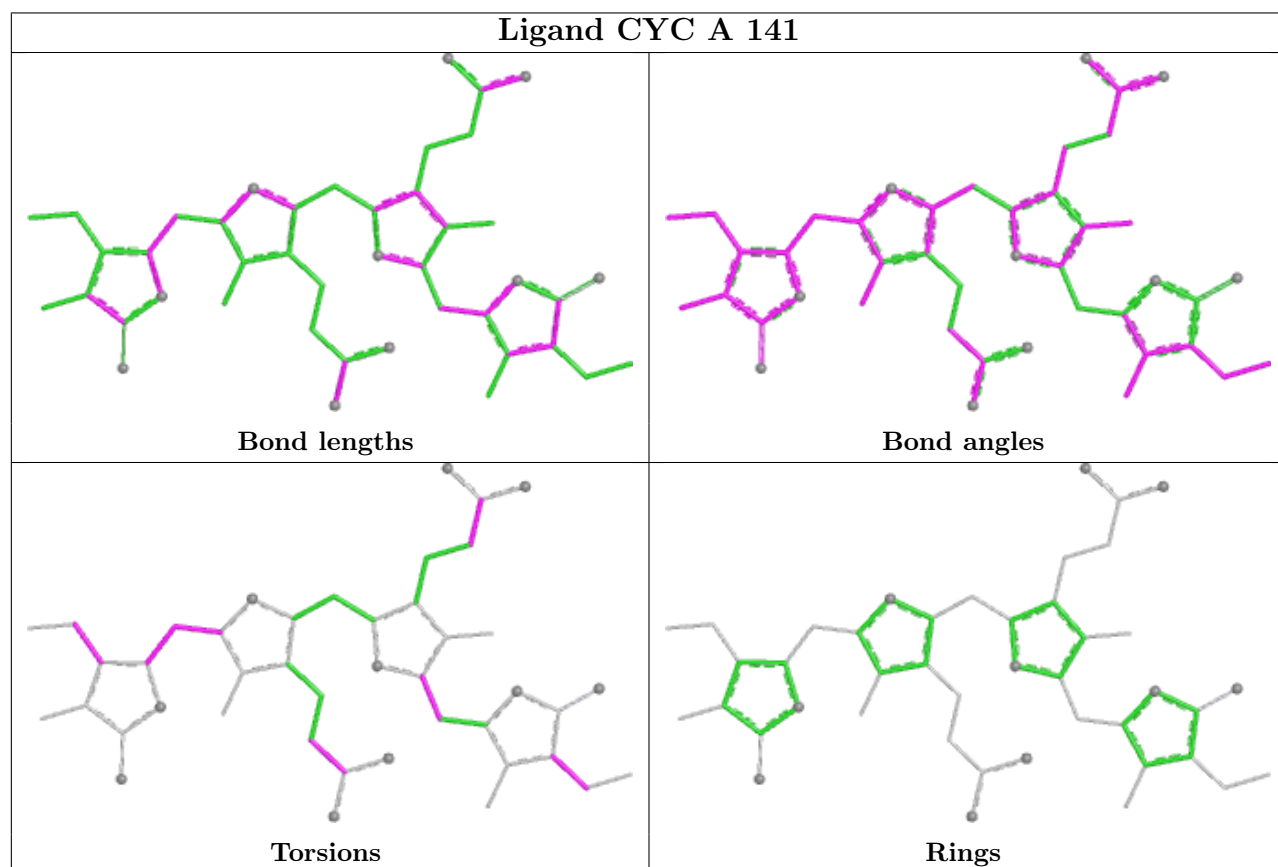
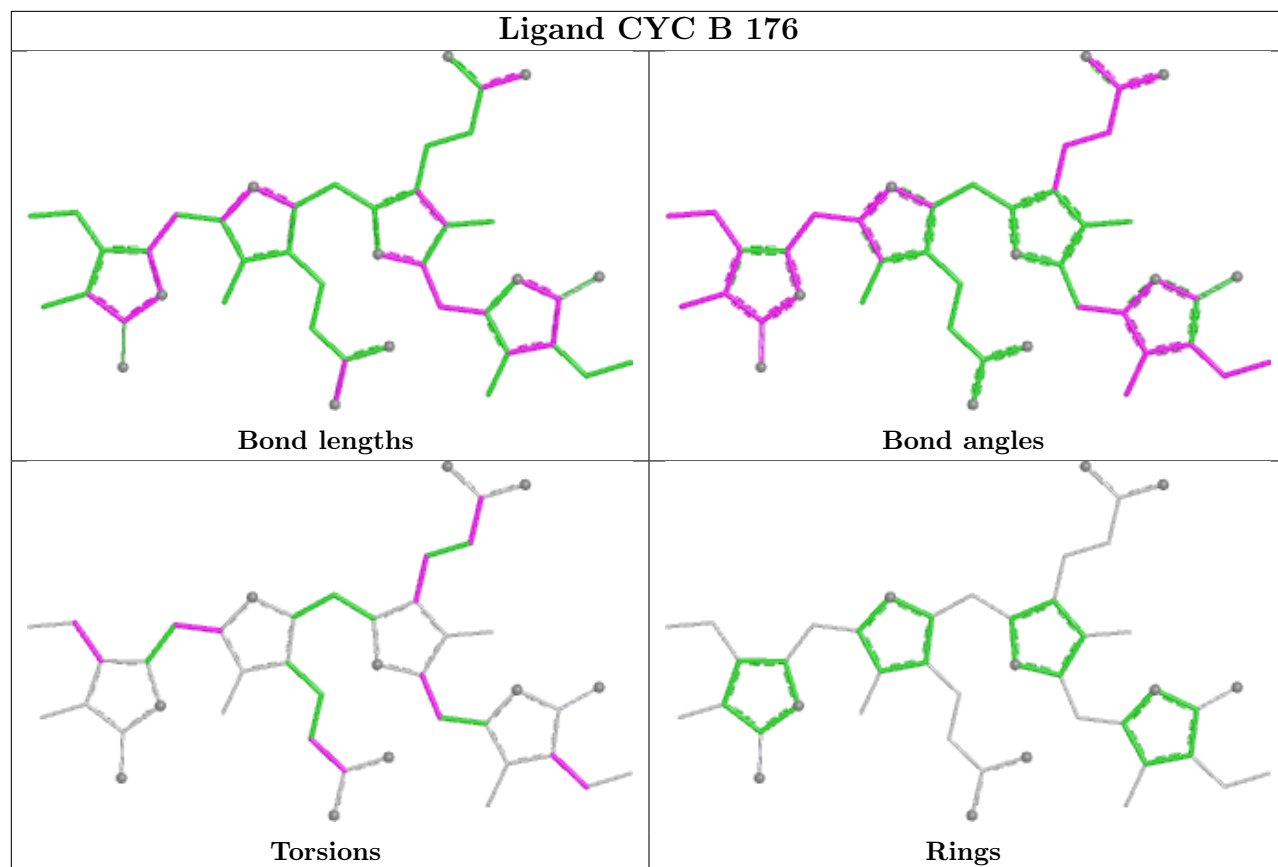


Ligand CYC B 175



Ligand CYC A 175





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.