



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 10:50 AM EDT

PDB ID : 1LIA
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

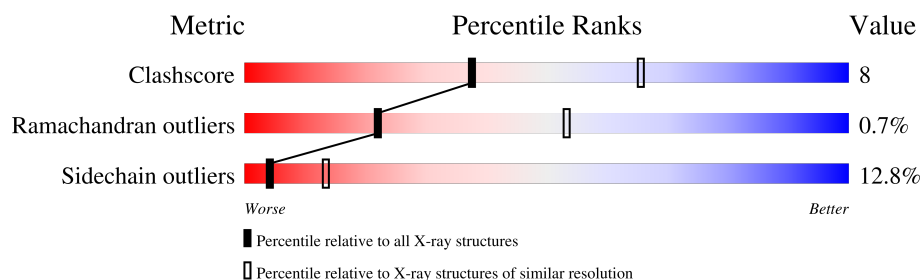
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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			

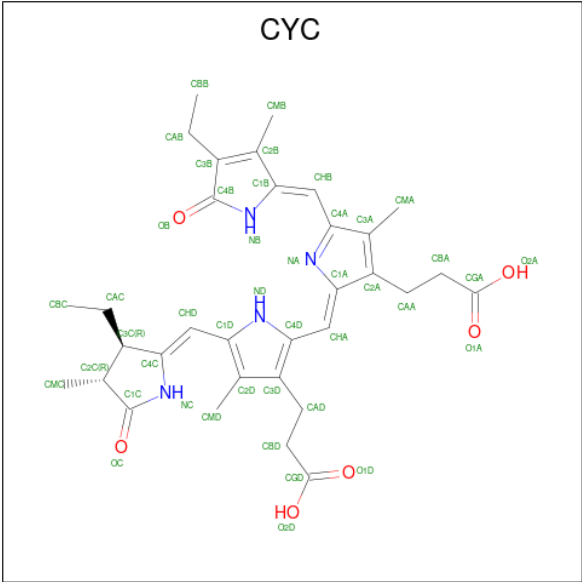
There are 2 discrepancies between the modelled and reference sequences:

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.

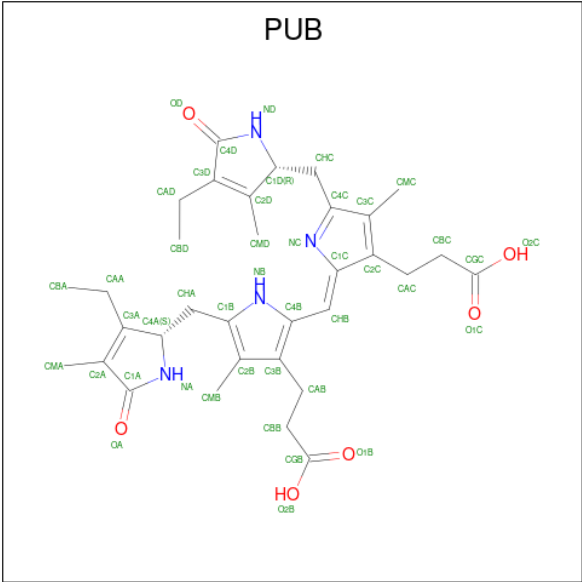
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1304	805	226	261	12			
2	L	177	Total	C	N	O	S	0	0	0
			1304	805	226	261	12			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: C₃₃H₄₀N₄O₆).



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

- Molecule 4 is PHYCOUROBILIN (three-letter code: PUB) (formula: C₃₃H₄₂N₄O₆).



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.

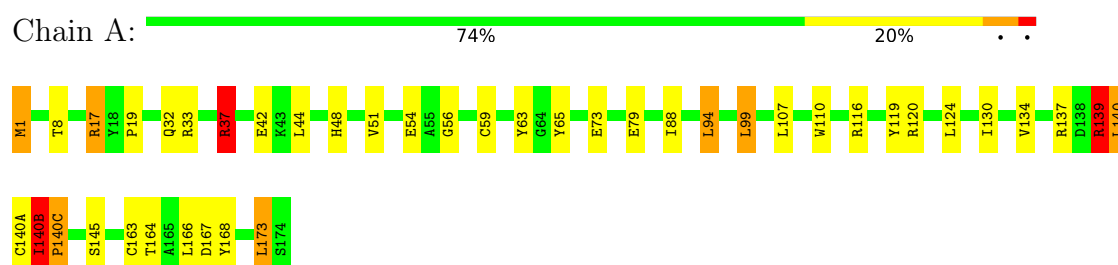
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		
5	B	22	Total	O	0	0
			22	22		
5	K	39	Total	O	0	0
			39	39		
5	L	32	Total	O	0	0
			32	32		

3 Residue-property plots

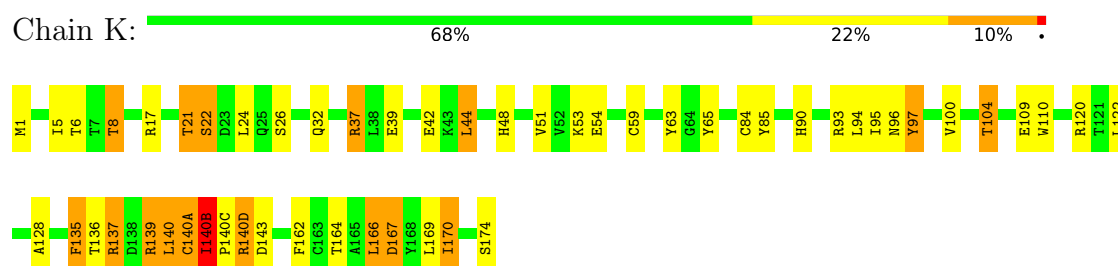
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

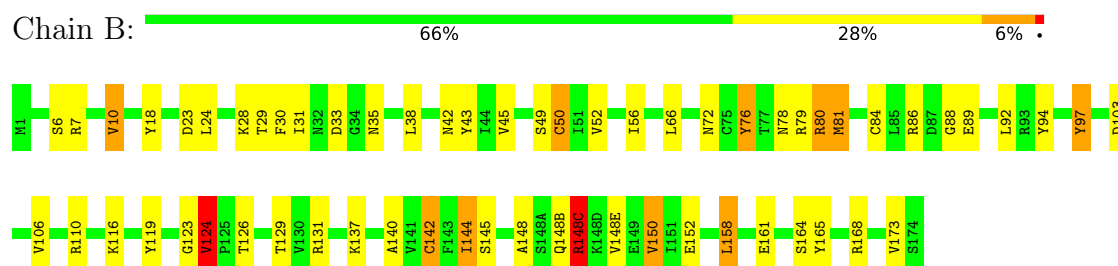
• Molecule 1: R-PHYCOERYTHRIN



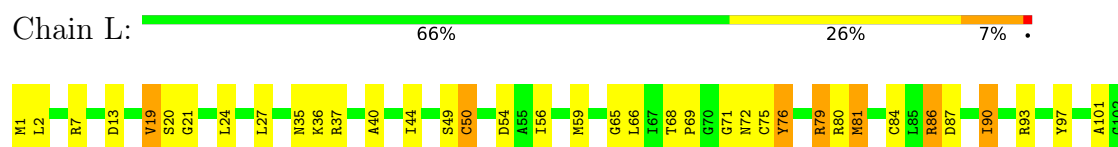
• Molecule 1: R-PHYCOERYTHRIN

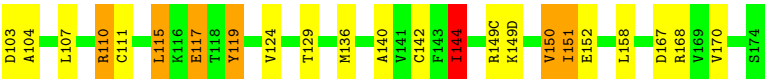


• Molecule 2: R-PHYCOERYTHRIN



• Molecule 2: R-PHYCOERYTHRIN





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 [i](#)

5.1 Standard geometry [i](#)

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	0.88	0/1273	1.68	17/1722 (1.0%)
1	K	0.97	1/1273 (0.1%)	1.72	27/1722 (1.6%)
2	B	0.93	2/1316 (0.2%)	1.76	26/1782 (1.5%)
2	L	0.98	1/1316 (0.1%)	1.86	31/1782 (1.7%)
All	All	0.94	4/5178 (0.1%)	1.76	101/7008 (1.4%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	148(B)	GLN	C-N	6.49	1.49	1.34
2	B	123	GLY	C-N	5.47	1.46	1.34
1	K	51	VAL	C-N	5.20	1.46	1.34
2	L	1	MET	C-N	-5.09	1.22	1.34

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	79	ARG	NE-CZ-NH2	-14.50	113.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	79	ARG	NE-CZ-NH1	11.81	126.20	120.30
2	B	97	TYR	CB-CG-CD1	10.98	127.59	121.00
2	L	93	ARG	NE-CZ-NH2	-10.96	114.82	120.30
2	B	97	TYR	CB-CG-CD2	-10.86	114.48	121.00
2	L	79	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	A	116	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	A	37	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	L	93	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	B	79	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	137	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	K	97	TYR	CB-CG-CD2	-8.60	115.84	121.00
2	L	76	TYR	C-N-CA	8.41	142.72	121.70
2	B	76	TYR	C-N-CA	8.16	142.09	121.70
2	L	37	ARG	NE-CZ-NH1	-7.92	116.34	120.30
2	B	81	MET	CG-SD-CE	7.92	112.87	100.20
1	A	139	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	K	17	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	33	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	K	139	ARG	NE-CZ-NH2	-7.49	116.56	120.30
2	B	50	CYS	CA-CB-SG	7.45	127.41	114.00
1	A	110	TRP	CE2-CD2-CG	-7.35	101.42	107.30
2	L	86	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	37	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	L	103	ASP	CB-CG-OD1	7.12	124.71	118.30
2	L	81	MET	CG-SD-CE	-6.96	89.06	100.20
2	L	7	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	B	30	PHE	CB-CG-CD2	-6.88	115.98	120.80
2	L	150	VAL	CB-CA-C	-6.81	98.47	111.40
1	A	110	TRP	CG-CD2-CE3	6.80	140.02	133.90
1	K	136	THR	C-N-CA	6.78	138.64	121.70
2	L	136	MET	CG-SD-CE	6.70	110.92	100.20
2	B	148(C)	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	K	137	ARG	NE-CZ-NH2	6.46	123.53	120.30
2	L	149(C)	ARG	CG-CD-NE	6.46	125.36	111.80
1	A	110	TRP	CD1-CG-CD2	6.45	111.46	106.30
2	B	88	GLY	C-N-CA	6.42	137.74	121.70
2	L	54	ASP	CB-CG-OD2	6.39	124.05	118.30
2	B	119	TYR	CB-CG-CD2	-6.38	117.17	121.00
2	B	168	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	L	97	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	L	90	ILE	CA-CB-CG2	-6.32	98.26	110.90
1	K	93	ARG	NE-CZ-NH2	-6.30	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	110	TRP	CE2-CD2-CG	-6.29	102.27	107.30
2	L	80	ARG	NE-CZ-NH2	-6.27	117.17	120.30
2	L	56	ILE	CG1-CB-CG2	-6.25	97.65	111.40
2	L	110	ARG	NE-CZ-NH1	6.15	123.37	120.30
2	L	90	ILE	CA-CB-CG1	6.14	122.66	111.00
2	B	161	GLU	CA-CB-CG	6.10	126.82	113.40
2	B	80	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	L	119	TYR	CB-CG-CD1	6.08	124.65	121.00
2	L	144	ILE	O-C-N	-6.05	113.02	122.70
1	K	110	TRP	CD1-CG-CD2	6.01	111.11	106.30
1	A	94	LEU	CA-CB-CG	6.00	129.10	115.30
1	K	174	SER	N-CA-CB	-6.00	101.51	110.50
2	B	131	ARG	NE-CZ-NH2	5.94	123.27	120.30
2	L	158	LEU	CA-CB-CG	5.91	128.89	115.30
2	L	87	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	140	LEU	CA-CB-CG	5.86	128.77	115.30
1	K	140(B)	ILE	CB-CA-C	-5.85	99.89	111.60
1	K	139	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	168	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	A	17	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	L	119	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	K	37	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	A	163	CYS	CA-CB-SG	5.77	124.39	114.00
1	K	140(B)	ILE	CG1-CB-CG2	5.74	124.03	111.40
2	B	18	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	B	45	VAL	N-CA-CB	-5.69	98.98	111.50
1	K	140(B)	ILE	CA-CB-CG2	-5.66	99.58	110.90
2	B	150	VAL	CB-CA-C	-5.66	100.66	111.40
1	K	85	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	K	17	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	K	140(D)	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	K	8	THR	N-CA-CB	-5.55	99.75	110.30
2	L	76	TYR	O-C-N	-5.52	113.87	122.70
2	L	168	ARG	CA-CB-CG	5.50	125.51	113.40
1	K	167	ASP	CB-CG-OD1	5.42	123.18	118.30
1	K	166	LEU	CA-CB-CG	5.42	127.77	115.30
2	B	165	TYR	CG-CD2-CE2	-5.42	116.97	121.30
1	K	140(A)	CYS	N-CA-CB	-5.38	100.92	110.60
2	L	50	CYS	CA-CB-SG	5.38	123.68	114.00
2	B	119	TYR	CB-CG-CD1	5.37	124.22	121.00
2	L	104	ALA	CB-CA-C	-5.35	102.07	110.10
1	K	140	LEU	CA-CB-CG	5.31	127.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	94	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	K	143	ASP	CB-CG-OD1	5.28	123.05	118.30
1	K	96	ASN	CB-CG-ND2	5.27	129.35	116.70
1	A	1	MET	CG-SD-CE	-5.26	91.78	100.20
1	A	119	TYR	CB-CG-CD2	-5.24	117.86	121.00
2	B	10	VAL	CG1-CB-CG2	-5.23	102.54	110.90
2	L	151	ILE	O-C-N	5.20	131.02	122.70
2	B	164	SER	N-CA-CB	-5.20	102.70	110.50
1	A	120	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	K	21	THR	OG1-CB-CG2	5.18	121.91	110.00
2	B	131	ARG	O-C-N	-5.16	114.44	122.70
2	L	86	ARG	CG-CD-NE	-5.16	100.97	111.80
2	B	158	LEU	CA-CB-CG	5.11	127.05	115.30
1	K	24	LEU	CA-CB-CG	5.04	126.89	115.30
2	B	137	LYS	CA-CB-CG	5.02	124.44	113.40
1	K	135	PHE	CB-CG-CD1	-5.01	117.29	120.80

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	16	0
1	K	1252	0	1224	20	0
2	B	1304	0	1308	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1304	0	1308	25	0
3	A	86	0	76	4	0
3	B	86	0	76	9	0
3	K	86	0	76	1	0
3	L	86	0	76	10	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	5440	85	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 (85) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:L:176:CYC:HMD2	3:L:176:CYC:HC	1.79	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:75:CYS:HB3	2:L:81:MET:HE2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLY:HA2	1:A:88:ILE:HD13	2.01	0.43
2:L:117:GLU:H	2:L:117:GLU:CD	2.22	0.42
2:B:28:LYS:HA	2:B:31:ILE:HD12	2.01	0.42
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
1:A:140(B):ILE:HG23	1:A:140(B):ILE:O	2.20	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:59:MET:HE2	2:L:59:MET:HB3	1.85	0.41
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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	13	39
1	K	162/164 (99%)	155 (96%)	5 (3%)	2 (1%)	13	39
2	B	175/177 (99%)	172 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	56
All	All	674/682 (99%)	653 (97%)	16 (2%)	5 (1%)	22	53

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%)	113 (88%)	16 (12%)	4	14
1	K	129/129 (100%)	111 (86%)	18 (14%)	3	11
2	B	144/144 (100%)	126 (88%)	18 (12%)	4	14
2	L	144/144 (100%)	126 (88%)	18 (12%)	4	14
All	All	546/546 (100%)	476 (87%)	70 (13%)	4	13

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	THR
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

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Mol	Chain	Res	Type
1	A	139	ARG
1	A	140	LEU
1	A	140(A)	CYS
1	A	140(B)	ILE
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	50	CYS
2	B	66	LEU
2	B	78	ASN
2	B	81	MET
2	B	92	LEU
2	B	124	VAL
2	B	142	CYS
2	B	144	ILE
2	B	145	SER
2	B	148(C)	ARG
2	B	148(E)	VAL
2	B	150	VAL
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	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
1	K	169	LEU

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Mol	Chain	Res	Type
1	K	170	ILE
2	L	2	LEU
2	L	19	VAL
2	L	20	SER
2	L	27	LEU
2	L	36	LYS
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	115	LEU
2	L	117	GLU
2	L	144	ILE
2	L	149(D)	LYS
2	L	150	VAL
2	L	151	ILE
2	L	152	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	171	ASN
2	B	35	ASN
2	B	72	ASN
2	L	35	ASN
2	L	47	ASN
2	L	72	ASN
2	L	149(B)	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	L	176	2	42,46,46	2.52	14 (33%)	50,67,67	2.32	20 (40%)
3	CYC	A	141	1	42,46,46	2.82	12 (28%)	50,67,67	2.23	17 (34%)
3	CYC	K	175	1	42,46,46	2.91	10 (23%)	50,67,67	2.37	24 (48%)
4	PUB	L	175	2	42,46,46	2.91	16 (38%)	37,67,67	2.95	15 (40%)
3	CYC	A	175	1	42,46,46	3.02	15 (35%)	50,67,67	2.26	18 (36%)
3	CYC	K	141	1	42,46,46	2.82	13 (30%)	50,67,67	2.49	22 (44%)
3	CYC	L	177	2	42,46,46	3.04	14 (33%)	50,67,67	2.74	21 (42%)
3	CYC	B	175	2	42,46,46	3.12	16 (38%)	50,67,67	2.63	19 (38%)
3	CYC	B	176	2	42,46,46	2.85	13 (30%)	50,67,67	2.48	17 (34%)
4	PUB	B	177	2	42,46,46	3.14	17 (40%)	37,67,67	3.27	12 (32%)

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	L	176	2	-	13/25/74/74	0/4/4/4
3	CYC	K	175	1	1/1/14/19	14/25/74/74	0/4/4/4
3	CYC	A	141	1	-	13/25/74/74	0/4/4/4
4	PUB	L	175	2	1/1/14/17	12/24/74/74	0/4/4/4
3	CYC	A	175	1	-	12/25/74/74	0/4/4/4
3	CYC	L	177	2	1/1/14/19	15/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	K	141	1	-	12/25/74/74	0/4/4/4
3	CYC	B	175	2	-	11/25/74/74	0/4/4/4
3	CYC	B	176	2	1/1/14/19	13/25/74/74	0/4/4/4
4	PUB	B	177	2	2/2/14/17	11/24/74/74	0/4/4/4

All (140) 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
3	B	175	CYC	CHA-C1A	9.10	1.42	1.35
4	B	177	PUB	C3A-C2A	8.94	1.44	1.34
4	L	175	PUB	CHB-C1C	8.56	1.42	1.35
4	B	177	PUB	CBA-CAA	-8.37	1.14	1.51
4	L	175	PUB	C3A-C2A	7.39	1.42	1.34
3	A	175	CYC	CHA-C1A	7.13	1.41	1.35
4	B	177	PUB	CHB-C1C	7.03	1.41	1.35
3	K	175	CYC	CHA-C1A	7.02	1.41	1.35
3	L	177	CYC	CHA-C1A	6.66	1.40	1.35
3	A	141	CYC	CHA-C1A	6.60	1.40	1.35
3	B	176	CYC	CHA-C1A	6.39	1.40	1.35
4	L	175	PUB	CHC-C4C	-6.39	1.43	1.50
4	B	177	PUB	CHC-C4C	-6.31	1.43	1.50
3	K	141	CYC	CHA-C1A	6.01	1.40	1.35
3	B	175	CYC	O2D-CGD	4.98	1.47	1.30
4	L	175	PUB	CHC-C1D	-4.94	1.43	1.53
3	B	176	CYC	C4B-C3B	-4.84	1.39	1.48
4	L	175	PUB	CHA-C4A	-4.84	1.42	1.54
4	B	177	PUB	O2C-CGC	4.76	1.46	1.30
3	A	141	CYC	O2A-CGA	4.69	1.46	1.30
3	B	176	CYC	O2A-CGA	4.48	1.45	1.30
4	L	175	PUB	CHA-C1B	-4.46	1.40	1.50
3	L	177	CYC	O2D-CGD	4.46	1.45	1.30
3	A	175	CYC	O2A-CGA	4.45	1.45	1.30
3	L	177	CYC	O2A-CGA	4.40	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	175	CYC	CAC-C3C	4.38	1.62	1.54
4	B	177	PUB	O2B-CGB	4.36	1.45	1.30
3	K	141	CYC	O2D-CGD	4.33	1.45	1.30
4	B	177	PUB	CHC-C1D	-4.31	1.44	1.53
3	L	176	CYC	O2A-CGA	4.30	1.45	1.30
3	L	176	CYC	O2D-CGD	4.29	1.45	1.30
3	A	175	CYC	O2D-CGD	4.24	1.45	1.30
4	B	177	PUB	C4D-C3D	-4.18	1.40	1.48
3	B	176	CYC	C1C-NC	-4.17	1.32	1.37
4	L	175	PUB	O2C-CGC	4.09	1.44	1.30
3	A	141	CYC	C4B-C3B	-4.05	1.40	1.48
3	B	176	CYC	O2D-CGD	4.01	1.44	1.30
3	K	175	CYC	O2D-CGD	3.97	1.44	1.30
3	B	176	CYC	C3B-C2B	3.96	1.45	1.36
4	B	177	PUB	C2C-C3C	3.89	1.45	1.36
3	L	176	CYC	C4B-C3B	-3.87	1.40	1.48
3	A	141	CYC	O2D-CGD	3.83	1.43	1.30
3	A	175	CYC	C2A-C3A	3.82	1.44	1.36
3	B	176	CYC	C2A-C3A	3.78	1.44	1.36
3	L	176	CYC	C2A-C3A	3.75	1.44	1.36
3	K	141	CYC	CAC-C3C	3.74	1.61	1.54
3	B	175	CYC	C4C-NC	3.71	1.45	1.37
3	K	141	CYC	C4C-NC	3.70	1.45	1.37
4	B	177	PUB	CHA-C4A	-3.69	1.44	1.54
3	K	141	CYC	O2A-CGA	3.67	1.43	1.30
3	A	141	CYC	C1B-NB	3.64	1.43	1.37
4	L	175	PUB	C4D-C3D	-3.61	1.41	1.48
3	K	175	CYC	C4C-NC	3.52	1.44	1.37
4	L	175	PUB	C4C-NC	3.48	1.41	1.35
3	K	175	CYC	C2A-C3A	3.44	1.44	1.36
4	L	175	PUB	O2B-CGB	3.42	1.42	1.30
3	B	175	CYC	O2A-CGA	3.41	1.42	1.30
3	A	175	CYC	C4B-C3B	-3.40	1.41	1.48
4	L	175	PUB	C4A-C3A	-3.33	1.40	1.50
4	L	175	PUB	C2C-C3C	3.29	1.43	1.36
3	B	175	CYC	C2A-C3A	3.26	1.43	1.36
3	L	177	CYC	C1B-NB	3.26	1.43	1.37
4	B	177	PUB	C4C-NC	3.23	1.41	1.35
3	A	175	CYC	CAC-C3C	3.22	1.60	1.54
3	L	177	CYC	C2A-C3A	3.22	1.43	1.36
3	K	175	CYC	O2A-CGA	3.20	1.41	1.30
3	A	175	CYC	C3B-C2B	3.19	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	175	CYC	C3C-C4C	3.19	1.55	1.50
3	L	176	CYC	C1A-C2A	-3.18	1.40	1.45
3	A	141	CYC	C3B-C2B	3.16	1.43	1.36
3	A	141	CYC	C4C-NC	3.16	1.44	1.37
3	L	176	CYC	C3B-C2B	3.09	1.43	1.36
3	B	175	CYC	C3B-C2B	3.06	1.43	1.36
3	L	177	CYC	C4C-NC	3.04	1.43	1.37
4	B	177	PUB	CHA-C1B	-3.03	1.44	1.50
3	K	141	CYC	C2A-C3A	3.02	1.43	1.36
3	K	175	CYC	C3B-C2B	3.00	1.43	1.36
3	A	141	CYC	CHB-C1B	2.99	1.45	1.38
3	B	175	CYC	CHD-C4C	2.90	1.45	1.38
3	K	141	CYC	C1B-NB	2.87	1.42	1.37
3	L	176	CYC	CHA-C1A	2.87	1.37	1.35
3	K	141	CYC	C3B-C2B	2.82	1.42	1.36
4	B	177	PUB	C4A-C3A	-2.82	1.41	1.50
3	A	175	CYC	C4C-NC	2.79	1.43	1.37
3	B	176	CYC	C4B-NB	-2.78	1.32	1.38
3	A	141	CYC	C2A-C3A	2.75	1.42	1.36
3	B	176	CYC	C4C-NC	2.72	1.43	1.37
4	L	175	PUB	C4A-NA	-2.65	1.41	1.45
3	L	176	CYC	C4B-NB	-2.64	1.32	1.38
3	L	176	CYC	C4C-NC	2.63	1.42	1.37
4	L	175	PUB	C1D-C2D	-2.61	1.42	1.50
3	B	175	CYC	CAC-C3C	2.61	1.59	1.54
3	K	141	CYC	CHD-C4C	2.55	1.44	1.38
3	L	177	CYC	CHD-C4C	2.51	1.44	1.38
3	B	176	CYC	CHB-C1B	2.50	1.43	1.38
3	L	176	CYC	CAD-C3D	2.49	1.55	1.52
4	L	175	PUB	C3B-C2B	2.48	1.45	1.37
4	B	177	PUB	C1A-C2A	-2.42	1.41	1.47
3	K	175	CYC	CHD-C4C	2.42	1.44	1.38
3	L	177	CYC	C3B-C2B	2.42	1.41	1.36
3	A	175	CYC	CHD-C4C	2.39	1.44	1.38
3	A	175	CYC	C3C-C4C	2.39	1.54	1.50
4	B	177	PUB	C3B-C2B	2.38	1.44	1.37
3	B	176	CYC	C4A-NA	2.34	1.42	1.36
3	A	175	CYC	C4A-NA	2.32	1.42	1.36
3	L	176	CYC	C3D-C2D	2.31	1.44	1.37
3	K	141	CYC	C3C-C4C	2.29	1.54	1.50
3	A	175	CYC	C4B-NB	-2.28	1.33	1.38
3	B	175	CYC	C4B-NB	-2.26	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	141	CYC	C4B-NB	-2.26	1.33	1.38
3	A	175	CYC	C1B-NB	2.25	1.41	1.37
3	A	141	CYC	CHD-C4C	2.25	1.43	1.38
3	B	175	CYC	C1B-NB	2.23	1.41	1.37
3	B	175	CYC	C1C-NC	-2.20	1.34	1.37
3	L	177	CYC	C4B-C3B	-2.19	1.44	1.48
3	B	176	CYC	CHB-C4A	2.17	1.45	1.40
3	A	175	CYC	C1C-NC	-2.11	1.34	1.37
3	K	175	CYC	C1B-NB	2.11	1.41	1.37
3	L	177	CYC	CHB-C1B	2.10	1.43	1.38
3	A	141	CYC	C1A-C2A	-2.10	1.42	1.45
3	L	176	CYC	CHD-C4C	2.10	1.43	1.38
4	B	177	PUB	C1D-C2D	-2.09	1.43	1.50
3	B	175	CYC	C3D-C2D	2.08	1.43	1.37
4	L	175	PUB	C1A-C2A	-2.06	1.42	1.47
4	B	177	PUB	C1C-C2C	-2.05	1.42	1.45
3	B	175	CYC	C1B-C2B	-2.05	1.41	1.45
3	K	141	CYC	C4A-NA	2.05	1.41	1.36
3	B	175	CYC	C4B-C3B	-2.05	1.44	1.48
3	L	177	CYC	C3D-C2D	2.05	1.43	1.37
3	L	177	CYC	C4B-NB	-2.04	1.33	1.38
3	L	176	CYC	C4A-NA	2.03	1.41	1.36
3	L	177	CYC	CMC-C2C	-2.02	1.48	1.53

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	177	PUB	CHA-C4A-NA	11.30	127.06	113.95
4	L	175	PUB	CHA-C4A-NA	9.88	125.42	113.95
3	B	175	CYC	C1B-C2B-C3B	-8.49	99.01	107.87
4	B	177	PUB	CHC-C1D-ND	8.41	124.37	113.72
4	L	175	PUB	CHC-C1D-ND	8.25	124.16	113.72
4	B	177	PUB	CAD-C3D-C4D	-7.58	109.40	121.38
3	L	177	CYC	C1B-C2B-C3B	-7.35	100.21	107.87
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
3	L	176	CYC	CMC-C2C-C1C	6.75	126.96	112.40
4	B	177	PUB	C1D-CHC-C4C	6.63	127.78	113.37
3	B	175	CYC	C1B-NB-C4B	-6.43	102.48	110.67
3	A	141	CYC	CBC-CAC-C3C	-6.36	99.31	113.47
3	A	141	CYC	CMC-C2C-C1C	6.31	126.00	112.40
3	A	175	CYC	CMC-C2C-C1C	5.91	125.14	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	177	CYC	CAC-C3C-C2C	-5.84	99.66	114.26
3	L	177	CYC	CAB-C3B-C4B	5.74	130.45	121.38
3	L	177	CYC	CMC-C2C-C1C	5.70	124.68	112.40
3	B	176	CYC	OC-C1C-NC	-5.61	118.15	124.94
3	L	177	CYC	CMB-C2B-C1B	5.50	131.04	124.17
3	K	141	CYC	C1B-C2B-C3B	-5.44	102.19	107.87
4	L	175	PUB	C1D-CHC-C4C	5.37	125.05	113.37
3	K	141	CYC	CMC-C2C-C1C	5.37	123.97	112.40
3	B	175	CYC	CMB-C2B-C1B	5.33	130.82	124.17
3	B	175	CYC	CMC-C2C-C1C	5.25	123.72	112.40
3	A	175	CYC	C1B-C2B-C3B	-5.18	102.46	107.87
3	B	176	CYC	CBB-CAB-C3B	5.18	126.71	112.43
3	L	176	CYC	CMB-C2B-C1B	5.17	130.63	124.17
3	K	175	CYC	C1B-C2B-C3B	-5.14	102.50	107.87
3	B	176	CYC	OC-C1C-C2C	5.07	130.21	126.17
3	L	177	CYC	C1B-NB-C4B	-5.01	104.29	110.67
3	K	175	CYC	CHD-C4C-NC	4.88	131.00	125.20
3	K	141	CYC	C1B-NB-C4B	-4.72	104.66	110.67
3	K	141	CYC	C2C-C1C-NC	4.56	112.20	108.27
3	B	175	CYC	CAB-C3B-C4B	4.52	128.52	121.38
3	L	177	CYC	CAC-C3C-C4C	4.49	124.20	112.67
3	K	141	CYC	CHD-C4C-NC	4.42	130.46	125.20
3	A	141	CYC	C1B-C2B-C3B	-4.37	103.31	107.87
3	A	175	CYC	C3B-C4B-NB	4.35	110.29	106.78
4	L	175	PUB	CAD-C3D-C4D	-4.32	114.55	121.38
3	B	176	CYC	C1B-NB-C4B	-4.30	105.19	110.67
3	K	141	CYC	CAB-C3B-C4B	4.29	128.16	121.38
3	K	141	CYC	CBC-CAC-C3C	-4.28	103.94	113.47
3	B	176	CYC	C1B-C2B-C3B	-4.25	103.44	107.87
3	A	141	CYC	CHD-C4C-NC	4.25	130.26	125.20
3	B	175	CYC	OB-C4B-C3B	4.24	132.65	128.04
3	A	175	CYC	CAC-C3C-C2C	-4.15	103.88	114.26
3	K	141	CYC	OC-C1C-C2C	-4.11	122.90	126.17
3	B	175	CYC	C2C-C1C-NC	4.01	111.73	108.27
4	L	175	PUB	CHB-C1C-NC	-3.99	123.29	128.83
3	A	175	CYC	CAC-C3C-C4C	3.93	122.76	112.67
3	B	176	CYC	C2C-C1C-NC	3.89	111.63	108.27
3	A	141	CYC	C4D-CHA-C1A	-3.82	124.25	128.81
3	B	176	CYC	CBC-CAC-C3C	-3.81	104.98	113.47
3	B	175	CYC	O2D-CGD-CBD	3.78	126.17	114.03
3	K	175	CYC	CAB-C3B-C4B	3.77	127.33	121.38
3	L	176	CYC	CBC-CAC-C3C	-3.73	105.17	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	176	CYC	CAC-C3C-C2C	-3.66	105.11	114.26
3	L	176	CYC	C1B-C2B-C3B	-3.65	104.06	107.87
4	B	177	PUB	O2B-CGB-CBB	3.64	125.74	114.03
4	B	177	PUB	CBA-CAA-C3A	-3.63	107.47	112.98
3	L	176	CYC	CAB-C3B-C4B	3.60	127.06	121.38
4	L	175	PUB	OD-C4D-C3D	3.59	131.93	128.04
3	A	175	CYC	CBC-CAC-C3C	-3.56	105.54	113.47
3	L	177	CYC	CBD-CAD-C3D	3.54	118.66	112.62
3	B	176	CYC	CAB-C3B-C2B	3.50	133.52	127.53
3	L	176	CYC	CBB-CAB-C3B	3.48	122.01	112.43
3	A	175	CYC	CMB-C2B-C1B	3.47	128.50	124.17
3	L	176	CYC	C1A-C2A-C3A	-3.45	102.97	106.78
3	L	177	CYC	O2D-CGD-CBD	3.37	124.86	114.03
3	A	175	CYC	O2A-CGA-O1A	-3.37	114.90	123.30
3	K	175	CYC	C1B-NB-C4B	-3.36	106.40	110.67
3	K	141	CYC	OB-C4B-C3B	3.35	131.68	128.04
3	L	176	CYC	CHB-C4A-NA	-3.34	117.94	124.93
3	A	141	CYC	OC-C1C-C2C	3.33	128.82	126.17
3	K	141	CYC	CBB-CAB-C3B	3.27	121.45	112.43
3	K	175	CYC	CMB-C2B-C1B	3.23	128.21	124.17
3	B	176	CYC	CBA-CAA-C2A	3.19	121.50	112.63
3	A	175	CYC	C1B-NB-C4B	-3.19	106.61	110.67
3	K	175	CYC	CMC-C2C-C3C	3.16	126.57	113.83
3	A	175	CYC	O2A-CGA-CBA	3.15	124.14	114.03
3	A	175	CYC	C4D-CHA-C1A	-3.14	125.06	128.81
4	B	177	PUB	O2B-CGB-O1B	-3.13	115.51	123.30
3	L	177	CYC	CHB-C4A-NA	-3.13	118.39	124.93
4	B	177	PUB	CHB-C1C-NC	-3.12	124.50	128.83
3	L	176	CYC	CHB-C4A-C3A	3.11	132.91	124.90
3	B	175	CYC	CMC-C2C-C3C	3.11	126.37	113.83
3	L	177	CYC	O2D-CGD-O1D	-3.07	115.65	123.30
3	K	175	CYC	O2A-CGA-O1A	-3.05	115.69	123.30
3	L	176	CYC	C1B-NB-C4B	-3.03	106.81	110.67
3	L	177	CYC	OB-C4B-C3B	3.01	131.31	128.04
4	L	175	PUB	O2C-CGC-CBC	3.01	123.71	114.03
4	L	175	PUB	CBB-CAB-C3B	-3.01	107.48	112.62
3	K	141	CYC	CMB-C2B-C1B	3.00	127.92	124.17
3	K	175	CYC	CBB-CAB-C3B	2.98	120.63	112.43
3	K	141	CYC	C1B-CHB-C4A	-2.97	120.82	128.08
3	K	175	CYC	O2A-CGA-CBA	2.97	123.58	114.03
3	A	141	CYC	O2D-CGD-CBD	2.95	123.50	114.03
4	B	177	PUB	C4B-CHB-C1C	-2.95	125.29	128.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	177	CYC	CHD-C4C-NC	2.94	128.71	125.20
3	K	141	CYC	C2B-C1B-NB	2.92	111.27	106.99
3	B	175	CYC	CAC-C3C-C2C	-2.90	107.01	114.26
3	L	177	CYC	CBB-CAB-C3B	2.90	120.43	112.43
3	B	176	CYC	CMB-C2B-C1B	2.90	127.79	124.17
3	L	177	CYC	CHA-C1A-NA	-2.89	124.82	128.83
3	A	175	CYC	CMC-C2C-C3C	2.87	125.41	113.83
3	A	141	CYC	C1A-NA-C4A	-2.86	101.13	106.51
3	L	177	CYC	O2A-CGA-O1A	-2.85	116.19	123.30
3	K	175	CYC	OB-C4B-C3B	2.85	131.13	128.04
3	A	175	CYC	CAA-CBA-CGA	2.84	119.72	113.60
3	A	175	CYC	O2D-CGD-CBD	2.82	123.09	114.03
3	A	141	CYC	CBB-CAB-C3B	2.79	120.11	112.43
3	A	141	CYC	O2A-CGA-CBA	2.76	122.88	114.03
3	B	175	CYC	CAC-C3C-C4C	2.75	119.72	112.67
3	B	175	CYC	CHB-C4A-NA	-2.74	119.21	124.93
3	L	177	CYC	O2A-CGA-CBA	2.73	122.80	114.03
3	L	177	CYC	CMC-C2C-C3C	2.69	124.67	113.83
3	L	176	CYC	CMA-C3A-C4A	2.68	129.20	125.06
3	L	176	CYC	C1A-NA-C4A	-2.67	101.47	106.51
3	B	176	CYC	O2A-CGA-CBA	2.67	122.60	114.03
4	L	175	PUB	CMA-C2A-C1A	2.67	127.67	121.39
3	K	175	CYC	CAD-CBD-CGD	-2.65	106.33	113.76
4	L	175	PUB	CBA-CAA-C3A	-2.65	108.96	112.98
3	B	175	CYC	O1D-CGD-CBD	-2.62	114.65	123.08
3	K	175	CYC	CMA-C3A-C4A	2.61	129.09	125.06
3	K	175	CYC	CHB-C4A-NA	-2.61	119.48	124.93
3	K	141	CYC	O2A-CGA-O1A	-2.60	116.83	123.30
3	K	141	CYC	C4A-C3A-C2A	-2.59	103.54	106.51
3	K	141	CYC	O2D-CGD-CBD	2.58	122.32	114.03
3	K	141	CYC	O2A-CGA-CBA	2.57	122.29	114.03
3	A	141	CYC	CMA-C3A-C4A	2.56	129.00	125.06
4	B	177	PUB	O2C-CGC-CBC	2.55	122.21	114.03
3	A	141	CYC	CAA-C2A-C1A	2.51	129.45	125.01
3	K	141	CYC	CMC-C2C-C3C	2.50	123.92	113.83
3	B	176	CYC	CHB-C1B-C2B	2.47	131.85	126.95
3	L	177	CYC	CBC-CAC-C3C	-2.47	107.97	113.47
3	K	141	CYC	CHB-C4A-NA	-2.47	119.77	124.93
3	A	175	CYC	CBB-CAB-C3B	2.44	119.17	112.43
3	B	175	CYC	CHD-C4C-NC	2.44	128.11	125.20
3	K	175	CYC	OC-C1C-C2C	-2.43	124.24	126.17
4	L	175	PUB	CAC-C2C-C1C	2.43	129.30	125.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	175	CYC	C3B-C4B-NB	2.42	108.73	106.78
3	L	176	CYC	C2C-C1C-NC	2.40	110.35	108.27
4	L	175	PUB	CAC-C2C-C3C	-2.39	123.44	127.88
3	K	175	CYC	C4A-C3A-C2A	-2.38	103.77	106.51
3	B	176	CYC	O2A-CGA-O1A	-2.38	117.37	123.30
3	B	176	CYC	CMC-C2C-C3C	2.38	123.41	113.83
3	L	177	CYC	CAB-C3B-C2B	-2.37	123.48	127.53
3	K	141	CYC	C1A-NA-C4A	-2.35	102.08	106.51
3	A	175	CYC	CHB-C4A-NA	-2.35	120.01	124.93
3	B	176	CYC	CHA-C1A-NA	-2.35	125.56	128.83
3	K	175	CYC	C2A-C1A-NA	-2.34	106.65	110.05
3	A	175	CYC	O1D-CGD-CBD	-2.31	115.65	123.08
3	L	176	CYC	OC-C1C-NC	-2.30	122.16	124.94
3	L	176	CYC	C4D-CHA-C1A	-2.27	126.10	128.81
3	L	176	CYC	OB-C4B-C3B	2.26	130.49	128.04
3	A	141	CYC	CMB-C2B-C1B	2.26	126.98	124.17
3	A	141	CYC	CBD-CAD-C3D	2.25	116.47	112.62
4	B	177	PUB	CHA-C1B-C2B	-2.24	126.51	130.34
3	A	175	CYC	CHA-C1A-NA	-2.23	125.74	128.83
4	L	175	PUB	O2B-CGB-CBB	2.21	121.12	114.03
3	K	141	CYC	OB-C4B-NB	-2.20	119.97	125.08
3	K	175	CYC	CAC-C3C-C4C	2.20	118.32	112.67
3	B	175	CYC	C2A-C1A-NA	-2.19	106.86	110.05
3	K	141	CYC	CAB-C3B-C2B	-2.17	123.81	127.53
3	A	141	CYC	CMC-C2C-C3C	2.17	122.58	113.83
3	B	175	CYC	O2A-CGA-O1A	-2.16	117.91	123.30
3	A	141	CYC	O2A-CGA-O1A	-2.16	117.93	123.30
3	K	175	CYC	C2B-C1B-NB	2.15	110.13	106.99
3	K	175	CYC	OB-C4B-NB	-2.13	120.13	125.08
3	B	176	CYC	CHD-C4C-NC	-2.10	122.71	125.20
4	B	177	PUB	CMB-C2B-C3B	2.07	128.84	124.94
3	A	141	CYC	C2C-C1C-NC	-2.06	106.50	108.27
3	B	175	CYC	CHA-C1A-NA	-2.06	125.97	128.83
3	L	176	CYC	C2A-C1A-NA	-2.05	107.06	110.05
3	B	175	CYC	CAB-C3B-C2B	-2.05	124.02	127.53
4	L	175	PUB	O1C-CGC-CBC	-2.04	116.52	123.08
3	B	175	CYC	OB-C4B-NB	-2.04	120.33	125.08
4	L	175	PUB	C3B-C2B-C1B	-2.03	103.23	111.33
3	L	176	CYC	O2A-CGA-CBA	2.03	120.54	114.03
3	K	175	CYC	CAA-CBA-CGA	2.02	117.95	113.60
3	L	177	CYC	OB-C4B-NB	-2.02	120.39	125.08
3	K	175	CYC	C1A-NA-C4A	-2.02	102.71	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	175	CYC	O2D-CGD-CBD	2.01	120.50	114.03
3	L	176	CYC	CHD-C4C-NC	2.01	127.59	125.20

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	C4A
4	B	177	PUB	C1D
4	L	175	PUB	C1D

All (126) 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	ND-C1D-CHD-C4C
3	A	175	CYC	C2D-C1D-CHD-C4C
3	A	141	CYC	C3D-C4D-CHA-C1A
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	ND-C1D-CHD-C4C
3	A	141	CYC	C2D-C1D-CHD-C4C
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	175	CYC	ND-C1D-CHD-C4C
3	B	175	CYC	C2D-C1D-CHD-C4C
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	B	176	CYC	ND-C1D-CHD-C4C
3	K	175	CYC	ND-C4D-CHA-C1A
3	K	175	CYC	NA-C4A-CHB-C1B
3	K	175	CYC	C3A-C4A-CHB-C1B
3	K	175	CYC	C2C-C3C-CAC-CBC

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

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Mol	Chain	Res	Type	Atoms
3	L	177	CYC	C2B-C1B-CHB-C4A
3	L	176	CYC	C4B-C3B-CAB-CBB
3	L	176	CYC	C2A-CAA-CBA-CGA
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	A	141	CYC	C4B-C3B-CAB-CBB
3	B	176	CYC	C2B-C3B-CAB-CBB
4	L	175	PUB	C3A-C4A-CHA-C1B
4	B	177	PUB	C3B-CAB-CBB-CGB
3	B	175	CYC	C2A-CAA-CBA-CGA
3	B	176	CYC	C4C-C3C-CAC-CBC
3	A	175	CYC	C3D-CAD-CBD-CGD
3	K	141	CYC	NA-C1A-CHA-C4D
4	B	177	PUB	C4A-C3A-CAA-CBA
3	A	141	CYC	C2B-C3B-CAB-CBB
3	L	177	CYC	CAD-CBD-CGD-O1D
3	B	175	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	CAB-CBB-CGB-O2B
3	K	141	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	C4A-C3A-CAA-CBA
3	B	176	CYC	CAD-CBD-CGD-O1D
3	A	141	CYC	CAD-CBD-CGD-O1D
3	B	175	CYC	CAD-CBD-CGD-O2D
3	K	175	CYC	CAA-CBA-CGA-O2A
3	L	176	CYC	CAD-CBD-CGD-O2D
3	L	177	CYC	CAA-CBA-CGA-O2A
3	B	176	CYC	CAA-CBA-CGA-O1A
3	B	175	CYC	CAA-CBA-CGA-O1A
3	B	176	CYC	CAD-CBD-CGD-O2D
3	K	141	CYC	CAA-CBA-CGA-O1A
3	B	175	CYC	CAD-CBD-CGD-O1D
3	K	175	CYC	CAD-CBD-CGD-O1D
3	L	176	CYC	CAD-CBD-CGD-O1D
4	L	175	PUB	CAB-CBB-CGB-O1B
3	A	175	CYC	CAD-CBD-CGD-O1D
3	A	141	CYC	CAA-CBA-CGA-O2A
4	L	175	PUB	CAC-CBC-CGC-O2C
3	B	176	CYC	CAA-CBA-CGA-O2A
3	K	175	CYC	CAA-CBA-CGA-O1A
3	K	141	CYC	CAD-CBD-CGD-O1D
3	L	176	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
3	A	175	CYC	CAD-CBD-CGD-O2D
4	L	175	PUB	CAC-CBC-CGC-O1C
3	A	175	CYC	CAA-CBA-CGA-O2A
3	A	141	CYC	CAA-CBA-CGA-O1A
3	K	141	CYC	CAD-CBD-CGD-O2D
3	A	141	CYC	CAD-CBD-CGD-O2D
3	L	177	CYC	CAA-CBA-CGA-O1A
3	L	176	CYC	C2A-C1A-CHA-C4D
3	L	176	CYC	CAA-CBA-CGA-O1A
3	A	175	CYC	CAA-CBA-CGA-O1A
3	L	177	CYC	CAD-CBD-CGD-O2D
4	B	177	PUB	CAC-CBC-CGC-O1C
4	B	177	PUB	CAC-CBC-CGC-O2C
4	L	175	PUB	C2D-C3D-CAD-CBD
3	K	175	CYC	CAD-CBD-CGD-O2D
3	B	176	CYC	C2C-C3C-CAC-CBC

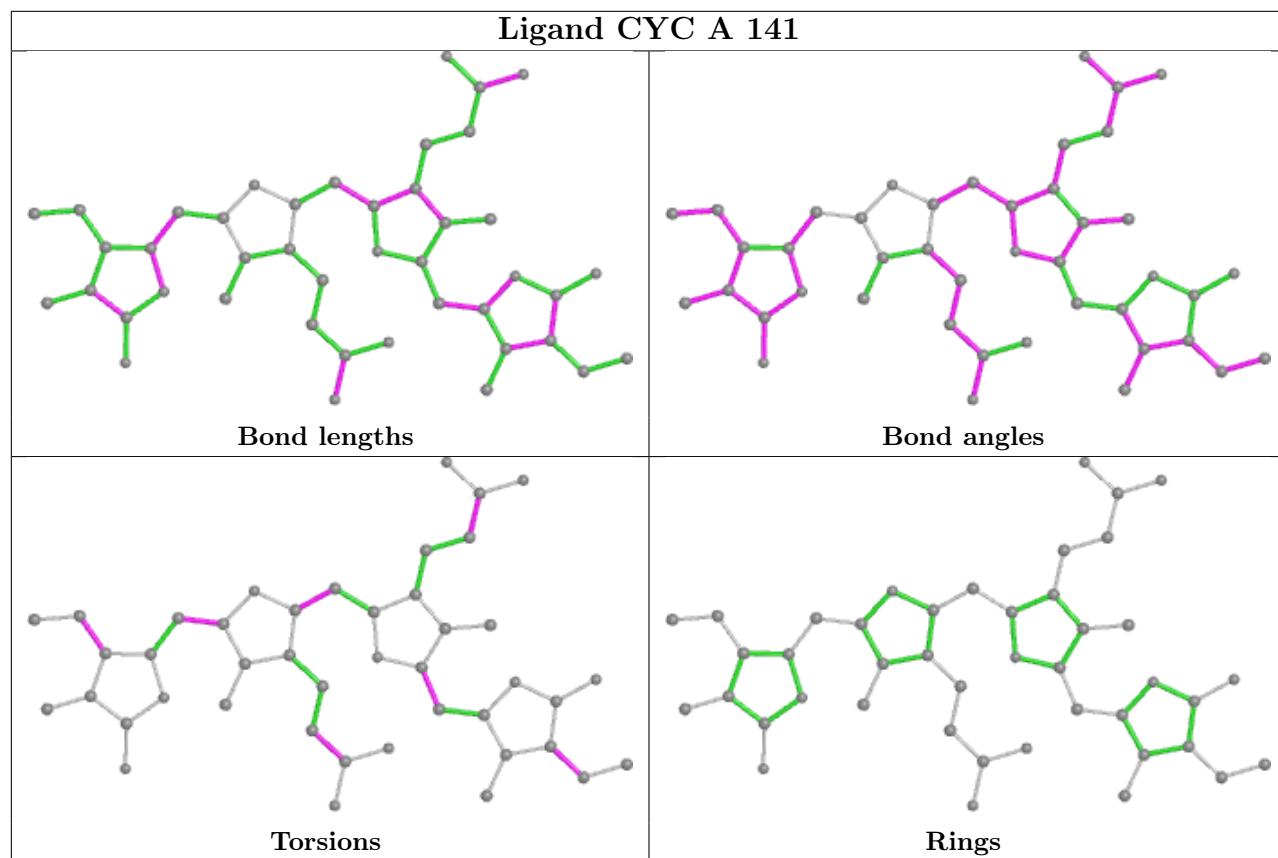
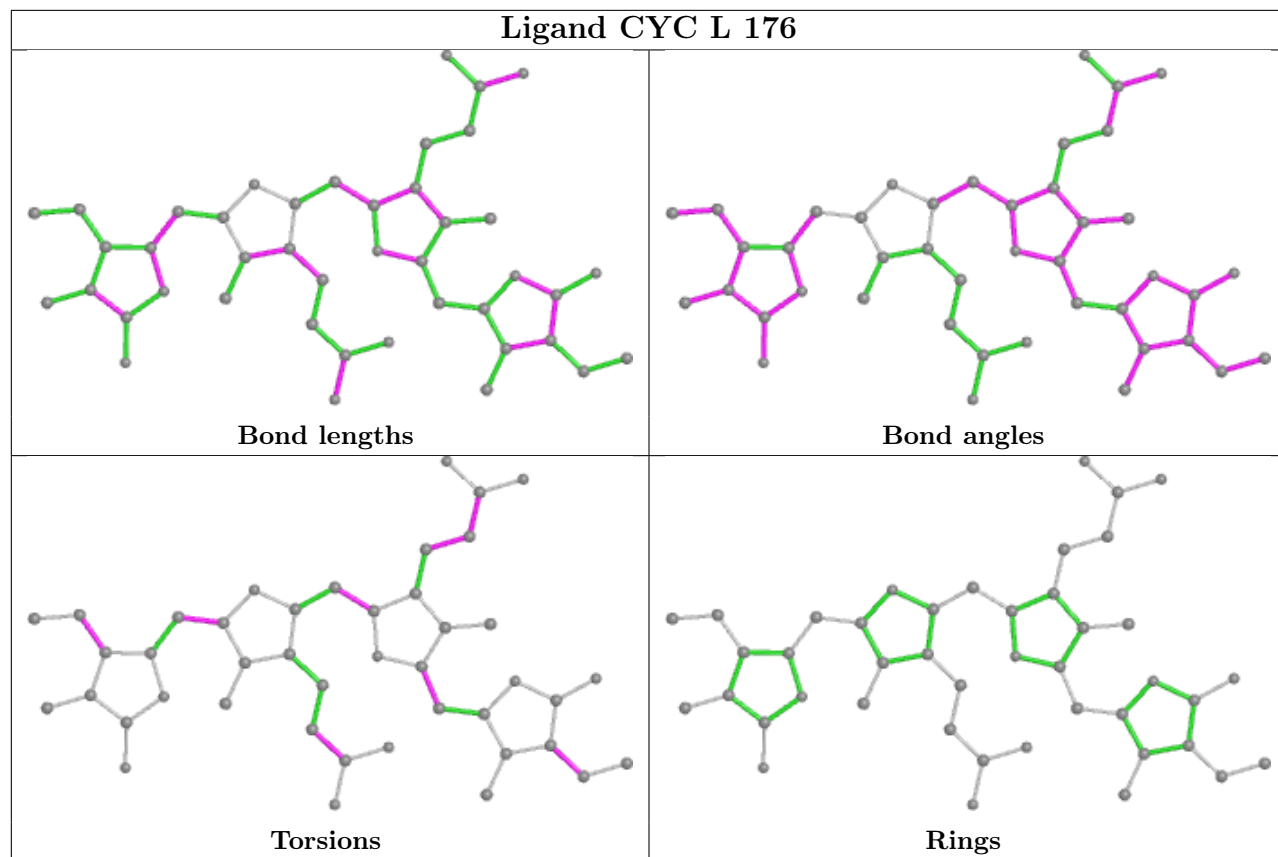
There are no ring outliers.

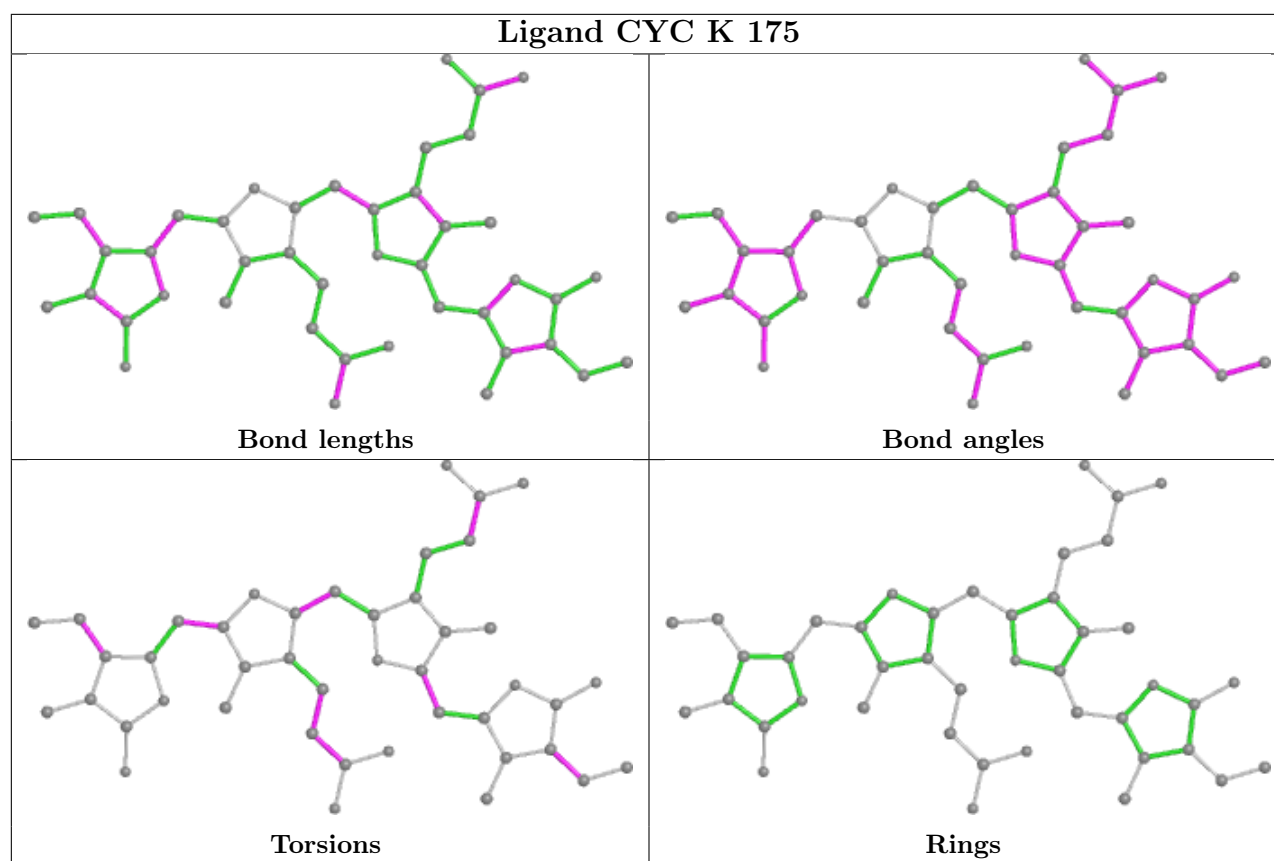
9 monomers are involved in 26 short contacts:

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

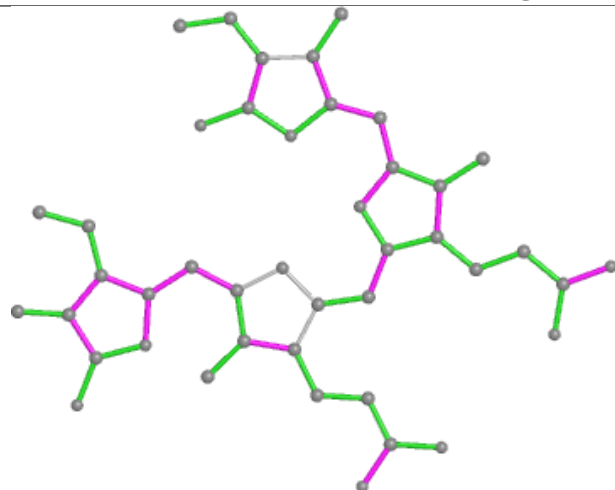
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

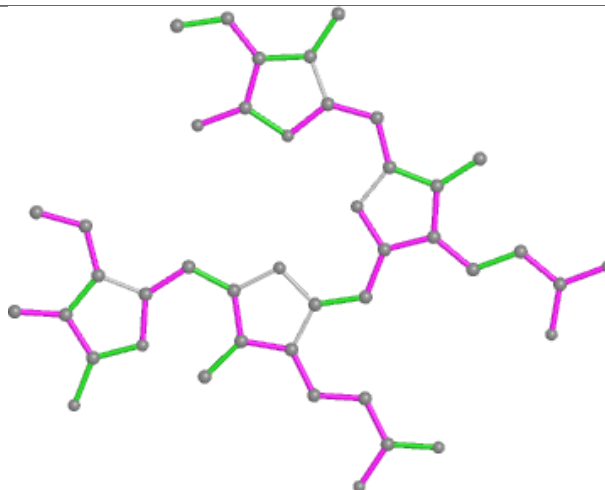




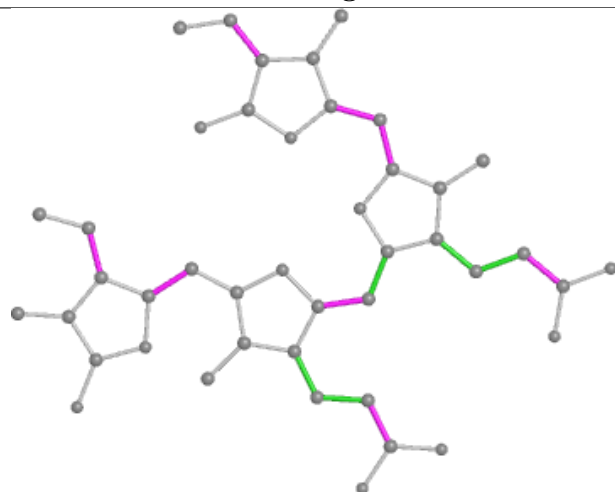
Ligand PUB L 175



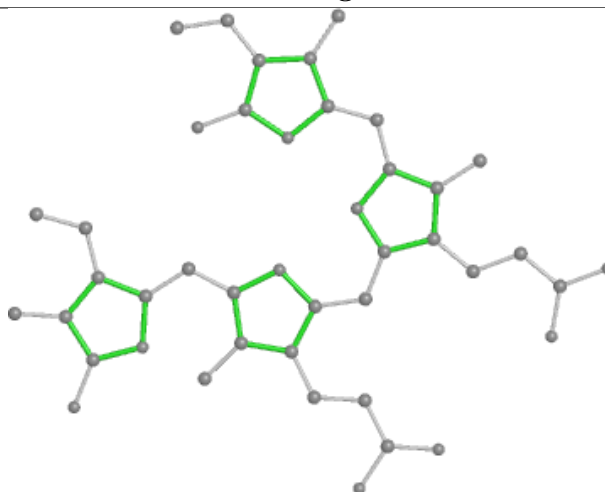
Bond lengths



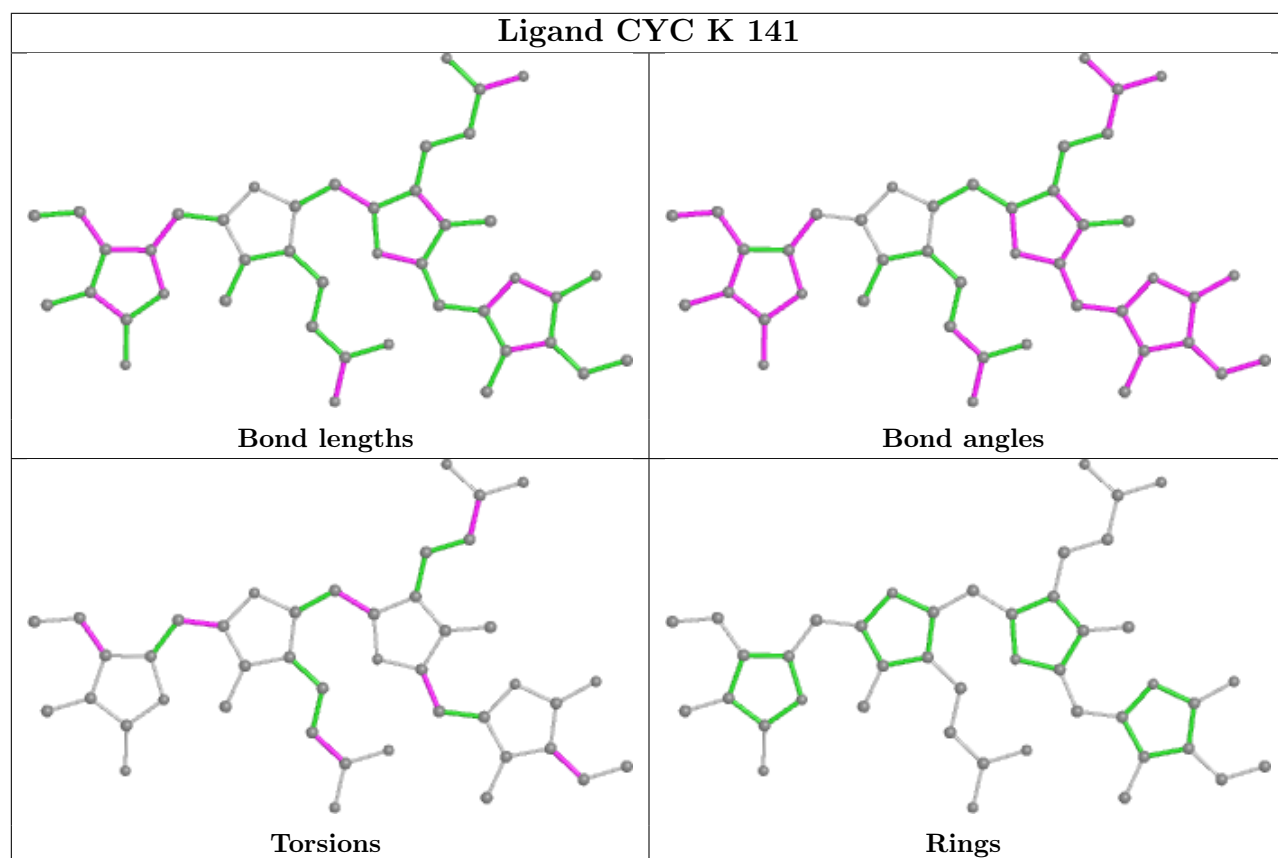
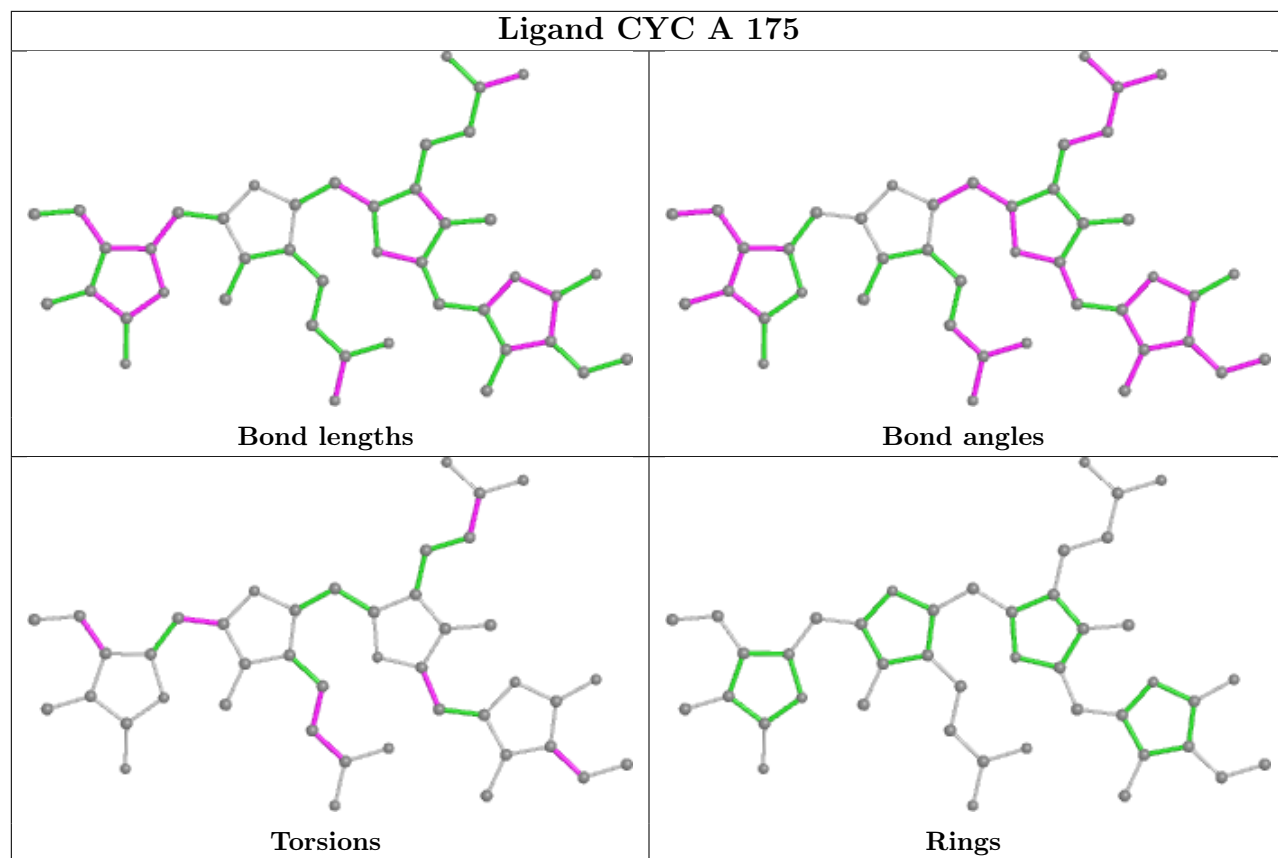
Bond angles



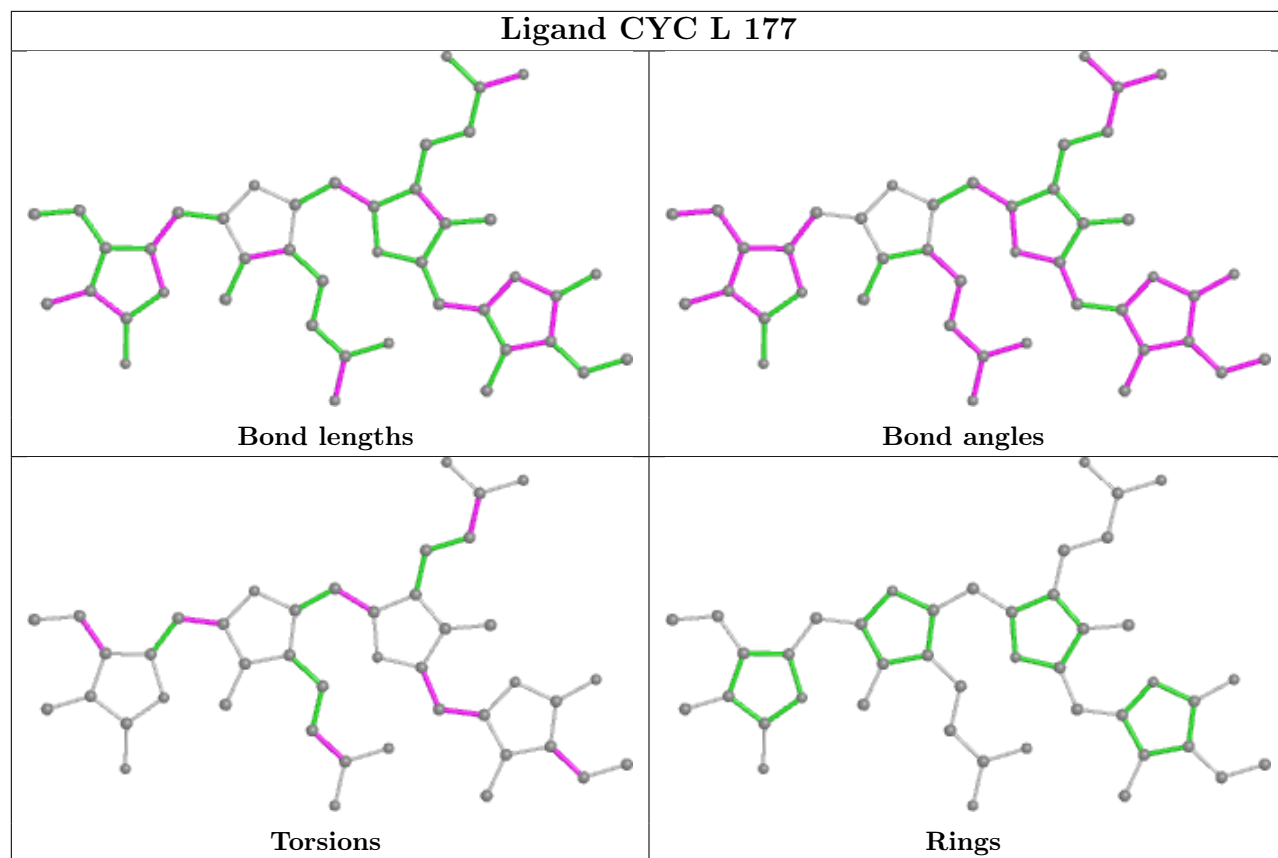
Torsions



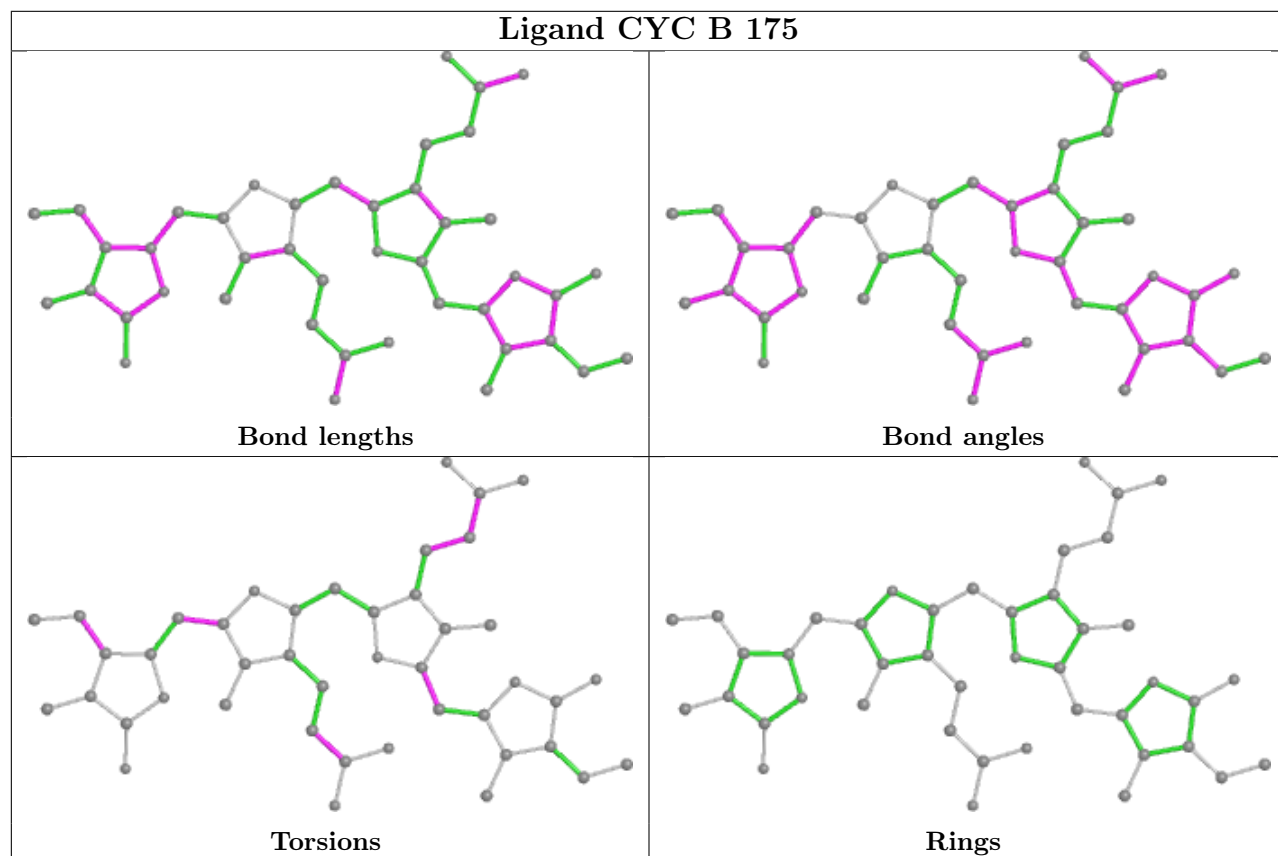
Rings

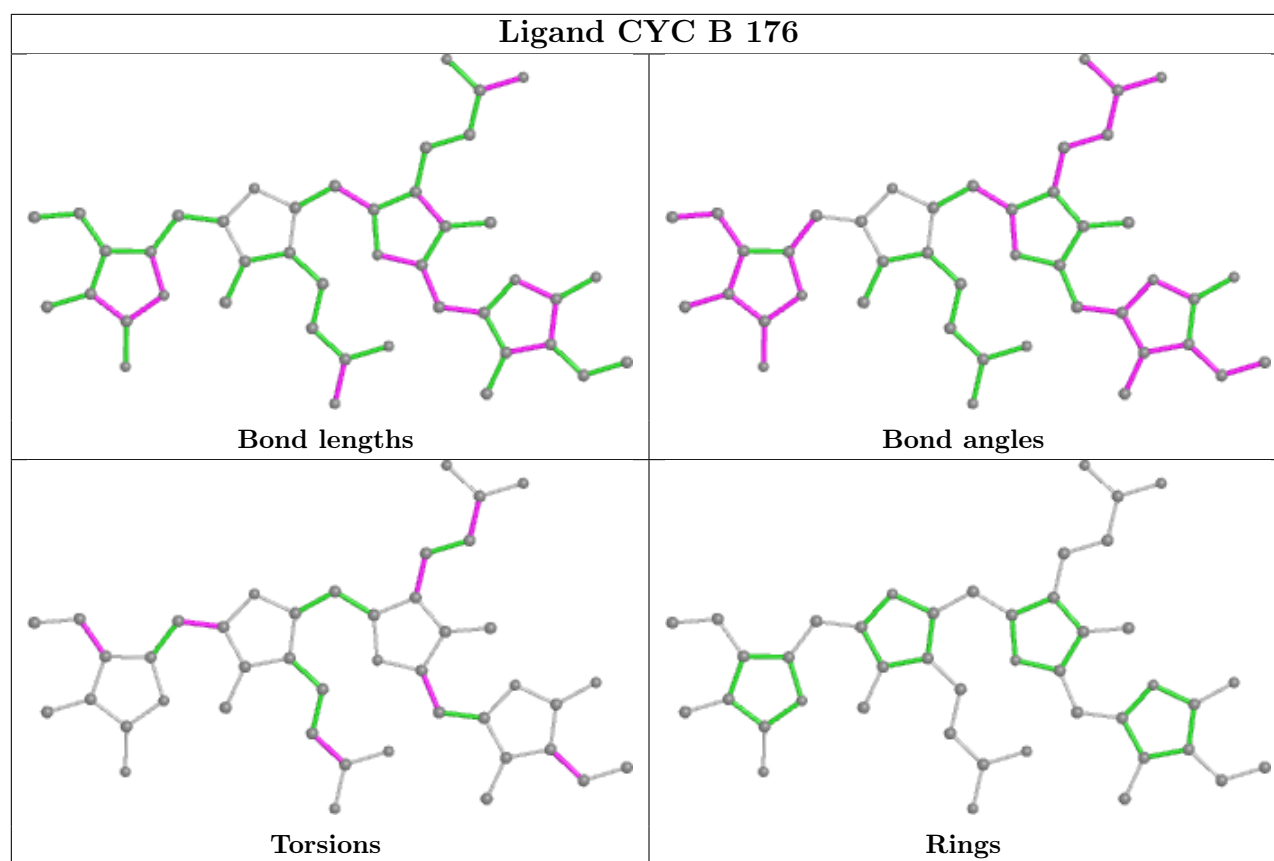


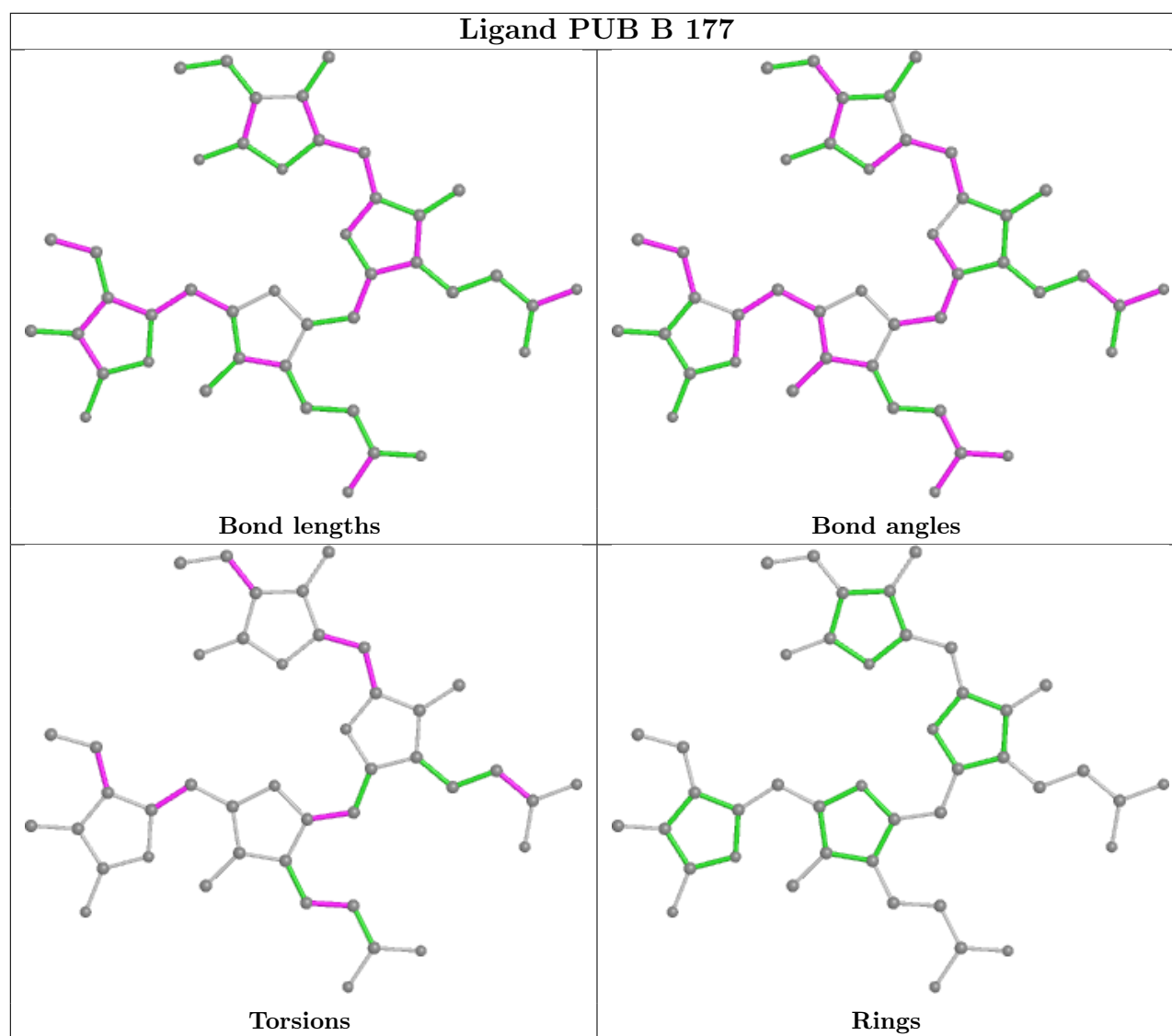
Ligand CYC L 177



Ligand CYC B 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.