



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:10 AM UTC

PDB ID : 1F99 / pdb_00001f99
Title : CRYSTAL STRUCTURE OF R-PHYCOCYANIN FROM POLYSIPHONIA
AT 2.4 Å RESOLUTION
Authors : Liang, D.C.; Jiang, T.; Chang, W.R.
Deposited on : 2000-07-09
Resolution : 2.40 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

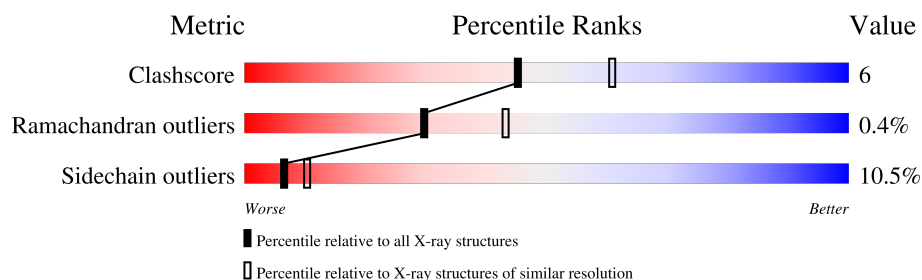
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	162	
1	K	162	
1	M	162	
2	B	172	
2	L	172	
2	N	172	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYC	A	384	X	-	-	-
3	CYC	K	386	X	-	-	-
4	PEB	B	355	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8209 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.

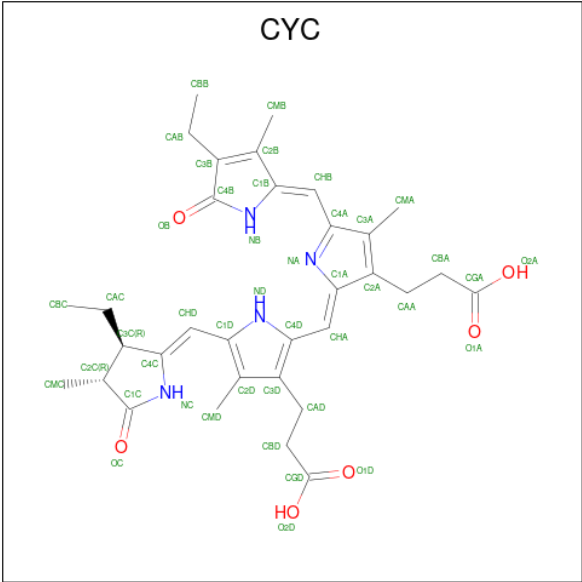
- Molecule 1 is a protein called R-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1235	776	208	245	6			
1	K	162	Total	C	N	O	S	0	0	0
			1235	776	208	245	6			
1	M	162	Total	C	N	O	S	0	0	0
			1235	776	208	245	6			

- Molecule 2 is a protein called R-PHYCOCYANIN.

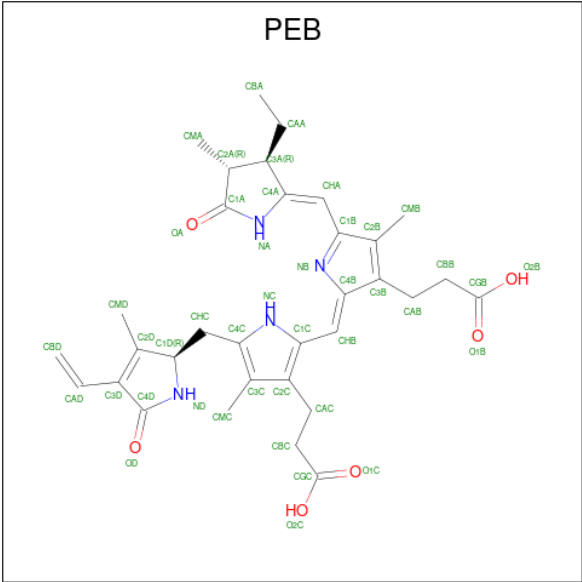
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1259	781	222	248	8			
2	L	172	Total	C	N	O	S	0	0	0
			1259	781	222	248	8			
2	N	172	Total	C	N	O	S	0	0	0
			1259	781	222	248	8			

- Molecule 3 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

- Molecule 4 is PHYCOERYTHROBILIN (CCD ID: PEB) (formula: C₃₃H₄₀N₄O₆).



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		
4	N	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	51	Total	O	0	0
			51	51		
5	K	59	Total	O	0	0
			59	59		
5	L	62	Total	O	0	0
			62	62		
5	M	46	Total	O	0	0
			46	46		
5	N	66	Total	O	0	0
			66	66		

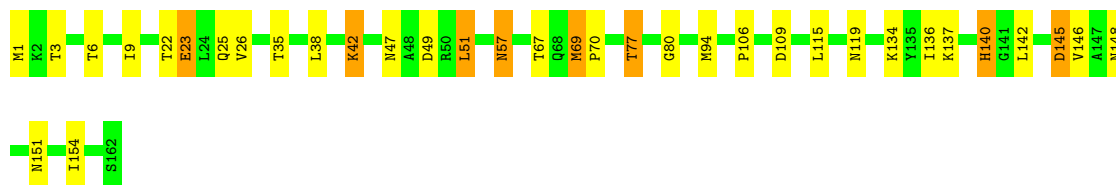
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

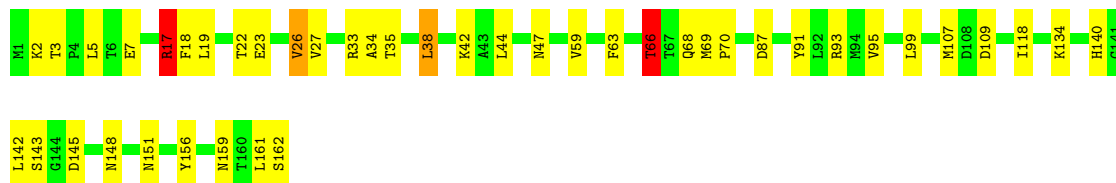
• Molecule 1: R-PHYCOCYANIN

Chain A: 



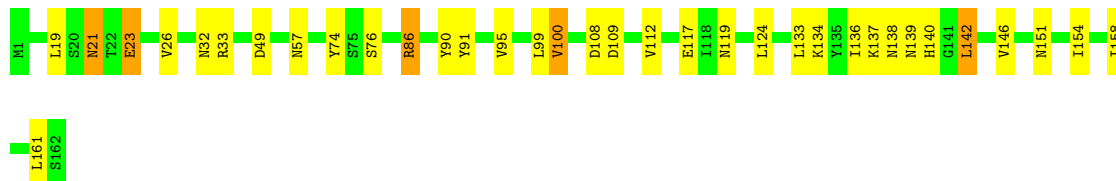
• Molecule 1: R-PHYCOCYANIN

Chain K: 



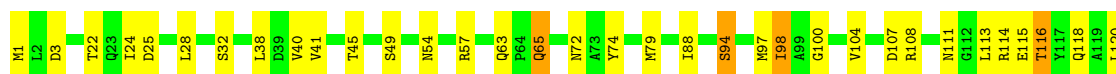
• Molecule 1: R-PHYCOCYANIN

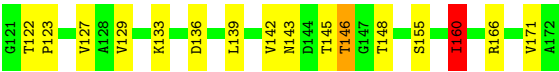
Chain M: 



• Molecule 2: R-PHYCOCYANIN

Chain B: 

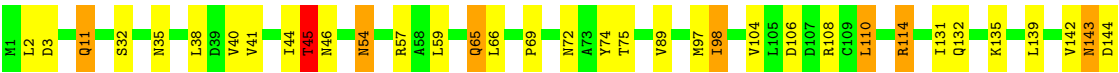




• Molecule 2: R-PHYCOCYANIN



• Molecule 2: R-PHYCOCYANIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	135.10Å 135.10Å 210.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	75.5 (8.00-2.40)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.189 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8209	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: CYC, PEB

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	0.66	0/1258	1.50	11/1709 (0.6%)
1	K	0.68	0/1258	1.58	17/1709 (1.0%)
1	M	0.67	0/1258	1.51	14/1709 (0.8%)
2	B	0.68	0/1271	1.62	22/1725 (1.3%)
2	L	0.68	0/1271	1.63	22/1725 (1.3%)
2	N	0.70	0/1271	1.70	30/1725 (1.7%)
All	All	0.68	0/7587	1.59	116/10302 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	160	ILE	CB-CA-C	-8.87	99.97	112.22
1	K	148	ASN	OD1-CG-ND2	-8.71	113.89	122.60
2	B	107	ASP	CA-CB-CG	8.41	121.01	112.60
1	M	109	ASP	CA-CB-CG	8.34	120.94	112.60
2	L	107	ASP	CA-CB-CG	8.07	120.67	112.60
2	N	160	ILE	N-CA-CB	8.07	122.69	110.58
2	N	144	ASP	CA-CB-CG	7.88	120.48	112.60
2	B	160	ILE	CB-CA-C	-7.86	101.54	112.14
2	L	51	ILE	CA-C-O	-7.84	112.80	120.95
2	N	3	ASP	CA-CB-CG	7.75	120.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	109	ASP	CA-CB-CG	7.74	120.34	112.60
2	B	3	ASP	CA-CB-CG	7.63	120.23	112.60
2	L	45	THR	N-CA-CB	-7.62	98.63	110.06
2	L	144	ASP	CA-CB-CG	7.43	120.03	112.60
2	N	45	THR	O-C-N	-7.40	113.77	122.20
1	K	66	THR	N-CA-CB	-7.37	97.80	110.32
1	M	57	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	K	47	ASN	OD1-CG-ND2	-7.05	115.55	122.60
2	B	74	TYR	CA-C-N	6.87	134.67	121.54
2	B	74	TYR	C-N-CA	6.87	134.67	121.54
1	K	68	GLN	OE1-CD-NE2	-6.84	115.76	122.60
1	A	109	ASP	CA-CB-CG	6.83	119.43	112.60
1	M	119	ASN	OD1-CG-ND2	-6.75	115.86	122.60
2	N	54	ASN	OD1-CG-ND2	-6.68	115.92	122.60
2	B	160	ILE	N-CA-CB	6.57	119.47	110.54
2	L	72	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	N	110	LEU	N-CA-C	6.51	119.37	111.82
1	A	69	MET	CA-C-N	6.49	126.40	119.85
1	A	69	MET	C-N-CA	6.49	126.40	119.85
1	M	139	ASN	N-CA-C	6.44	118.66	110.61
1	K	145	ASP	CA-CB-CG	-6.43	106.17	112.60
2	N	146	THR	CA-CB-OG1	-6.41	99.98	109.60
2	B	166	ARG	NE-CZ-NH1	-6.38	115.12	121.50
2	L	48	ALA	N-CA-C	6.38	118.23	111.28
2	L	35	ASN	OD1-CG-ND2	-6.36	116.24	122.60
2	L	37	ARG	NE-CZ-NH2	-6.32	113.51	119.20
1	K	26	VAL	N-CA-CB	-6.27	104.03	110.62
2	B	54	ASN	OD1-CG-ND2	-6.22	116.38	122.60
2	N	65	GLN	OE1-CD-NE2	-6.20	116.40	122.60
2	B	166	ARG	CG-CD-NE	-6.15	98.46	112.00
1	M	49	ASP	CA-CB-CG	-6.14	106.46	112.60
2	L	45	THR	CB-CA-C	6.10	121.06	110.68
1	M	26	VAL	N-CA-CB	-6.07	104.25	110.62
2	N	132	GLN	OE1-CD-NE2	-6.03	116.57	122.60
2	N	146	THR	CA-CB-CG2	6.01	120.72	110.50
2	B	143	ASN	OD1-CG-ND2	-6.01	116.59	122.60
2	L	25	ASP	CA-CB-CG	6.01	118.61	112.60
2	N	171	VAL	CA-C-N	5.97	132.45	121.70
2	N	171	VAL	C-N-CA	5.97	132.45	121.70
2	B	72	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	K	159	ASN	OD1-CG-ND2	-5.84	116.76	122.60
2	B	114	ARG	CA-C-O	-5.82	114.71	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	17	ARG	N-CA-CB	-5.80	101.46	111.55
2	N	148	THR	CA-C-N	5.80	125.99	119.90
2	N	148	THR	C-N-CA	5.80	125.99	119.90
2	N	35	ASN	OD1-CG-ND2	-5.80	116.80	122.60
2	B	166	ARG	NE-CZ-NH2	5.79	124.41	119.20
2	L	63	GLN	CA-C-N	5.79	125.46	119.56
2	L	63	GLN	C-N-CA	5.79	125.46	119.56
2	N	159	GLU	CA-C-O	-5.75	114.32	120.42
1	M	100	VAL	O-C-N	-5.72	113.99	121.82
1	M	161	LEU	O-C-N	5.67	130.19	122.37
1	K	3	THR	O-C-N	-5.63	116.53	121.32
2	L	111	ASN	CA-CB-CG	5.60	118.20	112.60
2	N	143	ASN	CA-CB-CG	-5.59	107.01	112.60
2	N	160	ILE	CA-CB-CG1	5.58	119.89	110.40
2	B	118	GLN	OE1-CD-NE2	-5.57	117.03	122.60
2	B	22	THR	CA-CB-OG1	-5.55	101.28	109.60
1	M	49	ASP	N-CA-C	5.53	117.39	111.36
1	K	161	LEU	CA-C-N	5.53	131.65	121.70
1	K	161	LEU	C-N-CA	5.53	131.65	121.70
2	L	74	TYR	CA-C-N	5.51	132.07	121.54
2	L	74	TYR	C-N-CA	5.51	132.07	121.54
2	B	79	MET	CG-SD-CE	-5.51	88.77	100.90
2	L	171	VAL	CA-C-N	5.46	131.53	121.70
2	L	171	VAL	C-N-CA	5.46	131.53	121.70
1	A	3	THR	CA-C-N	5.45	125.54	119.32
1	A	3	THR	C-N-CA	5.45	125.54	119.32
2	N	171	VAL	O-C-N	5.43	127.55	122.23
2	N	106	ASP	CB-CA-C	-5.42	102.36	110.88
1	K	148	ASN	CB-CG-ND2	5.40	124.50	116.40
1	A	25	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	M	161	LEU	CA-C-N	5.37	131.37	121.70
1	M	161	LEU	C-N-CA	5.37	131.37	121.70
2	B	49	SER	CA-CB-OG	-5.37	100.37	111.10
1	M	138	ASN	OD1-CG-ND2	-5.35	117.25	122.60
1	K	7	GLU	CA-CB-CG	-5.34	103.41	114.10
2	N	74	TYR	CA-C-N	5.33	131.73	121.54
2	N	74	TYR	C-N-CA	5.33	131.73	121.54
1	A	35	THR	CA-CB-OG1	-5.33	101.61	109.60
2	L	3	ASP	CA-CB-CG	5.33	117.92	112.60
2	B	116	THR	N-CA-C	-5.32	104.89	111.33
2	N	11	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	K	87	ASP	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	93	ARG	NE-CZ-NH2	-5.29	114.44	119.20
2	B	94	SER	CA-CB-OG	5.29	121.67	111.10
2	L	11	GLN	OE1-CD-NE2	-5.23	117.37	122.60
2	L	63	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	47	ASN	OD1-CG-ND2	-5.21	117.39	122.60
1	A	119	ASN	CB-CG-ND2	5.20	124.20	116.40
2	B	114	ARG	O-C-N	-5.19	116.48	122.09
2	B	136	ASP	CA-CB-CG	5.17	117.77	112.60
1	K	68	GLN	CG-CD-NE2	5.16	124.14	116.40
2	N	46	ASN	CB-CG-ND2	5.16	124.13	116.40
1	A	57	ASN	OD1-CG-ND2	-5.15	117.45	122.60
2	B	100	GLY	N-CA-C	-5.13	108.17	115.30
2	N	145	THR	CA-C-N	5.12	131.31	121.54
2	N	145	THR	C-N-CA	5.12	131.31	121.54
2	N	46	ASN	N-CA-C	5.11	119.52	113.28
1	A	67	THR	N-CA-CB	-5.10	102.93	110.53
1	M	21	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	L	47	ASN	OD1-CG-ND2	-5.08	117.52	122.60
2	L	136	ASP	CA-CB-CG	5.07	117.67	112.60
1	M	23	GLU	CA-CB-CG	-5.07	103.97	114.10
2	N	44	ILE	CA-C-N	5.03	127.72	120.38
2	N	44	ILE	C-N-CA	5.03	127.72	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	45	THR	Mainchain

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	1235	0	1212	15	0
1	K	1235	0	1212	15	0
1	M	1235	0	1212	10	0
2	B	1259	0	1271	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1259	0	1271	9	0
2	N	1259	0	1271	14	0
3	A	43	0	38	3	0
3	B	43	0	38	6	0
3	K	43	0	38	4	0
3	L	43	0	38	4	0
3	M	43	0	38	5	0
3	N	43	0	38	1	0
4	B	43	0	38	0	0
4	L	43	0	38	0	0
4	N	43	0	38	0	0
5	A	56	0	0	0	0
5	B	51	0	0	0	0
5	K	59	0	0	1	0
5	L	62	0	0	0	0
5	M	46	0	0	0	0
5	N	66	0	0	1	0
All	All	8209	0	7791	93	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 6.

All (93) 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)
3:B:385:CYC:HC	3:B:385:CYC:HMD1	1.39	0.88
2:N:89:VAL:HG11	2:N:131:ILE:HD12	1.61	0.82
3:B:385:CYC:HMA1	3:B:385:CYC:HB	1.52	0.73
1:M:142:LEU:HG	1:M:146:VAL:HG12	1.71	0.71
1:A:38:LEU:HD22	2:B:28:LEU:HG	1.73	0.71
2:B:40:VAL:HG11	2:B:97:MET:HE2	1.72	0.70
1:K:107:MET:HE3	1:K:156:TYR:HD2	1.57	0.69
3:B:385:CYC:HMA1	3:B:385:CYC:NB	2.08	0.68
3:K:386:CYC:HMA1	3:K:386:CYC:HB	1.62	0.65
1:M:137:LYS:HG3	1:M:154:ILE:HG21	1.78	0.65
3:B:385:CYC:HMD1	3:B:385:CYC:NC	2.10	0.64
3:A:384:CYC:HMA1	3:A:384:CYC:HB	1.63	0.64
2:N:54:ASN:HD22	2:N:57:ARG:HH21	1.46	0.63
2:N:54:ASN:ND2	2:N:57:ARG:HH21	1.98	0.61
1:K:140:HIS:HD2	1:K:142:LEU:H	1.50	0.59
1:A:22:THR:O	1:A:26:VAL:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LYS:HG3	2:B:24:ILE:HG21	1.85	0.58
1:K:34:ALA:O	1:K:38:LEU:HD22	2.03	0.58
2:B:88:ILE:HG21	3:B:385:CYC:HAB1	1.86	0.57
2:L:156:LEU:O	2:L:160:ILE:HG22	2.04	0.56
1:K:107:MET:HE3	1:K:156:TYR:CD2	2.41	0.56
3:A:384:CYC:HMA1	3:A:384:CYC:NB	2.21	0.55
1:K:63:PHE:O	1:K:66:THR:HB	2.07	0.55
2:B:1:MET:HE3	2:B:104:VAL:HB	1.89	0.54
1:A:142:LEU:HB3	1:A:146:VAL:HG23	1.89	0.54
1:A:145:ASP:HA	1:A:148:ASN:HB2	1.90	0.53
1:A:51:LEU:HG	1:A:136:ILE:HG23	1.91	0.52
1:A:140:HIS:HE1	1:A:151:ASN:OD1	1.92	0.52
2:L:41:VAL:HG21	2:L:98:ILE:HG12	1.91	0.52
1:A:23:GLU:O	1:A:26:VAL:HG22	2.10	0.51
1:M:140:HIS:HE1	1:M:151:ASN:OD1	1.93	0.51
2:L:60:PHE:CZ	2:L:79:MET:HE1	2.46	0.51
1:M:86:ARG:HD3	1:M:90:TYR:CE2	2.46	0.50
1:A:1:MET:SD	1:A:106:PRO:HG3	2.52	0.49
2:N:142:VAL:HG21	2:N:160:ILE:HD11	1.93	0.49
3:K:386:CYC:HMA1	3:K:386:CYC:NB	2.27	0.49
2:N:40:VAL:HG11	2:N:97:MET:HE2	1.94	0.49
3:L:387:CYC:HB	3:L:387:CYC:HMA3	1.77	0.49
2:N:108:ARG:HG2	5:N:446:HOH:O	2.12	0.49
1:K:17:ARG:HG2	1:K:18:PHE:O	2.13	0.48
1:A:77:THR:HG23	1:A:80:GLY:HA3	1.96	0.48
3:L:387:CYC:HMA3	3:L:387:CYC:NB	2.29	0.47
1:M:140:HIS:HD2	1:M:142:LEU:H	1.61	0.47
2:B:63:GLN:HB3	2:B:65:GLN:HE21	1.79	0.47
2:N:110:LEU:HG	2:N:170:ALA:HB3	1.95	0.47
2:N:135:LYS:O	2:N:139:LEU:HG	2.14	0.47
3:K:386:CYC:HBB2	2:N:75:THR:HA	1.95	0.47
3:M:388:CYC:HC	3:M:388:CYC:HMD2	1.79	0.47
1:M:95:VAL:HG21	1:M:154:ILE:HD13	1.97	0.46
2:B:145:THR:O	2:B:146:THR:CB	2.64	0.46
2:B:145:THR:O	2:B:146:THR:OG1	2.23	0.46
1:K:5:LEU:HD22	1:K:27:VAL:HG13	1.97	0.46
3:L:387:CYC:CMD	3:L:387:CYC:HC	2.30	0.45
1:A:9:ILE:HD11	2:B:98:ILE:HG22	1.99	0.45
3:M:388:CYC:HMC3	3:M:388:CYC:HAC2	1.86	0.44
1:M:134:LYS:HE2	1:M:158:ILE:HD13	2.00	0.44
2:L:79:MET:HE2	2:L:83:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:113:LEU:HD12	2:L:113:LEU:HA	1.78	0.43
1:K:2:LYS:HG2	5:K:427:HOH:O	2.18	0.43
1:K:140:HIS:HE1	1:K:151:ASN:OD1	2.00	0.43
2:L:97:MET:SD	2:L:160:ILE:HB	2.58	0.43
1:K:22:THR:O	1:K:26:VAL:HG23	2.17	0.43
1:A:94:MET:HE3	3:A:384:CYC:HBB1	2.00	0.43
2:B:123:PRO:O	2:B:127:VAL:HG23	2.19	0.43
2:B:129:VAL:O	2:B:133:LYS:HG2	2.19	0.43
1:K:91:TYR:O	1:K:95:VAL:HG23	2.18	0.43
1:M:74:TYR:HA	3:M:388:CYC:OC	2.17	0.43
1:M:108:ASP:HA	1:M:112:VAL:HB	2.00	0.43
2:B:120:LEU:HD11	3:B:385:CYC:HAA2	2.00	0.42
1:K:23:GLU:O	1:K:26:VAL:HB	2.19	0.42
3:L:387:CYC:HB	3:L:387:CYC:CMA	2.32	0.42
3:M:388:CYC:NB	3:M:388:CYC:HMA1	2.34	0.42
2:N:114:ARG:HG3	2:N:172:ALA:HB2	2.01	0.42
2:N:40:VAL:HG22	2:N:142:VAL:HG13	2.02	0.42
2:B:25:ASP:HA	2:B:28:LEU:HD12	2.02	0.42
2:B:116:THR:O	2:B:120:LEU:HG	2.20	0.42
1:A:69:MET:HA	1:A:70:PRO:HD3	1.80	0.41
2:B:57:ARG:NH2	3:M:388:CYC:O2D	2.53	0.41
2:B:113:LEU:HD23	2:B:171:VAL:HG12	2.02	0.41
2:N:160:ILE:HG21	2:N:160:ILE:HD13	1.80	0.41
1:A:1:MET:O	1:A:6:THR:HG21	2.21	0.41
2:B:41:VAL:HG11	2:B:98:ILE:HG12	2.01	0.41
2:L:91:ARG:O	2:L:94:SER:HB2	2.21	0.41
2:N:72:ASN:HD22	3:N:389:CYC:HC	1.68	0.41
1:K:118:ILE:HD12	3:K:386:CYC:HMA2	2.03	0.41
2:B:122:THR:HA	2:B:123:PRO:HD3	1.92	0.41
1:K:69:MET:HA	1:K:70:PRO:HD3	1.89	0.41
2:B:142:VAL:HG21	2:B:160:ILE:HD11	2.03	0.40
1:M:91:TYR:O	1:M:95:VAL:HG23	2.22	0.40
2:N:41:VAL:HG21	2:N:98:ILE:HG12	2.02	0.40
1:A:137:LYS:HD3	1:A:154:ILE:CG2	2.52	0.40
1:K:42:LYS:HE3	2:L:24:ILE:HG21	2.03	0.40
2:L:12:ALA:HA	2:L:15:ARG:HE	1.86	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	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	K	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	M	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
2	B	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	21	32
2	L	170/172 (99%)	164 (96%)	4 (2%)	2 (1%)	10	16
2	N	170/172 (99%)	166 (98%)	3 (2%)	1 (1%)	21	32
All	All	990/1002 (99%)	965 (98%)	21 (2%)	4 (0%)	30	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	146	THR
2	N	146	THR
2	L	111	ASN
2	L	146	THR

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%)	119 (92%)	10 (8%)	11	20
1	K	129/129 (100%)	117 (91%)	12 (9%)	8	14
1	M	129/129 (100%)	115 (89%)	14 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	127/127 (100%)	114 (90%)	13 (10%)	7	11
2	L	127/127 (100%)	113 (89%)	14 (11%)	6	9
2	N	127/127 (100%)	109 (86%)	18 (14%)	3	4
All	All	768/768 (100%)	687 (90%)	81 (10%)	6	10

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLU
1	A	42	LYS
1	A	49	ASP
1	A	51	LEU
1	A	57	ASN
1	A	77	THR
1	A	115	LEU
1	A	134	LYS
1	A	140	HIS
1	A	145	ASP
2	B	32	SER
2	B	38	LEU
2	B	45	THR
2	B	65	GLN
2	B	94	SER
2	B	98	ILE
2	B	108	ARG
2	B	111	ASN
2	B	115	GLU
2	B	139	LEU
2	B	148	THR
2	B	155	SER
2	B	160	ILE
1	K	17	ARG
1	K	19	LEU
1	K	33	ARG
1	K	35	THR
1	K	38	LEU
1	K	44	LEU
1	K	59	VAL
1	K	66	THR
1	K	99	LEU
1	K	134	LYS

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Mol	Chain	Res	Type
1	K	143	SER
1	K	162	SER
2	L	2	LEU
2	L	28	LEU
2	L	38	LEU
2	L	52	VAL
2	L	65	GLN
2	L	66	LEU
2	L	90	LEU
2	L	98	ILE
2	L	107	ASP
2	L	132	GLN
2	L	145	THR
2	L	146	THR
2	L	155	SER
2	L	160	ILE
1	M	19	LEU
1	M	21	ASN
1	M	23	GLU
1	M	32	ASN
1	M	33	ARG
1	M	76	SER
1	M	86	ARG
1	M	99	LEU
1	M	100	VAL
1	M	117	GLU
1	M	124	LEU
1	M	133	LEU
1	M	136	ILE
1	M	142	LEU
2	N	2	LEU
2	N	11	GLN
2	N	32	SER
2	N	38	LEU
2	N	45	THR
2	N	59	LEU
2	N	65	GLN
2	N	66	LEU
2	N	69	PRO
2	N	98	ILE
2	N	104	VAL
2	N	114	ARG

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Mol	Chain	Res	Type
2	N	143	ASN
2	N	145	THR
2	N	146	THR
2	N	148	THR
2	N	156	LEU
2	N	160	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	140	HIS
2	B	65	GLN
2	B	72	ASN
2	B	111	ASN
2	B	143	ASN
1	K	139	ASN
1	K	140	HIS
1	K	148	ASN
2	L	35	ASN
2	L	72	ASN
1	M	140	HIS
2	N	35	ASN
2	N	46	ASN
2	N	54	ASN
2	N	63	GLN
2	N	65	GLN
2	N	72	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

9 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	B	385	2	46,46,46	3.01	17 (36%)	63,67,67	2.78	29 (46%)
4	PEB	N	357	2	46,46,46	2.83	12 (26%)	56,67,67	2.42	23 (41%)
3	CYC	L	387	2	46,46,46	2.86	16 (34%)	63,67,67	2.60	33 (52%)
3	CYC	A	384	1	46,46,46	2.95	16 (34%)	63,67,67	2.78	27 (42%)
3	CYC	M	388	1	46,46,46	2.87	17 (36%)	63,67,67	2.81	26 (41%)
4	PEB	L	356	2	46,46,46	2.84	14 (30%)	56,67,67	2.33	20 (35%)
3	CYC	N	389	2	46,46,46	2.68	12 (26%)	63,67,67	2.40	28 (44%)
4	PEB	B	355	2	46,46,46	2.88	16 (34%)	56,67,67	2.51	25 (44%)
3	CYC	K	386	1	46,46,46	2.87	17 (36%)	63,67,67	3.08	30 (47%)

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	B	385	2	-	10/26/74/74	0/4/4/4
4	PEB	N	357	2	-	8/26/74/74	0/4/4/4
3	CYC	L	387	2	-	12/26/74/74	0/4/4/4
3	CYC	A	384	1	1/1/14/19	12/26/74/74	0/4/4/4
3	CYC	M	388	1	-	11/26/74/74	0/4/4/4
4	PEB	L	356	2	-	8/26/74/74	0/4/4/4
3	CYC	N	389	2	-	11/26/74/74	0/4/4/4
4	PEB	B	355	2	1/1/14/19	7/26/74/74	0/4/4/4
3	CYC	K	386	1	1/1/14/19	13/26/74/74	0/4/4/4

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	384	CYC	C2C-C1C	-13.53	1.40	1.52
3	K	386	CYC	C2C-C1C	-13.21	1.40	1.52
3	L	387	CYC	C2C-C1C	-13.12	1.40	1.52
3	N	389	CYC	C2C-C1C	-13.12	1.40	1.52
3	B	385	CYC	C2C-C1C	-12.85	1.40	1.52
4	B	355	PEB	C2A-C1A	-12.81	1.40	1.52
3	M	388	CYC	C2C-C1C	-12.78	1.40	1.52
4	L	356	PEB	C2A-C1A	-12.30	1.41	1.52
4	N	357	PEB	C2A-C1A	-11.43	1.41	1.52
3	B	385	CYC	C1A-C2A	-6.78	1.35	1.45
4	B	355	PEB	CHC-C4C	-6.12	1.42	1.50
4	N	357	PEB	C4C-C3C	6.08	1.46	1.38
3	A	384	CYC	C1A-C2A	-5.99	1.36	1.45
4	N	357	PEB	CHC-C4C	-5.99	1.42	1.50
3	L	387	CYC	C1A-C2A	-5.91	1.36	1.45
4	N	357	PEB	C2D-C3D	5.66	1.41	1.34
4	L	356	PEB	CHC-C4C	-5.62	1.43	1.50
3	B	385	CYC	C4B-C3B	-5.46	1.38	1.48
4	L	356	PEB	C2D-C3D	5.45	1.41	1.34
3	M	388	CYC	C4B-C3B	-5.44	1.38	1.48
3	A	384	CYC	C4B-C3B	-5.38	1.38	1.48
4	B	355	PEB	C2D-C3D	5.29	1.41	1.34
4	L	356	PEB	C4C-C3C	5.15	1.45	1.38
3	M	388	CYC	C1A-C2A	-5.11	1.37	1.45
4	L	356	PEB	CBD-CAD	4.86	1.53	1.30
4	N	357	PEB	CBD-CAD	4.85	1.53	1.30
4	B	355	PEB	CBD-CAD	4.81	1.53	1.30
3	B	385	CYC	C4A-C3A	4.77	1.56	1.45
3	K	386	CYC	C4B-C3B	-4.75	1.39	1.48
3	L	387	CYC	C4B-C3B	-4.72	1.39	1.48
3	K	386	CYC	C2A-C3A	4.71	1.46	1.36
3	M	388	CYC	CHD-C4C	4.62	1.44	1.36
3	N	389	CYC	C4B-C3B	-4.35	1.40	1.48
3	K	386	CYC	C1A-C2A	-4.31	1.39	1.45
4	N	357	PEB	O2B-CGB	4.18	1.44	1.30
3	N	389	CYC	O2D-CGD	4.11	1.44	1.30
3	L	387	CYC	CHD-C4C	4.07	1.43	1.36
3	M	388	CYC	C2A-C3A	4.06	1.45	1.36
4	B	355	PEB	O2B-CGB	4.00	1.44	1.30
3	N	389	CYC	CMA-C3A	3.97	1.58	1.50
3	A	384	CYC	CHD-C4C	3.92	1.43	1.36
4	L	356	PEB	O2C-CGC	3.92	1.43	1.30
4	N	357	PEB	O2C-CGC	3.90	1.43	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	386	CYC	C4A-NA	3.89	1.45	1.36
3	B	385	CYC	O2A-CGA	3.88	1.43	1.30
3	B	385	CYC	O2D-CGD	3.86	1.43	1.30
4	B	355	PEB	O2C-CGC	3.85	1.43	1.30
3	B	385	CYC	C1C-NC	-3.84	1.32	1.37
3	B	385	CYC	CHD-C4C	3.84	1.42	1.36
3	N	389	CYC	CHD-C4C	3.84	1.42	1.36
3	K	386	CYC	CHD-C4C	3.75	1.42	1.36
4	L	356	PEB	O2B-CGB	3.74	1.43	1.30
3	L	387	CYC	O2A-CGA	3.74	1.43	1.30
3	L	387	CYC	O2D-CGD	3.72	1.43	1.30
3	K	386	CYC	O2D-CGD	3.63	1.42	1.30
4	N	357	PEB	C1A-NA	-3.59	1.33	1.37
3	K	386	CYC	O2A-CGA	3.58	1.42	1.30
3	M	388	CYC	O2D-CGD	3.53	1.42	1.30
4	B	355	PEB	C1A-NA	-3.51	1.33	1.37
3	A	384	CYC	C4A-C3A	3.51	1.53	1.45
3	M	388	CYC	O2A-CGA	3.49	1.42	1.30
3	N	389	CYC	O2A-CGA	3.48	1.42	1.30
4	L	356	PEB	C1A-NA	-3.48	1.33	1.37
3	L	387	CYC	C2A-C3A	3.41	1.44	1.36
3	A	384	CYC	O2D-CGD	3.37	1.42	1.30
3	K	386	CYC	C4A-C3A	3.32	1.53	1.45
4	B	355	PEB	CMC-C3C	3.31	1.57	1.50
3	A	384	CYC	O2A-CGA	3.30	1.41	1.30
3	A	384	CYC	C2A-C3A	3.26	1.43	1.36
3	B	385	CYC	C2A-C3A	3.23	1.43	1.36
3	M	388	CYC	C4A-C3A	3.17	1.52	1.45
3	N	389	CYC	C3B-C2B	3.13	1.43	1.36
3	B	385	CYC	C4B-NB	-3.11	1.30	1.38
3	L	387	CYC	C1C-NC	-3.11	1.33	1.37
3	L	387	CYC	C3B-C2B	3.10	1.43	1.36
3	B	385	CYC	CAA-C2A	3.10	1.59	1.51
3	A	384	CYC	CAA-C2A	3.10	1.59	1.51
3	K	386	CYC	C1C-NC	-3.07	1.33	1.37
4	L	356	PEB	CHA-C4A	3.07	1.41	1.36
3	B	385	CYC	C3B-C2B	3.05	1.43	1.36
3	M	388	CYC	C4A-NA	3.03	1.43	1.36
3	A	384	CYC	C3B-C2B	3.00	1.43	1.36
4	B	355	PEB	CHA-C4A	2.99	1.41	1.36
3	L	387	CYC	C4B-NB	-2.92	1.31	1.38
3	A	384	CYC	C4A-NA	2.92	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	355	PEB	C3B-C2B	2.91	1.43	1.36
3	M	388	CYC	CAA-C2A	2.89	1.58	1.51
3	N	389	CYC	C1C-NC	-2.85	1.34	1.37
3	L	387	CYC	C4A-C3A	2.85	1.52	1.45
3	M	388	CYC	C1D-ND	2.84	1.42	1.37
3	K	386	CYC	CHB-C4A	2.84	1.47	1.40
3	A	384	CYC	C1C-NC	-2.82	1.34	1.37
4	L	356	PEB	CAA-C3A	-2.77	1.48	1.54
3	M	388	CYC	C4C-NC	2.75	1.42	1.37
4	B	355	PEB	CAC-C2C	-2.71	1.44	1.51
3	B	385	CYC	C4A-NA	2.68	1.42	1.36
3	M	388	CYC	C3B-C2B	2.68	1.42	1.36
3	K	386	CYC	C3B-C2B	2.65	1.42	1.36
4	L	356	PEB	C3B-C2B	2.59	1.42	1.36
3	K	386	CYC	C4C-NC	2.58	1.42	1.37
3	N	389	CYC	C4B-NB	-2.56	1.32	1.38
3	M	388	CYC	C1C-NC	-2.55	1.34	1.37
4	B	355	PEB	C4A-NA	2.54	1.42	1.37
3	M	388	CYC	C4D-ND	2.54	1.42	1.37
4	N	357	PEB	C3B-C2B	2.53	1.42	1.36
3	A	384	CYC	C4C-NC	2.53	1.42	1.37
4	N	357	PEB	CHA-C4A	2.52	1.40	1.36
3	A	384	CYC	C4B-NB	-2.44	1.32	1.38
3	A	384	CYC	C1D-ND	2.41	1.41	1.37
4	N	357	PEB	C4C-NC	2.38	1.42	1.37
3	K	386	CYC	C4B-NB	-2.36	1.32	1.38
3	N	389	CYC	C4C-NC	2.35	1.41	1.37
3	L	387	CYC	C4A-NA	2.29	1.41	1.36
3	N	389	CYC	C2A-C3A	2.29	1.41	1.36
4	N	357	PEB	C4A-NA	2.29	1.41	1.37
3	B	385	CYC	CMA-C3A	-2.29	1.46	1.50
3	B	385	CYC	C1D-ND	2.26	1.41	1.37
3	A	384	CYC	C4D-ND	2.24	1.41	1.37
3	L	387	CYC	C4C-NC	2.24	1.41	1.37
4	L	356	PEB	C4A-NA	2.24	1.41	1.37
3	K	386	CYC	C1D-ND	2.21	1.41	1.37
3	L	387	CYC	CAA-C2A	2.21	1.57	1.51
3	B	385	CYC	C4C-NC	2.20	1.41	1.37
3	K	386	CYC	C4D-ND	2.20	1.41	1.37
3	L	387	CYC	C1D-ND	2.18	1.41	1.37
3	B	385	CYC	C4D-ND	2.18	1.41	1.37
3	M	388	CYC	C1B-NB	2.15	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	387	CYC	C4D-ND	2.14	1.41	1.37
3	K	386	CYC	CAA-C2A	2.14	1.56	1.51
4	B	355	PEB	C4C-NC	2.13	1.41	1.37
4	B	355	PEB	C4B-C3B	-2.11	1.42	1.45
3	N	389	CYC	C1D-ND	2.11	1.41	1.37
4	L	356	PEB	C4B-C3B	-2.10	1.42	1.45
3	M	388	CYC	C4B-NB	-2.05	1.33	1.38
4	L	356	PEB	C4C-NC	2.05	1.41	1.37
4	B	355	PEB	CAD-C3D	2.04	1.52	1.47
4	B	355	PEB	C1C-NC	2.00	1.41	1.37

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	386	CYC	C4A-C3A-C2A	-10.67	94.37	106.48
3	M	388	CYC	C4A-C3A-C2A	-8.13	97.25	106.48
3	K	386	CYC	CAA-C2A-C3A	-8.03	112.83	127.87
3	B	385	CYC	C4A-C3A-C2A	-7.93	97.47	106.48
3	M	388	CYC	CAC-C3C-C4C	7.90	132.96	112.67
3	A	384	CYC	CAC-C3C-C4C	7.81	132.73	112.67
3	K	386	CYC	CAC-C3C-C4C	7.75	132.58	112.67
4	B	355	PEB	C1D-CHC-C4C	7.53	126.00	113.32
4	N	357	PEB	OD-C4D-ND	-7.44	115.80	126.02
3	A	384	CYC	C4A-C3A-C2A	-7.31	98.18	106.48
3	M	388	CYC	C3B-C4B-NB	7.28	112.57	106.77
3	K	386	CYC	C1A-C2A-C3A	6.95	114.25	106.73
4	L	356	PEB	C1D-CHC-C4C	6.93	125.00	113.32
3	A	384	CYC	C1A-C2A-C3A	6.90	114.19	106.73
3	B	385	CYC	C1A-C2A-C3A	6.87	114.17	106.73
4	L	356	PEB	OD-C4D-ND	-6.49	117.10	126.02
3	K	386	CYC	CMC-C2C-C1C	6.43	126.27	112.40
3	M	388	CYC	CMC-C2C-C1C	6.43	126.27	112.40
3	M	388	CYC	CAA-C2A-C3A	-6.41	115.87	127.87
3	A	384	CYC	CMC-C2C-C1C	6.27	125.92	112.40
3	A	384	CYC	C3B-C4B-NB	6.10	111.63	106.77
3	B	385	CYC	CAA-C2A-C3A	-6.05	116.53	127.87
3	B	385	CYC	C3B-C4B-NB	5.82	111.40	106.77
3	M	388	CYC	C1A-C2A-C3A	5.76	112.96	106.73
3	L	387	CYC	C4A-C3A-C2A	-5.69	100.02	106.48
4	B	355	PEB	CMA-C2A-C1A	5.50	124.25	112.40
3	L	387	CYC	C1A-C2A-C3A	5.39	112.56	106.73
3	A	384	CYC	CAA-C2A-C3A	-5.37	117.82	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	387	CYC	C3B-C4B-NB	5.31	111.00	106.77
3	N	389	CYC	C3B-C4B-NB	5.25	110.95	106.77
3	K	386	CYC	C3B-C4B-NB	5.22	110.93	106.77
3	N	389	CYC	CHB-C4A-NA	-5.21	113.71	124.95
3	B	385	CYC	CAC-C3C-C4C	5.20	126.03	112.67
3	N	389	CYC	CMC-C2C-C1C	5.16	123.53	112.40
3	K	386	CYC	CHB-C4A-NA	-5.16	113.81	124.95
4	N	357	PEB	C1D-CHC-C4C	5.05	121.83	113.32
4	B	355	PEB	C3C-C4C-NC	5.05	112.40	108.31
4	B	355	PEB	OD-C4D-ND	-5.00	119.15	126.02
3	N	389	CYC	CBC-CAC-C3C	-4.98	102.86	113.41
3	L	387	CYC	CMC-C2C-C1C	4.95	123.07	112.40
3	L	387	CYC	CAA-C2A-C3A	-4.94	118.62	127.87
3	N	389	CYC	CAC-C3C-C4C	4.85	125.13	112.67
4	N	357	PEB	OA-C1A-NA	-4.71	119.38	124.93
4	N	357	PEB	C1D-ND-C4D	-4.58	106.38	113.42
3	N	389	CYC	C1B-C2B-C3B	-4.57	103.17	107.86
4	L	356	PEB	CHC-C1D-ND	-4.55	108.14	113.73
4	L	356	PEB	CMA-C2A-C1A	4.51	122.12	112.40
3	L	387	CYC	CHB-C4A-NA	-4.46	115.31	124.95
3	B	385	CYC	CMB-C2B-C1B	4.44	129.56	124.16
4	N	357	PEB	CMA-C2A-C1A	4.39	121.87	112.40
3	M	388	CYC	CHB-C4A-NA	-4.36	115.54	124.95
4	N	357	PEB	CHC-C1D-ND	-4.36	108.39	113.73
4	B	355	PEB	CHB-C1C-C2C	-4.24	118.11	127.22
3	L	387	CYC	CMB-C2B-C1B	4.18	129.24	124.16
3	N	389	CYC	C2C-C1C-NC	4.16	111.75	108.29
3	B	385	CYC	C1B-C2B-C3B	-4.04	103.71	107.86
3	L	387	CYC	C1B-C2B-C3B	-4.03	103.72	107.86
4	N	357	PEB	OA-C1A-C2A	3.90	129.28	126.17
3	B	385	CYC	CMC-C2C-C1C	3.85	120.70	112.40
4	B	355	PEB	C1D-ND-C4D	-3.78	107.61	113.42
3	B	385	CYC	OC-C1C-NC	-3.76	120.50	124.93
3	A	384	CYC	CHB-C4A-NA	-3.75	116.85	124.95
3	B	385	CYC	CHB-C1B-NB	-3.74	118.08	126.06
4	L	356	PEB	OA-C1A-NA	-3.71	120.56	124.93
3	K	386	CYC	CBC-CAC-C3C	-3.71	105.55	113.41
3	M	388	CYC	C1B-NB-C4B	-3.70	106.12	110.66
4	N	357	PEB	C3D-C4D-ND	3.70	114.27	107.33
4	L	356	PEB	C1D-ND-C4D	-3.70	107.73	113.42
3	N	389	CYC	OC-C1C-NC	-3.65	120.63	124.93
3	B	385	CYC	CBB-CAB-C3B	3.64	122.29	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	357	PEB	C2A-C1A-NA	3.63	111.31	108.29
3	L	387	CYC	OC-C1C-NC	-3.63	120.65	124.93
3	A	384	CYC	CHD-C1D-ND	-3.56	117.26	125.29
4	B	355	PEB	O2B-CGB-CBB	3.53	125.15	114.00
3	B	385	CYC	CHB-C4A-NA	-3.53	117.33	124.95
3	L	387	CYC	CBC-CAC-C3C	-3.52	105.95	113.41
3	L	387	CYC	CBB-CAB-C3B	3.50	121.91	112.42
4	B	355	PEB	CHC-C4C-NC	-3.48	116.45	121.10
3	A	384	CYC	C2C-C1C-NC	3.47	111.17	108.29
3	K	386	CYC	CBB-CAB-C3B	3.45	121.79	112.42
3	K	386	CYC	C2C-C1C-NC	3.44	111.15	108.29
3	M	388	CYC	C2C-C1C-NC	3.42	111.14	108.29
3	L	387	CYC	CAC-C3C-C4C	3.40	121.42	112.67
4	L	356	PEB	C2A-C1A-NA	3.39	111.11	108.29
3	B	385	CYC	C2C-C1C-NC	3.39	111.11	108.29
3	B	385	CYC	C3D-C4D-ND	3.38	111.81	107.57
3	A	384	CYC	O2D-CGD-CBD	3.38	124.67	114.00
3	L	387	CYC	OB-C4B-NB	-3.37	117.17	125.08
3	N	389	CYC	C3D-C4D-ND	3.37	111.80	107.57
3	K	386	CYC	CHD-C1D-ND	-3.34	117.74	125.29
3	A	384	CYC	CBC-CAC-C3C	-3.33	106.35	113.41
3	K	386	CYC	O2D-CGD-CBD	3.33	124.51	114.00
3	N	389	CYC	CBB-CAB-C3B	3.33	121.44	112.42
3	L	387	CYC	C2C-C1C-NC	3.32	111.05	108.29
3	A	384	CYC	O2A-CGA-O1A	-3.32	114.80	123.33
3	B	385	CYC	O2D-CGD-CBD	3.31	124.46	114.00
3	A	384	CYC	C1B-C2B-C3B	-3.30	104.47	107.86
4	N	357	PEB	CBA-CAA-C3A	-3.29	106.43	113.41
3	B	385	CYC	OB-C4B-NB	-3.29	117.37	125.08
3	A	384	CYC	O2A-CGA-CBA	3.23	124.19	114.00
3	L	387	CYC	OB-C4B-C3B	3.22	131.42	128.03
3	L	387	CYC	CHB-C1B-NB	-3.18	119.28	126.06
3	L	387	CYC	O2D-CGD-CBD	3.18	124.04	114.00
3	L	387	CYC	O2A-CGA-CBA	3.18	124.03	114.00
4	N	357	PEB	CAC-CBC-CGC	-3.17	105.24	113.67
3	N	389	CYC	CHD-C1D-ND	-3.16	118.14	125.29
3	L	387	CYC	CHD-C1D-ND	-3.15	118.17	125.29
3	B	385	CYC	CBC-CAC-C3C	-3.14	106.75	113.41
4	N	357	PEB	O2B-CGB-CBB	3.11	123.83	114.00
3	L	387	CYC	CMD-C2D-C1D	3.11	130.14	125.62
4	B	355	PEB	CHA-C1B-NB	-3.10	118.26	124.95
3	A	384	CYC	CMC-C2C-C3C	3.10	125.95	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	384	CYC	CBB-CAB-C3B	3.09	120.81	112.42
4	B	355	PEB	CMA-C2A-C3A	3.08	125.89	113.98
3	N	389	CYC	O2D-CGD-CBD	3.08	123.72	114.00
3	M	388	CYC	C1B-C2B-C3B	-3.07	104.70	107.86
3	K	386	CYC	O2A-CGA-CBA	3.06	123.65	114.00
3	M	388	CYC	CHA-C4D-C3D	-3.05	120.67	127.22
4	L	356	PEB	C3D-C4D-ND	3.02	113.00	107.33
4	B	355	PEB	C1C-NC-C4C	-3.02	104.23	109.60
3	M	388	CYC	CBB-CAB-C3B	3.01	120.58	112.42
4	L	356	PEB	O2B-CGB-CBB	3.01	123.50	114.00
4	B	355	PEB	CAA-C3A-C4A	3.00	120.39	112.67
3	L	387	CYC	C3D-C4D-ND	3.00	111.33	107.57
4	B	355	PEB	CHC-C1D-ND	-3.00	110.05	113.73
3	K	386	CYC	CMC-C2C-C3C	3.00	125.57	113.98
3	K	386	CYC	OB-C4B-NB	-2.98	118.08	125.08
3	M	388	CYC	CBC-CAC-C3C	-2.98	107.09	113.41
4	L	356	PEB	O2C-CGC-CBC	2.95	123.33	114.00
3	B	385	CYC	OB-C4B-C3B	2.95	131.13	128.03
3	N	389	CYC	OB-C4B-NB	-2.94	118.20	125.08
3	K	386	CYC	CMD-C2D-C1D	2.89	129.82	125.62
3	B	385	CYC	CHD-C1D-ND	-2.89	118.77	125.29
3	B	385	CYC	CAB-C3B-C4B	2.85	125.78	121.37
3	A	384	CYC	CMB-C2B-C1B	2.82	127.59	124.16
4	B	355	PEB	C3D-C4D-ND	2.82	112.61	107.33
3	K	386	CYC	CMB-C2B-C1B	2.79	127.56	124.16
3	A	384	CYC	OB-C4B-NB	-2.79	118.53	125.08
4	L	356	PEB	CHA-C1B-NB	-2.79	118.92	124.95
3	N	389	CYC	C1B-NB-C4B	-2.79	107.24	110.66
3	B	385	CYC	OC-C1C-C2C	2.78	128.38	126.17
3	M	388	CYC	OB-C4B-NB	-2.76	118.61	125.08
3	K	386	CYC	O2A-CGA-O1A	-2.75	116.25	123.33
4	B	355	PEB	C2A-C1A-NA	2.75	110.57	108.29
4	N	357	PEB	CHA-C1B-NB	-2.72	119.08	124.95
4	L	356	PEB	OA-C1A-C2A	2.72	128.33	126.17
3	A	384	CYC	C1D-CHD-C4C	2.72	132.40	127.76
4	N	357	PEB	CMB-C2B-C1B	2.69	129.28	125.10
3	M	388	CYC	C1D-CHD-C4C	2.69	132.36	127.76
3	B	385	CYC	C4D-ND-C1D	-2.68	105.07	109.78
3	M	388	CYC	CMB-C2B-C1B	2.67	127.41	124.16
3	M	388	CYC	OC-C1C-NC	-2.67	121.78	124.93
3	N	389	CYC	OB-C4B-C3B	2.67	130.84	128.03
3	L	387	CYC	OC-C1C-C2C	2.67	128.29	126.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	389	CYC	CMA-C3A-C4A	2.66	129.24	125.10
3	K	386	CYC	OB-C4B-C3B	2.66	130.83	128.03
4	B	355	PEB	OA-C1A-NA	-2.66	121.80	124.93
3	M	388	CYC	CMC-C2C-C3C	2.65	124.25	113.98
3	L	387	CYC	CAB-C3B-C4B	2.64	125.46	121.37
3	L	387	CYC	CBD-CAD-C3D	2.64	119.84	112.53
4	B	355	PEB	O2C-CGC-CBC	2.62	122.27	114.00
3	N	389	CYC	CHB-C1B-NB	-2.62	120.48	126.06
4	L	356	PEB	CHB-C1C-C2C	-2.60	121.63	127.22
3	B	385	CYC	O2A-CGA-O1A	-2.59	116.67	123.33
3	K	386	CYC	C4D-ND-C1D	-2.58	105.25	109.78
4	N	357	PEB	O2C-CGC-CBC	2.58	122.15	114.00
3	B	385	CYC	O2A-CGA-CBA	2.56	122.07	114.00
3	N	389	CYC	C4D-ND-C1D	-2.55	105.31	109.78
3	K	386	CYC	OC-C1C-NC	-2.53	121.94	124.93
3	K	386	CYC	C1B-C2B-C3B	-2.52	105.27	107.86
4	L	356	PEB	CMB-C2B-C1B	2.52	129.01	125.10
4	L	356	PEB	CBA-CAA-C3A	-2.51	108.09	113.41
3	A	384	CYC	C4D-ND-C1D	-2.49	105.41	109.78
3	N	389	CYC	CHB-C4A-C3A	2.48	131.25	124.87
4	N	357	PEB	CAC-C2C-C3C	-2.48	121.52	127.07
3	N	389	CYC	O2A-CGA-CBA	2.46	121.77	114.00
3	A	384	CYC	C1B-NB-C4B	-2.45	107.66	110.66
4	B	355	PEB	CMD-C2D-C3D	-2.43	126.50	129.95
3	M	388	CYC	O2A-CGA-CBA	2.43	121.67	114.00
3	N	389	CYC	CMB-C2B-C1B	2.42	127.11	124.16
3	A	384	CYC	C3D-C4D-ND	2.42	110.60	107.57
3	M	388	CYC	CHD-C1D-ND	-2.42	119.83	125.29
3	K	386	CYC	CHA-C1A-NA	2.41	129.66	124.60
3	N	389	CYC	C1D-CHD-C4C	2.41	131.87	127.76
4	N	357	PEB	CBC-CAC-C2C	2.40	119.17	112.53
4	N	357	PEB	C3C-C4C-NC	2.39	110.25	108.31
4	L	356	PEB	CMD-C2D-C3D	-2.38	126.56	129.95
4	N	357	PEB	C1A-NA-C4A	-2.38	110.42	113.41
4	N	357	PEB	C1C-NC-C4C	-2.38	105.36	109.60
4	B	355	PEB	CMB-C2B-C1B	2.37	128.79	125.10
3	B	385	CYC	CHA-C4D-C3D	-2.37	122.14	127.22
3	L	387	CYC	O2A-CGA-O1A	-2.37	117.25	123.33
3	M	388	CYC	C4D-ND-C1D	-2.35	105.65	109.78
3	K	386	CYC	C3D-C4D-ND	2.35	110.52	107.57
3	N	389	CYC	CMD-C2D-C1D	2.33	129.00	125.62
3	L	387	CYC	CMC-C2C-C3C	2.32	122.97	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	384	CYC	CMD-C2D-C1D	2.32	128.99	125.62
3	L	387	CYC	O2D-CGD-O1D	-2.31	117.39	123.33
3	A	384	CYC	C2D-C1D-ND	2.29	110.56	107.43
3	N	389	CYC	CHA-C4D-C3D	-2.29	122.30	127.22
3	B	385	CYC	CMD-C2D-C1D	2.29	128.94	125.62
3	K	386	CYC	CHB-C4A-C3A	2.28	130.72	124.87
3	L	387	CYC	C1D-CHD-C4C	2.27	131.64	127.76
3	B	385	CYC	CAA-C2A-C1A	2.26	128.99	125.02
3	K	386	CYC	C2D-C1D-ND	2.26	110.51	107.43
3	M	388	CYC	O2D-CGD-CBD	2.26	121.13	114.00
3	M	388	CYC	C3D-C4D-ND	2.24	110.38	107.57
3	L	387	CYC	CHD-C1D-C2D	2.23	133.00	127.53
4	B	355	PEB	C2C-C1C-NC	2.23	110.36	107.57
4	B	355	PEB	CMC-C3C-C4C	2.19	129.32	126.97
3	M	388	CYC	C3C-C4C-NC	-2.19	105.12	107.94
3	N	389	CYC	C2B-C1B-NB	2.18	110.15	106.97
3	A	384	CYC	CHA-C4D-C3D	-2.17	122.55	127.22
3	N	389	CYC	O2A-CGA-O1A	-2.17	117.75	123.33
4	B	355	PEB	C1C-C2C-C3C	-2.17	105.09	107.62
4	L	356	PEB	C2C-C1C-NC	2.17	110.29	107.57
3	M	388	CYC	O2A-CGA-O1A	-2.17	117.75	123.33
4	B	355	PEB	O2B-CGB-O1B	-2.16	117.77	123.33
4	L	356	PEB	C1C-NC-C4C	-2.14	105.79	109.60
3	K	386	CYC	O1D-CGD-CBD	-2.14	116.31	123.09
3	K	386	CYC	CAB-C3B-C4B	2.13	124.67	121.37
3	L	387	CYC	CHA-C4D-C3D	-2.12	122.66	127.22
3	L	387	CYC	C4D-ND-C1D	-2.11	106.08	109.78
3	N	389	CYC	O2D-CGD-O1D	-2.11	117.91	123.33
3	N	389	CYC	CMC-C2C-C3C	2.10	122.12	113.98
3	A	384	CYC	O1D-CGD-CBD	-2.10	116.42	123.09
4	B	355	PEB	CHA-C1B-C2B	2.10	130.27	124.87
4	B	355	PEB	CBA-CAA-C3A	-2.09	108.97	113.41
4	N	357	PEB	O1B-CGB-CBB	-2.09	116.45	123.09
3	M	388	CYC	CHB-C4A-C3A	2.06	130.17	124.87
3	K	386	CYC	C1D-CHD-C4C	2.06	131.28	127.76
4	N	357	PEB	CMD-C2D-C3D	-2.05	127.04	129.95
3	B	385	CYC	CMC-C2C-C3C	2.05	121.92	113.98
4	L	356	PEB	O2C-CGC-O1C	-2.05	118.06	123.33
3	K	386	CYC	CBA-CAA-C2A	2.05	118.19	112.53
4	N	357	PEB	O2C-CGC-O1C	-2.04	118.08	123.33
3	L	387	CYC	CHB-C4A-C3A	2.04	130.10	124.87
3	B	385	CYC	O1D-CGD-CBD	-2.03	116.66	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	356	PEB	C1A-NA-C4A	-2.02	110.88	113.41
3	L	387	CYC	CMA-C3A-C4A	2.01	128.22	125.10
3	A	384	CYC	CAB-C3B-C4B	2.00	124.47	121.37

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	384	CYC	C2C
3	K	386	CYC	C2C
4	B	355	PEB	C2A

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	384	CYC	C3A-C4A-CHB-C1B
3	A	384	CYC	C2C-C3C-CAC-CBC
3	A	384	CYC	C4C-C3C-CAC-CBC
3	B	385	CYC	C3A-C4A-CHB-C1B
3	B	385	CYC	C4C-C3C-CAC-CBC
3	K	386	CYC	C3A-C2A-CAA-CBA
3	K	386	CYC	C3A-C4A-CHB-C1B
3	K	386	CYC	C2C-C3C-CAC-CBC
3	K	386	CYC	C4C-C3C-CAC-CBC
3	L	387	CYC	C3A-C4A-CHB-C1B
3	L	387	CYC	C2B-C3B-CAB-CBB
3	L	387	CYC	C4C-C3C-CAC-CBC
3	M	388	CYC	NA-C4A-CHB-C1B
3	M	388	CYC	C3A-C4A-CHB-C1B
3	M	388	CYC	C2C-C3C-CAC-CBC
3	N	389	CYC	NA-C4A-CHB-C1B
3	N	389	CYC	C3A-C4A-CHB-C1B
3	N	389	CYC	C2B-C3B-CAB-CBB
3	N	389	CYC	C4B-C3B-CAB-CBB
3	N	389	CYC	C4C-C3C-CAC-CBC
4	B	355	PEB	NB-C1B-CHA-C4A
4	B	355	PEB	C2B-C1B-CHA-C4A
4	L	356	PEB	C2A-C3A-CAA-CBA
4	L	356	PEB	C4A-C3A-CAA-CBA
4	L	356	PEB	NB-C1B-CHA-C4A
4	L	356	PEB	C2B-C1B-CHA-C4A
4	N	357	PEB	C2A-C3A-CAA-CBA
4	N	357	PEB	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
4	N	357	PEB	NB-C1B-CHA-C4A
4	N	357	PEB	C2B-C1B-CHA-C4A
3	B	385	CYC	C2B-C3B-CAB-CBB
3	K	386	CYC	C2B-C3B-CAB-CBB
3	M	388	CYC	C3A-C2A-CAA-CBA
3	A	384	CYC	C2B-C3B-CAB-CBB
3	M	388	CYC	C2D-C1D-CHD-C4C
3	N	389	CYC	C2A-CAA-CBA-CGA
3	M	388	CYC	C2B-C3B-CAB-CBB
3	B	385	CYC	ND-C1D-CHD-C4C
3	K	386	CYC	ND-C1D-CHD-C4C
3	L	387	CYC	ND-C1D-CHD-C4C
3	M	388	CYC	ND-C1D-CHD-C4C
3	N	389	CYC	ND-C1D-CHD-C4C
3	A	384	CYC	C2D-C1D-CHD-C4C
3	B	385	CYC	C2D-C1D-CHD-C4C
3	K	386	CYC	C2D-C1D-CHD-C4C
3	L	387	CYC	C2D-C1D-CHD-C4C
3	N	389	CYC	C2D-C1D-CHD-C4C
3	A	384	CYC	ND-C1D-CHD-C4C
3	B	385	CYC	C4B-C3B-CAB-CBB
3	K	386	CYC	C4B-C3B-CAB-CBB
3	L	387	CYC	C4B-C3B-CAB-CBB
3	A	384	CYC	NA-C4A-CHB-C1B
3	B	385	CYC	NA-C4A-CHB-C1B
3	K	386	CYC	NA-C4A-CHB-C1B
3	L	387	CYC	NA-C4A-CHB-C1B
3	A	384	CYC	C4B-C3B-CAB-CBB
3	M	388	CYC	C4B-C3B-CAB-CBB
3	B	385	CYC	C2C-C3C-CAC-CBC
3	L	387	CYC	C2C-C3C-CAC-CBC
3	N	389	CYC	C2C-C3C-CAC-CBC
3	A	384	CYC	C3A-C2A-CAA-CBA
3	M	388	CYC	C4C-C3C-CAC-CBC
4	B	355	PEB	C4A-C3A-CAA-CBA
3	L	387	CYC	C2D-C3D-CAD-CBD
3	L	387	CYC	C4D-C3D-CAD-CBD
3	B	385	CYC	C3A-C2A-CAA-CBA
3	L	387	CYC	CAA-CBA-CGA-O2A
4	B	355	PEB	CAB-CBB-CGB-O1B
4	B	355	PEB	CAC-CBC-CGC-O1C
4	N	357	PEB	CAC-CBC-CGC-O2C

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Mol	Chain	Res	Type	Atoms
4	B	355	PEB	CAB-CBB-CGB-O2B
3	B	385	CYC	C2A-CAA-CBA-CGA
3	N	389	CYC	CAA-CBA-CGA-O2A
3	A	384	CYC	CAA-CBA-CGA-O2A
4	N	357	PEB	CAC-CBC-CGC-O1C
3	A	384	CYC	CAA-CBA-CGA-O1A
4	L	356	PEB	CAB-CBB-CGB-O2B
3	L	387	CYC	CAA-CBA-CGA-O1A
4	N	357	PEB	CAB-CBB-CGB-O2B
4	B	355	PEB	CAC-CBC-CGC-O2C
3	N	389	CYC	CAA-CBA-CGA-O1A
4	N	357	PEB	CAB-CBB-CGB-O1B
3	K	386	CYC	CAA-CBA-CGA-O1A
3	K	386	CYC	CAA-CBA-CGA-O2A
4	L	356	PEB	CAB-CBB-CGB-O1B
4	L	356	PEB	CAC-CBC-CGC-O2C
3	M	388	CYC	CAA-CBA-CGA-O2A
3	M	388	CYC	CAA-CBA-CGA-O1A
3	K	386	CYC	CAD-CBD-CGD-O1D
4	L	356	PEB	C3C-C2C-CAC-CBC
3	K	386	CYC	CAD-CBD-CGD-O2D
3	A	384	CYC	CAD-CBD-CGD-O2D

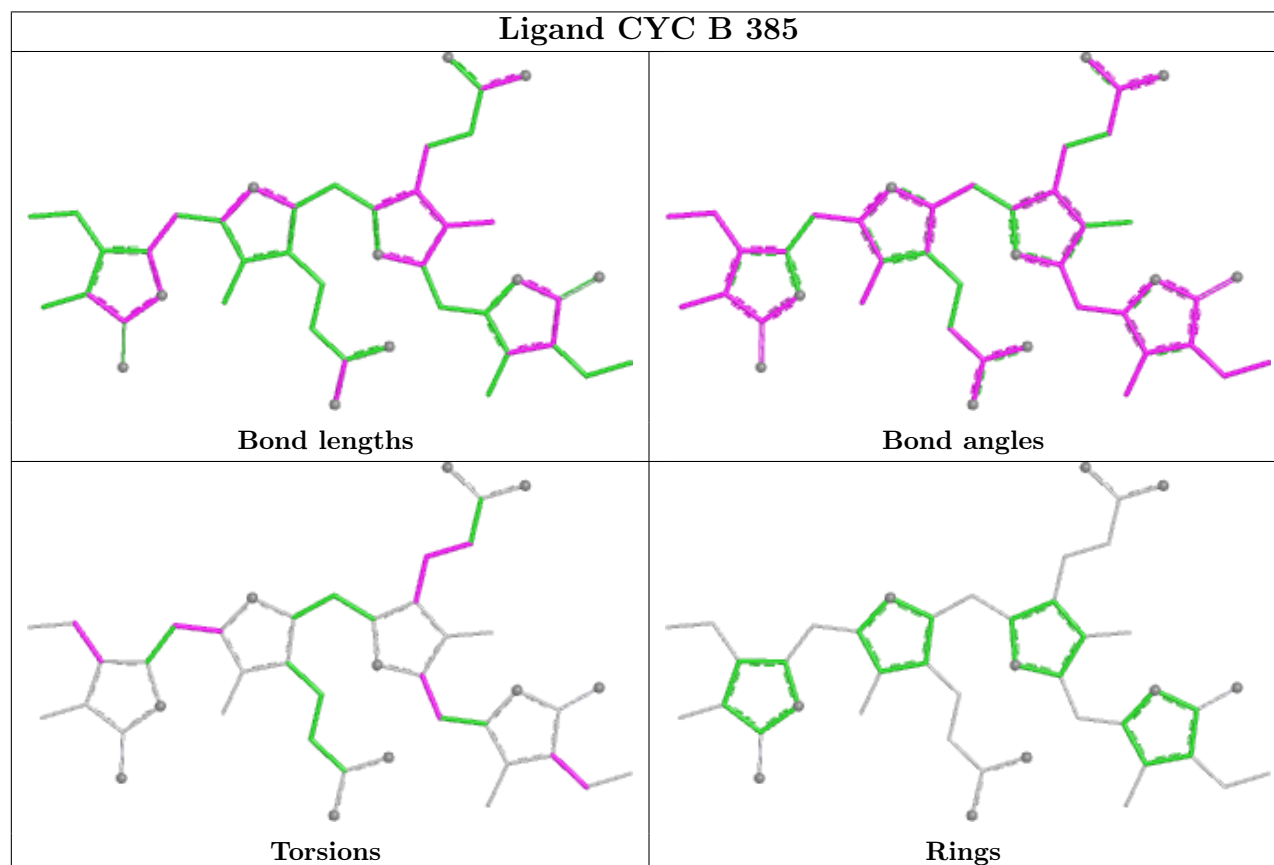
There are no ring outliers.

6 monomers are involved in 23 short contacts:

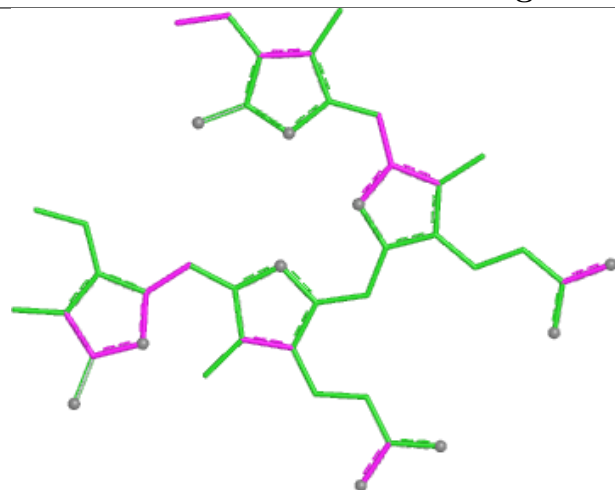
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	385	CYC	6	0
3	L	387	CYC	4	0
3	A	384	CYC	3	0
3	M	388	CYC	5	0
3	N	389	CYC	1	0
3	K	386	CYC	4	0

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

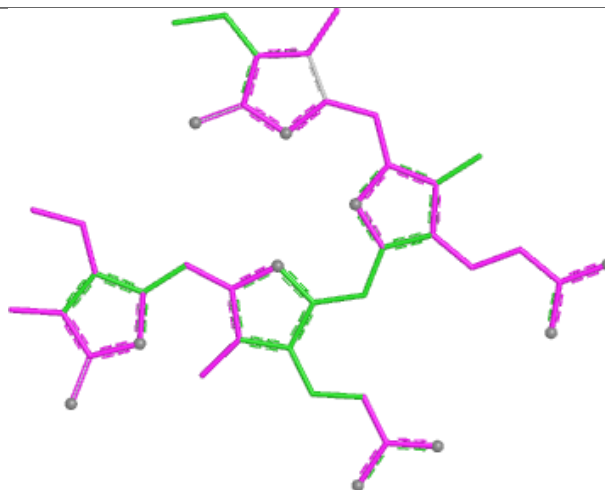
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



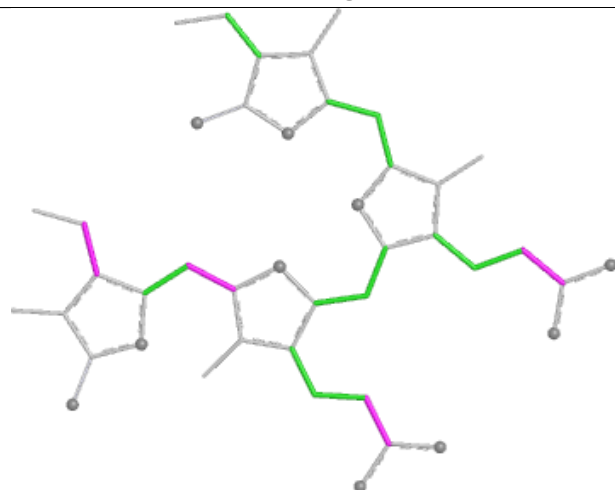
Ligand PEB N 357



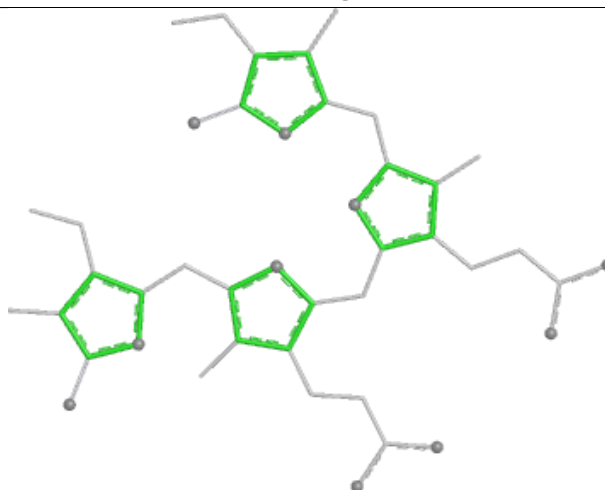
Bond lengths



Bond angles

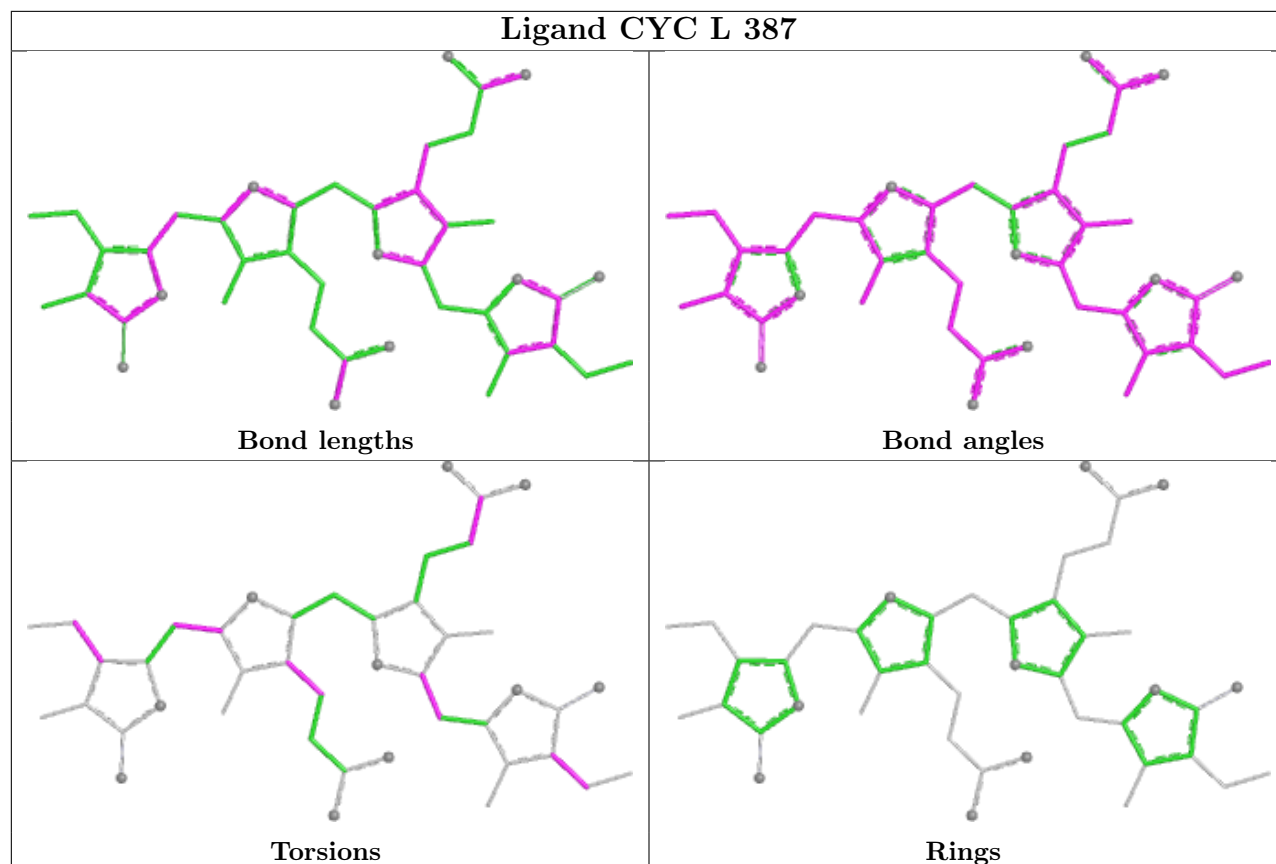


Torsions

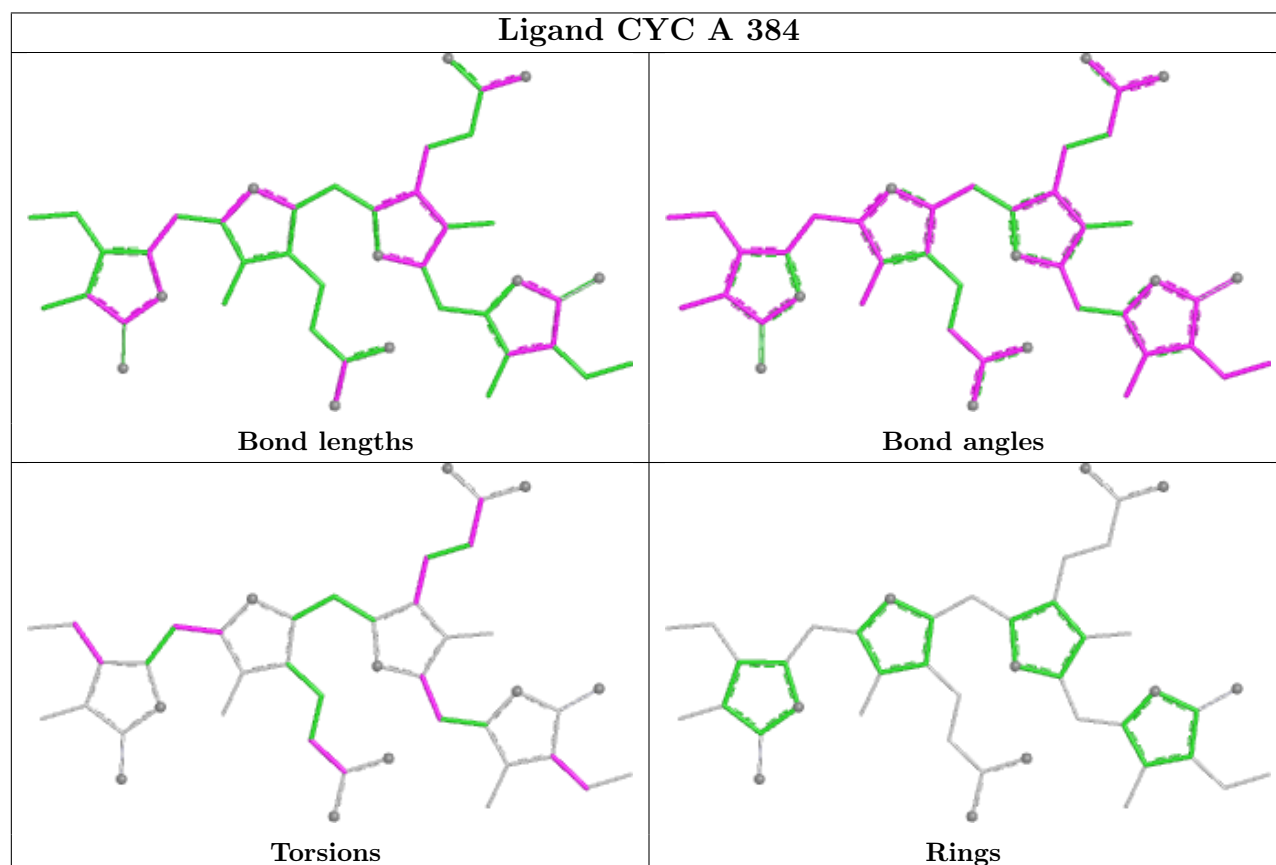


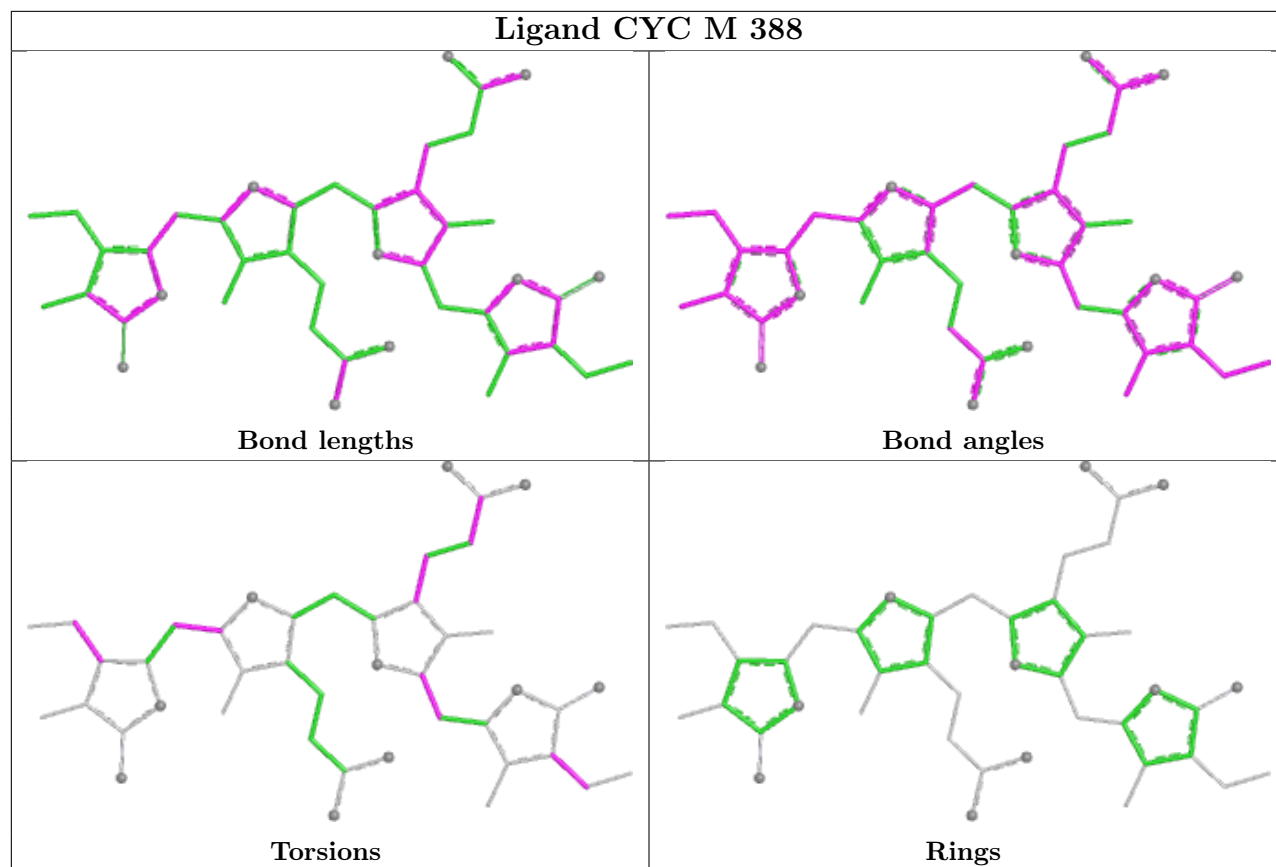
Rings

Ligand CYC L 387

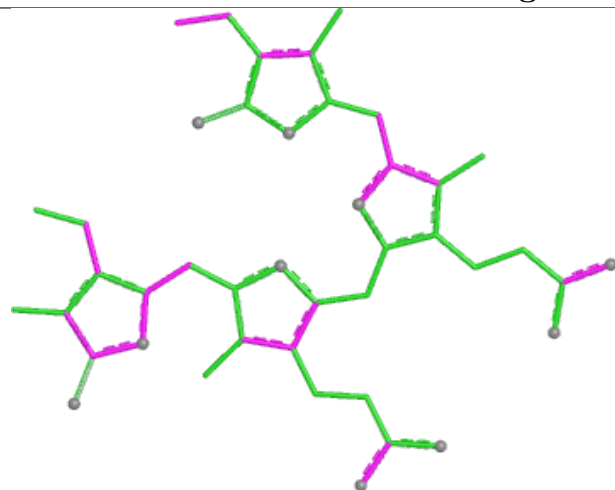


Ligand CYC A 384

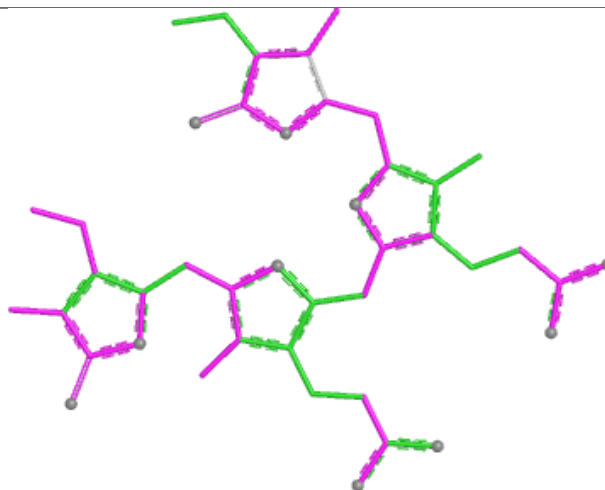




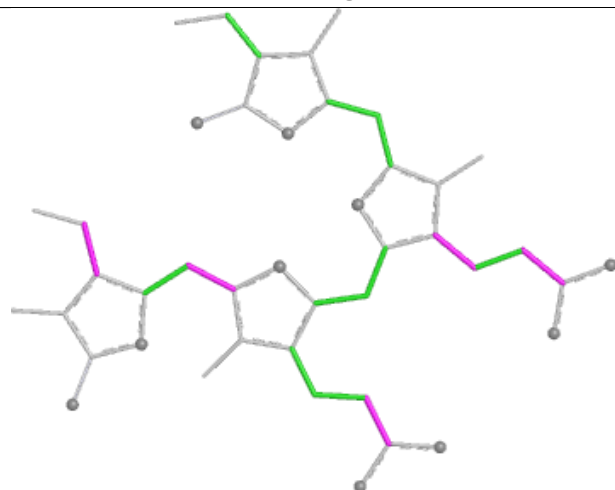
Ligand PEB L 356



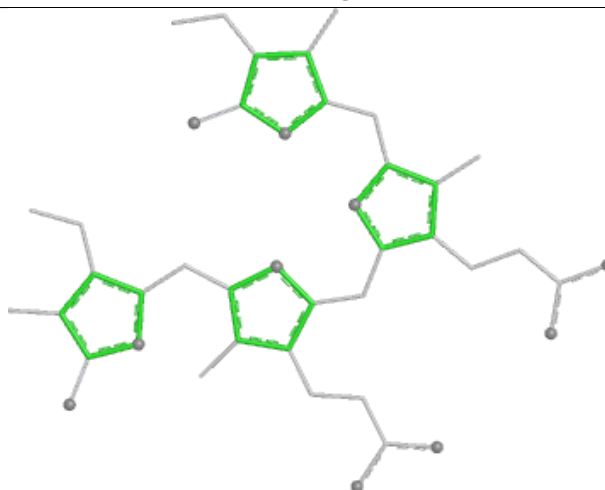
Bond lengths



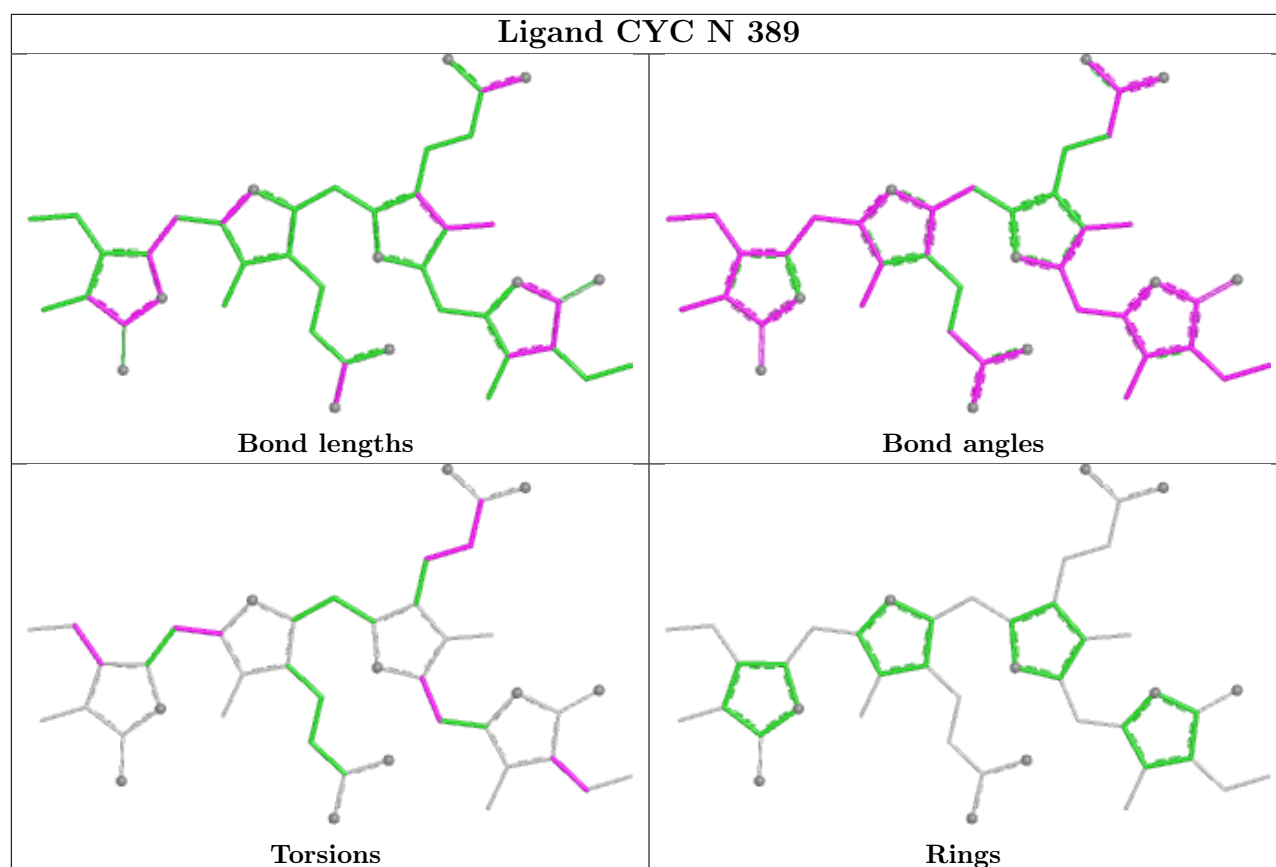
Bond angles



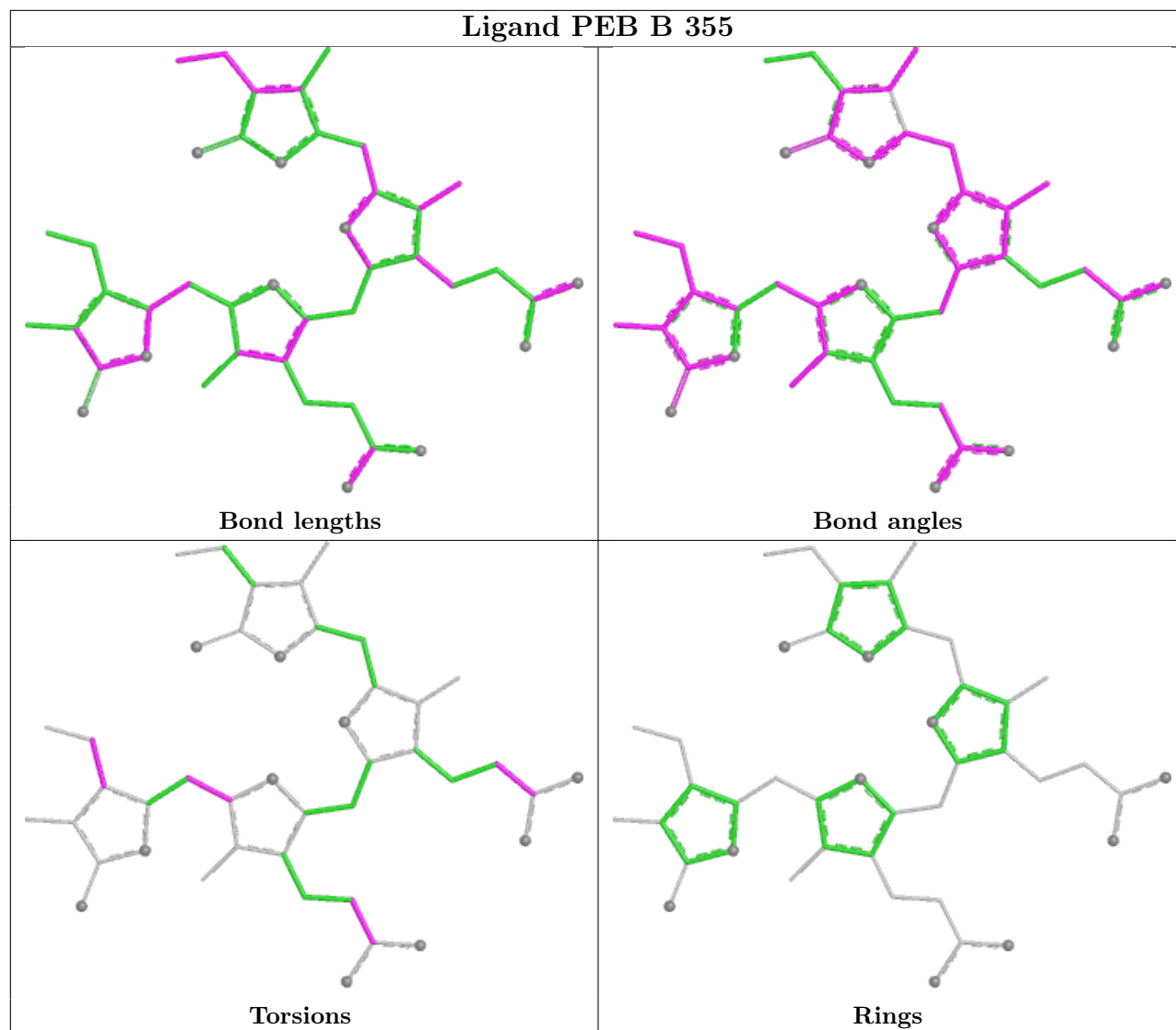
Torsions

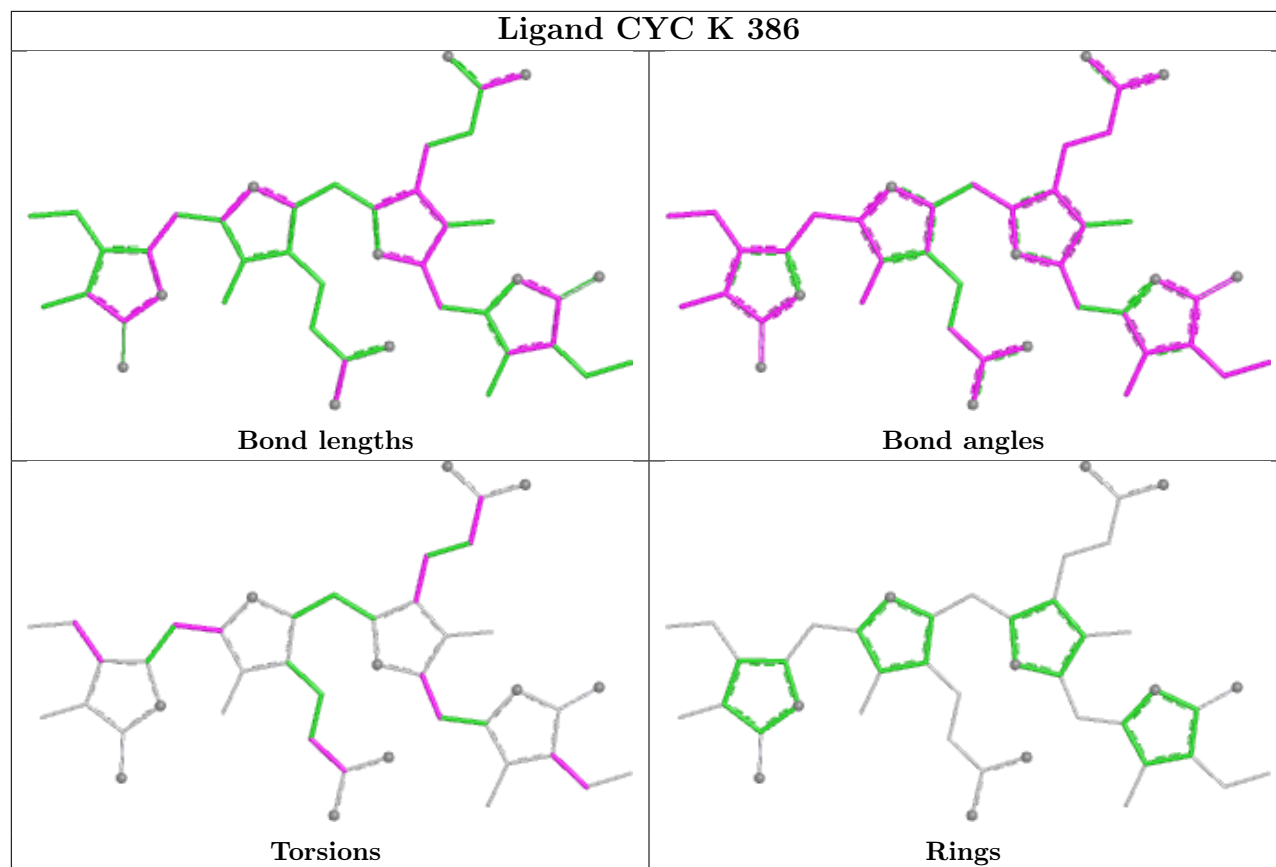


Rings



Ligand PEB B 355





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.