



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:24 PM UTC

PDB ID : 1B33 / pdb_00001b33
Title : STRUCTURE OF LIGHT HARVESTING COMPLEX OF ALLOPHY-
COCYANIN ALPHA AND BETA CHAINS/CORE-LINKER COMPLEX
AP*LC7.8
Authors : Reuter, W.; Wiegand, G.; Huber, R.; Than, M.E.
Deposited on : 1998-12-15
Resolution : 2.30 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

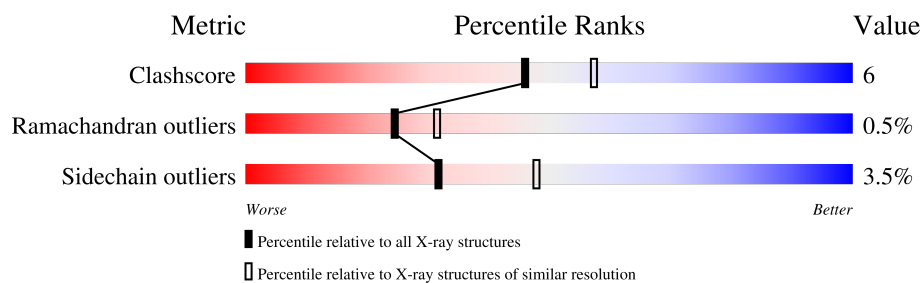
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	160	
1	C	160	
1	E	160	
1	H	160	
1	J	160	
1	L	160	
2	B	161	
2	D	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	161	 89% 9%
2	I	161	 89% 10%
2	K	161	 79% 20%
2	M	161	 85% 14%
3	N	67	 70% 22% 7%
3	O	67	 63% 30% 7%

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
4	CYC	A	201	X	-	-	-
4	CYC	B	202	X	-	-	-
4	CYC	C	203	X	-	-	-
4	CYC	D	204	X	-	-	-
4	CYC	E	205	X	-	-	-
4	CYC	F	206	X	-	-	-
4	CYC	H	207	X	-	-	-
4	CYC	I	208	X	-	-	-
4	CYC	J	209	X	-	-	-
4	CYC	K	210	X	-	-	-
4	CYC	L	211	X	-	-	-
4	CYC	M	212	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17502 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 ALLOPHYCOCYANIN, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	22	0	0
			1203	754	206	239	4			
1	C	160	Total	C	N	O	S	19	0	0
			1203	754	206	239	4			
1	E	160	Total	C	N	O	S	12	0	0
			1203	754	206	239	4			
1	H	160	Total	C	N	O	S	13	0	0
			1203	754	206	239	4			
1	J	160	Total	C	N	O	S	18	0	0
			1203	754	206	239	4			
1	L	160	Total	C	N	O	S	11	0	0
			1203	754	206	239	4			

- Molecule 2 is a protein called ALLOPHYCOCYANIN, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	21	0	0
			1219	769	202	241	7			
2	D	161	Total	C	N	O	S	6	0	0
			1219	769	202	241	7			
2	F	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	I	161	Total	C	N	O	S	8	0	0
			1219	769	202	241	7			
2	K	161	Total	C	N	O	S	10	0	0
			1219	769	202	241	7			
2	M	161	Total	C	N	O	S	13	0	0
			1219	769	202	241	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	MEN	ASN	modified residue	UNP P00318

Continued on next page...

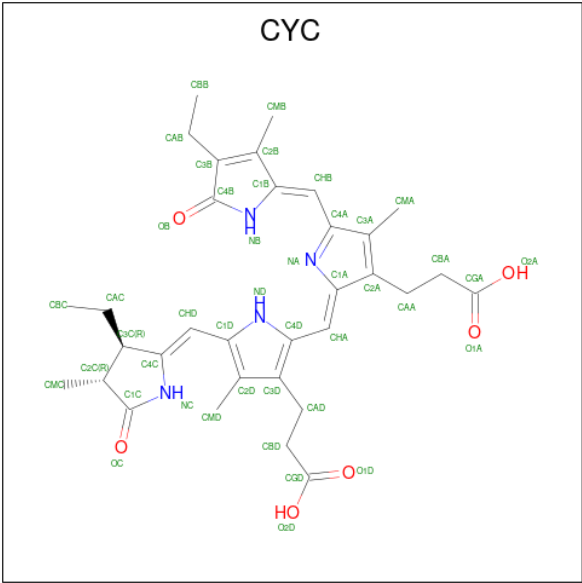
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	71	MEN	ASN	modified residue	UNP P00318
F	71	MEN	ASN	modified residue	UNP P00318
I	71	MEN	ASN	modified residue	UNP P00318
K	71	MEN	ASN	modified residue	UNP P00318
M	71	MEN	ASN	modified residue	UNP P00318

- Molecule 3 is a protein called PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	67	Total	C	N	O	S	13	0	0
			545	345	102	96	2			
3	O	67	Total	C	N	O	S	28	0	0
			545	345	102	96	2			

- Molecule 4 is PHYCOCYANOBILIN (CCD ID: CYC) (formula: C₃₃H₄₀N₄O₆).



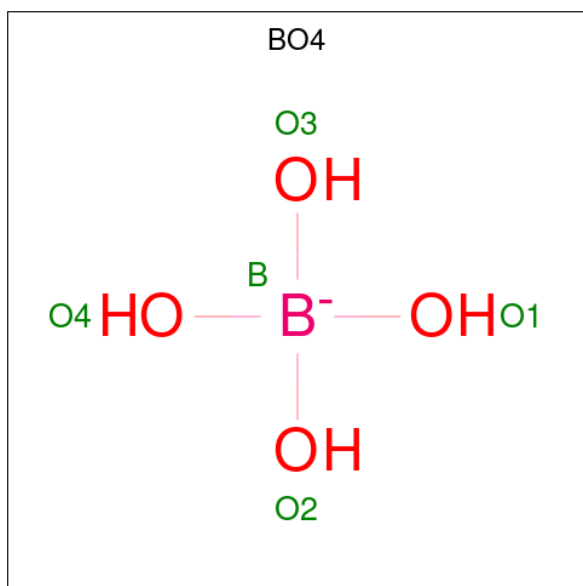
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			43	33	4	6		
4	B	1	Total	C	N	O	0	0
			43	33	4	6		
4	C	1	Total	C	N	O	0	0
			43	33	4	6		
4	D	1	Total	C	N	O	0	0
			43	33	4	6		
4	E	1	Total	C	N	O	0	0
			43	33	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total	C	N	O	0	0
			43	33	4	6		
4	H	1	Total	C	N	O	0	0
			43	33	4	6		
4	I	1	Total	C	N	O	0	0
			43	33	4	6		
4	J	1	Total	C	N	O	0	0
			43	33	4	6		
4	K	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	M	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is BORATE ION (CCD ID: BO4) (formula: BH_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	B	O	0	0
			5	1	4		
5	E	1	Total	B	O	0	0
			5	1	4		
5	J	1	Total	B	O	0	0
			5	1	4		
5	L	1	Total	B	O	0	0
			5	1	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	62	Total 62	O 62	0	0
6	B	81	Total 81	O 81	0	0
6	C	82	Total 82	O 82	0	0
6	D	145	Total 145	O 145	0	0
6	E	101	Total 101	O 101	0	0
6	F	127	Total 127	O 127	0	0
6	N	31	Total 31	O 31	0	0
6	H	99	Total 99	O 99	0	0
6	I	113	Total 113	O 113	0	0
6	J	109	Total 109	O 109	0	0
6	K	117	Total 117	O 117	0	0
6	L	126	Total 126	O 126	0	0
6	M	136	Total 136	O 136	0	0
6	O	15	Total 15	O 15	0	0

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.

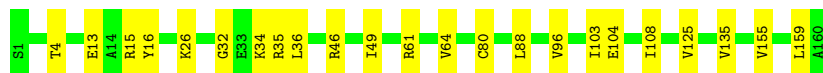
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain A: 



- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain C: 



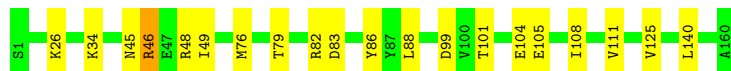
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain E: 



- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain H: 



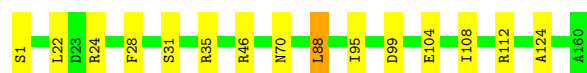
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain J: 



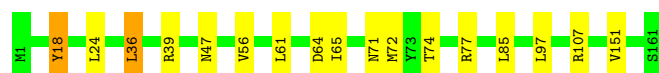
- Molecule 1: ALLOPHYCOCYANIN, ALPHA CHAIN

Chain L:  91% 9%



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain B:  89% 9%



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain D:  86% 13%



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain F:  89% 9%



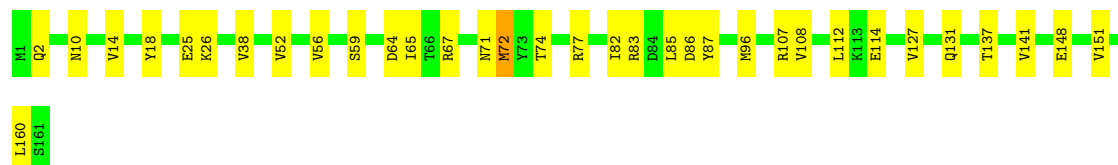
• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain I:  89% 10%



• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

Chain K:  79% 20%

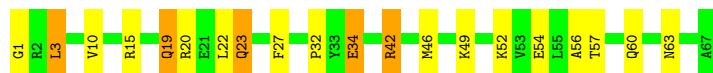


• Molecule 2: ALLOPHYCOCYANIN, BETA CHAIN

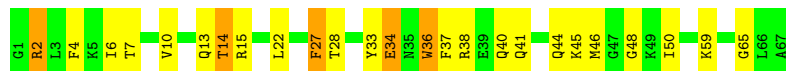
Chain M:  85% 14%



● Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain N:  70% 22% 7%

● Molecule 3: PHYCOBILISOME 7.8 KD LINKER POLYPEPTIDE

Chain O:  63% 30% 7%

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.12Å 151.90Å 137.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30	Depositor
% Data completeness (in resolution range)	96.5 (25.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.211 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17502	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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: BO4, MEN, 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	0.47	0/1218	0.94	1/1647 (0.1%)
1	C	0.51	0/1218	0.93	3/1647 (0.2%)
1	E	0.51	0/1218	0.95	1/1647 (0.1%)
1	H	0.54	0/1218	0.96	1/1647 (0.1%)
1	J	0.50	0/1218	0.93	0/1647
1	L	0.53	0/1218	0.95	1/1647 (0.1%)
2	B	0.52	0/1226	0.96	1/1659 (0.1%)
2	D	0.56	0/1226	0.98	5/1659 (0.3%)
2	F	0.52	0/1226	0.96	3/1659 (0.2%)
2	I	0.56	0/1226	1.00	7/1659 (0.4%)
2	K	0.54	0/1226	0.99	4/1659 (0.2%)
2	M	0.58	1/1226 (0.1%)	0.99	7/1659 (0.4%)
3	N	0.63	0/553	0.95	1/740 (0.1%)
3	O	0.65	0/553	1.08	4/740 (0.5%)
All	All	0.54	1/15770 (0.0%)	0.96	39/21316 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	74	THR	CA-CB	5.09	1.62	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	14	THR	N-CA-C	-8.34	102.66	113.17
2	I	18	TYR	N-CA-C	-7.74	100.32	110.53
2	D	18	TYR	N-CA-C	-7.42	100.53	110.55
2	M	18	TYR	N-CA-C	-6.73	102.13	110.41
2	F	18	TYR	N-CA-C	-6.50	101.34	110.50
2	F	3	ASP	N-CA-C	-6.38	100.76	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	59	LYS	N-CA-C	6.37	119.46	109.96
2	K	107	ARG	N-CA-C	6.16	120.82	112.88
2	M	112	LEU	N-CA-C	-6.14	104.58	111.28
2	I	142	GLY	CA-C-N	6.14	127.52	119.84
2	I	142	GLY	C-N-CA	6.14	127.52	119.84
1	C	46	ARG	N-CA-C	6.09	117.92	111.28
2	D	142	GLY	CA-C-N	5.96	125.44	119.24
2	D	142	GLY	C-N-CA	5.96	125.44	119.24
2	K	18	TYR	N-CA-C	-5.95	102.67	110.53
2	B	18	TYR	N-CA-C	-5.88	102.21	110.50
3	O	27	PHE	N-CA-C	5.87	118.11	109.24
2	M	109	LEU	N-CA-C	5.83	120.01	113.01
2	D	59	SER	N-CA-C	5.78	121.76	114.31
1	E	16	TYR	N-CA-C	-5.64	103.25	110.53
2	M	59	SER	N-CA-C	5.58	121.88	114.12
1	L	88	LEU	N-CA-C	-5.56	105.14	111.14
2	K	59	SER	N-CA-C	5.55	121.08	113.97
2	F	59	SER	N-CA-C	5.48	120.99	113.97
2	M	48	ALA	N-CA-C	5.47	117.67	111.11
1	H	125	VAL	N-CA-C	-5.44	105.22	110.72
1	C	16	TYR	N-CA-C	-5.41	103.25	110.55
3	N	27	PHE	N-CA-C	5.37	117.34	109.24
2	M	3	ASP	N-CA-C	-5.37	102.25	110.14
2	I	59	SER	N-CA-C	5.24	120.67	113.97
1	C	32	GLY	N-CA-C	5.21	118.94	112.64
2	M	153	PHE	N-CA-C	-5.19	105.53	111.14
2	I	106	GLU	N-CA-C	5.16	116.71	111.14
2	I	10	ASN	N-CA-C	5.15	116.90	111.28
2	I	153	PHE	N-CA-C	-5.13	105.58	111.07
3	O	36	TRP	N-CA-C	5.08	116.51	111.07
2	D	48	ALA	N-CA-C	5.08	117.21	111.11
2	K	114	GLU	N-CA-C	-5.07	105.45	110.97
1	A	105	GLU	N-CA-C	5.06	116.87	111.36

There are no chirality outliers.

There are no planarity outliers.

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	1203	0	1213	11	0
1	C	1203	0	1213	11	0
1	E	1203	0	1213	19	0
1	H	1203	0	1213	12	0
1	J	1203	0	1213	12	0
1	L	1203	0	1213	9	0
2	B	1219	0	1229	11	0
2	D	1219	0	1229	9	0
2	F	1219	0	1229	11	0
2	I	1219	0	1229	8	0
2	K	1219	0	1229	16	0
2	M	1219	0	1229	12	0
3	N	545	0	572	18	0
3	O	545	0	572	16	0
4	A	43	0	35	3	0
4	B	43	0	35	2	0
4	C	43	0	35	2	0
4	D	43	0	35	2	0
4	E	43	0	35	5	0
4	F	43	0	35	3	0
4	H	43	0	35	4	0
4	I	43	0	35	2	0
4	J	43	0	35	5	0
4	K	43	0	35	2	0
4	L	43	0	35	5	0
4	M	43	0	35	2	0
5	C	5	0	4	0	0
5	E	5	0	4	0	0
5	J	5	0	4	0	0
5	L	5	0	4	0	0
6	A	62	0	0	1	0
6	B	81	0	0	2	0
6	C	82	0	0	2	0
6	D	145	0	0	0	0
6	E	101	0	0	3	0
6	F	127	0	0	1	0
6	H	99	0	0	3	0
6	I	113	0	0	4	0
6	J	109	0	0	1	0
6	K	117	0	0	2	0
6	L	126	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	136	0	0	0	0
6	N	31	0	0	1	0
6	O	15	0	0	3	0
All	All	17502	0	16232	184	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 (184) 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)
4:E:205:CYC:HC	4:E:205:CYC:HMD1	1.35	0.92
2:F:110:ASN:HD21	3:N:56:ALA:HB1	1.33	0.91
1:J:48:ARG:HH21	1:J:139:ILE:HD11	1.38	0.88
4:H:207:CYC:HMA1	4:H:207:CYC:HB	1.42	0.85
1:J:70:ASN:HD22	4:J:209:CYC:HC	1.28	0.81
4:J:209:CYC:HC	4:J:209:CYC:HMD1	1.47	0.80
1:E:140:LEU:HD22	1:E:144:ASP:HB3	1.65	0.78
2:F:119:LEU:HD11	4:F:206:CYC:HAA2	1.69	0.74
4:E:205:CYC:HMA3	4:E:205:CYC:HB	1.52	0.73
1:H:76:MET:HE2	1:H:76:MET:HA	1.71	0.72
2:F:110:ASN:ND2	3:N:56:ALA:HB1	2.04	0.72
4:C:203:CYC:HMA1	4:C:203:CYC:HB	1.54	0.72
2:K:65:ILE:HG22	2:K:72:MET:HB2	1.74	0.70
4:J:209:CYC:HMA1	4:J:209:CYC:HB	1.56	0.69
2:B:65:ILE:HG22	2:B:72:MET:HB2	1.75	0.67
4:E:205:CYC:HMD1	4:E:205:CYC:NC	2.09	0.67
3:O:7:THR:HA	3:O:27:PHE:O	1.95	0.66
4:D:204:CYC:HB	4:D:204:CYC:HMA3	1.60	0.65
3:N:3:LEU:HD12	3:N:32:PRO:HA	1.79	0.64
1:A:14:ALA:HB2	3:N:19:GLN:HE21	1.63	0.64
6:C:2028:HOH:O	2:D:2:GLN:HA	1.98	0.64
1:C:104:GLU:HA	1:C:108:ILE:HB	1.79	0.64
4:J:209:CYC:HMD1	4:J:209:CYC:NC	2.11	0.63
3:N:34:GLU:H	3:N:34:GLU:CD	2.06	0.63
2:M:131:GLN:HE22	2:M:134:LYS:NZ	1.97	0.63
2:D:65:ILE:HG22	2:D:72:MET:HB2	1.81	0.62
1:J:101:THR:O	1:J:105:GLU:HG2	1.99	0.62
2:F:35:GLU:HG2	6:F:215:HOH:O	1.99	0.62
2:F:65:ILE:HG22	2:F:72:MET:HB2	1.83	0.61
2:I:65:ILE:HG22	2:I:72:MET:HB2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:H	1:A:75:GLU:CD	2.09	0.60
2:K:137:THR:O	2:K:141:VAL:HG22	2.02	0.60
3:O:34:GLU:H	3:O:34:GLU:CD	2.10	0.58
1:H:104:GLU:HA	1:H:108:ILE:HB	1.86	0.58
4:K:210:CYC:HC	4:K:210:CYC:CMD	2.17	0.58
1:E:104:GLU:HA	1:E:108:ILE:HB	1.85	0.58
3:N:3:LEU:HB2	3:N:57:THR:HG23	1.87	0.57
4:L:211:CYC:HMA3	4:L:211:CYC:HB	1.69	0.57
2:F:119:LEU:CD1	4:F:206:CYC:HAA2	2.34	0.57
1:C:35:ARG:HD3	6:C:2065:HOH:O	2.05	0.57
1:J:48:ARG:NH2	1:J:139:ILE:HD11	2.16	0.57
2:I:76:ARG:HD2	6:I:308:HOH:O	2.05	0.57
2:K:71:MEN:O	2:K:77:ARG:HD2	2.05	0.56
1:E:112:ARG:HD2	6:E:2071:HOH:O	2.05	0.56
1:E:61:ARG:O	1:E:64:VAL:HG22	2.06	0.56
6:J:2013:HOH:O	2:K:2:GLN:HA	2.06	0.56
1:C:4:THR:HG23	2:D:1:MET:HE2	1.88	0.56
3:O:40:GLN:O	3:O:44:GLN:HG3	2.07	0.55
3:N:52:LYS:HE3	3:N:54:GLU:HG2	1.89	0.55
1:E:45:ASN:OD1	1:E:139:ILE:HG12	2.07	0.54
2:D:10:ASN:O	2:D:14:VAL:HG23	2.07	0.54
1:L:24:ARG:NH1	6:L:2106:HOH:O	2.41	0.53
2:B:47:ASN:ND2	2:I:42:THR:HG21	2.24	0.53
1:J:70:ASN:ND2	4:J:209:CYC:HC	2.00	0.53
4:A:201:CYC:HB	4:A:201:CYC:HMA3	1.73	0.53
1:A:126:ALA:HB2	1:A:159:LEU:O	2.09	0.53
2:B:39:ARG:NH2	6:B:245:HOH:O	2.42	0.52
3:O:6:ILE:HG21	3:O:36:TRP:CH2	2.43	0.52
1:H:45:ASN:O	1:H:49:ILE:HG13	2.09	0.52
2:I:39:ARG:HB2	6:I:293:HOH:O	2.09	0.52
1:L:35:ARG:HD2	1:L:95:ILE:O	2.07	0.52
2:F:10:ASN:OD1	3:N:63:ASN:HB2	2.09	0.52
3:O:45:LYS:NZ	6:O:82:HOH:O	2.43	0.52
4:B:202:CYC:C4B	3:N:22:LEU:HB2	2.39	0.51
2:M:2:GLN:HG2	3:O:65:GLY:HA3	1.93	0.51
1:E:76:MET:HG2	6:E:2026:HOH:O	2.10	0.51
4:H:207:CYC:HAA1	2:M:61:LEU:HD22	1.93	0.51
2:M:2:GLN:HG3	6:O:71:HOH:O	2.11	0.51
1:E:49:ILE:HA	1:E:135:VAL:HG11	1.93	0.51
3:N:10:VAL:HG11	3:N:46:MET:HE3	1.93	0.50
2:K:83:ARG:O	2:K:87:TYR:HD1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:ARG:NH1	1:J:52:GLN:OE1	2.44	0.50
2:B:71:MEN:O	2:B:77:ARG:HD3	2.11	0.50
1:E:75:GLU:CD	1:E:75:GLU:H	2.20	0.50
1:C:26:LYS:HD2	2:D:35:GLU:HG2	1.94	0.49
1:L:112:ARG:HD2	6:L:2102:HOH:O	2.11	0.49
2:M:11:SER:O	2:M:14:VAL:HG12	2.12	0.49
1:A:46:ARG:HD3	2:B:18:TYR:CE1	2.46	0.49
3:O:10:VAL:HG11	3:O:46:MET:HE2	1.95	0.49
3:N:1:GLY:O	3:N:57:THR:HG21	2.13	0.48
1:L:70:ASN:HB3	4:L:211:CYC:OC	2.13	0.48
1:C:61:ARG:O	1:C:64:VAL:HG22	2.13	0.48
1:A:104:GLU:HA	1:A:108:ILE:HB	1.94	0.48
1:L:104:GLU:HA	1:L:108:ILE:HB	1.94	0.48
2:K:127:VAL:O	2:K:131:GLN:HG2	2.13	0.48
2:I:71:MEN:O	2:I:77:ARG:HD3	2.13	0.48
3:N:23:GLN:H	3:N:23:GLN:HG3	1.44	0.48
3:O:6:ILE:O	3:O:28:THR:HA	2.14	0.48
2:K:96:MET:HG2	2:K:148:GLU:HG3	1.95	0.48
3:N:15:ARG:NH1	6:N:1340:HOH:O	2.46	0.48
1:H:26:LYS:HE3	1:H:26:LYS:HB2	1.74	0.47
1:E:70:ASN:HD22	4:E:205:CYC:HC	1.61	0.47
4:A:201:CYC:CMD	4:A:201:CYC:HC	2.27	0.47
2:B:107:ARG:HH11	2:B:107:ARG:HG3	1.77	0.47
2:D:83:ARG:O	2:D:87:TYR:HD1	1.96	0.47
1:H:46:ARG:HD2	6:H:289:HOH:O	2.14	0.47
2:I:124:SER:HB3	6:I:266:HOH:O	2.15	0.47
2:M:131:GLN:HE22	2:M:134:LYS:HZ3	1.62	0.47
1:A:11:ASP:OD2	2:B:107:ARG:NH1	2.48	0.47
1:L:31:SER:OG	1:L:35:ARG:NH1	2.48	0.46
1:H:99:ASP:HB2	6:H:250:HOH:O	2.14	0.46
2:M:64:ASP:OD1	2:M:67:ARG:NH1	2.48	0.46
2:B:77:ARG:NH1	6:B:215:HOH:O	2.45	0.46
1:C:13:GLU:HB2	1:C:15:ARG:HG2	1.97	0.46
1:C:36:LEU:HD23	1:C:96:VAL:HG22	1.98	0.46
2:K:67:ARG:NH2	6:K:302:HOH:O	2.48	0.46
1:C:125:VAL:HG12	1:C:159:LEU:HD13	1.97	0.46
2:B:107:ARG:HG3	2:B:107:ARG:NH1	2.32	0.45
2:I:2:GLN:HA	6:I:236:HOH:O	2.14	0.45
2:B:56:VAL:HG12	2:B:61:LEU:HG	1.98	0.45
2:K:108:VAL:O	2:K:112:LEU:HB2	2.16	0.45
1:A:46:ARG:CG	1:A:47:GLU:N	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:GLY:HA2	1:E:113:GLU:OE1	2.17	0.45
1:E:131:ALA:O	1:E:135:VAL:HG23	2.17	0.45
1:J:4:THR:O	1:J:8:VAL:HG13	2.17	0.45
2:K:64:ASP:OD1	2:K:67:ARG:NH1	2.49	0.45
4:B:202:CYC:HC	4:B:202:CYC:CMD	2.30	0.45
2:D:75:THR:HG21	1:E:111:VAL:HG23	1.99	0.45
4:H:207:CYC:HMC1	4:H:207:CYC:HBC2	1.98	0.45
3:O:4:PHE:HE2	3:O:33:TYR:CD2	2.35	0.44
1:H:76:MET:HE1	2:M:62:TYR:OH	2.17	0.44
4:H:207:CYC:HMA1	4:H:207:CYC:NB	2.21	0.44
2:K:52:VAL:O	2:K:56:VAL:HG23	2.17	0.44
3:N:52:LYS:HE3	3:N:54:GLU:CG	2.46	0.44
1:J:103:ILE:HG21	1:J:155:VAL:HG22	1.99	0.44
3:O:2:ARG:HD3	6:O:72:HOH:O	2.17	0.44
2:K:83:ARG:O	2:K:86:ASP:HB2	2.17	0.44
4:E:205:CYC:HB	4:E:205:CYC:CMA	2.26	0.44
3:N:49:LYS:HE3	3:N:49:LYS:HB3	1.77	0.44
1:C:49:ILE:HA	1:C:135:VAL:HG11	1.99	0.44
2:D:77:ARG:HH22	3:N:63:ASN:HD21	1.65	0.44
1:H:79:THR:O	1:H:82:ARG:HB3	2.18	0.44
4:I:208:CYC:HC	4:I:208:CYC:CMD	2.31	0.44
1:A:35:ARG:NH1	6:A:255:HOH:O	2.42	0.44
4:F:206:CYC:CMD	4:F:206:CYC:HC	2.31	0.44
4:I:208:CYC:C4B	3:O:22:LEU:HB2	2.48	0.44
2:M:84:ASP:O	2:M:87:TYR:HB2	2.18	0.43
2:M:71:MEN:HB2	4:M:212:CYC:OC	2.19	0.43
2:I:85:LEU:HD12	2:I:85:LEU:HA	1.87	0.43
1:H:101:THR:O	1:H:105:GLU:HG3	2.19	0.42
4:D:204:CYC:HC	4:D:204:CYC:CMD	2.32	0.42
3:O:13:GLN:CG	3:O:14:THR:H	2.32	0.42
2:B:36:LEU:HD12	2:B:36:LEU:HA	1.83	0.42
1:J:61:ARG:O	1:J:64:VAL:HG22	2.19	0.42
4:K:210:CYC:HC	4:K:210:CYC:HMD2	1.85	0.42
1:C:80:CYS:HA	4:C:203:CYC:CHD	2.49	0.42
1:A:103:ILE:HG21	1:A:155:VAL:HG22	2.02	0.42
2:D:137:THR:O	2:D:141:VAL:HG22	2.20	0.42
2:F:71:MEN:O	2:F:77:ARG:HD3	2.20	0.42
1:C:103:ILE:HG21	1:C:155:VAL:HG22	2.01	0.42
3:N:42:ARG:NH2	3:N:46:MET:HE1	2.34	0.42
1:H:111:VAL:HG23	2:M:75:THR:HG21	2.01	0.42
1:J:75:GLU:H	1:J:75:GLU:CD	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:26:LYS:HD2	6:K:282:HOH:O	2.19	0.42
1:E:23:ASP:OD1	1:E:26:LYS:NZ	2.53	0.41
1:E:51:LYS:NZ	1:E:55:ASP:OD2	2.53	0.41
1:J:34:LYS:O	1:J:38:ILE:HG13	2.20	0.41
3:O:10:VAL:HG22	3:O:48:GLY:HA3	2.01	0.41
3:O:37:PHE:O	3:O:41:GLN:HG3	2.20	0.41
2:M:71:MEN:O	2:M:77:ARG:HD3	2.20	0.41
4:A:201:CYC:HC	4:A:201:CYC:HMD2	1.86	0.41
1:E:46:ARG:HD3	2:F:18:TYR:CE1	2.56	0.41
1:A:46:ARG:HG2	1:A:47:GLU:N	2.36	0.41
1:E:76:MET:HA	1:E:76:MET:HE2	2.01	0.41
3:N:20:ARG:HH12	3:N:22:LEU:HD23	1.85	0.41
3:O:40:GLN:HG3	3:O:50:ILE:CD1	2.50	0.41
4:L:211:CYC:CMD	4:L:211:CYC:HC	2.33	0.41
4:L:211:CYC:HB	4:L:211:CYC:CMA	2.33	0.41
1:A:143:GLU:HG3	1:A:144:ASP:N	2.36	0.41
2:F:88:TYR:HB2	2:F:133:MET:HE1	2.03	0.41
1:J:22:LEU:HD22	2:K:38:VAL:HG13	2.03	0.41
2:K:10:ASN:O	2:K:14:VAL:HG13	2.21	0.41
1:L:1:SER:HA	1:L:99:ASP:OD2	2.20	0.41
1:L:28:PHE:CE1	1:L:35:ARG:NH2	2.89	0.41
2:F:52:VAL:O	2:F:56:VAL:HG23	2.21	0.41
1:L:124:ALA:HB3	4:L:211:CYC:HMC3	2.03	0.41
1:E:75:GLU:CD	1:E:75:GLU:N	2.79	0.40
4:M:212:CYC:HBC2	4:M:212:CYC:HMC1	2.04	0.40
1:E:2:ILE:N	6:E:2080:HOH:O	2.49	0.40
1:E:41:ILE:HG13	1:E:42:LEU:N	2.36	0.40
1:H:34:LYS:NZ	6:H:267:HOH:O	2.55	0.40
3:O:13:GLN:CD	3:O:15:ARG:HG2	2.46	0.40
1:H:83:ASP:O	1:H:86:TYR:HB2	2.22	0.40
2:K:56:VAL:HG21	2:K:82:ILE:HG22	2.04	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	158/160 (99%)	153 (97%)	5 (3%)	0	100	100
1	C	158/160 (99%)	156 (99%)	2 (1%)	0	100	100
1	E	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
1	H	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
1	J	158/160 (99%)	154 (98%)	4 (2%)	0	100	100
1	L	158/160 (99%)	157 (99%)	1 (1%)	0	100	100
2	B	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	21	27
2	D	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	9	10
2	F	158/161 (98%)	152 (96%)	4 (2%)	2 (1%)	9	10
2	I	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	9	10
2	K	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	21	27
2	M	158/161 (98%)	154 (98%)	2 (1%)	2 (1%)	9	10
3	N	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
3	O	65/67 (97%)	60 (92%)	5 (8%)	0	100	100
All	All	2026/2060 (98%)	1975 (98%)	41 (2%)	10 (0%)	24	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	110	ASN
2	D	110	ASN
2	F	110	ASN
2	I	110	ASN
2	F	74	THR
2	K	74	THR
2	B	74	THR
2	I	74	THR
2	M	74	THR
2	D	74	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	125/125 (100%)	121 (97%)	4 (3%)	34	51
1	C	125/125 (100%)	123 (98%)	2 (2%)	55	73
1	E	125/125 (100%)	118 (94%)	7 (6%)	19	28
1	H	125/125 (100%)	121 (97%)	4 (3%)	34	51
1	J	125/125 (100%)	118 (94%)	7 (6%)	19	28
1	L	125/125 (100%)	122 (98%)	3 (2%)	43	62
2	B	126/126 (100%)	120 (95%)	6 (5%)	23	35
2	D	126/126 (100%)	122 (97%)	4 (3%)	34	51
2	F	126/126 (100%)	123 (98%)	3 (2%)	43	62
2	I	126/126 (100%)	124 (98%)	2 (2%)	55	73
2	K	126/126 (100%)	121 (96%)	5 (4%)	28	42
2	M	126/126 (100%)	125 (99%)	1 (1%)	73	86
3	N	58/58 (100%)	52 (90%)	6 (10%)	7	8
3	O	58/58 (100%)	55 (95%)	3 (5%)	21	31
All	All	1622/1622 (100%)	1565 (96%)	57 (4%)	32	48

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	75	GLU
1	A	88	LEU
1	A	90	LEU
2	B	24	LEU
2	B	36	LEU
2	B	64	ASP
2	B	85	LEU
2	B	97	LEU
2	B	151	VAL
1	C	34	LYS
1	C	88	LEU
2	D	35	GLU
2	D	68	PRO
2	D	85	LEU
2	D	135	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	24	ARG
1	E	41	ILE
1	E	46	ARG
1	E	51	LYS
1	E	86	TYR
1	E	88	LEU
1	E	90	LEU
2	F	35	GLU
2	F	85	LEU
2	F	97	LEU
3	N	3	LEU
3	N	19	GLN
3	N	23	GLN
3	N	34	GLU
3	N	42	ARG
3	N	60	GLN
1	H	46	ARG
1	H	48	ARG
1	H	88	LEU
1	H	140	LEU
2	I	72	MET
2	I	85	LEU
1	J	33	GLU
1	J	40	GLN
1	J	46	ARG
1	J	76	MET
1	J	88	LEU
1	J	90	LEU
1	J	96	VAL
2	K	25	GLU
2	K	72	MET
2	K	85	LEU
2	K	151	VAL
2	K	160	LEU
1	L	22	LEU
1	L	46	ARG
1	L	88	LEU
2	M	36	LEU
3	O	2	ARG
3	O	34	GLU
3	O	38	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
2	B	10	ASN
2	B	47	ASN
2	B	117	ASN
1	C	40	GLN
2	D	10	ASN
2	D	117	ASN
2	D	131	GLN
1	E	56	GLN
1	E	70	ASN
2	F	110	ASN
2	F	117	ASN
2	F	131	GLN
3	N	19	GLN
3	N	35	ASN
3	N	44	GLN
3	N	63	ASN
1	H	9	ASN
1	H	59	GLN
2	I	2	GLN
2	I	10	ASN
2	I	117	ASN
2	I	128	GLN
2	I	131	GLN
1	J	9	ASN
1	J	45	ASN
1	J	56	GLN
1	J	70	ASN
1	J	134	ASN
2	K	2	GLN
2	K	10	ASN
2	K	47	ASN
2	K	117	ASN
2	K	128	GLN
1	L	40	GLN
1	L	45	ASN
1	L	56	GLN
2	M	117	ASN
2	M	128	GLN
2	M	131	GLN
3	O	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MEN	F	71	2	7,8,9	0.60	0	4,9,11	0.68	0
2	MEN	I	71	2	7,8,9	0.55	0	4,9,11	0.50	0
2	MEN	D	71	2	7,8,9	0.56	0	4,9,11	0.58	0
2	MEN	B	71	2	7,8,9	0.53	0	4,9,11	0.34	0
2	MEN	K	71	2	7,8,9	0.51	0	4,9,11	0.30	0
2	MEN	M	71	2	7,8,9	0.41	0	4,9,11	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	F	71	2	-	2/7/8/10	-
2	MEN	I	71	2	-	2/7/8/10	-
2	MEN	D	71	2	-	2/7/8/10	-
2	MEN	B	71	2	-	2/7/8/10	-
2	MEN	K	71	2	-	2/7/8/10	-
2	MEN	M	71	2	-	2/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	71	MEN	CA-CB-CG-OD1
2	D	71	MEN	CA-CB-CG-OD1
2	F	71	MEN	CA-CB-CG-OD1
2	K	71	MEN	CA-CB-CG-OD1
2	M	71	MEN	CA-CB-CG-OD1
2	B	71	MEN	CA-CB-CG-ND2
2	I	71	MEN	CA-CB-CG-ND2
2	K	71	MEN	CA-CB-CG-ND2
2	F	71	MEN	CA-CB-CG-ND2
2	M	71	MEN	CA-CB-CG-ND2
2	I	71	MEN	CA-CB-CG-OD1
2	D	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	71	MEN	1	0
2	I	71	MEN	1	0
2	B	71	MEN	1	0
2	K	71	MEN	1	0
2	M	71	MEN	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	CYC	H	207	1	46,46,46	2.18	7 (15%)	63,67,67	1.90	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CYC	E	205	1	46,46,46	1.98	7 (15%)	63,67,67	2.19	14 (22%)
4	CYC	F	206	2	46,46,46	2.14	7 (15%)	63,67,67	2.64	20 (31%)
4	CYC	I	208	2	46,46,46	2.42	6 (13%)	63,67,67	2.51	21 (33%)
4	CYC	C	203	1	46,46,46	2.38	7 (15%)	63,67,67	2.11	19 (30%)
5	BO4	E	2004	-	4,4,4	0.71	0	6,6,6	0.58	0
4	CYC	J	209	1	46,46,46	2.21	6 (13%)	63,67,67	2.13	17 (26%)
4	CYC	K	210	2	46,46,46	2.60	8 (17%)	63,67,67	2.22	20 (31%)
4	CYC	B	202	2	46,46,46	2.31	7 (15%)	63,67,67	2.31	16 (25%)
5	BO4	J	2002	-	4,4,4	0.76	0	6,6,6	0.61	0
4	CYC	M	212	2	46,46,46	2.51	8 (17%)	63,67,67	2.54	21 (33%)
5	BO4	L	2001	-	4,4,4	1.07	0	6,6,6	1.03	1 (16%)
5	BO4	C	2003	-	4,4,4	0.82	0	6,6,6	0.85	0
4	CYC	L	211	1	46,46,46	2.14	6 (13%)	63,67,67	2.40	20 (31%)
4	CYC	D	204	2	46,46,46	2.19	6 (13%)	63,67,67	2.29	24 (38%)
4	CYC	A	201	1	46,46,46	2.17	7 (15%)	63,67,67	2.30	16 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYC	H	207	1	2/2/14/19	9/26/74/74	0/4/4/4
4	CYC	E	205	1	2/2/14/19	9/26/74/74	0/4/4/4
4	CYC	F	206	2	2/2/14/19	12/26/74/74	0/4/4/4
4	CYC	I	208	2	1/1/14/19	11/26/74/74	0/4/4/4
4	CYC	C	203	1	2/2/14/19	8/26/74/74	0/4/4/4
4	CYC	J	209	1	1/1/14/19	9/26/74/74	0/4/4/4
4	CYC	K	210	2	1/1/14/19	11/26/74/74	0/4/4/4
4	CYC	B	202	2	2/2/14/19	10/26/74/74	0/4/4/4
4	CYC	M	212	2	2/2/14/19	11/26/74/74	0/4/4/4
4	CYC	L	211	1	2/2/14/19	9/26/74/74	0/4/4/4
4	CYC	D	204	2	1/1/14/19	7/26/74/74	0/4/4/4
4	CYC	A	201	1	2/2/14/19	10/26/74/74	0/4/4/4

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	210	CYC	C2C-C1C	-12.22	1.41	1.52
4	I	208	CYC	C2C-C1C	-12.05	1.41	1.52
4	M	212	CYC	C2C-C1C	-11.91	1.41	1.52
4	C	203	CYC	C2C-C1C	-10.95	1.42	1.52
4	B	202	CYC	C2C-C1C	-10.43	1.42	1.52
4	L	211	CYC	C2C-C1C	-9.45	1.43	1.52
4	F	206	CYC	C2C-C1C	-9.16	1.43	1.52
4	J	209	CYC	C2C-C1C	-8.90	1.44	1.52
4	D	204	CYC	C2C-C1C	-8.38	1.44	1.52
4	A	201	CYC	C2C-C1C	-8.31	1.44	1.52
4	H	207	CYC	C2C-C1C	-7.52	1.45	1.52
4	E	205	CYC	C2C-C1C	-7.07	1.45	1.52
4	M	212	CYC	C2C-C3C	-6.75	1.36	1.54
4	B	202	CYC	C2C-C3C	-6.71	1.36	1.54
4	D	204	CYC	C2C-C3C	-6.55	1.36	1.54
4	K	210	CYC	C2C-C3C	-6.39	1.37	1.54
4	J	209	CYC	C2C-C3C	-6.22	1.37	1.54
4	A	201	CYC	C2C-C3C	-6.12	1.37	1.54
4	L	211	CYC	C2C-C3C	-5.79	1.38	1.54
4	I	208	CYC	C2C-C3C	-5.79	1.38	1.54
4	F	206	CYC	C2C-C3C	-5.77	1.38	1.54
4	H	207	CYC	OC-C1C	5.73	1.34	1.23
4	C	203	CYC	OB-C4B	5.65	1.34	1.23
4	E	205	CYC	C2C-C3C	-5.58	1.39	1.54
4	H	207	CYC	OB-C4B	5.53	1.34	1.23
4	I	208	CYC	OB-C4B	5.47	1.33	1.23
4	K	210	CYC	OB-C4B	5.44	1.33	1.23
4	D	204	CYC	OB-C4B	5.44	1.33	1.23
4	C	203	CYC	C2C-C3C	-5.38	1.39	1.54
4	M	212	CYC	OB-C4B	5.38	1.33	1.23
4	H	207	CYC	C2C-C3C	-5.36	1.40	1.54
4	K	210	CYC	OC-C1C	5.06	1.33	1.23
4	J	209	CYC	OB-C4B	4.97	1.33	1.23
4	D	204	CYC	CAB-C3B	-4.83	1.38	1.51
4	E	205	CYC	OC-C1C	4.83	1.32	1.23
4	B	202	CYC	OB-C4B	4.79	1.32	1.23
4	A	201	CYC	OB-C4B	4.73	1.32	1.23
4	J	209	CYC	CAB-C3B	-4.61	1.39	1.51
4	E	205	CYC	OB-C4B	4.54	1.32	1.23
4	L	211	CYC	OB-C4B	4.52	1.32	1.23
4	C	203	CYC	CAB-C3B	-4.51	1.39	1.51
4	A	201	CYC	CAB-C3B	-4.47	1.39	1.51
4	B	202	CYC	OC-C1C	4.46	1.32	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	212	CYC	CAB-C3B	-4.37	1.39	1.51
4	F	206	CYC	OB-C4B	4.31	1.31	1.23
4	A	201	CYC	OC-C1C	4.30	1.31	1.23
4	H	207	CYC	CAB-C3B	-4.27	1.40	1.51
4	F	206	CYC	CAB-C3B	-4.05	1.40	1.51
4	I	208	CYC	CAB-C3B	-4.04	1.40	1.51
4	C	203	CYC	OC-C1C	3.98	1.31	1.23
4	F	206	CYC	OC-C1C	3.96	1.31	1.23
4	L	211	CYC	OC-C1C	3.91	1.30	1.23
4	J	209	CYC	OC-C1C	3.85	1.30	1.23
4	B	202	CYC	CAB-C3B	-3.81	1.41	1.51
4	K	210	CYC	CAB-C3B	-3.72	1.41	1.51
4	D	204	CYC	OC-C1C	3.55	1.30	1.23
4	E	205	CYC	CAB-C3B	-3.39	1.42	1.51
4	I	208	CYC	OC-C1C	3.31	1.29	1.23
4	L	211	CYC	CAB-C3B	-3.26	1.42	1.51
4	H	207	CYC	C4B-C3B	-2.88	1.43	1.48
4	M	212	CYC	CBB-CAB	-2.83	1.39	1.51
4	I	208	CYC	CBB-CAB	-2.73	1.39	1.51
4	M	212	CYC	OC-C1C	2.70	1.28	1.23
4	F	206	CYC	CBB-CAB	-2.69	1.40	1.51
4	A	201	CYC	C3C-C4C	-2.67	1.45	1.50
4	J	209	CYC	C4B-C3B	-2.66	1.43	1.48
4	D	204	CYC	CBB-CAB	-2.61	1.40	1.51
4	M	212	CYC	C1D-C2D	2.55	1.47	1.41
4	K	210	CYC	CHD-C4C	2.52	1.40	1.36
4	H	207	CYC	CBB-CAB	-2.43	1.41	1.51
4	L	211	CYC	CHA-C1A	2.38	1.43	1.38
4	E	205	CYC	C3B-C2B	2.37	1.41	1.36
4	F	206	CYC	C1D-C2D	2.27	1.46	1.41
4	K	210	CYC	CBB-CAB	-2.24	1.42	1.51
4	C	203	CYC	CBB-CAB	-2.21	1.42	1.51
4	B	202	CYC	CHD-C4C	2.16	1.40	1.36
4	C	203	CYC	C1D-C2D	2.12	1.46	1.41
4	B	202	CYC	CBB-CAB	-2.11	1.42	1.51
4	E	205	CYC	C3C-C4C	-2.10	1.46	1.50
4	K	210	CYC	C1D-C2D	2.07	1.46	1.41
4	M	212	CYC	C3C-C4C	-2.06	1.46	1.50
4	A	201	CYC	CBB-CAB	-2.06	1.42	1.51

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	206	CYC	C1C-NC-C4C	-7.59	103.89	113.41
4	F	206	CYC	C3B-C4B-NB	7.45	112.71	106.77
4	A	201	CYC	C3B-C4B-NB	7.20	112.51	106.77
4	B	202	CYC	C3B-C4B-NB	7.11	112.44	106.77
4	M	212	CYC	C1C-NC-C4C	-7.04	104.58	113.41
4	D	204	CYC	C1C-NC-C4C	-7.02	104.60	113.41
4	M	212	CYC	C3B-C4B-NB	6.89	112.26	106.77
4	A	201	CYC	C1C-NC-C4C	-6.87	104.79	113.41
4	I	208	CYC	OC-C1C-C2C	-6.85	120.72	126.17
4	I	208	CYC	C1C-NC-C4C	-6.81	104.87	113.41
4	J	209	CYC	C1C-NC-C4C	-6.73	104.97	113.41
4	L	211	CYC	C1C-NC-C4C	-6.67	105.05	113.41
4	B	202	CYC	C1C-NC-C4C	-6.64	105.08	113.41
4	L	211	CYC	C3B-C4B-NB	6.60	112.03	106.77
4	F	206	CYC	OC-C1C-C2C	-6.38	121.10	126.17
4	E	205	CYC	C1C-NC-C4C	-6.37	105.42	113.41
4	M	212	CYC	CAB-C3B-C4B	6.32	131.15	121.37
4	C	203	CYC	C1C-NC-C4C	-6.16	105.68	113.41
4	E	205	CYC	C3B-C4B-NB	6.04	111.58	106.77
4	K	210	CYC	C1C-NC-C4C	-5.96	105.93	113.41
4	K	210	CYC	OC-C1C-C2C	-5.83	121.54	126.17
4	I	208	CYC	CAB-C3B-C4B	5.76	130.28	121.37
4	A	201	CYC	CMC-C2C-C1C	5.75	124.80	112.40
4	J	209	CYC	C3B-C4B-NB	5.75	111.35	106.77
4	J	209	CYC	CMC-C2C-C1C	5.66	124.60	112.40
4	K	210	CYC	C3B-C4B-NB	5.65	111.27	106.77
4	F	206	CYC	CMC-C2C-C1C	5.58	124.42	112.40
4	E	205	CYC	CMC-C2C-C1C	5.51	124.29	112.40
4	F	206	CYC	C1B-NB-C4B	-5.50	103.91	110.66
4	H	207	CYC	C1C-NC-C4C	-5.44	106.59	113.41
4	M	212	CYC	CMC-C2C-C1C	5.39	124.02	112.40
4	D	204	CYC	CMC-C2C-C1C	5.36	123.96	112.40
4	I	208	CYC	C2C-C1C-NC	5.33	112.72	108.29
4	F	206	CYC	C2C-C1C-NC	5.28	112.68	108.29
4	B	202	CYC	CMC-C2C-C1C	5.26	123.74	112.40
4	M	212	CYC	C2C-C1C-NC	5.20	112.61	108.29
4	L	211	CYC	CMC-C2C-C1C	5.13	123.46	112.40
4	K	210	CYC	CMC-C2C-C3C	5.08	133.60	113.98
4	M	212	CYC	CBB-CAB-C3B	5.00	125.99	112.42
4	F	206	CYC	CBB-CAB-C3B	5.00	125.97	112.42
4	B	202	CYC	C1B-NB-C4B	-4.89	104.66	110.66
4	M	212	CYC	C1B-NB-C4B	-4.89	104.66	110.66
4	I	208	CYC	CBB-CAB-C3B	4.85	125.57	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	206	CYC	CAB-C3B-C4B	4.83	128.84	121.37
4	I	208	CYC	CMC-C2C-C3C	4.82	132.62	113.98
4	C	203	CYC	CMC-C2C-C1C	4.76	122.66	112.40
4	B	202	CYC	CBB-CAB-C3B	4.72	125.20	112.42
4	E	205	CYC	CBB-CAB-C3B	4.71	125.19	112.42
4	I	208	CYC	CMC-C2C-C1C	4.71	122.55	112.40
4	H	207	CYC	CMC-C2C-C1C	4.71	122.55	112.40
4	L	211	CYC	CMC-C2C-C3C	4.62	131.84	113.98
4	M	212	CYC	CMC-C2C-C3C	4.51	131.40	113.98
4	B	202	CYC	CMC-C2C-C3C	4.44	131.16	113.98
4	F	206	CYC	CMC-C2C-C3C	4.39	130.94	113.98
4	L	211	CYC	CBB-CAB-C3B	4.38	124.30	112.42
4	A	201	CYC	C1B-NB-C4B	-4.37	105.30	110.66
4	H	207	CYC	C3B-C4B-NB	4.35	110.24	106.77
4	I	208	CYC	C3B-C4B-NB	4.33	110.22	106.77
4	D	204	CYC	CHB-C4A-NA	-4.33	115.60	124.95
4	A	201	CYC	CMB-C2B-C1B	4.32	129.42	124.16
4	L	211	CYC	CHD-C4C-NC	-4.30	120.27	125.63
4	I	208	CYC	OB-C4B-C3B	4.28	132.54	128.03
4	C	203	CYC	CMC-C2C-C3C	4.27	130.49	113.98
4	D	204	CYC	CMC-C2C-C3C	4.19	130.19	113.98
4	H	207	CYC	CMC-C2C-C3C	4.18	130.14	113.98
4	I	208	CYC	CMD-C2D-C1D	4.18	131.69	125.62
4	L	211	CYC	C2C-C1C-NC	4.16	111.75	108.29
4	L	211	CYC	CHB-C4A-NA	-4.15	116.00	124.95
4	L	211	CYC	C1B-NB-C4B	-4.10	105.62	110.66
4	L	211	CYC	CHB-C4A-C3A	4.08	135.36	124.87
4	M	212	CYC	C1D-CHD-C4C	4.07	134.72	127.76
4	E	205	CYC	CHB-C4A-NA	-4.06	116.19	124.95
4	E	205	CYC	CMC-C2C-C3C	4.01	129.49	113.98
4	C	203	CYC	C3B-C4B-NB	4.00	109.96	106.77
4	J	209	CYC	CMC-C2C-C3C	3.97	129.34	113.98
4	M	212	CYC	OC-C1C-C2C	-3.96	123.02	126.17
4	E	205	CYC	CHB-C4A-C3A	3.96	135.04	124.87
4	B	202	CYC	C2C-C1C-NC	3.95	111.58	108.29
4	D	204	CYC	C3B-C4B-NB	3.93	109.90	106.77
4	D	204	CYC	C2C-C1C-NC	3.93	111.56	108.29
4	C	203	CYC	C1B-NB-C4B	-3.92	105.85	110.66
4	D	204	CYC	C1B-NB-C4B	-3.90	105.87	110.66
4	A	201	CYC	CAB-C3B-C4B	3.87	127.35	121.37
4	A	201	CYC	CMC-C2C-C3C	3.85	128.86	113.98
4	A	201	CYC	C1B-CHB-C4A	3.80	137.39	128.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	203	CYC	CHB-C4A-NA	-3.80	116.76	124.95
4	D	204	CYC	CMB-C2B-C1B	3.75	128.72	124.16
4	L	211	CYC	CMA-C3A-C4A	3.74	130.91	125.10
4	K	210	CYC	CAB-C3B-C4B	3.73	127.14	121.37
4	H	207	CYC	CHB-C4A-NA	-3.69	116.98	124.95
4	D	204	CYC	CHB-C4A-C3A	3.66	134.26	124.87
4	K	210	CYC	CBB-CAB-C3B	3.64	122.30	112.42
4	B	202	CYC	OC-C1C-C2C	-3.64	123.28	126.17
4	A	201	CYC	CHB-C4A-NA	-3.61	117.15	124.95
4	J	209	CYC	C1B-CHB-C4A	3.60	136.89	128.06
4	K	210	CYC	C1B-CHB-C4A	3.56	136.81	128.06
4	J	209	CYC	CHD-C4C-NC	-3.56	121.18	125.63
4	C	203	CYC	CHD-C4C-NC	-3.56	121.19	125.63
4	C	203	CYC	CHB-C4A-C3A	3.53	133.94	124.87
4	H	207	CYC	CHB-C4A-C3A	3.53	133.94	124.87
4	A	201	CYC	CHB-C4A-C3A	3.51	133.88	124.87
4	I	208	CYC	C1B-NB-C4B	-3.49	106.37	110.66
4	D	204	CYC	C1B-CHB-C4A	3.49	136.61	128.06
4	C	203	CYC	CMA-C3A-C4A	3.48	130.50	125.10
4	C	203	CYC	C2B-C1B-NB	3.41	111.94	106.97
4	E	205	CYC	C1B-NB-C4B	-3.40	106.48	110.66
4	A	201	CYC	CMD-C2D-C1D	3.39	130.55	125.62
4	K	210	CYC	CHB-C4A-NA	-3.37	117.68	124.95
4	K	210	CYC	CHB-C4A-C3A	3.37	133.52	124.87
4	E	205	CYC	CAB-C3B-C4B	3.35	126.55	121.37
4	I	208	CYC	OB-C4B-NB	-3.35	117.24	125.08
4	K	210	CYC	CMA-C3A-C4A	3.33	130.26	125.10
4	C	203	CYC	C1B-CHB-C4A	3.32	136.22	128.06
4	B	202	CYC	CAB-C3B-C4B	3.32	126.50	121.37
4	E	205	CYC	CMD-C2D-C1D	3.31	130.43	125.62
4	B	202	CYC	C1D-CHD-C4C	3.30	133.39	127.76
4	D	204	CYC	OB-C4B-C3B	-3.27	124.59	128.03
4	F	206	CYC	CBA-CAA-C2A	3.27	121.57	112.53
4	E	205	CYC	C1B-CHB-C4A	3.24	136.02	128.06
4	H	207	CYC	OB-C4B-C3B	-3.22	124.64	128.03
4	M	212	CYC	CMA-C3A-C4A	3.22	130.10	125.10
4	B	202	CYC	CMD-C2D-C1D	3.19	130.25	125.62
4	K	210	CYC	C1B-NB-C4B	-3.16	106.78	110.66
4	J	209	CYC	C1B-NB-C4B	-3.14	106.81	110.66
4	F	206	CYC	C2B-C1B-NB	3.13	111.52	106.97
4	D	204	CYC	CHD-C1D-ND	-3.12	118.24	125.29
4	H	207	CYC	CBB-CAB-C3B	3.12	120.88	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	212	CYC	C2C-C3C-C4C	3.08	105.95	101.34
4	A	201	CYC	CMA-C3A-C4A	3.07	129.87	125.10
4	J	209	CYC	CAC-C3C-C4C	3.07	120.55	112.67
4	K	210	CYC	OB-C4B-C3B	-3.06	124.81	128.03
4	F	206	CYC	CAC-C3C-C4C	3.03	120.45	112.67
4	J	209	CYC	CHB-C4A-C3A	3.03	132.66	124.87
4	C	203	CYC	C2C-C1C-NC	3.01	110.79	108.29
4	C	203	CYC	CBB-CAB-C3B	3.00	120.56	112.42
4	D	204	CYC	CMD-C2D-C1D	2.98	129.96	125.62
4	L	211	CYC	C1B-CHB-C4A	2.97	135.34	128.06
4	F	206	CYC	CMD-C2D-C1D	2.95	129.91	125.62
4	D	204	CYC	CMA-C3A-C4A	2.93	129.65	125.10
4	H	207	CYC	C1B-NB-C4B	-2.91	107.09	110.66
4	D	204	CYC	C1D-CHD-C4C	2.89	132.69	127.76
4	B	202	CYC	C2C-C3C-C4C	2.87	105.64	101.34
4	H	207	CYC	CMD-C2D-C1D	2.86	129.78	125.62
4	L	211	CYC	CAC-C3C-C4C	2.84	119.97	112.67
4	J	209	CYC	CMD-C2D-C1D	2.82	129.72	125.62
4	J	209	CYC	CHB-C4A-NA	-2.82	118.87	124.95
4	C	203	CYC	CAC-C3C-C4C	2.81	119.90	112.67
4	K	210	CYC	OC-C1C-NC	2.81	128.24	124.93
4	C	203	CYC	C1B-C2B-C3B	-2.80	104.99	107.86
4	J	209	CYC	CMA-C3A-C4A	2.74	129.36	125.10
4	D	204	CYC	CAC-C3C-C4C	2.74	119.71	112.67
4	K	210	CYC	CMC-C2C-C1C	2.72	118.27	112.40
4	H	207	CYC	C1B-CHB-C4A	2.71	134.71	128.06
4	J	209	CYC	CAB-C3B-C4B	2.70	125.55	121.37
4	M	212	CYC	OB-C4B-NB	-2.70	118.74	125.08
4	M	212	CYC	CAC-C3C-C4C	2.70	119.61	112.67
4	J	209	CYC	C2C-C1C-NC	2.69	110.53	108.29
4	I	208	CYC	CHD-C1D-ND	-2.66	119.29	125.29
4	B	202	CYC	OB-C4B-C3B	-2.61	125.28	128.03
4	C	203	CYC	CMD-C2D-C1D	2.61	129.41	125.62
4	I	208	CYC	CAC-C3C-C4C	2.60	119.36	112.67
4	M	212	CYC	C2B-C1B-NB	2.59	110.74	106.97
4	H	207	CYC	C2C-C3C-C4C	2.58	105.21	101.34
4	K	210	CYC	CMB-C2B-C1B	2.57	127.28	124.16
4	I	208	CYC	CBA-CAA-C2A	2.57	119.63	112.53
4	D	204	CYC	C2B-C1B-NB	2.54	110.67	106.97
4	M	212	CYC	CMB-C2B-C1B	2.54	127.24	124.16
4	I	208	CYC	CMA-C3A-C4A	2.53	129.04	125.10
4	K	210	CYC	CAC-C3C-C4C	2.50	119.09	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	206	CYC	CMB-C2B-C1B	2.48	127.18	124.16
4	I	208	CYC	CHD-C1D-C2D	2.48	133.61	127.53
4	D	204	CYC	CAB-C3B-C4B	2.47	125.19	121.37
4	F	206	CYC	C2C-C3C-C4C	2.46	105.03	101.34
4	H	207	CYC	CAC-C3C-C4C	2.46	118.98	112.67
4	D	204	CYC	CHD-C4C-NC	-2.44	122.58	125.63
4	L	211	CYC	CMB-C2B-C1B	2.43	127.12	124.16
4	L	211	CYC	CAB-C3B-C4B	2.43	125.13	121.37
4	I	208	CYC	CMD-C2D-C3D	-2.42	120.50	125.62
4	E	205	CYC	CAA-C2A-C1A	-2.40	120.81	125.02
4	B	202	CYC	C2B-C1B-NB	2.39	110.45	106.97
4	J	209	CYC	OC-C1C-NC	-2.39	122.12	124.93
4	F	206	CYC	C1D-CHD-C4C	2.37	131.82	127.76
4	F	206	CYC	CHD-C1D-ND	-2.37	119.93	125.29
4	L	211	CYC	C2B-C1B-NB	2.37	110.42	106.97
4	M	212	CYC	CHD-C1D-ND	-2.36	119.97	125.29
4	C	203	CYC	CHB-C1B-C2B	-2.35	122.28	126.97
4	L	211	CYC	OB-C4B-C3B	-2.32	125.59	128.03
4	K	210	CYC	C2C-C1C-NC	2.32	110.22	108.29
4	I	208	CYC	C2B-C1B-NB	2.30	110.33	106.97
4	K	210	CYC	CHD-C4C-NC	-2.30	122.77	125.63
4	A	201	CYC	C2C-C3C-C4C	2.29	104.77	101.34
4	B	202	CYC	CMB-C2B-C1B	2.28	126.94	124.16
4	M	212	CYC	CBA-CAA-C2A	2.28	118.84	112.53
4	L	211	CYC	CHD-C1D-ND	-2.26	120.19	125.29
4	C	203	CYC	CAB-C3B-C4B	2.26	124.86	121.37
4	A	201	CYC	CBB-CAB-C3B	2.26	118.54	112.42
4	F	206	CYC	CAA-C2A-C1A	2.25	128.97	125.02
4	M	212	CYC	C3D-C4D-ND	2.25	110.39	107.57
4	C	203	CYC	C3D-C4D-ND	2.25	110.39	107.57
4	D	204	CYC	CBB-CAB-C3B	2.24	118.50	112.42
4	K	210	CYC	CBA-CAA-C2A	2.23	118.69	112.53
4	D	204	CYC	C2C-C3C-C4C	2.22	104.66	101.34
4	J	209	CYC	CBB-CAB-C3B	2.22	118.43	112.42
4	J	209	CYC	CHD-C1D-ND	-2.21	120.30	125.29
4	D	204	CYC	C3D-C4D-ND	2.21	110.34	107.57
4	B	202	CYC	CAC-C3C-C4C	2.21	118.34	112.67
4	F	206	CYC	CHB-C4A-NA	-2.20	120.19	124.95
4	E	205	CYC	CAC-C3C-C4C	2.19	118.31	112.67
4	E	205	CYC	C2B-C1B-NB	2.18	110.14	106.97
4	K	210	CYC	CMD-C2D-C1D	2.15	128.75	125.62
4	L	211	CYC	CMD-C2D-C1D	2.10	128.67	125.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	207	CYC	CMA-C3A-C4A	2.08	128.33	125.10
5	L	2001	BO4	O3-B-O2	-2.07	101.68	109.39
4	I	208	CYC	O2A-CGA-CBA	2.06	120.52	114.00
4	L	211	CYC	C2C-C3C-C4C	2.05	104.42	101.34
4	A	201	CYC	C2C-C1C-NC	2.05	109.99	108.29
4	A	201	CYC	C2B-C1B-NB	2.05	109.95	106.97
4	F	206	CYC	CHB-C4A-C3A	2.02	130.07	124.87
4	M	212	CYC	CHB-C4A-NA	-2.02	120.60	124.95
4	D	204	CYC	CHD-C1D-C2D	2.02	132.47	127.53
4	D	204	CYC	CHB-C1B-C2B	-2.02	122.95	126.97
4	I	208	CYC	CHB-C1B-NB	-2.01	121.76	126.06
4	M	212	CYC	CMD-C2D-C1D	2.00	128.53	125.62

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	201	CYC	C3C
4	A	201	CYC	C2C
4	B	202	CYC	C3C
4	B	202	CYC	C2C
4	C	203	CYC	C3C
4	C	203	CYC	C2C
4	D	204	CYC	C2C
4	E	205	CYC	C3C
4	E	205	CYC	C2C
4	F	206	CYC	C3C
4	F	206	CYC	C2C
4	H	207	CYC	C3C
4	H	207	CYC	C2C
4	I	208	CYC	C2C
4	J	209	CYC	C2C
4	K	210	CYC	C2C
4	L	211	CYC	C3C
4	L	211	CYC	C2C
4	M	212	CYC	C3C
4	M	212	CYC	C2C

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	201	CYC	C3A-C4A-CHB-C1B
4	A	201	CYC	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	202	CYC	NA-C4A-CHB-C1B
4	B	202	CYC	C3A-C4A-CHB-C1B
4	C	203	CYC	NA-C4A-CHB-C1B
4	C	203	CYC	C3A-C4A-CHB-C1B
4	C	203	CYC	C4C-C3C-CAC-CBC
4	D	204	CYC	C3A-C4A-CHB-C1B
4	D	204	CYC	C4C-C3C-CAC-CBC
4	E	205	CYC	C3A-C4A-CHB-C1B
4	E	205	CYC	C2C-C3C-CAC-CBC
4	F	206	CYC	NA-C4A-CHB-C1B
4	F	206	CYC	C3A-C4A-CHB-C1B
4	F	206	CYC	C4C-C3C-CAC-CBC
4	H	207	CYC	C3A-C4A-CHB-C1B
4	H	207	CYC	C4C-C3C-CAC-CBC
4	I	208	CYC	NA-C4A-CHB-C1B
4	I	208	CYC	C3A-C4A-CHB-C1B
4	J	209	CYC	NA-C4A-CHB-C1B
4	J	209	CYC	C3A-C4A-CHB-C1B
4	J	209	CYC	C4C-C3C-CAC-CBC
4	K	210	CYC	C2B-C3B-CAB-CBB
4	K	210	CYC	C4C-C3C-CAC-CBC
4	M	212	CYC	NA-C4A-CHB-C1B
4	M	212	CYC	C3A-C4A-CHB-C1B
4	M	212	CYC	C2B-C3B-CAB-CBB
4	M	212	CYC	C4B-C3B-CAB-CBB
4	M	212	CYC	C4C-C3C-CAC-CBC
4	F	206	CYC	C2B-C3B-CAB-CBB
4	A	201	CYC	ND-C1D-CHD-C4C
4	C	203	CYC	ND-C1D-CHD-C4C
4	H	207	CYC	ND-C1D-CHD-C4C
4	J	209	CYC	ND-C1D-CHD-C4C
4	L	211	CYC	ND-C1D-CHD-C4C
4	C	203	CYC	C2D-C1D-CHD-C4C
4	L	211	CYC	C2D-C1D-CHD-C4C
4	B	202	CYC	ND-C1D-CHD-C4C
4	E	205	CYC	ND-C1D-CHD-C4C
4	F	206	CYC	ND-C1D-CHD-C4C
4	I	208	CYC	ND-C1D-CHD-C4C
4	K	210	CYC	ND-C1D-CHD-C4C
4	M	212	CYC	ND-C1D-CHD-C4C
4	A	201	CYC	C2D-C1D-CHD-C4C
4	D	204	CYC	C2D-C1D-CHD-C4C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	205	CYC	C2D-C1D-CHD-C4C
4	F	206	CYC	C2D-C1D-CHD-C4C
4	H	207	CYC	C2D-C1D-CHD-C4C
4	I	208	CYC	C2D-C1D-CHD-C4C
4	J	209	CYC	C2D-C1D-CHD-C4C
4	K	210	CYC	C2D-C1D-CHD-C4C
4	D	204	CYC	ND-C1D-CHD-C4C
4	B	202	CYC	C2D-C1D-CHD-C4C
4	M	212	CYC	C2D-C1D-CHD-C4C
4	F	206	CYC	C4B-C3B-CAB-CBB
4	K	210	CYC	C4B-C3B-CAB-CBB
4	D	204	CYC	NA-C4A-CHB-C1B
4	E	205	CYC	NA-C4A-CHB-C1B
4	F	206	CYC	C2A-CAA-CBA-CGA
4	L	211	CYC	C3A-C4A-CHB-C1B
4	A	201	CYC	NA-C4A-CHB-C1B
4	H	207	CYC	NA-C4A-CHB-C1B
4	K	210	CYC	NA-C4A-CHB-C1B
4	L	211	CYC	NA-C4A-CHB-C1B
4	K	210	CYC	C3A-C4A-CHB-C1B
4	B	202	CYC	C2B-C3B-CAB-CBB
4	I	208	CYC	C2B-C3B-CAB-CBB
4	A	201	CYC	C2C-C3C-CAC-CBC
4	L	211	CYC	C2C-C3C-CAC-CBC
4	B	202	CYC	C4C-C3C-CAC-CBC
4	I	208	CYC	C4C-C3C-CAC-CBC
4	E	205	CYC	CAA-CBA-CGA-O2A
4	H	207	CYC	CAA-CBA-CGA-O2A
4	F	206	CYC	CAD-CBD-CGD-O1D
4	F	206	CYC	CAD-CBD-CGD-O2D
4	A	201	CYC	CAA-CBA-CGA-O2A
4	E	205	CYC	CAA-CBA-CGA-O1A
4	A	201	CYC	CAA-CBA-CGA-O1A
4	H	207	CYC	CAA-CBA-CGA-O1A
4	K	210	CYC	C1A-C2A-CAA-CBA
4	L	211	CYC	CAA-CBA-CGA-O2A
4	M	212	CYC	CAD-CBD-CGD-O1D
4	I	208	CYC	CAD-CBD-CGD-O1D
4	J	209	CYC	CAA-CBA-CGA-O1A
4	B	202	CYC	C4B-C3B-CAB-CBB
4	L	211	CYC	CAA-CBA-CGA-O1A
4	J	209	CYC	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	202	CYC	CAD-CBD-CGD-O1D
4	C	203	CYC	CAA-CBA-CGA-O2A
4	A	201	CYC	CAD-CBD-CGD-O2D
4	F	206	CYC	CAA-CBA-CGA-O2A
4	M	212	CYC	CAD-CBD-CGD-O2D
4	D	204	CYC	C3A-C2A-CAA-CBA
4	A	201	CYC	CAD-CBD-CGD-O1D
4	I	208	CYC	CAD-CBD-CGD-O2D
4	K	210	CYC	CAD-CBD-CGD-O1D
4	K	210	CYC	C3A-C2A-CAA-CBA
4	E	205	CYC	CAD-CBD-CGD-O1D
4	C	203	CYC	CAA-CBA-CGA-O1A
4	B	202	CYC	CAD-CBD-CGD-O2D
4	F	206	CYC	CAA-CBA-CGA-O1A
4	E	205	CYC	CAD-CBD-CGD-O2D
4	M	212	CYC	CAA-CBA-CGA-O1A
4	I	208	CYC	C2A-CAA-CBA-CGA
4	I	208	CYC	CAA-CBA-CGA-O1A
4	L	211	CYC	CAD-CBD-CGD-O1D
4	L	211	CYC	CAD-CBD-CGD-O2D
4	H	207	CYC	CAD-CBD-CGD-O1D
4	J	209	CYC	CAD-CBD-CGD-O1D
4	K	210	CYC	CAD-CBD-CGD-O2D
4	M	212	CYC	CAA-CBA-CGA-O2A
4	I	208	CYC	CAA-CBA-CGA-O2A
4	B	202	CYC	C2C-C3C-CAC-CBC
4	J	209	CYC	CAD-CBD-CGD-O2D
4	H	207	CYC	CAD-CBD-CGD-O2D
4	D	204	CYC	C1A-C2A-CAA-CBA
4	C	203	CYC	CAD-CBD-CGD-O2D

There are no ring outliers.

12 monomers are involved in 37 short contacts:

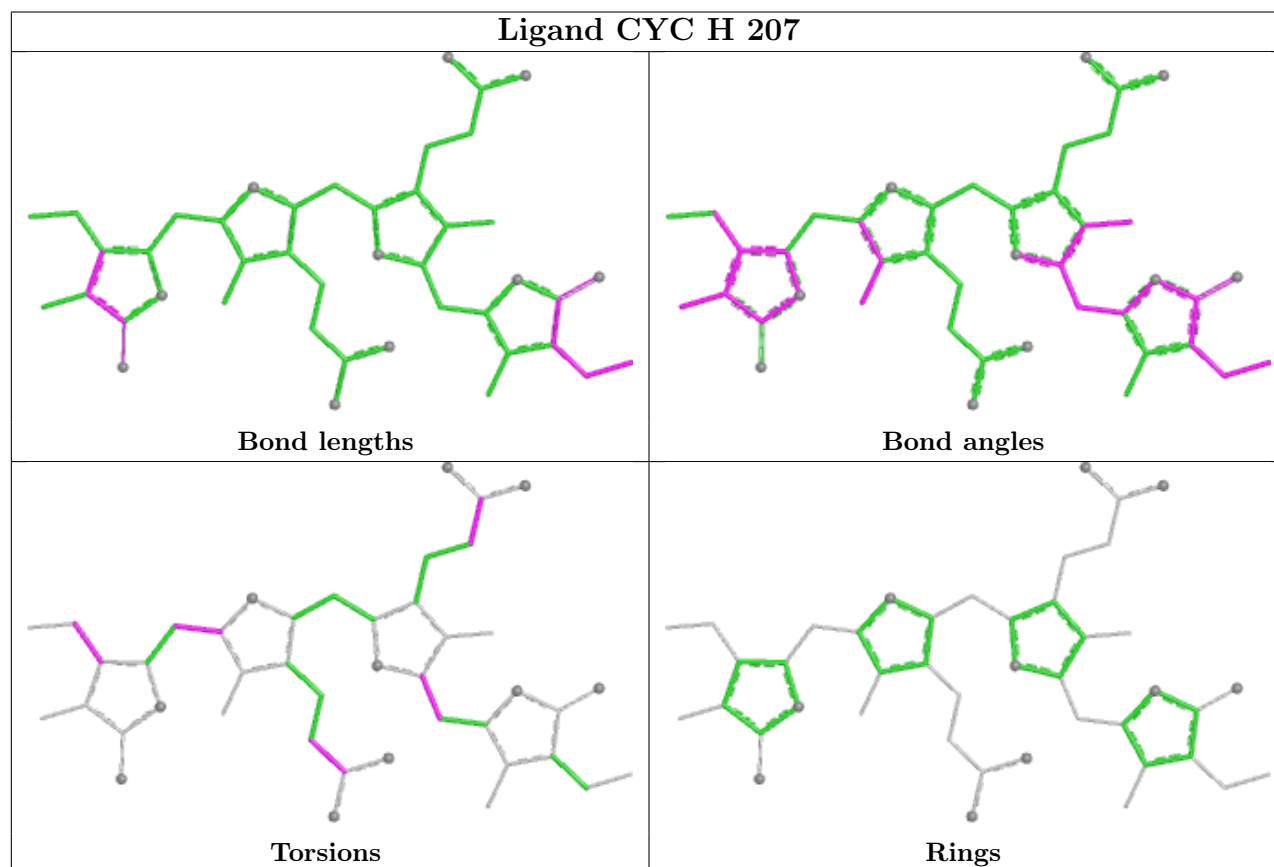
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	207	CYC	4	0
4	E	205	CYC	5	0
4	F	206	CYC	3	0
4	I	208	CYC	2	0
4	C	203	CYC	2	0
4	J	209	CYC	5	0
4	K	210	CYC	2	0

Continued on next page...

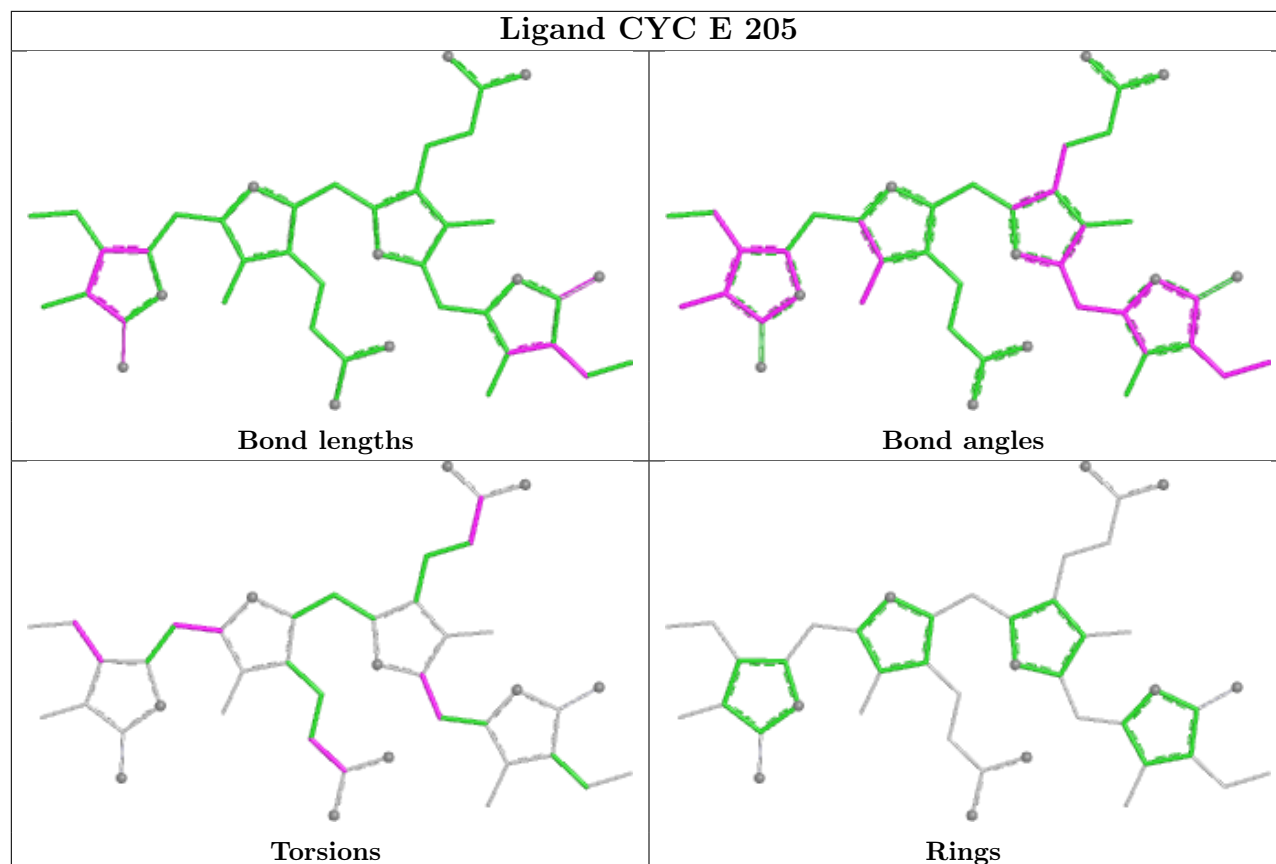
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	CYC	2	0
4	M	212	CYC	2	0
4	L	211	CYC	5	0
4	D	204	CYC	2	0
4	A	201	CYC	3	0

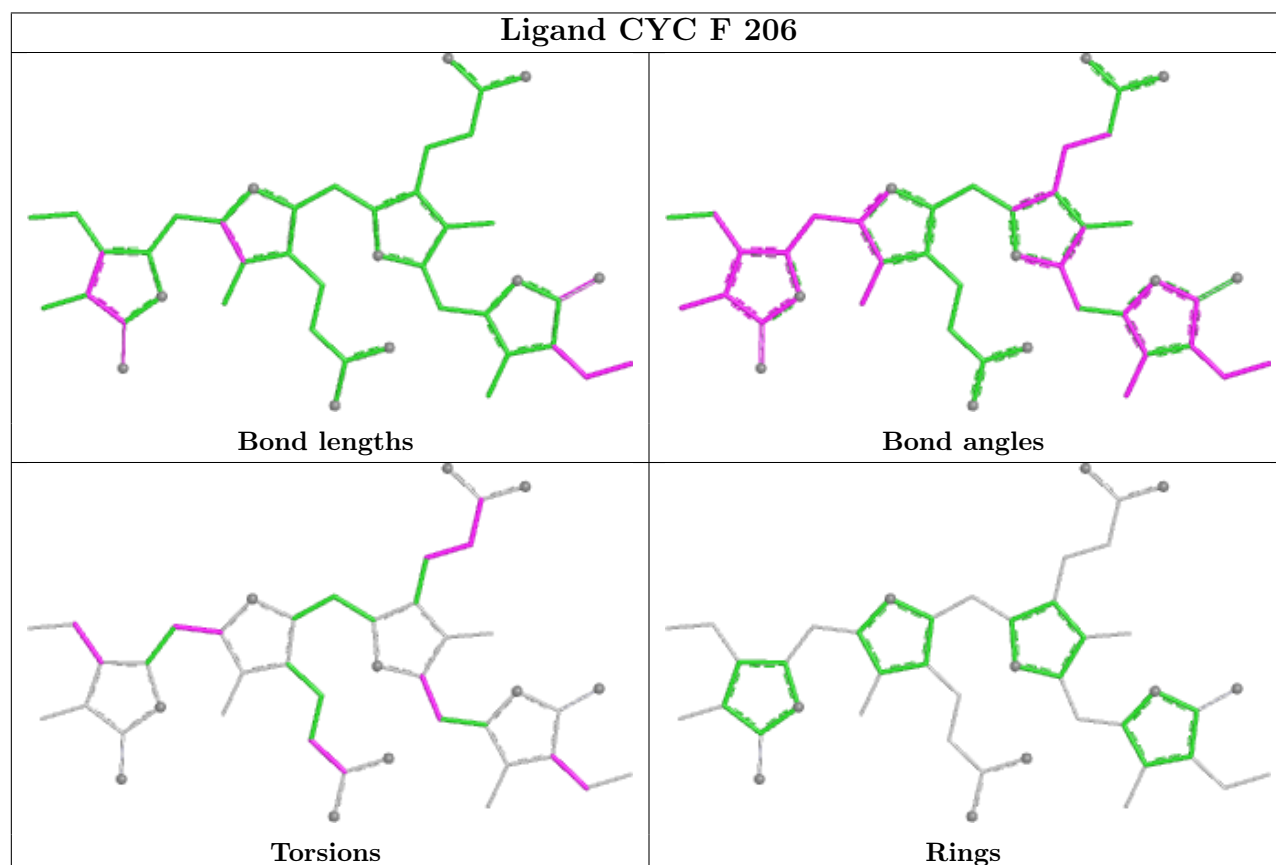
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



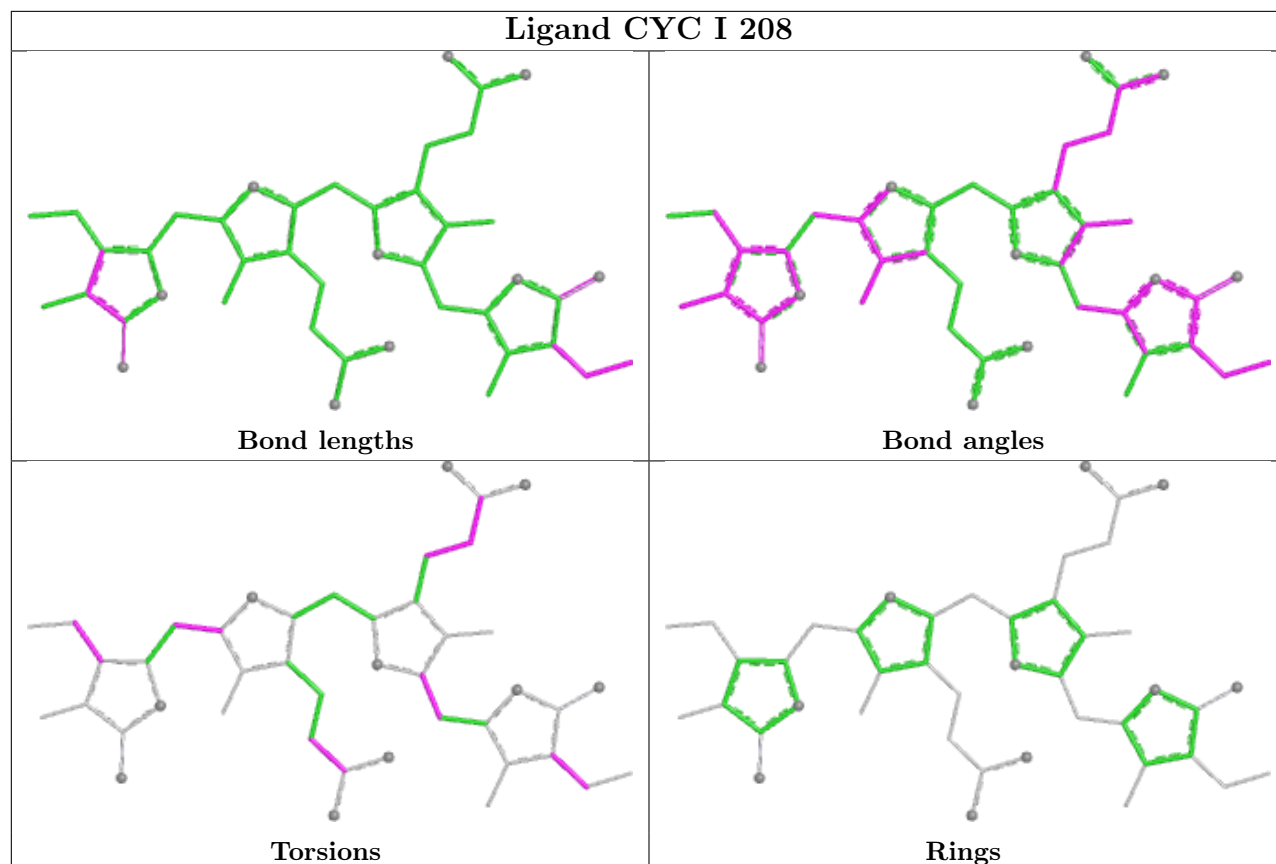
Ligand CYC E 205



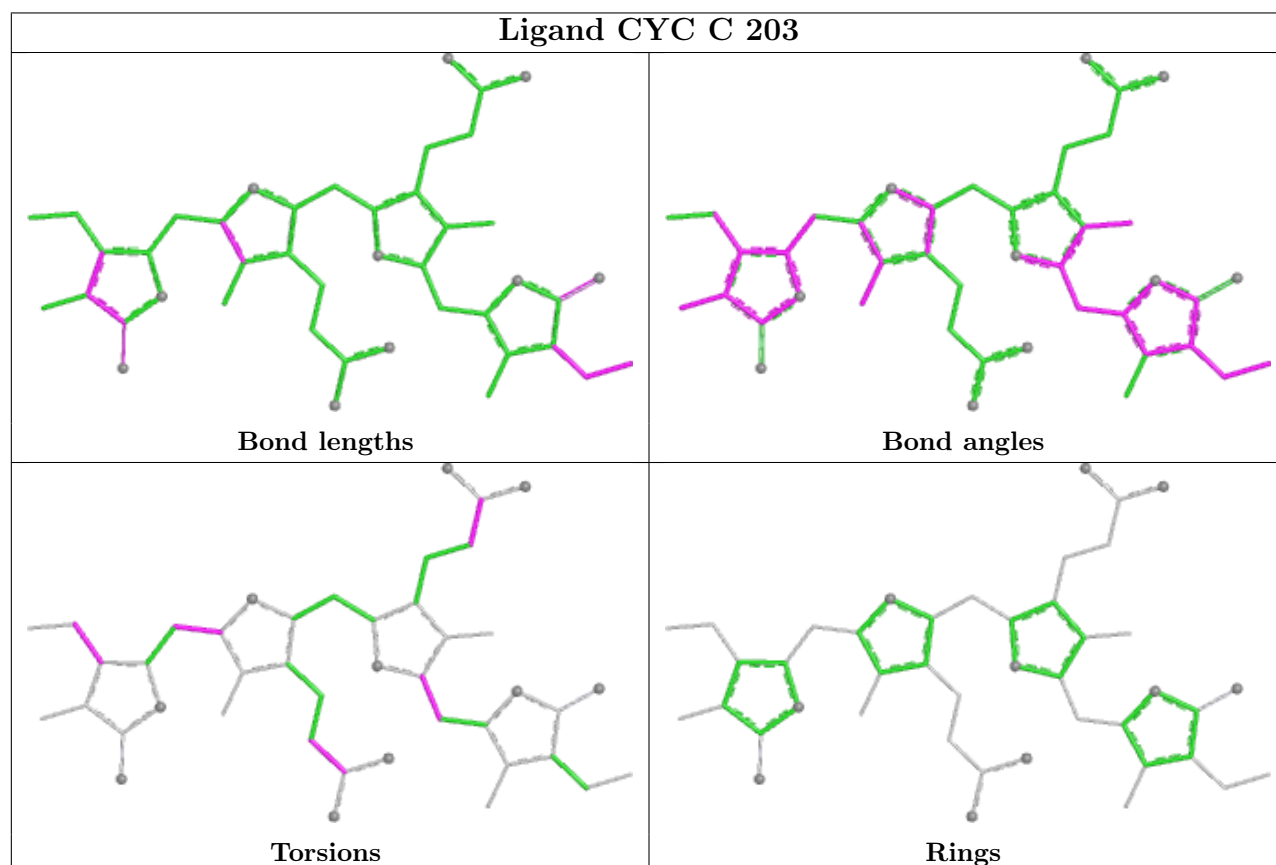
Ligand CYC F 206



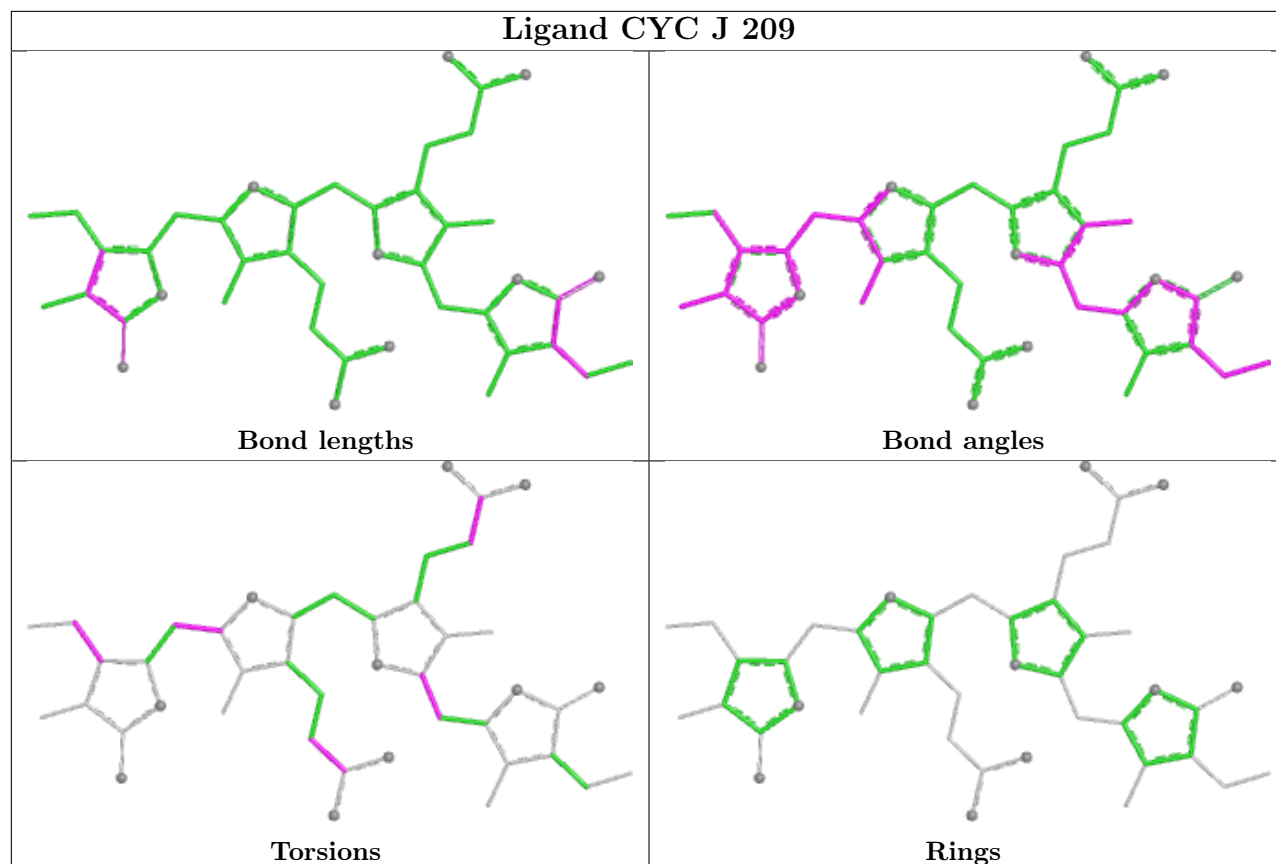
Ligand CYC I 208



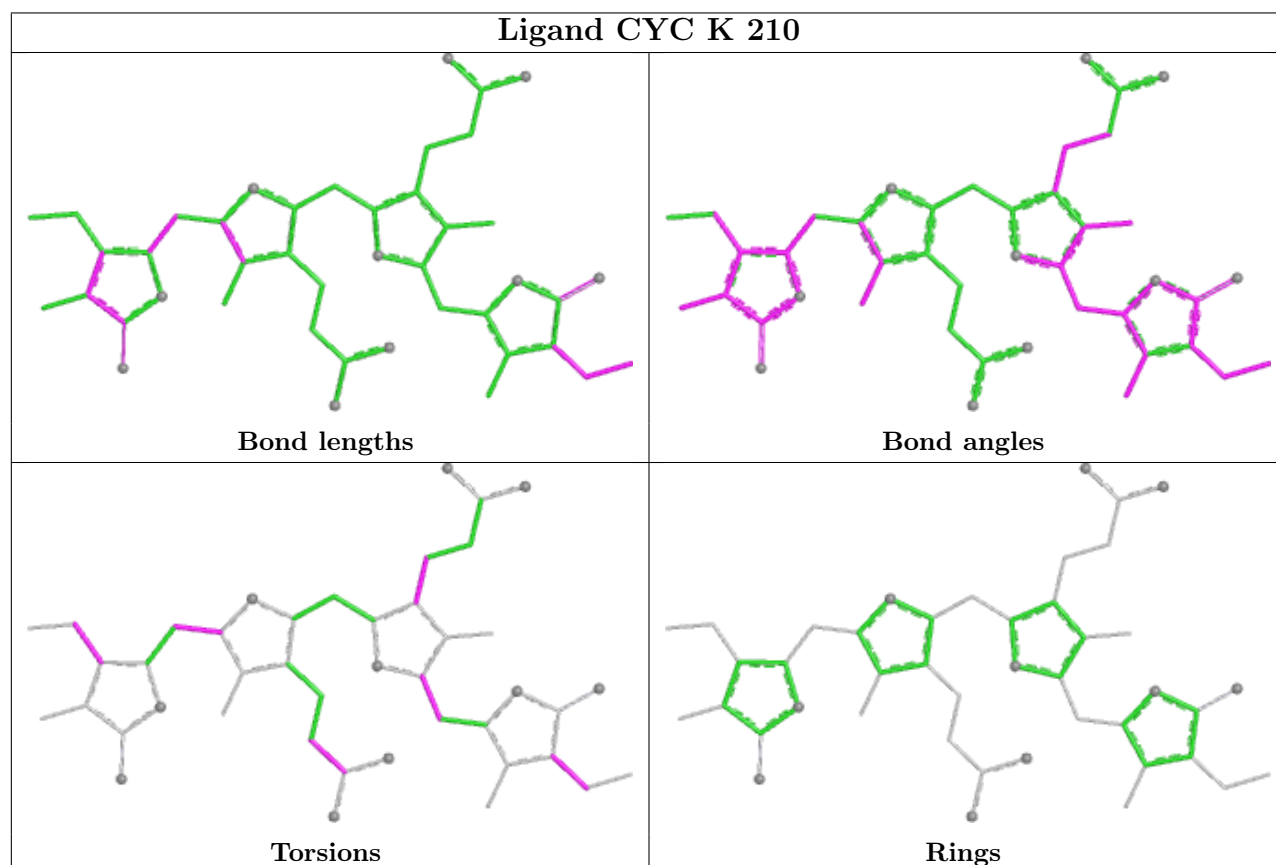
Ligand CYC C 203



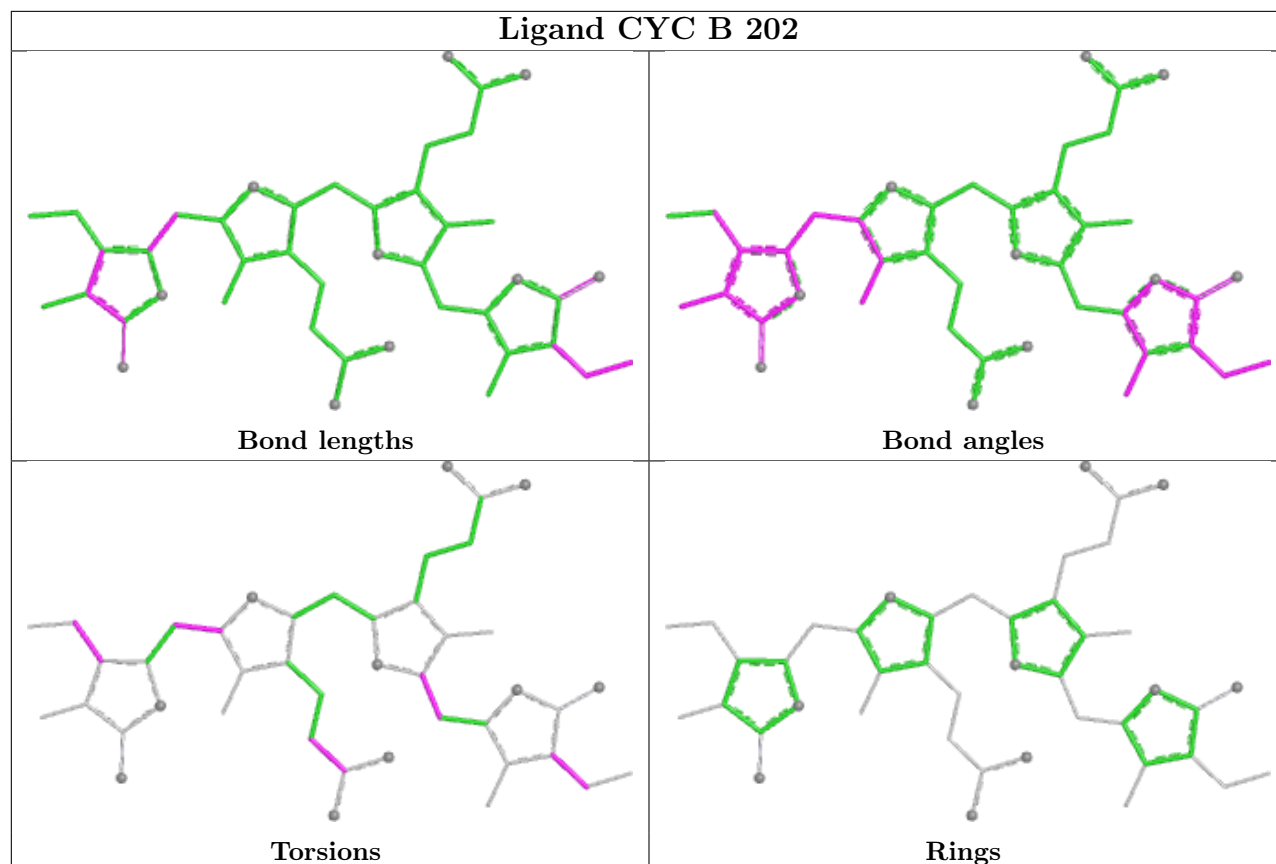
Ligand CYC J 209



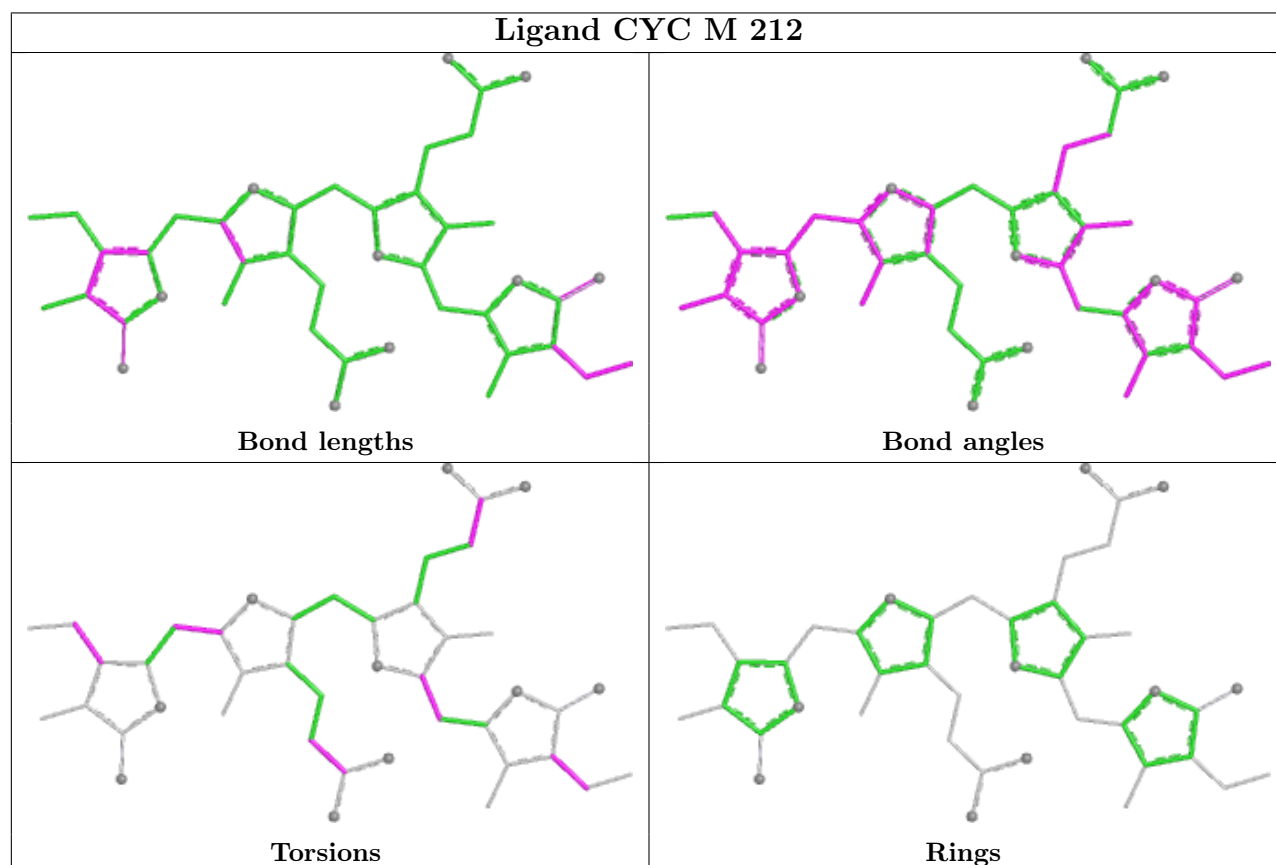
Ligand CYC K 210



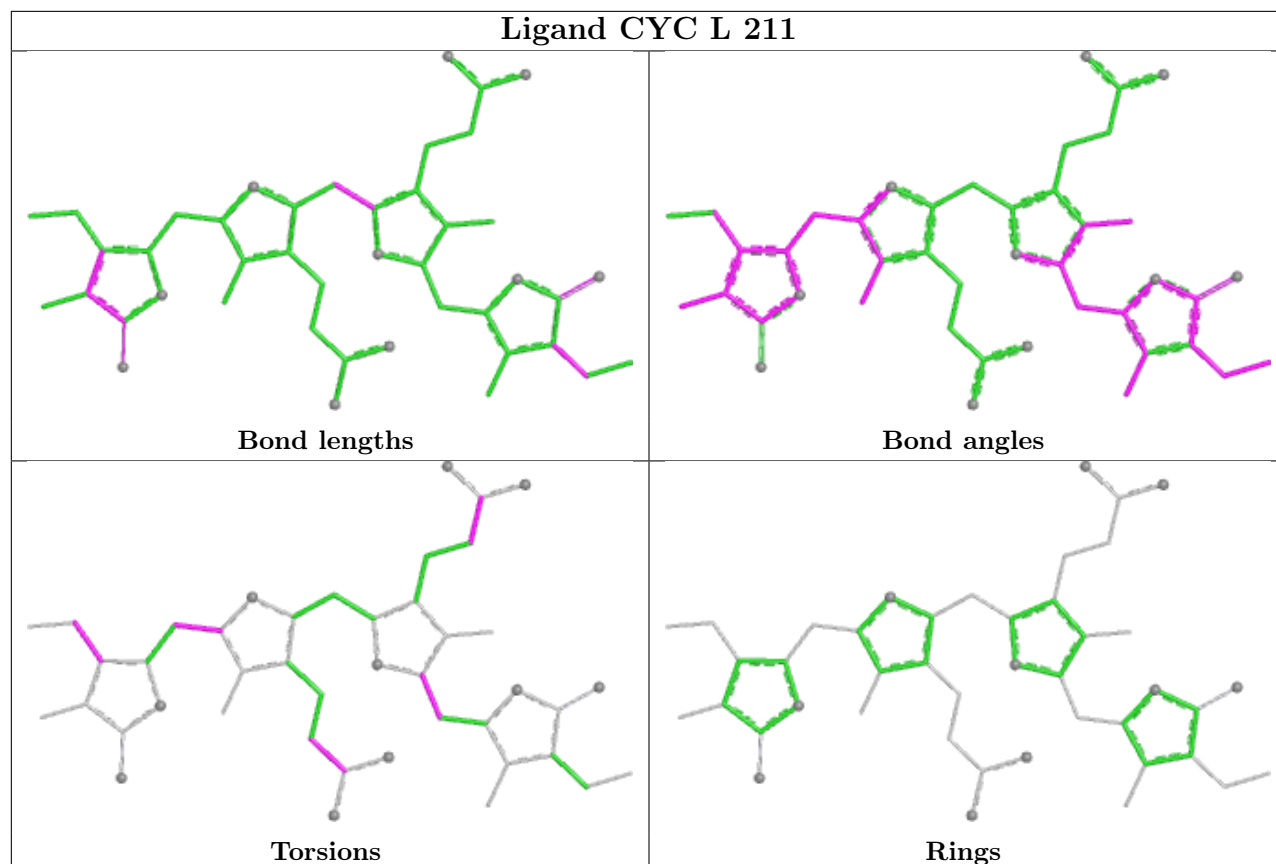
Ligand CYC B 202



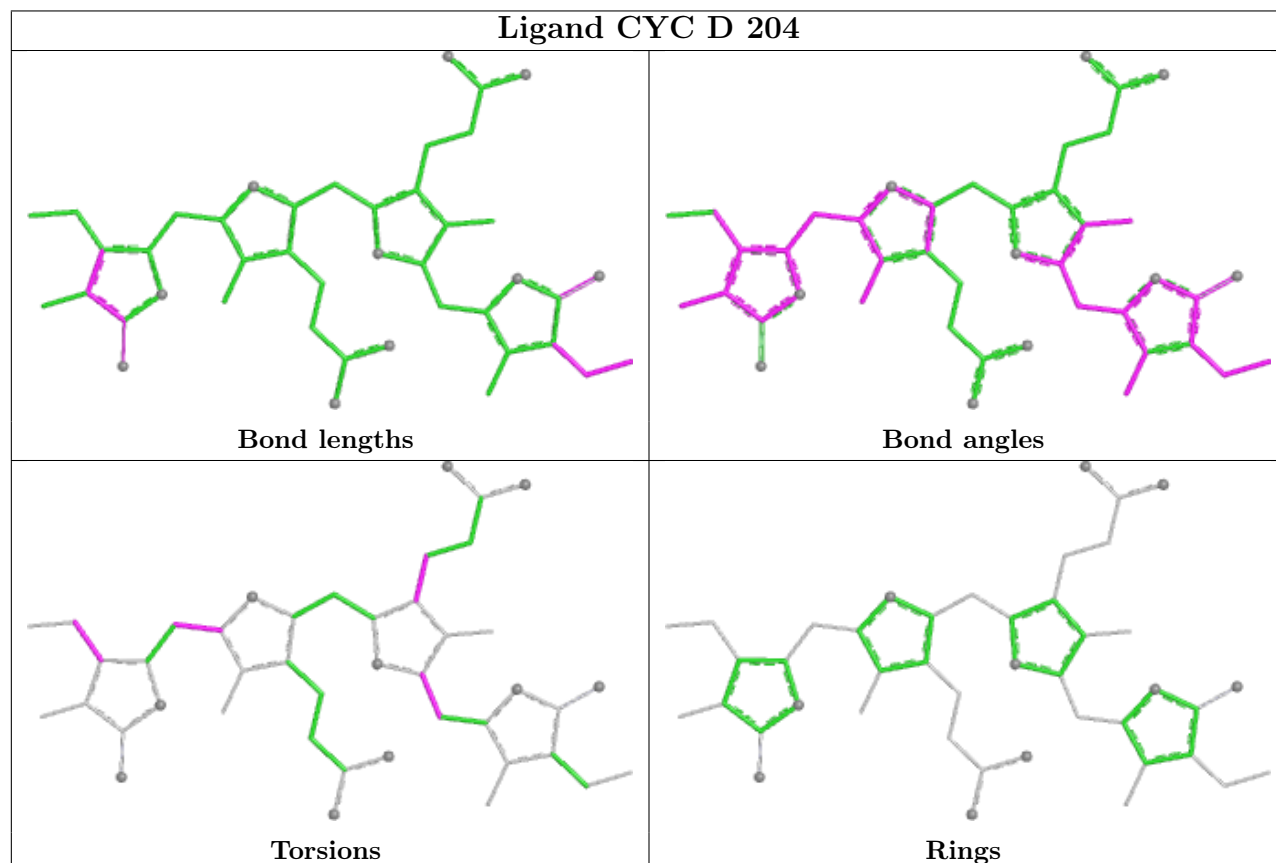
Ligand CYC M 212

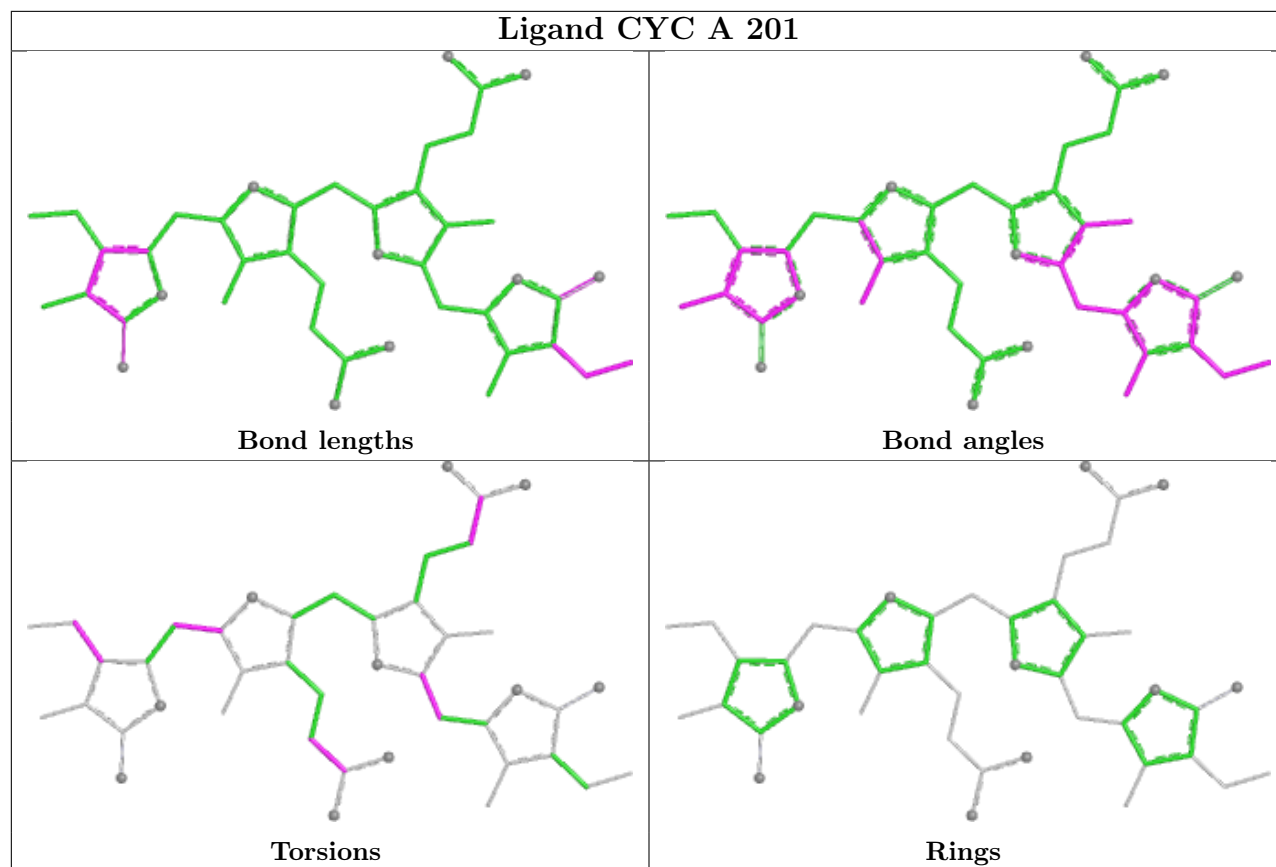


Ligand CYC L 211



Ligand CYC D 204





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.