



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 02:43 PM UTC

PDB ID : 3JBB / pdb_00003jbb
EMDB ID : EMD-6430
Title : Characterization of red-shifted phycobiliprotein complexes isolated from the chlorophyll f-containing cyanobacterium Halomicronema hongdechloris
Authors : Li, Y.; Lin, Y.; Garvey, C.; Birch, D.; Corkery, R.W.; Loughlin, P.C.; Scheer, H.; Willows, R.D.; Chen, M.
Deposited on : 2015-08-26
Resolution : 26.00 Å (reported)
Based on initial model : 4PO5

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

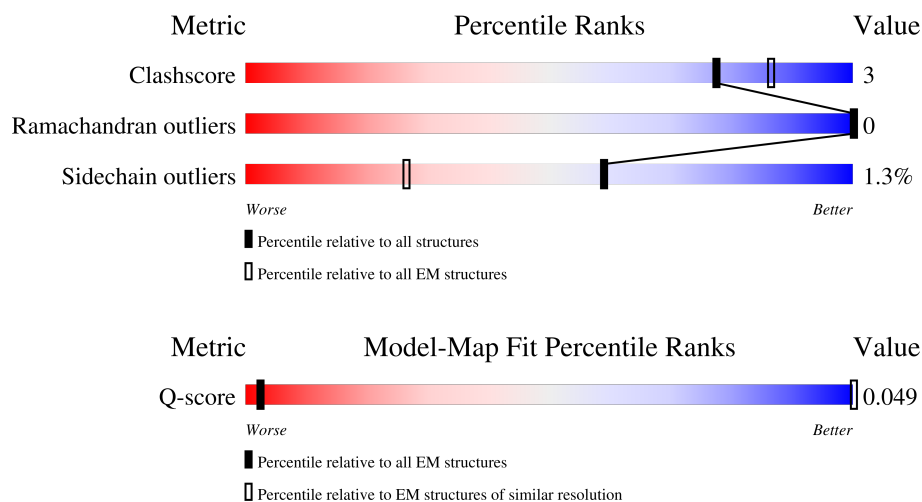
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 26.00 Å.

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



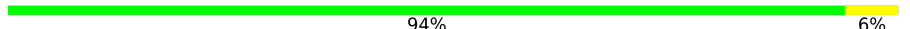
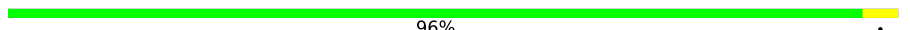
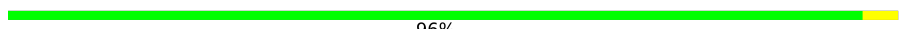
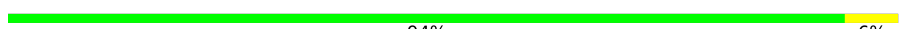
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8 (26.00 - 26.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	167	 89% 7% . .
1	C	167	 89% 8% .
1	E	167	 92% 5% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	167	 90%7% . .
1	I	167	 89%8% .
1	K	167	 92%5% . .
2	B	161	 94%6%
2	D	161	 96%. .
2	F	161	 96%. .
2	H	161	 94%6%
2	J	161	 96%. .
2	L	161	 96%. .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 18492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

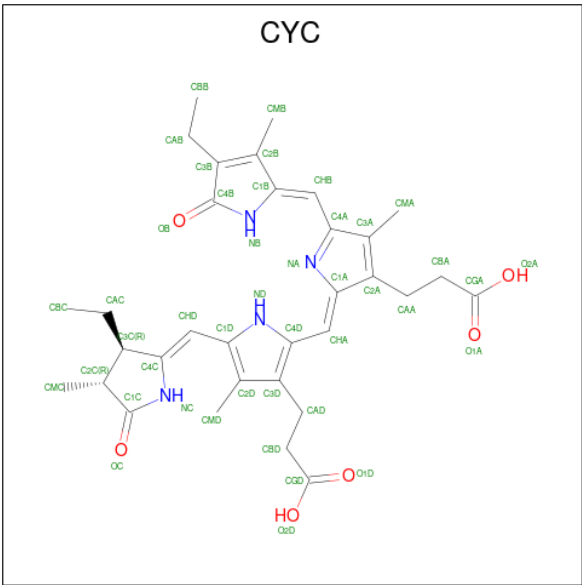
- Molecule 1 is a protein called allophycocyanin subunit alpha-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	C	162	Total	C	N	O	S	6	0
			1308	832	225	247	4		
1	E	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	G	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		
1	I	162	Total	C	N	O	S	6	0
			1308	832	225	247	4		
1	K	162	Total	C	N	O	S	5	0
			1302	829	224	245	4		

- Molecule 2 is a protein called allophycocyanin beta chain.

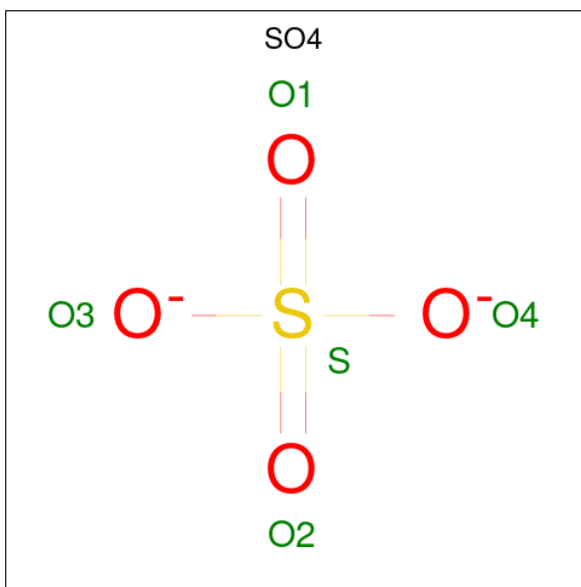
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	161	Total	C	N	O	S	9	0
			1257	789	212	249	7		
2	D	161	Total	C	N	O	S	9	0
			1259	789	213	250	7		
2	F	161	Total	C	N	O	S	7	0
			1248	782	210	249	7		
2	H	161	Total	C	N	O	S	9	0
			1257	789	212	249	7		
2	J	161	Total	C	N	O	S	9	0
			1259	789	213	250	7		
2	L	161	Total	C	N	O	S	7	0
			1248	782	210	249	7		

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



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	1
			46	34	4	8	
3	B	1	Total	C	N	O	0
			43	33	4	6	
3	C	1	Total	C	N	O	1
			46	34	4	8	
3	D	1	Total	C	N	O	0
			43	33	4	6	
3	E	1	Total	C	N	O	1
			46	34	4	8	
3	F	1	Total	C	N	O	0
			43	33	4	6	
3	G	1	Total	C	N	O	1
			46	34	4	8	
3	H	1	Total	C	N	O	0
			43	33	4	6	
3	I	1	Total	C	N	O	1
			46	34	4	8	
3	J	1	Total	C	N	O	0
			43	33	4	6	
3	K	1	Total	C	N	O	1
			46	34	4	8	
3	L	1	Total	C	N	O	0
			43	33	4	6	

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	O	S	0
			5	4	1	
4	A	1	Total	O	S	0
			5	4	1	
4	B	1	Total	O	S	0
			5	4	1	
4	B	1	Total	O	S	0
			5	4	1	
4	B	1	Total	O	S	0
			5	4	1	
4	B	1	Total	O	S	0
			5	4	1	
4	C	1	Total	O	S	0
			5	4	1	
4	C	1	Total	O	S	0
			5	4	1	
4	D	1	Total	O	S	0
			5	4	1	
4	D	1	Total	O	S	0
			5	4	1	
4	D	1	Total	O	S	0
			5	4	1	
4	D	1	Total	O	S	0
			5	4	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	E	1	Total 5	O 4	S 1	0
4	E	1	Total 5	O 4	S 1	0
4	F	1	Total 5	O 4	S 1	0
4	F	1	Total 5	O 4	S 1	0
4	F	1	Total 5	O 4	S 1	0
4	F	1	Total 5	O 4	S 1	0
4	F	1	Total 5	O 4	S 1	0
4	G	1	Total 5	O 4	S 1	0
4	G	1	Total 5	O 4	S 1	0
4	H	1	Total 5	O 4	S 1	0
4	H	1	Total 5	O 4	S 1	0
4	H	1	Total 5	O 4	S 1	0
4	H	1	Total 5	O 4	S 1	0
4	H	1	Total 5	O 4	S 1	0
4	I	1	Total 5	O 4	S 1	0
4	I	1	Total 5	O 4	S 1	0
4	J	1	Total 5	O 4	S 1	0
4	J	1	Total 5	O 4	S 1	0
4	J	1	Total 5	O 4	S 1	0
4	J	1	Total 5	O 4	S 1	0
4	J	1	Total 5	O 4	S 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
4	K	1	Total	O	S	0
			5	4	1	
4	K	1	Total	O	S	0
			5	4	1	
4	L	1	Total	O	S	0
			5	4	1	
4	L	1	Total	O	S	0
			5	4	1	
4	L	1	Total	O	S	0
			5	4	1	
4	L	1	Total	O	S	0
			5	4	1	

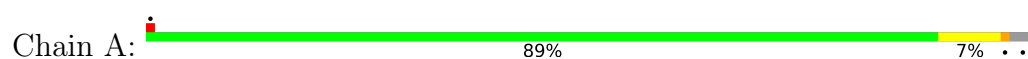
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	177	Total	O	0
			177	177	
5	B	218	Total	O	0
			218	218	
5	C	188	Total	O	0
			188	188	
5	D	212	Total	O	0
			212	212	
5	E	185	Total	O	0
			185	185	
5	F	218	Total	O	0
			218	218	
5	G	178	Total	O	0
			178	178	
5	H	217	Total	O	0
			217	217	
5	I	188	Total	O	0
			188	188	
5	J	212	Total	O	0
			212	212	
5	K	185	Total	O	0
			185	185	
5	L	218	Total	O	0
			218	218	

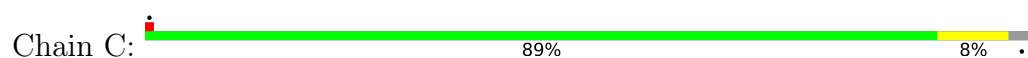
3 Residue-property plots [i](#)

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

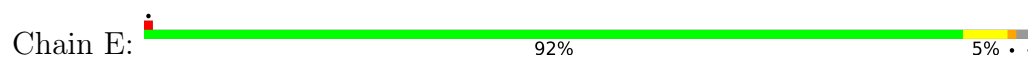
- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B



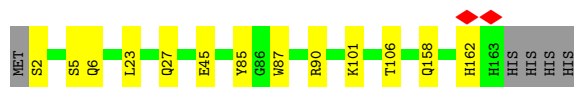
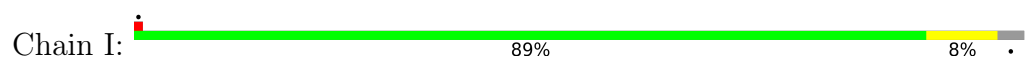
- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B



- Molecule 1: allophycocyanin subunit alpha-B

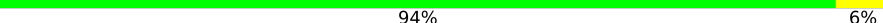


- Molecule 1: allophycocyanin subunit alpha-B

Chain K:  92% 5% ..

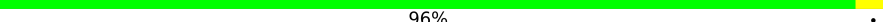


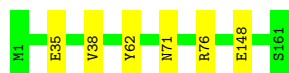
- Molecule 2: allophycocyanin beta chain

Chain B:  94% 6%

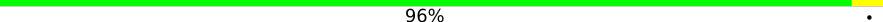


- Molecule 2: allophycocyanin beta chain

Chain D:  96% .

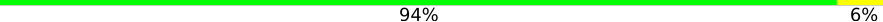


- Molecule 2: allophycocyanin beta chain

Chain F:  96% .

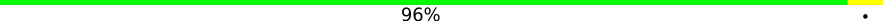


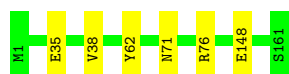
- Molecule 2: allophycocyanin beta chain

Chain H:  94% 6%

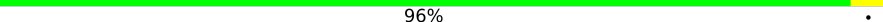


- Molecule 2: allophycocyanin beta chain

Chain J:  96% .



- Molecule 2: allophycocyanin beta chain

Chain L:  96% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	420	Depositor
Resolution determination method	FSC 0.33 CUT-OFF	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI/PHILIPS CM10	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	3000	Depositor
Magnification	180000	Depositor
Image detector	GENERIC IMAGE PLATES	Depositor
Maximum map value	1.131	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.077	Depositor
Map value standard deviation	0.247	Depositor
Recommended contour level	0.86	Depositor
Map size ($\text{\AA}$)	273.6, 273.6, 273.6	wwPDB
Map dimensions	72, 72, 72	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	3.8000002, 3.8000002, 3.8000002	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CYC, MEN

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	0.45	0/1342	0.68	0/1817
1	C	0.45	0/1348	0.70	0/1825
1	E	0.44	0/1342	0.71	0/1817
1	G	0.45	0/1342	0.68	0/1817
1	I	0.45	0/1348	0.70	0/1825
1	K	0.44	0/1342	0.71	0/1817
2	B	0.44	0/1279	0.70	0/1726
2	D	0.43	0/1278	0.69	0/1725
2	F	0.43	0/1261	0.70	0/1703
2	H	0.44	0/1279	0.70	0/1726
2	J	0.43	0/1278	0.69	0/1725
2	L	0.44	0/1261	0.70	0/1703
All	All	0.44	0/15700	0.70	0/21226

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1302	0	1311	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1308	0	1315	9	0
1	E	1302	0	1311	7	0
1	G	1302	0	1311	9	0
1	I	1308	0	1315	9	0
1	K	1302	0	1311	7	0
2	B	1257	0	1284	7	0
2	D	1259	0	1282	5	0
2	F	1248	0	1264	4	0
2	H	1257	0	1284	7	0
2	J	1259	0	1282	6	0
2	L	1248	0	1264	4	0
3	A	46	0	4	1	0
3	B	43	0	35	2	0
3	C	46	0	4	1	0
3	D	43	0	35	4	0
3	E	46	0	4	1	0
3	F	43	0	35	2	0
3	G	46	0	4	1	0
3	H	43	0	35	2	0
3	I	46	0	4	1	0
3	J	43	0	35	3	0
3	K	46	0	4	1	0
3	L	43	0	35	2	0
4	A	10	0	0	0	0
4	B	25	0	0	0	0
4	C	10	0	0	0	0
4	D	25	0	0	0	0
4	E	10	0	0	0	0
4	F	25	0	0	0	0
4	G	10	0	0	0	0
4	H	25	0	0	0	0
4	I	10	0	0	0	0
4	J	25	0	0	0	0
4	K	10	0	0	0	0
4	L	25	0	0	0	0
5	A	177	0	0	2	0
5	B	218	0	0	2	0
5	C	188	0	0	3	0
5	D	212	0	0	1	0
5	E	185	0	0	1	0
5	F	218	0	0	2	0
5	G	178	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	217	0	0	2	0
5	I	188	0	0	3	0
5	J	212	0	0	1	0
5	K	185	0	0	1	0
5	L	218	0	0	2	0
All	All	18492	0	15768	82	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 3.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:TYR:OH	3:C:201[B]:CYC:O1D	2.12	0.67
2:D:62:TYR:OH	3:E:201[B]:CYC:O1D	2.12	0.66
2:J:62:TYR:OH	3:K:201[B]:CYC:O1D	2.12	0.66
2:H:62:TYR:OH	3:I:201[B]:CYC:O1D	2.12	0.66
3:G:201[B]:CYC:O1D	2:L:62:TYR:OH	2.14	0.62
3:A:201[B]:CYC:O1D	2:F:62:TYR:OH	2.14	0.62
3:D:201:CYC:NB	3:D:201:CYC:HMA1	2.18	0.59
3:J:201:CYC:HMA1	3:J:201:CYC:NB	2.18	0.59
3:B:201:CYC:NB	3:B:201:CYC:HMA1	2.18	0.58
3:H:201:CYC:NB	3:H:201:CYC:HMA1	2.18	0.58
3:L:201:CYC:NB	3:L:201:CYC:HMA1	2.19	0.57
3:F:201:CYC:NB	3:F:201:CYC:HMA1	2.19	0.57
1:G:117:ASN:ND2	5:G:456:HOH:O	2.38	0.55
1:A:117:ASN:ND2	5:A:456:HOH:O	2.38	0.55
1:K:45:GLU:HG3	5:K:345:HOH:O	2.10	0.51
1:E:45:GLU:HG3	5:E:345:HOH:O	2.10	0.51
1:C:6:GLN:NE2	5:C:420:HOH:O	2.45	0.50
1:I:6:GLN:NE2	5:I:420:HOH:O	2.45	0.50
1:E:162:HIS:HB3	1:E:163:HIS:CD2	2.46	0.50
2:D:76[B]:ARG:NH1	1:E:106:THR:O	2.45	0.49
1:K:162:HIS:HB3	1:K:163:HIS:CD2	2.46	0.49
2:H:131[B]:GLN:OE1	5:H:326:HOH:O	2.20	0.49
2:J:76[B]:ARG:NH1	1:K:106:THR:O	2.45	0.49
2:B:76[B]:ARG:NH1	1:C:106:THR:O	2.45	0.49
2:H:76[B]:ARG:NH1	1:I:106:THR:O	2.45	0.49
2:H:148:GLU:OE2	5:H:491:HOH:O	2.19	0.49
2:B:131[B]:GLN:OE1	5:B:327:HOH:O	2.20	0.49
1:C:2:SER:N	1:C:5[B]:SER:HG	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:GLU:OE2	5:B:492:HOH:O	2.20	0.49
1:A:45:GLU:HG3	5:A:336:HOH:O	2.12	0.48
1:E:163:HIS:CD2	1:E:163:HIS:N	2.80	0.48
1:I:2:SER:N	1:I:5[B]:SER:HG	2.11	0.48
1:K:163:HIS:CD2	1:K:163:HIS:N	2.80	0.48
1:G:45:GLU:HG3	5:G:336:HOH:O	2.12	0.48
2:L:148:GLU:OE2	5:L:385:HOH:O	2.20	0.48
1:G:101[A]:LYS:HD2	1:G:155:TYR:CE1	2.49	0.48
1:A:101[A]:LYS:HD2	1:A:155:TYR:CE1	2.49	0.48
2:F:148:GLU:OE2	5:F:385:HOH:O	2.19	0.48
2:D:148:GLU:OE2	5:D:508:HOH:O	2.20	0.47
1:C:45:GLU:HG3	5:C:331:HOH:O	2.15	0.47
1:I:45:GLU:HG3	5:I:331:HOH:O	2.15	0.47
2:J:148:GLU:OE2	5:J:508:HOH:O	2.20	0.47
1:K:101[A]:LYS:HD2	1:K:155:TYR:CE1	2.50	0.46
1:E:101[A]:LYS:HD2	1:E:155:TYR:CE1	2.50	0.46
1:I:162:HIS:HA	5:I:468:HOH:O	2.16	0.45
1:C:162:HIS:HA	5:C:468:HOH:O	2.16	0.45
1:E:87:TRP:CD1	1:E:90:ARG:HH21	2.35	0.45
1:K:87:TRP:CD1	1:K:90:ARG:HH21	2.35	0.45
1:A:23:LEU:HB3	2:B:38[B]:VAL:HG23	1.98	0.45
1:G:23:LEU:HB3	2:H:38[B]:VAL:HG23	1.98	0.45
1:C:27[B]:GLN:NE2	2:D:35:GLU:HA	2.32	0.45
1:I:27[B]:GLN:NE2	2:J:35:GLU:HA	2.33	0.44
1:C:87:TRP:CD1	1:C:90:ARG:HH21	2.34	0.44
1:I:87:TRP:CD1	1:I:90:ARG:HH21	2.34	0.44
1:A:106:THR:O	2:F:76[B]:ARG:NH1	2.51	0.44
1:G:106:THR:O	2:L:76[B]:ARG:NH1	2.51	0.44
1:A:27[B]:GLN:NE2	2:B:35:GLU:HA	2.35	0.42
1:A:87:TRP:CD1	1:A:90:ARG:HH21	2.37	0.42
1:G:27[B]:GLN:HE21	2:H:38[B]:VAL:HG11	1.85	0.42
1:G:27[B]:GLN:NE2	2:H:35:GLU:HA	2.35	0.42
1:A:27[B]:GLN:HE21	2:B:38[B]:VAL:HG11	1.85	0.42
2:F:2:GLN:OE1	5:F:512:HOH:O	2.21	0.42
1:G:87:TRP:CD1	1:G:90:ARG:HH21	2.37	0.42
1:I:23:LEU:HB3	2:J:38[B]:VAL:HG23	2.01	0.41
2:L:2:GLN:OE1	5:L:512:HOH:O	2.21	0.41
1:A:2:SER:HB2	1:A:98:ALA:O	2.21	0.41
1:C:23:LEU:HB3	2:D:38[B]:VAL:HG23	2.01	0.41
3:F:201:CYC:HMA3	3:F:201:CYC:HBA1	2.02	0.41
1:G:2:SER:HB2	1:G:98:ALA:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:201:CYC:HMA3	3:B:201:CYC:HBA1	2.03	0.41
3:J:201:CYC:HBA1	3:J:201:CYC:HMA3	2.02	0.41
3:L:201:CYC:HBA1	3:L:201:CYC:HMA3	2.02	0.41
3:D:201:CYC:HBA1	3:D:201:CYC:HMA3	2.02	0.41
3:H:201:CYC:HBA1	3:H:201:CYC:HMA3	2.03	0.41
3:D:201:CYC:HMA1	3:D:201:CYC:HB	1.85	0.40
1:E:101[A]:LYS:HD2	1:E:155:TYR:CZ	2.57	0.40
1:K:101[A]:LYS:HD2	1:K:155:TYR:CZ	2.56	0.40
1:A:2:SER:N	1:A:5:SER:HG	2.20	0.40
3:J:201:CYC:HMA1	3:J:201:CYC:HB	1.85	0.40
3:D:201:CYC:HB	3:D:201:CYC:CMA	2.35	0.40
1:I:27[B]:GLN:HE21	2:J:38[B]:VAL:HG11	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	165/167 (99%)	165 (100%)	0	0	100	100
1	C	166/167 (99%)	166 (100%)	0	0	100	100
1	E	165/167 (99%)	165 (100%)	0	0	100	100
1	G	165/167 (99%)	165 (100%)	0	0	100	100
1	I	166/167 (99%)	166 (100%)	0	0	100	100
1	K	165/167 (99%)	165 (100%)	0	0	100	100
2	B	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	D	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	F	165/161 (102%)	163 (99%)	2 (1%)	0	100	100
2	H	167/161 (104%)	165 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	167/161 (104%)	165 (99%)	2 (1%)	0	100	100
2	L	165/161 (102%)	163 (99%)	2 (1%)	0	100	100
All	All	1990/1968 (101%)	1978 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	139/139 (100%)	136 (98%)	3 (2%)	45	64
1	C	140/139 (101%)	136 (97%)	4 (3%)	37	58
1	E	139/139 (100%)	137 (99%)	2 (1%)	59	72
1	G	139/139 (100%)	136 (98%)	3 (2%)	45	64
1	I	140/139 (101%)	136 (97%)	4 (3%)	37	58
1	K	139/139 (100%)	137 (99%)	2 (1%)	59	72
2	B	133/124 (107%)	131 (98%)	2 (2%)	57	72
2	D	133/124 (107%)	133 (100%)	0	100	100
2	F	131/124 (106%)	130 (99%)	1 (1%)	73	80
2	H	133/124 (107%)	131 (98%)	2 (2%)	57	72
2	J	133/124 (107%)	133 (100%)	0	100	100
2	L	131/124 (106%)	130 (99%)	1 (1%)	73	80
All	All	1630/1578 (103%)	1606 (98%)	24 (2%)	59	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	101[A]	LYS
1	A	101[B]	LYS
2	B	36	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	113	LYS
1	C	85	TYR
1	C	101[A]	LYS
1	C	101[B]	LYS
1	C	158	GLN
1	E	85	TYR
1	E	163	HIS
2	F	36	LEU
1	G	85	TYR
1	G	101[A]	LYS
1	G	101[B]	LYS
2	H	36	LEU
2	H	113	LYS
1	I	85	TYR
1	I	101[A]	LYS
1	I	101[B]	LYS
1	I	158	GLN
1	K	85	TYR
1	K	163	HIS
2	L	36	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	15	GLN
1	E	158	GLN
1	E	163	HIS
2	H	15	GLN
1	K	158	GLN
1	K	163	HIS

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	J	71	2	7,8,9	0.84	0	4,9,11	1.50	1 (25%)
2	MEN	H	71	2	7,8,9	0.75	0	4,9,11	1.47	1 (25%)
2	MEN	B	71	2	7,8,9	0.77	0	4,9,11	1.44	1 (25%)
2	MEN	D	71	2	7,8,9	0.82	0	4,9,11	1.47	1 (25%)
2	MEN	L	71	2	7,8,9	0.84	0	4,9,11	1.30	1 (25%)
2	MEN	F	71	2	7,8,9	0.82	0	4,9,11	1.31	1 (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
2	MEN	J	71	2	-	2/7/8/10	-
2	MEN	H	71	2	-	2/7/8/10	-
2	MEN	B	71	2	-	2/7/8/10	-
2	MEN	D	71	2	-	2/7/8/10	-
2	MEN	L	71	2	-	2/7/8/10	-
2	MEN	F	71	2	-	2/7/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	71	MEN	CB-CG-ND2	2.28	118.51	115.53
2	B	71	MEN	CB-CG-ND2	2.24	118.46	115.53
2	J	71	MEN	CB-CG-ND2	2.22	118.42	115.53
2	D	71	MEN	CB-CG-ND2	2.20	118.40	115.53
2	L	71	MEN	CB-CG-ND2	2.09	118.26	115.53
2	F	71	MEN	CB-CG-ND2	2.08	118.25	115.53

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	H	71	MEN	CA-CB-CG-OD1
2	J	71	MEN	CA-CB-CG-OD1
2	F	71	MEN	CA-CB-CG-OD1
2	L	71	MEN	CA-CB-CG-OD1
2	F	71	MEN	CA-CB-CG-ND2
2	J	71	MEN	CA-CB-CG-ND2
2	L	71	MEN	CA-CB-CG-ND2
2	B	71	MEN	CA-CB-CG-ND2
2	D	71	MEN	CA-CB-CG-ND2
2	H	71	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	SO4	J	205	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	J	203	-	4,4,4	0.21	0	6,6,6	0.18	0
4	SO4	K	202	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	D	206	-	4,4,4	0.25	0	6,6,6	0.07	0
3	CYC	K	201[B]	-	46,46,46	4.04	13 (28%)	63,67,67	2.19	26 (41%)
3	CYC	A	201[B]	-	46,46,46	4.00	12 (26%)	63,67,67	2.18	26 (41%)
3	CYC	G	201[B]	-	46,46,46	4.00	12 (26%)	63,67,67	2.17	26 (41%)
4	SO4	C	202	-	4,4,4	0.24	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	L	204	-	4,4,4	0.24	0	6,6,6	0.10	0
3	CYC	E	201[B]	-	46,46,46	4.02	14 (30%)	63,67,67	2.19	25 (39%)
4	SO4	B	206	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	A	203	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	B	202	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	F	204	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	L	202	-	4,4,4	0.22	0	6,6,6	0.07	0
4	SO4	H	203	-	4,4,4	0.22	0	6,6,6	0.16	0
3	CYC	B	201	2	46,46,46	4.27	16 (34%)	63,67,67	2.31	22 (34%)
3	CYC	F	201	2	46,46,46	4.22	15 (32%)	63,67,67	2.13	20 (31%)
4	SO4	J	202	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	H	202	-	4,4,4	0.24	0	6,6,6	0.07	0
3	CYC	D	201	2	46,46,46	4.28	15 (32%)	63,67,67	2.30	20 (31%)
4	SO4	J	206	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	F	202	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	J	204	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	E	203	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	D	204	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	F	203	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	D	203	-	4,4,4	0.20	0	6,6,6	0.17	0
4	SO4	G	203	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	I	203	-	4,4,4	0.26	0	6,6,6	0.07	0
3	CYC	C	201[A]	-	46,46,46	4.08	13 (28%)	63,67,67	2.25	30 (47%)
4	SO4	L	205	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	I	202	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	B	205	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	H	204	-	4,4,4	0.24	0	6,6,6	0.09	0
3	CYC	I	201[A]	-	46,46,46	4.06	13 (28%)	63,67,67	2.25	30 (47%)
4	SO4	C	203	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	D	205	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	L	206	-	4,4,4	0.24	0	6,6,6	0.09	0
3	CYC	L	201	2	46,46,46	4.23	15 (32%)	63,67,67	2.13	20 (31%)
4	SO4	G	202	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	H	206	-	4,4,4	0.24	0	6,6,6	0.09	0
3	CYC	C	201[B]	-	46,46,46	4.09	13 (28%)	63,67,67	2.23	29 (46%)
3	CYC	H	201	2	46,46,46	4.28	17 (36%)	63,67,67	2.31	23 (36%)
4	SO4	H	205	-	4,4,4	0.24	0	6,6,6	0.08	0
3	CYC	I	201[B]	-	46,46,46	4.07	13 (28%)	63,67,67	2.23	29 (46%)
4	SO4	F	205	-	4,4,4	0.23	0	6,6,6	0.07	0
3	CYC	J	201	2	46,46,46	4.27	16 (34%)	63,67,67	2.30	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	202	-	4,4,4	0.25	0	6,6,6	0.10	0
4	SO4	B	204	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	L	203	-	4,4,4	0.22	0	6,6,6	0.18	0
4	SO4	E	202	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	F	206	-	4,4,4	0.25	0	6,6,6	0.09	0
3	CYC	K	201[A]	-	46,46,46	4.03	13 (28%)	63,67,67	2.21	27 (42%)
3	CYC	A	201[A]	-	46,46,46	3.99	12 (26%)	63,67,67	2.20	27 (42%)
4	SO4	B	203	-	4,4,4	0.22	0	6,6,6	0.15	0
3	CYC	G	201[A]	-	46,46,46	4.00	12 (26%)	63,67,67	2.20	27 (42%)
3	CYC	E	201[A]	-	46,46,46	4.01	14 (30%)	63,67,67	2.21	26 (41%)
4	SO4	A	202	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	K	203	-	4,4,4	0.26	0	6,6,6	0.07	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
3	CYC	B	201	2	-	10/26/74/74	0/4/4/4
3	CYC	F	201	2	-	10/26/74/74	0/4/4/4
3	CYC	H	201	2	-	10/26/74/74	0/4/4/4
3	CYC	D	201	2	-	11/26/74/74	0/4/4/4
3	CYC	C	201[A]	-	-	8/26/74/74	0/4/4/4
3	CYC	I	201[B]	-	-	6/26/74/74	0/4/4/4
3	CYC	J	201	2	-	11/26/74/74	0/4/4/4
3	CYC	K	201[B]	-	-	6/26/74/74	0/4/4/4
3	CYC	A	201[B]	-	-	6/26/74/74	0/4/4/4
3	CYC	G	201[B]	-	-	6/26/74/74	0/4/4/4
3	CYC	I	201[A]	-	-	8/26/74/74	0/4/4/4
3	CYC	E	201[A]	-	-	7/26/74/74	0/4/4/4
3	CYC	K	201[A]	-	-	7/26/74/74	0/4/4/4
3	CYC	A	201[A]	-	-	7/26/74/74	0/4/4/4
3	CYC	E	201[B]	-	-	6/26/74/74	0/4/4/4
3	CYC	G	201[A]	-	-	7/26/74/74	0/4/4/4
3	CYC	L	201	2	-	10/26/74/74	0/4/4/4
3	CYC	C	201[B]	-	-	6/26/74/74	0/4/4/4

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	201	CYC	C2C-C1C	-20.51	1.33	1.52
3	J	201	CYC	C2C-C1C	-20.51	1.33	1.52
3	H	201	CYC	C2C-C1C	-20.39	1.33	1.52
3	B	201	CYC	C2C-C1C	-20.34	1.34	1.52
3	F	201	CYC	C2C-C1C	-20.08	1.34	1.52
3	L	201	CYC	C2C-C1C	-20.07	1.34	1.52
3	C	201[A]	CYC	C2C-C1C	-19.88	1.34	1.52
3	C	201[B]	CYC	C2C-C1C	-19.88	1.34	1.52
3	I	201[A]	CYC	C2C-C1C	-19.68	1.34	1.52
3	I	201[B]	CYC	C2C-C1C	-19.68	1.34	1.52
3	K	201[A]	CYC	C2C-C1C	-19.50	1.34	1.52
3	K	201[B]	CYC	C2C-C1C	-19.50	1.34	1.52
3	E	201[A]	CYC	C2C-C1C	-19.32	1.34	1.52
3	E	201[B]	CYC	C2C-C1C	-19.32	1.34	1.52
3	G	201[A]	CYC	C2C-C1C	-19.07	1.35	1.52
3	G	201[B]	CYC	C2C-C1C	-19.07	1.35	1.52
3	A	201[A]	CYC	C2C-C1C	-19.05	1.35	1.52
3	A	201[B]	CYC	C2C-C1C	-19.05	1.35	1.52
3	I	201[A]	CYC	C4B-C3B	-8.17	1.33	1.48
3	I	201[B]	CYC	C4B-C3B	-8.17	1.33	1.48
3	A	201[A]	CYC	C4B-C3B	-8.15	1.33	1.48
3	A	201[B]	CYC	C4B-C3B	-8.15	1.33	1.48
3	G	201[A]	CYC	C4B-C3B	-8.15	1.33	1.48
3	G	201[B]	CYC	C4B-C3B	-8.15	1.33	1.48
3	H	201	CYC	C4B-C3B	-8.12	1.33	1.48
3	C	201[A]	CYC	C4B-C3B	-8.11	1.33	1.48
3	C	201[B]	CYC	C4B-C3B	-8.11	1.33	1.48
3	B	201	CYC	C4B-C3B	-8.05	1.33	1.48
3	L	201	CYC	C4B-C3B	-7.94	1.33	1.48
3	K	201[A]	CYC	C4B-C3B	-7.92	1.33	1.48
3	K	201[B]	CYC	C4B-C3B	-7.92	1.33	1.48
3	E	201[A]	CYC	C4B-C3B	-7.92	1.33	1.48
3	E	201[B]	CYC	C4B-C3B	-7.92	1.33	1.48
3	F	201	CYC	C4B-C3B	-7.92	1.33	1.48
3	D	201	CYC	C4B-C3B	-7.89	1.33	1.48
3	J	201	CYC	C4B-C3B	-7.84	1.33	1.48
3	J	201	CYC	CAB-C3B	-6.91	1.33	1.51
3	L	201	CYC	OB-C4B	6.90	1.36	1.23
3	B	201	CYC	CAB-C3B	-6.89	1.33	1.51
3	H	201	CYC	OB-C4B	6.87	1.36	1.23
3	D	201	CYC	CAB-C3B	-6.87	1.33	1.51
3	D	201	CYC	OB-C4B	6.86	1.36	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	CYC	CAB-C3B	-6.85	1.33	1.51
3	J	201	CYC	OB-C4B	6.83	1.36	1.23
3	B	201	CYC	OB-C4B	6.82	1.36	1.23
3	F	201	CYC	OB-C4B	6.79	1.36	1.23
3	F	201	CYC	CAB-C3B	-6.78	1.33	1.51
3	L	201	CYC	CAB-C3B	-6.76	1.33	1.51
3	G	201[A]	CYC	OB-C4B	6.74	1.36	1.23
3	G	201[B]	CYC	OB-C4B	6.74	1.36	1.23
3	A	201[A]	CYC	OB-C4B	6.68	1.36	1.23
3	A	201[B]	CYC	OB-C4B	6.68	1.36	1.23
3	L	201	CYC	C1A-C2A	-6.61	1.35	1.45
3	C	201[A]	CYC	OB-C4B	6.58	1.36	1.23
3	C	201[B]	CYC	OB-C4B	6.58	1.36	1.23
3	K	201[A]	CYC	OB-C4B	6.57	1.36	1.23
3	K	201[B]	CYC	OB-C4B	6.57	1.36	1.23
3	J	201	CYC	C1A-C2A	-6.56	1.35	1.45
3	F	201	CYC	C1A-C2A	-6.55	1.35	1.45
3	I	201[A]	CYC	OB-C4B	6.55	1.36	1.23
3	I	201[B]	CYC	OB-C4B	6.55	1.36	1.23
3	E	201[A]	CYC	OB-C4B	6.54	1.36	1.23
3	E	201[B]	CYC	OB-C4B	6.54	1.36	1.23
3	H	201	CYC	C2C-C3C	-6.54	1.36	1.54
3	D	201	CYC	C1A-C2A	-6.52	1.35	1.45
3	B	201	CYC	C2C-C3C	-6.52	1.36	1.54
3	C	201[A]	CYC	C2C-C3C	-6.50	1.36	1.54
3	C	201[B]	CYC	C2C-C3C	-6.50	1.36	1.54
3	B	201	CYC	C1A-C2A	-6.49	1.35	1.45
3	H	201	CYC	C1A-C2A	-6.49	1.35	1.45
3	I	201[A]	CYC	C2C-C3C	-6.48	1.36	1.54
3	I	201[B]	CYC	C2C-C3C	-6.48	1.36	1.54
3	F	201	CYC	C2C-C3C	-6.42	1.37	1.54
3	A	201[A]	CYC	C2C-C3C	-6.42	1.37	1.54
3	A	201[B]	CYC	C2C-C3C	-6.42	1.37	1.54
3	G	201[A]	CYC	C2C-C3C	-6.40	1.37	1.54
3	G	201[B]	CYC	C2C-C3C	-6.40	1.37	1.54
3	L	201	CYC	C2C-C3C	-6.38	1.37	1.54
3	D	201	CYC	C2C-C3C	-6.34	1.37	1.54
3	E	201[A]	CYC	C2C-C3C	-6.32	1.37	1.54
3	E	201[B]	CYC	C2C-C3C	-6.32	1.37	1.54
3	J	201	CYC	C2C-C3C	-6.29	1.37	1.54
3	K	201[A]	CYC	C2C-C3C	-6.29	1.37	1.54
3	K	201[B]	CYC	C2C-C3C	-6.29	1.37	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201[A]	CYC	C1A-C2A	-6.20	1.36	1.45
3	A	201[B]	CYC	C1A-C2A	-6.20	1.36	1.45
3	C	201[A]	CYC	C1A-C2A	-6.20	1.36	1.45
3	C	201[B]	CYC	C1A-C2A	-6.20	1.36	1.45
3	G	201[A]	CYC	C1A-C2A	-6.19	1.36	1.45
3	G	201[B]	CYC	C1A-C2A	-6.19	1.36	1.45
3	I	201[A]	CYC	C1A-C2A	-6.16	1.36	1.45
3	I	201[B]	CYC	C1A-C2A	-6.16	1.36	1.45
3	K	201[A]	CYC	CAB-C3B	-6.13	1.35	1.51
3	K	201[B]	CYC	CAB-C3B	-6.13	1.35	1.51
3	E	201[A]	CYC	CAB-C3B	-6.12	1.35	1.51
3	E	201[B]	CYC	CAB-C3B	-6.12	1.35	1.51
3	C	201[A]	CYC	CAB-C3B	-6.11	1.35	1.51
3	C	201[B]	CYC	CAB-C3B	-6.11	1.35	1.51
3	K	201[A]	CYC	C1A-C2A	-6.10	1.36	1.45
3	K	201[B]	CYC	C1A-C2A	-6.10	1.36	1.45
3	I	201[A]	CYC	CAB-C3B	-6.08	1.35	1.51
3	I	201[B]	CYC	CAB-C3B	-6.08	1.35	1.51
3	E	201[A]	CYC	C1A-C2A	-6.07	1.36	1.45
3	E	201[B]	CYC	C1A-C2A	-6.07	1.36	1.45
3	L	201	CYC	C1B-C2B	-6.04	1.34	1.45
3	A	201[A]	CYC	CAB-C3B	-6.02	1.35	1.51
3	A	201[B]	CYC	CAB-C3B	-6.02	1.35	1.51
3	I	201[A]	CYC	C3C-C4C	-6.02	1.38	1.50
3	I	201[B]	CYC	C3C-C4C	-6.02	1.38	1.50
3	D	201	CYC	C1B-C2B	-6.01	1.34	1.45
3	E	201[A]	CYC	C3C-C4C	-6.00	1.38	1.50
3	E	201[B]	CYC	C3C-C4C	-6.00	1.38	1.50
3	K	201[A]	CYC	C3C-C4C	-6.00	1.38	1.50
3	K	201[B]	CYC	C3C-C4C	-6.00	1.38	1.50
3	F	201	CYC	C1B-C2B	-6.00	1.34	1.45
3	G	201[A]	CYC	CAB-C3B	-5.99	1.35	1.51
3	G	201[B]	CYC	CAB-C3B	-5.99	1.35	1.51
3	B	201	CYC	C1B-C2B	-5.99	1.34	1.45
3	H	201	CYC	C1B-C2B	-5.98	1.34	1.45
3	B	201	CYC	C3C-C4C	-5.96	1.38	1.50
3	H	201	CYC	C3C-C4C	-5.96	1.38	1.50
3	J	201	CYC	C1B-C2B	-5.94	1.34	1.45
3	C	201[A]	CYC	C3C-C4C	-5.92	1.38	1.50
3	C	201[B]	CYC	C3C-C4C	-5.92	1.38	1.50
3	L	201	CYC	C3C-C4C	-5.90	1.38	1.50
3	D	201	CYC	C3C-C4C	-5.86	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	CYC	C3C-C4C	-5.84	1.38	1.50
3	G	201[A]	CYC	C3C-C4C	-5.83	1.38	1.50
3	G	201[B]	CYC	C3C-C4C	-5.83	1.38	1.50
3	A	201[A]	CYC	C3C-C4C	-5.81	1.38	1.50
3	A	201[B]	CYC	C3C-C4C	-5.81	1.38	1.50
3	J	201	CYC	C3C-C4C	-5.77	1.38	1.50
3	E	201[A]	CYC	C1B-C2B	-4.79	1.36	1.45
3	E	201[B]	CYC	C1B-C2B	-4.79	1.36	1.45
3	K	201[A]	CYC	C1B-C2B	-4.72	1.36	1.45
3	K	201[B]	CYC	C1B-C2B	-4.72	1.36	1.45
3	H	201	CYC	C4A-C3A	-4.71	1.35	1.45
3	B	201	CYC	C4A-C3A	-4.67	1.35	1.45
3	A	201[A]	CYC	C1B-C2B	-4.62	1.36	1.45
3	A	201[B]	CYC	C1B-C2B	-4.62	1.36	1.45
3	C	201[A]	CYC	C1B-C2B	-4.62	1.36	1.45
3	C	201[B]	CYC	C1B-C2B	-4.62	1.36	1.45
3	G	201[A]	CYC	C1B-C2B	-4.60	1.36	1.45
3	G	201[B]	CYC	C1B-C2B	-4.60	1.36	1.45
3	I	201[A]	CYC	C1B-C2B	-4.59	1.36	1.45
3	I	201[B]	CYC	C1B-C2B	-4.59	1.36	1.45
3	F	201	CYC	C4A-C3A	-4.57	1.35	1.45
3	L	201	CYC	C4A-C3A	-4.54	1.36	1.45
3	D	201	CYC	C4A-C3A	-4.53	1.36	1.45
3	J	201	CYC	C4A-C3A	-4.53	1.36	1.45
3	G	201[A]	CYC	C4A-C3A	-4.46	1.36	1.45
3	G	201[B]	CYC	C4A-C3A	-4.46	1.36	1.45
3	A	201[A]	CYC	C4A-C3A	-4.39	1.36	1.45
3	A	201[B]	CYC	C4A-C3A	-4.39	1.36	1.45
3	I	201[A]	CYC	C4A-C3A	-4.35	1.36	1.45
3	I	201[B]	CYC	C4A-C3A	-4.35	1.36	1.45
3	C	201[A]	CYC	C4A-C3A	-4.32	1.36	1.45
3	C	201[B]	CYC	C4A-C3A	-4.32	1.36	1.45
3	E	201[A]	CYC	C4A-C3A	-4.21	1.36	1.45
3	E	201[B]	CYC	C4A-C3A	-4.21	1.36	1.45
3	K	201[A]	CYC	C4A-C3A	-4.18	1.36	1.45
3	K	201[B]	CYC	C4A-C3A	-4.18	1.36	1.45
3	B	201	CYC	C4D-C3D	-3.19	1.35	1.42
3	H	201	CYC	C4D-C3D	-3.18	1.35	1.42
3	L	201	CYC	C4D-C3D	-3.16	1.35	1.42
3	B	201	CYC	C1C-NC	-3.15	1.33	1.37
3	F	201	CYC	C4D-C3D	-3.12	1.35	1.42
3	H	201	CYC	C1C-NC	-3.11	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	201	CYC	C1C-NC	-3.05	1.33	1.37
3	J	201	CYC	C1C-NC	-3.02	1.33	1.37
3	L	201	CYC	C1C-NC	-3.01	1.33	1.37
3	D	201	CYC	C1C-NC	-3.00	1.33	1.37
3	K	201[A]	CYC	CMD-C2D	2.97	1.56	1.50
3	K	201[B]	CYC	CMD-C2D	2.97	1.56	1.50
3	J	201	CYC	C4D-C3D	-2.95	1.36	1.42
3	C	201[A]	CYC	C4D-C3D	-2.91	1.36	1.42
3	C	201[B]	CYC	C4D-C3D	-2.91	1.36	1.42
3	D	201	CYC	C4D-C3D	-2.90	1.36	1.42
3	E	201[A]	CYC	CMD-C2D	2.89	1.56	1.50
3	E	201[B]	CYC	CMD-C2D	2.89	1.56	1.50
3	I	201[A]	CYC	C4D-C3D	-2.86	1.36	1.42
3	I	201[B]	CYC	C4D-C3D	-2.86	1.36	1.42
3	G	201[A]	CYC	C4D-C3D	-2.82	1.36	1.42
3	G	201[B]	CYC	C4D-C3D	-2.82	1.36	1.42
3	A	201[A]	CYC	C4D-C3D	-2.79	1.36	1.42
3	A	201[B]	CYC	C4D-C3D	-2.79	1.36	1.42
3	D	201	CYC	CMA-C3A	2.79	1.56	1.50
3	J	201	CYC	CMA-C3A	2.71	1.56	1.50
3	A	201[A]	CYC	C1C-NC	-2.70	1.34	1.37
3	A	201[B]	CYC	C1C-NC	-2.70	1.34	1.37
3	G	201[A]	CYC	CMD-C2D	2.69	1.56	1.50
3	G	201[B]	CYC	CMD-C2D	2.69	1.56	1.50
3	A	201[A]	CYC	CMD-C2D	2.68	1.56	1.50
3	A	201[B]	CYC	CMD-C2D	2.68	1.56	1.50
3	H	201	CYC	CMA-C3A	2.68	1.56	1.50
3	B	201	CYC	CMA-C3A	2.66	1.56	1.50
3	G	201[A]	CYC	C1C-NC	-2.66	1.34	1.37
3	G	201[B]	CYC	C1C-NC	-2.66	1.34	1.37
3	K	201[A]	CYC	C1C-NC	-2.61	1.34	1.37
3	K	201[B]	CYC	C1C-NC	-2.61	1.34	1.37
3	C	201[A]	CYC	C1C-NC	-2.60	1.34	1.37
3	C	201[B]	CYC	C1C-NC	-2.60	1.34	1.37
3	K	201[A]	CYC	C4D-C3D	-2.57	1.37	1.42
3	K	201[B]	CYC	C4D-C3D	-2.57	1.37	1.42
3	E	201[A]	CYC	C4D-C3D	-2.57	1.37	1.42
3	E	201[B]	CYC	C4D-C3D	-2.57	1.37	1.42
3	I	201[A]	CYC	C1C-NC	-2.54	1.34	1.37
3	I	201[B]	CYC	C1C-NC	-2.54	1.34	1.37
3	E	201[A]	CYC	C1C-NC	-2.50	1.34	1.37
3	E	201[B]	CYC	C1C-NC	-2.50	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	201	CYC	CMA-C3A	2.49	1.55	1.50
3	F	201	CYC	CMA-C3A	2.47	1.55	1.50
3	D	201	CYC	CMD-C2D	2.40	1.55	1.50
3	J	201	CYC	CMD-C2D	2.31	1.55	1.50
3	H	201	CYC	C1A-NA	-2.29	1.33	1.38
3	J	201	CYC	CBD-CGD	2.27	1.55	1.50
3	C	201[A]	CYC	CMD-C2D	2.26	1.55	1.50
3	C	201[B]	CYC	CMD-C2D	2.26	1.55	1.50
3	I	201[A]	CYC	CMD-C2D	2.26	1.55	1.50
3	I	201[B]	CYC	CMD-C2D	2.26	1.55	1.50
3	B	201	CYC	C1A-NA	-2.25	1.33	1.38
3	D	201	CYC	CBD-CGD	2.24	1.55	1.50
3	L	201	CYC	C1D-C2D	-2.24	1.36	1.41
3	H	201	CYC	CBD-CGD	2.23	1.55	1.50
3	B	201	CYC	CBD-CGD	2.21	1.55	1.50
3	J	201	CYC	C1D-C2D	-2.21	1.36	1.41
3	K	201[A]	CYC	CMA-C3A	2.19	1.55	1.50
3	K	201[B]	CYC	CMA-C3A	2.19	1.55	1.50
3	L	201	CYC	CMD-C2D	2.19	1.55	1.50
3	F	201	CYC	C1D-C2D	-2.18	1.36	1.41
3	H	201	CYC	C1D-C2D	-2.18	1.36	1.41
3	D	201	CYC	C1D-C2D	-2.17	1.36	1.41
3	L	201	CYC	CBD-CGD	2.14	1.55	1.50
3	E	201[A]	CYC	CMA-C3A	2.14	1.55	1.50
3	E	201[B]	CYC	CMA-C3A	2.14	1.55	1.50
3	F	201	CYC	CMD-C2D	2.14	1.55	1.50
3	F	201	CYC	CBD-CGD	2.13	1.55	1.50
3	B	201	CYC	C1D-C2D	-2.10	1.36	1.41
3	I	201[A]	CYC	CMA-C3A	2.10	1.55	1.50
3	I	201[B]	CYC	CMA-C3A	2.10	1.55	1.50
3	C	201[A]	CYC	CMA-C3A	2.09	1.55	1.50
3	C	201[B]	CYC	CMA-C3A	2.09	1.55	1.50
3	H	201	CYC	CMD-C2D	2.07	1.55	1.50
3	H	201	CYC	C1B-NB	-2.05	1.34	1.37
3	B	201	CYC	C1B-NB	-2.04	1.34	1.37
3	J	201	CYC	C1A-NA	-2.03	1.34	1.38
3	E	201[A]	CYC	CMB-C2B	2.03	1.54	1.50
3	E	201[B]	CYC	CMB-C2B	2.03	1.54	1.50

All (453) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	CYC	CBB-CAB-C3B	11.27	142.98	112.42
3	J	201	CYC	CBB-CAB-C3B	11.24	142.88	112.42
3	H	201	CYC	CBB-CAB-C3B	11.17	142.70	112.42
3	B	201	CYC	CBB-CAB-C3B	11.15	142.65	112.42
3	F	201	CYC	CBB-CAB-C3B	8.54	135.57	112.42
3	L	201	CYC	CBB-CAB-C3B	8.49	135.44	112.42
3	I	201[A]	CYC	C1C-NC-C4C	-5.11	107.00	113.41
3	I	201[B]	CYC	C1C-NC-C4C	-5.11	107.00	113.41
3	C	201[A]	CYC	C1C-NC-C4C	-5.06	107.06	113.41
3	C	201[B]	CYC	C1C-NC-C4C	-5.06	107.06	113.41
3	C	201[A]	CYC	CBB-CAB-C3B	5.00	125.97	112.42
3	C	201[B]	CYC	CBB-CAB-C3B	5.00	125.97	112.42
3	I	201[A]	CYC	CBB-CAB-C3B	4.99	125.96	112.42
3	I	201[B]	CYC	CBB-CAB-C3B	4.99	125.96	112.42
3	E	201[A]	CYC	C1C-NC-C4C	-4.99	107.15	113.41
3	E	201[B]	CYC	C1C-NC-C4C	-4.99	107.15	113.41
3	K	201[A]	CYC	C1C-NC-C4C	-4.97	107.17	113.41
3	K	201[B]	CYC	C1C-NC-C4C	-4.97	107.17	113.41
3	G	201[A]	CYC	C1C-NC-C4C	-4.86	107.31	113.41
3	G	201[B]	CYC	C1C-NC-C4C	-4.86	107.31	113.41
3	A	201[A]	CYC	C1C-NC-C4C	-4.85	107.32	113.41
3	A	201[B]	CYC	C1C-NC-C4C	-4.85	107.32	113.41
3	A	201[A]	CYC	CBB-CAB-C3B	4.83	125.51	112.42
3	A	201[B]	CYC	CBB-CAB-C3B	4.83	125.51	112.42
3	G	201[A]	CYC	CBB-CAB-C3B	4.82	125.50	112.42
3	G	201[B]	CYC	CBB-CAB-C3B	4.82	125.50	112.42
3	I	201[A]	CYC	CHB-C4A-C3A	4.74	137.05	124.87
3	I	201[B]	CYC	CHB-C4A-C3A	4.74	137.05	124.87
3	C	201[A]	CYC	CHB-C4A-C3A	4.71	136.98	124.87
3	C	201[B]	CYC	CHB-C4A-C3A	4.71	136.98	124.87
3	E	201[A]	CYC	CHB-C4A-C3A	4.68	136.90	124.87
3	E	201[B]	CYC	CHB-C4A-C3A	4.68	136.90	124.87
3	K	201[A]	CYC	CHB-C4A-C3A	4.68	136.90	124.87
3	K	201[B]	CYC	CHB-C4A-C3A	4.68	136.90	124.87
3	G	201[A]	CYC	CHB-C4A-C3A	4.59	136.66	124.87
3	G	201[B]	CYC	CHB-C4A-C3A	4.59	136.66	124.87
3	F	201	CYC	C1C-NC-C4C	-4.54	107.71	113.41
3	A	201[A]	CYC	CHB-C4A-C3A	4.54	136.53	124.87
3	A	201[B]	CYC	CHB-C4A-C3A	4.54	136.53	124.87
3	L	201	CYC	C1C-NC-C4C	-4.49	107.78	113.41
3	H	201	CYC	C1C-NC-C4C	-4.46	107.81	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	CYC	C1C-NC-C4C	-4.46	107.82	113.41
3	D	201	CYC	C1C-NC-C4C	-4.22	108.11	113.41
3	E	201[A]	CYC	C2C-C3C-C4C	4.21	107.64	101.34
3	E	201[B]	CYC	C2C-C3C-C4C	4.21	107.64	101.34
3	K	201[A]	CYC	C2C-C3C-C4C	4.20	107.63	101.34
3	K	201[B]	CYC	C2C-C3C-C4C	4.20	107.63	101.34
3	L	201	CYC	C2C-C3C-C4C	4.17	107.59	101.34
3	I	201[A]	CYC	C2C-C3C-C4C	4.13	107.52	101.34
3	I	201[B]	CYC	C2C-C3C-C4C	4.13	107.52	101.34
3	C	201[A]	CYC	C2C-C3C-C4C	4.12	107.52	101.34
3	C	201[B]	CYC	C2C-C3C-C4C	4.12	107.52	101.34
3	D	201	CYC	C2C-C3C-C4C	4.12	107.51	101.34
3	J	201	CYC	C1C-NC-C4C	-4.12	108.24	113.41
3	F	201	CYC	C2C-C3C-C4C	4.11	107.50	101.34
3	J	201	CYC	C2C-C3C-C4C	4.11	107.49	101.34
3	B	201	CYC	C2C-C3C-C4C	4.07	107.43	101.34
3	H	201	CYC	C2C-C3C-C4C	4.05	107.41	101.34
3	A	201[A]	CYC	C2C-C3C-C4C	3.98	107.30	101.34
3	A	201[B]	CYC	C2C-C3C-C4C	3.98	107.30	101.34
3	G	201[A]	CYC	C2C-C3C-C4C	3.98	107.30	101.34
3	G	201[B]	CYC	C2C-C3C-C4C	3.98	107.30	101.34
3	I	201[A]	CYC	CHB-C4A-NA	-3.59	117.20	124.95
3	I	201[B]	CYC	CHB-C4A-NA	-3.59	117.20	124.95
3	C	201[A]	CYC	CHB-C4A-NA	-3.56	117.26	124.95
3	C	201[B]	CYC	CHB-C4A-NA	-3.56	117.26	124.95
3	E	201[A]	CYC	C2A-C1A-NA	-3.54	105.03	110.04
3	E	201[B]	CYC	C2A-C1A-NA	-3.54	105.03	110.04
3	I	201[A]	CYC	C3B-C4B-NB	3.54	109.59	106.77
3	I	201[B]	CYC	C3B-C4B-NB	3.54	109.59	106.77
3	C	201[A]	CYC	C3B-C4B-NB	3.53	109.58	106.77
3	C	201[B]	CYC	C3B-C4B-NB	3.53	109.58	106.77
3	K	201[A]	CYC	CBB-CAB-C3B	3.52	121.97	112.42
3	K	201[B]	CYC	CBB-CAB-C3B	3.52	121.97	112.42
3	K	201[A]	CYC	C2A-C1A-NA	-3.50	105.09	110.04
3	K	201[B]	CYC	C2A-C1A-NA	-3.50	105.09	110.04
3	E	201[A]	CYC	CBB-CAB-C3B	3.49	121.89	112.42
3	E	201[B]	CYC	CBB-CAB-C3B	3.49	121.89	112.42
3	E	201[A]	CYC	C3B-C4B-NB	3.48	109.54	106.77
3	E	201[B]	CYC	C3B-C4B-NB	3.48	109.54	106.77
3	E	201[A]	CYC	CHB-C4A-NA	-3.48	117.44	124.95
3	E	201[B]	CYC	CHB-C4A-NA	-3.48	117.44	124.95
3	K	201[A]	CYC	CHB-C4A-NA	-3.47	117.47	124.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	201[B]	CYC	CHB-C4A-NA	-3.47	117.47	124.95
3	G	201[A]	CYC	C3B-C4B-NB	3.46	109.53	106.77
3	G	201[B]	CYC	C3B-C4B-NB	3.46	109.53	106.77
3	F	201	CYC	CMA-C3A-C4A	3.45	130.45	125.10
3	K	201[A]	CYC	C3B-C4B-NB	3.44	109.51	106.77
3	K	201[B]	CYC	C3B-C4B-NB	3.44	109.51	106.77
3	A	201[A]	CYC	CHD-C1D-C2D	3.44	135.95	127.53
3	A	201[B]	CYC	CHD-C1D-C2D	3.44	135.95	127.53
3	A	201[A]	CYC	C3B-C4B-NB	3.43	109.50	106.77
3	A	201[B]	CYC	C3B-C4B-NB	3.43	109.50	106.77
3	L	201	CYC	CMA-C3A-C4A	3.43	130.42	125.10
3	G	201[A]	CYC	CHD-C1D-C2D	3.42	135.90	127.53
3	G	201[B]	CYC	CHD-C1D-C2D	3.42	135.90	127.53
3	E	201[A]	CYC	CAD-C3D-C4D	-3.42	120.35	125.77
3	E	201[B]	CYC	CAD-C3D-C4D	-3.42	120.35	125.77
3	E	201[A]	CYC	CHD-C1D-C2D	3.40	135.85	127.53
3	E	201[B]	CYC	CHD-C1D-C2D	3.40	135.85	127.53
3	K	201[A]	CYC	CHD-C1D-C2D	3.39	135.84	127.53
3	K	201[B]	CYC	CHD-C1D-C2D	3.39	135.84	127.53
3	K	201[A]	CYC	CAD-C3D-C4D	-3.39	120.39	125.77
3	K	201[B]	CYC	CAD-C3D-C4D	-3.39	120.39	125.77
3	A	201[A]	CYC	CHB-C1B-NB	3.38	133.28	126.06
3	A	201[B]	CYC	CHB-C1B-NB	3.38	133.28	126.06
3	G	201[A]	CYC	CHB-C4A-NA	-3.37	117.67	124.95
3	G	201[B]	CYC	CHB-C4A-NA	-3.37	117.67	124.95
3	G	201[A]	CYC	CHB-C1B-NB	3.37	133.24	126.06
3	G	201[B]	CYC	CHB-C1B-NB	3.37	133.24	126.06
3	A	201[A]	CYC	CHB-C4A-NA	-3.32	117.77	124.95
3	A	201[B]	CYC	CHB-C4A-NA	-3.32	117.77	124.95
3	C	201[A]	CYC	C2A-C1A-NA	-3.30	105.37	110.04
3	C	201[B]	CYC	C2A-C1A-NA	-3.30	105.37	110.04
3	I	201[A]	CYC	C2A-C1A-NA	-3.29	105.39	110.04
3	I	201[B]	CYC	C2A-C1A-NA	-3.29	105.39	110.04
3	E	201[A]	CYC	CHD-C1D-ND	-3.28	117.88	125.29
3	E	201[B]	CYC	CHD-C1D-ND	-3.28	117.88	125.29
3	H	201	CYC	CHD-C1D-C2D	3.27	135.54	127.53
3	K	201[A]	CYC	CHD-C1D-ND	-3.25	117.94	125.29
3	K	201[B]	CYC	CHD-C1D-ND	-3.25	117.94	125.29
3	F	201	CYC	C2A-C1A-NA	-3.24	105.45	110.04
3	L	201	CYC	CHD-C1D-C2D	3.24	135.47	127.53
3	B	201	CYC	C2A-C1A-NA	-3.23	105.47	110.04
3	D	201	CYC	CHD-C1D-C2D	3.23	135.45	127.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	CYC	CHD-C1D-C2D	3.23	135.44	127.53
3	B	201	CYC	CHD-C1D-C2D	3.21	135.40	127.53
3	L	201	CYC	C2A-C1A-NA	-3.21	105.50	110.04
3	A	201[A]	CYC	CHD-C1D-ND	-3.19	118.08	125.29
3	A	201[B]	CYC	CHD-C1D-ND	-3.19	118.08	125.29
3	J	201	CYC	CHD-C1D-C2D	3.19	135.34	127.53
3	A	201[A]	CYC	C2A-C1A-NA	-3.17	105.55	110.04
3	A	201[B]	CYC	C2A-C1A-NA	-3.17	105.55	110.04
3	E	201[A]	CYC	C1A-C2A-C3A	3.16	110.15	106.73
3	E	201[B]	CYC	C1A-C2A-C3A	3.16	110.15	106.73
3	G	201[A]	CYC	CHD-C1D-ND	-3.16	118.15	125.29
3	G	201[B]	CYC	CHD-C1D-ND	-3.16	118.15	125.29
3	D	201	CYC	C2A-C1A-NA	-3.16	105.57	110.04
3	J	201	CYC	C2A-C1A-NA	-3.15	105.59	110.04
3	D	201	CYC	CMA-C3A-C4A	3.14	129.98	125.10
3	J	201	CYC	CMA-C3A-C4A	3.14	129.97	125.10
3	E	201[A]	CYC	CAB-C3B-C4B	3.14	126.22	121.37
3	E	201[B]	CYC	CAB-C3B-C4B	3.14	126.22	121.37
3	I	201[A]	CYC	CHD-C1D-C2D	3.13	135.19	127.53
3	I	201[B]	CYC	CHD-C1D-C2D	3.13	135.19	127.53
3	K	201[A]	CYC	C1A-C2A-C3A	3.12	110.11	106.73
3	K	201[B]	CYC	C1A-C2A-C3A	3.12	110.11	106.73
3	K	201[A]	CYC	CHB-C1B-NB	3.12	132.72	126.06
3	K	201[B]	CYC	CHB-C1B-NB	3.12	132.72	126.06
3	K	201[A]	CYC	CAB-C3B-C4B	3.12	126.20	121.37
3	K	201[B]	CYC	CAB-C3B-C4B	3.12	126.20	121.37
3	H	201	CYC	C2A-C1A-NA	-3.12	105.63	110.04
3	C	201[A]	CYC	CHB-C1B-NB	3.11	132.69	126.06
3	C	201[B]	CYC	CHB-C1B-NB	3.11	132.69	126.06
3	A	201[A]	CYC	CHB-C1B-C2B	-3.10	120.79	126.97
3	A	201[B]	CYC	CHB-C1B-C2B	-3.10	120.79	126.97
3	G	201[A]	CYC	C2A-C1A-NA	-3.08	105.68	110.04
3	G	201[B]	CYC	C2A-C1A-NA	-3.08	105.68	110.04
3	I	201[A]	CYC	CHB-C1B-NB	3.08	132.63	126.06
3	I	201[B]	CYC	CHB-C1B-NB	3.08	132.63	126.06
3	C	201[A]	CYC	CHD-C1D-C2D	3.08	135.08	127.53
3	C	201[B]	CYC	CHD-C1D-C2D	3.08	135.08	127.53
3	E	201[A]	CYC	CHB-C1B-NB	3.07	132.60	126.06
3	E	201[B]	CYC	CHB-C1B-NB	3.07	132.60	126.06
3	K	201[A]	CYC	C2C-C1C-NC	3.07	110.84	108.29
3	K	201[B]	CYC	C2C-C1C-NC	3.07	110.84	108.29
3	B	201	CYC	CMA-C3A-C4A	3.07	129.86	125.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201[A]	CYC	CAD-C3D-C4D	-3.05	120.93	125.77
3	G	201[B]	CYC	CAD-C3D-C4D	-3.05	120.93	125.77
3	G	201[A]	CYC	CHB-C1B-C2B	-3.05	120.89	126.97
3	G	201[B]	CYC	CHB-C1B-C2B	-3.05	120.89	126.97
3	A	201[A]	CYC	CAD-C3D-C4D	-3.04	120.94	125.77
3	A	201[B]	CYC	CAD-C3D-C4D	-3.04	120.94	125.77
3	H	201	CYC	CMA-C3A-C4A	3.04	129.81	125.10
3	K	201[A]	CYC	CHB-C1B-C2B	-3.03	120.94	126.97
3	K	201[B]	CYC	CHB-C1B-C2B	-3.03	120.94	126.97
3	I	201[A]	CYC	CAD-C3D-C4D	-3.01	121.00	125.77
3	I	201[B]	CYC	CAD-C3D-C4D	-3.01	121.00	125.77
3	E	201[A]	CYC	CHB-C1B-C2B	-3.00	120.99	126.97
3	E	201[B]	CYC	CHB-C1B-C2B	-3.00	120.99	126.97
3	C	201[A]	CYC	CAD-C3D-C4D	-2.99	121.03	125.77
3	C	201[B]	CYC	CAD-C3D-C4D	-2.99	121.03	125.77
3	E	201[A]	CYC	C2C-C1C-NC	2.95	110.75	108.29
3	E	201[B]	CYC	C2C-C1C-NC	2.95	110.75	108.29
3	F	201	CYC	OC-C1C-C2C	-2.95	123.83	126.17
3	L	201	CYC	CHD-C1D-ND	-2.95	118.64	125.29
3	C	201[A]	CYC	C2C-C1C-NC	2.93	110.73	108.29
3	C	201[B]	CYC	C2C-C1C-NC	2.93	110.73	108.29
3	C	201[A]	CYC	C1D-CHD-C4C	2.92	132.76	127.76
3	C	201[B]	CYC	C1D-CHD-C4C	2.92	132.76	127.76
3	C	201[A]	CYC	CHB-C1B-C2B	-2.91	121.16	126.97
3	C	201[B]	CYC	CHB-C1B-C2B	-2.91	121.16	126.97
3	I	201[A]	CYC	CAB-C3B-C4B	2.91	125.88	121.37
3	I	201[B]	CYC	CAB-C3B-C4B	2.91	125.88	121.37
3	F	201	CYC	C2C-C1C-NC	2.91	110.71	108.29
3	I	201[A]	CYC	CHB-C1B-C2B	-2.91	121.17	126.97
3	I	201[B]	CYC	CHB-C1B-C2B	-2.91	121.17	126.97
3	C	201[A]	CYC	OC-C1C-C2C	-2.90	123.86	126.17
3	C	201[B]	CYC	OC-C1C-C2C	-2.90	123.86	126.17
3	B	201	CYC	OC-C1C-C2C	-2.90	123.86	126.17
3	I	201[A]	CYC	CHD-C1D-ND	-2.90	118.73	125.29
3	I	201[B]	CYC	CHD-C1D-ND	-2.90	118.73	125.29
3	J	201	CYC	OC-C1C-C2C	-2.90	123.87	126.17
3	A	201[A]	CYC	CAB-C3B-C4B	2.90	125.85	121.37
3	A	201[B]	CYC	CAB-C3B-C4B	2.90	125.85	121.37
3	F	201	CYC	CHD-C1D-ND	-2.90	118.75	125.29
3	L	201	CYC	OC-C1C-C2C	-2.89	123.88	126.17
3	I	201[A]	CYC	C1D-CHD-C4C	2.89	132.69	127.76
3	I	201[B]	CYC	C1D-CHD-C4C	2.89	132.69	127.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	201[A]	CYC	C1B-NB-C4B	-2.88	107.13	110.66
3	E	201[B]	CYC	C1B-NB-C4B	-2.88	107.13	110.66
3	I	201[A]	CYC	C2C-C1C-NC	2.87	110.68	108.29
3	I	201[B]	CYC	C2C-C1C-NC	2.87	110.68	108.29
3	C	201[A]	CYC	CAB-C3B-C4B	2.87	125.81	121.37
3	C	201[B]	CYC	CAB-C3B-C4B	2.87	125.81	121.37
3	I	201[A]	CYC	C1B-NB-C4B	-2.87	107.14	110.66
3	I	201[B]	CYC	C1B-NB-C4B	-2.87	107.14	110.66
3	C	201[A]	CYC	CHD-C1D-ND	-2.86	118.83	125.29
3	C	201[B]	CYC	CHD-C1D-ND	-2.86	118.83	125.29
3	L	201	CYC	C2C-C1C-NC	2.86	110.66	108.29
3	G	201[A]	CYC	CAB-C3B-C4B	2.85	125.79	121.37
3	G	201[B]	CYC	CAB-C3B-C4B	2.85	125.79	121.37
3	H	201	CYC	CHD-C1D-ND	-2.85	118.85	125.29
3	I	201[A]	CYC	OC-C1C-C2C	-2.85	123.91	126.17
3	I	201[B]	CYC	OC-C1C-C2C	-2.85	123.91	126.17
3	J	201	CYC	CHD-C1D-ND	-2.83	118.89	125.29
3	C	201[A]	CYC	C1B-NB-C4B	-2.83	107.19	110.66
3	C	201[B]	CYC	C1B-NB-C4B	-2.83	107.19	110.66
3	H	201	CYC	OC-C1C-C2C	-2.82	123.93	126.17
3	K	201[A]	CYC	C1B-NB-C4B	-2.82	107.21	110.66
3	K	201[B]	CYC	C1B-NB-C4B	-2.82	107.21	110.66
3	D	201	CYC	OC-C1C-C2C	-2.81	123.94	126.17
3	D	201	CYC	CHD-C1D-ND	-2.81	118.95	125.29
3	G	201[A]	CYC	C1B-NB-C4B	-2.80	107.22	110.66
3	G	201[B]	CYC	C1B-NB-C4B	-2.80	107.22	110.66
3	C	201[A]	CYC	C1A-C2A-C3A	2.80	109.76	106.73
3	C	201[B]	CYC	C1A-C2A-C3A	2.80	109.76	106.73
3	A	201[A]	CYC	C1B-NB-C4B	-2.79	107.24	110.66
3	A	201[B]	CYC	C1B-NB-C4B	-2.79	107.24	110.66
3	B	201	CYC	CHD-C1D-ND	-2.78	119.01	125.29
3	I	201[A]	CYC	C1A-C2A-C3A	2.76	109.72	106.73
3	I	201[B]	CYC	C1A-C2A-C3A	2.76	109.72	106.73
3	E	201[A]	CYC	C1B-CHB-C4A	2.76	134.82	128.06
3	E	201[B]	CYC	C1B-CHB-C4A	2.76	134.82	128.06
3	L	201	CYC	CAB-C3B-C4B	2.73	125.60	121.37
3	K	201[A]	CYC	C1D-CHD-C4C	2.73	132.43	127.76
3	K	201[B]	CYC	C1D-CHD-C4C	2.73	132.43	127.76
3	K	201[A]	CYC	C1B-CHB-C4A	2.73	134.75	128.06
3	K	201[B]	CYC	C1B-CHB-C4A	2.73	134.75	128.06
3	B	201	CYC	CHB-C4A-C3A	2.73	131.88	124.87
3	H	201	CYC	CHB-C4A-C3A	2.72	131.86	124.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201[A]	CYC	C1D-CHD-C4C	2.72	132.40	127.76
3	G	201[B]	CYC	C1D-CHD-C4C	2.72	132.40	127.76
3	E	201[A]	CYC	C1D-CHD-C4C	2.69	132.35	127.76
3	E	201[B]	CYC	C1D-CHD-C4C	2.69	132.35	127.76
3	J	201	CYC	CAB-C3B-C4B	2.69	125.52	121.37
3	D	201	CYC	CHB-C4A-C3A	2.68	131.75	124.87
3	J	201	CYC	CHB-C4A-C3A	2.68	131.75	124.87
3	K	201[A]	CYC	C1A-NA-C4A	2.68	111.43	106.52
3	K	201[B]	CYC	C1A-NA-C4A	2.68	111.43	106.52
3	E	201[A]	CYC	C1A-NA-C4A	2.67	111.43	106.52
3	E	201[B]	CYC	C1A-NA-C4A	2.67	111.43	106.52
3	J	201	CYC	C1A-C2A-C3A	2.66	109.61	106.73
3	B	201	CYC	C1A-C2A-C3A	2.66	109.61	106.73
3	D	201	CYC	CMC-C2C-C3C	2.65	124.23	113.98
3	J	201	CYC	CMC-C2C-C3C	2.65	124.22	113.98
3	C	201[A]	CYC	C1B-CHB-C4A	2.65	134.55	128.06
3	C	201[B]	CYC	C1B-CHB-C4A	2.65	134.55	128.06
3	D	201	CYC	CAB-C3B-C4B	2.65	125.46	121.37
3	F	201	CYC	C1A-C2A-C3A	2.64	109.59	106.73
3	I	201[A]	CYC	C1B-CHB-C4A	2.64	134.54	128.06
3	I	201[B]	CYC	C1B-CHB-C4A	2.64	134.54	128.06
3	L	201	CYC	C1A-C2A-C3A	2.64	109.58	106.73
3	A	201[A]	CYC	C1D-CHD-C4C	2.63	132.25	127.76
3	A	201[B]	CYC	C1D-CHD-C4C	2.63	132.25	127.76
3	A	201[A]	CYC	C1A-C2A-C3A	2.62	109.56	106.73
3	A	201[B]	CYC	C1A-C2A-C3A	2.62	109.56	106.73
3	C	201[A]	CYC	C1A-NA-C4A	2.61	111.31	106.52
3	C	201[B]	CYC	C1A-NA-C4A	2.61	111.31	106.52
3	A	201[A]	CYC	C2C-C1C-NC	2.61	110.46	108.29
3	A	201[B]	CYC	C2C-C1C-NC	2.61	110.46	108.29
3	I	201[A]	CYC	C1A-NA-C4A	2.61	111.31	106.52
3	I	201[B]	CYC	C1A-NA-C4A	2.61	111.31	106.52
3	H	201	CYC	CAB-C3B-C4B	2.60	125.40	121.37
3	F	201	CYC	CAB-C3B-C4B	2.60	125.39	121.37
3	G	201[A]	CYC	C2C-C1C-NC	2.59	110.44	108.29
3	G	201[B]	CYC	C2C-C1C-NC	2.59	110.44	108.29
3	B	201	CYC	CAB-C3B-C4B	2.59	125.37	121.37
3	D	201	CYC	C2C-C1C-NC	2.57	110.43	108.29
3	D	201	CYC	C1A-C2A-C3A	2.57	109.51	106.73
3	B	201	CYC	C2C-C1C-NC	2.57	110.43	108.29
3	J	201	CYC	C2C-C1C-NC	2.55	110.41	108.29
3	L	201	CYC	CHB-C4A-C3A	2.53	131.36	124.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	CYC	CHB-C4A-C3A	2.52	131.35	124.87
3	K	201[A]	CYC	O1D-CGD-CBD	-2.52	115.09	123.09
3	H	201	CYC	C2C-C1C-NC	2.52	110.38	108.29
3	I	201[A]	CYC	O1D-CGD-CBD	-2.50	115.15	123.09
3	L	201	CYC	CMC-C2C-C3C	2.50	123.66	113.98
3	C	201[A]	CYC	CHD-C4C-NC	2.50	128.75	125.63
3	C	201[B]	CYC	CHD-C4C-NC	2.50	128.75	125.63
3	H	201	CYC	C1A-C2A-C3A	2.50	109.43	106.73
3	F	201	CYC	CMC-C2C-C3C	2.50	123.63	113.98
3	C	201[A]	CYC	O1D-CGD-CBD	-2.49	115.20	123.09
3	A	201[A]	CYC	C1B-CHB-C4A	2.48	134.15	128.06
3	A	201[B]	CYC	C1B-CHB-C4A	2.48	134.15	128.06
3	E	201[A]	CYC	O1D-CGD-CBD	-2.48	115.23	123.09
3	A	201[A]	CYC	CMA-C3A-C4A	2.47	128.94	125.10
3	A	201[B]	CYC	CMA-C3A-C4A	2.47	128.94	125.10
3	G	201[A]	CYC	C1B-CHB-C4A	2.47	134.11	128.06
3	G	201[B]	CYC	C1B-CHB-C4A	2.47	134.11	128.06
3	B	201	CYC	CMC-C2C-C3C	2.47	123.52	113.98
3	H	201	CYC	CMC-C2C-C3C	2.47	123.51	113.98
3	A	201[A]	CYC	O1D-CGD-CBD	-2.46	115.28	123.09
3	A	201[A]	CYC	C1A-NA-C4A	2.46	111.03	106.52
3	A	201[B]	CYC	C1A-NA-C4A	2.46	111.03	106.52
3	G	201[A]	CYC	O1D-CGD-CBD	-2.46	115.29	123.09
3	C	201[A]	CYC	CMB-C2B-C1B	2.46	127.15	124.16
3	C	201[B]	CYC	CMB-C2B-C1B	2.46	127.15	124.16
3	H	201	CYC	CHB-C4A-NA	-2.46	119.65	124.95
3	G	201[A]	CYC	C1A-NA-C4A	2.45	111.02	106.52
3	G	201[B]	CYC	C1A-NA-C4A	2.45	111.02	106.52
3	B	201	CYC	CHB-C4A-NA	-2.45	119.65	124.95
3	G	201[A]	CYC	C1A-C2A-C3A	2.45	109.38	106.73
3	G	201[B]	CYC	C1A-C2A-C3A	2.45	109.38	106.73
3	I	201[A]	CYC	CMB-C2B-C1B	2.45	127.14	124.16
3	I	201[B]	CYC	CMB-C2B-C1B	2.45	127.14	124.16
3	C	201[A]	CYC	CMA-C3A-C4A	2.44	128.89	125.10
3	C	201[B]	CYC	CMA-C3A-C4A	2.44	128.89	125.10
3	G	201[A]	CYC	CMA-C3A-C4A	2.43	128.87	125.10
3	G	201[B]	CYC	CMA-C3A-C4A	2.43	128.87	125.10
3	I	201[A]	CYC	CMA-C3A-C4A	2.43	128.87	125.10
3	I	201[B]	CYC	CMA-C3A-C4A	2.43	128.87	125.10
3	A	201[A]	CYC	CMB-C2B-C1B	2.43	127.11	124.16
3	A	201[B]	CYC	CMB-C2B-C1B	2.43	127.11	124.16
3	K	201[A]	CYC	CMB-C2B-C1B	2.42	127.10	124.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	201[B]	CYC	CMB-C2B-C1B	2.42	127.10	124.16
3	I	201[A]	CYC	CHD-C4C-NC	2.41	128.65	125.63
3	I	201[B]	CYC	CHD-C4C-NC	2.41	128.65	125.63
3	J	201	CYC	CHB-C4A-NA	-2.41	119.74	124.95
3	E	201[A]	CYC	CMB-C2B-C1B	2.40	127.07	124.16
3	E	201[B]	CYC	CMB-C2B-C1B	2.40	127.07	124.16
3	D	201	CYC	CHB-C4A-NA	-2.39	119.78	124.95
3	A	201[A]	CYC	CHA-C4D-ND	2.39	130.68	125.29
3	A	201[B]	CYC	CHA-C4D-ND	2.39	130.68	125.29
3	E	201[A]	CYC	CHA-C4D-ND	2.38	130.66	125.29
3	E	201[B]	CYC	CHA-C4D-ND	2.38	130.66	125.29
3	G	201[A]	CYC	CHA-C4D-ND	2.38	130.66	125.29
3	G	201[B]	CYC	CHA-C4D-ND	2.38	130.66	125.29
3	H	201	CYC	CHA-C4D-ND	2.37	130.65	125.29
3	B	201	CYC	CMB-C2B-C1B	2.37	127.04	124.16
3	B	201	CYC	CHA-C4D-ND	2.34	130.58	125.29
3	K	201[A]	CYC	CHA-C4D-ND	2.33	130.56	125.29
3	K	201[B]	CYC	CHA-C4D-ND	2.33	130.56	125.29
3	I	201[A]	CYC	CHA-C4D-ND	2.32	130.54	125.29
3	I	201[B]	CYC	CHA-C4D-ND	2.32	130.54	125.29
3	H	201	CYC	CMB-C2B-C1B	2.32	126.98	124.16
3	C	201[A]	CYC	CHA-C4D-ND	2.30	130.49	125.29
3	C	201[B]	CYC	CHA-C4D-ND	2.30	130.49	125.29
3	G	201[A]	CYC	CMB-C2B-C1B	2.30	126.95	124.16
3	G	201[B]	CYC	CMB-C2B-C1B	2.30	126.95	124.16
3	F	201	CYC	C1D-CHD-C4C	2.29	131.68	127.76
3	K	201[A]	CYC	O1A-CGA-CBA	-2.28	115.87	123.09
3	K	201[B]	CYC	O1A-CGA-CBA	-2.28	115.87	123.09
3	E	201[A]	CYC	O1A-CGA-CBA	-2.27	115.89	123.09
3	E	201[B]	CYC	O1A-CGA-CBA	-2.27	115.89	123.09
3	K	201[A]	CYC	C3A-C4A-NA	-2.27	105.63	110.58
3	K	201[B]	CYC	C3A-C4A-NA	-2.27	105.63	110.58
3	L	201	CYC	C1D-CHD-C4C	2.27	131.63	127.76
3	E	201[A]	CYC	C3A-C4A-NA	-2.26	105.65	110.58
3	E	201[B]	CYC	C3A-C4A-NA	-2.26	105.65	110.58
3	G	201[A]	CYC	C3A-C4A-NA	-2.25	105.66	110.58
3	G	201[B]	CYC	C3A-C4A-NA	-2.25	105.66	110.58
3	L	201	CYC	CHB-C4A-NA	-2.25	120.09	124.95
3	F	201	CYC	CHA-C4D-ND	2.25	130.36	125.29
3	A	201[A]	CYC	C3A-C4A-NA	-2.24	105.69	110.58
3	A	201[B]	CYC	C3A-C4A-NA	-2.24	105.69	110.58
3	F	201	CYC	CHB-C4A-NA	-2.24	120.12	124.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201[A]	CYC	C1B-C2B-C3B	2.24	110.16	107.86
3	G	201[B]	CYC	C1B-C2B-C3B	2.24	110.16	107.86
3	G	201[A]	CYC	OB-C4B-C3B	-2.23	125.68	128.03
3	G	201[B]	CYC	OB-C4B-C3B	-2.23	125.68	128.03
3	J	201	CYC	CMB-C2B-C1B	2.23	126.87	124.16
3	B	201	CYC	C1A-NA-C4A	2.23	110.61	106.52
3	A	201[A]	CYC	OB-C4B-C3B	-2.22	125.70	128.03
3	A	201[B]	CYC	OB-C4B-C3B	-2.22	125.70	128.03
3	I	201[A]	CYC	C3A-C4A-NA	-2.22	105.73	110.58
3	I	201[B]	CYC	C3A-C4A-NA	-2.22	105.73	110.58
3	C	201[A]	CYC	C3A-C4A-NA	-2.21	105.75	110.58
3	C	201[B]	CYC	C3A-C4A-NA	-2.21	105.75	110.58
3	A	201[A]	CYC	O1A-CGA-CBA	-2.20	116.11	123.09
3	A	201[B]	CYC	O1A-CGA-CBA	-2.20	116.11	123.09
3	G	201[A]	CYC	O1A-CGA-CBA	-2.19	116.14	123.09
3	G	201[B]	CYC	O1A-CGA-CBA	-2.19	116.14	123.09
3	L	201	CYC	CHA-C4D-ND	2.19	130.23	125.29
3	K	201[A]	CYC	CMA-C3A-C4A	2.18	128.49	125.10
3	K	201[B]	CYC	CMA-C3A-C4A	2.18	128.49	125.10
3	L	201	CYC	CMB-C2B-C1B	2.18	126.81	124.16
3	H	201	CYC	C1A-NA-C4A	2.18	110.52	106.52
3	H	201	CYC	CMD-C2D-C1D	2.18	128.79	125.62
3	C	201[A]	CYC	C1B-C2B-C3B	2.18	110.10	107.86
3	C	201[B]	CYC	C1B-C2B-C3B	2.18	110.10	107.86
3	F	201	CYC	C1A-NA-C4A	2.18	110.51	106.52
3	D	201	CYC	C1A-NA-C4A	2.17	110.50	106.52
3	B	201	CYC	CMD-C2D-C1D	2.16	128.76	125.62
3	E	201[A]	CYC	CMA-C3A-C4A	2.16	128.46	125.10
3	E	201[B]	CYC	CMA-C3A-C4A	2.16	128.46	125.10
3	A	201[A]	CYC	C1B-C2B-C3B	2.16	110.08	107.86
3	A	201[B]	CYC	C1B-C2B-C3B	2.16	110.08	107.86
3	L	201	CYC	C1A-NA-C4A	2.16	110.48	106.52
3	B	201	CYC	C1D-CHD-C4C	2.15	131.43	127.76
3	L	201	CYC	C3A-C4A-NA	-2.14	105.91	110.58
3	D	201	CYC	CMB-C2B-C1B	2.13	126.75	124.16
3	F	201	CYC	C3A-C4A-NA	-2.13	105.94	110.58
3	J	201	CYC	C1A-NA-C4A	2.13	110.42	106.52
3	H	201	CYC	CAC-C3C-C4C	2.13	118.13	112.67
3	E	201[A]	CYC	CHA-C1A-NA	2.11	129.04	124.60
3	E	201[B]	CYC	CHA-C1A-NA	2.11	129.04	124.60
3	I	201[A]	CYC	C1B-C2B-C3B	2.11	110.04	107.86
3	I	201[B]	CYC	C1B-C2B-C3B	2.11	110.04	107.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201[A]	CYC	O1A-CGA-CBA	-2.11	116.40	123.09
3	C	201[B]	CYC	O1A-CGA-CBA	-2.11	116.40	123.09
3	B	201	CYC	CAC-C3C-C4C	2.10	118.07	112.67
3	I	201[A]	CYC	CHA-C1A-NA	2.10	129.01	124.60
3	I	201[B]	CYC	CHA-C1A-NA	2.10	129.01	124.60
3	B	201	CYC	C3A-C4A-NA	-2.09	106.01	110.58
3	D	201	CYC	CHA-C4D-ND	2.09	130.00	125.29
3	H	201	CYC	C1D-CHD-C4C	2.08	131.32	127.76
3	I	201[A]	CYC	O1A-CGA-CBA	-2.08	116.50	123.09
3	I	201[B]	CYC	O1A-CGA-CBA	-2.08	116.50	123.09
3	J	201	CYC	CHA-C4D-ND	2.08	129.98	125.29
3	K	201[A]	CYC	CHA-C1A-NA	2.08	128.96	124.60
3	K	201[B]	CYC	CHA-C1A-NA	2.08	128.96	124.60
3	F	201	CYC	CMB-C2B-C1B	2.07	126.68	124.16
3	B	201	CYC	O1A-CGA-CBA	-2.07	116.53	123.09
3	C	201[A]	CYC	CHA-C1A-NA	2.07	128.94	124.60
3	C	201[B]	CYC	CHA-C1A-NA	2.07	128.94	124.60
3	H	201	CYC	C3A-C4A-NA	-2.07	106.06	110.58
3	D	201	CYC	C1D-CHD-C4C	2.06	131.28	127.76
3	C	201[A]	CYC	C4D-C3D-C2D	2.06	110.01	107.62
3	C	201[B]	CYC	C4D-C3D-C2D	2.06	110.01	107.62
3	J	201	CYC	C1D-CHD-C4C	2.05	131.27	127.76
3	D	201	CYC	C3A-C4A-NA	-2.05	106.10	110.58
3	H	201	CYC	O1A-CGA-CBA	-2.05	116.59	123.09
3	L	201	CYC	O1A-CGA-CBA	-2.04	116.61	123.09
3	I	201[A]	CYC	C4D-C3D-C2D	2.04	109.99	107.62
3	I	201[B]	CYC	C4D-C3D-C2D	2.04	109.99	107.62
3	J	201	CYC	O1A-CGA-CBA	-2.03	116.66	123.09
3	F	201	CYC	O1A-CGA-CBA	-2.02	116.67	123.09
3	D	201	CYC	O1A-CGA-CBA	-2.02	116.68	123.09
3	K	201[A]	CYC	CHD-C4C-NC	2.02	128.15	125.63
3	K	201[B]	CYC	CHD-C4C-NC	2.02	128.15	125.63
3	J	201	CYC	C3A-C4A-NA	-2.02	106.18	110.58
3	H	201	CYC	C3D-C4D-ND	-2.01	105.05	107.57

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201[A]	CYC	NA-C4A-CHB-C1B
3	A	201[A]	CYC	C3A-C4A-CHB-C1B
3	A	201[B]	CYC	NA-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	201[B]	CYC	C3A-C4A-CHB-C1B
3	B	201	CYC	C3A-C4A-CHB-C1B
3	B	201	CYC	NC-C4C-CHD-C1D
3	C	201[A]	CYC	NA-C4A-CHB-C1B
3	C	201[A]	CYC	C3A-C4A-CHB-C1B
3	C	201[B]	CYC	NA-C4A-CHB-C1B
3	C	201[B]	CYC	C3A-C4A-CHB-C1B
3	D	201	CYC	C3A-C4A-CHB-C1B
3	D	201	CYC	NC-C4C-CHD-C1D
3	E	201[A]	CYC	NA-C4A-CHB-C1B
3	E	201[A]	CYC	C3A-C4A-CHB-C1B
3	E	201[B]	CYC	NA-C4A-CHB-C1B
3	E	201[B]	CYC	C3A-C4A-CHB-C1B
3	F	201	CYC	C3A-C4A-CHB-C1B
3	F	201	CYC	NC-C4C-CHD-C1D
3	G	201[A]	CYC	NA-C4A-CHB-C1B
3	G	201[A]	CYC	C3A-C4A-CHB-C1B
3	G	201[B]	CYC	NA-C4A-CHB-C1B
3	G	201[B]	CYC	C3A-C4A-CHB-C1B
3	H	201	CYC	C3A-C4A-CHB-C1B
3	H	201	CYC	NC-C4C-CHD-C1D
3	I	201[A]	CYC	NA-C4A-CHB-C1B
3	I	201[A]	CYC	C3A-C4A-CHB-C1B
3	I	201[B]	CYC	NA-C4A-CHB-C1B
3	I	201[B]	CYC	C3A-C4A-CHB-C1B
3	J	201	CYC	C3A-C4A-CHB-C1B
3	J	201	CYC	NC-C4C-CHD-C1D
3	K	201[A]	CYC	NA-C4A-CHB-C1B
3	K	201[A]	CYC	C3A-C4A-CHB-C1B
3	K	201[B]	CYC	NA-C4A-CHB-C1B
3	K	201[B]	CYC	C3A-C4A-CHB-C1B
3	L	201	CYC	C3A-C4A-CHB-C1B
3	L	201	CYC	NC-C4C-CHD-C1D
3	A	201[A]	CYC	C2D-C1D-CHD-C4C
3	A	201[B]	CYC	C2D-C1D-CHD-C4C
3	B	201	CYC	C2D-C1D-CHD-C4C
3	C	201[A]	CYC	C2D-C1D-CHD-C4C
3	C	201[B]	CYC	C2D-C1D-CHD-C4C
3	D	201	CYC	C2D-C1D-CHD-C4C
3	E	201[A]	CYC	C2D-C1D-CHD-C4C
3	E	201[B]	CYC	C2D-C1D-CHD-C4C
3	F	201	CYC	C2D-C1D-CHD-C4C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	G	201[A]	CYC	C2D-C1D-CHD-C4C
3	G	201[B]	CYC	C2D-C1D-CHD-C4C
3	H	201	CYC	C2D-C1D-CHD-C4C
3	I	201[A]	CYC	C2D-C1D-CHD-C4C
3	I	201[B]	CYC	C2D-C1D-CHD-C4C
3	J	201	CYC	C2D-C1D-CHD-C4C
3	K	201[A]	CYC	C2D-C1D-CHD-C4C
3	K	201[B]	CYC	C2D-C1D-CHD-C4C
3	L	201	CYC	C2D-C1D-CHD-C4C
3	A	201[A]	CYC	ND-C1D-CHD-C4C
3	A	201[B]	CYC	ND-C1D-CHD-C4C
3	B	201	CYC	ND-C1D-CHD-C4C
3	C	201[A]	CYC	ND-C1D-CHD-C4C
3	C	201[B]	CYC	ND-C1D-CHD-C4C
3	E	201[A]	CYC	ND-C1D-CHD-C4C
3	E	201[B]	CYC	ND-C1D-CHD-C4C
3	G	201[A]	CYC	ND-C1D-CHD-C4C
3	G	201[B]	CYC	ND-C1D-CHD-C4C
3	H	201	CYC	ND-C1D-CHD-C4C
3	I	201[A]	CYC	ND-C1D-CHD-C4C
3	I	201[B]	CYC	ND-C1D-CHD-C4C
3	K	201[A]	CYC	ND-C1D-CHD-C4C
3	K	201[B]	CYC	ND-C1D-CHD-C4C
3	D	201	CYC	ND-C1D-CHD-C4C
3	F	201	CYC	ND-C1D-CHD-C4C
3	J	201	CYC	ND-C1D-CHD-C4C
3	L	201	CYC	ND-C1D-CHD-C4C
3	B	201	CYC	NA-C4A-CHB-C1B
3	D	201	CYC	NA-C4A-CHB-C1B
3	F	201	CYC	NA-C4A-CHB-C1B
3	H	201	CYC	NA-C4A-CHB-C1B
3	J	201	CYC	NA-C4A-CHB-C1B
3	L	201	CYC	NA-C4A-CHB-C1B
3	J	201	CYC	C2B-C3B-CAB-CBB
3	D	201	CYC	C2B-C3B-CAB-CBB
3	D	201	CYC	CAD-CBD-CGD-O1D
3	J	201	CYC	CAD-CBD-CGD-O1D
3	D	201	CYC	CAA-CBA-CGA-O1A
3	D	201	CYC	CAD-CBD-CGD-O2D
3	J	201	CYC	CAD-CBD-CGD-O2D
3	J	201	CYC	CAA-CBA-CGA-O1A
3	B	201	CYC	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	H	201	CYC	CAD-CBD-CGD-O2D
3	L	201	CYC	CAD-CBD-CGD-O2D
3	F	201	CYC	CAD-CBD-CGD-O2D
3	H	201	CYC	CAA-CBA-CGA-O1A
3	B	201	CYC	CAA-CBA-CGA-O1A
3	B	201	CYC	CAD-CBD-CGD-O1D
3	H	201	CYC	CAD-CBD-CGD-O1D
3	B	201	CYC	C1A-C2A-CAA-CBA
3	H	201	CYC	C1A-C2A-CAA-CBA
3	F	201	CYC	CAA-CBA-CGA-O1A
3	L	201	CYC	CAA-CBA-CGA-O1A
3	F	201	CYC	CAD-CBD-CGD-O1D
3	L	201	CYC	CAD-CBD-CGD-O1D
3	F	201	CYC	CAA-CBA-CGA-O2A
3	L	201	CYC	CAA-CBA-CGA-O2A
3	D	201	CYC	CAA-CBA-CGA-O2A
3	J	201	CYC	CAA-CBA-CGA-O2A
3	E	201[A]	CYC	CAA-CBA-CGA-O2A
3	E	201[B]	CYC	CAA-CBA-CGA-O2A
3	K	201[A]	CYC	CAA-CBA-CGA-O2A
3	K	201[B]	CYC	CAA-CBA-CGA-O2A
3	C	201[A]	CYC	CAA-CBA-CGA-O2A
3	C	201[B]	CYC	CAA-CBA-CGA-O2A
3	I	201[A]	CYC	CAA-CBA-CGA-O2A
3	I	201[B]	CYC	CAA-CBA-CGA-O2A
3	B	201	CYC	CAA-CBA-CGA-O2A
3	C	201[A]	CYC	CAA-CBA-CGA-O1A
3	C	201[B]	CYC	CAA-CBA-CGA-O1A
3	E	201[A]	CYC	CAA-CBA-CGA-O1A
3	E	201[B]	CYC	CAA-CBA-CGA-O1A
3	H	201	CYC	CAA-CBA-CGA-O2A
3	K	201[A]	CYC	CAA-CBA-CGA-O1A
3	K	201[B]	CYC	CAA-CBA-CGA-O1A
3	I	201[A]	CYC	CAA-CBA-CGA-O1A
3	I	201[B]	CYC	CAA-CBA-CGA-O1A
3	A	201[A]	CYC	CAA-CBA-CGA-O1A
3	A	201[B]	CYC	CAA-CBA-CGA-O1A
3	G	201[A]	CYC	CAA-CBA-CGA-O1A
3	G	201[B]	CYC	CAA-CBA-CGA-O1A
3	D	201	CYC	C1A-C2A-CAA-CBA
3	J	201	CYC	C1A-C2A-CAA-CBA
3	A	201[A]	CYC	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	201[B]	CYC	CAA-CBA-CGA-O2A
3	G	201[A]	CYC	CAA-CBA-CGA-O2A
3	G	201[B]	CYC	CAA-CBA-CGA-O2A
3	F	201	CYC	C1A-C2A-CAA-CBA
3	L	201	CYC	C1A-C2A-CAA-CBA
3	C	201[A]	CYC	CAD-CBD-CGD-O1D
3	I	201[A]	CYC	CAD-CBD-CGD-O1D
3	G	201[A]	CYC	CAD-CBD-CGD-O1D
3	A	201[A]	CYC	CAD-CBD-CGD-O1D
3	E	201[A]	CYC	CAD-CBD-CGD-O1D
3	K	201[A]	CYC	CAD-CBD-CGD-O1D
3	C	201[A]	CYC	CAD-CBD-CGD-O2D
3	I	201[A]	CYC	CAD-CBD-CGD-O2D

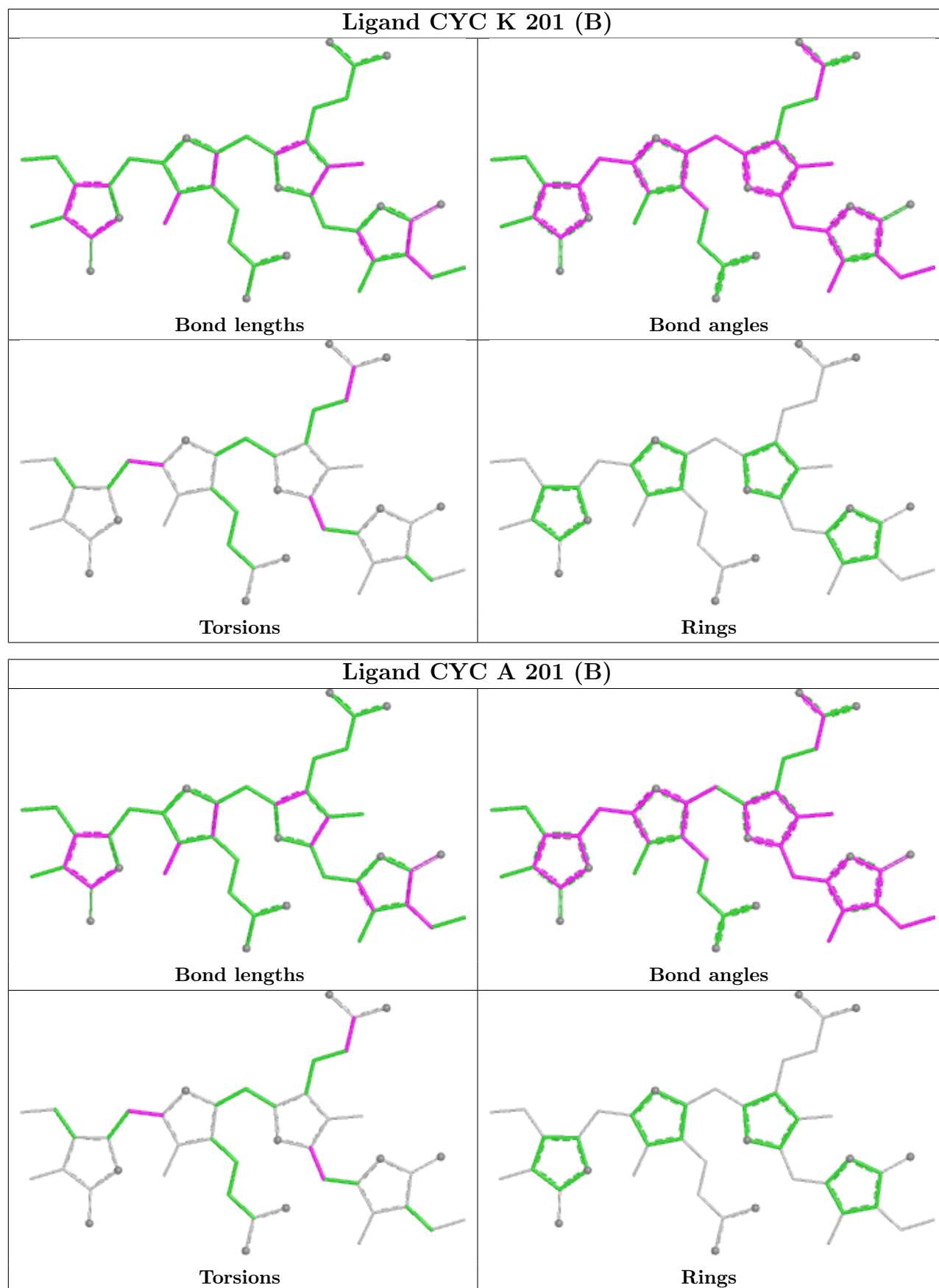
There are no ring outliers.

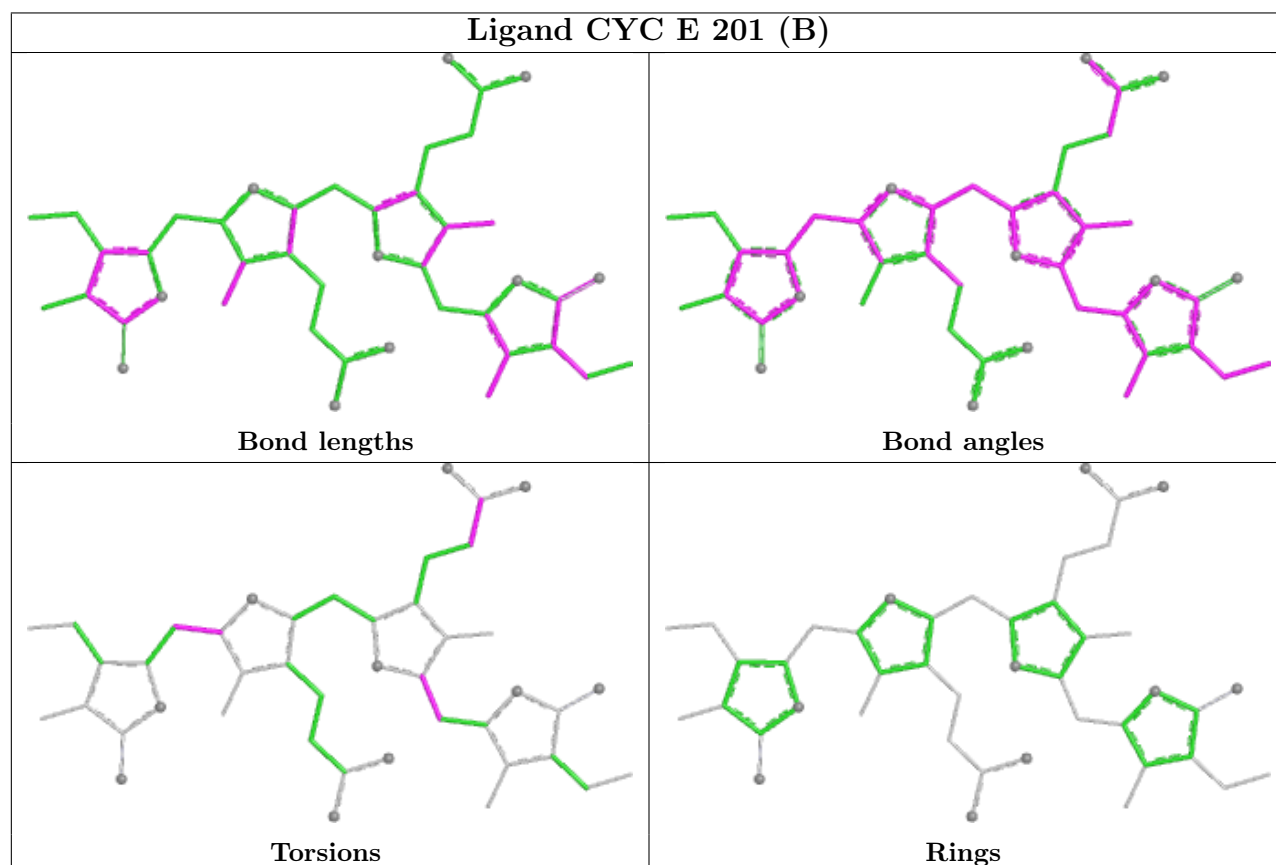
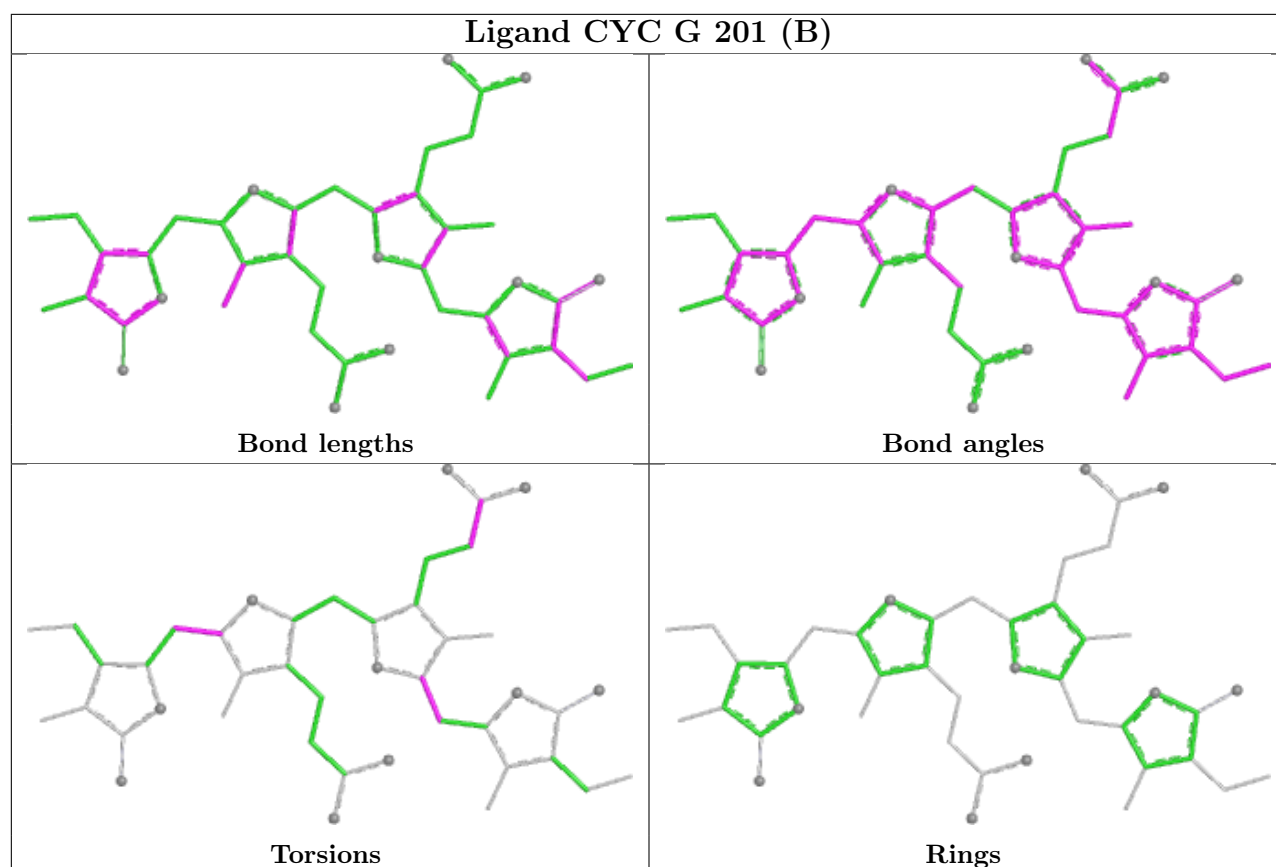
12 monomers are involved in 21 short contacts:

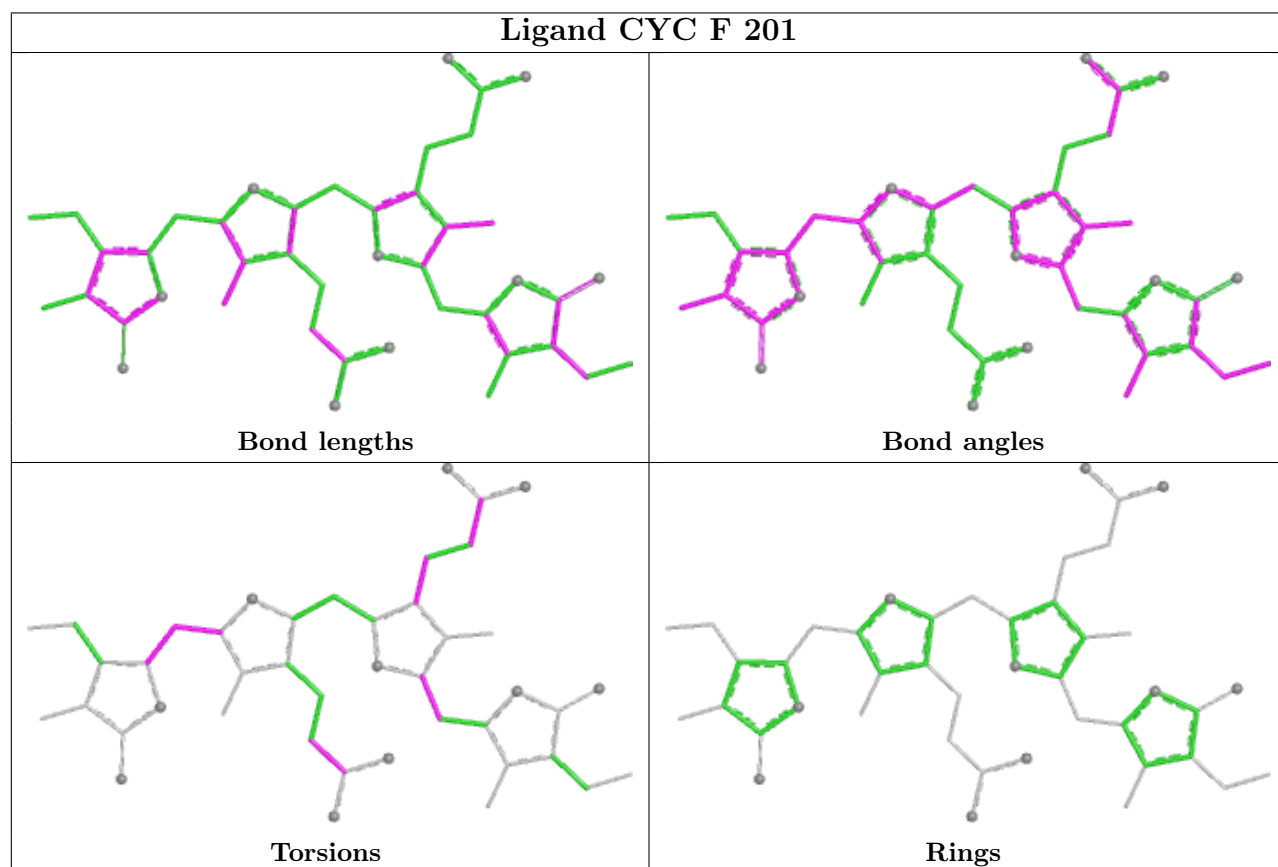
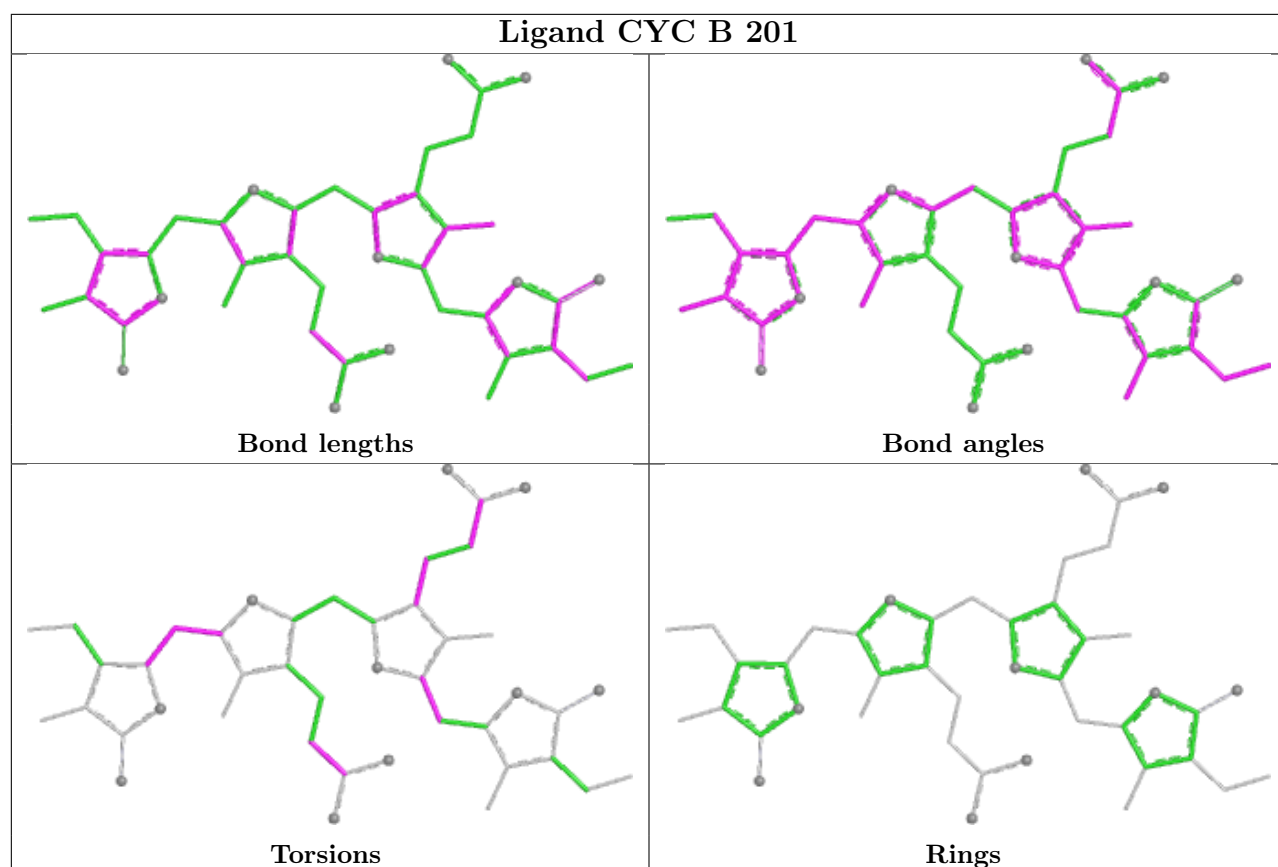
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	201[B]	CYC	1	0
3	A	201[B]	CYC	1	0
3	G	201[B]	CYC	1	0
3	E	201[B]	CYC	1	0
3	B	201	CYC	2	0
3	F	201	CYC	2	0
3	D	201	CYC	4	0
3	L	201	CYC	2	0
3	C	201[B]	CYC	1	0
3	H	201	CYC	2	0
3	I	201[B]	CYC	1	0
3	J	201	CYC	3	0

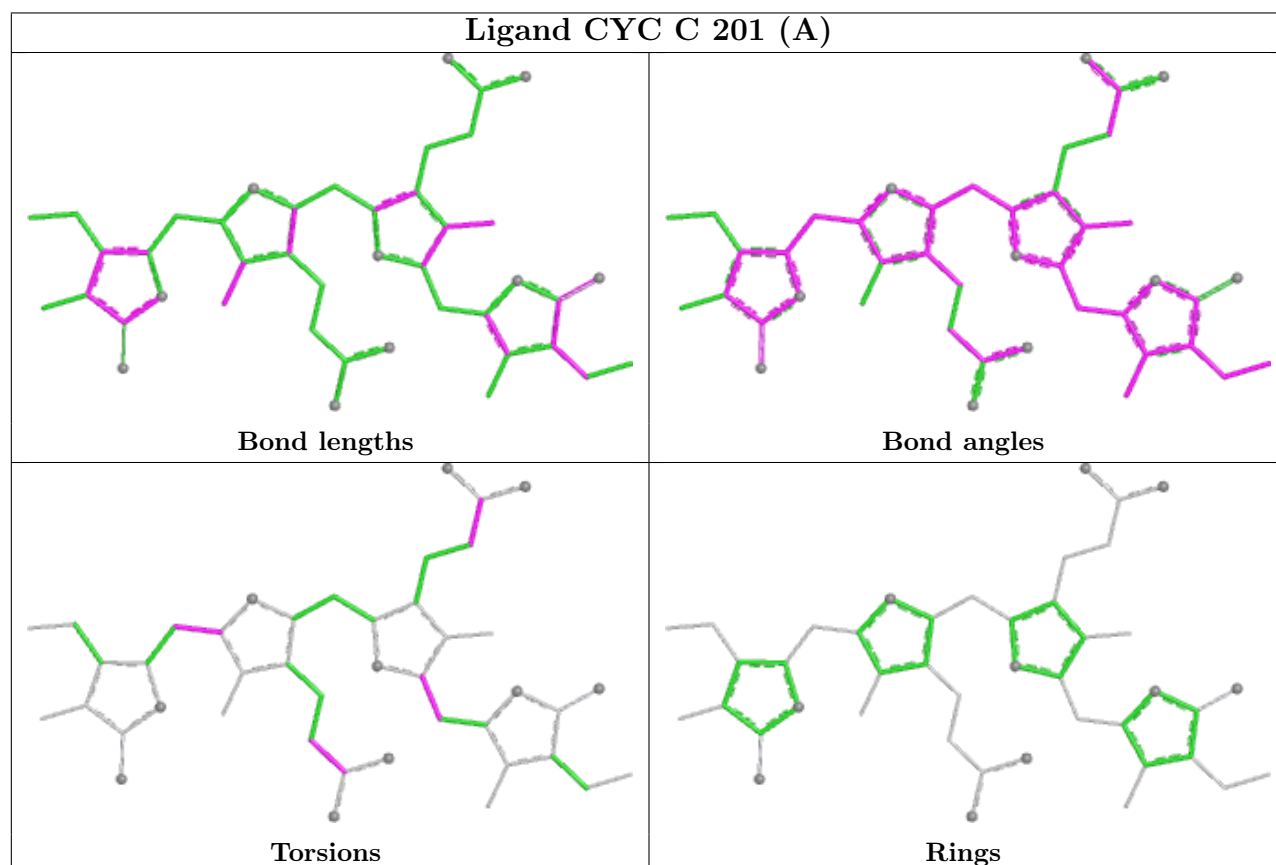
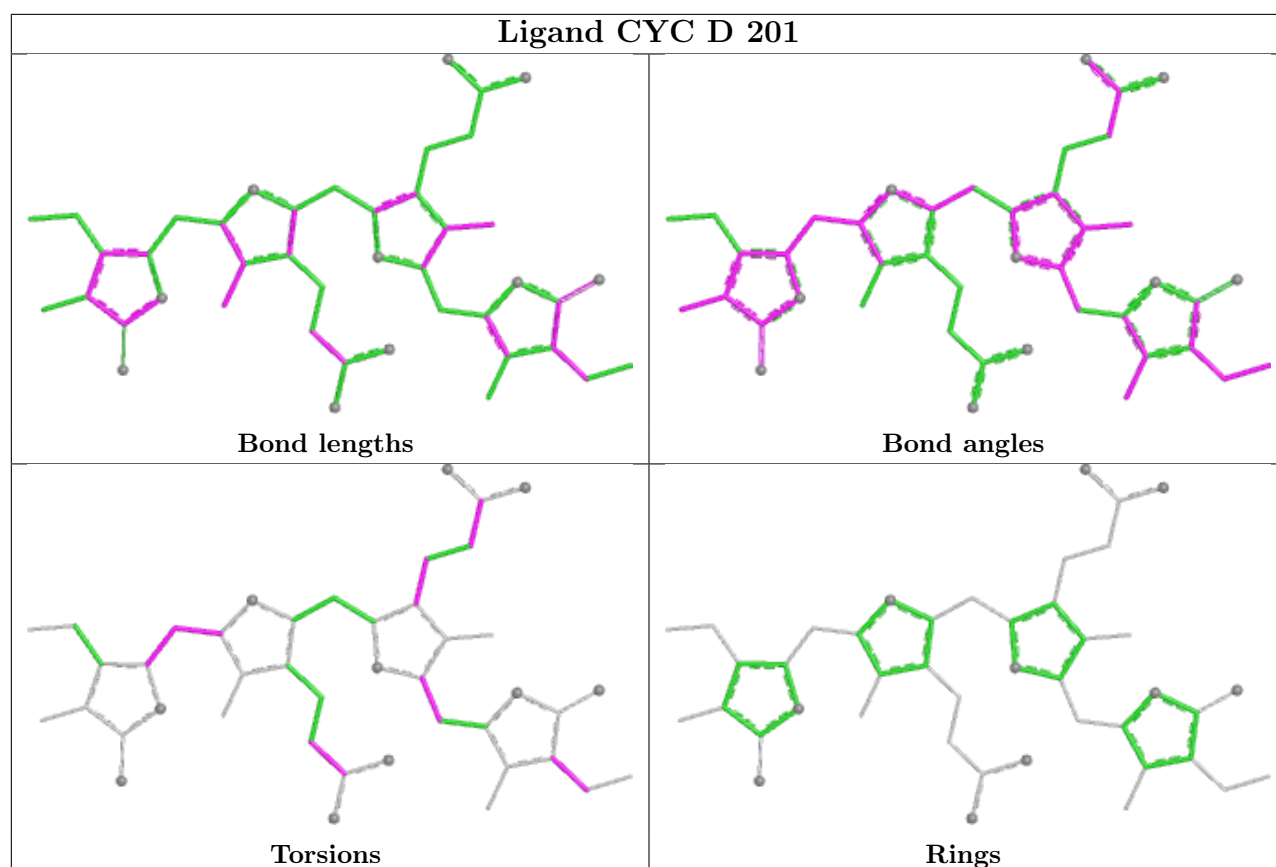
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

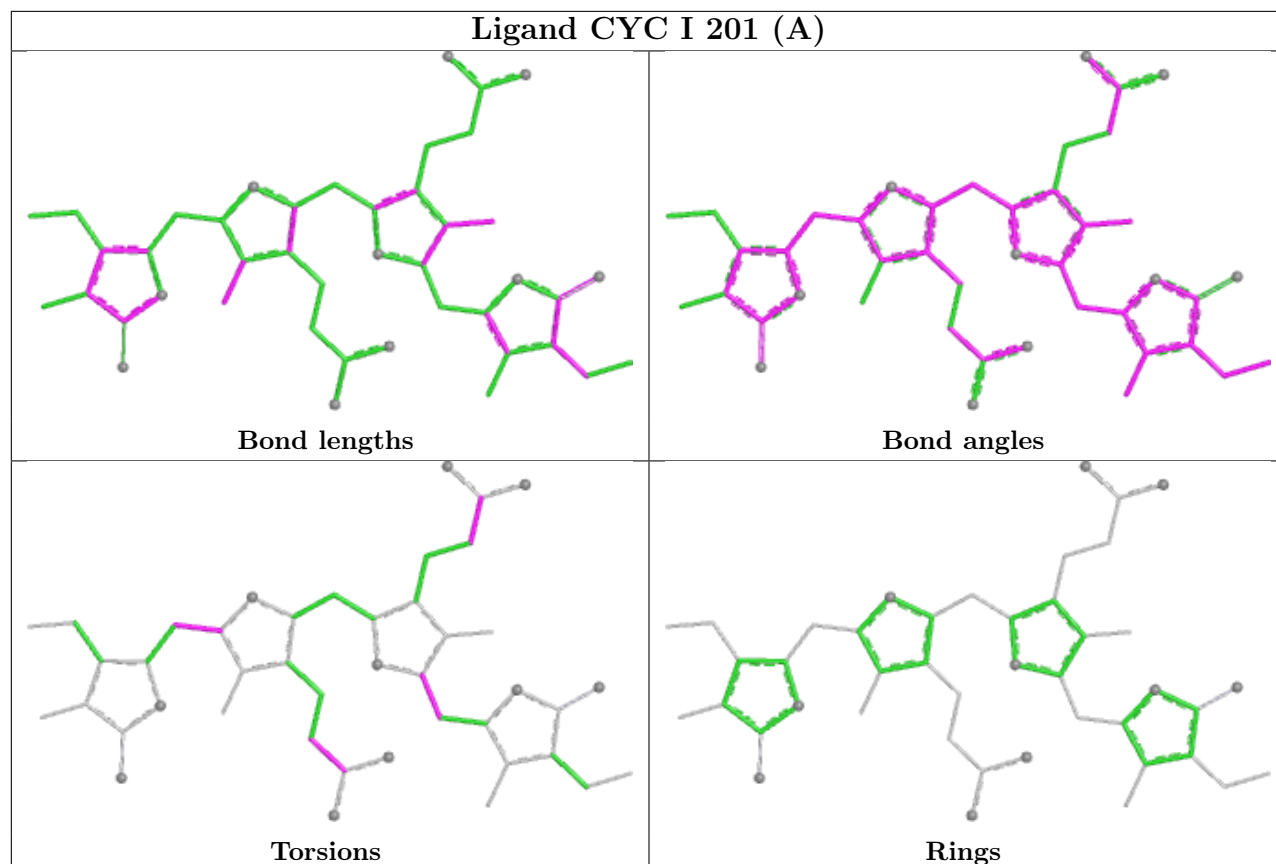




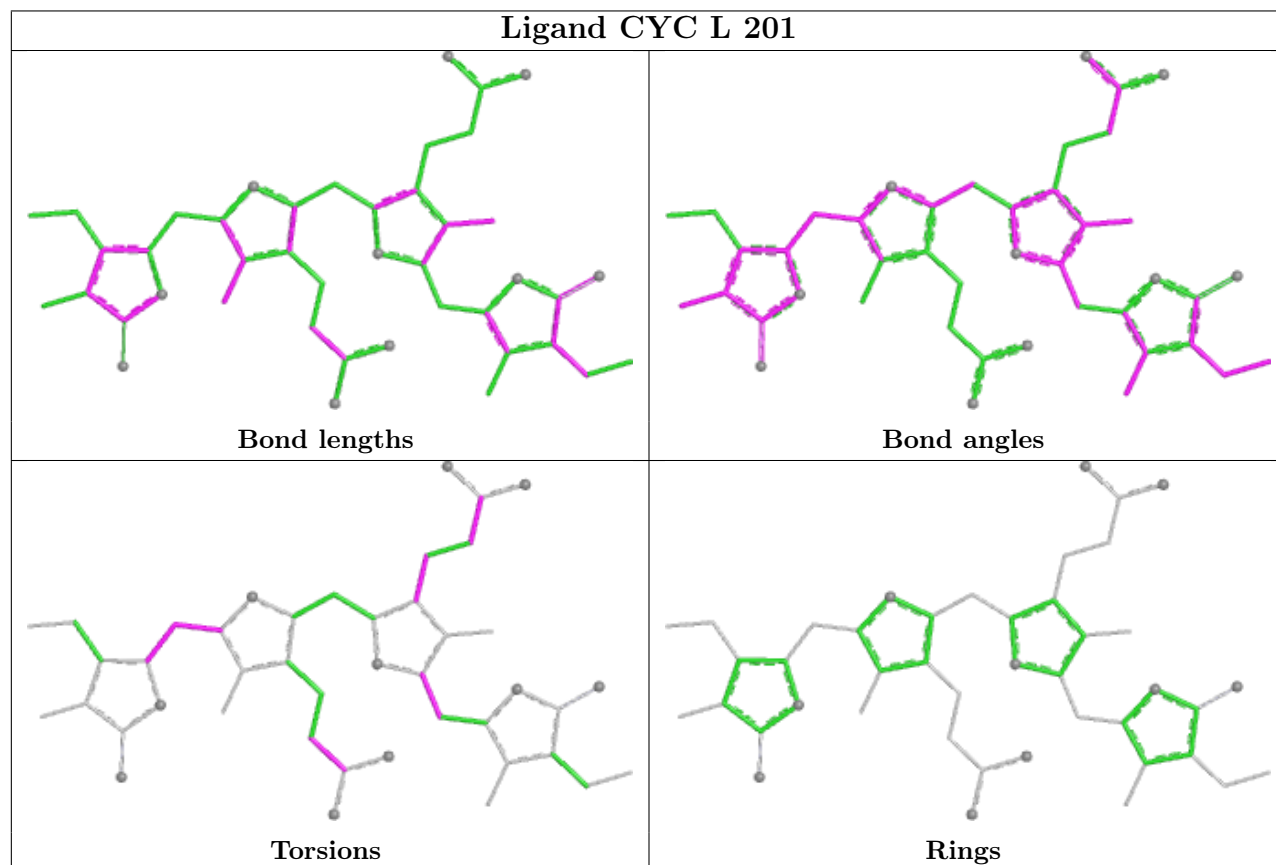


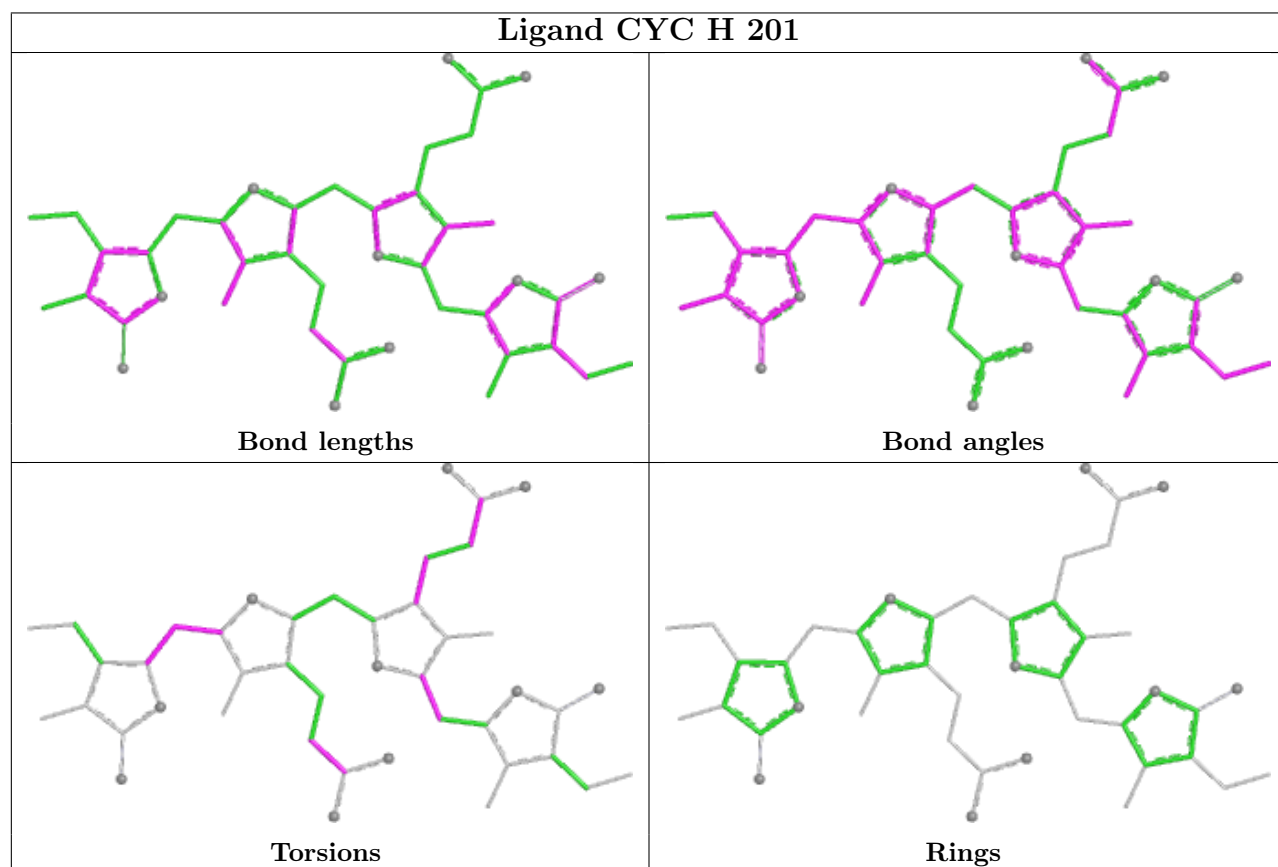
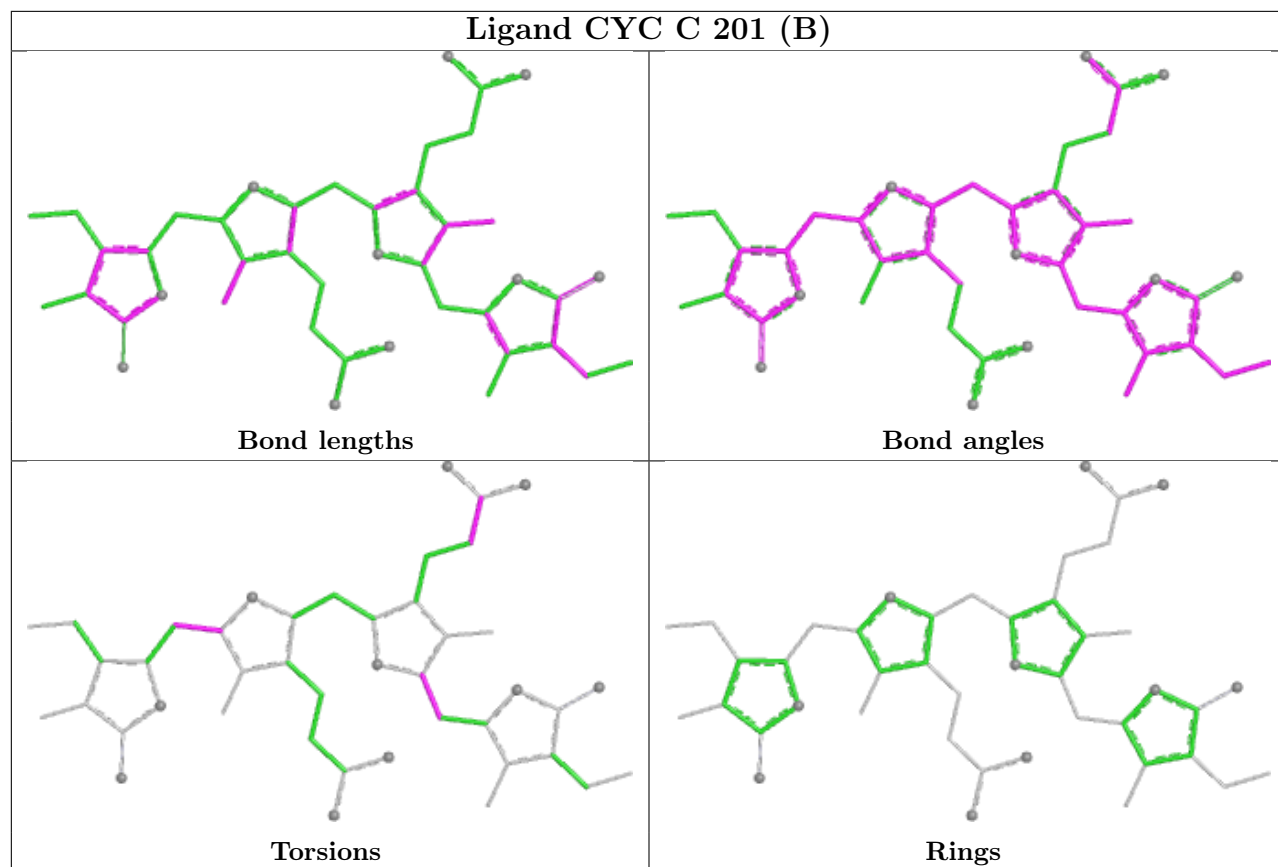


Ligand CYC I 201 (A)

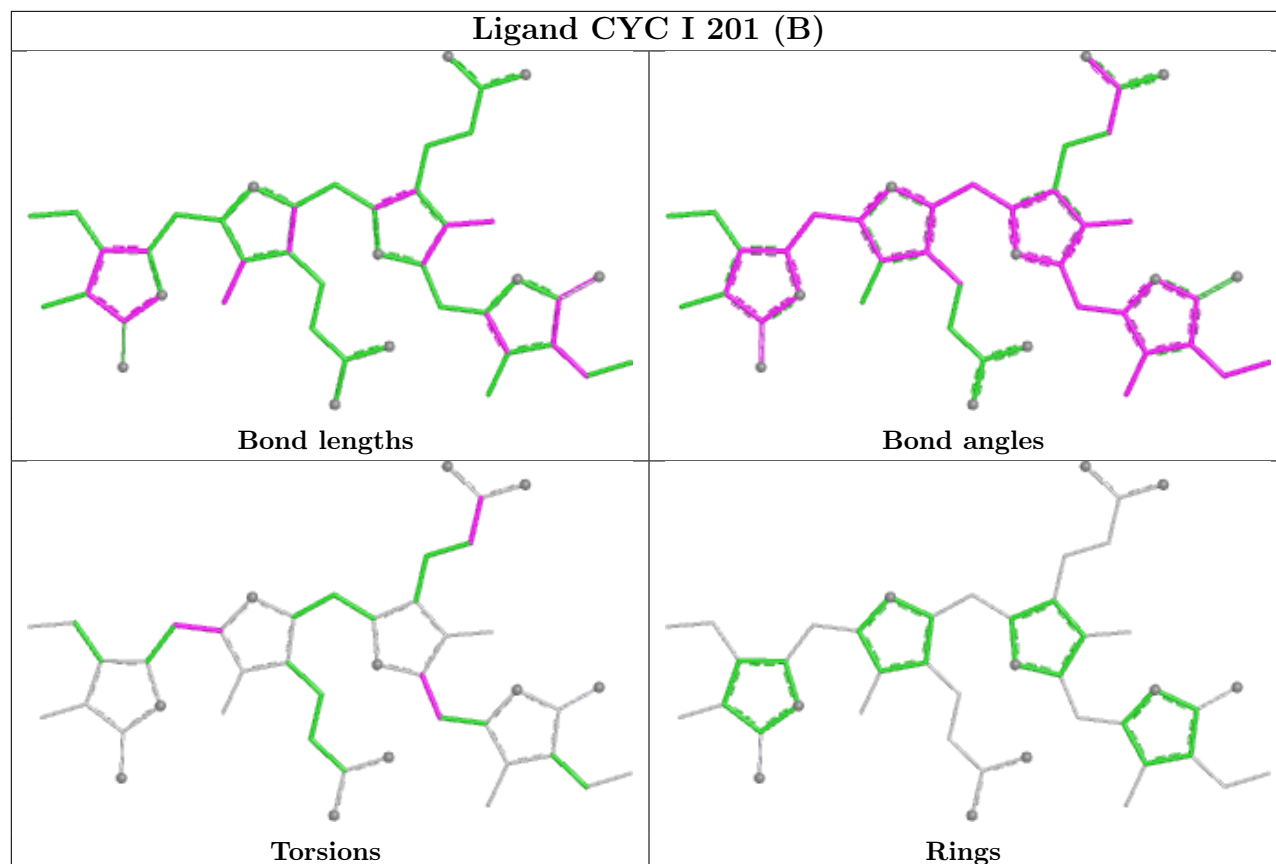


Ligand CYC L 201

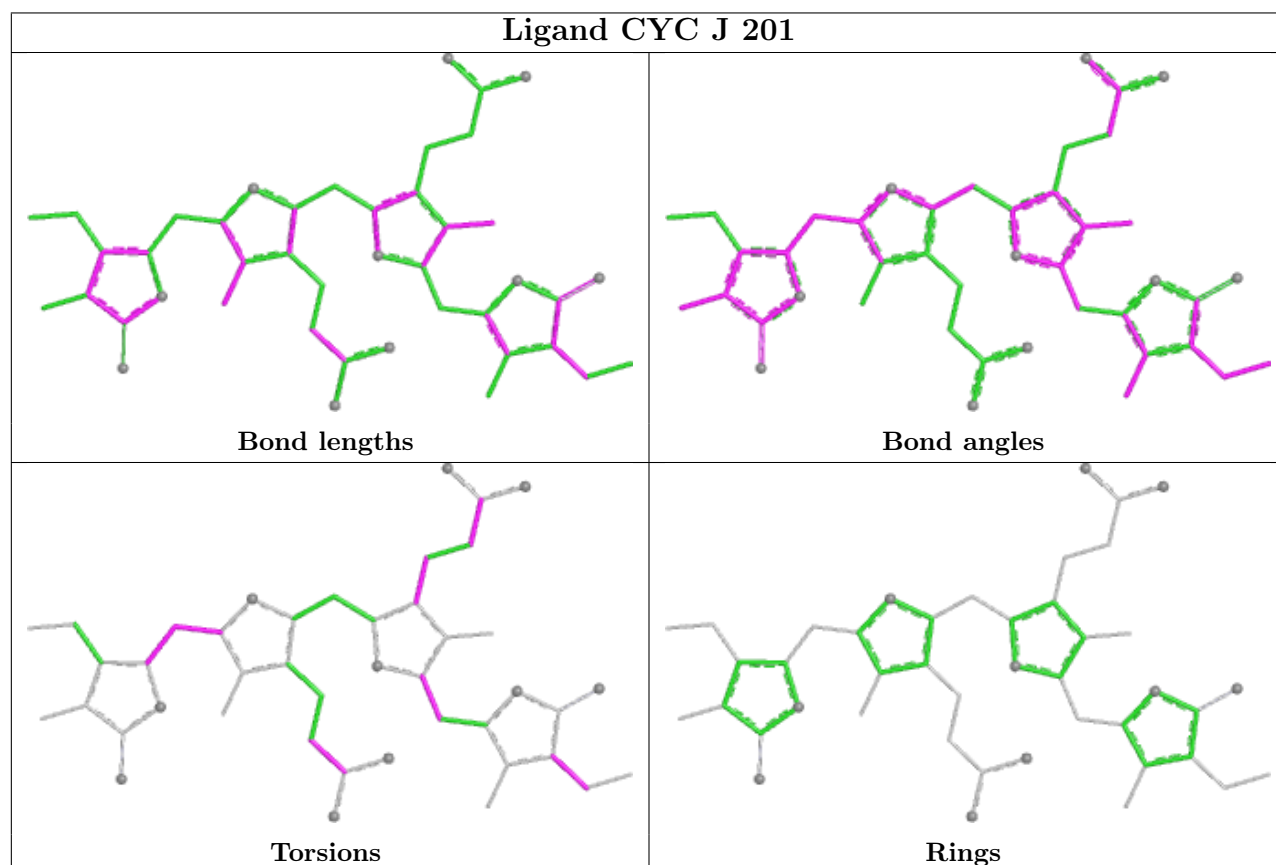


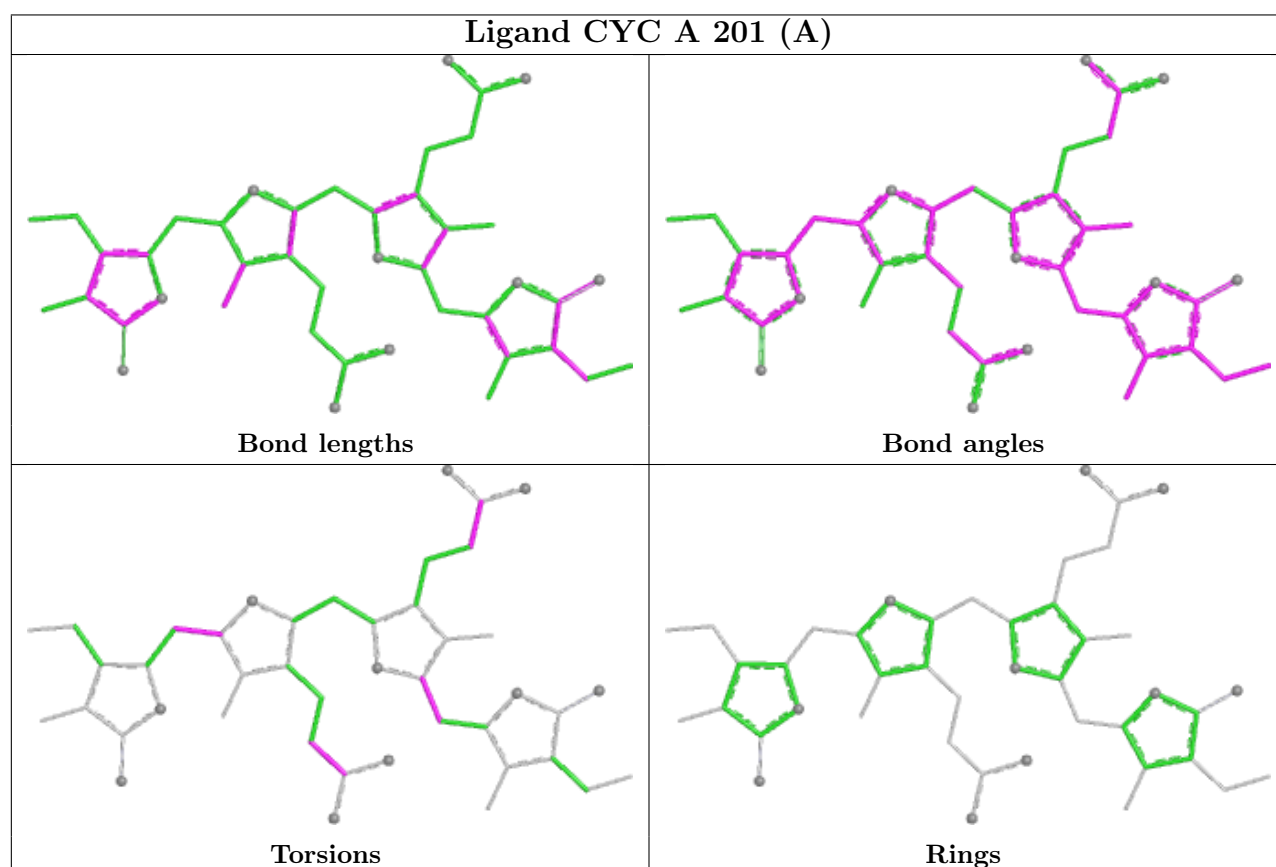
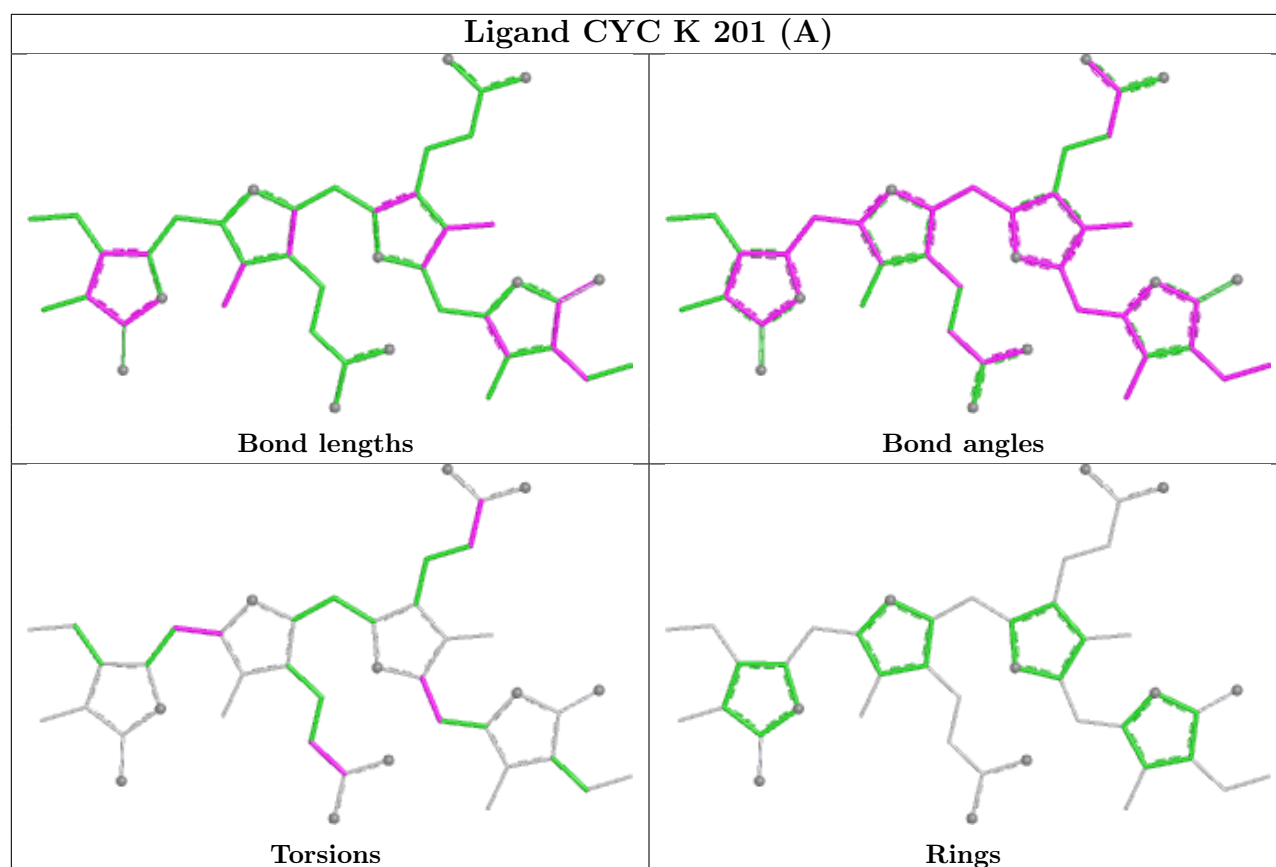


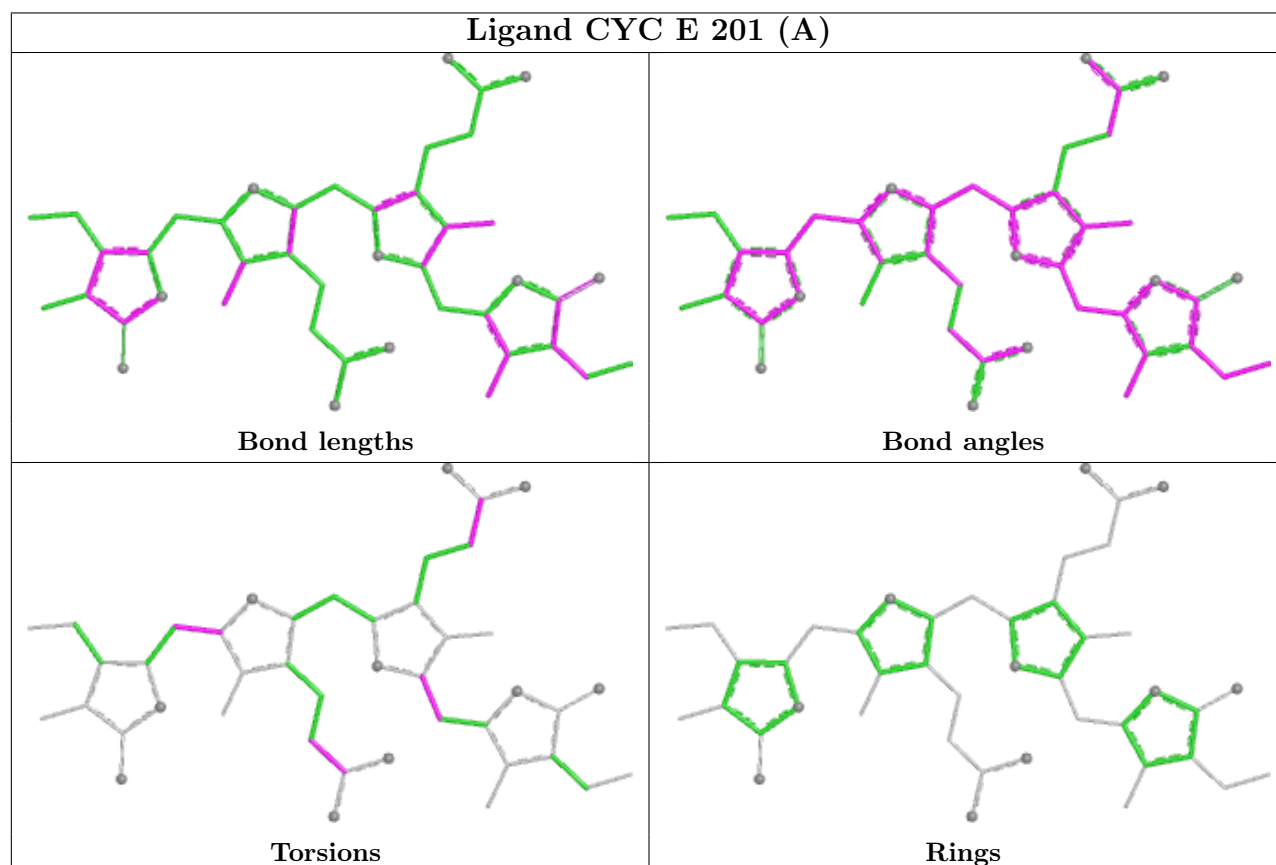
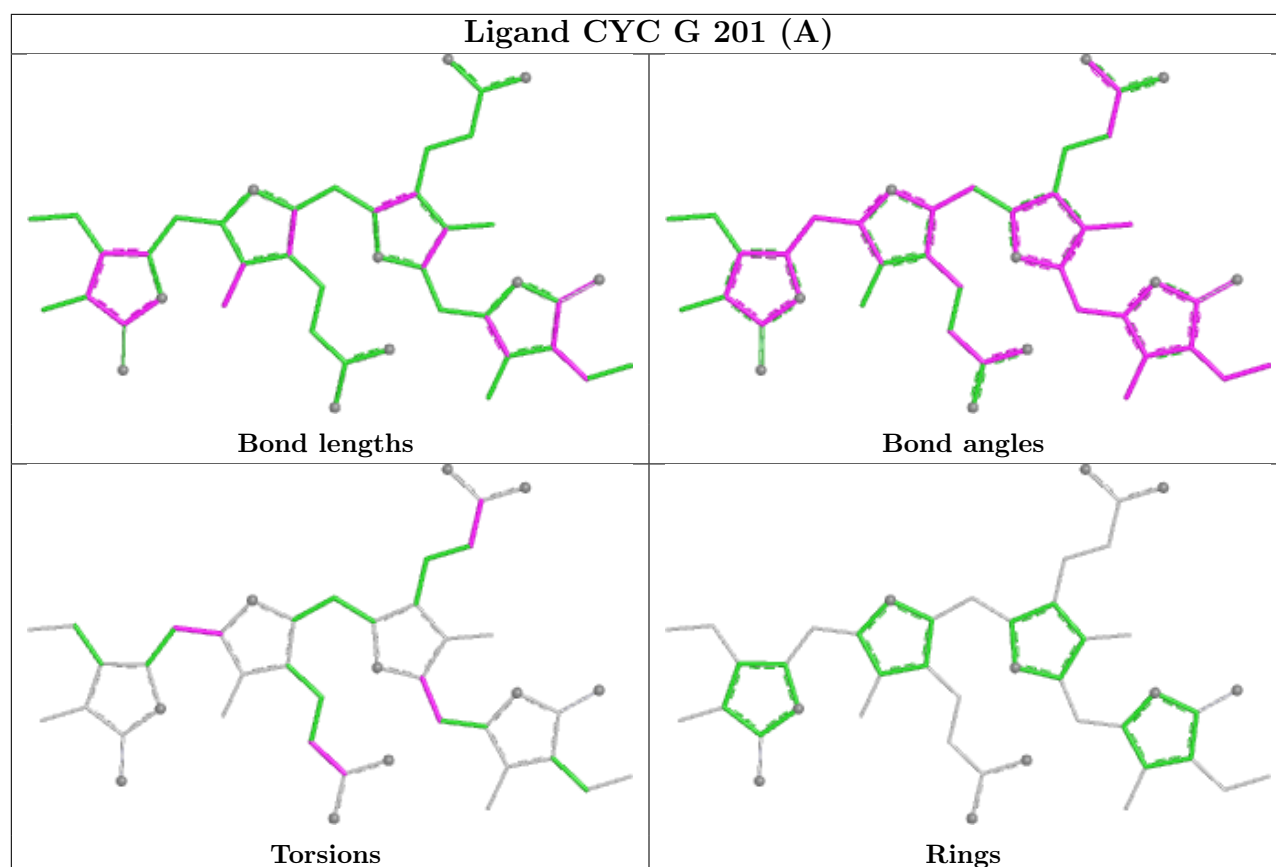
Ligand CYC I 201 (B)



Ligand CYC J 201







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.

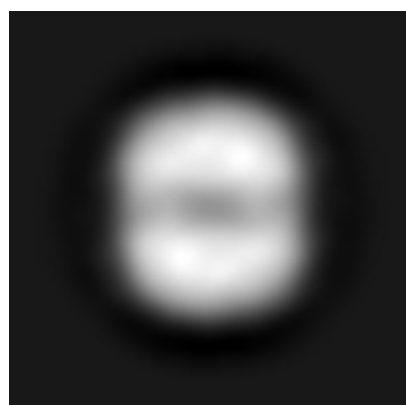
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6430. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

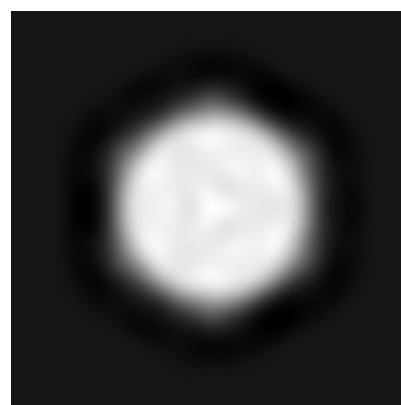
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

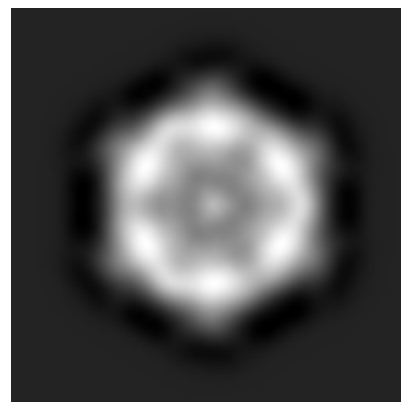
6.2.1 Primary map



X Index: 36



Y Index: 36



Z Index: 36

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 36



Y Index: 36

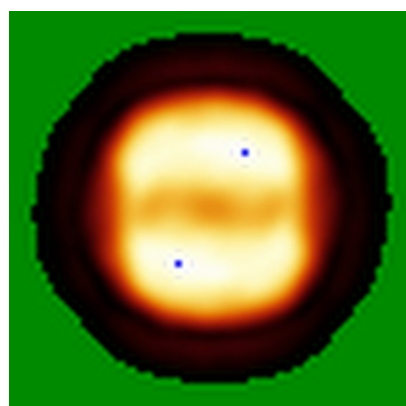


Z Index: 27

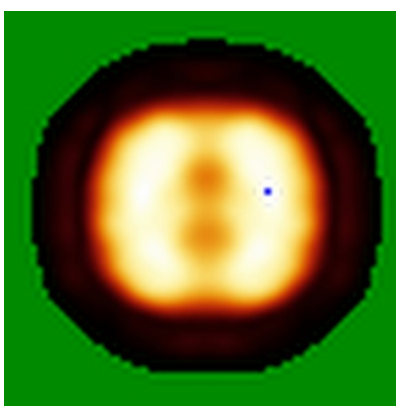
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

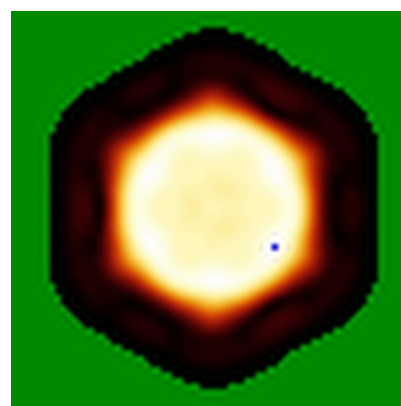
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.86. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

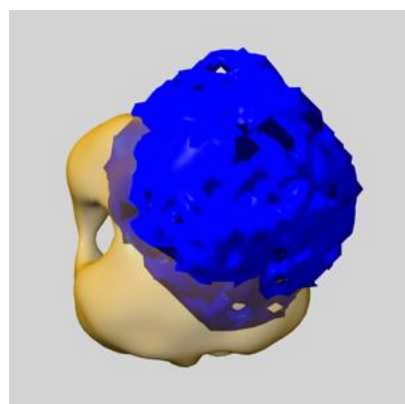
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

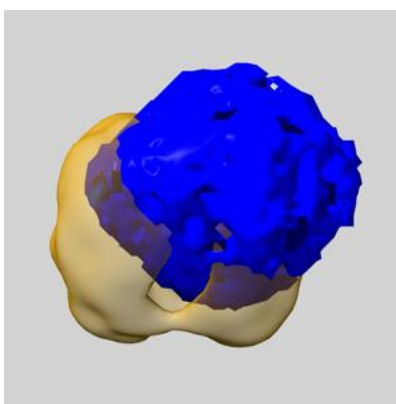
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

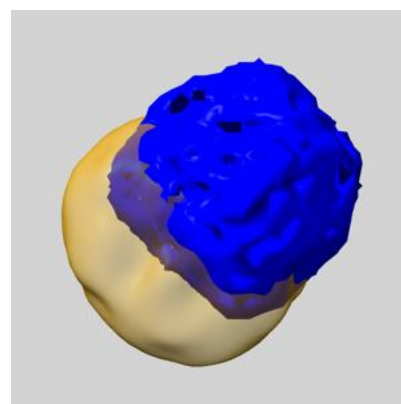
6.6.1 emd_6430_msk_1.map [i](#)



X



Y

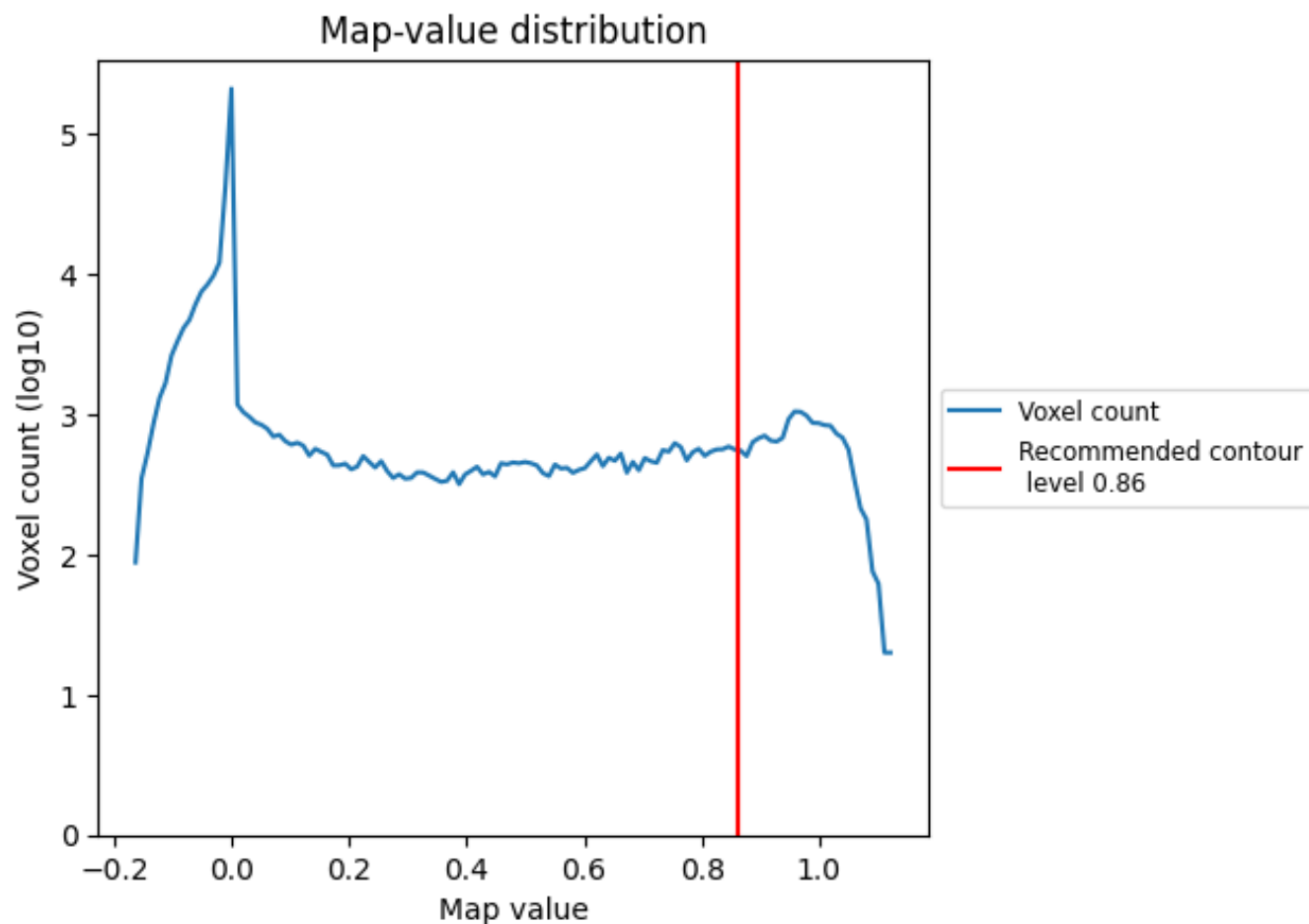


Z

7 Map analysis [i](#)

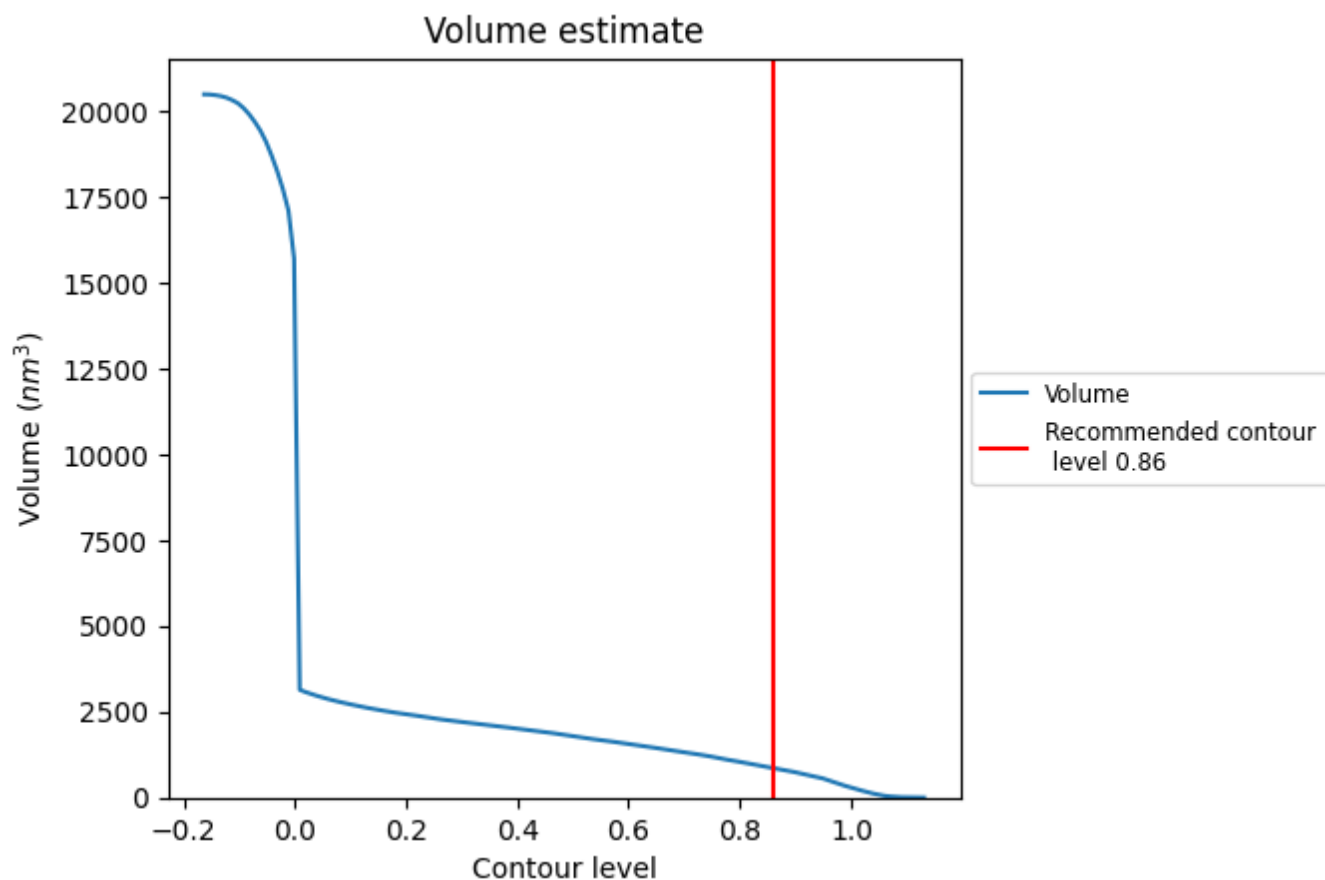
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

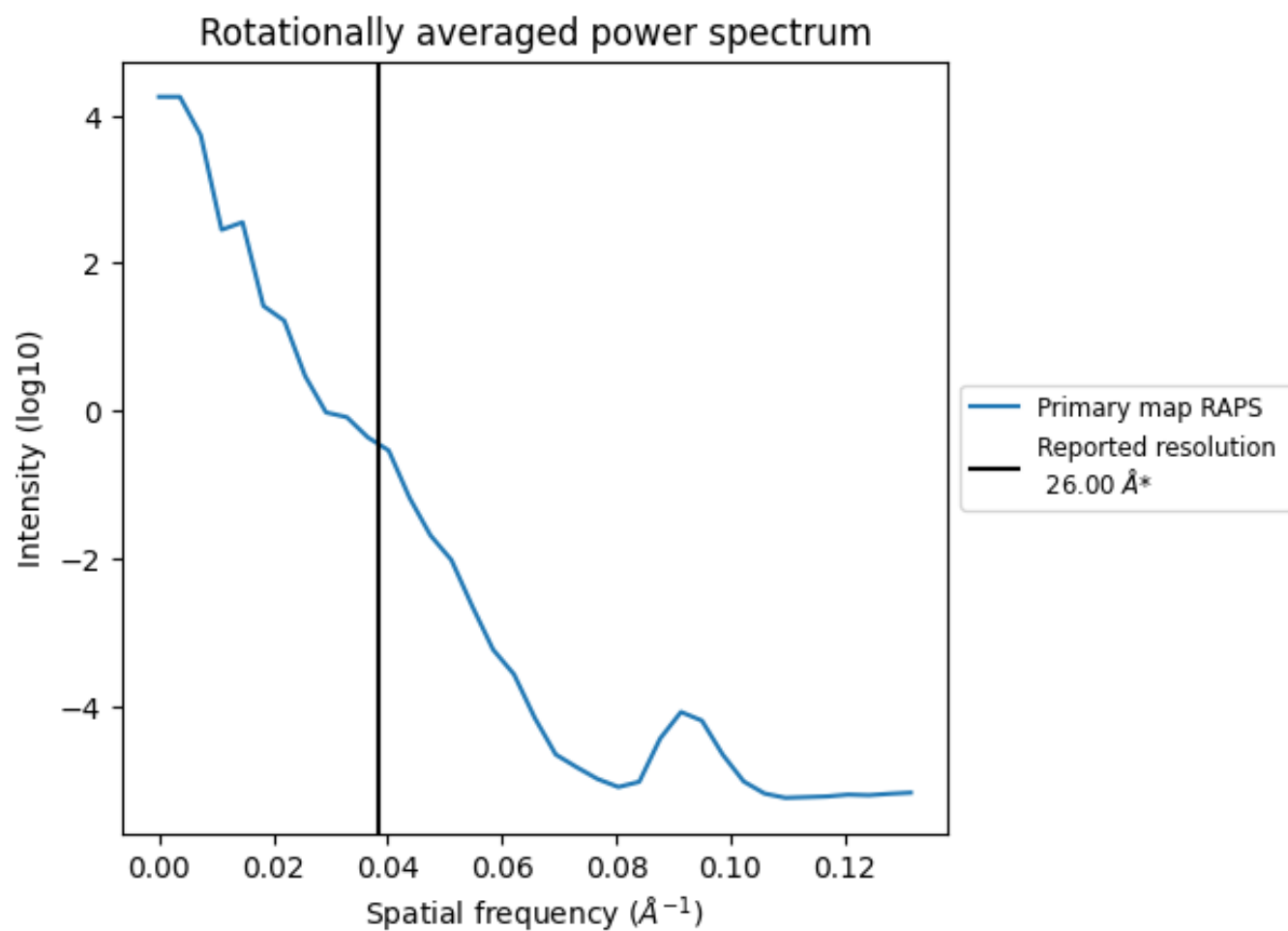
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 858 nm³; this corresponds to an approximate mass of 775 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

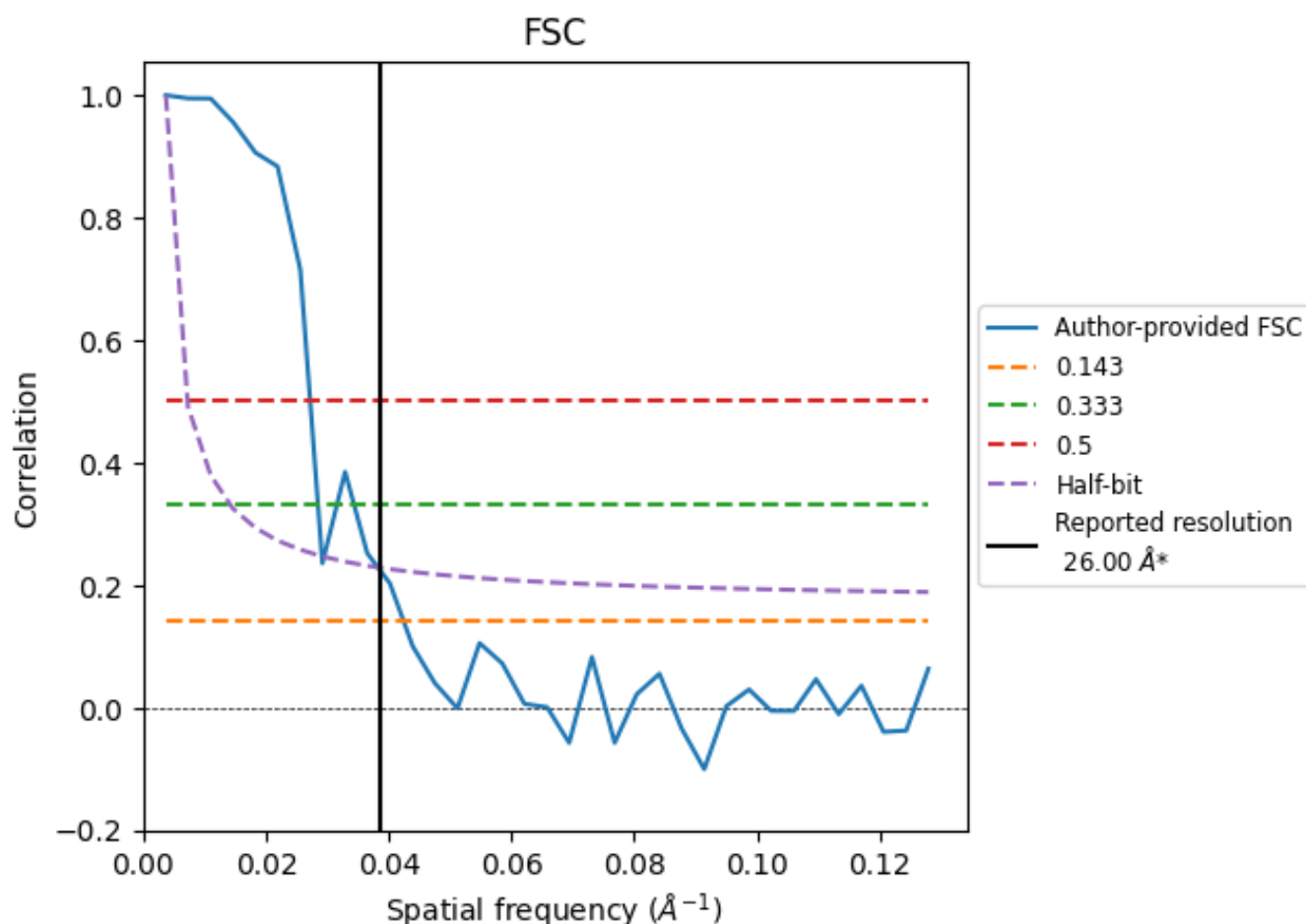


*Reported resolution corresponds to spatial frequency of 0.038 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.038 Å⁻¹

8.2 Resolution estimates [i](#)

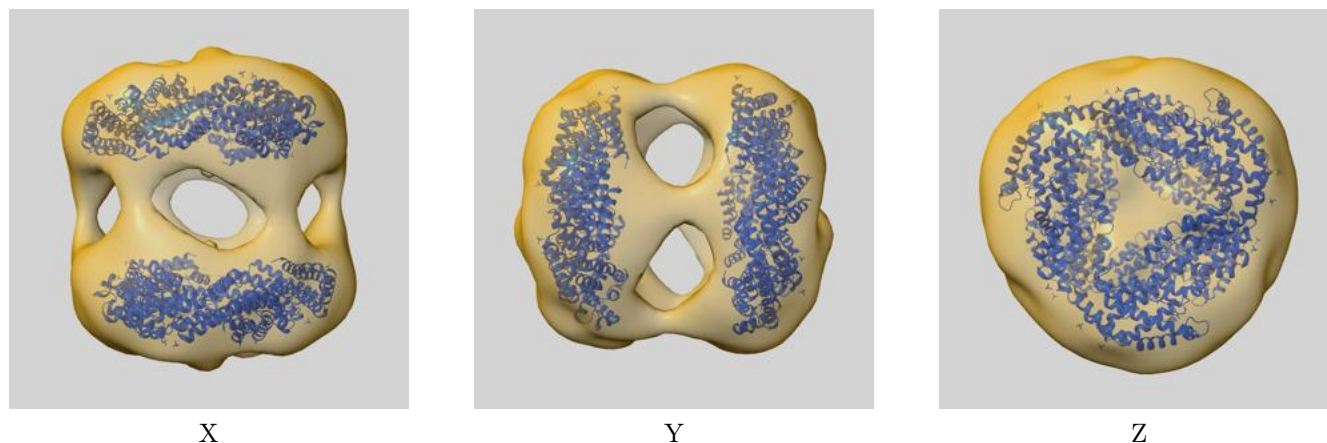
Resolution estimate (Å)	Estimation criterion (FSC cut-off)			
	0.143	0.5	Half-bit	0.333
Reported by author	-	-	-	26.00
Author-provided FSC curve	23.64	36.76	34.25	35.09
Unmasked-calculated*	-	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.33 CUT-OFF 35.09 differs from the reported value 26.0 by more than 10 %

9 Map-model fit [i](#)

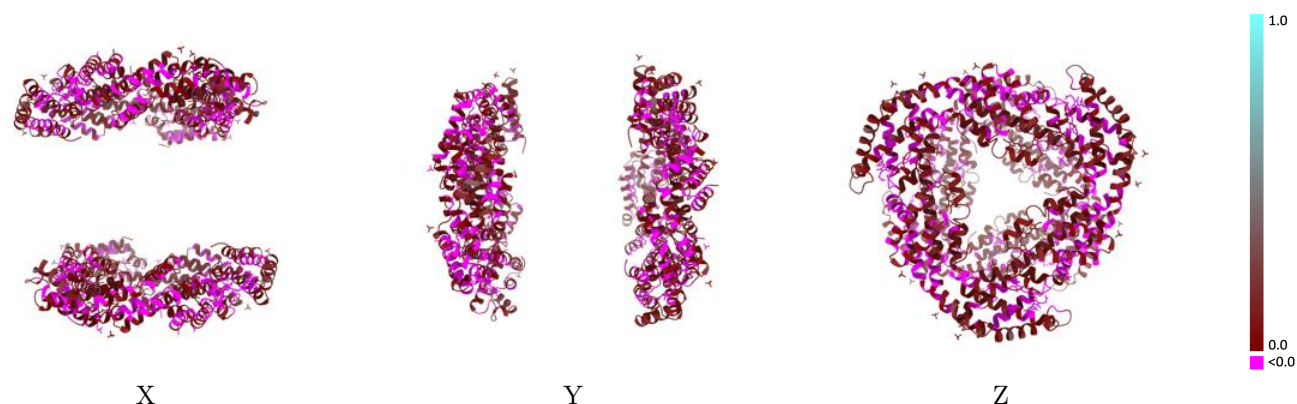
This section contains information regarding the fit between EMDB map EMD-6430 and PDB model 3JBB. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



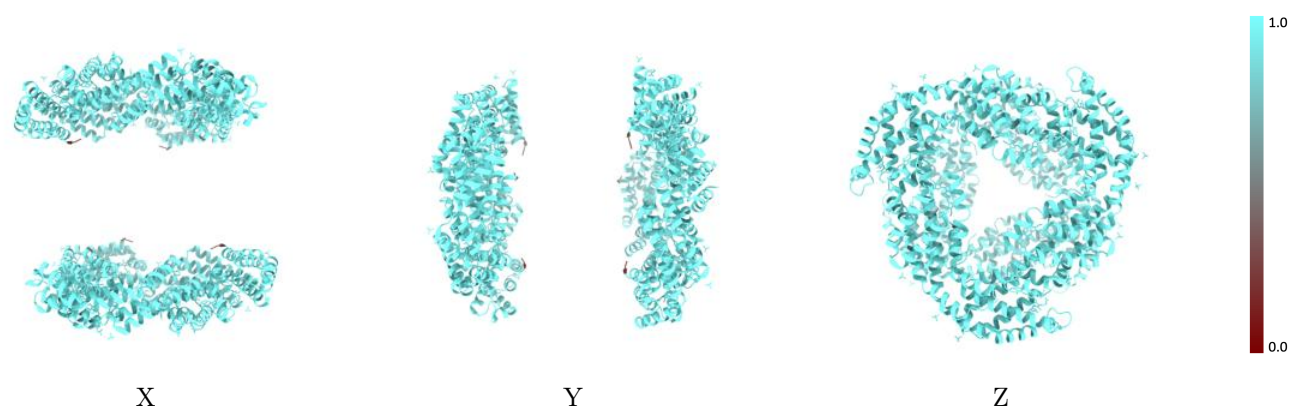
The images above show the 3D surface view of the map at the recommended contour level 0.86 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



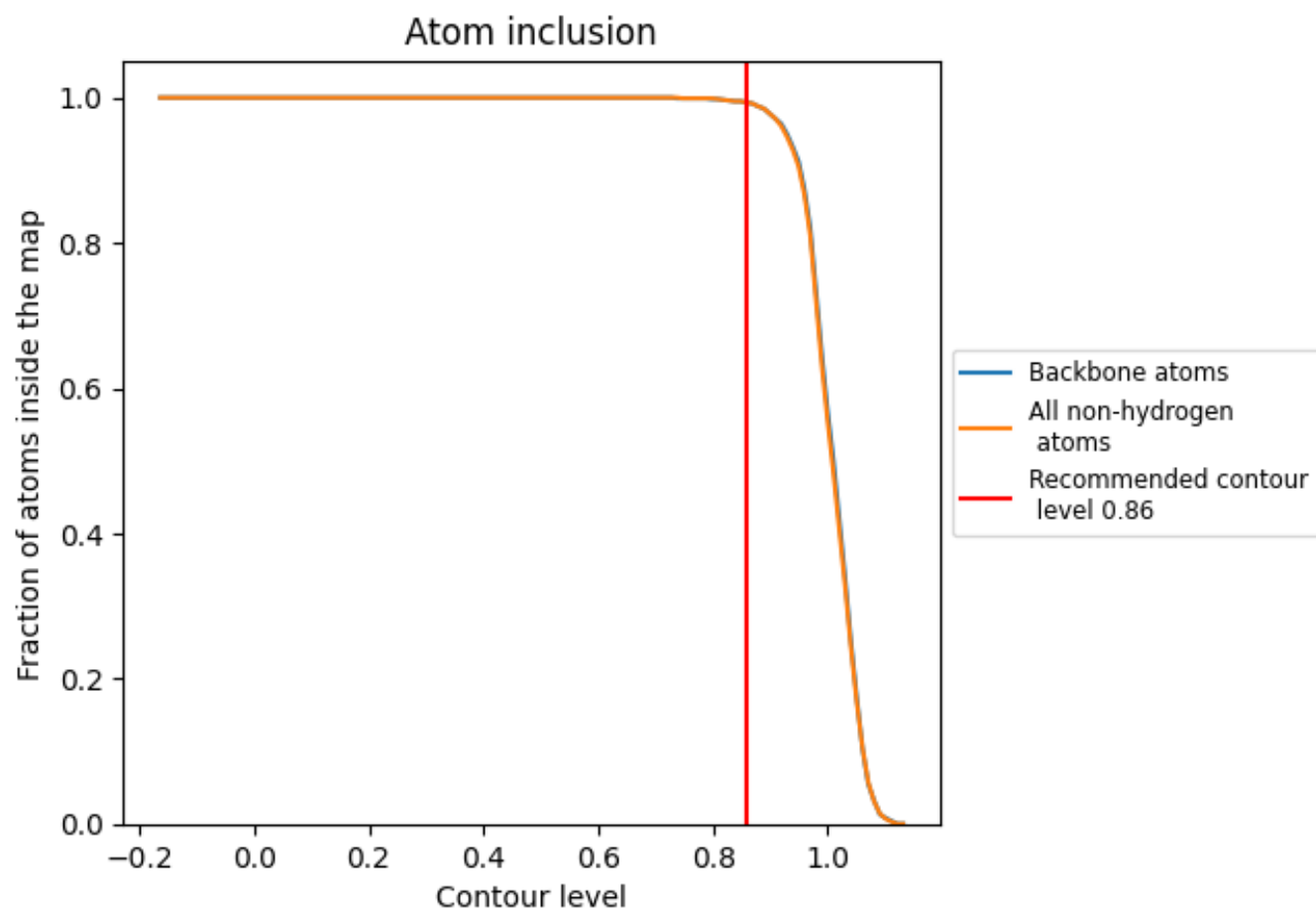
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.86).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9930	0.0490
A	0.9850	0.0530
B	1.0000	0.0450
C	0.9850	0.0510
D	1.0000	0.0440
E	0.9860	0.0610
F	1.0000	0.0470
G	0.9880	0.0620
H	0.9990	0.0320
I	0.9850	0.0580
J	0.9990	0.0300
K	0.9860	0.0650
L	1.0000	0.0360

1.0

0.0

<0.0