



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:35 am BST

PDB ID : 2UUN  
Title : Crystal structure of C-phycoyanin from Phormidium, Lyngbya spp. (Marine) and Spirulina sp. (Fresh water) shows two different ways of energy transfer between two hexamers.  
Authors : Satyanarayana, L.; Patel, A.; Mishra, S.; K Ghosh, P.; Suresh, C.G.  
Deposited on : 2007-03-05  
Resolution : 3.00 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

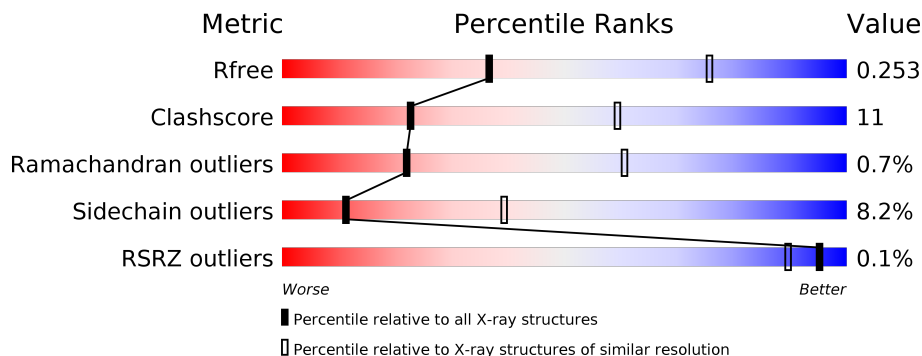
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	81% 15% .
1	C	162	78% 16% . .
1	E	162	% 82% 15% .
1	G	162	84% 13% . .
1	I	162	80% 18% .
1	K	162	% 81% 15% . .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	162	 79% 19% ..
1	O	162	 81% 15% .
1	Q	162	 79% 17% .
1	S	162	 79% 17% .
1	U	162	 81% 18% ..
1	W	162	 83% 12% .
2	B	172	 76% 21% ..
2	F	172	 80% 19% .
2	H	172	 79% 17% .
2	J	172	 82% 16% .
2	L	172	 82% 16% .
2	N	172	 81% 17% .
2	P	172	 78% 19% .
2	R	172	 75% 23% .
2	T	172	 80% 18% .
2	V	172	 80% 18% .
2	X	172	 81% 17% .
3	D	172	 72% 24% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 31361 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 C-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	162	1211	761	203	240	7	0	0	0
1	C	162	1211	761	203	240	7	0	0	0
1	E	162	1211	761	203	240	7	0	0	0
1	G	162	1211	761	203	240	7	0	0	0
1	I	162	1211	761	203	240	7	0	0	0
1	K	162	1211	761	203	240	7	0	0	0
1	M	162	1211	761	203	240	7	0	0	0
1	O	162	1211	761	203	240	7	0	0	0
1	Q	162	1211	761	203	240	7	0	0	0
1	S	162	1211	761	203	240	7	0	0	0
1	U	162	1211	761	203	240	7	0	0	0
1	W	162	1211	761	203	240	7	0	0	0

- Molecule 2 is a protein called C-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1242	768	218	247	9	0	0	0
2	F	172	1242	768	218	247	9	0	0	0

*Continued on next page...*

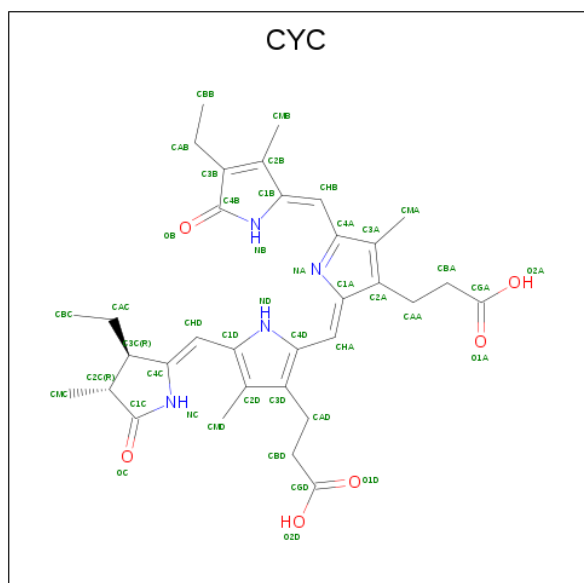
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	J	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	L	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	N	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	P	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	R	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	T	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	V	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0
2	X	172	Total 1242	C 768	N 218	O 247	S 9	0	0	0

- Molecule 3 is a protein called C-PHYCOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	172	Total 1244	C 770	N 218	O 247	S 9	0	0	0

- Molecule 4 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ).



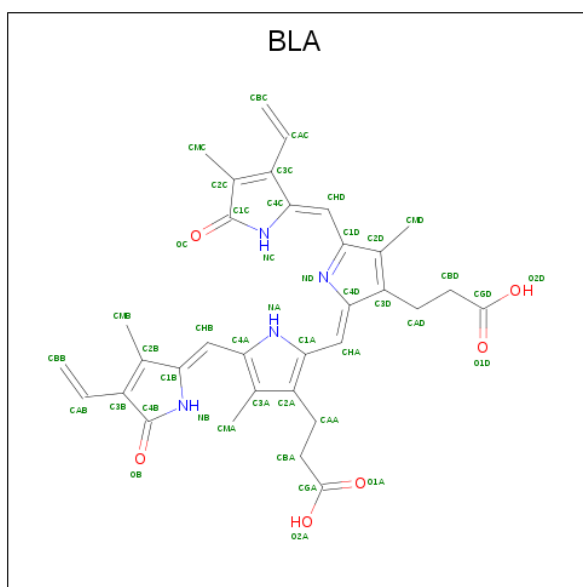
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 43	C 33	N 4	O 6	0	0
4	B	1	Total 43	C 33	N 4	O 6	0	0
4	C	1	Total 43	C 33	N 4	O 6	0	0
4	D	1	Total 43	C 33	N 4	O 6	0	0
4	D	1	Total 43	C 33	N 4	O 6	0	0
4	E	1	Total 43	C 33	N 4	O 6	0	0
4	F	1	Total 43	C 33	N 4	O 6	0	0
4	F	1	Total 43	C 33	N 4	O 6	0	0
4	G	1	Total 43	C 33	N 4	O 6	0	0
4	H	1	Total 43	C 33	N 4	O 6	0	0
4	H	1	Total 43	C 33	N 4	O 6	0	0
4	I	1	Total 43	C 33	N 4	O 6	0	0
4	J	1	Total 43	C 33	N 4	O 6	0	0
4	J	1	Total 43	C 33	N 4	O 6	0	0
4	K	1	Total 43	C 33	N 4	O 6	0	0
4	L	1	Total 43	C 33	N 4	O 6	0	0
4	L	1	Total 43	C 33	N 4	O 6	0	0
4	M	1	Total 43	C 33	N 4	O 6	0	0
4	N	1	Total 43	C 33	N 4	O 6	0	0
4	N	1	Total 43	C 33	N 4	O 6	0	0
4	O	1	Total 43	C 33	N 4	O 6	0	0
4	P	1	Total 43	C 33	N 4	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	0	0
			43	33	4	6		
4	Q	1	Total	C	N	O	0	0
			43	33	4	6		
4	R	1	Total	C	N	O	0	0
			43	33	4	6		
4	R	1	Total	C	N	O	0	0
			43	33	4	6		
4	S	1	Total	C	N	O	0	0
			43	33	4	6		
4	T	1	Total	C	N	O	0	0
			43	33	4	6		
4	T	1	Total	C	N	O	0	0
			43	33	4	6		
4	U	1	Total	C	N	O	0	0
			43	33	4	6		
4	V	1	Total	C	N	O	0	0
			43	33	4	6		
4	V	1	Total	C	N	O	0	0
			43	33	4	6		
4	W	1	Total	C	N	O	0	0
			43	33	4	6		
4	X	1	Total	C	N	O	0	0
			43	33	4	6		
4	X	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 5 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula:  $C_{33}H_{34}N_4O_6$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	C	31	Total	O	0	0
			31	31		
6	D	13	Total	O	0	0
			13	13		
6	E	8	Total	O	0	0
			8	8		
6	F	39	Total	O	0	0
			39	39		
6	I	40	Total	O	0	0
			40	40		
6	J	15	Total	O	0	0
			15	15		
6	K	9	Total	O	0	0
			9	9		
6	L	31	Total	O	0	0
			31	31		
6	M	40	Total	O	0	0
			40	40		
6	N	13	Total	O	0	0
			13	13		

*Continued on next page...*




*Continued from previous page...*

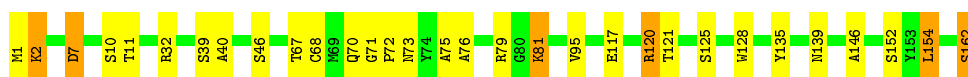
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	O	13	Total 13	O 13	0	0
6	P	27	Total 27	O 27	0	0
6	Q	2	Total 2	O 2	0	0
6	R	3	Total 3	O 3	0	0
6	S	6	Total 6	O 6	0	0
6	T	30	Total 30	O 30	0	0
6	W	34	Total 34	O 34	0	0
6	X	19	Total 19	O 19	0	0

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: C-PHYCOCYANIN

Chain A: 




- Molecule 1: C-PHYCOCYANIN

Chain C: 




- Molecule 1: C-PHYCOCYANIN

Chain E: 




- Molecule 1: C-PHYCOCYANIN

Chain G: 




- Molecule 1: C-PHYCOCYANIN

Chain I: 

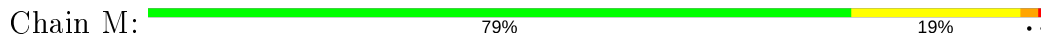


- Molecule 1: C-PHYCOCYANIN

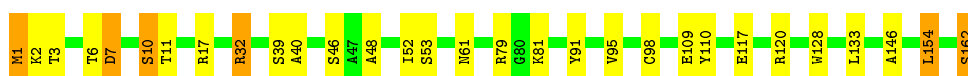
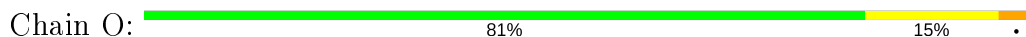
Chain K: 



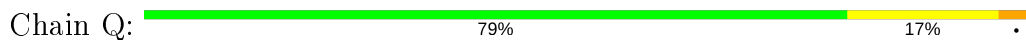
- Molecule 1: C-PHYCOCYANIN



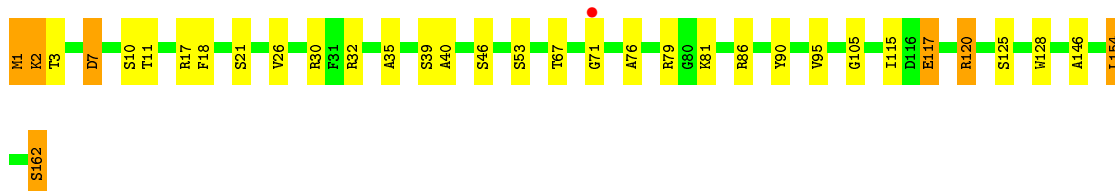
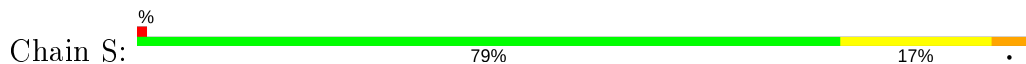
- Molecule 1: C-PHYCOCYANIN



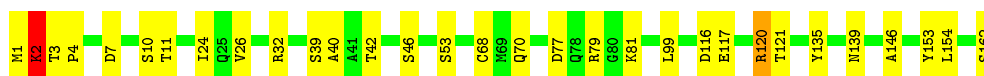
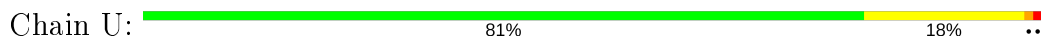
- Molecule 1: C-PHYCOCYANIN



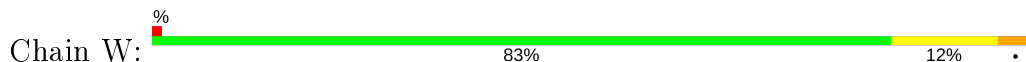
- Molecule 1: C-PHYCOCYANIN



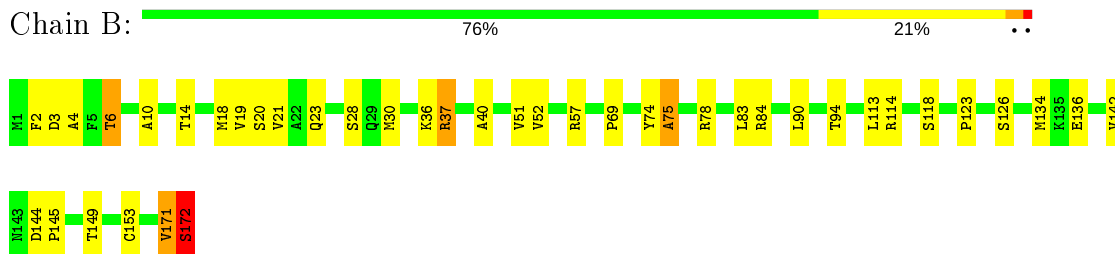
- Molecule 1: C-PHYCOCYANIN



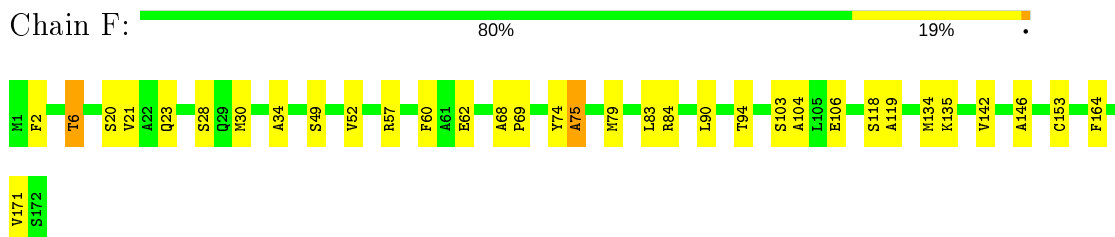
- Molecule 1: C-PHYCOCYANIN



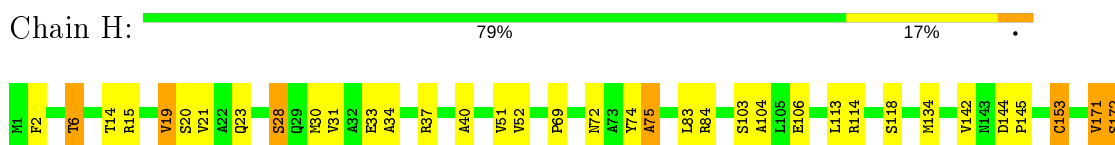
- Molecule 2: C-PHYCOCYANIN



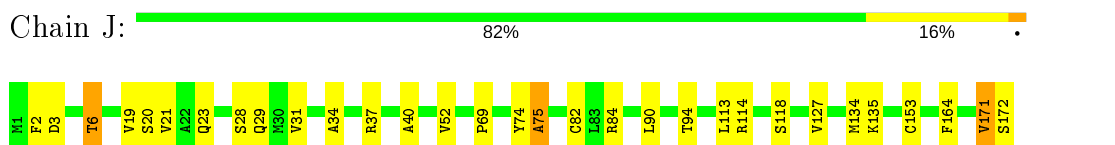
- Molecule 2: C-PHYCOCYANIN



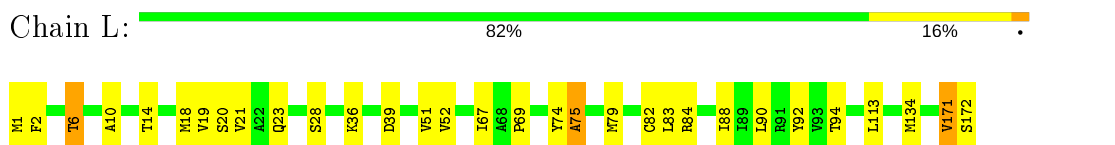
- Molecule 2: C-PHYCOCYANIN



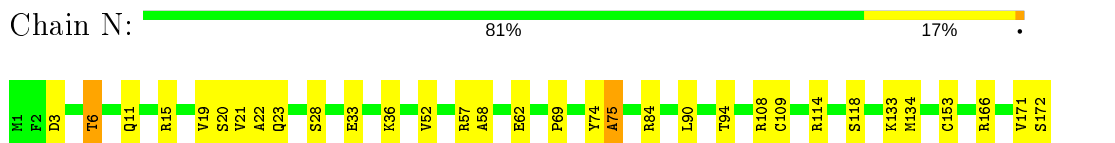
- Molecule 2: C-PHYCOCYANIN



- Molecule 2: C-PHYCOCYANIN



- Molecule 2: C-PHYCOCYANIN



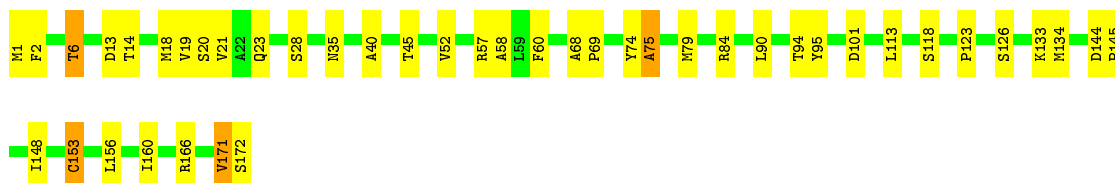
- Molecule 2: C-PHYCOCYANIN





- Molecule 2: C-PHYCOCYANIN

Chain R: 75% 23%



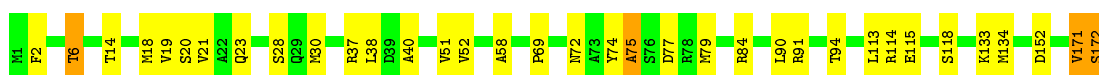
- Molecule 2: C-PHYCOCYANIN

Chain T: 80% 18%



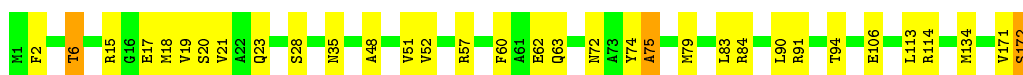
- Molecule 2: C-PHYCOCYANIN

Chain V: 80% 18%



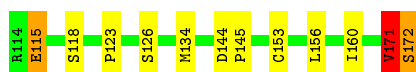
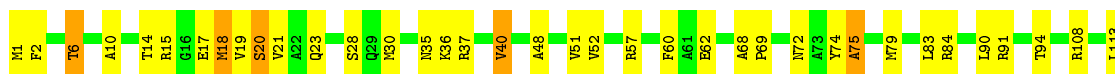
- Molecule 2: C-PHYCOCYANIN

Chain X: 81% 17%



- Molecule 3: C-PHYCOCYANIN

Chain D: 72% 24%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.46Å 115.33Å 183.37Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	182.57 – 3.00 24.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (182.57-3.00) 96.2 (24.86-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.99Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.213 , 0.262 0.208 , 0.253	Depositor DCC
$R_{free}$ test set	4359 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 14.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	31361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	2.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CYC, BLA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.14	3/1234 (0.2%)	0.93	3/1676 (0.2%)
1	C	1.13	6/1234 (0.5%)	0.99	6/1676 (0.4%)
1	E	1.24	3/1234 (0.2%)	1.06	9/1676 (0.5%)
1	G	1.13	4/1234 (0.3%)	0.95	5/1676 (0.3%)
1	I	1.05	0/1234	0.90	0/1676
1	K	1.17	6/1234 (0.5%)	0.98	6/1676 (0.4%)
1	M	1.05	2/1234 (0.2%)	0.88	2/1676 (0.1%)
1	O	1.13	6/1234 (0.5%)	0.96	1/1676 (0.1%)
1	Q	1.14	4/1234 (0.3%)	0.94	2/1676 (0.1%)
1	S	1.16	7/1234 (0.6%)	0.99	3/1676 (0.2%)
1	U	1.12	4/1234 (0.3%)	0.93	4/1676 (0.2%)
1	W	1.14	3/1234 (0.2%)	0.96	3/1676 (0.2%)
2	B	1.08	2/1256 (0.2%)	0.97	5/1704 (0.3%)
2	F	1.14	3/1256 (0.2%)	0.96	2/1704 (0.1%)
2	H	1.12	4/1256 (0.3%)	0.96	3/1704 (0.2%)
2	J	1.07	1/1256 (0.1%)	0.95	3/1704 (0.2%)
2	L	1.07	0/1256	0.99	1/1704 (0.1%)
2	N	1.13	1/1256 (0.1%)	0.95	0/1704
2	P	1.07	2/1256 (0.2%)	0.98	2/1704 (0.1%)
2	R	1.13	2/1256 (0.2%)	1.01	4/1704 (0.2%)
2	T	1.09	3/1256 (0.2%)	0.96	0/1704
2	V	1.09	1/1256 (0.1%)	0.97	5/1704 (0.3%)
2	X	1.06	2/1256 (0.2%)	0.94	2/1704 (0.1%)
3	D	1.13	4/1258 (0.3%)	0.96	2/1707 (0.1%)
All	All	1.12	73/29882 (0.2%)	0.96	73/40563 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	S	0	1
1	W	0	1
All	All	0	8

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	68	CYS	CB-SG	-15.62	1.55	1.82
1	E	161	LEU	C-O	-13.97	0.96	1.23
2	F	171	VAL	C-O	-11.88	1.00	1.23
2	R	171	VAL	C-O	-9.22	1.05	1.23
2	J	153	CYS	CB-SG	-8.24	1.68	1.82
1	C	68	CYS	CB-SG	7.71	1.95	1.82
1	A	68	CYS	CB-SG	7.51	1.95	1.82
1	O	98	CYS	CB-SG	-7.24	1.70	1.82
1	A	162	SER	CB-OG	-7.17	1.32	1.42
1	C	162	SER	CB-OG	-7.03	1.33	1.42
1	S	117	GLU	CD-OE1	6.74	1.33	1.25
1	Q	47	ALA	CA-CB	6.71	1.66	1.52
2	P	82	CYS	CB-SG	-6.67	1.71	1.82
1	C	117	GLU	CD-OE1	6.65	1.32	1.25
3	D	171	VAL	C-O	-6.63	1.10	1.23
2	H	153	CYS	CB-SG	-6.60	1.71	1.82
1	G	162	SER	CB-OG	-6.49	1.33	1.42
1	W	162	SER	CB-OG	-6.47	1.33	1.42
2	N	62	GLU	CD-OE2	6.46	1.32	1.25
1	O	109	GLU	CD-OE1	6.43	1.32	1.25
2	T	17	GLU	CD-OE1	6.38	1.32	1.25
3	D	17	GLU	CD-OE1	6.32	1.32	1.25
1	O	109	GLU	CD-OE2	6.28	1.32	1.25
2	F	106	GLU	CD-OE1	6.26	1.32	1.25
1	C	161	LEU	C-O	-6.23	1.11	1.23
2	R	153	CYS	CB-SG	-6.16	1.71	1.82
1	M	162	SER	CB-OG	-6.15	1.34	1.42
1	W	84	CYS	CB-SG	-6.04	1.72	1.82
2	X	106	GLU	CD-OE1	6.01	1.32	1.25
1	K	162	SER	CA-CB	-5.96	1.44	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	162	SER	CB-OG	-5.91	1.34	1.42
1	C	117	GLU	CD-OE2	5.89	1.32	1.25
1	Q	149	GLU	CD-OE2	5.84	1.32	1.25
1	K	162	SER	CB-OG	-5.78	1.34	1.42
1	U	70	GLN	CG-CD	5.70	1.64	1.51
1	C	42	THR	CA-CB	5.68	1.68	1.53
1	O	162	SER	CA-CB	-5.65	1.44	1.52
3	D	20	SER	CB-OG	5.64	1.49	1.42
2	V	77	ASP	CB-CG	5.59	1.63	1.51
1	K	117	GLU	CD-OE2	5.57	1.31	1.25
1	S	117	GLU	CD-OE2	5.57	1.31	1.25
3	D	153	CYS	CB-SG	-5.53	1.72	1.81
1	O	162	SER	CB-OG	-5.50	1.35	1.42
1	E	162	SER	CB-OG	-5.49	1.35	1.42
1	U	120	ARG	CG-CD	5.48	1.65	1.51
1	G	162	SER	CA-CB	-5.47	1.44	1.52
1	U	42	THR	CA-CB	5.42	1.67	1.53
2	F	153	CYS	CB-SG	-5.41	1.73	1.81
1	G	120	ARG	CZ-NH1	5.38	1.40	1.33
1	S	35	ALA	CA-CB	5.38	1.63	1.52
2	H	106	GLU	CD-OE1	5.34	1.31	1.25
2	B	136	GLU	CD-OE1	5.28	1.31	1.25
1	K	47	ALA	CA-CB	5.28	1.63	1.52
2	T	136	GLU	CD-OE1	5.28	1.31	1.25
1	S	79	ARG	CZ-NH1	5.25	1.39	1.33
2	H	33	GLU	CD-OE1	5.24	1.31	1.25
1	S	120	ARG	CG-CD	5.22	1.65	1.51
1	W	42	THR	CA-CB	5.22	1.67	1.53
2	T	2	PHE	CE2-CZ	5.21	1.47	1.37
1	U	162	SER	CB-OG	-5.20	1.35	1.42
2	P	17	GLU	CD-OE1	5.19	1.31	1.25
1	A	120	ARG	CG-CD	5.15	1.64	1.51
1	O	120	ARG	CG-CD	5.14	1.64	1.51
1	S	162	SER	CB-OG	-5.12	1.35	1.42
1	G	123	GLU	CD-OE2	5.10	1.31	1.25
1	Q	98	CYS	CB-SG	-5.10	1.73	1.81
2	X	17	GLU	CD-OE1	5.08	1.31	1.25
1	S	79	ARG	CZ-NH2	5.07	1.39	1.33
2	H	106	GLU	CD-OE2	5.07	1.31	1.25
1	M	84	CYS	CB-SG	-5.06	1.73	1.81
1	K	65	TYR	CD1-CE1	5.03	1.46	1.39
1	K	117	GLU	CG-CD	5.03	1.59	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	SER	CA-CB	5.00	1.60	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	LEU	CA-C-N	8.91	136.80	117.20
1	E	161	LEU	O-C-N	-8.31	109.41	122.70
1	O	120	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	K	30	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	E	162	SER	N-CA-C	-7.46	90.86	111.00
2	R	171	VAL	CA-C-N	7.35	133.36	117.20
1	E	68	CYS	CB-CA-C	-7.30	95.80	110.40
2	F	171	VAL	O-C-N	-7.26	111.08	122.70
1	C	116	ASP	CB-CG-OD1	7.08	124.67	118.30
1	E	30	ARG	NE-CZ-NH1	6.95	123.78	120.30
2	F	171	VAL	CA-C-N	6.83	132.23	117.20
1	S	120	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	K	116	ASP	CB-CG-OD1	6.77	124.40	118.30
2	R	171	VAL	CB-CA-C	-6.68	98.70	111.40
2	B	114	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	U	77	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	U	77	ASP	CB-CG-OD1	6.44	124.10	118.30
2	R	171	VAL	O-C-N	-6.28	112.65	122.70
2	X	114	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	G	120	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	E	161	LEU	N-CA-C	-6.05	94.65	111.00
1	Q	120	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	Q	116	ASP	CB-CG-OD1	5.94	123.64	118.30
1	K	93	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	68	CYS	CA-CB-SG	5.93	124.68	114.00
1	S	30	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	116	ASP	CB-CG-OD1	5.87	123.58	118.30
1	G	79	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	W	93	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	U	116	ASP	CB-CG-OD1	5.78	123.50	118.30
1	G	87	ASP	CB-CG-OD1	5.78	123.50	118.30
1	G	120	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	K	120	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	X	91	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	L	171	VAL	N-CA-C	-5.74	95.51	111.00
1	C	161	LEU	N-CA-C	-5.73	95.53	111.00
2	H	114	ARG	NE-CZ-NH2	-5.73	117.44	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	161	LEU	CB-CG-CD2	-5.70	101.31	111.00
2	B	37	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	B	171	VAL	N-CA-C	-5.64	95.77	111.00
1	C	161	LEU	CA-C-N	5.63	129.59	117.20
2	J	171	VAL	N-CA-C	-5.60	95.87	111.00
1	A	120	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	W	120	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	171	VAL	CB-CA-C	-5.51	100.92	111.40
2	P	171	VAL	N-CA-C	-5.51	96.12	111.00
1	A	79	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	M	68	CYS	CA-CB-SG	5.48	123.86	114.00
2	R	101	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	G	116	ASP	CB-CG-OD1	5.44	123.20	118.30
2	V	114	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	P	91	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	D	171	VAL	CA-C-N	5.41	129.10	117.20
1	E	79	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	V	91	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	7	ASP	CB-CG-OD2	-5.31	113.53	118.30
2	J	114	ARG	NE-CZ-NH2	-5.31	117.65	120.30
2	B	78	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	K	30	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	K	7	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	V	152	ASP	CB-CG-OD2	5.15	122.94	118.30
2	V	79	MET	CG-SD-CE	-5.15	91.96	100.20
2	H	19	VAL	CB-CA-C	5.14	121.17	111.40
2	H	171	VAL	N-CA-C	-5.12	97.17	111.00
1	U	120	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	W	161	LEU	CB-CA-C	-5.09	100.52	110.20
2	J	171	VAL	CA-C-N	5.09	128.40	117.20
1	C	161	LEU	C-N-CA	-5.08	109.00	121.70
1	A	7	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	S	86	ARG	NE-CZ-NH2	-5.05	117.78	120.30
3	D	15	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	M	116	ASP	CB-CG-OD1	5.01	122.81	118.30
2	V	171	VAL	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	GLY	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	C	71	GLY	Peptide
1	E	71	GLY	Peptide
1	G	71	GLY	Peptide
1	I	71	GLY	Peptide
1	M	71	GLY	Peptide
1	S	71	GLY	Peptide
1	W	71	GLY	Peptide

## 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	1211	0	1172	13	0
1	C	1211	0	1172	22	0
1	E	1211	0	1172	18	1
1	G	1211	0	1172	12	0
1	I	1211	0	1172	18	0
1	K	1211	0	1172	16	0
1	M	1211	0	1172	25	0
1	O	1211	0	1172	15	1
1	Q	1211	0	1172	23	0
1	S	1211	0	1172	19	0
1	U	1211	0	1172	12	0
1	W	1211	0	1172	13	0
2	B	1242	0	1234	35	0
2	F	1242	0	1233	22	0
2	H	1242	0	1234	28	1
2	J	1242	0	1234	24	0
2	L	1242	0	1234	37	0
2	N	1242	0	1233	33	1
2	P	1242	0	1233	26	0
2	R	1242	0	1234	41	0
2	T	1242	0	1235	37	1
2	V	1242	0	1233	18	0
2	X	1242	0	1233	25	0
3	D	1244	0	1237	38	1
4	A	43	0	37	6	0
4	B	43	0	37	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	43	0	37	5	0
4	D	86	0	72	16	0
4	E	43	0	37	6	0
4	F	86	0	73	9	0
4	G	43	0	37	6	0
4	H	86	0	75	18	0
4	I	43	0	37	4	0
4	J	86	0	74	20	0
4	K	43	0	36	5	0
4	L	86	0	75	27	0
4	M	43	0	36	3	0
4	N	86	0	74	18	0
4	O	43	0	37	6	0
4	P	86	0	73	24	0
4	Q	43	0	37	6	0
4	R	86	0	74	20	0
4	S	43	0	37	11	0
4	T	86	0	76	27	0
4	U	43	0	37	5	0
4	V	86	0	74	13	0
4	W	43	0	37	5	0
4	X	86	0	72	9	0
5	B	43	0	32	16	0
6	A	2	0	0	1	0
6	C	31	0	0	3	0
6	D	13	0	0	2	0
6	E	8	0	0	2	0
6	F	39	0	0	5	0
6	I	40	0	0	3	0
6	J	15	0	0	1	0
6	K	9	0	0	3	0
6	L	31	0	0	2	0
6	M	40	0	0	5	0
6	N	13	0	0	6	0
6	O	13	0	0	3	0
6	P	27	0	0	4	0
6	Q	2	0	0	1	0
6	R	3	0	0	0	0
6	S	6	0	0	0	0
6	T	30	0	0	4	0
6	W	34	0	0	3	0
6	X	19	0	0	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31361	0	30194	699	3

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 11.

All (699) 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:R:153:CYS:SG	4:R:255:CYC:HAC1	1.18	1.71
2:J:82:CYS:SG	4:J:184:CYC:HAC2	1.15	1.66
2:H:153:CYS:SG	4:H:255:CYC:HAC1	1.15	1.64
2:T:153:CYS:SG	4:T:255:CYC:HAC1	1.41	1.58
2:T:82:CYS:SG	4:T:184:CYC:HAC2	1.42	1.58
2:B:153:CYS:SG	5:B:255:BLA:HAC	1.45	1.54
2:H:153:CYS:SG	4:H:255:CYC:CAC	2.11	1.37
2:R:153:CYS:SG	4:R:255:CYC:CAC	2.12	1.36
2:B:153:CYS:SG	5:B:255:BLA:CAC	2.12	1.36
2:T:153:CYS:SG	4:T:255:CYC:CAC	2.14	1.34
2:T:82:CYS:SG	4:T:184:CYC:CAC	2.24	1.26
2:L:82:CYS:SG	4:L:184:CYC:HAC2	1.76	1.25
2:L:82:CYS:SG	4:L:184:CYC:CBC	2.27	1.22
4:J:255:CYC:CMA	4:J:255:CYC:HMB3	1.69	1.19
2:N:15:ARG:HD2	6:N:2004:HOH:O	1.43	1.18
2:L:82:CYS:SG	4:L:184:CYC:CAC	2.31	1.18
1:C:120:ARG:HD2	1:I:162:SER:O	1.39	1.17
5:B:255:BLA:HMA1	5:B:255:BLA:NB	1.58	1.17
5:B:255:BLA:HMA1	5:B:255:BLA:HB	1.05	1.17
4:P:184:CYC:HC	4:P:184:CYC:HMD2	1.11	1.14
2:N:171:VAL:O	2:N:172:SER:CB	1.92	1.14
1:K:32:ARG:HD2	6:K:2004:HOH:O	1.49	1.12
2:L:82:CYS:SG	4:L:184:CYC:HBC2	1.88	1.09
4:J:255:CYC:HMA1	4:J:255:CYC:HMB3	1.28	1.07
4:L:255:CYC:HMB1	4:L:255:CYC:HBB2	1.35	1.07
2:L:171:VAL:O	2:L:172:SER:HB2	1.47	1.07
4:S:184:CYC:HHA	4:S:184:CYC:HBD1	1.33	1.06
5:B:255:BLA:CMA	5:B:255:BLA:HB	1.68	1.06
4:P:255:CYC:HBC3	4:P:255:CYC:HHB	1.08	1.06
2:L:171:VAL:O	2:L:172:SER:CB	1.96	1.05
2:V:171:VAL:O	2:V:172:SER:HB3	1.50	1.05
2:J:171:VAL:O	2:J:172:SER:HB2	1.50	1.05
2:B:171:VAL:O	2:B:172:SER:HB3	1.32	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:171:VAL:O	2:P:172:SER:CB	2.04	1.04
2:P:171:VAL:O	2:P:172:SER:HB3	1.29	1.04
2:H:171:VAL:O	2:H:172:SER:HB3	1.53	1.03
4:X:184:CYC:CMD	4:X:184:CYC:HC	1.72	1.03
2:R:171:VAL:O	2:R:171:VAL:HG23	1.53	1.02
2:X:171:VAL:O	2:X:172:SER:HB3	1.58	1.02
4:B:184:CYC:HMD2	4:B:184:CYC:HC	1.17	1.02
2:J:171:VAL:O	2:J:172:SER:CB	2.06	1.01
4:R:184:CYC:HC	4:R:184:CYC:HMD2	1.22	1.01
4:D:184:CYC:HMD2	4:D:184:CYC:HC	1.25	1.00
4:B:184:CYC:CMD	4:B:184:CYC:HC	1.75	0.99
3:D:40:VAL:CG1	3:D:156:LEU:HD21	1.91	0.99
1:M:6:THR:HG21	6:N:2002:HOH:O	1.61	0.99
3:D:40:VAL:HG11	3:D:156:LEU:HD21	1.41	0.99
2:P:20:SER:H	2:P:23:GLN:HE21	1.10	0.98
4:V:255:CYC:HMA1	4:V:255:CYC:NB	1.79	0.98
2:L:20:SER:H	2:L:23:GLN:HE21	1.05	0.98
1:C:32:ARG:HD2	6:C:2005:HOH:O	1.63	0.97
2:X:62:GLU:HG2	6:X:2011:HOH:O	1.64	0.97
2:N:20:SER:H	2:N:23:GLN:HE21	1.03	0.97
2:N:36:LYS:HD3	4:N:255:CYC:HMD3	1.47	0.97
2:L:88:ILE:HG21	4:L:184:CYC:HBB3	1.47	0.97
2:B:20:SER:H	2:B:23:GLN:NE2	1.63	0.96
1:W:1:MET:HB2	6:W:2001:HOH:O	1.65	0.96
2:B:171:VAL:O	2:B:172:SER:CB	2.13	0.96
3:D:20:SER:H	3:D:23:GLN:HE21	1.08	0.95
4:P:184:CYC:HC	4:P:184:CYC:CMD	1.78	0.95
2:H:20:SER:H	2:H:23:GLN:HE21	0.97	0.95
2:H:113:LEU:HD13	4:H:184:CYC:HMB3	1.49	0.95
4:S:184:CYC:HMD2	4:S:184:CYC:HC	1.32	0.95
2:N:171:VAL:O	2:N:172:SER:HB2	1.63	0.95
4:X:184:CYC:HMD2	4:X:184:CYC:HC	1.30	0.94
2:V:20:SER:H	2:V:23:GLN:HE21	1.12	0.94
2:J:20:SER:H	2:J:23:GLN:HE21	1.11	0.93
4:P:255:CYC:HBC3	4:P:255:CYC:CHD	1.91	0.93
2:R:20:SER:H	2:R:23:GLN:HE21	1.13	0.93
2:X:20:SER:H	2:X:23:GLN:HE21	1.12	0.93
2:N:171:VAL:O	2:N:172:SER:HB3	1.69	0.92
2:T:153:CYS:HG	4:T:255:CYC:HAC1	1.16	0.91
2:B:20:SER:H	2:B:23:GLN:HE21	0.92	0.91
4:D:184:CYC:HC	4:D:184:CYC:CMD	1.84	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:20:SER:H	2:F:23:GLN:HE21	1.05	0.91
1:C:120:ARG:CD	1:I:162:SER:O	2.19	0.90
1:E:162:SER:O	1:G:120:ARG:HG2	1.71	0.90
2:T:171:VAL:O	2:T:172:SER:HB3	1.70	0.90
2:T:20:SER:H	2:T:23:GLN:HE21	1.00	0.90
4:J:255:CYC:OB	4:J:255:CYC:HBB3	1.69	0.89
2:N:153:CYS:SG	4:N:255:CYC:C3C	2.60	0.89
4:S:184:CYC: CBD	4:S:184:CYC:HHA	2.03	0.88
4:P:255:CYC:HBA1	4:P:255:CYC:HHA	1.55	0.88
4:H:255:CYC:HMA1	4:H:255:CYC:NB	1.90	0.87
2:R:171:VAL:O	2:R:171:VAL:CG2	2.13	0.87
2:P:20:SER:H	2:P:23:GLN:NE2	1.73	0.87
4:R:255:CYC:NB	4:R:255:CYC:HMA1	1.89	0.87
2:B:153:CYS:HG	5:B:255:BLA:HAC	1.04	0.85
2:H:20:SER:H	2:H:23:GLN:NE2	1.74	0.85
4:V:184:CYC:HMD2	4:V:184:CYC:HC	1.41	0.85
2:J:113:LEU:HD13	4:J:184:CYC:HMB3	1.57	0.85
2:T:82:CYS:SG	4:T:184:CYC:CBC	2.65	0.84
4:H:255:CYC:HMA1	4:H:255:CYC:HB	1.41	0.84
4:R:184:CYC:CMD	4:R:184:CYC:HC	1.90	0.84
4:V:255:CYC:HMA1	4:V:255:CYC:HB	1.38	0.84
2:F:20:SER:H	2:F:23:GLN:NE2	1.75	0.84
2:T:82:CYS:CB	4:T:184:CYC:HAC2	2.07	0.83
4:T:255:CYC:HBB2	4:T:255:CYC:OB	1.77	0.83
2:N:20:SER:H	2:N:23:GLN:NE2	1.77	0.83
2:T:153:CYS:SG	4:T:255:CYC:HAC2	2.19	0.83
2:T:20:SER:H	2:T:23:GLN:NE2	1.77	0.82
2:R:113:LEU:HD13	4:R:184:CYC:HMB3	1.58	0.82
1:M:162:SER:O	1:W:120:ARG:HG2	1.78	0.82
4:V:255:CYC:CMA	4:V:255:CYC:HB	1.93	0.81
4:U:184:CYC:HMD2	4:U:184:CYC:HC	1.46	0.80
4:P:184:CYC:HMA1	4:P:184:CYC:NB	1.96	0.80
2:T:76:SER:HB2	6:W:2021:HOH:O	1.82	0.80
4:P:255:CYC:HHD	4:P:255:CYC:CBC	1.95	0.80
4:P:184:CYC:NC	4:P:184:CYC:HMD2	1.94	0.79
4:T:184:CYC:NB	4:T:184:CYC:HMA1	1.97	0.79
2:V:113:LEU:HD13	4:V:184:CYC:HMB3	1.64	0.79
2:P:36:LYS:HE3	6:P:2027:HOH:O	1.80	0.79
2:R:20:SER:H	2:R:23:GLN:NE2	1.81	0.78
2:R:52:VAL:HG22	2:R:134:MET:CE	2.13	0.78
4:L:184:CYC:HMD2	4:L:184:CYC:HC	1.49	0.78

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:SER:H	2:L:23:GLN:NE2	1.79	0.78
4:W:184:CYC:HC	4:W:184:CYC:HMD2	1.48	0.78
2:B:20:SER:OG	2:B:23:GLN:HG3	1.84	0.78
4:D:255:CYC:NB	4:D:255:CYC:HMA1	1.99	0.78
3:D:20:SER:H	3:D:23:GLN:NE2	1.81	0.78
4:J:255:CYC:HMA2	4:J:255:CYC:HMB3	1.66	0.78
2:X:20:SER:H	2:X:23:GLN:NE2	1.81	0.78
1:C:11:THR:HB	6:K:2001:HOH:O	1.84	0.78
2:B:20:SER:N	2:B:23:GLN:HE21	1.77	0.77
1:M:83:LYS:HG2	6:M:2022:HOH:O	1.82	0.77
4:P:255:CYC:CBA	4:P:255:CYC:HHA	2.13	0.77
4:S:184:CYC:HC	4:S:184:CYC:CMD	1.98	0.77
3:D:40:VAL:HG11	3:D:156:LEU:CD2	2.14	0.76
2:L:82:CYS:CB	4:L:184:CYC:HAC2	2.15	0.76
4:L:255:CYC:HMA1	4:L:255:CYC:NB	2.02	0.75
2:T:20:SER:OG	2:T:23:GLN:HG3	1.86	0.75
2:J:20:SER:H	2:J:23:GLN:NE2	1.83	0.75
2:B:57:ARG:HD3	4:E:184:CYC:O2D	1.86	0.75
2:N:11:GLN:HA	6:N:2003:HOH:O	1.86	0.75
1:G:111:LEU:HD12	4:G:184:CYC:HBB3	1.69	0.75
2:R:35:ASN:HB2	4:R:255:CYC:O2D	1.87	0.74
4:M:184:CYC:O1D	2:P:57:ARG:NH1	2.21	0.74
4:T:184:CYC:HMD2	4:T:184:CYC:HC	1.53	0.74
2:B:57:ARG:NH1	4:E:184:CYC:O1D	2.21	0.73
2:N:20:SER:OG	2:N:23:GLN:HG3	1.88	0.73
2:V:20:SER:H	2:V:23:GLN:NE2	1.86	0.73
2:X:15:ARG:HD2	6:X:2003:HOH:O	1.88	0.73
2:X:113:LEU:HD13	4:X:184:CYC:HMB3	1.71	0.73
2:P:170:ALA:HB1	6:P:2018:HOH:O	1.89	0.73
2:B:113:LEU:HD13	4:B:184:CYC:HMB3	1.71	0.73
2:J:29:GLN:HG2	6:J:2005:HOH:O	1.88	0.73
4:H:255:CYC:CMA	4:H:255:CYC:HB	2.02	0.72
4:S:184:CYC:CBD	4:S:184:CYC:CHA	2.68	0.72
4:U:184:CYC:NB	4:U:184:CYC:HMA1	2.05	0.72
4:P:184:CYC:HHA	4:P:184:CYC:HBD2	1.72	0.72
5:B:255:BLA:HMA2	1:G:145:ASP:OD1	1.89	0.71
2:V:20:SER:OG	2:V:23:GLN:HG3	1.90	0.71
2:V:171:VAL:O	2:V:172:SER:CB	2.28	0.71
4:D:255:CYC:HB	4:D:255:CYC:HMA1	1.56	0.71
1:E:162:SER:O	1:G:120:ARG:CG	2.39	0.70
2:P:20:SER:OG	2:P:23:GLN:HG3	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:153:CYS:HG	4:R:255:CYC:HAC1	1.52	0.70
2:L:36:LYS:HD3	4:L:255:CYC:HMD3	1.73	0.70
4:P:184:CYC:HB	4:P:184:CYC:CMA	2.04	0.70
5:B:255:BLA:HBA1	5:B:255:BLA:HHA	1.74	0.70
1:E:161:LEU:O	1:E:162:SER:HB2	1.91	0.70
2:R:74:TYR:O	2:R:75:ALA:HB3	1.91	0.70
4:X:184:CYC:HMD2	4:X:184:CYC:NC	2.04	0.70
1:A:120:ARG:HD2	1:K:162:SER:O	1.91	0.70
4:B:184:CYC:NC	4:B:184:CYC:CMD	2.54	0.69
4:D:255:CYC:HB	4:D:255:CYC:CMA	2.04	0.69
2:L:88:ILE:CG2	4:L:184:CYC:HBB3	2.21	0.69
2:N:57:ARG:NH1	4:Q:184:CYC:O1D	2.25	0.69
2:F:20:SER:N	2:F:23:GLN:HE21	1.87	0.69
2:R:20:SER:OG	2:R:23:GLN:HG3	1.93	0.69
1:C:68:CYS:HB2	1:M:68:CYS:HB2	1.74	0.69
4:N:184:CYC:HMB1	4:N:184:CYC:HBB2	1.75	0.68
4:C:184:CYC:HC	4:C:184:CYC:HMD2	1.56	0.68
3:D:1:MET:SD	6:D:2009:HOH:O	2.51	0.68
4:H:184:CYC:HC	4:H:184:CYC:HMD2	1.58	0.68
2:N:33:GLU:HG3	6:N:2007:HOH:O	1.93	0.68
2:F:52:VAL:HG22	2:F:134:MET:CE	2.24	0.68
1:O:32:ARG:HA	6:O:2008:HOH:O	1.94	0.68
1:E:33:GLN:NE2	4:J:255:CYC:HBB1	2.08	0.67
4:B:184:CYC:NC	4:B:184:CYC:HMD2	2.01	0.67
4:W:184:CYC:CMD	4:W:184:CYC:HC	2.06	0.67
5:B:255:BLA:OB	5:B:255:BLA:HBB1	1.94	0.67
4:R:255:CYC:HB	4:R:255:CYC:HMA1	1.58	0.67
2:N:153:CYS:SG	4:N:255:CYC:HAC2	2.28	0.67
2:X:171:VAL:O	2:X:172:SER:CB	2.33	0.67
1:S:128:TRP:CE3	4:S:184:CYC:HMC3	2.29	0.66
2:N:52:VAL:HG22	2:N:134:MET:CE	2.25	0.66
1:A:162:SER:O	1:K:120:ARG:HD2	1.95	0.66
4:Q:184:CYC:HC	4:Q:184:CYC:HMD2	1.61	0.66
2:J:20:SER:OG	2:J:23:GLN:HG3	1.95	0.66
4:L:184:CYC:CMD	4:L:184:CYC:HC	2.09	0.66
2:N:19:VAL:CG1	2:N:23:GLN:HB2	2.26	0.66
2:R:74:TYR:O	2:R:75:ALA:CB	2.44	0.66
4:L:255:CYC:HHD	4:L:255:CYC:HBC3	1.76	0.65
1:M:35:ALA:HA	6:M:2008:HOH:O	1.96	0.65
3:D:40:VAL:HG21	3:D:160:ILE:HD11	1.79	0.65
4:G:184:CYC:HBC2	4:G:184:CYC:HMC1	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:153:CYS:SG	4:T:255:CYC:H2C	2.36	0.65
2:F:146:ALA:HA	6:F:2032:HOH:O	1.95	0.65
4:L:255:CYC:CMB	4:L:255:CYC:HBB2	2.17	0.65
4:J:255:CYC:CMA	4:J:255:CYC:CMB	2.62	0.65
4:R:255:CYC:CMA	4:R:255:CYC:HB	2.09	0.65
2:P:37:ARG:O	2:P:40:ALA:HB3	1.97	0.64
3:D:51:VAL:HG12	3:D:134:MET:HG2	1.79	0.64
1:S:3:THR:O	1:S:7:ASP:HB2	1.97	0.64
4:L:255:CYC:HMA1	4:L:255:CYC:HB	1.63	0.64
2:P:20:SER:N	2:P:23:GLN:HE21	1.89	0.64
2:N:74:TYR:O	2:N:75:ALA:HB3	1.98	0.64
4:U:184:CYC:O1D	2:X:57:ARG:NH1	2.31	0.63
4:Q:184:CYC:NC	4:Q:184:CYC:HMD2	2.13	0.63
4:V:255:CYC:HHH	4:V:255:CYC:HBC3	1.80	0.63
4:F:184:CYC:HC	4:F:184:CYC:HMD2	1.63	0.63
2:T:19:VAL:CG1	2:T:23:GLN:HB2	2.29	0.63
2:X:63:GLN:HG3	6:X:2011:HOH:O	1.97	0.63
4:J:255:CYC:HHA	4:J:255:CYC:O1A	1.98	0.63
2:L:171:VAL:O	2:L:172:SER:HB3	1.92	0.63
1:U:40:ALA:HB2	1:U:146:ALA:HB1	1.79	0.63
1:E:40:ALA:HB2	1:E:146:ALA:HB1	1.79	0.63
2:P:74:TYR:O	2:P:75:ALA:HB3	1.99	0.63
4:A:184:CYC:HMA1	4:A:184:CYC:NB	2.14	0.62
4:K:184:CYC:HMA1	4:K:184:CYC:NB	2.15	0.62
4:F:255:CYC:HBB2	4:F:255:CYC:OB	2.00	0.62
1:Q:120:ARG:HD2	1:S:162:SER:O	1.99	0.61
2:N:6:THR:HG21	6:N:2002:HOH:O	2.00	0.61
4:T:184:CYC:HB	4:T:184:CYC:CMA	2.13	0.61
1:M:24:ILE:HG21	4:N:255:CYC:HBB2	1.81	0.61
6:M:2037:HOH:O	1:S:21:SER:HB3	2.00	0.61
2:B:37:ARG:O	2:B:40:ALA:HB3	2.01	0.61
4:P:255:CYC:HBD2	6:P:2027:HOH:O	2.00	0.61
2:T:152:ASP:HB3	6:T:2027:HOH:O	2.00	0.61
3:D:20:SER:OG	3:D:23:GLN:HG3	2.01	0.61
4:P:184:CYC:HB	4:P:184:CYC:HMA1	1.62	0.61
4:I:184:CYC:HMD2	4:I:184:CYC:HC	1.66	0.60
3:D:18:MET:HB3	6:D:2004:HOH:O	1.99	0.60
1:C:73:ASN:HA	4:C:184:CYC:HBD2	1.83	0.60
4:D:255:CYC:HBC3	4:D:255:CYC:HHH	1.84	0.60
2:F:20:SER:OG	2:F:23:GLN:HG3	2.01	0.60
4:T:184:CYC:NB	4:T:184:CYC:CMA	2.64	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:255:CYC:HBC3	4:J:255:CYC:HHD	1.84	0.59
1:Q:3:THR:O	1:Q:7:ASP:HB2	2.02	0.59
2:N:74:TYR:O	2:N:75:ALA:CB	2.50	0.59
4:Q:184:CYC:NB	4:Q:184:CYC:HMA1	2.17	0.59
4:V:184:CYC:CMD	4:V:184:CYC:HC	2.11	0.59
2:H:171:VAL:O	2:H:172:SER:CB	2.31	0.59
4:A:184:CYC:HC	4:A:184:CYC:HMD2	1.66	0.59
1:A:95:VAL:HG21	1:A:154:LEU:HD13	1.85	0.59
1:Q:120:ARG:HG2	1:S:162:SER:O	2.03	0.59
4:H:255:CYC:HBC3	4:H:255:CYC:HHD	1.83	0.59
4:L:184:CYC:HBB2	6:L:2030:HOH:O	2.01	0.59
1:M:120:ARG:HG2	1:W:162:SER:O	2.02	0.59
2:B:36:LYS:HD3	5:B:255:BLA:HMD3	1.83	0.59
1:K:40:ALA:HB2	1:K:146:ALA:HB1	1.84	0.59
2:H:52:VAL:HG22	2:H:134:MET:CE	2.32	0.59
1:I:6:THR:HG23	2:J:3:ASP:OD2	2.03	0.59
2:F:6:THR:HG21	6:F:2002:HOH:O	2.02	0.58
2:H:153:CYS:SG	4:H:255:CYC:C3C	2.87	0.58
1:A:40:ALA:HB2	1:A:146:ALA:HB1	1.84	0.58
2:L:90:LEU:O	2:L:94:THR:HG23	2.03	0.58
1:Q:67:THR:HB	6:Q:2002:HOH:O	2.03	0.58
4:X:184:CYC:CMD	4:X:184:CYC:NC	2.55	0.58
2:J:52:VAL:HG22	2:J:134:MET:CE	2.33	0.58
4:N:255:CYC:HMB1	4:N:255:CYC:HBB3	1.84	0.58
4:O:184:CYC:O1D	2:R:57:ARG:NH1	2.35	0.58
4:N:255:CYC:NB	4:N:255:CYC:HMA1	2.19	0.58
2:L:20:SER:OG	2:L:23:GLN:HG3	2.03	0.58
3:D:19:VAL:CG1	3:D:23:GLN:HB2	2.34	0.58
4:H:255:CYC:CGA	4:H:255:CYC:HHA	2.33	0.58
4:L:255:CYC:HMB1	4:L:255:CYC:CBB	2.21	0.58
1:S:90:TYR:CD2	4:S:184:CYC:HBB3	2.39	0.58
1:Q:162:SER:O	1:S:120:ARG:HD2	2.03	0.58
2:R:60:PHE:HE2	2:R:79:MET:HE1	1.69	0.57
2:X:52:VAL:HG22	2:X:134:MET:CE	2.33	0.57
4:K:184:CYC:HMD2	4:K:184:CYC:HC	1.69	0.57
4:R:255:CYC:HHD	4:R:255:CYC:HBC3	1.85	0.57
1:E:145:ASP:OD1	4:J:255:CYC:CMB	2.53	0.57
2:N:108:ARG:O	4:N:184:CYC:HBB1	2.05	0.57
1:O:162:SER:O	1:U:120:ARG:HG2	2.05	0.57
4:D:255:CYC:HBD1	4:D:255:CYC:CHA	2.34	0.57
2:R:113:LEU:CD1	4:R:184:CYC:HMB3	2.32	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:184:CYC:HC	4:G:184:CYC:HMD2	1.70	0.57
2:X:35:ASN:ND2	6:X:2007:HOH:O	2.38	0.57
2:T:82:CYS:SG	4:T:184:CYC:H2C	2.44	0.56
1:S:128:TRP:CD2	4:S:184:CYC:HMC3	2.41	0.56
1:C:40:ALA:HB2	1:C:146:ALA:HB1	1.87	0.56
2:B:52:VAL:HG22	2:B:134:MET:CE	2.35	0.56
3:D:171:VAL:HG23	3:D:172:SER:N	2.21	0.56
4:F:255:CYC:HMA1	4:F:255:CYC:HB	1.71	0.56
2:B:171:VAL:O	2:B:171:VAL:CG2	2.54	0.56
4:N:255:CYC:HMA1	4:N:255:CYC:HB	1.71	0.56
1:G:72:PRO:HB2	4:G:184:CYC:O1D	2.06	0.56
4:F:184:CYC:HC	4:F:184:CYC:CMD	2.18	0.56
4:T:255:CYC:HHH	4:T:255:CYC:HBC3	1.88	0.56
4:X:184:CYC:HMD3	4:X:184:CYC:HC	1.66	0.56
2:J:74:TYR:O	2:J:75:ALA:HB3	2.06	0.56
1:O:17:ARG:HB2	6:O:2003:HOH:O	2.06	0.56
3:D:113:LEU:HD13	4:D:184:CYC:HMB3	1.87	0.55
4:L:255:CYC:CMA	4:L:255:CYC:HB	2.19	0.55
2:H:113:LEU:CD1	4:H:184:CYC:HMB3	2.29	0.55
4:J:255:CYC:C3A	4:J:255:CYC:HMB3	2.34	0.55
4:T:184:CYC:CMD	4:T:184:CYC:HC	2.19	0.55
2:V:19:VAL:CG1	2:V:23:GLN:HB2	2.36	0.55
4:C:184:CYC:HMA1	4:C:184:CYC:NB	2.22	0.55
3:D:40:VAL:CG1	3:D:156:LEU:CD2	2.75	0.55
1:I:142:LEU:HD23	6:I:2034:HOH:O	2.06	0.55
1:Q:18:PHE:HB3	2:R:45:THR:HG23	1.87	0.55
2:L:36:LYS:CD	4:L:255:CYC:HMD3	2.35	0.55
4:M:184:CYC:NB	4:M:184:CYC:HMA1	2.21	0.55
2:N:153:CYS:SG	4:N:255:CYC:C4C	2.95	0.55
2:P:110:LEU:O	6:P:2018:HOH:O	2.18	0.55
1:A:125:SER:HB3	1:A:128:TRP:CE2	2.42	0.55
1:Q:40:ALA:HB2	1:Q:146:ALA:HB1	1.89	0.55
1:C:3:THR:O	1:C:7:ASP:HB2	2.07	0.54
4:F:255:CYC:HMA1	4:F:255:CYC:NB	2.22	0.54
4:H:184:CYC:HC	4:H:184:CYC:CMD	2.19	0.54
1:E:120:ARG:HG2	1:G:162:SER:O	2.07	0.54
2:H:153:CYS:SG	4:H:255:CYC:CBC	2.92	0.54
2:L:74:TYR:O	2:L:75:ALA:HB3	2.08	0.54
2:T:153:CYS:SG	4:T:255:CYC:C3C	2.92	0.54
1:I:95:VAL:HG21	1:I:154:LEU:HD13	1.90	0.54
1:I:28:PHE:HE2	4:J:255:CYC:HBB2	1.73	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:184:CYC:HMD2	4:N:184:CYC:HC	1.73	0.54
2:N:36:LYS:CD	4:N:255:CYC:HMD3	2.30	0.54
4:G:184:CYC:NB	4:G:184:CYC:HMA1	2.22	0.54
2:R:90:LEU:O	2:R:94:THR:HG23	2.07	0.54
6:C:2004:HOH:O	1:K:32:ARG:HG3	2.08	0.54
1:M:61:ASN:HB2	6:M:2015:HOH:O	2.08	0.54
1:S:67:THR:O	1:S:76:ALA:HA	2.09	0.53
2:B:74:TYR:O	2:B:75:ALA:HB3	2.07	0.53
2:F:62:GLU:HG2	6:F:2018:HOH:O	2.09	0.53
1:M:120:ARG:HD2	1:W:162:SER:O	2.08	0.53
4:E:184:CYC:HC	4:E:184:CYC:HMD2	1.74	0.53
2:H:83:LEU:HD13	1:K:121:THR:HG21	1.90	0.53
4:O:184:CYC:NB	4:O:184:CYC:HMA1	2.23	0.53
2:P:2:PHE:HA	2:P:6:THR:HG22	1.89	0.53
1:E:145:ASP:OD1	4:J:255:CYC:HMB1	2.08	0.53
2:T:153:CYS:SG	4:T:255:CYC:C2C	2.97	0.53
5:B:255:BLA:CMA	5:B:255:BLA:NB	2.40	0.53
4:D:184:CYC:CMD	4:D:184:CYC:NC	2.65	0.53
1:A:73:ASN:HA	4:A:184:CYC:HBD2	1.91	0.53
3:D:52:VAL:HG22	3:D:134:MET:CE	2.39	0.53
2:R:19:VAL:CG1	2:R:23:GLN:HB2	2.38	0.53
1:I:111:LEU:HG	4:I:184:CYC:HMB1	1.90	0.53
1:S:95:VAL:HG21	1:S:154:LEU:HD13	1.90	0.53
2:R:52:VAL:HG22	2:R:134:MET:HE3	1.88	0.53
2:V:58:ALA:HB3	2:V:133:LYS:HD3	1.91	0.53
1:W:95:VAL:HG21	1:W:154:LEU:HD13	1.91	0.53
2:L:20:SER:N	2:L:23:GLN:HE21	1.90	0.52
4:D:255:CYC:HBD1	4:D:255:CYC:HHA	1.89	0.52
2:F:74:TYR:O	2:F:75:ALA:HB3	2.09	0.52
1:M:72:PRO:O	4:M:184:CYC:HBD2	2.09	0.52
1:S:40:ALA:HB2	1:S:146:ALA:HB1	1.91	0.52
1:G:3:THR:O	1:G:7:ASP:HB2	2.10	0.52
2:T:52:VAL:HG22	2:T:134:MET:CE	2.40	0.52
2:T:20:SER:N	2:T:23:GLN:HE21	1.86	0.52
2:R:60:PHE:CE2	2:R:79:MET:HE1	2.45	0.52
1:G:40:ALA:HB2	1:G:146:ALA:HB1	1.92	0.52
2:H:153:CYS:SG	4:H:255:CYC:H2C	2.50	0.52
2:P:46:ALA:HA	6:W:2030:HOH:O	2.09	0.52
1:W:3:THR:O	1:W:7:ASP:HB2	2.10	0.52
4:E:184:CYC:HHA	4:E:184:CYC:HBD1	1.92	0.51
4:P:184:CYC:NC	4:P:184:CYC:CMD	2.58	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:184:CYC:HBB2	4:T:184:CYC:OB	2.09	0.51
2:L:92:TYR:CE2	4:L:184:CYC:HBB1	2.46	0.51
4:J:255:CYC:HMA1	4:J:255:CYC:CMB	2.20	0.51
2:B:153:CYS:SG	5:B:255:BLA:C3C	2.93	0.51
2:B:2:PHE:HA	2:B:6:THR:HG22	1.91	0.51
1:O:40:ALA:HB2	1:O:146:ALA:HB1	1.91	0.51
2:T:62:GLU:HG2	6:T:2013:HOH:O	2.10	0.51
2:R:148:ILE:HG21	4:R:255:CYC:HMC3	1.91	0.51
3:D:37:ARG:O	3:D:40:VAL:HG13	2.11	0.51
2:N:109:CYS:HA	4:N:184:CYC:CBB	2.41	0.51
1:O:95:VAL:HG21	1:O:154:LEU:HD13	1.92	0.51
1:K:74:TYR:HA	4:K:184:CYC:OC	2.11	0.51
2:N:90:LEU:O	2:N:94:THR:HG23	2.11	0.51
4:A:184:CYC:O1D	3:D:57:ARG:NH1	2.43	0.51
2:J:19:VAL:CG1	2:J:23:GLN:HB2	2.41	0.51
2:T:82:CYS:SG	4:T:184:CYC:HBC2	2.49	0.51
1:E:145:ASP:CG	4:J:255:CYC:HMB1	2.31	0.50
2:P:74:TYR:O	2:P:75:ALA:CB	2.59	0.50
2:T:113:LEU:HD13	4:T:184:CYC:HMB3	1.93	0.50
3:D:19:VAL:HG13	3:D:23:GLN:HB2	1.93	0.50
1:E:95:VAL:HG21	1:E:154:LEU:HD13	1.92	0.50
1:C:91:TYR:O	1:C:95:VAL:HG23	2.12	0.50
1:E:35:ALA:HA	6:F:2006:HOH:O	2.10	0.50
4:J:255:CYC:CBB	4:J:255:CYC:OB	2.45	0.50
2:L:82:CYS:SG	4:L:184:CYC:HBC1	2.40	0.50
2:N:74:TYR:OH	2:R:13:ASP:OD1	2.21	0.50
4:R:255:CYC:HBA1	4:R:255:CYC:HHA	1.93	0.50
3:D:69:PRO:HA	3:D:74:TYR:CG	2.46	0.50
4:P:255:CYC:HBA1	4:P:255:CYC:HAD1	1.93	0.50
2:T:151:GLY:HA3	4:T:255:CYC:CMD	2.41	0.50
4:V:184:CYC:HMA1	4:V:184:CYC:NB	2.26	0.50
4:W:184:CYC:NB	4:W:184:CYC:HMA1	2.27	0.50
2:F:60:PHE:HE2	2:F:79:MET:HE1	1.77	0.50
1:O:3:THR:O	1:O:7:ASP:HB2	2.12	0.50
4:V:255:CYC:CMA	4:V:255:CYC:NB	2.56	0.50
1:W:125:SER:HB3	1:W:128:TRP:CE2	2.47	0.50
4:B:184:CYC:HMA1	4:B:184:CYC:NB	2.27	0.50
1:K:3:THR:O	1:K:7:ASP:HB2	2.11	0.50
2:P:48:ALA:O	2:P:52:VAL:HG23	2.12	0.50
2:V:74:TYR:O	2:V:75:ALA:HB3	2.10	0.50
2:H:72:ASN:HB3	4:H:184:CYC:OC	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:123:PRO:O	2:R:126:SER:HB2	2.12	0.50
1:W:72:PRO:HB2	4:W:184:CYC:O1D	2.12	0.50
3:D:68:ALA:O	3:D:69:PRO:C	2.48	0.50
2:H:51:VAL:HG12	2:H:134:MET:HG2	1.93	0.50
1:Q:120:ARG:CG	1:S:162:SER:O	2.60	0.50
1:I:125:SER:HB3	1:I:128:TRP:CE2	2.47	0.50
2:N:153:CYS:SG	4:N:255:CYC:C2C	3.00	0.50
2:H:19:VAL:CG1	2:H:23:GLN:HB2	2.41	0.49
2:L:82:CYS:CA	4:L:184:CYC:HAC2	2.42	0.49
1:S:1:MET:O	1:S:3:THR:HG23	2.11	0.49
1:E:161:LEU:O	1:E:162:SER:CB	2.47	0.49
2:R:153:CYS:SG	4:R:255:CYC:C3C	2.95	0.49
4:R:255:CYC:CMA	4:R:255:CYC:NB	2.64	0.49
2:X:79:MET:HE2	2:X:83:LEU:HG	1.93	0.49
4:U:184:CYC:CMD	4:U:184:CYC:HC	2.21	0.49
2:V:90:LEU:O	2:V:94:THR:HG23	2.12	0.49
2:X:51:VAL:HG12	2:X:134:MET:HG2	1.93	0.49
1:I:3:THR:HB	6:I:2001:HOH:O	2.12	0.49
2:R:60:PHE:CE2	2:R:79:MET:CE	2.95	0.49
1:M:24:ILE:HG21	4:N:255:CYC:CBB	2.43	0.49
2:V:51:VAL:HG12	2:V:134:MET:HG2	1.95	0.49
1:O:110:TYR:O	2:R:75:ALA:HA	2.12	0.48
2:H:20:SER:OG	2:H:23:GLN:HG3	2.13	0.48
4:P:184:CYC:HBB2	4:P:184:CYC:OB	2.13	0.48
4:K:184:CYC:HMD2	4:K:184:CYC:NC	2.28	0.48
3:D:35:ASN:HB2	4:D:255:CYC:O1D	2.13	0.48
1:M:125:SER:HB3	1:M:128:TRP:CE2	2.48	0.48
2:R:2:PHE:HA	2:R:6:THR:HG22	1.94	0.48
4:T:255:CYC:NB	4:T:255:CYC:HMA1	2.28	0.48
2:L:69:PRO:HA	2:L:74:TYR:CG	2.49	0.48
2:P:19:VAL:HG13	2:P:23:GLN:HB2	1.96	0.48
2:X:90:LEU:O	2:X:94:THR:HG23	2.12	0.48
1:C:17:ARG:NH2	1:K:2:LYS:HD2	2.28	0.48
2:L:79:MET:HE2	2:L:83:LEU:HG	1.95	0.48
2:T:68:ALA:HB1	6:T:2014:HOH:O	2.14	0.48
2:T:19:VAL:HG12	2:T:23:GLN:HB2	1.95	0.48
4:X:184:CYC:OB	4:X:184:CYC:HBB2	2.13	0.48
4:A:184:CYC:HMA1	4:A:184:CYC:HB	1.79	0.47
2:J:135:LYS:HG3	2:J:164:PHE:CB	2.44	0.47
1:Q:26:VAL:HG22	1:U:26:VAL:HG22	1.96	0.47
2:B:153:CYS:SG	5:B:255:BLA:C2C	3.03	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:121:THR:HG21	2:L:83:LEU:HD13	1.95	0.47
2:L:39:ASP:OD1	4:L:255:CYC:HHB	2.15	0.47
4:R:255:CYC:CBA	4:R:255:CYC:HHA	2.45	0.47
1:U:24:ILE:HG23	2:V:38:LEU:HD22	1.96	0.47
2:R:68:ALA:O	2:R:69:PRO:C	2.50	0.47
2:V:19:VAL:HG13	2:V:23:GLN:HB2	1.96	0.47
2:X:74:TYR:O	2:X:75:ALA:HB3	2.15	0.47
2:B:123:PRO:O	2:B:126:SER:HB2	2.14	0.47
4:D:255:CYC:NB	4:D:255:CYC:CMA	2.70	0.47
3:D:90:LEU:O	3:D:94:THR:HG23	2.13	0.47
1:Q:95:VAL:HG21	1:Q:154:LEU:HD13	1.97	0.47
2:R:40:ALA:HB2	2:R:156:LEU:HD21	1.96	0.47
2:T:74:TYR:O	2:T:75:ALA:HB3	2.15	0.47
3:D:171:VAL:O	3:D:172:SER:CB	2.59	0.47
1:U:121:THR:HG21	2:X:83:LEU:HD13	1.95	0.47
1:A:67:THR:O	1:A:76:ALA:HA	2.15	0.47
4:H:255:CYC:O1A	4:H:255:CYC:HHA	2.15	0.47
2:H:2:PHE:HA	2:H:6:THR:HG22	1.95	0.47
2:P:90:LEU:O	2:P:94:THR:HG23	2.15	0.47
2:N:20:SER:N	2:N:23:GLN:HE21	1.88	0.47
4:P:255:CYC:CGA	4:P:255:CYC:HHA	2.44	0.47
1:C:121:THR:HG21	2:F:83:LEU:HD13	1.97	0.47
1:K:6:THR:HA	2:L:1:MET:HE1	1.97	0.47
2:V:69:PRO:HA	2:V:74:TYR:CG	2.50	0.47
4:C:184:CYC:NC	4:C:184:CYC:HMD2	2.29	0.46
1:I:48:ALA:O	1:I:52:ILE:HG13	2.15	0.46
2:T:19:VAL:HG13	2:T:23:GLN:HB2	1.97	0.46
4:U:184:CYC:NB	4:U:184:CYC:CMA	2.76	0.46
3:D:36:LYS:O	3:D:40:VAL:HG12	2.15	0.46
2:L:52:VAL:HG22	2:L:134:MET:CE	2.45	0.46
1:C:68:CYS:HB2	1:M:68:CYS:O	2.16	0.46
1:I:120:ARG:HH11	1:I:120:ARG:HG3	1.79	0.46
1:C:68:CYS:HB2	1:M:68:CYS:C	2.35	0.46
4:P:255:CYC:CHA	4:P:255:CYC:O1A	2.63	0.46
4:R:255:CYC:C1B	4:R:255:CYC:HMA1	2.43	0.46
1:A:72:PRO:O	4:A:184:CYC:HBD2	2.15	0.46
4:O:184:CYC:HMA1	4:O:184:CYC:HB	1.79	0.46
2:P:2:PHE:HA	2:P:6:THR:CG2	2.45	0.46
2:R:19:VAL:HG13	2:R:23:GLN:HB2	1.97	0.46
1:Q:6:THR:HG22	2:R:1:MET:HE2	1.97	0.46
2:T:171:VAL:O	2:T:172:SER:CB	2.43	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:184:CYC:C2D	4:B:184:CYC:HC	2.29	0.46
3:D:2:PHE:HA	3:D:6:THR:HG22	1.97	0.46
1:E:10:SER:CA	6:E:2002:HOH:O	2.63	0.46
1:G:95:VAL:HG21	1:G:154:LEU:HD13	1.98	0.46
2:T:90:LEU:O	2:T:94:THR:HG23	2.16	0.46
1:U:135:TYR:CE2	1:U:139:ASN:ND2	2.84	0.46
4:F:184:CYC:HMA1	4:F:184:CYC:NB	2.30	0.46
2:R:69:PRO:HA	2:R:74:TYR:CG	2.50	0.46
1:O:6:THR:O	1:O:10:SER:HB2	2.16	0.46
4:V:255:CYC:HHA	4:V:255:CYC:HAD1	1.76	0.46
1:C:18:PHE:CE2	3:D:91:ARG:HA	2.51	0.46
1:E:10:SER:N	6:E:2002:HOH:O	2.49	0.46
2:V:72:ASN:HB3	4:V:184:CYC:OC	2.15	0.46
2:B:19:VAL:CG1	2:B:23:GLN:HB2	2.46	0.46
1:E:162:SER:O	1:G:120:ARG:HD2	2.16	0.46
1:K:1:MET:O	1:K:3:THR:HG23	2.16	0.46
2:R:144:ASP:HA	2:R:145:PRO:HD3	1.82	0.46
4:D:184:CYC:HMD2	4:D:184:CYC:NC	2.09	0.46
4:N:184:CYC:NB	4:N:184:CYC:HMA1	2.31	0.46
2:N:22:ALA:HA	6:N:2006:HOH:O	2.14	0.46
2:B:3:ASP:O	2:B:4:ALA:C	2.53	0.45
2:L:113:LEU:HD13	4:L:184:CYC:HMB3	1.98	0.45
4:L:255:CYC:CMB	4:L:255:CYC:CBB	2.87	0.45
2:N:19:VAL:HG13	2:N:23:GLN:HB2	1.95	0.45
4:P:184:CYC:HC	4:P:184:CYC:C2D	2.27	0.45
2:F:60:PHE:CE2	2:F:79:MET:HE1	2.51	0.45
4:T:255:CYC:HAD1	6:T:2030:HOH:O	2.16	0.45
2:X:20:SER:OG	2:X:23:GLN:HG3	2.16	0.45
1:C:13:ASP:OD2	3:D:108:ARG:HD2	2.17	0.45
4:C:184:CYC:O1D	2:F:57:ARG:NH1	2.47	0.45
1:C:79:ARG:HG3	6:C:2015:HOH:O	2.15	0.45
1:Q:6:THR:O	1:Q:10:SER:HB2	2.16	0.45
4:B:184:CYC:HMA1	4:B:184:CYC:C1B	2.46	0.45
2:F:49:SER:HB3	6:I:2039:HOH:O	2.17	0.45
2:J:135:LYS:HG3	2:J:164:PHE:HB2	1.98	0.45
4:J:184:CYC:HC	4:J:184:CYC:CMD	2.29	0.45
2:X:72:ASN:HB3	4:X:184:CYC:OC	2.16	0.45
1:M:40:ALA:HB2	1:M:146:ALA:HB1	1.99	0.45
1:M:13:ASP:OD2	2:N:108:ARG:HD2	2.17	0.45
2:R:40:ALA:HB1	2:R:160:ILE:HD11	1.98	0.45
4:E:184:CYC:NC	4:E:184:CYC:HMD2	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:90:LEU:O	2:J:94:THR:HG23	2.17	0.45
1:M:2:LYS:HD2	1:S:17:ARG:NH2	2.32	0.45
1:W:73:ASN:O	4:W:184:CYC:HMD2	2.15	0.45
1:A:135:TYR:CE2	1:A:139:ASN:ND2	2.85	0.45
2:B:69:PRO:HA	2:B:74:TYR:CG	2.51	0.45
1:K:13:ASP:OD1	2:L:92:TYR:OH	2.28	0.45
2:B:113:LEU:HG	2:B:171:VAL:HG12	1.98	0.45
1:C:125:SER:HB3	1:C:128:TRP:CE2	2.51	0.45
2:F:2:PHE:HA	2:F:6:THR:CG2	2.47	0.45
4:S:184:CYC:NB	4:S:184:CYC:HMA1	2.32	0.45
1:W:130:ILE:HD11	1:W:161:LEU:O	2.17	0.45
1:I:68:CYS:HB2	1:W:60:TYR:HB3	1.99	0.45
1:E:162:SER:O	1:G:120:ARG:CD	2.65	0.44
2:N:19:VAL:HG12	2:N:23:GLN:HB2	1.96	0.44
1:Q:120:ARG:CD	1:S:162:SER:O	2.65	0.44
2:T:2:PHE:HA	2:T:6:THR:HG22	1.99	0.44
2:V:52:VAL:HG22	2:V:134:MET:CE	2.47	0.44
2:L:92:TYR:HE2	4:L:184:CYC:HBB1	1.80	0.44
2:P:115:GLU:CD	2:P:115:GLU:H	2.21	0.44
2:V:2:PHE:HA	2:V:6:THR:HG22	1.99	0.44
2:X:60:PHE:HE2	2:X:79:MET:HE1	1.82	0.44
2:H:103:SER:O	2:H:104:ALA:C	2.55	0.44
4:V:184:CYC:HAD2	4:V:184:CYC:HHA	1.73	0.44
2:B:144:ASP:HA	2:B:145:PRO:HD3	1.88	0.44
2:L:51:VAL:HG12	2:L:134:MET:HG2	2.00	0.44
1:M:121:THR:HG21	2:P:83:LEU:HD13	1.99	0.44
2:B:90:LEU:O	2:B:94:THR:HG23	2.17	0.44
4:F:255:CYC:CBB	4:F:255:CYC:OB	2.65	0.44
1:C:120:ARG:CG	1:I:162:SER:O	2.65	0.44
4:P:184:CYC:OB	4:P:184:CYC:CBB	2.66	0.44
4:R:184:CYC:NC	4:R:184:CYC:CMD	2.69	0.44
2:X:79:MET:CE	2:X:83:LEU:HG	2.48	0.44
1:C:1:MET:O	1:C:3:THR:HG23	2.17	0.44
2:H:2:PHE:HA	2:H:6:THR:CG2	2.48	0.44
2:J:31:VAL:O	2:J:34:ALA:HB2	2.17	0.44
1:A:70:GLN:HG3	6:A:2002:HOH:O	2.17	0.44
4:D:184:CYC:HMA1	4:D:184:CYC:NB	2.33	0.44
2:J:19:VAL:HG12	2:J:23:GLN:HB2	2.00	0.44
2:N:58:ALA:HB3	2:N:133:LYS:HD3	2.00	0.44
4:S:184:CYC:OB	4:S:184:CYC:HBB2	2.18	0.44
2:J:171:VAL:O	2:J:172:SER:HB3	2.10	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:74:TYR:O	2:L:75:ALA:CB	2.66	0.43
2:B:52:VAL:HG22	2:B:134:MET:HE3	1.99	0.43
3:D:74:TYR:O	3:D:75:ALA:HB3	2.18	0.43
1:I:128:TRP:CE3	4:I:184:CYC:HMC3	2.52	0.43
1:O:91:TYR:CD2	1:O:133:LEU:HD21	2.54	0.43
1:Q:79:ARG:HB3	1:Q:79:ARG:HE	1.72	0.43
1:U:79:ARG:HB3	1:U:79:ARG:HE	1.72	0.43
2:N:69:PRO:HA	2:N:74:TYR:CG	2.52	0.43
4:B:184:CYC:HAD1	4:B:184:CYC:HMD1	1.90	0.43
4:O:184:CYC:HAA2	4:O:184:CYC:HHA	1.87	0.43
4:T:255:CYC:HB	4:T:255:CYC:HMA1	1.82	0.43
2:P:52:VAL:HG22	2:P:134:MET:CE	2.48	0.43
2:J:74:TYR:O	2:J:75:ALA:CB	2.66	0.43
2:L:19:VAL:CG1	2:L:23:GLN:HB2	2.49	0.43
4:X:184:CYC:HHA	4:X:184:CYC:CBD	2.49	0.43
2:B:74:TYR:O	2:B:75:ALA:CB	2.66	0.43
1:C:104:THR:O	1:C:105:GLY:C	2.57	0.43
1:Q:125:SER:HB3	1:Q:128:TRP:CE2	2.54	0.43
2:T:82:CYS:CA	4:T:184:CYC:HAC2	2.48	0.43
1:O:162:SER:O	1:U:120:ARG:HD2	2.18	0.43
3:D:40:VAL:HG12	3:D:156:LEU:HD21	1.94	0.43
3:D:60:PHE:HE2	3:D:79:MET:HE1	1.83	0.43
2:F:103:SER:O	2:F:104:ALA:C	2.57	0.43
2:H:28:SER:O	2:H:31:VAL:HB	2.19	0.43
2:X:19:VAL:CG1	2:X:23:GLN:HB2	2.49	0.43
3:D:48:ALA:O	3:D:52:VAL:HG23	2.19	0.42
4:F:255:CYC:HB	4:F:255:CYC:CMA	2.32	0.42
2:H:74:TYR:O	2:H:75:ALA:HB3	2.18	0.42
4:N:255:CYC:HHA	4:N:255:CYC:HBA1	2.01	0.42
1:M:120:ARG:CG	1:W:162:SER:O	2.67	0.42
3:D:10:ALA:O	3:D:14:THR:HG23	2.20	0.42
2:L:10:ALA:O	2:L:14:THR:HG23	2.20	0.42
2:P:51:VAL:HG12	2:P:134:MET:HG2	2.01	0.42
2:T:79:MET:HE2	2:T:83:LEU:HG	2.00	0.42
2:P:114:ARG:HB2	2:P:170:ALA:O	2.19	0.42
1:E:115:ILE:HD12	1:E:115:ILE:HA	1.87	0.42
2:F:68:ALA:O	2:F:69:PRO:C	2.57	0.42
2:H:37:ARG:O	2:H:40:ALA:HB3	2.19	0.42
1:K:91:TYR:O	1:K:95:VAL:HG23	2.19	0.42
2:L:79:MET:CE	2:L:83:LEU:HG	2.49	0.42
2:P:19:VAL:CG1	2:P:23:GLN:HB2	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:GLU:CD	3:D:115:GLU:H	2.23	0.42
2:F:2:PHE:HA	2:F:6:THR:HG22	2.02	0.42
1:K:33:GLN:N	6:K:2004:HOH:O	2.51	0.42
4:L:255:CYC:CMA	4:L:255:CYC:NB	2.78	0.42
1:O:79:ARG:HE	1:O:79:ARG:HB3	1.71	0.42
4:S:184:CYC:NC	4:S:184:CYC:CMD	2.75	0.42
2:B:2:PHE:HA	2:B:6:THR:CG2	2.49	0.42
2:J:37:ARG:O	2:J:40:ALA:HB3	2.19	0.42
2:R:153:CYS:SG	4:R:255:CYC:H2C	2.59	0.42
2:X:113:LEU:CD2	2:X:171:VAL:HG12	2.50	0.42
2:X:48:ALA:O	2:X:52:VAL:HG23	2.19	0.42
1:A:75:ALA:O	1:A:81:LYS:HD3	2.20	0.42
1:S:125:SER:HB3	1:S:128:TRP:CE2	2.55	0.42
2:T:124:GLY:HA3	2:T:172:SER:H	1.85	0.42
2:B:171:VAL:O	2:B:171:VAL:HG23	2.16	0.42
2:T:74:TYR:O	2:T:75:ALA:CB	2.68	0.42
4:H:255:CYC:CGA	4:H:255:CYC:CHA	2.97	0.42
1:I:74:TYR:HA	4:I:184:CYC:OC	2.20	0.42
1:M:162:SER:O	1:W:120:ARG:CG	2.57	0.42
1:O:1:MET:O	1:O:3:THR:HG23	2.20	0.42
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.85	0.42
5:B:255:BLA:NC	5:B:255:BLA:HMD2	2.34	0.42
2:L:2:PHE:HA	2:L:6:THR:HG22	2.02	0.42
2:J:2:PHE:HA	2:J:6:THR:HG22	2.02	0.41
4:K:184:CYC:HMA1	4:K:184:CYC:HB	1.85	0.41
4:P:255:CYC:HMA1	4:P:255:CYC:HB	1.85	0.41
4:Q:184:CYC:NC	4:Q:184:CYC:CMD	2.81	0.41
1:S:115:ILE:HA	1:S:115:ILE:HD12	1.78	0.41
2:B:83:LEU:HD13	1:E:121:THR:HG21	2.01	0.41
1:M:26:VAL:HG13	1:S:26:VAL:HG22	2.02	0.41
1:O:48:ALA:O	1:O:52:ILE:HG13	2.19	0.41
5:B:255:BLA:HMA1	5:B:255:BLA:C1B	2.40	0.41
4:D:184:CYC:OB	4:D:184:CYC:CBB	2.67	0.41
4:E:184:CYC:HAC1	4:E:184:CYC:HHD	1.91	0.41
1:M:5:LEU:HB2	2:N:3:ASP:OD2	2.19	0.41
1:Q:74:TYR:HA	4:Q:184:CYC:OC	2.20	0.41
3:D:171:VAL:HG23	3:D:172:SER:H	1.86	0.41
2:F:119:ALA:HA	6:F:2026:HOH:O	2.20	0.41
2:F:90:LEU:O	2:F:94:THR:HG23	2.20	0.41
2:H:113:LEU:HG	2:H:171:VAL:HG12	2.03	0.41
2:L:67:ILE:O	6:L:2012:HOH:O	2.22	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:TRP:CE3	4:O:184:CYC:HMC3	2.55	0.41
1:Q:99:LEU:HD23	1:Q:153:TYR:HE2	1.85	0.41
4:B:184:CYC:HBB2	4:B:184:CYC:OB	2.20	0.41
4:P:184:CYC:NB	4:P:184:CYC:CMA	2.64	0.41
2:B:51:VAL:HG12	2:B:134:MET:HG2	2.03	0.41
2:J:127:VAL:HG22	4:J:184:CYC:H3C	2.03	0.41
2:J:82:CYS:SG	4:J:184:CYC:C3C	3.00	0.41
1:M:3:THR:O	1:M:7:ASP:HB2	2.21	0.41
4:N:255:CYC:CMA	4:N:255:CYC:HB	2.33	0.41
1:O:17:ARG:CB	6:O:2003:HOH:O	2.64	0.41
1:Q:6:THR:HA	2:R:1:MET:HE1	2.02	0.41
2:F:74:TYR:O	2:F:75:ALA:CB	2.68	0.41
4:P:255:CYC:HB	4:P:255:CYC:CMA	2.34	0.41
2:X:2:PHE:HA	2:X:6:THR:HG22	2.02	0.41
3:D:144:ASP:HA	3:D:145:PRO:HD3	1.95	0.41
1:K:73:ASN:N	1:K:73:ASN:OD1	2.52	0.41
1:Q:6:THR:HG22	2:R:1:MET:CE	2.50	0.41
2:R:113:LEU:HG	2:R:171:VAL:HG12	2.03	0.41
3:D:123:PRO:O	3:D:126:SER:HB2	2.21	0.41
4:F:184:CYC:HB	4:F:184:CYC:CMA	2.34	0.41
1:G:72:PRO:O	4:G:184:CYC:HBD2	2.21	0.41
2:R:58:ALA:HB3	2:R:133:LYS:HD3	2.02	0.41
1:Q:13:ASP:HA	2:R:95:TYR:OH	2.21	0.41
1:C:24:ILE:HG23	1:C:24:ILE:HD12	1.74	0.40
2:H:144:ASP:HA	2:H:145:PRO:HD3	1.90	0.40
2:H:31:VAL:O	2:H:34:ALA:HB2	2.21	0.40
1:I:67:THR:O	1:I:76:ALA:HA	2.21	0.40
1:M:39:SER:HB3	6:M:2009:HOH:O	2.20	0.40
2:P:144:ASP:HA	2:P:145:PRO:HD3	1.89	0.40
1:Q:17:ARG:CZ	1:U:2:LYS:HD2	2.51	0.40
2:V:37:ARG:O	2:V:40:ALA:HB3	2.22	0.40
1:I:77:ASP:O	1:I:81:LYS:HB2	2.22	0.40
2:J:69:PRO:HA	2:J:74:TYR:CG	2.56	0.40
1:Q:26:VAL:HG13	1:U:26:VAL:HG22	2.03	0.40
1:U:99:LEU:HD23	1:U:153:TYR:HE2	1.85	0.40
2:B:10:ALA:O	2:B:14:THR:HG23	2.21	0.40
2:B:149:THR:OG1	5:B:255:BLA:O1A	2.26	0.40
2:H:153:CYS:SG	4:H:255:CYC:C2C	3.09	0.40
1:M:115:ILE:HD12	1:M:115:ILE:HA	1.94	0.40
4:O:184:CYC:HBD1	4:O:184:CYC:HHA	2.04	0.40
1:Q:115:ILE:HD12	1:Q:115:ILE:HA	1.94	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:3:THR:O	1:U:4:PRO:C	2.58	0.40
4:V:255:CYC:C1B	4:V:255:CYC:HMA1	2.48	0.40
2:X:79:MET:HE2	2:X:83:LEU:CG	2.51	0.40
1:C:2:LYS:HD2	1:K:17:ARG:NH2	2.35	0.40
2:F:135:LYS:HG3	2:F:164:PHE:HB2	2.03	0.40
3:D:72:ASN:HB3	4:D:184:CYC:OC	2.22	0.40
1:A:121:THR:HG21	3:D:83:LEU:HD13	2.04	0.40
2:H:69:PRO:HA	2:H:74:TYR:CG	2.55	0.40
4:P:255:CYC:CBC	4:P:255:CYC:CHD	2.66	0.40
1:S:18:PHE:CE2	2:T:91:ARG:HA	2.56	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:62:GLU:OE1	2:H:23:GLN:CG[2_746]	2.05	0.15
1:E:67:THR:O	1:O:61:ASN:CG[1_554]	2.07	0.13
2:N:114:ARG:NH1	2:T:15:ARG:NH2[2_547]	2.19	0.01

## 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	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25 64
1	C	160/162 (99%)	152 (95%)	6 (4%)	2 (1%)	12 45
1	E	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	25 64
1	G	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	25 64
1	I	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25 64
1	K	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	25 64
1	M	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	25 64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25	64
1	Q	160/162 (99%)	155 (97%)	4 (2%)	1 (1%)	25	64
1	S	160/162 (99%)	154 (96%)	4 (2%)	2 (1%)	12	45
1	U	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25	64
1	W	160/162 (99%)	153 (96%)	6 (4%)	1 (1%)	25	64
2	B	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	25	64
2	F	170/172 (99%)	164 (96%)	4 (2%)	2 (1%)	13	48
2	H	170/172 (99%)	161 (95%)	8 (5%)	1 (1%)	25	64
2	J	170/172 (99%)	165 (97%)	4 (2%)	1 (1%)	25	64
2	L	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	25	64
2	N	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	25	64
2	P	170/172 (99%)	164 (96%)	5 (3%)	1 (1%)	25	64
2	R	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
2	T	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	13	48
2	V	170/172 (99%)	163 (96%)	6 (4%)	1 (1%)	25	64
2	X	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	25	64
3	D	170/172 (99%)	162 (95%)	6 (4%)	2 (1%)	13	48
All	All	3960/4008 (99%)	3813 (96%)	118 (3%)	29 (1%)	22	60

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	LYS
1	G	2	LYS
1	M	2	LYS
1	O	2	LYS
1	Q	2	LYS
1	A	2	LYS
1	C	2	LYS
3	D	171	VAL
1	I	2	LYS
1	K	2	LYS
1	S	2	LYS
1	U	2	LYS
1	W	2	LYS
2	N	75	ALA

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
2	R	75	ALA
3	D	75	ALA
2	F	34	ALA
2	H	75	ALA
2	L	75	ALA
2	P	75	ALA
2	T	75	ALA
2	B	75	ALA
2	F	75	ALA
2	J	75	ALA
2	V	75	ALA
2	X	75	ALA
1	C	105	GLY
1	S	105	GLY
2	T	171	VAL

### 5.3.2 Protein sidechains [i](#)

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	120/120 (100%)	108 (90%)	12 (10%)	7	29
1	C	120/120 (100%)	107 (89%)	13 (11%)	6	26
1	E	120/120 (100%)	108 (90%)	12 (10%)	7	29
1	G	120/120 (100%)	107 (89%)	13 (11%)	6	26
1	I	120/120 (100%)	107 (89%)	13 (11%)	6	26
1	K	120/120 (100%)	109 (91%)	11 (9%)	9	34
1	M	120/120 (100%)	109 (91%)	11 (9%)	9	34
1	O	120/120 (100%)	109 (91%)	11 (9%)	9	34
1	Q	120/120 (100%)	109 (91%)	11 (9%)	9	34
1	S	120/120 (100%)	108 (90%)	12 (10%)	7	29
1	U	120/120 (100%)	107 (89%)	13 (11%)	6	26
1	W	120/120 (100%)	108 (90%)	12 (10%)	7	29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	123/123 (100%)	114 (93%)	9 (7%)	14	44
2	F	123/123 (100%)	116 (94%)	7 (6%)	20	56
2	H	123/123 (100%)	113 (92%)	10 (8%)	11	40
2	J	123/123 (100%)	118 (96%)	5 (4%)	30	67
2	L	123/123 (100%)	118 (96%)	5 (4%)	30	67
2	N	123/123 (100%)	117 (95%)	6 (5%)	25	61
2	P	123/123 (100%)	114 (93%)	9 (7%)	14	44
2	R	123/123 (100%)	114 (93%)	9 (7%)	14	44
2	T	123/123 (100%)	115 (94%)	8 (6%)	17	50
2	V	123/123 (100%)	113 (92%)	10 (8%)	11	40
2	X	123/123 (100%)	117 (95%)	6 (5%)	25	61
3	D	124/124 (100%)	114 (92%)	10 (8%)	11	40
All	All	2917/2917 (100%)	2679 (92%)	238 (8%)	11	39

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	LYS
1	A	7	ASP
1	A	10	SER
1	A	11	THR
1	A	32	ARG
1	A	39	SER
1	A	46	SER
1	A	81	LYS
1	A	117	GLU
1	A	152	SER
1	A	154	LEU
2	B	6	THR
2	B	18	MET
2	B	21	VAL
2	B	28	SER
2	B	30	MET
2	B	84	ARG
2	B	118	SER
2	B	142	VAL
2	B	172	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	1	MET
1	C	2	LYS
1	C	7	ASP
1	C	10	SER
1	C	11	THR
1	C	32	ARG
1	C	39	SER
1	C	53	SER
1	C	81	LYS
1	C	117	GLU
1	C	152	SER
1	C	154	LEU
1	C	162	SER
3	D	6	THR
3	D	18	MET
3	D	21	VAL
3	D	28	SER
3	D	30	MET
3	D	40	VAL
3	D	84	ARG
3	D	115	GLU
3	D	118	SER
3	D	172	SER
1	E	1	MET
1	E	2	LYS
1	E	10	SER
1	E	11	THR
1	E	32	ARG
1	E	39	SER
1	E	46	SER
1	E	53	SER
1	E	81	LYS
1	E	117	GLU
1	E	152	SER
1	E	154	LEU
2	F	6	THR
2	F	21	VAL
2	F	28	SER
2	F	30	MET
2	F	84	ARG
2	F	118	SER
2	F	142	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	1	MET
1	G	2	LYS
1	G	7	ASP
1	G	10	SER
1	G	11	THR
1	G	32	ARG
1	G	39	SER
1	G	53	SER
1	G	81	LYS
1	G	117	GLU
1	G	152	SER
1	G	154	LEU
1	G	162	SER
2	H	6	THR
2	H	14	THR
2	H	15	ARG
2	H	21	VAL
2	H	28	SER
2	H	30	MET
2	H	84	ARG
2	H	118	SER
2	H	142	VAL
2	H	172	SER
1	I	1	MET
1	I	2	LYS
1	I	7	ASP
1	I	10	SER
1	I	11	THR
1	I	32	ARG
1	I	39	SER
1	I	46	SER
1	I	53	SER
1	I	81	LYS
1	I	117	GLU
1	I	152	SER
1	I	154	LEU
2	J	6	THR
2	J	21	VAL
2	J	28	SER
2	J	84	ARG
2	J	118	SER
1	K	1	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	2	LYS
1	K	10	SER
1	K	11	THR
1	K	32	ARG
1	K	39	SER
1	K	46	SER
1	K	53	SER
1	K	81	LYS
1	K	117	GLU
1	K	154	LEU
2	L	6	THR
2	L	18	MET
2	L	21	VAL
2	L	28	SER
2	L	84	ARG
1	M	1	MET
1	M	2	LYS
1	M	7	ASP
1	M	10	SER
1	M	11	THR
1	M	32	ARG
1	M	46	SER
1	M	53	SER
1	M	81	LYS
1	M	117	GLU
1	M	154	LEU
2	N	6	THR
2	N	21	VAL
2	N	28	SER
2	N	84	ARG
2	N	118	SER
2	N	166	ARG
1	O	1	MET
1	O	7	ASP
1	O	10	SER
1	O	11	THR
1	O	32	ARG
1	O	39	SER
1	O	46	SER
1	O	53	SER
1	O	81	LYS
1	O	117	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	154	LEU
2	P	6	THR
2	P	18	MET
2	P	21	VAL
2	P	28	SER
2	P	30	MET
2	P	84	ARG
2	P	118	SER
2	P	166	ARG
2	P	172	SER
1	Q	1	MET
1	Q	2	LYS
1	Q	7	ASP
1	Q	10	SER
1	Q	11	THR
1	Q	32	ARG
1	Q	39	SER
1	Q	53	SER
1	Q	81	LYS
1	Q	117	GLU
1	Q	154	LEU
2	R	6	THR
2	R	14	THR
2	R	18	MET
2	R	21	VAL
2	R	28	SER
2	R	84	ARG
2	R	118	SER
2	R	166	ARG
2	R	172	SER
1	S	1	MET
1	S	2	LYS
1	S	7	ASP
1	S	10	SER
1	S	11	THR
1	S	32	ARG
1	S	39	SER
1	S	46	SER
1	S	53	SER
1	S	81	LYS
1	S	117	GLU
1	S	154	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	T	6	THR
2	T	18	MET
2	T	21	VAL
2	T	28	SER
2	T	30	MET
2	T	84	ARG
2	T	118	SER
2	T	166	ARG
1	U	1	MET
1	U	2	LYS
1	U	7	ASP
1	U	10	SER
1	U	11	THR
1	U	32	ARG
1	U	39	SER
1	U	46	SER
1	U	53	SER
1	U	68	CYS
1	U	81	LYS
1	U	117	GLU
1	U	154	LEU
2	V	6	THR
2	V	14	THR
2	V	18	MET
2	V	21	VAL
2	V	28	SER
2	V	30	MET
2	V	84	ARG
2	V	115	GLU
2	V	118	SER
2	V	172	SER
1	W	1	MET
1	W	2	LYS
1	W	7	ASP
1	W	10	SER
1	W	11	THR
1	W	32	ARG
1	W	39	SER
1	W	53	SER
1	W	81	LYS
1	W	117	GLU
1	W	152	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	W	154	LEU
2	X	6	THR
2	X	18	MET
2	X	21	VAL
2	X	28	SER
2	X	84	ARG
2	X	172	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	139	ASN
2	B	23	GLN
2	B	35	ASN
1	C	139	ASN
3	D	23	GLN
3	D	35	ASN
1	E	70	GLN
2	F	23	GLN
2	F	35	ASN
1	G	139	ASN
2	H	23	GLN
2	H	35	ASN
1	I	139	ASN
2	J	23	GLN
2	J	35	ASN
1	K	139	ASN
2	L	23	GLN
2	L	35	ASN
2	N	23	GLN
2	N	35	ASN
1	O	139	ASN
2	P	23	GLN
2	P	35	ASN
1	Q	139	ASN
2	R	23	GLN
2	R	35	ASN
1	S	139	ASN
2	T	23	GLN
2	T	35	ASN
1	U	139	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	V	23	GLN
2	V	35	ASN
1	W	139	ASN
2	X	23	GLN
2	X	35	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

36 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	I	184	1	36,46,46	3.94	12 (33%)	44,67,67	3.02	19 (43%)
4	CYC	J	255	2	36,46,46	3.88	15 (41%)	44,67,67	3.24	21 (47%)
4	CYC	O	184	1	36,46,46	3.56	12 (33%)	44,67,67	2.75	15 (34%)
4	CYC	R	184	2	36,46,46	4.24	12 (33%)	44,67,67	3.05	21 (47%)
4	CYC	E	184	1	36,46,46	3.45	13 (36%)	44,67,67	3.08	13 (29%)
4	CYC	L	184	-	36,46,46	4.03	12 (33%)	44,67,67	3.05	18 (40%)
4	CYC	V	255	2	36,46,46	4.12	16 (44%)	44,67,67	3.41	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CYC	Q	184	1	36,46,46	3.58	15 (41%)	44,67,67	2.71	14 (31%)
4	CYC	B	184	2	36,46,46	4.00	11 (30%)	44,67,67	3.04	16 (36%)
4	CYC	S	184	1	36,46,46	4.04	14 (38%)	44,67,67	3.48	20 (45%)
4	CYC	D	255	3	36,46,46	3.82	13 (36%)	44,67,67	2.81	20 (45%)
4	CYC	W	184	1	36,46,46	3.83	15 (41%)	44,67,67	2.56	13 (29%)
4	CYC	X	184	2	36,46,46	4.75	13 (36%)	44,67,67	2.62	16 (36%)
4	CYC	K	184	1	36,46,46	4.05	12 (33%)	44,67,67	2.75	15 (34%)
4	CYC	M	184	1	36,46,46	4.06	13 (36%)	44,67,67	3.22	20 (45%)
4	CYC	N	255	2	36,46,46	3.98	13 (36%)	44,67,67	2.64	14 (31%)
4	CYC	P	184	2	36,46,46	4.56	12 (33%)	44,67,67	3.03	21 (47%)
4	CYC	A	184	1	36,46,46	4.03	13 (36%)	44,67,67	2.83	20 (45%)
4	CYC	C	184	1	36,46,46	3.66	12 (33%)	44,67,67	2.95	18 (40%)
4	CYC	T	184	-	36,46,46	3.63	14 (38%)	44,67,67	3.27	17 (38%)
4	CYC	V	184	2	36,46,46	3.66	14 (38%)	44,67,67	3.03	15 (34%)
5	BLA	B	255	-	36,46,46	4.89	14 (38%)	47,67,67	3.00	20 (42%)
4	CYC	U	184	1	36,46,46	3.80	15 (41%)	44,67,67	3.15	22 (50%)
4	CYC	F	255	2	36,46,46	4.39	14 (38%)	44,67,67	2.67	17 (38%)
4	CYC	L	255	2	36,46,46	4.13	12 (33%)	44,67,67	2.83	17 (38%)
4	CYC	T	255	-	36,46,46	3.52	14 (38%)	44,67,67	2.42	13 (29%)
4	CYC	X	255	2	36,46,46	3.61	11 (30%)	44,67,67	2.71	16 (36%)
4	CYC	H	255	-	36,46,46	3.67	14 (38%)	44,67,67	2.84	18 (40%)
4	CYC	P	255	2	36,46,46	3.45	12 (33%)	44,67,67	3.02	17 (38%)
4	CYC	R	255	-	36,46,46	4.20	10 (27%)	44,67,67	3.23	18 (40%)
4	CYC	G	184	1	36,46,46	3.53	15 (41%)	44,67,67	2.65	13 (29%)
4	CYC	H	184	2	36,46,46	4.44	12 (33%)	44,67,67	3.16	12 (27%)
4	CYC	J	184	2	36,46,46	3.49	13 (36%)	44,67,67	3.33	14 (31%)
4	CYC	N	184	2	36,46,46	3.90	14 (38%)	44,67,67	2.61	14 (31%)
4	CYC	D	184	3	36,46,46	4.21	12 (33%)	44,67,67	3.20	20 (45%)
4	CYC	F	184	2	36,46,46	4.22	14 (38%)	44,67,67	2.56	16 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYC	I	184	1	-	5/21/74/74	0/4/4/4
4	CYC	J	255	2	-	13/21/74/74	0/4/4/4
4	CYC	O	184	1	-	6/21/74/74	0/4/4/4
4	CYC	R	184	2	-	10/21/74/74	0/4/4/4
4	CYC	E	184	1	-	11/21/74/74	0/4/4/4
4	CYC	L	184	-	-	9/21/74/74	0/4/4/4
4	CYC	V	255	2	-	5/21/74/74	0/4/4/4
4	CYC	Q	184	1	-	6/21/74/74	0/4/4/4
4	CYC	B	184	2	-	10/21/74/74	0/4/4/4
4	CYC	S	184	1	-	10/21/74/74	0/4/4/4
4	CYC	D	255	3	-	11/21/74/74	0/4/4/4
4	CYC	W	184	1	-	8/21/74/74	0/4/4/4
4	CYC	X	184	2	-	13/21/74/74	0/4/4/4
4	CYC	K	184	1	-	7/21/74/74	0/4/4/4
4	CYC	M	184	1	-	5/21/74/74	0/4/4/4
4	CYC	N	255	2	-	12/21/74/74	0/4/4/4
4	CYC	P	184	2	-	10/21/74/74	0/4/4/4
4	CYC	A	184	1	-	9/21/74/74	0/4/4/4
4	CYC	C	184	1	-	6/21/74/74	0/4/4/4
4	CYC	T	184	-	-	6/21/74/74	0/4/4/4
4	CYC	V	184	2	-	9/21/74/74	0/4/4/4
5	BLA	B	255	-	-	11/22/74/74	0/4/4/4
4	CYC	U	184	1	-	7/21/74/74	0/4/4/4
4	CYC	F	255	2	-	8/21/74/74	0/4/4/4
4	CYC	L	255	2	-	11/21/74/74	0/4/4/4
4	CYC	T	255	-	-	8/21/74/74	0/4/4/4
4	CYC	X	255	2	-	7/21/74/74	0/4/4/4
4	CYC	H	255	-	-	4/21/74/74	0/4/4/4
4	CYC	P	255	2	-	12/21/74/74	0/4/4/4
4	CYC	R	255	-	-	9/21/74/74	0/4/4/4
4	CYC	G	184	1	-	8/21/74/74	0/4/4/4
4	CYC	H	184	2	-	8/21/74/74	0/4/4/4
4	CYC	J	184	2	-	10/21/74/74	0/4/4/4
4	CYC	N	184	2	-	8/21/74/74	0/4/4/4
4	CYC	D	184	3	-	11/21/74/74	0/4/4/4

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CYC	F	184	2	-	6/21/74/74	0/4/4/4

All (472) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	184	CYC	CHA-C1A	25.35	1.56	1.35
4	P	184	CYC	CHA-C1A	23.26	1.54	1.35
4	H	184	CYC	CHA-C1A	23.19	1.54	1.35
5	B	255	BLA	CHA-C4D	23.15	1.54	1.35
4	F	255	CYC	CHA-C1A	22.44	1.53	1.35
4	R	255	CYC	CHA-C1A	21.99	1.53	1.35
4	F	184	CYC	CHA-C1A	21.64	1.53	1.35
4	R	184	CYC	CHA-C1A	21.44	1.53	1.35
4	L	255	CYC	CHA-C1A	21.42	1.53	1.35
4	D	184	CYC	CHA-C1A	21.36	1.53	1.35
4	B	184	CYC	CHA-C1A	21.09	1.52	1.35
4	K	184	CYC	CHA-C1A	20.82	1.52	1.35
4	A	184	CYC	CHA-C1A	20.68	1.52	1.35
4	M	184	CYC	CHA-C1A	20.46	1.52	1.35
4	L	184	CYC	CHA-C1A	19.99	1.51	1.35
4	V	255	CYC	CHA-C1A	19.90	1.51	1.35
4	N	255	CYC	CHA-C1A	19.38	1.51	1.35
4	I	184	CYC	CHA-C1A	19.30	1.51	1.35
4	S	184	CYC	CHA-C1A	19.05	1.51	1.35
4	N	184	CYC	CHA-C1A	18.94	1.50	1.35
4	J	255	CYC	CHA-C1A	18.25	1.50	1.35
4	D	255	CYC	CHA-C1A	18.15	1.50	1.35
4	U	184	CYC	CHA-C1A	18.07	1.50	1.35
4	W	184	CYC	CHA-C1A	17.70	1.49	1.35
4	H	255	CYC	CHA-C1A	17.04	1.49	1.35
4	V	184	CYC	CHA-C1A	16.91	1.49	1.35
4	T	184	CYC	CHA-C1A	16.78	1.49	1.35
4	X	255	CYC	CHA-C1A	16.75	1.49	1.35
4	O	184	CYC	CHA-C1A	16.67	1.49	1.35
4	C	184	CYC	CHA-C1A	16.59	1.49	1.35
4	J	184	CYC	CHA-C1A	16.52	1.48	1.35
4	P	255	CYC	CHA-C1A	16.48	1.48	1.35
4	G	184	CYC	CHA-C1A	15.91	1.48	1.35
4	T	255	CYC	CHA-C1A	15.85	1.48	1.35
4	Q	184	CYC	CHA-C1A	15.39	1.48	1.35
4	E	184	CYC	CHA-C1A	14.55	1.47	1.35
5	B	255	BLA	CHB-C1B	8.49	1.52	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	255	BLA	C3C-C2C	8.28	1.54	1.37
4	S	184	CYC	C4B-C3B	-7.80	1.33	1.48
4	Q	184	CYC	CHB-C1B	7.01	1.54	1.38
4	N	255	CYC	CHB-C1B	6.54	1.53	1.38
4	F	255	CYC	C4B-C3B	-6.53	1.35	1.48
4	J	255	CYC	C4B-C3B	-6.45	1.35	1.48
4	C	184	CYC	C4B-C3B	-6.43	1.36	1.48
4	I	184	CYC	C4B-C3B	-6.35	1.36	1.48
4	V	184	CYC	CHB-C1B	6.25	1.52	1.38
4	G	184	CYC	C1A-C2A	-6.22	1.35	1.45
4	V	184	CYC	CHB-C4A	6.22	1.55	1.40
4	T	255	CYC	C4B-C3B	-6.21	1.36	1.48
4	T	255	CYC	CHB-C1B	6.17	1.52	1.38
4	O	184	CYC	CHB-C1B	6.16	1.52	1.38
4	E	184	CYC	C2C-C1C	-6.16	1.46	1.52
4	W	184	CYC	C4B-C3B	-6.09	1.36	1.48
4	L	255	CYC	C4B-C3B	-6.04	1.36	1.48
4	D	184	CYC	CHB-C4A	6.01	1.54	1.40
4	F	184	CYC	CHB-C1B	6.00	1.52	1.38
4	R	184	CYC	CHB-C1B	5.97	1.52	1.38
4	V	255	CYC	CHB-C4A	5.93	1.54	1.40
4	J	255	CYC	CHB-C1B	5.89	1.52	1.38
4	K	184	CYC	C4B-C3B	-5.87	1.37	1.48
4	A	184	CYC	CHB-C1B	5.84	1.51	1.38
4	E	184	CYC	CHB-C1B	5.84	1.51	1.38
4	S	184	CYC	CHB-C1B	5.83	1.51	1.38
4	V	255	CYC	CHB-C1B	5.82	1.51	1.38
4	F	184	CYC	CHB-C4A	5.64	1.53	1.40
4	W	184	CYC	C1A-C2A	-5.60	1.36	1.45
4	X	255	CYC	CHB-C1B	5.58	1.51	1.38
4	T	184	CYC	CHB-C1B	5.56	1.51	1.38
4	E	184	CYC	C4B-C3B	-5.52	1.37	1.48
4	P	184	CYC	CHB-C1B	5.48	1.51	1.38
4	X	255	CYC	CHB-C4A	5.47	1.53	1.40
4	N	184	CYC	CHB-C1B	5.47	1.51	1.38
4	H	184	CYC	CHB-C1B	5.47	1.51	1.38
4	L	184	CYC	CHB-C1B	5.45	1.51	1.38
4	D	255	CYC	CHB-C1B	5.37	1.50	1.38
4	P	184	CYC	C4B-C3B	-5.36	1.38	1.48
4	Q	184	CYC	CHB-C4A	5.35	1.52	1.40
4	U	184	CYC	C4B-C3B	-5.35	1.38	1.48
4	G	184	CYC	CHB-C1B	5.31	1.50	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	184	CYC	CHB-C1B	5.31	1.50	1.38
4	G	184	CYC	CHB-C4A	5.30	1.52	1.40
5	B	255	BLA	C3D-C2D	5.29	1.48	1.36
4	X	255	CYC	C4B-C3B	-5.28	1.38	1.48
4	H	255	CYC	CHB-C1B	5.26	1.50	1.38
4	X	255	CYC	C1A-C2A	-5.26	1.37	1.45
4	Q	184	CYC	C4B-C3B	-5.26	1.38	1.48
4	R	255	CYC	CHB-C1B	5.24	1.50	1.38
4	O	184	CYC	CHB-C4A	5.23	1.52	1.40
4	L	184	CYC	C4B-C3B	-5.17	1.38	1.48
4	W	184	CYC	CHB-C1B	5.17	1.50	1.38
4	T	184	CYC	C2C-C1C	-5.16	1.47	1.52
5	B	255	BLA	C4D-C3D	5.16	1.53	1.45
4	I	184	CYC	CHB-C1B	5.16	1.50	1.38
4	V	184	CYC	C4B-C3B	-5.15	1.38	1.48
4	H	255	CYC	CHB-C4A	5.14	1.52	1.40
4	F	255	CYC	CHB-C1B	5.13	1.50	1.38
4	N	184	CYC	CHB-C4A	5.13	1.52	1.40
4	D	255	CYC	C2C-C1C	-5.13	1.47	1.52
4	R	184	CYC	CHB-C4A	5.12	1.52	1.40
4	I	184	CYC	CHB-C4A	5.08	1.52	1.40
4	E	184	CYC	CHB-C4A	5.08	1.52	1.40
4	X	184	CYC	C4B-C3B	-5.07	1.38	1.48
4	N	255	CYC	CHB-C4A	5.06	1.52	1.40
4	M	184	CYC	C4B-C3B	-5.02	1.38	1.48
4	R	255	CYC	C4B-C3B	-5.01	1.38	1.48
4	P	184	CYC	C1C-NC	-4.99	1.31	1.37
4	S	184	CYC	CHB-C4A	4.99	1.52	1.40
4	Q	184	CYC	C1A-C2A	-4.99	1.37	1.45
4	H	184	CYC	C4B-C3B	-4.97	1.38	1.48
4	T	184	CYC	C4B-C3B	-4.96	1.38	1.48
4	M	184	CYC	CHB-C1B	4.95	1.49	1.38
4	U	184	CYC	CHB-C1B	4.89	1.49	1.38
4	J	255	CYC	CHB-C4A	4.87	1.51	1.40
4	W	184	CYC	CHB-C4A	4.87	1.51	1.40
4	J	184	CYC	C4B-C3B	-4.86	1.39	1.48
4	O	184	CYC	C1A-C2A	-4.82	1.38	1.45
4	C	184	CYC	CHB-C1B	4.81	1.49	1.38
4	N	184	CYC	C3D-C2D	4.79	1.51	1.37
4	X	255	CYC	OB-C4B	4.75	1.32	1.23
4	D	255	CYC	CHB-C4A	4.75	1.51	1.40
4	T	255	CYC	CHB-C4A	4.75	1.51	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	184	CYC	CHB-C4A	4.73	1.51	1.40
4	N	255	CYC	OB-C4B	4.73	1.32	1.23
4	C	184	CYC	C2C-C1C	-4.66	1.47	1.52
4	D	255	CYC	C4B-C3B	-4.66	1.39	1.48
4	P	184	CYC	C2C-C1C	-4.62	1.48	1.52
4	D	184	CYC	C4B-C3B	-4.61	1.39	1.48
4	V	255	CYC	C4B-C3B	-4.59	1.39	1.48
4	P	255	CYC	C4B-C3B	-4.58	1.39	1.48
4	W	184	CYC	C1B-C2B	-4.58	1.36	1.45
4	L	184	CYC	CHB-C4A	4.56	1.51	1.40
4	P	255	CYC	CHB-C1B	4.53	1.48	1.38
4	H	255	CYC	C4B-C3B	-4.46	1.39	1.48
4	T	184	CYC	CHB-C4A	4.45	1.50	1.40
4	H	184	CYC	CHB-C4A	4.45	1.50	1.40
4	X	184	CYC	OB-C4B	4.45	1.32	1.23
4	N	184	CYC	C4B-C3B	-4.43	1.39	1.48
4	O	184	CYC	C4B-C3B	-4.39	1.39	1.48
4	C	184	CYC	C1B-C2B	-4.38	1.37	1.45
4	L	184	CYC	C1C-NC	-4.37	1.31	1.37
4	H	255	CYC	OB-C4B	4.36	1.31	1.23
5	B	255	BLA	CHD-C1D	4.35	1.50	1.40
4	C	184	CYC	CHB-C4A	4.35	1.50	1.40
4	R	255	CYC	C3D-C2D	4.35	1.50	1.37
4	T	255	CYC	OB-C4B	4.34	1.31	1.23
4	B	184	CYC	C4B-C3B	-4.34	1.40	1.48
4	K	184	CYC	CHB-C4A	4.31	1.50	1.40
4	X	184	CYC	CHB-C1B	4.30	1.48	1.38
4	P	184	CYC	CHB-C4A	4.27	1.50	1.40
5	B	255	BLA	CBB-CAB	4.25	1.51	1.30
4	G	184	CYC	C4B-C3B	-4.23	1.40	1.48
4	U	184	CYC	CHB-C4A	4.22	1.50	1.40
4	V	255	CYC	C1A-C2A	-4.22	1.39	1.45
4	L	255	CYC	CHB-C1B	4.21	1.48	1.38
4	R	255	CYC	CHB-C4A	4.21	1.50	1.40
4	P	184	CYC	C1A-C2A	-4.20	1.39	1.45
4	D	255	CYC	C1B-C2B	-4.18	1.37	1.45
4	R	255	CYC	C2C-C1C	-4.18	1.48	1.52
4	H	184	CYC	C1C-NC	-4.14	1.32	1.37
4	K	184	CYC	CHB-C1B	4.12	1.47	1.38
4	U	184	CYC	C3D-C2D	4.11	1.49	1.37
4	M	184	CYC	CHB-C4A	4.07	1.50	1.40
4	J	184	CYC	CHB-C1B	4.07	1.47	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	184	CYC	C1B-C2B	-4.07	1.37	1.45
4	N	184	CYC	OB-C4B	4.05	1.31	1.23
4	W	184	CYC	C3D-C2D	4.05	1.49	1.37
4	J	184	CYC	CHB-C4A	4.04	1.49	1.40
4	J	184	CYC	C1A-C2A	-4.00	1.39	1.45
4	N	184	CYC	C1A-C2A	-3.99	1.39	1.45
4	H	255	CYC	C1B-C2B	-3.98	1.37	1.45
4	N	255	CYC	C4B-C3B	-3.98	1.40	1.48
4	N	255	CYC	C3D-C2D	3.97	1.49	1.37
4	B	184	CYC	CHB-C1B	3.97	1.47	1.38
5	B	255	BLA	CBC-CAC	3.96	1.49	1.30
4	M	184	CYC	C3D-C2D	3.95	1.49	1.37
4	P	255	CYC	CHB-C4A	3.94	1.49	1.40
4	I	184	CYC	C1A-C2A	-3.94	1.39	1.45
4	L	255	CYC	CHB-C4A	3.94	1.49	1.40
4	X	184	CYC	C1C-NC	-3.93	1.32	1.37
4	H	184	CYC	C2C-C1C	-3.91	1.48	1.52
4	D	184	CYC	C3D-C2D	3.90	1.49	1.37
5	B	255	BLA	C4C-NC	-3.89	1.31	1.37
4	I	184	CYC	OB-C4B	3.89	1.31	1.23
4	C	184	CYC	C3D-C2D	3.88	1.49	1.37
4	V	184	CYC	C3D-C2D	3.88	1.49	1.37
4	T	184	CYC	OB-C4B	3.87	1.31	1.23
4	X	184	CYC	CHB-C4A	3.87	1.49	1.40
4	E	184	CYC	C1A-C2A	-3.87	1.39	1.45
4	C	184	CYC	C1C-NC	-3.86	1.32	1.37
4	F	184	CYC	C4B-C3B	-3.83	1.41	1.48
4	M	184	CYC	C1A-C2A	-3.81	1.39	1.45
4	H	255	CYC	C1C-NC	-3.81	1.32	1.37
4	F	255	CYC	C1B-C2B	-3.77	1.38	1.45
4	F	255	CYC	C3D-C2D	3.75	1.48	1.37
4	F	255	CYC	CHB-C4A	3.74	1.49	1.40
4	L	184	CYC	C2C-C1C	-3.73	1.48	1.52
4	J	255	CYC	OB-C4B	3.73	1.30	1.23
4	D	255	CYC	C3D-C2D	3.71	1.48	1.37
4	G	184	CYC	C1A-NA	-3.70	1.30	1.38
4	S	184	CYC	C1B-C2B	-3.70	1.38	1.45
4	S	184	CYC	C3D-C2D	3.68	1.48	1.37
4	V	255	CYC	C3B-C2B	3.67	1.44	1.36
4	K	184	CYC	C3D-C2D	3.67	1.48	1.37
4	R	184	CYC	C4B-C3B	-3.66	1.41	1.48
4	L	255	CYC	C1B-C2B	-3.65	1.38	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	184	CYC	OB-C4B	3.65	1.30	1.23
4	B	184	CYC	CHB-C4A	3.65	1.49	1.40
4	S	184	CYC	C1A-C2A	-3.65	1.39	1.45
4	L	184	CYC	C3D-C2D	3.65	1.48	1.37
4	L	255	CYC	C3D-C2D	3.65	1.48	1.37
4	R	184	CYC	C1C-NC	-3.64	1.32	1.37
4	M	184	CYC	C2C-C1C	-3.64	1.48	1.52
4	H	184	CYC	C3D-C2D	3.64	1.48	1.37
4	F	255	CYC	C1A-C2A	-3.63	1.39	1.45
4	J	184	CYC	C1C-NC	-3.61	1.32	1.37
4	X	184	CYC	C4D-CHA	3.60	1.55	1.41
4	J	255	CYC	C4D-CHA	3.59	1.55	1.41
4	A	184	CYC	C3D-C2D	3.59	1.48	1.37
4	H	255	CYC	C2C-C1C	-3.55	1.48	1.52
4	R	184	CYC	C1A-C2A	-3.55	1.40	1.45
4	P	184	CYC	C3D-C2D	3.55	1.48	1.37
4	H	255	CYC	C1A-C2A	-3.54	1.40	1.45
4	R	184	CYC	C4D-CHA	3.54	1.54	1.41
4	U	184	CYC	C1C-NC	-3.53	1.33	1.37
4	H	184	CYC	C4D-CHA	3.53	1.54	1.41
4	T	255	CYC	C3D-C2D	3.50	1.48	1.37
4	V	255	CYC	CAD-C3D	-3.49	1.46	1.52
4	R	184	CYC	C1D-CHD	3.47	1.54	1.41
4	F	184	CYC	C1C-NC	-3.47	1.33	1.37
4	P	255	CYC	C1B-C2B	-3.46	1.38	1.45
4	U	184	CYC	C1A-C2A	-3.46	1.40	1.45
4	L	184	CYC	OB-C4B	3.44	1.30	1.23
4	R	184	CYC	C3D-C2D	3.44	1.47	1.37
4	A	184	CYC	OB-C4B	3.41	1.30	1.23
4	B	184	CYC	C1C-NC	-3.41	1.33	1.37
4	K	184	CYC	OB-C4B	3.40	1.30	1.23
4	E	184	CYC	C1A-NA	-3.39	1.31	1.38
4	J	255	CYC	C1B-C2B	-3.38	1.39	1.45
4	E	184	CYC	C3D-C2D	3.36	1.47	1.37
4	I	184	CYC	C3D-C2D	3.35	1.47	1.37
4	P	255	CYC	C3D-C2D	3.34	1.47	1.37
4	V	255	CYC	C1C-NC	-3.34	1.33	1.37
4	N	255	CYC	C1C-NC	-3.34	1.33	1.37
4	K	184	CYC	C1A-C2A	-3.32	1.40	1.45
4	S	184	CYC	C4D-CHA	3.31	1.54	1.41
4	L	255	CYC	C2C-C1C	-3.28	1.49	1.52
4	U	184	CYC	C4D-CHA	3.25	1.53	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	255	CYC	OB-C4B	3.25	1.29	1.23
4	D	184	CYC	C1D-CHD	3.23	1.53	1.41
4	U	184	CYC	C1D-CHD	3.22	1.53	1.41
4	P	255	CYC	C4A-C3A	3.21	1.52	1.45
4	L	184	CYC	C4A-C3A	3.21	1.52	1.45
4	X	255	CYC	C3D-C2D	3.20	1.47	1.37
4	Q	184	CYC	C4C-NC	-3.19	1.30	1.37
4	Q	184	CYC	C1B-C2B	-3.19	1.39	1.45
5	B	255	BLA	OB-C4B	3.19	1.29	1.23
4	B	184	CYC	C4D-CHA	3.18	1.53	1.41
4	R	184	CYC	C2C-C1C	-3.18	1.49	1.52
4	D	184	CYC	OB-C4B	3.17	1.29	1.23
4	F	184	CYC	C4C-NC	-3.16	1.30	1.37
4	H	184	CYC	C4C-NC	-3.16	1.30	1.37
4	N	255	CYC	C1A-C2A	-3.15	1.40	1.45
4	J	184	CYC	C3D-C2D	3.15	1.47	1.37
4	I	184	CYC	C4D-CHA	3.14	1.53	1.41
4	G	184	CYC	C3D-C2D	3.13	1.46	1.37
4	J	184	CYC	C1B-C2B	-3.12	1.39	1.45
4	H	255	CYC	C3D-C2D	3.12	1.46	1.37
4	T	184	CYC	C3D-C2D	3.11	1.46	1.37
4	X	184	CYC	C1D-CHD	3.11	1.53	1.41
4	O	184	CYC	C3D-C2D	3.09	1.46	1.37
4	P	184	CYC	C4C-NC	-3.08	1.30	1.37
4	F	255	CYC	C4D-CHA	3.08	1.53	1.41
4	T	255	CYC	C1A-C2A	-3.07	1.40	1.45
4	M	184	CYC	C1D-CHD	3.07	1.53	1.41
4	R	184	CYC	C4C-NC	-3.06	1.30	1.37
4	P	184	CYC	C4D-CHA	3.06	1.53	1.41
4	B	184	CYC	C2C-C1C	-3.05	1.49	1.52
4	C	184	CYC	C1D-CHD	3.05	1.53	1.41
4	K	184	CYC	C4D-CHA	3.04	1.52	1.41
4	F	184	CYC	C4D-CHA	3.04	1.52	1.41
4	D	255	CYC	C1D-CHD	3.02	1.52	1.41
4	D	184	CYC	C4D-CHA	3.00	1.52	1.41
4	B	184	CYC	C1B-C2B	-3.00	1.39	1.45
4	L	255	CYC	C1C-NC	-2.99	1.33	1.37
4	P	255	CYC	OB-C4B	2.98	1.29	1.23
4	V	184	CYC	C1C-NC	-2.98	1.33	1.37
4	L	255	CYC	C4C-NC	-2.97	1.31	1.37
4	W	184	CYC	OB-C4B	2.97	1.29	1.23
4	A	184	CYC	C1C-NC	-2.97	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	184	CYC	C1A-NA	-2.95	1.32	1.38
4	X	184	CYC	C3D-C2D	2.95	1.46	1.37
4	Q	184	CYC	C3D-C2D	2.94	1.46	1.37
4	A	184	CYC	C1A-C2A	-2.94	1.41	1.45
4	V	184	CYC	C1A-C2A	-2.94	1.41	1.45
4	N	184	CYC	C2C-C1C	-2.93	1.49	1.52
4	X	184	CYC	C2C-C1C	-2.93	1.49	1.52
4	J	255	CYC	C1A-C2A	-2.93	1.41	1.45
4	K	184	CYC	C1D-CHD	2.93	1.52	1.41
4	R	255	CYC	OB-C4B	2.92	1.29	1.23
4	N	255	CYC	C4C-NC	-2.91	1.31	1.37
4	M	184	CYC	C4D-CHA	2.91	1.52	1.41
4	M	184	CYC	OB-C4B	2.89	1.29	1.23
4	J	184	CYC	C4D-CHA	2.89	1.52	1.41
4	R	184	CYC	OB-C4B	2.89	1.29	1.23
4	G	184	CYC	OB-C4B	2.87	1.29	1.23
4	N	184	CYC	C4D-CHA	2.86	1.52	1.41
4	V	255	CYC	C4D-CHA	2.85	1.52	1.41
4	J	255	CYC	C2C-C1C	-2.84	1.49	1.52
4	T	255	CYC	C4C-NC	-2.84	1.31	1.37
4	I	184	CYC	C1B-C2B	-2.84	1.40	1.45
4	V	184	CYC	C1D-CHD	2.84	1.52	1.41
4	B	184	CYC	OB-C4B	2.84	1.29	1.23
4	V	184	CYC	C4B-NB	-2.83	1.32	1.38
4	J	184	CYC	C4C-NC	-2.82	1.31	1.37
4	L	184	CYC	C1A-C2A	-2.82	1.41	1.45
4	M	184	CYC	C1B-C2B	-2.82	1.40	1.45
4	D	255	CYC	OB-C4B	2.81	1.28	1.23
4	L	184	CYC	C4D-CHA	2.80	1.52	1.41
4	E	184	CYC	C4D-CHA	2.80	1.52	1.41
4	G	184	CYC	C1C-NC	-2.79	1.34	1.37
4	N	255	CYC	C4D-CHA	2.78	1.51	1.41
4	J	184	CYC	C1A-NA	-2.78	1.32	1.38
4	D	255	CYC	C1A-C2A	-2.77	1.41	1.45
4	F	184	CYC	C1D-CHD	2.77	1.51	1.41
4	B	184	CYC	C3D-C2D	2.77	1.45	1.37
4	D	184	CYC	C2A-C3A	2.77	1.42	1.36
5	B	255	BLA	C1A-CHA	2.76	1.51	1.41
4	V	255	CYC	C1B-C2B	-2.74	1.40	1.45
4	U	184	CYC	C2C-C1C	-2.74	1.49	1.52
4	H	184	CYC	C1D-CHD	2.74	1.51	1.41
4	I	184	CYC	C3C-C4C	2.73	1.54	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	184	CYC	C3B-C2B	2.73	1.42	1.36
4	N	184	CYC	C1D-CHD	2.72	1.51	1.41
4	U	184	CYC	C1A-NA	-2.71	1.32	1.38
4	X	184	CYC	C1B-C2B	-2.71	1.40	1.45
4	C	184	CYC	C4B-NB	-2.71	1.32	1.38
4	V	255	CYC	C3D-C2D	2.71	1.45	1.37
4	P	255	CYC	C1A-NA	-2.69	1.32	1.38
4	F	184	CYC	OB-C4B	2.69	1.28	1.23
4	E	184	CYC	C1D-CHD	2.68	1.51	1.41
4	M	184	CYC	C3B-C2B	2.68	1.42	1.36
4	V	255	CYC	C1A-NA	-2.66	1.32	1.38
4	F	255	CYC	C1B-NB	-2.66	1.33	1.37
4	T	184	CYC	C1A-C2A	-2.65	1.41	1.45
4	V	184	CYC	C4A-C3A	2.63	1.51	1.45
4	H	255	CYC	C1D-CHD	2.62	1.51	1.41
4	S	184	CYC	C1C-NC	-2.60	1.34	1.37
4	H	255	CYC	C4C-NC	-2.60	1.31	1.37
4	N	184	CYC	C1B-C2B	-2.60	1.40	1.45
4	V	184	CYC	OB-C4B	2.60	1.28	1.23
4	E	184	CYC	C1B-C2B	-2.60	1.40	1.45
4	J	184	CYC	C2C-C1C	-2.58	1.49	1.52
4	X	184	CYC	C4C-NC	-2.58	1.31	1.37
4	J	255	CYC	C4C-NC	-2.58	1.31	1.37
4	R	255	CYC	C1B-C2B	-2.58	1.40	1.45
4	J	255	CYC	C1C-NC	-2.57	1.34	1.37
4	R	255	CYC	C4D-CHA	2.57	1.51	1.41
4	S	184	CYC	C4A-C3A	2.56	1.51	1.45
4	T	184	CYC	C1C-NC	-2.55	1.34	1.37
4	N	255	CYC	C1D-CHD	2.54	1.51	1.41
4	O	184	CYC	C2C-C1C	-2.53	1.49	1.52
4	T	184	CYC	C4A-C3A	2.53	1.51	1.45
5	B	255	BLA	C1C-NC	-2.53	1.32	1.38
4	G	184	CYC	C4B-NB	-2.53	1.32	1.38
4	Q	184	CYC	C2C-C1C	-2.52	1.49	1.52
4	T	255	CYC	C1B-C2B	-2.52	1.40	1.45
4	S	184	CYC	C1D-CHD	2.51	1.50	1.41
4	O	184	CYC	OB-C4B	2.51	1.28	1.23
4	A	184	CYC	C4D-CHA	2.51	1.50	1.41
4	T	184	CYC	C4D-CHA	2.50	1.50	1.41
4	D	184	CYC	C1A-C2A	-2.50	1.41	1.45
4	F	255	CYC	C4B-NB	-2.50	1.32	1.38
4	D	184	CYC	C4A-C3A	2.49	1.51	1.45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	255	CYC	C3D-C2D	2.48	1.45	1.37
4	Q	184	CYC	C4B-NB	-2.48	1.32	1.38
4	T	255	CYC	C4A-C3A	2.47	1.51	1.45
4	G	184	CYC	C1D-CHD	2.47	1.50	1.41
4	N	184	CYC	C4C-NC	-2.47	1.32	1.37
5	B	255	BLA	C3B-C4B	-2.45	1.40	1.47
5	B	255	BLA	C4A-CHB	2.45	1.50	1.41
4	J	255	CYC	CMB-C2B	-2.44	1.45	1.50
4	O	184	CYC	C1D-CHD	2.44	1.50	1.41
4	N	255	CYC	CAD-C3D	2.43	1.55	1.52
4	J	255	CYC	C3B-C2B	-2.42	1.31	1.36
4	Q	184	CYC	C4A-C3A	2.41	1.51	1.45
4	F	184	CYC	C3D-C2D	2.41	1.44	1.37
4	E	184	CYC	C1C-NC	-2.41	1.34	1.37
4	Q	184	CYC	C1D-CHD	2.41	1.50	1.41
4	U	184	CYC	C4B-NB	-2.39	1.32	1.38
4	S	184	CYC	C4C-NC	-2.39	1.32	1.37
4	I	184	CYC	C4A-C3A	2.38	1.50	1.45
4	W	184	CYC	C1A-NA	-2.37	1.33	1.38
4	W	184	CYC	C1D-CHD	2.37	1.50	1.41
4	A	184	CYC	C4C-NC	-2.37	1.32	1.37
4	Q	184	CYC	C1C-NC	-2.36	1.34	1.37
4	H	184	CYC	C1A-C2A	-2.36	1.42	1.45
4	B	184	CYC	C1D-CHD	2.36	1.50	1.41
4	C	184	CYC	C4D-CHA	2.36	1.50	1.41
4	S	184	CYC	OB-C4B	2.36	1.28	1.23
4	G	184	CYC	C1B-C2B	-2.35	1.40	1.45
4	F	184	CYC	C4B-NB	-2.34	1.33	1.38
4	L	255	CYC	C1D-CHD	2.34	1.50	1.41
4	A	184	CYC	C4B-C3B	-2.33	1.43	1.48
4	V	184	CYC	C4D-CHA	2.33	1.50	1.41
4	K	184	CYC	C4C-NC	-2.33	1.32	1.37
4	N	255	CYC	C2A-C3A	2.32	1.41	1.36
4	W	184	CYC	C4D-CHA	2.31	1.50	1.41
4	M	184	CYC	C3C-C4C	2.31	1.54	1.50
4	T	184	CYC	C1D-CHD	2.31	1.50	1.41
4	D	255	CYC	C4D-CHA	2.31	1.50	1.41
4	W	184	CYC	C4C-NC	-2.30	1.32	1.37
4	D	255	CYC	C1A-NA	-2.29	1.33	1.38
4	F	184	CYC	C3C-C4C	-2.28	1.47	1.50
4	J	184	CYC	C1D-CHD	2.28	1.50	1.41
4	S	184	CYC	C2C-C1C	2.27	1.54	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	184	CYC	C1B-C2B	-2.26	1.41	1.45
4	C	184	CYC	C4A-C3A	2.26	1.50	1.45
4	J	255	CYC	C1A-NA	-2.25	1.33	1.38
4	N	184	CYC	C4A-C3A	2.25	1.50	1.45
4	V	255	CYC	C2C-C1C	-2.24	1.50	1.52
4	F	255	CYC	C4A-NA	-2.23	1.31	1.36
4	P	255	CYC	C1D-CHD	2.23	1.49	1.41
4	P	184	CYC	C1D-CHD	2.22	1.49	1.41
4	P	255	CYC	C1A-C2A	-2.22	1.42	1.45
4	T	255	CYC	C1C-NC	-2.22	1.34	1.37
4	X	184	CYC	C1A-C2A	-2.21	1.42	1.45
4	L	184	CYC	C4C-NC	-2.21	1.32	1.37
4	F	255	CYC	CAD-C3D	-2.20	1.48	1.52
4	N	184	CYC	C3B-C2B	2.19	1.41	1.36
4	X	255	CYC	C4A-C3A	2.19	1.50	1.45
4	T	184	CYC	C4C-NC	-2.18	1.32	1.37
4	H	255	CYC	C4D-CHA	2.18	1.49	1.41
4	F	255	CYC	C1D-CHD	2.17	1.49	1.41
4	H	184	CYC	OB-C4B	2.17	1.27	1.23
4	O	184	CYC	C4D-CHA	2.17	1.49	1.41
4	F	184	CYC	C2C-C1C	-2.16	1.50	1.52
4	E	184	CYC	C4B-NB	-2.16	1.33	1.38
4	K	184	CYC	C1C-NC	-2.16	1.34	1.37
4	U	184	CYC	C4A-C3A	2.15	1.50	1.45
4	F	184	CYC	C1A-C2A	-2.15	1.42	1.45
4	L	255	CYC	C4B-NB	-2.15	1.33	1.38
4	P	255	CYC	C1C-NC	-2.14	1.34	1.37
4	X	255	CYC	C1D-CHD	2.14	1.49	1.41
4	U	184	CYC	CAC-C3C	-2.14	1.49	1.54
4	T	184	CYC	CAA-C2A	2.13	1.56	1.51
4	G	184	CYC	C4D-CHA	2.12	1.49	1.41
4	A	184	CYC	CAD-C3D	-2.12	1.48	1.52
4	X	255	CYC	C1B-C2B	-2.11	1.41	1.45
4	W	184	CYC	C3C-C4C	2.10	1.53	1.50
4	V	255	CYC	C4C-NC	-2.10	1.32	1.37
4	T	255	CYC	C3B-C2B	2.10	1.41	1.36
4	V	255	CYC	C4B-NB	-2.09	1.33	1.38
4	P	184	CYC	CAD-C3D	-2.08	1.49	1.52
4	I	184	CYC	C1D-CHD	2.08	1.49	1.41
4	T	255	CYC	C4D-CHA	2.08	1.49	1.41
4	H	255	CYC	C1A-NA	-2.07	1.34	1.38
4	V	184	CYC	C4C-NC	-2.07	1.33	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	255	CYC	C1A-C2A	-2.07	1.42	1.45
4	D	255	CYC	C1C-NC	-2.06	1.34	1.37
4	W	184	CYC	C1B-NB	-2.06	1.34	1.37
4	T	255	CYC	CHD-C4C	-2.05	1.32	1.38
4	X	255	CYC	C4D-CHA	2.05	1.49	1.41
4	Q	184	CYC	C4D-CHA	2.05	1.49	1.41
4	A	184	CYC	C1D-CHD	2.04	1.49	1.41
4	G	184	CYC	C2C-C1C	-2.03	1.50	1.52
4	V	255	CYC	CMA-C3A	2.02	1.55	1.50
4	A	184	CYC	C4A-C3A	2.02	1.50	1.45
4	G	184	CYC	C4C-NC	-2.01	1.33	1.37
4	L	255	CYC	C3B-C2B	2.01	1.41	1.36
4	D	184	CYC	C1C-NC	-2.00	1.35	1.37
4	W	184	CYC	C4B-NB	-2.00	1.33	1.38
4	V	184	CYC	C1B-C2B	-2.00	1.41	1.45

All (609) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	255	CYC	C3B-C4B-NB	12.86	117.17	106.78
4	J	184	CYC	C3B-C4B-NB	12.74	117.07	106.78
4	H	184	CYC	C3B-C4B-NB	12.46	116.84	106.78
4	S	184	CYC	OB-C4B-C3B	-12.43	114.55	128.04
4	E	184	CYC	C3B-C4B-NB	11.68	116.21	106.78
4	U	184	CYC	C3B-C4B-NB	11.32	115.92	106.78
4	S	184	CYC	C3B-C4B-NB	11.20	115.82	106.78
4	M	184	CYC	OC-C1C-C2C	-10.95	117.47	126.17
4	R	255	CYC	C3B-C4B-NB	10.93	115.61	106.78
4	D	184	CYC	C3B-C4B-NB	10.88	115.57	106.78
4	G	184	CYC	C3B-C4B-NB	10.87	115.56	106.78
4	V	184	CYC	C4D-CHA-C1A	-10.78	115.93	128.81
4	C	184	CYC	C3B-C4B-NB	10.57	115.32	106.78
4	R	184	CYC	C3B-C4B-NB	10.43	115.20	106.78
4	K	184	CYC	C3B-C4B-NB	10.32	115.11	106.78
4	B	184	CYC	C3B-C4B-NB	10.19	115.01	106.78
4	P	184	CYC	C3B-C4B-NB	9.91	114.78	106.78
4	L	184	CYC	C3B-C4B-NB	9.89	114.77	106.78
4	O	184	CYC	C3B-C4B-NB	9.77	114.67	106.78
4	P	255	CYC	C3B-C4B-NB	9.73	114.64	106.78
4	T	184	CYC	OC-C1C-C2C	-9.71	118.45	126.17
4	T	184	CYC	C3B-C4B-NB	9.49	114.44	106.78
4	X	255	CYC	C3B-C4B-NB	9.40	114.37	106.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	184	CYC	C3B-C4B-NB	9.35	114.33	106.78
4	J	255	CYC	C3B-C4B-NB	9.23	114.23	106.78
4	Q	184	CYC	C4D-CHA-C1A	-9.17	117.85	128.81
4	H	255	CYC	C3B-C4B-NB	9.14	114.16	106.78
4	W	184	CYC	C3B-C4B-NB	9.00	114.05	106.78
4	F	184	CYC	C3B-C4B-NB	8.98	114.03	106.78
4	D	255	CYC	C3B-C4B-NB	8.93	113.99	106.78
4	R	184	CYC	CAB-C3B-C4B	8.93	135.48	121.38
4	N	255	CYC	C3B-C4B-NB	8.72	113.82	106.78
4	M	184	CYC	C3B-C4B-NB	8.69	113.80	106.78
5	B	255	BLA	C1A-CHA-C4D	-8.61	118.52	128.81
4	X	184	CYC	C3B-C4B-NB	8.57	113.70	106.78
4	Q	184	CYC	C3B-C4B-NB	8.57	113.70	106.78
4	V	255	CYC	CAA-CBA-CGA	-8.44	98.51	112.67
4	L	255	CYC	C3B-C4B-NB	8.42	113.58	106.78
4	F	255	CYC	C3B-C4B-NB	8.00	113.24	106.78
4	I	184	CYC	C3B-C4B-NB	7.93	113.19	106.78
4	J	184	CYC	CAA-CBA-CGA	-7.86	99.49	112.67
4	K	184	CYC	OB-C4B-C3B	-7.75	119.62	128.04
4	J	255	CYC	OB-C4B-C3B	-7.73	119.65	128.04
4	L	255	CYC	C4D-CHA-C1A	-7.64	119.69	128.81
4	I	184	CYC	OB-C4B-C3B	-7.62	119.77	128.04
5	B	255	BLA	C3B-C4B-NB	7.61	114.79	106.19
4	R	255	CYC	CAB-C3B-C4B	7.53	133.27	121.38
4	N	184	CYC	C3B-C4B-NB	7.46	112.80	106.78
4	A	184	CYC	C3B-C4B-NB	7.41	112.77	106.78
4	T	255	CYC	C4D-CHA-C1A	-7.35	120.03	128.81
4	O	184	CYC	OC-C1C-C2C	-7.32	120.35	126.17
4	R	255	CYC	OB-C4B-C3B	-7.26	120.16	128.04
4	A	184	CYC	CAB-C3B-C4B	7.24	132.81	121.38
4	H	184	CYC	OB-C4B-C3B	-7.14	120.29	128.04
4	X	255	CYC	OB-C4B-C3B	-7.00	120.44	128.04
4	D	184	CYC	CBD-CAD-C3D	6.97	125.33	112.49
4	R	255	CYC	OC-C1C-C2C	-6.92	120.67	126.17
4	J	184	CYC	CAB-C3B-C4B	6.85	132.19	121.38
4	H	184	CYC	C1B-NB-C4B	-6.77	102.04	110.67
4	B	184	CYC	C1B-NB-C4B	-6.77	102.05	110.67
4	P	255	CYC	OB-C4B-C3B	-6.70	120.77	128.04
4	V	255	CYC	C1B-NB-C4B	-6.51	102.38	110.67
4	E	184	CYC	OC-C1C-C2C	-6.48	121.02	126.17
4	F	255	CYC	C4D-CHA-C1A	-6.47	121.08	128.81
4	H	255	CYC	CAB-C3B-C4B	6.46	131.57	121.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	255	CYC	CAB-C3B-C4B	6.45	131.56	121.38
4	J	255	CYC	C1B-NB-C4B	-6.42	102.49	110.67
4	K	184	CYC	C1B-NB-C4B	-6.40	102.52	110.67
4	U	184	CYC	C1B-NB-C4B	-6.38	102.55	110.67
4	J	184	CYC	C1B-NB-C4B	-6.35	102.58	110.67
4	U	184	CYC	CAB-C3B-C4B	6.30	131.33	121.38
5	B	255	BLA	C1B-NB-C4B	-6.27	102.69	110.67
5	B	255	BLA	CAC-C3C-C4C	-6.25	105.42	123.54
4	J	255	CYC	CHA-C1A-NA	-6.24	120.17	128.83
4	W	184	CYC	C4D-CHA-C1A	-6.24	121.36	128.81
4	E	184	CYC	C1B-NB-C4B	-6.23	102.73	110.67
4	S	184	CYC	C4D-CHA-C1A	-6.23	121.37	128.81
4	N	184	CYC	C4D-CHA-C1A	-6.19	121.42	128.81
4	N	255	CYC	C4D-CHA-C1A	-6.18	121.42	128.81
4	D	255	CYC	C4D-CHA-C1A	-6.18	121.42	128.81
4	U	184	CYC	C1B-CHB-C4A	-6.15	113.07	128.08
4	H	184	CYC	CAB-C3B-C4B	6.13	131.06	121.38
4	V	255	CYC	OB-C4B-C3B	-6.11	121.41	128.04
4	I	184	CYC	C2C-C1C-NC	6.10	113.53	108.27
4	D	184	CYC	C2C-C1C-NC	6.08	113.51	108.27
4	P	184	CYC	C2C-C1C-NC	6.05	113.49	108.27
4	A	184	CYC	OC-C1C-C2C	-6.04	121.37	126.17
4	T	255	CYC	C3B-C4B-NB	5.95	111.58	106.78
4	N	184	CYC	CBD-CAD-C3D	5.93	123.42	112.49
4	D	184	CYC	OC-C1C-C2C	-5.89	121.49	126.17
4	I	184	CYC	CBD-CAD-C3D	-5.84	101.71	112.49
4	N	255	CYC	OB-C4B-C3B	-5.84	121.70	128.04
4	L	184	CYC	CBD-CAD-C3D	5.83	123.24	112.49
4	N	184	CYC	OC-C1C-C2C	-5.83	121.54	126.17
4	F	184	CYC	CAB-C3B-C4B	5.81	130.55	121.38
4	R	255	CYC	C1B-NB-C4B	-5.77	103.32	110.67
4	L	184	CYC	CMA-C3A-C4A	5.77	133.95	125.06
4	X	184	CYC	C1B-NB-C4B	-5.73	103.37	110.67
4	P	184	CYC	OB-C4B-C3B	-5.73	121.83	128.04
4	B	184	CYC	OB-C4B-C3B	-5.70	121.86	128.04
4	P	255	CYC	C1B-NB-C4B	-5.70	103.42	110.67
4	R	184	CYC	C1B-NB-C4B	-5.69	103.42	110.67
4	H	255	CYC	C1B-NB-C4B	-5.69	103.43	110.67
4	F	255	CYC	CBD-CAD-C3D	-5.69	102.00	112.49
4	C	184	CYC	C1B-NB-C4B	-5.67	103.45	110.67
4	X	255	CYC	C4D-CHA-C1A	-5.67	122.04	128.81
4	J	255	CYC	CBB-CAB-C3B	-5.67	96.81	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	184	CYC	C4D-CHA-C1A	-5.65	122.06	128.81
4	V	184	CYC	CAD-CBD-CGD	-5.65	103.19	112.67
4	L	255	CYC	OB-C4B-C3B	-5.65	121.91	128.04
4	L	184	CYC	CAD-CBD-CGD	-5.65	103.20	112.67
4	M	184	CYC	CAC-C3C-C4C	5.64	127.17	112.67
4	X	184	CYC	OB-C4B-C3B	-5.62	121.94	128.04
4	J	184	CYC	OC-C1C-C2C	-5.61	121.71	126.17
4	T	184	CYC	OB-C4B-C3B	-5.59	121.97	128.04
4	A	184	CYC	CBD-CAD-C3D	-5.59	102.18	112.49
4	I	184	CYC	C4D-CHA-C1A	-5.58	122.14	128.81
4	F	184	CYC	CMB-C2B-C1B	5.58	131.13	124.17
4	G	184	CYC	C1B-NB-C4B	-5.54	103.62	110.67
4	I	184	CYC	OC-C1C-C2C	-5.54	121.77	126.17
4	D	184	CYC	C4D-CHA-C1A	-5.53	122.20	128.81
4	M	184	CYC	C1B-CHB-C4A	-5.47	114.71	128.08
4	V	184	CYC	CAB-C3B-C4B	5.46	130.01	121.38
4	T	184	CYC	C2C-C1C-NC	5.46	112.98	108.27
4	D	184	CYC	C1B-NB-C4B	-5.44	103.75	110.67
4	J	184	CYC	C2C-C1C-NC	5.42	112.94	108.27
4	T	255	CYC	OB-C4B-C3B	-5.36	122.23	128.04
4	L	184	CYC	C1B-NB-C4B	-5.29	103.93	110.67
4	E	184	CYC	CAD-CBD-CGD	5.28	121.53	112.67
4	O	184	CYC	C2C-C1C-NC	5.26	112.81	108.27
4	P	255	CYC	C1B-CHB-C4A	-5.25	115.25	128.08
4	N	255	CYC	CBD-CAD-C3D	5.24	122.15	112.49
4	S	184	CYC	CAD-CBD-CGD	-5.21	103.93	112.67
4	P	184	CYC	C1B-CHB-C4A	-5.18	115.42	128.08
4	C	184	CYC	C4D-CHA-C1A	-5.15	122.65	128.81
4	V	255	CYC	CBD-CAD-C3D	-5.12	103.04	112.49
4	S	184	CYC	C1B-NB-C4B	-5.12	104.15	110.67
4	J	255	CYC	CHB-C4A-C3A	5.11	138.04	124.90
4	L	184	CYC	OB-C4B-C3B	-5.11	122.50	128.04
4	H	184	CYC	CHD-C4C-NC	-5.10	119.14	125.20
4	B	184	CYC	C2C-C1C-NC	5.10	112.67	108.27
4	A	184	CYC	C2C-C1C-NC	5.06	112.63	108.27
4	A	184	CYC	C4D-CHA-C1A	-5.00	122.84	128.81
4	T	184	CYC	CAD-CBD-CGD	-5.00	104.29	112.67
4	H	255	CYC	C4D-CHA-C1A	-4.99	122.85	128.81
4	B	184	CYC	CAB-C3B-C4B	4.95	129.21	121.38
4	X	184	CYC	CHD-C4C-NC	-4.94	119.33	125.20
4	C	184	CYC	OC-C1C-C2C	-4.94	122.25	126.17
4	L	255	CYC	CMA-C3A-C4A	4.93	132.65	125.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	255	CYC	CAB-C3B-C4B	4.92	129.14	121.38
5	B	255	BLA	CAA-CBA-CGA	-4.91	104.43	112.67
4	V	184	CYC	C2C-C1C-NC	4.89	112.49	108.27
4	T	184	CYC	C4D-CHA-C1A	-4.85	123.01	128.81
4	E	184	CYC	OB-C4B-C3B	-4.82	122.81	128.04
4	O	184	CYC	CAB-C3B-C4B	4.82	128.99	121.38
4	J	184	CYC	CAD-CBD-CGD	-4.81	104.60	112.67
4	D	184	CYC	OB-C4B-C3B	-4.80	122.83	128.04
4	E	184	CYC	C4D-CHA-C1A	-4.80	123.08	128.81
4	C	184	CYC	CMA-C3A-C4A	4.78	132.42	125.06
4	N	184	CYC	C1B-CHB-C4A	-4.77	116.43	128.08
4	T	184	CYC	C1B-CHB-C4A	-4.76	116.45	128.08
4	F	184	CYC	C1B-NB-C4B	-4.73	104.65	110.67
4	P	184	CYC	CAA-CBA-CGA	-4.72	104.75	112.67
5	B	255	BLA	CMC-C2C-C1C	-4.71	110.32	121.39
4	Q	184	CYC	CAB-C3B-C4B	4.70	128.81	121.38
4	F	255	CYC	CHB-C4A-C3A	4.70	136.99	124.90
4	P	255	CYC	OC-C1C-C2C	-4.68	122.45	126.17
4	P	184	CYC	C4D-CHA-C1A	-4.68	123.21	128.81
4	W	184	CYC	CAB-C3B-C4B	4.67	128.75	121.38
4	M	184	CYC	OC-C1C-NC	4.66	130.58	124.94
4	C	184	CYC	C2C-C1C-NC	4.64	112.28	108.27
4	V	255	CYC	C1B-CHB-C4A	-4.64	116.75	128.08
4	C	184	CYC	C1B-CHB-C4A	-4.63	116.76	128.08
4	N	255	CYC	C1B-NB-C4B	-4.59	104.82	110.67
4	L	184	CYC	CAB-C3B-C4B	4.58	128.62	121.38
4	P	255	CYC	CHB-C1B-C2B	-4.58	117.87	126.95
4	X	255	CYC	C1B-NB-C4B	-4.58	104.84	110.67
4	T	184	CYC	C1B-NB-C4B	-4.56	104.86	110.67
4	C	184	CYC	CAB-C3B-C4B	4.55	128.56	121.38
4	D	255	CYC	C1B-CHB-C4A	-4.54	116.99	128.08
4	S	184	CYC	CHD-C4C-NC	-4.52	119.83	125.20
4	P	184	CYC	C1B-NB-C4B	-4.49	104.95	110.67
4	M	184	CYC	C1B-NB-C4B	-4.48	104.97	110.67
4	I	184	CYC	CMB-C2B-C1B	4.48	129.76	124.17
4	T	184	CYC	CMB-C2B-C1B	4.45	129.73	124.17
4	E	184	CYC	CAB-C3B-C4B	4.45	128.41	121.38
4	P	255	CYC	CHB-C4A-NA	-4.45	115.62	124.93
4	T	255	CYC	CMA-C3A-C4A	4.44	131.91	125.06
4	F	255	CYC	CAD-CBD-CGD	4.42	120.08	112.67
4	B	184	CYC	OC-C1C-C2C	-4.41	122.67	126.17
4	T	184	CYC	CBD-CAD-C3D	4.41	120.61	112.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	255	CYC	C1B-NB-C4B	-4.41	105.06	110.67
4	B	184	CYC	CAD-CBD-CGD	-4.39	105.30	112.67
4	H	184	CYC	C2C-C1C-NC	4.37	112.04	108.27
4	W	184	CYC	OB-C4B-C3B	-4.37	123.30	128.04
4	W	184	CYC	C1B-NB-C4B	-4.34	105.14	110.67
4	B	184	CYC	C1B-CHB-C4A	-4.34	117.47	128.08
4	P	184	CYC	CAB-C3B-C4B	4.33	128.22	121.38
4	J	255	CYC	OC-C1C-C2C	-4.33	122.73	126.17
4	B	184	CYC	C4D-CHA-C1A	-4.31	123.66	128.81
4	G	184	CYC	CAA-CBA-CGA	-4.29	105.47	112.67
4	V	255	CYC	CHB-C1B-C2B	-4.29	118.45	126.95
4	O	184	CYC	C4D-CHA-C1A	-4.29	123.69	128.81
4	E	184	CYC	OC-C1C-NC	4.29	130.13	124.94
4	M	184	CYC	C2C-C1C-NC	4.26	111.94	108.27
4	X	184	CYC	C4D-CHA-C1A	-4.25	123.74	128.81
4	V	255	CYC	CAB-C3B-C2B	4.23	134.76	127.53
4	H	255	CYC	OC-C1C-C2C	-4.22	122.81	126.17
4	R	184	CYC	OC-C1C-C2C	-4.21	122.83	126.17
4	A	184	CYC	C1B-NB-C4B	-4.17	105.36	110.67
4	F	255	CYC	CMA-C3A-C4A	4.15	131.46	125.06
4	U	184	CYC	CHA-C1A-NA	-4.15	123.08	128.83
4	H	255	CYC	OB-C4B-C3B	-4.14	123.54	128.04
4	X	255	CYC	CHB-C4A-C3A	4.14	135.55	124.90
5	B	255	BLA	CMC-C2C-C3C	-4.14	118.18	128.30
4	D	255	CYC	OC-C1C-C2C	-4.11	122.90	126.17
4	N	184	CYC	CAD-C3D-C2D	4.11	139.05	127.25
4	W	184	CYC	C1B-CHB-C4A	-4.10	118.05	128.08
4	R	184	CYC	C4D-CHA-C1A	-4.10	123.91	128.81
4	L	184	CYC	C2C-C1C-NC	4.09	111.80	108.27
4	B	184	CYC	CBD-CAD-C3D	4.08	120.00	112.49
4	M	184	CYC	OB-C4B-C3B	-4.06	123.63	128.04
4	H	255	CYC	CHB-C1B-C2B	-4.06	118.90	126.95
4	V	184	CYC	C1B-CHB-C4A	-4.06	118.17	128.08
4	T	255	CYC	CBB-CAB-C3B	-4.06	101.25	112.43
4	J	255	CYC	CMB-C2B-C1B	4.05	129.22	124.17
4	P	255	CYC	CHA-C1A-NA	-4.04	123.22	128.83
4	P	184	CYC	CHD-C4C-NC	-4.04	120.40	125.20
4	H	184	CYC	CMB-C2B-C1B	4.04	129.21	124.17
4	J	255	CYC	CAB-C3B-C4B	3.99	127.68	121.38
4	F	255	CYC	CHB-C4A-NA	-3.98	116.60	124.93
4	L	184	CYC	CMB-C2B-C1B	3.98	129.13	124.17
4	H	255	CYC	C1B-CHB-C4A	-3.97	118.39	128.08

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	184	CYC	CMA-C3A-C4A	3.95	131.14	125.06
4	Q	184	CYC	C1B-CHB-C4A	-3.94	118.45	128.08
4	K	184	CYC	CMB-C2B-C1B	3.94	129.08	124.17
4	F	184	CYC	C4D-CHA-C1A	-3.93	124.12	128.81
4	L	255	CYC	CAA-C2A-C3A	-3.92	120.57	127.88
4	I	184	CYC	C1B-NB-C4B	-3.92	105.68	110.67
4	R	184	CYC	C2C-C1C-NC	3.92	111.65	108.27
4	R	184	CYC	CAC-C3C-C2C	-3.90	104.51	114.26
5	B	255	BLA	CAC-C3C-C2C	-3.90	115.75	128.60
4	I	184	CYC	CAB-C3B-C4B	3.89	127.52	121.38
4	G	184	CYC	C4D-CHA-C1A	-3.85	124.21	128.81
4	R	255	CYC	C1B-CHB-C4A	-3.85	118.68	128.08
4	Q	184	CYC	C2C-C1C-NC	3.85	111.59	108.27
4	X	184	CYC	CAB-C3B-C4B	3.83	127.44	121.38
4	O	184	CYC	OB-C4B-C3B	-3.83	123.89	128.04
4	E	184	CYC	CHA-C1A-NA	-3.82	123.52	128.83
4	H	255	CYC	C2C-C1C-NC	3.82	111.57	108.27
4	D	255	CYC	C1B-NB-C4B	-3.82	105.81	110.67
4	M	184	CYC	CAD-CBD-CGD	3.81	119.07	112.67
4	Q	184	CYC	OC-C1C-C2C	-3.79	123.16	126.17
4	H	255	CYC	CHD-C4C-NC	-3.78	120.71	125.20
4	D	255	CYC	CAD-CBD-CGD	-3.78	106.33	112.67
4	D	184	CYC	CAD-CBD-CGD	-3.78	106.34	112.67
4	T	184	CYC	CAB-C3B-C4B	3.77	127.33	121.38
4	F	255	CYC	C1B-NB-C4B	-3.77	105.87	110.67
4	B	184	CYC	C2B-C1B-NB	3.75	112.48	106.99
4	J	255	CYC	CHB-C4A-NA	-3.75	117.09	124.93
4	V	255	CYC	CMB-C2B-C1B	-3.74	119.49	124.17
4	J	255	CYC	C2C-C1C-NC	3.73	111.48	108.27
4	L	255	CYC	CHB-C1B-C2B	-3.73	119.57	126.95
4	T	255	CYC	CAD-CBD-CGD	3.72	118.91	112.67
4	V	255	CYC	C4D-CHA-C1A	-3.72	124.37	128.81
4	N	255	CYC	CHD-C4C-NC	-3.70	120.81	125.20
4	W	184	CYC	C2C-C1C-NC	3.69	111.45	108.27
4	P	255	CYC	CHB-C4A-C3A	3.68	134.36	124.90
4	L	184	CYC	C4D-CHA-C1A	-3.65	124.45	128.81
4	B	184	CYC	CHB-C1B-C2B	-3.62	119.78	126.95
4	J	184	CYC	C1B-CHB-C4A	-3.61	119.27	128.08
4	F	184	CYC	CAA-CBA-CGA	-3.60	106.62	112.67
4	P	255	CYC	C2C-C1C-NC	3.58	111.36	108.27
4	S	184	CYC	CAA-CBA-CGA	-3.57	106.67	112.67
4	H	184	CYC	C4D-CHA-C1A	-3.55	124.57	128.81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	184	CYC	C2B-C1B-NB	3.55	112.19	106.99
4	N	184	CYC	C2C-C1C-NC	3.54	111.33	108.27
4	T	184	CYC	CMC-C2C-C1C	-3.54	104.77	112.40
4	R	255	CYC	CMC-C2C-C1C	-3.54	104.77	112.40
4	A	184	CYC	CAA-CBA-CGA	-3.54	106.73	112.67
4	E	184	CYC	CMC-C2C-C1C	-3.53	104.79	112.40
4	R	184	CYC	CMB-C2B-C1B	3.52	128.57	124.17
4	O	184	CYC	C1B-NB-C4B	-3.51	106.20	110.67
5	B	255	BLA	CAD-CBD-CGD	-3.51	106.79	112.67
4	R	184	CYC	CHD-C4C-NC	-3.50	121.04	125.20
4	M	184	CYC	C4D-CHA-C1A	-3.49	124.64	128.81
4	N	184	CYC	C1B-NB-C4B	-3.48	106.24	110.67
4	L	184	CYC	CHB-C4A-C3A	3.48	133.85	124.90
4	L	255	CYC	C1B-CHB-C4A	-3.47	119.59	128.08
4	L	255	CYC	CAA-C2A-C1A	3.47	131.14	125.01
4	X	255	CYC	C3A-C4A-NA	-3.46	103.14	110.53
4	U	184	CYC	CHB-C1B-C2B	-3.46	120.10	126.95
4	X	255	CYC	C2C-C1C-NC	3.45	111.25	108.27
4	F	184	CYC	CHD-C4C-NC	-3.44	121.11	125.20
4	F	255	CYC	C1B-CHB-C4A	-3.44	119.69	128.08
4	X	184	CYC	CMC-C2C-C1C	-3.43	105.00	112.40
4	L	184	CYC	C1B-CHB-C4A	-3.43	119.70	128.08
4	B	184	CYC	CHA-C1A-NA	-3.43	124.07	128.83
4	U	184	CYC	OB-C4B-C3B	-3.42	124.33	128.04
5	B	255	BLA	OB-C4B-C3B	-3.41	121.72	129.46
4	G	184	CYC	CAB-C3B-C4B	3.41	126.77	121.38
4	Q	184	CYC	C1B-NB-C4B	-3.41	106.33	110.67
4	L	255	CYC	C2C-C1C-NC	3.40	111.20	108.27
4	R	255	CYC	CMD-C2D-C3D	3.39	131.34	124.94
4	G	184	CYC	OB-C4B-NB	-3.39	117.19	125.08
4	D	184	CYC	CMB-C2B-C1B	3.39	128.40	124.17
4	D	184	CYC	CAA-CBA-CGA	3.38	118.34	112.67
4	V	184	CYC	C1B-NB-C4B	-3.38	106.37	110.67
4	G	184	CYC	C1B-CHB-C4A	-3.36	119.86	128.08
4	S	184	CYC	CMA-C3A-C4A	3.36	130.24	125.06
4	V	255	CYC	C2B-C1B-NB	3.36	111.90	106.99
4	J	255	CYC	CAA-C2A-C1A	3.36	130.95	125.01
4	N	255	CYC	C1A-NA-C4A	3.35	112.83	106.51
4	S	184	CYC	C1B-CHB-C4A	-3.35	119.90	128.08
4	V	184	CYC	CHD-C4C-NC	-3.34	121.23	125.20
4	M	184	CYC	CBB-CAB-C3B	-3.32	103.27	112.43
4	R	184	CYC	CAB-C3B-C2B	-3.32	121.85	127.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	184	CYC	CMA-C3A-C4A	3.31	130.17	125.06
4	G	184	CYC	CHB-C4A-C3A	3.30	133.39	124.90
4	R	255	CYC	CHB-C1B-C2B	-3.30	120.42	126.95
4	N	184	CYC	OB-C4B-C3B	-3.29	124.47	128.04
4	D	255	CYC	CMA-C3A-C4A	3.28	130.12	125.06
5	B	255	BLA	CAD-C3D-C4D	3.28	130.80	125.01
4	X	255	CYC	C1A-NA-C4A	3.27	112.68	106.51
4	L	255	CYC	CBB-CAB-C3B	-3.25	103.48	112.43
4	D	255	CYC	OB-C4B-C3B	-3.24	124.53	128.04
4	P	184	CYC	CAD-CBD-CGD	-3.24	107.24	112.67
4	X	184	CYC	CAD-CBD-CGD	-3.23	107.25	112.67
4	J	184	CYC	OB-C4B-C3B	-3.22	124.55	128.04
5	B	255	BLA	CBB-CAB-C3B	-3.21	111.63	127.62
4	K	184	CYC	C2B-C1B-NB	3.21	111.69	106.99
4	G	184	CYC	C2B-C1B-NB	3.21	111.68	106.99
4	R	255	CYC	C4D-CHA-C1A	-3.20	124.98	128.81
4	E	184	CYC	CHD-C4C-NC	3.19	129.00	125.20
4	R	255	CYC	C1B-C2B-C3B	3.17	111.18	107.87
4	T	255	CYC	CHD-C4C-NC	-3.17	121.44	125.20
4	P	255	CYC	C2A-C1A-NA	3.17	114.65	110.05
4	J	255	CYC	C1A-NA-C4A	3.16	112.47	106.51
4	X	184	CYC	CAA-CBA-CGA	-3.15	107.39	112.67
4	P	184	CYC	CMB-C2B-C1B	3.15	128.09	124.17
4	L	184	CYC	CHB-C4A-NA	-3.13	118.38	124.93
4	S	184	CYC	CAB-C3B-C2B	3.13	132.88	127.53
4	D	184	CYC	CAC-C3C-C2C	-3.12	106.46	114.26
4	G	184	CYC	CBB-CAB-C3B	3.12	121.02	112.43
4	D	184	CYC	CAB-C3B-C4B	3.10	126.28	121.38
4	M	184	CYC	CMD-C2D-C3D	3.09	130.77	124.94
4	P	255	CYC	C2B-C1B-NB	3.09	111.51	106.99
4	J	255	CYC	CMA-C3A-C4A	3.08	129.81	125.06
5	B	255	BLA	CBC-CAC-C3C	-3.08	112.31	127.62
4	N	255	CYC	C2C-C1C-NC	3.07	110.92	108.27
4	X	255	CYC	CBB-CAB-C3B	3.05	120.85	112.43
4	O	184	CYC	CHB-C4A-C3A	3.05	132.74	124.90
4	Q	184	CYC	CBD-CAD-C3D	-3.05	106.87	112.49
4	R	255	CYC	CAA-C2A-C3A	-3.04	122.22	127.88
4	N	184	CYC	CAB-C3B-C4B	3.03	126.16	121.38
4	V	255	CYC	CMB-C2B-C3B	3.02	134.31	126.12
4	D	184	CYC	C1B-CHB-C4A	-3.01	120.72	128.08
4	I	184	CYC	C1B-CHB-C4A	-3.00	120.75	128.08
4	O	184	CYC	CHD-C4C-NC	2.99	128.76	125.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	255	CYC	C2B-C1B-NB	2.99	111.37	106.99
4	P	184	CYC	CMA-C3A-C4A	2.98	129.66	125.06
4	U	184	CYC	CHB-C4A-C3A	2.98	132.56	124.90
4	A	184	CYC	OB-C4B-NB	-2.98	118.16	125.08
4	U	184	CYC	CBD-CAD-C3D	-2.97	107.00	112.49
4	L	255	CYC	CAB-C3B-C4B	2.97	126.07	121.38
4	D	255	CYC	CAC-C3C-C4C	-2.97	105.06	112.67
4	R	184	CYC	CBD-CAD-C3D	2.96	117.95	112.49
4	X	184	CYC	CBD-CAD-C3D	2.96	117.94	112.49
4	T	184	CYC	OC-C1C-NC	2.96	128.53	124.94
4	R	255	CYC	OC-C1C-NC	2.96	128.53	124.94
4	C	184	CYC	CHA-C1A-NA	-2.95	124.73	128.83
4	L	255	CYC	CAC-C3C-C2C	-2.95	106.89	114.26
4	I	184	CYC	CHB-C4A-C3A	2.95	132.49	124.90
4	K	184	CYC	CAC-C3C-C4C	2.95	120.25	112.67
4	M	184	CYC	C2C-C3C-C4C	2.95	105.75	101.34
4	C	184	CYC	CHB-C1B-C2B	-2.95	121.11	126.95
5	B	255	BLA	CMB-C2B-C1B	2.94	127.83	124.17
4	V	184	CYC	OB-C4B-NB	-2.94	118.25	125.08
4	A	184	CYC	CHB-C1B-C2B	-2.94	121.13	126.95
4	I	184	CYC	CBB-CAB-C3B	-2.93	104.34	112.43
4	I	184	CYC	CMA-C3A-C4A	2.93	129.57	125.06
5	B	255	BLA	C4B-C3B-C2B	-2.91	104.18	107.92
4	C	184	CYC	OB-C4B-NB	-2.91	118.31	125.08
4	K	184	CYC	C2C-C1C-NC	2.91	110.78	108.27
4	Q	184	CYC	CHD-C4C-NC	-2.91	121.74	125.20
4	H	255	CYC	CAA-CBA-CGA	-2.91	107.79	112.67
4	P	184	CYC	C1A-NA-C4A	2.91	111.99	106.51
4	W	184	CYC	CHD-C4C-NC	-2.90	121.75	125.20
4	P	184	CYC	CHB-C4A-C3A	2.90	132.35	124.90
4	X	255	CYC	CMA-C3A-C4A	2.89	129.51	125.06
4	I	184	CYC	CBC-CAC-C3C	-2.88	107.05	113.47
4	J	184	CYC	OB-C4B-NB	-2.88	118.38	125.08
4	D	255	CYC	CHB-C1B-C2B	-2.88	121.24	126.95
4	R	184	CYC	CAC-C3C-C4C	2.86	120.02	112.67
4	T	184	CYC	CAA-CBA-CGA	-2.86	107.87	112.67
4	J	255	CYC	CBC-CAC-C3C	-2.85	107.11	113.47
4	R	184	CYC	OB-C4B-NB	-2.85	118.45	125.08
4	X	255	CYC	CAB-C3B-C2B	2.85	132.40	127.53
4	J	184	CYC	CHB-C1B-C2B	-2.84	121.31	126.95
4	J	184	CYC	C2B-C1B-NB	2.84	111.15	106.99
4	F	255	CYC	C1A-NA-C4A	2.83	111.84	106.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	255	CYC	CAB-C3B-C2B	2.83	132.36	127.53
4	B	184	CYC	CHD-C4C-NC	-2.82	121.85	125.20
4	F	184	CYC	C1B-CHB-C4A	-2.82	121.19	128.08
4	D	255	CYC	C2C-C3C-C4C	2.81	105.56	101.34
4	S	184	CYC	CHB-C1B-C2B	-2.81	121.37	126.95
4	K	184	CYC	CBB-CAB-C3B	-2.81	104.68	112.43
4	F	184	CYC	C2B-C1B-NB	2.81	111.10	106.99
4	F	255	CYC	OB-C4B-C3B	-2.81	124.99	128.04
4	H	255	CYC	CHA-C1A-NA	-2.81	124.93	128.83
4	R	255	CYC	C2C-C1C-NC	2.81	110.69	108.27
4	M	184	CYC	CHD-C4C-NC	2.80	128.53	125.20
4	J	255	CYC	CAA-CBA-CGA	-2.78	108.00	112.67
4	S	184	CYC	CHB-C4A-C3A	2.78	132.05	124.90
4	T	255	CYC	OC-C1C-C2C	-2.77	123.97	126.17
4	S	184	CYC	C2C-C1C-NC	2.77	110.66	108.27
4	O	184	CYC	CAD-CBD-CGD	-2.76	108.04	112.67
4	P	255	CYC	C4A-C3A-C2A	-2.76	103.34	106.51
4	T	255	CYC	CAB-C3B-C2B	2.75	132.24	127.53
5	B	255	BLA	C2B-C1B-NB	2.75	111.01	106.99
4	F	255	CYC	CAA-CBA-CGA	2.74	117.27	112.67
4	A	184	CYC	CMA-C3A-C4A	2.74	129.28	125.06
4	W	184	CYC	CAD-CBD-CGD	-2.73	108.09	112.67
4	D	184	CYC	C2B-C1B-NB	2.73	110.98	106.99
4	D	255	CYC	C1B-C2B-C3B	2.73	110.72	107.87
4	V	255	CYC	C1A-NA-C4A	2.72	111.64	106.51
4	L	255	CYC	C2C-C3C-C4C	2.72	105.41	101.34
4	R	184	CYC	CAA-CBA-CGA	-2.72	108.11	112.67
4	A	184	CYC	C1B-CHB-C4A	-2.71	121.45	128.08
4	M	184	CYC	C2B-C1B-NB	2.71	110.95	106.99
4	F	184	CYC	CBD-CAD-C3D	2.70	117.47	112.49
4	J	255	CYC	CAA-C2A-C3A	-2.69	122.86	127.88
4	Q	184	CYC	CHA-C1A-C2A	-2.69	119.11	125.32
4	U	184	CYC	C4A-C3A-C2A	-2.68	103.43	106.51
4	K	184	CYC	C1B-CHB-C4A	-2.67	121.56	128.08
4	F	255	CYC	CAB-C3B-C4B	2.67	125.59	121.38
4	L	255	CYC	CBD-CAD-C3D	-2.66	107.58	112.49
4	P	184	CYC	OC-C1C-C2C	-2.66	124.06	126.17
4	J	255	CYC	C3A-C4A-NA	-2.65	104.86	110.53
4	G	184	CYC	C1A-NA-C4A	2.65	111.50	106.51
4	C	184	CYC	CMB-C2B-C1B	-2.65	120.86	124.17
4	W	184	CYC	OC-C1C-C2C	-2.64	124.07	126.17
4	K	184	CYC	CHB-C4A-C3A	2.63	131.68	124.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	184	CYC	CBC-CAC-C3C	-2.63	107.61	113.47
4	A	184	CYC	CAC-C3C-C4C	2.63	119.42	112.67
4	H	255	CYC	CBD-CAD-C3D	-2.63	107.64	112.49
4	U	184	CYC	C2C-C1C-NC	2.62	110.53	108.27
4	W	184	CYC	CHB-C1B-C2B	-2.61	121.77	126.95
4	D	255	CYC	C4A-C3A-C2A	-2.61	103.51	106.51
4	P	255	CYC	CMA-C3A-C4A	2.60	129.07	125.06
4	A	184	CYC	CAB-C3B-C2B	-2.59	123.10	127.53
4	T	255	CYC	C1B-NB-C4B	-2.58	107.38	110.67
4	N	255	CYC	C3A-C4A-NA	-2.57	105.03	110.53
4	G	184	CYC	C3A-C4A-NA	-2.57	105.03	110.53
4	C	184	CYC	CBD-CAD-C3D	-2.57	107.74	112.49
4	T	255	CYC	CHB-C1B-C2B	-2.57	121.86	126.95
4	R	184	CYC	CMD-C2D-C3D	2.57	129.78	124.94
4	N	255	CYC	CHB-C1B-C2B	-2.56	121.87	126.95
4	A	184	CYC	CHA-C1A-C2A	-2.56	119.40	125.32
4	V	184	CYC	CMB-C2B-C1B	2.56	127.36	124.17
4	X	255	CYC	OC-C1C-NC	-2.56	121.84	124.94
4	G	184	CYC	CAC-C3C-C4C	2.56	119.24	112.67
4	P	184	CYC	CAD-C3D-C2D	-2.55	119.91	127.25
4	V	184	CYC	CBD-CAD-C3D	2.55	117.19	112.49
4	S	184	CYC	CAC-C3C-C4C	2.54	119.20	112.67
4	W	184	CYC	CAC-C3C-C4C	2.54	119.19	112.67
4	L	184	CYC	CAD-C3D-C2D	2.54	134.54	127.25
4	F	184	CYC	OB-C4B-NB	-2.54	119.18	125.08
4	D	184	CYC	C2C-C3C-C4C	2.53	105.13	101.34
4	J	255	CYC	C2C-C3C-C4C	2.53	105.13	101.34
5	B	255	BLA	C1D-C2D-C3D	-2.53	103.60	106.51
4	U	184	CYC	CHB-C4A-NA	-2.52	119.66	124.93
4	X	184	CYC	CMB-C2B-C1B	2.52	127.31	124.17
4	X	184	CYC	OC-C1C-C2C	-2.52	124.17	126.17
4	N	184	CYC	CMC-C2C-C1C	-2.51	106.98	112.40
4	R	184	CYC	C1B-CHB-C4A	-2.51	121.94	128.08
4	U	184	CYC	CMD-C2D-C3D	2.51	129.68	124.94
4	T	255	CYC	C1B-CHB-C4A	-2.51	121.95	128.08
4	C	184	CYC	C2B-C1B-NB	2.50	110.65	106.99
4	U	184	CYC	C2B-C1B-NB	2.50	110.65	106.99
4	V	255	CYC	CHD-C4C-NC	-2.50	122.23	125.20
4	F	255	CYC	C2C-C3C-C4C	2.49	105.08	101.34
4	E	184	CYC	C1B-CHB-C4A	-2.49	121.99	128.08
4	D	255	CYC	OC-C1C-NC	2.49	127.95	124.94
4	Q	184	CYC	CAA-CBA-CGA	-2.48	108.51	112.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	184	CYC	CAC-C3C-C2C	-2.48	108.06	114.26
4	A	184	CYC	C2B-C1B-NB	2.48	110.62	106.99
5	B	255	BLA	CHB-C1B-C2B	-2.47	122.09	126.97
4	S	184	CYC	OC-C1C-NC	-2.47	121.95	124.94
4	X	184	CYC	C2C-C1C-NC	2.45	110.39	108.27
4	C	184	CYC	CHB-C4A-C3A	2.45	131.20	124.90
4	N	255	CYC	CAC-C3C-C4C	2.45	118.97	112.67
4	Q	184	CYC	OB-C4B-NB	-2.45	119.38	125.08
4	L	255	CYC	C2B-C1B-NB	2.45	110.57	106.99
4	D	184	CYC	C1A-NA-C4A	2.45	111.12	106.51
4	V	255	CYC	C4A-C3A-C2A	-2.44	103.71	106.51
4	S	184	CYC	CBB-CAB-C3B	-2.43	105.72	112.43
4	A	184	CYC	CMD-C2D-C3D	2.43	129.53	124.94
4	E	184	CYC	C2B-C1B-NB	2.43	110.54	106.99
4	B	184	CYC	CAD-C3D-C2D	-2.43	120.27	127.25
4	D	184	CYC	CHB-C1B-NB	-2.43	120.85	126.06
4	D	255	CYC	CMB-C2B-C1B	-2.42	121.15	124.17
4	K	184	CYC	C1A-NA-C4A	2.41	111.05	106.51
4	R	255	CYC	CAA-C2A-C1A	2.41	129.27	125.01
4	N	184	CYC	CMD-C2D-C3D	2.41	129.48	124.94
4	R	184	CYC	C1A-NA-C4A	2.40	111.03	106.51
4	J	184	CYC	CHA-C1A-NA	-2.40	125.50	128.83
4	U	184	CYC	OC-C1C-C2C	-2.39	124.27	126.17
4	V	184	CYC	CAD-C3D-C2D	2.39	134.13	127.25
4	K	184	CYC	CAB-C3B-C4B	2.39	125.15	121.38
4	I	184	CYC	C2C-C3C-C4C	2.38	104.91	101.34
4	X	255	CYC	CBC-CAC-C3C	-2.37	108.20	113.47
4	L	184	CYC	CBB-CAB-C3B	-2.36	105.92	112.43
4	K	184	CYC	CMD-C2D-C3D	2.36	129.39	124.94
4	P	184	CYC	C3A-C4A-NA	-2.36	105.48	110.53
4	F	184	CYC	OC-C1C-NC	2.36	127.80	124.94
4	Q	184	CYC	C2A-C1A-NA	2.35	113.47	110.05
4	C	184	CYC	CAA-C2A-C3A	-2.35	123.51	127.88
4	U	184	CYC	CAD-CBD-CGD	2.34	116.60	112.67
4	C	184	CYC	CHB-C4A-NA	-2.34	120.04	124.93
4	N	184	CYC	CMA-C3A-C4A	2.34	128.67	125.06
4	F	184	CYC	CHB-C1B-NB	-2.34	121.04	126.06
4	K	184	CYC	C4D-CHA-C1A	-2.33	126.03	128.81
4	D	255	CYC	CMC-C2C-C1C	-2.32	107.39	112.40
4	N	255	CYC	CHB-C4A-C3A	2.32	130.87	124.90
4	X	184	CYC	CAD-C3D-C2D	-2.32	120.58	127.25
4	R	255	CYC	C1A-NA-C4A	2.32	110.88	106.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	255	BLA	CAD-C3D-C2D	-2.32	123.56	127.88
4	S	184	CYC	C1A-NA-C4A	2.31	110.86	106.51
4	D	184	CYC	CHB-C4A-C3A	2.31	130.83	124.90
4	L	255	CYC	CHD-C4C-NC	-2.30	122.47	125.20
4	H	255	CYC	CAC-C3C-C4C	2.30	118.58	112.67
4	I	184	CYC	C1A-C2A-C3A	2.30	109.33	106.78
4	U	184	CYC	OB-C4B-NB	-2.30	119.74	125.08
4	R	184	CYC	CHA-C1A-NA	-2.29	125.65	128.83
4	R	184	CYC	CHB-C1B-C2B	-2.28	122.42	126.95
4	M	184	CYC	CAB-C3B-C4B	2.28	124.98	121.38
4	H	184	CYC	C2B-C1B-NB	2.28	110.33	106.99
4	O	184	CYC	CBB-CAB-C3B	-2.28	106.15	112.43
4	R	255	CYC	CHB-C1B-NB	2.28	130.94	126.06
4	O	184	CYC	CMA-C3A-C4A	2.27	128.57	125.06
4	H	184	CYC	OC-C1C-C2C	-2.27	124.37	126.17
4	J	255	CYC	C4D-CHA-C1A	-2.27	126.10	128.81
4	V	184	CYC	CHA-C1A-NA	-2.27	125.68	128.83
4	F	184	CYC	CMA-C3A-C4A	2.25	128.53	125.06
4	X	184	CYC	CHB-C1B-C2B	-2.25	122.50	126.95
4	U	184	CYC	CAA-C2A-C3A	-2.24	123.71	127.88
4	L	184	CYC	CAA-CBA-CGA	-2.23	108.93	112.67
4	P	255	CYC	CAC-C3C-C4C	-2.22	106.96	112.67
4	H	255	CYC	CBC-CAC-C3C	2.22	118.41	113.47
4	R	255	CYC	CBC-CAC-C3C	2.21	118.39	113.47
4	J	255	CYC	CHA-C1A-C2A	2.21	130.43	125.32
4	R	184	CYC	C2B-C1B-NB	2.21	110.22	106.99
4	T	184	CYC	CHA-C1A-NA	-2.21	125.76	128.83
4	F	255	CYC	CAC-C3C-C4C	-2.20	107.01	112.67
4	B	184	CYC	C4A-C3A-C2A	-2.20	103.98	106.51
4	L	184	CYC	CHA-C1A-C2A	-2.20	120.25	125.32
4	D	255	CYC	CMD-C2D-C3D	2.19	129.07	124.94
4	N	184	CYC	C2C-C3C-C4C	2.19	104.62	101.34
4	I	184	CYC	C1A-NA-C4A	2.19	110.64	106.51
4	N	255	CYC	OC-C1C-NC	-2.19	122.29	124.94
4	L	184	CYC	C4A-C3A-C2A	-2.19	104.00	106.51
4	C	184	CYC	CAC-C3C-C4C	2.18	118.27	112.67
5	B	255	BLA	C3C-C4C-NC	2.18	110.20	106.80
4	A	184	CYC	CHB-C4A-C3A	2.17	130.48	124.90
4	H	184	CYC	C1B-CHB-C4A	-2.17	122.78	128.08
4	T	184	CYC	CBB-CAB-C3B	-2.17	106.46	112.43
4	D	184	CYC	CAD-C3D-C2D	-2.17	121.02	127.25
4	Q	184	CYC	CAC-C3C-C4C	2.17	118.23	112.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	184	CYC	CHA-C1A-C2A	-2.16	120.32	125.32
4	V	184	CYC	CMA-C3A-C4A	2.16	128.39	125.06
4	M	184	CYC	CHB-C4A-C3A	2.16	130.45	124.90
4	P	184	CYC	CAA-C2A-C3A	-2.15	123.88	127.88
4	O	184	CYC	CAA-CBA-CGA	-2.15	109.07	112.67
4	T	255	CYC	CHA-C1A-C2A	-2.14	120.38	125.32
4	A	184	CYC	CHB-C4A-NA	-2.12	120.49	124.93
4	O	184	CYC	CHB-C4A-NA	-2.12	120.50	124.93
4	S	184	CYC	CHA-C1A-NA	-2.12	125.89	128.83
4	S	184	CYC	CAB-C3B-C4B	2.12	124.73	121.38
4	J	184	CYC	CAD-C3D-C2D	2.12	133.33	127.25
4	K	184	CYC	CHD-C4C-NC	-2.11	122.69	125.20
4	P	255	CYC	CHB-C1B-NB	2.11	130.59	126.06
4	D	255	CYC	CAA-C2A-C3A	-2.11	123.94	127.88
4	D	184	CYC	CAB-C3B-C2B	2.11	131.13	127.53
4	H	255	CYC	CMA-C3A-C4A	2.10	128.30	125.06
4	W	184	CYC	CHB-C4A-C3A	2.10	130.30	124.90
4	M	184	CYC	CHB-C1B-C2B	-2.10	122.79	126.95
4	X	255	CYC	CHA-C1A-C2A	-2.09	120.50	125.32
4	U	184	CYC	C1A-NA-C4A	2.08	110.43	106.51
4	H	255	CYC	CHB-C4A-C3A	2.08	130.24	124.90
4	I	184	CYC	CHB-C1B-C2B	-2.06	122.86	126.95
4	P	184	CYC	OC-C1C-NC	-2.06	122.44	124.94
4	X	255	CYC	C1B-CHB-C4A	-2.06	123.04	128.08
4	A	184	CYC	CBB-CAB-C3B	-2.06	106.75	112.43
4	D	255	CYC	CBD-CAD-C3D	2.06	116.28	112.49
4	F	255	CYC	CMD-C2D-C3D	2.05	128.81	124.94
4	I	184	CYC	C4A-C3A-C2A	-2.05	104.16	106.51
4	T	184	CYC	CMA-C3A-C4A	2.04	128.21	125.06
4	M	184	CYC	CMA-C3A-C4A	2.04	128.20	125.06
4	F	184	CYC	CMD-C2D-C3D	-2.04	121.11	124.94
4	R	184	CYC	C3A-C4A-NA	-2.03	106.19	110.53
4	V	255	CYC	C1A-C2A-C3A	2.03	109.03	106.78
4	O	184	CYC	C1B-CHB-C4A	-2.02	123.14	128.08
4	P	184	CYC	C1A-C2A-C3A	2.02	109.02	106.78
4	X	255	CYC	CMB-C2B-C1B	2.02	126.69	124.17
4	V	184	CYC	CMD-C2D-C3D	2.01	128.74	124.94
4	M	184	CYC	CAD-C3D-C2D	2.01	133.02	127.25
4	S	184	CYC	C3A-C4A-NA	-2.01	106.23	110.53
4	F	255	CYC	C3A-C4A-NA	-2.00	106.25	110.53

There are no chirality outliers.

All (309) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	184	CYC	NA-C4A-CHB-C1B
4	I	184	CYC	C3A-C4A-CHB-C1B
4	I	184	CYC	C4C-C3C-CAC-CBC
4	I	184	CYC	ND-C1D-CHD-C4C
4	I	184	CYC	C2D-C1D-CHD-C4C
4	J	255	CYC	ND-C4D-CHA-C1A
4	J	255	CYC	C3D-C4D-CHA-C1A
4	J	255	CYC	NA-C4A-CHB-C1B
4	J	255	CYC	C3A-C4A-CHB-C1B
4	J	255	CYC	C2B-C1B-CHB-C4A
4	J	255	CYC	C4B-C3B-CAB-CBB
4	J	255	CYC	C2C-C3C-CAC-CBC
4	J	255	CYC	C4C-C3C-CAC-CBC
4	J	255	CYC	C2D-C1D-CHD-C4C
4	O	184	CYC	NA-C4A-CHB-C1B
4	O	184	CYC	C4C-C3C-CAC-CBC
4	R	184	CYC	NA-C4A-CHB-C1B
4	R	184	CYC	C3A-C4A-CHB-C1B
4	R	184	CYC	C2C-C3C-CAC-CBC
4	R	184	CYC	C4C-C3C-CAC-CBC
4	R	184	CYC	ND-C1D-CHD-C4C
4	R	184	CYC	C2D-C1D-CHD-C4C
4	R	184	CYC	C2D-C3D-CAD-CBD
4	R	184	CYC	C4D-C3D-CAD-CBD
4	E	184	CYC	NA-C4A-CHB-C1B
4	E	184	CYC	C3A-C4A-CHB-C1B
4	E	184	CYC	C4B-C3B-CAB-CBB
4	E	184	CYC	C2C-C3C-CAC-CBC
4	E	184	CYC	C4C-C3C-CAC-CBC
4	E	184	CYC	ND-C1D-CHD-C4C
4	E	184	CYC	C2D-C1D-CHD-C4C
4	L	184	CYC	NA-C4A-CHB-C1B
4	L	184	CYC	C3A-C4A-CHB-C1B
4	L	184	CYC	C2C-C3C-CAC-CBC
4	L	184	CYC	C4C-C3C-CAC-CBC
4	L	184	CYC	ND-C1D-CHD-C4C
4	L	184	CYC	C2D-C1D-CHD-C4C
4	L	184	CYC	C2D-C3D-CAD-CBD
4	L	184	CYC	C4D-C3D-CAD-CBD
4	V	255	CYC	NA-C4A-CHB-C1B
4	Q	184	CYC	NA-C4A-CHB-C1B
4	Q	184	CYC	C3A-C4A-CHB-C1B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	Q	184	CYC	C4B-C3B-CAB-CBB
4	Q	184	CYC	ND-C1D-CHD-C4C
4	B	184	CYC	NA-C4A-CHB-C1B
4	B	184	CYC	C3A-C4A-CHB-C1B
4	B	184	CYC	ND-C1D-CHD-C4C
4	B	184	CYC	C2D-C1D-CHD-C4C
4	B	184	CYC	C2D-C3D-CAD-CBD
4	B	184	CYC	C4D-C3D-CAD-CBD
4	S	184	CYC	NA-C4A-CHB-C1B
4	S	184	CYC	C3A-C4A-CHB-C1B
4	S	184	CYC	C4C-C3C-CAC-CBC
4	S	184	CYC	ND-C1D-CHD-C4C
4	S	184	CYC	C2D-C1D-CHD-C4C
4	S	184	CYC	C2D-C3D-CAD-CBD
4	S	184	CYC	C4D-C3D-CAD-CBD
4	D	255	CYC	ND-C4D-CHA-C1A
4	D	255	CYC	C3D-C4D-CHA-C1A
4	D	255	CYC	NA-C4A-CHB-C1B
4	D	255	CYC	C3A-C4A-CHB-C1B
4	D	255	CYC	C2C-C3C-CAC-CBC
4	D	255	CYC	C4C-C3C-CAC-CBC
4	D	255	CYC	C2D-C3D-CAD-CBD
4	D	255	CYC	C4D-C3D-CAD-CBD
4	W	184	CYC	NA-C4A-CHB-C1B
4	W	184	CYC	C3A-C4A-CHB-C1B
4	W	184	CYC	ND-C1D-CHD-C4C
4	W	184	CYC	C2D-C1D-CHD-C4C
4	X	184	CYC	NA-C4A-CHB-C1B
4	X	184	CYC	C3A-C4A-CHB-C1B
4	X	184	CYC	C2C-C3C-CAC-CBC
4	X	184	CYC	C4C-C3C-CAC-CBC
4	X	184	CYC	ND-C1D-CHD-C4C
4	X	184	CYC	C2D-C1D-CHD-C4C
4	X	184	CYC	C2D-C3D-CAD-CBD
4	X	184	CYC	C4D-C3D-CAD-CBD
4	K	184	CYC	NA-C4A-CHB-C1B
4	K	184	CYC	C3A-C4A-CHB-C1B
4	K	184	CYC	C2C-C3C-CAC-CBC
4	K	184	CYC	C4C-C3C-CAC-CBC
4	K	184	CYC	ND-C1D-CHD-C4C
4	K	184	CYC	C2D-C1D-CHD-C4C
4	M	184	CYC	NA-C4A-CHB-C1B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	M	184	CYC	C3A-C4A-CHB-C1B
4	M	184	CYC	C2C-C3C-CAC-CBC
4	M	184	CYC	C4C-C3C-CAC-CBC
4	M	184	CYC	ND-C1D-CHD-C4C
4	N	255	CYC	ND-C4D-CHA-C1A
4	N	255	CYC	C3D-C4D-CHA-C1A
4	N	255	CYC	NA-C4A-CHB-C1B
4	N	255	CYC	C3A-C4A-CHB-C1B
4	N	255	CYC	C4B-C3B-CAB-CBB
4	N	255	CYC	C2C-C3C-CAC-CBC
4	N	255	CYC	C2D-C3D-CAD-CBD
4	N	255	CYC	C4D-C3D-CAD-CBD
4	P	184	CYC	NA-C4A-CHB-C1B
4	P	184	CYC	C2B-C3B-CAB-CBB
4	P	184	CYC	C2C-C3C-CAC-CBC
4	P	184	CYC	C4C-C3C-CAC-CBC
4	P	184	CYC	ND-C1D-CHD-C4C
4	P	184	CYC	C2D-C1D-CHD-C4C
4	P	184	CYC	C2D-C3D-CAD-CBD
4	P	184	CYC	C4D-C3D-CAD-CBD
4	A	184	CYC	NA-C4A-CHB-C1B
4	A	184	CYC	C4B-C3B-CAB-CBB
4	A	184	CYC	C2C-C3C-CAC-CBC
4	A	184	CYC	C4C-C3C-CAC-CBC
4	A	184	CYC	C2D-C1D-CHD-C4C
4	C	184	CYC	NA-C4A-CHB-C1B
4	C	184	CYC	C4C-C3C-CAC-CBC
4	C	184	CYC	ND-C1D-CHD-C4C
4	C	184	CYC	C2D-C1D-CHD-C4C
4	T	184	CYC	NA-C4A-CHB-C1B
4	T	184	CYC	C3A-C4A-CHB-C1B
4	T	184	CYC	C4B-C3B-CAB-CBB
4	T	184	CYC	ND-C1D-CHD-C4C
4	T	184	CYC	C2D-C1D-CHD-C4C
4	V	184	CYC	NA-C4A-CHB-C1B
4	V	184	CYC	C3A-C4A-CHB-C1B
4	V	184	CYC	ND-C1D-CHD-C4C
4	V	184	CYC	C2D-C1D-CHD-C4C
4	V	184	CYC	C4D-C3D-CAD-CBD
5	B	255	BLA	C1A-C2A-CAA-CBA
5	B	255	BLA	C3A-C2A-CAA-CBA
5	B	255	BLA	NA-C4A-CHB-C1B

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	B	255	BLA	C3A-C4A-CHB-C1B
5	B	255	BLA	C2C-C3C-CAC-CBC
5	B	255	BLA	ND-C1D-CHD-C4C
5	B	255	BLA	C2D-C1D-CHD-C4C
5	B	255	BLA	C2D-C3D-CAD-CBD
4	U	184	CYC	C2C-C3C-CAC-CBC
4	U	184	CYC	C4C-C3C-CAC-CBC
4	U	184	CYC	ND-C1D-CHD-C4C
4	U	184	CYC	C2D-C1D-CHD-C4C
4	F	255	CYC	ND-C4D-CHA-C1A
4	F	255	CYC	C2A-CAA-CBA-CGA
4	F	255	CYC	C4C-C3C-CAC-CBC
4	L	255	CYC	ND-C4D-CHA-C1A
4	L	255	CYC	C3D-C4D-CHA-C1A
4	L	255	CYC	NA-C4A-CHB-C1B
4	L	255	CYC	C2A-CAA-CBA-CGA
4	L	255	CYC	C4B-C3B-CAB-CBB
4	L	255	CYC	ND-C1D-CHD-C4C
4	L	255	CYC	C2D-C1D-CHD-C4C
4	T	255	CYC	ND-C4D-CHA-C1A
4	T	255	CYC	C3D-C4D-CHA-C1A
4	T	255	CYC	NA-C4A-CHB-C1B
4	T	255	CYC	C3A-C4A-CHB-C1B
4	T	255	CYC	C4C-C3C-CAC-CBC
4	X	255	CYC	ND-C4D-CHA-C1A
4	X	255	CYC	C4C-C3C-CAC-CBC
4	H	255	CYC	NA-C4A-CHB-C1B
4	H	255	CYC	C3A-C4A-CHB-C1B
4	P	255	CYC	ND-C4D-CHA-C1A
4	P	255	CYC	C3D-C4D-CHA-C1A
4	P	255	CYC	NA-C4A-CHB-C1B
4	P	255	CYC	C3A-C4A-CHB-C1B
4	P	255	CYC	ND-C1D-CHD-C4C
4	P	255	CYC	C2D-C1D-CHD-C4C
4	R	255	CYC	ND-C4D-CHA-C1A
4	R	255	CYC	C3D-C4D-CHA-C1A
4	R	255	CYC	C1A-C2A-CAA-CBA
4	R	255	CYC	C3A-C2A-CAA-CBA
4	R	255	CYC	NA-C4A-CHB-C1B
4	G	184	CYC	NA-C4A-CHB-C1B
4	G	184	CYC	C3A-C4A-CHB-C1B
4	G	184	CYC	C4B-C3B-CAB-CBB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	G	184	CYC	C4C-C3C-CAC-CBC
4	G	184	CYC	ND-C1D-CHD-C4C
4	G	184	CYC	C2D-C1D-CHD-C4C
4	H	184	CYC	NA-C4A-CHB-C1B
4	H	184	CYC	C3A-C4A-CHB-C1B
4	H	184	CYC	C2B-C3B-CAB-CBB
4	H	184	CYC	C4B-C3B-CAB-CBB
4	H	184	CYC	ND-C1D-CHD-C4C
4	H	184	CYC	C2D-C1D-CHD-C4C
4	J	184	CYC	NA-C4A-CHB-C1B
4	J	184	CYC	C3A-C4A-CHB-C1B
4	J	184	CYC	C4B-C3B-CAB-CBB
4	J	184	CYC	ND-C1D-CHD-C4C
4	J	184	CYC	C2D-C1D-CHD-C4C
4	J	184	CYC	C2D-C3D-CAD-CBD
4	J	184	CYC	C4D-C3D-CAD-CBD
4	N	184	CYC	NA-C4A-CHB-C1B
4	N	184	CYC	C3A-C4A-CHB-C1B
4	N	184	CYC	C4B-C3B-CAB-CBB
4	N	184	CYC	ND-C1D-CHD-C4C
4	N	184	CYC	C2D-C1D-CHD-C4C
4	N	184	CYC	C2D-C3D-CAD-CBD
4	N	184	CYC	C4D-C3D-CAD-CBD
4	D	184	CYC	NA-C4A-CHB-C1B
4	D	184	CYC	C3A-C4A-CHB-C1B
4	D	184	CYC	C2B-C3B-CAB-CBB
4	D	184	CYC	C4B-C3B-CAB-CBB
4	D	184	CYC	C2C-C3C-CAC-CBC
4	D	184	CYC	C4C-C3C-CAC-CBC
4	D	184	CYC	ND-C1D-CHD-C4C
4	D	184	CYC	C2D-C1D-CHD-C4C
4	D	184	CYC	C2D-C3D-CAD-CBD
4	D	184	CYC	C4D-C3D-CAD-CBD
4	F	184	CYC	NA-C4A-CHB-C1B
4	F	184	CYC	C3A-C4A-CHB-C1B
4	F	184	CYC	ND-C1D-CHD-C4C
4	F	184	CYC	C2D-C1D-CHD-C4C
4	R	184	CYC	C2B-C3B-CAB-CBB
4	E	184	CYC	C2B-C3B-CAB-CBB
4	B	184	CYC	C2B-C3B-CAB-CBB
4	X	184	CYC	C2B-C3B-CAB-CBB
4	F	255	CYC	C2B-C3B-CAB-CBB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	H	255	CYC	C2B-C3B-CAB-CBB
4	R	255	CYC	C2B-C3B-CAB-CBB
4	F	184	CYC	C2B-C3B-CAB-CBB
4	N	255	CYC	C2B-C3B-CAB-CBB
4	L	255	CYC	C2B-C3B-CAB-CBB
4	V	255	CYC	C2B-C3B-CAB-CBB
4	N	184	CYC	C2B-C3B-CAB-CBB
4	A	184	CYC	C2B-C3B-CAB-CBB
4	T	184	CYC	C2B-C3B-CAB-CBB
4	J	184	CYC	C2B-C3B-CAB-CBB
4	P	255	CYC	C3A-C2A-CAA-CBA
4	J	255	CYC	C2B-C3B-CAB-CBB
4	T	255	CYC	C2B-C3B-CAB-CBB
5	B	255	BLA	C4D-C3D-CAD-CBD
4	P	255	CYC	C1A-C2A-CAA-CBA
4	G	184	CYC	C2B-C3B-CAB-CBB
4	D	255	CYC	C2B-C3B-CAB-CBB
4	O	184	CYC	C3A-C4A-CHB-C1B
4	V	255	CYC	C3A-C4A-CHB-C1B
4	P	184	CYC	C3A-C4A-CHB-C1B
4	A	184	CYC	C3A-C4A-CHB-C1B
4	C	184	CYC	C3A-C4A-CHB-C1B
4	R	255	CYC	C3A-C4A-CHB-C1B
4	P	255	CYC	C2B-C3B-CAB-CBB
4	E	184	CYC	C2A-CAA-CBA-CGA
4	X	255	CYC	C2A-CAA-CBA-CGA
4	J	255	CYC	NA-C1A-CHA-C4D
4	W	184	CYC	NA-C1A-CHA-C4D
4	K	184	CYC	NA-C1A-CHA-C4D
4	N	255	CYC	NA-C1A-CHA-C4D
5	B	255	BLA	ND-C4D-CHA-C1A
4	P	255	CYC	NA-C1A-CHA-C4D
4	J	184	CYC	NA-C1A-CHA-C4D
4	R	184	CYC	C4B-C3B-CAB-CBB
4	V	255	CYC	C4B-C3B-CAB-CBB
4	B	184	CYC	C4B-C3B-CAB-CBB
4	X	184	CYC	C4B-C3B-CAB-CBB
4	P	184	CYC	C4B-C3B-CAB-CBB
4	F	255	CYC	C4B-C3B-CAB-CBB
4	T	255	CYC	C4B-C3B-CAB-CBB
4	H	255	CYC	C4B-C3B-CAB-CBB
4	R	255	CYC	C4B-C3B-CAB-CBB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	F	184	CYC	C4B-C3B-CAB-CBB
4	V	184	CYC	C2B-C3B-CAB-CBB
4	Q	184	CYC	C2B-C3B-CAB-CBB
4	U	184	CYC	NA-C4A-CHB-C1B
4	F	255	CYC	NA-C4A-CHB-C1B
4	X	255	CYC	NA-C4A-CHB-C1B
4	U	184	CYC	C3A-C4A-CHB-C1B
4	F	255	CYC	C3A-C4A-CHB-C1B
4	L	255	CYC	C3A-C4A-CHB-C1B
4	X	255	CYC	C3A-C4A-CHB-C1B
4	V	184	CYC	C2A-CAA-CBA-CGA
4	Q	184	CYC	NA-C1A-CHA-C4D
4	O	184	CYC	C1A-C2A-CAA-CBA
4	J	255	CYC	NB-C1B-CHB-C4A
4	N	255	CYC	C2A-CAA-CBA-CGA
4	C	184	CYC	C2C-C3C-CAC-CBC
4	F	255	CYC	C2C-C3C-CAC-CBC
4	X	255	CYC	C2C-C3C-CAC-CBC
4	L	255	CYC	NA-C1A-CHA-C4D
4	H	184	CYC	NA-C1A-CHA-C4D
4	O	184	CYC	C3A-C2A-CAA-CBA
4	J	255	CYC	C2A-C1A-CHA-C4D
4	W	184	CYC	C2A-C1A-CHA-C4D
4	R	255	CYC	C2A-CAA-CBA-CGA
4	E	184	CYC	NA-C1A-CHA-C4D
4	G	184	CYC	NA-C1A-CHA-C4D
4	W	184	CYC	C2B-C3B-CAB-CBB
4	W	184	CYC	C4C-C3C-CAC-CBC
4	N	255	CYC	C4C-C3C-CAC-CBC
4	H	184	CYC	C2A-CAA-CBA-CGA
4	S	184	CYC	NA-C1A-CHA-C4D
4	X	255	CYC	NA-C1A-CHA-C4D
4	D	255	CYC	C4B-C3B-CAB-CBB
4	V	255	CYC	C3D-CAD-CBD-CGD
4	O	184	CYC	C2C-C3C-CAC-CBC
4	S	184	CYC	C2C-C3C-CAC-CBC
4	X	184	CYC	C2A-CAA-CBA-CGA
4	P	255	CYC	C2A-CAA-CBA-CGA
4	D	184	CYC	NA-C1A-CHA-C4D
4	V	184	CYC	C2D-C3D-CAD-CBD
4	S	184	CYC	C2B-C3B-CAB-CBB
4	E	184	CYC	C2A-C1A-CHA-C4D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	X	184	CYC	NA-C1A-CHA-C4D
4	A	184	CYC	C1A-C2A-CAA-CBA
4	V	184	CYC	NB-C1B-CHB-C4A
4	L	184	CYC	NA-C1A-CHA-C4D
4	X	184	CYC	NB-C1B-CHB-C4A
4	A	184	CYC	C3A-C2A-CAA-CBA
4	T	255	CYC	C2C-C3C-CAC-CBC
5	B	255	BLA	C3D-C4D-CHA-C1A
4	P	255	CYC	C2A-C1A-CHA-C4D
4	D	255	CYC	NA-C1A-CHA-C4D
4	L	255	CYC	C3D-CAD-CBD-CGD
4	J	184	CYC	C2A-C1A-CHA-C4D
4	U	184	CYC	NB-C1B-CHB-C4A
4	B	184	CYC	NB-C1B-CHB-C4A
4	B	184	CYC	NA-C1A-CHA-C4D

There are no ring outliers.

35 monomers are involved in 295 short contacts:

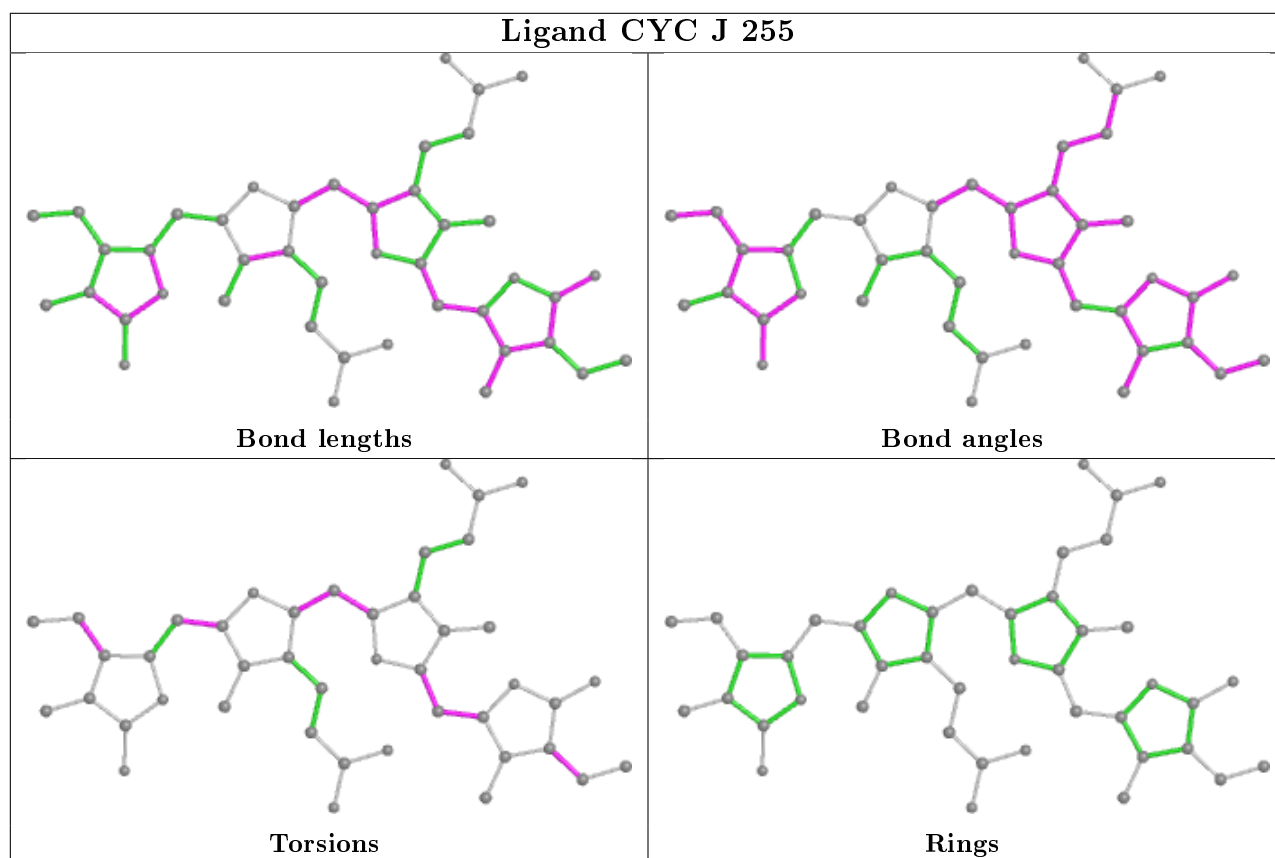
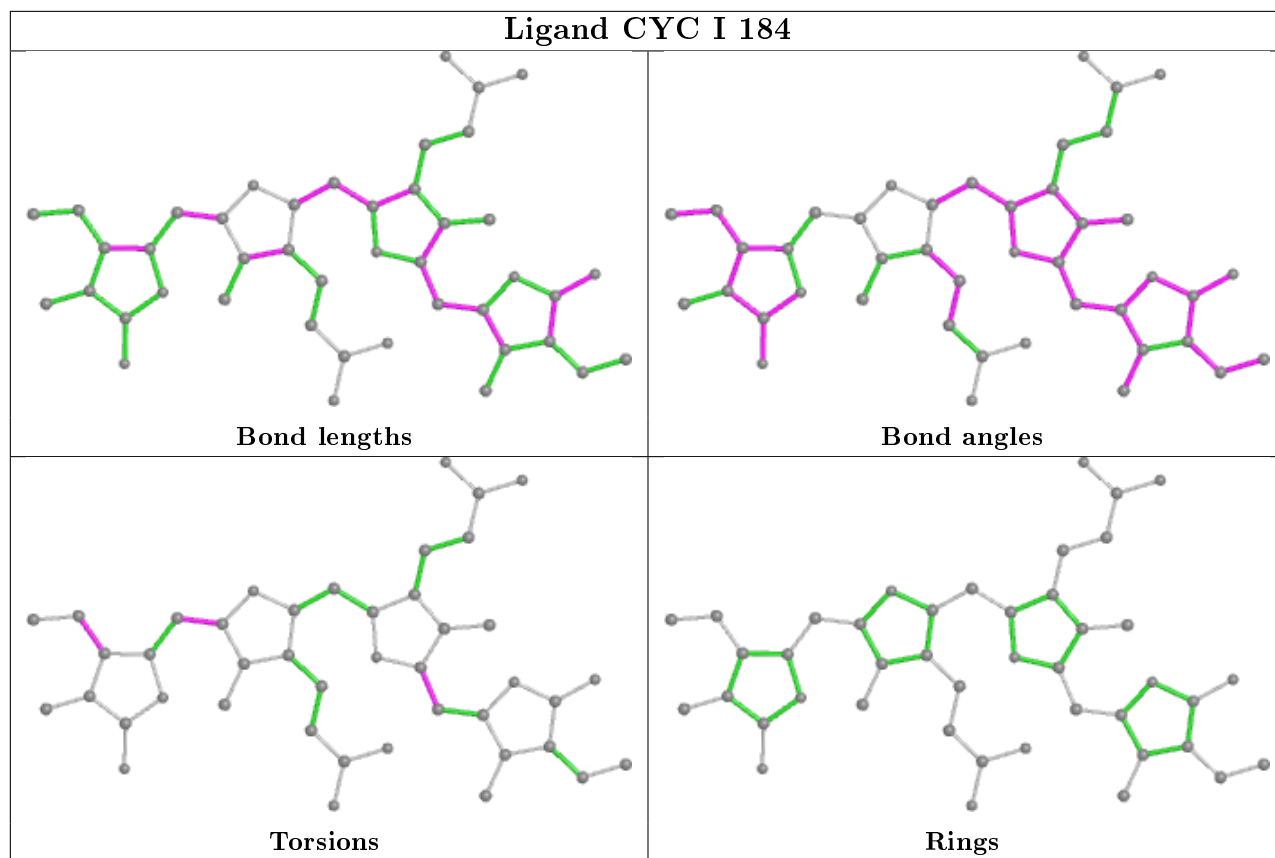
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	184	CYC	4	0
4	J	255	CYC	15	0
4	O	184	CYC	6	0
4	R	184	CYC	5	0
4	E	184	CYC	6	0
4	L	184	CYC	15	0
4	V	255	CYC	7	0
4	Q	184	CYC	6	0
4	B	184	CYC	10	0
4	S	184	CYC	11	0
4	D	255	CYC	8	0
4	W	184	CYC	5	0
4	X	184	CYC	9	0
4	K	184	CYC	5	0
4	M	184	CYC	3	0
4	N	255	CYC	13	0
4	P	184	CYC	12	0
4	A	184	CYC	6	0
4	C	184	CYC	5	0
4	T	184	CYC	14	0
4	V	184	CYC	6	0
5	B	255	BLA	16	0

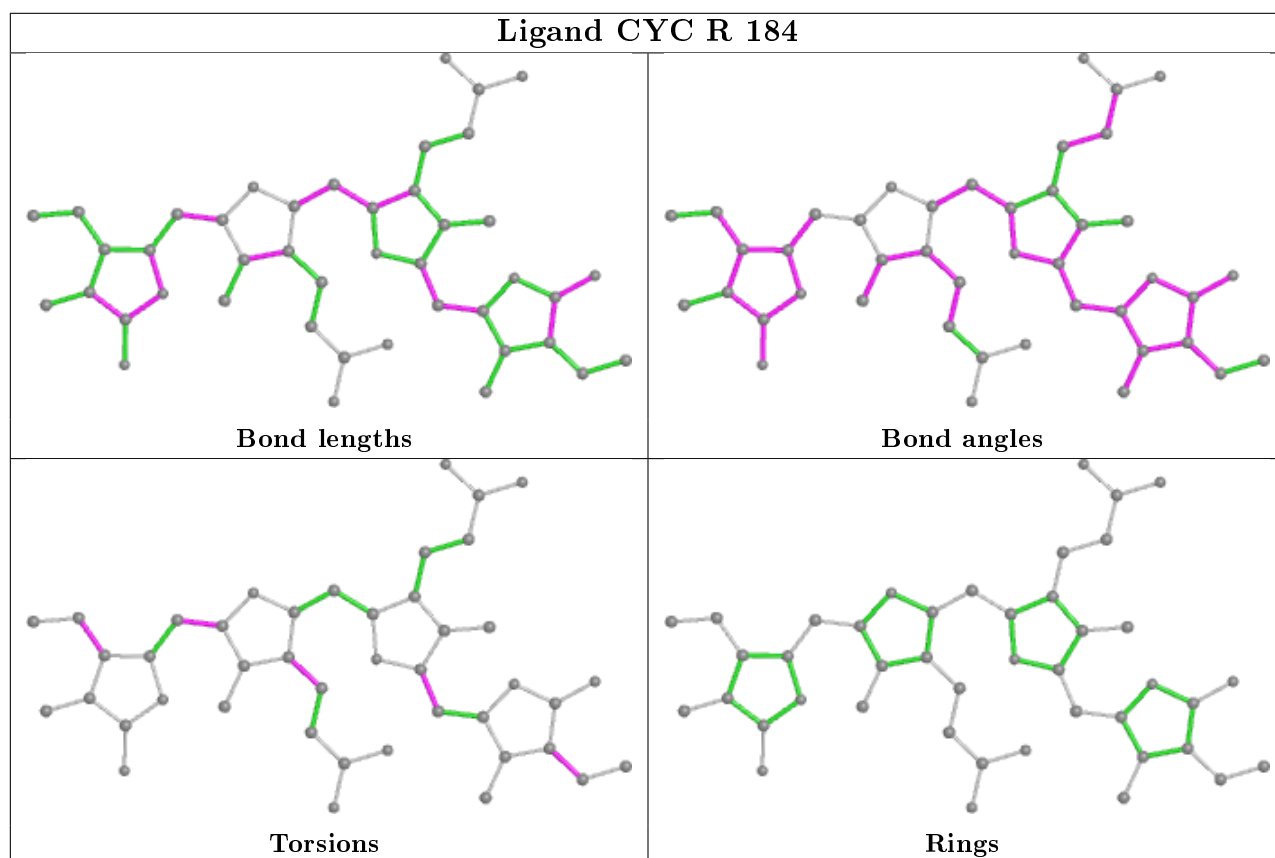
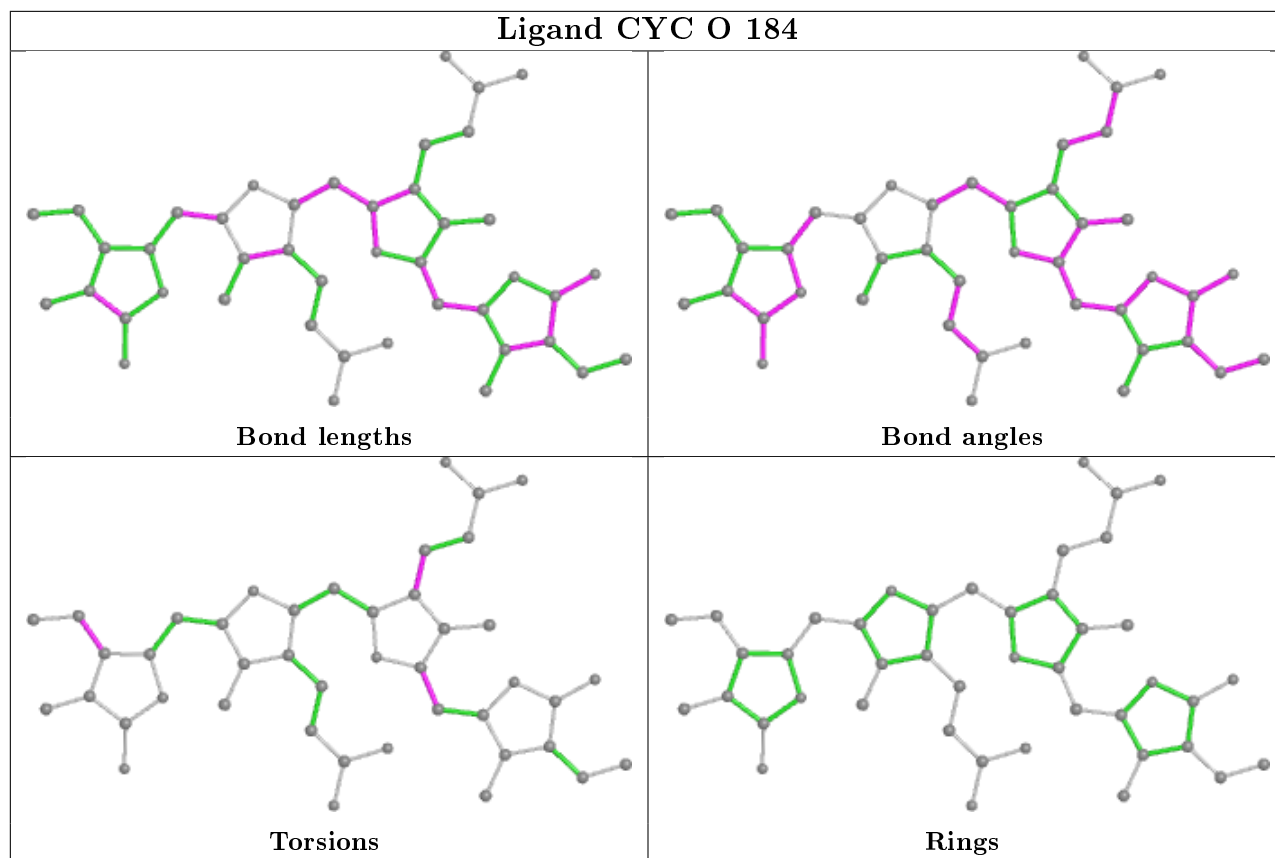
*Continued on next page...*

*Continued from previous page...*

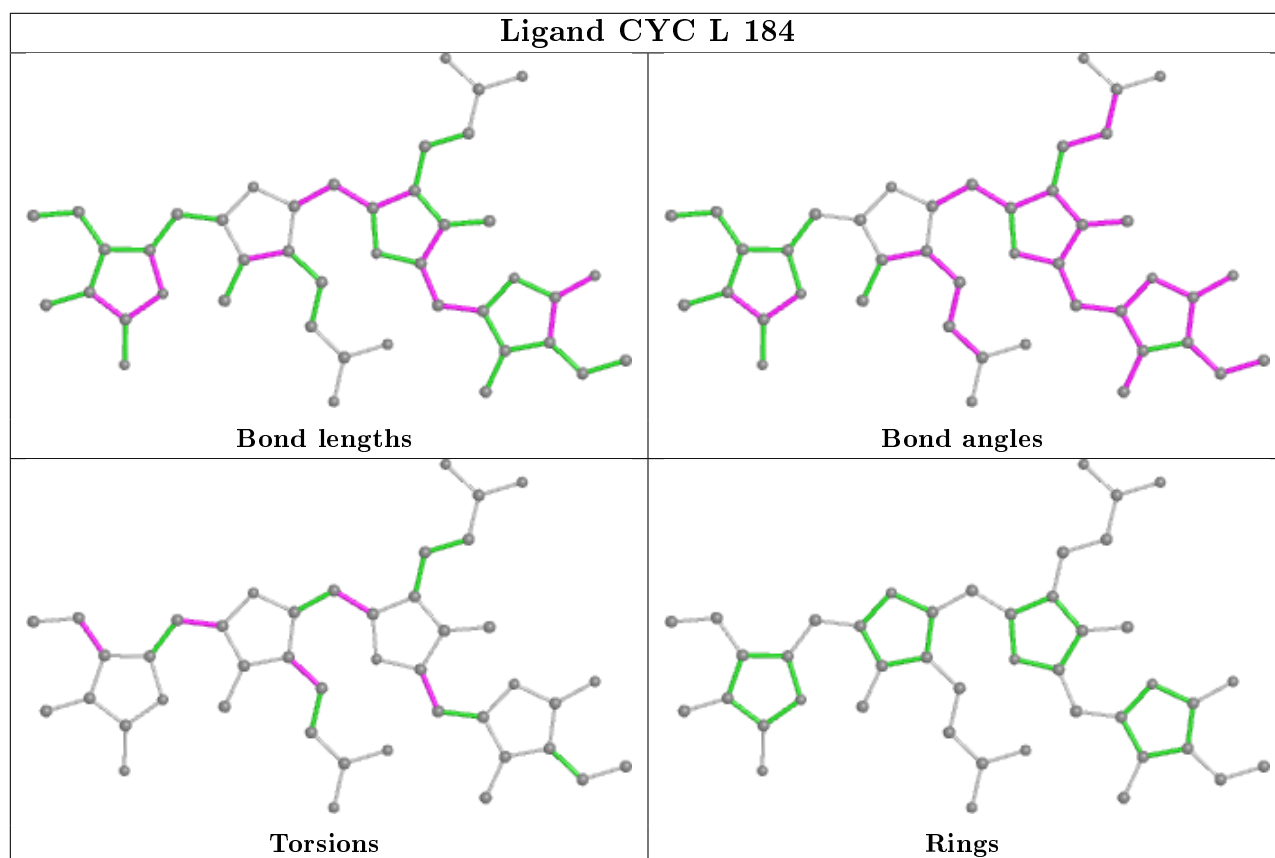
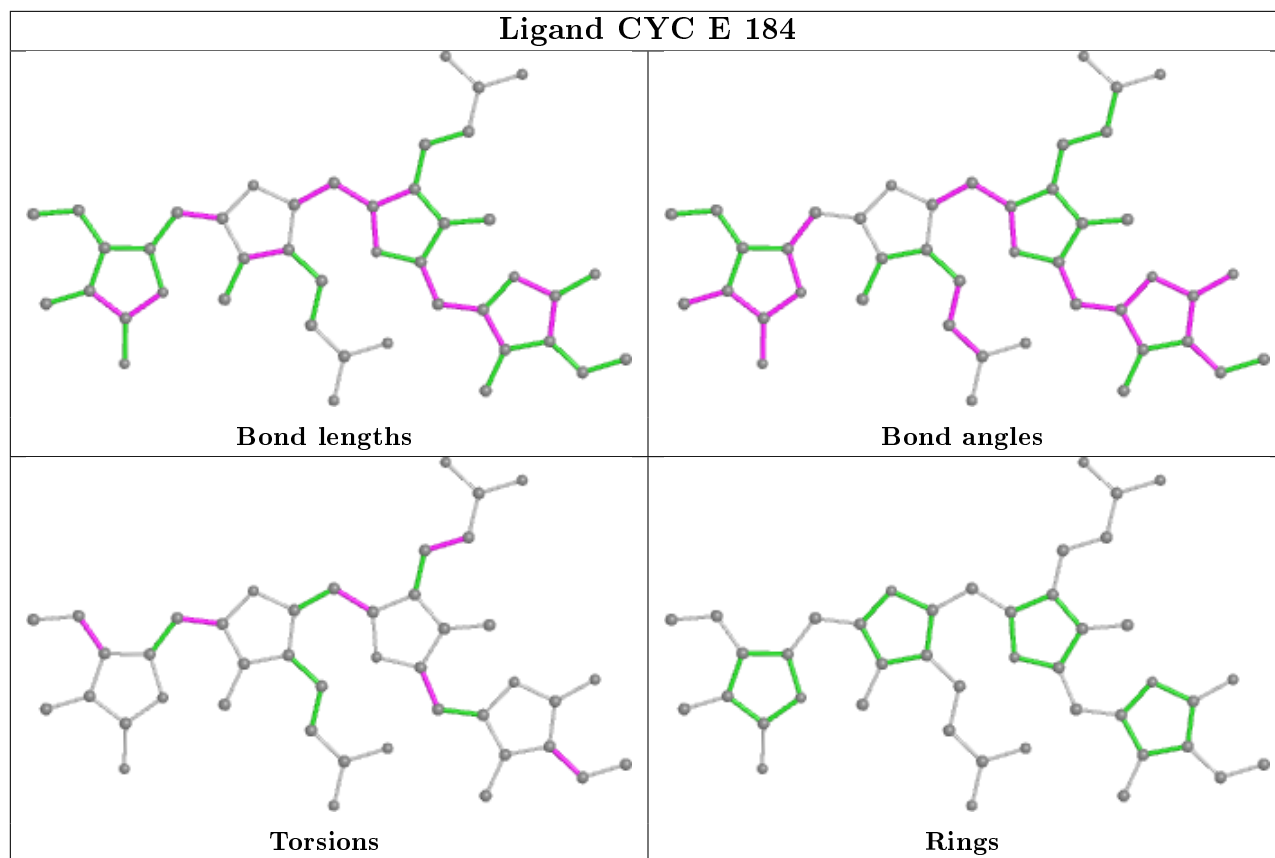
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	184	CYC	5	0
4	F	255	CYC	5	0
4	L	255	CYC	12	0
4	T	255	CYC	13	0
4	H	255	CYC	13	0
4	P	255	CYC	12	0
4	R	255	CYC	15	0
4	G	184	CYC	6	0
4	H	184	CYC	5	0
4	J	184	CYC	5	0
4	N	184	CYC	5	0
4	D	184	CYC	8	0
4	F	184	CYC	4	0

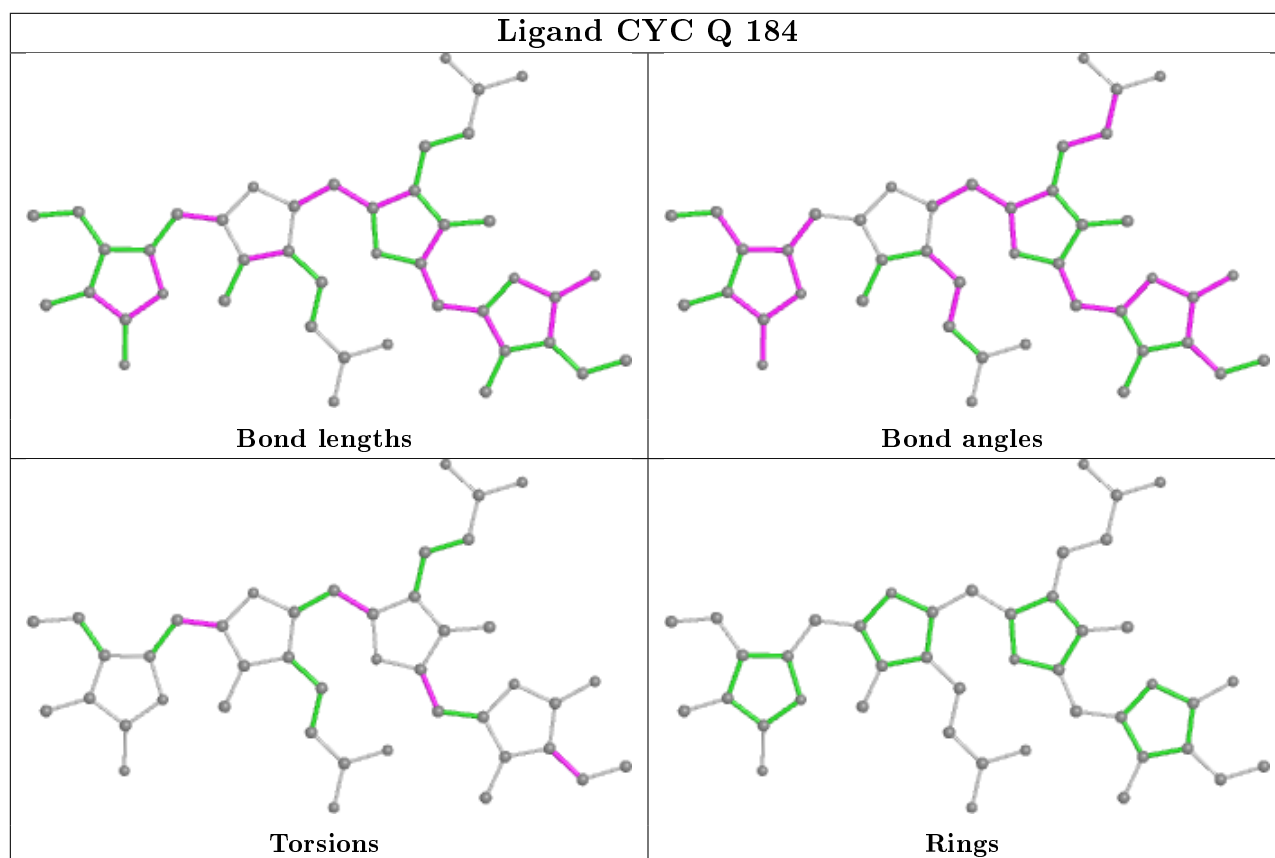
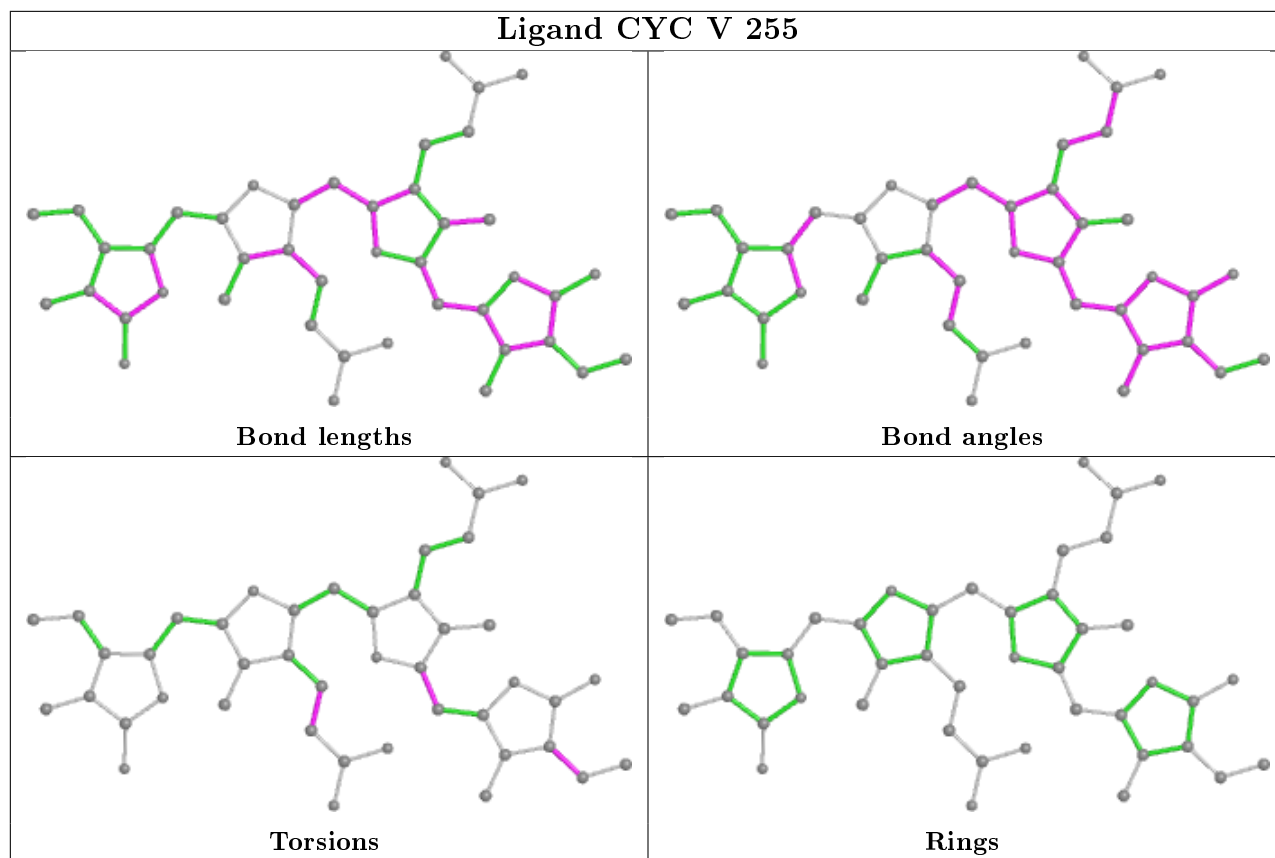
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

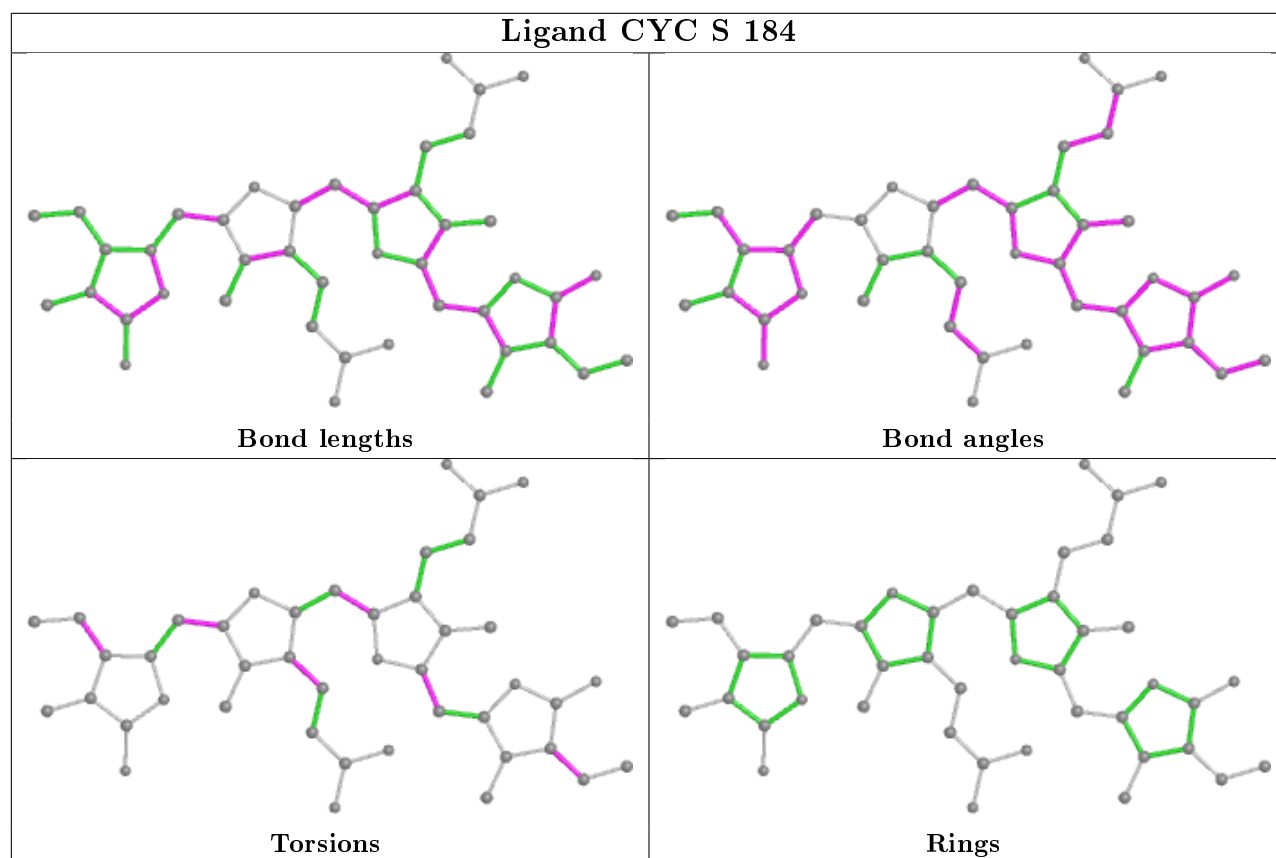
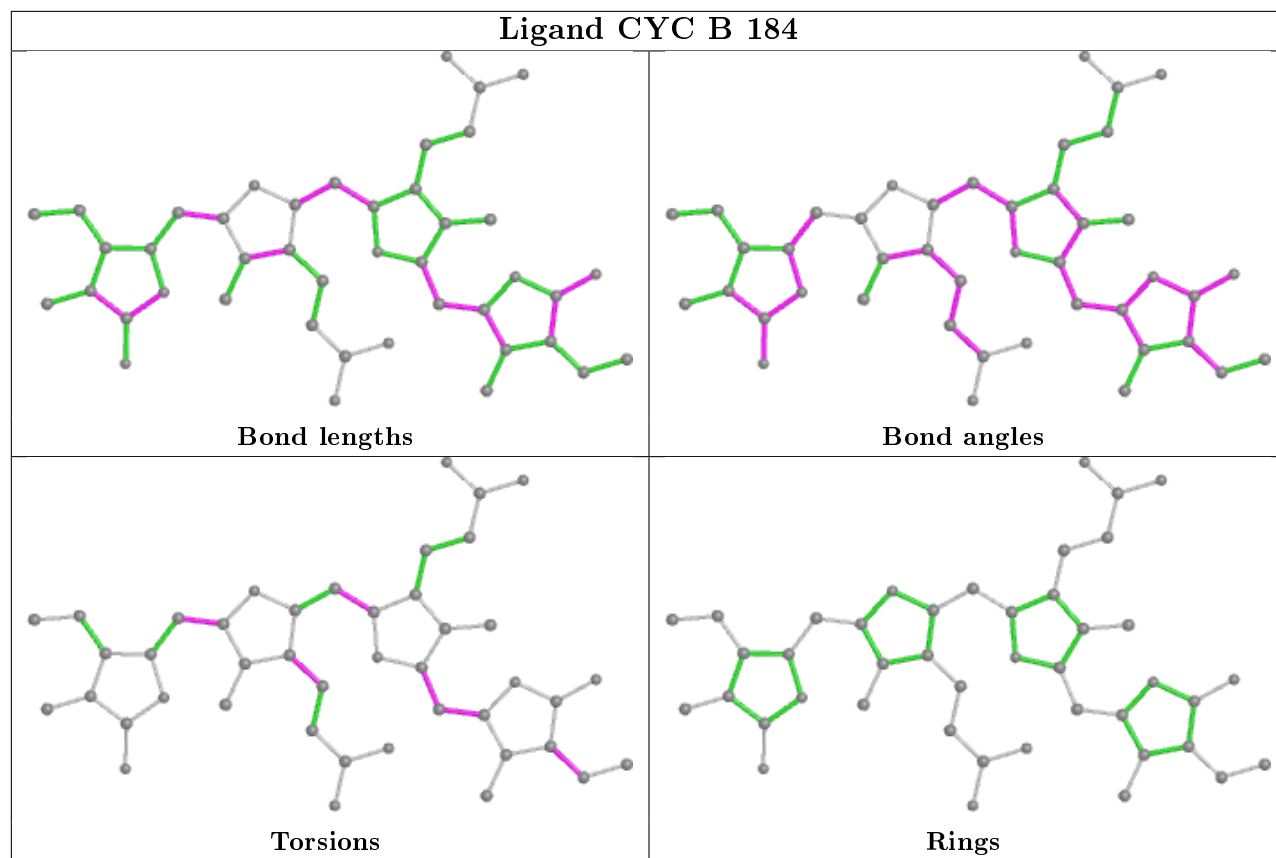


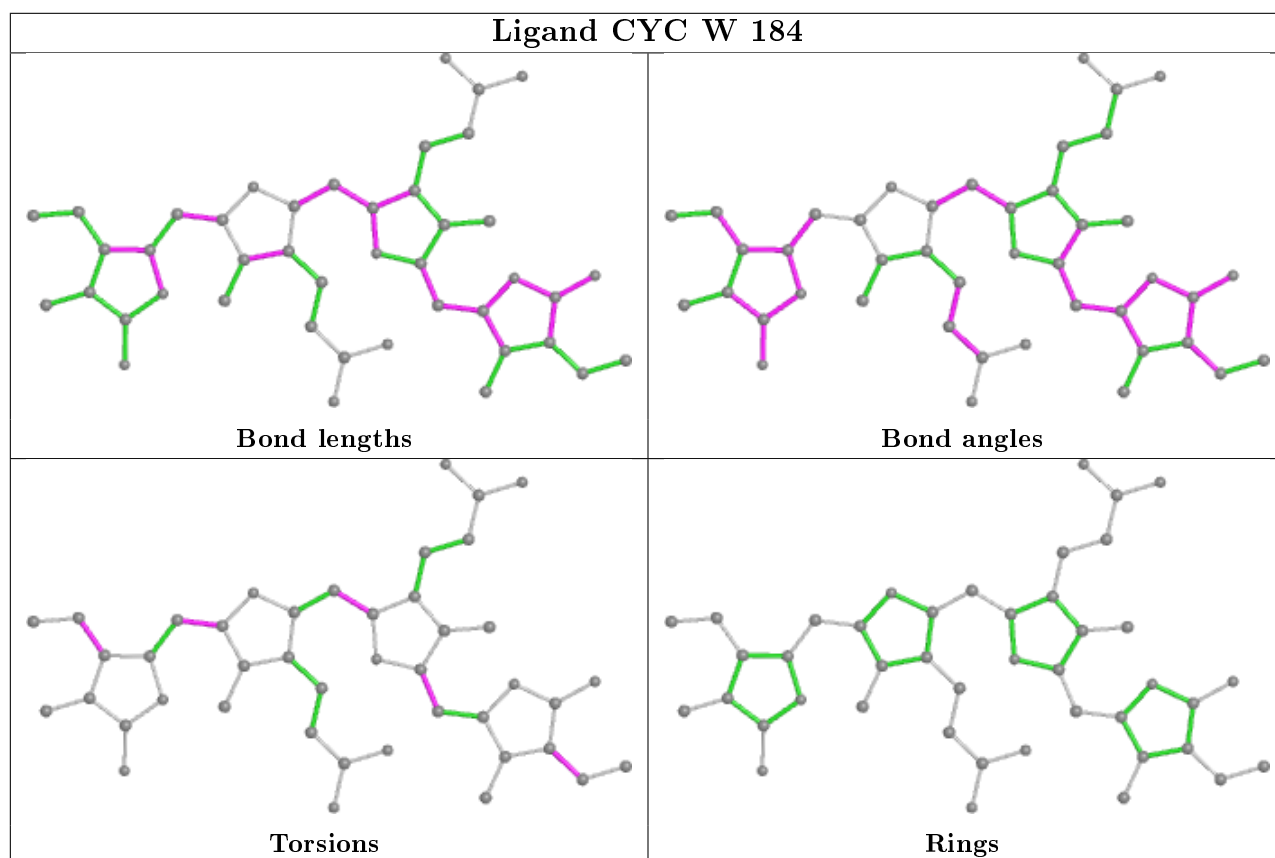
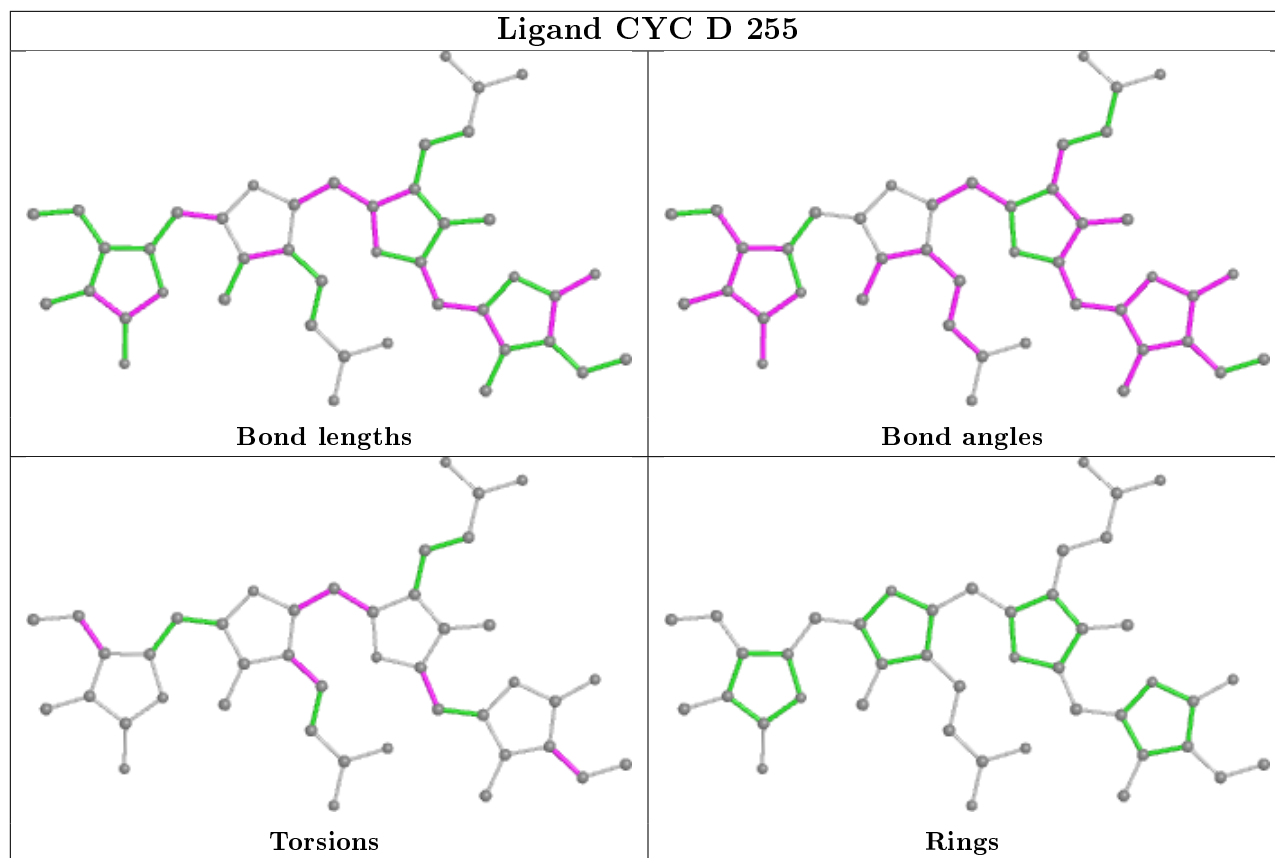


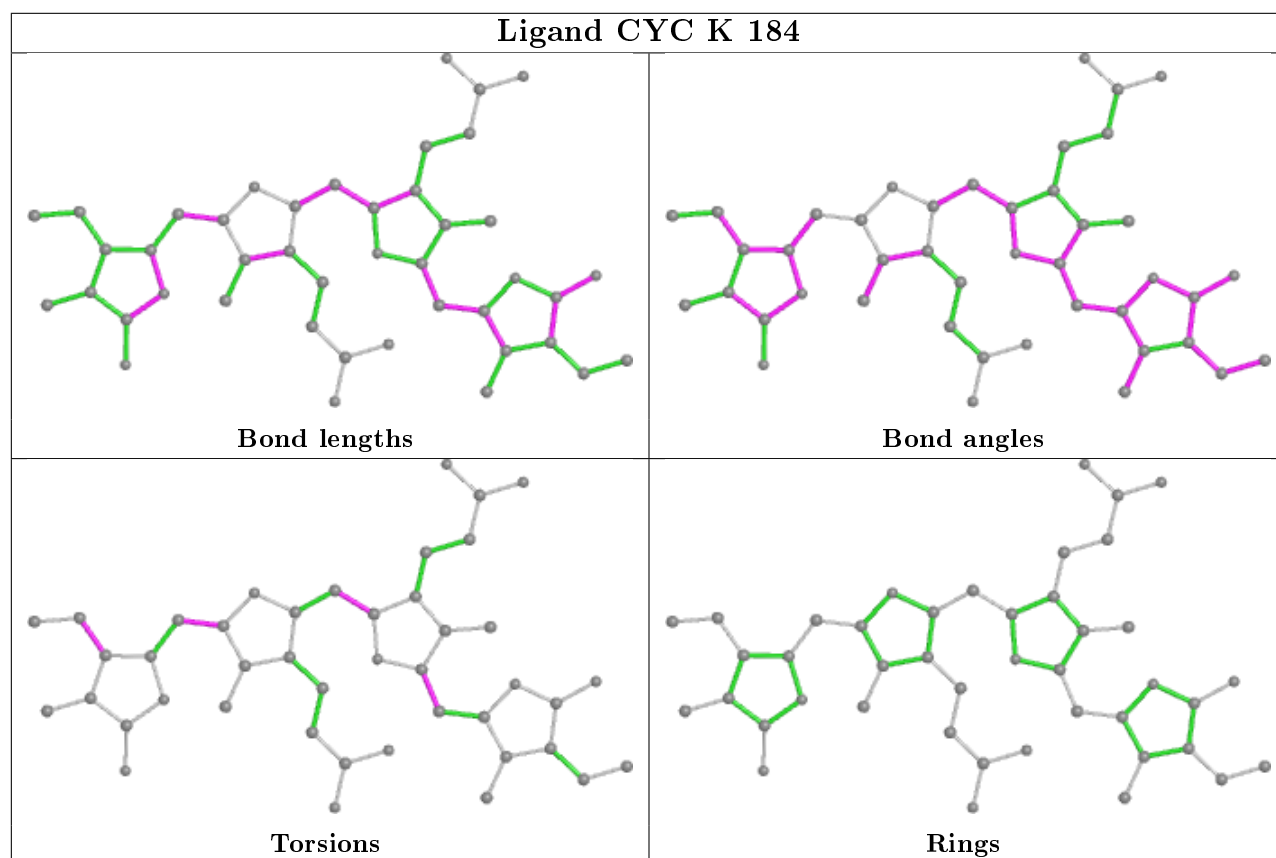
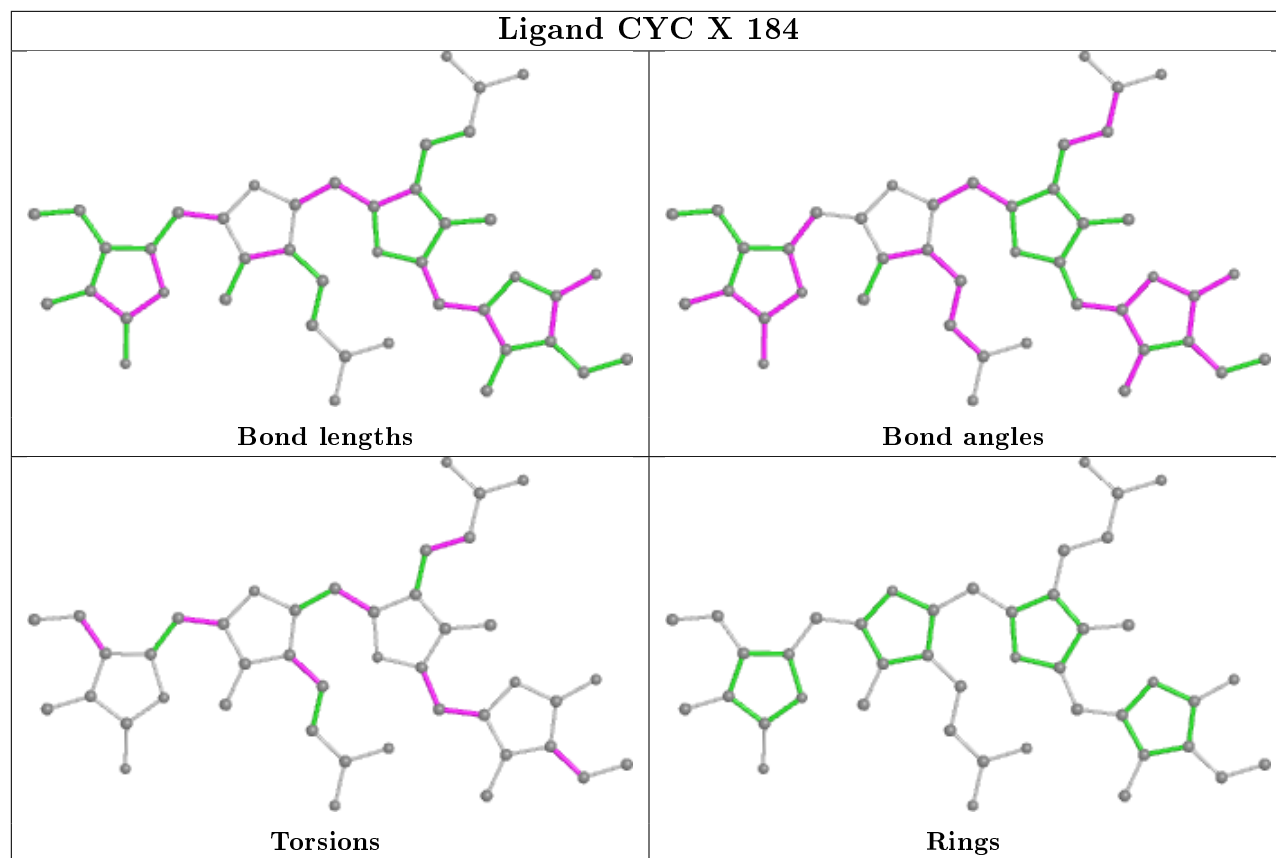


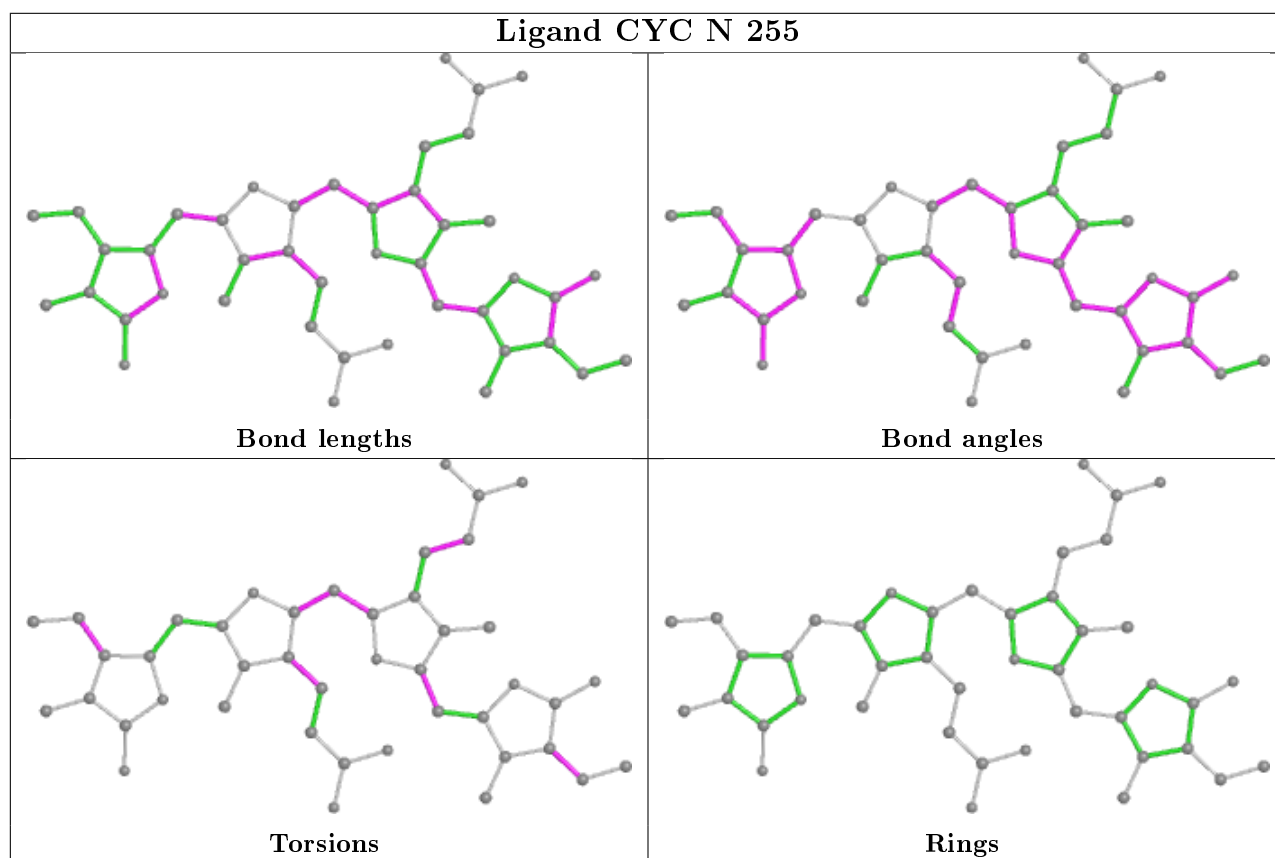
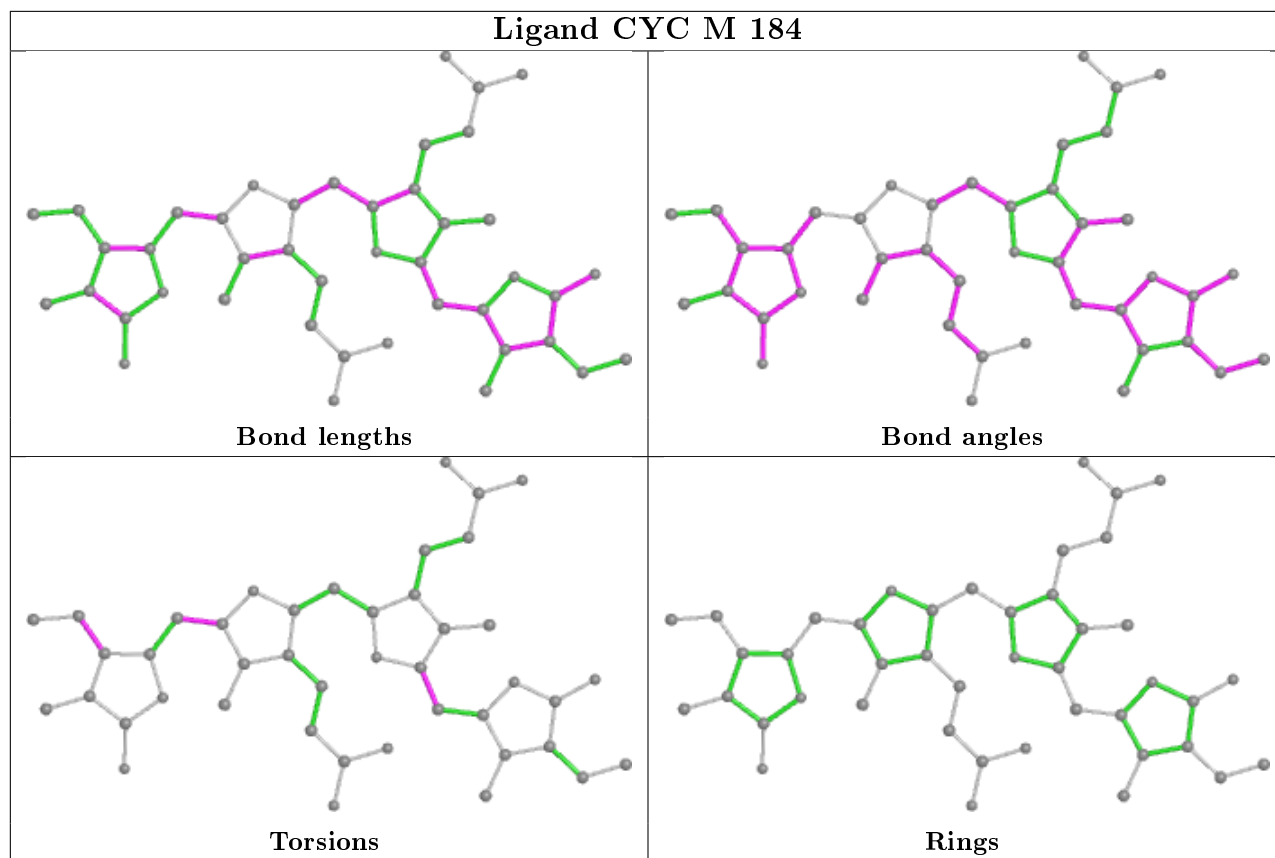


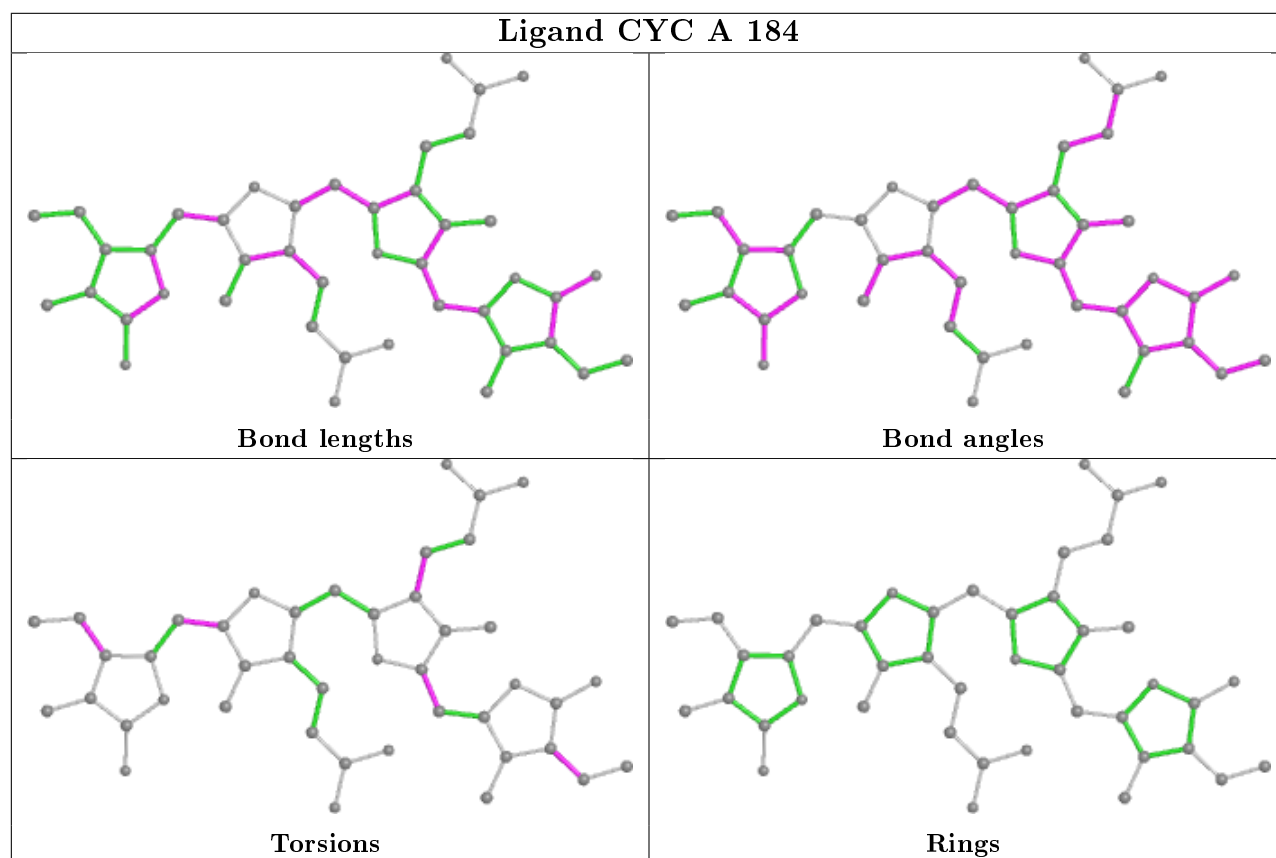
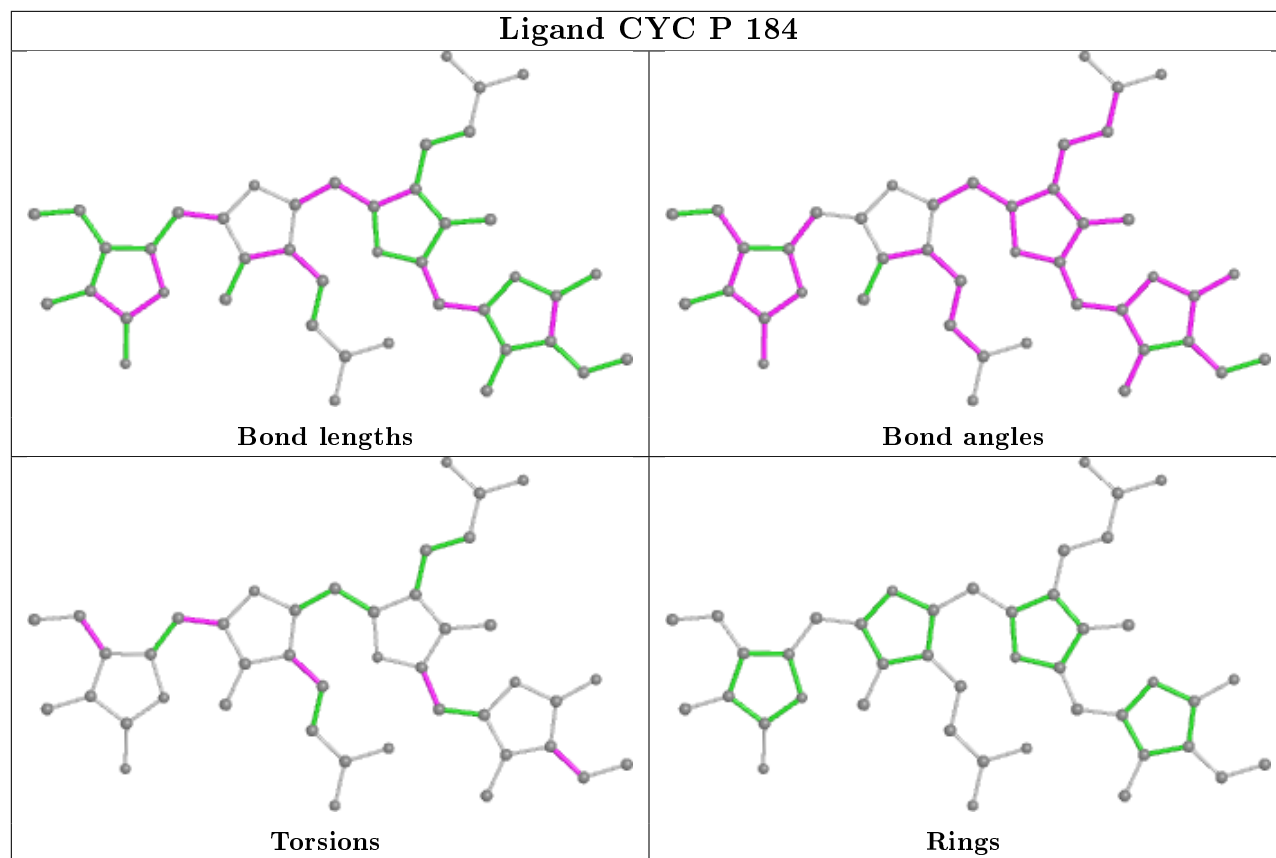


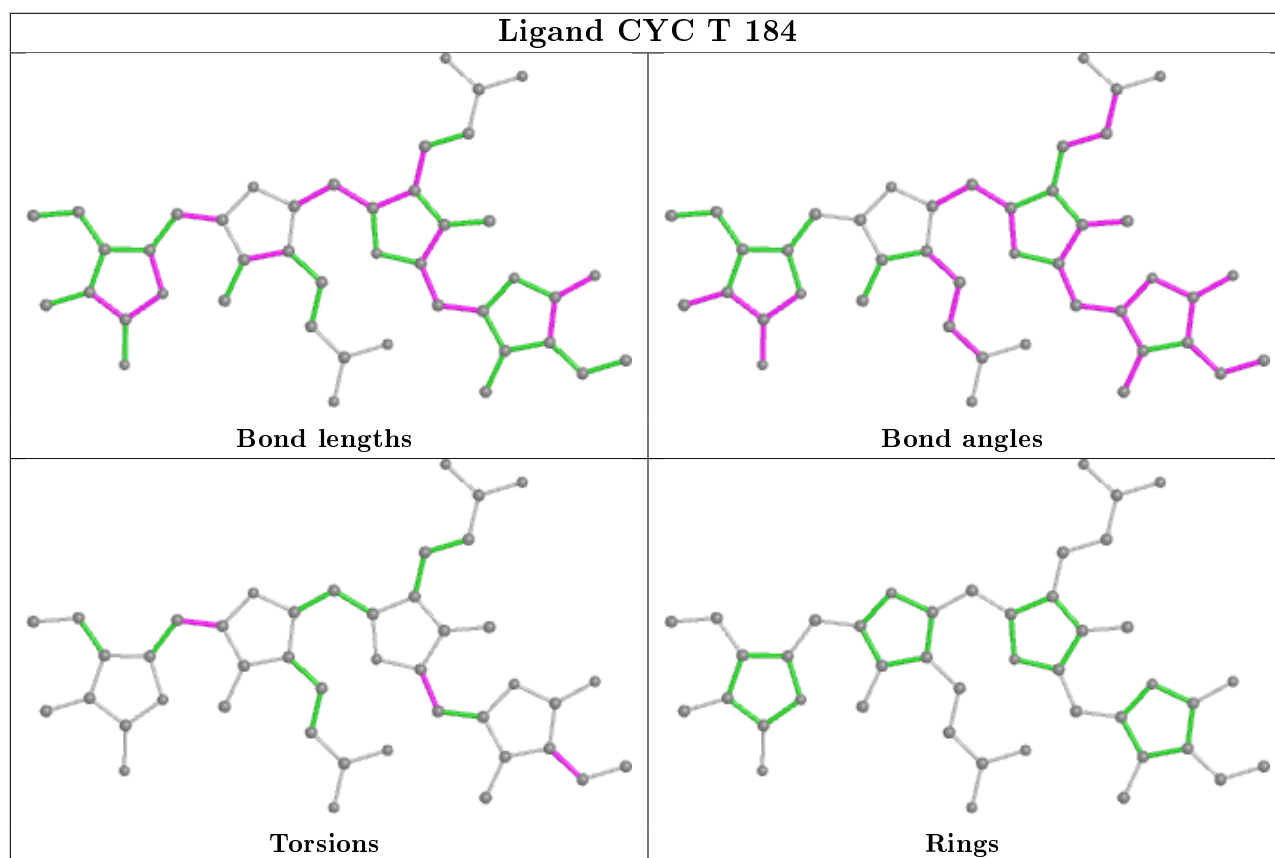
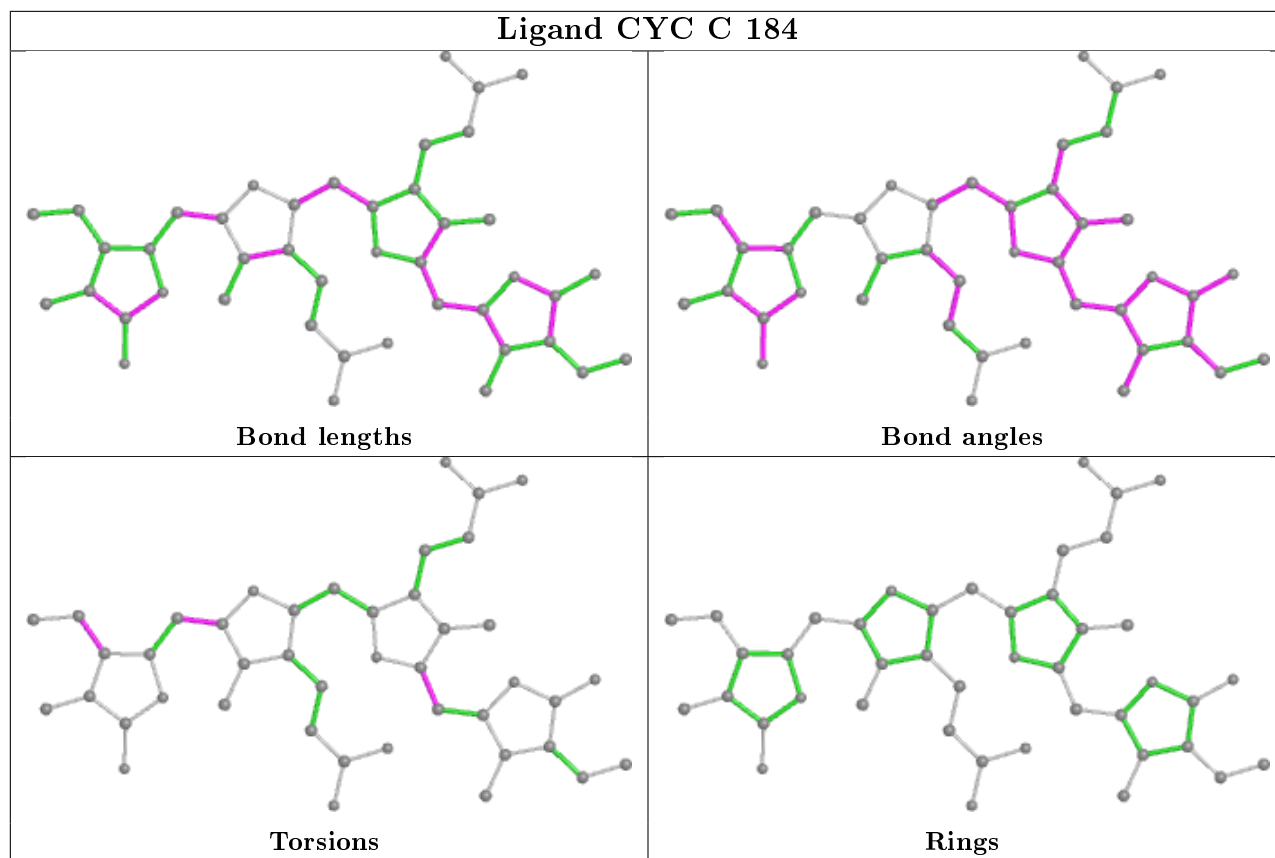




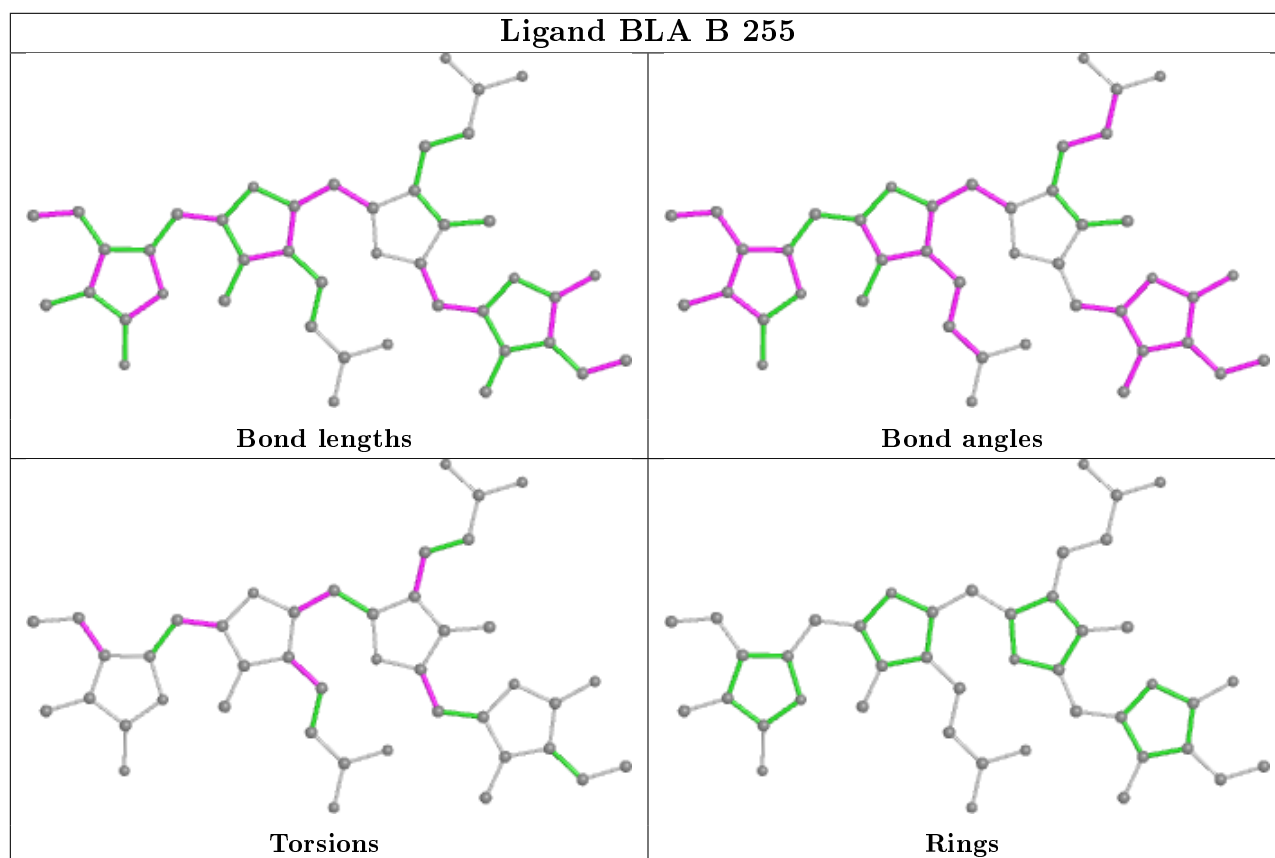
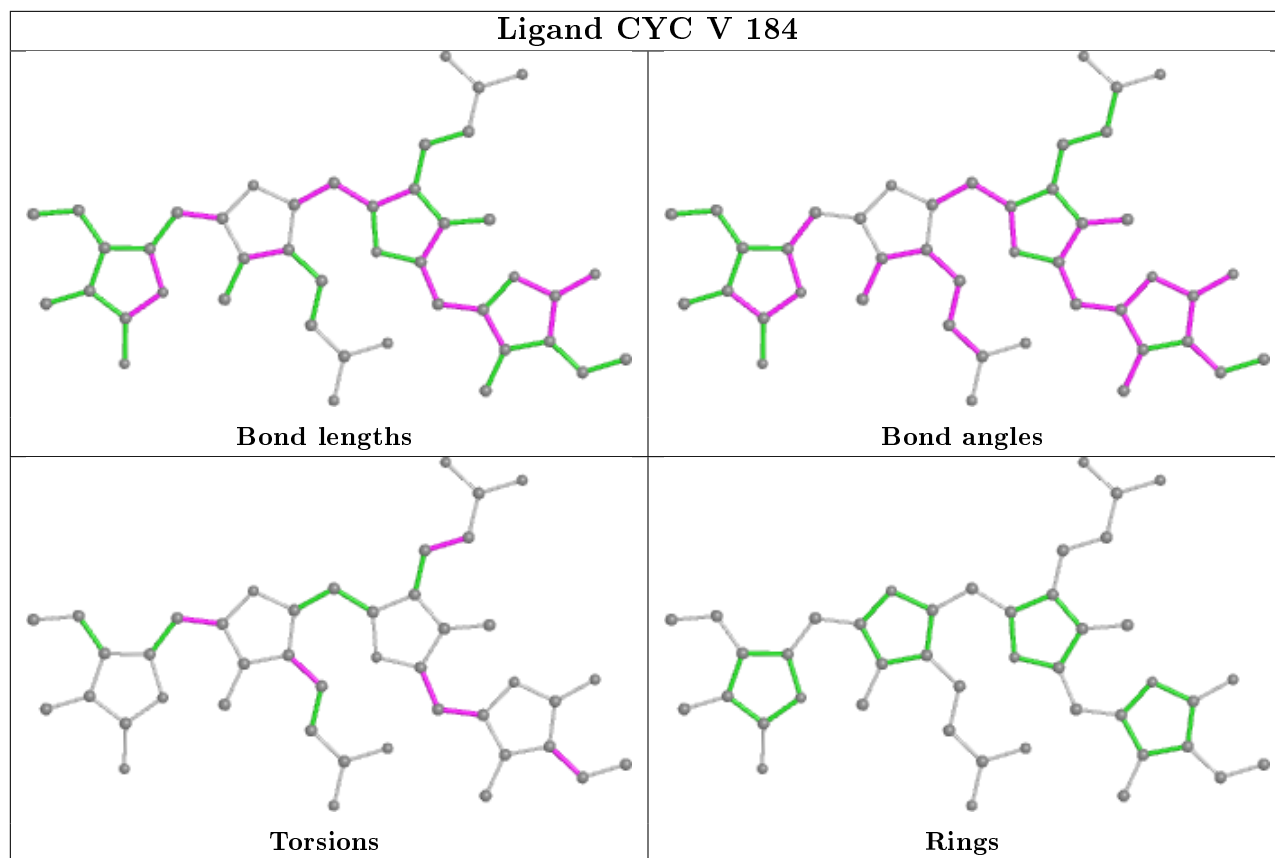


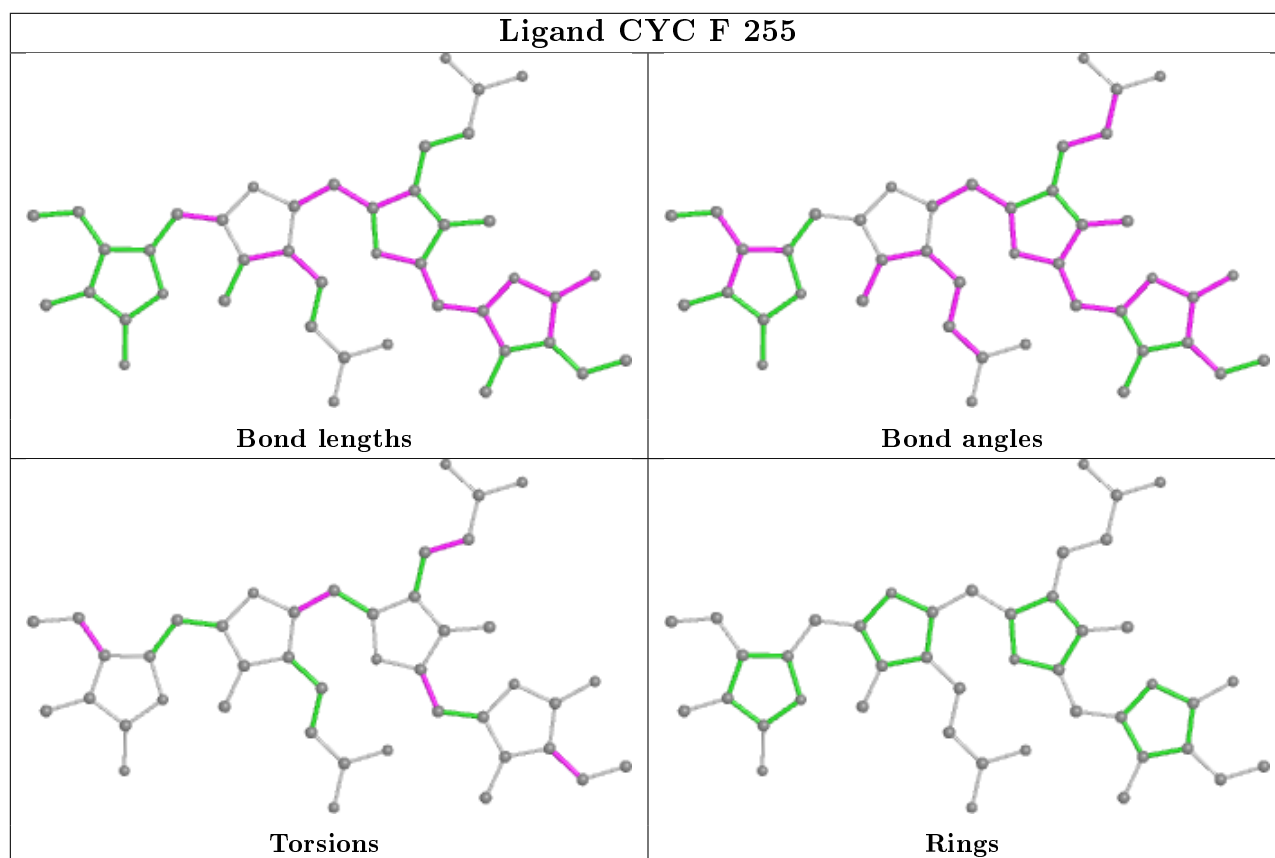
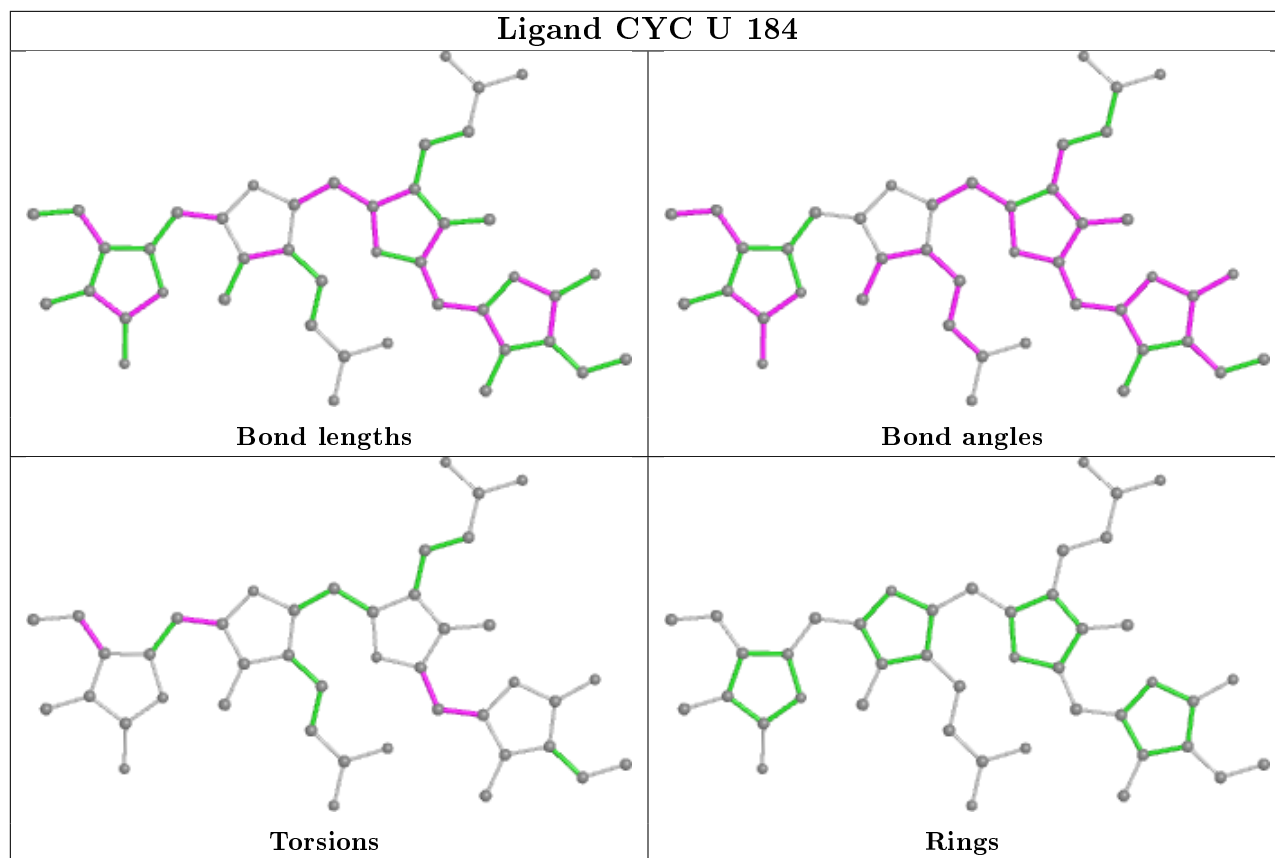


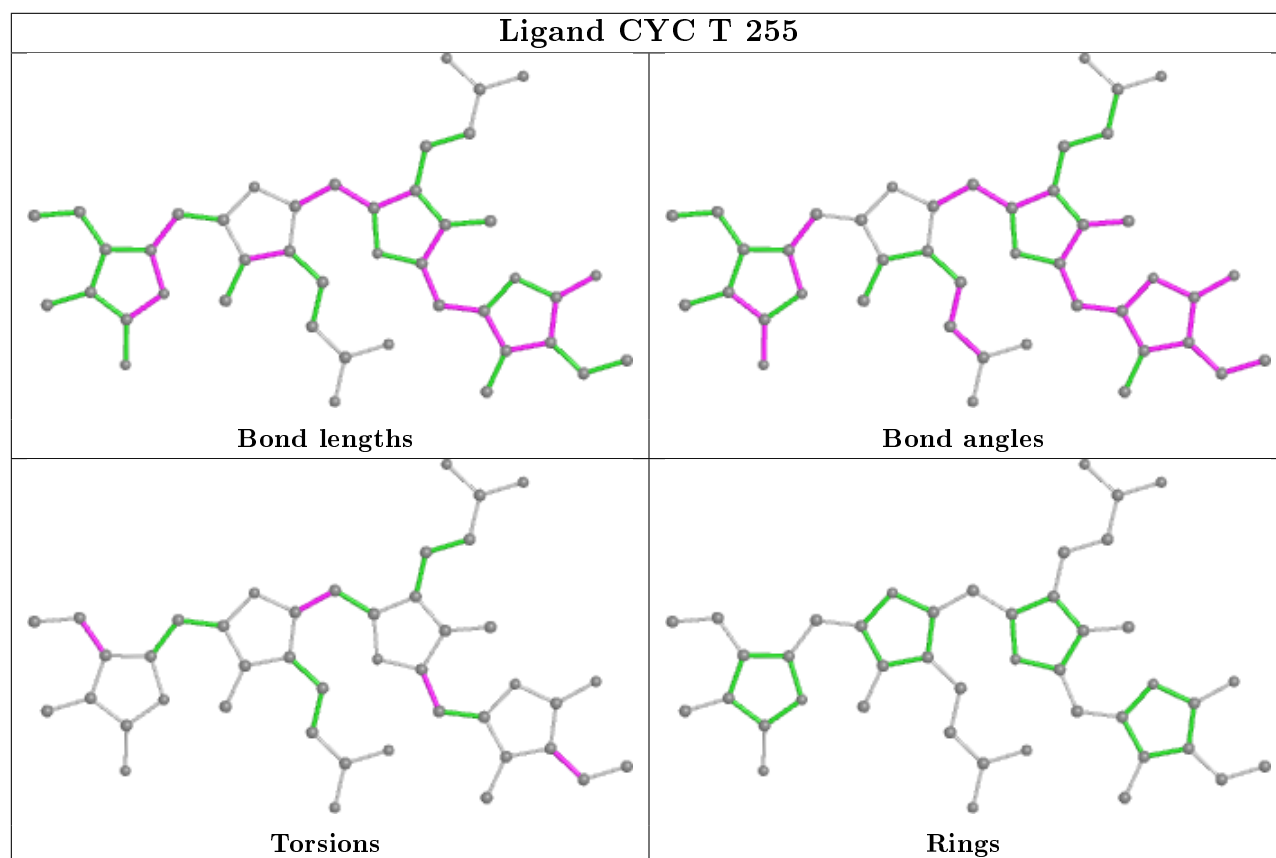
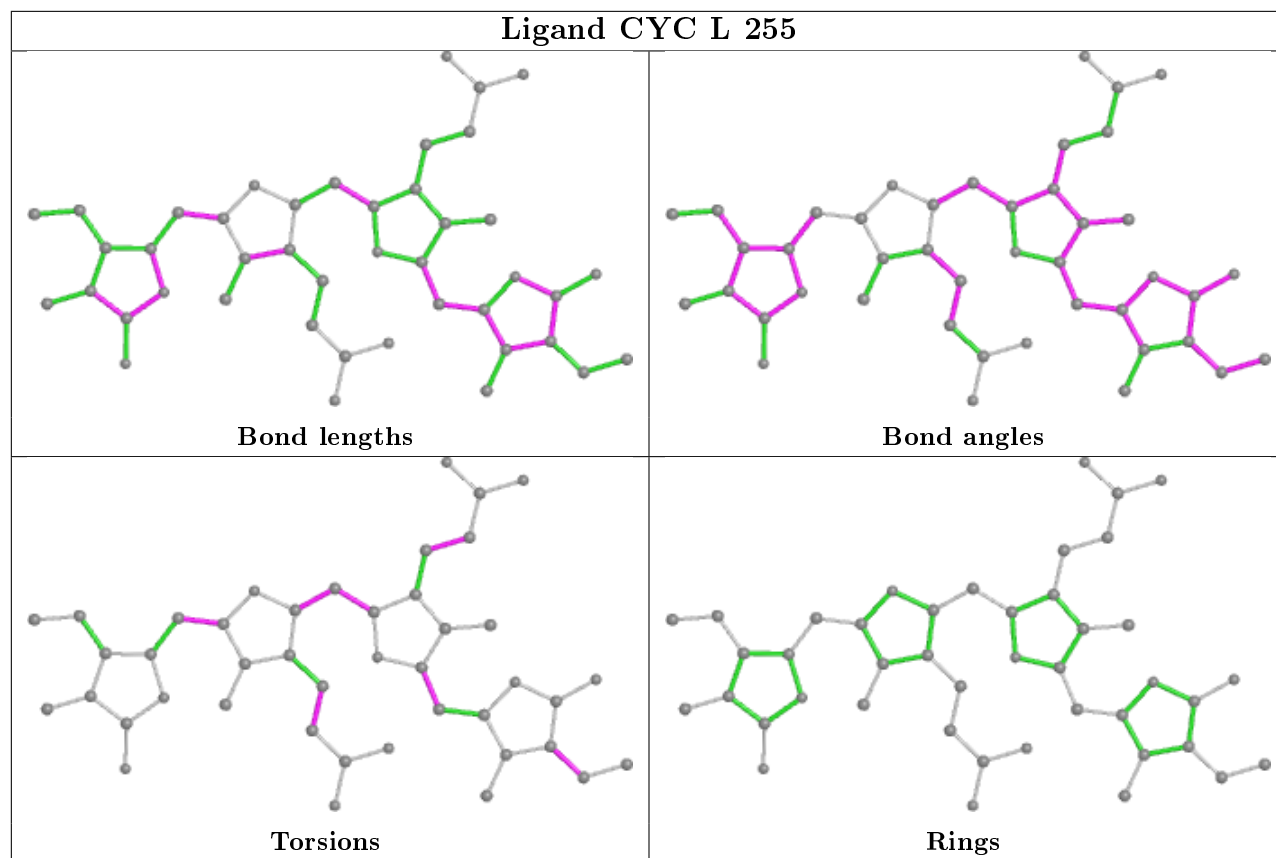


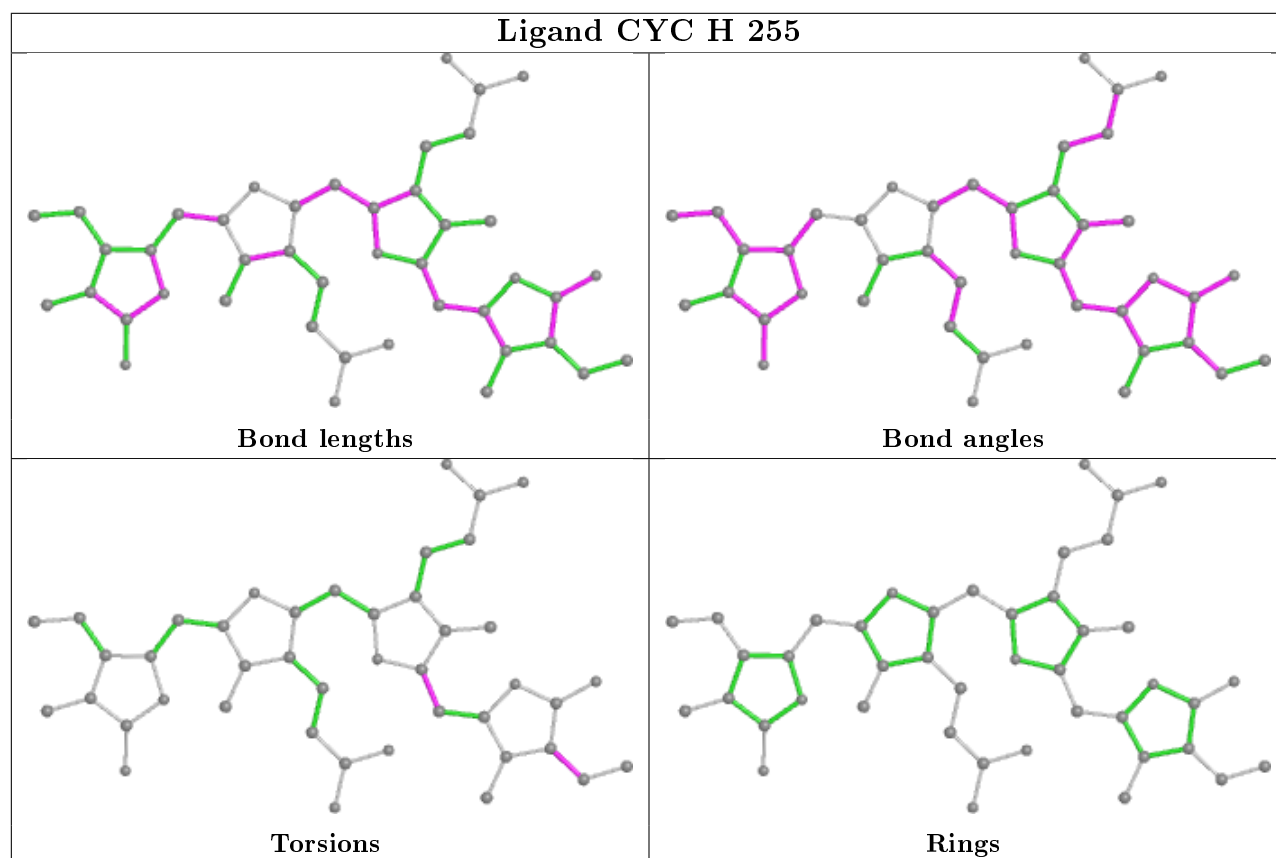
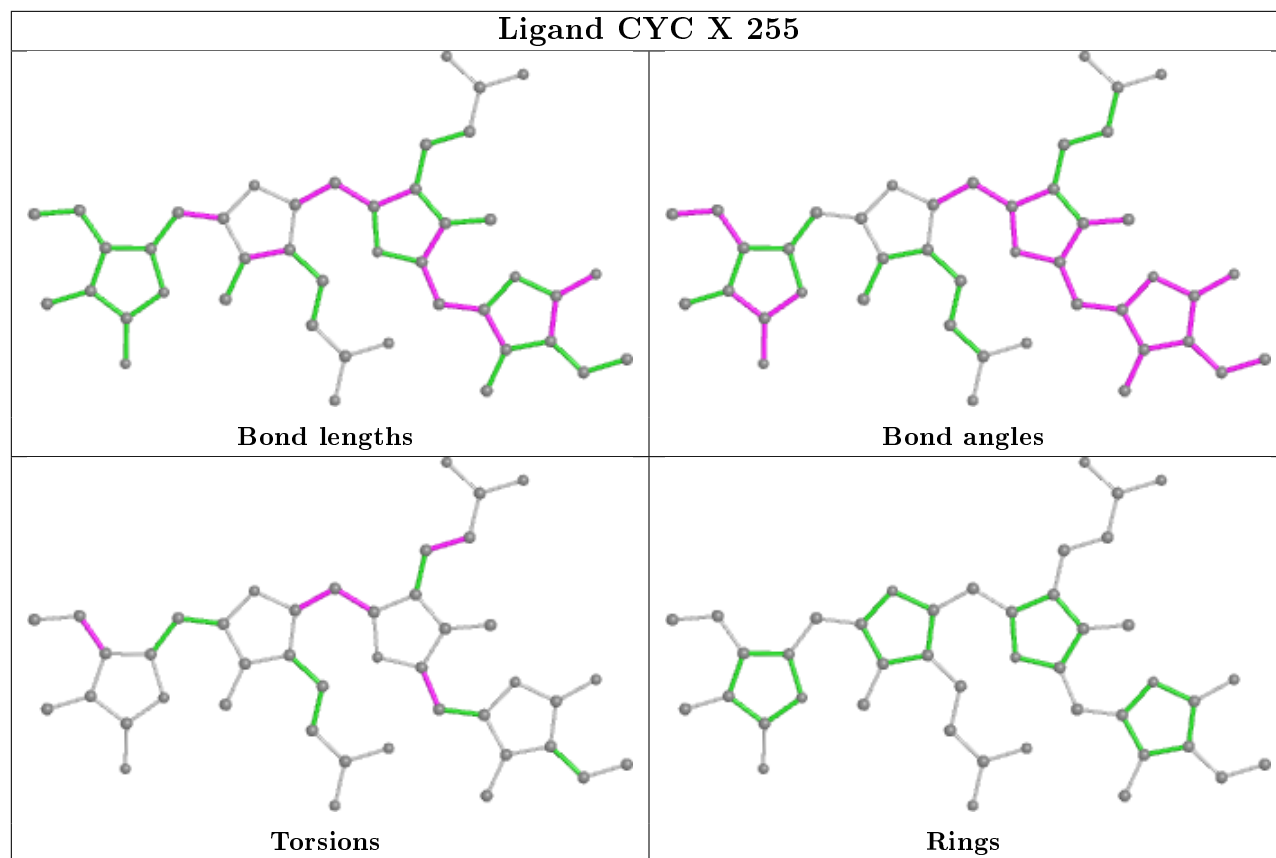


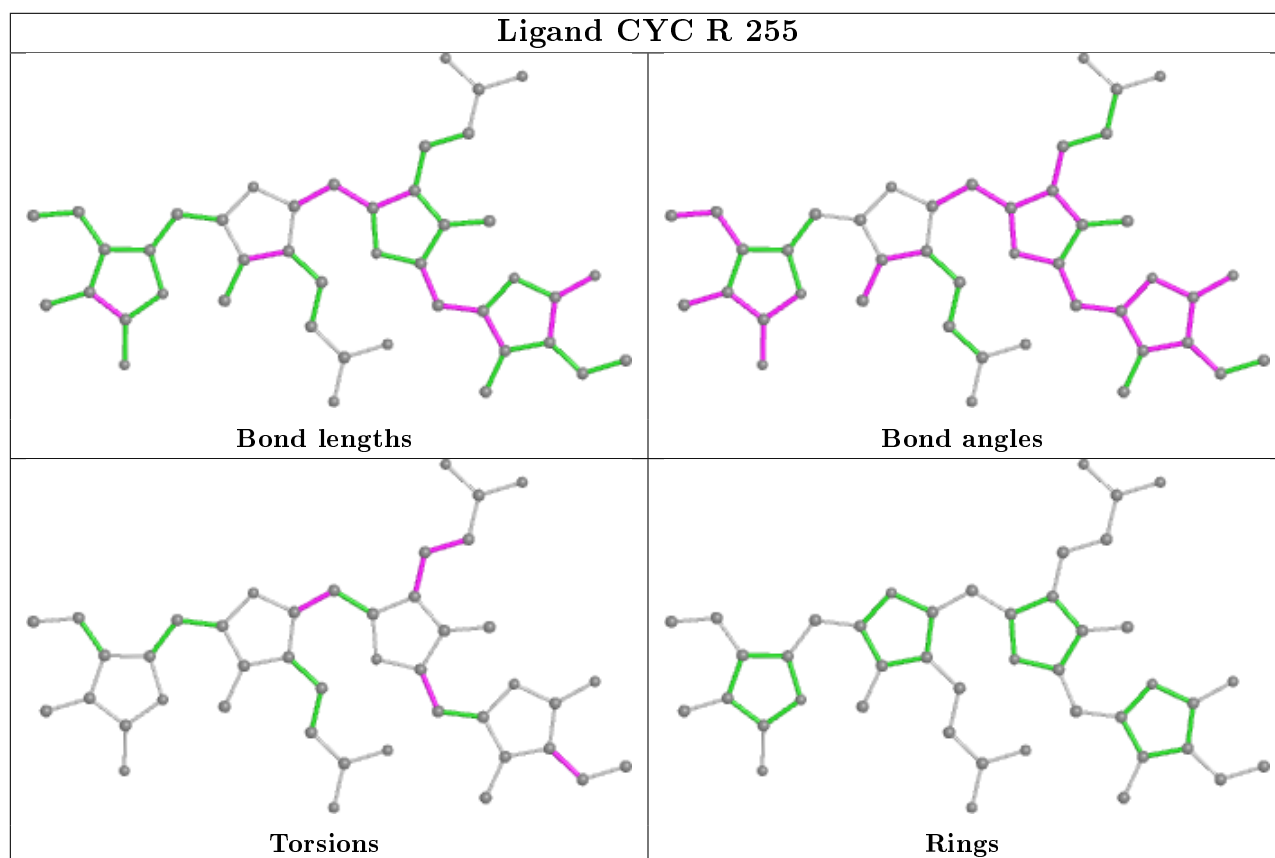
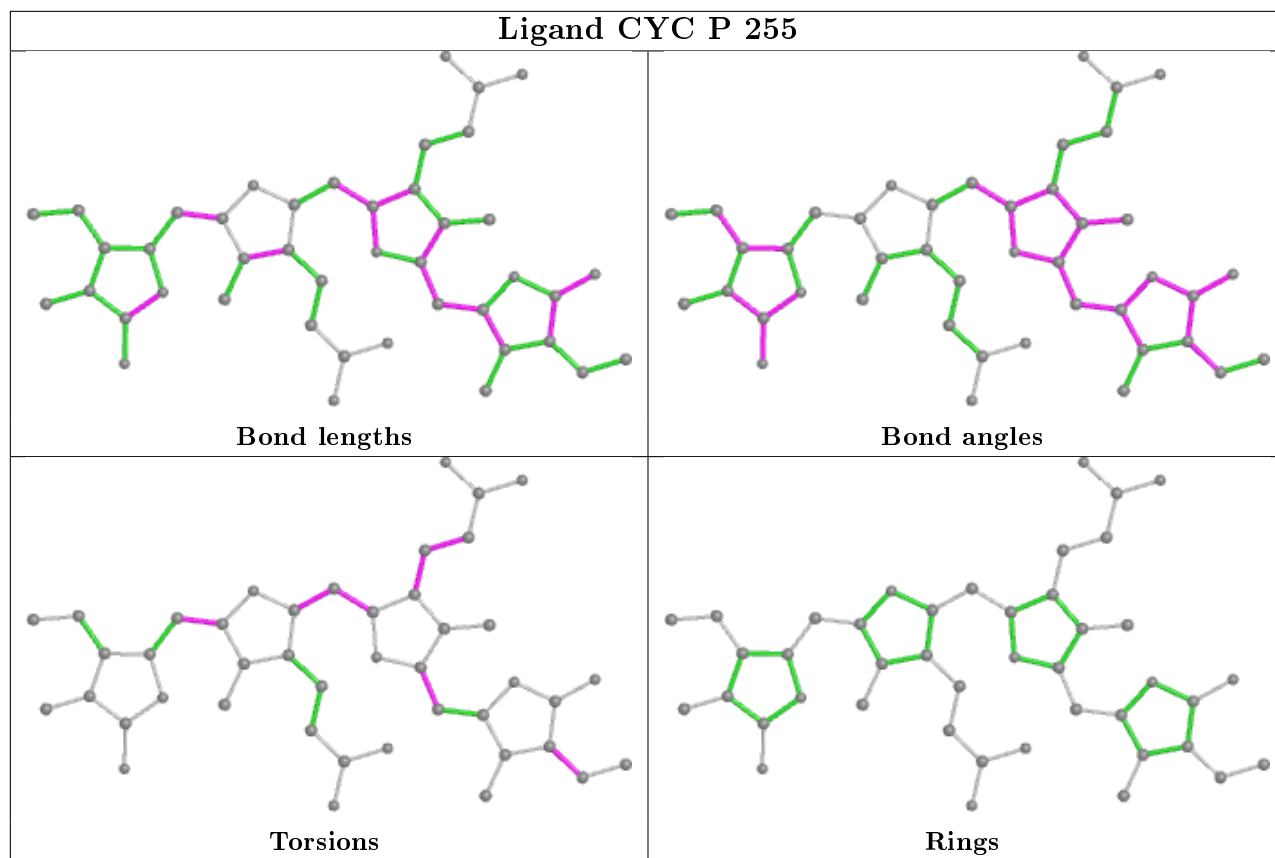


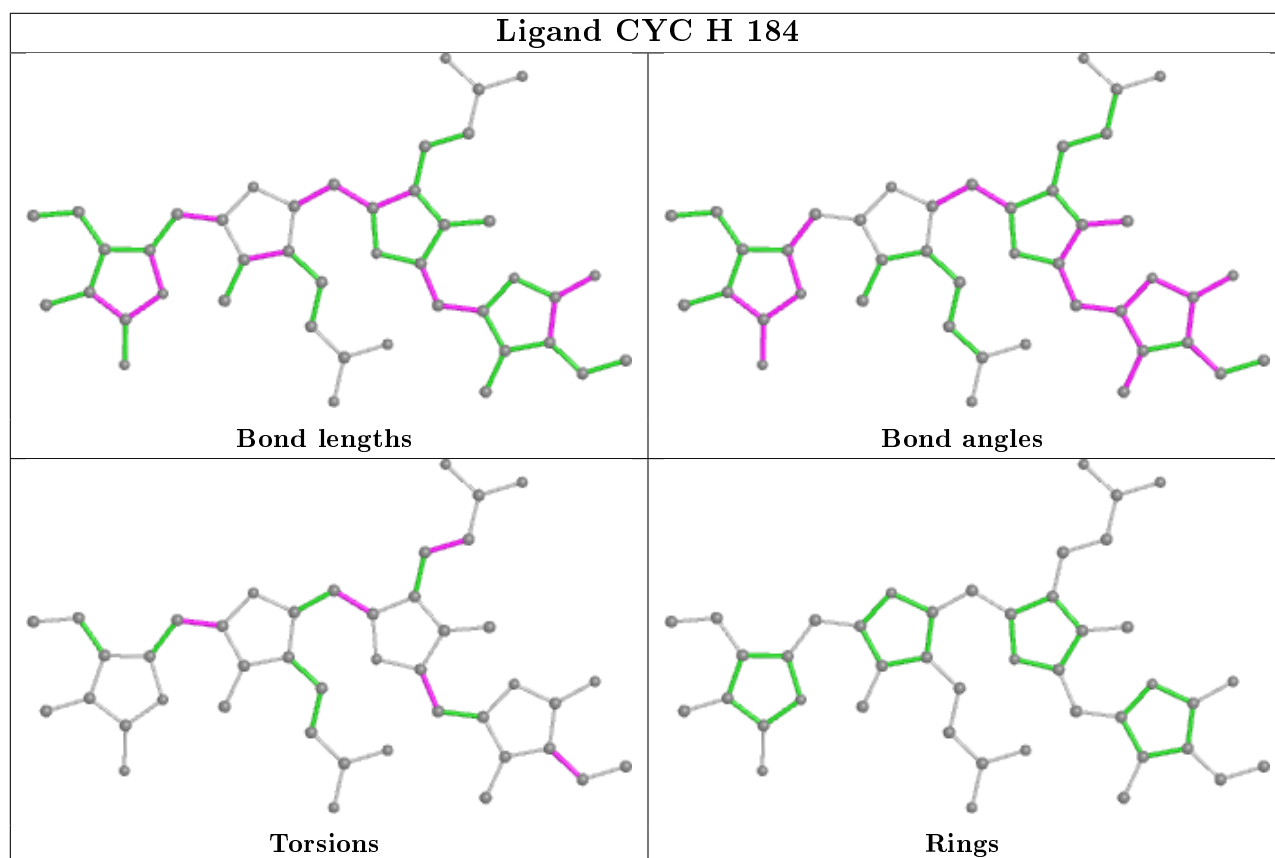
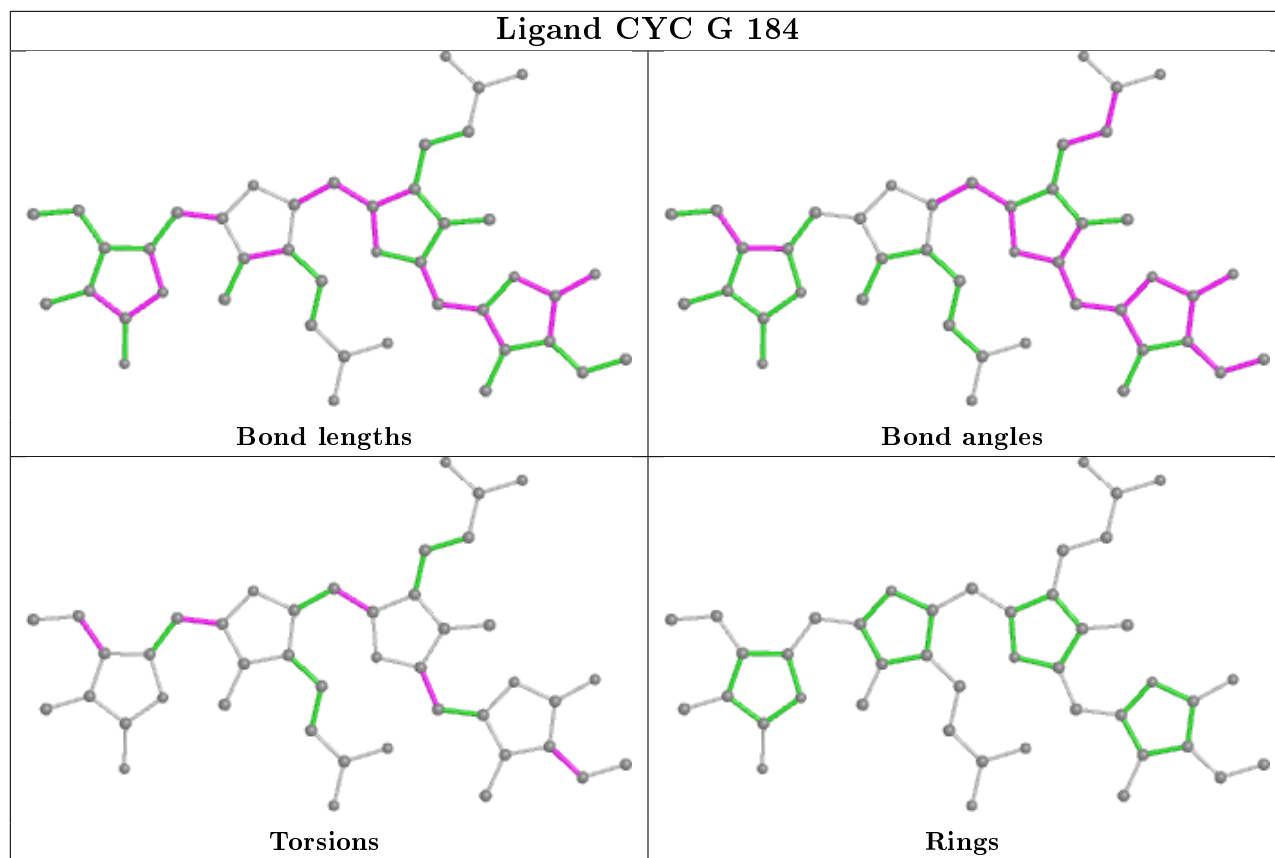


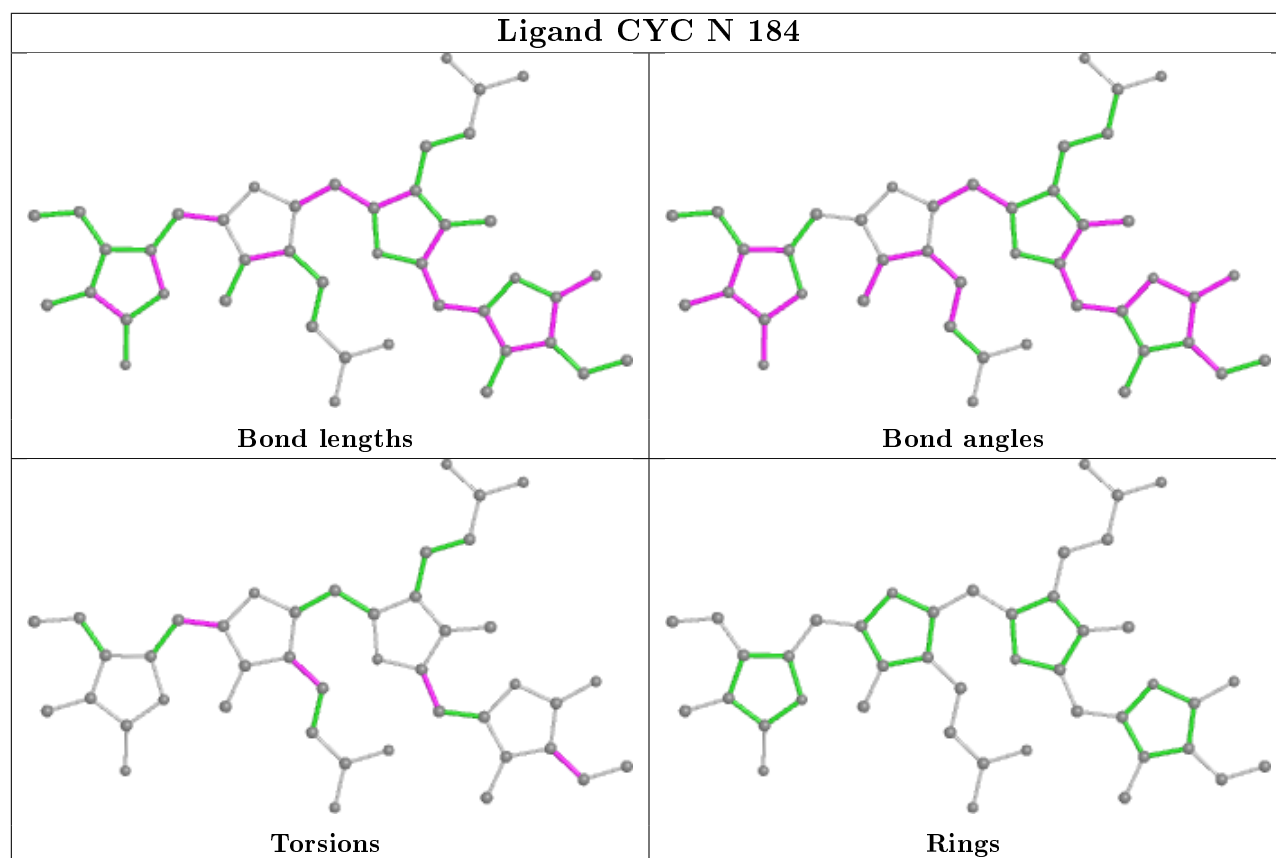
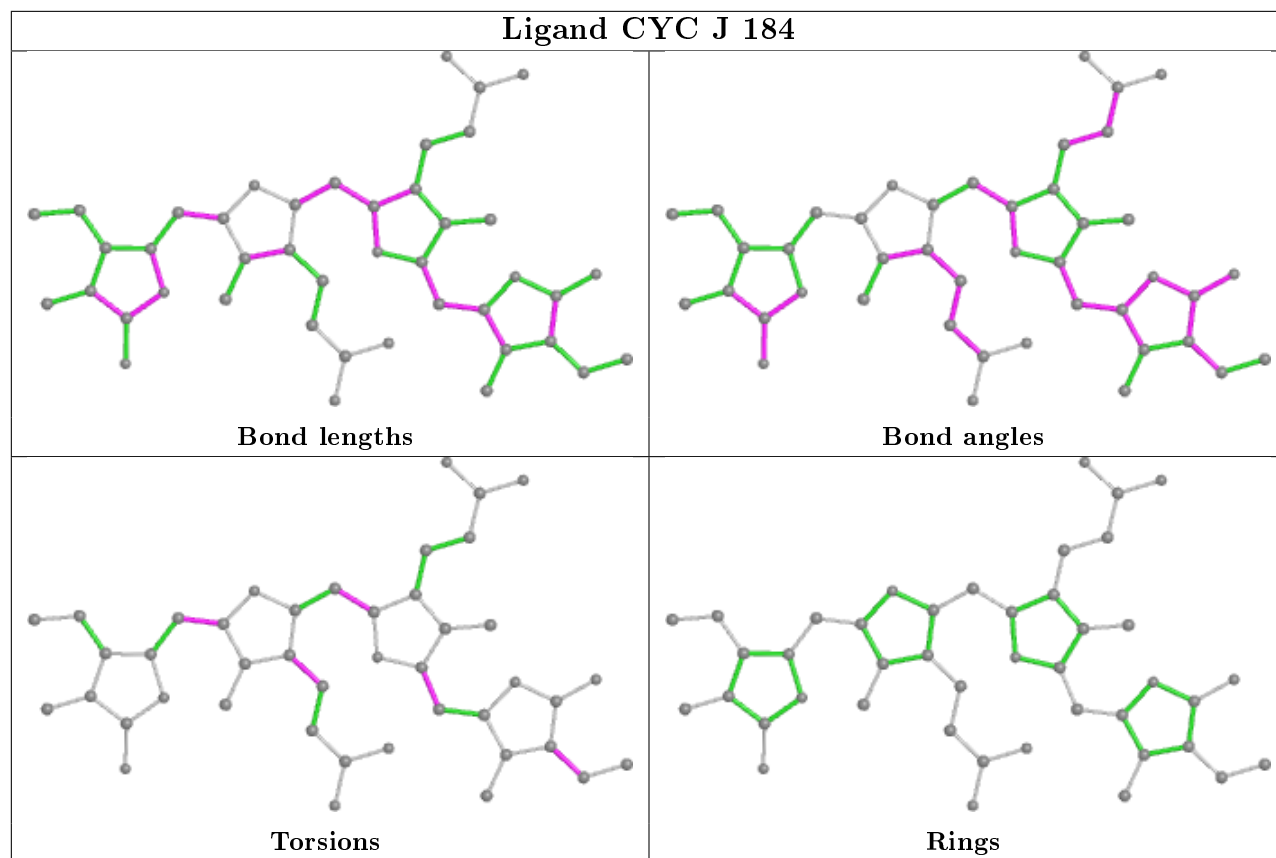


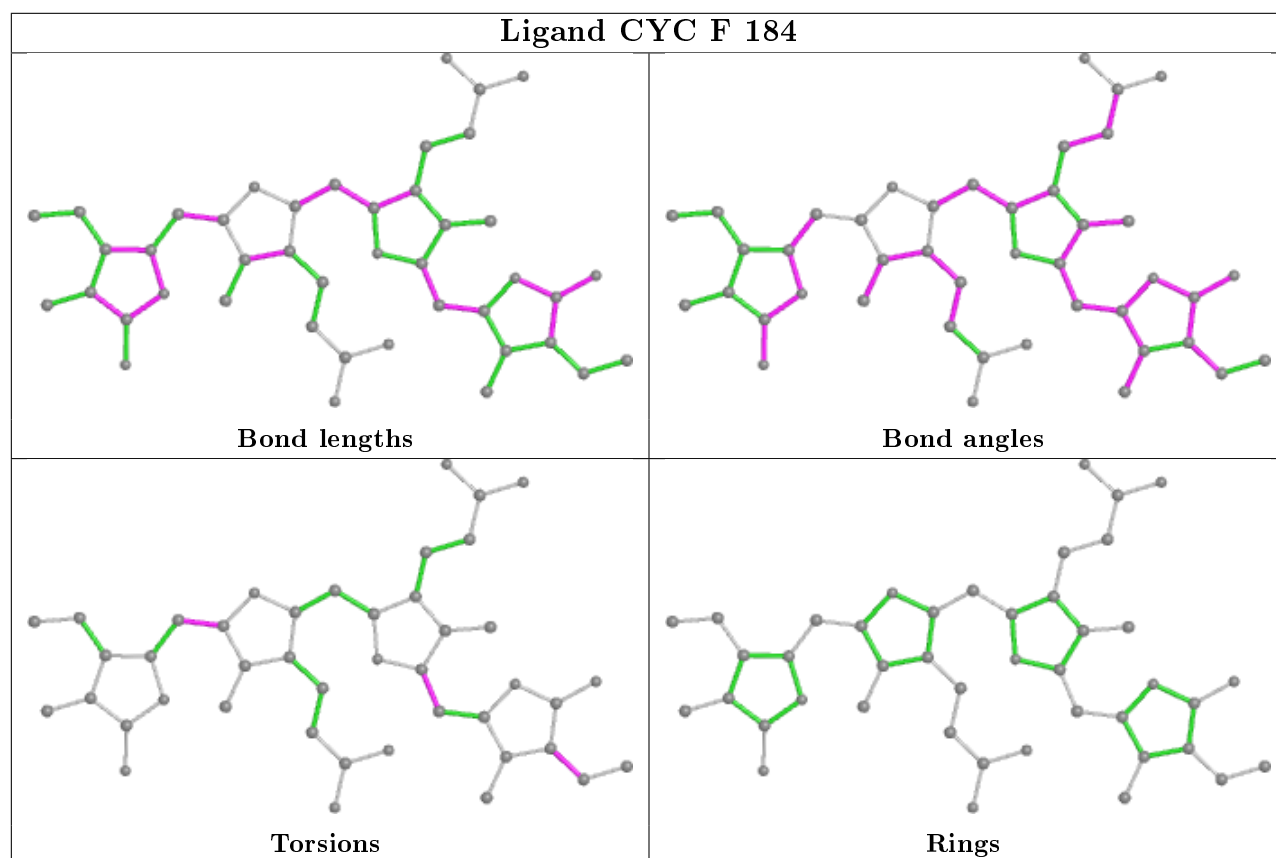
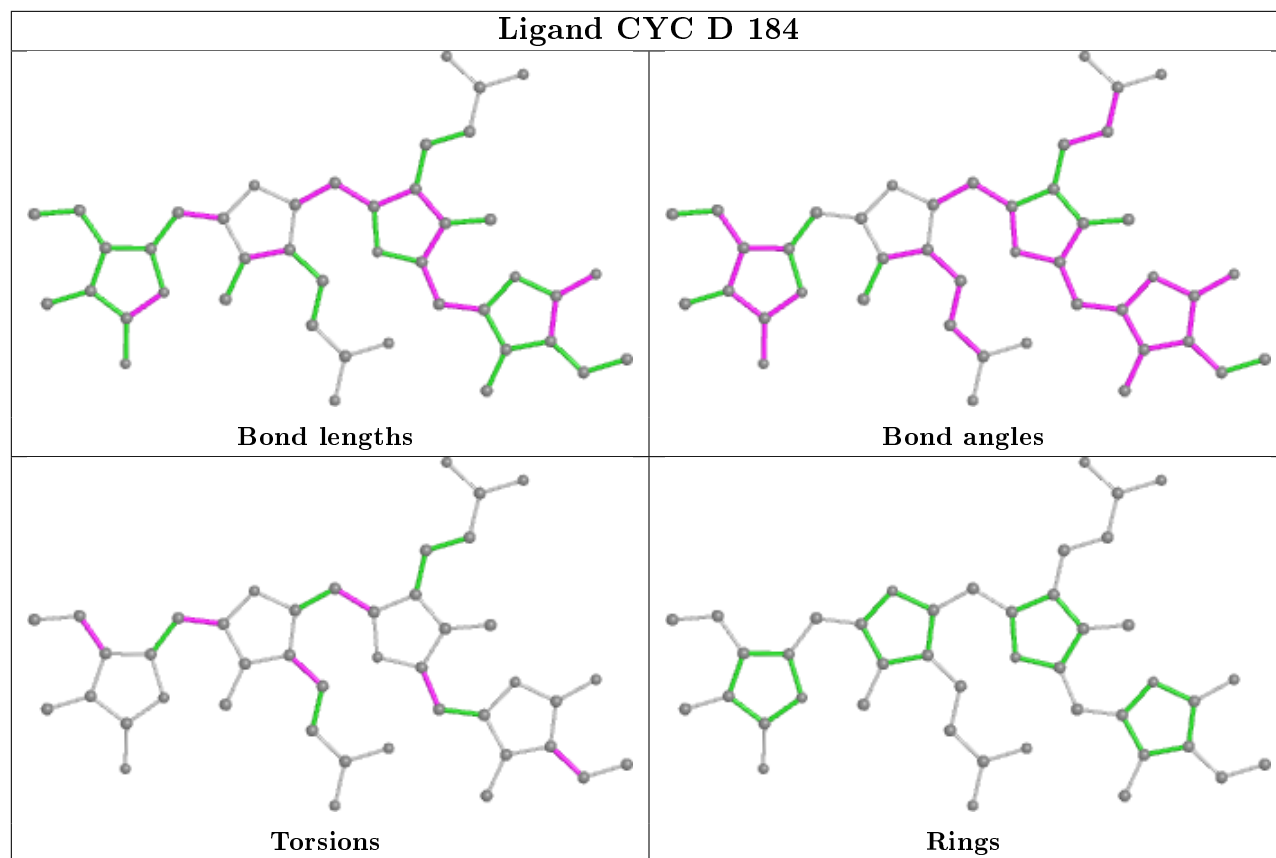














## 5.7 Other polymers [i](#)

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 i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	162/162 (100%)	-0.51	0 100 100	2, 2, 2, 10	0
1	C	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	E	162/162 (100%)	-0.62	1 (0%) 89 72	2, 2, 2, 10	0
1	G	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	I	162/162 (100%)	-0.59	0 100 100	2, 2, 2, 10	0
1	K	162/162 (100%)	-0.55	1 (0%) 89 72	2, 2, 2, 10	0
1	M	162/162 (100%)	-0.61	0 100 100	2, 2, 2, 10	0
1	O	162/162 (100%)	-0.58	0 100 100	2, 2, 2, 10	0
1	Q	162/162 (100%)	-0.47	0 100 100	2, 2, 2, 10	0
1	S	162/162 (100%)	-0.42	1 (0%) 89 72	2, 2, 2, 10	0
1	U	162/162 (100%)	-0.56	0 100 100	2, 2, 2, 10	0
1	W	162/162 (100%)	-0.59	1 (0%) 89 72	2, 2, 2, 10	0
2	B	172/172 (100%)	-0.42	0 100 100	2, 2, 2, 11	0
2	F	172/172 (100%)	-0.59	0 100 100	2, 2, 2, 11	0
2	H	172/172 (100%)	-0.54	0 100 100	2, 2, 2, 11	0
2	J	172/172 (100%)	-0.53	0 100 100	2, 2, 2, 11	0
2	L	172/172 (100%)	-0.59	0 100 100	2, 2, 2, 11	0
2	N	172/172 (100%)	-0.43	0 100 100	2, 2, 2, 11	0
2	P	172/172 (100%)	-0.47	0 100 100	2, 2, 2, 11	0
2	R	172/172 (100%)	-0.47	0 100 100	2, 2, 2, 11	0
2	T	172/172 (100%)	-0.50	0 100 100	2, 2, 2, 11	0
2	V	172/172 (100%)	-0.39	0 100 100	2, 2, 2, 11	0
2	X	172/172 (100%)	-0.51	0 100 100	2, 2, 2, 11	0
3	D	172/172 (100%)	-0.43	0 100 100	2, 2, 2, 11	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4008/4008 (100%)	-0.52	4 (0%) 95 89	2, 2, 2, 11	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	162	SER	2.3
1	E	162	SER	2.1
1	S	71	GLY	2.1
1	W	162	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CYC	V	184	43/43	0.90	0.23	7,16,24,29	0
4	CYC	B	184	43/43	0.91	0.18	2,3,10,13	0
4	CYC	X	184	43/43	0.91	0.20	2,2,7,10	0
4	CYC	T	184	43/43	0.91	0.19	2,3,10,15	0
4	CYC	R	184	43/43	0.91	0.20	2,4,19,24	0
4	CYC	D	184	43/43	0.91	0.21	2,11,23,26	0
4	CYC	N	184	43/43	0.92	0.18	2,5,12,14	0
4	CYC	N	255	43/43	0.92	0.22	2,10,23,28	0
4	CYC	F	184	43/43	0.92	0.19	2,2,13,15	0
5	BLA	B	255	43/43	0.93	0.18	2,4,9,15	0
4	CYC	H	184	43/43	0.93	0.19	2,6,19,28	0
4	CYC	V	255	43/43	0.93	0.17	2,2,10,15	0
4	CYC	J	255	43/43	0.93	0.20	2,2,2,7	0

Continued on next page...

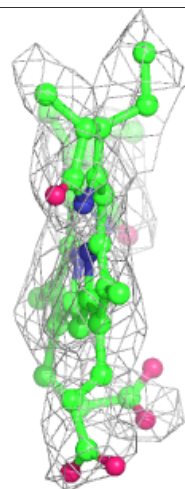
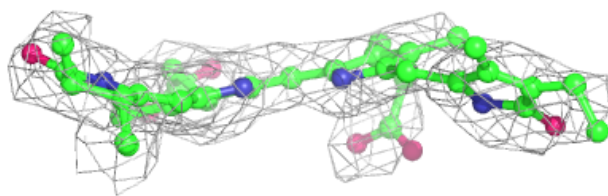
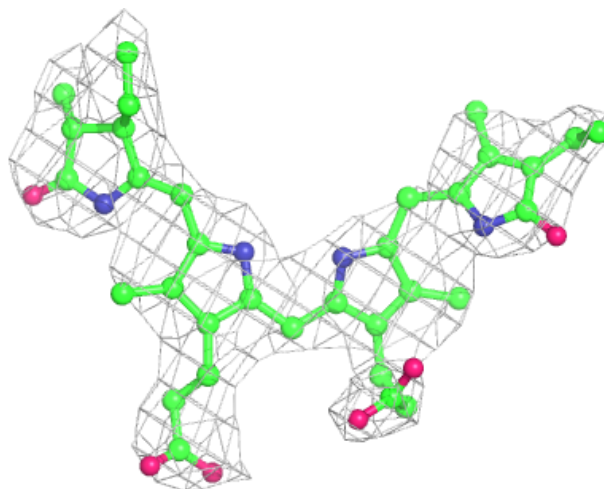
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CYC	L	184	43/43	0.93	0.17	2,5,15,23	0
4	CYC	X	255	43/43	0.94	0.20	2,2,7,10	0
4	CYC	M	184	43/43	0.94	0.17	2,2,3,5	0
4	CYC	J	184	43/43	0.94	0.18	2,2,9,10	0
4	CYC	D	255	43/43	0.94	0.18	3,8,17,18	0
4	CYC	P	184	43/43	0.94	0.18	2,2,11,18	0
4	CYC	L	255	43/43	0.94	0.19	2,2,2,11	0
4	CYC	I	184	43/43	0.95	0.17	2,2,2,3	0
4	CYC	T	255	43/43	0.95	0.17	2,2,5,8	0
4	CYC	A	184	43/43	0.95	0.15	2,2,2,3	0
4	CYC	H	255	43/43	0.95	0.17	2,2,7,10	0
4	CYC	P	255	43/43	0.95	0.16	2,3,10,11	0
4	CYC	R	255	43/43	0.95	0.16	2,2,7,9	0
4	CYC	C	184	43/43	0.95	0.17	2,2,3,4	0
4	CYC	K	184	43/43	0.95	0.16	2,2,3,6	0
4	CYC	S	184	43/43	0.95	0.15	2,6,11,14	0
4	CYC	Q	184	43/43	0.95	0.15	2,2,5,7	0
4	CYC	F	255	43/43	0.95	0.15	2,2,2,2	0
4	CYC	U	184	43/43	0.96	0.15	2,2,2,5	0
4	CYC	O	184	43/43	0.96	0.15	2,2,2,2	0
4	CYC	G	184	43/43	0.96	0.17	2,2,2,2	0
4	CYC	E	184	43/43	0.96	0.14	2,2,2,2	0
4	CYC	W	184	43/43	0.97	0.14	2,2,2,2	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

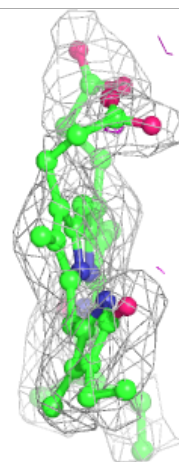
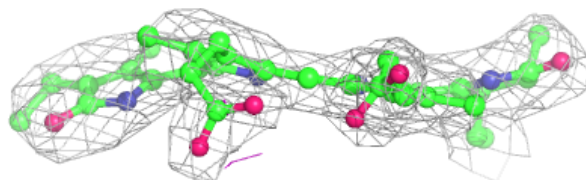
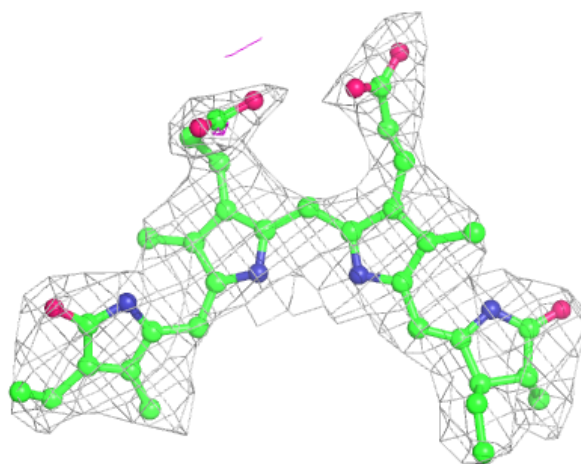
**Electron density around CYC V 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



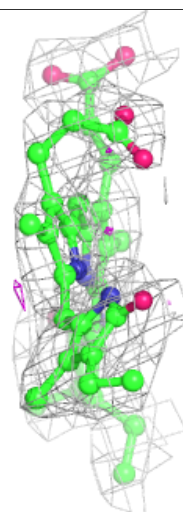
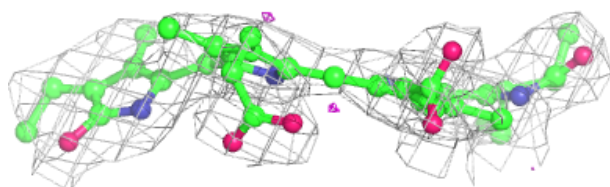
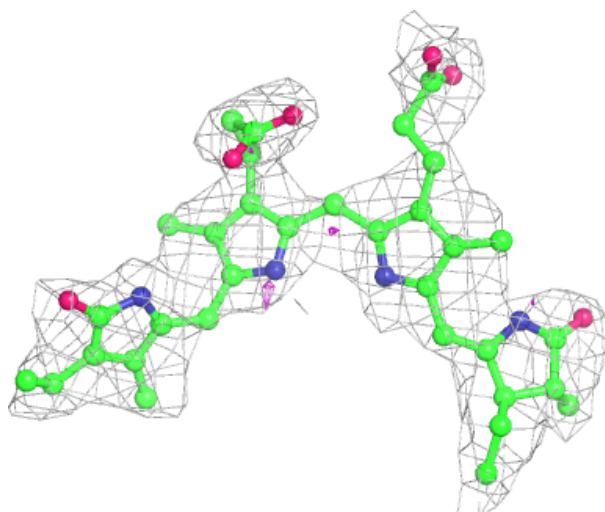
**Electron density around CYC B 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



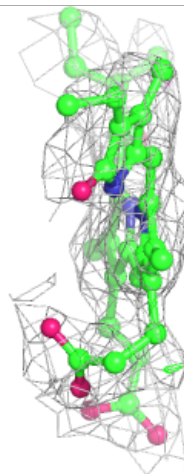
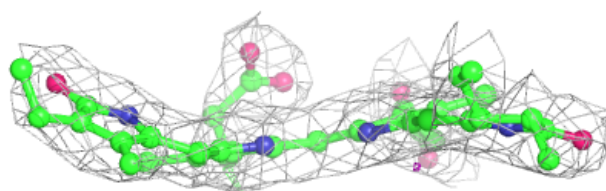
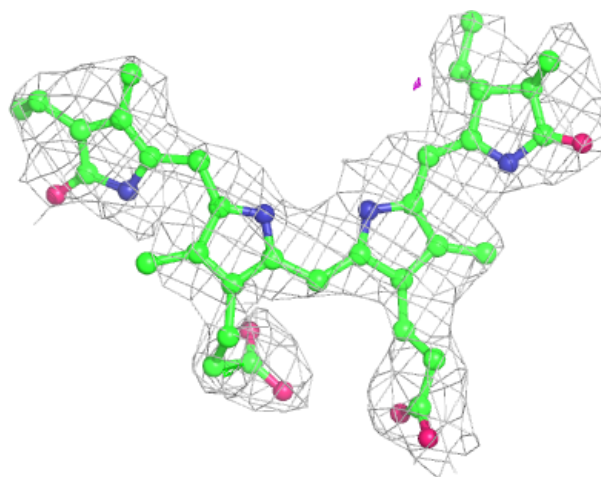
**Electron density around CYC X 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CYC T 184:**

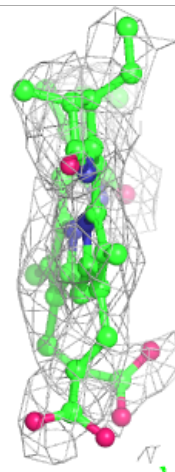
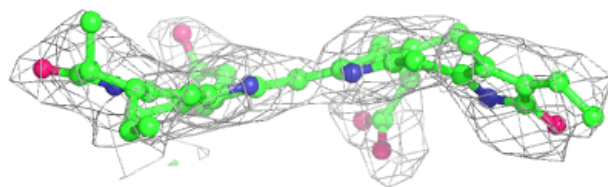
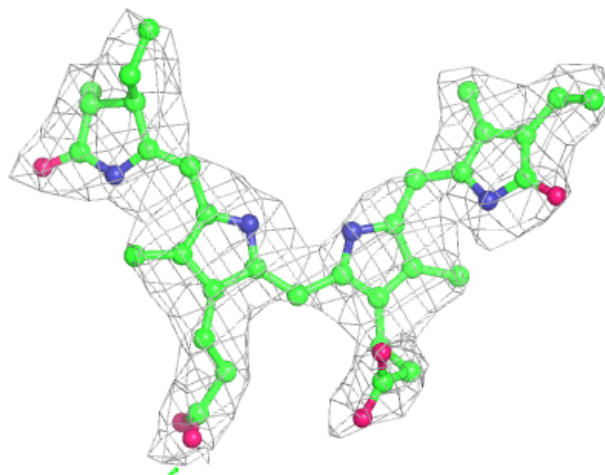
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





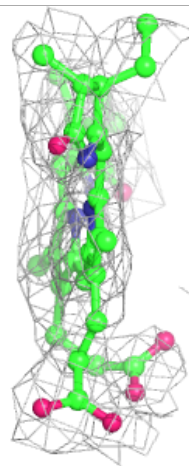
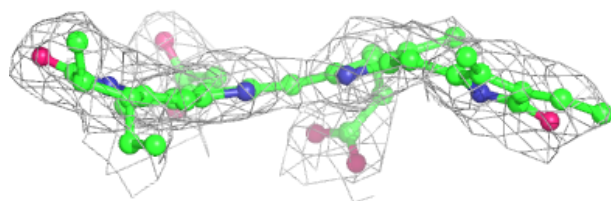
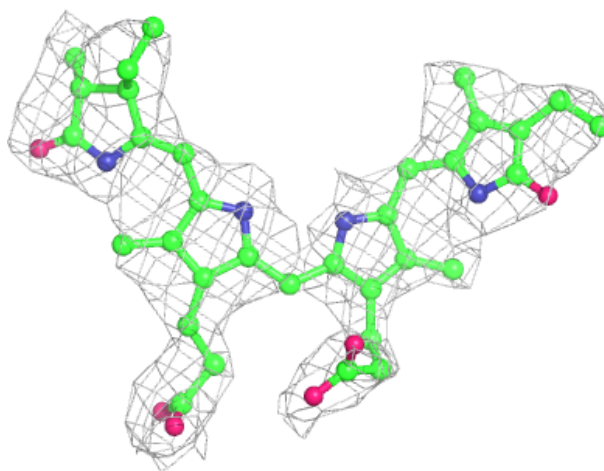
**Electron density around CYC R 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



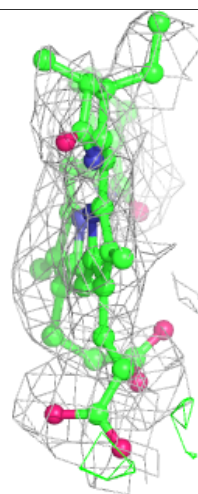
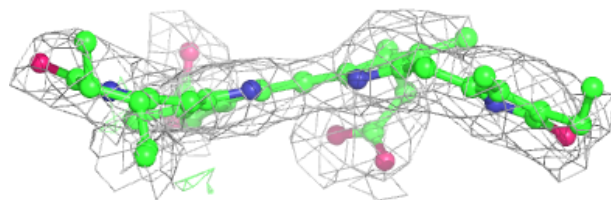
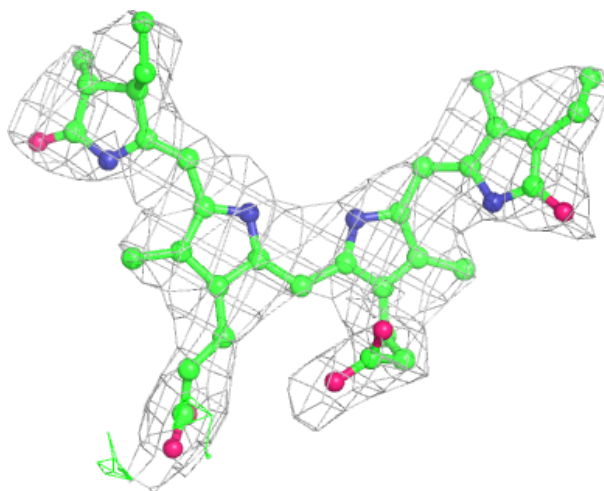
**Electron density around CYC D 184:**

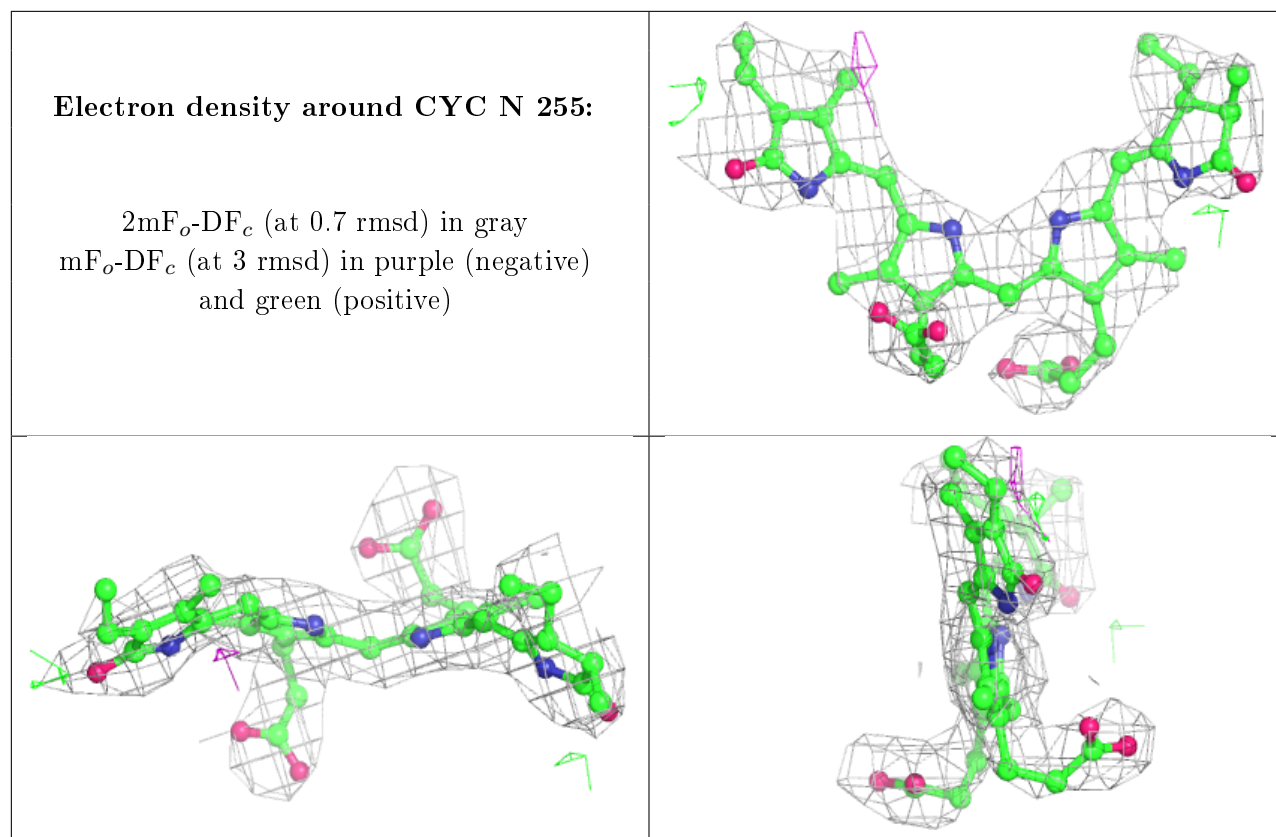
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

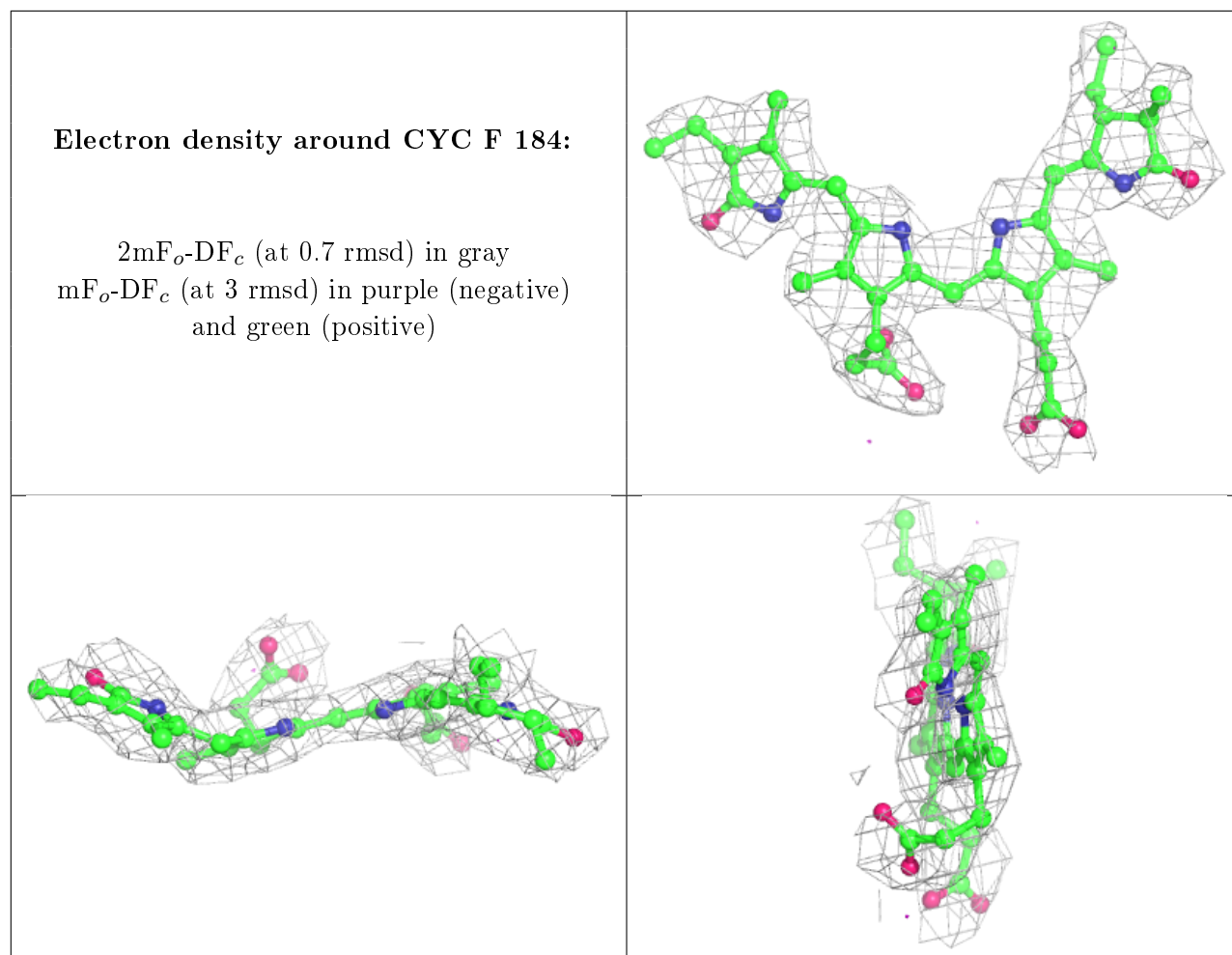


**Electron density around CYC N 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

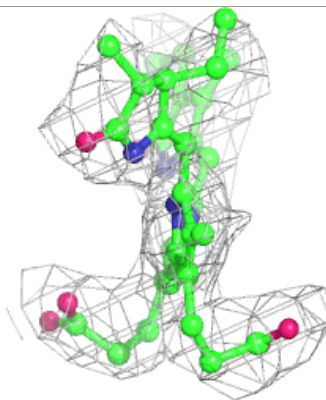
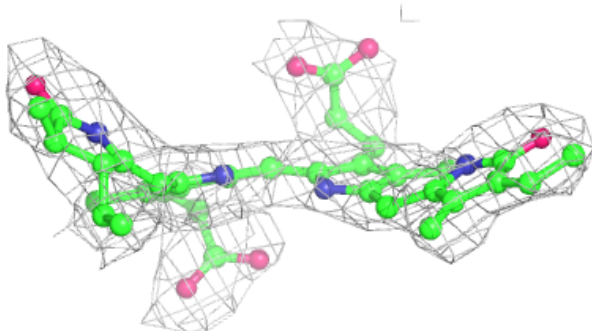
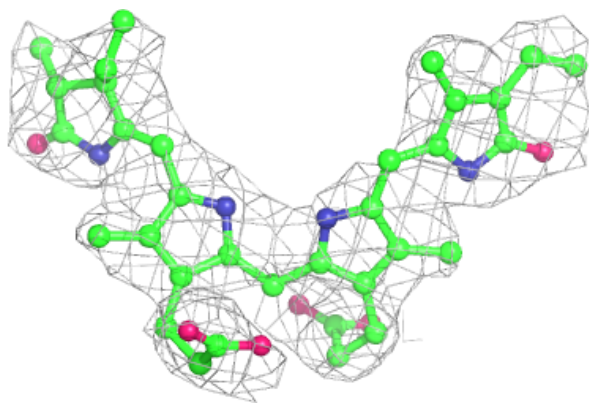






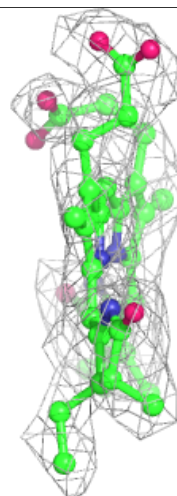
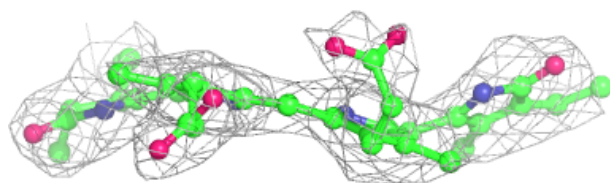
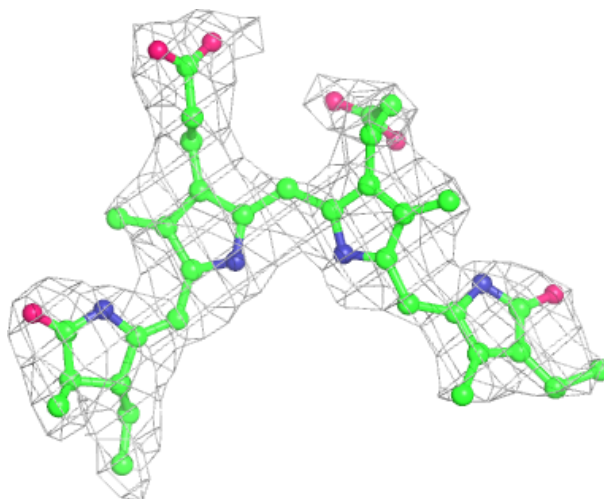
**Electron density around BLA B 255:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



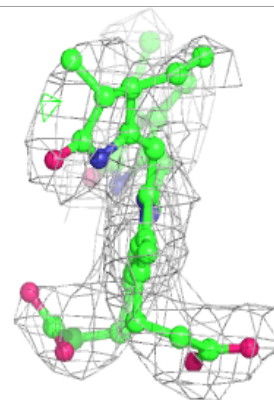
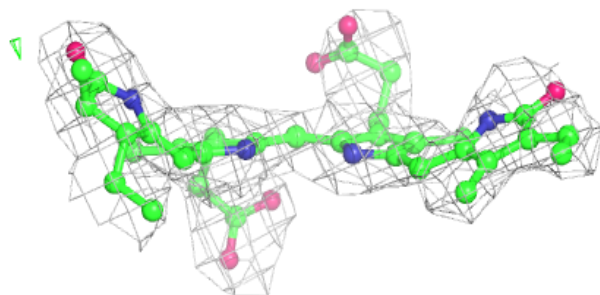
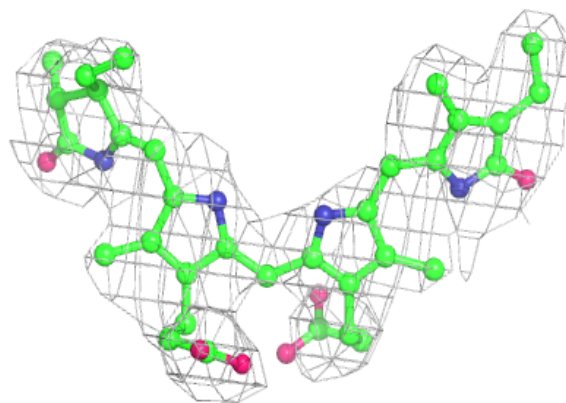
**Electron density around CYC H 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

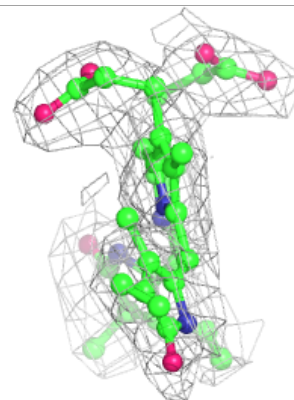
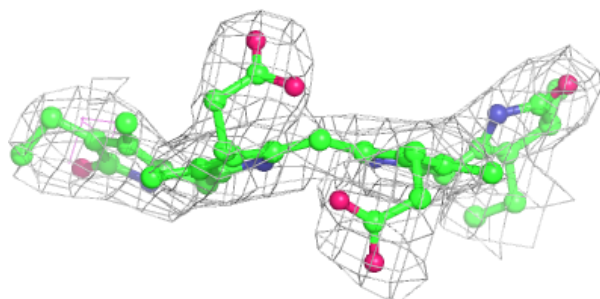
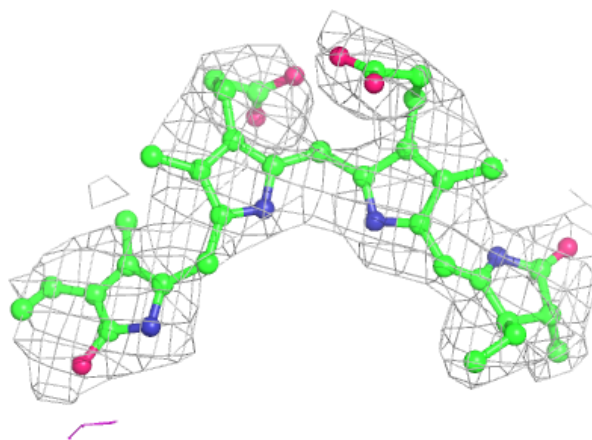


**Electron density around CYC V 255:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CYC J 255:**

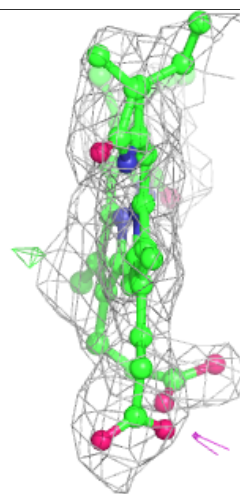
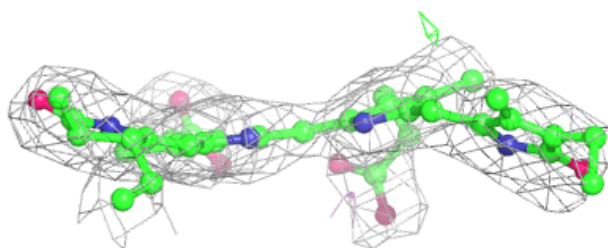
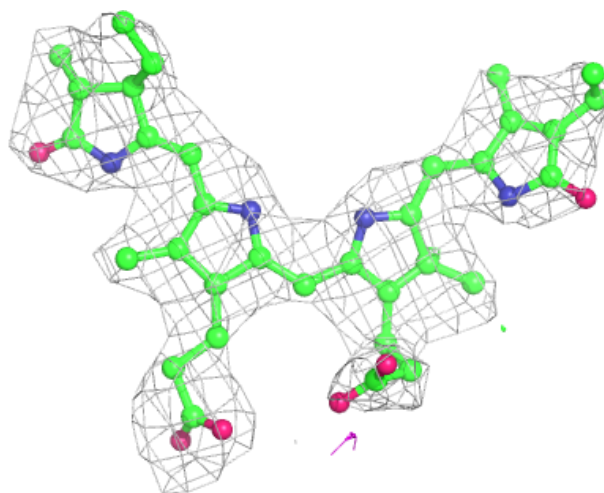
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

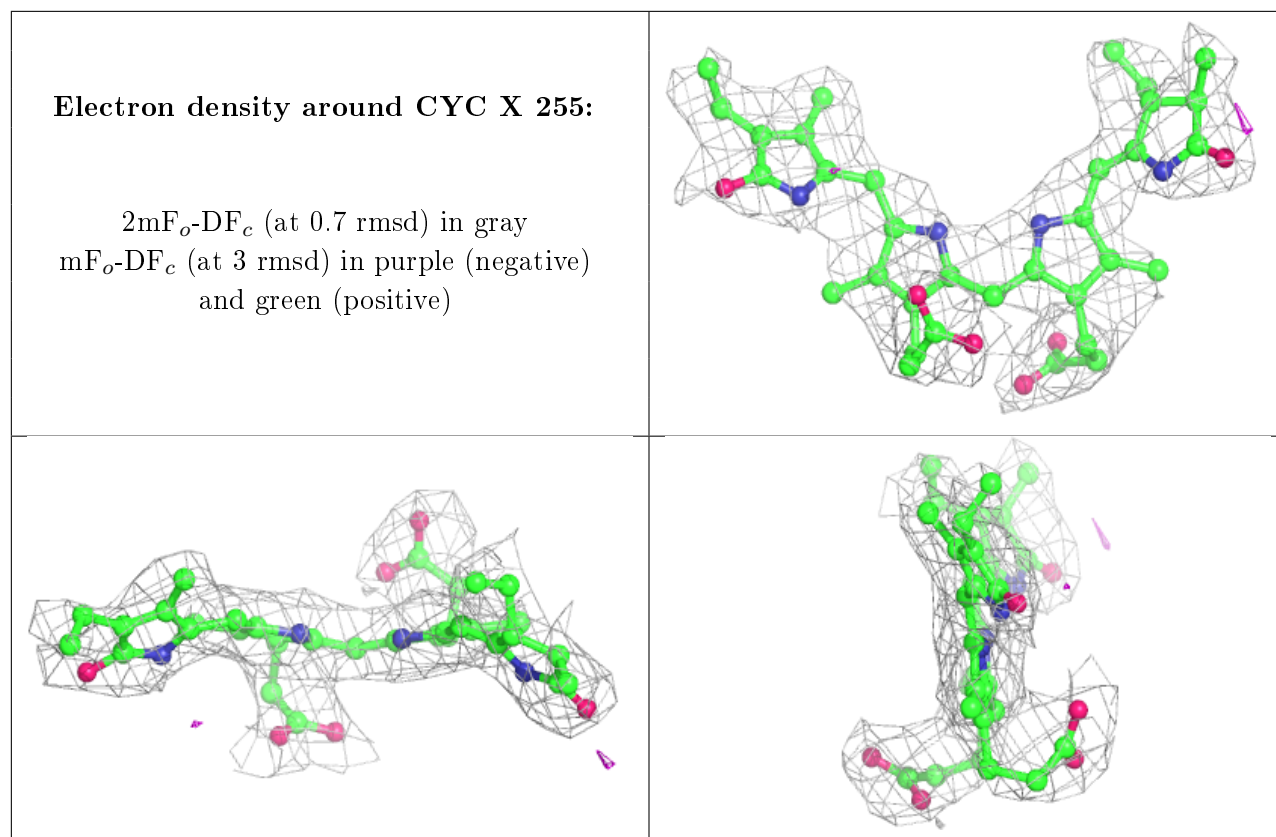




**Electron density around CYC L 184:**

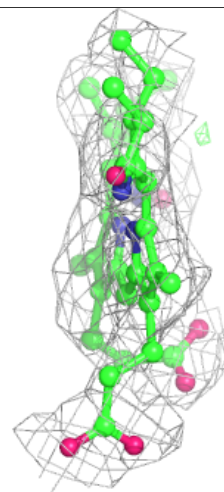
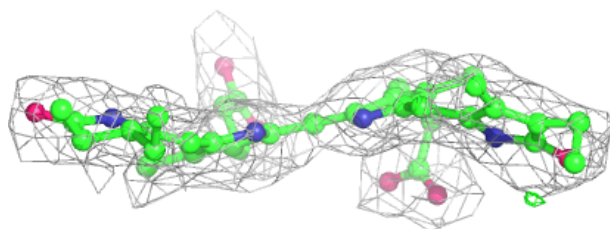
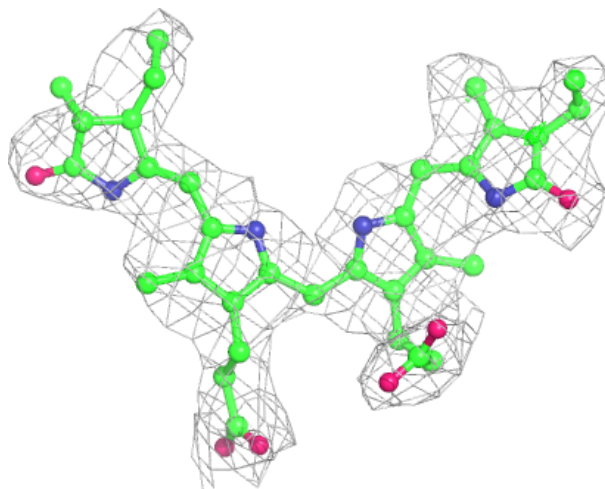
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





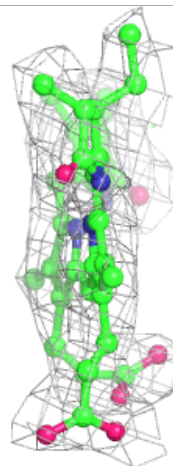
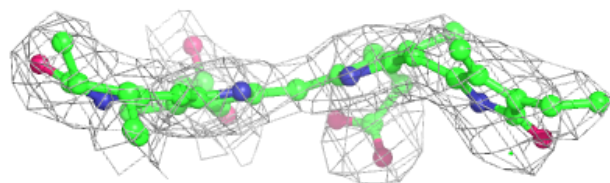
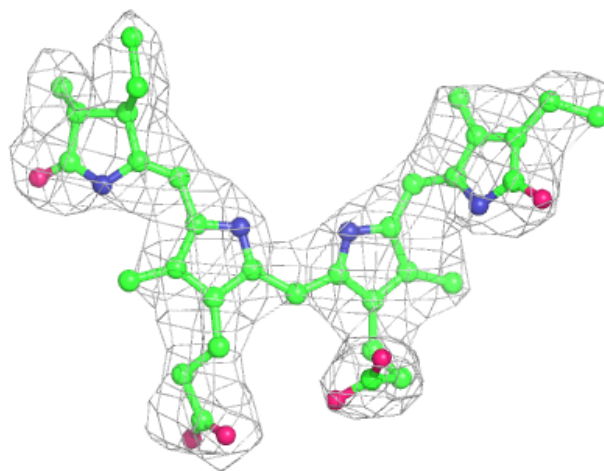
**Electron density around CYC M 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



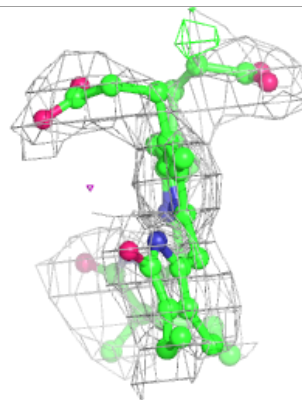
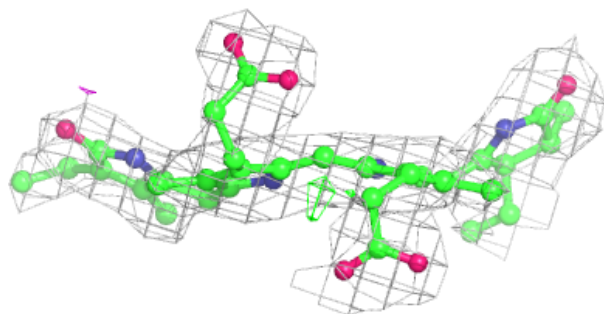
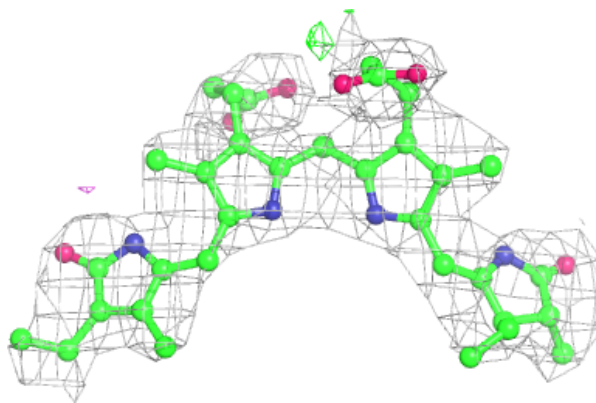
**Electron density around CYC J 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



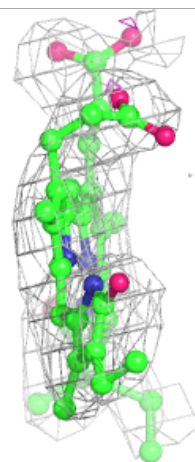
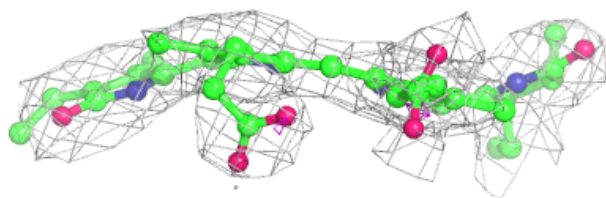
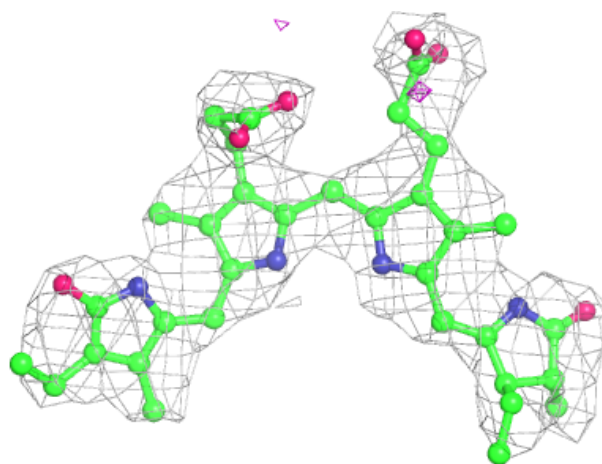
**Electron density around CYC D 255:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



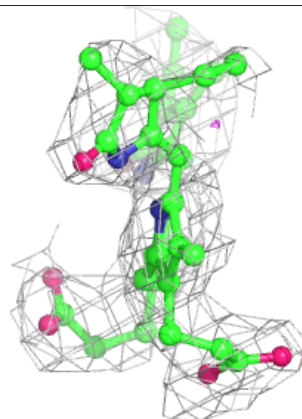
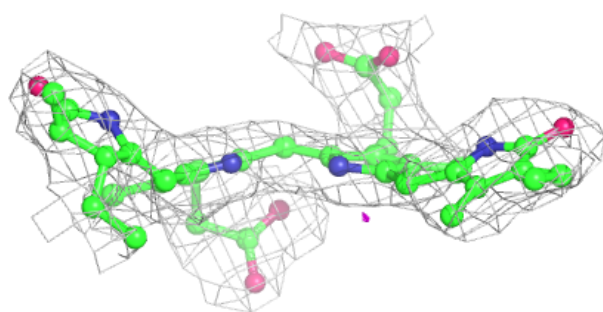
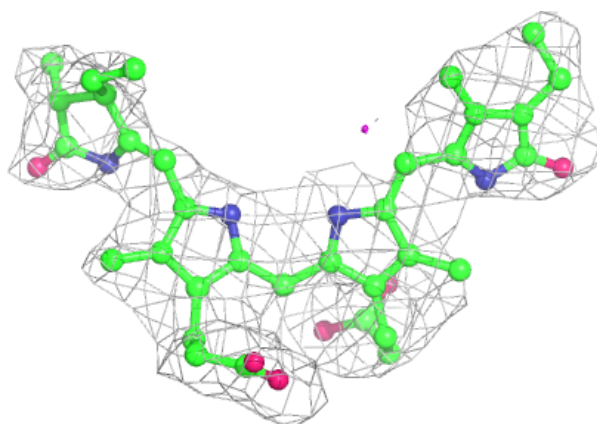
**Electron density around CYC P 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



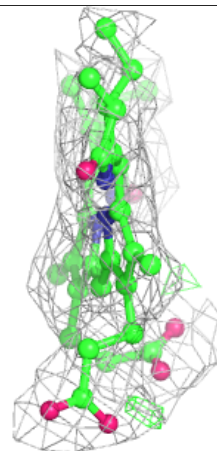
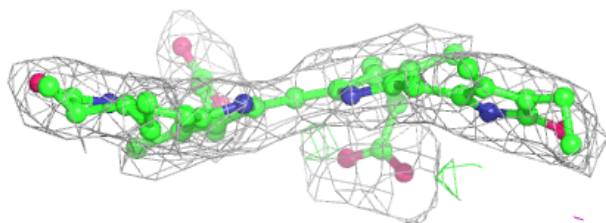
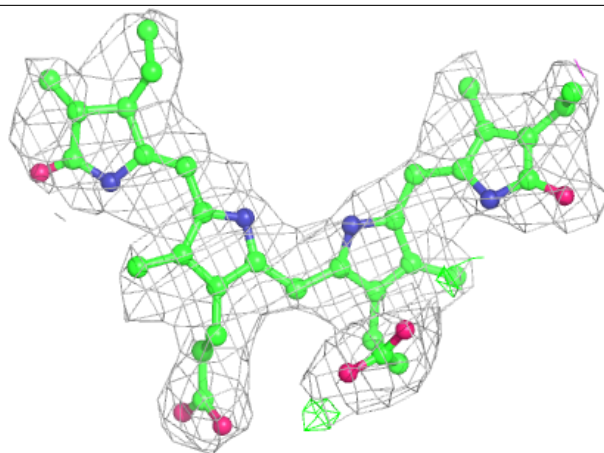
**Electron density around CYC L 255:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

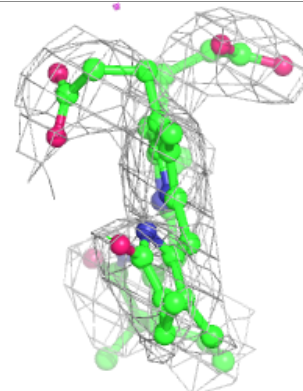
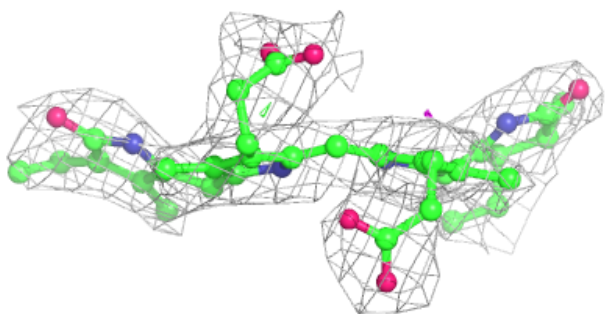
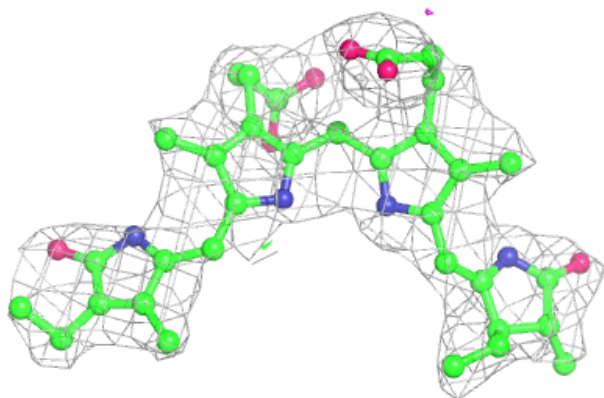


**Electron density around CYC I 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CYC T 255:**

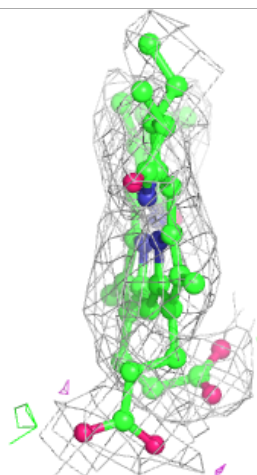
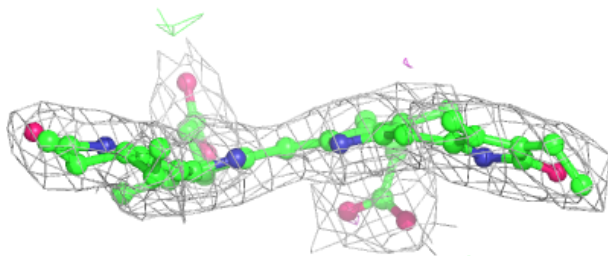
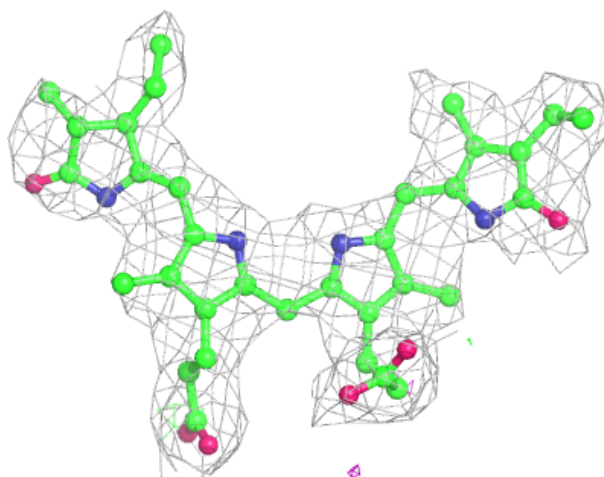
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





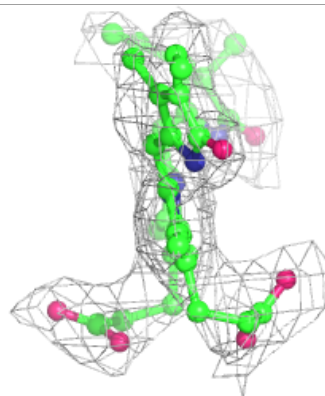
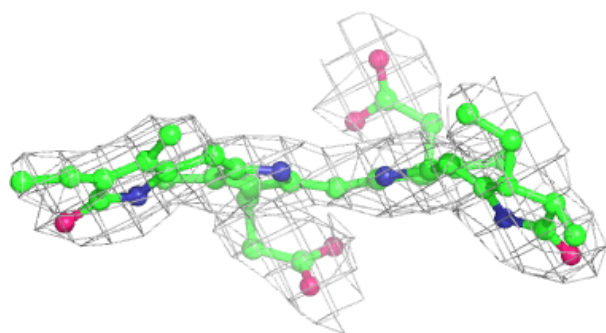
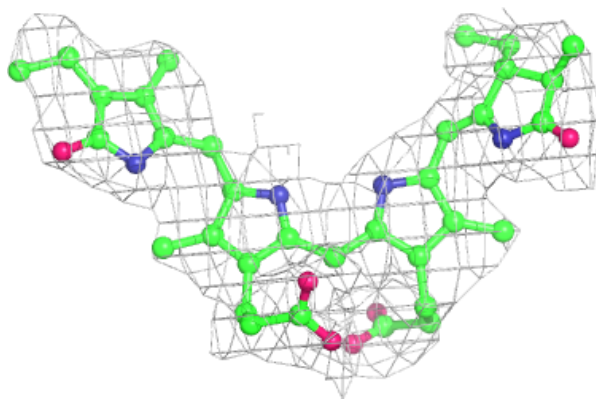
**Electron density around CYC A 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

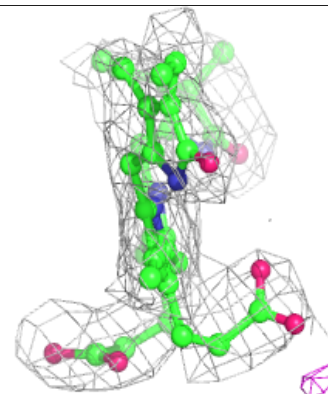
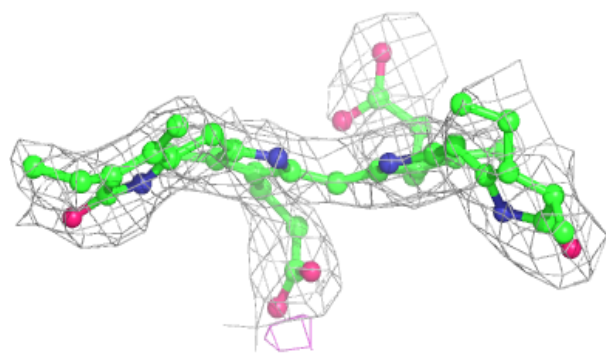
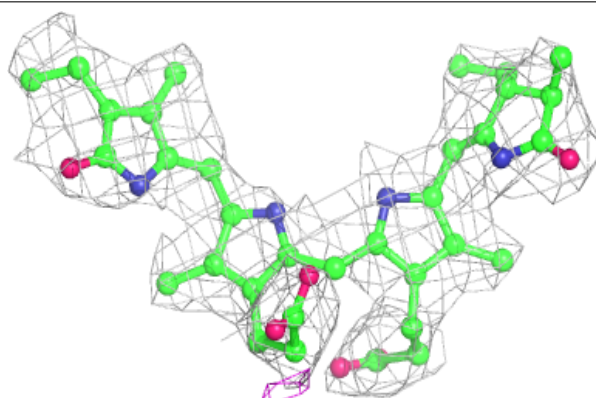


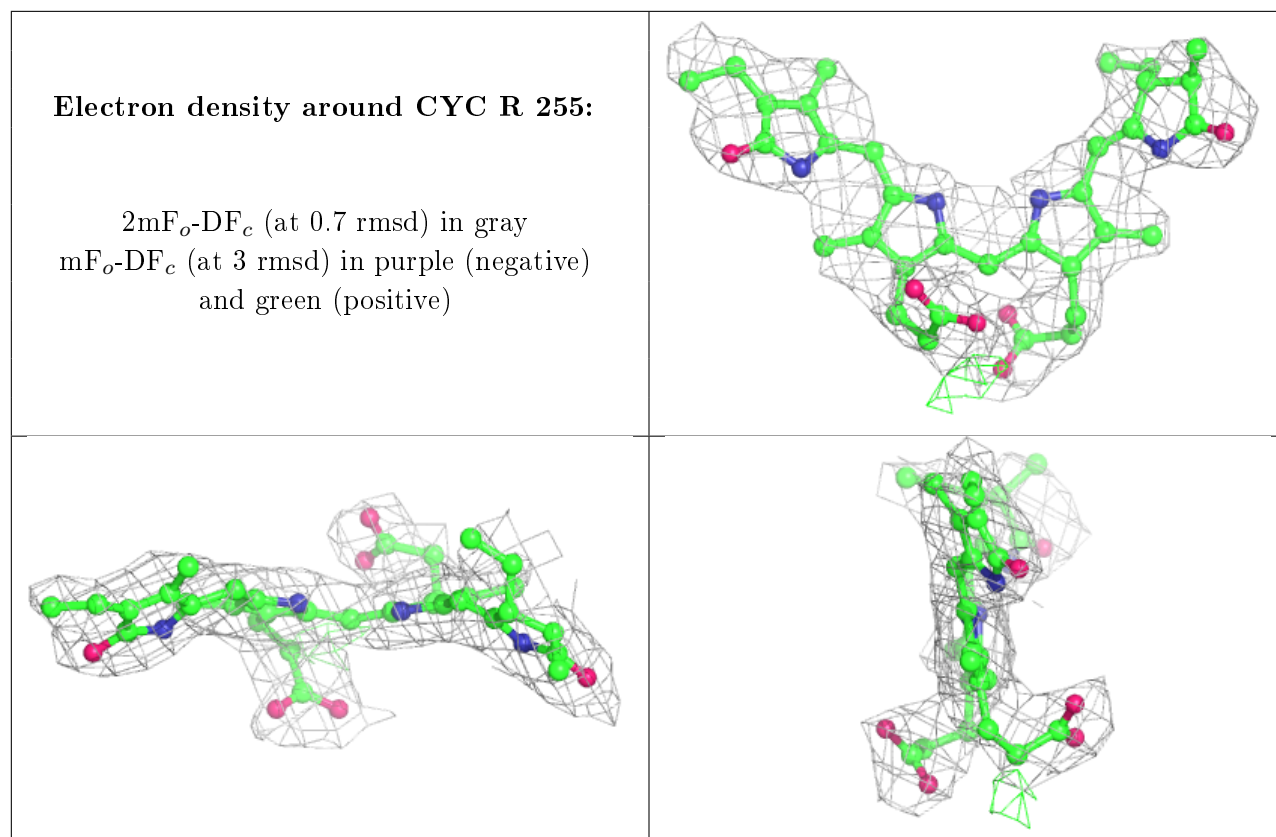
**Electron density around CYC H 255:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CYC P 255:**

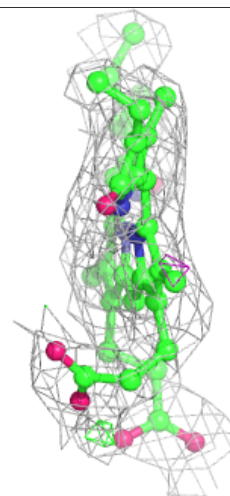
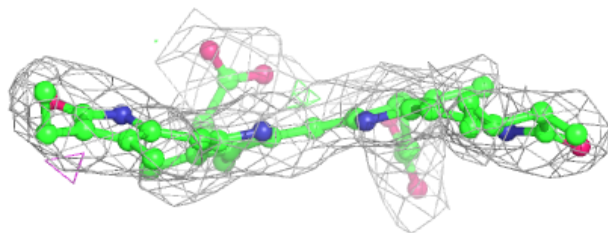
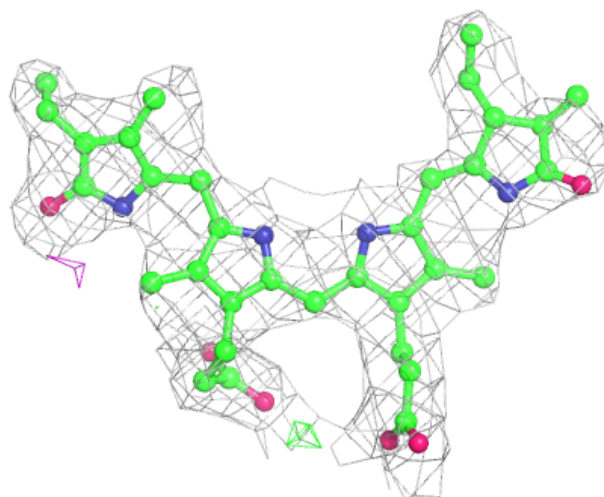
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





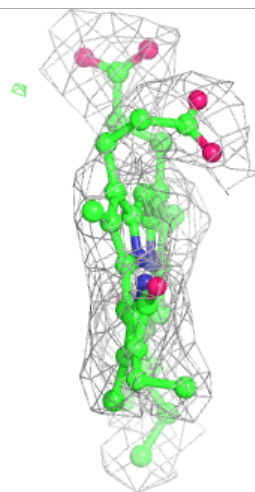
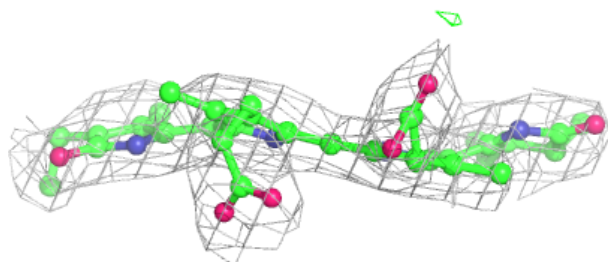
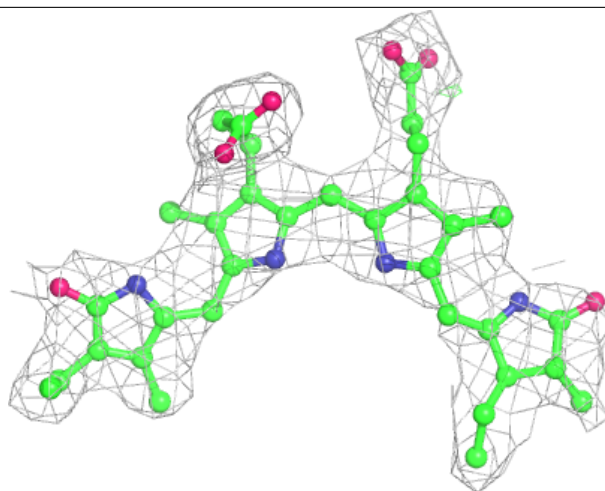
**Electron density around CYC C 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



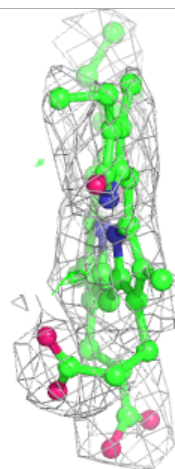
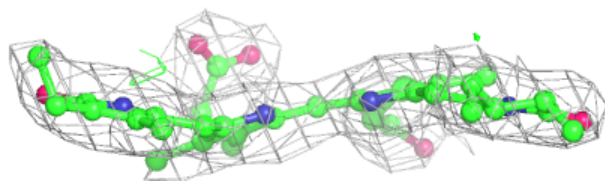
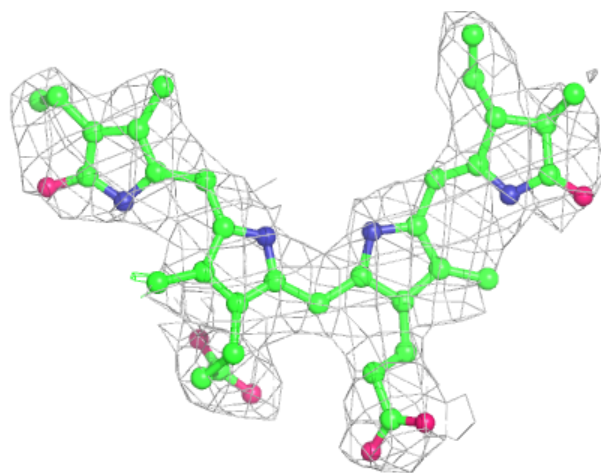
**Electron density around CYC K 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



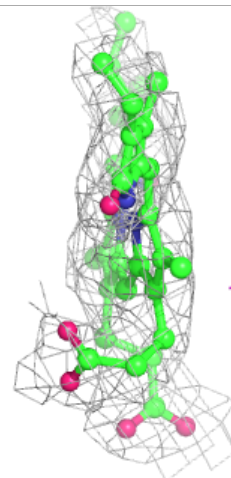
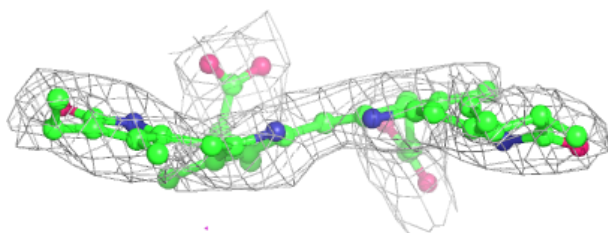
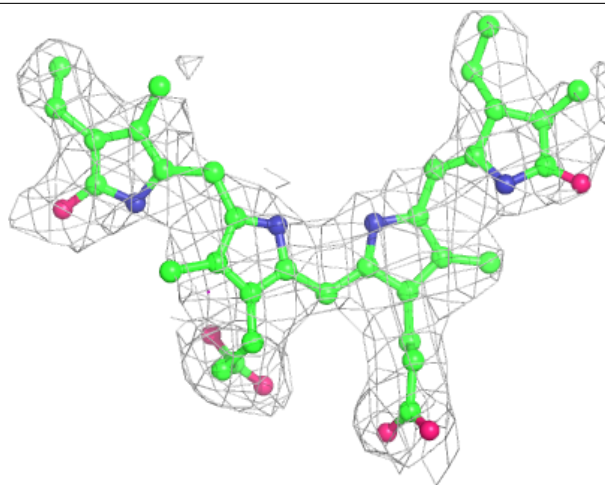
**Electron density around CYC S 184:**

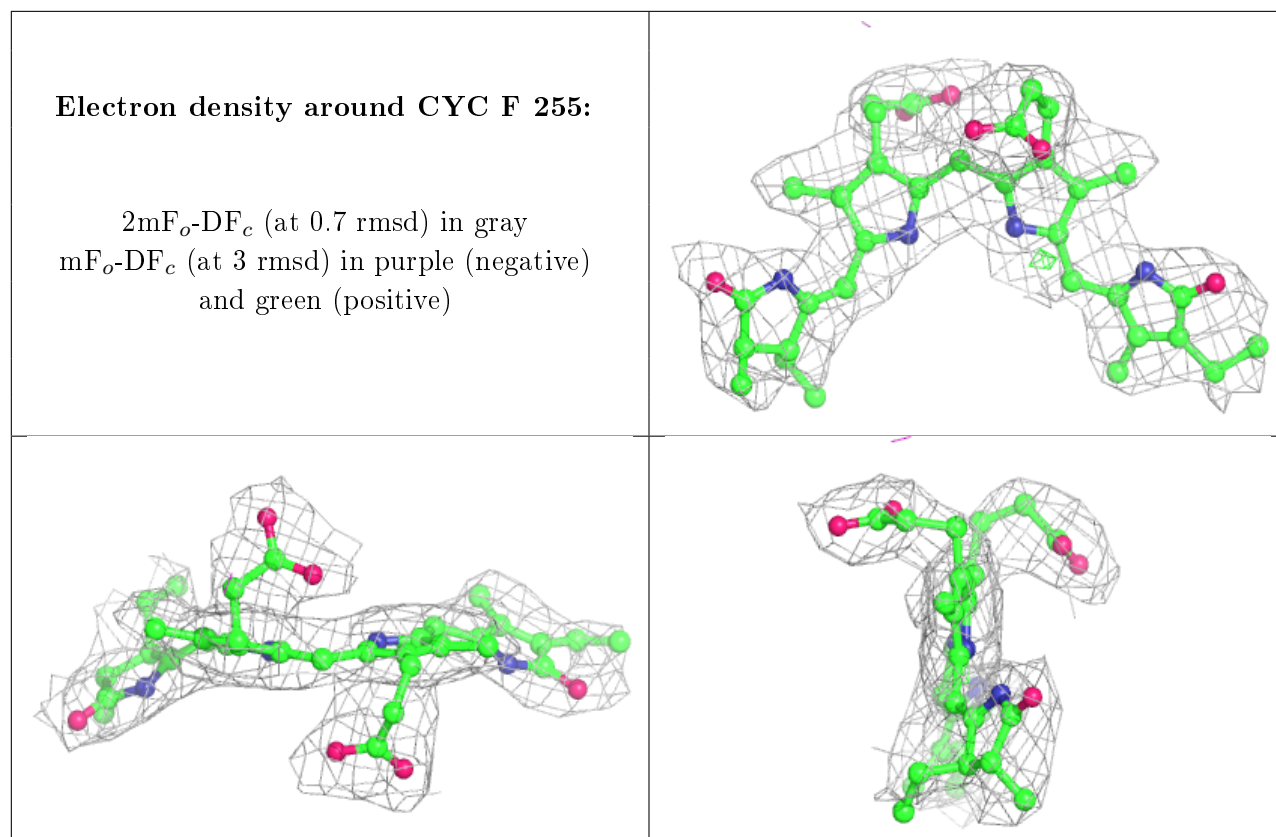
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CYC Q 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

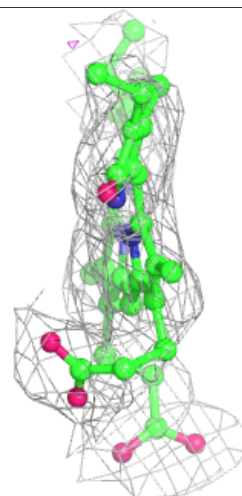
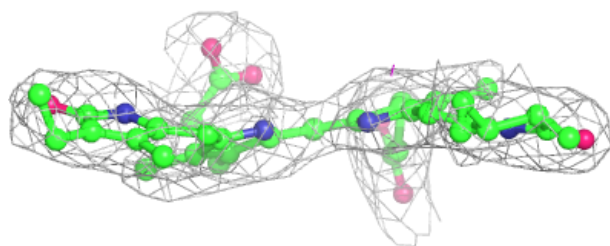
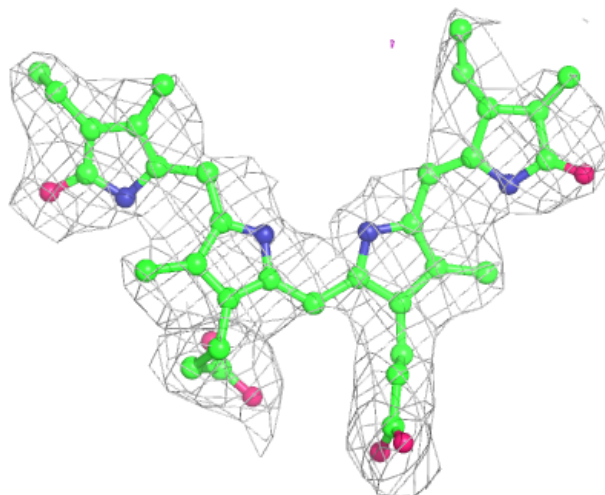






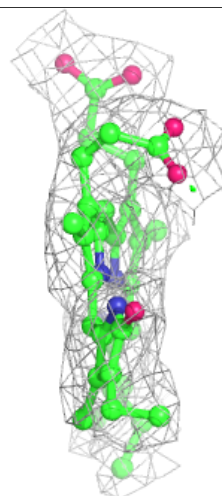
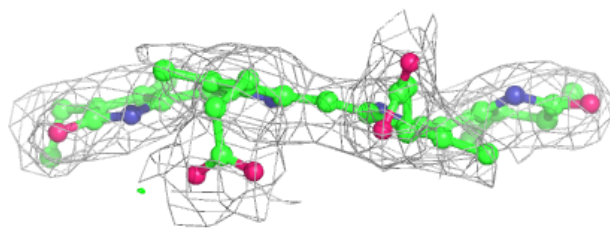
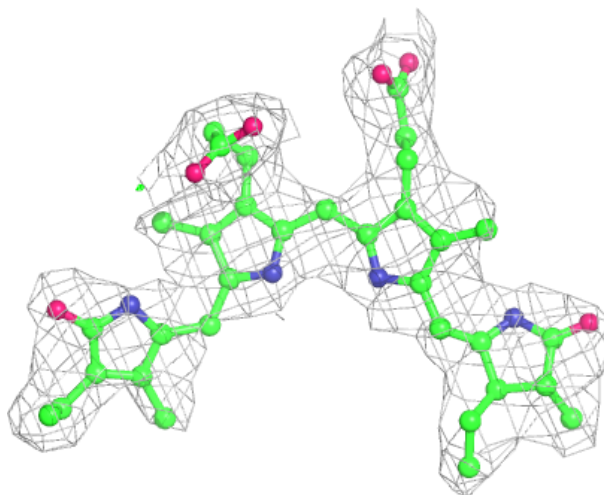
**Electron density around CYC U 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



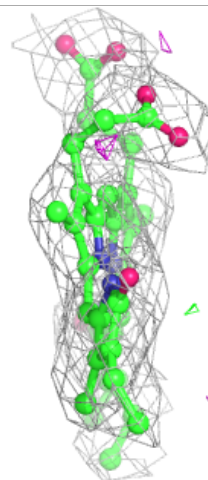
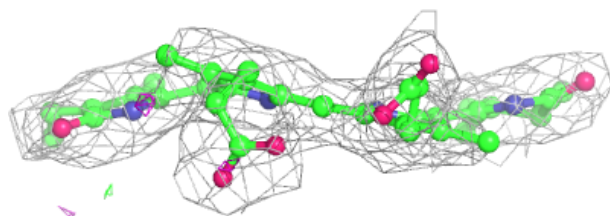
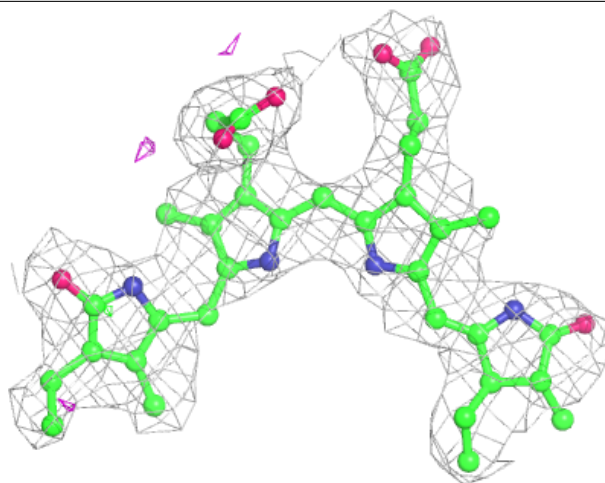
**Electron density around CYC O 184:**

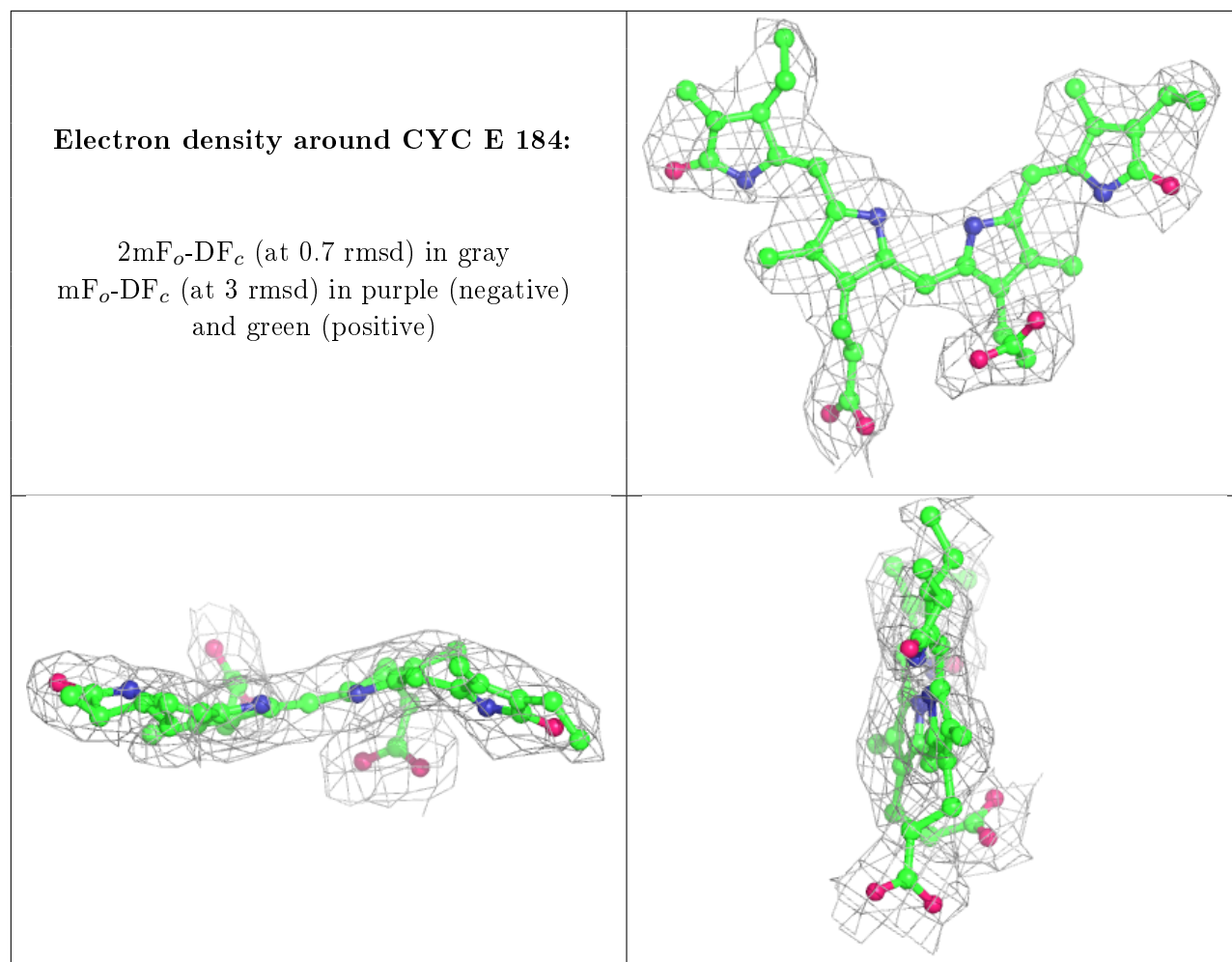
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

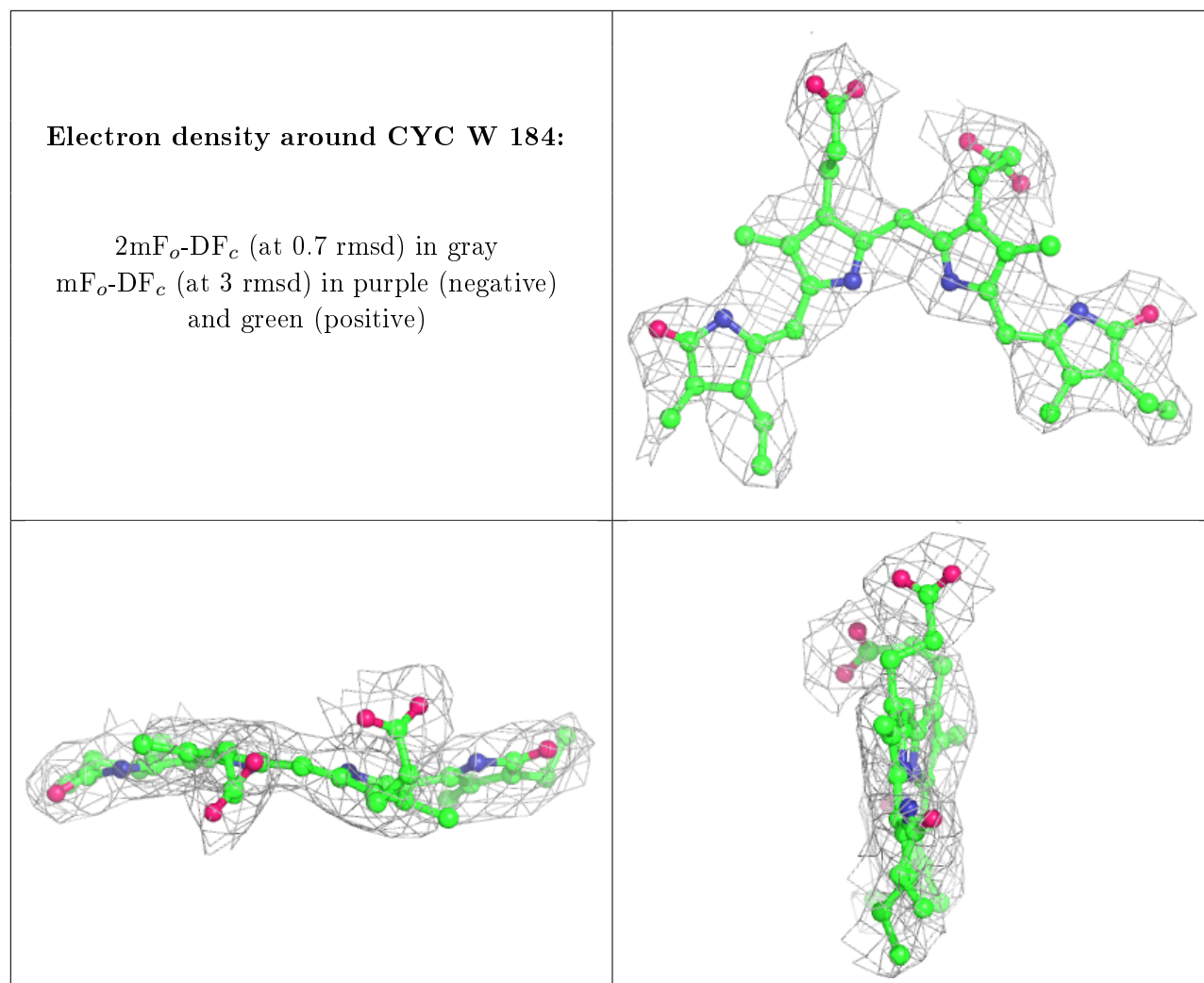


**Electron density around CYC G 184:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.