



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 05:34 am BST

PDB ID : 2BV8  
Title : The crystal structure of Phycocyanin from Gracilaria chilensis.  
Authors : Contreras-Martel, C.; Martinez-Oyanedel, J.; Poo-Caama, G.; Bruna, C.; Bunker, M.  
Deposited on : 2005-06-23  
Resolution : 2.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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

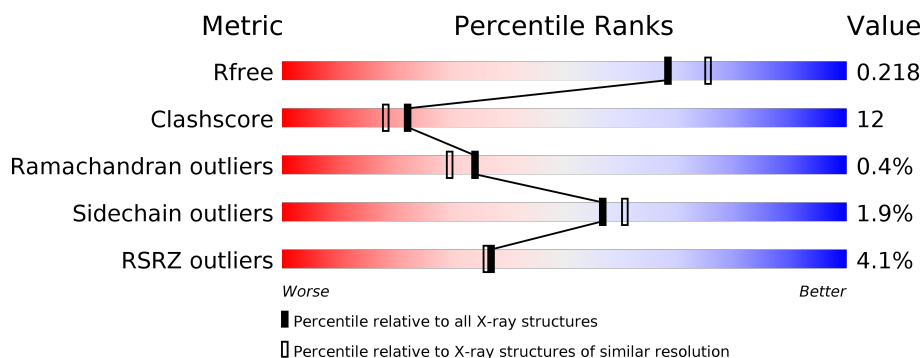
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	<div> <div>7%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	C	162	<div> <div>7%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
1	E	162	<div> <div>7%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
1	K	162	<div> <div>7%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
1	M	162	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	O	162	<div> <div>7%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	172	 90% 9% •
2	D	172	 84% 15% •
2	F	172	 85% 14% •
2	L	172	 83% 16% •
2	N	172	 85% 13% •
2	P	172	 85% 13% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEB	B	1175	X	-	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16812 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 ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			
1	C	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			
1	E	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			
1	K	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			
1	M	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			
1	O	162	Total	C	N	O	S	0	0	0
			1235	771	209	249	6			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	THR	SER	conflict	UNP Q6B8L6
A	49	GLU	GLN	conflict	UNP Q6B8L6
A	53	SER	THR	conflict	UNP Q6B8L6
A	61	SER	THR	conflict	UNP Q6B8L6
A	65	TYR	PHE	conflict	UNP Q6B8L6
A	70	GLN	PRO	conflict	UNP Q6B8L6
A	73	ASN	THR	conflict	UNP Q6B8L6
A	76	ALA	SER	conflict	UNP Q6B8L6
A	77	ASP	SER	conflict	UNP Q6B8L6
A	79	THR	ILE	conflict	UNP Q6B8L6
A	95	VAL	THR	conflict	UNP Q6B8L6
A	116	SER	GLU	conflict	UNP Q6B8L6
A	134	GLU	GLN	conflict	UNP Q6B8L6
A	138	ASP	ASN	conflict	UNP Q6B8L6
A	141	ALA	SER	conflict	UNP Q6B8L6
C	35	THR	SER	conflict	UNP Q6B8L6
C	49	GLU	GLN	conflict	UNP Q6B8L6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	53	SER	THR	conflict	UNP Q6B8L6
C	61	SER	THR	conflict	UNP Q6B8L6
C	65	TYR	PHE	conflict	UNP Q6B8L6
C	70	GLN	PRO	conflict	UNP Q6B8L6
C	73	ASN	THR	conflict	UNP Q6B8L6
C	76	ALA	SER	conflict	UNP Q6B8L6
C	77	ASP	SER	conflict	UNP Q6B8L6
C	79	THR	ILE	conflict	UNP Q6B8L6
C	95	VAL	THR	conflict	UNP Q6B8L6
C	116	SER	GLU	conflict	UNP Q6B8L6
C	134	GLU	GLN	conflict	UNP Q6B8L6
C	138	ASP	ASN	conflict	UNP Q6B8L6
C	141	ALA	SER	conflict	UNP Q6B8L6
E	35	THR	SER	conflict	UNP Q6B8L6
E	49	GLU	GLN	conflict	UNP Q6B8L6
E	53	SER	THR	conflict	UNP Q6B8L6
E	61	SER	THR	conflict	UNP Q6B8L6
E	65	TYR	PHE	conflict	UNP Q6B8L6
E	70	GLN	PRO	conflict	UNP Q6B8L6
E	73	ASN	THR	conflict	UNP Q6B8L6
E	76	ALA	SER	conflict	UNP Q6B8L6
E	77	ASP	SER	conflict	UNP Q6B8L6
E	79	THR	ILE	conflict	UNP Q6B8L6
E	95	VAL	THR	conflict	UNP Q6B8L6
E	116	SER	GLU	conflict	UNP Q6B8L6
E	134	GLU	GLN	conflict	UNP Q6B8L6
E	138	ASP	ASN	conflict	UNP Q6B8L6
E	141	ALA	SER	conflict	UNP Q6B8L6
K	35	THR	SER	conflict	UNP Q6B8L6
K	49	GLU	GLN	conflict	UNP Q6B8L6
K	53	SER	THR	conflict	UNP Q6B8L6
K	61	SER	THR	conflict	UNP Q6B8L6
K	65	TYR	PHE	conflict	UNP Q6B8L6
K	70	GLN	PRO	conflict	UNP Q6B8L6
K	73	ASN	THR	conflict	UNP Q6B8L6
K	76	ALA	SER	conflict	UNP Q6B8L6
K	77	ASP	SER	conflict	UNP Q6B8L6
K	79	THR	ILE	conflict	UNP Q6B8L6
K	95	VAL	THR	conflict	UNP Q6B8L6
K	116	SER	GLU	conflict	UNP Q6B8L6
K	134	GLU	GLN	conflict	UNP Q6B8L6
K	138	ASP	ASN	conflict	UNP Q6B8L6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	141	ALA	SER	conflict	UNP Q6B8L6
M	35	THR	SER	conflict	UNP Q6B8L6
M	49	GLU	GLN	conflict	UNP Q6B8L6
M	53	SER	THR	conflict	UNP Q6B8L6
M	61	SER	THR	conflict	UNP Q6B8L6
M	65	TYR	PHE	conflict	UNP Q6B8L6
M	70	GLN	PRO	conflict	UNP Q6B8L6
M	73	ASN	THR	conflict	UNP Q6B8L6
M	76	ALA	SER	conflict	UNP Q6B8L6
M	77	ASP	SER	conflict	UNP Q6B8L6
M	79	THR	ILE	conflict	UNP Q6B8L6
M	95	VAL	THR	conflict	UNP Q6B8L6
M	116	SER	GLU	conflict	UNP Q6B8L6
M	134	GLU	GLN	conflict	UNP Q6B8L6
M	138	ASP	ASN	conflict	UNP Q6B8L6
M	141	ALA	SER	conflict	UNP Q6B8L6
O	35	THR	SER	conflict	UNP Q6B8L6
O	49	GLU	GLN	conflict	UNP Q6B8L6
O	53	SER	THR	conflict	UNP Q6B8L6
O	61	SER	THR	conflict	UNP Q6B8L6
O	65	TYR	PHE	conflict	UNP Q6B8L6
O	70	GLN	PRO	conflict	UNP Q6B8L6
O	73	ASN	THR	conflict	UNP Q6B8L6
O	76	ALA	SER	conflict	UNP Q6B8L6
O	77	ASP	SER	conflict	UNP Q6B8L6
O	79	THR	ILE	conflict	UNP Q6B8L6
O	95	VAL	THR	conflict	UNP Q6B8L6
O	116	SER	GLU	conflict	UNP Q6B8L6
O	134	GLU	GLN	conflict	UNP Q6B8L6
O	138	ASP	ASN	conflict	UNP Q6B8L6
O	141	ALA	SER	conflict	UNP Q6B8L6

- Molecule 2 is a protein called C-PHYCOCYANIN BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			
2	D	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			
2	F	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			
2	L	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			
2	P	172	Total	C	N	O	S	0	0	0
			1270	773	226	263	8			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	31	ILE	VAL	conflict	UNP Q6B8L7
B	43	ARG	LYS	conflict	UNP Q6B8L7
B	52	VAL	ILE	conflict	UNP Q6B8L7
B	53	SER	THR	conflict	UNP Q6B8L7
B	58	ALA	SER	conflict	UNP Q6B8L7
B	67	ILE	VAL	conflict	UNP Q6B8L7
B	97	GLU	MET	conflict	UNP Q6B8L7
B	125	SER	THR	conflict	UNP Q6B8L7
B	132	GLU	GLN	conflict	UNP Q6B8L7
B	141	ASP	LEU	conflict	UNP Q6B8L7
B	146	SER	ASN	conflict	UNP Q6B8L7
B	150	SER	ILE	conflict	UNP Q6B8L7
B	157	SER	THR	conflict	UNP Q6B8L7
B	162	THR	VAL	conflict	UNP Q6B8L7
B	169	SER	VAL	conflict	UNP Q6B8L7
B	172	SER	VAL	conflict	UNP Q6B8L7
D	31	ILE	VAL	conflict	UNP Q6B8L7
D	43	ARG	LYS	conflict	UNP Q6B8L7
D	52	VAL	ILE	conflict	UNP Q6B8L7
D	53	SER	THR	conflict	UNP Q6B8L7
D	58	ALA	SER	conflict	UNP Q6B8L7
D	67	ILE	VAL	conflict	UNP Q6B8L7
D	97	GLU	MET	conflict	UNP Q6B8L7
D	125	SER	THR	conflict	UNP Q6B8L7
D	132	GLU	GLN	conflict	UNP Q6B8L7
D	141	ASP	LEU	conflict	UNP Q6B8L7
D	146	SER	ASN	conflict	UNP Q6B8L7
D	150	SER	ILE	conflict	UNP Q6B8L7
D	157	SER	THR	conflict	UNP Q6B8L7
D	162	THR	VAL	conflict	UNP Q6B8L7
D	169	SER	VAL	conflict	UNP Q6B8L7
D	172	SER	VAL	conflict	UNP Q6B8L7
F	31	ILE	VAL	conflict	UNP Q6B8L7
F	43	ARG	LYS	conflict	UNP Q6B8L7

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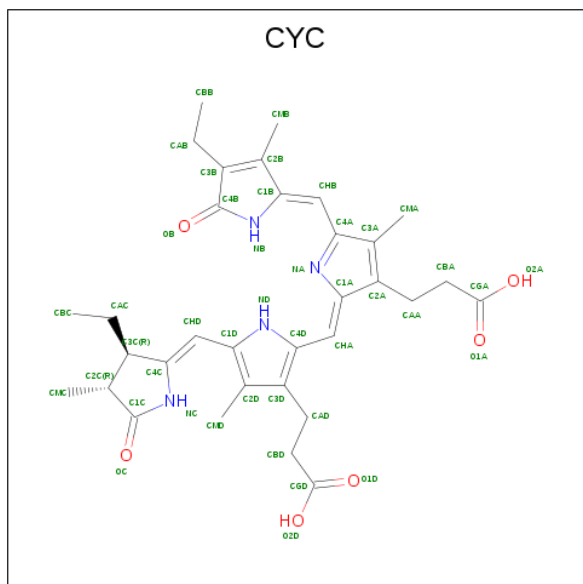
Chain	Residue	Modelled	Actual	Comment	Reference
F	52	VAL	ILE	conflict	UNP Q6B8L7
F	53	SER	THR	conflict	UNP Q6B8L7
F	58	ALA	SER	conflict	UNP Q6B8L7
F	67	ILE	VAL	conflict	UNP Q6B8L7
F	97	GLU	MET	conflict	UNP Q6B8L7
F	125	SER	THR	conflict	UNP Q6B8L7
F	132	GLU	GLN	conflict	UNP Q6B8L7
F	141	ASP	LEU	conflict	UNP Q6B8L7
F	146	SER	ASN	conflict	UNP Q6B8L7
F	150	SER	ILE	conflict	UNP Q6B8L7
F	157	SER	THR	conflict	UNP Q6B8L7
F	162	THR	VAL	conflict	UNP Q6B8L7
F	169	SER	VAL	conflict	UNP Q6B8L7
F	172	SER	VAL	conflict	UNP Q6B8L7
L	31	ILE	VAL	conflict	UNP Q6B8L7
L	43	ARG	LYS	conflict	UNP Q6B8L7
L	52	VAL	ILE	conflict	UNP Q6B8L7
L	53	SER	THR	conflict	UNP Q6B8L7
L	58	ALA	SER	conflict	UNP Q6B8L7
L	67	ILE	VAL	conflict	UNP Q6B8L7
L	97	GLU	MET	conflict	UNP Q6B8L7
L	125	SER	THR	conflict	UNP Q6B8L7
L	132	GLU	GLN	conflict	UNP Q6B8L7
L	141	ASP	LEU	conflict	UNP Q6B8L7
L	146	SER	ASN	conflict	UNP Q6B8L7
L	150	SER	ILE	conflict	UNP Q6B8L7
L	157	SER	THR	conflict	UNP Q6B8L7
L	162	THR	VAL	conflict	UNP Q6B8L7
L	169	SER	VAL	conflict	UNP Q6B8L7
L	172	SER	VAL	conflict	UNP Q6B8L7
N	31	ILE	VAL	conflict	UNP Q6B8L7
N	43	ARG	LYS	conflict	UNP Q6B8L7
N	52	VAL	ILE	conflict	UNP Q6B8L7
N	53	SER	THR	conflict	UNP Q6B8L7
N	58	ALA	SER	conflict	UNP Q6B8L7
N	67	ILE	VAL	conflict	UNP Q6B8L7
N	97	GLU	MET	conflict	UNP Q6B8L7
N	125	SER	THR	conflict	UNP Q6B8L7
N	132	GLU	GLN	conflict	UNP Q6B8L7
N	141	ASP	LEU	conflict	UNP Q6B8L7
N	146	SER	ASN	conflict	UNP Q6B8L7
N	150	SER	ILE	conflict	UNP Q6B8L7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	157	SER	THR	conflict	UNP Q6B8L7
N	162	THR	VAL	conflict	UNP Q6B8L7
N	169	SER	VAL	conflict	UNP Q6B8L7
N	172	SER	VAL	conflict	UNP Q6B8L7
P	31	ILE	VAL	conflict	UNP Q6B8L7
P	43	ARG	LYS	conflict	UNP Q6B8L7
P	52	VAL	ILE	conflict	UNP Q6B8L7
P	53	SER	THR	conflict	UNP Q6B8L7
P	58	ALA	SER	conflict	UNP Q6B8L7
P	67	ILE	VAL	conflict	UNP Q6B8L7
P	97	GLU	MET	conflict	UNP Q6B8L7
P	125	SER	THR	conflict	UNP Q6B8L7
P	132	GLU	GLN	conflict	UNP Q6B8L7
P	141	ASP	LEU	conflict	UNP Q6B8L7
P	146	SER	ASN	conflict	UNP Q6B8L7
P	150	SER	ILE	conflict	UNP Q6B8L7
P	157	SER	THR	conflict	UNP Q6B8L7
P	162	THR	VAL	conflict	UNP Q6B8L7
P	169	SER	VAL	conflict	UNP Q6B8L7
P	172	SER	VAL	conflict	UNP Q6B8L7

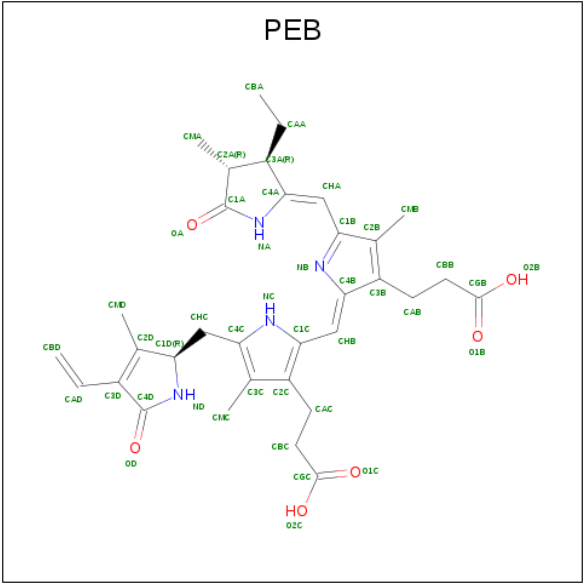
- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ).



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

- Molecule 4 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	81	Total	O	0	0
			81	81		
5	B	114	Total	O	0	0
			114	114		
5	C	83	Total	O	0	0
			83	83		
5	D	80	Total	O	0	0
			80	80		
5	E	100	Total	O	0	0
			100	100		
5	F	66	Total	O	0	0
			66	66		
5	K	95	Total	O	0	0
			95	95		
5	L	85	Total	O	0	0
			85	85		
5	M	91	Total	O	0	0
			91	91		
5	N	99	Total	O	0	0
			99	99		
5	O	59	Total	O	0	0
			59	59		

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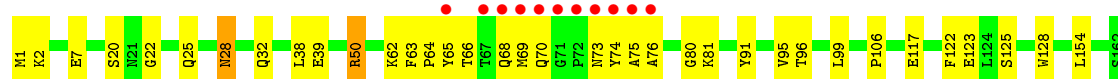
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	55	Total	O	0	0
			55	55		

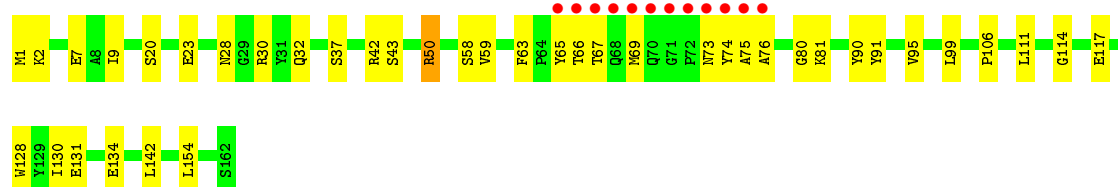
### 3 Residue-property plots [i](#)

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.

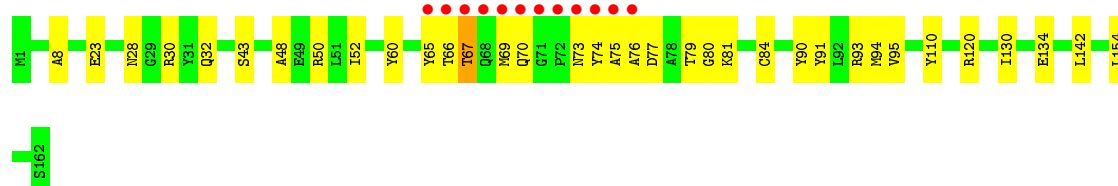
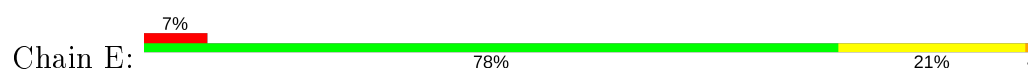
#### • Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



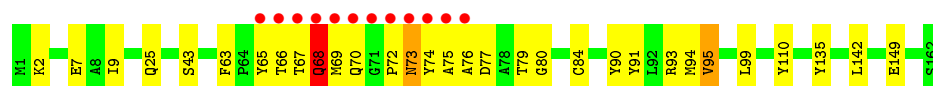
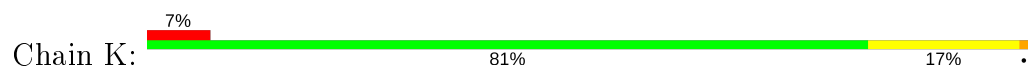
#### • Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



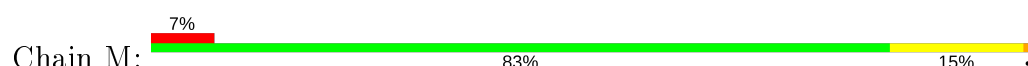
#### • Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



#### • Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

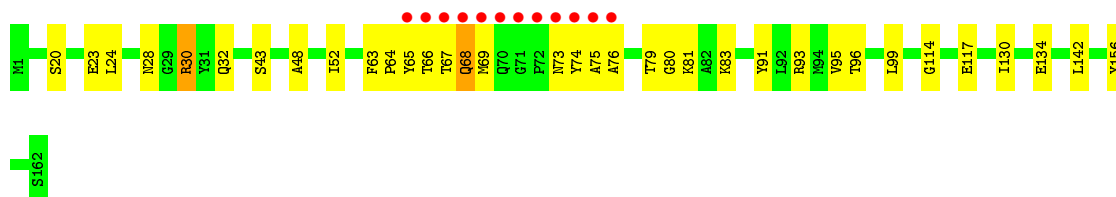
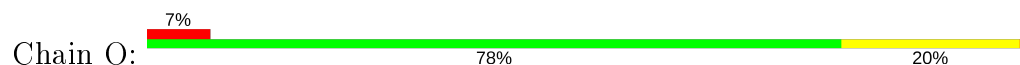


#### • Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

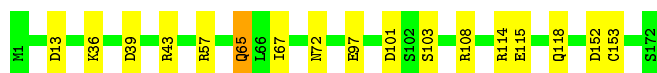




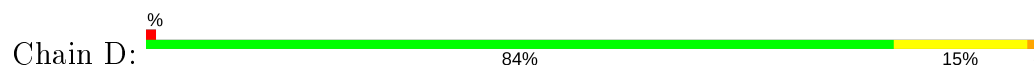
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT



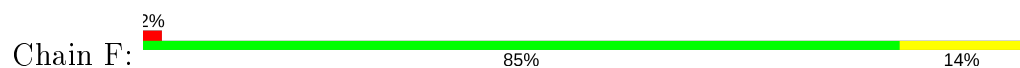
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



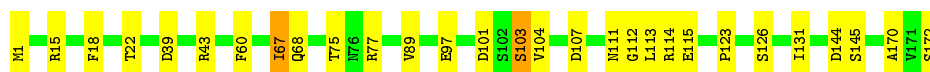
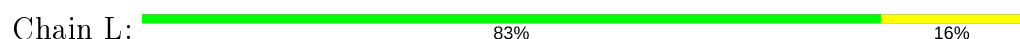
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



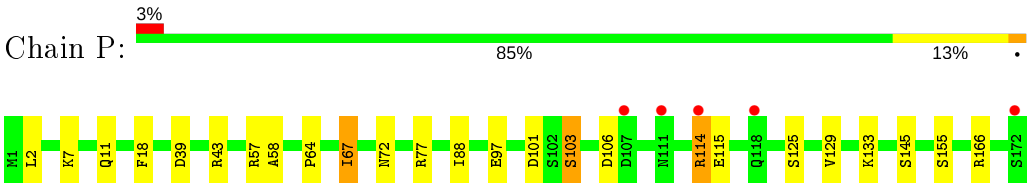
• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.98Å 151.80Å 101.55Å 90.00° 117.45° 90.00°	Depositor
Resolution (Å)	52.83 – 2.01 52.83 – 2.01	Depositor EDS
% Data completeness (in resolution range)	97.7 (52.83-2.01) 97.9 (52.83-2.01)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.199 , 0.231 0.190 , 0.218	Depositor DCC
$R_{free}$ test set	7100 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for l,k,-h-l 0.008 for -h-l,k,h 0.028 for -h-l,-k,l 0.023 for h,-k,-h-l 0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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, MEN, PEB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.82	0/1257	0.78	0/1703
1	C	0.79	0/1257	0.78	0/1703
1	E	0.86	0/1257	0.81	0/1703
1	K	0.85	1/1257 (0.1%)	0.83	0/1703
1	M	0.86	1/1257 (0.1%)	0.88	1/1703 (0.1%)
1	O	0.73	0/1257	0.77	0/1703
2	B	0.95	2/1272 (0.2%)	0.85	1/1717 (0.1%)
2	D	0.76	1/1272 (0.1%)	0.81	0/1717
2	F	0.82	2/1272 (0.2%)	0.81	0/1717
2	L	0.84	1/1272 (0.1%)	0.80	0/1717
2	N	0.88	1/1272 (0.1%)	0.87	1/1717 (0.1%)
2	P	0.76	1/1272 (0.1%)	0.80	0/1717
All	All	0.83	10/15174 (0.1%)	0.82	3/20520 (0.0%)

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	K	0	1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	97	GLU	CD-OE1	-9.87	1.14	1.25
2	B	97	GLU	CD-OE1	-8.84	1.16	1.25
2	N	97	GLU	CD-OE1	-8.32	1.16	1.25
2	B	153	CYS	CB-SG	-6.59	1.71	1.82
1	M	94	MET	SD-CE	-6.11	1.43	1.77

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	94	MET	CG-SD-CE	-7.80	87.71	100.20
2	B	13	ASP	CB-CG-OD2	5.19	122.97	118.30
2	N	97	GLU	OE1-CD-OE2	-5.01	117.28	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	135	TYR	Sidechain

## 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	1235	0	1199	33	0
1	C	1235	0	1199	35	0
1	E	1235	0	1199	34	0
1	K	1235	0	1199	37	0
1	M	1235	0	1199	26	0
1	O	1235	0	1199	30	0
2	B	1270	0	1243	13	0
2	D	1270	0	1243	18	0
2	F	1270	0	1243	30	0
2	L	1270	0	1243	25	0
2	N	1270	0	1243	23	0
2	P	1270	0	1243	24	0
3	A	43	0	37	6	0
3	B	43	0	37	4	0
3	C	43	0	37	9	0
3	D	86	0	74	11	0
3	E	43	0	37	7	0
3	F	86	0	74	8	0
3	K	43	0	37	7	0
3	L	86	0	74	11	0
3	M	43	0	37	5	0
3	N	86	0	74	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	43	0	37	7	0
3	P	86	0	74	9	0
4	B	43	0	36	2	0
5	A	81	0	0	3	0
5	B	114	0	0	0	0
5	C	83	0	0	1	0
5	D	80	0	0	1	0
5	E	100	0	0	3	0
5	F	66	0	0	1	0
5	K	95	0	0	2	0
5	L	85	0	0	0	0
5	M	91	0	0	0	0
5	N	99	0	0	1	0
5	O	59	0	0	1	0
5	P	55	0	0	0	0
All	All	16812	0	15317	365	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 365 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)
1:C:75:ALA:HB1	1:C:81:LYS:HG3	1.28	1.14
1:C:73:ASN:HA	3:C:1163:CYC:HBD2	1.24	1.12
1:E:73:ASN:HB3	5:E:2098:HOH:O	1.56	1.04
1:K:94:MET:HE1	1:K:110:TYR:HB2	1.39	1.04
1:K:73:ASN:HB3	5:K:2095:HOH:O	1.65	0.96

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	C	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	E	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25	19
1	K	160/162 (99%)	153 (96%)	5 (3%)	2 (1%)	12	6
1	M	160/162 (99%)	156 (98%)	2 (1%)	2 (1%)	12	6
1	O	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
2	B	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	D	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
2	F	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	L	169/172 (98%)	167 (99%)	1 (1%)	1 (1%)	25	19
2	N	169/172 (98%)	167 (99%)	1 (1%)	1 (1%)	25	19
2	P	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	1974/2004 (98%)	1929 (98%)	38 (2%)	7 (0%)	34	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	70	GLN
1	M	69	MET
1	K	68	GLN
2	L	75	THR
2	N	75	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/127 (100%)	123 (97%)	4 (3%)	40	40
1	C	127/127 (100%)	126 (99%)	1 (1%)	81	86
1	E	127/127 (100%)	126 (99%)	1 (1%)	81	86
1	K	127/127 (100%)	124 (98%)	3 (2%)	49	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	127/127 (100%)	127 (100%)	0	100	100
1	O	127/127 (100%)	125 (98%)	2 (2%)	62	67
2	B	133/133 (100%)	132 (99%)	1 (1%)	81	86
2	D	133/133 (100%)	129 (97%)	4 (3%)	41	41
2	F	133/133 (100%)	130 (98%)	3 (2%)	50	53
2	L	133/133 (100%)	130 (98%)	3 (2%)	50	53
2	N	133/133 (100%)	129 (97%)	4 (3%)	41	41
2	P	133/133 (100%)	129 (97%)	4 (3%)	41	41
All	All	1560/1560 (100%)	1530 (98%)	30 (2%)	57	61

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	155	SER
1	K	73	ASN
2	P	103	SER
1	K	68	GLN
2	L	22	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	68	GLN
2	L	111	ASN
2	P	11	GLN
2	L	11	GLN
2	L	68	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MEN	L	72	2	7,8,9	0.78	0	6,9,11	0.24	0
2	MEN	F	72	2	7,8,9	0.73	0	6,9,11	0.67	0
2	MEN	B	72	2	7,8,9	0.62	0	6,9,11	0.55	0
2	MEN	D	72	2	7,8,9	0.81	0	6,9,11	0.74	0
2	MEN	P	72	2	7,8,9	1.18	1 (14%)	6,9,11	0.43	0
2	MEN	N	72	2	7,8,9	1.13	1 (14%)	6,9,11	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	L	72	2	-	2/7/8/10	-
2	MEN	F	72	2	-	3/7/8/10	-
2	MEN	B	72	2	-	3/7/8/10	-
2	MEN	D	72	2	-	2/7/8/10	-
2	MEN	P	72	2	-	3/7/8/10	-
2	MEN	N	72	2	-	3/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	72	MEN	CE2-ND2	2.67	1.50	1.45
2	P	72	MEN	CE2-ND2	2.30	1.49	1.45

There are no bond angle outliers.

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	CA-CB-CG-OD1
2	F	72	MEN	CA-CB-CG-ND2

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Mol	Chain	Res	Type	Atoms
2	L	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-OD1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	72	MEN	1	0
2	B	72	MEN	1	0
2	P	72	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	PEB	B	1175	2	37,46,46	3.29	21 (56%)	39,67,67	3.50	19 (48%)
3	CYC	E	1163	1	36,46,46	3.33	18 (50%)	44,67,67	2.50	16 (36%)
3	CYC	P	1175	2	36,46,46	2.92	13 (36%)	44,67,67	2.20	15 (34%)
3	CYC	B	1174	2	36,46,46	3.21	16 (44%)	44,67,67	2.53	16 (36%)
3	CYC	A	1163	1	36,46,46	3.30	14 (38%)	44,67,67	2.33	15 (34%)
3	CYC	D	1174	2	36,46,46	3.33	17 (47%)	44,67,67	2.55	17 (38%)
3	CYC	C	1163	1	36,46,46	3.44	14 (38%)	44,67,67	2.47	14 (31%)
3	CYC	F	1174	2	36,46,46	3.06	13 (36%)	44,67,67	2.75	13 (29%)
3	CYC	M	1163	1	36,46,46	3.53	17 (47%)	44,67,67	2.24	14 (31%)
3	CYC	O	1163	1	36,46,46	3.64	20 (55%)	44,67,67	2.36	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	CYC	D	1175	2	36,46,46	3.11	18 (50%)	44,67,67	2.91	18 (40%)
3	CYC	L	1174	2	36,46,46	2.75	13 (36%)	44,67,67	2.50	19 (43%)
3	CYC	K	1163	1	36,46,46	3.04	19 (52%)	44,67,67	2.67	18 (40%)
3	CYC	N	1174	2	36,46,46	4.00	18 (50%)	44,67,67	2.73	18 (40%)
3	CYC	P	1174	2	36,46,46	3.54	17 (47%)	44,67,67	2.53	16 (36%)
3	CYC	L	1175	2	36,46,46	3.39	18 (50%)	44,67,67	2.40	15 (34%)
3	CYC	N	1175	2	36,46,46	3.30	18 (50%)	44,67,67	2.45	14 (31%)
3	CYC	F	1175	2	36,46,46	3.30	20 (55%)	44,67,67	2.64	23 (52%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	L	1175	2	-	9/21/74/74	0/4/4/4
3	CYC	E	1163	1	-	8/21/74/74	0/4/4/4
3	CYC	P	1175	2	-	9/21/74/74	0/4/4/4
3	CYC	B	1174	2	-	5/21/74/74	0/4/4/4
3	CYC	A	1163	1	-	9/21/74/74	0/4/4/4
3	CYC	D	1174	2	-	6/21/74/74	0/4/4/4
3	CYC	C	1163	1	-	8/21/74/74	0/4/4/4
3	CYC	F	1174	2	-	5/21/74/74	0/4/4/4
3	CYC	M	1163	1	-	8/21/74/74	0/4/4/4
3	CYC	O	1163	1	-	10/21/74/74	0/4/4/4
3	CYC	D	1175	2	-	9/21/74/74	0/4/4/4
3	CYC	L	1174	2	-	5/21/74/74	0/4/4/4
3	CYC	K	1163	1	-	10/21/74/74	0/4/4/4
3	CYC	N	1174	2	-	8/21/74/74	0/4/4/4
3	CYC	P	1174	2	-	8/21/74/74	0/4/4/4
4	PEB	B	1175	2	1/1/14/19	5/20/74/74	0/4/4/4
3	CYC	N	1175	2	-	11/21/74/74	0/4/4/4
3	CYC	F	1175	2	-	8/21/74/74	0/4/4/4

The worst 5 of 304 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1175	CYC	CHA-C1A	12.51	1.45	1.35
3	O	1163	CYC	C3C-C4C	11.16	1.67	1.50
3	N	1174	CYC	CHA-C1A	10.66	1.44	1.35
3	C	1163	CYC	CMB-C2B	10.08	1.72	1.50
3	B	1174	CYC	C2C-C1C	-9.96	1.43	1.52

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1175	PEB	CHC-C1D-ND	13.11	129.17	113.95
3	D	1175	CYC	CAB-C3B-C4B	10.00	137.18	121.38
3	O	1163	CYC	OC-C1C-C2C	-9.05	118.98	126.17
3	F	1174	CYC	C2C-C1C-NC	8.77	115.83	108.27
3	P	1174	CYC	C2C-C1C-NC	7.89	115.07	108.27

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	1175	PEB	C1D

5 of 141 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1175	PEB	ND-C1D-CHC-C4C
4	B	1175	PEB	NA-C4A-CHA-C1B
4	B	1175	PEB	NB-C1B-CHA-C4A
3	E	1163	CYC	NC-C4C-CHD-C1D
3	E	1163	CYC	ND-C1D-CHD-C4C

There are no ring outliers.

18 monomers are involved in 93 short contacts:

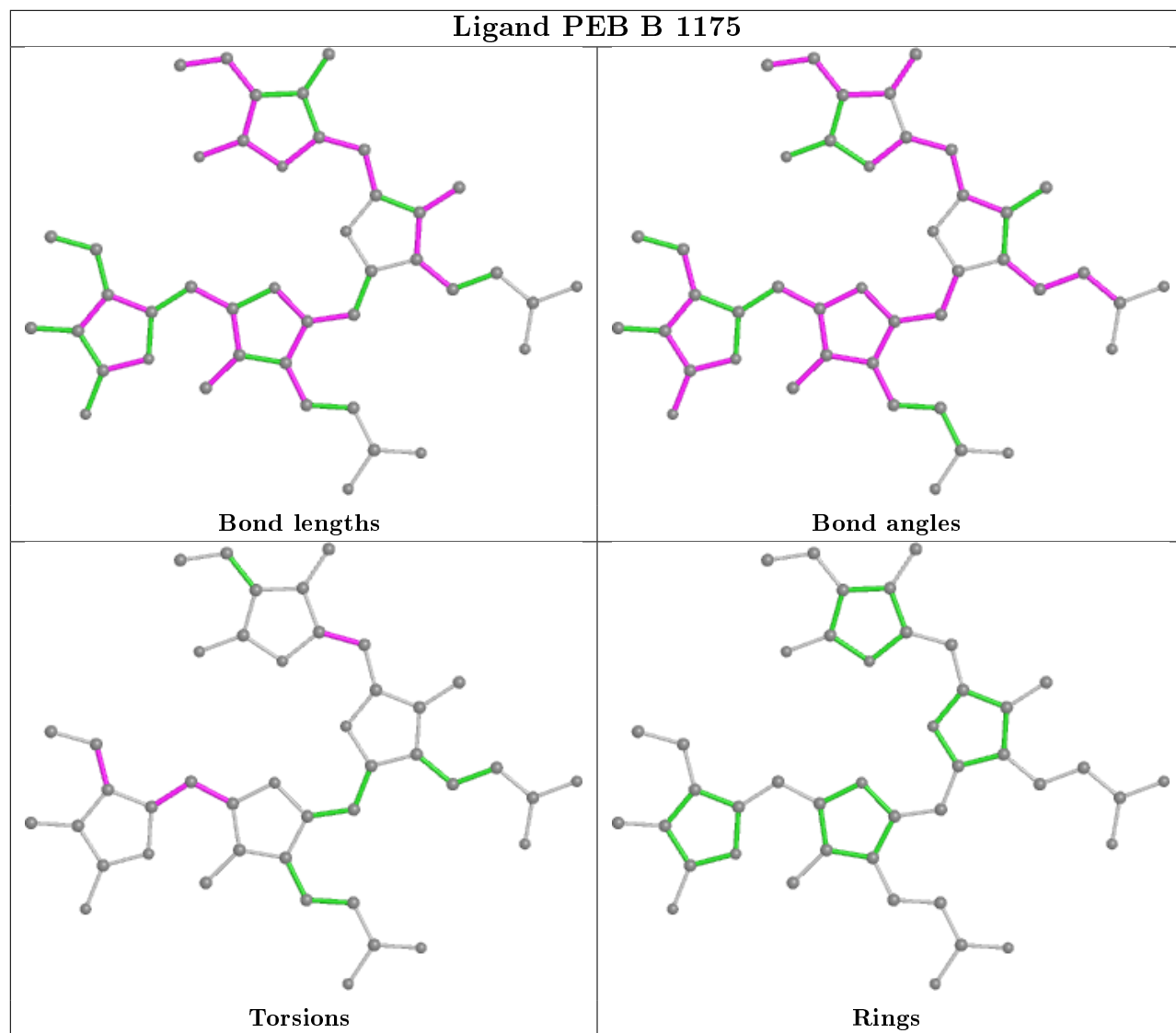
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1175	PEB	2	0
3	E	1163	CYC	7	0
3	P	1175	CYC	4	0
3	B	1174	CYC	4	0
3	A	1163	CYC	6	0
3	D	1174	CYC	7	0
3	C	1163	CYC	9	0
3	F	1174	CYC	5	0
3	M	1163	CYC	5	0

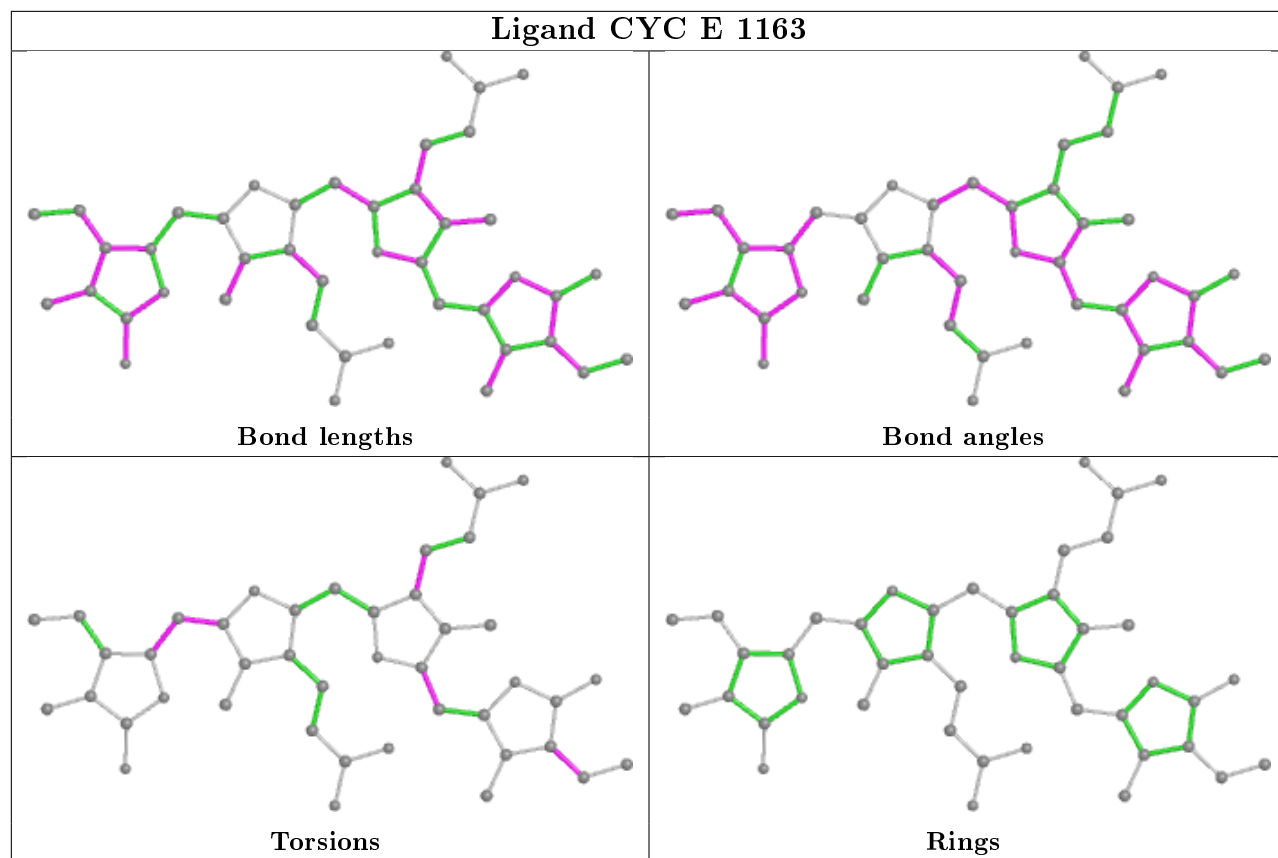
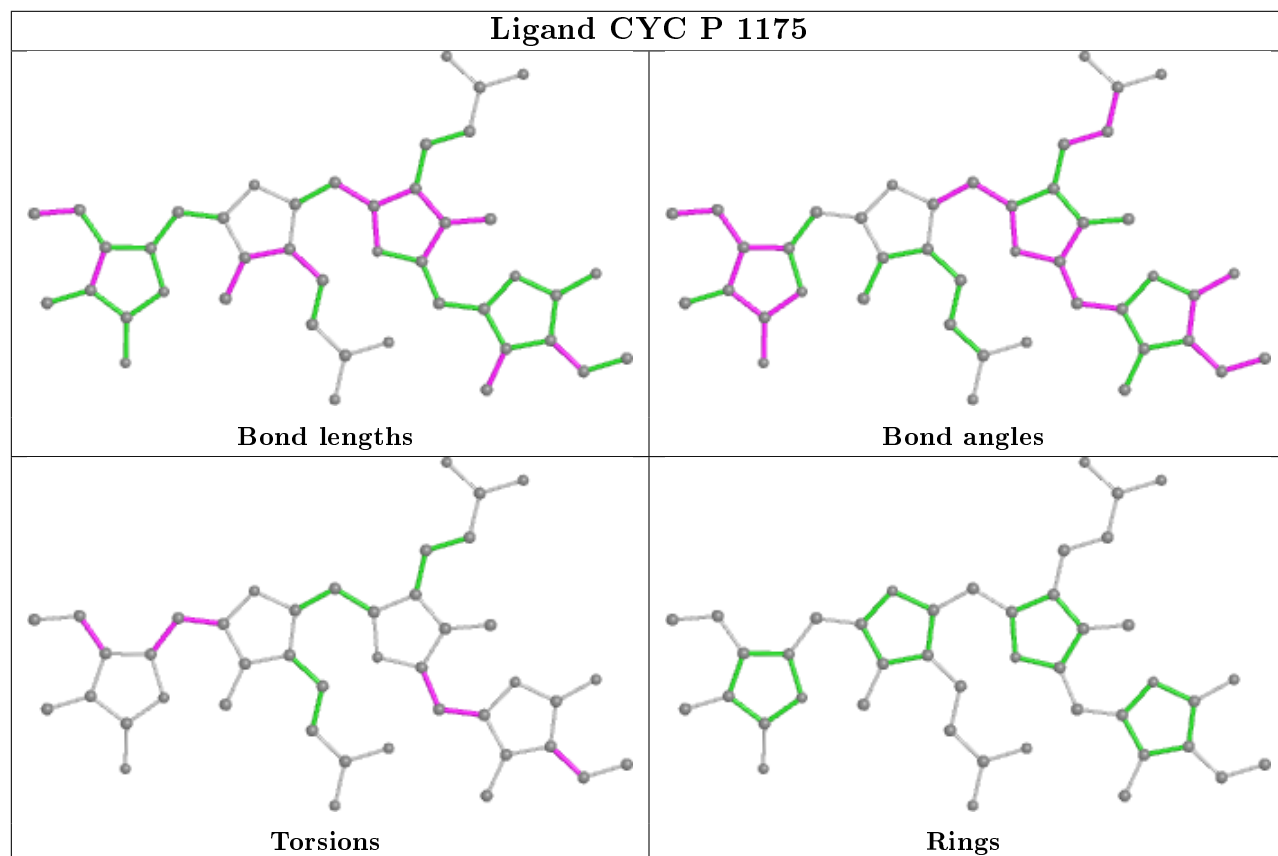
*Continued on next page...*

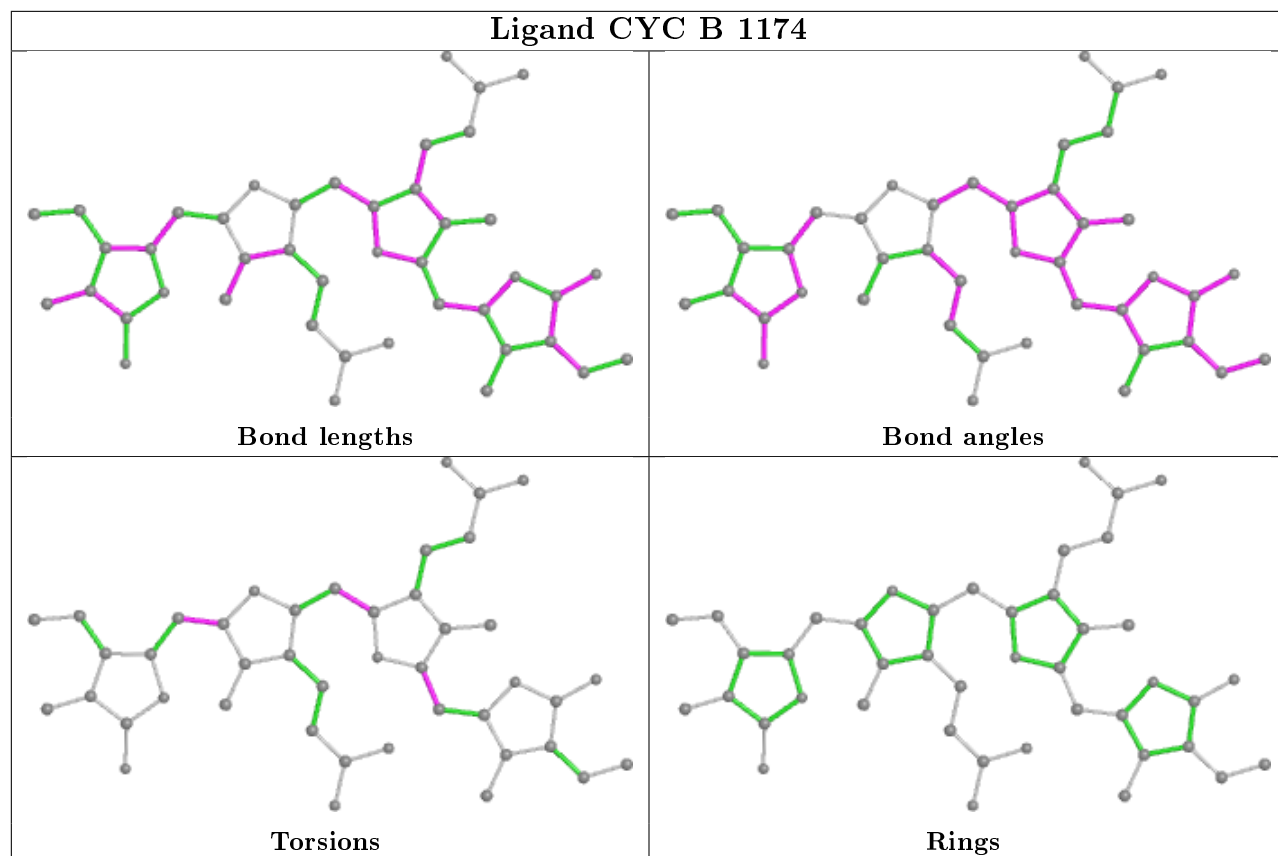
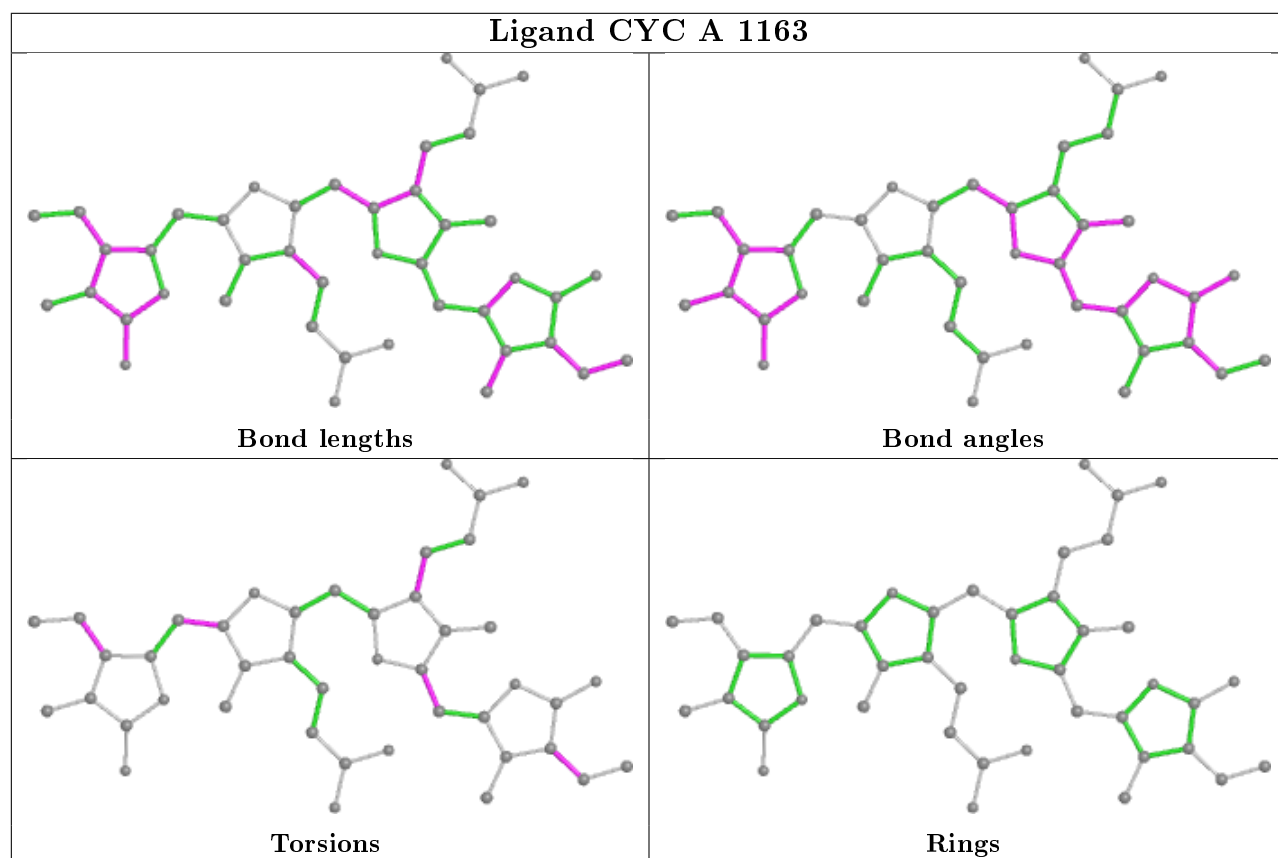
*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	1163	CYC	7	0
3	D	1175	CYC	4	0
3	L	1174	CYC	6	0
3	K	1163	CYC	7	0
3	N	1174	CYC	4	0
3	P	1174	CYC	5	0
3	L	1175	CYC	5	0
3	N	1175	CYC	3	0
3	F	1175	CYC	3	0

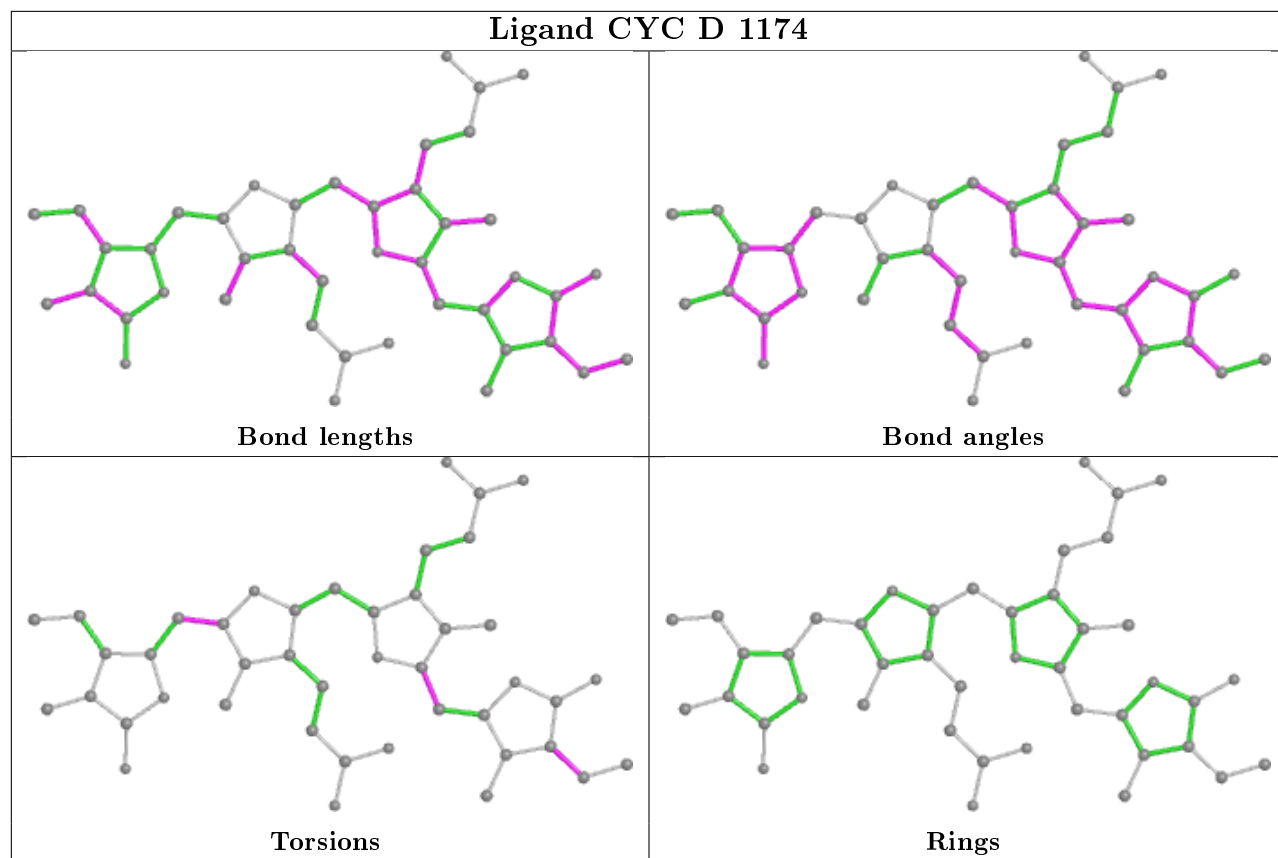
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



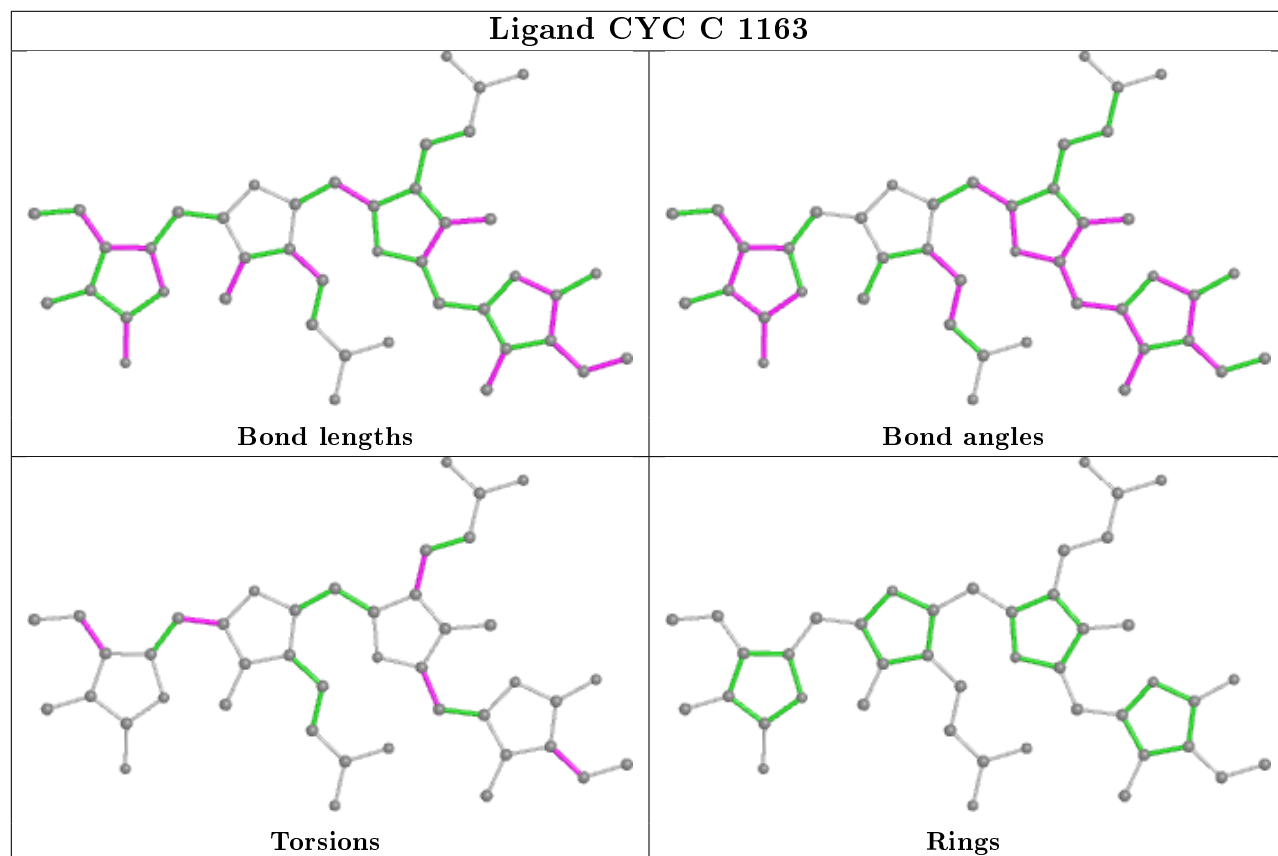
**Ligand CYC E 1163****Ligand CYC P 1175**

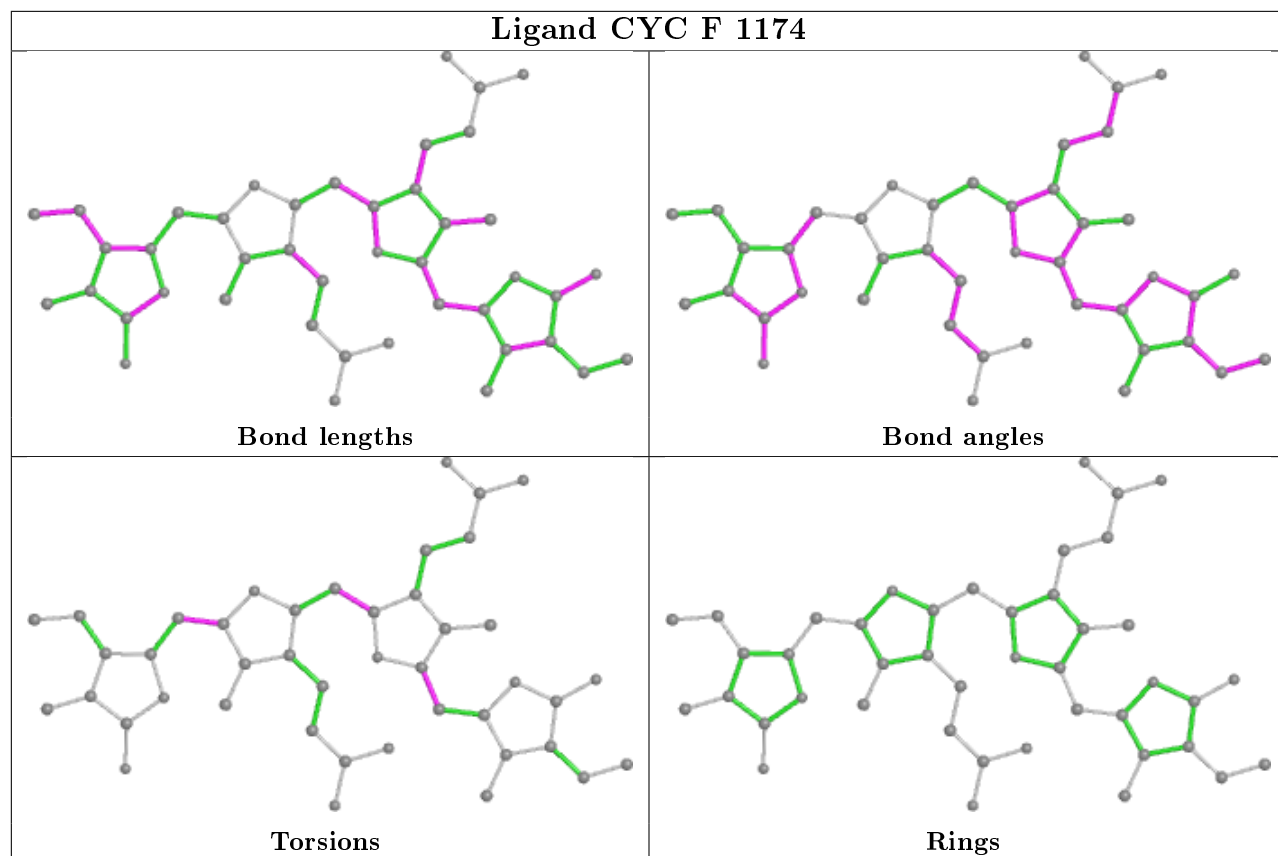
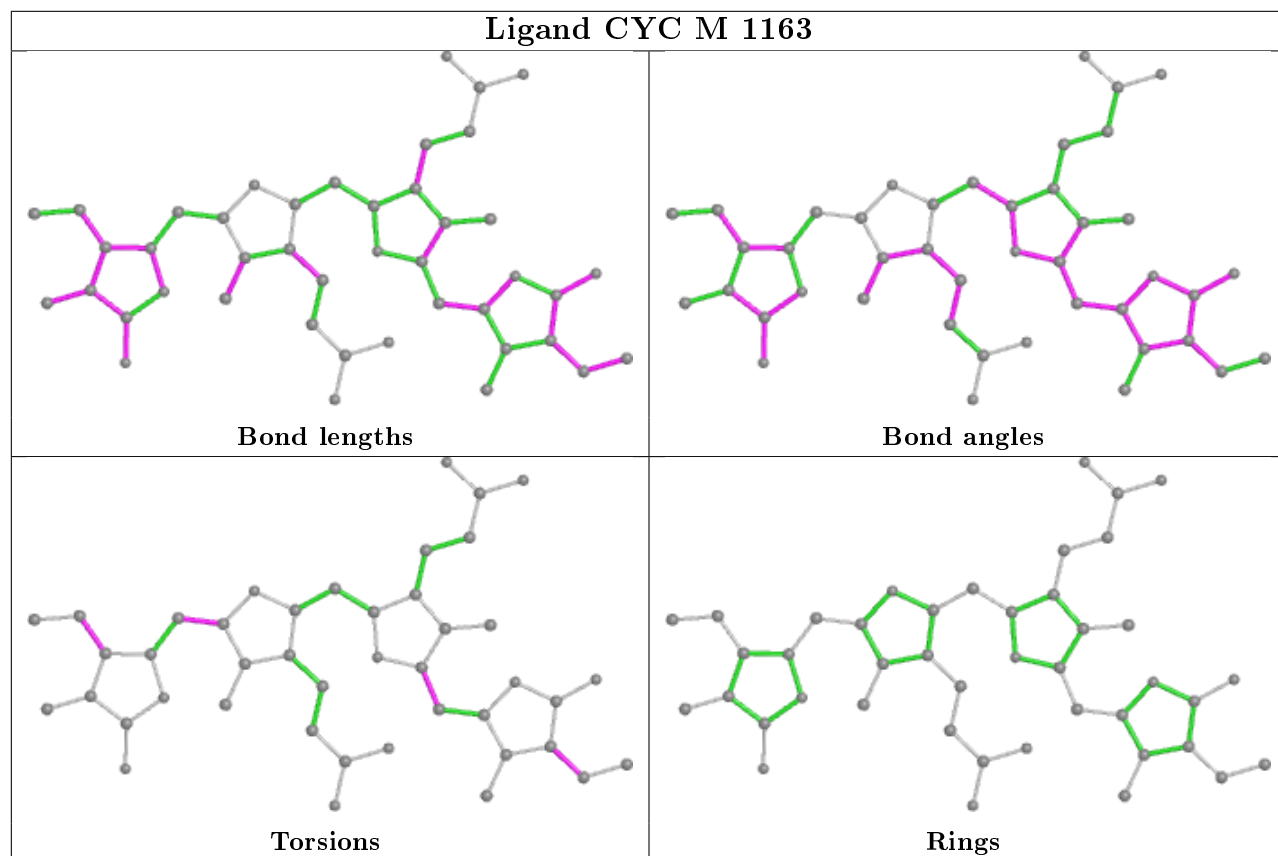
**Ligand CYC B 1174****Ligand CYC A 1163**

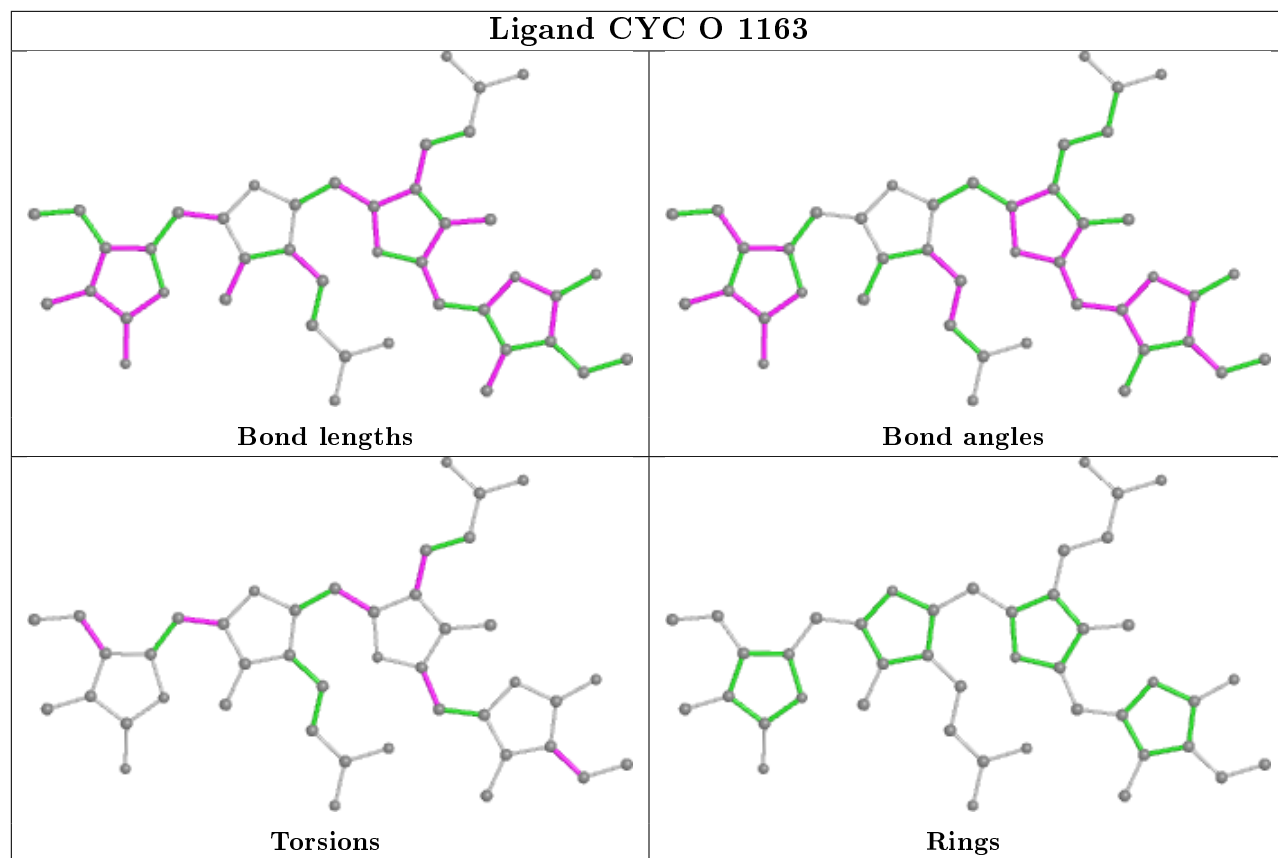
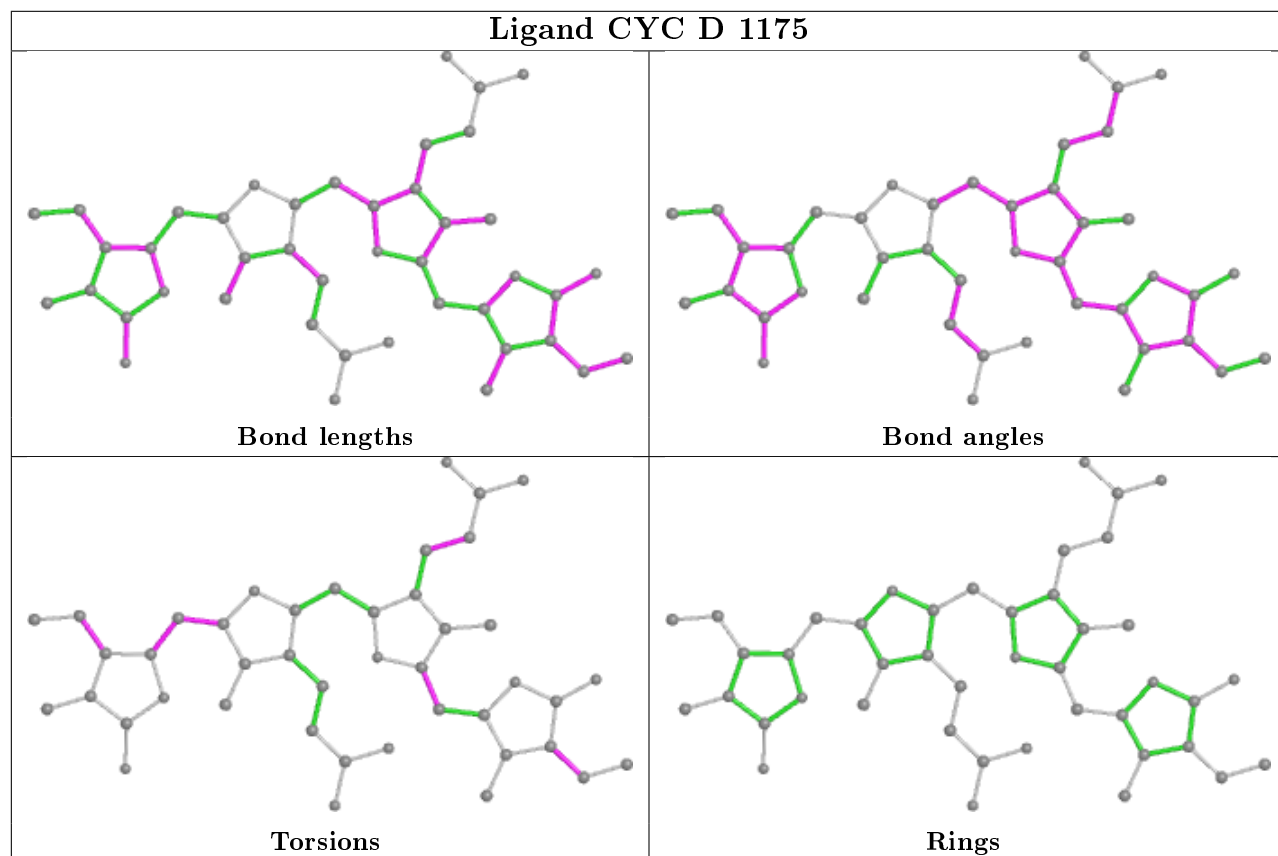
## Ligand CYC D 1174



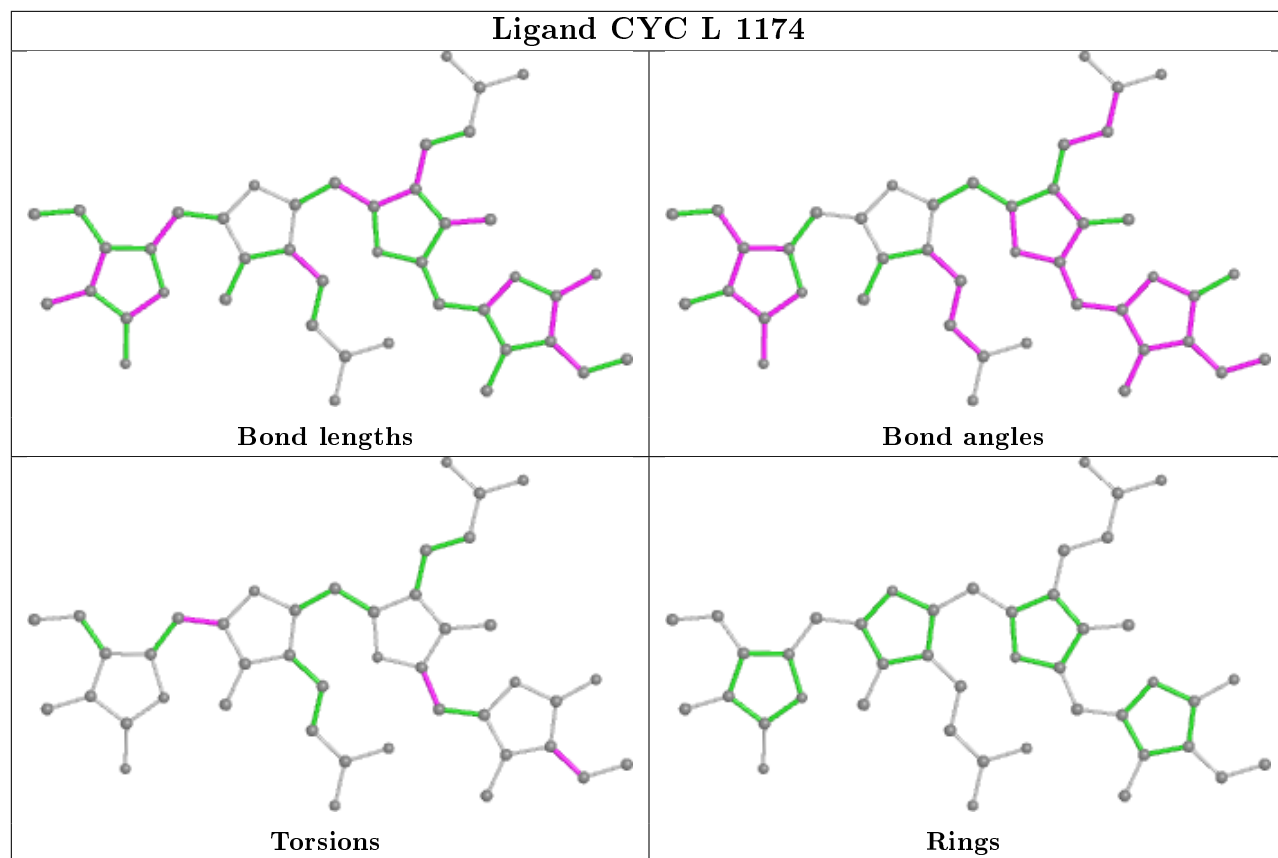
## Ligand CYC C 1163



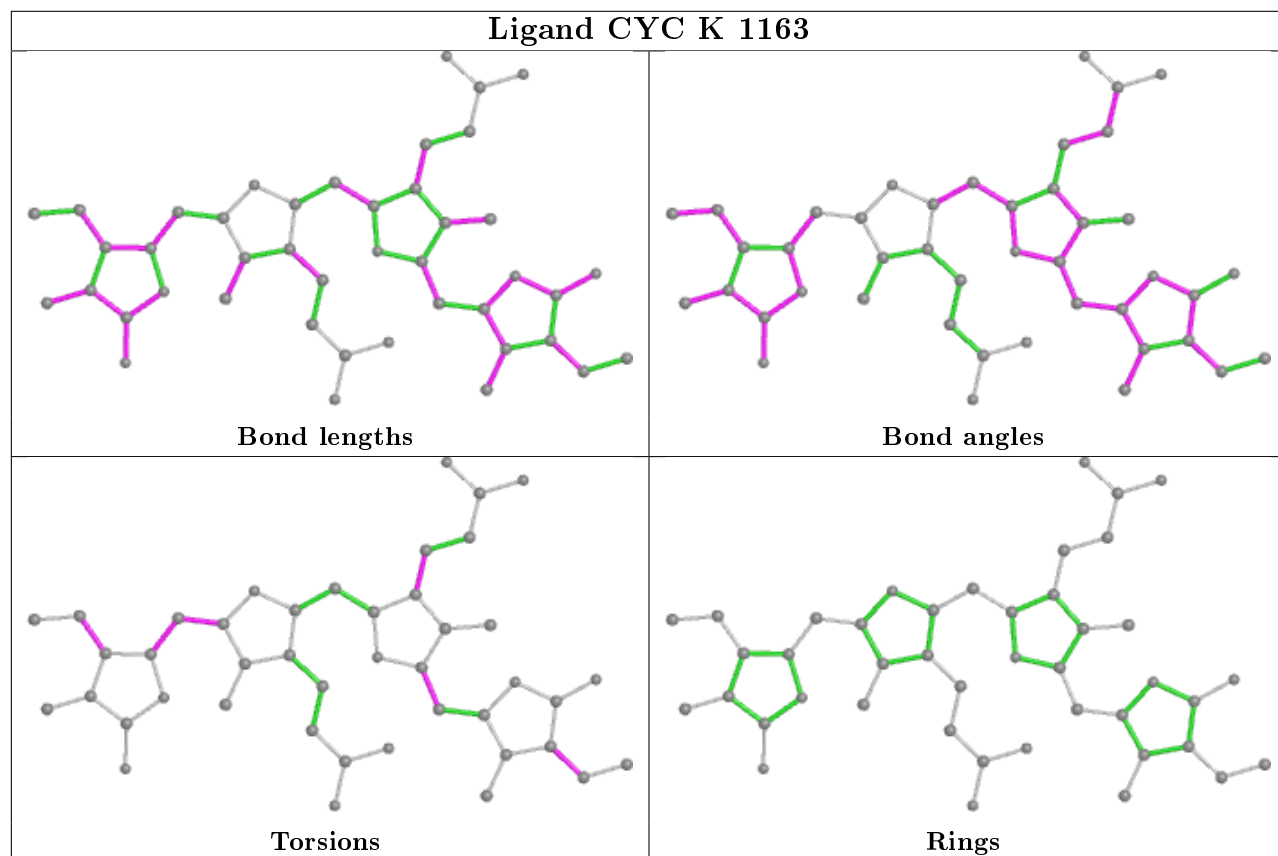
**Ligand CYC F 1174****Ligand CYC M 1163**

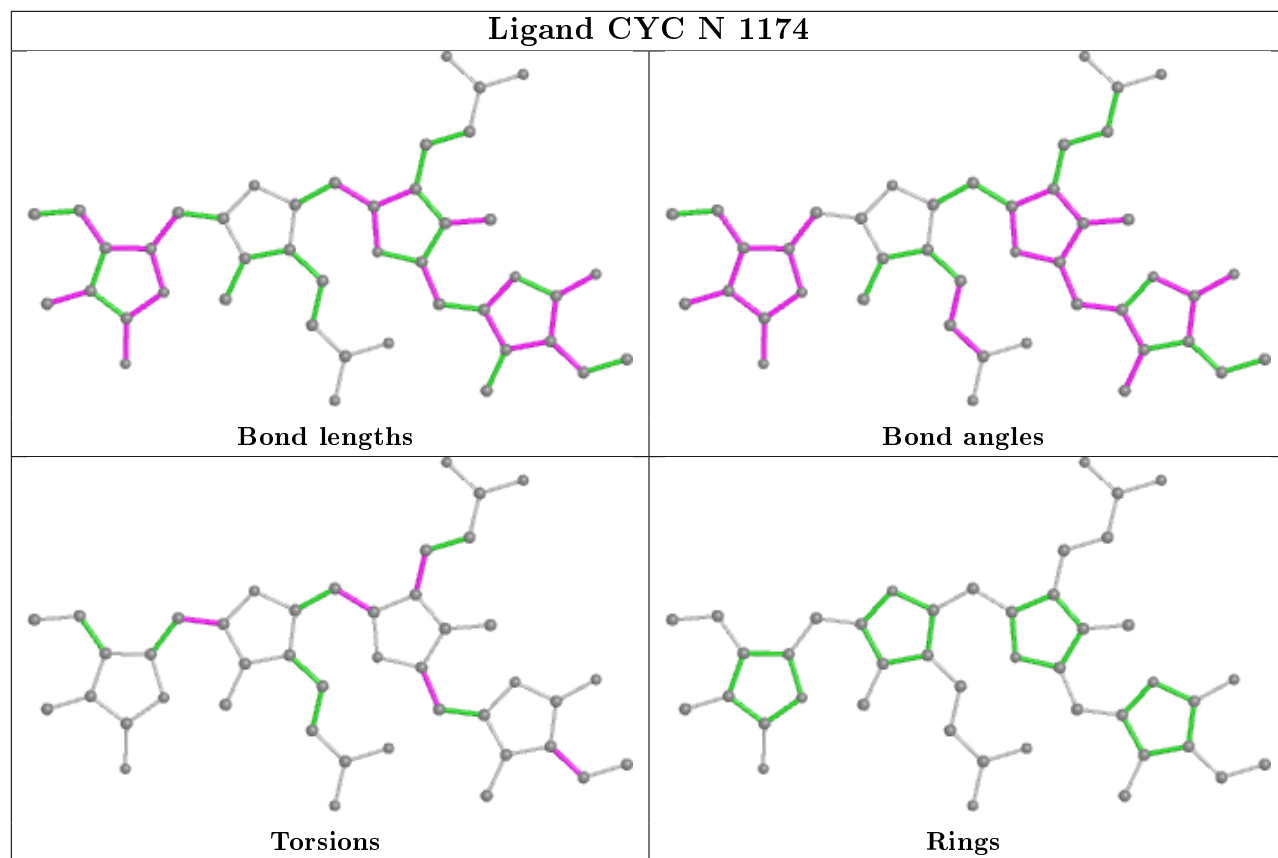
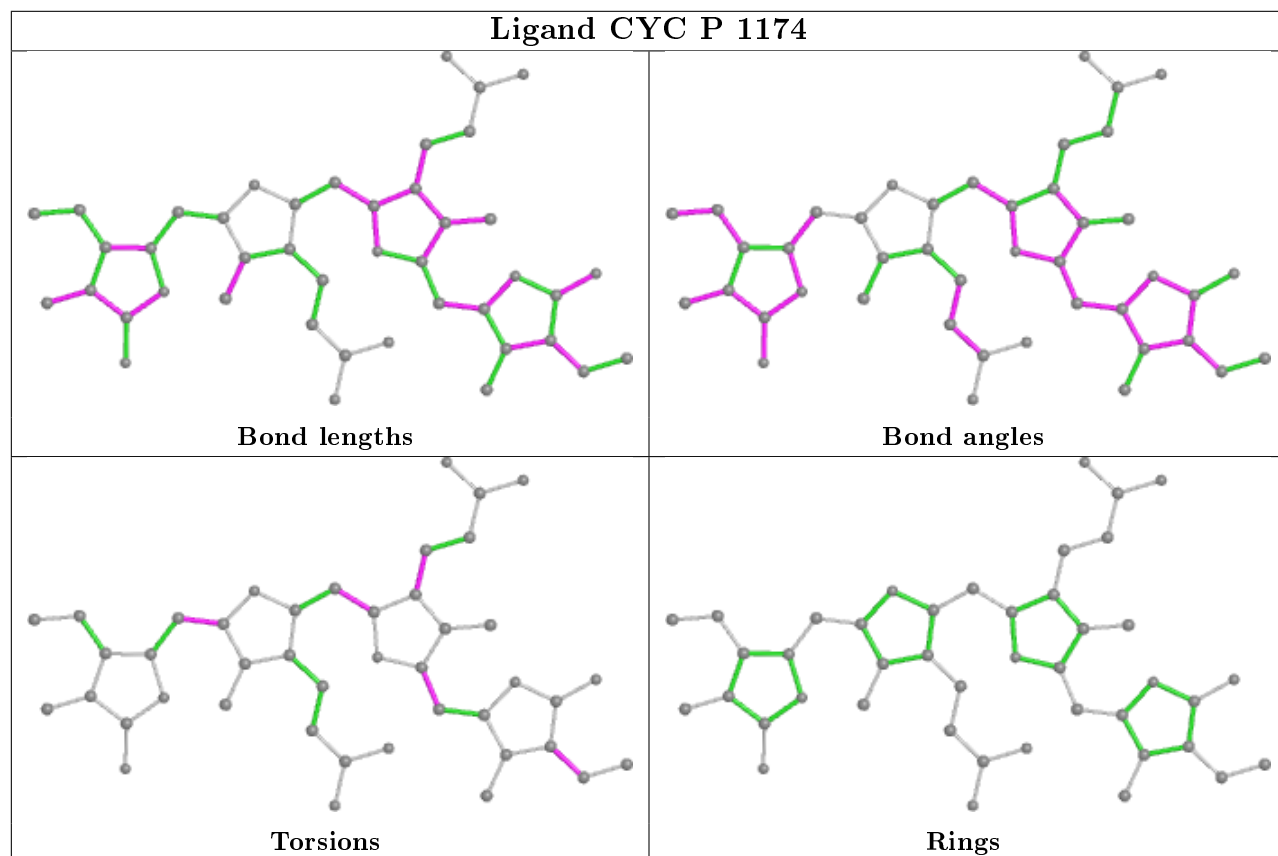
**Ligand CYC O 1163****Ligand CYC D 1175**

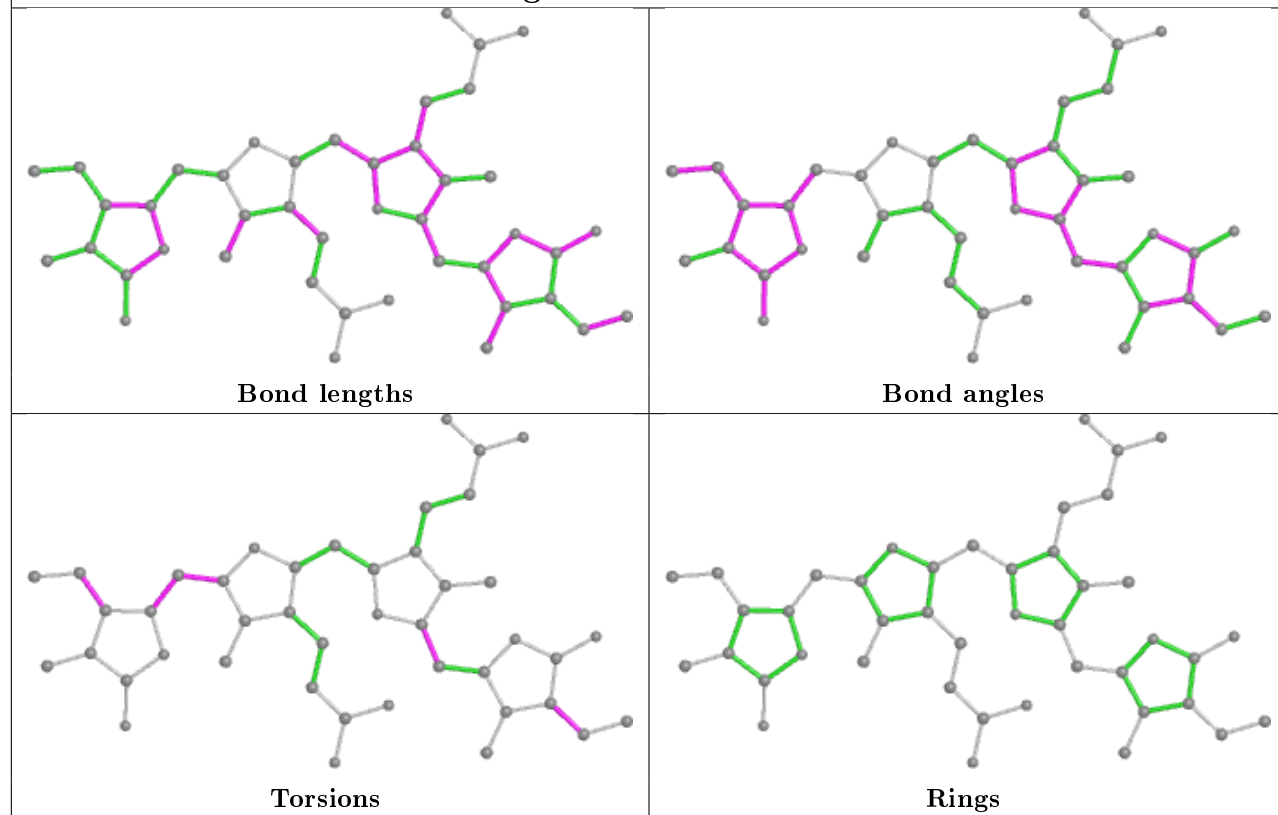
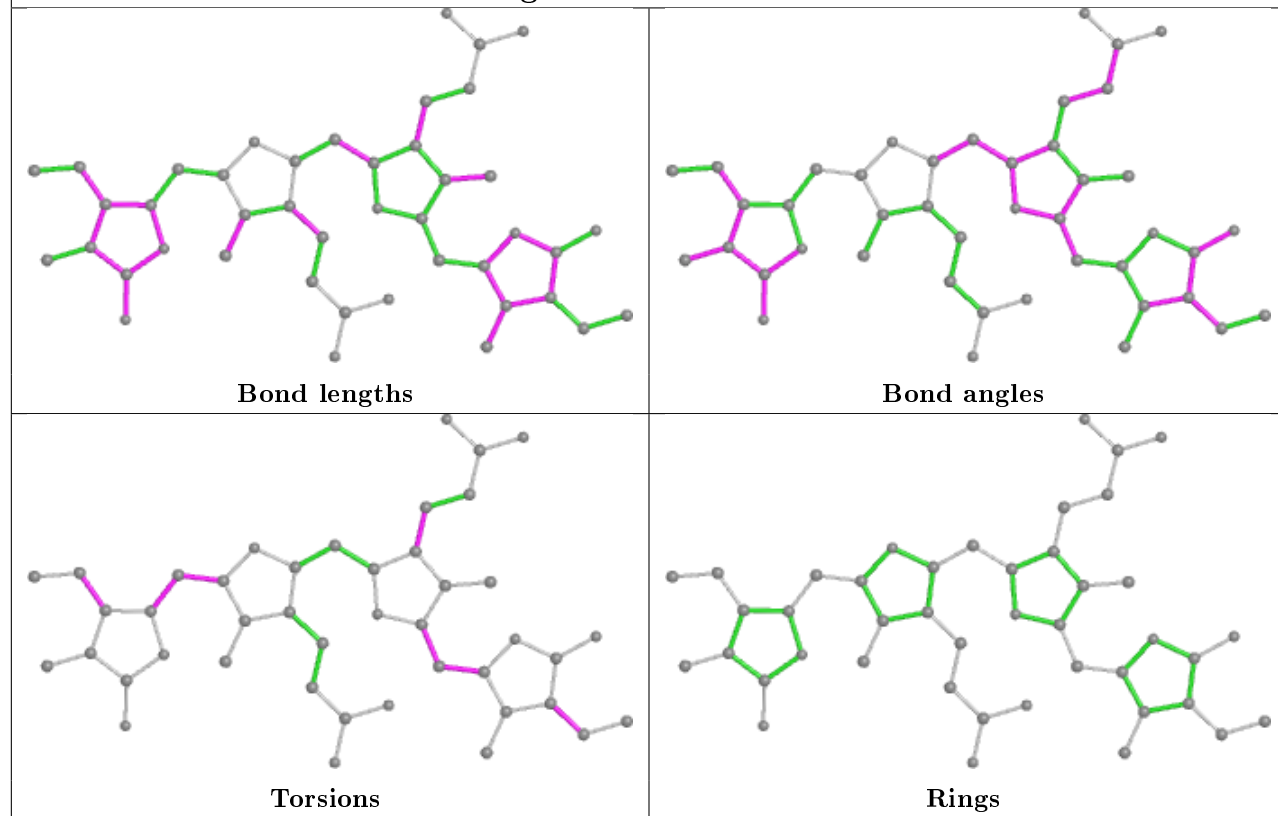
## Ligand CYC L 1174

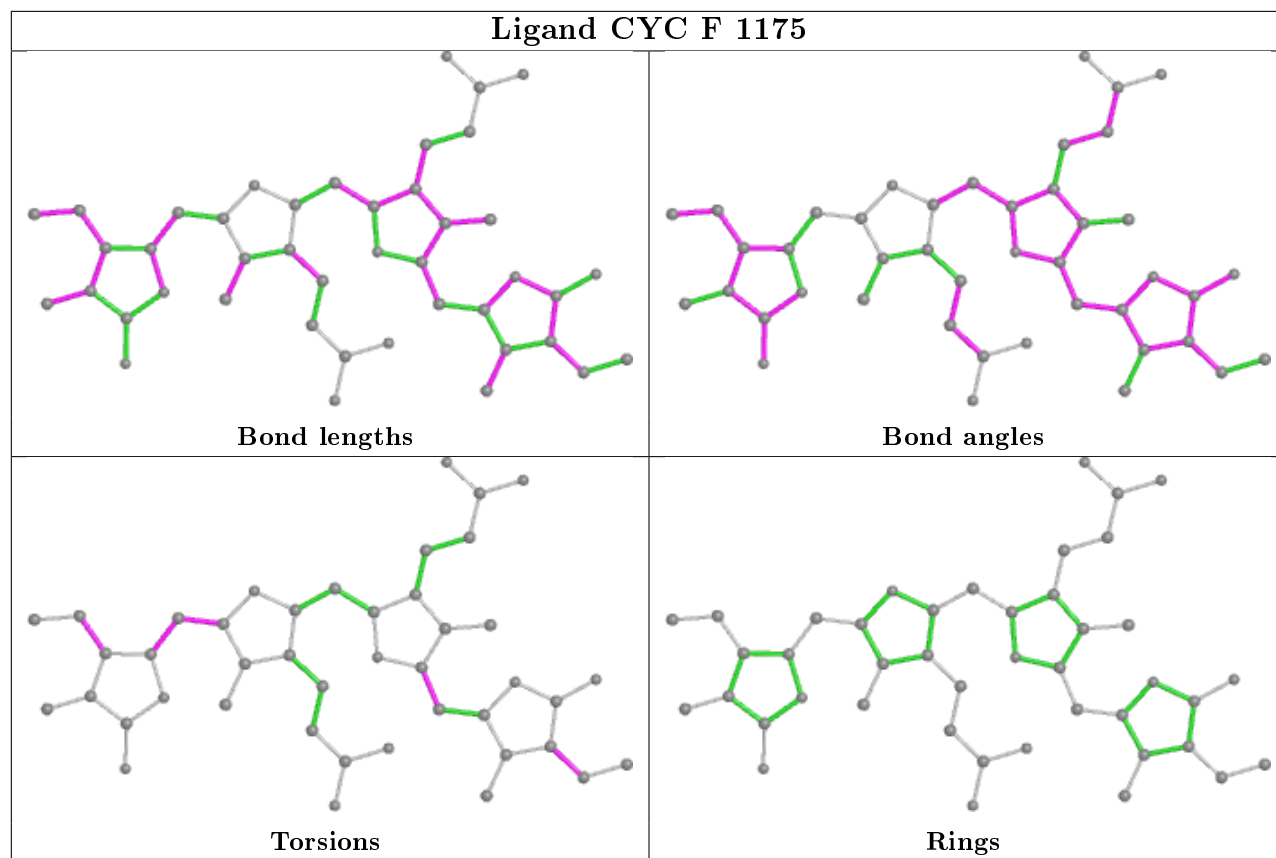


## Ligand CYC K 1163



**Ligand CYC N 1174****Ligand CYC P 1174**

**Ligand CYC L 1175****Ligand CYC N 1175**



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.15	11 (6%) 17 16	16, 23, 76, 94	0
1	C	162/162 (100%)	0.04	12 (7%) 14 13	17, 26, 80, 98	0
1	E	162/162 (100%)	0.04	12 (7%) 14 13	15, 21, 75, 102	0
1	K	162/162 (100%)	0.15	12 (7%) 14 13	14, 21, 74, 98	0
1	M	162/162 (100%)	-0.27	12 (7%) 14 13	14, 22, 71, 96	0
1	O	162/162 (100%)	0.04	12 (7%) 14 13	17, 26, 79, 96	0
2	B	171/172 (99%)	-0.52	0 100 100	14, 22, 36, 46	0
2	D	171/172 (99%)	-0.45	2 (1%) 79 78	15, 25, 39, 52	0
2	F	171/172 (99%)	-0.42	4 (2%) 60 59	17, 28, 41, 58	0
2	L	171/172 (99%)	-0.55	0 100 100	16, 24, 40, 49	0
2	N	171/172 (99%)	-0.48	0 100 100	14, 21, 34, 40	0
2	P	171/172 (99%)	-0.33	5 (2%) 51 50	17, 28, 46, 57	0
All	All	1998/2004 (99%)	-0.25	82 (4%) 37 36	14, 24, 49, 102	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	75	ALA	10.7
1	K	72	PRO	10.3
1	C	67	THR	9.9
1	A	74	TYR	9.7
1	C	73	ASN	9.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
2	MEN	D	72	9/10	0.97	0.10	19,23,25,27	0
2	MEN	N	72	9/10	0.97	0.08	16,19,23,27	0
2	MEN	L	72	9/10	0.98	0.08	16,20,24,25	0
2	MEN	P	72	9/10	0.98	0.08	21,22,25,26	0
2	MEN	B	72	9/10	0.98	0.06	14,18,22,23	0
2	MEN	F	72	9/10	0.99	0.09	21,26,27,34	0

### 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.

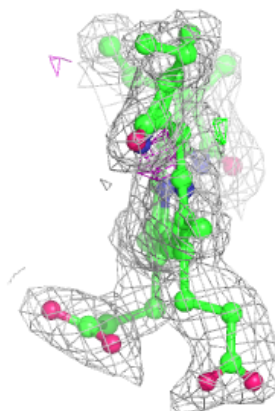
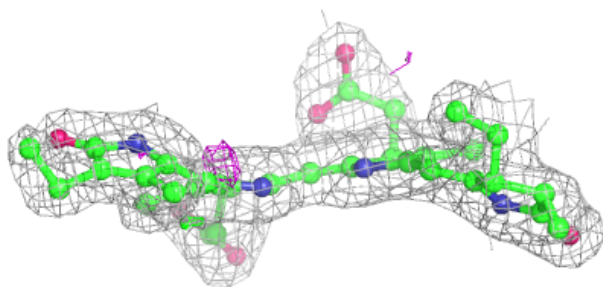
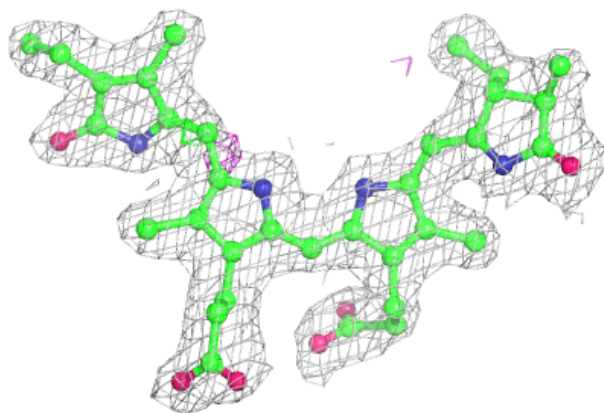
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	CYC	P	1175	43/43	0.94	0.10	20,31,49,52	0
3	CYC	P	1174	43/43	0.94	0.13	19,29,44,47	0
3	CYC	F	1174	43/43	0.95	0.13	16,29,45,49	0
3	CYC	L	1174	43/43	0.95	0.10	15,31,40,49	0
3	CYC	B	1174	43/43	0.95	0.10	9,21,35,39	0
3	CYC	L	1175	43/43	0.95	0.10	17,24,40,52	0
3	CYC	O	1163	43/43	0.96	0.08	14,23,37,45	0
3	CYC	D	1175	43/43	0.96	0.08	14,23,38,56	0
3	CYC	A	1163	43/43	0.96	0.08	14,25,39,46	0
3	CYC	F	1175	43/43	0.96	0.10	14,24,41,63	0
3	CYC	N	1174	43/43	0.96	0.10	9,24,38,44	0
3	CYC	D	1174	43/43	0.96	0.11	13,34,47,53	0
3	CYC	E	1163	43/43	0.96	0.12	12,18,28,38	0
3	CYC	N	1175	43/43	0.96	0.09	14,24,51,59	0
3	CYC	M	1163	43/43	0.97	0.08	15,23,32,40	0
3	CYC	C	1163	43/43	0.97	0.08	13,22,35,37	0
4	PEB	B	1175	43/43	0.97	0.08	11,22,44,52	0
3	CYC	K	1163	43/43	0.97	0.12	13,20,29,36	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.

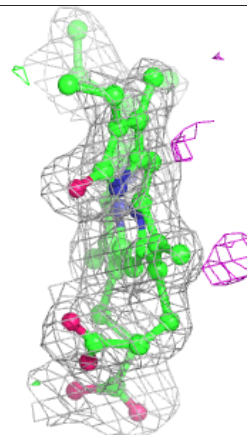
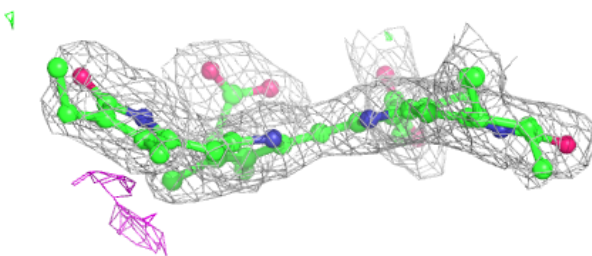
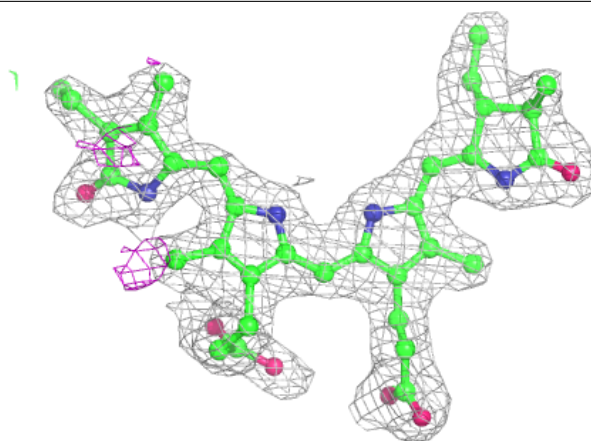
**Electron density around CYC P 1175:**

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



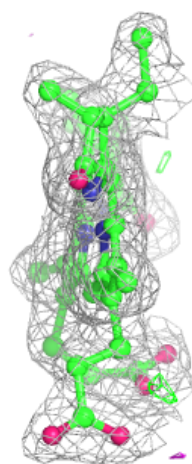
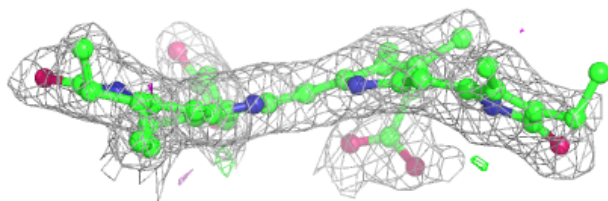
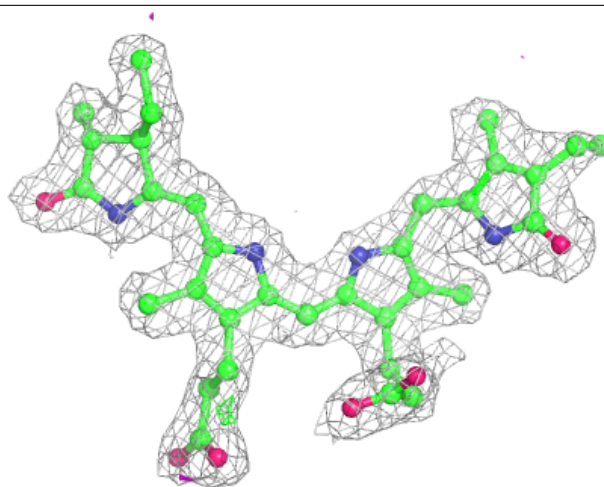
**Electron density around CYC P 1174:**

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and green (positive)



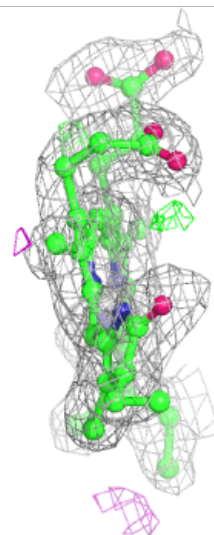
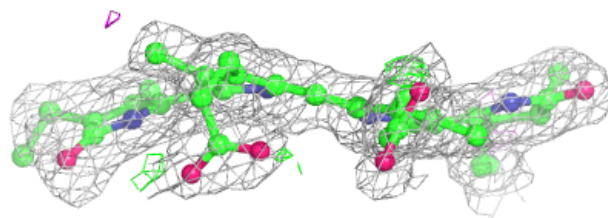
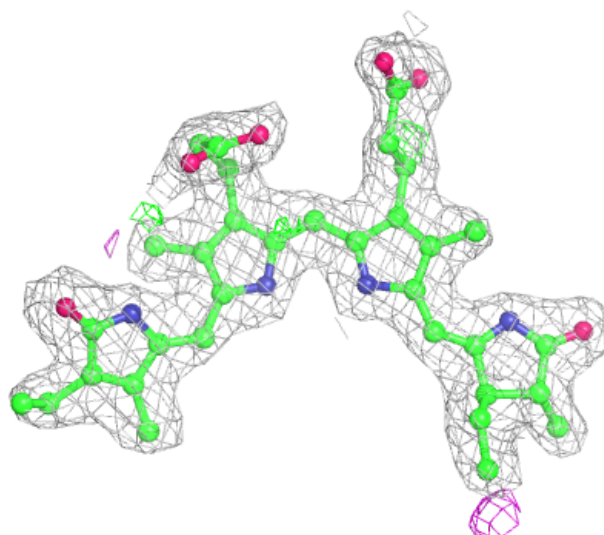
**Electron density around CYC F 1174:**

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and green (positive)



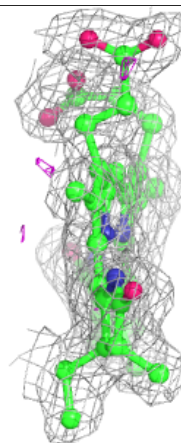
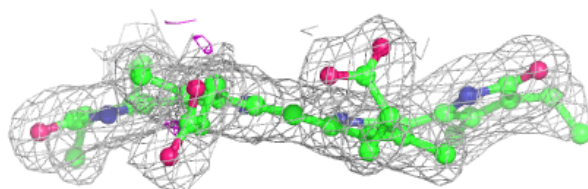
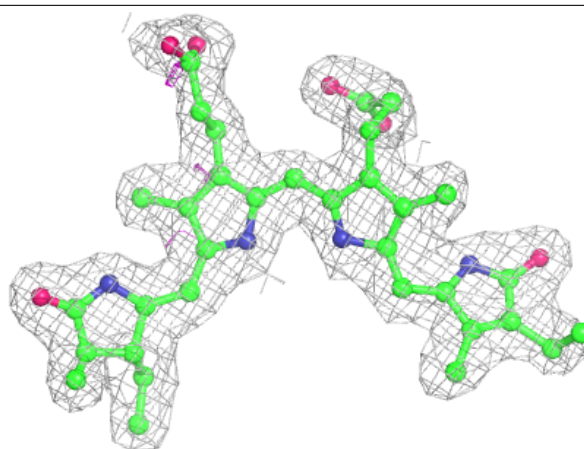
**Electron density around CYC L 1174:**

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and green (positive)

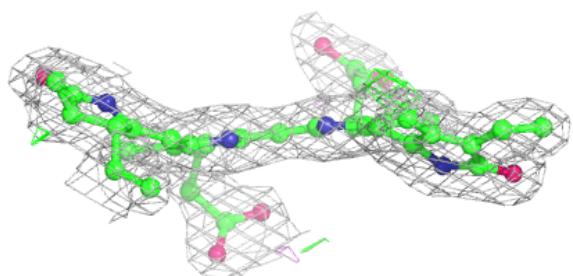
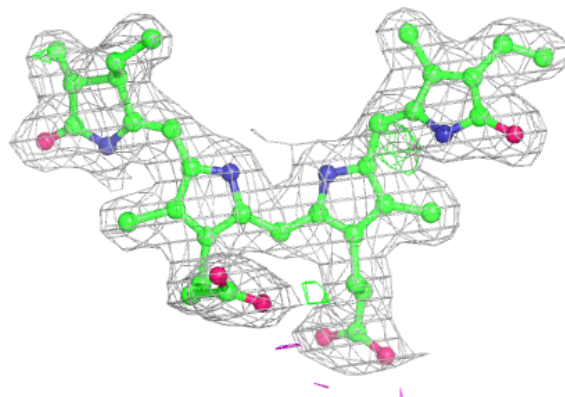


**Electron density around CYC B 1174:**

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and green (positive)

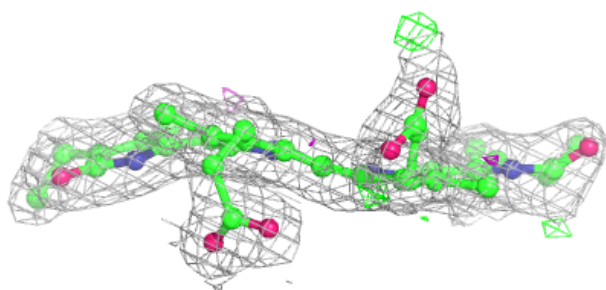
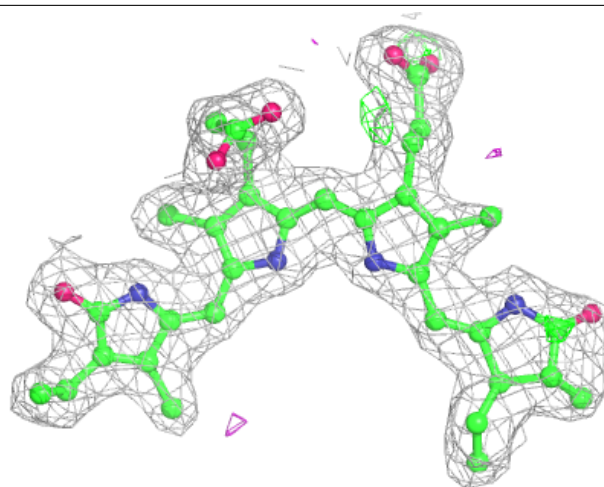
**Electron density around CYC L 1175:**

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and green (positive)



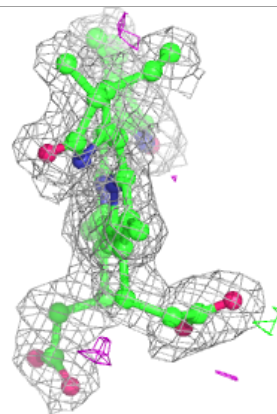
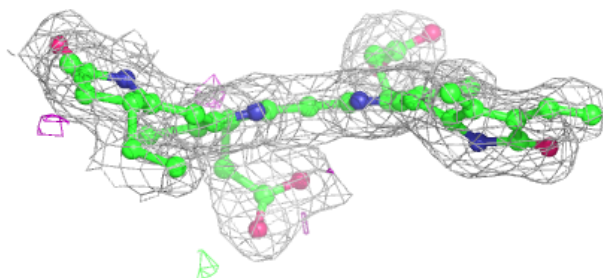
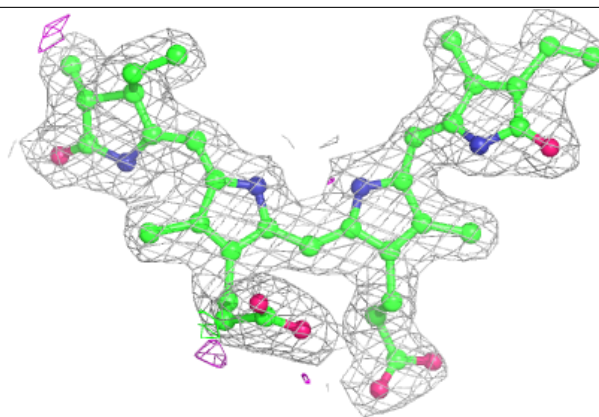
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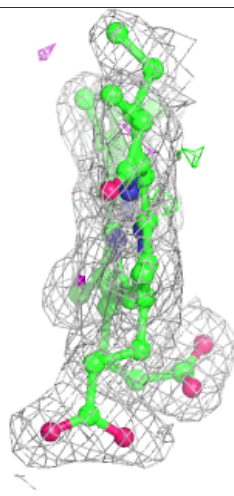
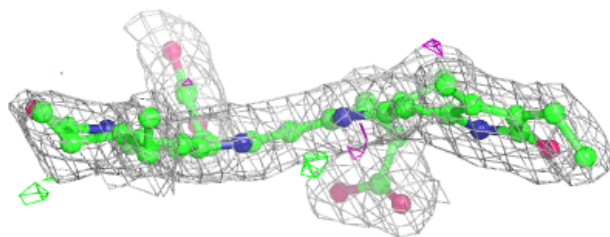
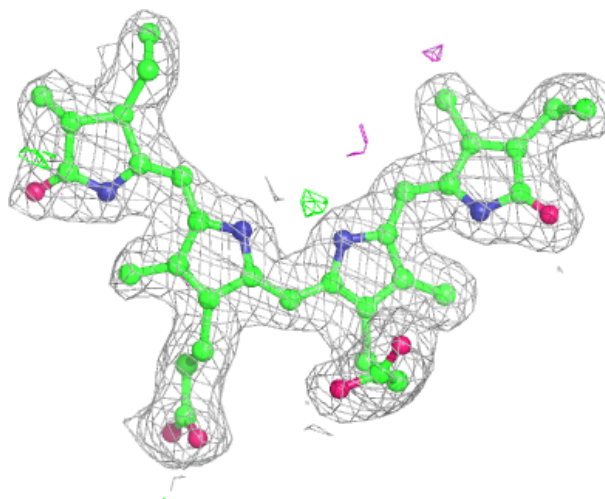
**Electron density around CYC D 1175:**

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and green (positive)



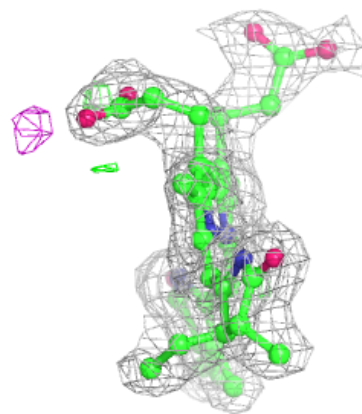
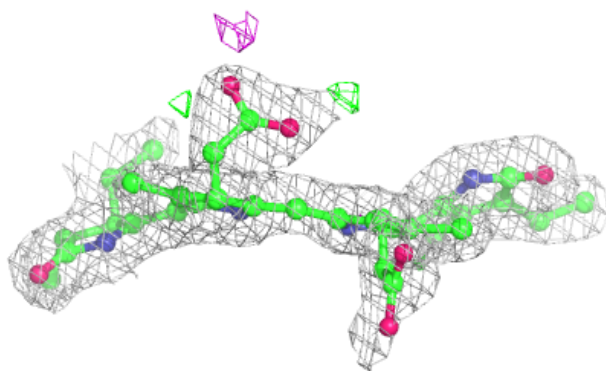
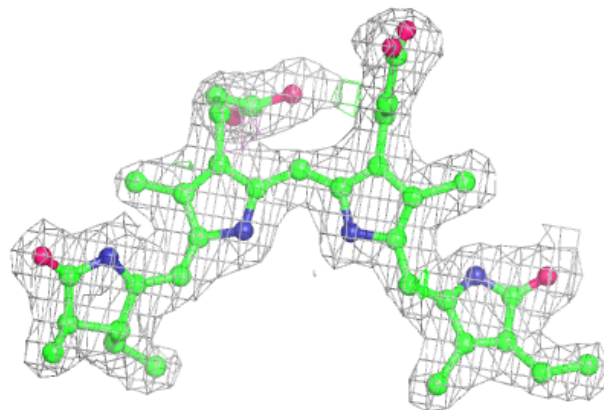
**Electron density around CYC A 1163:**

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and green (positive)



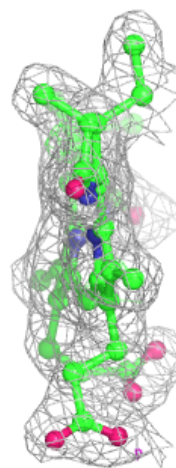
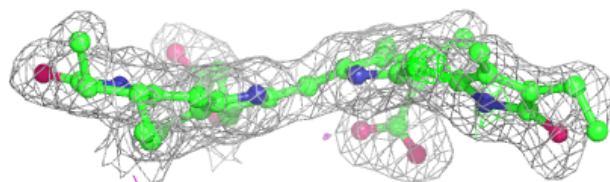
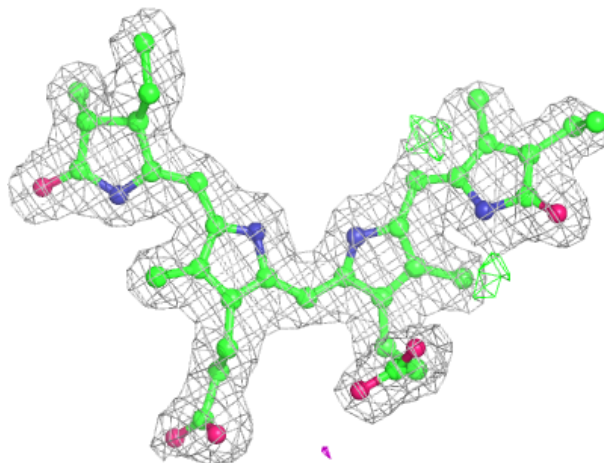
**Electron density around CYC F 1175:**

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and green (positive)



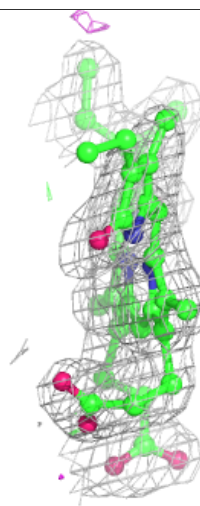
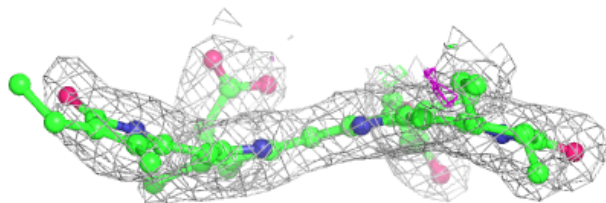
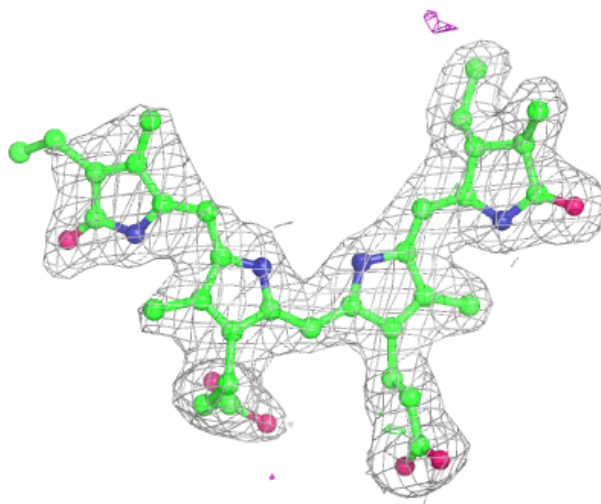
**Electron density around CYC N 1174:**

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



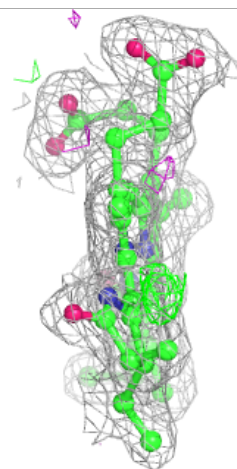
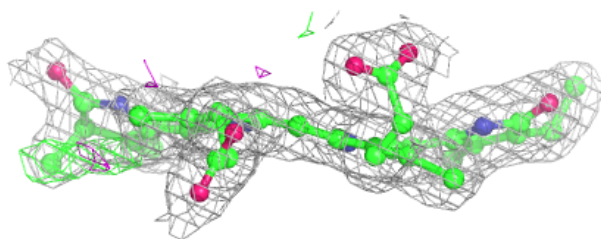
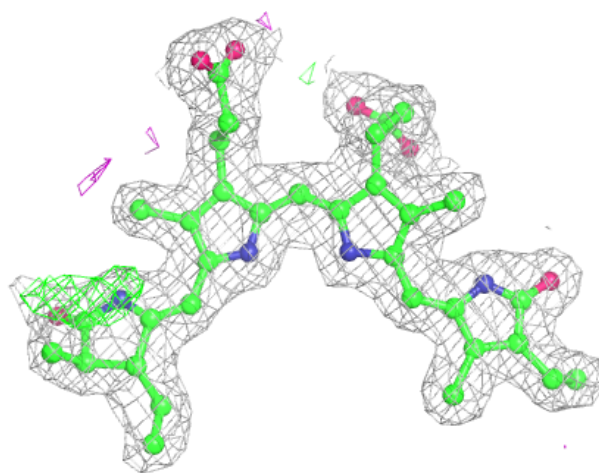
**Electron density around CYC D 1174:**

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



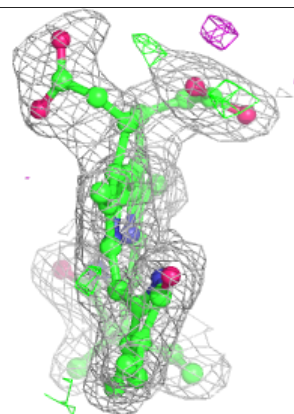
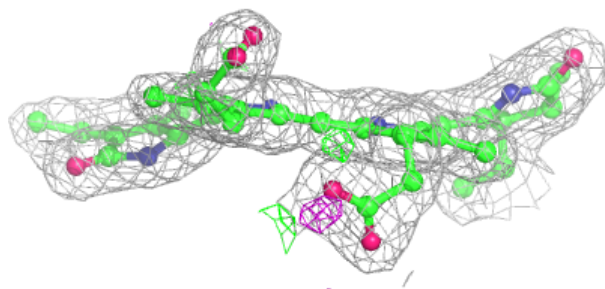
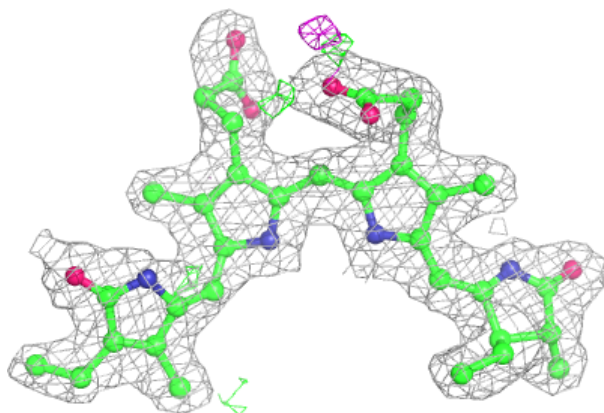
**Electron density around CYC E 1163:**

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



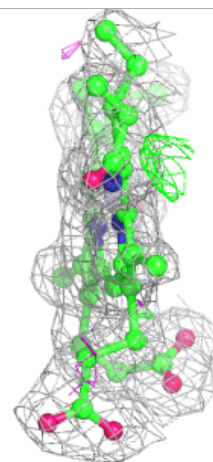
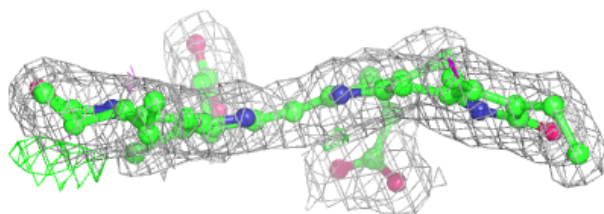
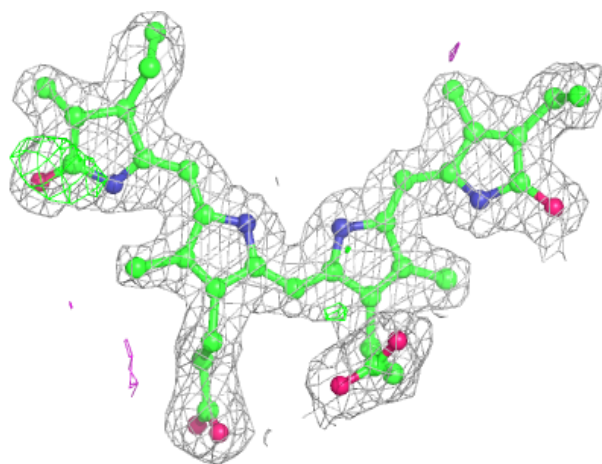
**Electron density around CYC N 1175:**

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



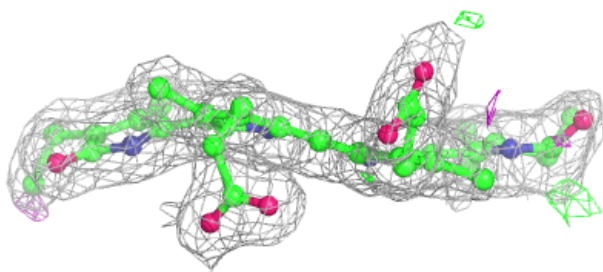
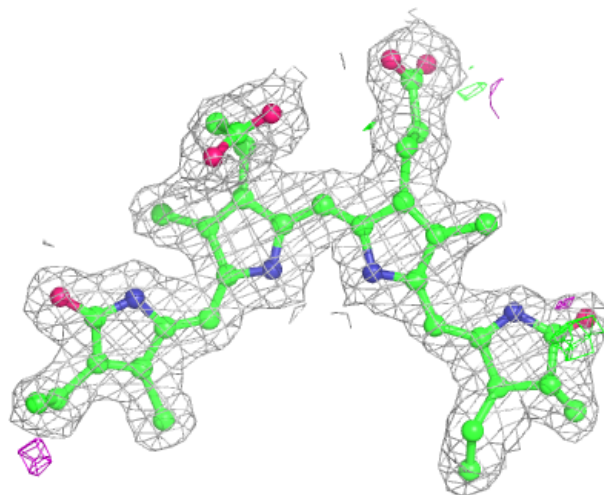
**Electron density around CYC M 1163:**

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



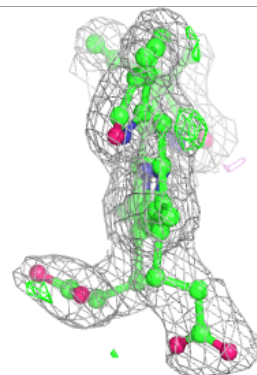
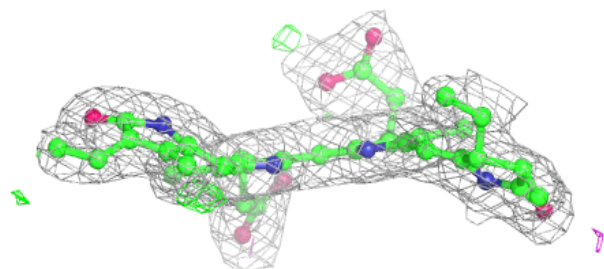
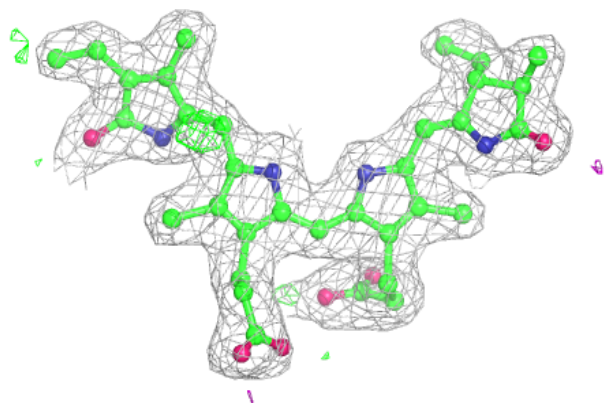
**Electron density around CYC C 1163:**

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

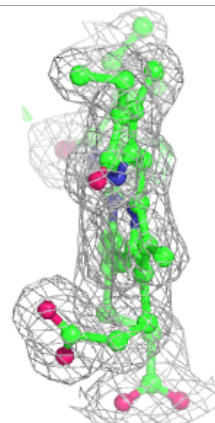
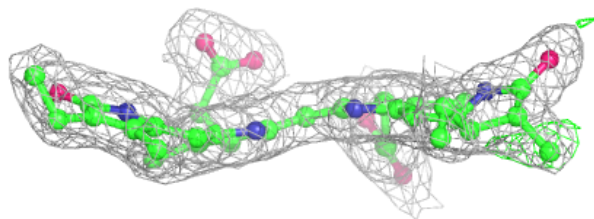
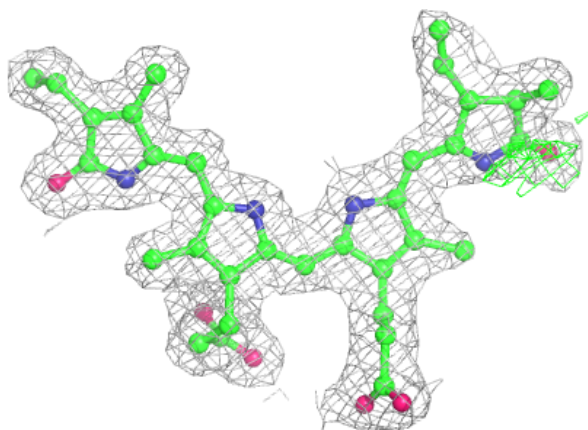


**Electron density around PEB B 1175:**

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

**Electron density around CYC K 1163:**

$2mF_o-DF_c$  (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.