Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 08:36 PM EST

PDB ID	:	1GH0
Title	:	CRYSTAL STRUCTURE OF C-PHYCOCYANIN FROM SPIRULINA PLATENSIS
Authors	:	Liang, D.-C.; Chang, W.-R.; Wang, X.-Q.
Deposited on	:	2000-10-29
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

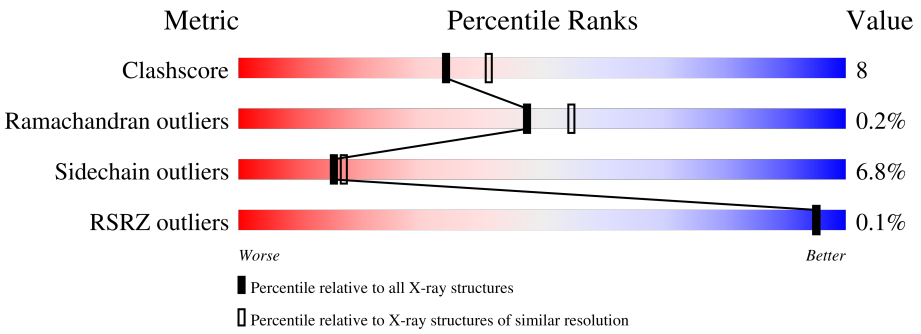
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	85% 14% •
1	C	162	80% 18% •
1	E	162	86% 12% •
1	G	162	80% 19% •
1	I	162	81% 16% •
1	K	162	86% 14% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	162	%, 80%, 18%
1	O	162	82%, 16%
1	Q	162	75%, 21%
1	S	162	79%, 18%
1	U	162	83%, 17%
1	W	162	85%, 13%
2	B	172	82%, 17%
2	D	172	81%, 17%
2	F	172	%, 84%, 14%
2	H	172	78%, 21%
2	J	172	81%, 17%
2	L	172	%, 82%, 17%
2	N	172	85%, 14%
2	P	172	%, 74%, 23%
2	R	172	79%, 17%
2	T	172	77%, 19%
2	V	172	85%, 14%
2	X	172	81%, 18%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32493 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
			Total	C	N	O	S			
1	A	162	1237	781	208	242	6	8	0	0
1	C	162	1237	781	208	242	6	12	0	0
1	E	162	1237	781	208	242	6	4	0	0
1	G	162	1237	781	208	242	6	8	0	0
1	I	162	1237	781	208	242	6	4	0	0
1	K	162	1237	781	208	242	6	4	0	0
1	M	162	1237	781	208	242	6	4	0	0
1	O	162	1237	781	208	242	6	12	0	0
1	Q	162	1237	781	208	242	6	4	0	0
1	S	162	1237	781	208	242	6	8	0	0
1	U	162	1237	781	208	242	6	4	0	0
1	W	162	1237	781	208	242	6	4	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	VAL	ILE	see remark 999	UNP P72509
A	51	LEU	ARG	see remark 999	UNP P72509
A	148	VAL	GLY	see remark 999	UNP P72509
C	11	VAL	ILE	see remark 999	UNP P72509
C	51	LEU	ARG	see remark 999	UNP P72509

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	148	VAL	GLY	see remark 999	UNP P72509
E	11	VAL	ILE	see remark 999	UNP P72509
E	51	LEU	ARG	see remark 999	UNP P72509
E	148	VAL	GLY	see remark 999	UNP P72509
G	11	VAL	ILE	see remark 999	UNP P72509
G	51	LEU	ARG	see remark 999	UNP P72509
G	148	VAL	GLY	see remark 999	UNP P72509
I	11	VAL	ILE	see remark 999	UNP P72509
I	51	LEU	ARG	see remark 999	UNP P72509
I	148	VAL	GLY	see remark 999	UNP P72509
K	11	VAL	ILE	see remark 999	UNP P72509
K	51	LEU	ARG	see remark 999	UNP P72509
K	148	VAL	GLY	see remark 999	UNP P72509
M	11	VAL	ILE	see remark 999	UNP P72509
M	51	LEU	ARG	see remark 999	UNP P72509
M	148	VAL	GLY	see remark 999	UNP P72509
O	11	VAL	ILE	see remark 999	UNP P72509
O	51	LEU	ARG	see remark 999	UNP P72509
O	148	VAL	GLY	see remark 999	UNP P72509
Q	11	VAL	ILE	see remark 999	UNP P72509
Q	51	LEU	ARG	see remark 999	UNP P72509
Q	148	VAL	GLY	see remark 999	UNP P72509
S	11	VAL	ILE	see remark 999	UNP P72509
S	51	LEU	ARG	see remark 999	UNP P72509
S	148	VAL	GLY	see remark 999	UNP P72509
U	11	VAL	ILE	see remark 999	UNP P72509
U	51	LEU	ARG	see remark 999	UNP P72509
U	148	VAL	GLY	see remark 999	UNP P72509
W	11	VAL	ILE	see remark 999	UNP P72509
W	51	LEU	ARG	see remark 999	UNP P72509
W	148	VAL	GLY	see remark 999	UNP P72509

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	172	1263	782	221	251	9	0	0	0
			Total	C	N	O	S			
2	D	172	1263	782	221	251	9	0	0	0
			Total	C	N	O	S			
2	F	172	1263	782	221	251	9	4	0	0
			Total	C	N	O	S			
2	H	172	1263	782	221	251	9	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	J	172	1263	782	221	251	9	0	0	0
2	L	172	1263	782	221	251	9	0	0	0
2	N	172	1263	782	221	251	9	0	0	0
2	P	172	1263	782	221	251	9	0	0	0
2	R	172	1263	782	221	251	9	4	0	0
2	T	172	1263	782	221	251	9	4	0	0
2	V	172	1263	782	221	251	9	4	0	0
2	X	172	1263	782	221	251	9	4	0	0

There are 60 discrepancies between the modelled and reference sequences:

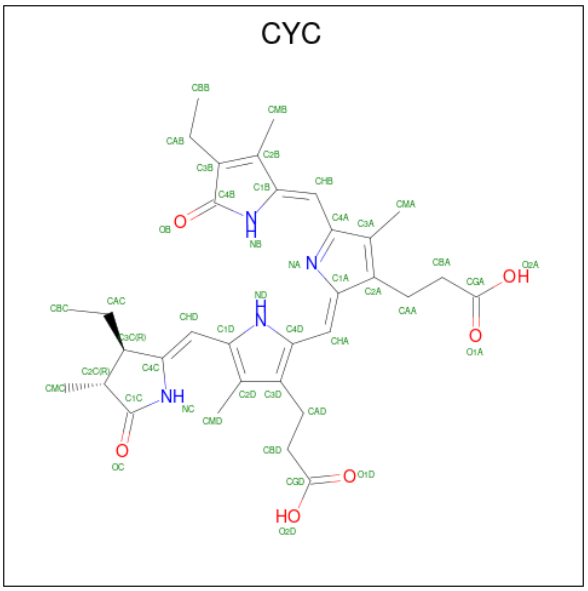
Chain	Residue	Modelled	Actual	Comment	Reference
B	40	VAL	ALA	see remark 999	UNP P72508
B	72	MEN	ASN	modified residue	UNP P72508
B	76	SER	ASN	see remark 999	UNP P72508
B	162	GLY	SER	see remark 999	UNP P72508
B	168	ALA	CYS	see remark 999	UNP P72508
D	40	VAL	ALA	see remark 999	UNP P72508
D	72	MEN	ASN	modified residue	UNP P72508
D	76	SER	ASN	see remark 999	UNP P72508
D	162	GLY	SER	see remark 999	UNP P72508
D	168	ALA	CYS	see remark 999	UNP P72508
F	40	VAL	ALA	see remark 999	UNP P72508
F	72	MEN	ASN	modified residue	UNP P72508
F	76	SER	ASN	see remark 999	UNP P72508
F	162	GLY	SER	see remark 999	UNP P72508
F	168	ALA	CYS	see remark 999	UNP P72508
H	40	VAL	ALA	see remark 999	UNP P72508
H	72	MEN	ASN	modified residue	UNP P72508
H	76	SER	ASN	see remark 999	UNP P72508
H	162	GLY	SER	see remark 999	UNP P72508
H	168	ALA	CYS	see remark 999	UNP P72508
J	40	VAL	ALA	see remark 999	UNP P72508
J	72	MEN	ASN	modified residue	UNP P72508
J	76	SER	ASN	see remark 999	UNP P72508

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	162	GLY	SER	see remark 999	UNP P72508
J	168	ALA	CYS	see remark 999	UNP P72508
L	40	VAL	ALA	see remark 999	UNP P72508
L	72	MEN	ASN	modified residue	UNP P72508
L	76	SER	ASN	see remark 999	UNP P72508
L	162	GLY	SER	see remark 999	UNP P72508
L	168	ALA	CYS	see remark 999	UNP P72508
N	40	VAL	ALA	see remark 999	UNP P72508
N	72	MEN	ASN	modified residue	UNP P72508
N	76	SER	ASN	see remark 999	UNP P72508
N	162	GLY	SER	see remark 999	UNP P72508
N	168	ALA	CYS	see remark 999	UNP P72508
P	40	VAL	ALA	see remark 999	UNP P72508
P	72	MEN	ASN	modified residue	UNP P72508
P	76	SER	ASN	see remark 999	UNP P72508
P	162	GLY	SER	see remark 999	UNP P72508
P	168	ALA	CYS	see remark 999	UNP P72508
R	40	VAL	ALA	see remark 999	UNP P72508
R	72	MEN	ASN	modified residue	UNP P72508
R	76	SER	ASN	see remark 999	UNP P72508
R	162	GLY	SER	see remark 999	UNP P72508
R	168	ALA	CYS	see remark 999	UNP P72508
T	40	VAL	ALA	see remark 999	UNP P72508
T	72	MEN	ASN	modified residue	UNP P72508
T	76	SER	ASN	see remark 999	UNP P72508
T	162	GLY	SER	see remark 999	UNP P72508
T	168	ALA	CYS	see remark 999	UNP P72508
V	40	VAL	ALA	see remark 999	UNP P72508
V	72	MEN	ASN	modified residue	UNP P72508
V	76	SER	ASN	see remark 999	UNP P72508
V	162	GLY	SER	see remark 999	UNP P72508
V	168	ALA	CYS	see remark 999	UNP P72508
X	40	VAL	ALA	see remark 999	UNP P72508
X	72	MEN	ASN	modified residue	UNP P72508
X	76	SER	ASN	see remark 999	UNP P72508
X	162	GLY	SER	see remark 999	UNP P72508
X	168	ALA	CYS	see remark 999	UNP P72508

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	36	36	36	0	0
4	B	60	60	60	0	0
4	C	39	39	39	0	0
4	D	47	47	47	0	0
4	E	53	53	53	0	0
4	F	29	29	29	0	0
4	G	40	40	40	0	0
4	H	41	41	41	0	0
4	I	39	39	39	0	0
4	J	26	26	26	0	0
4	K	57	57	57	0	0
4	L	32	32	32	0	0
4	M	31	31	31	0	0
4	N	42	42	42	0	0
4	O	35	35	35	0	0
4	P	30	30	30	0	0
4	Q	40	40	40	0	0
4	R	39	39	39	0	0

Continued on next page...

Continued from previous page...

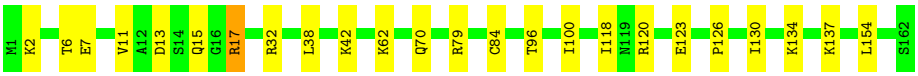
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	S	45	45	45	0	0
			Total	O		
4	T	29	29	29	0	0
			Total	O		
4	U	33	33	33	0	0
			Total	O		
4	V	48	48	48	0	0
			Total	O		
4	W	49	49	49	0	0
			Total	O		
4	X	25	25	25	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

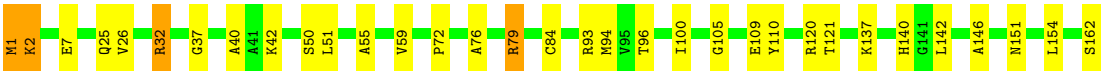
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain A:



• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain C:

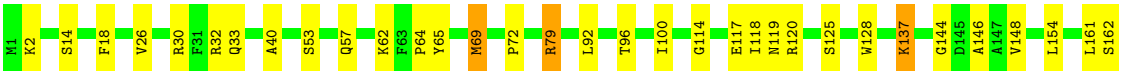


• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain E:

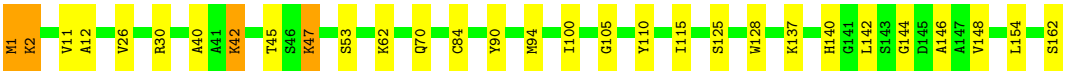
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain G:



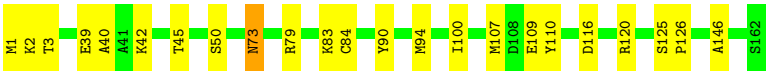
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain I:



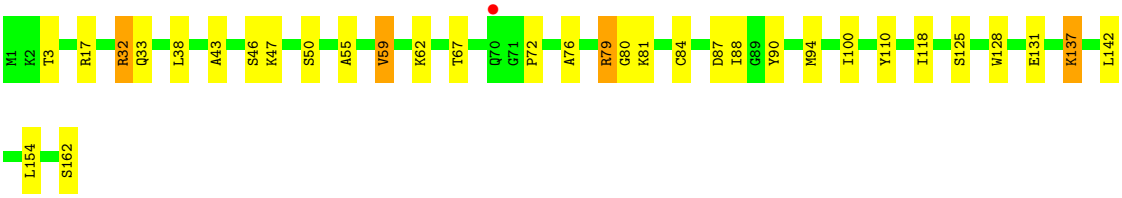
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain K:



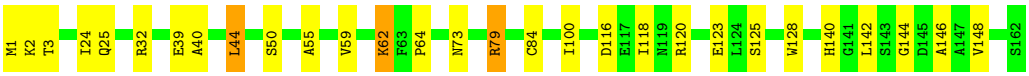
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain M:



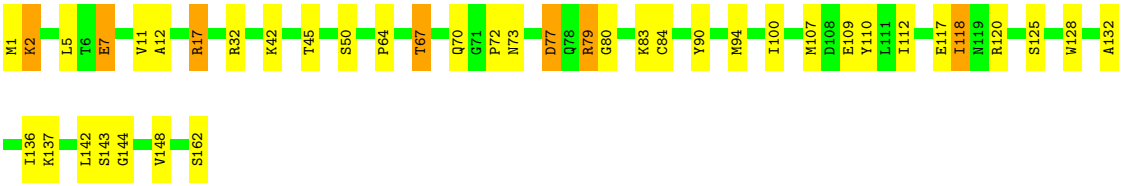
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain O:



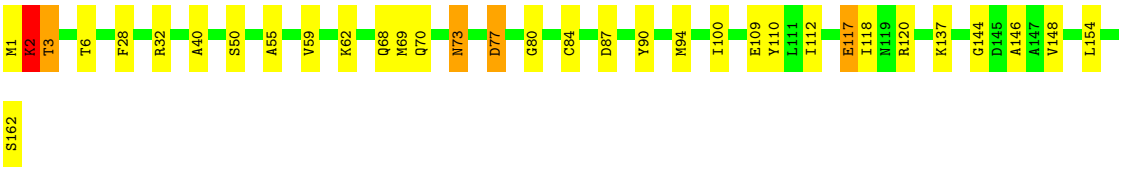
• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain Q:



• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain S:

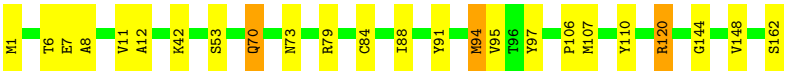


• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain U:

• Molecule 1: C-PHYCOCYANIN ALPHA SUBUNIT

Chain W:



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain B:

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

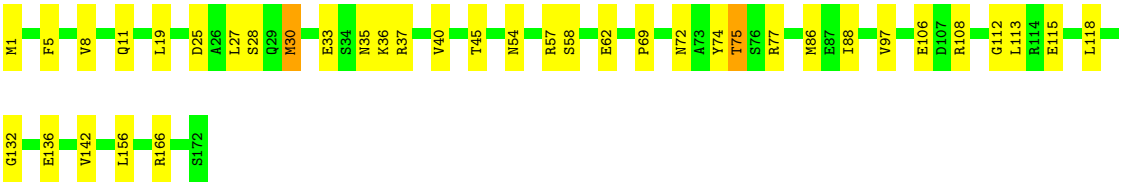
Chain D:

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain F:

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain H:

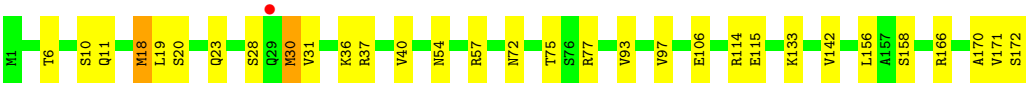


• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain J:

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain L:



• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain N: 85% 14%

M1 F2 D3 R15 G16 E17 M18 L19 S20 Q23 M30 R37 V40 N72 T75 V93 V97 N111 G112 L113 R114 E115 L118 P123 S126 V142 L156 A157 S158 S172

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain P: % 74% 23%

M1 T6 K7 V8 R15 G16 E17 M18 L19 S28 Q29 M30 R37 L38 D39 V40 V41 T50 S53 A56 R57 E62 Q63 P64 Q65 N72 T75 S76 R77 R78 M79 L83 M86 V97 V104 L105 E106 L113 R114 E115 T116 L120 S125

S126 V127 A128 V131 L139 D144 P145 I148 L156 R166 V171 S172

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain R: 79% 17%

M1 A4 K7 Q11 R15 M18 L19 S20 Q23 I24 S28 Q29 M30 V31 K36 R37 V40 S49 S53 Q65 N72 A73 Y74 T75 D85 I89 E106 D107 R108 G112 L113 R114 E115 V142 N143 D144 P145 I148 G151

L156 R166 S172

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain T: 77% 19%

M1 F2 D3 T6 K7 V8 L19 S20 Q23 M30 K36 R37 L38 D39 V40 S49 F60 Q63 P64 Q65 G70 G71 N72 R77 R78 M79 L83 R84 A102 G112 L113 R114 E115 L118 T122 S125 V129 A138 V142 N143 D144

P145 A146 G147 I148 L156 A157 S158 R166 S172

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain V: 85% 14%

M1 S10 R15 G16 E17 S20 Q23 S28 Q29 M30 N35 K36 R37 V40 T50 Q63 P64 Q65 L66 M79 E106 D107 R108 L113 S125 V129 A137 I141 V142 I148 G151 R166 S172

• Molecule 2: C-PHYCOCYANIN BETA SUBUNIT

Chain X: 81% 18%

M1 K7 S10 T14 R15 G16 E17 T21 S28 Q29 M30 V31 S34 V40 V41 S58 Q63 P64 Q65 Y74 R77 R78 L90 T94 V104 L105 E106 G112 L113 R114 E115 T116 L120 A128 K133 I141 R166 V171 S172

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.00Å 117.50Å 185.00Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.20) 90.9 (19.98-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.189 , 0.237 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32493	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MEN, CYC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.35	0/1260	0.52	0/1703
1	C	0.34	0/1260	0.52	0/1703
1	E	0.36	0/1260	0.52	0/1703
1	G	0.38	0/1260	0.54	0/1703
1	I	0.36	0/1260	0.50	0/1703
1	K	0.43	0/1260	0.68	3/1703 (0.2%)
1	M	0.35	0/1260	0.52	0/1703
1	O	0.33	0/1260	0.51	0/1703
1	Q	0.36	0/1260	0.56	0/1703
1	S	0.35	0/1260	0.54	0/1703
1	U	0.34	0/1260	0.52	0/1703
1	W	0.35	0/1260	0.52	0/1703
2	B	0.36	0/1267	0.58	1/1714 (0.1%)
2	D	0.35	0/1267	0.54	0/1714
2	F	0.34	0/1267	0.56	0/1714
2	H	0.36	0/1267	0.63	2/1714 (0.1%)
2	J	0.34	0/1267	0.56	0/1714
2	L	0.35	0/1267	0.56	0/1714
2	N	0.34	0/1267	0.57	0/1714
2	P	0.34	0/1267	0.54	0/1714
2	R	0.33	0/1267	0.55	0/1714
2	T	0.34	0/1267	0.55	0/1714
2	V	0.34	0/1267	0.56	0/1714
2	X	0.35	0/1267	0.54	0/1714
All	All	0.35	0/30324	0.55	6/41004 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	79	ARG	NE-CZ-NH1	-14.14	113.23	120.30
2	H	25	ASP	CB-CG-OD2	9.61	126.94	118.30
1	K	79	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	K	79	ARG	CD-NE-CZ	-6.66	114.27	123.60
2	H	25	ASP	CB-CG-OD1	-5.79	113.09	118.30
2	B	92	TYR	CA-CB-CG	-5.26	103.41	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1237	0	1216	18	0
1	C	1237	0	1216	30	0
1	E	1237	0	1216	12	0
1	G	1237	0	1216	17	0
1	I	1237	0	1216	25	0
1	K	1237	0	1216	19	0
1	M	1237	0	1216	19	0
1	O	1237	0	1216	19	0
1	Q	1237	0	1216	33	0
1	S	1237	0	1216	23	0
1	U	1237	0	1216	13	0
1	W	1237	0	1216	20	0
2	B	1263	0	1265	20	0
2	D	1263	0	1265	28	0
2	F	1263	0	1265	21	0
2	H	1263	0	1265	24	0
2	J	1263	0	1265	23	0
2	L	1263	0	1265	24	0
2	N	1263	0	1265	16	0
2	P	1263	0	1265	30	0
2	R	1263	0	1265	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	1263	0	1265	39	0
2	V	1263	0	1265	18	0
2	X	1263	0	1265	15	0
3	A	43	0	37	2	0
3	B	86	0	74	3	0
3	C	43	0	37	2	0
3	D	86	0	73	6	0
3	E	43	0	37	2	0
3	F	86	0	74	8	0
3	G	43	0	37	1	0
3	H	86	0	74	6	0
3	I	43	0	37	1	0
3	J	86	0	74	3	0
3	K	43	0	37	2	0
3	L	86	0	74	5	0
3	M	43	0	37	3	0
3	N	86	0	74	5	0
3	O	43	0	37	3	0
3	P	86	0	74	5	0
3	Q	43	0	37	4	0
3	R	86	0	74	6	0
3	S	43	0	37	2	0
3	T	86	0	73	10	0
3	U	43	0	37	1	0
3	V	86	0	73	5	0
3	W	43	0	37	3	0
3	X	86	0	74	5	0
4	A	36	0	0	1	0
4	B	60	0	0	2	0
4	C	39	0	0	4	0
4	D	47	0	0	0	0
4	E	53	0	0	1	0
4	F	29	0	0	3	0
4	G	40	0	0	0	0
4	H	41	0	0	0	0
4	I	39	0	0	1	0
4	J	26	0	0	0	0
4	K	57	0	0	2	0
4	L	32	0	0	0	0
4	M	31	0	0	1	0
4	N	42	0	0	0	0
4	O	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	30	0	0	0	0
4	Q	40	0	0	1	0
4	R	39	0	0	1	0
4	S	45	0	0	0	0
4	T	29	0	0	3	0
4	U	33	0	0	0	0
4	V	48	0	0	1	0
4	W	49	0	0	1	0
4	X	25	0	0	3	0
All	All	32493	0	31101	525	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 8.

All (525) 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:K:73:ASN:H	1:K:73:ASN:HD22	1.04	1.00
2:L:20:SER:H	2:L:23:GLN:HE21	1.10	0.99
2:T:20:SER:H	2:T:23:GLN:HE21	1.09	0.98
1:Q:100:ILE:HD13	2:R:19:LEU:HD22	1.43	0.97
1:S:73:ASN:HD22	1:S:73:ASN:H	1.08	0.94
2:N:20:SER:H	2:N:23:GLN:HE21	1.15	0.92
2:B:20:SER:H	2:B:23:GLN:HE21	1.19	0.90
1:M:94:MET:HE1	1:M:110:TYR:HD2	1.35	0.90
1:K:100:ILE:HD13	2:L:19:LEU:HD22	1.55	0.88
1:C:140:HIS:HD2	1:C:142:LEU:H	1.22	0.88
2:T:37:ARG:O	2:T:40:VAL:HG22	1.76	0.85
2:F:36:LYS:O	2:F:40:VAL:HG13	1.76	0.85
2:F:166:ARG:HD3	4:F:1165:HOH:O	1.75	0.85
2:N:37:ARG:O	2:N:40:VAL:HG22	1.77	0.84
2:J:37:ARG:HA	2:J:156:LEU:HD21	1.59	0.84
2:J:20:SER:H	2:J:23:GLN:HE21	1.25	0.83
1:E:26:VAL:HG22	1:G:26:VAL:HG22	1.59	0.82
1:O:100:ILE:HD13	2:P:19:LEU:HD22	1.62	0.82
1:Q:64:PRO:O	1:Q:67:THR:HG22	1.80	0.82
2:B:37:ARG:O	2:B:40:VAL:HG22	1.78	0.82
2:H:37:ARG:O	2:H:40:VAL:HG22	1.79	0.81
2:V:40:VAL:HG12	2:V:142:VAL:HG13	1.63	0.79
2:X:15:ARG:HD2	2:X:17:GLU:OE2	1.81	0.79
2:R:37:ARG:O	2:R:40:VAL:HG22	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:THR:HG21	4:F:1160:HOH:O	1.81	0.78
1:I:94:MET:HE1	1:I:110:TYR:HD2	1.48	0.78
1:I:100:ILE:HD13	2:J:19:LEU:HD22	1.65	0.78
2:R:20:SER:H	2:R:23:GLN:NE2	1.81	0.77
2:J:37:ARG:O	2:J:40:VAL:HG22	1.85	0.77
2:L:37:ARG:O	2:L:40:VAL:HG22	1.85	0.76
2:J:20:SER:OG	2:J:23:GLN:HG3	1.86	0.75
2:F:37:ARG:O	2:F:40:VAL:HG22	1.87	0.74
2:V:50:THR:HG22	4:V:1161:HOH:O	1.86	0.74
2:V:37:ARG:O	2:V:40:VAL:HG22	1.86	0.74
2:B:37:ARG:HA	2:B:156:LEU:HD21	1.69	0.74
1:S:40:ALA:HB2	1:S:146:ALA:HB1	1.69	0.74
2:P:127:VAL:O	2:P:131:VAL:HG12	1.86	0.73
2:T:2:PHE:HD1	2:T:6:THR:CG2	2.01	0.73
2:H:106:GLU:OE2	2:H:166:ARG:HD3	1.89	0.73
2:H:37:ARG:HA	2:H:156:LEU:HD21	1.70	0.72
1:K:73:ASN:H	1:K:73:ASN:ND2	1.84	0.72
2:L:114:ARG:HG3	2:L:170:ALA:O	1.90	0.72
2:T:37:ARG:HA	2:T:156:LEU:HD21	1.70	0.71
2:P:79:MET:HE2	2:P:79:MET:O	1.91	0.71
2:T:8:VAL:HG12	2:T:19:LEU:HD11	1.71	0.71
2:T:79:MET:HE2	2:T:83:LEU:HG	1.73	0.71
2:R:36:LYS:O	2:R:40:VAL:HG13	1.91	0.71
2:N:20:SER:H	2:N:23:GLN:NE2	1.90	0.70
1:S:73:ASN:H	1:S:73:ASN:ND2	1.85	0.70
1:M:72:PRO:O	1:M:79:ARG:NH2	2.25	0.70
1:G:117:GLU:HG3	1:G:120:ARG:HH12	1.57	0.69
2:V:106:GLU:OE2	2:V:166:ARG:HD3	1.93	0.69
2:H:54:ASN:ND2	2:H:57:ARG:HH21	1.90	0.68
1:S:6:THR:HG21	4:T:1156:HOH:O	1.92	0.68
1:C:140:HIS:HE1	1:C:151:ASN:OD1	1.76	0.68
1:Q:77:ASP:OD2	1:Q:79:ARG:HG2	1.92	0.68
1:K:73:ASN:HD22	1:K:73:ASN:N	1.81	0.67
1:M:94:MET:HE1	1:M:110:TYR:CD2	2.24	0.67
1:K:94:MET:HE1	1:K:110:TYR:HD2	1.60	0.67
1:G:100:ILE:HD13	2:H:19:LEU:HD22	1.78	0.66
2:F:37:ARG:HA	2:F:156:LEU:HD21	1.78	0.66
1:M:162:SER:O	1:U:120:ARG:HD2	1.95	0.66
2:D:40:VAL:HG11	2:D:97:VAL:HG11	1.78	0.65
2:T:20:SER:H	2:T:23:GLN:NE2	1.89	0.65
2:R:112:GLY:O	2:R:115:GLU:HG2	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:MET:HG3	2:F:31:VAL:N	2.10	0.65
1:W:94:MET:CE	1:W:110:TYR:HD2	2.10	0.65
2:L:20:SER:H	2:L:23:GLN:NE2	1.87	0.65
2:J:113:LEU:HD13	3:J:1082:CYC:HMB3	1.77	0.64
2:T:113:LEU:HD13	3:T:1082:CYC:HMB3	1.78	0.64
2:B:113:LEU:HD13	3:B:1082:CYC:HMB3	1.79	0.64
1:S:77:ASP:HB3	1:S:80:GLY:H	1.62	0.64
1:S:73:ASN:HD22	1:S:73:ASN:N	1.89	0.64
2:V:63:GLN:HG2	2:V:65:GLN:NE2	2.14	0.63
1:I:40:ALA:HB2	1:I:146:ALA:HB1	1.80	0.63
2:N:37:ARG:HA	2:N:156:LEU:HD21	1.80	0.63
1:C:72:PRO:O	1:C:79:ARG:NH2	2.30	0.63
2:V:40:VAL:HG12	2:V:142:VAL:CG1	2.27	0.63
1:G:53:SER:O	1:G:57:GLN:HG2	1.98	0.62
1:Q:100:ILE:CD1	2:R:19:LEU:HD22	2.23	0.62
2:N:113:LEU:HD13	3:N:1082:CYC:HMB3	1.82	0.62
1:I:42:LYS:HD2	2:J:24:ILE:HG21	1.82	0.62
1:U:47:LYS:O	1:U:51:LEU:HB2	1.99	0.62
2:F:113:LEU:HD13	3:F:1082:CYC:HMB3	1.80	0.61
2:F:27:LEU:O	2:F:31:VAL:HG23	2.00	0.61
2:R:20:SER:H	2:R:23:GLN:HE21	1.45	0.61
2:T:148:ILE:HG21	3:T:1153:CYC:HMC3	1.82	0.61
1:M:62:LYS:HD2	1:M:131:GLU:CD	2.21	0.61
1:U:75:ALA:HB1	1:U:81:LYS:HG3	1.83	0.61
1:U:78:GLN:HA	1:U:78:GLN:NE2	2.15	0.61
2:D:40:VAL:CG1	2:D:97:VAL:HG11	2.30	0.61
2:H:113:LEU:HD13	3:H:1082:CYC:HMB3	1.83	0.60
1:Q:2:LYS:O	1:Q:2:LYS:HG3	2.00	0.60
2:R:7:LYS:O	2:R:11:GLN:HG3	2.01	0.60
2:F:58:SER:HB3	2:F:133:LYS:HD3	1.83	0.60
2:T:20:SER:N	2:T:23:GLN:HE21	1.91	0.60
1:K:90:TYR:O	1:K:94:MET:HG2	2.01	0.60
2:R:113:LEU:HD13	3:R:1082:CYC:HMB3	1.83	0.60
2:L:37:ARG:HA	2:L:156:LEU:HD21	1.84	0.60
1:S:1:MET:O	1:S:3:THR:HG23	2.01	0.60
2:H:36:LYS:O	2:H:40:VAL:HG13	2.02	0.59
1:W:94:MET:HE1	1:W:110:TYR:HD2	1.66	0.59
2:V:20:SER:OG	2:V:23:GLN:HG3	2.03	0.59
2:X:128:ALA:HB2	2:X:172:SER:HB3	1.84	0.59
2:X:106:GLU:OE2	2:X:166:ARG:HD3	2.02	0.59
1:Q:32:ARG:HH22	3:T:1153:CYC:HMA3	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:144:GLY:O	1:I:148:VAL:HG23	2.03	0.58
2:J:77:ARG:HH11	2:J:77:ARG:HG2	1.67	0.58
2:T:102:ALA:HB3	2:T:166:ARG:NH1	2.17	0.58
2:N:114:ARG:NH1	2:N:172:SER:O	2.36	0.58
2:D:25:ASP:O	2:D:28:SER:HB2	2.03	0.58
1:Q:79:ARG:HH11	1:Q:79:ARG:CG	2.17	0.58
1:S:6:THR:HG22	2:T:3:ASP:HB3	1.85	0.58
1:U:114:GLY:O	1:U:118:ILE:HD13	2.02	0.58
2:T:36:LYS:O	2:T:40:VAL:HG13	2.05	0.57
1:G:144:GLY:O	1:G:148:VAL:HG23	2.04	0.57
2:T:125:SER:O	2:T:129:VAL:HG23	2.04	0.57
1:C:1:MET:HE2	2:D:6:THR:HB	1.87	0.57
1:C:25:GLN:HE21	1:I:30:ARG:HA	1.70	0.57
1:Q:79:ARG:NH1	1:Q:79:ARG:HG3	2.20	0.57
1:C:96:THR:HG21	2:D:18:MET:HE2	1.86	0.57
1:Q:79:ARG:HG3	1:Q:80:GLY:N	2.20	0.57
2:F:72:MEN:HE22	3:F:1082:CYC:HBD2	1.86	0.57
1:C:1:MET:HB2	1:C:105:GLY:HA3	1.86	0.56
2:L:36:LYS:O	2:L:40:VAL:HG13	2.04	0.56
2:L:54:ASN:HD22	2:L:57:ARG:HH21	1.53	0.56
1:W:94:MET:HE1	1:W:97:TYR:HD2	1.70	0.56
2:P:15:ARG:HB2	2:P:17:GLU:HG2	1.87	0.56
2:D:58:SER:OG	2:D:133:LYS:HE2	2.05	0.56
2:L:20:SER:N	2:L:23:GLN:HE21	1.92	0.56
2:N:40:VAL:HG12	2:N:142:VAL:HG13	1.88	0.56
1:O:84:CYS:HA	3:O:1084:CYC:HHD	1.88	0.56
1:Q:72:PRO:O	1:Q:79:ARG:NH2	2.36	0.56
1:A:120:ARG:HD2	1:I:162:SER:O	2.05	0.56
3:F:1082:CYC:HMD2	3:F:1082:CYC:HC	1.71	0.56
1:I:47:LYS:HE2	1:I:140:HIS:O	2.06	0.56
4:C:1090:HOH:O	1:I:2:LYS:HE2	2.04	0.56
1:Q:77:ASP:HB3	1:Q:80:GLY:H	1.69	0.56
2:R:106:GLU:OE2	2:R:166:ARG:HD3	2.05	0.56
1:C:140:HIS:CD2	1:C:142:LEU:H	2.12	0.56
1:K:83:LYS:HE2	4:K:1111:HOH:O	2.05	0.56
2:T:2:PHE:CD1	2:T:6:THR:CG2	2.86	0.55
2:J:137:ALA:O	2:J:141:ILE:HD12	2.05	0.55
1:U:90:TYR:O	1:U:94:MET:HG2	2.06	0.55
1:C:100:ILE:HD13	2:D:19:LEU:HD22	1.88	0.55
1:C:137:LYS:HG3	1:C:154:LEU:HD13	1.89	0.55
2:D:65:GLN:CD	2:D:65:GLN:H	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:79:ARG:HH11	1:Q:79:ARG:HG3	1.72	0.55
2:P:148:ILE:HG21	3:P:1153:CYC:HMC3	1.88	0.55
2:T:72:MEN:HE23	2:T:122:THR:HG22	1.87	0.55
2:P:128:ALA:HA	2:P:131:VAL:CG1	2.36	0.54
2:H:5:PHE:O	2:H:8:VAL:HG12	2.07	0.54
2:N:72:MEN:HE22	3:N:1082:CYC:HBD2	1.88	0.54
1:K:45:THR:HA	2:L:18:MET:HE1	1.89	0.54
2:H:88:ILE:HG21	3:H:1082:CYC:HAB1	1.88	0.54
2:H:132:GLY:O	2:H:136:GLU:HG3	2.08	0.54
2:P:77:ARG:HG3	2:P:78:ARG:N	2.21	0.54
2:X:10:SER:O	2:X:14:THR:HG23	2.07	0.54
1:M:55:ALA:O	1:M:59:VAL:HG13	2.07	0.54
2:R:65:GLN:HB2	4:R:1164:HOH:O	2.08	0.54
2:T:2:PHE:CD1	2:T:6:THR:HG22	2.43	0.54
2:L:20:SER:OG	2:L:23:GLN:HG3	2.08	0.53
3:L:1153:CYC:HB	3:L:1153:CYC:HMA1	1.73	0.53
1:Q:94:MET:HE1	1:Q:110:TYR:HD2	1.71	0.53
3:J:1082:CYC:HC	3:J:1082:CYC:HMD2	1.73	0.53
2:T:112:GLY:HA2	2:T:115:GLU:OE1	2.09	0.53
1:W:91:TYR:O	1:W:95:VAL:HG23	2.07	0.53
1:S:100:ILE:HD12	2:T:19:LEU:HD22	1.90	0.53
3:D:1153:CYC:HB	3:D:1153:CYC:HMA1	1.74	0.53
2:F:11:GLN:O	2:F:15:ARG:NH1	2.41	0.53
2:J:15:ARG:HD2	2:J:17:GLU:OE2	2.08	0.53
2:B:40:VAL:HG12	2:B:142:VAL:HG13	1.90	0.53
1:C:76:ALA:HB3	4:C:1109:HOH:O	2.08	0.53
2:F:40:VAL:HG11	2:F:156:LEU:CD2	2.38	0.53
2:J:93:VAL:O	2:J:97:VAL:HG23	2.09	0.53
2:D:10:SER:O	2:D:14:THR:HG23	2.08	0.53
1:I:45:THR:HG23	2:J:18:MET:HE3	1.91	0.53
2:V:63:GLN:CG	2:V:65:GLN:NE2	2.72	0.53
2:H:37:ARG:HD3	2:H:97:VAL:O	2.09	0.53
2:R:37:ARG:HA	2:R:156:LEU:HD21	1.91	0.53
2:H:8:VAL:HG11	2:H:27:LEU:HD11	1.91	0.53
2:P:115:GLU:N	2:P:115:GLU:OE1	2.40	0.53
1:C:2:LYS:HB2	4:C:1116:HOH:O	2.10	0.52
1:S:120:ARG:HG2	1:S:120:ARG:HH11	1.75	0.52
1:C:93:ARG:HA	2:D:18:MET:HE3	1.90	0.52
3:D:1082:CYC:HMD2	3:D:1082:CYC:HC	1.74	0.52
1:W:6:THR:HG21	4:X:1161:HOH:O	2.09	0.52
1:A:70:GLN:OE1	1:A:70:GLN:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:84:CYS:HA	3:W:1084:CYC:HHD	1.91	0.52
2:D:37:ARG:HA	2:D:156:LEU:HD21	1.91	0.52
2:D:113:LEU:HD13	3:D:1082:CYC:HMB3	1.92	0.52
1:A:137:LYS:HG3	1:A:154:LEU:HD13	1.91	0.52
2:R:49:SER:O	2:R:53:SER:HB2	2.10	0.52
1:K:40:ALA:HB2	1:K:146:ALA:HB1	1.92	0.52
2:T:79:MET:HE2	2:T:83:LEU:CG	2.40	0.52
2:B:20:SER:OG	2:B:23:GLN:HG3	2.10	0.51
3:N:1082:CYC:HMD2	3:N:1082:CYC:HC	1.75	0.51
1:S:94:MET:HE1	1:S:110:TYR:HD2	1.75	0.51
1:A:96:THR:O	1:A:100:ILE:HG12	2.10	0.51
1:C:26:VAL:HG22	1:I:26:VAL:HG22	1.91	0.51
1:M:94:MET:HE2	1:M:110:TYR:HB2	1.92	0.51
1:U:84:CYS:HA	3:U:1084:CYC:HHD	1.91	0.51
3:V:1082:CYC:HC	3:V:1082:CYC:HMD2	1.74	0.51
2:L:30:MET:HG3	2:L:31:VAL:N	2.23	0.51
2:X:112:GLY:HA2	2:X:115:GLU:OE1	2.11	0.51
2:D:36:LYS:HE3	2:D:152:ASP:O	2.10	0.51
3:B:1082:CYC:HMD2	3:B:1082:CYC:HC	1.76	0.51
3:H:1153:CYC:HMA1	3:H:1153:CYC:HB	1.74	0.51
2:N:40:VAL:HG12	2:N:142:VAL:CG1	2.40	0.51
2:J:20:SER:N	2:J:23:GLN:HE21	2.03	0.51
1:Q:45:THR:HA	2:R:18:MET:HE2	1.92	0.51
1:S:28:PHE:CE1	2:T:38:LEU:HD12	2.45	0.51
1:W:79:ARG:HD2	4:W:1128:HOH:O	2.09	0.51
2:P:116:THR:HG22	2:P:120:LEU:HD11	1.93	0.51
1:A:11:VAL:HG21	4:K:1136:HOH:O	2.11	0.51
1:O:1:MET:CE	2:P:6:THR:HB	2.41	0.51
1:W:70:GLN:HE21	1:W:70:GLN:N	2.09	0.50
2:P:113:LEU:HD13	2:P:171:VAL:HG11	1.92	0.50
2:R:40:VAL:HG12	2:R:142:VAL:HG13	1.92	0.50
2:T:20:SER:OG	2:T:23:GLN:HG3	2.11	0.50
2:T:114:ARG:NH1	2:T:172:SER:C	2.64	0.50
1:C:25:GLN:HE22	1:I:30:ARG:HH11	1.60	0.50
3:C:1084:CYC:NB	3:C:1084:CYC:HMA1	2.27	0.50
1:E:94:MET:HE1	1:E:110:TYR:HD2	1.77	0.50
1:G:114:GLY:O	1:G:118:ILE:HD13	2.12	0.50
1:O:79:ARG:HG3	1:O:79:ARG:HH11	1.77	0.50
1:S:68:GLN:HG2	1:S:69:MET:N	2.26	0.50
1:W:73:ASN:HA	3:W:1084:CYC:HBD2	1.94	0.50
1:S:68:GLN:CG	1:S:69:MET:N	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:VAL:HG23	1:I:12:ALA:N	2.27	0.50
1:I:90:TYR:O	1:I:94:MET:HG2	2.12	0.50
2:L:106:GLU:OE2	2:L:166:ARG:HD3	2.12	0.49
2:P:79:MET:HE2	2:P:83:LEU:HG	1.94	0.49
2:J:40:VAL:HG12	2:J:142:VAL:HG13	1.92	0.49
2:R:72:MEN:HB2	3:R:1082:CYC:OC	2.12	0.49
1:A:6:THR:HA	2:B:1:MET:HE1	1.93	0.49
2:T:79:MET:CE	2:T:83:LEU:HG	2.41	0.49
2:V:15:ARG:NH1	2:V:17:GLU:OE1	2.43	0.49
1:I:84:CYS:HA	3:I:1084:CYC:HHD	1.94	0.49
1:Q:162:SER:O	1:W:120:ARG:NH1	2.45	0.49
2:B:10:SER:O	2:B:14:THR:HG23	2.12	0.49
2:V:65:GLN:HG2	2:V:66:LEU:N	2.28	0.49
1:W:94:MET:CE	1:W:97:TYR:HD2	2.26	0.49
2:D:40:VAL:HG11	2:D:160:ILE:HD11	1.94	0.49
1:Q:42:LYS:HE2	2:R:24:ILE:HG21	1.93	0.49
1:Q:120:ARG:HD2	1:W:162:SER:O	2.12	0.49
2:T:138:ALA:O	2:T:142:VAL:HG13	2.12	0.49
3:X:1153:CYC:HMA1	3:X:1153:CYC:HB	1.77	0.49
2:H:8:VAL:HA	2:H:11:GLN:NE2	2.27	0.49
1:E:7:GLU:O	1:E:11:VAL:HG23	2.13	0.49
1:Q:90:TYR:O	1:Q:94:MET:HG2	2.12	0.49
2:T:70:GLY:HA2	4:T:1169:HOH:O	2.11	0.49
2:V:63:GLN:CG	2:V:65:GLN:HE22	2.25	0.49
2:D:36:LYS:HG2	2:D:153:CYS:SG	2.52	0.49
1:Q:45:THR:HA	2:R:18:MET:CE	2.43	0.49
1:C:84:CYS:HA	3:C:1084:CYC:HHD	1.94	0.48
3:H:1153:CYC:HMA1	3:H:1153:CYC:NB	2.28	0.48
2:J:10:SER:O	2:J:14:THR:HG23	2.13	0.48
2:D:56:ALA:HB2	2:D:86:MET:CE	2.44	0.48
3:G:1084:CYC:HMA1	3:G:1084:CYC:NB	2.29	0.48
2:F:112:GLY:O	2:F:116:THR:HG23	2.13	0.48
1:G:137:LYS:HG3	1:G:154:LEU:HD13	1.96	0.48
2:B:50:THR:HG22	4:B:1186:HOH:O	2.14	0.48
1:I:45:THR:HG23	2:J:18:MET:CE	2.44	0.48
2:J:125:SER:O	2:J:129:VAL:HG23	2.13	0.48
1:O:1:MET:HG2	2:P:6:THR:HG21	1.96	0.48
1:O:55:ALA:O	1:O:59:VAL:HG23	2.14	0.48
2:T:144:ASP:OD2	2:T:146:ALA:HB3	2.14	0.48
1:E:90:TYR:O	1:E:94:MET:HG2	2.14	0.48
1:I:45:THR:HA	2:J:18:MET:HE3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:72:MEN:HE22	3:L:1082:CYC:HBD2	1.95	0.48
1:A:84:CYS:HA	3:A:1084:CYC:HHD	1.95	0.48
2:X:63:GLN:HB3	2:X:65:GLN:NE2	2.28	0.48
2:D:40:VAL:CG1	2:D:160:ILE:HD11	2.43	0.48
1:M:125:SER:HB3	1:M:128:TRP:CE2	2.49	0.48
1:A:13:ASP:OD1	2:B:92:TYR:OH	2.22	0.47
2:P:106:GLU:OE2	2:P:166:ARG:NH1	2.47	0.47
2:R:30:MET:HG3	2:R:31:VAL:N	2.28	0.47
1:Q:125:SER:HB3	1:Q:128:TRP:CE2	2.49	0.47
1:U:96:THR:O	1:U:100:ILE:HD12	2.14	0.47
1:W:11:VAL:HG23	1:W:12:ALA:N	2.28	0.47
2:X:40:VAL:HG12	2:X:41:VAL:N	2.29	0.47
2:R:85:ASP:O	2:R:89:ILE:HG13	2.14	0.47
2:D:15:ARG:HB3	2:D:17:GLU:HG3	1.95	0.47
1:M:84:CYS:HA	3:M:1084:CYC:HHD	1.97	0.47
3:R:1153:CYC:HC	3:R:1153:CYC:HMD2	1.79	0.47
2:B:152:ASP:OD1	2:B:154:SER:HB2	2.14	0.47
2:X:171:VAL:HG23	2:X:172:SER:N	2.30	0.47
2:J:77:ARG:HG2	2:J:77:ARG:NH1	2.30	0.47
1:Q:70:GLN:HA	1:Q:70:GLN:OE1	2.14	0.47
1:Q:118:ILE:N	1:Q:118:ILE:HD13	2.29	0.47
2:V:148:ILE:HG21	3:V:1153:CYC:HMC3	1.97	0.47
1:A:118:ILE:HD11	2:D:79:MET:HB3	1.97	0.47
1:E:84:CYS:HA	3:E:1084:CYC:HHD	1.97	0.47
1:A:130:ILE:O	1:A:134:LYS:HG3	2.15	0.47
1:C:25:GLN:HE22	1:I:30:ARG:HD2	1.79	0.47
3:L:1153:CYC:HMA1	3:L:1153:CYC:NB	2.30	0.47
1:G:92:LEU:O	1:G:96:THR:HG23	2.15	0.46
2:H:35:ASN:HB2	3:H:1153:CYC:O2D	2.16	0.46
3:S:1084:CYC:HMA1	3:S:1084:CYC:NB	2.31	0.46
2:T:6:THR:HG21	4:T:1156:HOH:O	2.16	0.46
1:K:116:ASP:OD1	1:K:116:ASP:N	2.49	0.46
2:R:40:VAL:HG11	2:R:156:LEU:CD2	2.45	0.46
1:A:130:ILE:HG22	1:A:134:LYS:HE2	1.97	0.46
1:C:32:ARG:HE	1:C:32:ARG:HB2	1.50	0.46
1:G:18:PHE:HB3	2:H:45:THR:HG23	1.97	0.46
2:L:93:VAL:O	2:L:97:VAL:HG23	2.15	0.46
2:T:72:MEN:HE22	3:T:1082:CYC:HBD2	1.97	0.46
2:F:148:ILE:HD12	4:F:1172:HOH:O	2.16	0.46
1:G:40:ALA:HB2	1:G:146:ALA:HB1	1.97	0.46
1:O:144:GLY:O	1:O:148:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1082:CYC:HC	3:L:1082:CYC:HMD2	1.81	0.46
1:M:67:THR:O	1:M:76:ALA:HA	2.15	0.46
1:Q:83:LYS:HE3	4:Q:1122:HOH:O	2.15	0.46
1:W:8:ALA:O	1:W:11:VAL:HG22	2.16	0.46
1:W:94:MET:HE2	1:W:106:PRO:O	2.15	0.46
2:X:104:VAL:CG2	4:X:1164:HOH:O	2.63	0.46
2:X:104:VAL:HG22	4:X:1164:HOH:O	2.15	0.46
1:C:94:MET:HE1	1:C:110:TYR:HD2	1.80	0.46
2:T:63:GLN:HB3	2:T:65:GLN:NE2	2.31	0.46
2:V:137:ALA:O	2:V:141:ILE:HG13	2.15	0.46
3:D:1153:CYC:HMA1	3:D:1153:CYC:NB	2.30	0.46
1:C:1:MET:CE	2:D:6:THR:HB	2.45	0.46
3:M:1084:CYC:HMA1	3:M:1084:CYC:NB	2.31	0.45
3:D:1153:CYC:HMD2	3:D:1153:CYC:HC	1.80	0.45
3:X:1082:CYC:HMD2	3:X:1082:CYC:HC	1.80	0.45
2:P:40:VAL:HG12	2:P:41:VAL:N	2.30	0.45
2:N:20:SER:OG	2:N:23:GLN:HG3	2.16	0.45
2:P:128:ALA:HA	2:P:131:VAL:HG13	1.98	0.45
2:D:40:VAL:HG12	2:D:41:VAL:N	2.31	0.45
2:L:54:ASN:ND2	2:L:57:ARG:HH21	2.12	0.45
1:Q:11:VAL:HG13	1:Q:12:ALA:N	2.32	0.45
1:Q:132:ALA:O	1:Q:136:ILE:HG13	2.17	0.45
2:R:148:ILE:HG21	3:R:1153:CYC:HMC3	1.99	0.45
1:S:137:LYS:HG3	1:S:154:LEU:HD13	1.97	0.45
2:T:77:ARG:NH2	3:T:1082:CYC:O2D	2.50	0.45
2:J:19:LEU:HA	2:J:23:GLN:NE2	2.32	0.45
3:O:1084:CYC:NB	3:O:1084:CYC:HMA1	2.32	0.45
3:P:1153:CYC:HMD2	3:P:1153:CYC:HC	1.80	0.45
2:R:144:ASP:OD1	2:R:145:PRO:HD2	2.16	0.45
1:U:125:SER:HB3	1:U:128:TRP:CE2	2.50	0.45
3:X:1153:CYC:HMD2	3:X:1153:CYC:HC	1.82	0.45
1:I:1:MET:HG3	1:I:105:GLY:HA3	1.99	0.45
2:V:63:GLN:HG3	2:V:65:GLN:HE22	1.82	0.45
3:V:1153:CYC:HB	3:V:1153:CYC:HMA1	1.81	0.45
2:P:104:VAL:HG13	2:P:105:LEU:N	2.31	0.45
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.82	0.45
2:B:135:LYS:HG3	2:B:164:PHE:CB	2.47	0.45
1:M:38:LEU:HD23	1:M:100:ILE:CD1	2.47	0.45
2:P:40:VAL:CG1	2:P:97:VAL:HG11	2.46	0.45
3:A:1084:CYC:HMA1	3:A:1084:CYC:NB	2.32	0.45
1:G:62:LYS:C	1:G:64:PRO:HD3	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:118:LEU:HD23	2:T:118:LEU:HA	1.84	0.45
2:H:40:VAL:HG12	2:H:142:VAL:HG13	1.97	0.44
2:H:58:SER:O	2:H:62:GLU:HG3	2.17	0.44
1:A:42:LYS:HE3	2:B:21:THR:HG22	1.99	0.44
2:H:1:MET:HE3	2:H:108:ARG:NH2	2.33	0.44
1:M:137:LYS:HG3	1:M:154:LEU:HD13	1.98	0.44
2:P:56:ALA:HB2	2:P:86:MET:CE	2.48	0.44
1:Q:73:ASN:HA	3:Q:1084:CYC:HBD2	1.99	0.44
2:R:74:TYR:O	2:R:75:THR:HG23	2.18	0.44
1:A:6:THR:HG21	4:B:1168:HOH:O	2.16	0.44
1:C:1:MET:HB2	1:C:105:GLY:CA	2.47	0.44
1:W:84:CYS:O	1:W:88:ILE:HG13	2.16	0.44
2:L:40:VAL:HG11	2:L:156:LEU:CD2	2.48	0.44
2:P:39:ASP:OD2	3:P:1153:CYC:NA	2.50	0.44
1:A:126:PRO:HD2	4:A:1096:HOH:O	2.18	0.44
2:B:135:LYS:HG3	2:B:164:PHE:HB2	1.98	0.44
1:O:1:MET:HE3	2:P:6:THR:HB	1.99	0.44
3:V:1153:CYC:HMA1	3:V:1153:CYC:NB	2.33	0.44
1:G:65:TYR:O	1:G:69:MET:HG3	2.18	0.44
1:I:140:HIS:CE1	1:I:142:LEU:HB2	2.53	0.44
2:T:114:ARG:NH1	2:T:172:SER:O	2.51	0.44
3:W:1084:CYC:HMA1	3:W:1084:CYC:NB	2.31	0.44
2:F:77:ARG:NH2	3:F:1082:CYC:O2D	2.51	0.44
1:M:43:ALA:HB3	1:M:142:LEU:HD21	2.00	0.44
1:O:39:GLU:HG3	1:O:40:ALA:N	2.33	0.44
1:O:140:HIS:CE1	1:O:142:LEU:HB2	2.52	0.44
2:T:60:PHE:HE2	2:T:79:MET:HE1	1.83	0.44
1:I:125:SER:HB3	1:I:128:TRP:CE2	2.52	0.44
2:N:15:ARG:HD2	2:N:17:GLU:OE2	2.18	0.44
1:Q:32:ARG:NH2	3:T:1153:CYC:HMA3	2.32	0.44
2:B:104:VAL:HG13	2:B:105:LEU:N	2.33	0.43
1:U:130:ILE:O	1:U:134:LYS:HG3	2.18	0.43
1:U:144:GLY:O	1:U:148:VAL:HG23	2.17	0.43
2:X:31:VAL:O	2:X:34:SER:HB3	2.17	0.43
2:D:114:ARG:HB2	2:D:170:ALA:O	2.17	0.43
2:L:171:VAL:HG23	2:L:172:SER:N	2.33	0.43
2:N:123:PRO:O	2:N:126:SER:HB2	2.19	0.43
1:O:73:ASN:HA	3:O:1084:CYC:HBD2	1.99	0.43
2:X:74:TYR:O	2:X:78:ARG:HB2	2.18	0.43
3:L:1153:CYC:HAA1	3:L:1153:CYC:HHA	1.88	0.43
2:N:112:GLY:HA2	2:N:115:GLU:OE1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:144:ASP:HA	2:P:145:PRO:HD3	1.89	0.43
1:C:93:ARG:HA	2:D:18:MET:CE	2.49	0.43
2:V:125:SER:O	2:V:129:VAL:HG23	2.17	0.43
2:F:168:ALA:O	2:F:172:SER:HB3	2.19	0.43
3:F:1153:CYC:HB	3:F:1153:CYC:HMA1	1.84	0.43
1:Q:2:LYS:HD3	1:Q:7:GLU:OE2	2.19	0.43
2:D:56:ALA:HB2	2:D:86:MET:HE3	2.01	0.43
2:J:72:MEN:HE22	3:J:1082:CYC:HBD2	2.01	0.43
2:J:106:GLU:OE2	2:J:166:ARG:HD3	2.18	0.43
1:K:3:THR:HG21	2:L:6:THR:CG2	2.49	0.43
1:O:40:ALA:HB2	1:O:146:ALA:HB1	2.00	0.43
3:T:1082:CYC:HC	3:T:1082:CYC:HMD2	1.84	0.43
2:H:112:GLY:HA2	2:H:115:GLU:OE1	2.18	0.43
1:W:94:MET:HE2	1:W:110:TYR:HD2	1.84	0.43
2:X:128:ALA:CB	2:X:172:SER:HB3	2.47	0.43
1:C:96:THR:HG21	2:D:18:MET:CE	2.49	0.43
1:K:45:THR:HA	2:L:18:MET:CE	2.48	0.43
1:Q:144:GLY:O	1:Q:148:VAL:HG23	2.19	0.43
3:Q:1084:CYC:NB	3:Q:1084:CYC:HMA1	2.33	0.43
1:S:87:ASP:O	1:S:90:TYR:HB2	2.19	0.43
1:O:1:MET:HG2	2:P:6:THR:CG2	2.49	0.43
2:T:72:MEN:OD1	2:T:122:THR:HB	2.19	0.43
1:C:120:ARG:HG2	1:C:120:ARG:HH11	1.83	0.42
2:F:112:GLY:O	2:F:116:THR:CG2	2.67	0.42
2:J:30:MET:HG3	2:J:31:VAL:N	2.32	0.42
1:C:40:ALA:HB2	1:C:146:ALA:HB1	2.00	0.42
2:P:8:VAL:CG1	2:P:19:LEU:HD21	2.49	0.42
2:D:125:SER:O	2:D:129:VAL:HG23	2.18	0.42
1:O:62:LYS:C	1:O:64:PRO:HD3	2.40	0.42
1:S:94:MET:HE3	1:S:94:MET:HA	1.99	0.42
3:X:1153:CYC:HMA1	3:X:1153:CYC:NB	2.35	0.42
1:A:2:LYS:HE3	1:A:7:GLU:OE1	2.19	0.42
2:D:39:ASP:OD2	3:D:1153:CYC:NA	2.52	0.42
2:H:74:TYR:O	2:H:75:THR:HG23	2.19	0.42
1:G:118:ILE:HG22	1:G:119:ASN:N	2.33	0.42
1:K:3:THR:HG21	2:L:6:THR:HG21	2.01	0.42
2:L:40:VAL:HG12	2:L:142:VAL:HG13	2.02	0.42
1:O:3:THR:HG21	2:P:6:THR:CG2	2.48	0.42
2:B:36:LYS:O	2:B:40:VAL:HG13	2.19	0.42
1:E:125:SER:HA	1:E:126:PRO:HD3	1.92	0.42
1:G:72:PRO:O	1:G:79:ARG:NH2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:93:VAL:O	2:N:97:VAL:HG23	2.18	0.42
1:Q:84:CYS:HA	3:Q:1084:CYC:HHD	2.01	0.42
1:S:118:ILE:HD11	2:V:79:MET:HB3	2.02	0.42
2:T:40:VAL:HG11	2:T:156:LEU:HD23	2.01	0.42
1:A:2:LYS:HE3	1:A:7:GLU:CD	2.40	0.42
2:H:30:MET:HE2	2:H:30:MET:HB2	1.89	0.42
1:I:115:ILE:HD12	1:I:115:ILE:HA	1.87	0.42
1:K:125:SER:HA	1:K:126:PRO:HD3	1.95	0.42
2:T:114:ARG:HH12	2:T:172:SER:C	2.23	0.42
1:W:94:MET:HE1	1:W:97:TYR:CD2	2.52	0.42
1:C:55:ALA:O	1:C:59:VAL:HG23	2.20	0.42
1:G:33:GLN:O	1:G:33:GLN:HG3	2.20	0.42
1:K:73:ASN:HA	3:K:1084:CYC:HBD2	2.02	0.42
3:X:1153:CYC:HAA1	3:X:1153:CYC:HHA	1.90	0.42
2:L:40:VAL:HG11	2:L:156:LEU:HD23	2.02	0.42
1:M:32:ARG:NH1	1:M:33:GLN:OE1	2.53	0.42
1:M:87:ASP:O	1:M:90:TYR:HB2	2.18	0.42
2:X:90:LEU:O	2:X:94:THR:HG23	2.20	0.42
1:E:79:ARG:HE	1:E:79:ARG:HB3	1.58	0.42
1:G:125:SER:HB3	1:G:128:TRP:CE2	2.55	0.42
2:L:30:MET:HE2	2:L:30:MET:HB2	1.91	0.42
2:N:113:LEU:CD1	3:N:1082:CYC:HMB3	2.48	0.42
1:S:117:GLU:HG3	1:S:120:ARG:HH21	1.85	0.42
1:W:144:GLY:O	1:W:148:VAL:HG23	2.19	0.42
2:B:72:MEN:HB2	3:B:1082:CYC:OC	2.20	0.41
3:F:1153:CYC:HMA1	3:F:1153:CYC:NB	2.35	0.41
1:O:44:LEU:HD12	1:O:44:LEU:HA	1.85	0.41
2:R:18:MET:H	2:R:18:MET:HG2	1.64	0.41
2:T:40:VAL:HG11	2:T:156:LEU:CD2	2.50	0.41
2:R:4:ALA:HB3	2:R:30:MET:CE	2.51	0.41
2:V:35:ASN:HD22	2:V:35:ASN:HA	1.67	0.41
1:M:79:ARG:HG3	1:M:80:GLY:N	2.35	0.41
1:E:37:GLY:HA3	4:E:1092:HOH:O	2.21	0.41
1:E:162:SER:O	1:K:120:ARG:HD2	2.21	0.41
2:P:79:MET:CE	2:P:83:LEU:HG	2.50	0.41
2:B:77:ARG:NH2	1:E:109:GLU:OE2	2.54	0.41
2:F:40:VAL:HG11	2:F:156:LEU:HD23	2.02	0.41
1:I:137:LYS:HG3	1:I:154:LEU:HD13	2.01	0.41
1:K:94:MET:HE2	1:K:107:MET:HA	2.02	0.41
1:O:44:LEU:HD11	1:O:140:HIS:HB2	2.02	0.41
2:R:151:GLY:HA3	3:R:1153:CYC:CMD	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:1153:CYC:HHA	3:R:1153:CYC:HAA1	1.87	0.41
3:E:1084:CYC:HC	3:E:1084:CYC:HMD2	1.86	0.41
2:F:7:LYS:HA	2:F:7:LYS:HD3	1.87	0.41
3:P:1153:CYC:HAA1	3:P:1153:CYC:HHA	1.90	0.41
2:R:7:LYS:HZ3	2:R:7:LYS:HA	1.84	0.41
1:W:94:MET:HG3	1:W:107:MET:HA	2.02	0.41
2:B:58:SER:O	2:B:62:GLU:HG3	2.21	0.41
1:C:2:LYS:HE2	4:I:1089:HOH:O	2.20	0.41
1:C:121:THR:HG21	2:F:83:LEU:HD13	2.02	0.41
2:F:135:LYS:HG3	2:F:139:LEU:HD11	2.02	0.41
2:X:114:ARG:HH12	2:X:172:SER:C	2.24	0.41
1:M:94:MET:CE	1:M:110:TYR:HB2	2.49	0.41
3:M:1084:CYC:HC	3:M:1084:CYC:HMD2	1.85	0.41
1:Q:17:ARG:CZ	1:S:2:LYS:HD3	2.50	0.41
3:T:1153:CYC:HMA1	3:T:1153:CYC:HB	1.86	0.41
2:H:118:LEU:HD12	2:H:118:LEU:HA	1.91	0.41
1:K:1:MET:O	1:K:3:THR:HG23	2.21	0.41
2:P:37:ARG:HA	2:P:156:LEU:HD21	2.03	0.41
2:P:40:VAL:HG11	2:P:97:VAL:HG11	2.03	0.41
2:P:62:GLU:O	2:P:64:PRO:HD3	2.21	0.41
1:S:55:ALA:O	1:S:59:VAL:HG23	2.21	0.41
1:U:94:MET:HE2	1:U:107:MET:HA	2.03	0.41
2:B:112:GLY:HA2	2:B:115:GLU:OE1	2.21	0.41
1:I:70:GLN:OE1	1:I:70:GLN:HA	2.21	0.41
2:N:3:ASP:OD1	2:N:3:ASP:C	2.59	0.41
3:N:1153:CYC:HMA1	3:N:1153:CYC:HB	1.86	0.41
1:S:144:GLY:O	1:S:148:VAL:HG23	2.21	0.41
2:V:151:GLY:HA3	3:V:1153:CYC:CMD	2.51	0.41
3:H:1082:CYC:HHA	3:H:1082:CYC:HAD2	1.94	0.40
1:O:125:SER:HB3	1:O:128:TRP:CE2	2.56	0.40
1:M:84:CYS:O	1:M:88:ILE:HG13	2.22	0.40
2:T:36:LYS:HE2	3:T:1153:CYC:HMD3	2.03	0.40
1:C:25:GLN:NE2	1:I:30:ARG:HD2	2.36	0.40
1:C:37:GLY:HA3	4:C:1098:HOH:O	2.20	0.40
2:F:113:LEU:CD1	3:F:1082:CYC:HMB3	2.48	0.40
2:H:69:PRO:HA	2:H:74:TYR:CG	2.55	0.40
1:Q:83:LYS:HE2	3:Q:1084:CYC:O2A	2.22	0.40
1:A:15:GLN:HB2	1:A:17:ARG:HG3	2.04	0.40
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.76	0.40
1:E:25:GLN:OE1	1:G:30:ARG:HD2	2.21	0.40
1:K:84:CYS:HA	3:K:1084:CYC:HHD	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:1153:CYC:HMA1	3:P:1153:CYC:NB	2.37	0.40
1:Q:107:MET:O	1:Q:112:ILE:HG12	2.22	0.40
3:F:1153:CYC:HHA	3:F:1153:CYC:HAA1	1.88	0.40
2:H:40:VAL:HG11	2:H:156:LEU:HG	2.03	0.40
1:M:47:LYS:HE3	4:M:1110:HOH:O	2.22	0.40
1:O:25:GLN:O	1:U:29:GLY:HA3	2.22	0.40
2:P:57:ARG:HH11	2:P:57:ARG:HG2	1.85	0.40
1:S:84:CYS:HA	3:S:1084:CYC:HHD	2.04	0.40
3:T:1153:CYC:HMA1	3:T:1153:CYC:NB	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	C	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	E	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	26
1	G	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	I	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
1	K	160/162 (99%)	157 (98%)	2 (1%)	1 (1%)	25	26
1	M	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
1	O	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	Q	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	S	160/162 (99%)	156 (98%)	3 (2%)	1 (1%)	25	26
1	U	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	W	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
2	B	169/172 (98%)	166 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	F	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	H	169/172 (98%)	166 (98%)	2 (1%)	1 (1%)	25	26
2	J	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	L	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	N	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	P	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	26
2	R	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	26
2	T	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
2	V	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
2	X	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
All	All	3948/4008 (98%)	3856 (98%)	83 (2%)	9 (0%)	47	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	2	LYS
2	L	75	THR
2	R	75	THR
1	S	2	LYS
1	E	2	LYS
2	H	75	THR
2	J	75	THR
2	P	75	THR
2	N	75	THR

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	125/125 (100%)	119 (95%)	6 (5%)	25	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	125/125 (100%)	115 (92%)	10 (8%)	12	12
1	E	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	G	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	I	125/125 (100%)	119 (95%)	6 (5%)	25	32
1	K	125/125 (100%)	120 (96%)	5 (4%)	31	40
1	M	125/125 (100%)	115 (92%)	10 (8%)	12	12
1	O	125/125 (100%)	114 (91%)	11 (9%)	10	10
1	Q	125/125 (100%)	110 (88%)	15 (12%)	5	4
1	S	125/125 (100%)	113 (90%)	12 (10%)	8	8
1	U	125/125 (100%)	117 (94%)	8 (6%)	17	20
1	W	125/125 (100%)	118 (94%)	7 (6%)	21	25
2	B	130/130 (100%)	124 (95%)	6 (5%)	27	34
2	D	130/130 (100%)	125 (96%)	5 (4%)	33	42
2	F	130/130 (100%)	122 (94%)	8 (6%)	18	21
2	H	130/130 (100%)	125 (96%)	5 (4%)	33	42
2	J	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	L	130/130 (100%)	121 (93%)	9 (7%)	15	16
2	N	130/130 (100%)	124 (95%)	6 (5%)	27	34
2	P	130/130 (100%)	116 (89%)	14 (11%)	6	6
2	R	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	T	130/130 (100%)	120 (92%)	10 (8%)	13	13
2	V	130/130 (100%)	123 (95%)	7 (5%)	22	26
2	X	130/130 (100%)	118 (91%)	12 (9%)	9	9
All	All	3060/3060 (100%)	2852 (93%)	208 (7%)	16	17

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	32	ARG
1	A	38	LEU
1	A	62	LYS
1	A	79	ARG
1	A	123	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	19	LEU
2	B	24	ILE
2	B	30	MET
2	B	118	LEU
2	B	154	SER
2	B	172	SER
1	C	1	MET
1	C	2	LYS
1	C	7	GLU
1	C	32	ARG
1	C	42	LYS
1	C	50	SER
1	C	51	LEU
1	C	79	ARG
1	C	109	GLU
1	C	162	SER
2	D	11	GLN
2	D	40	VAL
2	D	118	LEU
2	D	125	SER
2	D	139	LEU
1	E	1	MET
1	E	17	ARG
1	E	32	ARG
1	E	50	SER
1	E	57	GLN
1	E	79	ARG
1	E	109	GLU
1	E	143	SER
2	F	7	LYS
2	F	10	SER
2	F	18	MET
2	F	30	MET
2	F	116	THR
2	F	120	LEU
2	F	125	SER
2	F	133	LYS
1	G	2	LYS
1	G	14	SER
1	G	32	ARG
1	G	69	MET
1	G	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	137	LYS
1	G	161	LEU
1	G	162	SER
2	H	28	SER
2	H	30	MET
2	H	33	GLU
2	H	77	ARG
2	H	86	MET
1	I	1	MET
1	I	2	LYS
1	I	42	LYS
1	I	47	LYS
1	I	53	SER
1	I	62	LYS
2	J	7	LYS
2	J	10	SER
2	J	11	GLN
2	J	18	MET
2	J	30	MET
2	J	33	GLU
2	J	59	LEU
2	J	125	SER
2	J	136	GLU
2	J	158	SER
1	K	39	GLU
1	K	42	LYS
1	K	50	SER
1	K	73	ASN
1	K	109	GLU
2	L	10	SER
2	L	11	GLN
2	L	18	MET
2	L	28	SER
2	L	30	MET
2	L	77	ARG
2	L	115	GLU
2	L	133	LYS
2	L	158	SER
1	M	3	THR
1	M	17	ARG
1	M	32	ARG
1	M	46	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	50	SER
1	M	59	VAL
1	M	79	ARG
1	M	81	LYS
1	M	118	ILE
1	M	137	LYS
2	N	18	MET
2	N	30	MET
2	N	111	ASN
2	N	118	LEU
2	N	158	SER
2	N	172	SER
1	O	2	LYS
1	O	24	ILE
1	O	32	ARG
1	O	44	LEU
1	O	50	SER
1	O	62	LYS
1	O	79	ARG
1	O	116	ASP
1	O	118	ILE
1	O	120	ARG
1	O	123	GLU
2	P	18	MET
2	P	28	SER
2	P	30	MET
2	P	50	THR
2	P	53	SER
2	P	57	ARG
2	P	65	GLN
2	P	77	ARG
2	P	86	MET
2	P	113	LEU
2	P	120	LEU
2	P	125	SER
2	P	131	VAL
2	P	139	LEU
1	Q	1	MET
1	Q	2	LYS
1	Q	5	LEU
1	Q	7	GLU
1	Q	17	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	50	SER
1	Q	67	THR
1	Q	77	ASP
1	Q	79	ARG
1	Q	109	GLU
1	Q	117	GLU
1	Q	118	ILE
1	Q	137	LYS
1	Q	142	LEU
1	Q	143	SER
2	R	1	MET
2	R	7	LYS
2	R	15	ARG
2	R	18	MET
2	R	28	SER
2	R	30	MET
2	R	53	SER
2	R	65	GLN
2	R	108	ARG
2	R	115	GLU
1	S	2	LYS
1	S	3	THR
1	S	32	ARG
1	S	50	SER
1	S	62	LYS
1	S	70	GLN
1	S	73	ASN
1	S	77	ASP
1	S	109	GLU
1	S	112	ILE
1	S	117	GLU
1	S	162	SER
2	T	6	THR
2	T	30	MET
2	T	49	SER
2	T	84	ARG
2	T	114	ARG
2	T	122	THR
2	T	125	SER
2	T	142	VAL
2	T	158	SER
2	T	172	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	1	MET
1	U	2	LYS
1	U	42	LYS
1	U	50	SER
1	U	51	LEU
1	U	79	ARG
1	U	143	SER
1	U	154	LEU
2	V	10	SER
2	V	28	SER
2	V	30	MET
2	V	50	THR
2	V	63	GLN
2	V	108	ARG
2	V	113	LEU
1	W	1	MET
1	W	7	GLU
1	W	42	LYS
1	W	53	SER
1	W	70	GLN
1	W	94	MET
1	W	120	ARG
2	X	7	LYS
2	X	21	THR
2	X	28	SER
2	X	30	MET
2	X	58	SER
2	X	77	ARG
2	X	104	VAL
2	X	106	GLU
2	X	116	THR
2	X	120	LEU
2	X	133	LYS
2	X	141	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	23	GLN
2	B	35	ASN
2	B	47	ASN
1	C	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	140	HIS
2	D	35	ASN
2	F	35	ASN
1	G	68	GLN
2	H	35	ASN
2	H	47	ASN
2	H	54	ASN
2	J	23	GLN
2	J	35	ASN
2	J	47	ASN
1	K	61	ASN
1	K	73	ASN
2	L	23	GLN
2	L	35	ASN
2	L	47	ASN
2	L	54	ASN
2	N	23	GLN
2	N	35	ASN
2	N	47	ASN
2	N	111	ASN
2	P	11	GLN
1	Q	78	GLN
2	R	23	GLN
2	R	35	ASN
1	S	70	GLN
1	S	73	ASN
2	T	23	GLN
2	T	35	ASN
2	T	47	ASN
1	U	78	GLN
2	V	35	ASN
1	W	70	GLN
2	X	35	ASN
2	X	47	ASN
2	X	143	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)

12 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	N	72	2	7,8,9	0.82	0	6,9,11	0.55	0
2	MEN	R	72	2	7,8,9	0.77	0	6,9,11	0.56	0
2	MEN	D	72	2	7,8,9	0.79	0	6,9,11	0.57	0
2	MEN	P	72	2	7,8,9	0.90	1 (14%)	6,9,11	0.45	0
2	MEN	X	72	2	7,8,9	0.87	0	6,9,11	0.48	0
2	MEN	J	72	2	7,8,9	0.86	0	6,9,11	0.60	0
2	MEN	F	72	2	7,8,9	0.84	0	6,9,11	0.53	0
2	MEN	L	72	2	7,8,9	0.86	0	6,9,11	0.53	0
2	MEN	V	72	2	7,8,9	0.88	0	6,9,11	0.60	0
2	MEN	B	72	2	7,8,9	0.74	0	6,9,11	0.52	0
2	MEN	T	72	2	7,8,9	0.93	1 (14%)	6,9,11	0.54	0
2	MEN	H	72	2	7,8,9	0.89	1 (14%)	6,9,11	0.64	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	N	72	2	-	3/7/8/10	-
2	MEN	R	72	2	-	3/7/8/10	-
2	MEN	D	72	2	-	3/7/8/10	-
2	MEN	P	72	2	-	2/7/8/10	-
2	MEN	X	72	2	-	4/7/8/10	-
2	MEN	J	72	2	-	2/7/8/10	-
2	MEN	F	72	2	-	3/7/8/10	-
2	MEN	L	72	2	-	3/7/8/10	-
2	MEN	V	72	2	-	3/7/8/10	-
2	MEN	B	72	2	-	3/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	T	72	2	-	2/7/8/10	-
2	MEN	H	72	2	-	2/7/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	72	MEN	CE2-ND2	-2.16	1.41	1.45
2	P	72	MEN	CE2-ND2	-2.08	1.41	1.45
2	H	72	MEN	CE2-ND2	-2.07	1.41	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	72	MEN	N-CA-CB-CG
2	F	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	CA-CB-CG-OD1
2	L	72	MEN	CA-CB-CG-OD1
2	N	72	MEN	CA-CB-CG-OD1
2	P	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	CA-CB-CG-ND2
2	L	72	MEN	CA-CB-CG-ND2
2	P	72	MEN	CA-CB-CG-ND2
2	B	72	MEN	CA-CB-CG-OD1
2	H	72	MEN	CA-CB-CG-OD1
2	J	72	MEN	CA-CB-CG-OD1
2	R	72	MEN	CA-CB-CG-OD1
2	V	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2
2	H	72	MEN	CA-CB-CG-ND2
2	V	72	MEN	CA-CB-CG-ND2
2	X	72	MEN	C-CA-CB-CG
2	T	72	MEN	CA-CB-CG-OD1
2	F	72	MEN	CA-CB-CG-ND2
2	J	72	MEN	CA-CB-CG-ND2
2	N	72	MEN	CA-CB-CG-ND2
2	R	72	MEN	CA-CB-CG-ND2
2	T	72	MEN	CA-CB-CG-ND2
2	X	72	MEN	CA-CB-CG-ND2
2	R	72	MEN	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	X	72	MEN	CA-CB-CG-OD1
2	D	72	MEN	N-CA-CB-CG
2	F	72	MEN	N-CA-CB-CG
2	L	72	MEN	N-CA-CB-CG
2	N	72	MEN	N-CA-CB-CG
2	V	72	MEN	N-CA-CB-CG
2	B	72	MEN	N-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	72	MEN	1	0
2	R	72	MEN	1	0
2	J	72	MEN	1	0
2	F	72	MEN	1	0
2	L	72	MEN	1	0
2	B	72	MEN	1	0
2	T	72	MEN	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	CYC	I	1084	1	42,46,46	2.04	8 (19%)	50,67,67	1.72	10 (20%)
3	CYC	M	1084	1	42,46,46	1.99	8 (19%)	50,67,67	1.70	8 (16%)
3	CYC	Q	1084	1	42,46,46	1.96	8 (19%)	50,67,67	1.66	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CYC	R	1153	2	42,46,46	1.86	7 (16%)	50,67,67	1.84	14 (28%)
3	CYC	X	1082	2	42,46,46	2.06	11 (26%)	50,67,67	1.78	11 (22%)
3	CYC	X	1153	2	42,46,46	1.88	9 (21%)	50,67,67	1.90	11 (22%)
3	CYC	H	1082	2	42,46,46	1.99	8 (19%)	50,67,67	1.76	10 (20%)
3	CYC	F	1082	2	42,46,46	1.92	7 (16%)	50,67,67	1.74	10 (20%)
3	CYC	B	1082	2	42,46,46	2.04	7 (16%)	50,67,67	1.74	10 (20%)
3	CYC	V	1153	2	42,46,46	1.88	10 (23%)	50,67,67	2.10	13 (26%)
3	CYC	N	1153	2	42,46,46	1.73	9 (21%)	50,67,67	1.83	12 (24%)
3	CYC	S	1084	1	42,46,46	1.97	8 (19%)	50,67,67	1.70	9 (18%)
3	CYC	A	1084	1	42,46,46	1.92	8 (19%)	50,67,67	1.70	9 (18%)
3	CYC	L	1153	2	42,46,46	1.78	9 (21%)	50,67,67	1.93	13 (26%)
3	CYC	O	1084	1	42,46,46	1.99	9 (21%)	50,67,67	1.65	8 (16%)
3	CYC	D	1153	2	42,46,46	1.74	7 (16%)	50,67,67	1.93	12 (24%)
3	CYC	G	1084	1	42,46,46	1.92	7 (16%)	50,67,67	1.68	9 (18%)
3	CYC	C	1084	1	42,46,46	2.08	8 (19%)	50,67,67	1.68	8 (16%)
3	CYC	E	1084	1	42,46,46	1.99	9 (21%)	50,67,67	1.72	8 (16%)
3	CYC	F	1153	2	42,46,46	1.76	10 (23%)	50,67,67	1.79	11 (22%)
3	CYC	B	1153	2	42,46,46	1.98	9 (21%)	50,67,67	1.91	13 (26%)
3	CYC	P	1153	2	42,46,46	1.65	9 (21%)	50,67,67	1.87	11 (22%)
3	CYC	J	1082	2	42,46,46	1.92	8 (19%)	50,67,67	1.73	10 (20%)
3	CYC	H	1153	2	42,46,46	1.61	8 (19%)	50,67,67	1.88	11 (22%)
3	CYC	J	1153	2	42,46,46	1.69	7 (16%)	50,67,67	1.85	10 (20%)
3	CYC	W	1084	1	42,46,46	1.99	10 (23%)	50,67,67	1.68	9 (18%)
3	CYC	T	1153	2	42,46,46	1.74	9 (21%)	50,67,67	1.93	12 (24%)
3	CYC	K	1084	1	42,46,46	2.12	9 (21%)	50,67,67	1.68	8 (16%)
3	CYC	R	1082	2	42,46,46	2.44	15 (35%)	50,67,67	1.89	12 (24%)
3	CYC	P	1082	2	42,46,46	1.91	8 (19%)	50,67,67	1.88	12 (24%)
3	CYC	N	1082	2	42,46,46	1.98	8 (19%)	50,67,67	1.73	10 (20%)
3	CYC	D	1082	2	42,46,46	1.91	8 (19%)	50,67,67	1.71	11 (22%)
3	CYC	U	1084	1	42,46,46	2.05	9 (21%)	50,67,67	1.73	7 (14%)
3	CYC	L	1082	2	42,46,46	2.05	9 (21%)	50,67,67	1.69	9 (18%)
3	CYC	T	1082	2	42,46,46	2.05	7 (16%)	50,67,67	1.79	9 (18%)
3	CYC	V	1082	2	42,46,46	2.01	7 (16%)	50,67,67	1.74	11 (22%)

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	I	1084	1	-	11/25/74/74	0/4/4/4
3	CYC	M	1084	1	-	10/25/74/74	0/4/4/4
3	CYC	Q	1084	1	-	8/25/74/74	0/4/4/4
3	CYC	R	1153	2	-	10/25/74/74	0/4/4/4
3	CYC	X	1082	2	-	7/25/74/74	0/4/4/4
3	CYC	X	1153	2	-	6/25/74/74	0/4/4/4
3	CYC	H	1082	2	-	10/25/74/74	0/4/4/4
3	CYC	F	1082	2	-	6/25/74/74	0/4/4/4
3	CYC	B	1082	2	-	9/25/74/74	0/4/4/4
3	CYC	V	1153	2	-	6/25/74/74	0/4/4/4
3	CYC	N	1153	2	-	6/25/74/74	0/4/4/4
3	CYC	S	1084	1	-	6/25/74/74	0/4/4/4
3	CYC	A	1084	1	-	10/25/74/74	0/4/4/4
3	CYC	L	1153	2	-	7/25/74/74	0/4/4/4
3	CYC	O	1084	1	-	10/25/74/74	0/4/4/4
3	CYC	D	1153	2	-	8/25/74/74	0/4/4/4
3	CYC	G	1084	1	-	7/25/74/74	0/4/4/4
3	CYC	C	1084	1	-	8/25/74/74	0/4/4/4
3	CYC	E	1084	1	-	10/25/74/74	0/4/4/4
3	CYC	F	1153	2	-	7/25/74/74	0/4/4/4
3	CYC	B	1153	2	-	7/25/74/74	0/4/4/4
3	CYC	P	1153	2	-	8/25/74/74	0/4/4/4
3	CYC	J	1082	2	-	8/25/74/74	0/4/4/4
3	CYC	H	1153	2	-	8/25/74/74	0/4/4/4
3	CYC	J	1153	2	-	10/25/74/74	0/4/4/4
3	CYC	W	1084	1	-	10/25/74/74	0/4/4/4
3	CYC	T	1153	2	-	8/25/74/74	0/4/4/4
3	CYC	K	1084	1	-	11/25/74/74	0/4/4/4
3	CYC	R	1082	2	-	7/25/74/74	0/4/4/4
3	CYC	P	1082	2	-	7/25/74/74	0/4/4/4
3	CYC	N	1082	2	-	9/25/74/74	0/4/4/4
3	CYC	D	1082	2	-	8/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	U	1084	1	-	9/25/74/74	0/4/4/4
3	CYC	L	1082	2	-	8/25/74/74	0/4/4/4
3	CYC	T	1082	2	-	9/25/74/74	0/4/4/4
3	CYC	V	1082	2	-	8/25/74/74	0/4/4/4

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1082	CYC	CHA-C1A	9.73	1.43	1.35
3	K	1084	CYC	CHA-C1A	8.93	1.42	1.35
3	T	1082	CYC	CHA-C1A	8.85	1.42	1.35
3	B	1082	CYC	CHA-C1A	8.50	1.42	1.35
3	V	1082	CYC	CHA-C1A	8.42	1.42	1.35
3	C	1084	CYC	CHA-C1A	8.40	1.42	1.35
3	U	1084	CYC	CHA-C1A	8.32	1.42	1.35
3	I	1084	CYC	CHA-C1A	8.19	1.42	1.35
3	S	1084	CYC	CHA-C1A	8.13	1.41	1.35
3	M	1084	CYC	CHA-C1A	8.00	1.41	1.35
3	N	1082	CYC	CHA-C1A	7.94	1.41	1.35
3	L	1082	CYC	CHA-C1A	7.92	1.41	1.35
3	G	1084	CYC	CHA-C1A	7.72	1.41	1.35
3	A	1084	CYC	CHA-C1A	7.71	1.41	1.35
3	O	1084	CYC	CHA-C1A	7.69	1.41	1.35
3	H	1082	CYC	CHA-C1A	7.65	1.41	1.35
3	F	1082	CYC	CHA-C1A	7.47	1.41	1.35
3	B	1153	CYC	CHA-C1A	7.42	1.41	1.35
3	D	1082	CYC	CHA-C1A	7.40	1.41	1.35
3	J	1082	CYC	CHA-C1A	7.36	1.41	1.35
3	E	1084	CYC	CHA-C1A	7.31	1.41	1.35
3	Q	1084	CYC	CHA-C1A	7.12	1.41	1.35
3	W	1084	CYC	CHA-C1A	7.09	1.41	1.35
3	X	1082	CYC	CHA-C1A	7.01	1.41	1.35
3	X	1153	CYC	CHA-C1A	6.78	1.40	1.35
3	P	1082	CYC	CHA-C1A	6.68	1.40	1.35
3	V	1153	CYC	CHA-C1A	5.86	1.40	1.35
3	R	1153	CYC	CHA-C1A	5.65	1.39	1.35
3	N	1153	CYC	CHA-C1A	5.44	1.39	1.35
3	L	1153	CYC	CHA-C1A	5.35	1.39	1.35
3	D	1153	CYC	CHA-C1A	5.29	1.39	1.35
3	R	1082	CYC	CAC-C3C	5.02	1.63	1.54
3	T	1153	CYC	CHA-C1A	4.95	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1082	CYC	C2A-C3A	4.77	1.46	1.36
3	B	1082	CYC	C1C-NC	-4.55	1.31	1.37
3	J	1153	CYC	CHA-C1A	4.52	1.38	1.35
3	E	1084	CYC	CAC-C3C	4.51	1.62	1.54
3	Q	1084	CYC	CAC-C3C	4.51	1.62	1.54
3	P	1082	CYC	C1C-NC	-4.40	1.31	1.37
3	K	1084	CYC	CAC-C3C	4.31	1.62	1.54
3	R	1153	CYC	C3B-C2B	4.29	1.45	1.36
3	H	1082	CYC	CAC-C3C	4.27	1.62	1.54
3	V	1153	CYC	C4B-NB	-4.26	1.29	1.38
3	K	1084	CYC	C2A-C3A	4.23	1.45	1.36
3	F	1082	CYC	C1C-NC	-4.20	1.32	1.37
3	O	1084	CYC	CAC-C3C	4.16	1.62	1.54
3	R	1082	CYC	C1C-NC	-4.15	1.32	1.37
3	W	1084	CYC	CAC-C3C	4.14	1.62	1.54
3	M	1084	CYC	CAC-C3C	4.13	1.62	1.54
3	C	1084	CYC	CAC-C3C	4.11	1.62	1.54
3	X	1082	CYC	C1C-NC	-4.09	1.32	1.37
3	I	1084	CYC	CAC-C3C	4.05	1.62	1.54
3	F	1082	CYC	CAC-C3C	4.04	1.61	1.54
3	U	1084	CYC	CAC-C3C	4.03	1.61	1.54
3	L	1082	CYC	CAC-C3C	4.03	1.61	1.54
3	D	1153	CYC	C3B-C2B	4.01	1.45	1.36
3	A	1084	CYC	CAC-C3C	4.01	1.61	1.54
3	E	1084	CYC	C2A-C3A	4.00	1.45	1.36
3	B	1153	CYC	C1C-NC	-4.00	1.32	1.37
3	N	1082	CYC	C2A-C3A	3.98	1.45	1.36
3	S	1084	CYC	CAC-C3C	3.98	1.61	1.54
3	I	1084	CYC	C2A-C3A	3.98	1.45	1.36
3	W	1084	CYC	C2A-C3A	3.95	1.45	1.36
3	P	1153	CYC	C3B-C2B	3.95	1.45	1.36
3	J	1082	CYC	C2A-C3A	3.94	1.45	1.36
3	B	1082	CYC	CAC-C3C	3.93	1.61	1.54
3	R	1082	CYC	C3D-C2D	3.91	1.49	1.37
3	L	1082	CYC	C2A-C3A	3.91	1.45	1.36
3	T	1153	CYC	C3B-C2B	3.91	1.45	1.36
3	J	1153	CYC	C3B-C2B	3.90	1.45	1.36
3	J	1153	CYC	C1A-C2A	-3.90	1.39	1.45
3	T	1153	CYC	C1A-C2A	-3.90	1.39	1.45
3	H	1153	CYC	C3B-C2B	3.87	1.44	1.36
3	G	1084	CYC	CAC-C3C	3.87	1.61	1.54
3	R	1153	CYC	C1C-NC	-3.86	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	1082	CYC	C2A-C3A	3.86	1.44	1.36
3	F	1153	CYC	CHA-C1A	3.85	1.38	1.35
3	U	1084	CYC	C2A-C3A	3.83	1.44	1.36
3	P	1082	CYC	C2A-C3A	3.82	1.44	1.36
3	S	1084	CYC	C2A-C3A	3.81	1.44	1.36
3	M	1084	CYC	C2A-C3A	3.80	1.44	1.36
3	J	1082	CYC	C1C-NC	-3.78	1.32	1.37
3	R	1153	CYC	C1A-C2A	-3.76	1.39	1.45
3	R	1082	CYC	C2A-C3A	3.76	1.44	1.36
3	Q	1084	CYC	C2A-C3A	3.75	1.44	1.36
3	P	1082	CYC	CAC-C3C	3.73	1.61	1.54
3	V	1082	CYC	C1C-NC	-3.73	1.32	1.37
3	X	1082	CYC	CAC-C3C	3.73	1.61	1.54
3	T	1082	CYC	C2A-C3A	3.72	1.44	1.36
3	D	1082	CYC	C2A-C3A	3.70	1.44	1.36
3	O	1084	CYC	C2A-C3A	3.69	1.44	1.36
3	F	1153	CYC	C3B-C2B	3.69	1.44	1.36
3	J	1082	CYC	CAC-C3C	3.67	1.61	1.54
3	T	1082	CYC	CAC-C3C	3.66	1.61	1.54
3	G	1084	CYC	C2A-C3A	3.66	1.44	1.36
3	D	1082	CYC	CAC-C3C	3.66	1.61	1.54
3	A	1084	CYC	C2A-C3A	3.65	1.44	1.36
3	X	1153	CYC	C3B-C2B	3.65	1.44	1.36
3	C	1084	CYC	C2A-C3A	3.65	1.44	1.36
3	T	1082	CYC	C1C-NC	-3.64	1.32	1.37
3	L	1082	CYC	C3B-C2B	3.64	1.44	1.36
3	V	1082	CYC	CAC-C3C	3.63	1.61	1.54
3	P	1153	CYC	C1A-C2A	-3.63	1.39	1.45
3	N	1082	CYC	C1C-NC	-3.61	1.32	1.37
3	C	1084	CYC	C1C-NC	-3.60	1.32	1.37
3	D	1082	CYC	C1C-NC	-3.59	1.33	1.37
3	H	1082	CYC	C1C-NC	-3.59	1.33	1.37
3	F	1082	CYC	C2A-C3A	3.58	1.44	1.36
3	H	1082	CYC	C2A-C3A	3.57	1.44	1.36
3	L	1153	CYC	C3B-C2B	3.56	1.44	1.36
3	P	1153	CYC	CHA-C1A	3.56	1.38	1.35
3	X	1153	CYC	C1C-NC	-3.55	1.33	1.37
3	H	1153	CYC	C1A-C2A	-3.55	1.40	1.45
3	L	1082	CYC	C1C-NC	-3.53	1.33	1.37
3	B	1153	CYC	C3B-C2B	3.53	1.44	1.36
3	N	1082	CYC	CAC-C3C	3.53	1.60	1.54
3	V	1153	CYC	C1A-C2A	-3.52	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1153	CYC	C3B-C2B	3.51	1.44	1.36
3	H	1153	CYC	C4B-NB	-3.51	1.30	1.38
3	T	1153	CYC	C1C-NC	-3.51	1.33	1.37
3	G	1084	CYC	C3B-C2B	3.49	1.44	1.36
3	F	1153	CYC	C1A-C2A	-3.49	1.40	1.45
3	W	1084	CYC	C2C-C1C	3.47	1.55	1.52
3	W	1084	CYC	C1C-NC	-3.45	1.33	1.37
3	B	1153	CYC	C2A-C3A	3.44	1.44	1.36
3	O	1084	CYC	C1C-NC	-3.44	1.33	1.37
3	I	1084	CYC	C3B-C2B	3.42	1.44	1.36
3	U	1084	CYC	C3B-C2B	3.39	1.43	1.36
3	O	1084	CYC	C3B-C2B	3.38	1.43	1.36
3	L	1153	CYC	C1A-C2A	-3.37	1.40	1.45
3	B	1082	CYC	C2A-C3A	3.36	1.43	1.36
3	P	1153	CYC	C1C-NC	-3.35	1.33	1.37
3	K	1084	CYC	C3B-C2B	3.35	1.43	1.36
3	S	1084	CYC	C3B-C2B	3.34	1.43	1.36
3	E	1084	CYC	C1C-NC	-3.32	1.33	1.37
3	E	1084	CYC	C3B-C2B	3.31	1.43	1.36
3	X	1153	CYC	C1A-C2A	-3.30	1.40	1.45
3	J	1153	CYC	C1C-NC	-3.29	1.33	1.37
3	R	1082	CYC	C3B-C2B	3.29	1.43	1.36
3	T	1082	CYC	C3B-C2B	3.27	1.43	1.36
3	F	1153	CYC	C4B-NB	-3.27	1.31	1.38
3	H	1082	CYC	C3B-C2B	3.26	1.43	1.36
3	W	1084	CYC	C3B-C2B	3.25	1.43	1.36
3	C	1084	CYC	C3B-C2B	3.25	1.43	1.36
3	P	1082	CYC	C3B-C2B	3.23	1.43	1.36
3	U	1084	CYC	C1C-NC	-3.22	1.33	1.37
3	N	1153	CYC	C1A-C2A	-3.20	1.40	1.45
3	X	1082	CYC	C3B-C2B	3.20	1.43	1.36
3	D	1082	CYC	C3B-C2B	3.19	1.43	1.36
3	Q	1084	CYC	C2C-C1C	3.16	1.54	1.52
3	B	1153	CYC	C1A-C2A	-3.16	1.40	1.45
3	N	1082	CYC	C3B-C2B	3.14	1.43	1.36
3	D	1153	CYC	C4B-NB	-3.12	1.31	1.38
3	Q	1084	CYC	C3B-C2B	3.12	1.43	1.36
3	V	1153	CYC	C3B-C2B	3.10	1.43	1.36
3	M	1084	CYC	C1C-NC	-3.09	1.33	1.37
3	F	1153	CYC	C2A-C3A	3.09	1.43	1.36
3	X	1153	CYC	C2A-C3A	3.07	1.43	1.36
3	H	1153	CYC	CHA-C1A	3.07	1.37	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	1082	CYC	C3B-C2B	3.04	1.43	1.36
3	C	1084	CYC	C2C-C1C	2.99	1.54	1.52
3	D	1153	CYC	C1C-NC	-2.98	1.33	1.37
3	I	1084	CYC	C1C-NC	-2.97	1.33	1.37
3	A	1084	CYC	C3B-C2B	2.97	1.43	1.36
3	P	1153	CYC	C4B-NB	-2.95	1.31	1.38
3	A	1084	CYC	C1C-NC	-2.95	1.33	1.37
3	J	1082	CYC	C3B-C2B	2.94	1.43	1.36
3	L	1153	CYC	C4B-NB	-2.94	1.31	1.38
3	X	1153	CYC	C4B-NB	-2.94	1.31	1.38
3	N	1153	CYC	C1C-NC	-2.94	1.33	1.37
3	B	1082	CYC	C3B-C2B	2.91	1.42	1.36
3	V	1153	CYC	C1C-NC	-2.90	1.33	1.37
3	D	1153	CYC	C1A-C2A	-2.89	1.41	1.45
3	M	1084	CYC	C3B-C2B	2.86	1.42	1.36
3	N	1153	CYC	C2A-C3A	2.82	1.42	1.36
3	L	1153	CYC	C1C-NC	-2.81	1.34	1.37
3	T	1153	CYC	C4B-NB	-2.81	1.32	1.38
3	R	1153	CYC	C2A-C3A	2.79	1.42	1.36
3	F	1082	CYC	C3B-C2B	2.79	1.42	1.36
3	K	1084	CYC	C1C-NC	-2.78	1.34	1.37
3	X	1082	CYC	C1A-C2A	-2.77	1.41	1.45
3	I	1084	CYC	C2C-C1C	2.76	1.54	1.52
3	J	1153	CYC	C2A-C3A	2.76	1.42	1.36
3	K	1084	CYC	C2C-C1C	2.74	1.54	1.52
3	R	1153	CYC	C4B-NB	-2.73	1.32	1.38
3	S	1084	CYC	C1C-NC	-2.72	1.34	1.37
3	P	1153	CYC	C2A-C3A	2.72	1.42	1.36
3	N	1153	CYC	C4B-NB	-2.69	1.32	1.38
3	D	1153	CYC	C2A-C3A	2.69	1.42	1.36
3	F	1153	CYC	C1C-NC	-2.69	1.34	1.37
3	Q	1084	CYC	C4C-NC	2.69	1.43	1.37
3	Q	1084	CYC	C1C-NC	-2.68	1.34	1.37
3	L	1153	CYC	C2A-C3A	2.67	1.42	1.36
3	B	1153	CYC	C4B-NB	-2.67	1.32	1.38
3	V	1153	CYC	C2A-C3A	2.67	1.42	1.36
3	G	1084	CYC	C1C-NC	-2.62	1.34	1.37
3	J	1153	CYC	C4B-NB	-2.62	1.32	1.38
3	M	1084	CYC	C2C-C1C	2.61	1.54	1.52
3	R	1082	CYC	O1D-CGD	2.59	1.30	1.22
3	A	1084	CYC	C2C-C1C	2.56	1.54	1.52
3	R	1082	CYC	C4C-NC	2.56	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1153	CYC	C4C-NC	2.54	1.42	1.37
3	T	1153	CYC	C2A-C3A	2.52	1.42	1.36
3	H	1082	CYC	C3D-C2D	2.52	1.45	1.37
3	V	1082	CYC	C3D-C2D	2.49	1.45	1.37
3	X	1082	CYC	CBA-CAA	2.48	1.59	1.52
3	V	1153	CYC	CBB-CAB	2.44	1.62	1.51
3	L	1153	CYC	C4C-NC	2.40	1.42	1.37
3	L	1082	CYC	C1A-C2A	-2.36	1.42	1.45
3	S	1084	CYC	C4C-NC	2.36	1.42	1.37
3	R	1082	CYC	CAD-CBD	2.35	1.64	1.52
3	M	1084	CYC	C4C-NC	2.35	1.42	1.37
3	U	1084	CYC	CHB-C1B	2.35	1.43	1.38
3	P	1082	CYC	C1A-C2A	-2.35	1.42	1.45
3	H	1153	CYC	C1C-NC	-2.35	1.34	1.37
3	M	1084	CYC	C3D-C2D	2.34	1.44	1.37
3	E	1084	CYC	C2C-C1C	2.34	1.54	1.52
3	V	1082	CYC	C4C-NC	2.34	1.42	1.37
3	P	1082	CYC	C3D-C2D	2.33	1.44	1.37
3	N	1082	CYC	C4C-NC	2.33	1.42	1.37
3	R	1082	CYC	C1A-NA	2.32	1.43	1.38
3	V	1153	CYC	C4C-NC	2.31	1.42	1.37
3	X	1082	CYC	C2C-C1C	2.31	1.54	1.52
3	H	1082	CYC	C1A-C2A	-2.31	1.42	1.45
3	L	1082	CYC	C4C-NC	2.30	1.42	1.37
3	H	1153	CYC	C2A-C3A	2.29	1.41	1.36
3	U	1084	CYC	C2C-C1C	2.28	1.54	1.52
3	R	1082	CYC	CHB-C1B	2.27	1.43	1.38
3	L	1082	CYC	CHB-C1B	2.27	1.43	1.38
3	O	1084	CYC	C4C-NC	2.26	1.42	1.37
3	F	1153	CYC	CHD-C4C	2.25	1.43	1.38
3	X	1082	CYC	C3D-C2D	2.25	1.44	1.37
3	B	1082	CYC	C3D-C2D	2.25	1.44	1.37
3	F	1153	CYC	CAC-C3C	2.23	1.58	1.54
3	X	1082	CYC	C1A-NA	2.22	1.43	1.38
3	K	1084	CYC	C3D-C2D	2.22	1.44	1.37
3	J	1153	CYC	CAD-C3D	-2.21	1.48	1.52
3	E	1084	CYC	CHB-C1B	2.21	1.43	1.38
3	D	1082	CYC	C4C-NC	2.21	1.42	1.37
3	J	1082	CYC	C4C-NC	2.21	1.42	1.37
3	H	1153	CYC	O2D-CGD	-2.20	1.23	1.30
3	L	1082	CYC	C3D-C2D	2.20	1.44	1.37
3	B	1153	CYC	C2C-C1C	2.20	1.54	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1153	CYC	CHD-C4C	2.20	1.43	1.38
3	I	1084	CYC	CHB-C1B	2.19	1.43	1.38
3	X	1153	CYC	CBA-CGA	2.19	1.55	1.50
3	H	1153	CYC	CHD-C4C	2.19	1.43	1.38
3	T	1153	CYC	O1A-CGA	2.17	1.29	1.22
3	N	1082	CYC	C3D-C2D	2.17	1.44	1.37
3	E	1084	CYC	C4C-NC	2.17	1.41	1.37
3	F	1153	CYC	CBA-CGA	2.16	1.55	1.50
3	A	1084	CYC	C4C-NC	2.16	1.41	1.37
3	R	1082	CYC	CAD-C3D	2.16	1.55	1.52
3	R	1082	CYC	CHD-C4C	2.15	1.43	1.38
3	B	1153	CYC	C4C-NC	2.15	1.41	1.37
3	W	1084	CYC	C4C-NC	2.15	1.41	1.37
3	S	1084	CYC	C3D-C2D	2.15	1.44	1.37
3	T	1153	CYC	CBA-CGA	2.14	1.55	1.50
3	P	1153	CYC	C4C-NC	2.14	1.41	1.37
3	O	1084	CYC	C3D-C2D	2.13	1.44	1.37
3	R	1082	CYC	C1A-C2A	-2.13	1.42	1.45
3	L	1153	CYC	CAD-C3D	-2.13	1.48	1.52
3	F	1082	CYC	C3D-C2D	2.13	1.44	1.37
3	O	1084	CYC	CBA-CGA	2.12	1.55	1.50
3	N	1153	CYC	C4C-NC	2.12	1.41	1.37
3	W	1084	CYC	C4B-NB	-2.11	1.33	1.38
3	B	1082	CYC	C4C-NC	2.11	1.41	1.37
3	D	1153	CYC	C4C-NC	2.11	1.41	1.37
3	D	1082	CYC	C3D-C2D	2.10	1.43	1.37
3	C	1084	CYC	C4C-NC	2.10	1.41	1.37
3	N	1082	CYC	C1A-C2A	-2.10	1.42	1.45
3	H	1082	CYC	CHB-C1B	2.10	1.43	1.38
3	T	1082	CYC	C3D-C2D	2.10	1.43	1.37
3	N	1153	CYC	CBA-CGA	2.09	1.55	1.50
3	G	1084	CYC	C3D-C2D	2.09	1.43	1.37
3	K	1084	CYC	CHB-C1B	2.09	1.42	1.38
3	U	1084	CYC	C3D-C2D	2.08	1.43	1.37
3	R	1082	CYC	C2C-C1C	2.08	1.53	1.52
3	T	1082	CYC	C4C-NC	2.08	1.41	1.37
3	P	1082	CYC	CHB-C1B	2.07	1.42	1.38
3	K	1084	CYC	C4C-NC	2.07	1.41	1.37
3	P	1153	CYC	O1A-CGA	2.07	1.29	1.22
3	U	1084	CYC	C4C-NC	2.06	1.41	1.37
3	A	1084	CYC	C3D-C2D	2.06	1.43	1.37
3	J	1082	CYC	C1A-C2A	-2.06	1.42	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	1082	CYC	C4C-NC	2.06	1.41	1.37
3	J	1082	CYC	C3D-C2D	2.06	1.43	1.37
3	C	1084	CYC	CHB-C1B	2.05	1.42	1.38
3	S	1084	CYC	C2C-C1C	2.04	1.53	1.52
3	F	1082	CYC	C1A-C2A	-2.04	1.42	1.45
3	W	1084	CYC	CMC-C2C	2.03	1.57	1.53
3	O	1084	CYC	CHB-C1B	2.03	1.42	1.38
3	G	1084	CYC	C4C-NC	2.03	1.41	1.37
3	V	1153	CYC	C1B-NB	2.03	1.41	1.37
3	L	1153	CYC	O1A-CGA	2.03	1.28	1.22
3	I	1084	CYC	C3D-C2D	2.02	1.43	1.37
3	W	1084	CYC	C3D-C2D	2.02	1.43	1.37
3	R	1153	CYC	C4B-C3B	2.02	1.52	1.48
3	D	1082	CYC	C1A-C2A	-2.02	1.42	1.45
3	P	1153	CYC	CHD-C4C	2.01	1.43	1.38
3	E	1084	CYC	C1A-C2A	-2.01	1.42	1.45
3	V	1153	CYC	CBA-CAA	2.01	1.58	1.52
3	T	1153	CYC	CHD-C4C	2.01	1.43	1.38
3	X	1153	CYC	C4C-NC	2.01	1.41	1.37
3	B	1153	CYC	O1A-CGA	2.00	1.28	1.22
3	Q	1084	CYC	C1A-C2A	-2.00	1.42	1.45
3	X	1153	CYC	O1A-CGA	2.00	1.28	1.22

All (371) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	1153	CYC	C2C-C1C-NC	5.93	113.39	108.27
3	R	1082	CYC	C2C-C1C-NC	5.74	113.22	108.27
3	X	1153	CYC	C2C-C1C-NC	5.66	113.15	108.27
3	B	1153	CYC	C2C-C1C-NC	5.66	113.15	108.27
3	T	1153	CYC	C2C-C1C-NC	5.65	113.14	108.27
3	C	1084	CYC	C3B-C4B-NB	5.61	111.31	106.78
3	L	1153	CYC	C4D-CHA-C1A	5.52	135.40	128.81
3	L	1153	CYC	C2C-C1C-NC	5.50	113.02	108.27
3	P	1153	CYC	C2C-C1C-NC	5.50	113.02	108.27
3	F	1153	CYC	C2C-C1C-NC	5.50	113.01	108.27
3	V	1153	CYC	C2C-C1C-NC	5.49	113.00	108.27
3	N	1153	CYC	C2C-C1C-NC	5.49	113.00	108.27
3	I	1084	CYC	C3B-C4B-NB	5.47	111.20	106.78
3	E	1084	CYC	C3B-C4B-NB	5.46	111.19	106.78
3	A	1084	CYC	C3B-C4B-NB	5.45	111.18	106.78
3	J	1153	CYC	C2C-C1C-NC	5.39	112.92	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1082	CYC	C3B-C4B-NB	5.37	111.12	106.78
3	M	1084	CYC	C3B-C4B-NB	5.37	111.11	106.78
3	Q	1084	CYC	C3B-C4B-NB	5.36	111.10	106.78
3	S	1084	CYC	C3B-C4B-NB	5.36	111.10	106.78
3	D	1153	CYC	C2C-C1C-NC	5.35	112.88	108.27
3	T	1153	CYC	C4D-CHA-C1A	5.31	135.15	128.81
3	J	1082	CYC	C3B-C4B-NB	5.30	111.06	106.78
3	W	1084	CYC	C3B-C4B-NB	5.30	111.06	106.78
3	P	1082	CYC	C2C-C1C-NC	5.28	112.82	108.27
3	G	1084	CYC	C3B-C4B-NB	5.27	111.03	106.78
3	O	1084	CYC	C3B-C4B-NB	5.26	111.02	106.78
3	R	1082	CYC	C3B-C4B-NB	5.24	111.01	106.78
3	B	1082	CYC	C2C-C1C-NC	5.20	112.75	108.27
3	T	1082	CYC	C3B-C4B-NB	5.19	110.97	106.78
3	L	1082	CYC	C2C-C1C-NC	5.19	112.75	108.27
3	P	1082	CYC	C3B-C4B-NB	5.17	110.95	106.78
3	B	1082	CYC	C3B-C4B-NB	5.16	110.94	106.78
3	F	1082	CYC	C3B-C4B-NB	5.15	110.94	106.78
3	V	1082	CYC	C3B-C4B-NB	5.13	110.92	106.78
3	H	1082	CYC	C2C-C1C-NC	5.12	112.69	108.27
3	R	1153	CYC	C2C-C1C-NC	5.09	112.66	108.27
3	K	1084	CYC	C3B-C4B-NB	5.09	110.89	106.78
3	N	1082	CYC	C3B-C4B-NB	5.07	110.88	106.78
3	X	1082	CYC	C2C-C1C-NC	5.05	112.63	108.27
3	U	1084	CYC	C3B-C4B-NB	5.05	110.86	106.78
3	D	1082	CYC	C2C-C1C-NC	5.04	112.62	108.27
3	D	1082	CYC	C3B-C4B-NB	5.04	110.85	106.78
3	N	1082	CYC	C2C-C1C-NC	5.03	112.61	108.27
3	X	1082	CYC	C3B-C4B-NB	5.02	110.83	106.78
3	L	1082	CYC	C3B-C4B-NB	5.00	110.82	106.78
3	J	1082	CYC	C2C-C1C-NC	4.94	112.53	108.27
3	F	1082	CYC	C2C-C1C-NC	4.94	112.53	108.27
3	T	1082	CYC	C2C-C1C-NC	4.91	112.50	108.27
3	D	1153	CYC	C4D-CHA-C1A	4.87	134.63	128.81
3	V	1082	CYC	C2C-C1C-NC	4.86	112.46	108.27
3	V	1153	CYC	CBB-CAB-C3B	4.83	125.75	112.43
3	V	1153	CYC	C4D-CHA-C1A	4.78	134.52	128.81
3	T	1082	CYC	CAB-C3B-C4B	4.74	128.87	121.38
3	X	1153	CYC	C4D-CHA-C1A	4.65	134.36	128.81
3	U	1084	CYC	C4D-CHA-C1A	4.64	134.35	128.81
3	B	1153	CYC	C4D-CHA-C1A	4.59	134.29	128.81
3	P	1153	CYC	C4D-CHA-C1A	4.58	134.28	128.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	U	1084	CYC	CAB-C3B-C4B	4.55	128.57	121.38
3	J	1153	CYC	C4D-CHA-C1A	4.45	134.12	128.81
3	M	1084	CYC	CAB-C3B-C4B	4.43	128.38	121.38
3	I	1084	CYC	CAB-C3B-C4B	4.37	128.28	121.38
3	S	1084	CYC	C4D-CHA-C1A	4.35	134.00	128.81
3	H	1082	CYC	CAB-C3B-C4B	4.32	128.20	121.38
3	C	1084	CYC	C4D-CHA-C1A	4.32	133.97	128.81
3	R	1153	CYC	C4D-CHA-C1A	4.31	133.95	128.81
3	P	1082	CYC	CBD-CAD-C3D	4.30	119.96	112.62
3	H	1153	CYC	OC-C1C-C2C	-4.27	122.77	126.17
3	Q	1084	CYC	CAB-C3B-C4B	4.27	128.12	121.38
3	A	1084	CYC	C4D-CHA-C1A	4.25	133.88	128.81
3	A	1084	CYC	CAB-C3B-C4B	4.23	128.05	121.38
3	K	1084	CYC	CAB-C3B-C4B	4.22	128.05	121.38
3	H	1153	CYC	C2C-C3C-C4C	4.21	107.65	101.34
3	N	1153	CYC	C2C-C3C-C4C	4.20	107.64	101.34
3	B	1153	CYC	C3B-C4B-NB	4.17	110.14	106.78
3	D	1153	CYC	C3B-C4B-NB	4.10	110.09	106.78
3	W	1084	CYC	CAB-C3B-C4B	4.10	127.86	121.38
3	P	1082	CYC	CAB-C3B-C4B	4.05	127.78	121.38
3	I	1084	CYC	C4D-CHA-C1A	4.04	133.63	128.81
3	K	1084	CYC	C4D-CHA-C1A	4.03	133.63	128.81
3	C	1084	CYC	CAB-C3B-C4B	4.03	127.75	121.38
3	F	1082	CYC	CAB-C3B-C4B	4.03	127.75	121.38
3	G	1084	CYC	CAB-C3B-C4B	4.03	127.74	121.38
3	V	1153	CYC	C1B-C2B-C3B	-4.02	103.68	107.87
3	E	1084	CYC	C2C-C1C-NC	4.00	111.72	108.27
3	J	1082	CYC	CAB-C3B-C4B	3.98	127.66	121.38
3	E	1084	CYC	CAB-C3B-C4B	3.96	127.64	121.38
3	D	1153	CYC	OC-C1C-C2C	-3.96	123.02	126.17
3	M	1084	CYC	C4D-CHA-C1A	3.90	133.47	128.81
3	R	1082	CYC	CAB-C3B-C4B	3.90	127.53	121.38
3	N	1082	CYC	CAB-C3B-C4B	3.88	127.51	121.38
3	O	1084	CYC	C4D-CHA-C1A	3.88	133.44	128.81
3	G	1084	CYC	C4D-CHA-C1A	3.87	133.43	128.81
3	S	1084	CYC	CAB-C3B-C4B	3.86	127.47	121.38
3	U	1084	CYC	C2C-C1C-NC	3.85	111.59	108.27
3	O	1084	CYC	CAB-C3B-C4B	3.82	127.41	121.38
3	V	1153	CYC	OC-C1C-C2C	-3.82	123.14	126.17
3	T	1153	CYC	C2C-C3C-C4C	3.82	107.06	101.34
3	L	1153	CYC	C2C-C3C-C4C	3.80	107.03	101.34
3	J	1153	CYC	C3B-C4B-NB	3.79	109.84	106.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1153	CYC	C3B-C4B-NB	3.77	109.82	106.78
3	P	1153	CYC	C2C-C3C-C4C	3.77	106.98	101.34
3	I	1084	CYC	C2C-C1C-NC	3.76	111.51	108.27
3	P	1153	CYC	C3B-C4B-NB	3.76	109.81	106.78
3	F	1153	CYC	C2C-C3C-C4C	3.75	106.95	101.34
3	D	1153	CYC	C2C-C3C-C4C	3.75	106.95	101.34
3	H	1153	CYC	C3B-C4B-NB	3.75	109.80	106.78
3	R	1082	CYC	CHD-C4C-NC	-3.75	120.75	125.20
3	B	1082	CYC	CAB-C3B-C4B	3.74	127.28	121.38
3	N	1153	CYC	C3B-C4B-NB	3.73	109.79	106.78
3	D	1082	CYC	CAB-C3B-C4B	3.73	127.27	121.38
3	N	1153	CYC	OC-C1C-C2C	-3.72	123.22	126.17
3	X	1082	CYC	CAB-C3B-C4B	3.71	127.24	121.38
3	L	1082	CYC	CAB-C3B-C4B	3.70	127.22	121.38
3	L	1153	CYC	OC-C1C-C2C	-3.70	123.23	126.17
3	K	1084	CYC	C2C-C1C-NC	3.68	111.45	108.27
3	V	1082	CYC	CAB-C3B-C4B	3.68	127.18	121.38
3	J	1153	CYC	C2C-C3C-C4C	3.63	106.78	101.34
3	R	1153	CYC	C3B-C4B-NB	3.63	109.71	106.78
3	F	1153	CYC	C3B-C4B-NB	3.61	109.69	106.78
3	V	1153	CYC	CMB-C2B-C1B	3.59	128.65	124.17
3	X	1153	CYC	C2C-C3C-C4C	3.59	106.72	101.34
3	H	1153	CYC	CMA-C3A-C4A	3.58	130.58	125.06
3	V	1153	CYC	CMA-C3A-C4A	3.56	130.54	125.06
3	E	1084	CYC	C4D-CHA-C1A	3.56	133.06	128.81
3	O	1084	CYC	C2C-C1C-NC	3.56	111.34	108.27
3	F	1153	CYC	OC-C1C-C2C	-3.55	123.35	126.17
3	W	1084	CYC	C2C-C1C-NC	3.55	111.33	108.27
3	T	1153	CYC	OC-C1C-C2C	-3.54	123.36	126.17
3	T	1082	CYC	C4D-CHA-C1A	3.53	133.03	128.81
3	G	1084	CYC	C2C-C1C-NC	3.53	111.31	108.27
3	X	1153	CYC	OC-C1C-C2C	-3.53	123.37	126.17
3	R	1082	CYC	C4D-CHA-C1A	3.52	133.02	128.81
3	B	1153	CYC	C2C-C3C-C4C	3.52	106.61	101.34
3	R	1153	CYC	C2C-C3C-C4C	3.51	106.60	101.34
3	V	1153	CYC	C2C-C3C-C4C	3.51	106.60	101.34
3	W	1084	CYC	C4D-CHA-C1A	3.51	133.00	128.81
3	X	1153	CYC	C3B-C4B-NB	3.50	109.61	106.78
3	T	1153	CYC	C3B-C4B-NB	3.49	109.59	106.78
3	S	1084	CYC	C2C-C1C-NC	3.49	111.28	108.27
3	M	1084	CYC	C2C-C1C-NC	3.49	111.28	108.27
3	F	1082	CYC	CHD-C4C-NC	-3.48	121.07	125.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1153	CYC	C4D-CHA-C1A	3.42	132.90	128.81
3	P	1153	CYC	OC-C1C-C2C	-3.41	123.46	126.17
3	B	1082	CYC	CHD-C4C-NC	-3.35	121.22	125.20
3	F	1153	CYC	C4D-CHA-C1A	3.35	132.81	128.81
3	A	1084	CYC	C2C-C1C-NC	3.32	111.14	108.27
3	R	1153	CYC	CAB-C3B-C4B	3.32	126.63	121.38
3	W	1084	CYC	CHD-C4C-NC	-3.30	121.28	125.20
3	R	1082	CYC	C2C-C3C-C4C	3.29	106.27	101.34
3	H	1153	CYC	C4D-CHA-C1A	3.29	132.74	128.81
3	C	1084	CYC	C2C-C1C-NC	3.27	111.09	108.27
3	L	1153	CYC	CMA-C3A-C4A	3.27	130.10	125.06
3	E	1084	CYC	CHD-C4C-NC	-3.26	121.33	125.20
3	D	1153	CYC	CMA-C3A-C4A	3.23	130.04	125.06
3	Q	1084	CYC	C4D-CHA-C1A	3.22	132.66	128.81
3	P	1153	CYC	CMA-C3A-C4A	3.21	130.01	125.06
3	J	1153	CYC	OC-C1C-C2C	-3.21	123.62	126.17
3	X	1153	CYC	CMA-C3A-C4A	3.20	129.99	125.06
3	B	1153	CYC	CAB-C3B-C4B	3.20	126.43	121.38
3	B	1153	CYC	OC-C1C-C2C	-3.20	123.63	126.17
3	T	1153	CYC	CMA-C3A-C4A	3.19	129.98	125.06
3	J	1082	CYC	CHD-C4C-NC	-3.19	121.42	125.20
3	F	1153	CYC	CAB-C3B-C4B	3.17	126.39	121.38
3	K	1084	CYC	CHD-C4C-NC	-3.17	121.44	125.20
3	Q	1084	CYC	C2C-C1C-NC	3.16	111.00	108.27
3	N	1153	CYC	CMA-C3A-C4A	3.16	129.92	125.06
3	R	1153	CYC	CMA-C3A-C4A	3.15	129.91	125.06
3	F	1153	CYC	CMA-C3A-C4A	3.13	129.88	125.06
3	N	1082	CYC	C2C-C3C-C4C	3.12	106.01	101.34
3	P	1082	CYC	CHD-C4C-NC	-3.12	121.50	125.20
3	U	1084	CYC	CHD-C4C-NC	-3.10	121.52	125.20
3	X	1153	CYC	CAB-C3B-C4B	3.10	126.27	121.38
3	L	1153	CYC	CAB-C3B-C4B	3.09	126.25	121.38
3	X	1082	CYC	CHD-C4C-NC	-3.07	121.55	125.20
3	W	1084	CYC	C2B-C1B-NB	3.07	111.48	106.99
3	V	1082	CYC	CHD-C4C-NC	-3.06	121.57	125.20
3	O	1084	CYC	CHD-C4C-NC	-3.05	121.57	125.20
3	T	1082	CYC	C2C-C3C-C4C	3.03	105.88	101.34
3	H	1082	CYC	CHD-C4C-NC	-3.02	121.62	125.20
3	D	1153	CYC	CAB-C3B-C4B	2.98	126.08	121.38
3	M	1084	CYC	C2B-C1B-NB	2.98	111.35	106.99
3	J	1153	CYC	CAB-C3B-C4B	2.96	126.05	121.38
3	M	1084	CYC	CHD-C4C-NC	-2.96	121.69	125.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1082	CYC	C4D-CHA-C1A	2.96	132.34	128.81
3	T	1082	CYC	CHD-C4C-NC	-2.95	121.69	125.20
3	T	1153	CYC	CAB-C3B-C4B	2.95	126.03	121.38
3	D	1082	CYC	C2C-C3C-C4C	2.95	105.75	101.34
3	L	1082	CYC	C2C-C3C-C4C	2.95	105.75	101.34
3	C	1084	CYC	CHD-C4C-NC	-2.93	121.73	125.20
3	V	1082	CYC	C2C-C3C-C4C	2.92	105.72	101.34
3	A	1084	CYC	C2B-C1B-NB	2.92	111.26	106.99
3	X	1082	CYC	C2C-C3C-C4C	2.91	105.70	101.34
3	H	1082	CYC	C2C-C3C-C4C	2.91	105.70	101.34
3	S	1084	CYC	C2B-C1B-NB	2.91	111.25	106.99
3	R	1082	CYC	CAD-CBD-CGD	-2.91	105.60	113.76
3	D	1082	CYC	C2B-C1B-NB	2.91	111.24	106.99
3	L	1082	CYC	CHD-C4C-NC	-2.90	121.76	125.20
3	P	1153	CYC	CAB-C3B-C4B	2.89	125.94	121.38
3	J	1153	CYC	CMA-C3A-C4A	2.88	129.50	125.06
3	J	1082	CYC	C2C-C3C-C4C	2.87	105.63	101.34
3	N	1153	CYC	CAB-C3B-C4B	2.84	125.87	121.38
3	R	1153	CYC	CBD-CAD-C3D	2.84	117.47	112.62
3	F	1082	CYC	C2B-C1B-NB	2.84	111.14	106.99
3	N	1082	CYC	C2B-C1B-NB	2.83	111.13	106.99
3	P	1082	CYC	C2C-C3C-C4C	2.81	105.55	101.34
3	D	1082	CYC	C4D-CHA-C1A	2.80	132.15	128.81
3	X	1153	CYC	CHB-C4A-C3A	2.79	132.08	124.90
3	B	1153	CYC	CMA-C3A-C4A	2.79	129.36	125.06
3	G	1084	CYC	CHD-C4C-NC	-2.78	121.89	125.20
3	B	1153	CYC	C1B-CHB-C4A	2.78	134.88	128.08
3	D	1153	CYC	CHB-C4A-C3A	2.78	132.05	124.90
3	H	1153	CYC	CAB-C3B-C4B	2.78	125.77	121.38
3	U	1084	CYC	C2B-C1B-NB	2.77	111.05	106.99
3	B	1082	CYC	C2B-C1B-NB	2.77	111.04	106.99
3	V	1153	CYC	CHB-C4A-C3A	2.77	132.02	124.90
3	E	1084	CYC	C2B-C1B-NB	2.77	111.04	106.99
3	J	1082	CYC	C2B-C1B-NB	2.76	111.03	106.99
3	V	1082	CYC	C2B-C1B-NB	2.76	111.02	106.99
3	N	1082	CYC	CHD-C4C-NC	-2.75	121.93	125.20
3	O	1084	CYC	C2B-C1B-NB	2.75	111.01	106.99
3	D	1082	CYC	CHD-C4C-NC	-2.74	121.95	125.20
3	V	1153	CYC	OB-C4B-C3B	-2.73	125.08	128.04
3	N	1082	CYC	OC-C1C-C2C	-2.72	124.01	126.17
3	T	1082	CYC	C2B-C1B-NB	2.72	110.97	106.99
3	I	1084	CYC	CHD-C4C-NC	-2.72	121.97	125.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1084	CYC	C2B-C1B-NB	2.72	110.97	106.99
3	Q	1084	CYC	C2B-C1B-NB	2.72	110.96	106.99
3	L	1082	CYC	OC-C1C-C2C	-2.72	124.01	126.17
3	F	1082	CYC	C2C-C3C-C4C	2.71	105.40	101.34
3	R	1082	CYC	C2B-C1B-NB	2.71	110.95	106.99
3	P	1082	CYC	C2B-C1B-NB	2.70	110.94	106.99
3	B	1082	CYC	C2C-C3C-C4C	2.70	105.38	101.34
3	R	1153	CYC	OC-C1C-C2C	-2.69	124.03	126.17
3	A	1084	CYC	CHD-C4C-NC	-2.69	122.01	125.20
3	K	1084	CYC	C2B-C1B-NB	2.68	110.90	106.99
3	D	1153	CYC	CHB-C4A-NA	-2.65	119.40	124.93
3	T	1153	CYC	CBD-CAD-C3D	2.64	117.12	112.62
3	J	1153	CYC	CHB-C4A-C3A	2.63	131.66	124.90
3	H	1082	CYC	C2B-C1B-NB	2.63	110.83	106.99
3	X	1082	CYC	CBA-CAA-C2A	2.63	119.92	112.63
3	X	1082	CYC	C2B-C1B-NB	2.62	110.82	106.99
3	R	1153	CYC	CHB-C4A-C3A	2.62	131.63	124.90
3	Q	1084	CYC	CHD-C4C-NC	-2.60	122.11	125.20
3	C	1084	CYC	C2B-C1B-NB	2.60	110.79	106.99
3	L	1153	CYC	CHB-C4A-C3A	2.60	131.58	124.90
3	S	1084	CYC	C1B-NB-C4B	-2.60	107.36	110.67
3	F	1153	CYC	CHB-C4A-C3A	2.58	131.55	124.90
3	I	1084	CYC	C2B-C1B-NB	2.57	110.76	106.99
3	M	1084	CYC	C1B-NB-C4B	-2.57	107.39	110.67
3	X	1153	CYC	C1B-CHB-C4A	2.57	134.36	128.08
3	H	1153	CYC	CHB-C4A-C3A	2.57	131.51	124.90
3	V	1153	CYC	C3B-C4B-NB	2.56	108.84	106.78
3	V	1153	CYC	CHB-C4A-NA	-2.56	119.58	124.93
3	V	1082	CYC	C1B-NB-C4B	-2.56	107.41	110.67
3	V	1082	CYC	C4D-CHA-C1A	2.55	131.85	128.81
3	A	1084	CYC	C1B-NB-C4B	-2.55	107.43	110.67
3	L	1082	CYC	C2B-C1B-NB	2.54	110.70	106.99
3	H	1082	CYC	OC-C1C-C2C	-2.54	124.16	126.17
3	X	1153	CYC	CHB-C4A-NA	-2.52	119.66	124.93
3	N	1153	CYC	CHB-C4A-C3A	2.51	131.35	124.90
3	V	1082	CYC	OC-C1C-C2C	-2.49	124.19	126.17
3	F	1082	CYC	C1B-NB-C4B	-2.49	107.50	110.67
3	F	1082	CYC	OC-C1C-C2C	-2.48	124.20	126.17
3	J	1082	CYC	C1B-NB-C4B	-2.48	107.52	110.67
3	P	1082	CYC	C1B-NB-C4B	-2.47	107.53	110.67
3	T	1153	CYC	CHB-C4A-C3A	2.45	131.20	124.90
3	D	1082	CYC	OC-C1C-C2C	-2.45	124.23	126.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1082	CYC	C1B-NB-C4B	-2.44	107.56	110.67
3	B	1153	CYC	CHB-C4A-C3A	2.44	131.18	124.90
3	J	1153	CYC	C1B-CHB-C4A	2.43	134.01	128.08
3	Q	1084	CYC	C1B-NB-C4B	-2.42	107.59	110.67
3	H	1082	CYC	CMB-C2B-C1B	2.41	127.18	124.17
3	T	1153	CYC	C1B-CHB-C4A	2.41	133.97	128.08
3	P	1153	CYC	CHB-C4A-C3A	2.41	131.09	124.90
3	J	1082	CYC	OC-C1C-C2C	-2.40	124.26	126.17
3	F	1153	CYC	CHB-C4A-NA	-2.40	119.92	124.93
3	R	1082	CYC	C1B-NB-C4B	-2.38	107.63	110.67
3	H	1153	CYC	C1B-C2B-C3B	-2.38	105.38	107.87
3	J	1153	CYC	CHB-C4A-NA	-2.38	119.95	124.93
3	R	1153	CYC	CHB-C4A-NA	-2.37	119.97	124.93
3	T	1082	CYC	OC-C1C-C2C	-2.37	124.29	126.17
3	L	1153	CYC	C1B-CHB-C4A	2.36	133.85	128.08
3	O	1084	CYC	C1B-NB-C4B	-2.36	107.67	110.67
3	U	1084	CYC	C1B-NB-C4B	-2.35	107.67	110.67
3	L	1153	CYC	CHB-C4A-NA	-2.35	120.02	124.93
3	W	1084	CYC	C1B-NB-C4B	-2.35	107.68	110.67
3	D	1082	CYC	C1B-NB-C4B	-2.35	107.68	110.67
3	S	1084	CYC	CHD-C4C-NC	-2.34	122.42	125.20
3	R	1082	CYC	OC-C1C-C2C	-2.33	124.32	126.17
3	X	1082	CYC	C1B-NB-C4B	-2.33	107.71	110.67
3	J	1082	CYC	CHA-C1A-NA	-2.32	125.61	128.83
3	B	1082	CYC	C4D-CHA-C1A	2.31	131.57	128.81
3	P	1153	CYC	C1B-C2B-C3B	-2.30	105.47	107.87
3	K	1084	CYC	C1B-NB-C4B	-2.30	107.74	110.67
3	C	1084	CYC	C1B-NB-C4B	-2.30	107.74	110.67
3	T	1153	CYC	CHA-C1A-C2A	-2.30	120.01	125.32
3	F	1082	CYC	CHA-C1A-NA	-2.30	125.64	128.83
3	V	1082	CYC	CHA-C1A-NA	-2.29	125.64	128.83
3	J	1082	CYC	C4D-CHA-C1A	2.28	131.53	128.81
3	E	1084	CYC	C1B-NB-C4B	-2.27	107.78	110.67
3	N	1082	CYC	C1B-NB-C4B	-2.27	107.78	110.67
3	F	1082	CYC	C4D-CHA-C1A	2.26	131.51	128.81
3	T	1082	CYC	C1B-NB-C4B	-2.25	107.80	110.67
3	D	1153	CYC	C1B-C2B-C3B	-2.25	105.52	107.87
3	F	1153	CYC	C1B-C2B-C3B	-2.25	105.52	107.87
3	R	1153	CYC	CBB-CAB-C3B	2.25	118.62	112.43
3	H	1082	CYC	CHA-C1A-NA	-2.24	125.71	128.83
3	B	1082	CYC	OC-C1C-C2C	-2.24	124.39	126.17
3	X	1082	CYC	OC-C1C-C2C	-2.24	124.39	126.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	1082	CYC	CHA-C1A-NA	-2.24	125.72	128.83
3	H	1153	CYC	CHB-C4A-NA	-2.22	120.29	124.93
3	I	1084	CYC	CMA-C3A-C4A	2.22	128.48	125.06
3	N	1153	CYC	C1B-CHB-C4A	2.21	133.47	128.08
3	P	1153	CYC	CHB-C4A-NA	-2.20	120.33	124.93
3	L	1082	CYC	CHA-C1A-NA	-2.20	125.78	128.83
3	P	1082	CYC	OC-C1C-C2C	-2.19	124.43	126.17
3	X	1082	CYC	C4D-CHA-C1A	2.19	131.43	128.81
3	Q	1084	CYC	CMA-C3A-C4A	2.18	128.43	125.06
3	E	1084	CYC	O1D-CGD-CBD	-2.18	116.08	123.08
3	F	1153	CYC	C2B-C1B-NB	2.17	110.16	106.99
3	N	1082	CYC	CMB-C2B-C1B	2.17	126.88	124.17
3	L	1153	CYC	C1B-C2B-C3B	-2.16	105.62	107.87
3	B	1153	CYC	CMB-C2B-C1B	2.16	126.86	124.17
3	B	1153	CYC	CBB-CAB-C3B	2.15	118.36	112.43
3	R	1153	CYC	C2B-C1B-NB	2.15	110.13	106.99
3	N	1153	CYC	CHB-C4A-NA	-2.14	120.46	124.93
3	G	1084	CYC	C1B-NB-C4B	-2.14	107.95	110.67
3	D	1153	CYC	C1B-CHB-C4A	2.13	133.30	128.08
3	V	1153	CYC	C2B-C1B-NB	2.13	110.10	106.99
3	P	1082	CYC	CAD-CBD-CGD	-2.12	107.81	113.76
3	D	1082	CYC	CHA-C1A-NA	-2.12	125.89	128.83
3	G	1084	CYC	CMA-C3A-C4A	2.11	128.31	125.06
3	X	1153	CYC	C1B-C2B-C3B	-2.10	105.68	107.87
3	I	1084	CYC	CMB-C2B-C1B	2.09	126.78	124.17
3	N	1153	CYC	CBD-CAD-C3D	2.09	116.19	112.62
3	T	1153	CYC	CHB-C4A-NA	-2.09	120.56	124.93
3	I	1084	CYC	O1D-CGD-CBD	-2.08	116.39	123.08
3	H	1082	CYC	C1B-NB-C4B	-2.08	108.02	110.67
3	D	1153	CYC	C2B-C1B-NB	2.08	110.03	106.99
3	K	1084	CYC	CMA-C3A-C4A	2.08	128.26	125.06
3	B	1153	CYC	CHB-C4A-NA	-2.07	120.59	124.93
3	O	1084	CYC	CMA-C3A-C4A	2.07	128.25	125.06
3	B	1153	CYC	C1B-C2B-C3B	-2.07	105.71	107.87
3	I	1084	CYC	C1B-NB-C4B	-2.07	108.03	110.67
3	M	1084	CYC	CMA-C3A-C4A	2.07	128.25	125.06
3	A	1084	CYC	CMA-C3A-C4A	2.07	128.25	125.06
3	R	1082	CYC	OC-C1C-NC	-2.05	122.45	124.94
3	X	1082	CYC	CMB-C2B-C1B	2.05	126.73	124.17
3	D	1082	CYC	C1B-C2B-C3B	-2.05	105.73	107.87
3	S	1084	CYC	O1D-CGD-CBD	-2.05	116.49	123.08
3	R	1153	CYC	C1B-C2B-C3B	-2.05	105.73	107.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	1153	CYC	C1B-C2B-C3B	-2.04	105.74	107.87
3	L	1153	CYC	CHA-C1A-C2A	-2.04	120.61	125.32
3	H	1153	CYC	CMB-C2B-C1B	2.04	126.71	124.17
3	R	1082	CYC	CAA-CBA-CGA	-2.04	109.22	113.60
3	W	1084	CYC	CMA-C3A-C4A	2.04	128.20	125.06
3	C	1084	CYC	CMA-C3A-C4A	2.04	128.20	125.06
3	S	1084	CYC	CMA-C3A-C4A	2.03	128.19	125.06
3	P	1153	CYC	C2B-C1B-NB	2.03	109.96	106.99
3	W	1084	CYC	C1B-C2B-C3B	-2.03	105.76	107.87
3	P	1082	CYC	CHA-C1A-NA	-2.02	126.02	128.83
3	G	1084	CYC	O1D-CGD-CBD	-2.02	116.58	123.08
3	Q	1084	CYC	O1D-CGD-CBD	-2.02	116.58	123.08
3	R	1153	CYC	C1B-CHB-C4A	2.02	133.02	128.08
3	L	1082	CYC	C1B-NB-C4B	-2.02	108.10	110.67
3	L	1153	CYC	C2B-C1B-NB	2.01	109.94	106.99
3	V	1082	CYC	O1D-CGD-CBD	-2.01	116.62	123.08
3	Q	1084	CYC	CHA-C1A-NA	-2.01	126.04	128.83
3	B	1082	CYC	CMB-C2B-C1B	2.01	126.67	124.17
3	A	1084	CYC	O1D-CGD-CBD	-2.00	116.65	123.08

There are no chirality outliers.

All (297) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1084	CYC	NA-C4A-CHB-C1B
3	A	1084	CYC	C3A-C4A-CHB-C1B
3	A	1084	CYC	C2C-C3C-CAC-CBC
3	A	1084	CYC	C4C-C3C-CAC-CBC
3	B	1082	CYC	NA-C4A-CHB-C1B
3	B	1082	CYC	C3A-C4A-CHB-C1B
3	B	1082	CYC	ND-C1D-CHD-C4C
3	B	1082	CYC	C2D-C1D-CHD-C4C
3	B	1153	CYC	NA-C4A-CHB-C1B
3	B	1153	CYC	C3A-C4A-CHB-C1B
3	B	1153	CYC	C2C-C3C-CAC-CBC
3	B	1153	CYC	C4C-C3C-CAC-CBC
3	C	1084	CYC	NA-C4A-CHB-C1B
3	C	1084	CYC	C3A-C4A-CHB-C1B
3	C	1084	CYC	C2C-C3C-CAC-CBC
3	C	1084	CYC	C4C-C3C-CAC-CBC
3	D	1082	CYC	NA-C4A-CHB-C1B
3	D	1082	CYC	C3A-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	1082	CYC	C4C-C3C-CAC-CBC
3	D	1082	CYC	ND-C1D-CHD-C4C
3	D	1082	CYC	C2D-C1D-CHD-C4C
3	D	1153	CYC	NA-C4A-CHB-C1B
3	D	1153	CYC	C2C-C3C-CAC-CBC
3	D	1153	CYC	C4C-C3C-CAC-CBC
3	D	1153	CYC	ND-C1D-CHD-C4C
3	E	1084	CYC	NA-C4A-CHB-C1B
3	E	1084	CYC	C3A-C4A-CHB-C1B
3	E	1084	CYC	C2C-C3C-CAC-CBC
3	E	1084	CYC	C4C-C3C-CAC-CBC
3	F	1082	CYC	NA-C4A-CHB-C1B
3	F	1082	CYC	C3A-C4A-CHB-C1B
3	F	1082	CYC	ND-C1D-CHD-C4C
3	F	1153	CYC	NA-C4A-CHB-C1B
3	F	1153	CYC	C3A-C4A-CHB-C1B
3	F	1153	CYC	C2C-C3C-CAC-CBC
3	F	1153	CYC	C4C-C3C-CAC-CBC
3	G	1084	CYC	NA-C4A-CHB-C1B
3	G	1084	CYC	C3A-C4A-CHB-C1B
3	G	1084	CYC	C2C-C3C-CAC-CBC
3	G	1084	CYC	C4C-C3C-CAC-CBC
3	H	1082	CYC	NA-C4A-CHB-C1B
3	H	1082	CYC	C3A-C4A-CHB-C1B
3	H	1082	CYC	C4B-C3B-CAB-CBB
3	H	1082	CYC	ND-C1D-CHD-C4C
3	H	1082	CYC	C2D-C1D-CHD-C4C
3	H	1153	CYC	NA-C4A-CHB-C1B
3	H	1153	CYC	C3A-C4A-CHB-C1B
3	H	1153	CYC	C2C-C3C-CAC-CBC
3	H	1153	CYC	C4C-C3C-CAC-CBC
3	I	1084	CYC	NA-C4A-CHB-C1B
3	I	1084	CYC	C3A-C4A-CHB-C1B
3	I	1084	CYC	C4B-C3B-CAB-CBB
3	I	1084	CYC	C2C-C3C-CAC-CBC
3	I	1084	CYC	C4C-C3C-CAC-CBC
3	J	1082	CYC	NA-C4A-CHB-C1B
3	J	1082	CYC	C3A-C4A-CHB-C1B
3	J	1082	CYC	ND-C1D-CHD-C4C
3	J	1082	CYC	C2D-C1D-CHD-C4C
3	J	1153	CYC	NA-C4A-CHB-C1B
3	J	1153	CYC	C3A-C4A-CHB-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	J	1153	CYC	C2C-C3C-CAC-CBC
3	J	1153	CYC	C4C-C3C-CAC-CBC
3	K	1084	CYC	NA-C4A-CHB-C1B
3	K	1084	CYC	C3A-C4A-CHB-C1B
3	K	1084	CYC	C2C-C3C-CAC-CBC
3	K	1084	CYC	C4C-C3C-CAC-CBC
3	L	1082	CYC	NA-C4A-CHB-C1B
3	L	1082	CYC	C3A-C4A-CHB-C1B
3	L	1082	CYC	ND-C1D-CHD-C4C
3	L	1082	CYC	C2D-C1D-CHD-C4C
3	L	1153	CYC	NA-C4A-CHB-C1B
3	L	1153	CYC	C2C-C3C-CAC-CBC
3	L	1153	CYC	C4C-C3C-CAC-CBC
3	M	1084	CYC	NA-C4A-CHB-C1B
3	M	1084	CYC	C3A-C4A-CHB-C1B
3	M	1084	CYC	C4B-C3B-CAB-CBB
3	M	1084	CYC	C2C-C3C-CAC-CBC
3	M	1084	CYC	C4C-C3C-CAC-CBC
3	N	1082	CYC	NA-C4A-CHB-C1B
3	N	1082	CYC	C3A-C4A-CHB-C1B
3	N	1082	CYC	C4C-C3C-CAC-CBC
3	N	1082	CYC	ND-C1D-CHD-C4C
3	N	1082	CYC	C2D-C1D-CHD-C4C
3	N	1153	CYC	NA-C4A-CHB-C1B
3	N	1153	CYC	C3A-C4A-CHB-C1B
3	N	1153	CYC	C2C-C3C-CAC-CBC
3	N	1153	CYC	C4C-C3C-CAC-CBC
3	O	1084	CYC	NA-C4A-CHB-C1B
3	O	1084	CYC	C3A-C4A-CHB-C1B
3	O	1084	CYC	C2C-C3C-CAC-CBC
3	O	1084	CYC	C4C-C3C-CAC-CBC
3	P	1082	CYC	NA-C4A-CHB-C1B
3	P	1082	CYC	C3A-C4A-CHB-C1B
3	P	1082	CYC	ND-C1D-CHD-C4C
3	P	1082	CYC	C2D-C1D-CHD-C4C
3	P	1153	CYC	NA-C4A-CHB-C1B
3	P	1153	CYC	C3A-C4A-CHB-C1B
3	P	1153	CYC	C2C-C3C-CAC-CBC
3	P	1153	CYC	C4C-C3C-CAC-CBC
3	Q	1084	CYC	NA-C4A-CHB-C1B
3	Q	1084	CYC	C3A-C4A-CHB-C1B
3	Q	1084	CYC	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	Q	1084	CYC	C4C-C3C-CAC-CBC
3	R	1082	CYC	NA-C4A-CHB-C1B
3	R	1082	CYC	C3A-C4A-CHB-C1B
3	R	1082	CYC	ND-C1D-CHD-C4C
3	R	1082	CYC	C2D-C1D-CHD-C4C
3	R	1153	CYC	NA-C4A-CHB-C1B
3	R	1153	CYC	C3A-C4A-CHB-C1B
3	R	1153	CYC	C4B-C3B-CAB-CBB
3	R	1153	CYC	C2C-C3C-CAC-CBC
3	R	1153	CYC	C4C-C3C-CAC-CBC
3	S	1084	CYC	NA-C4A-CHB-C1B
3	S	1084	CYC	C3A-C4A-CHB-C1B
3	S	1084	CYC	C2C-C3C-CAC-CBC
3	S	1084	CYC	C4C-C3C-CAC-CBC
3	T	1082	CYC	NA-C4A-CHB-C1B
3	T	1082	CYC	C3A-C4A-CHB-C1B
3	T	1082	CYC	C2B-C3B-CAB-CBB
3	T	1082	CYC	C4C-C3C-CAC-CBC
3	T	1082	CYC	ND-C1D-CHD-C4C
3	T	1153	CYC	NA-C4A-CHB-C1B
3	T	1153	CYC	C3A-C4A-CHB-C1B
3	T	1153	CYC	C2C-C3C-CAC-CBC
3	T	1153	CYC	C4C-C3C-CAC-CBC
3	U	1084	CYC	NA-C4A-CHB-C1B
3	U	1084	CYC	C3A-C4A-CHB-C1B
3	U	1084	CYC	C2C-C3C-CAC-CBC
3	U	1084	CYC	C4C-C3C-CAC-CBC
3	V	1082	CYC	NA-C4A-CHB-C1B
3	V	1082	CYC	C3A-C4A-CHB-C1B
3	V	1082	CYC	ND-C1D-CHD-C4C
3	V	1082	CYC	C2D-C1D-CHD-C4C
3	V	1153	CYC	NA-C4A-CHB-C1B
3	V	1153	CYC	C3A-C4A-CHB-C1B
3	V	1153	CYC	C2C-C3C-CAC-CBC
3	W	1084	CYC	NA-C4A-CHB-C1B
3	W	1084	CYC	C3A-C4A-CHB-C1B
3	W	1084	CYC	C2C-C3C-CAC-CBC
3	W	1084	CYC	C4C-C3C-CAC-CBC
3	X	1082	CYC	NA-C4A-CHB-C1B
3	X	1082	CYC	C3A-C4A-CHB-C1B
3	X	1082	CYC	ND-C1D-CHD-C4C
3	X	1082	CYC	C2D-C1D-CHD-C4C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	X	1153	CYC	NA-C4A-CHB-C1B
3	X	1153	CYC	C2C-C3C-CAC-CBC
3	H	1082	CYC	C2B-C3B-CAB-CBB
3	R	1153	CYC	C2B-C3B-CAB-CBB
3	I	1084	CYC	C2B-C3B-CAB-CBB
3	M	1084	CYC	C2B-C3B-CAB-CBB
3	N	1082	CYC	C2B-C3B-CAB-CBB
3	D	1153	CYC	C3A-C4A-CHB-C1B
3	L	1153	CYC	C3A-C4A-CHB-C1B
3	X	1153	CYC	C3A-C4A-CHB-C1B
3	K	1084	CYC	C2B-C3B-CAB-CBB
3	J	1082	CYC	C2B-C3B-CAB-CBB
3	J	1153	CYC	C2B-C3B-CAB-CBB
3	D	1153	CYC	C3D-CAD-CBD-CGD
3	T	1082	CYC	C4B-C3B-CAB-CBB
3	E	1084	CYC	C2B-C3B-CAB-CBB
3	L	1082	CYC	C2B-C3B-CAB-CBB
3	U	1084	CYC	C2B-C3B-CAB-CBB
3	W	1084	CYC	C2B-C3B-CAB-CBB
3	F	1153	CYC	C3D-CAD-CBD-CGD
3	A	1084	CYC	C2B-C3B-CAB-CBB
3	X	1082	CYC	C2A-CAA-CBA-CGA
3	G	1084	CYC	C2B-C3B-CAB-CBB
3	O	1084	CYC	C2B-C3B-CAB-CBB
3	F	1082	CYC	C2B-C3B-CAB-CBB
3	T	1082	CYC	C2C-C3C-CAC-CBC
3	K	1084	CYC	C4B-C3B-CAB-CBB
3	N	1082	CYC	C4B-C3B-CAB-CBB
3	Q	1084	CYC	C2B-C3B-CAB-CBB
3	V	1082	CYC	C4C-C3C-CAC-CBC
3	V	1153	CYC	C4C-C3C-CAC-CBC
3	X	1153	CYC	C4C-C3C-CAC-CBC
3	R	1082	CYC	C2B-C3B-CAB-CBB
3	B	1153	CYC	C2B-C3B-CAB-CBB
3	P	1082	CYC	C2B-C3B-CAB-CBB
3	J	1082	CYC	C4B-C3B-CAB-CBB
3	J	1153	CYC	C4B-C3B-CAB-CBB
3	C	1084	CYC	C2B-C3B-CAB-CBB
3	V	1082	CYC	C2B-C3B-CAB-CBB
3	C	1084	CYC	NC-C4C-CHD-C1D
3	I	1084	CYC	NC-C4C-CHD-C1D
3	K	1084	CYC	NC-C4C-CHD-C1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	M	1084	CYC	NC-C4C-CHD-C1D
3	O	1084	CYC	NC-C4C-CHD-C1D
3	U	1084	CYC	NC-C4C-CHD-C1D
3	E	1084	CYC	C4B-C3B-CAB-CBB
3	X	1082	CYC	CAA-CBA-CGA-O1A
3	T	1082	CYC	CAA-CBA-CGA-O1A
3	K	1084	CYC	CAA-CBA-CGA-O2A
3	U	1084	CYC	CAA-CBA-CGA-O2A
3	A	1084	CYC	CAA-CBA-CGA-O1A
3	C	1084	CYC	CAA-CBA-CGA-O1A
3	E	1084	CYC	CAA-CBA-CGA-O1A
3	G	1084	CYC	CAA-CBA-CGA-O1A
3	I	1084	CYC	CAA-CBA-CGA-O1A
3	W	1084	CYC	CAA-CBA-CGA-O1A
3	K	1084	CYC	CAA-CBA-CGA-O1A
3	O	1084	CYC	CAA-CBA-CGA-O2A
3	V	1082	CYC	CAA-CBA-CGA-O1A
3	I	1084	CYC	CAA-CBA-CGA-O2A
3	O	1084	CYC	CAA-CBA-CGA-O1A
3	M	1084	CYC	CAA-CBA-CGA-O1A
3	M	1084	CYC	CAA-CBA-CGA-O2A
3	B	1082	CYC	C2B-C3B-CAB-CBB
3	A	1084	CYC	CAA-CBA-CGA-O2A
3	L	1153	CYC	CAA-CBA-CGA-O2A
3	L	1082	CYC	C4B-C3B-CAB-CBB
3	E	1084	CYC	CAA-CBA-CGA-O2A
3	P	1153	CYC	CAA-CBA-CGA-O2A
3	T	1082	CYC	CAA-CBA-CGA-O2A
3	Q	1084	CYC	CAA-CBA-CGA-O1A
3	R	1082	CYC	CAA-CBA-CGA-O1A
3	C	1084	CYC	CAA-CBA-CGA-O2A
3	G	1084	CYC	CAA-CBA-CGA-O2A
3	S	1084	CYC	CAA-CBA-CGA-O1A
3	V	1082	CYC	CAA-CBA-CGA-O2A
3	W	1084	CYC	CAA-CBA-CGA-O2A
3	X	1082	CYC	CAA-CBA-CGA-O2A
3	D	1082	CYC	C2B-C3B-CAB-CBB
3	P	1153	CYC	CAA-CBA-CGA-O1A
3	P	1082	CYC	CAA-CBA-CGA-O1A
3	Q	1084	CYC	CAA-CBA-CGA-O2A
3	S	1084	CYC	CAA-CBA-CGA-O2A
3	L	1153	CYC	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	R	1082	CYC	CAA-CBA-CGA-O2A
3	R	1153	CYC	CAA-CBA-CGA-O2A
3	A	1084	CYC	NC-C4C-CHD-C1D
3	E	1084	CYC	NC-C4C-CHD-C1D
3	W	1084	CYC	NC-C4C-CHD-C1D
3	P	1082	CYC	CAA-CBA-CGA-O2A
3	D	1082	CYC	C1A-C2A-CAA-CBA
3	U	1084	CYC	CAA-CBA-CGA-O1A
3	D	1153	CYC	CAA-CBA-CGA-O2A
3	H	1082	CYC	CAA-CBA-CGA-O1A
3	J	1153	CYC	CAD-CBD-CGD-O1D
3	U	1084	CYC	C4B-C3B-CAB-CBB
3	W	1084	CYC	C4B-C3B-CAB-CBB
3	F	1153	CYC	CAA-CBA-CGA-O2A
3	J	1153	CYC	CAA-CBA-CGA-O2A
3	D	1082	CYC	C3A-C2A-CAA-CBA
3	H	1153	CYC	CAA-CBA-CGA-O2A
3	K	1084	CYC	CAD-CBD-CGD-O2D
3	R	1153	CYC	CAA-CBA-CGA-O1A
3	P	1153	CYC	CAD-CBD-CGD-O1D
3	K	1084	CYC	CAD-CBD-CGD-O1D
3	J	1082	CYC	CAA-CBA-CGA-O1A
3	J	1153	CYC	CAA-CBA-CGA-O1A
3	N	1082	CYC	CAA-CBA-CGA-O1A
3	L	1153	CYC	C3D-CAD-CBD-CGD
3	B	1153	CYC	CAA-CBA-CGA-O2A
3	D	1153	CYC	CAA-CBA-CGA-O1A
3	H	1153	CYC	CAD-CBD-CGD-O2D
3	N	1153	CYC	CAA-CBA-CGA-O2A
3	O	1084	CYC	CAD-CBD-CGD-O2D
3	O	1084	CYC	CAD-CBD-CGD-O1D
3	B	1082	CYC	CAA-CBA-CGA-O2A
3	F	1153	CYC	CAA-CBA-CGA-O1A
3	T	1153	CYC	CAA-CBA-CGA-O2A
3	X	1153	CYC	CAA-CBA-CGA-O2A
3	B	1082	CYC	CAA-CBA-CGA-O1A
3	T	1153	CYC	CAA-CBA-CGA-O1A
3	V	1153	CYC	CAA-CBA-CGA-O2A
3	H	1153	CYC	CAA-CBA-CGA-O1A
3	H	1153	CYC	CAD-CBD-CGD-O1D
3	L	1082	CYC	CAA-CBA-CGA-O1A
3	R	1153	CYC	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	X	1153	CYC	CAA-CBA-CGA-O1A
3	H	1082	CYC	CAD-CBD-CGD-O2D
3	L	1082	CYC	CAA-CBA-CGA-O2A
3	N	1153	CYC	CAA-CBA-CGA-O1A
3	R	1153	CYC	CAD-CBD-CGD-O2D
3	B	1153	CYC	CAA-CBA-CGA-O1A
3	V	1153	CYC	CAA-CBA-CGA-O1A
3	F	1082	CYC	CAD-CBD-CGD-O1D
3	H	1082	CYC	CAA-CBA-CGA-O2A
3	N	1082	CYC	CAA-CBA-CGA-O2A
3	B	1082	CYC	CAD-CBD-CGD-O1D
3	J	1082	CYC	CAA-CBA-CGA-O2A
3	T	1153	CYC	CAD-CBD-CGD-O1D
3	J	1153	CYC	CAD-CBD-CGD-O2D
3	P	1153	CYC	CAD-CBD-CGD-O2D
3	F	1082	CYC	CAD-CBD-CGD-O2D
3	I	1084	CYC	CAD-CBD-CGD-O2D
3	H	1082	CYC	CAD-CBD-CGD-O1D
3	T	1153	CYC	CAD-CBD-CGD-O2D
3	Q	1084	CYC	CAD-CBD-CGD-O2D
3	A	1084	CYC	CAD-CBD-CGD-O2D
3	E	1084	CYC	CAD-CBD-CGD-O2D
3	I	1084	CYC	CAD-CBD-CGD-O1D
3	B	1082	CYC	CAD-CBD-CGD-O2D
3	M	1084	CYC	CAD-CBD-CGD-O2D
3	W	1084	CYC	CAD-CBD-CGD-O2D
3	A	1084	CYC	CAD-CBD-CGD-O1D

There are no ring outliers.

33 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	1084	CYC	1	0
3	M	1084	CYC	3	0
3	Q	1084	CYC	4	0
3	R	1153	CYC	4	0
3	X	1082	CYC	1	0
3	X	1153	CYC	4	0
3	H	1082	CYC	3	0
3	F	1082	CYC	5	0
3	B	1082	CYC	3	0
3	V	1153	CYC	4	0

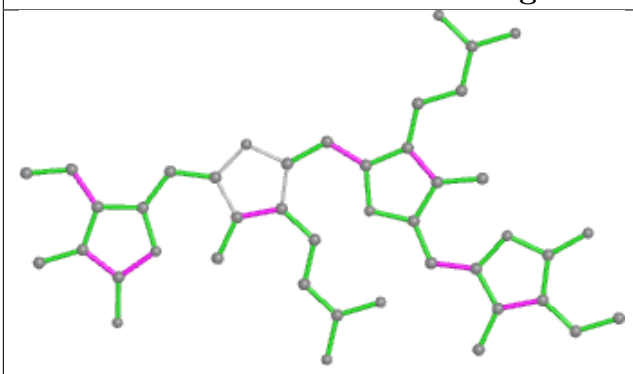
Continued on next page...

Continued from previous page...

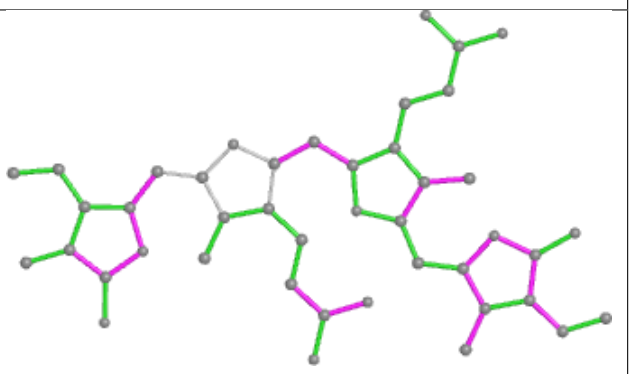
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1153	CYC	1	0
3	S	1084	CYC	2	0
3	A	1084	CYC	2	0
3	L	1153	CYC	3	0
3	O	1084	CYC	3	0
3	D	1153	CYC	4	0
3	G	1084	CYC	1	0
3	C	1084	CYC	2	0
3	E	1084	CYC	2	0
3	F	1153	CYC	3	0
3	P	1153	CYC	5	0
3	J	1082	CYC	3	0
3	H	1153	CYC	3	0
3	W	1084	CYC	3	0
3	T	1153	CYC	6	0
3	K	1084	CYC	2	0
3	R	1082	CYC	2	0
3	N	1082	CYC	4	0
3	D	1082	CYC	2	0
3	U	1084	CYC	1	0
3	L	1082	CYC	2	0
3	T	1082	CYC	4	0
3	V	1082	CYC	1	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

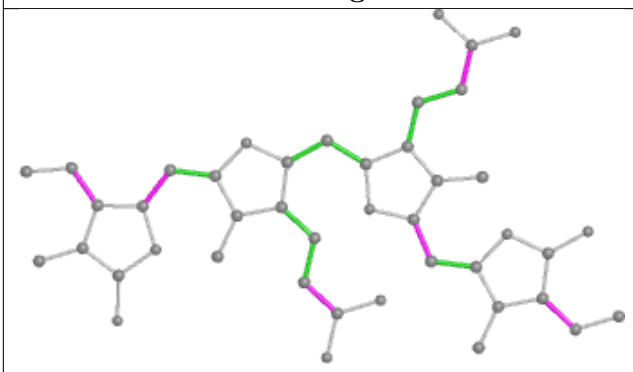
Ligand CYC I 1084



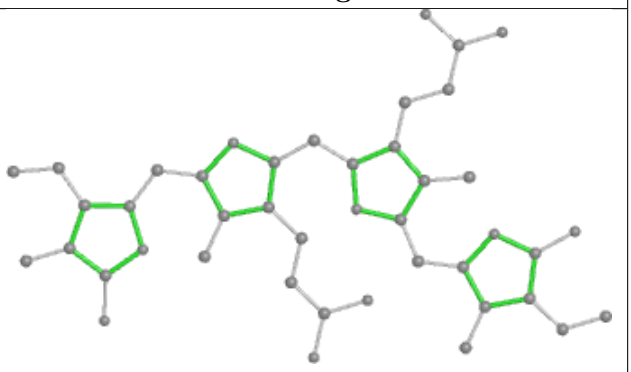
Bond lengths



Bond angles

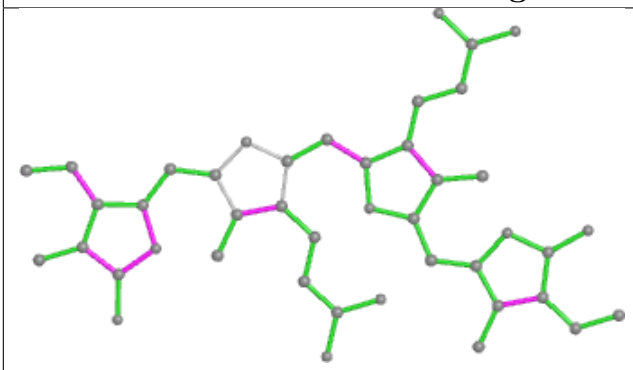


Torsions

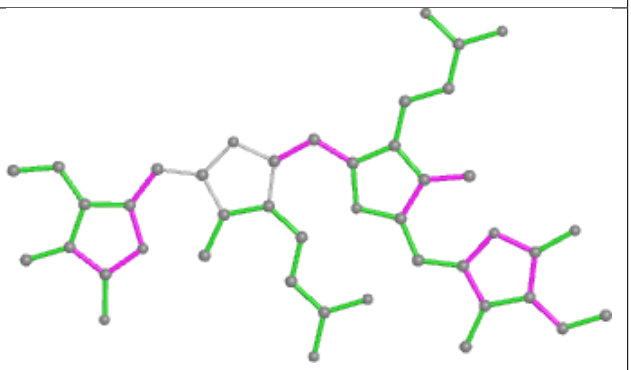


Rings

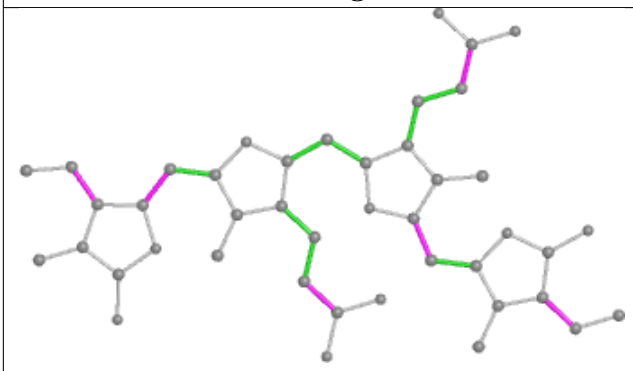
Ligand CYC M 1084



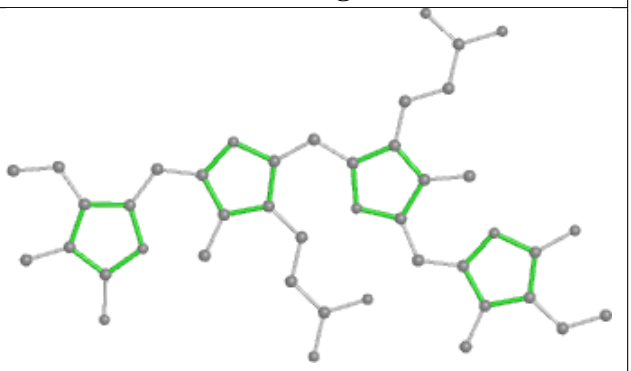
Bond lengths



Bond angles

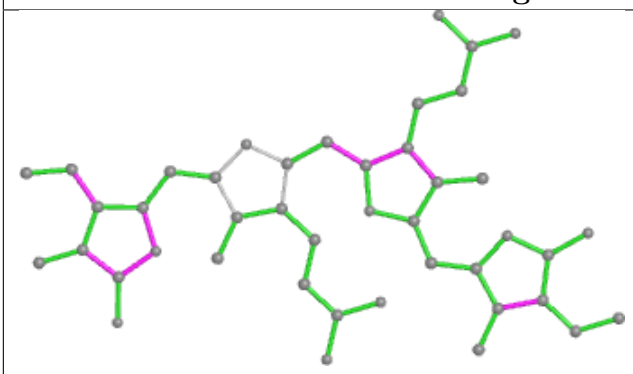


Torsions

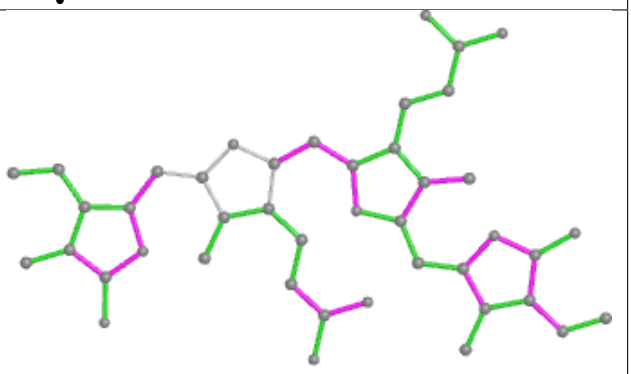


Rings

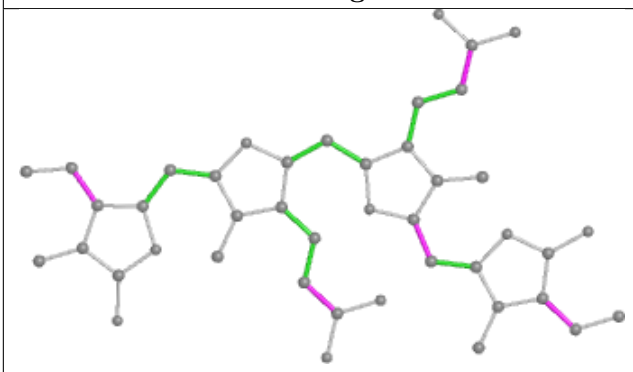
Ligand CYC Q 1084



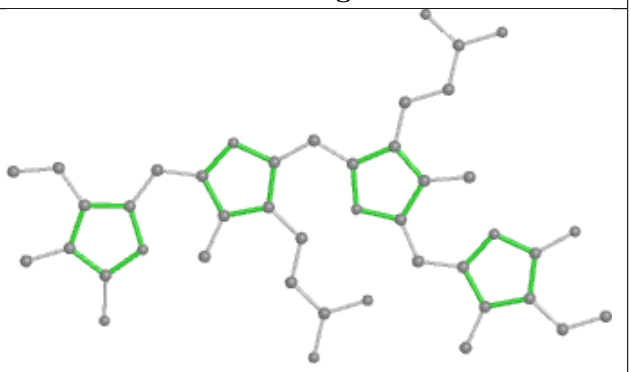
Bond lengths



Bond angles

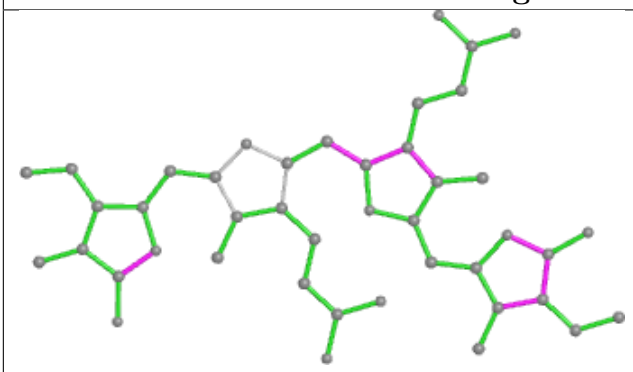


Torsions

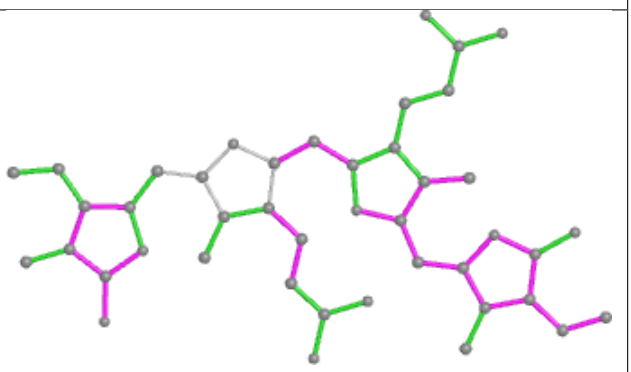


Rings

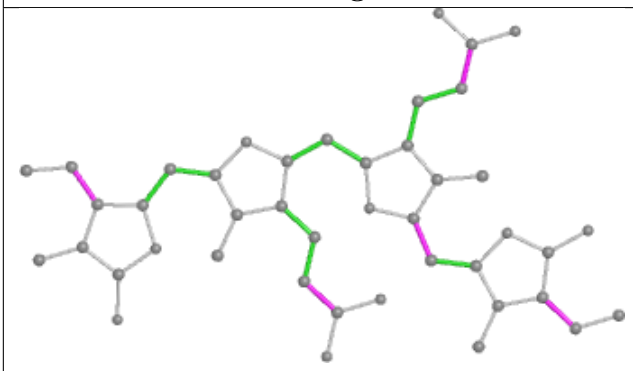
Ligand CYC R 1153



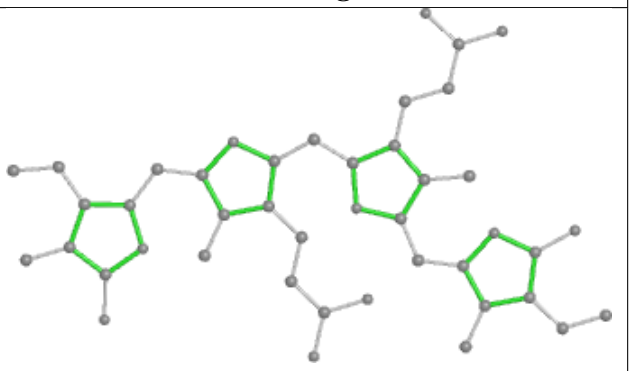
Bond lengths



Bond angles

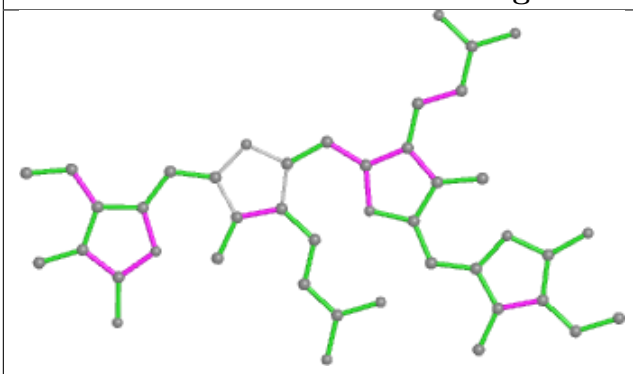


Torsions

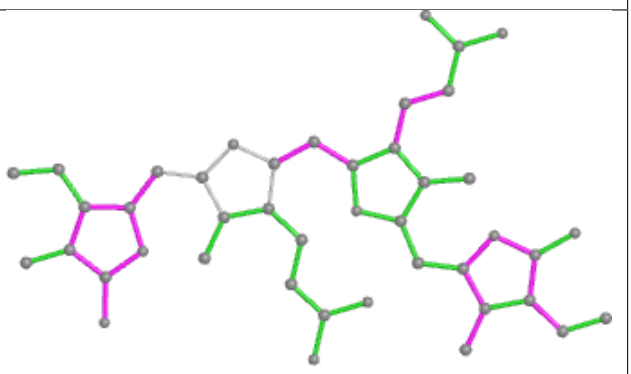


Rings

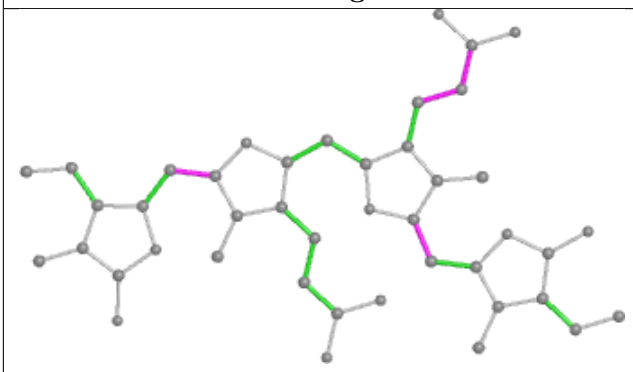
Ligand CYC X 1082



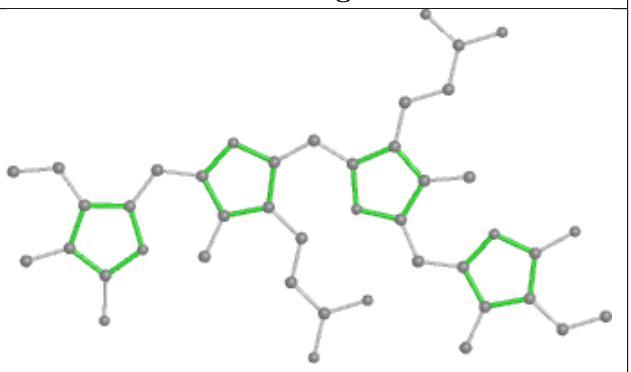
Bond lengths



Bond angles

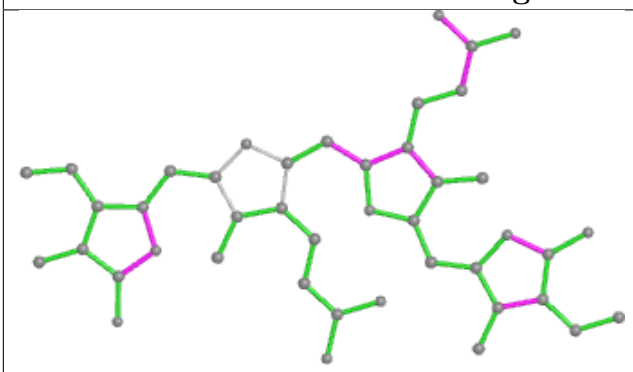


Torsions

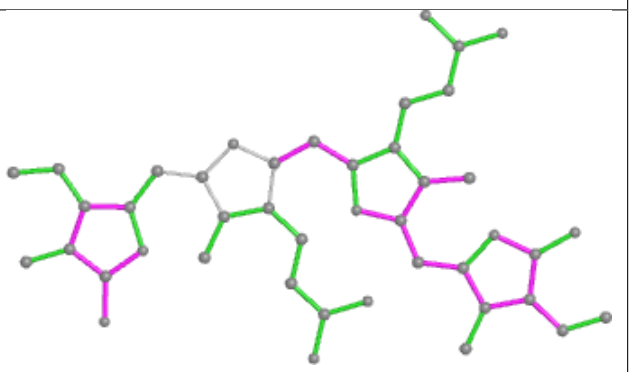


Rings

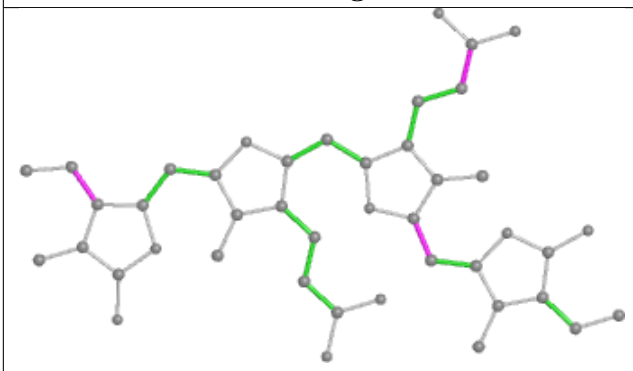
Ligand CYC X 1153



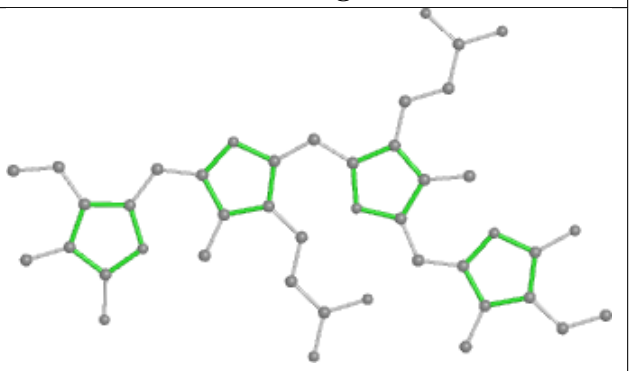
Bond lengths



Bond angles

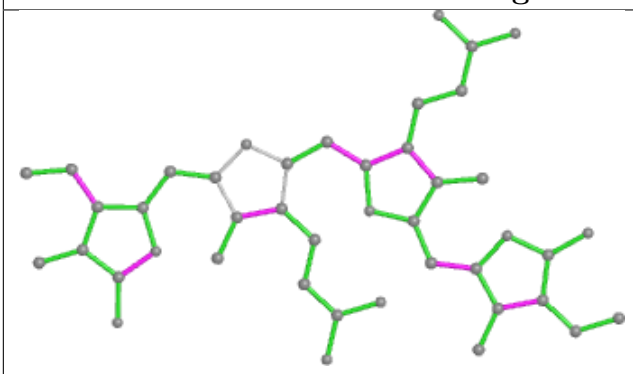


Torsions

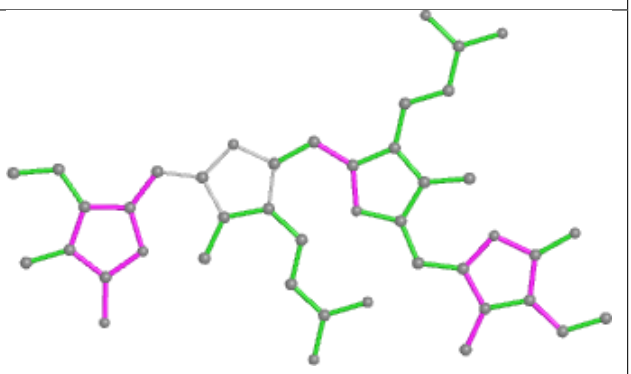


Rings

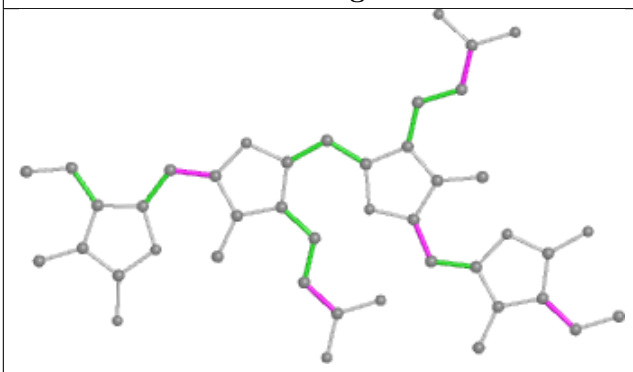
Ligand CYC H 1082



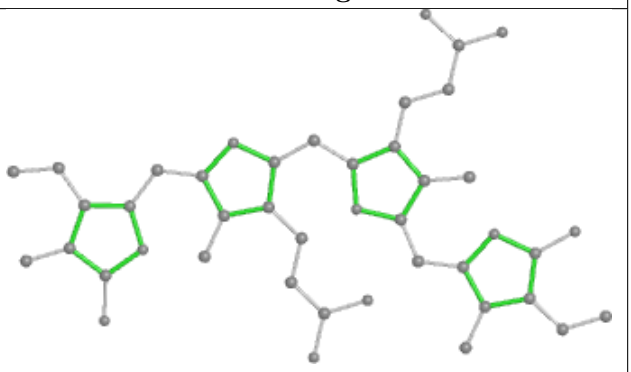
Bond lengths



Bond angles

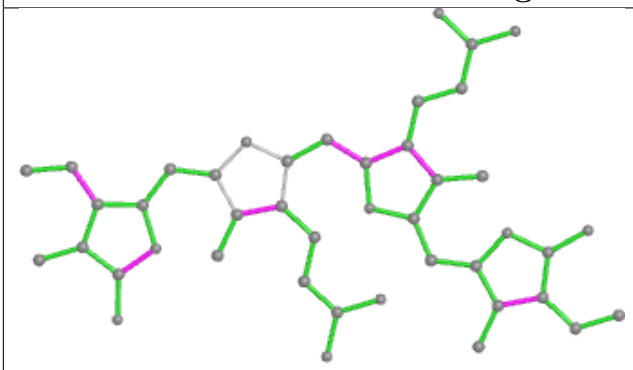


Torsions

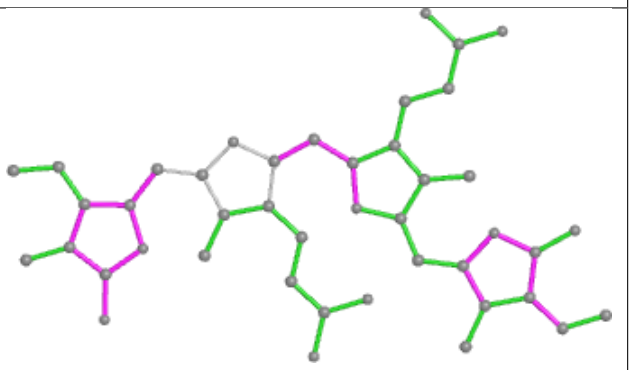


Rings

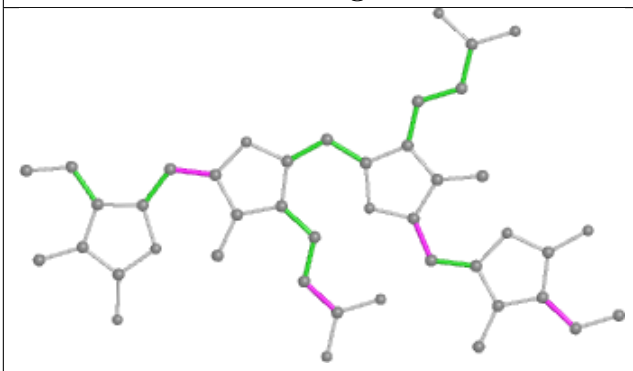
Ligand CYC F 1082



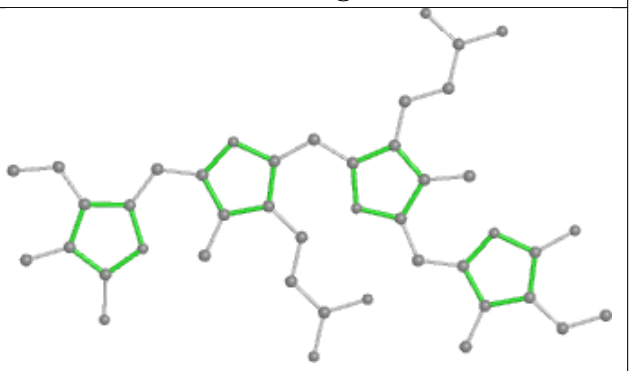
Bond lengths



Bond angles

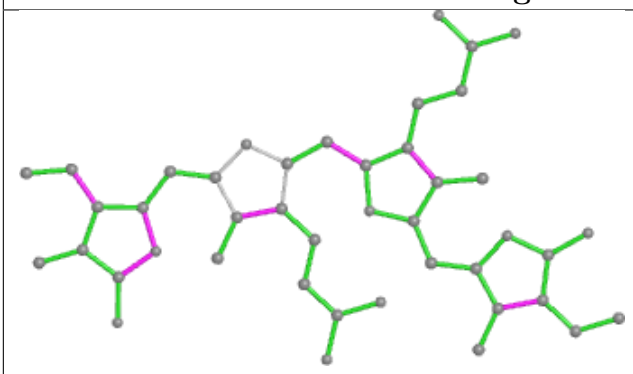


Torsions

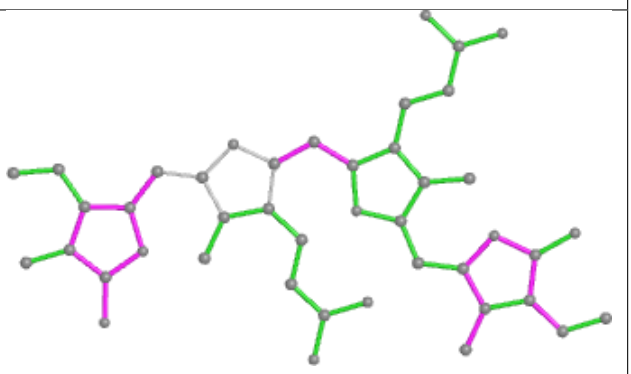


Rings

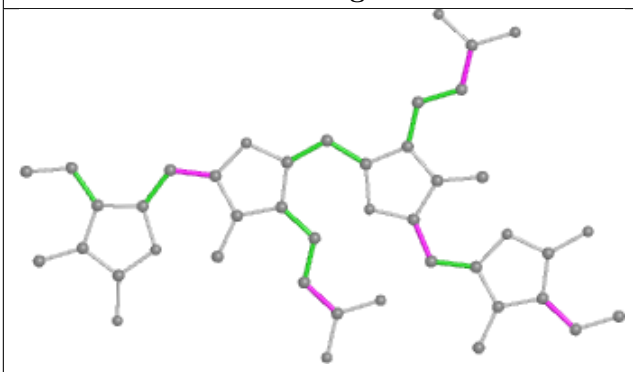
Ligand CYC B 1082



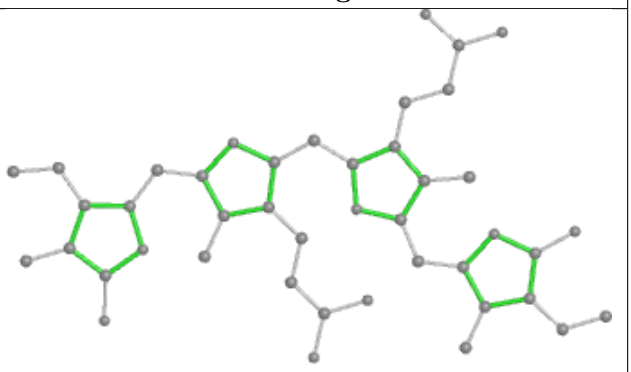
Bond lengths



Bond angles

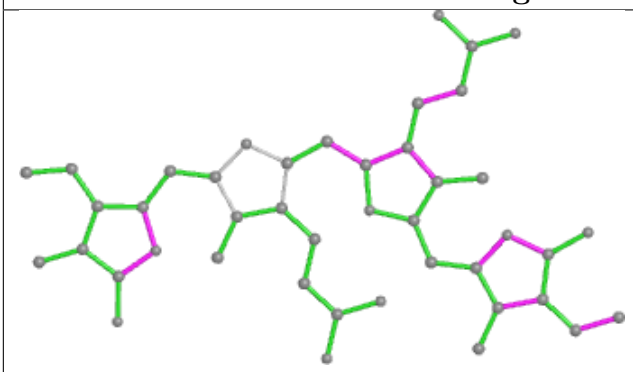


Torsions

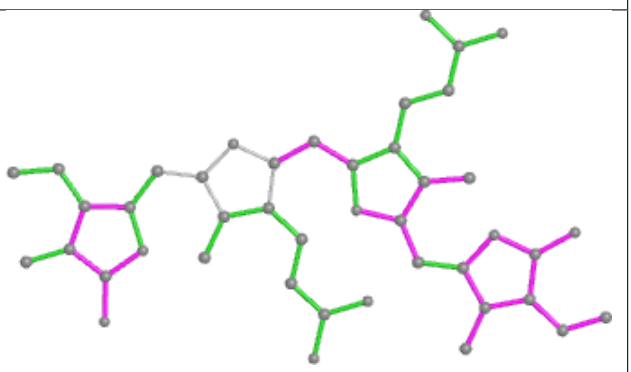


Rings

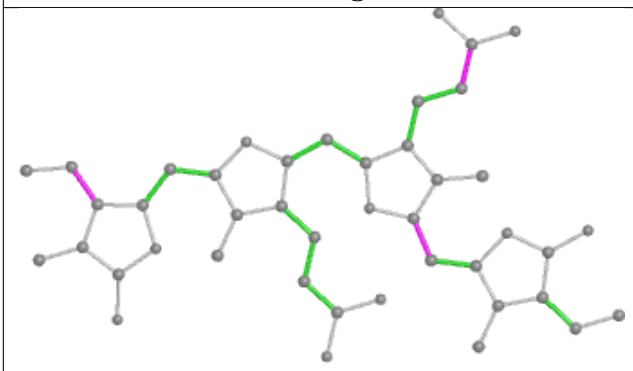
Ligand CYC V 1153



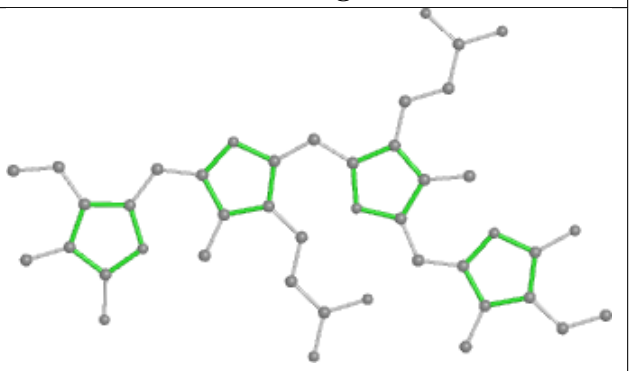
Bond lengths



Bond angles

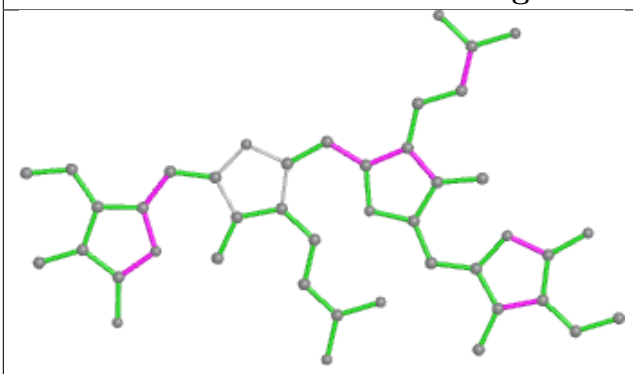


Torsions

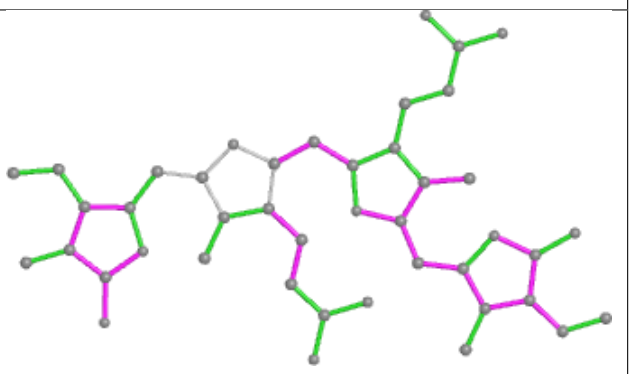


Rings

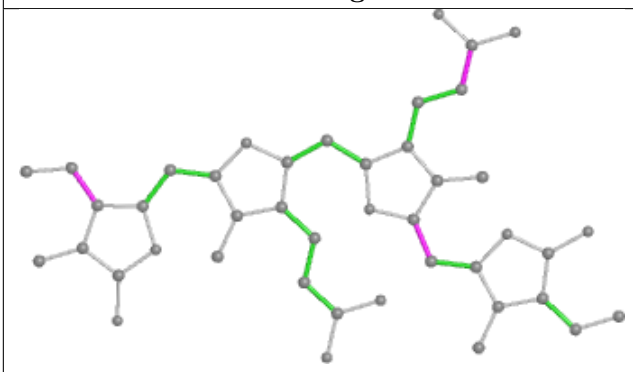
Ligand CYC N 1153



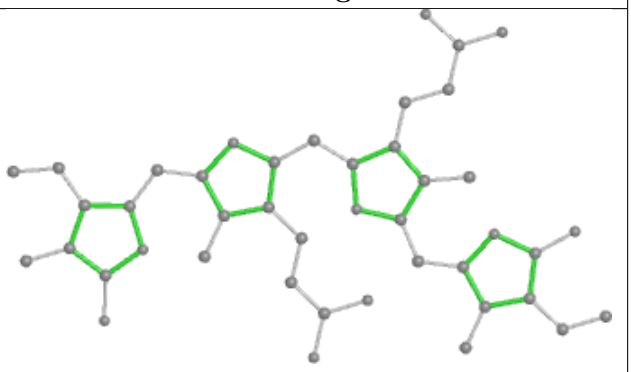
Bond lengths



Bond angles

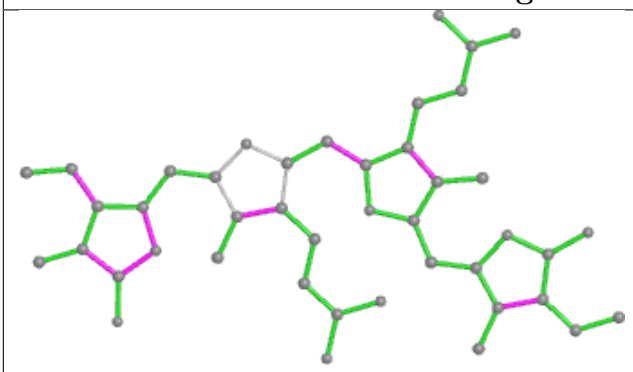


Torsions

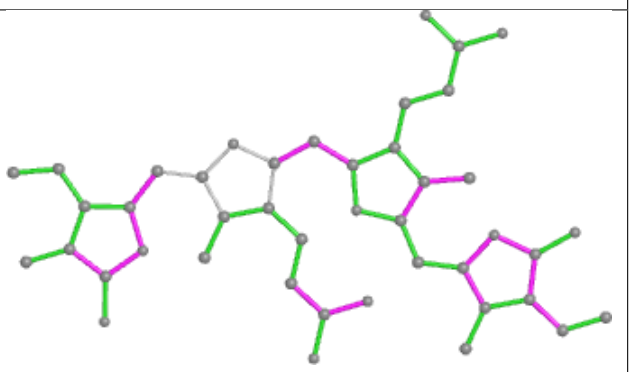


Rings

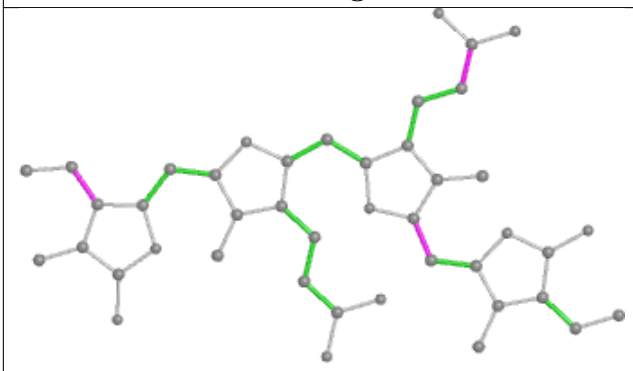
Ligand CYC S 1084



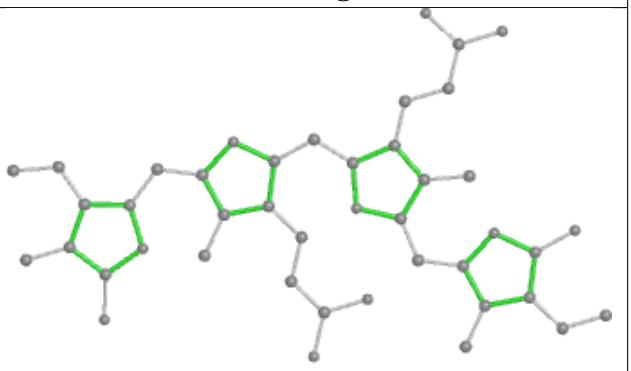
Bond lengths



Bond angles

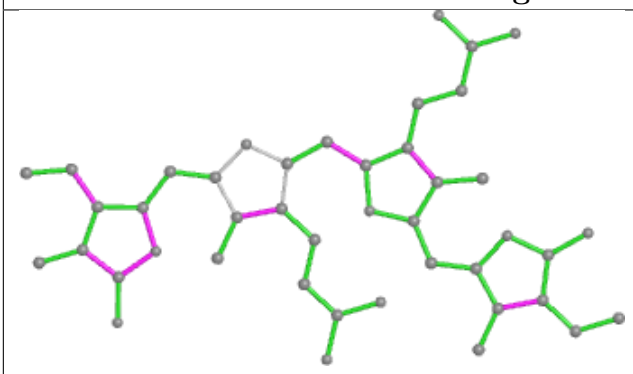


Torsions

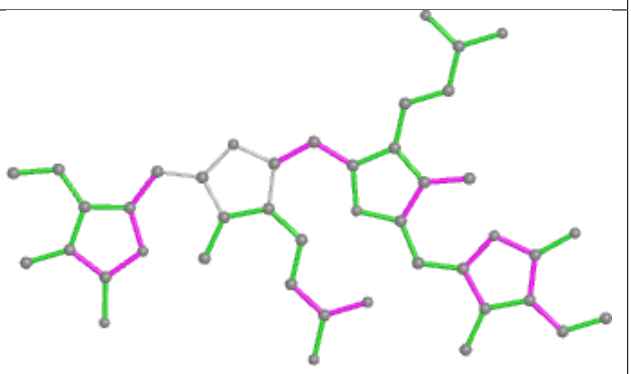


Rings

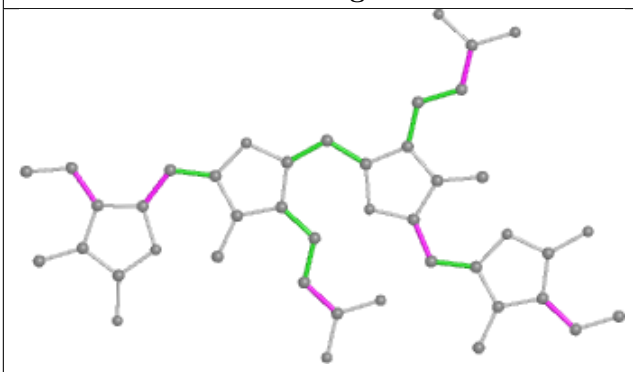
Ligand CYC A 1084



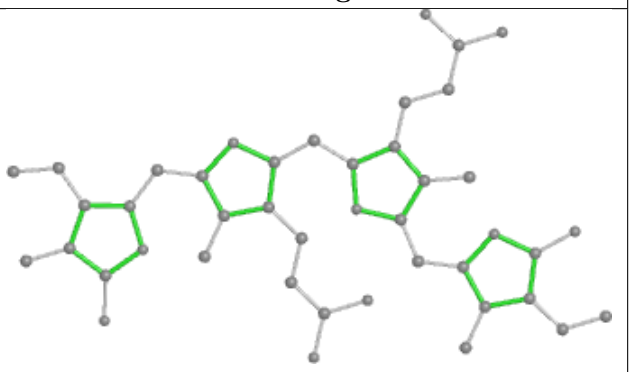
Bond lengths



Bond angles

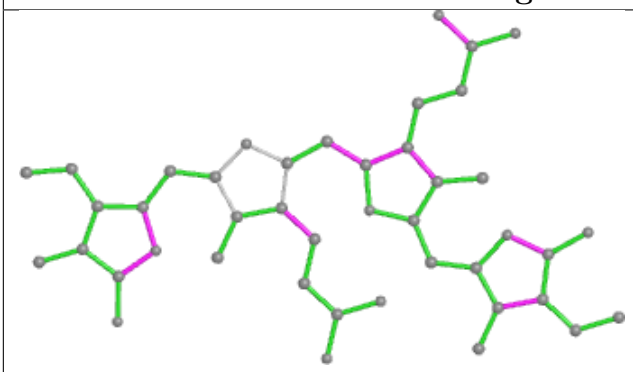


Torsions

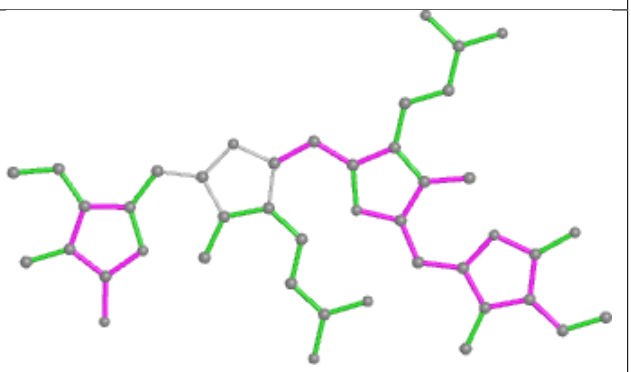


Rings

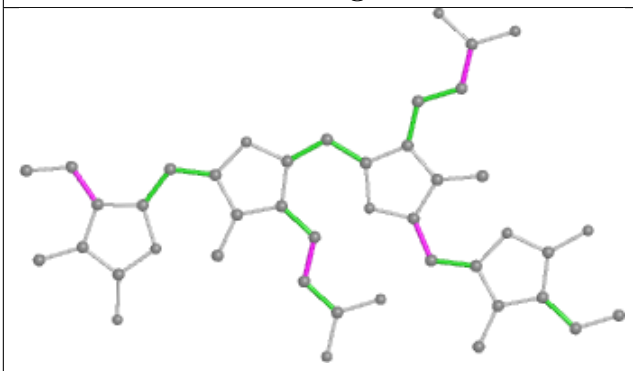
Ligand CYC L 1153



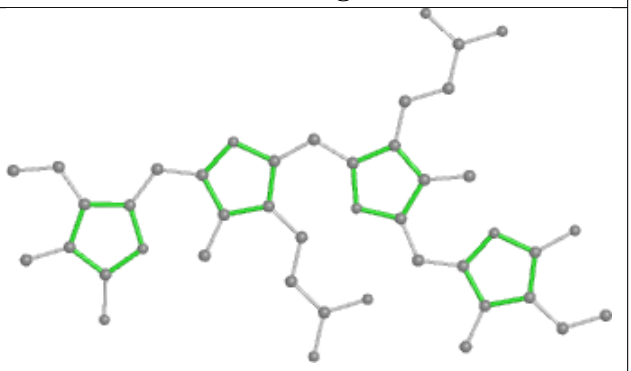
Bond lengths



Bond angles

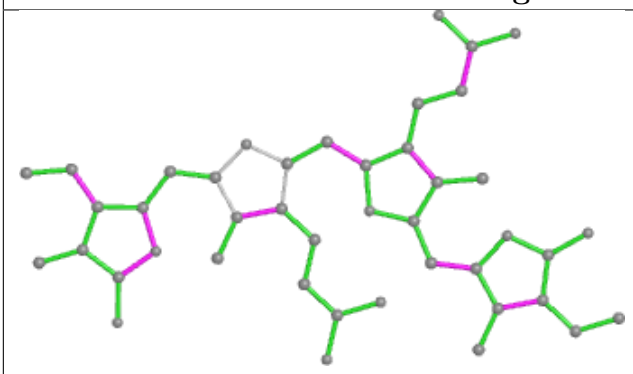


Torsions

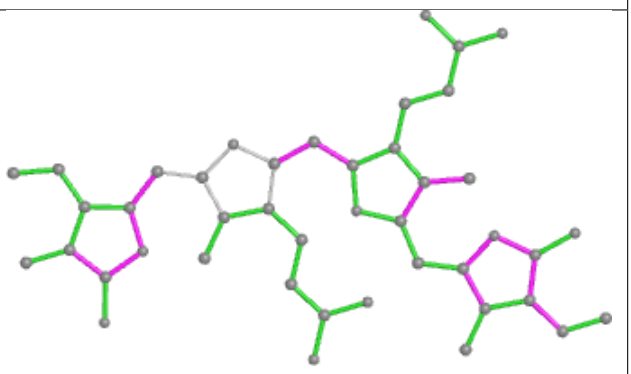


Rings

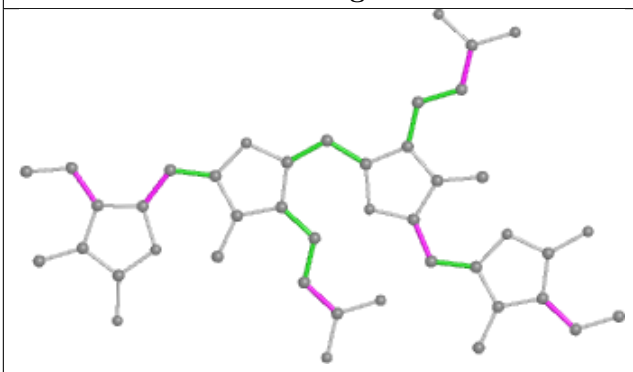
Ligand CYC O 1084



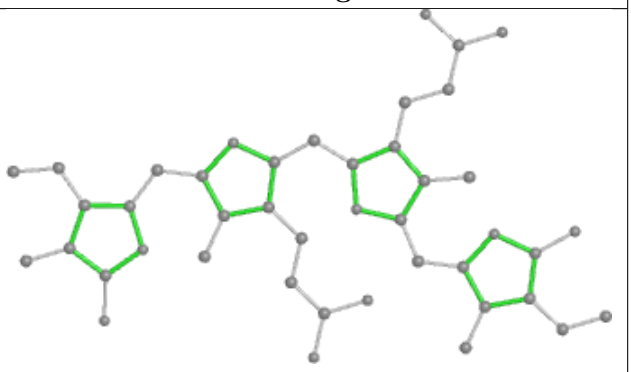
Bond lengths



Bond angles

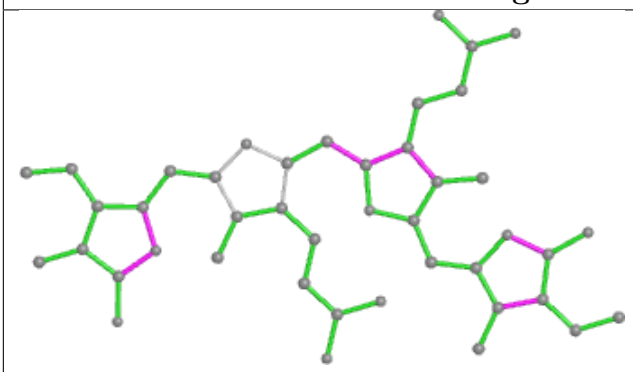


Torsions

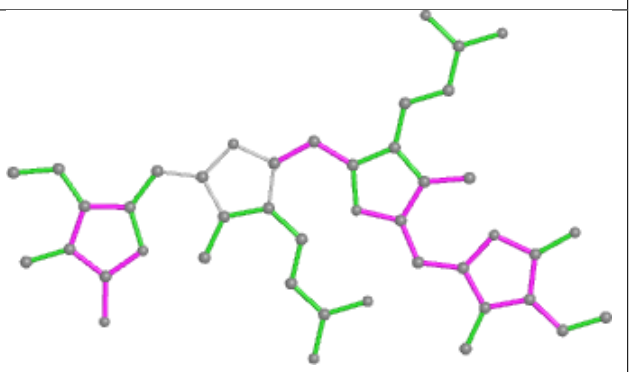


Rings

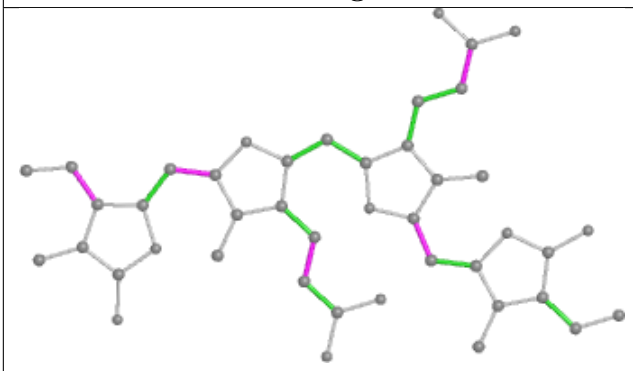
Ligand CYC D 1153



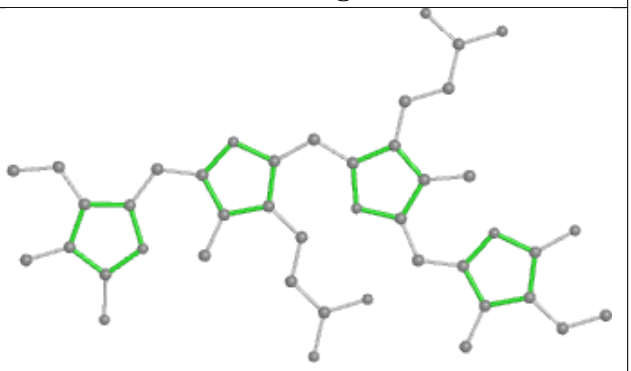
Bond lengths



Bond angles

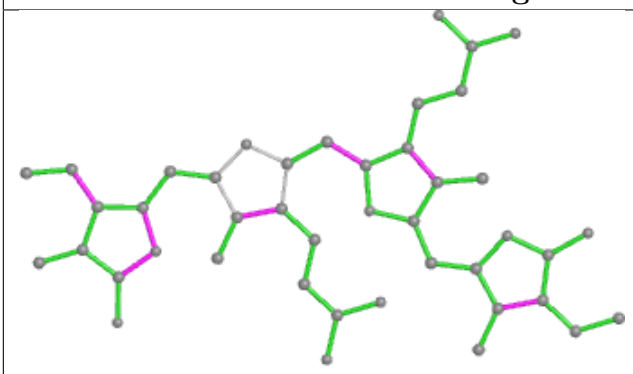


Torsions

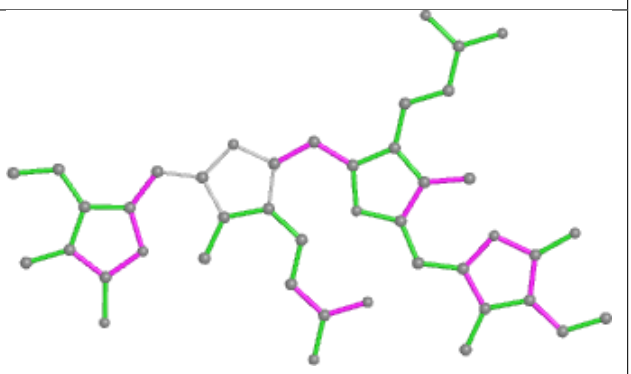


Rings

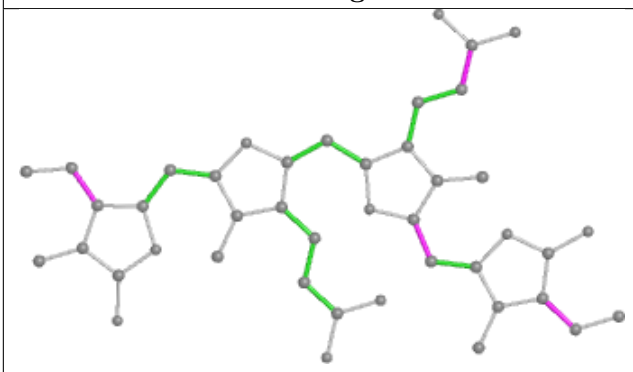
Ligand CYC G 1084



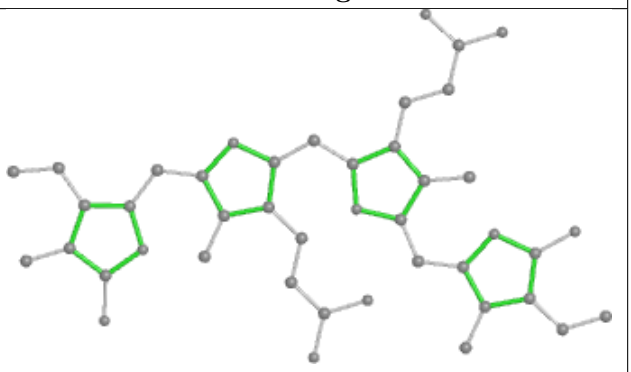
Bond lengths



Bond angles

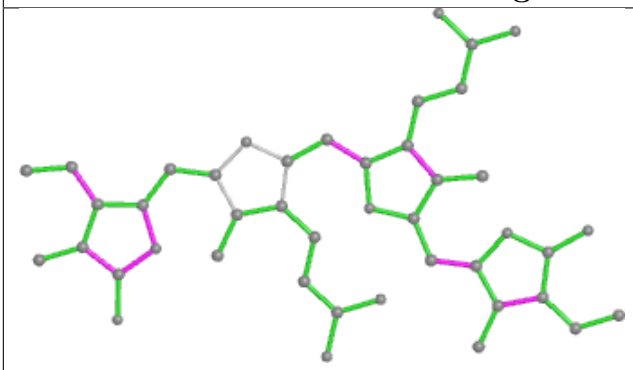


Torsions

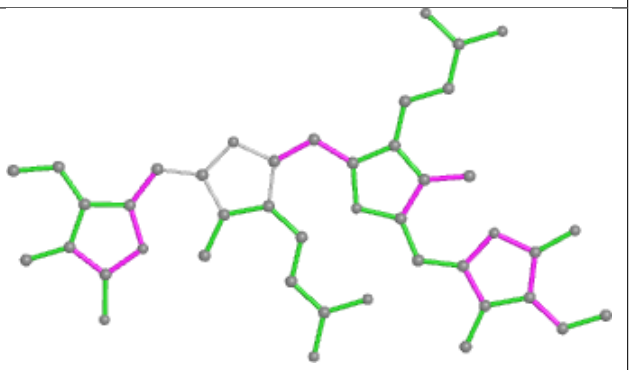


Rings

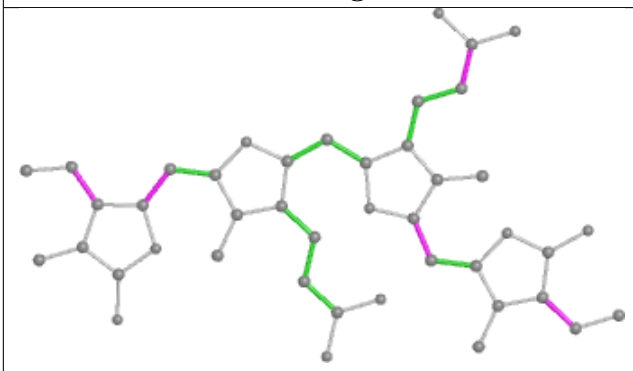
Ligand CYC C 1084



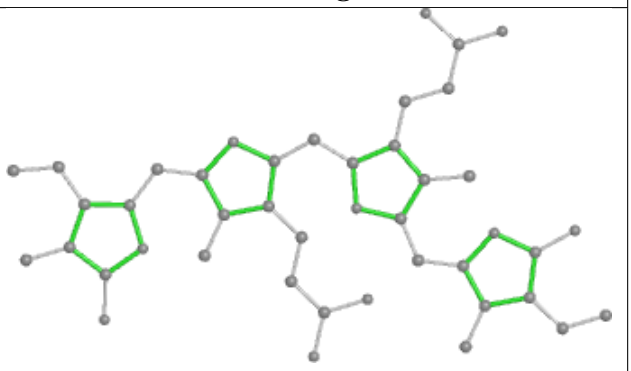
Bond lengths



Bond angles

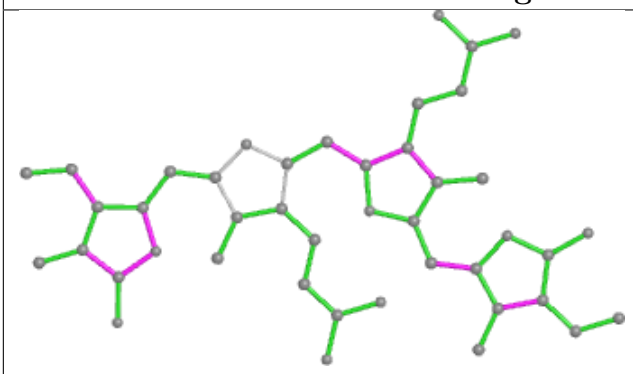


Torsions

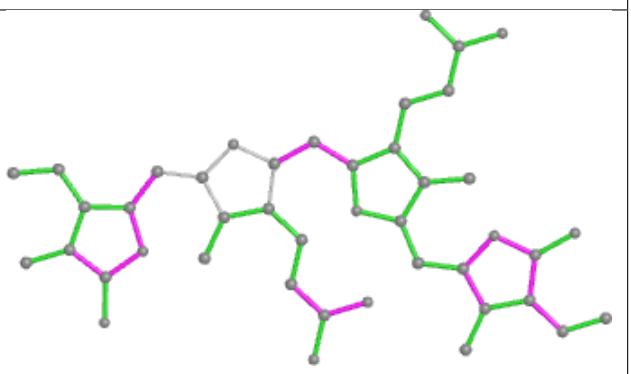


Rings

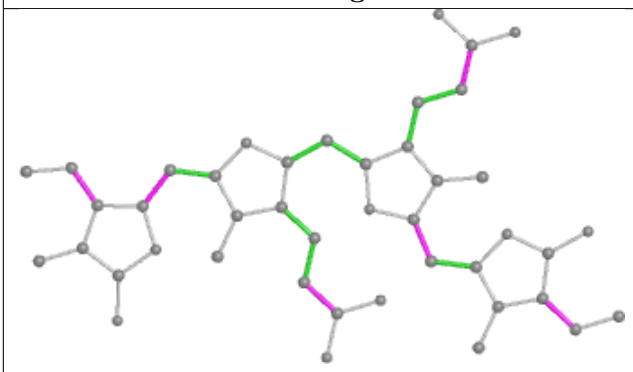
Ligand CYC E 1084



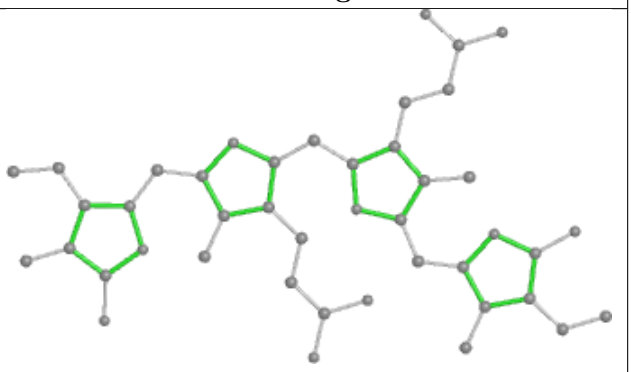
Bond lengths



Bond angles

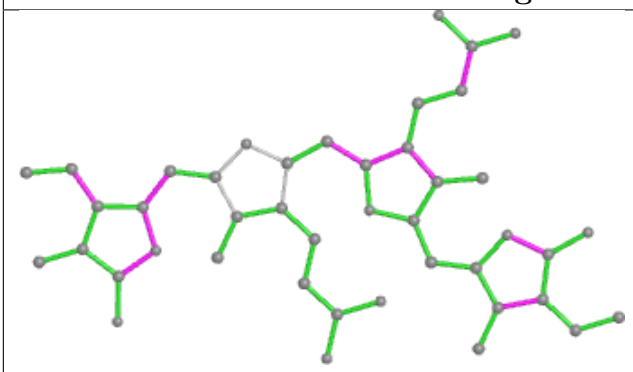


Torsions

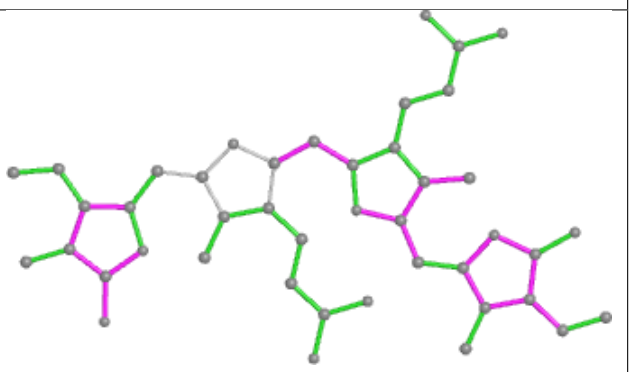


Rings

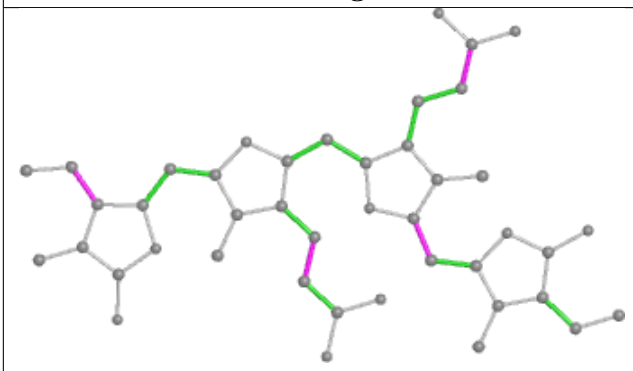
Ligand CYC F 1153



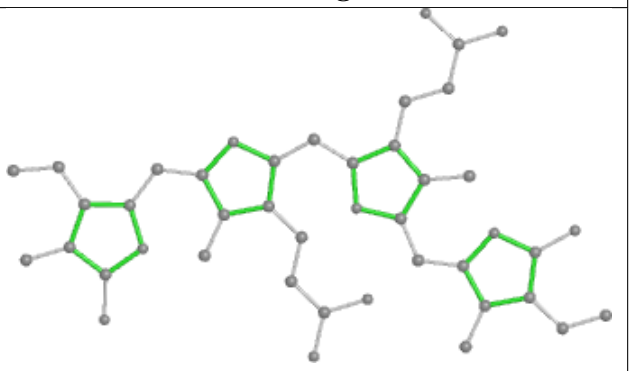
Bond lengths



Bond angles

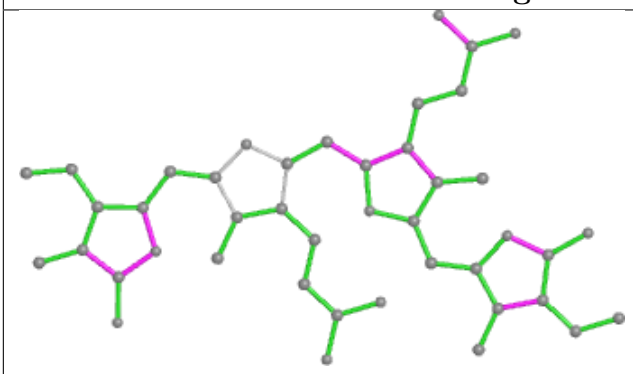


Torsions

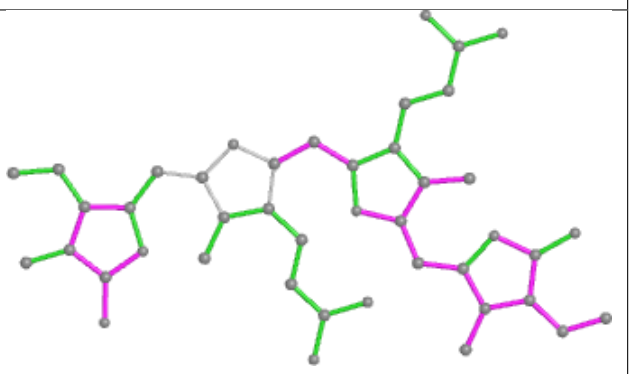


Rings

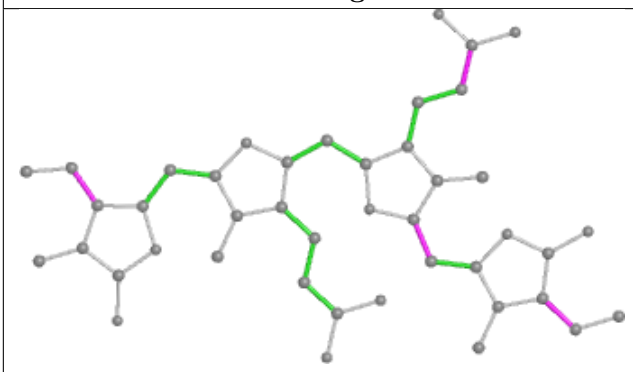
Ligand CYC B 1153



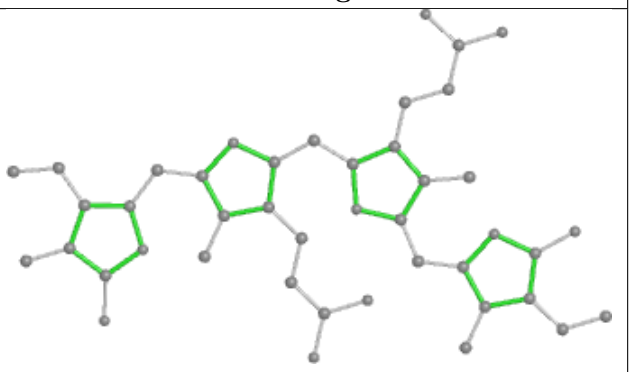
Bond lengths



Bond angles

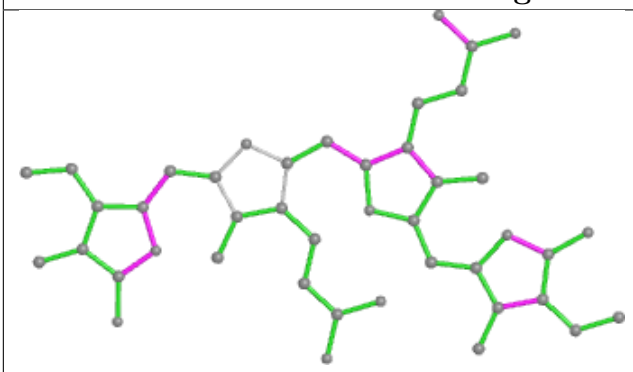


Torsions

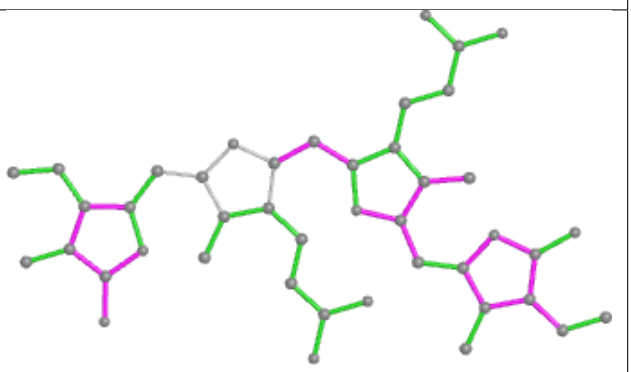


Rings

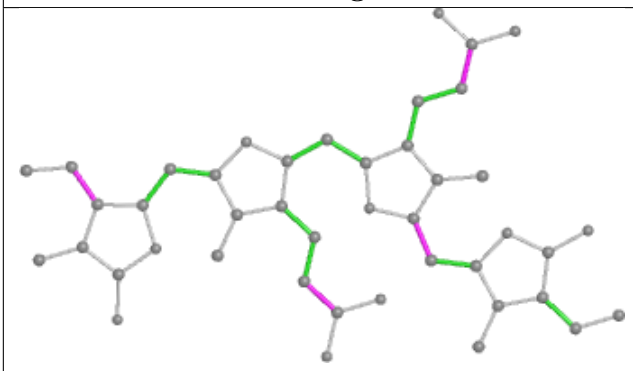
Ligand CYC P 1153



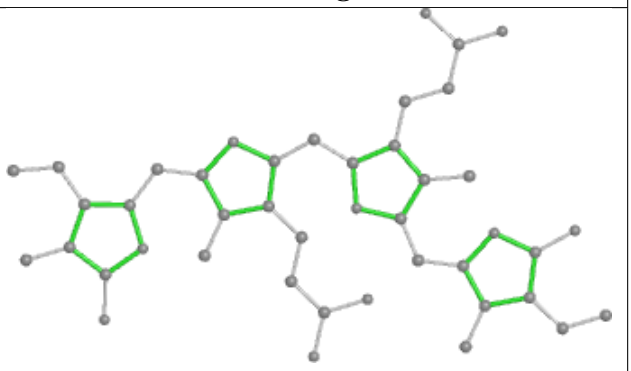
Bond lengths



Bond angles

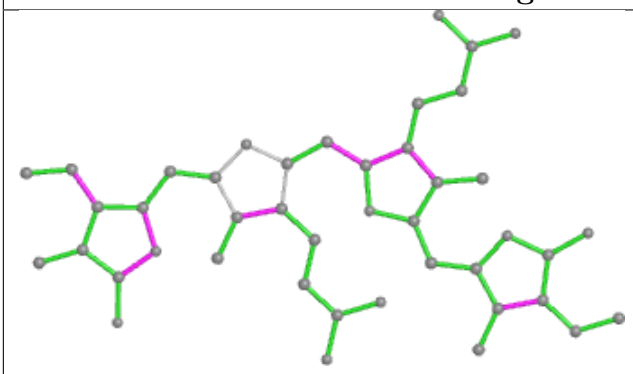


Torsions

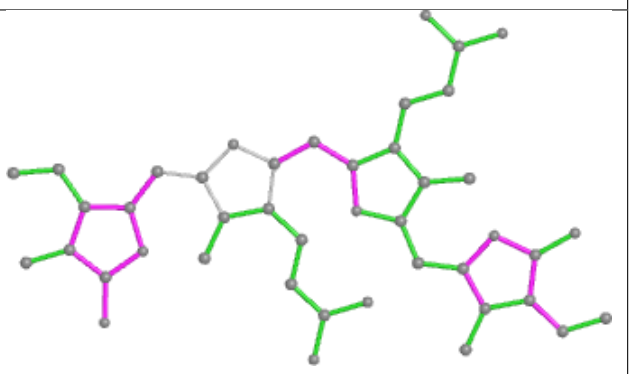


Rings

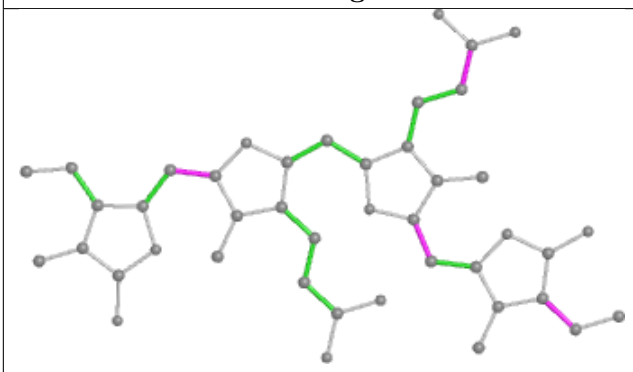
Ligand CYC J 1082



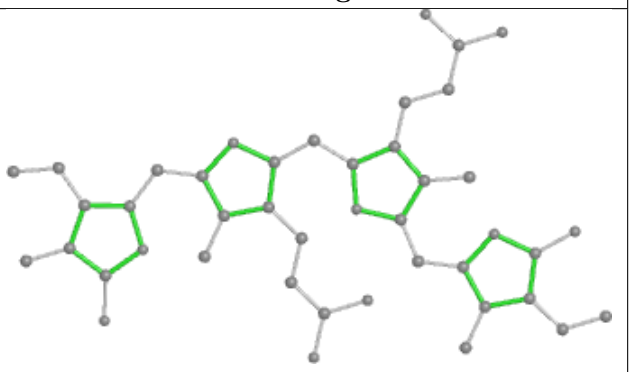
Bond lengths



Bond angles

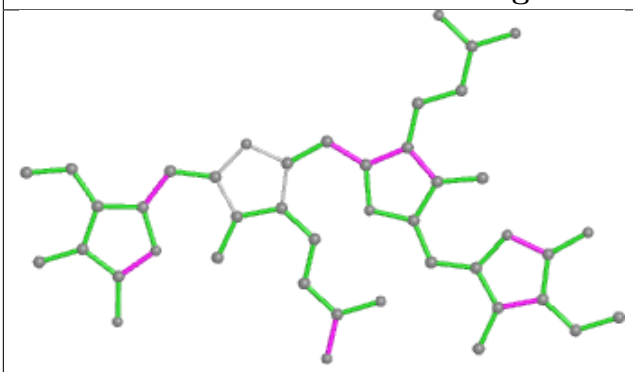


Torsions

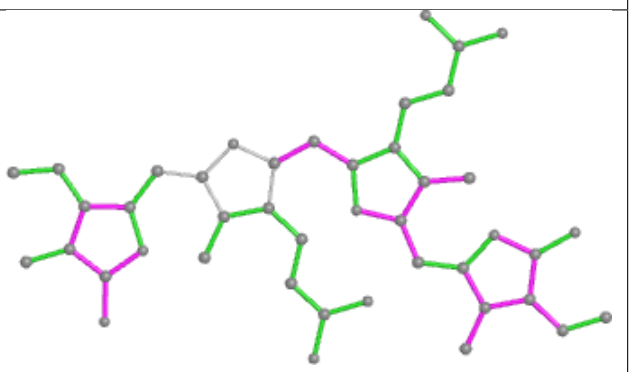


Rings

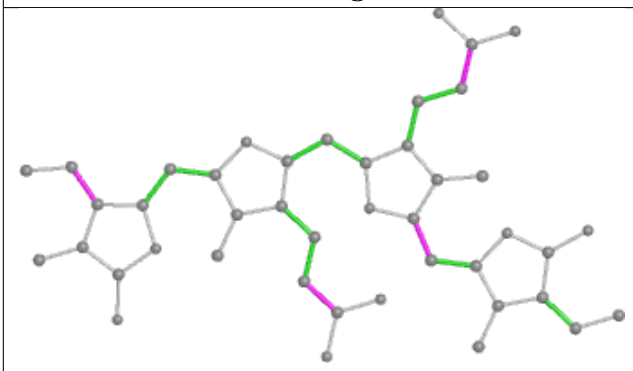
Ligand CYC H 1153



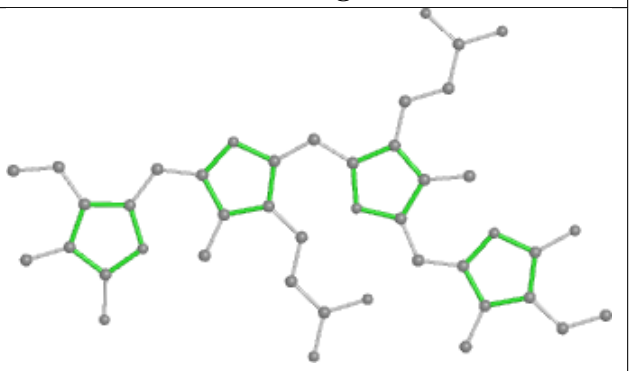
Bond lengths



Bond angles

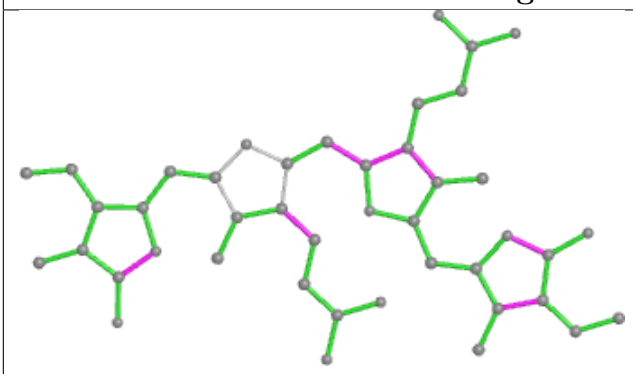


Torsions

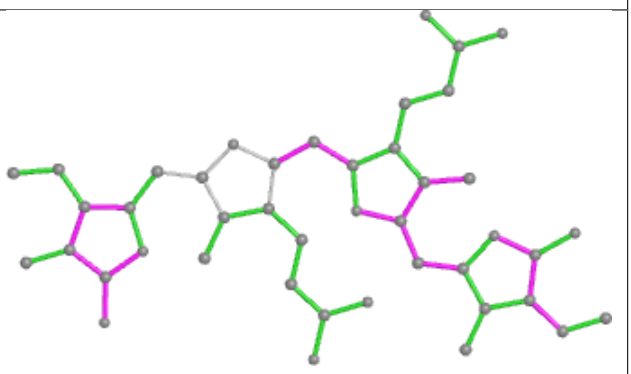


Rings

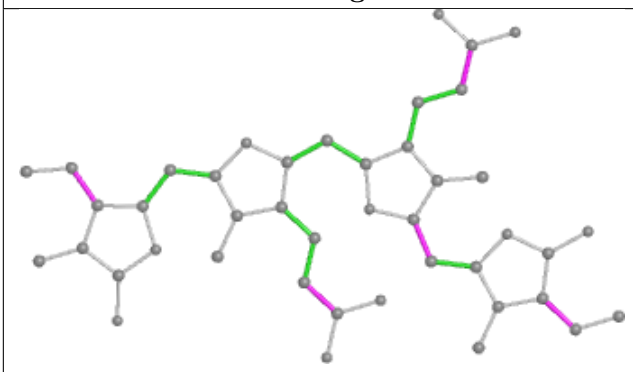
Ligand CYC J 1153



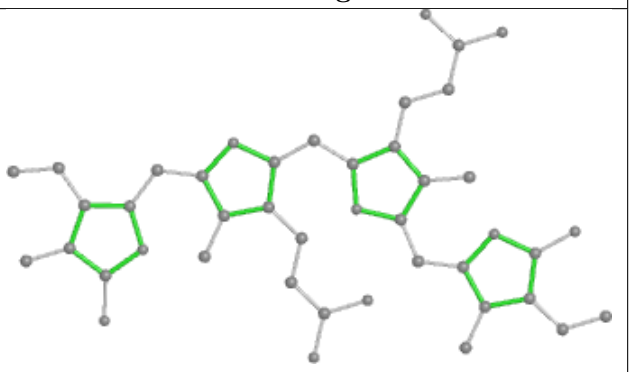
Bond lengths



Bond angles

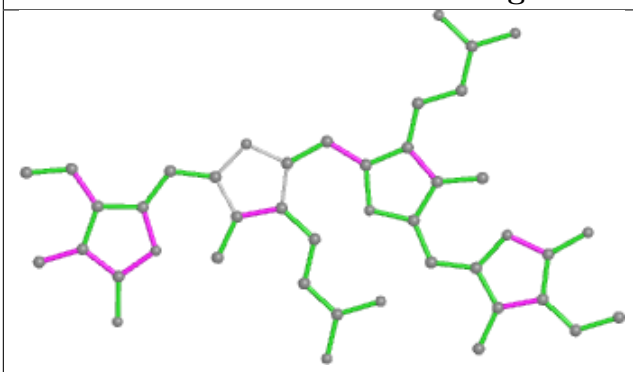


Torsions

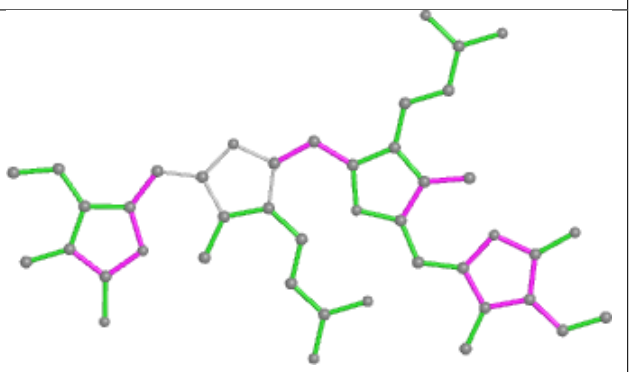


Rings

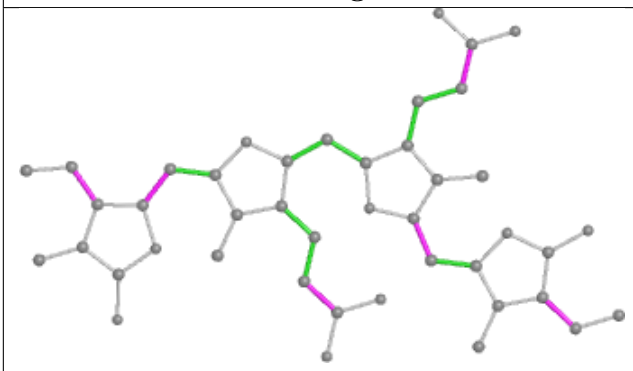
Ligand CYC W 1084



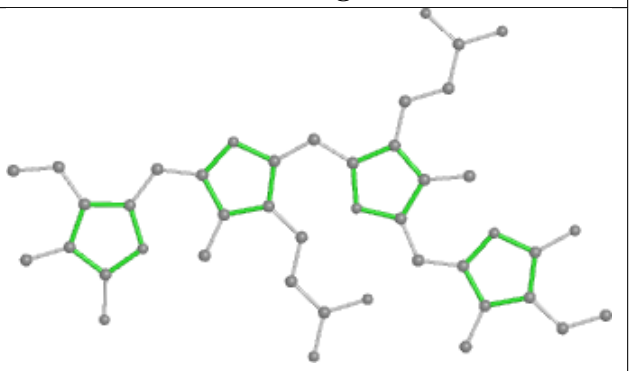
Bond lengths



Bond angles

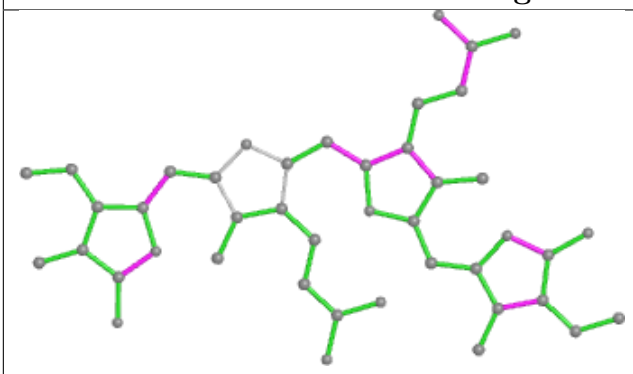


Torsions

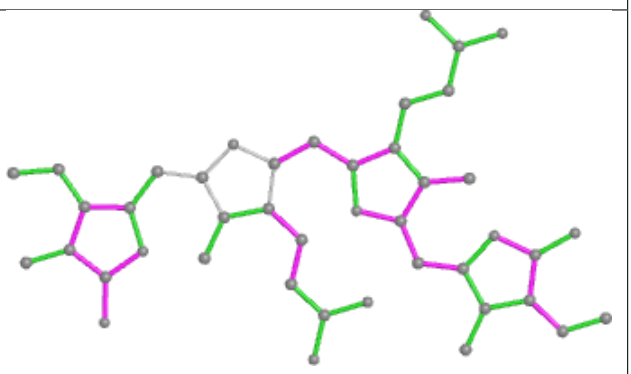


Rings

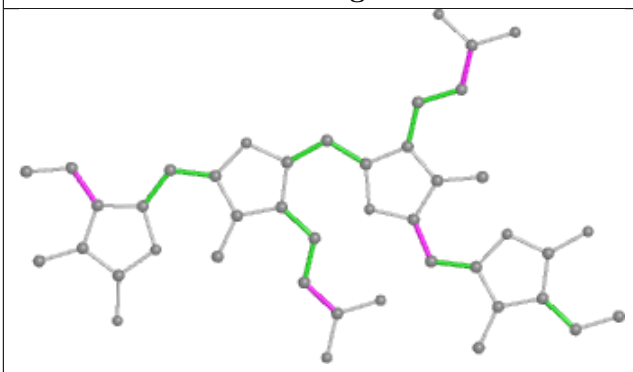
Ligand CYC T 1153



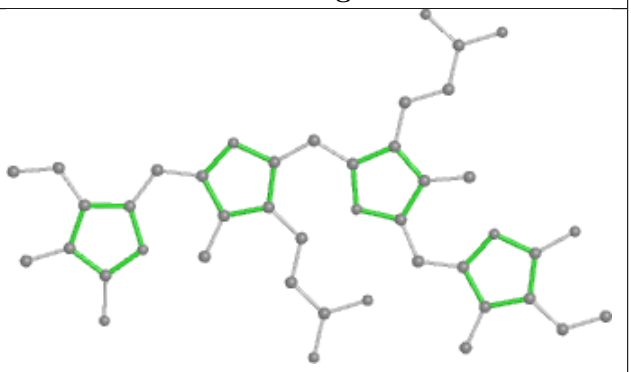
Bond lengths



Bond angles

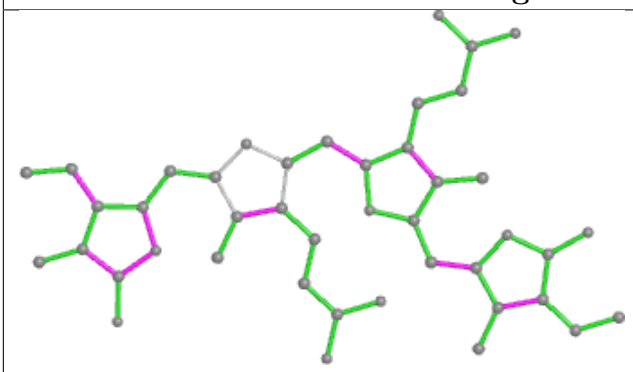


Torsions

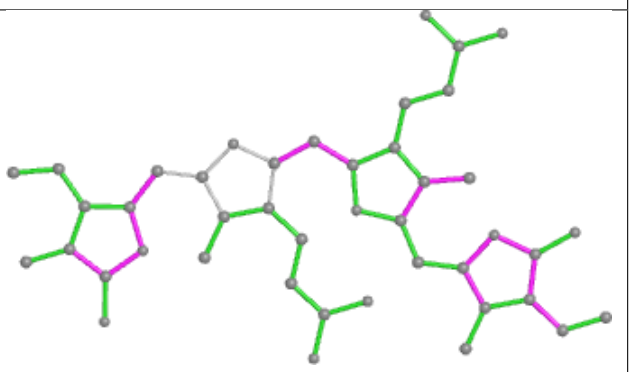


Rings

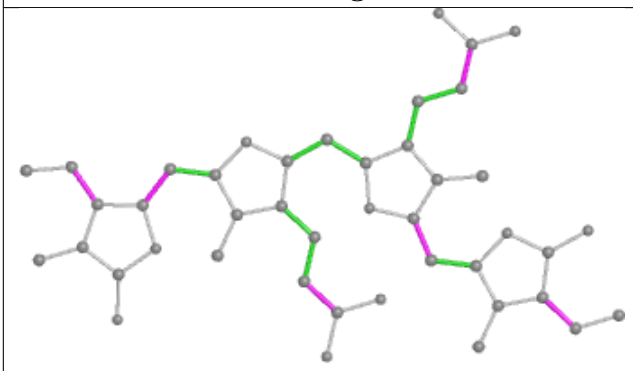
Ligand CYC K 1084



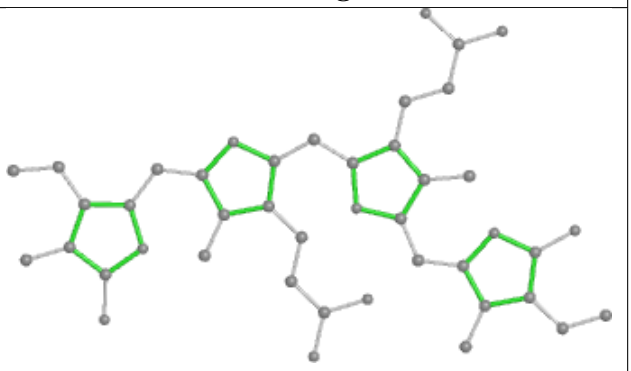
Bond lengths



Bond angles

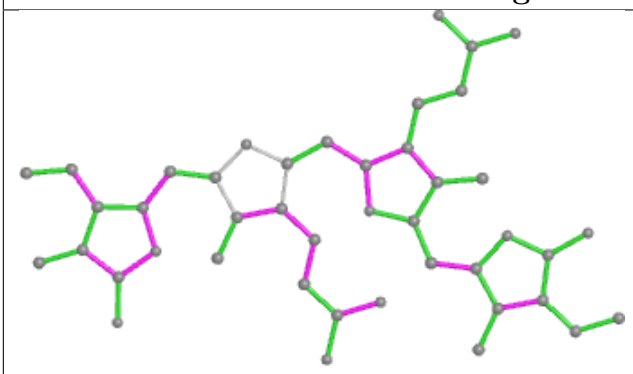


Torsions

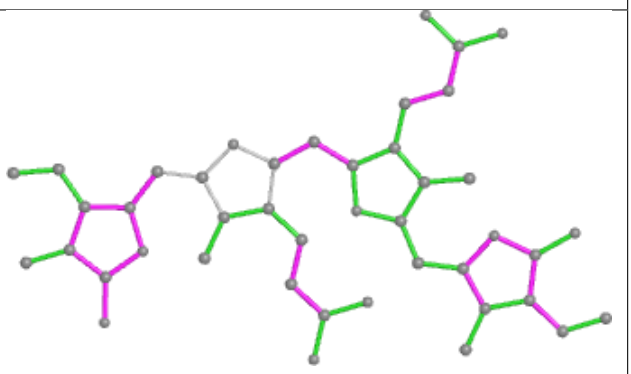


Rings

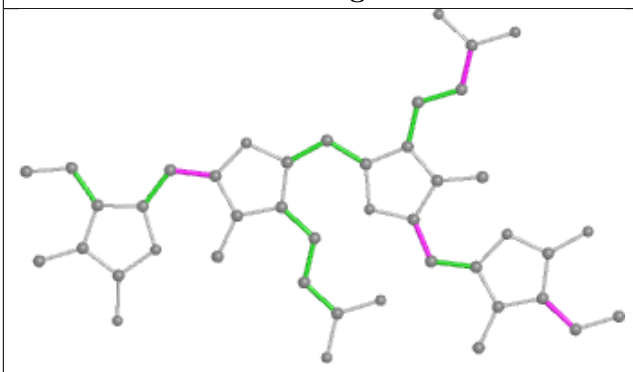
Ligand CYC R 1082



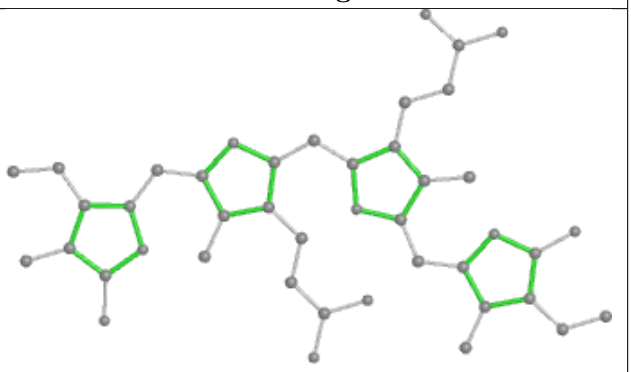
Bond lengths



Bond angles

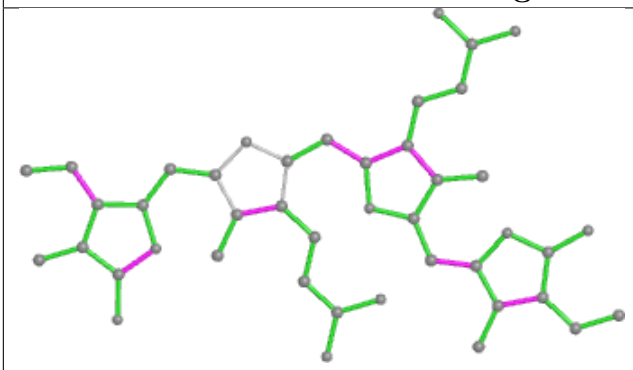


Torsions

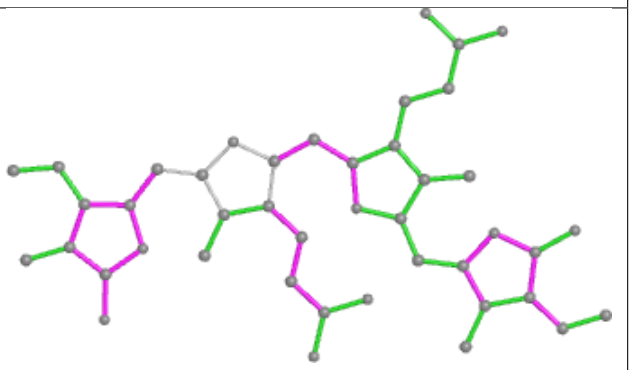


Rings

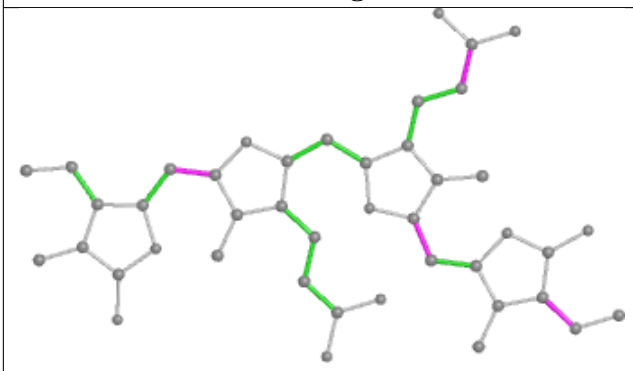
Ligand CYC P 1082



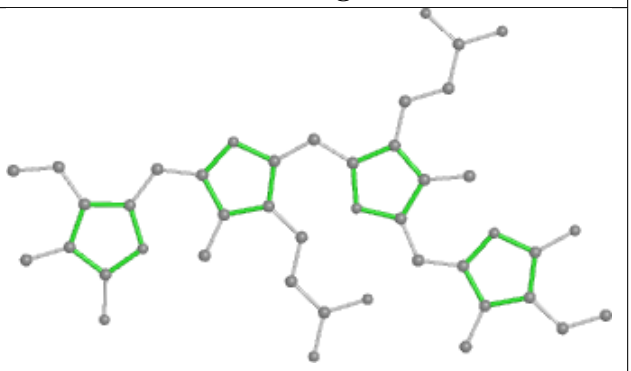
Bond lengths



Bond angles

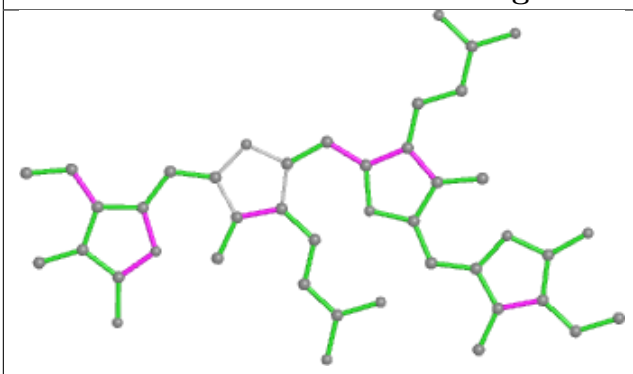


Torsions

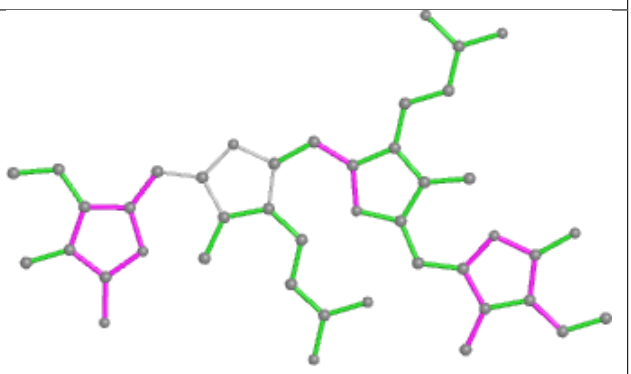


Rings

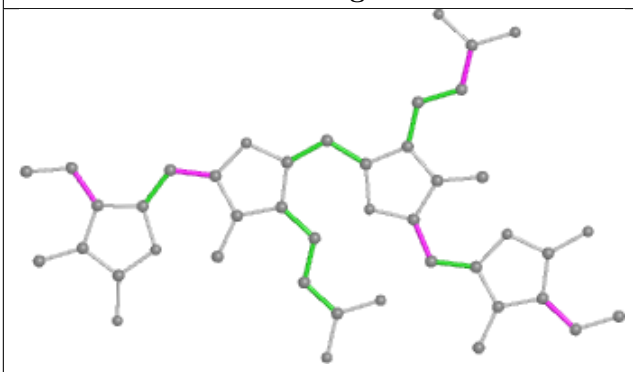
Ligand CYC N 1082



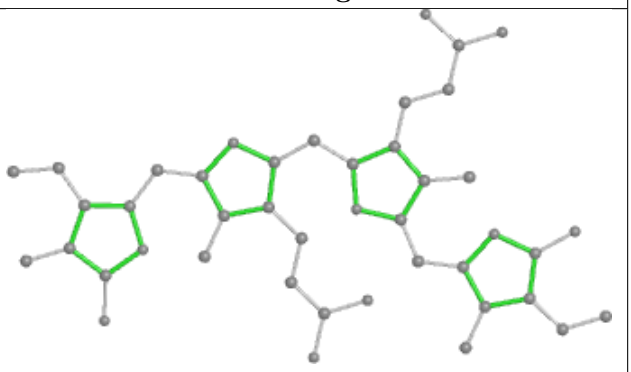
Bond lengths



Bond angles

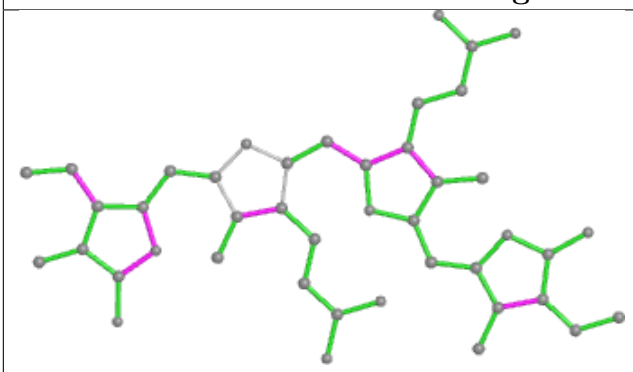


Torsions

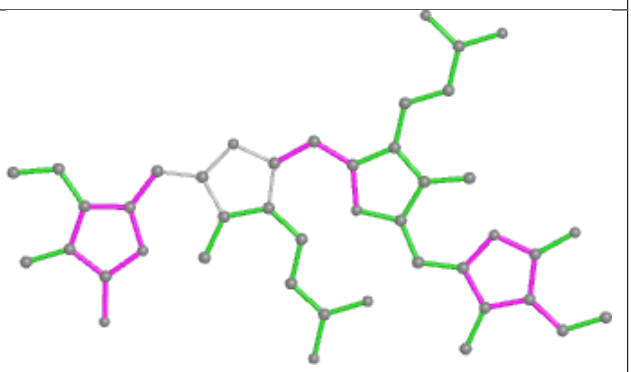


Rings

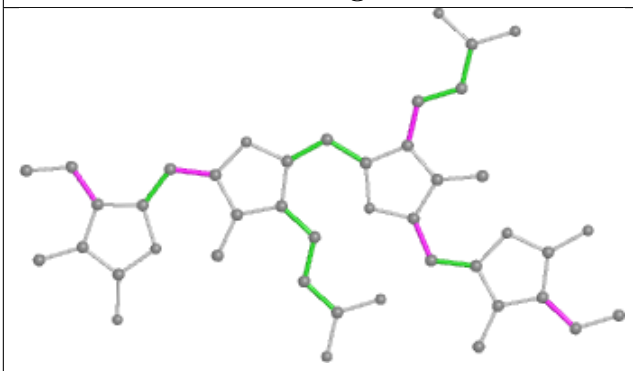
Ligand CYC D 1082



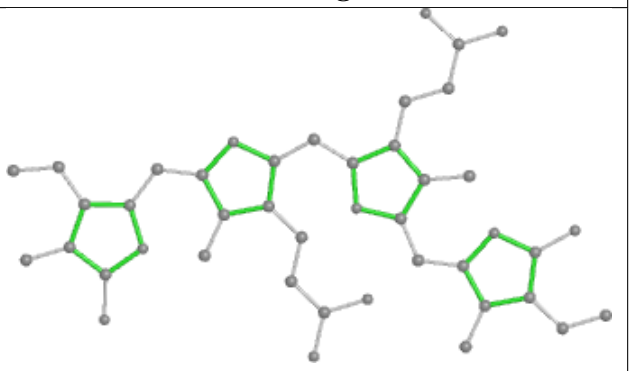
Bond lengths



Bond angles

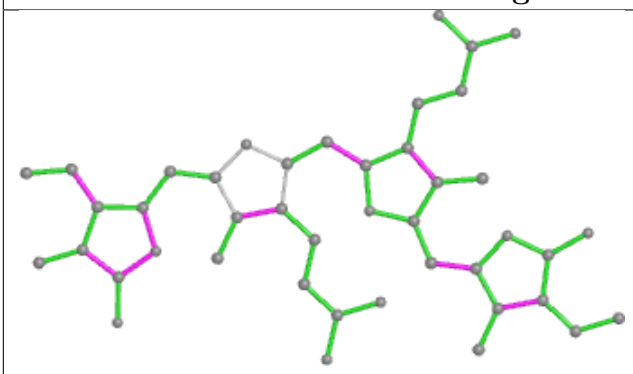


Torsions

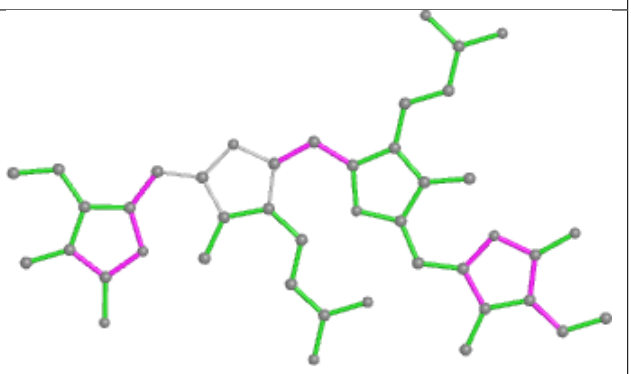


Rings

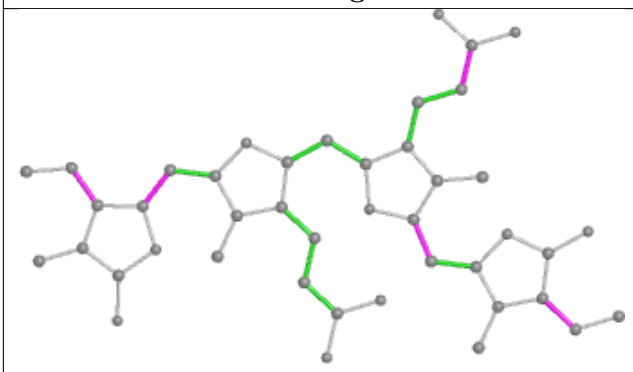
Ligand CYC U 1084



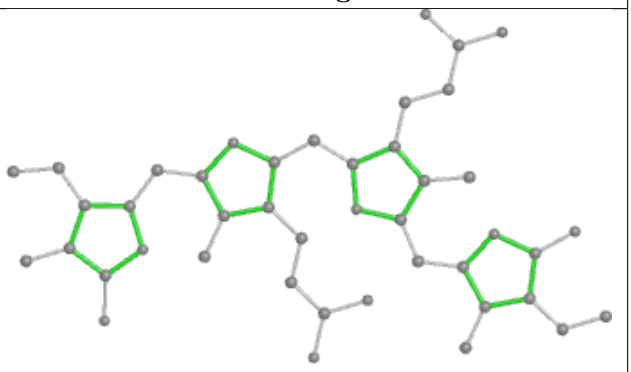
Bond lengths



Bond angles

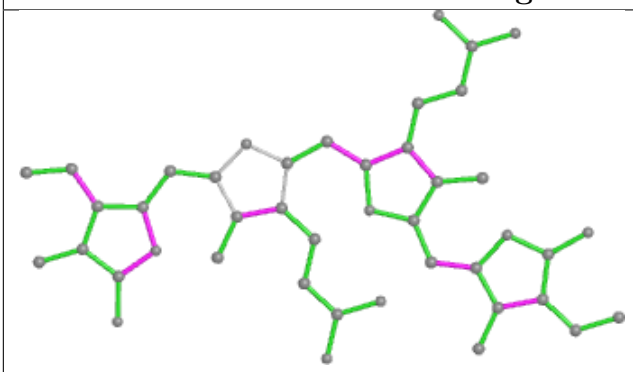


Torsions

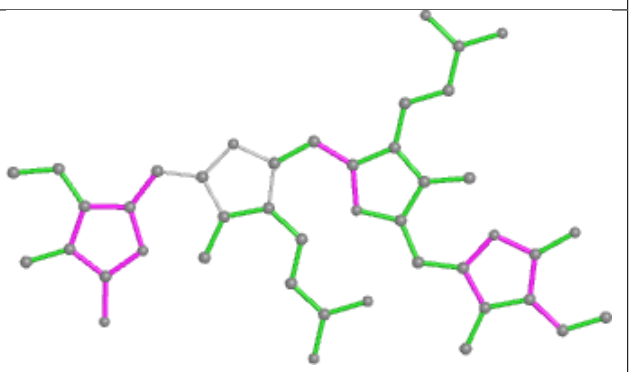


Rings

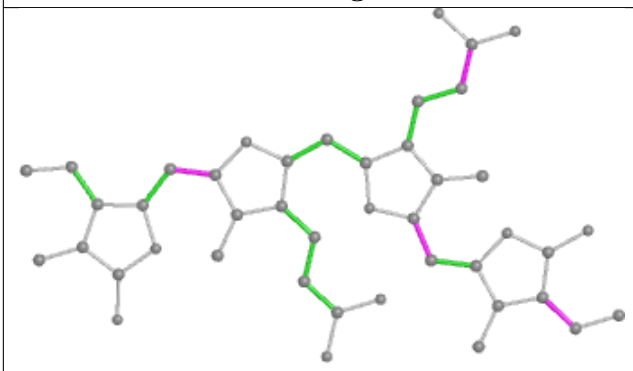
Ligand CYC L 1082



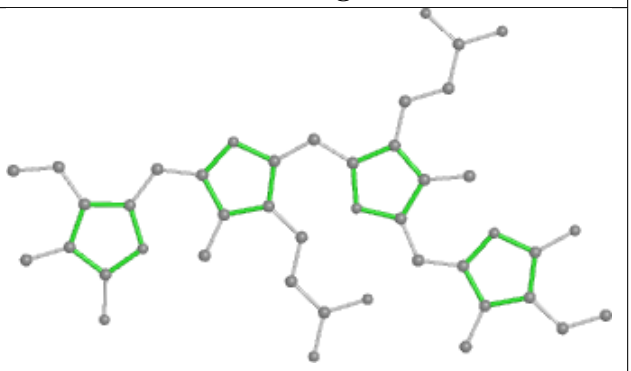
Bond lengths



Bond angles

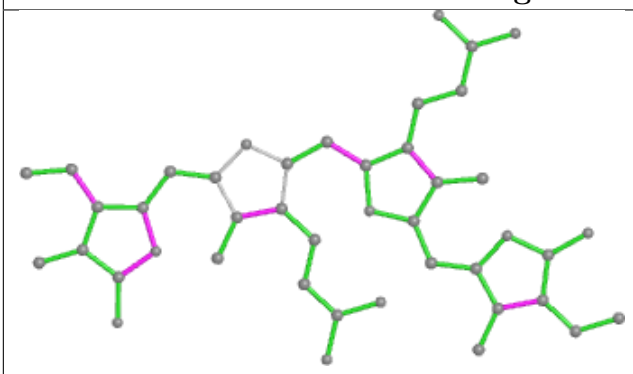


Torsions

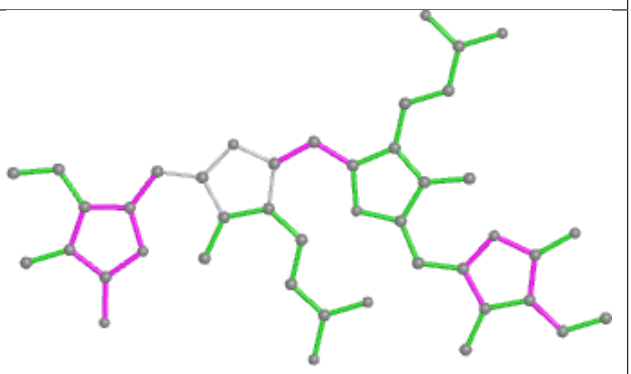


Rings

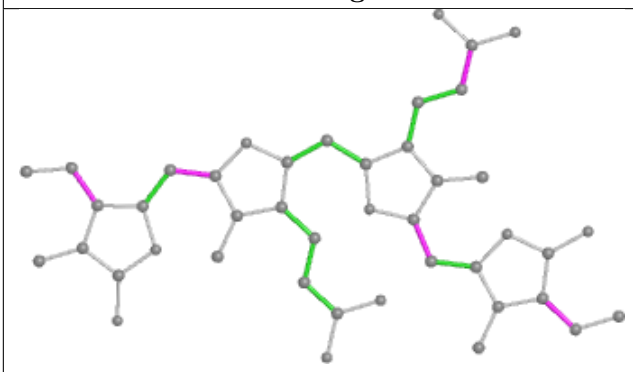
Ligand CYC T 1082



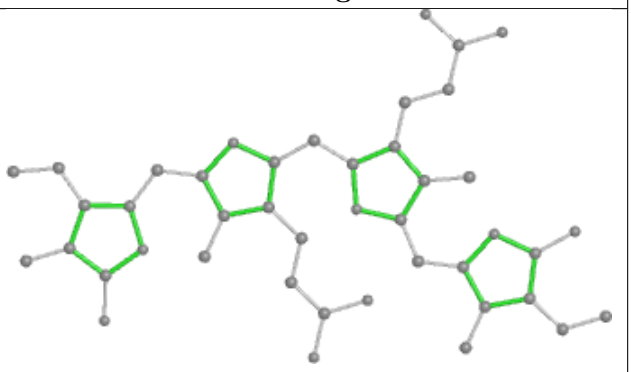
Bond lengths



Bond angles

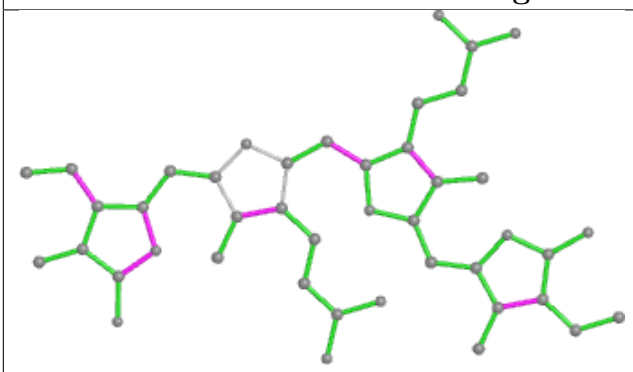


Torsions

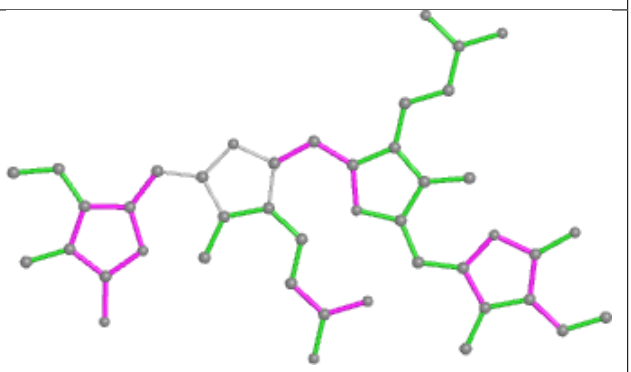


Rings

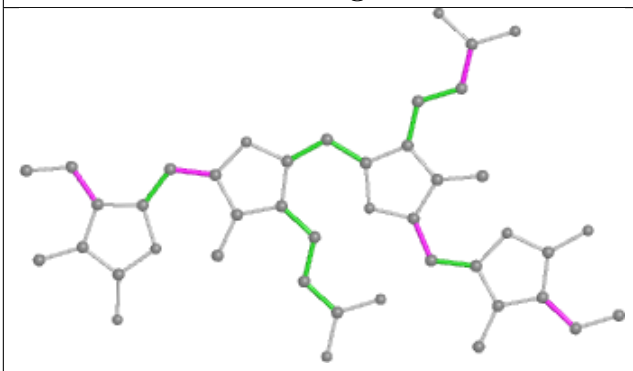
Ligand CYC V 1082



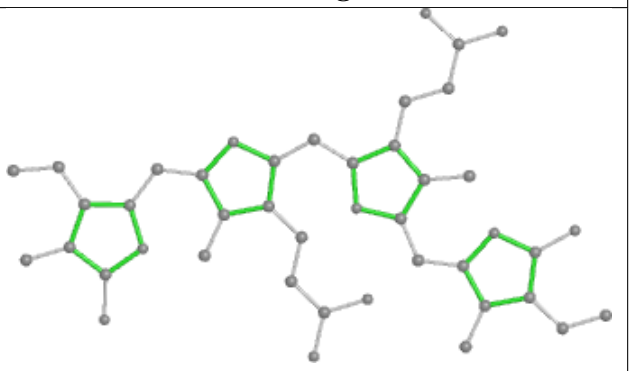
Bond lengths



Bond angles



Torsions



Rings

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, 95th 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^2)	Q<0.9
1	A	162/162 (100%)	-0.77	0 100 100	10, 17, 32, 43	2 (1%)
1	C	162/162 (100%)	-0.69	0 100 100	12, 21, 34, 47	3 (1%)
1	E	162/162 (100%)	-0.80	0 100 100	8, 17, 30, 39	1 (0%)
1	G	162/162 (100%)	-0.71	0 100 100	12, 20, 34, 41	2 (1%)
1	I	162/162 (100%)	-0.72	0 100 100	12, 20, 34, 43	1 (0%)
1	K	162/162 (100%)	-0.76	0 100 100	10, 17, 29, 43	1 (0%)
1	M	162/162 (100%)	-0.55	1 (0%) 89 88	12, 23, 37, 52	1 (0%)
1	O	162/162 (100%)	-0.73	0 100 100	12, 21, 34, 44	3 (1%)
1	Q	162/162 (100%)	-0.74	0 100 100	11, 18, 32, 45	1 (0%)
1	S	162/162 (100%)	-0.75	0 100 100	12, 19, 33, 45	2 (1%)
1	U	162/162 (100%)	-0.64	0 100 100	13, 22, 37, 44	1 (0%)
1	W	162/162 (100%)	-0.72	0 100 100	13, 20, 32, 45	1 (0%)
2	B	171/172 (99%)	-0.80	0 100 100	8, 17, 32, 39	0
2	D	171/172 (99%)	-0.68	0 100 100	12, 22, 37, 44	0
2	F	171/172 (99%)	-0.57	1 (0%) 89 88	13, 24, 36, 50	1 (0%)
2	H	171/172 (99%)	-0.65	0 100 100	11, 21, 35, 45	1 (0%)
2	J	171/172 (99%)	-0.61	0 100 100	13, 22, 35, 49	0
2	L	171/172 (99%)	-0.64	1 (0%) 89 88	11, 20, 35, 56	0
2	N	171/172 (99%)	-0.67	0 100 100	10, 20, 35, 49	0
2	P	171/172 (99%)	-0.43	1 (0%) 89 88	17, 28, 41, 57	0
2	R	171/172 (99%)	-0.59	0 100 100	13, 23, 38, 43	1 (0%)
2	T	171/172 (99%)	-0.61	0 100 100	14, 23, 36, 47	1 (0%)
2	V	171/172 (99%)	-0.74	0 100 100	9, 19, 33, 42	1 (0%)
2	X	171/172 (99%)	-0.48	0 100 100	15, 25, 38, 49	1 (0%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3996/4008 (99%)	-0.67	4 (0%)	95	95	8, 21, 36, 57	25 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	70	GLN	2.5
2	F	172	SER	2.3
2	P	172	SER	2.2
2	L	29	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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^2)	Q<0.9
2	MEN	P	72	9/10	0.91	0.11	26,28,33,36	0
2	MEN	X	72	9/10	0.94	0.09	22,24,31,31	0
2	MEN	H	72	9/10	0.96	0.09	17,19,25,25	0
2	MEN	J	72	9/10	0.96	0.07	21,23,23,27	0
2	MEN	B	72	9/10	0.96	0.08	14,16,19,21	0
2	MEN	T	72	9/10	0.96	0.08	21,24,26,30	0
2	MEN	F	72	9/10	0.96	0.08	18,19,21,23	0
2	MEN	N	72	9/10	0.97	0.07	16,18,25,27	0
2	MEN	V	72	9/10	0.97	0.08	16,18,21,22	0
2	MEN	D	72	9/10	0.97	0.08	15,18,26,28	0
2	MEN	R	72	9/10	0.98	0.07	20,21,27,27	0
2	MEN	L	72	9/10	0.98	0.06	16,19,22,24	0

6.3 Carbohydrates (i)

There are no monosaccharides 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,

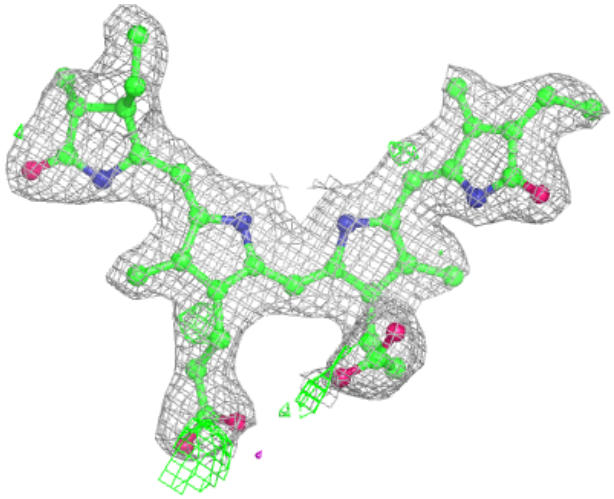
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

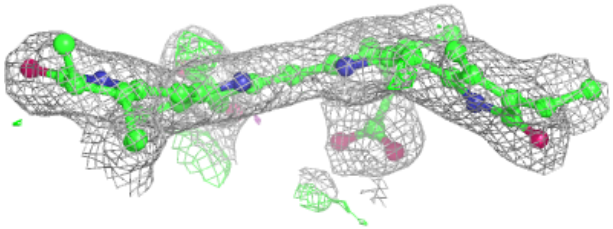
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CYC	P	1082	43/43	0.85	0.16	26,39,47,49	0
3	CYC	J	1082	43/43	0.86	0.15	18,29,37,42	0
3	CYC	T	1082	43/43	0.87	0.16	20,30,37,39	0
3	CYC	X	1082	43/43	0.87	0.14	20,30,39,43	0
3	CYC	F	1082	43/43	0.88	0.15	18,29,39,42	0
3	CYC	R	1082	43/43	0.88	0.15	18,28,34,43	0
3	CYC	L	1082	43/43	0.89	0.13	13,23,33,37	0
3	CYC	H	1082	43/43	0.90	0.13	11,25,31,37	0
3	CYC	N	1082	43/43	0.90	0.13	17,27,35,37	0
3	CYC	V	1082	43/43	0.90	0.14	12,24,30,36	0
3	CYC	B	1082	43/43	0.90	0.14	1,23,30,36	0
3	CYC	X	1153	43/43	0.90	0.12	23,29,40,45	0
3	CYC	D	1082	43/43	0.91	0.13	17,28,32,35	0
3	CYC	L	1153	43/43	0.92	0.11	18,25,37,44	0
3	CYC	R	1153	43/43	0.92	0.12	17,23,32,39	0
3	CYC	B	1153	43/43	0.93	0.11	11,16,23,30	0
3	CYC	N	1153	43/43	0.93	0.11	15,18,26,32	0
3	CYC	T	1153	43/43	0.93	0.11	17,22,32,39	0
3	CYC	U	1084	43/43	0.93	0.13	15,21,23,25	0
3	CYC	F	1153	43/43	0.93	0.11	17,22,34,42	0
3	CYC	P	1153	43/43	0.93	0.11	19,27,40,44	0
3	CYC	D	1153	43/43	0.93	0.12	17,21,28,36	0
3	CYC	H	1153	43/43	0.94	0.10	12,18,30,36	0
3	CYC	J	1153	43/43	0.94	0.11	15,21,28,34	0
3	CYC	M	1084	43/43	0.94	0.13	18,21,25,28	0
3	CYC	W	1084	43/43	0.95	0.11	11,17,21,24	0
3	CYC	I	1084	43/43	0.95	0.13	7,14,17,19	0
3	CYC	V	1153	43/43	0.95	0.10	9,17,25,30	0
3	CYC	C	1084	43/43	0.96	0.11	13,19,22,23	0
3	CYC	O	1084	43/43	0.96	0.12	12,15,18,19	0
3	CYC	K	1084	43/43	0.96	0.11	7,13,15,18	0
3	CYC	G	1084	43/43	0.96	0.11	8,16,20,23	0
3	CYC	Q	1084	43/43	0.96	0.09	5,13,16,19	0
3	CYC	S	1084	43/43	0.97	0.10	11,13,16,17	0
3	CYC	A	1084	43/43	0.97	0.11	11,14,18,20	0
3	CYC	E	1084	43/43	0.97	0.10	5,10,14,15	0

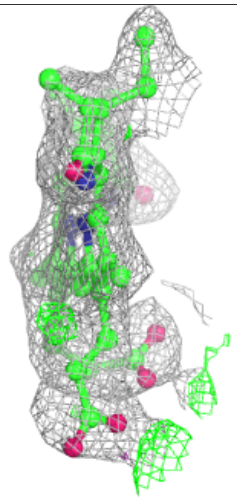
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC P 1082:

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

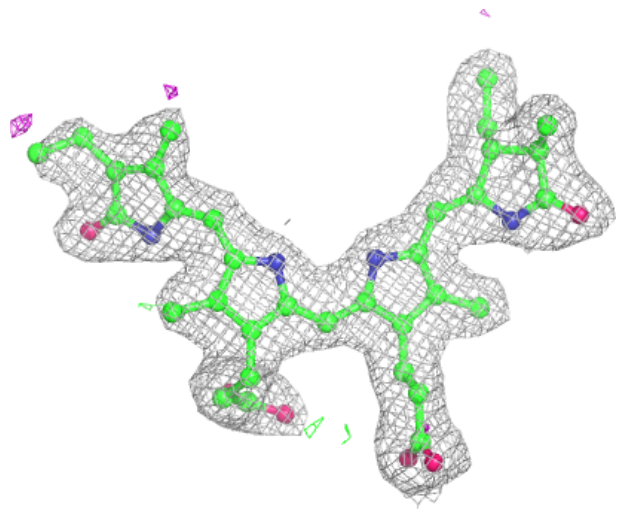


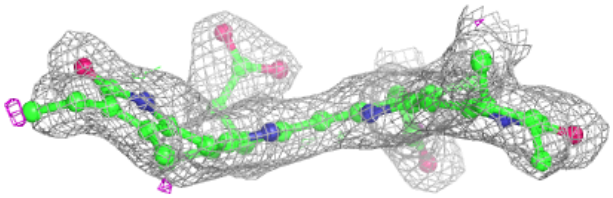


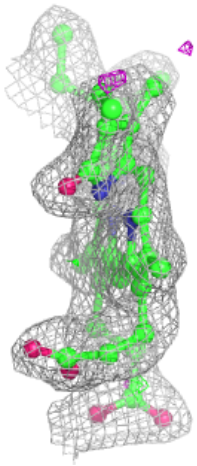


Electron density around CYC J 1082:

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

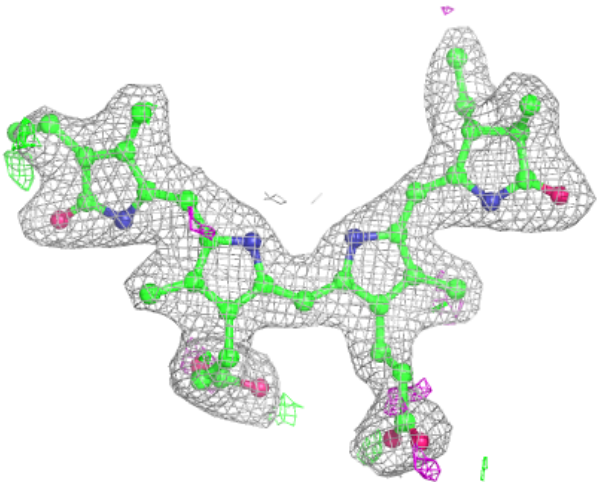


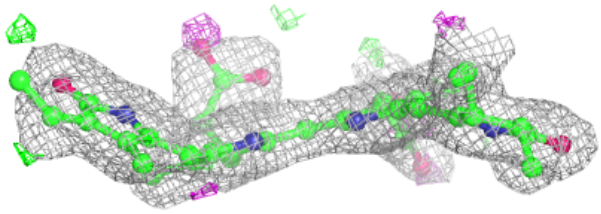


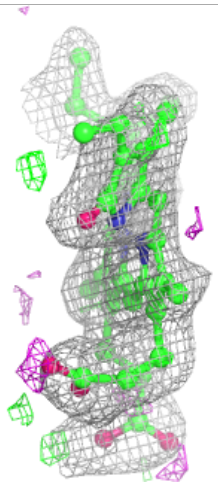


Electron density around CYC T 1082:

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

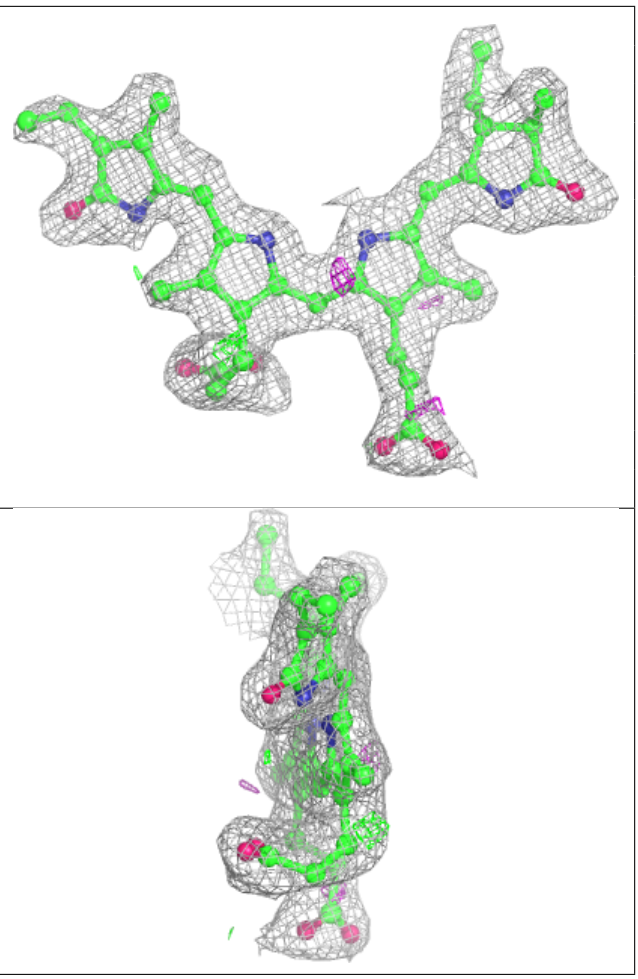






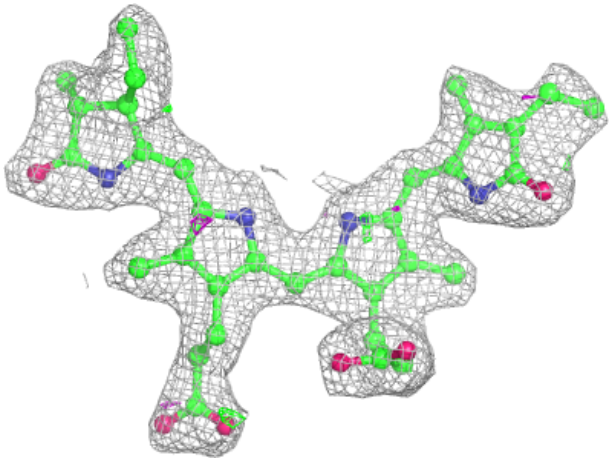
Electron density around CYC X 1082:

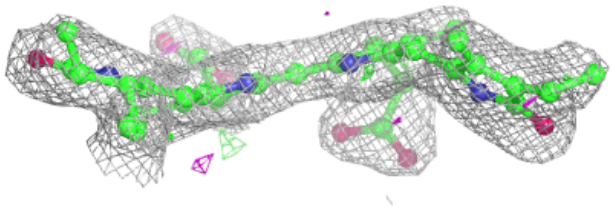
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

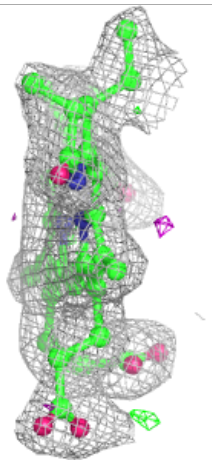


Electron density around CYC F 1082:

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

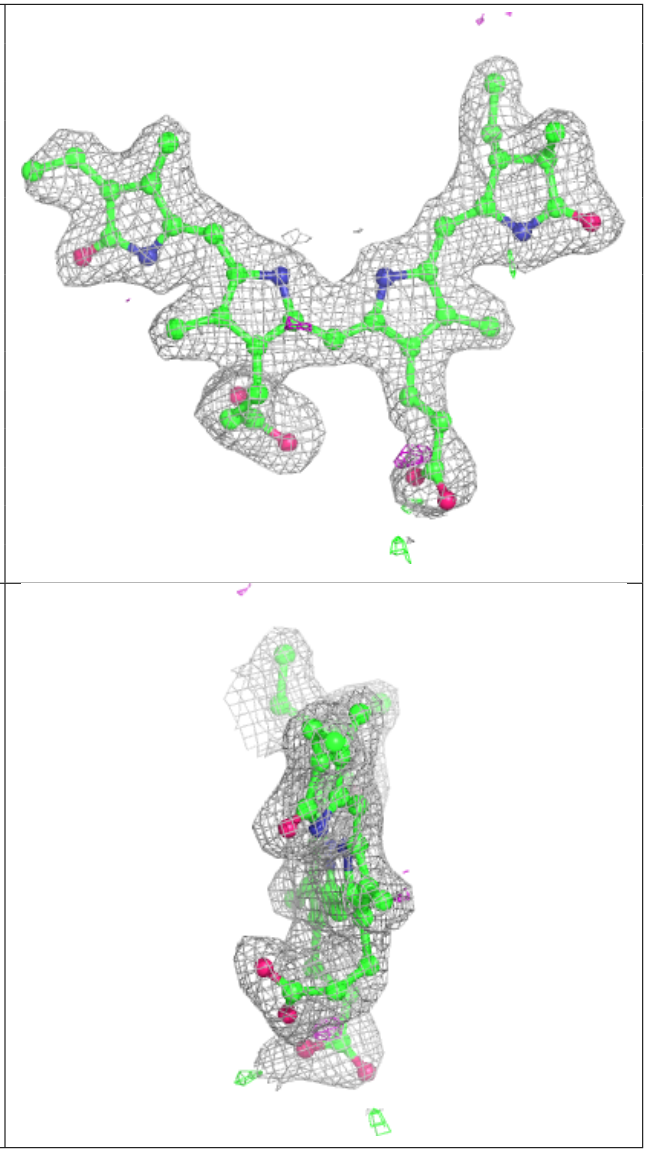






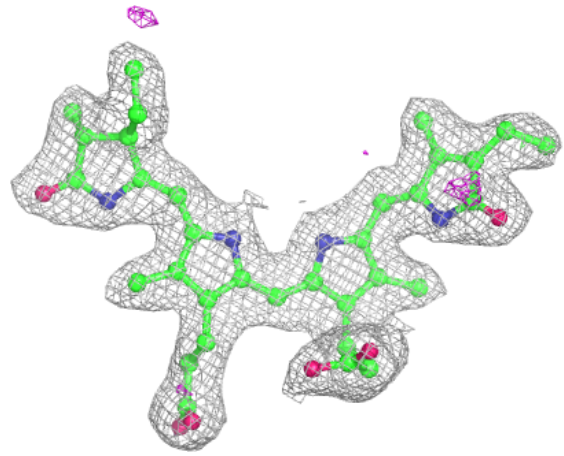
Electron density around CYC R 1082:

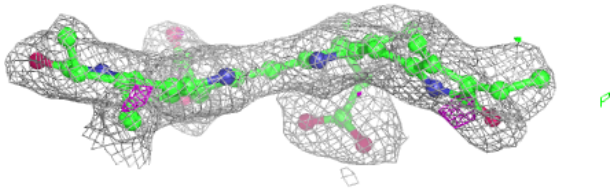
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

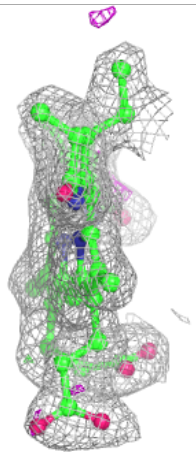


Electron density around CYC L 1082:

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

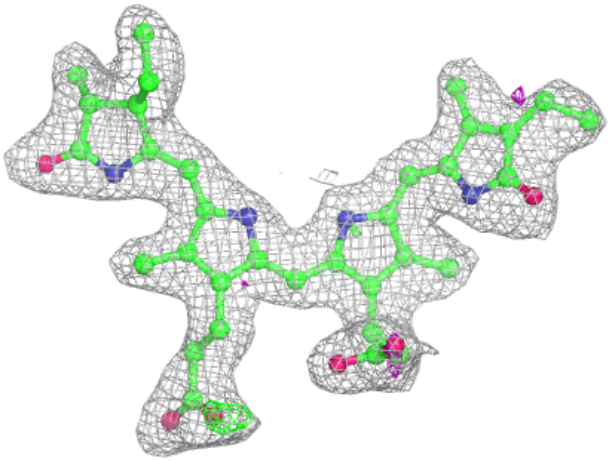


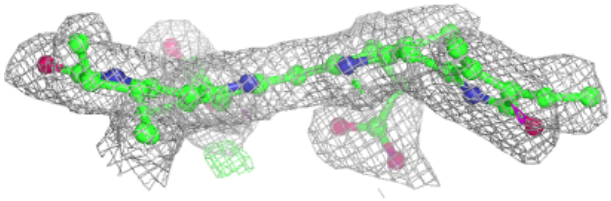


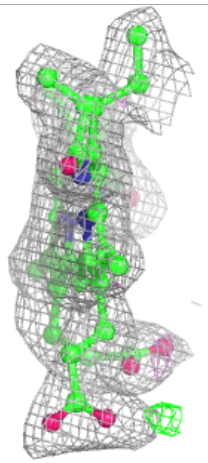


Electron density around CYC H 1082:

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

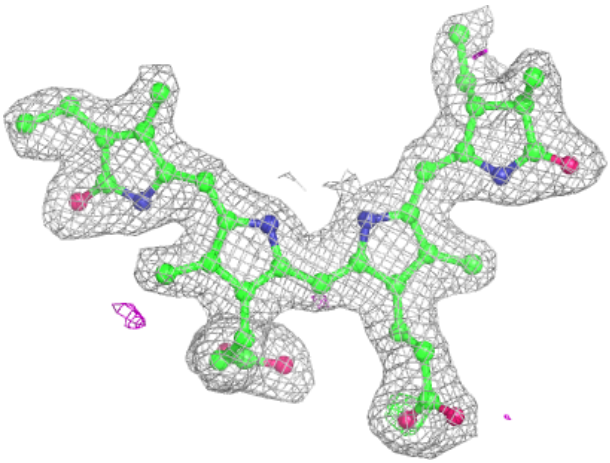


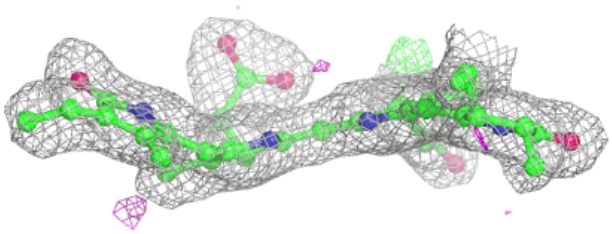




Electron density around CYC N 1082:

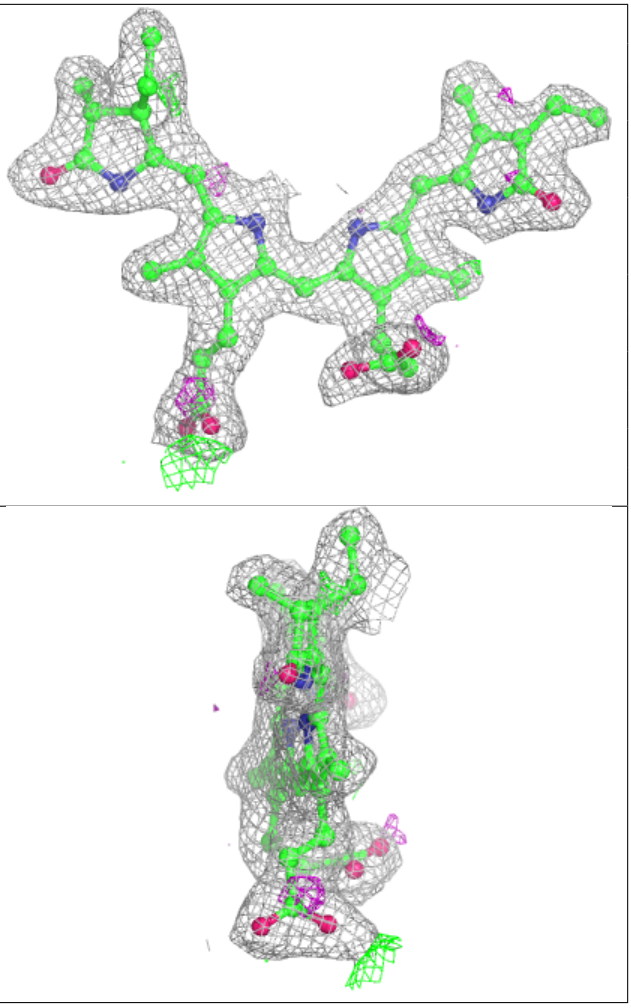
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





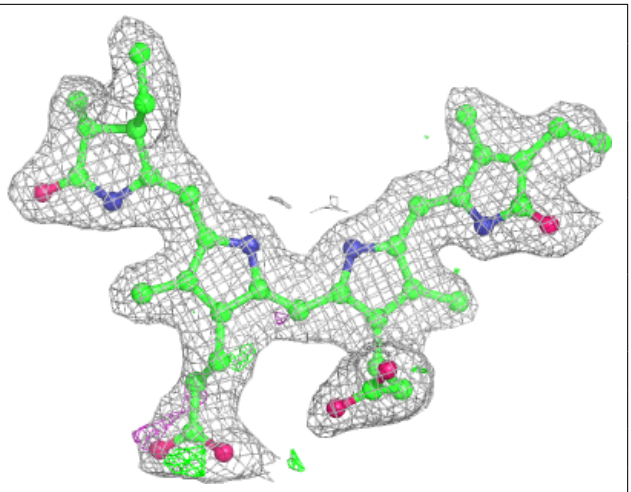
Electron density around CYC V 1082:

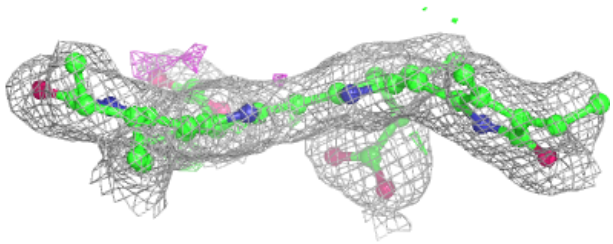
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

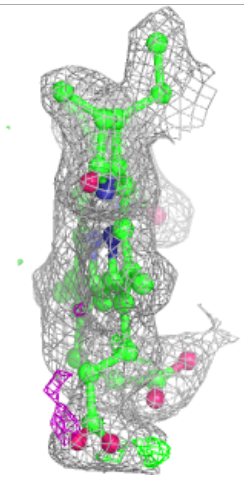


Electron density around CYC B 1082:

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

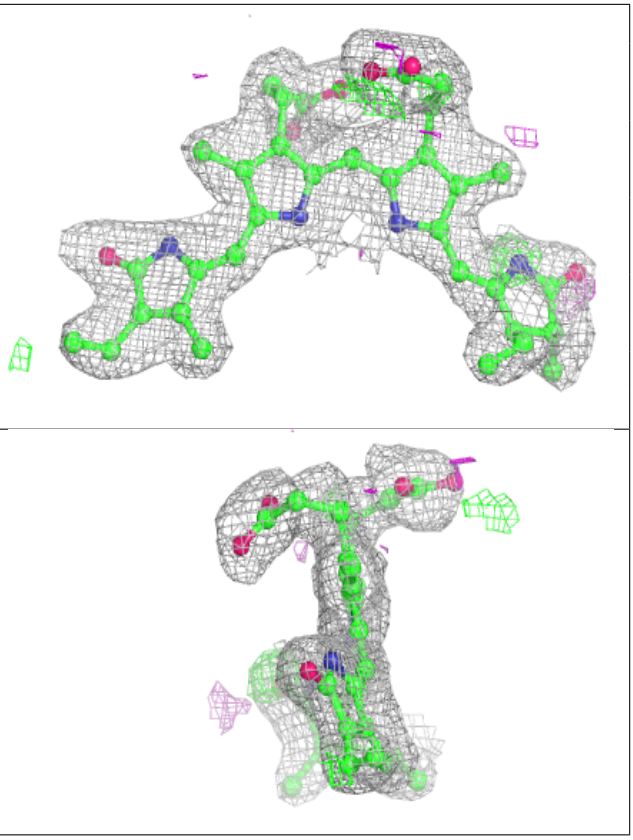






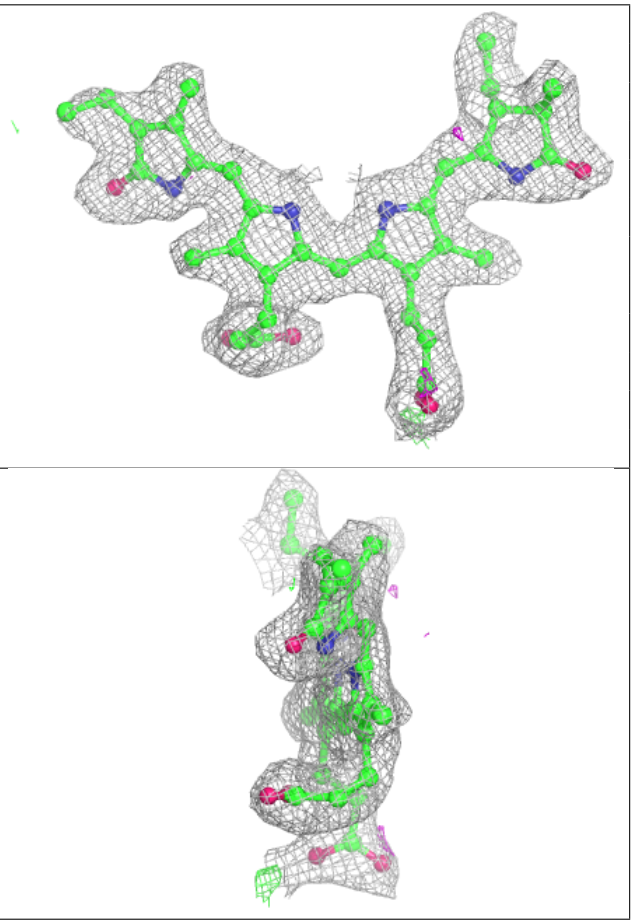
Electron density around CYC X 1153:

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



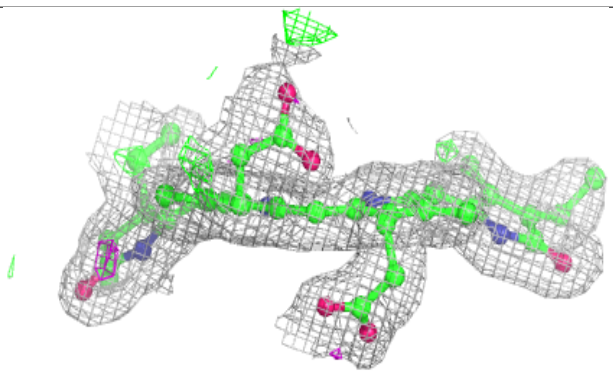
Electron density around CYC D 1082:

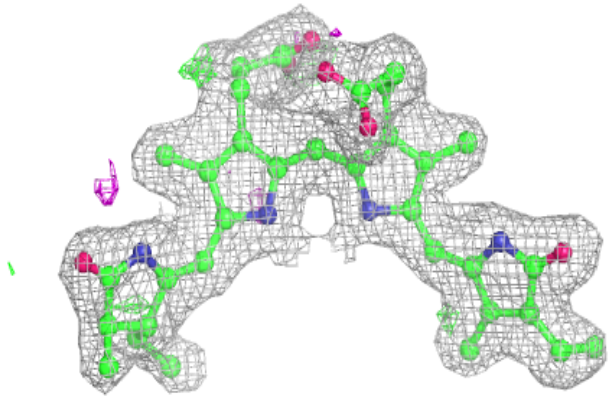
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

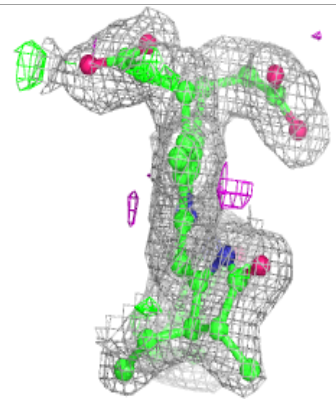


Electron density around CYC L 1153:

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

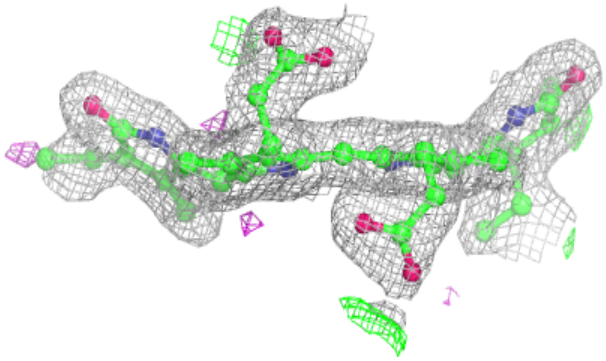


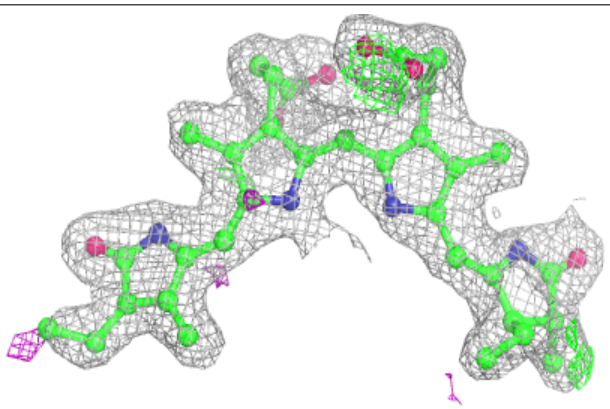


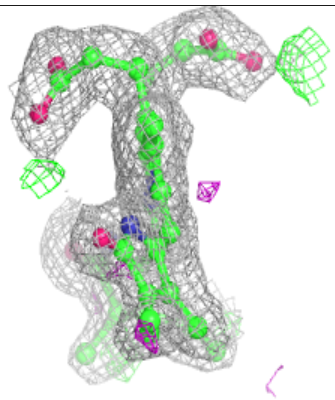


Electron density around CYC R 1153:

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

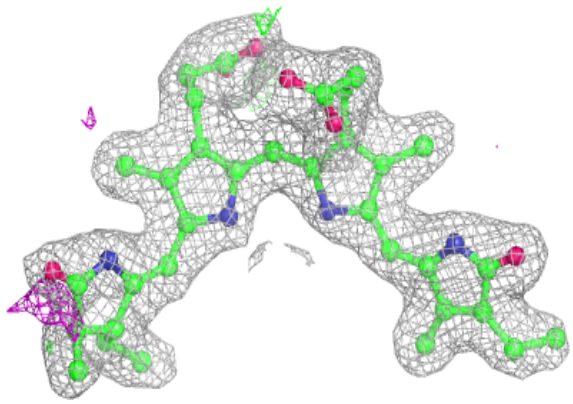


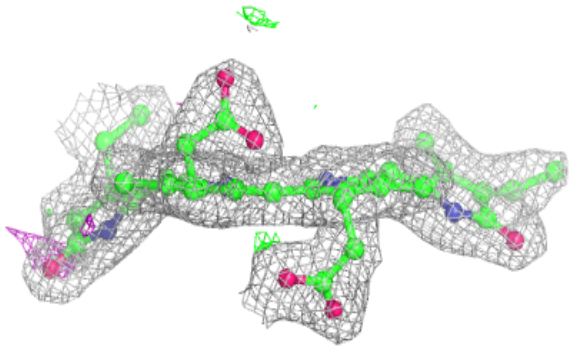


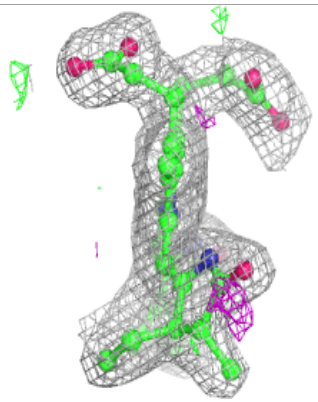


Electron density around CYC B 1153:

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

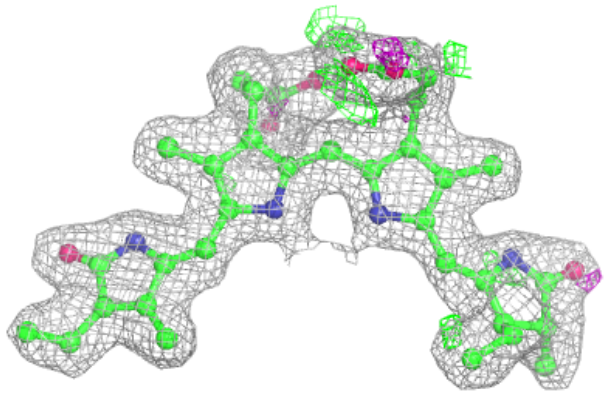


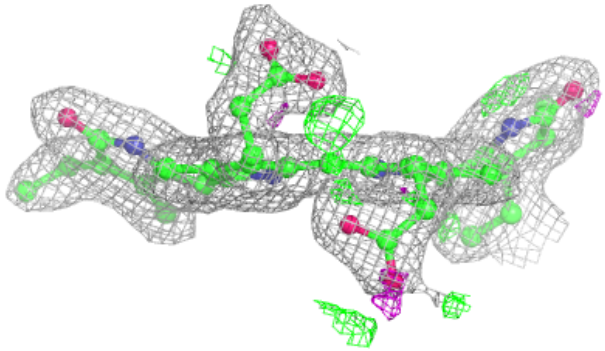


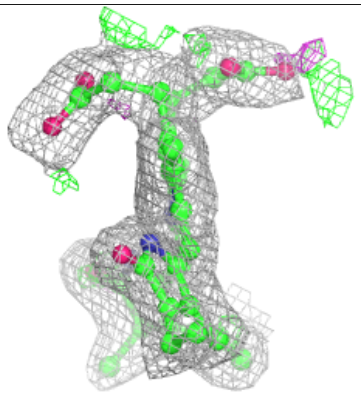


Electron density around CYC N 1153:

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

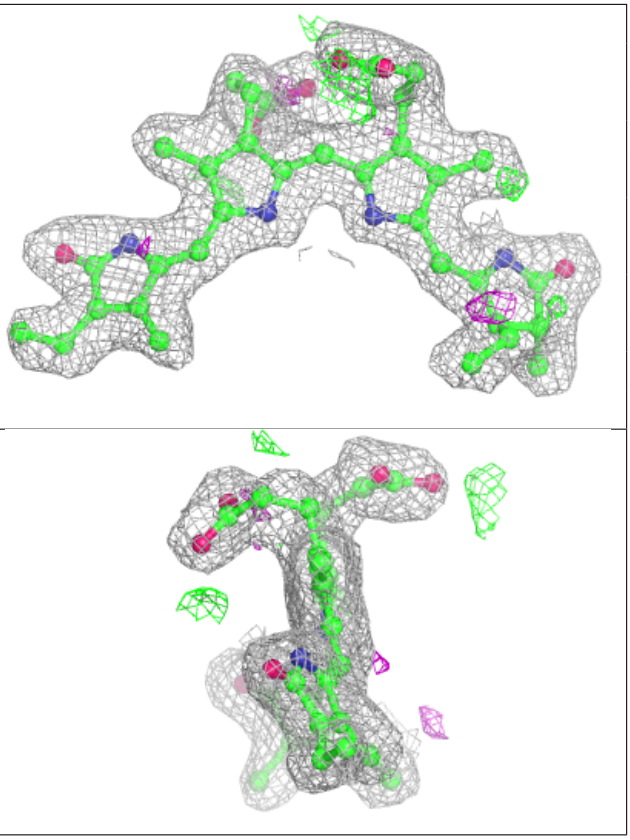






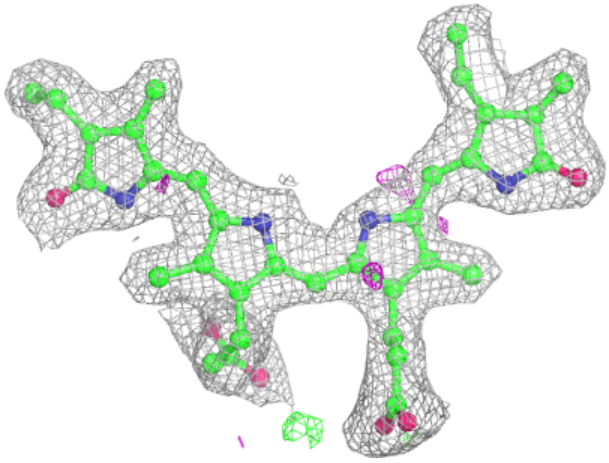
Electron density around CYC T 1153:

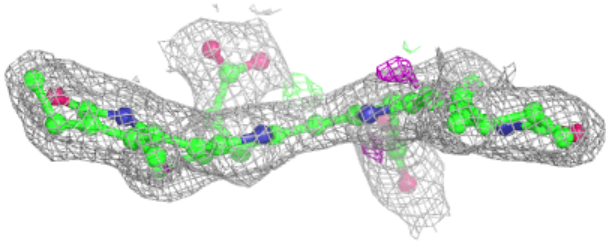
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

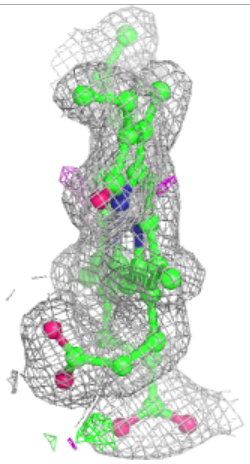


Electron density around CYC U 1084:

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

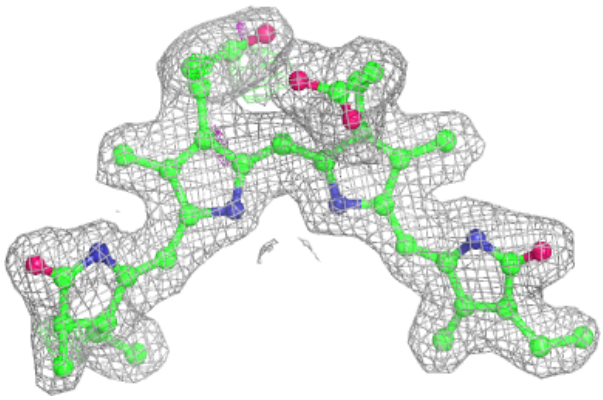


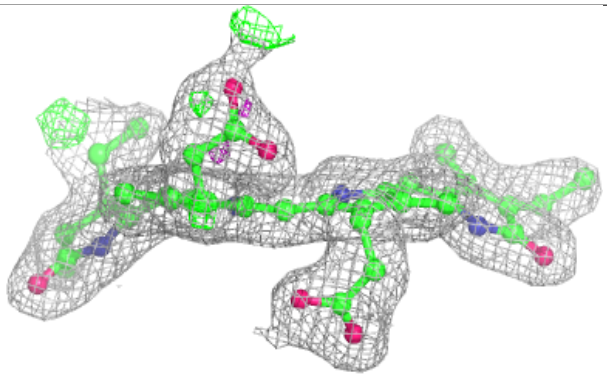


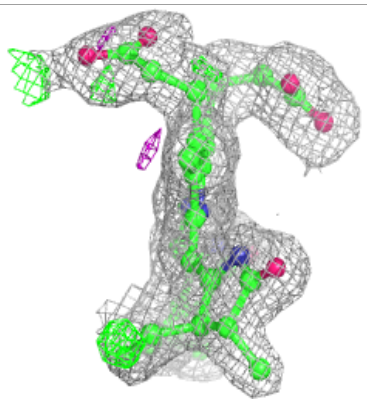


Electron density around CYC F 1153:

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

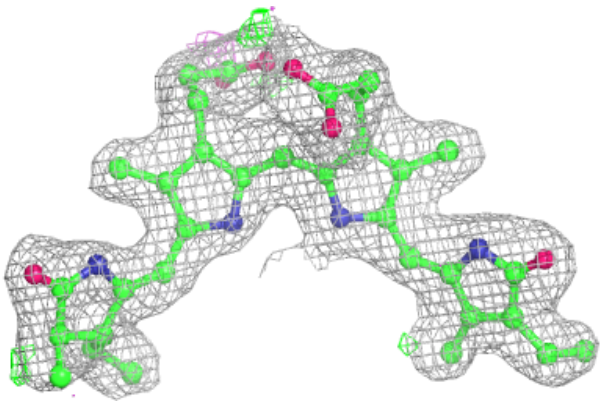


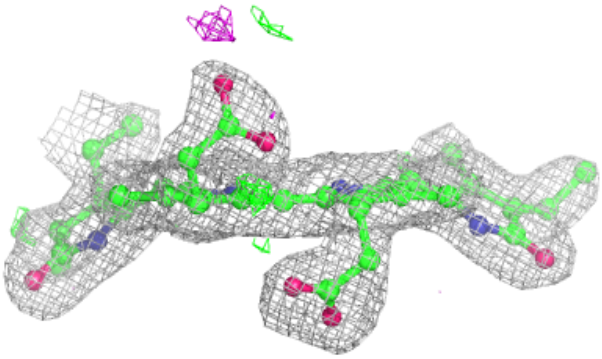


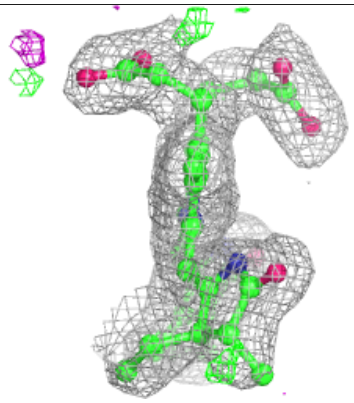


Electron density around CYC P 1153:

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

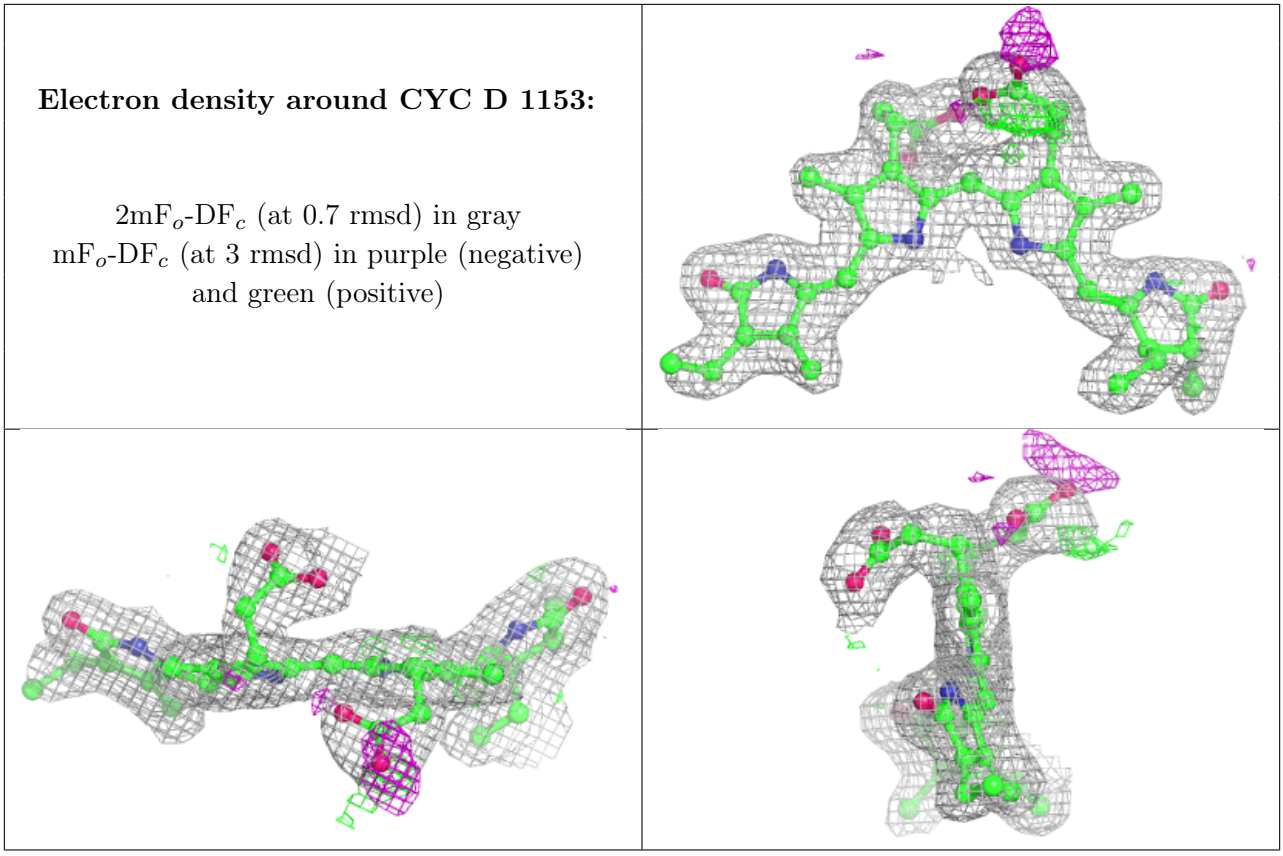






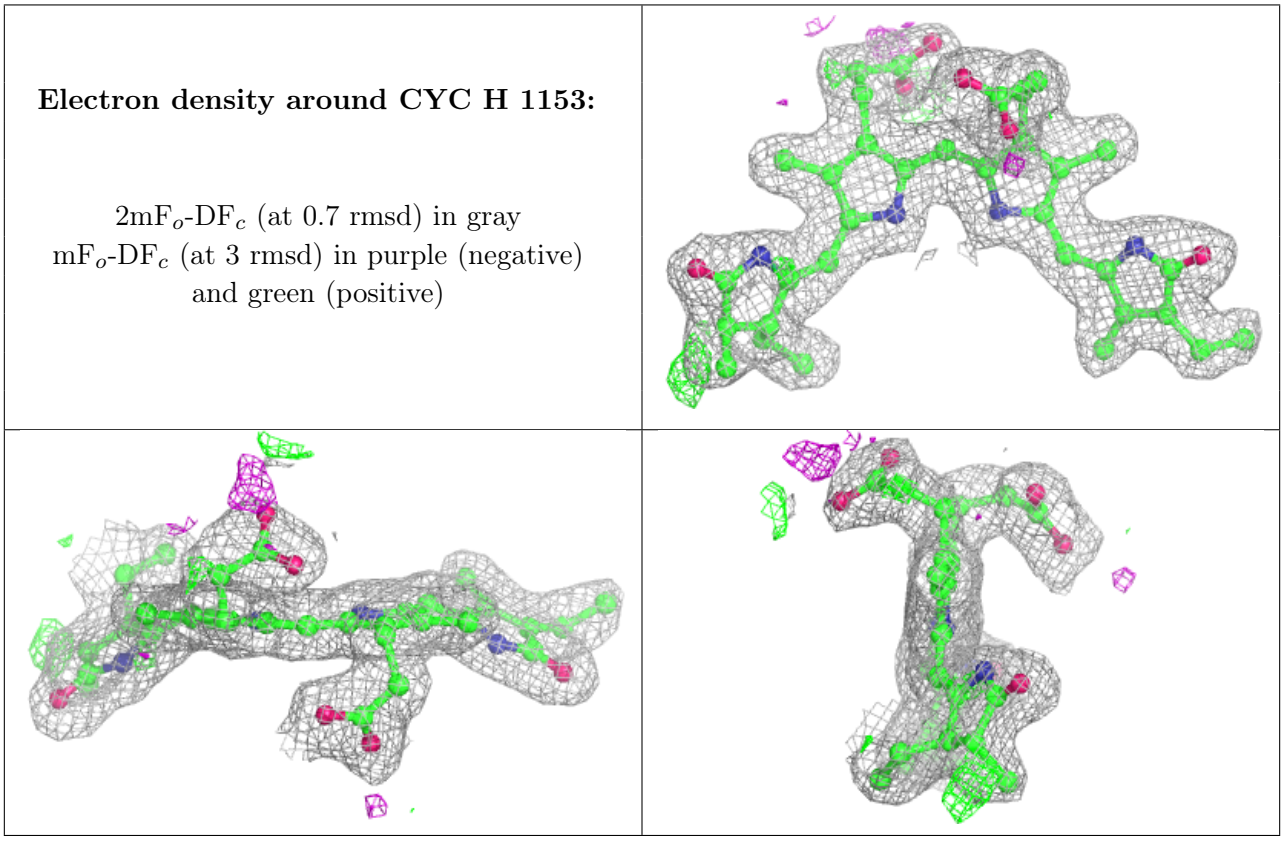
Electron density around CYC D 1153:

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



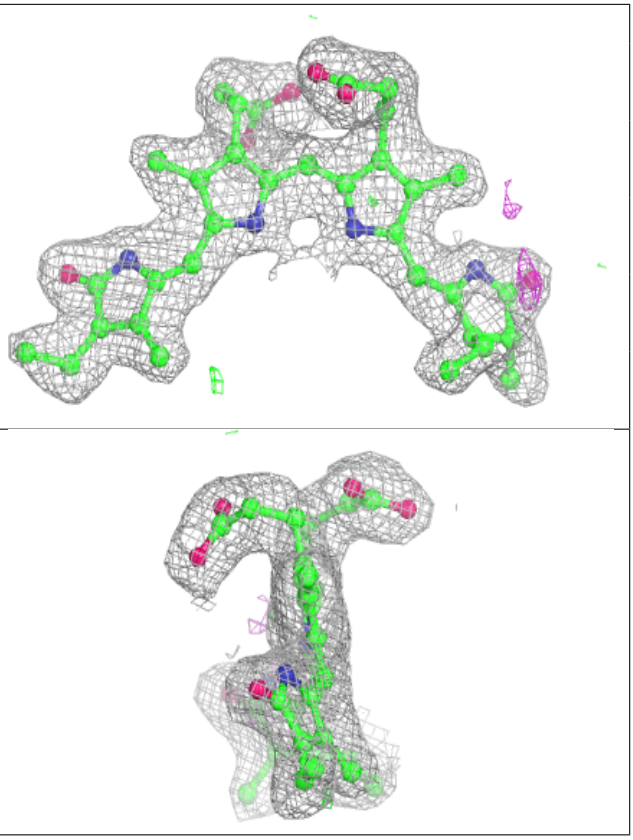
Electron density around CYC H 1153:

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



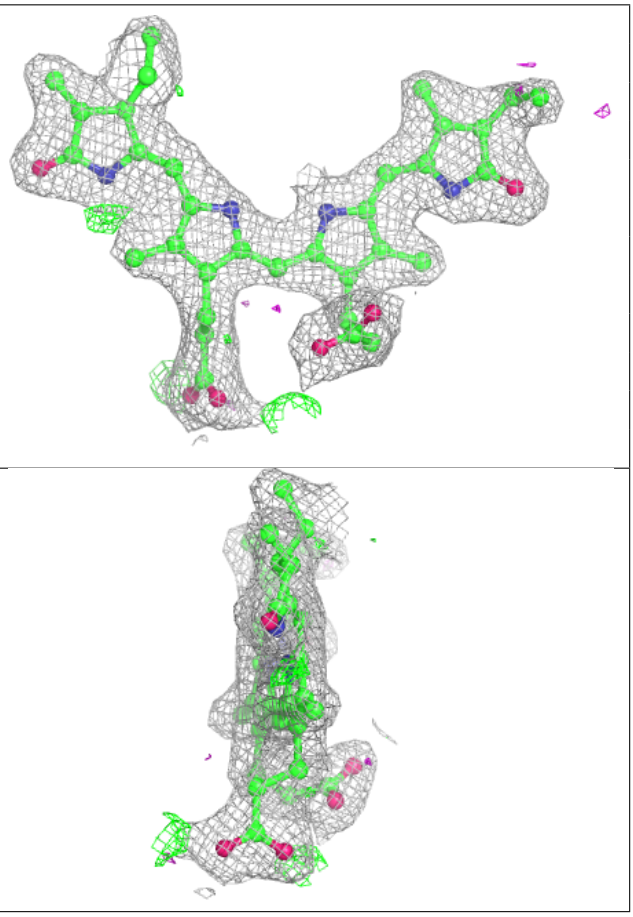
Electron density around CYC J 1153:

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



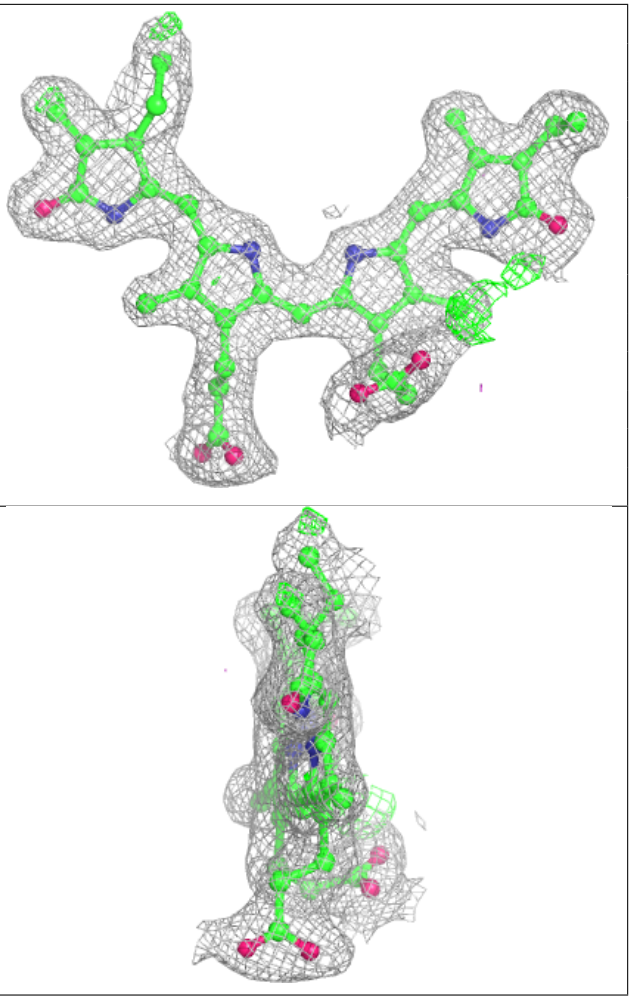
Electron density around CYC M 1084:

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



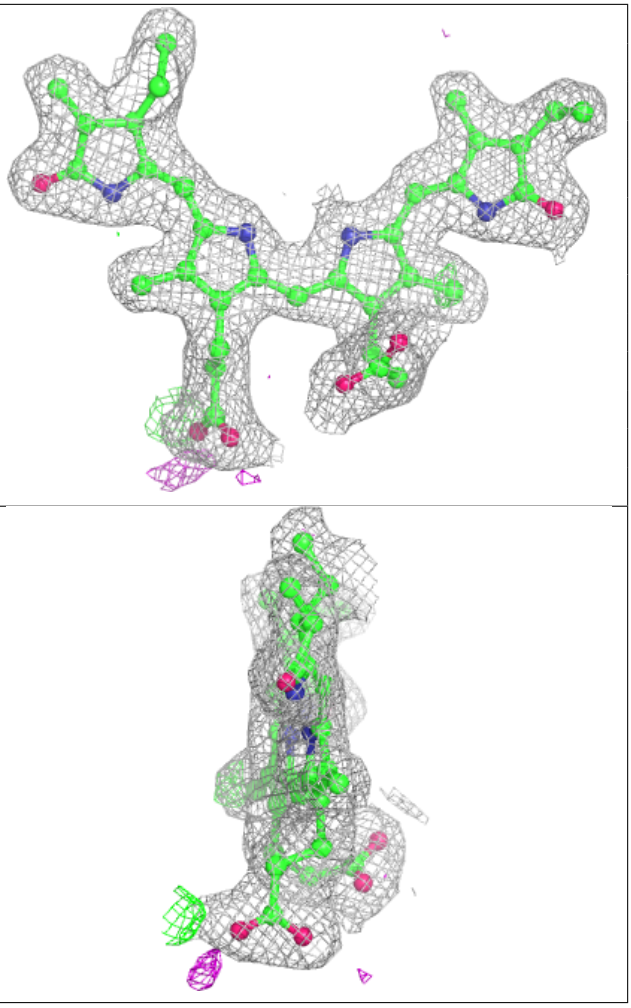
Electron density around CYC W 1084:

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



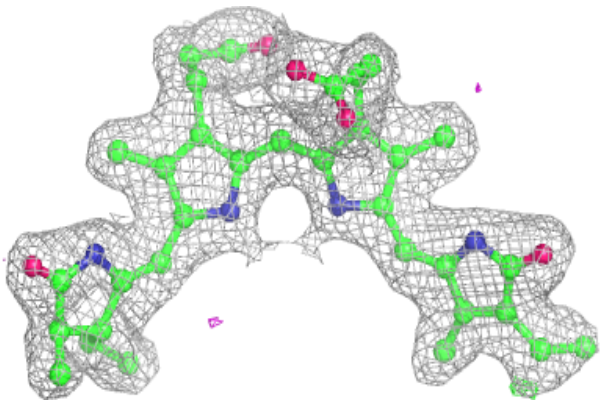
Electron density around CYC I 1084:

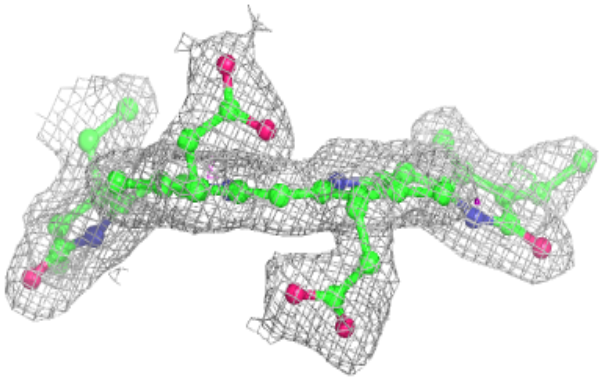
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

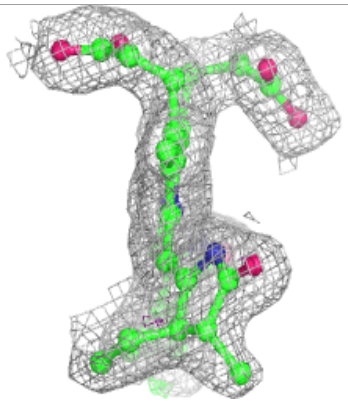


Electron density around CYC V 1153:

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

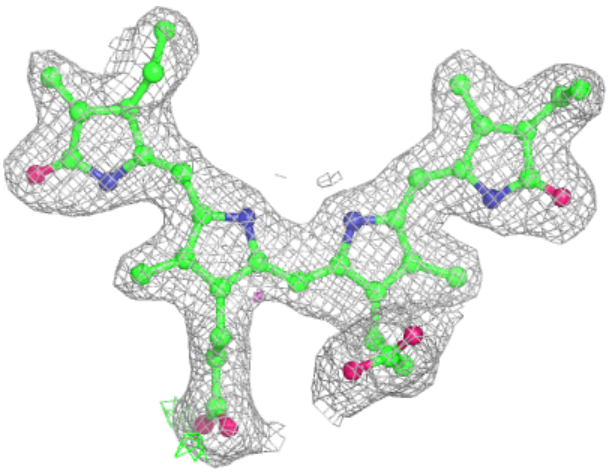


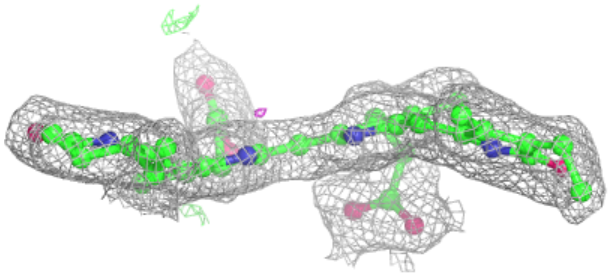


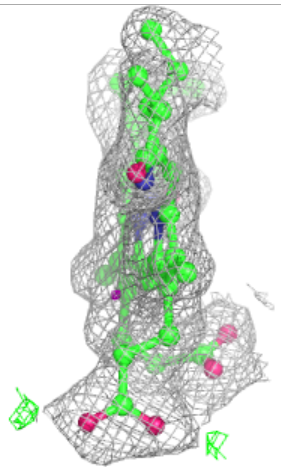


Electron density around CYC C 1084:

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

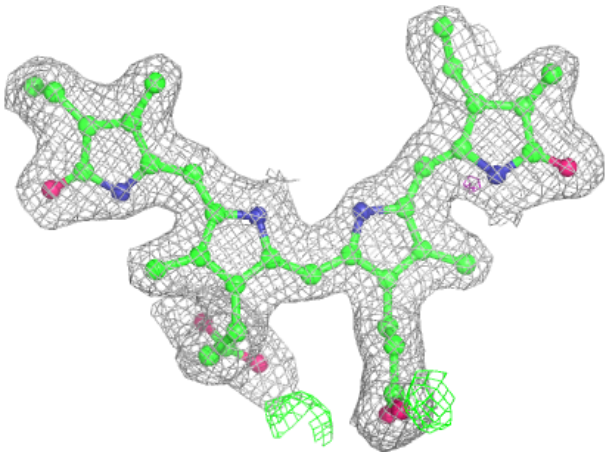


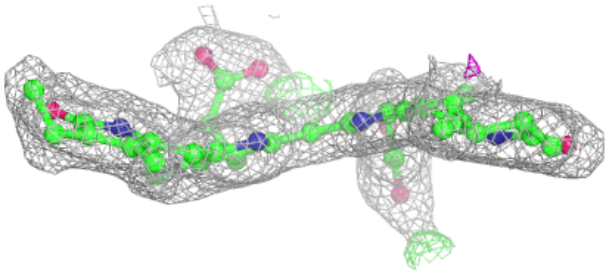


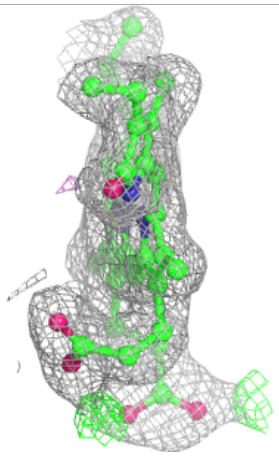


Electron density around CYC O 1084:

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

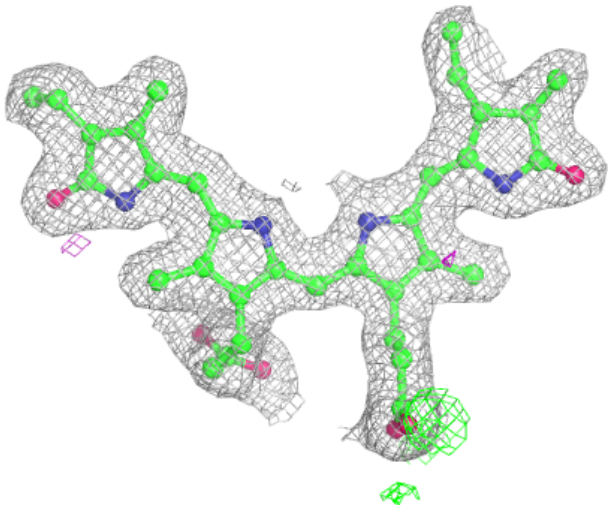


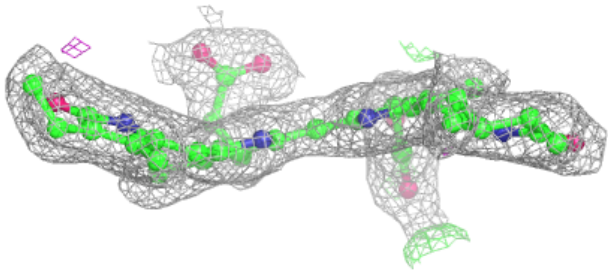


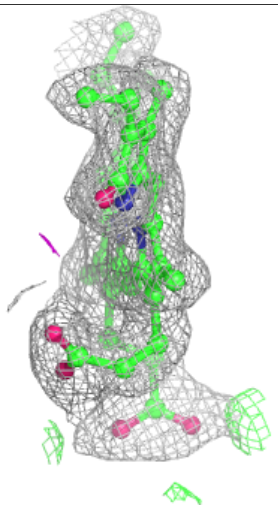


Electron density around CYC K 1084:

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

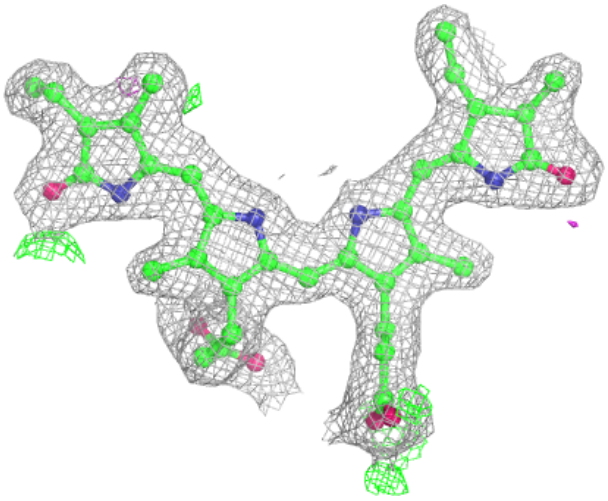


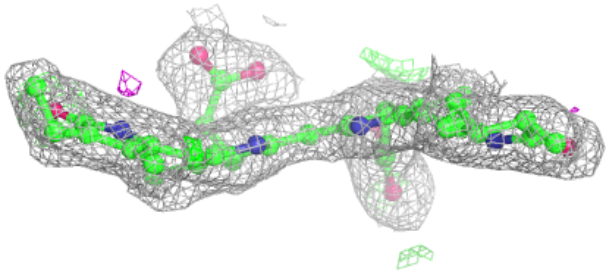


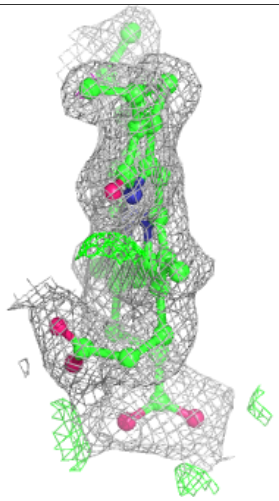


Electron density around CYC G 1084:

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

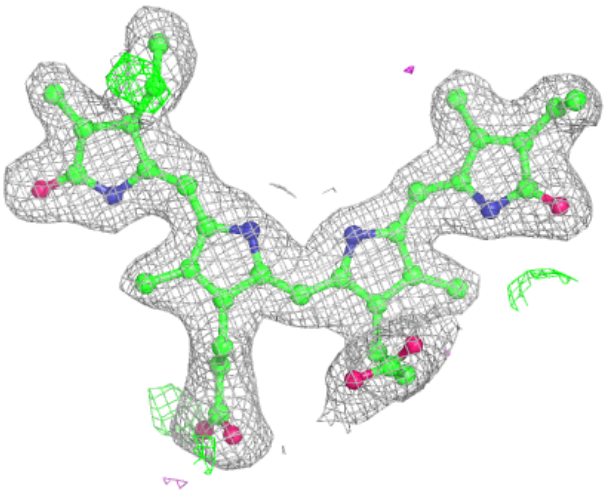


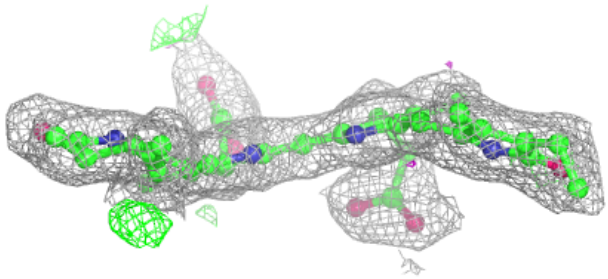


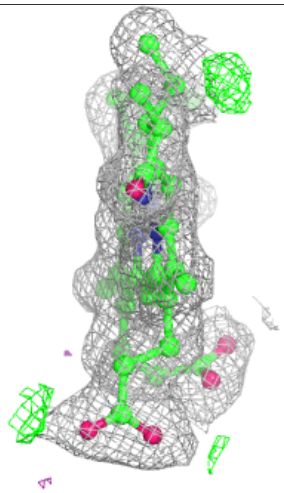


Electron density around CYC Q 1084:

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

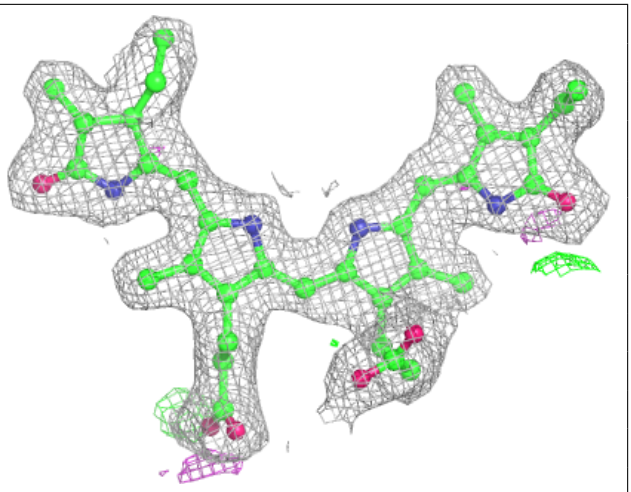


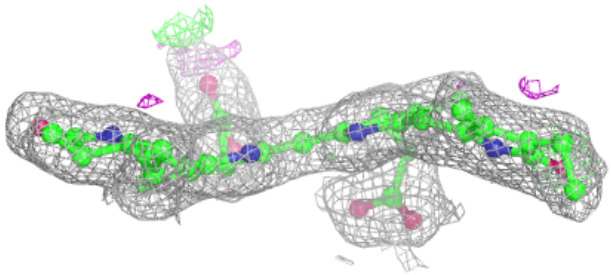


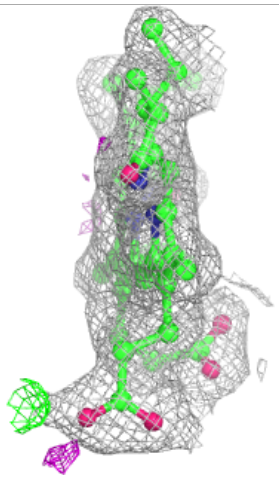


Electron density around CYC S 1084:

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

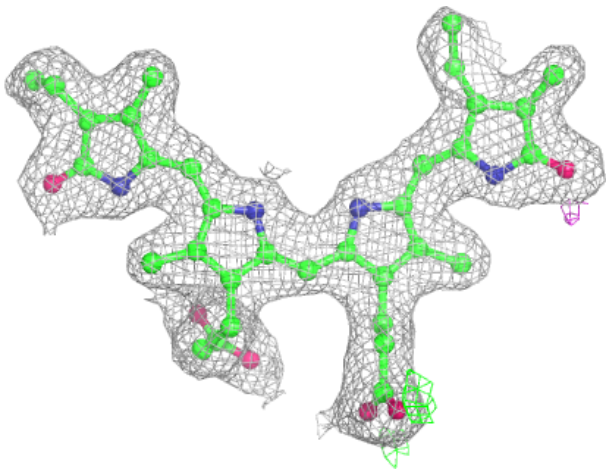


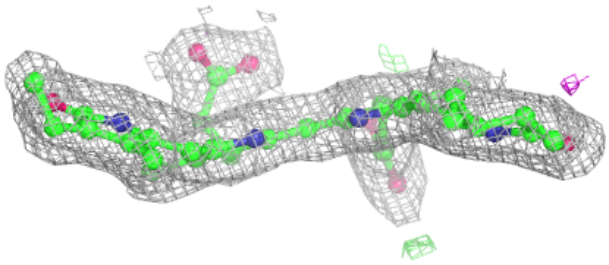


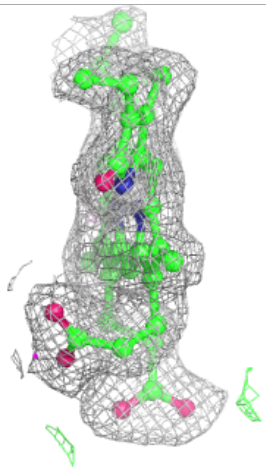


Electron density around CYC A 1084:

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

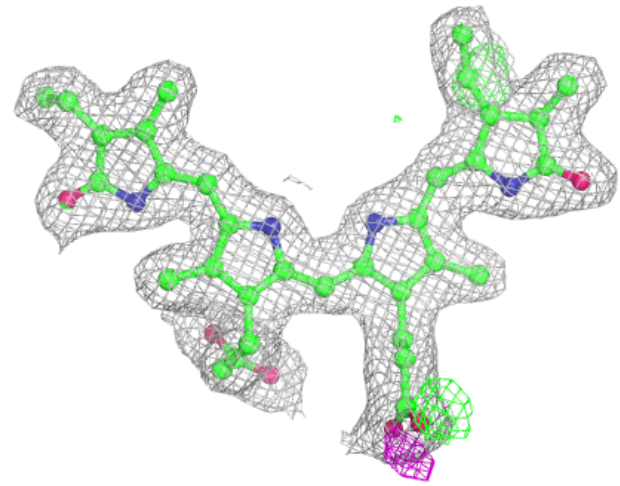


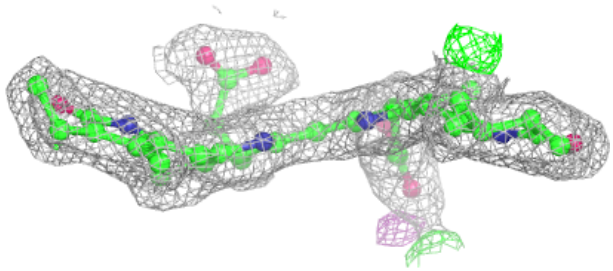


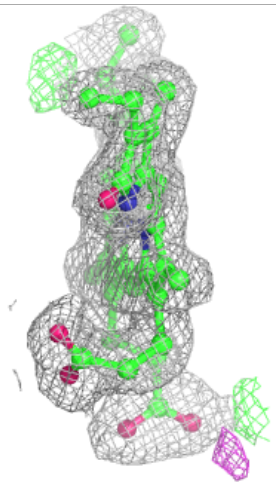


Electron density around CYC E 1084:

$2mF_o$-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.