Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 07:51 pm GMT

PDB ID	:	2UUL
Title	:	Crystal structure of C-phycocyanin from Phormidium, Lyngbya spp. (Marine) and Spirulina sp. (Fresh water) shows two different ways of energy transfer between two hexamers.
Authors	:	Satyanarayana, L.; Patel, A.; Mishra, S.; K Ghosh, P.; Suresh, C.G.
Deposited on	:	2007-03-04
Resolution	:	3.10 Å(reported)

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

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

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

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

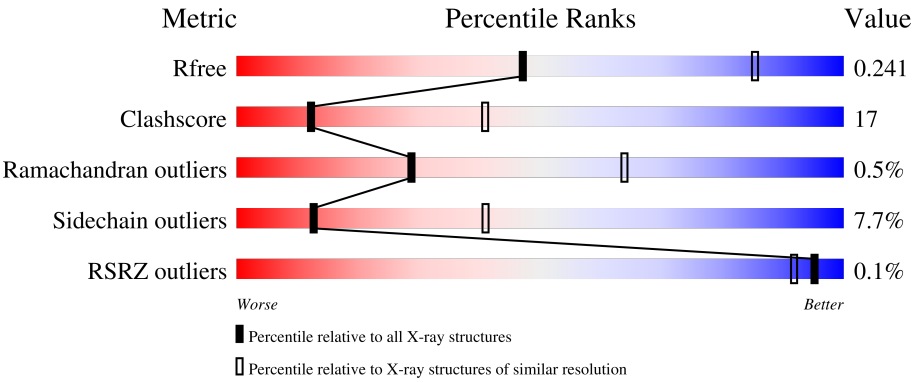
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	75% 22%
1	E	162	77% 21%
1	G	162	% 77% 22%
1	I	162	78% 20%

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Mol	Chain	Length	Quality of chain
1	K	162	69% 30%
1	M	162	77% 22%
1	O	162	79% 17%
1	Q	162	75% 23%
1	S	162	73% 23%
1	U	162	77% 22%
1	W	162	80% 16%
2	B	172	79% 19%
2	F	172	78% 20%
2	J	172	76% 23%
2	L	172	81% 17%
2	N	172	79% 19%
2	P	172	80% 17%
2	R	172	73% 25%
2	T	172	77% 20%
2	V	172	79% 19%
2	X	172	81% 18%
3	C	162	75% 23%
4	D	172	74% 25%
5	H	172	80% 18%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CYC	J	255	-	-	X	-
6	CYC	L	184	-	-	X	-
6	CYC	L	255	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CYC	N	184	-	-	X	-
6	CYC	Q	184	-	-	X	-
6	CYC	T	255	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31131 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 CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	E	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	G	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	I	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	K	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	M	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	O	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	Q	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	S	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	U	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			
1	W	162	Total	C	N	O	S	0	0	0
			1210	761	204	238	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	F	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	J	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	N	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	P	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	R	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	T	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	V	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			
2	X	172	Total	C	N	O	S	0	0	0
			1243	769	219	246	9			

- Molecule 3 is a protein called C-PHYCOCYANIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	162	Total	C	N	O	S	0	0	0
			1213	763	204	239	7			

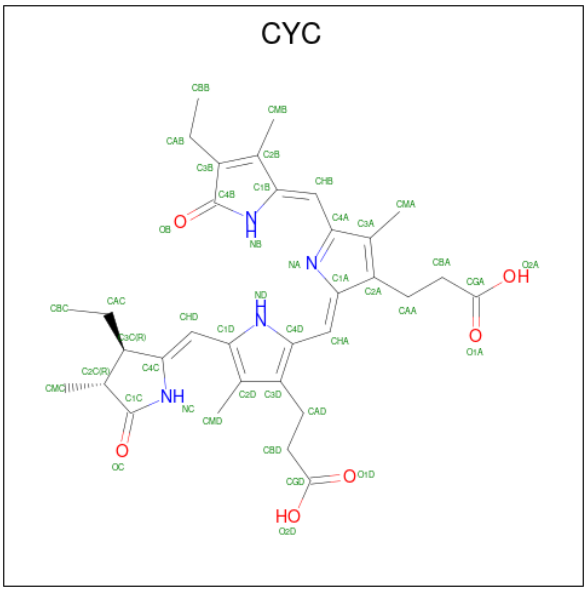
- Molecule 4 is a protein called C-PHYCOCYANIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	172	Total	C	N	O	S	0	0	0
			1252	775	219	249	9			

- Molecule 5 is a protein called C-PHYCOCYANIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	172	Total	C	N	O	S	0	0	0
			1239	764	219	247	9			

- Molecule 6 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

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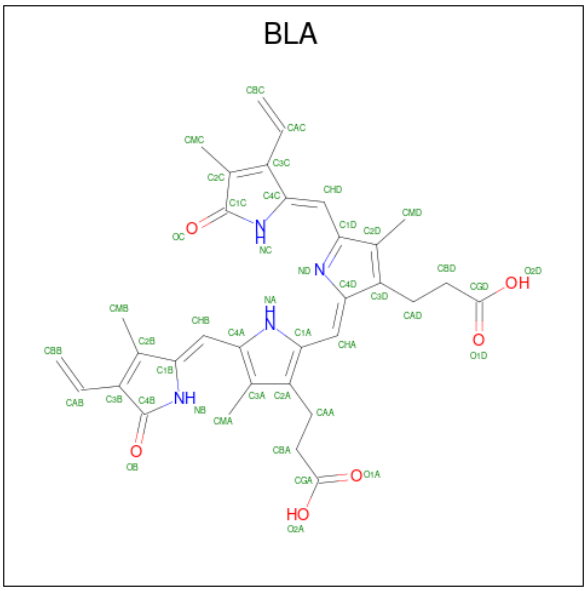
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			43	33	4	6		
6	M	1	Total	C	N	O	0	0
			43	33	4	6		
6	N	1	Total	C	N	O	0	0
			43	33	4	6		
6	N	1	Total	C	N	O	0	0
			43	33	4	6		
6	O	1	Total	C	N	O	0	0
			43	33	4	6		
6	P	1	Total	C	N	O	0	0
			43	33	4	6		
6	P	1	Total	C	N	O	0	0
			43	33	4	6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

- Molecule 7 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	11	Total O 11 11	0	0
8	D	4	Total O 4 4	0	0
8	E	4	Total O 4 4	0	0
8	F	15	Total O 15 15	0	0
8	I	18	Total O 18 18	0	0
8	J	6	Total O 6 6	0	0
8	K	3	Total O 3 3	0	0
8	L	10	Total O 10 10	0	0
8	M	12	Total O 12 12	0	0

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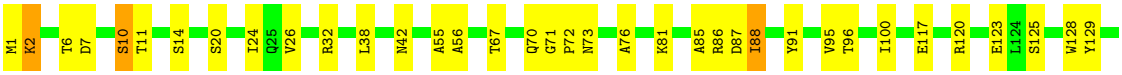
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	N	7	Total O 7 7	0	0
8	O	2	Total O 2 2	0	0
8	P	15	Total O 15 15	0	0
8	S	1	Total O 1 1	0	0
8	T	8	Total O 8 8	0	0
8	W	17	Total O 17 17	0	0
8	X	6	Total O 6 6	0	0

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.

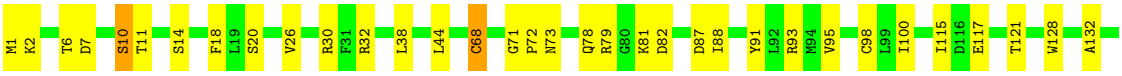
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain A:



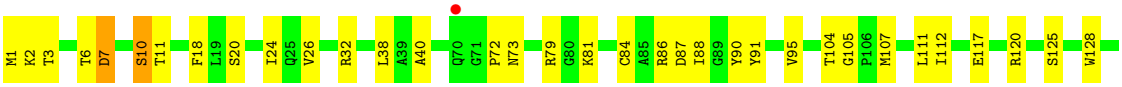
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain E:



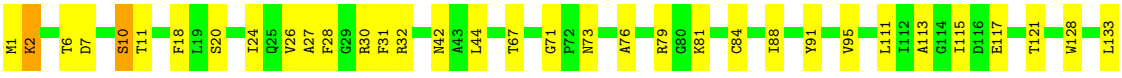
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain G:



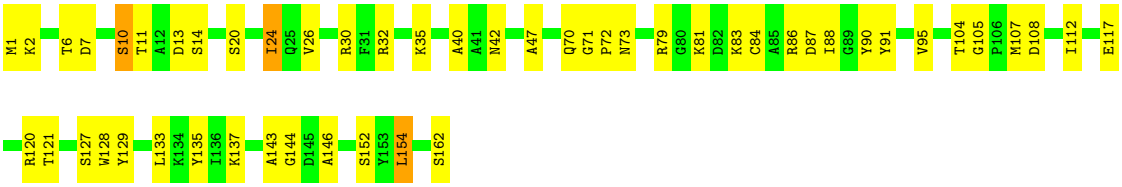
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain I:



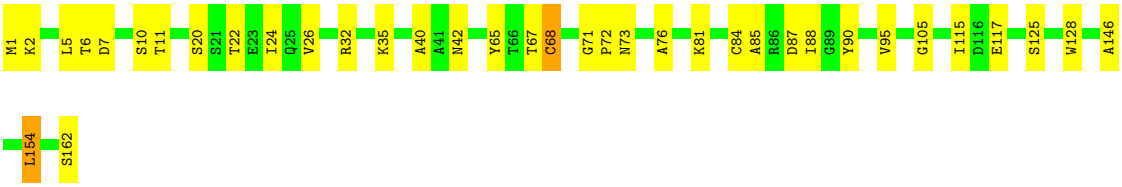
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain K:



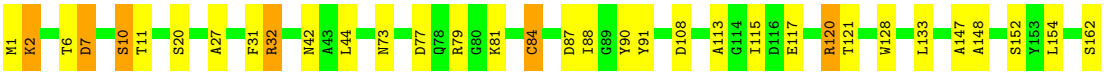
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain M:



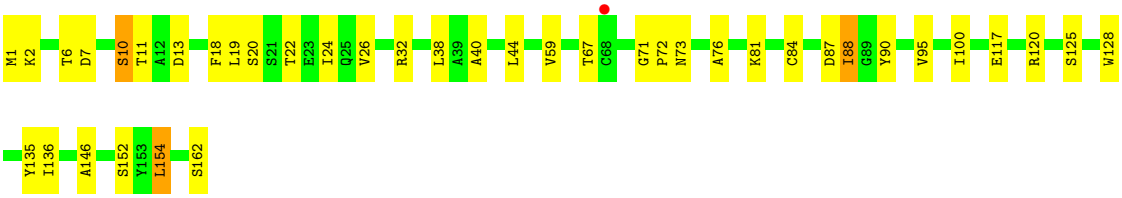
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain O:



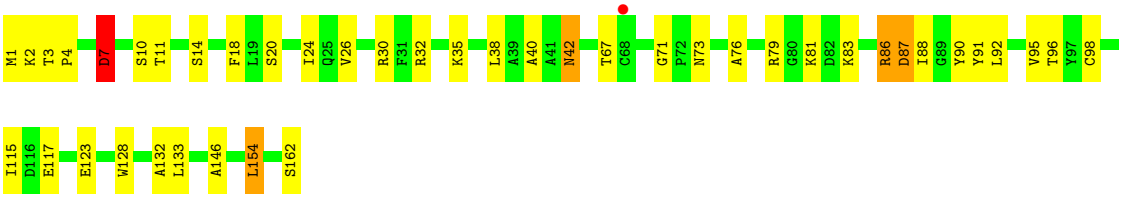
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain Q:



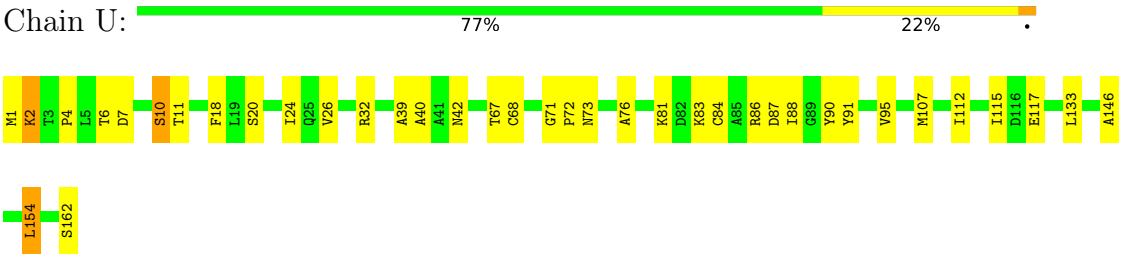
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain S:



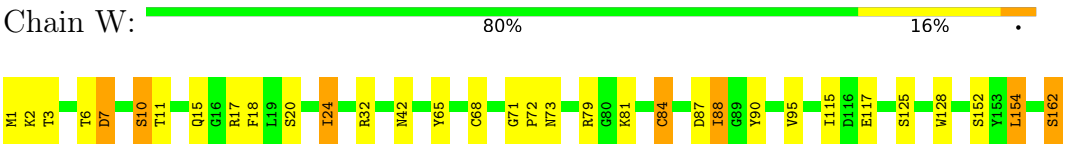
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain U:



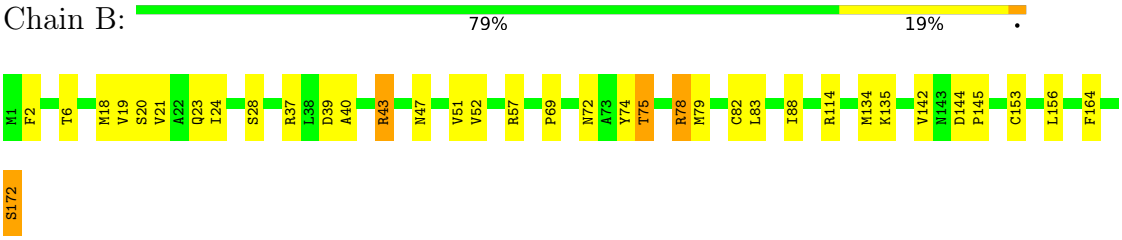
• Molecule 1: C-PHYCOCYANIN ALPHA CHAIN

Chain W:



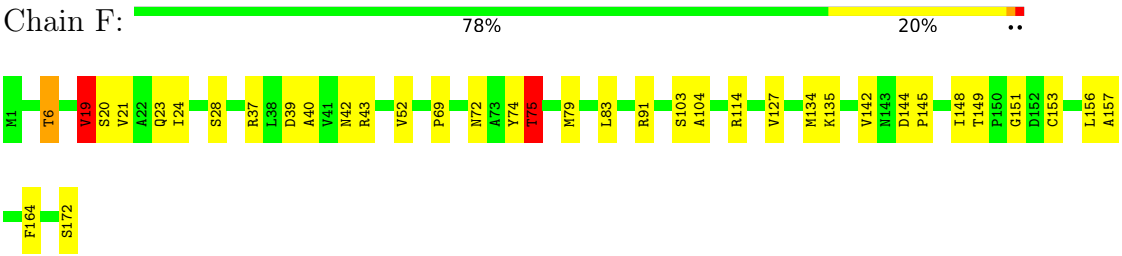
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain B:



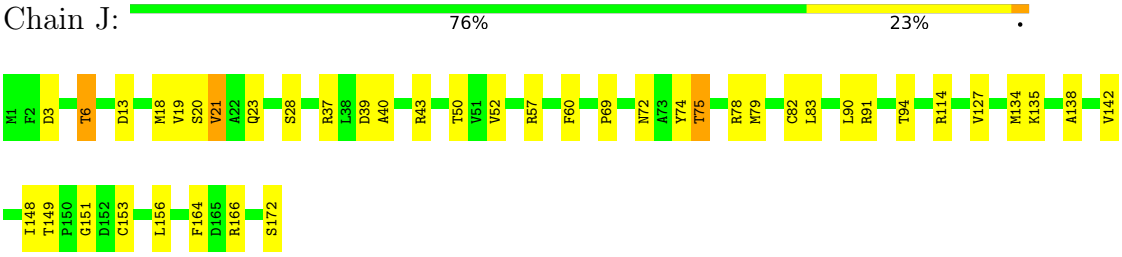
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain F:



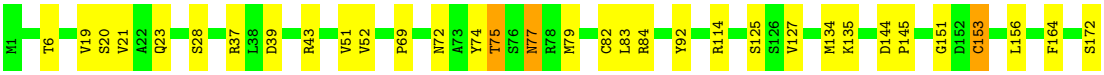
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain J:



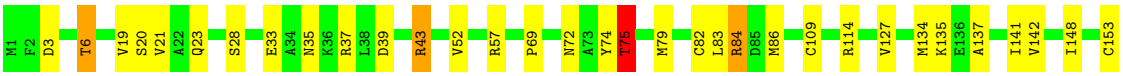
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

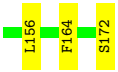
Chain L:



• Molecule 2: C-PHYCOCYANIN BETA CHAIN

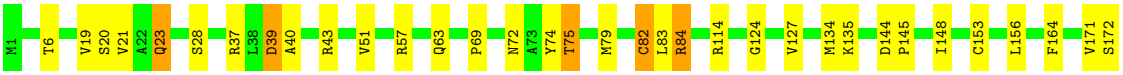
Chain N:





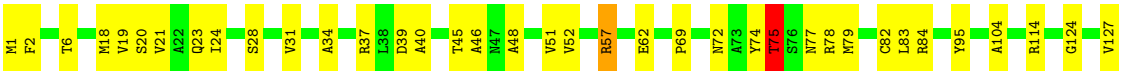
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain P:



• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain R:

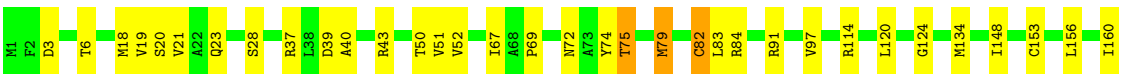


• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain T:

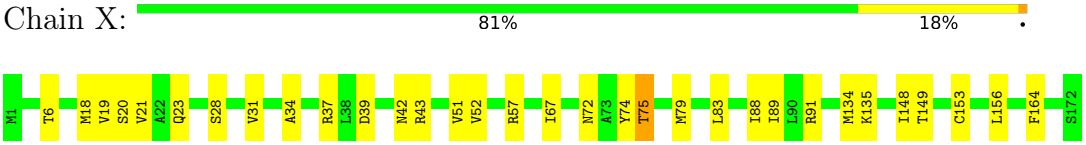
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain V:



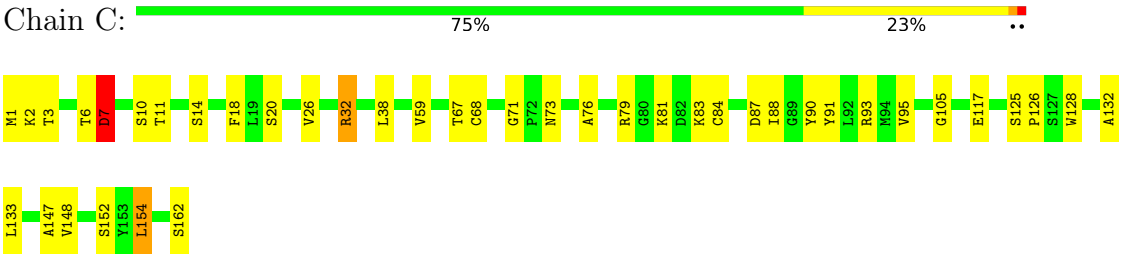
• Molecule 2: C-PHYCOCYANIN BETA CHAIN

Chain X:



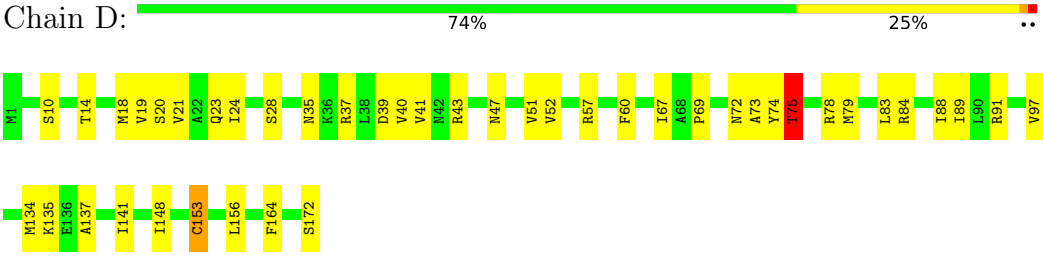
• Molecule 3: C-PHYCOCYANIN ALPHA CHAIN

Chain C:



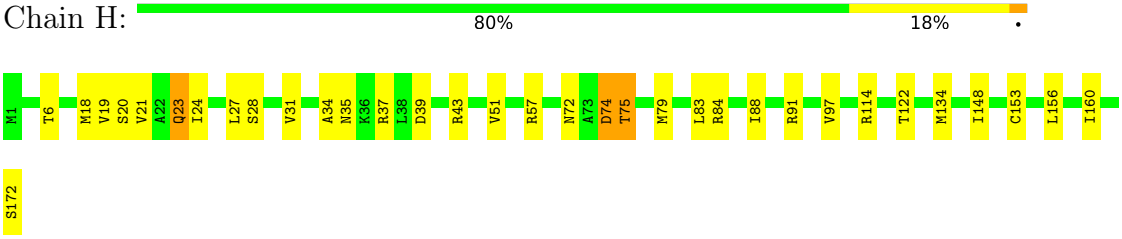
• Molecule 4: C-PHYCOCYANIN BETA CHAIN

Chain D:



• Molecule 5: C-PHYCOCYANIN BETA CHAIN

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.88Å 115.78Å 183.55Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	25.00 – 3.10 24.22 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.5 (25.00-3.10) 92.5 (24.22-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 3.11Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.245 0.197 , 0.241	Depositor DCC
R_{free} test set	3825 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	31131	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.89% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BLA, 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	1.02	2/1233 (0.2%)	0.91	1/1675 (0.1%)
1	E	1.18	2/1233 (0.2%)	1.02	6/1675 (0.4%)
1	G	1.02	0/1233	0.96	2/1675 (0.1%)
1	I	1.03	0/1233	0.96	3/1675 (0.2%)
1	K	1.03	2/1233 (0.2%)	0.97	4/1675 (0.2%)
1	M	1.03	0/1233	0.92	1/1675 (0.1%)
1	O	0.99	1/1233 (0.1%)	0.93	6/1675 (0.4%)
1	Q	1.08	0/1233	0.92	0/1675
1	S	1.17	4/1233 (0.3%)	1.00	6/1675 (0.4%)
1	U	1.00	1/1233 (0.1%)	0.92	1/1675 (0.1%)
1	W	1.02	1/1233 (0.1%)	0.97	1/1675 (0.1%)
2	B	0.94	0/1257	0.88	1/1706 (0.1%)
2	F	0.98	0/1257	0.92	1/1706 (0.1%)
2	J	0.97	1/1257 (0.1%)	0.90	1/1706 (0.1%)
2	L	1.02	2/1257 (0.2%)	0.94	2/1706 (0.1%)
2	N	1.03	0/1257	0.93	2/1706 (0.1%)
2	P	0.94	1/1257 (0.1%)	0.95	2/1706 (0.1%)
2	R	1.04	3/1257 (0.2%)	0.92	1/1706 (0.1%)
2	T	1.04	2/1257 (0.2%)	0.95	1/1706 (0.1%)
2	V	1.04	1/1257 (0.1%)	0.95	2/1706 (0.1%)
2	X	0.95	0/1257	0.90	0/1706
3	C	1.05	0/1236	0.96	2/1679 (0.1%)
4	D	1.02	1/1266 (0.1%)	0.93	1/1718 (0.1%)
5	H	1.00	1/1252 (0.1%)	0.95	1/1699 (0.1%)
All	All	1.03	25/29887 (0.1%)	0.94	48/40581 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	I	0	1
1	K	0	1
1	M	0	1
1	Q	0	1
1	S	0	1
1	U	0	1
1	W	0	1
3	C	0	1
All	All	0	10

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	68	CYS	CB-SG	-17.95	1.51	1.82
4	D	153	CYS	CB-SG	-10.08	1.65	1.82
2	T	153	CYS	CB-SG	-8.71	1.67	1.82
2	R	153	CYS	CB-SG	-7.82	1.69	1.82
5	H	74	ASP	CB-CG	7.23	1.67	1.51
1	S	98	CYS	CB-SG	-7.02	1.70	1.82
1	E	98	CYS	CB-SG	-6.77	1.70	1.82
1	W	84	CYS	CB-SG	-6.67	1.71	1.82
2	L	153	CYS	CB-SG	-6.57	1.71	1.82
1	A	42	ASN	CG-ND2	-6.48	1.16	1.32
1	O	84	CYS	CB-SG	-6.35	1.71	1.82
2	R	46	ALA	CA-CB	6.25	1.65	1.52
1	A	42	ASN	CG-OD1	-6.25	1.10	1.24
2	J	82	CYS	CB-SG	-6.11	1.71	1.82
1	U	39	ALA	CA-CB	5.55	1.64	1.52
1	S	42	ASN	CB-CG	-5.47	1.38	1.51
2	P	82	CYS	CB-SG	-5.37	1.73	1.81
1	K	47	ALA	CA-CB	5.36	1.63	1.52
2	V	82	CYS	CB-SG	-5.36	1.73	1.81
1	K	135	TYR	CE2-CZ	-5.29	1.31	1.38
2	R	82	CYS	CB-SG	-5.11	1.73	1.81
1	S	123	GLU	CG-CD	5.11	1.59	1.51
2	L	77	ASN	CB-CG	5.09	1.62	1.51
1	S	7	ASP	CB-CG	5.05	1.62	1.51
2	T	46	ALA	CA-CB	5.04	1.63	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	30	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	E	68	CYS	CA-CB-SG	8.83	129.89	114.00
5	H	74	ASP	CB-CG-OD1	8.56	126.00	118.30
1	S	87	ASP	CB-CG-OD1	8.20	125.68	118.30
1	E	68	CYS	CB-CA-C	-7.70	94.99	110.40
2	T	39	ASP	CB-CG-OD1	7.01	124.61	118.30
3	C	7	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	L	84	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	S	42	ASN	CB-CA-C	6.67	123.73	110.40
1	W	42	ASN	CB-CA-C	-6.25	97.91	110.40
2	N	84	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	O	42	ASN	CB-CA-C	-6.20	97.99	110.40
1	G	120	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	K	30	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	I	30	ARG	NE-CZ-NH1	5.99	123.29	120.30
2	V	79	MET	CG-SD-CE	-5.99	90.62	100.20
1	U	42	ASN	CB-CA-C	-5.98	98.44	110.40
1	K	30	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	K	120	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	L	84	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	79	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	K	42	ASN	CB-CA-C	-5.75	98.89	110.40
1	O	120	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	O	32	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	D	78	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	O	108	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	N	84	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	E	93	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	P	84	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	S	86	ARG	NE-CZ-NH2	-5.42	117.59	120.30
3	C	93	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	S	79	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	S	7	ASP	CB-CG-OD1	5.30	123.07	118.30
1	O	7	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	I	42	ASN	CB-CA-C	-5.28	99.84	110.40
2	P	39	ASP	CB-CG-OD1	5.27	123.05	118.30
2	F	19	VAL	CG1-CB-CG2	-5.26	102.49	110.90
1	G	79	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	V	82	CYS	CA-CB-SG	-5.23	104.59	114.00
1	O	77	ASP	CB-CG-OD1	5.20	122.98	118.30
2	R	57	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	120	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	I	30	ARG	NE-CZ-NH2	-5.14	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	42	ASN	CB-CA-C	-5.09	100.23	110.40
1	E	87	ASP	CB-CG-OD1	5.05	122.84	118.30
2	J	166	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	S	30	ARG	NE-CZ-NH2	-5.01	117.79	120.30
2	B	78	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	71	GLY	Peptide
3	C	71	GLY	Peptide
1	E	71	GLY	Peptide
1	I	71	GLY	Peptide
1	K	71	GLY	Peptide
1	M	71	GLY	Peptide
1	Q	71	GLY	Peptide
1	S	71	GLY	Peptide
1	U	71	GLY	Peptide
1	W	71	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1210	0	1168	21	0
1	E	1210	0	1168	16	0
1	G	1210	0	1168	22	0
1	I	1210	0	1168	19	0
1	K	1210	0	1168	26	0
1	M	1210	0	1168	24	0
1	O	1210	0	1168	20	0
1	Q	1210	0	1169	28	0
1	S	1210	0	1168	22	0
1	U	1210	0	1168	17	0
1	W	1210	0	1168	19	0
2	B	1243	0	1238	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1243	0	1238	37	0
2	J	1243	0	1238	39	0
2	L	1243	0	1239	42	1
2	N	1243	0	1239	44	1
2	P	1243	0	1239	43	0
2	R	1243	0	1238	47	1
2	T	1243	0	1238	43	1
2	V	1243	0	1239	39	0
2	X	1243	0	1238	30	0
3	C	1213	0	1172	27	0
4	D	1252	0	1250	48	0
5	H	1239	0	1233	36	0
6	A	43	0	36	14	0
6	C	43	0	35	16	0
6	D	43	0	37	15	0
6	E	43	0	36	19	0
6	F	86	0	75	29	0
6	G	43	0	35	13	0
6	H	86	0	75	24	0
6	I	43	0	36	12	0
6	J	86	0	75	36	0
6	K	43	0	36	18	0
6	L	86	0	76	45	0
6	M	43	0	37	16	0
6	N	86	0	76	41	0
6	O	43	0	35	19	0
6	P	86	0	76	34	0
6	Q	43	0	37	23	0
6	R	86	0	75	28	0
6	S	43	0	36	15	0
6	T	86	0	75	40	0
6	U	43	0	36	20	0
6	V	86	0	76	25	0
6	W	43	0	35	13	0
6	X	86	0	75	28	0
7	B	86	0	63	26	0
7	D	43	0	32	17	0
8	C	11	0	0	3	0
8	D	4	0	0	0	0
8	E	4	0	0	1	0
8	F	15	0	0	2	0
8	I	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	6	0	0	1	0
8	K	3	0	0	0	0
8	L	10	0	0	2	0
8	M	12	0	0	3	0
8	N	7	0	0	2	0
8	O	2	0	0	0	0
8	P	15	0	0	3	0
8	S	1	0	0	0	0
8	T	8	0	0	1	0
8	W	17	0	0	2	0
8	X	6	0	0	0	0
All	All	31131	0	30204	1037	2

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 17.

All (1037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:82:CYS:SG	6:V:184:CYC:HAC2	1.21	1.75
2:J:153:CYS:SG	6:J:255:CYC:HBC3	1.22	1.73
2:R:153:CYS:SG	6:R:255:CYC:HBC3	1.15	1.71
2:N:82:CYS:SG	6:N:184:CYC:HAC2	1.30	1.68
2:P:82:CYS:SG	6:P:184:CYC:HAC2	1.17	1.68
1:Q:84:CYS:SG	6:Q:184:CYC:HAC2	1.28	1.64
2:V:153:CYS:SG	6:V:255:CYC:HBC3	1.34	1.62
2:X:153:CYS:SG	6:X:255:CYC:HAC1	1.41	1.57
2:L:82:CYS:SG	6:L:184:CYC:HAC2	1.49	1.52
2:F:153:CYS:SG	6:F:255:CYC:HAC2	1.52	1.49
5:H:153:CYS:SG	6:H:255:CYC:HAC2	1.58	1.41
2:T:153:CYS:SG	6:T:255:CYC:HAC1	1.63	1.38
6:J:184:CYC:HMA1	6:J:184:CYC:NB	1.37	1.37
2:P:153:CYS:SG	6:P:255:CYC:CBC	2.16	1.33
6:J:184:CYC:HB	6:J:184:CYC:CMA	1.40	1.33
6:N:184:CYC:HMA1	6:N:184:CYC:NB	1.40	1.32
2:V:82:CYS:SG	6:V:184:CYC:CAC	2.16	1.32
6:N:184:CYC:HB	6:N:184:CYC:CMA	1.41	1.31
2:L:82:CYS:SG	6:L:184:CYC:CBC	2.18	1.30
2:R:74:TYR:O	2:R:75:THR:HG23	1.31	1.29
2:P:153:CYS:SG	6:P:255:CYC:HBC3	1.73	1.29
1:Q:84:CYS:SG	6:Q:184:CYC:CAC	2.20	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:153:CYS:SG	6:X:255:CYC:CAC	2.20	1.28
6:E:184:CYC:HMA1	6:E:184:CYC:NB	1.46	1.28
2:N:153:CYS:SG	6:N:255:CYC:HAC1	1.75	1.26
2:R:74:TYR:O	2:R:75:THR:CG2	1.83	1.26
7:D:255:BLA:HMA1	7:D:255:BLA:NB	1.48	1.25
6:G:184:CYC:HMA1	6:G:184:CYC:NB	1.50	1.24
6:V:255:CYC:HMA1	6:V:255:CYC:NB	1.52	1.24
6:E:184:CYC:HB	6:E:184:CYC:CMA	1.52	1.22
6:P:184:CYC:HC	6:P:184:CYC:CMD	1.51	1.21
6:J:255:CYC:HMA1	6:J:255:CYC:CMB	1.71	1.20
2:V:153:CYS:SG	6:V:255:CYC:CBC	2.30	1.20
6:I:184:CYC:HMA1	6:I:184:CYC:NB	1.55	1.20
6:L:184:CYC:HB	6:L:184:CYC:CMA	1.55	1.19
6:L:184:CYC:HMA1	6:L:184:CYC:NB	1.55	1.19
6:D:184:CYC:HMA1	6:D:184:CYC:NB	1.57	1.18
7:D:255:BLA:HB	7:D:255:BLA:CMA	1.54	1.18
6:G:184:CYC:HB	6:G:184:CYC:CMA	1.55	1.17
6:H:184:CYC:HB	6:H:184:CYC:CMA	1.59	1.15
6:X:184:CYC:HC	6:X:184:CYC:CMD	1.60	1.15
6:A:184:CYC:HMA1	6:A:184:CYC:NB	1.63	1.14
2:P:74:TYR:O	2:P:75:THR:HG23	1.44	1.13
6:F:184:CYC:HMA1	6:F:184:CYC:NB	1.64	1.13
6:S:184:CYC:HB	6:S:184:CYC:HMA1	0.97	1.13
2:X:74:TYR:O	2:X:75:THR:HG23	1.46	1.13
6:I:184:CYC:HB	6:I:184:CYC:CMA	1.60	1.12
6:H:255:CYC:HMA1	6:H:255:CYC:NB	1.63	1.12
6:R:255:CYC:HMA1	6:R:255:CYC:NB	1.62	1.12
6:T:184:CYC:CMA	6:T:184:CYC:HB	1.61	1.12
2:V:74:TYR:O	2:V:75:THR:HG23	1.48	1.12
2:T:74:TYR:O	2:T:75:THR:HG23	1.48	1.12
6:V:255:CYC:HB	6:V:255:CYC:CMA	1.62	1.11
6:X:255:CYC:HMA1	6:X:255:CYC:NB	1.64	1.11
2:B:74:TYR:O	2:B:75:THR:HG23	1.51	1.11
6:H:184:CYC:HMA1	6:H:184:CYC:NB	1.62	1.11
6:R:184:CYC:HC	6:R:184:CYC:CMD	1.64	1.11
6:T:184:CYC:HMA1	6:T:184:CYC:NB	1.64	1.10
7:B:184:BLA:HMA1	7:B:184:BLA:HB	1.04	1.10
6:D:184:CYC:HC	6:D:184:CYC:CMD	1.64	1.10
6:F:184:CYC:CMD	6:F:184:CYC:HC	1.64	1.10
6:M:184:CYC:HMA1	6:M:184:CYC:NB	1.64	1.10
6:N:255:CYC:HB	6:N:255:CYC:HMA1	1.02	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:184:CYC:HB	6:D:184:CYC:CMA	1.65	1.10
6:R:184:CYC:NB	6:R:184:CYC:HMA1	1.66	1.09
6:W:184:CYC:HB	6:W:184:CYC:HMA1	1.05	1.09
6:X:184:CYC:HB	6:X:184:CYC:HMA1	1.12	1.09
6:M:184:CYC:CMA	6:M:184:CYC:HB	1.64	1.09
2:J:74:TYR:O	2:J:75:THR:HG23	1.51	1.09
6:F:184:CYC:HB	6:F:184:CYC:CMA	1.65	1.09
6:J:255:CYC:HMA1	6:J:255:CYC:HMB2	1.33	1.09
6:Q:184:CYC:HC	6:Q:184:CYC:CMD	1.65	1.09
6:T:255:CYC:HB	6:T:255:CYC:HMA1	0.94	1.08
2:F:153:CYS:SG	6:F:255:CYC:CAC	2.42	1.08
2:F:74:TYR:O	2:F:75:THR:HG23	1.54	1.06
2:L:82:CYS:SG	6:L:184:CYC:HBC2	1.88	1.06
6:V:184:CYC:HMA1	6:V:184:CYC:NB	1.69	1.06
6:C:184:CYC:HMA1	6:C:184:CYC:NB	1.67	1.06
6:U:184:CYC:HMA1	6:U:184:CYC:NB	1.70	1.06
6:O:184:CYC:HMA1	6:O:184:CYC:NB	1.71	1.06
6:P:184:CYC:HMA1	6:P:184:CYC:NB	1.68	1.06
6:R:184:CYC:HB	6:R:184:CYC:CMA	1.67	1.06
2:T:153:CYS:SG	6:T:255:CYC:CAC	2.43	1.06
6:A:184:CYC:HB	6:A:184:CYC:CMA	1.68	1.05
6:K:184:CYC:HMA1	6:K:184:CYC:NB	1.71	1.05
6:L:184:CYC:HC	6:L:184:CYC:CMD	1.69	1.05
2:T:39:ASP:OD1	6:T:255:CYC:HHB	1.56	1.05
6:T:184:CYC:HB	6:T:184:CYC:HMA1	0.94	1.05
6:L:255:CYC:HMA1	6:L:255:CYC:NB	1.71	1.05
6:Q:184:CYC:HB	6:Q:184:CYC:HMA1	0.94	1.04
6:U:184:CYC:HC	6:U:184:CYC:CMD	1.70	1.04
2:P:74:TYR:O	2:P:75:THR:CG2	2.04	1.03
6:K:184:CYC:HMA1	6:K:184:CYC:HB	0.87	1.03
6:U:184:CYC:HMA1	6:U:184:CYC:HB	0.86	1.03
2:L:74:TYR:O	2:L:75:THR:HG23	1.58	1.03
5:H:153:CYS:SG	6:H:255:CYC:CAC	2.47	1.02
6:H:255:CYC:HB	6:H:255:CYC:CMA	1.71	1.02
6:O:184:CYC:HMA1	6:O:184:CYC:HB	0.86	1.02
6:P:184:CYC:HB	6:P:184:CYC:CMA	1.72	1.02
2:V:74:TYR:O	2:V:75:THR:CG2	2.06	1.02
2:B:74:TYR:O	2:B:75:THR:CG2	2.07	1.02
6:T:184:CYC:HC	6:T:184:CYC:CMD	1.72	1.02
6:U:184:CYC:HB	6:U:184:CYC:CMA	1.72	1.02
6:V:184:CYC:HB	6:V:184:CYC:CMA	1.72	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:184:CYC:HBD1	6:U:184:CYC:HHA	1.41	1.01
6:X:255:CYC:HB	6:X:255:CYC:CMA	1.72	1.01
6:H:184:CYC:HB	6:H:184:CYC:HMA1	0.85	1.01
6:M:184:CYC:HMA1	6:M:184:CYC:HB	0.86	1.01
1:Q:84:CYS:HG	6:Q:184:CYC:HAC2	1.26	1.00
1:W:128:TRP:CE3	6:W:184:CYC:HMC3	1.95	1.00
6:K:184:CYC:HB	6:K:184:CYC:CMA	1.74	1.00
6:L:255:CYC:HMA1	6:L:255:CYC:HB	0.85	0.99
6:P:184:CYC:HMA1	6:P:184:CYC:HB	0.82	0.99
2:P:153:CYS:SG	6:P:255:CYC:CAC	2.50	0.99
6:C:184:CYC:HMA1	6:C:184:CYC:HB	0.82	0.99
4:D:74:TYR:O	4:D:75:THR:CG2	2.10	0.99
6:L:255:CYC:HB	6:L:255:CYC:CMA	1.75	0.99
6:F:184:CYC:HMA1	6:F:184:CYC:HB	0.82	0.99
5:H:74:ASP:O	5:H:75:THR:HG23	1.64	0.98
6:R:184:CYC:HMA1	6:R:184:CYC:HB	0.86	0.98
6:V:184:CYC:HMA1	6:V:184:CYC:HB	0.84	0.98
6:C:184:CYC:HC	6:C:184:CYC:CMD	1.77	0.98
6:P:255:CYC:HBC2	6:P:255:CYC:CHD	1.90	0.98
6:Q:184:CYC:HMA1	6:Q:184:CYC:NB	1.79	0.98
2:X:74:TYR:O	2:X:75:THR:CG2	2.09	0.97
1:K:84:CYS:HA	6:K:184:CYC:HBC3	1.44	0.97
6:R:255:CYC:HB	6:R:255:CYC:CMA	1.76	0.97
2:J:74:TYR:O	2:J:75:THR:CG2	2.13	0.97
2:N:82:CYS:SG	6:N:184:CYC:CBC	2.53	0.97
2:T:74:TYR:O	2:T:75:THR:CG2	2.12	0.97
2:B:153:CYS:SG	7:B:255:BLA:HAC	2.04	0.96
2:T:20:SER:H	2:T:23:GLN:HE21	1.11	0.96
2:P:172:SER:HB3	8:P:2015:HOH:O	1.64	0.96
6:O:184:CYC:HC	6:O:184:CYC:CMD	1.77	0.95
6:C:184:CYC:HB	6:C:184:CYC:CMA	1.77	0.95
6:J:255:CYC:HMA1	6:J:255:CYC:HMB3	1.46	0.95
1:O:73:ASN:O	6:O:184:CYC:HMD2	1.67	0.95
2:B:82:CYS:SG	7:B:184:BLA:CBC	2.55	0.95
2:B:153:CYS:SG	7:B:255:BLA:CAC	2.55	0.95
6:N:184:CYC:HC	6:N:184:CYC:CMD	1.78	0.95
1:O:128:TRP:CE3	6:O:184:CYC:HMC3	2.02	0.95
6:T:255:CYC:HMA1	6:T:255:CYC:NB	1.80	0.95
6:P:184:CYC:HC	6:P:184:CYC:HMD2	1.33	0.94
2:N:74:TYR:O	2:N:75:THR:HG23	1.66	0.94
6:S:184:CYC:HMA1	6:S:184:CYC:NB	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:184:CYC:HB	6:L:184:CYC:HMA1	0.77	0.93
4:D:153:CYS:SG	7:D:255:BLA:CAC	2.57	0.93
6:M:184:CYC:O1D	2:P:57:ARG:NH1	2.02	0.93
2:F:74:TYR:O	2:F:75:THR:CG2	2.17	0.93
2:P:153:CYS:SG	6:P:255:CYC:HAC1	2.07	0.92
6:O:184:CYC:HB	6:O:184:CYC:CMA	1.81	0.92
2:N:153:CYS:SG	6:N:255:CYC:CAC	2.58	0.92
6:P:184:CYC:HC	6:P:184:CYC:HMD3	1.32	0.92
2:B:20:SER:H	2:B:23:GLN:HE21	1.12	0.91
6:E:184:CYC:HC	6:E:184:CYC:CMD	1.83	0.91
4:D:40:VAL:CG1	4:D:156:LEU:HD21	2.00	0.91
5:H:20:SER:H	5:H:23:GLN:HE21	1.12	0.91
6:T:255:CYC:HB	6:T:255:CYC:CMA	1.83	0.91
6:A:184:CYC:HMA1	6:A:184:CYC:HB	0.77	0.91
5:H:39:ASP:OD1	6:H:255:CYC:HHB	1.70	0.90
2:N:20:SER:H	2:N:23:GLN:HE21	1.20	0.90
2:F:72:ASN:OD1	6:F:184:CYC:HMD2	1.71	0.90
2:X:20:SER:H	2:X:23:GLN:HE21	1.14	0.90
2:R:74:TYR:O	2:R:75:THR:HG22	1.71	0.89
7:B:184:BLA:HMA1	7:B:184:BLA:NB	1.87	0.88
6:H:255:CYC:HMA1	6:H:255:CYC:HB	0.77	0.88
2:L:153:CYS:SG	6:L:255:CYC:HBC3	2.13	0.88
4:D:39:ASP:OD1	7:D:255:BLA:HHB	1.74	0.88
6:Q:184:CYC:HC	6:Q:184:CYC:HMD2	1.37	0.88
2:R:20:SER:H	2:R:23:GLN:HE21	1.15	0.88
6:X:255:CYC:HMA1	6:X:255:CYC:HB	0.78	0.88
6:N:255:CYC:HMA1	6:N:255:CYC:NB	1.88	0.88
1:K:73:ASN:O	6:K:184:CYC:HMD2	1.73	0.88
1:M:35:LYS:HA	8:M:2003:HOH:O	1.72	0.88
6:P:255:CYC:HB	6:P:255:CYC:HMA1	1.38	0.88
2:J:20:SER:H	2:J:23:GLN:HE21	1.17	0.87
4:D:74:TYR:O	4:D:75:THR:HG22	1.72	0.87
2:L:20:SER:H	2:L:23:GLN:HE21	1.20	0.87
6:S:184:CYC:HC	6:S:184:CYC:CMD	1.86	0.87
2:P:20:SER:H	2:P:23:GLN:HE21	1.16	0.87
7:B:184:BLA:HB	7:B:184:BLA:CMA	1.86	0.86
5:H:74:ASP:O	5:H:75:THR:CG2	2.23	0.86
6:R:184:CYC:HC	6:R:184:CYC:HMD2	1.38	0.86
2:B:153:CYS:SG	7:B:255:BLA:C1C	2.64	0.86
6:P:184:CYC:CMD	6:P:184:CYC:NC	2.37	0.86
6:J:255:CYC:OB	6:J:255:CYC:HBB3	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:184:CYC:HC	6:R:184:CYC:HMD3	1.39	0.85
6:D:184:CYC:HC	6:D:184:CYC:HMD2	1.40	0.85
2:F:20:SER:H	2:F:23:GLN:HE21	1.21	0.85
1:E:128:TRP:CE3	6:E:184:CYC:HMC3	2.11	0.85
1:U:73:ASN:O	6:U:184:CYC:HMD2	1.76	0.85
6:R:255:CYC:HMA1	6:R:255:CYC:HB	0.79	0.85
6:U:184:CYC:HC	6:U:184:CYC:HMD2	1.41	0.85
5:H:57:ARG:NH1	6:K:184:CYC:O1D	2.10	0.85
4:D:37:ARG:O	4:D:40:VAL:HG13	1.77	0.84
6:Q:184:CYC:HC	6:Q:184:CYC:HMD3	1.39	0.84
6:F:255:CYC:HB	6:F:255:CYC:HMA1	1.41	0.84
6:X:184:CYC:HC	6:X:184:CYC:HMD3	1.43	0.84
2:N:69:PRO:HA	2:N:74:TYR:CD2	2.12	0.84
2:L:82:CYS:CB	6:L:184:CYC:HAC2	2.07	0.84
1:S:128:TRP:CE3	6:S:184:CYC:HMC3	2.12	0.83
6:N:184:CYC:HMA1	6:N:184:CYC:HB	0.68	0.83
2:P:153:CYS:SG	6:P:255:CYC:HBC1	2.18	0.83
2:J:153:CYS:SG	6:J:255:CYC:CAC	2.67	0.83
6:P:184:CYC:HBD1	6:P:184:CYC:HHA	1.59	0.83
6:F:184:CYC:HC	6:F:184:CYC:HMD2	1.42	0.83
7:B:184:BLA:HC	7:B:184:BLA:CMD	1.92	0.83
2:B:20:SER:H	2:B:23:GLN:NE2	1.75	0.83
6:N:255:CYC:HBD1	6:N:255:CYC:HHA	1.61	0.83
6:O:184:CYC:HC	6:O:184:CYC:HMD2	1.42	0.82
6:X:184:CYC:HMA1	6:X:184:CYC:NB	1.94	0.82
6:L:184:CYC:HC	6:L:184:CYC:HMD2	1.43	0.82
4:D:40:VAL:CG2	4:D:97:VAL:HG11	2.08	0.82
2:L:74:TYR:O	2:L:75:THR:CG2	2.26	0.82
6:A:184:CYC:CMD	6:A:184:CYC:HC	1.93	0.82
2:T:20:SER:H	2:T:23:GLN:NE2	1.77	0.82
6:X:184:CYC:HC	6:X:184:CYC:HMD2	1.43	0.82
2:T:72:ASN:OD1	6:T:184:CYC:HMD2	1.77	0.82
6:S:184:CYC:HBD2	6:S:184:CYC:HHA	1.60	0.81
6:L:255:CYC:CHD	6:L:255:CYC:HBC2	2.10	0.81
6:U:184:CYC:HC	6:U:184:CYC:HMD3	1.46	0.81
6:X:184:CYC:HB	6:X:184:CYC:CMA	1.91	0.81
2:V:39:ASP:OD1	6:V:255:CYC:HHB	1.80	0.81
6:F:184:CYC:HC	6:F:184:CYC:HMD3	1.44	0.81
2:L:153:CYS:SG	6:L:255:CYC:CBC	2.69	0.81
4:D:74:TYR:O	4:D:75:THR:HG23	1.78	0.81
2:L:153:CYS:SG	6:L:255:CYC:HAC1	2.20	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:255:CYC:HB	6:N:255:CYC:CMA	1.91	0.80
6:C:184:CYC:HC	6:C:184:CYC:HMD2	1.46	0.80
2:N:74:TYR:O	2:N:75:THR:CG2	2.29	0.80
6:D:184:CYC:HC	6:D:184:CYC:HMD3	1.46	0.80
6:I:184:CYC:HMA1	6:I:184:CYC:HB	0.70	0.80
1:Q:73:ASN:O	6:Q:184:CYC:HMD2	1.81	0.80
6:W:184:CYC:HMA1	6:W:184:CYC:NB	1.91	0.80
2:V:148:ILE:HD13	6:V:255:CYC:HHD	1.64	0.80
6:V:184:CYC:HC	6:V:184:CYC:CMD	1.95	0.80
5:H:20:SER:H	5:H:23:GLN:NE2	1.81	0.79
6:T:255:CYC:HC	6:T:255:CYC:CMD	1.94	0.79
4:D:40:VAL:HG11	4:D:156:LEU:HD21	1.64	0.79
2:P:20:SER:H	2:P:23:GLN:NE2	1.80	0.79
4:D:40:VAL:HG21	4:D:97:VAL:HG11	1.64	0.78
6:H:184:CYC:HC	6:H:184:CYC:CMD	1.97	0.78
2:F:6:THR:HG21	8:F:2001:HOH:O	1.83	0.78
6:T:184:CYC:HC	6:T:184:CYC:HMD2	1.46	0.78
2:X:20:SER:H	2:X:23:GLN:NE2	1.81	0.78
2:X:153:CYS:SG	6:X:255:CYC:HAC2	2.23	0.78
6:D:184:CYC:HMA1	6:D:184:CYC:HB	0.72	0.78
2:R:74:TYR:C	2:R:75:THR:CG2	2.51	0.78
6:L:184:CYC:HC	6:L:184:CYC:HMD3	1.46	0.78
1:S:73:ASN:O	6:S:184:CYC:HMD2	1.84	0.78
3:C:73:ASN:O	6:C:184:CYC:HMD2	1.83	0.77
2:J:13:ASP:OD1	2:L:74:TYR:OH	2.02	0.77
2:J:72:ASN:OD1	6:J:184:CYC:HMD2	1.82	0.77
6:Q:184:CYC:HB	6:Q:184:CYC:CMA	1.88	0.77
2:R:20:SER:H	2:R:23:GLN:NE2	1.81	0.77
2:J:153:CYS:HG	6:J:255:CYC:HBC3	0.96	0.77
6:N:184:CYC:HC	6:N:184:CYC:HMD2	1.50	0.77
4:D:20:SER:H	4:D:23:GLN:HE21	1.32	0.77
2:J:20:SER:H	2:J:23:GLN:NE2	1.81	0.77
3:C:83:LYS:HE3	8:C:2007:HOH:O	1.84	0.76
3:C:68:CYS:HB2	1:M:68:CYS:O	1.86	0.76
2:V:20:SER:H	2:V:23:GLN:HE21	1.33	0.76
7:D:255:BLA:HC	7:D:255:BLA:CMD	1.98	0.76
2:L:153:CYS:SG	6:L:255:CYC:CAC	2.73	0.76
6:I:184:CYC:HC	6:I:184:CYC:CMD	1.97	0.76
7:B:255:BLA:HB	7:B:255:BLA:HMA1	1.49	0.76
6:O:184:CYC:HBD2	6:O:184:CYC:HHA	1.65	0.76
2:X:39:ASP:OD1	6:X:255:CYC:HHB	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:184:CYC:HB	6:T:184:CYC:C3A	1.96	0.76
7:D:255:BLA:HBD1	7:D:255:BLA:HHA	1.68	0.75
2:P:153:CYS:HG	6:P:255:CYC:HBC3	1.47	0.75
6:T:184:CYC:HC	6:T:184:CYC:HMD3	1.50	0.75
6:L:255:CYC:CHD	6:L:255:CYC:CBC	2.64	0.75
6:N:184:CYC:HB	6:N:184:CYC:C3A	1.96	0.75
2:R:39:ASP:OD1	6:R:255:CYC:HHB	1.87	0.75
2:L:39:ASP:OD1	6:L:255:CYC:HHB	1.85	0.75
6:N:184:CYC:HC	6:N:184:CYC:HMD3	1.52	0.74
2:P:82:CYS:SG	6:P:184:CYC:CBC	2.74	0.74
1:W:73:ASN:O	6:W:184:CYC:HMD2	1.86	0.74
1:M:73:ASN:HA	6:M:184:CYC:HBD2	1.70	0.74
2:V:19:VAL:HG12	2:V:23:GLN:HB2	1.69	0.74
6:G:184:CYC:HMA1	6:G:184:CYC:HB	0.65	0.74
2:J:153:CYS:HG	6:J:255:CYC:CBC	1.72	0.74
7:D:255:BLA:CHD	7:D:255:BLA:HBC1	2.17	0.73
6:J:184:CYC:HC	6:J:184:CYC:CMD	2.00	0.73
2:N:20:SER:H	2:N:23:GLN:NE2	1.85	0.73
2:P:172:SER:CB	8:P:2015:HOH:O	2.30	0.73
6:J:255:CYC:OB	6:J:255:CYC:CBB	2.35	0.73
6:E:184:CYC:HC	6:E:184:CYC:HMD2	1.53	0.73
2:F:39:ASP:OD1	6:F:255:CYC:HHB	1.88	0.73
2:P:74:TYR:C	2:P:75:THR:CG2	2.53	0.73
6:R:184:CYC:CMD	6:R:184:CYC:NC	2.48	0.73
6:C:184:CYC:HC	6:C:184:CYC:HMD3	1.51	0.73
1:K:72:PRO:O	6:K:184:CYC:HBD2	1.89	0.73
6:L:255:CYC:HC	6:L:255:CYC:CMD	2.02	0.72
1:I:128:TRP:CE3	6:I:184:CYC:HMC3	2.23	0.72
6:I:184:CYC:HMD1	6:I:184:CYC:HBD1	1.71	0.72
2:L:72:ASN:OD1	6:L:184:CYC:HMD2	1.89	0.72
6:E:184:CYC:CBD	6:E:184:CYC:HHA	2.19	0.72
1:M:73:ASN:O	6:M:184:CYC:HMD2	1.89	0.72
6:J:184:CYC:HMA1	6:J:184:CYC:HB	0.60	0.72
2:P:74:TYR:C	2:P:75:THR:HG22	2.10	0.72
6:J:184:CYC:HB	6:J:184:CYC:C3A	2.03	0.71
6:P:255:CYC:CBC	6:P:255:CYC:CHD	2.57	0.71
2:T:153:CYS:SG	6:T:255:CYC:CBC	2.79	0.71
2:F:157:ALA:HB1	8:F:2012:HOH:O	1.89	0.71
4:D:19:VAL:HG12	4:D:23:GLN:HB2	1.73	0.71
2:R:153:CYS:SG	6:R:255:CYC:CAC	2.78	0.71
2:V:74:TYR:C	2:V:75:THR:CG2	2.59	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:255:BLA:HBD1	7:B:255:BLA:HHA	1.71	0.71
4:D:153:CYS:SG	7:D:255:BLA:CBC	2.79	0.71
6:T:255:CYC:HBA1	6:T:255:CYC:HHA	1.71	0.70
2:B:72:ASN:OD1	7:B:184:BLA:HMD2	1.91	0.70
6:O:184:CYC:HC	6:O:184:CYC:HMD3	1.54	0.70
6:W:184:CYC:HB	6:W:184:CYC:CMA	1.93	0.70
2:F:20:SER:H	2:F:23:GLN:NE2	1.90	0.70
6:O:184:CYC:HHA	6:O:184:CYC:CBD	2.22	0.69
6:E:184:CYC:HC	6:E:184:CYC:HMD3	1.56	0.69
6:K:184:CYC:CMD	6:K:184:CYC:HC	2.05	0.69
1:S:128:TRP:CD2	6:S:184:CYC:HMC3	2.28	0.69
2:N:39:ASP:OD1	6:N:255:CYC:HHB	1.92	0.69
1:A:72:PRO:O	6:A:184:CYC:HBD1	1.93	0.69
2:J:74:TYR:C	2:J:75:THR:CG2	2.60	0.69
6:X:255:CYC:HC	6:X:255:CYC:CMD	2.06	0.69
3:C:148:VAL:HG11	6:L:255:CYC:HMB3	1.73	0.69
6:R:255:CYC:HC	6:R:255:CYC:CMD	2.06	0.69
2:N:19:VAL:HG12	2:N:23:GLN:HB2	1.74	0.68
2:N:127:VAL:HG22	6:N:184:CYC:H3C	1.75	0.68
2:N:6:THR:HG21	8:N:2002:HOH:O	1.93	0.68
6:Q:184:CYC:CMD	6:Q:184:CYC:NC	2.48	0.68
2:R:74:TYR:C	2:R:75:THR:HG22	2.11	0.68
1:O:73:ASN:O	6:O:184:CYC:CMD	2.41	0.68
6:E:184:CYC:HMA1	6:E:184:CYC:HB	0.62	0.68
2:R:72:ASN:OD1	6:R:184:CYC:HMD2	1.93	0.67
2:L:20:SER:H	2:L:23:GLN:NE2	1.90	0.67
6:S:184:CYC:HC	6:S:184:CYC:HMD3	1.59	0.67
2:T:37:ARG:O	2:T:40:ALA:HB3	1.94	0.67
2:F:74:TYR:C	2:F:75:THR:CG2	2.63	0.67
6:G:184:CYC:O1D	2:J:57:ARG:HD3	1.95	0.67
1:Q:84:CYS:SG	6:Q:184:CYC:C3C	2.82	0.67
2:V:51:VAL:HG12	2:V:134:MET:HG2	1.75	0.67
2:X:74:TYR:C	2:X:75:THR:CG2	2.61	0.67
2:V:153:CYS:HG	6:V:255:CYC:HBC3	1.55	0.67
7:D:255:BLA:HMA1	7:D:255:BLA:HB	0.62	0.66
6:J:255:CYC:HC	6:J:255:CYC:CMD	2.07	0.66
6:A:184:CYC:O2D	4:D:57:ARG:HD3	1.96	0.66
5:H:74:ASP:C	5:H:75:THR:CG2	2.63	0.66
6:F:184:CYC:CMD	6:F:184:CYC:NC	2.50	0.66
1:M:6:THR:HG21	8:N:2002:HOH:O	1.95	0.66
6:P:184:CYC:HMD2	6:P:184:CYC:NC	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:184:CYC:HMA1	6:N:184:CYC:C4B	2.22	0.66
6:U:184:CYC:CMA	6:U:184:CYC:HBA1	2.27	0.66
4:D:40:VAL:HG12	4:D:156:LEU:HD21	1.79	0.65
6:S:184:CYC:HHA	6:S:184:CYC:CBD	2.25	0.65
6:A:184:CYC:HC	6:A:184:CYC:HMD2	1.61	0.65
6:H:184:CYC:HB	6:H:184:CYC:C3A	2.06	0.65
3:C:68:CYS:O	1:M:68:CYS:HB2	1.95	0.65
6:X:184:CYC:CMD	6:X:184:CYC:NC	2.46	0.65
2:F:37:ARG:O	2:F:40:ALA:HB3	1.96	0.65
4:D:20:SER:H	4:D:23:GLN:NE2	1.94	0.65
6:G:184:CYC:HMC1	6:G:184:CYC:HBC2	1.77	0.65
1:E:73:ASN:O	6:E:184:CYC:HMD2	1.96	0.65
6:D:184:CYC:CMD	6:D:184:CYC:NC	2.49	0.65
2:J:37:ARG:O	2:J:40:ALA:HB3	1.96	0.65
6:U:184:CYC:HBA1	6:U:184:CYC:HMA3	1.78	0.65
2:V:74:TYR:O	2:V:75:THR:HG22	1.97	0.65
2:R:79:MET:HE2	2:R:83:LEU:HG	1.79	0.65
2:T:19:VAL:HG12	2:T:23:GLN:HB2	1.79	0.64
6:U:184:CYC:CMD	6:U:184:CYC:NC	2.53	0.64
2:V:74:TYR:C	2:V:75:THR:HG22	2.18	0.64
6:L:255:CYC:HBC2	6:L:255:CYC:HHD	1.79	0.64
2:N:82:CYS:SG	6:N:184:CYC:HBC2	2.36	0.64
2:V:20:SER:H	2:V:23:GLN:NE2	1.94	0.64
1:Q:67:THR:O	1:Q:76:ALA:HA	1.96	0.64
6:F:184:CYC:HBB2	6:F:184:CYC:OB	1.98	0.64
1:U:72:PRO:O	6:U:184:CYC:HAD1	1.98	0.64
6:S:184:CYC:HC	6:S:184:CYC:HMD2	1.61	0.63
2:B:153:CYS:SG	7:B:255:BLA:C2C	2.86	0.63
2:P:127:VAL:HG22	6:P:184:CYC:H3C	1.81	0.63
2:L:82:CYS:CA	6:L:184:CYC:HAC2	2.29	0.63
6:L:184:CYC:HB	6:L:184:CYC:C3A	2.09	0.63
2:P:72:ASN:OD1	6:P:184:CYC:HMD2	1.99	0.63
6:P:184:CYC:HMD3	6:P:184:CYC:NC	2.06	0.63
1:Q:18:PHE:HB3	2:R:45:THR:HG23	1.80	0.63
2:R:69:PRO:HA	2:R:74:TYR:CG	2.34	0.63
1:W:128:TRP:CD2	6:W:184:CYC:HMC3	2.33	0.63
6:F:255:CYC:HBB2	6:F:255:CYC:OB	1.99	0.63
6:L:184:CYC:CMD	6:L:184:CYC:NC	2.53	0.63
1:Q:128:TRP:CE3	6:Q:184:CYC:HMC3	2.34	0.63
6:Q:184:CYC:HMD3	6:Q:184:CYC:NC	2.12	0.63
7:B:255:BLA:HBB1	7:B:255:BLA:OB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:153:CYS:SG	6:T:255:CYC:C2C	2.86	0.62
6:C:184:CYC:HHA	6:C:184:CYC:CBD	2.28	0.62
1:G:24:ILE:HG21	6:H:255:CYC:HBB2	1.81	0.62
2:R:19:VAL:HG12	2:R:23:GLN:HB2	1.81	0.62
1:K:83:LYS:HE2	1:K:86:ARG:NH1	2.15	0.62
1:O:128:TRP:CD2	6:O:184:CYC:HMC3	2.34	0.62
2:B:74:TYR:O	2:B:75:THR:HG22	1.97	0.62
2:T:79:MET:HE2	2:T:83:LEU:HG	1.81	0.62
2:T:74:TYR:C	2:T:75:THR:CG2	2.67	0.62
6:I:184:CYC:HMA3	8:L:2007:HOH:O	2.00	0.62
6:O:184:CYC:CMD	6:O:184:CYC:NC	2.59	0.62
6:F:255:CYC:OB	6:F:255:CYC:CBB	2.46	0.61
2:V:148:ILE:CD1	6:V:255:CYC:HHD	2.28	0.61
4:D:35:ASN:HB2	7:D:255:BLA:O2D	1.99	0.61
6:G:184:CYC:HC	6:G:184:CYC:CMD	2.13	0.61
2:B:74:TYR:C	2:B:75:THR:CG2	2.66	0.61
2:N:82:CYS:SG	6:N:184:CYC:C2C	2.89	0.61
1:E:26:VAL:HG22	1:I:26:VAL:HG22	1.80	0.61
2:L:82:CYS:SG	6:L:184:CYC:H2C	2.41	0.61
2:N:82:CYS:SG	6:N:184:CYC:C3C	2.88	0.61
8:W:2003:HOH:O	2:X:42:ASN:HA	2.01	0.61
2:X:19:VAL:HG12	2:X:23:GLN:HB2	1.82	0.61
5:H:74:ASP:C	5:H:75:THR:HG22	2.21	0.61
1:I:73:ASN:O	6:I:184:CYC:HMD2	2.00	0.61
2:N:114:ARG:HH21	2:N:172:SER:C	2.05	0.61
1:G:72:PRO:HB2	6:G:184:CYC:O1D	2.01	0.60
6:Q:184:CYC:HBC2	6:Q:184:CYC:HMC1	1.83	0.60
6:W:184:CYC:CMD	6:W:184:CYC:HC	2.14	0.60
2:F:19:VAL:HG12	2:F:23:GLN:HB2	1.83	0.60
2:J:74:TYR:C	2:J:75:THR:HG22	2.20	0.60
2:X:79:MET:HE2	2:X:83:LEU:HG	1.83	0.60
2:J:19:VAL:HG12	2:J:23:GLN:HB2	1.83	0.60
6:N:255:CYC:CMD	6:N:255:CYC:HC	2.14	0.60
6:J:184:CYC:HMA1	6:J:184:CYC:C4B	2.26	0.60
6:J:255:CYC:HMA2	6:J:255:CYC:HBA2	1.84	0.60
2:T:57:ARG:HD3	6:W:184:CYC:O2D	2.00	0.60
2:L:19:VAL:HG12	2:L:23:GLN:HB2	1.82	0.60
2:R:78:ARG:HD2	6:R:184:CYC:HBD1	1.84	0.60
7:B:184:BLA:HC	7:B:184:BLA:HMD3	1.66	0.60
6:E:184:CYC:HHA	6:E:184:CYC:HBD2	1.83	0.60
2:J:78:ARG:HD2	6:J:184:CYC:HBD1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:255:CYC:HMB2	6:J:255:CYC:CMA	2.21	0.60
6:V:184:CYC:HC	6:V:184:CYC:HMD2	1.66	0.60
2:B:79:MET:HE2	2:B:83:LEU:HG	1.84	0.60
7:B:184:BLA:HC	7:B:184:BLA:HMD2	1.67	0.60
2:P:79:MET:HE2	2:P:83:LEU:HG	1.84	0.60
6:Q:184:CYC:HHA	6:Q:184:CYC:HBD1	1.83	0.60
1:S:95:VAL:HG21	1:S:154:LEU:CD1	2.32	0.60
4:D:40:VAL:HG22	4:D:41:VAL:N	2.17	0.60
8:E:2002:HOH:O	2:F:42:ASN:HA	2.02	0.60
2:N:79:MET:HE2	2:N:83:LEU:HG	1.84	0.60
1:W:72:PRO:O	6:W:184:CYC:HBD1	2.02	0.60
4:D:69:PRO:HA	4:D:74:TYR:CG	2.36	0.59
2:F:79:MET:HE2	2:F:83:LEU:HG	1.83	0.59
2:F:135:LYS:HG3	2:F:164:PHE:CB	2.31	0.59
2:V:72:ASN:OD1	6:V:184:CYC:HMD2	2.02	0.59
6:T:255:CYC:HHA	6:T:255:CYC:CBA	2.29	0.59
6:T:184:CYC:HMA1	6:T:184:CYC:C4B	2.32	0.59
6:T:255:CYC:HC	6:T:255:CYC:HMD2	1.66	0.59
2:L:82:CYS:SG	6:L:184:CYC:C2C	2.90	0.59
1:Q:128:TRP:HB3	6:Q:184:CYC:HBC3	1.84	0.59
2:F:74:TYR:C	2:F:75:THR:HG22	2.23	0.59
6:M:184:CYC:HB	6:M:184:CYC:C3A	2.15	0.59
2:P:63:GLN:HG2	8:P:2009:HOH:O	2.03	0.59
2:T:153:CYS:SG	6:T:255:CYC:C1C	2.90	0.59
2:V:69:PRO:HA	2:V:74:TYR:CD1	2.38	0.59
1:A:26:VAL:HG22	1:G:26:VAL:HG22	1.84	0.59
6:A:184:CYC:HC	6:A:184:CYC:HMD3	1.66	0.59
2:B:82:CYS:SG	7:B:184:BLA:C2C	2.91	0.59
7:B:255:BLA:CMD	7:B:255:BLA:HC	2.16	0.59
2:L:69:PRO:HA	2:L:74:TYR:CG	2.37	0.59
2:L:82:CYS:SG	6:L:184:CYC:C3C	2.90	0.59
1:Q:128:TRP:CD2	6:Q:184:CYC:HMC3	2.37	0.59
6:M:184:CYC:HC	6:M:184:CYC:CMD	2.15	0.59
2:F:153:CYS:SG	6:F:255:CYC:CBC	2.90	0.58
1:M:73:ASN:C	6:M:184:CYC:HMD2	2.24	0.58
5:H:79:MET:HE2	5:H:83:LEU:HG	1.85	0.58
6:L:255:CYC:HC	6:L:255:CYC:HMD2	1.68	0.58
1:S:90:TYR:CD2	6:S:184:CYC:HBB3	2.38	0.58
2:P:39:ASP:OD1	6:P:255:CYC:HHB	2.03	0.58
6:T:184:CYC:CMD	6:T:184:CYC:NC	2.57	0.58
1:M:128:TRP:CE3	6:M:184:CYC:HMC3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:SER:N	2:B:23:GLN:HE21	1.91	0.58
2:P:37:ARG:O	2:P:40:ALA:HB3	2.03	0.58
2:R:37:ARG:O	2:R:40:ALA:HB3	2.03	0.58
1:G:40:ALA:HB2	1:G:146:ALA:HB1	1.86	0.58
6:H:184:CYC:HC	6:H:184:CYC:HMD2	1.68	0.58
6:U:184:CYC:HBD1	6:U:184:CYC:CHA	2.21	0.58
6:V:255:CYC:HMA1	6:V:255:CYC:HB	0.67	0.58
1:A:67:THR:O	1:A:76:ALA:HA	2.04	0.57
4:D:20:SER:OG	4:D:23:GLN:HG3	2.04	0.57
2:F:72:ASN:OD1	6:F:184:CYC:CMD	2.50	0.57
2:P:74:TYR:O	2:P:75:THR:HG22	1.96	0.57
1:S:67:THR:O	1:S:76:ALA:HA	2.04	0.57
2:X:149:THR:O	6:X:255:CYC:HMD2	2.04	0.57
2:N:135:LYS:HG3	2:N:164:PHE:CB	2.34	0.57
2:R:114:ARG:HH21	2:R:172:SER:C	2.08	0.57
2:N:82:CYS:SG	6:N:184:CYC:H2C	2.43	0.57
2:L:79:MET:HE2	2:L:83:LEU:HG	1.86	0.57
1:U:84:CYS:O	1:U:88:ILE:HG13	2.04	0.57
4:D:114:ARG:HH21	4:D:172:SER:C	2.08	0.57
7:D:255:BLA:HC	7:D:255:BLA:HMD2	1.67	0.57
6:D:184:CYC:HBD2	6:D:184:CYC:HHA	1.87	0.57
1:I:6:THR:O	1:I:10:SER:HB2	2.05	0.57
2:J:148:ILE:HG21	6:J:255:CYC:H3C	1.86	0.57
4:D:51:VAL:HG12	4:D:134:MET:HG2	1.87	0.57
1:E:38:LEU:HD22	2:F:24:ILE:HG23	1.87	0.57
2:N:153:CYS:SG	6:N:255:CYC:C1C	2.93	0.57
1:Q:59:VAL:HG11	6:Q:184:CYC:HBC2	1.86	0.57
6:I:184:CYC:HC	6:I:184:CYC:HMD2	1.68	0.56
6:R:184:CYC:HMD3	6:R:184:CYC:NC	2.13	0.56
4:D:79:MET:HE2	4:D:83:LEU:HG	1.86	0.56
1:Q:26:VAL:HG22	1:U:26:VAL:HG22	1.87	0.56
6:C:184:CYC:CMD	6:C:184:CYC:NC	2.59	0.56
6:M:184:CYC:HMC1	6:M:184:CYC:HBC2	1.87	0.56
6:J:184:CYC:HMD2	6:J:184:CYC:HC	1.71	0.56
2:L:153:CYS:SG	6:L:255:CYC:C1C	2.94	0.56
2:N:37:ARG:HA	2:N:156:LEU:HD21	1.87	0.56
2:V:20:SER:OG	2:V:23:GLN:HG3	2.06	0.56
1:A:128:TRP:CE3	6:A:184:CYC:HMC3	2.40	0.56
1:K:84:CYS:HA	6:K:184:CYC:CBC	2.28	0.56
2:J:151:GLY:O	6:J:255:CYC:OC	2.24	0.56
6:X:255:CYC:HC	6:X:255:CYC:HMD2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:52:VAL:HG22	2:R:134:MET:CE	2.36	0.56
2:X:72:ASN:OD1	6:X:184:CYC:HMD2	2.05	0.56
6:X:184:CYC:HMD3	6:X:184:CYC:NC	2.17	0.56
1:I:121:THR:HG21	2:L:83:LEU:HD13	1.86	0.56
6:I:184:CYC:HC	6:I:184:CYC:HMD3	1.69	0.56
2:T:153:CYS:SG	6:T:255:CYC:H2C	2.45	0.56
2:X:52:VAL:HG22	2:X:134:MET:CE	2.36	0.56
1:S:18:PHE:CE2	2:T:91:ARG:HA	2.42	0.55
2:B:82:CYS:SG	7:B:184:BLA:C3C	2.91	0.55
1:W:24:ILE:HG21	6:X:255:CYC:CBB	2.36	0.55
2:B:69:PRO:HA	2:B:74:TYR:CG	2.41	0.55
2:J:52:VAL:HG22	2:J:134:MET:CE	2.37	0.55
2:N:135:LYS:HG3	2:N:164:PHE:HB2	1.89	0.55
2:V:148:ILE:HD13	6:V:255:CYC:CHD	2.36	0.55
2:V:79:MET:HE2	2:V:83:LEU:HG	1.89	0.55
2:X:74:TYR:C	2:X:75:THR:HG22	2.27	0.55
2:T:20:SER:OG	2:T:23:GLN:HG3	2.07	0.55
6:X:184:CYC:HC	6:X:184:CYC:C2D	2.19	0.55
2:B:74:TYR:C	2:B:75:THR:HG22	2.27	0.55
6:C:184:CYC:HHA	6:C:184:CYC:HBD1	1.89	0.55
1:K:73:ASN:C	6:K:184:CYC:HMD2	2.27	0.55
2:L:37:ARG:HA	2:L:156:LEU:HD21	1.88	0.55
2:F:148:ILE:CD1	6:F:255:CYC:HHD	2.37	0.55
1:A:73:ASN:O	6:A:184:CYC:HMD2	2.07	0.55
2:J:135:LYS:HG3	2:J:164:PHE:CB	2.37	0.54
2:P:148:ILE:HD13	6:P:255:CYC:HHD	1.90	0.54
4:D:84:ARG:NH2	6:D:184:CYC:C4A	2.70	0.54
2:B:78:ARG:HD2	7:B:184:BLA:HBD1	1.89	0.54
5:H:153:CYS:HG	6:H:255:CYC:HAC2	1.65	0.54
6:H:184:CYC:HC	6:H:184:CYC:HMD3	1.72	0.54
6:I:184:CYC:CMA	8:L:2007:HOH:O	2.55	0.54
1:K:95:VAL:HG21	1:K:154:LEU:CD1	2.37	0.54
1:W:6:THR:O	1:W:10:SER:HB2	2.06	0.54
4:D:52:VAL:HG22	4:D:134:MET:CE	2.38	0.54
1:I:67:THR:O	1:I:76:ALA:HA	2.07	0.54
2:B:114:ARG:HH21	2:B:172:SER:C	2.11	0.54
4:D:148:ILE:HD13	7:D:255:BLA:HHD	1.89	0.54
2:R:153:CYS:SG	6:R:255:CYC:C1C	2.95	0.54
1:S:86:ARG:NH1	6:S:184:CYC:O1A	2.41	0.54
1:U:87:ASP:O	1:U:90:TYR:HB2	2.07	0.54
4:D:60:PHE:HE2	4:D:79:MET:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:153:CYS:SG	6:H:255:CYC:CBC	2.96	0.54
2:T:69:PRO:HA	2:T:74:TYR:CG	2.43	0.54
6:X:184:CYC:HMA3	6:X:184:CYC:O1A	2.08	0.54
2:N:153:CYS:SG	6:N:255:CYC:C2C	2.96	0.53
3:C:26:VAL:HG22	1:K:26:VAL:HG22	1.90	0.53
2:N:69:PRO:HA	2:N:74:TYR:CG	2.42	0.53
1:K:40:ALA:HB2	1:K:146:ALA:HB1	1.89	0.53
2:F:149:THR:O	6:F:255:CYC:HMD2	2.08	0.53
6:F:184:CYC:HB	6:F:184:CYC:C3A	2.21	0.53
2:N:148:ILE:HD13	6:N:255:CYC:HHD	1.89	0.53
6:T:255:CYC:HC	6:T:255:CYC:HMD3	1.73	0.53
6:V:255:CYC:HC	6:V:255:CYC:CMD	2.21	0.53
5:H:72:ASN:OD1	6:H:184:CYC:HMD2	2.08	0.53
3:C:84:CYS:O	3:C:88:ILE:HG13	2.08	0.53
7:D:255:BLA:HC	7:D:255:BLA:HMD3	1.71	0.53
6:K:184:CYC:HMD2	6:K:184:CYC:HC	1.74	0.53
2:L:74:TYR:C	2:L:75:THR:CG2	2.75	0.53
2:P:79:MET:CE	2:P:83:LEU:HG	2.38	0.53
1:Q:100:ILE:HD12	2:R:19:VAL:HG21	1.90	0.53
2:T:37:ARG:HA	2:T:156:LEU:HD21	1.91	0.53
6:U:184:CYC:HMD3	6:U:184:CYC:NC	2.21	0.53
3:C:18:PHE:CE2	4:D:91:ARG:HA	2.43	0.53
6:D:184:CYC:HMD2	6:D:184:CYC:NC	2.18	0.53
2:F:52:VAL:HG22	2:F:134:MET:CE	2.39	0.53
2:P:37:ARG:HA	2:P:156:LEU:HD21	1.89	0.53
1:E:95:VAL:HG21	1:E:154:LEU:CD1	2.39	0.53
1:G:73:ASN:O	6:G:184:CYC:HMD2	2.08	0.53
2:P:82:CYS:CB	6:P:184:CYC:HAC2	2.28	0.53
2:B:19:VAL:HG12	2:B:23:GLN:HB2	1.91	0.52
2:F:114:ARG:HH21	2:F:172:SER:C	2.12	0.52
2:V:3:ASP:OD1	2:V:3:ASP:C	2.47	0.52
2:X:148:ILE:HD13	6:X:255:CYC:HHD	1.90	0.52
2:L:82:CYS:SG	6:L:184:CYC:HBC1	2.38	0.52
1:O:90:TYR:CD2	6:O:184:CYC:HBB3	2.45	0.52
1:A:70:GLN:HA	1:A:70:GLN:NE2	2.23	0.52
4:D:40:VAL:HG22	4:D:97:VAL:HG11	1.91	0.52
6:J:184:CYC:HC	6:J:184:CYC:HMD3	1.72	0.52
1:W:87:ASP:O	1:W:90:TYR:HB2	2.10	0.52
6:C:184:CYC:CMA	6:C:184:CYC:HBA1	2.40	0.52
4:D:74:TYR:C	4:D:75:THR:HG22	2.30	0.52
1:O:87:ASP:O	1:O:90:TYR:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:LYS:HG3	2:F:164:PHE:HB2	1.91	0.52
2:L:114:ARG:HH21	2:L:172:SER:C	2.14	0.52
6:V:184:CYC:HC	6:V:184:CYC:HMD3	1.70	0.52
6:K:184:CYC:HC	6:K:184:CYC:HMD3	1.75	0.52
2:T:151:GLY:HA3	6:T:255:CYC:CMD	2.39	0.51
1:A:125:SER:HB3	1:A:128:TRP:CE2	2.45	0.51
3:C:91:TYR:CD2	3:C:133:LEU:HD21	2.45	0.51
1:E:128:TRP:CD2	6:E:184:CYC:HMC3	2.45	0.51
6:J:255:CYC:HC	6:J:255:CYC:HMD2	1.72	0.51
6:R:184:CYC:HMD2	6:R:184:CYC:NC	2.16	0.51
4:D:72:ASN:OD1	6:D:184:CYC:HMD2	2.10	0.51
5:H:153:CYS:SG	6:H:255:CYC:C1C	2.98	0.51
5:H:20:SER:N	5:H:23:GLN:HE21	1.95	0.51
6:L:255:CYC:HC	6:L:255:CYC:HMD3	1.75	0.51
1:G:86:ARG:NH1	6:G:184:CYC:O1A	2.33	0.51
1:A:123:GLU:HG2	1:K:127:SER:OG	2.10	0.51
4:D:60:PHE:CE2	4:D:79:MET:HE1	2.45	0.51
2:J:3:ASP:OD1	2:J:6:THR:HB	2.11	0.51
4:D:137:ALA:O	4:D:141:ILE:HG13	2.10	0.51
2:T:74:TYR:O	2:T:75:THR:HG22	2.07	0.51
6:D:184:CYC:HMD3	6:D:184:CYC:NC	2.21	0.51
1:M:85:ALA:HB3	8:M:2009:HOH:O	2.11	0.51
1:Q:73:ASN:O	6:Q:184:CYC:CMD	2.57	0.51
1:A:70:GLN:HA	1:A:70:GLN:HE21	1.75	0.50
2:R:31:VAL:O	2:R:34:ALA:HB2	2.12	0.50
2:T:39:ASP:HA	8:T:2003:HOH:O	2.11	0.50
1:G:18:PHE:CE2	5:H:91:ARG:HA	2.46	0.50
6:I:184:CYC:HBB2	6:I:184:CYC:OB	2.12	0.50
2:N:52:VAL:HG22	2:N:134:MET:CE	2.41	0.50
2:B:57:ARG:HD3	6:E:184:CYC:O2D	2.10	0.50
6:Q:184:CYC:HMD2	6:Q:184:CYC:NC	2.16	0.50
2:T:114:ARG:HH21	2:T:172:SER:C	2.14	0.50
2:T:135:LYS:HG3	2:T:164:PHE:HB2	1.94	0.50
6:U:184:CYC:O1D	2:X:57:ARG:NH1	2.44	0.50
2:V:37:ARG:O	2:V:40:ALA:HB3	2.12	0.50
2:F:148:ILE:HD13	6:F:255:CYC:HHD	1.92	0.50
6:F:255:CYC:HC	6:F:255:CYC:CMD	2.24	0.50
2:J:135:LYS:HG3	2:J:164:PHE:HB2	1.93	0.50
6:T:184:CYC:NB	6:T:184:CYC:C3A	2.72	0.50
6:U:184:CYC:HHA	6:U:184:CYC:CBD	2.29	0.50
1:K:24:ILE:HG21	6:L:255:CYC:HBB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:148:ILE:HG21	6:V:255:CYC:H3C	1.93	0.50
3:C:68:CYS:CB	1:M:68:CYS:O	2.59	0.50
6:S:184:CYC:HBD2	6:S:184:CYC:CHA	2.36	0.50
2:T:127:VAL:HG22	6:T:184:CYC:H3C	1.93	0.50
2:V:69:PRO:HA	2:V:74:TYR:CG	2.47	0.50
2:L:127:VAL:HG22	6:L:184:CYC:H3C	1.94	0.50
2:P:148:ILE:HG21	6:P:255:CYC:H3C	1.92	0.50
2:T:135:LYS:HG3	2:T:164:PHE:CB	2.42	0.50
1:U:73:ASN:O	6:U:184:CYC:CMD	2.55	0.50
1:G:125:SER:HB3	1:G:128:TRP:CE2	2.47	0.50
2:J:127:VAL:HG22	6:J:184:CYC:H3C	1.94	0.50
2:N:74:TYR:C	2:N:75:THR:CG2	2.79	0.50
6:F:184:CYC:HMD3	6:F:184:CYC:NC	2.20	0.49
1:M:84:CYS:O	1:M:88:ILE:HG13	2.12	0.49
2:N:109:CYS:HA	6:N:184:CYC:HBB1	1.93	0.49
6:O:184:CYC:HMD3	6:O:184:CYC:NC	2.25	0.49
2:R:153:CYS:SG	6:R:255:CYC:C2C	3.00	0.49
2:F:69:PRO:HA	2:F:74:TYR:CG	2.47	0.49
1:S:95:VAL:HG21	1:S:154:LEU:HD13	1.94	0.49
2:X:88:ILE:O	2:X:89:ILE:C	2.49	0.49
6:X:184:CYC:HMD2	6:X:184:CYC:NC	2.18	0.49
1:O:6:THR:O	1:O:10:SER:HB2	2.13	0.49
2:T:74:TYR:C	2:T:75:THR:HG22	2.32	0.49
2:B:39:ASP:HB2	7:B:255:BLA:HBC1	1.93	0.49
6:S:184:CYC:HB	6:S:184:CYC:CMA	1.92	0.49
2:B:37:ARG:HA	2:B:156:LEU:HD21	1.93	0.49
4:D:73:ALA:HB2	6:D:184:CYC:OC	2.13	0.49
2:N:39:ASP:O	2:N:43:ARG:HB2	2.13	0.49
2:T:39:ASP:CG	6:T:255:CYC:HHB	2.28	0.49
4:D:148:ILE:CD1	7:D:255:BLA:HHD	2.42	0.49
6:F:184:CYC:HMD2	6:F:184:CYC:NC	2.20	0.49
2:X:135:LYS:HG3	2:X:164:PHE:CB	2.43	0.49
1:A:95:VAL:HG21	1:A:154:LEU:CD1	2.42	0.49
2:N:57:ARG:NH1	6:Q:184:CYC:O1D	2.46	0.49
6:T:255:CYC:CBA	6:T:255:CYC:CHA	2.90	0.49
2:V:114:ARG:HH21	2:V:172:SER:C	2.16	0.49
1:A:91:TYR:O	1:A:95:VAL:HG23	2.13	0.49
3:C:125:SER:HB3	3:C:128:TRP:CE2	2.48	0.49
1:Q:40:ALA:HB2	1:Q:146:ALA:HB1	1.95	0.49
2:T:151:GLY:O	6:T:255:CYC:OC	2.31	0.49
1:M:72:PRO:O	6:M:184:CYC:HMD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:137:ALA:O	2:N:141:ILE:HG13	2.13	0.49
1:S:3:THR:O	1:S:7:ASP:HB2	2.13	0.49
2:V:84:ARG:NH2	6:V:184:CYC:C4A	2.76	0.49
4:D:40:VAL:CG2	4:D:41:VAL:N	2.73	0.48
2:J:74:TYR:O	2:J:75:THR:HG22	2.07	0.48
6:N:184:CYC:NB	6:N:184:CYC:C3A	2.68	0.48
2:L:151:GLY:HA3	6:L:255:CYC:CMD	2.42	0.48
1:E:6:THR:O	1:E:10:SER:HB2	2.13	0.48
2:L:52:VAL:HG22	2:L:134:MET:CE	2.44	0.48
2:N:86:MET:HB3	2:N:134:MET:HE3	1.95	0.48
6:E:184:CYC:CMD	6:E:184:CYC:NC	2.65	0.48
2:N:35:ASN:OD1	6:N:255:CYC:HAA1	2.14	0.48
1:O:113:ALA:O	2:R:77:ASN:N	2.46	0.48
1:W:125:SER:HB3	1:W:128:TRP:CE2	2.49	0.48
1:M:26:VAL:HG22	1:S:26:VAL:HG22	1.96	0.48
2:R:51:VAL:HG12	2:R:134:MET:HG2	1.95	0.48
1:G:95:VAL:HG21	1:G:154:LEU:CD1	2.44	0.48
3:C:87:ASP:O	3:C:90:TYR:HB2	2.14	0.48
5:H:74:ASP:O	5:H:75:THR:HG22	2.13	0.48
2:P:19:VAL:HG12	2:P:23:GLN:HB2	1.95	0.48
5:H:19:VAL:HG12	5:H:23:GLN:HB2	1.96	0.47
5:H:37:ARG:HA	5:H:156:LEU:HD21	1.95	0.47
6:P:184:CYC:HBD1	6:P:184:CYC:CHA	2.38	0.47
2:R:79:MET:CE	2:R:83:LEU:HG	2.44	0.47
2:T:69:PRO:HA	2:T:74:TYR:CD1	2.49	0.47
1:W:162:SER:C	8:W:2017:HOH:O	2.52	0.47
2:B:57:ARG:NH1	6:E:184:CYC:O1D	2.48	0.47
2:F:74:TYR:O	2:F:75:THR:HG22	2.09	0.47
1:I:28:PHE:CZ	6:J:255:CYC:HMB3	2.49	0.47
2:T:20:SER:N	2:T:23:GLN:HE21	1.95	0.47
6:U:184:CYC:O1A	2:X:67:ILE:HD12	2.15	0.47
4:D:153:CYS:SG	7:D:255:BLA:HAC	2.51	0.47
1:G:104:THR:O	1:G:105:GLY:C	2.53	0.47
6:L:184:CYC:HMD3	6:L:184:CYC:NC	2.22	0.47
2:N:43:ARG:NH1	2:N:142:VAL:O	2.48	0.47
6:O:184:CYC:HMD2	6:O:184:CYC:NC	2.22	0.47
3:C:6:THR:O	3:C:10:SER:HB2	2.15	0.47
2:L:135:LYS:HG3	2:L:164:PHE:CB	2.45	0.47
3:C:67:THR:O	3:C:76:ALA:HA	2.15	0.47
4:D:84:ARG:HH22	6:D:184:CYC:C4A	2.27	0.47
1:I:18:PHE:CE2	2:J:91:ARG:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:184:CYC:H2C	6:J:184:CYC:HBC2	1.48	0.47
1:M:40:ALA:HB2	1:M:146:ALA:HB1	1.97	0.47
6:P:255:CYC:HHA	6:P:255:CYC:CBA	2.44	0.47
6:U:184:CYC:HMD2	6:U:184:CYC:NC	2.19	0.47
3:C:95:VAL:HG21	3:C:154:LEU:CD1	2.45	0.47
2:N:153:CYS:SG	6:N:255:CYC:CBC	3.02	0.47
2:T:153:CYS:SG	6:T:255:CYC:HBC3	2.55	0.47
4:D:37:ARG:HA	4:D:40:VAL:HG13	1.96	0.47
2:J:60:PHE:CE2	2:J:79:MET:HE1	2.49	0.47
2:J:114:ARG:HH21	2:J:172:SER:C	2.18	0.47
1:M:87:ASP:O	1:M:90:TYR:HB2	2.15	0.47
4:D:135:LYS:HG3	4:D:164:PHE:CB	2.46	0.47
2:X:51:VAL:HG12	2:X:134:MET:HG2	1.97	0.47
1:G:73:ASN:C	6:G:184:CYC:HMD2	2.35	0.46
1:K:128:TRP:CE3	6:K:184:CYC:HMC3	2.49	0.46
1:W:24:ILE:HG21	6:X:255:CYC:HBB3	1.96	0.46
7:B:255:BLA:O2A	7:B:255:BLA:CHA	2.63	0.46
2:R:69:PRO:HA	2:R:74:TYR:CD2	2.50	0.46
2:R:79:MET:HE2	2:R:83:LEU:CG	2.44	0.46
2:J:79:MET:HE2	2:J:83:LEU:HG	1.95	0.46
1:K:72:PRO:O	6:K:184:CYC:HMD1	2.16	0.46
2:L:20:SER:OG	2:L:23:GLN:HG3	2.16	0.46
2:L:135:LYS:HG3	2:L:164:PHE:HB2	1.98	0.46
1:M:65:TYR:HB3	8:M:2005:HOH:O	2.14	0.46
6:T:255:CYC:CBC	6:T:255:CYC:CHD	2.91	0.46
2:B:83:LEU:HD13	1:E:121:THR:HG21	1.96	0.46
1:E:91:TYR:O	1:E:95:VAL:HG23	2.16	0.46
1:E:115:ILE:HD12	1:E:115:ILE:HA	1.83	0.46
2:J:90:LEU:O	2:J:94:THR:HG23	2.15	0.46
6:L:184:CYC:HMD2	6:L:184:CYC:NC	2.21	0.46
1:M:125:SER:HB3	1:M:128:TRP:CE2	2.50	0.46
6:N:255:CYC:HHA	6:N:255:CYC:CBA	2.45	0.46
1:Q:72:PRO:O	6:Q:184:CYC:HAD1	2.15	0.46
1:S:38:LEU:HD22	2:T:24:ILE:HG23	1.97	0.46
2:V:79:MET:CE	2:V:83:LEU:HG	2.46	0.46
2:B:135:LYS:HG3	2:B:164:PHE:CB	2.46	0.46
1:G:107:MET:SD	1:G:112:ILE:HD11	2.56	0.46
2:J:153:CYS:SG	6:J:255:CYC:HAC1	2.53	0.46
1:K:13:ASP:OD1	2:L:92:TYR:OH	2.28	0.46
2:P:20:SER:OG	2:P:23:GLN:HG3	2.15	0.46
2:R:148:ILE:HD13	6:R:255:CYC:HHD	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:74:TYR:O	2:X:75:THR:HG22	2.09	0.46
3:C:147:ALA:O	3:C:148:VAL:C	2.53	0.46
1:G:87:ASP:O	1:G:90:TYR:HB2	2.15	0.46
1:K:79:ARG:HE	1:K:79:ARG:HB3	1.57	0.46
6:R:184:CYC:HAD1	6:R:184:CYC:HHA	1.72	0.46
3:C:148:VAL:HG11	6:L:255:CYC:CMB	2.42	0.46
2:J:69:PRO:HA	2:J:74:TYR:CG	2.49	0.46
6:J:255:CYC:HMB3	6:J:255:CYC:CMA	2.31	0.46
2:N:20:SER:OG	2:N:23:GLN:HG3	2.15	0.46
1:Q:84:CYS:O	1:Q:88:ILE:HG13	2.16	0.46
5:H:79:MET:CE	5:H:83:LEU:HG	2.45	0.46
6:J:184:CYC:NB	6:J:184:CYC:CMA	2.26	0.46
5:H:84:ARG:HH12	6:H:184:CYC:HBA1	1.81	0.46
6:A:184:CYC:O2A	4:D:67:ILE:HD12	2.15	0.45
6:N:184:CYC:CMD	6:N:184:CYC:NC	2.62	0.45
6:V:255:CYC:HMB1	6:V:255:CYC:HBB3	1.98	0.45
6:C:184:CYC:HMD2	6:C:184:CYC:NC	2.24	0.45
4:D:69:PRO:HA	4:D:74:TYR:CD2	2.52	0.45
1:O:73:ASN:C	6:O:184:CYC:CMD	2.84	0.45
2:R:2:PHE:HD1	2:R:6:THR:HG22	1.81	0.45
2:R:37:ARG:HA	2:R:156:LEU:HD21	1.97	0.45
6:X:255:CYC:HC	6:X:255:CYC:HMD3	1.78	0.45
2:F:142:VAL:O	6:F:255:CYC:HBC3	2.17	0.45
2:L:82:CYS:HA	6:L:184:CYC:HAC2	1.98	0.45
1:O:121:THR:HG21	2:R:83:LEU:HD13	1.99	0.45
1:W:18:PHE:CE2	2:X:91:ARG:HA	2.51	0.45
6:H:255:CYC:HC	6:H:255:CYC:CMD	2.29	0.45
3:C:38:LEU:HD22	4:D:24:ILE:HG23	1.97	0.45
1:U:40:ALA:HB2	1:U:146:ALA:HB1	1.99	0.45
1:U:107:MET:SD	1:U:112:ILE:HD11	2.57	0.45
2:B:51:VAL:HG12	2:B:134:MET:HG2	1.98	0.45
1:I:95:VAL:HG21	1:I:154:LEU:CD1	2.47	0.45
1:I:111:LEU:C	1:I:111:LEU:HD23	2.37	0.45
1:M:22:THR:HG23	1:S:4:PRO:HG3	1.98	0.45
6:M:184:CYC:HMD2	6:M:184:CYC:HC	1.81	0.45
6:N:184:CYC:NB	6:N:184:CYC:CMA	2.26	0.45
2:V:120:LEU:HD22	6:V:184:CYC:HBD1	1.99	0.45
2:F:127:VAL:HG22	6:F:184:CYC:H3C	1.97	0.45
2:F:151:GLY:O	6:F:255:CYC:OC	2.35	0.45
1:G:6:THR:O	1:G:10:SER:HB2	2.16	0.45
5:H:97:VAL:CG2	5:H:160:ILE:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:39:ASP:OD2	6:L:255:CYC:NA	2.50	0.45
6:R:255:CYC:HC	6:R:255:CYC:HMD2	1.77	0.45
2:J:148:ILE:HD13	6:J:255:CYC:HHD	1.98	0.45
1:O:84:CYS:O	1:O:88:ILE:HG13	2.17	0.45
1:Q:87:ASP:O	1:Q:90:TYR:HB2	2.16	0.45
1:W:79:ARG:HE	1:W:79:ARG:HB3	1.73	0.45
1:A:55:ALA:O	1:A:56:ALA:C	2.55	0.45
1:A:96:THR:O	1:A:100:ILE:HG13	2.16	0.44
6:E:184:CYC:CBD	6:E:184:CYC:CHA	2.94	0.44
2:F:79:MET:CE	2:F:83:LEU:HG	2.47	0.44
1:G:111:LEU:HG	6:G:184:CYC:HAB1	1.99	0.44
5:H:51:VAL:HG12	5:H:134:MET:HG2	1.99	0.44
2:P:144:ASP:HA	2:P:145:PRO:HD3	1.78	0.44
1:S:115:ILE:HD12	1:S:115:ILE:HA	1.84	0.44
6:W:184:CYC:HAD1	6:W:184:CYC:HHA	1.55	0.44
6:W:184:CYC:HHA	6:W:184:CYC:HAA2	1.82	0.44
2:F:37:ARG:HA	2:F:156:LEU:HD21	1.99	0.44
6:O:184:CYC:O1D	2:R:57:ARG:NH1	2.45	0.44
5:H:31:VAL:O	5:H:34:ALA:HB2	2.17	0.44
1:K:91:TYR:CD2	1:K:133:LEU:HD21	2.52	0.44
7:B:255:BLA:OB	7:B:255:BLA:CBB	2.64	0.44
4:D:39:ASP:OD2	7:D:255:BLA:NA	2.49	0.44
2:P:148:ILE:HD13	6:P:255:CYC:H3C	1.99	0.44
1:U:18:PHE:CE2	2:V:91:ARG:HA	2.53	0.44
2:B:52:VAL:HG22	2:B:134:MET:CE	2.47	0.44
1:E:72:PRO:O	6:E:184:CYC:HAD1	2.17	0.44
5:H:39:ASP:OD2	6:H:255:CYC:NA	2.51	0.44
2:N:109:CYS:HA	6:N:184:CYC:CBB	2.48	0.44
6:R:255:CYC:HC	6:R:255:CYC:HMD3	1.83	0.44
2:T:39:ASP:OD2	6:T:255:CYC:NA	2.50	0.44
2:T:78:ARG:HD2	6:T:184:CYC:HBD2	1.99	0.44
5:H:88:ILE:HG21	6:H:184:CYC:HBB3	2.00	0.44
2:N:82:CYS:CB	6:N:184:CYC:HAC2	2.38	0.44
1:W:95:VAL:HG21	1:W:154:LEU:CD1	2.47	0.44
1:A:6:THR:O	1:A:10:SER:HB2	2.17	0.44
3:C:79:ARG:HE	3:C:79:ARG:HB3	1.64	0.44
6:E:184:CYC:HMD3	6:E:184:CYC:NC	2.30	0.44
1:I:2:LYS:HE3	1:I:2:LYS:HB2	1.87	0.44
6:J:184:CYC:HHA	6:J:184:CYC:HAD1	1.73	0.44
1:K:87:ASP:O	1:K:90:TYR:HB2	2.18	0.44
1:K:107:MET:SD	1:K:112:ILE:HD11	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:148:ILE:CD1	6:P:255:CYC:HHD	2.48	0.44
2:R:1:MET:HE3	2:R:104:ALA:HB2	2.00	0.44
2:T:8:VAL:C	2:T:10:ALA:H	2.21	0.44
1:A:87:ASP:OD2	1:A:129:TYR:OH	2.30	0.43
5:H:72:ASN:OD1	5:H:122:THR:HA	2.18	0.43
1:K:6:THR:O	1:K:10:SER:HB2	2.18	0.43
6:T:184:CYC:HBC2	6:T:184:CYC:H2C	1.70	0.43
6:W:184:CYC:HC	6:W:184:CYC:HMD3	1.82	0.43
6:H:184:CYC:HHA	6:H:184:CYC:HAD2	1.63	0.43
6:L:184:CYC:CMA	6:L:184:CYC:NB	2.41	0.43
2:N:153:CYS:SG	6:N:255:CYC:H2C	2.57	0.43
2:B:20:SER:OG	2:B:23:GLN:HG3	2.19	0.43
2:B:39:ASP:OD1	7:B:255:BLA:HHB	2.19	0.43
1:G:90:TYR:CD2	6:G:184:CYC:HBB3	2.53	0.43
5:H:27:LEU:O	5:H:31:VAL:HG23	2.18	0.43
1:M:95:VAL:HG21	1:M:154:LEU:CD1	2.48	0.43
1:O:27:ALA:HB1	1:O:31:PHE:CE2	2.53	0.43
1:A:2:LYS:HE3	1:A:2:LYS:HB2	1.86	0.43
1:A:38:LEU:HD22	2:B:24:ILE:HG23	2.00	0.43
2:L:144:ASP:HA	2:L:145:PRO:HD3	1.89	0.43
1:Q:13:ASP:HA	2:R:95:TYR:OH	2.18	0.43
2:R:84:ARG:NH2	6:R:184:CYC:C4A	2.82	0.43
6:T:184:CYC:HMD3	6:T:184:CYC:NC	2.26	0.43
3:C:126:PRO:HB2	8:C:2009:HOH:O	2.17	0.43
6:C:184:CYC:HMD3	6:C:184:CYC:NC	2.25	0.43
6:K:184:CYC:HHA	6:K:184:CYC:HAA2	1.78	0.43
1:U:83:LYS:HE2	1:U:86:ARG:NH1	2.33	0.43
1:U:95:VAL:HG21	1:U:154:LEU:CD1	2.48	0.43
4:D:37:ARG:C	4:D:40:VAL:HG13	2.36	0.43
2:J:37:ARG:HA	2:J:156:LEU:HD21	1.98	0.43
1:M:67:THR:O	1:M:76:ALA:HA	2.19	0.43
2:B:79:MET:CE	2:B:83:LEU:HG	2.49	0.43
4:D:37:ARG:HA	4:D:40:VAL:CG1	2.49	0.43
2:J:60:PHE:HE2	2:J:79:MET:HE1	1.84	0.43
6:N:255:CYC:HC	6:N:255:CYC:HMD2	1.83	0.43
2:R:127:VAL:HG22	6:R:184:CYC:H3C	2.01	0.43
1:S:83:LYS:HE2	1:S:86:ARG:NH1	2.34	0.43
6:T:184:CYC:HMD2	6:T:184:CYC:NC	2.25	0.43
2:B:43:ARG:NH1	2:B:142:VAL:O	2.52	0.43
3:C:88:ILE:HD13	3:C:132:ALA:CB	2.48	0.43
1:E:18:PHE:CE2	2:F:91:ARG:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:103:SER:O	2:F:104:ALA:C	2.57	0.43
2:J:39:ASP:OD1	6:J:255:CYC:HHB	2.19	0.43
1:M:115:ILE:HD12	1:M:115:ILE:HA	1.78	0.43
6:M:184:CYC:CMA	6:M:184:CYC:HBA1	2.48	0.43
2:P:84:ARG:NH2	6:P:184:CYC:C4A	2.82	0.43
1:W:84:CYS:O	1:W:88:ILE:HG13	2.18	0.43
1:Q:44:LEU:HD23	1:Q:44:LEU:HA	1.88	0.43
1:Q:100:ILE:HD12	2:R:19:VAL:CG2	2.48	0.43
2:B:47:ASN:O	2:B:51:VAL:HG23	2.18	0.42
3:C:88:ILE:HD13	3:C:132:ALA:HB1	2.01	0.42
1:O:91:TYR:CD2	1:O:133:LEU:HD21	2.54	0.42
1:Q:125:SER:HB3	1:Q:128:TRP:CE2	2.54	0.42
6:U:184:CYC:CHA	6:U:184:CYC:CBD	2.94	0.42
5:H:97:VAL:HG21	5:H:160:ILE:HG12	2.01	0.42
1:M:128:TRP:CD2	6:M:184:CYC:HMC3	2.54	0.42
2:P:135:LYS:HG3	2:P:164:PHE:CB	2.49	0.42
2:X:148:ILE:CD1	6:X:255:CYC:HHD	2.49	0.42
1:A:85:ALA:O	1:A:86:ARG:C	2.58	0.42
1:A:128:TRP:CD2	6:A:184:CYC:HMC3	2.55	0.42
3:C:90:TYR:CD2	6:C:184:CYC:HBB3	2.55	0.42
6:E:184:CYC:HHA	6:E:184:CYC:HBD1	1.95	0.42
6:J:255:CYC:HAD1	6:J:255:CYC:HHA	1.65	0.42
6:S:184:CYC:O1A	2:V:67:ILE:HD12	2.19	0.42
1:M:5:LEU:HB2	2:N:3:ASP:OD2	2.19	0.42
2:R:48:ALA:O	2:R:52:VAL:HG23	2.19	0.42
2:X:79:MET:CE	2:X:83:LEU:HG	2.48	0.42
5:H:83:LEU:HD13	1:K:121:THR:HG21	2.02	0.42
2:J:138:ALA:O	2:J:142:VAL:HG13	2.20	0.42
2:V:39:ASP:O	2:V:40:ALA:C	2.58	0.42
2:B:88:ILE:HG21	7:B:184:BLA:HMB1	2.02	0.42
1:G:3:THR:O	1:G:7:ASP:HB2	2.20	0.42
1:K:143:ALA:O	1:K:144:GLY:C	2.57	0.42
6:N:255:CYC:HHA	6:N:255:CYC:HBA1	2.01	0.42
1:U:2:LYS:HB2	1:U:2:LYS:HE3	1.87	0.42
2:B:88:ILE:HG21	7:B:184:BLA:CMB	2.50	0.42
2:L:51:VAL:HG12	2:L:134:MET:HG2	2.00	0.42
1:M:65:TYR:CD2	1:W:65:TYR:CD2	3.06	0.42
2:N:72:ASN:OD1	6:N:184:CYC:HMD2	2.20	0.42
1:S:92:LEU:O	1:S:96:THR:HG23	2.19	0.42
1:A:73:ASN:C	6:A:184:CYC:HMD2	2.40	0.42
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:149:THR:O	6:J:255:CYC:HMD2	2.20	0.42
2:L:153:CYS:SG	6:L:255:CYC:C2C	3.08	0.42
2:N:84:ARG:NH2	6:N:184:CYC:C4A	2.82	0.42
2:R:2:PHE:HD1	2:R:6:THR:CG2	2.33	0.42
1:S:91:TYR:CD2	1:S:133:LEU:HD21	2.55	0.42
2:T:144:ASP:HA	2:T:145:PRO:HD3	1.91	0.42
2:B:2:PHE:HD1	2:B:6:THR:HG22	1.84	0.42
1:G:111:LEU:C	1:G:111:LEU:HD23	2.40	0.42
6:G:184:CYC:HC	6:G:184:CYC:HMD2	1.82	0.42
1:K:137:LYS:HG3	1:K:154:LEU:HD23	2.02	0.42
1:O:73:ASN:C	6:O:184:CYC:HMD1	2.40	0.42
6:T:184:CYC:HBD2	6:T:184:CYC:HMD1	2.02	0.42
6:A:184:CYC:HBD1	6:A:184:CYC:HMD1	2.02	0.42
3:C:3:THR:O	3:C:7:ASP:HB2	2.20	0.42
2:R:144:ASP:HA	2:R:145:PRO:HD3	1.82	0.42
1:U:115:ILE:HD12	1:U:115:ILE:HA	1.90	0.42
2:V:97:VAL:CG2	2:V:160:ILE:HG12	2.50	0.42
3:C:59:VAL:HG11	6:C:184:CYC:HMC1	2.02	0.41
4:D:47:ASN:O	4:D:51:VAL:HG23	2.20	0.41
1:I:84:CYS:O	1:I:88:ILE:HG13	2.20	0.41
2:J:21:VAL:HG13	8:J:2002:HOH:O	2.19	0.41
1:K:104:THR:O	1:K:105:GLY:C	2.57	0.41
2:R:135:LYS:HG3	2:R:164:PHE:CB	2.50	0.41
2:V:153:CYS:SG	6:V:255:CYC:C1C	3.08	0.41
5:H:79:MET:HE2	5:H:83:LEU:CG	2.48	0.41
1:I:67:THR:OG1	1:W:68:CYS:HB3	2.20	0.41
1:I:79:ARG:HE	1:I:79:ARG:HB3	1.71	0.41
2:B:2:PHE:HD1	2:B:6:THR:CG2	2.33	0.41
1:I:113:ALA:O	2:L:77:ASN:N	2.52	0.41
6:M:184:CYC:O2D	2:P:57:ARG:HD3	2.20	0.41
1:Q:19:LEU:O	2:R:45:THR:HG21	2.20	0.41
7:D:255:BLA:HHA	7:D:255:BLA:HAA1	1.86	0.41
1:O:73:ASN:OD1	1:O:73:ASN:N	2.53	0.41
6:W:184:CYC:HMD2	6:W:184:CYC:HC	1.86	0.41
2:X:39:ASP:CG	2:X:148:ILE:HD11	2.41	0.41
6:P:184:CYC:HBC2	6:P:184:CYC:H2C	1.88	0.41
1:Q:6:THR:O	1:Q:10:SER:HB2	2.20	0.41
1:Q:22:THR:HG23	1:U:4:PRO:HG3	2.02	0.41
2:R:124:GLY:HA3	2:R:171:VAL:O	2.20	0.41
1:U:91:TYR:CD2	1:U:133:LEU:HD21	2.55	0.41
3:C:32:ARG:NH1	8:C:2002:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:184:CYC:OB	6:D:184:CYC:HBB2	2.20	0.41
6:F:255:CYC:HBC2	6:F:255:CYC:H2C	1.83	0.41
1:O:79:ARG:HE	1:O:79:ARG:HB3	1.69	0.41
1:S:86:ARG:NH2	1:S:87:ASP:OD1	2.40	0.41
4:D:88:ILE:O	4:D:89:ILE:C	2.59	0.41
1:I:115:ILE:HA	1:I:115:ILE:HD12	1.86	0.41
1:K:105:GLY:O	1:K:108:ASP:HB2	2.21	0.41
1:S:87:ASP:O	1:S:90:TYR:HB2	2.20	0.41
1:U:6:THR:O	1:U:10:SER:HB2	2.20	0.41
2:V:97:VAL:HG21	2:V:160:ILE:HG12	2.02	0.41
2:X:153:CYS:SG	6:X:255:CYC:C2C	3.09	0.41
2:F:144:ASP:HA	2:F:145:PRO:HD3	1.87	0.41
5:H:35:ASN:HD22	5:H:35:ASN:HA	1.74	0.41
1:I:44:LEU:HD23	1:I:44:LEU:HA	1.95	0.41
2:P:20:SER:N	2:P:23:GLN:HE21	1.99	0.41
2:P:51:VAL:HG12	2:P:134:MET:HG2	2.03	0.41
2:P:114:ARG:HH21	2:P:172:SER:C	2.23	0.41
2:R:84:ARG:NH1	6:R:184:CYC:O1A	2.41	0.41
2:B:144:ASP:HA	2:B:145:PRO:HD3	1.84	0.41
1:E:100:ILE:HD12	2:F:19:VAL:HG21	2.02	0.41
6:F:255:CYC:HAA1	6:F:255:CYC:HHA	1.85	0.41
5:H:114:ARG:HH21	5:H:172:SER:C	2.24	0.41
2:J:20:SER:OG	2:J:23:GLN:HG3	2.21	0.41
6:K:184:CYC:HBD2	6:K:184:CYC:HMD1	2.01	0.41
6:L:184:CYC:NB	6:L:184:CYC:C3A	2.80	0.41
2:N:84:ARG:HH22	6:N:184:CYC:C1A	2.33	0.41
1:O:115:ILE:HA	1:O:115:ILE:HD12	1.83	0.41
2:P:69:PRO:HA	2:P:74:TYR:CG	2.55	0.41
2:P:124:GLY:HA3	2:P:171:VAL:O	2.21	0.41
1:S:90:TYR:O	1:S:91:TYR:C	2.57	0.41
2:T:8:VAL:C	2:T:10:ALA:N	2.73	0.41
2:T:148:ILE:HD13	6:T:255:CYC:HHD	2.03	0.41
1:U:67:THR:O	1:U:76:ALA:HA	2.21	0.41
2:V:124:GLY:HA3	2:V:171:VAL:O	2.20	0.41
1:W:15:GLN:HB2	1:W:17:ARG:HG2	2.03	0.41
2:X:37:ARG:HA	2:X:156:LEU:HD21	2.01	0.41
1:I:91:TYR:CD2	1:I:133:LEU:HD21	2.56	0.41
1:K:129:TYR:CZ	6:K:184:CYC:HBC2	2.56	0.41
2:L:79:MET:CE	2:L:83:LEU:HG	2.50	0.41
2:R:20:SER:OG	2:R:23:GLN:HG3	2.20	0.41
2:V:37:ARG:HA	2:V:156:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:O	2:B:40:ALA:HB3	2.20	0.40
1:G:90:TYR:O	1:G:91:TYR:C	2.59	0.40
7:B:184:BLA:HHA	7:B:184:BLA:HAD1	1.64	0.40
3:C:73:ASN:O	6:C:184:CYC:CMD	2.61	0.40
6:E:184:CYC:HBD2	6:E:184:CYC:CHA	2.51	0.40
1:G:38:LEU:HD22	5:H:24:ILE:HG23	2.03	0.40
1:G:84:CYS:O	1:G:88:ILE:HG13	2.21	0.40
5:H:148:ILE:HD13	6:H:255:CYC:H3C	2.04	0.40
6:R:255:CYC:NB	6:R:255:CYC:CMA	2.56	0.40
1:S:40:ALA:HB2	1:S:146:ALA:HB1	2.03	0.40
2:V:114:ARG:NH2	2:V:172:SER:H	2.19	0.40
1:W:3:THR:O	1:W:7:ASP:HB2	2.22	0.40
1:A:88:ILE:HD13	1:A:132:ALA:HB1	2.02	0.40
1:G:73:ASN:OD1	1:G:73:ASN:N	2.54	0.40
1:I:27:ALA:HB1	1:I:31:PHE:CE2	2.56	0.40
1:O:2:LYS:HE3	1:O:2:LYS:HB2	1.97	0.40
1:O:147:ALA:O	1:O:148:ALA:C	2.59	0.40
2:P:82:CYS:SG	6:P:184:CYC:C2C	3.10	0.40
1:Q:38:LEU:HD22	2:R:24:ILE:HG23	2.03	0.40
1:Q:135:TYR:O	1:Q:136:ILE:C	2.58	0.40
1:S:88:ILE:HD13	1:S:132:ALA:HB1	2.03	0.40
2:T:43:ARG:HH11	2:T:43:ARG:HD3	1.76	0.40
1:K:70:GLN:HA	1:K:70:GLN:NE2	2.37	0.40
6:K:184:CYC:HHA	6:K:184:CYC:HAD2	1.90	0.40
1:O:44:LEU:HD23	1:O:44:LEU:HA	1.92	0.40
1:Q:95:VAL:HG21	1:Q:154:LEU:CD1	2.51	0.40
1:W:115:ILE:HD12	1:W:115:ILE:HA	1.85	0.40
2:X:31:VAL:O	2:X:34:ALA:HB2	2.22	0.40
1:E:78:GLN:NE2	1:E:82:ASP:OD1	2.55	0.40
1:E:88:ILE:HD13	1:E:132:ALA:HB1	2.04	0.40
2:T:52:VAL:HG22	2:T:134:MET:CE	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:125:SER:OG	2:R:62:GLU:OE1[2_657]	1.92	0.28
2:N:114:ARG:NH1	2:T:15:ARG:NH2[2_547]	2.04	0.16

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%)	144 (90%)	15 (9%)	1 (1%)	25	59
1	E	160/162 (99%)	150 (94%)	9 (6%)	1 (1%)	25	59
1	G	160/162 (99%)	152 (95%)	7 (4%)	1 (1%)	25	59
1	I	160/162 (99%)	150 (94%)	9 (6%)	1 (1%)	25	59
1	K	160/162 (99%)	149 (93%)	9 (6%)	2 (1%)	12	42
1	M	160/162 (99%)	150 (94%)	8 (5%)	2 (1%)	12	42
1	O	160/162 (99%)	151 (94%)	8 (5%)	1 (1%)	25	59
1	Q	160/162 (99%)	146 (91%)	13 (8%)	1 (1%)	25	59
1	S	160/162 (99%)	150 (94%)	8 (5%)	2 (1%)	12	42
1	U	160/162 (99%)	150 (94%)	9 (6%)	1 (1%)	25	59
1	W	160/162 (99%)	150 (94%)	9 (6%)	1 (1%)	25	59
2	B	170/172 (99%)	160 (94%)	10 (6%)	0	100	100
2	F	170/172 (99%)	162 (95%)	7 (4%)	1 (1%)	25	59
2	J	170/172 (99%)	162 (95%)	8 (5%)	0	100	100
2	L	170/172 (99%)	157 (92%)	13 (8%)	0	100	100
2	N	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	25	59
2	P	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
2	R	170/172 (99%)	159 (94%)	10 (6%)	1 (1%)	25	59
2	T	170/172 (99%)	159 (94%)	11 (6%)	0	100	100
2	V	170/172 (99%)	159 (94%)	10 (6%)	1 (1%)	25	59
2	X	170/172 (99%)	159 (94%)	11 (6%)	0	100	100
3	C	160/162 (99%)	150 (94%)	8 (5%)	2 (1%)	12	42
4	D	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	25	59
5	H	170/172 (99%)	164 (96%)	6 (4%)	0	100	100
All	All	3960/4008 (99%)	3714 (94%)	225 (6%)	21 (0%)	29	64

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
3	C	2	LYS
1	G	2	LYS
1	M	2	LYS
1	O	2	LYS
1	S	2	LYS
1	U	2	LYS
1	E	2	LYS
1	I	2	LYS
1	K	2	LYS
1	Q	2	LYS
1	W	2	LYS
1	S	35	LYS
1	K	35	LYS
2	R	75	THR
4	D	75	THR
2	N	75	THR
2	F	75	THR
1	M	105	GLY
3	C	105	GLY
2	V	52	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	119/120 (99%)	105 (88%)	14 (12%)	5 21
1	E	119/120 (99%)	106 (89%)	13 (11%)	6 25
1	G	119/120 (99%)	108 (91%)	11 (9%)	9 33
1	I	119/120 (99%)	108 (91%)	11 (9%)	9 33
1	K	119/120 (99%)	105 (88%)	14 (12%)	5 21
1	M	119/120 (99%)	107 (90%)	12 (10%)	7 28
1	O	119/120 (99%)	107 (90%)	12 (10%)	7 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Q	119/120 (99%)	105 (88%)	14 (12%)	5 21
1	S	119/120 (99%)	106 (89%)	13 (11%)	6 25
1	U	119/120 (99%)	107 (90%)	12 (10%)	7 28
1	W	119/120 (99%)	106 (89%)	13 (11%)	6 25
2	B	124/124 (100%)	118 (95%)	6 (5%)	25 58
2	F	124/124 (100%)	118 (95%)	6 (5%)	25 58
2	J	124/124 (100%)	117 (94%)	7 (6%)	21 52
2	L	124/124 (100%)	119 (96%)	5 (4%)	31 65
2	N	124/124 (100%)	118 (95%)	6 (5%)	25 58
2	P	124/124 (100%)	118 (95%)	6 (5%)	25 58
2	R	124/124 (100%)	119 (96%)	5 (4%)	31 65
2	T	124/124 (100%)	117 (94%)	7 (6%)	21 52
2	V	124/124 (100%)	117 (94%)	7 (6%)	21 52
2	X	124/124 (100%)	118 (95%)	6 (5%)	25 58
3	C	121/122 (99%)	110 (91%)	11 (9%)	9 33
4	D	130/130 (100%)	122 (94%)	8 (6%)	18 49
5	H	124/124 (100%)	117 (94%)	7 (6%)	21 52
All	All	2924/2936 (100%)	2698 (92%)	226 (8%)	13 41

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	ASP
1	A	10	SER
1	A	11	THR
1	A	14	SER
1	A	20	SER
1	A	24	ILE
1	A	32	ARG
1	A	81	LYS
1	A	88	ILE
1	A	117	GLU
1	A	152	SER
1	A	154	LEU
1	A	162	SER

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Mol	Chain	Res	Type
2	B	18	MET
2	B	21	VAL
2	B	28	SER
2	B	43	ARG
2	B	75	THR
2	B	172	SER
3	C	1	MET
3	C	7	ASP
3	C	11	THR
3	C	14	SER
3	C	20	SER
3	C	32	ARG
3	C	81	LYS
3	C	117	GLU
3	C	152	SER
3	C	154	LEU
3	C	162	SER
4	D	10	SER
4	D	14	THR
4	D	18	MET
4	D	21	VAL
4	D	28	SER
4	D	43	ARG
4	D	75	THR
4	D	104	VAL
1	E	1	MET
1	E	7	ASP
1	E	10	SER
1	E	11	THR
1	E	14	SER
1	E	20	SER
1	E	32	ARG
1	E	68	CYS
1	E	81	LYS
1	E	117	GLU
1	E	152	SER
1	E	154	LEU
1	E	162	SER
2	F	6	THR
2	F	19	VAL
2	F	21	VAL
2	F	28	SER

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Mol	Chain	Res	Type
2	F	43	ARG
2	F	75	THR
1	G	1	MET
1	G	7	ASP
1	G	10	SER
1	G	11	THR
1	G	20	SER
1	G	32	ARG
1	G	81	LYS
1	G	117	GLU
1	G	152	SER
1	G	154	LEU
1	G	162	SER
5	H	6	THR
5	H	18	MET
5	H	21	VAL
5	H	23	GLN
5	H	28	SER
5	H	43	ARG
5	H	75	THR
1	I	1	MET
1	I	7	ASP
1	I	10	SER
1	I	11	THR
1	I	20	SER
1	I	24	ILE
1	I	32	ARG
1	I	81	LYS
1	I	117	GLU
1	I	154	LEU
1	I	162	SER
2	J	6	THR
2	J	18	MET
2	J	21	VAL
2	J	28	SER
2	J	43	ARG
2	J	50	THR
2	J	75	THR
1	K	1	MET
1	K	7	ASP
1	K	10	SER
1	K	11	THR

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Mol	Chain	Res	Type
1	K	14	SER
1	K	20	SER
1	K	24	ILE
1	K	32	ARG
1	K	81	LYS
1	K	88	ILE
1	K	117	GLU
1	K	152	SER
1	K	154	LEU
1	K	162	SER
2	L	6	THR
2	L	21	VAL
2	L	28	SER
2	L	43	ARG
2	L	75	THR
1	M	1	MET
1	M	7	ASP
1	M	10	SER
1	M	11	THR
1	M	20	SER
1	M	24	ILE
1	M	32	ARG
1	M	68	CYS
1	M	81	LYS
1	M	117	GLU
1	M	154	LEU
1	M	162	SER
2	N	6	THR
2	N	21	VAL
2	N	28	SER
2	N	33	GLU
2	N	43	ARG
2	N	75	THR
1	O	1	MET
1	O	7	ASP
1	O	10	SER
1	O	11	THR
1	O	20	SER
1	O	32	ARG
1	O	81	LYS
1	O	117	GLU
1	O	120	ARG

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Mol	Chain	Res	Type
1	O	152	SER
1	O	154	LEU
1	O	162	SER
2	P	6	THR
2	P	21	VAL
2	P	23	GLN
2	P	28	SER
2	P	43	ARG
2	P	75	THR
1	Q	1	MET
1	Q	7	ASP
1	Q	10	SER
1	Q	11	THR
1	Q	20	SER
1	Q	24	ILE
1	Q	32	ARG
1	Q	81	LYS
1	Q	88	ILE
1	Q	117	GLU
1	Q	120	ARG
1	Q	152	SER
1	Q	154	LEU
1	Q	162	SER
2	R	18	MET
2	R	21	VAL
2	R	28	SER
2	R	75	THR
2	R	172	SER
1	S	1	MET
1	S	7	ASP
1	S	10	SER
1	S	11	THR
1	S	14	SER
1	S	20	SER
1	S	24	ILE
1	S	32	ARG
1	S	42	ASN
1	S	81	LYS
1	S	117	GLU
1	S	154	LEU
1	S	162	SER
2	T	6	THR

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Mol	Chain	Res	Type
2	T	14	THR
2	T	18	MET
2	T	21	VAL
2	T	28	SER
2	T	43	ARG
2	T	75	THR
1	U	1	MET
1	U	7	ASP
1	U	10	SER
1	U	11	THR
1	U	20	SER
1	U	24	ILE
1	U	32	ARG
1	U	68	CYS
1	U	81	LYS
1	U	117	GLU
1	U	154	LEU
1	U	162	SER
2	V	6	THR
2	V	18	MET
2	V	21	VAL
2	V	28	SER
2	V	43	ARG
2	V	50	THR
2	V	75	THR
1	W	1	MET
1	W	7	ASP
1	W	10	SER
1	W	11	THR
1	W	20	SER
1	W	24	ILE
1	W	32	ARG
1	W	81	LYS
1	W	88	ILE
1	W	117	GLU
1	W	152	SER
1	W	154	LEU
1	W	162	SER
2	X	6	THR
2	X	18	MET
2	X	21	VAL
2	X	28	SER

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Mol	Chain	Res	Type
2	X	43	ARG
2	X	75	THR

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

Mol	Chain	Res	Type
1	A	70	GLN
2	B	23	GLN
2	B	35	ASN
3	C	70	GLN
4	D	23	GLN
4	D	42	ASN
1	E	70	GLN
2	F	23	GLN
2	F	35	ASN
1	G	70	GLN
1	G	139	ASN
5	H	23	GLN
5	H	35	ASN
5	H	42	ASN
1	I	70	GLN
2	J	23	GLN
2	J	35	ASN
1	K	70	GLN
1	K	139	ASN
2	L	23	GLN
1	M	70	GLN
2	N	23	GLN
2	P	23	GLN
2	P	35	ASN
1	Q	70	GLN
1	Q	139	ASN
2	R	23	GLN
2	R	35	ASN
2	T	23	GLN
2	T	42	ASN
1	U	70	GLN
2	V	23	GLN
2	V	35	ASN
1	W	70	GLN
2	X	23	GLN
2	X	35	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	$\#\|Z\| > 2$
6	CYC	O	184	1	42,46,46	3.13	13 (30%)	50,67,67	4.07	26 (52%)
6	CYC	S	184	1	42,46,46	3.45	14 (33%)	50,67,67	3.41	25 (50%)
6	CYC	N	255	-	42,46,46	3.41	12 (28%)	50,67,67	3.31	25 (50%)
6	CYC	X	184	2	42,46,46	2.97	15 (35%)	50,67,67	4.14	26 (52%)
6	CYC	E	184	1	42,46,46	2.97	13 (30%)	50,67,67	4.02	28 (56%)
6	CYC	C	184	3	42,46,46	3.07	13 (30%)	50,67,67	3.38	25 (50%)
6	CYC	X	255	-	42,46,46	2.86	12 (28%)	50,67,67	3.95	29 (58%)
6	CYC	D	184	4	42,46,46	3.24	13 (30%)	50,67,67	4.12	25 (50%)
6	CYC	A	184	1	42,46,46	2.94	15 (35%)	50,67,67	3.79	29 (58%)
6	CYC	Q	184	-	42,46,46	3.12	10 (23%)	50,67,67	3.12	23 (46%)
6	CYC	W	184	1	42,46,46	3.09	14 (33%)	50,67,67	4.38	29 (58%)
6	CYC	V	255	-	42,46,46	3.40	11 (26%)	50,67,67	3.69	20 (40%)
6	CYC	J	184	2	42,46,46	3.24	15 (35%)	50,67,67	4.21	34 (68%)
6	CYC	K	184	1	42,46,46	3.08	17 (40%)	50,67,67	4.22	29 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	CYC	N	184	2	42,46,46	2.91	13 (30%)	50,67,67	3.84	33 (66%)
6	CYC	R	184	2	42,46,46	3.30	17 (40%)	50,67,67	3.98	26 (52%)
6	CYC	P	184	2	42,46,46	3.30	11 (26%)	50,67,67	3.79	28 (56%)
6	CYC	L	184	2	42,46,46	3.16	13 (30%)	50,67,67	3.67	25 (50%)
7	BLA	B	184	2	42,46,46	3.68	17 (40%)	53,67,67	3.42	28 (52%)
6	CYC	P	255	-	42,46,46	3.06	13 (30%)	50,67,67	4.68	30 (60%)
7	BLA	B	255	-	42,46,46	3.66	18 (42%)	53,67,67	3.60	26 (49%)
6	CYC	I	184	1	42,46,46	2.65	16 (38%)	50,67,67	3.96	31 (62%)
6	CYC	R	255	2	42,46,46	2.88	13 (30%)	50,67,67	4.47	26 (52%)
6	CYC	M	184	1	42,46,46	2.96	15 (35%)	50,67,67	3.91	27 (54%)
6	CYC	L	255	-	42,46,46	3.36	14 (33%)	50,67,67	4.06	25 (50%)
6	CYC	T	255	-	42,46,46	3.24	15 (35%)	50,67,67	3.85	25 (50%)
6	CYC	V	184	-	42,46,46	3.26	14 (33%)	50,67,67	3.29	27 (54%)
6	CYC	F	184	2	42,46,46	3.45	13 (30%)	50,67,67	3.65	25 (50%)
6	CYC	H	255	-	42,46,46	3.24	14 (33%)	50,67,67	3.53	24 (48%)
6	CYC	H	184	5	42,46,46	3.11	18 (42%)	50,67,67	4.28	30 (60%)
7	BLA	D	255	-	42,46,46	3.23	13 (30%)	53,67,67	3.81	28 (52%)
6	CYC	J	255	2	42,46,46	3.20	14 (33%)	50,67,67	4.46	33 (66%)
6	CYC	G	184	1	42,46,46	3.12	14 (33%)	50,67,67	4.35	32 (64%)
6	CYC	U	184	1	42,46,46	3.13	16 (38%)	50,67,67	4.02	24 (48%)
6	CYC	F	255	-	42,46,46	2.86	13 (30%)	50,67,67	4.23	25 (50%)
6	CYC	T	184	2	42,46,46	3.09	15 (35%)	50,67,67	4.09	30 (60%)

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
6	CYC	O	184	1	-	14/25/74/74	0/4/4/4
6	CYC	S	184	1	-	14/25/74/74	0/4/4/4
6	CYC	N	255	-	-	15/25/74/74	0/4/4/4
6	CYC	X	184	2	-	7/25/74/74	0/4/4/4
6	CYC	E	184	1	-	14/25/74/74	0/4/4/4
6	CYC	C	184	3	-	14/25/74/74	0/4/4/4
6	CYC	X	255	-	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	CYC	D	184	4	-	15/25/74/74	0/4/4/4
6	CYC	A	184	1	-	15/25/74/74	0/4/4/4
6	CYC	Q	184	-	-	12/25/74/74	0/4/4/4
6	CYC	W	184	1	-	16/25/74/74	0/4/4/4
6	CYC	V	255	-	-	10/25/74/74	0/4/4/4
6	CYC	J	184	2	-	10/25/74/74	0/4/4/4
6	CYC	K	184	1	-	13/25/74/74	0/4/4/4
6	CYC	N	184	2	-	11/25/74/74	0/4/4/4
6	CYC	R	184	2	-	12/25/74/74	0/4/4/4
6	CYC	P	184	2	-	13/25/74/74	0/4/4/4
6	CYC	L	184	2	-	11/25/74/74	0/4/4/4
7	BLA	B	184	2	-	15/26/74/74	0/4/4/4
6	CYC	P	255	-	-	11/25/74/74	0/4/4/4
7	BLA	B	255	-	-	10/26/74/74	0/4/4/4
6	CYC	I	184	1	-	14/25/74/74	0/4/4/4
6	CYC	R	255	2	-	14/25/74/74	0/4/4/4
6	CYC	M	184	1	-	8/25/74/74	0/4/4/4
6	CYC	L	255	-	-	9/25/74/74	0/4/4/4
6	CYC	T	255	-	-	11/25/74/74	0/4/4/4
6	CYC	V	184	-	-	11/25/74/74	0/4/4/4
6	CYC	F	184	2	-	12/25/74/74	0/4/4/4
6	CYC	H	255	-	-	8/25/74/74	0/4/4/4
6	CYC	H	184	5	-	9/25/74/74	0/4/4/4
7	BLA	D	255	-	-	13/26/74/74	0/4/4/4
6	CYC	J	255	2	-	14/25/74/74	0/4/4/4
6	CYC	G	184	1	-	12/25/74/74	0/4/4/4
6	CYC	U	184	1	-	14/25/74/74	0/4/4/4
6	CYC	F	255	-	-	8/25/74/74	0/4/4/4
6	CYC	T	184	2	-	10/25/74/74	0/4/4/4

All (506) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	184	CYC	CHA-C1A	18.03	1.50	1.35
7	B	184	BLA	CHA-C4D	17.65	1.49	1.35
6	N	255	CYC	CHA-C1A	17.27	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	V	255	CYC	CHA-C1A	16.57	1.49	1.35
6	L	255	CYC	CHA-C1A	16.54	1.48	1.35
6	Q	184	CYC	CHA-C1A	16.09	1.48	1.35
6	L	184	CYC	CHA-C1A	16.00	1.48	1.35
6	F	184	CYC	CHA-C1A	15.96	1.48	1.35
7	B	255	BLA	CHA-C4D	15.93	1.48	1.35
6	P	184	CYC	CHA-C1A	15.66	1.48	1.35
6	R	184	CYC	CHA-C1A	15.48	1.48	1.35
6	D	184	CYC	CHA-C1A	15.48	1.48	1.35
6	V	184	CYC	CHA-C1A	14.93	1.47	1.35
6	K	184	CYC	CHA-C1A	14.87	1.47	1.35
6	O	184	CYC	CHA-C1A	14.75	1.47	1.35
6	H	255	CYC	CHA-C1A	14.60	1.47	1.35
6	U	184	CYC	CHA-C1A	14.40	1.47	1.35
6	J	184	CYC	CHA-C1A	14.10	1.46	1.35
6	N	184	CYC	CHA-C1A	14.06	1.46	1.35
6	G	184	CYC	CHA-C1A	14.06	1.46	1.35
6	J	255	CYC	CHA-C1A	13.86	1.46	1.35
6	H	184	CYC	CHA-C1A	13.84	1.46	1.35
6	C	184	CYC	CHA-C1A	13.70	1.46	1.35
6	T	255	CYC	CHA-C1A	13.62	1.46	1.35
7	D	255	BLA	CHA-C4D	13.47	1.46	1.35
6	P	255	CYC	CHA-C1A	13.26	1.46	1.35
6	M	184	CYC	CHA-C1A	13.25	1.46	1.35
6	A	184	CYC	CHA-C1A	13.10	1.46	1.35
6	W	184	CYC	CHA-C1A	12.97	1.46	1.35
6	E	184	CYC	CHA-C1A	12.64	1.45	1.35
6	X	255	CYC	CHA-C1A	12.32	1.45	1.35
6	R	255	CYC	CHA-C1A	12.14	1.45	1.35
6	T	184	CYC	CHA-C1A	12.03	1.45	1.35
6	X	184	CYC	CHA-C1A	11.48	1.44	1.35
6	F	255	CYC	CHA-C1A	10.71	1.44	1.35
6	I	184	CYC	CHA-C1A	10.70	1.44	1.35
6	J	255	CYC	C4B-C3B	-8.49	1.32	1.48
6	F	255	CYC	C4B-C3B	-7.79	1.33	1.48
6	J	184	CYC	C2C-C1C	-7.42	1.45	1.52
6	T	184	CYC	C2C-C1C	-7.38	1.45	1.52
6	R	255	CYC	C4B-C3B	-7.35	1.34	1.48
6	G	184	CYC	C1A-C2A	-7.05	1.34	1.45
7	B	255	BLA	CHB-C1B	6.94	1.48	1.34
7	D	255	BLA	C3C-C2C	6.89	1.51	1.37
7	D	255	BLA	CHB-C1B	6.84	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	255	CYC	C4B-C3B	-6.78	1.35	1.48
7	B	184	BLA	C3C-C2C	6.69	1.50	1.37
6	W	184	CYC	C4B-C3B	-6.55	1.35	1.48
6	H	255	CYC	C4B-C3B	-6.49	1.35	1.48
6	X	255	CYC	C4B-C3B	-6.45	1.35	1.48
6	F	184	CYC	C1C-NC	-6.45	1.29	1.37
6	F	184	CYC	C2C-C1C	-6.44	1.46	1.52
6	V	255	CYC	C4B-C3B	-6.42	1.36	1.48
6	O	184	CYC	C4B-C3B	-6.39	1.36	1.48
6	F	255	CYC	C1A-C2A	-6.38	1.35	1.45
6	H	255	CYC	C2C-C1C	-6.37	1.46	1.52
6	C	184	CYC	C4B-C3B	-6.33	1.36	1.48
6	P	255	CYC	C4B-C3B	-6.22	1.36	1.48
6	G	184	CYC	C4B-C3B	-6.18	1.36	1.48
6	P	184	CYC	C4B-C3B	-6.08	1.36	1.48
6	L	255	CYC	C4B-C3B	-6.05	1.36	1.48
7	B	255	BLA	C4C-NC	-6.01	1.27	1.37
6	E	184	CYC	C1A-C2A	-6.00	1.36	1.45
6	L	255	CYC	C2C-C1C	-5.98	1.46	1.52
7	B	184	BLA	CHB-C1B	5.95	1.46	1.34
6	T	184	CYC	C4B-C3B	-5.92	1.36	1.48
6	I	184	CYC	C4B-C3B	-5.92	1.37	1.48
6	O	184	CYC	C1A-C2A	-5.92	1.36	1.45
6	M	184	CYC	C1A-C2A	-5.89	1.36	1.45
6	E	184	CYC	C2C-C1C	-5.82	1.46	1.52
6	X	184	CYC	C1C-NC	-5.82	1.30	1.37
6	J	184	CYC	C1C-NC	-5.81	1.30	1.37
6	K	184	CYC	C4B-C3B	-5.80	1.37	1.48
6	X	255	CYC	C1A-C2A	-5.79	1.36	1.45
6	U	184	CYC	C4B-C3B	-5.75	1.37	1.48
7	B	255	BLA	C3C-C2C	5.74	1.48	1.37
6	T	255	CYC	C2C-C1C	-5.70	1.47	1.52
6	R	184	CYC	C4B-C3B	-5.61	1.37	1.48
6	V	255	CYC	CHB-C1B	5.61	1.51	1.38
6	V	255	CYC	C2C-C1C	-5.50	1.47	1.52
6	V	184	CYC	C2C-C1C	-5.49	1.47	1.52
6	C	184	CYC	CHB-C1B	5.45	1.51	1.38
6	V	184	CYC	C4B-C3B	-5.43	1.37	1.48
6	H	184	CYC	C1C-NC	-5.40	1.30	1.37
6	H	184	CYC	C4B-C3B	-5.38	1.38	1.48
6	J	184	CYC	C4B-C3B	-5.38	1.38	1.48
6	D	184	CYC	C1C-NC	-5.36	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	255	CYC	C2C-C1C	-5.30	1.47	1.52
6	P	255	CYC	C2C-C1C	-5.30	1.47	1.52
6	R	184	CYC	CHB-C4A	5.28	1.52	1.40
6	N	255	CYC	CHB-C1B	5.26	1.50	1.38
6	R	255	CYC	C1A-C2A	-5.22	1.37	1.45
6	C	184	CYC	C1C-NC	-5.20	1.30	1.37
6	L	184	CYC	C4B-C3B	-5.19	1.38	1.48
6	X	184	CYC	C1B-NB	-5.14	1.29	1.37
6	D	184	CYC	CHB-C1B	5.12	1.50	1.38
6	T	255	CYC	C1A-C2A	-5.11	1.37	1.45
6	N	255	CYC	C4B-C3B	-5.10	1.38	1.48
6	F	184	CYC	C4B-C3B	-5.09	1.38	1.48
6	P	255	CYC	C1A-C2A	-5.07	1.37	1.45
6	P	184	CYC	C1C-NC	-5.06	1.31	1.37
6	S	184	CYC	CHB-C1B	5.04	1.50	1.38
6	D	184	CYC	C4B-C3B	-4.99	1.38	1.48
6	A	184	CYC	C4B-C3B	-4.94	1.38	1.48
6	S	184	CYC	C4B-C3B	-4.88	1.38	1.48
6	P	184	CYC	CHB-C1B	4.87	1.49	1.38
7	B	255	BLA	CHD-C1D	4.85	1.51	1.40
6	H	255	CYC	C1A-C2A	-4.83	1.38	1.45
6	Q	184	CYC	CHB-C1B	4.82	1.49	1.38
6	P	184	CYC	C2C-C1C	-4.81	1.47	1.52
6	X	184	CYC	C2C-C1C	-4.80	1.47	1.52
6	H	255	CYC	CHB-C1B	4.78	1.49	1.38
6	X	255	CYC	C2C-C1C	-4.77	1.47	1.52
6	V	184	CYC	CHB-C4A	4.77	1.51	1.40
6	S	184	CYC	C1C-NC	-4.77	1.31	1.37
6	T	184	CYC	CHB-C4A	4.76	1.51	1.40
6	T	255	CYC	C4C-NC	-4.74	1.27	1.37
6	O	184	CYC	CHB-C1B	4.74	1.49	1.38
6	F	184	CYC	CHB-C1B	4.73	1.49	1.38
6	V	255	CYC	C1A-C2A	-4.71	1.38	1.45
6	E	184	CYC	C4B-C3B	-4.68	1.39	1.48
6	X	184	CYC	OB-C4B	4.67	1.32	1.23
6	R	184	CYC	CHB-C1B	4.64	1.49	1.38
6	X	184	CYC	C4B-C3B	-4.62	1.39	1.48
7	B	255	BLA	CBB-CAB	4.62	1.53	1.30
6	A	184	CYC	C1C-NC	-4.62	1.31	1.37
6	J	255	CYC	C1A-C2A	-4.61	1.38	1.45
7	B	184	BLA	CBB-CAB	4.56	1.52	1.30
6	M	184	CYC	C4B-C3B	-4.52	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	184	CYC	CHB-C4A	4.51	1.51	1.40
6	U	184	CYC	C1A-C2A	-4.51	1.38	1.45
6	J	255	CYC	C2C-C1C	-4.48	1.48	1.52
6	Q	184	CYC	C4B-C3B	-4.42	1.39	1.48
6	C	184	CYC	CHB-C4A	4.41	1.50	1.40
6	R	184	CYC	C1C-NC	-4.41	1.31	1.37
6	T	184	CYC	C1C-NC	-4.40	1.31	1.37
6	N	184	CYC	C4B-C3B	-4.39	1.39	1.48
6	U	184	CYC	CHB-C1B	4.38	1.48	1.38
6	A	184	CYC	C1B-C2B	-4.37	1.37	1.45
7	D	255	BLA	CBB-CAB	4.37	1.51	1.30
6	J	255	CYC	CHB-C1B	4.34	1.48	1.38
7	B	255	BLA	CBC-CAC	4.32	1.51	1.30
6	V	184	CYC	CHB-C1B	4.29	1.48	1.38
7	D	255	BLA	CBC-CAC	4.28	1.51	1.30
6	T	255	CYC	C1C-NC	-4.28	1.32	1.37
6	U	184	CYC	CHB-C4A	4.28	1.50	1.40
6	T	255	CYC	CHB-C1B	4.26	1.48	1.38
6	E	184	CYC	CHB-C1B	4.25	1.48	1.38
6	S	184	CYC	CHB-C4A	4.24	1.50	1.40
6	I	184	CYC	C1A-C2A	-4.24	1.39	1.45
6	N	184	CYC	C1A-C2A	-4.23	1.39	1.45
6	N	255	CYC	CHB-C4A	4.23	1.50	1.40
6	F	184	CYC	CHB-C4A	4.23	1.50	1.40
7	B	184	BLA	CHD-C1D	4.22	1.50	1.40
6	M	184	CYC	C2C-C1C	-4.22	1.48	1.52
6	L	184	CYC	C1C-NC	-4.22	1.32	1.37
6	I	184	CYC	CHB-C4A	4.21	1.50	1.40
6	V	255	CYC	CHB-C4A	4.18	1.50	1.40
6	D	184	CYC	CHB-C4A	4.18	1.50	1.40
7	B	184	BLA	CBC-CAC	4.17	1.51	1.30
6	D	184	CYC	C1A-C2A	-4.16	1.39	1.45
6	J	255	CYC	C1B-C2B	-4.15	1.37	1.45
6	T	184	CYC	C4A-C3A	4.13	1.54	1.45
6	N	184	CYC	C2C-C1C	-4.12	1.48	1.52
6	V	184	CYC	C1B-C2B	-4.11	1.37	1.45
6	M	184	CYC	CHB-C4A	4.10	1.50	1.40
7	D	255	BLA	C4C-NC	-4.09	1.31	1.37
7	B	255	BLA	C3B-C4B	-4.09	1.35	1.47
6	G	184	CYC	CHB-C4A	4.06	1.49	1.40
6	F	255	CYC	CHB-C1B	4.06	1.47	1.38
6	K	184	CYC	C1B-NB	-4.06	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	184	CYC	CHB-C4A	4.05	1.49	1.40
6	G	184	CYC	CHB-C1B	4.04	1.47	1.38
6	I	184	CYC	CHB-C1B	4.03	1.47	1.38
6	X	255	CYC	C1B-C2B	-4.03	1.37	1.45
6	M	184	CYC	CHB-C1B	4.03	1.47	1.38
6	J	184	CYC	CHB-C1B	4.02	1.47	1.38
6	T	184	CYC	C1A-C2A	-4.02	1.39	1.45
6	R	184	CYC	C2C-C1C	-4.00	1.48	1.52
6	A	184	CYC	C1A-C2A	-3.99	1.39	1.45
6	A	184	CYC	CHB-C1B	3.97	1.47	1.38
6	F	255	CYC	C1B-C2B	-3.97	1.38	1.45
6	H	255	CYC	CHB-C4A	3.96	1.49	1.40
6	W	184	CYC	C2C-C1C	-3.96	1.48	1.52
6	W	184	CYC	CHB-C4A	3.96	1.49	1.40
6	Q	184	CYC	CHB-C4A	3.94	1.49	1.40
7	D	255	BLA	CHD-C1D	3.93	1.49	1.40
6	P	184	CYC	C4C-NC	-3.92	1.29	1.37
6	W	184	CYC	C1B-C2B	-3.92	1.38	1.45
6	L	184	CYC	CHB-C1B	3.92	1.47	1.38
6	L	255	CYC	CHB-C1B	3.92	1.47	1.38
6	W	184	CYC	CHB-C1B	3.91	1.47	1.38
6	T	184	CYC	CHB-C1B	3.89	1.47	1.38
6	V	184	CYC	C1C-NC	-3.89	1.32	1.37
6	W	184	CYC	C1C-NC	-3.89	1.32	1.37
6	F	184	CYC	OB-C4B	3.86	1.30	1.23
6	F	255	CYC	C4C-NC	-3.86	1.29	1.37
6	L	255	CYC	C1B-NB	-3.86	1.31	1.37
6	E	184	CYC	CHB-C4A	3.85	1.49	1.40
6	W	184	CYC	C1B-NB	-3.84	1.31	1.37
6	X	255	CYC	CHB-C1B	3.83	1.47	1.38
6	W	184	CYC	C1A-C2A	-3.82	1.39	1.45
6	R	184	CYC	C1B-NB	-3.82	1.31	1.37
7	B	184	BLA	OB-C4B	3.82	1.30	1.23
6	K	184	CYC	C1A-C2A	-3.82	1.39	1.45
6	A	184	CYC	CHB-C4A	3.81	1.49	1.40
6	P	255	CYC	CBA-CGA	3.80	1.59	1.50
6	R	255	CYC	C2C-C1C	-3.79	1.48	1.52
6	S	184	CYC	C4C-NC	-3.79	1.29	1.37
6	C	184	CYC	C1B-C2B	-3.76	1.38	1.45
6	J	184	CYC	C4C-NC	-3.76	1.29	1.37
6	H	184	CYC	C4C-NC	-3.75	1.29	1.37
6	L	184	CYC	C2C-C1C	-3.75	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	255	CYC	C1B-NB	-3.72	1.31	1.37
6	N	255	CYC	C1A-C2A	-3.72	1.39	1.45
7	D	255	BLA	C3B-C4B	-3.71	1.36	1.47
6	T	255	CYC	CHB-C4A	3.71	1.49	1.40
6	W	184	CYC	C4B-NB	-3.67	1.30	1.38
6	D	184	CYC	C4C-NC	-3.66	1.29	1.37
6	U	184	CYC	C1B-NB	-3.66	1.31	1.37
6	R	255	CYC	CHB-C1B	3.65	1.46	1.38
6	I	184	CYC	C1C-NC	-3.63	1.32	1.37
6	P	255	CYC	CHB-C1B	3.63	1.46	1.38
6	G	184	CYC	C1D-CHD	3.63	1.55	1.41
6	L	184	CYC	C1B-NB	-3.60	1.31	1.37
6	A	184	CYC	C4C-NC	-3.58	1.29	1.37
6	H	184	CYC	CHB-C1B	3.58	1.46	1.38
6	F	184	CYC	C4C-NC	-3.58	1.29	1.37
6	L	255	CYC	C4C-NC	-3.57	1.29	1.37
6	J	255	CYC	C4C-NC	-3.56	1.29	1.37
6	P	184	CYC	C1A-C2A	-3.55	1.40	1.45
6	U	184	CYC	C2C-C1C	-3.54	1.48	1.52
6	X	184	CYC	CHB-C1B	3.52	1.46	1.38
7	B	255	BLA	C1C-NC	-3.51	1.30	1.38
6	W	184	CYC	C4C-NC	-3.50	1.30	1.37
6	J	184	CYC	C1A-C2A	-3.50	1.40	1.45
6	K	184	CYC	CHB-C1B	3.49	1.46	1.38
7	B	255	BLA	C1B-NB	-3.49	1.32	1.37
6	H	184	CYC	C2C-C1C	-3.48	1.49	1.52
7	B	184	BLA	C3C-C4C	3.48	1.51	1.45
7	B	255	BLA	C3C-C4C	3.48	1.51	1.45
7	D	255	BLA	C1B-NB	-3.47	1.32	1.37
6	X	184	CYC	CHB-C4A	3.47	1.48	1.40
6	X	184	CYC	C4C-NC	-3.47	1.30	1.37
6	U	184	CYC	C1C-NC	-3.46	1.33	1.37
6	D	184	CYC	OB-C4B	3.45	1.30	1.23
6	V	184	CYC	C4A-C3A	3.44	1.53	1.45
6	R	255	CYC	C1A-NA	-3.44	1.31	1.38
6	H	184	CYC	C1B-NB	-3.44	1.32	1.37
7	B	184	BLA	C4C-NC	-3.43	1.32	1.37
6	I	184	CYC	C2C-C1C	-3.42	1.49	1.52
6	G	184	CYC	C3C-C4C	3.42	1.55	1.50
6	H	255	CYC	C1B-NB	-3.40	1.32	1.37
6	N	255	CYC	C1C-NC	-3.39	1.33	1.37
6	H	184	CYC	C1B-C2B	-3.39	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	184	CYC	C1B-C2B	-3.38	1.39	1.45
6	W	184	CYC	C4A-C3A	3.36	1.53	1.45
6	L	255	CYC	C1A-C2A	-3.36	1.40	1.45
6	L	255	CYC	C1C-NC	-3.35	1.33	1.37
6	E	184	CYC	C1A-NA	-3.32	1.31	1.38
6	L	184	CYC	CHB-C4A	3.31	1.48	1.40
6	X	184	CYC	C1A-C2A	-3.30	1.40	1.45
6	O	184	CYC	CHB-C4A	3.28	1.48	1.40
6	P	255	CYC	C4C-NC	-3.27	1.30	1.37
6	H	184	CYC	CHB-C4A	3.27	1.48	1.40
6	O	184	CYC	C2C-C1C	-3.26	1.49	1.52
6	F	255	CYC	C1B-NB	-3.26	1.32	1.37
6	R	255	CYC	C1C-NC	-3.25	1.33	1.37
6	U	184	CYC	OB-C4B	3.24	1.29	1.23
6	W	184	CYC	C1D-CHD	3.23	1.53	1.41
6	Q	184	CYC	C1B-C2B	-3.23	1.39	1.45
6	N	184	CYC	C4C-NC	-3.22	1.30	1.37
6	V	184	CYC	OB-C4B	3.21	1.29	1.23
6	N	184	CYC	OB-C4B	3.20	1.29	1.23
7	B	184	BLA	C1B-NB	-3.20	1.32	1.37
6	T	184	CYC	C1B-NB	-3.19	1.32	1.37
6	I	184	CYC	C1B-C2B	-3.18	1.39	1.45
6	N	184	CYC	C1B-NB	-3.17	1.32	1.37
6	N	184	CYC	CHB-C4A	3.16	1.47	1.40
6	M	184	CYC	C4A-C3A	3.15	1.52	1.45
6	F	255	CYC	C4B-NB	-3.14	1.31	1.38
6	J	255	CYC	C1B-NB	-3.14	1.32	1.37
6	N	184	CYC	CHB-C1B	3.13	1.45	1.38
6	M	184	CYC	C1D-CHD	3.13	1.53	1.41
6	H	184	CYC	C1A-C2A	-3.13	1.40	1.45
6	E	184	CYC	C1B-C2B	-3.12	1.39	1.45
6	R	184	CYC	C4B-NB	-3.09	1.31	1.38
6	G	184	CYC	C4B-NB	-3.08	1.31	1.38
6	K	184	CYC	C4C-NC	-3.08	1.30	1.37
6	P	184	CYC	C4A-C3A	3.08	1.52	1.45
6	P	255	CYC	C4A-C3A	3.08	1.52	1.45
6	X	184	CYC	C4A-C3A	3.07	1.52	1.45
6	Q	184	CYC	C1A-C2A	-3.07	1.40	1.45
6	T	255	CYC	C1B-NB	-3.06	1.32	1.37
6	R	255	CYC	C1B-C2B	-3.06	1.39	1.45
6	M	184	CYC	OB-C4B	3.06	1.29	1.23
6	N	255	CYC	C4C-NC	-3.06	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	184	CYC	C1A-C2A	-3.05	1.40	1.45
6	R	255	CYC	C4C-NC	-3.04	1.31	1.37
6	J	184	CYC	C1B-NB	-3.04	1.32	1.37
6	P	255	CYC	CHB-C4A	3.01	1.47	1.40
6	E	184	CYC	OB-C4B	3.01	1.29	1.23
6	L	184	CYC	C4A-C3A	3.01	1.52	1.45
6	Q	184	CYC	OB-C4B	3.00	1.29	1.23
6	A	184	CYC	OB-C4B	3.00	1.29	1.23
6	J	255	CYC	CHB-C4A	2.99	1.47	1.40
6	C	184	CYC	C1D-CHD	2.97	1.52	1.41
6	C	184	CYC	C4A-C3A	2.95	1.52	1.45
6	H	184	CYC	C4B-NB	-2.95	1.31	1.38
6	S	184	CYC	OB-C4B	2.94	1.29	1.23
6	H	184	CYC	C4A-C3A	2.93	1.52	1.45
6	J	184	CYC	CHB-C4A	2.93	1.47	1.40
6	R	255	CYC	OB-C4B	2.92	1.29	1.23
6	G	184	CYC	C1B-NB	-2.92	1.32	1.37
6	V	255	CYC	C4C-NC	-2.91	1.31	1.37
6	L	255	CYC	CBA-CGA	2.89	1.57	1.50
6	C	184	CYC	C1A-C2A	-2.88	1.41	1.45
6	X	184	CYC	C1D-CHD	2.88	1.52	1.41
6	F	255	CYC	C4A-C3A	2.88	1.52	1.45
6	S	184	CYC	C1B-C2B	-2.88	1.39	1.45
6	J	255	CYC	C4B-NB	-2.87	1.31	1.38
6	Q	184	CYC	C1D-CHD	2.87	1.52	1.41
6	N	255	CYC	C1B-NB	-2.87	1.33	1.37
7	B	184	BLA	C1B-C2B	-2.87	1.39	1.45
6	R	184	CYC	C1D-CHD	2.86	1.52	1.41
6	N	184	CYC	C1B-C2B	-2.86	1.39	1.45
6	J	255	CYC	CBA-CGA	2.86	1.57	1.50
6	S	184	CYC	C1D-CHD	2.85	1.52	1.41
6	F	255	CYC	C4A-NA	-2.85	1.30	1.36
6	V	184	CYC	C1B-NB	-2.85	1.33	1.37
6	M	184	CYC	C1C-NC	-2.83	1.33	1.37
6	U	184	CYC	C4A-C3A	2.83	1.51	1.45
6	H	255	CYC	C4C-NC	-2.82	1.31	1.37
6	U	184	CYC	C1B-C2B	-2.81	1.40	1.45
6	L	184	CYC	C4C-NC	-2.80	1.31	1.37
6	T	184	CYC	C4B-NB	-2.79	1.32	1.38
6	K	184	CYC	C1B-C2B	-2.79	1.40	1.45
6	E	184	CYC	C1B-NB	-2.79	1.33	1.37
7	D	255	BLA	C3C-C4C	2.78	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	184	CYC	C2C-C1C	-2.78	1.49	1.52
6	V	184	CYC	C1D-CHD	2.76	1.51	1.41
6	H	255	CYC	C1B-C2B	-2.76	1.40	1.45
7	B	255	BLA	C1B-C2B	-2.75	1.40	1.45
6	K	184	CYC	C1D-CHD	2.75	1.51	1.41
6	J	184	CYC	C1B-C2B	-2.74	1.40	1.45
6	X	255	CYC	C1A-NA	-2.74	1.32	1.38
6	V	184	CYC	C1A-C2A	-2.74	1.41	1.45
6	A	184	CYC	C4A-C3A	2.74	1.51	1.45
6	R	184	CYC	C4C-NC	-2.72	1.31	1.37
6	V	184	CYC	C4C-NC	-2.72	1.31	1.37
6	S	184	CYC	C4A-C3A	2.71	1.51	1.45
6	N	255	CYC	C4A-C3A	2.70	1.51	1.45
6	T	255	CYC	C4A-C3A	2.70	1.51	1.45
6	Q	184	CYC	C4A-C3A	2.69	1.51	1.45
6	P	184	CYC	OB-C4B	2.69	1.28	1.23
6	X	184	CYC	C1B-C2B	-2.69	1.40	1.45
6	R	184	CYC	C1A-C2A	-2.69	1.41	1.45
6	T	184	CYC	C4C-NC	-2.68	1.31	1.37
6	K	184	CYC	C2A-C3A	2.68	1.42	1.36
6	G	184	CYC	C1B-C2B	-2.68	1.40	1.45
6	R	255	CYC	C1D-CHD	2.68	1.51	1.41
6	J	184	CYC	C1D-CHD	2.67	1.51	1.41
6	T	255	CYC	CHD-C4C	-2.67	1.31	1.38
6	L	255	CYC	OB-C4B	2.66	1.28	1.23
6	X	255	CYC	C1B-NB	-2.65	1.33	1.37
6	I	184	CYC	C1B-NB	-2.65	1.33	1.37
6	X	255	CYC	O2A-CGA	-2.63	1.21	1.30
6	F	184	CYC	C1B-NB	-2.63	1.33	1.37
6	N	255	CYC	OB-C4B	2.63	1.28	1.23
7	D	255	BLA	OB-C4B	2.62	1.28	1.23
6	L	184	CYC	OB-C4B	2.61	1.28	1.23
6	D	184	CYC	C1B-NB	-2.59	1.33	1.37
6	D	184	CYC	C4A-C3A	2.58	1.51	1.45
6	E	184	CYC	C1D-CHD	2.58	1.51	1.41
7	B	184	BLA	C3B-C4B	-2.57	1.40	1.47
6	I	184	CYC	OB-C4B	2.55	1.28	1.23
6	N	184	CYC	C1C-NC	-2.55	1.34	1.37
6	K	184	CYC	O2D-CGD	-2.54	1.22	1.30
6	J	184	CYC	C1A-NA	-2.53	1.33	1.38
7	B	255	BLA	C4D-C3D	2.53	1.49	1.45
6	G	184	CYC	C1A-NA	-2.52	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	184	CYC	C2A-C3A	2.51	1.42	1.36
6	L	255	CYC	C1B-C2B	-2.51	1.40	1.45
6	I	184	CYC	C1A-NA	-2.51	1.33	1.38
6	P	255	CYC	C1A-NA	-2.51	1.33	1.38
6	J	184	CYC	C4B-NB	-2.50	1.32	1.38
6	N	184	CYC	C1D-CHD	2.50	1.50	1.41
6	F	184	CYC	C4D-CHA	2.50	1.50	1.41
6	K	184	CYC	C3C-C4C	2.50	1.54	1.50
6	M	184	CYC	C3C-C4C	2.49	1.54	1.50
7	B	184	BLA	C1D-C2D	2.49	1.51	1.45
6	V	255	CYC	C1D-CHD	2.48	1.50	1.41
6	P	255	CYC	CBA-CAA	2.48	1.59	1.52
6	F	255	CYC	C1D-CHD	2.48	1.50	1.41
6	O	184	CYC	C4A-C3A	2.48	1.51	1.45
6	P	255	CYC	C1B-C2B	-2.47	1.40	1.45
6	L	255	CYC	CHB-C4A	2.47	1.46	1.40
6	I	184	CYC	CAD-C3D	-2.47	1.48	1.52
6	K	184	CYC	O1A-CGA	2.46	1.30	1.22
6	S	184	CYC	C2A-C3A	2.46	1.41	1.36
6	F	184	CYC	C4A-C3A	2.45	1.51	1.45
6	I	184	CYC	C1D-CHD	2.44	1.50	1.41
6	D	184	CYC	C2C-C1C	-2.44	1.49	1.52
6	R	184	CYC	C4A-C3A	2.44	1.51	1.45
6	R	184	CYC	C1A-NA	-2.44	1.33	1.38
6	T	184	CYC	C3C-C4C	-2.43	1.47	1.50
6	H	184	CYC	C3C-C4C	2.43	1.54	1.50
6	K	184	CYC	C4B-NB	-2.42	1.32	1.38
6	E	184	CYC	C4B-NB	-2.42	1.32	1.38
6	J	255	CYC	C1A-NA	-2.42	1.33	1.38
6	X	255	CYC	CHB-C4A	2.42	1.46	1.40
6	O	184	CYC	C1D-CHD	2.42	1.50	1.41
6	U	184	CYC	C1D-CHD	2.41	1.50	1.41
7	B	184	BLA	C4A-CHB	2.40	1.50	1.41
6	L	184	CYC	C1A-C2A	-2.40	1.41	1.45
6	M	184	CYC	C1B-NB	-2.39	1.33	1.37
6	R	184	CYC	C2A-C3A	2.39	1.41	1.36
6	C	184	CYC	C4C-NC	-2.38	1.32	1.37
6	T	255	CYC	C3C-C4C	-2.38	1.47	1.50
6	S	184	CYC	C4D-CHA	2.38	1.50	1.41
6	V	255	CYC	C4B-NB	-2.38	1.32	1.38
6	H	184	CYC	CBD-CGD	2.38	1.56	1.50
6	P	184	CYC	C1B-NB	-2.37	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	184	CYC	OB-C4B	2.37	1.28	1.23
6	T	184	CYC	C1D-CHD	2.36	1.50	1.41
6	K	184	CYC	C1A-NA	-2.36	1.33	1.38
6	A	184	CYC	C1D-CHD	2.35	1.50	1.41
6	Q	184	CYC	C2A-C3A	2.35	1.41	1.36
7	B	255	BLA	OB-C4B	2.35	1.28	1.23
6	X	255	CYC	OB-C4B	2.33	1.28	1.23
6	C	184	CYC	C2A-C3A	2.33	1.41	1.36
6	E	184	CYC	C1C-NC	-2.33	1.34	1.37
6	T	255	CYC	C1B-C2B	-2.33	1.40	1.45
6	H	184	CYC	C1D-CHD	2.32	1.50	1.41
6	H	255	CYC	C1C-NC	-2.32	1.34	1.37
6	I	184	CYC	C4C-NC	-2.31	1.32	1.37
6	S	184	CYC	C2C-C1C	-2.31	1.50	1.52
6	R	255	CYC	C1B-NB	-2.30	1.34	1.37
6	F	184	CYC	C1D-CHD	2.30	1.50	1.41
6	F	255	CYC	CHB-C4A	2.29	1.45	1.40
6	M	184	CYC	C2A-C3A	2.29	1.41	1.36
6	N	184	CYC	C4D-CHA	2.28	1.50	1.41
6	X	255	CYC	C1D-CHD	2.26	1.49	1.41
6	U	184	CYC	C4D-CHA	2.26	1.49	1.41
7	D	255	BLA	CAC-C3C	2.26	1.53	1.47
6	U	184	CYC	OC-C1C	-2.25	1.18	1.23
7	B	184	BLA	C1C-NC	-2.25	1.33	1.38
7	D	255	BLA	C4A-CHB	2.25	1.49	1.41
6	C	184	CYC	C4B-NB	-2.25	1.33	1.38
6	J	184	CYC	C4D-CHA	2.24	1.49	1.41
6	G	184	CYC	O1A-CGA	2.23	1.29	1.22
6	R	184	CYC	C4D-CHA	2.22	1.49	1.41
6	I	184	CYC	C4A-C3A	2.22	1.50	1.45
6	W	184	CYC	C1A-NA	-2.22	1.33	1.38
6	K	184	CYC	OB-C4B	2.22	1.27	1.23
6	H	184	CYC	OC-C1C	-2.21	1.19	1.23
7	B	255	BLA	C1D-C2D	2.21	1.50	1.45
6	K	184	CYC	C4A-C3A	2.20	1.50	1.45
6	O	184	CYC	C4A-NA	-2.20	1.31	1.36
6	L	184	CYC	C1B-C2B	-2.19	1.41	1.45
6	R	184	CYC	CAA-C2A	2.19	1.57	1.51
6	L	255	CYC	C1D-CHD	2.18	1.49	1.41
6	H	255	CYC	CBA-CGA	2.16	1.55	1.50
6	A	184	CYC	C1B-NB	-2.16	1.34	1.37
6	O	184	CYC	O1A-CGA	2.15	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	X	184	CYC	O1A-CGA	2.15	1.29	1.22
6	H	184	CYC	OB-C4B	2.15	1.27	1.23
6	O	184	CYC	OB-C4B	2.14	1.27	1.23
6	J	255	CYC	C1D-CHD	2.14	1.49	1.41
6	J	184	CYC	OC-C1C	-2.13	1.19	1.23
6	U	184	CYC	C4B-NB	-2.13	1.33	1.38
6	J	255	CYC	C3C-C4C	2.12	1.54	1.50
6	U	184	CYC	C3C-C4C	2.12	1.53	1.50
6	T	255	CYC	C1D-CHD	2.12	1.49	1.41
6	I	184	CYC	C4B-NB	-2.12	1.33	1.38
6	L	184	CYC	C4B-NB	-2.10	1.33	1.38
6	D	184	CYC	C1D-CHD	2.09	1.49	1.41
6	M	184	CYC	C1A-NA	-2.08	1.34	1.38
6	V	184	CYC	C4B-NB	-2.08	1.33	1.38
6	H	255	CYC	O2A-CGA	-2.07	1.23	1.30
6	A	184	CYC	C3B-C2B	2.07	1.41	1.36
6	H	184	CYC	C4D-CHA	2.06	1.49	1.41
6	A	184	CYC	C1A-NA	-2.06	1.34	1.38
6	O	184	CYC	C4C-NC	-2.06	1.33	1.37
6	F	255	CYC	C2C-C1C	-2.06	1.50	1.52
6	M	184	CYC	C4B-NB	-2.05	1.33	1.38
7	B	184	BLA	CAB-C3B	2.05	1.53	1.47
6	L	255	CYC	CBA-CAA	2.05	1.58	1.52
6	V	255	CYC	C1B-NB	-2.05	1.34	1.37
6	H	255	CYC	CBA-CAA	2.05	1.58	1.52
6	C	184	CYC	O1A-CGA	2.05	1.28	1.22
6	G	184	CYC	C4C-NC	-2.05	1.33	1.37
6	T	255	CYC	OB-C4B	2.04	1.27	1.23
6	N	255	CYC	C1D-CHD	2.04	1.49	1.41
7	B	184	BLA	O2D-CGD	-2.04	1.23	1.30
6	R	255	CYC	CBA-CAA	2.04	1.58	1.52
6	H	255	CYC	OB-C4B	2.03	1.27	1.23
6	X	184	CYC	CAA-C2A	2.03	1.56	1.51
7	B	255	BLA	CAB-C3B	2.03	1.53	1.47
7	B	255	BLA	C4D-ND	-2.03	1.34	1.38
6	T	184	CYC	C1B-C2B	-2.02	1.41	1.45
6	V	255	CYC	C1C-NC	-2.01	1.35	1.37
6	T	184	CYC	C3B-C2B	2.01	1.41	1.36
6	G	184	CYC	C1C-NC	-2.01	1.35	1.37
6	S	184	CYC	C1A-C2A	-2.01	1.42	1.45
7	B	255	BLA	C1A-CHA	2.00	1.48	1.41

All (981) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	184	CYC	CAA-CBA-CGA	-17.52	75.89	113.60
6	R	255	CYC	OB-C4B-C3B	-16.03	110.65	128.04
6	F	255	CYC	C3B-C4B-NB	15.70	119.47	106.78
6	V	255	CYC	C3B-C4B-NB	15.52	119.32	106.78
6	R	255	CYC	C3B-C4B-NB	15.18	119.05	106.78
6	T	255	CYC	C3B-C4B-NB	14.46	118.46	106.78
6	P	255	CYC	C3B-C4B-NB	14.33	118.36	106.78
6	D	184	CYC	C3B-C4B-NB	14.00	118.09	106.78
6	R	184	CYC	C3B-C4B-NB	13.96	118.06	106.78
6	L	255	CYC	C3B-C4B-NB	13.84	117.96	106.78
6	K	184	CYC	C3B-C4B-NB	13.69	117.84	106.78
6	O	184	CYC	C3B-C4B-NB	13.69	117.84	106.78
6	L	184	CYC	C3B-C4B-NB	13.11	117.37	106.78
6	T	184	CYC	C3B-C4B-NB	12.98	117.27	106.78
6	J	184	CYC	C3B-C4B-NB	12.97	117.26	106.78
6	D	184	CYC	CAA-CBA-CGA	-12.85	85.94	113.60
6	H	255	CYC	C3B-C4B-NB	12.65	117.00	106.78
6	X	255	CYC	C3B-C4B-NB	12.51	116.89	106.78
6	J	255	CYC	C3B-C4B-NB	12.49	116.87	106.78
6	W	184	CYC	C3B-C4B-NB	12.41	116.80	106.78
6	G	184	CYC	C3B-C4B-NB	12.01	116.48	106.78
6	P	184	CYC	C3B-C4B-NB	11.76	116.28	106.78
7	B	255	BLA	CAC-C3C-C2C	-11.67	90.14	128.60
6	U	184	CYC	CAA-CBA-CGA	-11.59	88.66	113.60
6	E	184	CYC	C3B-C4B-NB	11.58	116.13	106.78
6	N	255	CYC	C3B-C4B-NB	11.57	116.13	106.78
6	X	184	CYC	C3B-C4B-NB	11.34	115.94	106.78
6	H	184	CYC	C3B-C4B-NB	11.31	115.91	106.78
6	S	184	CYC	CAA-CBA-CGA	-11.30	89.30	113.60
6	U	184	CYC	C3B-C4B-NB	11.28	115.89	106.78
6	P	255	CYC	OC-C1C-C2C	-11.18	117.29	126.17
6	F	184	CYC	C3B-C4B-NB	11.10	115.74	106.78
7	D	255	BLA	CMC-C2C-C1C	-11.09	95.33	121.39
6	T	255	CYC	OB-C4B-C3B	-11.05	116.05	128.04
6	J	255	CYC	OB-C4B-C3B	-11.02	116.08	128.04
6	H	184	CYC	CBD-CAD-C3D	11.01	131.40	112.62
6	M	184	CYC	C3B-C4B-NB	10.95	115.63	106.78
6	J	255	CYC	OC-C1C-C2C	-10.91	117.50	126.17
6	F	255	CYC	OB-C4B-C3B	-10.90	116.20	128.04
6	O	184	CYC	OB-C4B-C3B	-10.86	116.25	128.04
6	I	184	CYC	C3B-C4B-NB	10.80	115.50	106.78
6	R	184	CYC	CHA-C1A-NA	-10.54	114.20	128.83
6	C	184	CYC	C3B-C4B-NB	10.52	115.28	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	255	BLA	C3B-C4B-NB	10.46	118.01	106.19
6	H	184	CYC	C2C-C1C-NC	10.37	117.22	108.27
6	N	184	CYC	C3B-C4B-NB	10.35	115.14	106.78
6	E	184	CYC	CAA-CBA-CGA	-10.23	91.58	113.60
6	R	255	CYC	C1B-NB-C4B	-10.16	97.74	110.67
6	E	184	CYC	OC-C1C-C2C	-10.07	118.17	126.17
6	K	184	CYC	CAA-CBA-CGA	-9.96	92.17	113.60
6	X	255	CYC	OC-C1C-C2C	-9.75	118.42	126.17
6	Q	184	CYC	C3B-C4B-NB	9.70	114.61	106.78
6	V	184	CYC	C3B-C4B-NB	9.61	114.54	106.78
7	B	255	BLA	CMC-C2C-C1C	-9.60	98.82	121.39
7	B	255	BLA	C3B-C4B-NB	9.54	116.97	106.19
6	A	184	CYC	CAA-CBA-CGA	-9.30	93.59	113.60
6	X	184	CYC	CHA-C1A-NA	-9.28	115.96	128.83
7	D	255	BLA	CAC-C3C-C2C	-9.15	98.45	128.60
6	U	184	CYC	OC-C1C-C2C	-9.12	118.92	126.17
6	M	184	CYC	CAA-CBA-CGA	-8.97	94.29	113.60
6	P	184	CYC	CAA-CBA-CGA	-8.97	94.30	113.60
6	W	184	CYC	OC-C1C-C2C	-8.96	119.05	126.17
6	L	184	CYC	CHA-C1A-NA	-8.87	116.53	128.83
6	H	255	CYC	OC-C1C-C2C	-8.84	119.14	126.17
6	I	184	CYC	CHA-C1A-NA	-8.81	116.61	128.83
6	L	255	CYC	OB-C4B-C3B	-8.79	118.50	128.04
6	X	255	CYC	OB-C4B-C3B	-8.63	118.67	128.04
6	D	184	CYC	OB-C4B-C3B	-8.62	118.69	128.04
6	A	184	CYC	C2C-C1C-NC	8.60	115.69	108.27
6	L	255	CYC	C2C-C1C-NC	8.59	115.68	108.27
6	S	184	CYC	C3B-C4B-NB	8.58	113.71	106.78
6	L	255	CYC	C1B-NB-C4B	-8.55	99.79	110.67
6	D	184	CYC	C1B-NB-C4B	-8.51	99.83	110.67
6	L	255	CYC	OC-C1C-C2C	-8.44	119.46	126.17
6	J	184	CYC	CAA-CBA-CGA	-8.44	95.44	113.60
6	F	255	CYC	CHB-C4A-NA	-8.42	107.31	124.93
6	P	255	CYC	OB-C4B-C3B	-8.42	118.90	128.04
6	K	184	CYC	C1B-NB-C4B	-8.41	99.96	110.67
6	F	255	CYC	C1B-NB-C4B	-8.40	99.97	110.67
6	P	255	CYC	C4D-CHA-C1A	8.38	138.82	128.81
6	V	255	CYC	OC-C1C-C2C	-8.36	119.52	126.17
6	O	184	CYC	OC-C1C-C2C	-8.34	119.54	126.17
6	I	184	CYC	OB-C4B-C3B	-8.28	119.05	128.04
6	P	184	CYC	OB-C4B-C3B	-8.27	119.06	128.04
6	Q	184	CYC	CAA-CBA-CGA	-8.25	95.84	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	W	184	CYC	CAA-CBA-CGA	-8.22	95.91	113.60
6	P	255	CYC	CHB-C4A-NA	-8.19	107.80	124.93
6	X	184	CYC	C2A-C1A-NA	8.16	121.91	110.05
6	A	184	CYC	C3B-C4B-NB	8.16	113.37	106.78
6	N	184	CYC	CHA-C1A-NA	-8.14	117.54	128.83
6	O	184	CYC	C1B-NB-C4B	-8.13	100.33	110.67
6	J	184	CYC	CHA-C1A-NA	-8.10	117.59	128.83
7	B	184	BLA	CMC-C2C-C3C	-8.07	108.53	128.30
6	F	184	CYC	CHA-C1A-NA	-8.07	117.64	128.83
6	J	184	CYC	C1B-NB-C4B	-8.05	100.42	110.67
6	N	255	CYC	OC-C1C-C2C	-8.02	119.79	126.17
6	X	255	CYC	C1B-NB-C4B	-8.01	100.47	110.67
6	W	184	CYC	C2C-C1C-NC	7.96	115.14	108.27
6	O	184	CYC	CAA-CBA-CGA	-7.96	96.47	113.60
6	T	255	CYC	C1B-NB-C4B	-7.95	100.55	110.67
6	A	184	CYC	CHA-C1A-NA	-7.93	117.83	128.83
6	T	184	CYC	OC-C1C-C2C	-7.92	119.87	126.17
6	E	184	CYC	C1B-NB-C4B	-7.87	100.65	110.67
6	W	184	CYC	C1B-NB-C4B	-7.87	100.65	110.67
6	X	184	CYC	CHB-C4A-NA	-7.86	108.50	124.93
7	D	255	BLA	CMC-C2C-C3C	-7.85	109.08	128.30
6	M	184	CYC	OC-C1C-C2C	-7.81	119.96	126.17
6	P	255	CYC	C1B-NB-C4B	-7.79	100.76	110.67
6	J	184	CYC	C2C-C1C-NC	7.77	114.97	108.27
6	T	184	CYC	CHB-C1B-NB	-7.77	109.38	126.06
7	B	184	BLA	C3B-C4B-NB	7.77	114.96	106.19
6	V	255	CYC	OB-C4B-C3B	-7.76	119.62	128.04
6	V	255	CYC	C1B-NB-C4B	-7.75	100.81	110.67
7	B	184	BLA	CMC-C2C-C1C	-7.70	103.29	121.39
6	R	184	CYC	CHB-C1B-NB	-7.69	109.55	126.06
6	U	184	CYC	C2C-C1C-NC	7.65	114.86	108.27
6	X	255	CYC	CAC-C3C-C2C	-7.49	95.55	114.26
6	A	184	CYC	OC-C1C-C2C	-7.48	120.23	126.17
6	N	184	CYC	OC-C1C-C2C	-7.47	120.23	126.17
6	R	184	CYC	C1B-NB-C4B	-7.39	101.26	110.67
6	X	184	CYC	CHB-C1B-NB	-7.37	110.24	126.06
6	X	184	CYC	C1B-NB-C4B	-7.37	101.29	110.67
6	W	184	CYC	C2A-C1A-NA	7.37	120.77	110.05
6	J	255	CYC	CMA-C3A-C4A	7.36	136.40	125.06
6	F	184	CYC	CAA-CBA-CGA	-7.29	97.90	113.60
6	I	184	CYC	CAA-CBA-CGA	-7.29	97.91	113.60
6	H	184	CYC	CHA-C1A-NA	-7.29	118.71	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	184	CYC	CHB-C1B-NB	-7.27	110.46	126.06
6	L	184	CYC	C1B-NB-C4B	-7.24	101.45	110.67
7	D	255	BLA	C1B-NB-C4B	-7.23	101.46	110.67
6	U	184	CYC	C1B-NB-C4B	-7.23	101.46	110.67
6	G	184	CYC	C1B-NB-C4B	-7.23	101.47	110.67
6	H	255	CYC	OB-C4B-C3B	-7.23	120.20	128.04
6	J	255	CYC	CHB-C1B-NB	-7.21	110.59	126.06
6	W	184	CYC	CHA-C1A-NA	-7.18	118.86	128.83
6	P	184	CYC	CMB-C2B-C1B	7.18	133.13	124.17
6	T	184	CYC	CHA-C1A-NA	-7.17	118.88	128.83
6	D	184	CYC	C2C-C1C-NC	7.17	114.45	108.27
6	M	184	CYC	C1B-NB-C4B	-7.14	101.58	110.67
6	H	184	CYC	CMA-C3A-C4A	7.13	136.04	125.06
6	H	184	CYC	C1B-NB-C4B	-7.12	101.61	110.67
6	E	184	CYC	CHA-C1A-NA	-7.11	118.96	128.83
6	X	184	CYC	CAA-CBA-CGA	-7.07	98.39	113.60
7	B	255	BLA	C1B-NB-C4B	-7.07	101.67	110.67
6	F	184	CYC	CHB-C1B-NB	-7.05	110.91	126.06
6	A	184	CYC	C2A-C1A-NA	7.05	120.30	110.05
6	I	184	CYC	C1B-NB-C4B	-7.04	101.71	110.67
6	N	184	CYC	C1B-NB-C4B	-7.01	101.75	110.67
6	P	255	CYC	C2C-C1C-NC	6.99	114.30	108.27
6	N	255	CYC	CAC-C3C-C2C	-6.97	96.84	114.26
6	W	184	CYC	CAC-C3C-C4C	6.92	130.43	112.67
6	C	184	CYC	CAA-CBA-CGA	-6.90	98.76	113.60
6	J	255	CYC	C1B-NB-C4B	-6.88	101.91	110.67
6	F	255	CYC	CMA-C3A-C4A	6.80	135.54	125.06
6	P	184	CYC	C1B-NB-C4B	-6.76	102.06	110.67
6	W	184	CYC	CHB-C4A-NA	-6.76	110.80	124.93
6	V	255	CYC	CMC-C2C-C1C	-6.74	97.88	112.40
6	Q	184	CYC	CHA-C1A-NA	-6.74	119.48	128.83
6	V	184	CYC	CBD-CAD-C3D	6.72	124.08	112.62
6	F	184	CYC	C1B-NB-C4B	-6.71	102.12	110.67
6	P	184	CYC	C2C-C1C-NC	6.67	114.03	108.27
7	B	184	BLA	CAC-C3C-C2C	-6.63	106.77	128.60
6	T	184	CYC	C2A-C1A-NA	6.63	119.69	110.05
6	K	184	CYC	CAC-C3C-C4C	6.60	129.62	112.67
6	X	255	CYC	CHA-C1A-NA	-6.59	119.68	128.83
6	V	184	CYC	OC-C1C-C2C	-6.58	120.94	126.17
6	C	184	CYC	C2A-C1A-NA	6.58	119.61	110.05
6	F	255	CYC	C2A-C1A-NA	6.56	119.59	110.05
6	U	184	CYC	CHA-C1A-NA	-6.54	119.75	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	184	CYC	C1B-NB-C4B	-6.53	102.36	110.67
6	C	184	CYC	C1B-NB-C4B	-6.52	102.37	110.67
6	I	184	CYC	CMB-C2B-C1B	6.51	132.30	124.17
6	J	255	CYC	CBA-CAA-C2A	-6.51	94.53	112.63
6	K	184	CYC	CHB-C1B-NB	-6.46	112.18	126.06
6	J	255	CYC	C2C-C1C-NC	6.45	113.83	108.27
6	R	255	CYC	CHA-C1A-NA	-6.44	119.89	128.83
6	H	255	CYC	C1B-NB-C4B	-6.44	102.47	110.67
6	M	184	CYC	CMB-C2B-C1B	6.43	132.20	124.17
6	N	184	CYC	CHB-C1B-NB	-6.41	112.30	126.06
7	B	255	BLA	CMC-C2C-C3C	-6.39	112.65	128.30
6	C	184	CYC	C2C-C1C-NC	6.39	113.78	108.27
6	J	184	CYC	CHB-C1B-NB	-6.31	112.51	126.06
6	J	184	CYC	OC-C1C-C2C	-6.30	121.17	126.17
6	S	184	CYC	C2C-C1C-NC	6.25	113.67	108.27
6	T	255	CYC	CAC-C3C-C2C	-6.23	98.69	114.26
6	S	184	CYC	C1B-NB-C4B	-6.23	102.73	110.67
6	R	255	CYC	C2B-C1B-NB	6.23	116.11	106.99
7	B	184	BLA	CAA-CBA-CGA	-6.22	96.33	113.76
7	D	255	BLA	CHA-C4D-ND	-6.21	120.21	128.83
6	H	255	CYC	CAC-C3C-C4C	-6.15	96.87	112.67
6	V	184	CYC	CHA-C1A-NA	-6.14	120.31	128.83
6	H	184	CYC	CAA-CBA-CGA	-6.13	100.41	113.60
6	I	184	CYC	C2A-C1A-NA	6.11	118.94	110.05
6	J	184	CYC	CBD-CAD-C3D	6.11	123.04	112.62
6	X	184	CYC	CMC-C2C-C1C	-6.09	99.27	112.40
6	N	184	CYC	C2C-C1C-NC	6.09	113.53	108.27
6	L	184	CYC	CHB-C1B-NB	-6.07	113.02	126.06
6	K	184	CYC	CHA-C1A-NA	-6.04	120.45	128.83
6	K	184	CYC	OC-C1C-C2C	-5.99	121.41	126.17
7	B	184	BLA	C1B-NB-C4B	-5.98	103.05	110.67
6	L	184	CYC	CBD-CAD-C3D	5.97	122.80	112.62
6	M	184	CYC	CHA-C1A-NA	-5.95	120.57	128.83
6	K	184	CYC	CHB-C4A-NA	-5.93	112.52	124.93
6	L	255	CYC	CMA-C3A-C4A	5.91	134.17	125.06
6	P	184	CYC	CHA-C1A-NA	-5.90	120.64	128.83
6	P	255	CYC	O2A-CGA-O1A	-5.88	108.64	123.30
6	U	184	CYC	CMB-C2B-C1B	5.84	131.47	124.17
6	P	255	CYC	CHD-C4C-NC	5.83	132.14	125.20
6	O	184	CYC	CHA-C1A-NA	-5.83	120.75	128.83
6	F	184	CYC	OB-C4B-C3B	-5.82	121.73	128.04
6	P	255	CYC	C2A-C1A-NA	5.81	118.50	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	255	CYC	CMC-C2C-C1C	-5.81	99.89	112.40
6	R	184	CYC	CMB-C2B-C1B	5.81	131.42	124.17
6	R	255	CYC	CAB-C3B-C2B	5.78	137.42	127.53
6	T	184	CYC	CHB-C4A-NA	-5.76	112.87	124.93
6	Q	184	CYC	CAB-C3B-C4B	5.76	130.48	121.38
6	P	255	CYC	CHB-C4A-C3A	5.75	139.68	124.90
6	H	184	CYC	CHB-C1B-NB	-5.74	113.73	126.06
6	V	255	CYC	C2C-C1C-NC	5.72	113.20	108.27
6	G	184	CYC	CMB-C2B-C1B	5.71	131.29	124.17
6	D	184	CYC	CMB-C2B-C1B	5.70	131.28	124.17
6	P	255	CYC	CMA-C3A-C4A	5.69	133.82	125.06
6	E	184	CYC	CAB-C3B-C4B	5.68	130.35	121.38
6	N	255	CYC	C2C-C1C-NC	5.67	113.16	108.27
7	D	255	BLA	OB-C4B-C3B	-5.63	116.70	129.46
6	K	184	CYC	C2B-C1B-NB	5.63	115.23	106.99
6	X	184	CYC	C2B-C1B-NB	5.60	115.19	106.99
6	M	184	CYC	CHB-C4A-NA	-5.59	113.24	124.93
6	R	255	CYC	CHB-C4A-NA	-5.58	113.26	124.93
6	V	184	CYC	C1B-NB-C4B	-5.58	103.56	110.67
6	Q	184	CYC	C1B-NB-C4B	-5.57	103.58	110.67
6	F	255	CYC	CHB-C4A-C3A	5.56	139.20	124.90
6	I	184	CYC	CAD-CBD-CGD	-5.56	98.18	113.76
7	D	255	BLA	CAC-C3C-C4C	-5.55	107.43	123.54
6	K	184	CYC	C4D-CHA-C1A	5.55	135.44	128.81
6	W	184	CYC	CBD-CAD-C3D	5.54	122.07	112.62
6	N	184	CYC	CAA-CBA-CGA	-5.51	101.74	113.60
6	S	184	CYC	CHA-C1A-NA	-5.51	121.18	128.83
6	G	184	CYC	CAA-C2A-C3A	5.51	138.14	127.88
6	J	255	CYC	CAC-C3C-C2C	-5.51	100.50	114.26
6	F	184	CYC	C2C-C1C-NC	5.51	113.02	108.27
6	J	184	CYC	C2B-C1B-NB	5.50	115.04	106.99
6	N	184	CYC	C2B-C1B-NB	5.50	115.04	106.99
6	U	184	CYC	CAB-C3B-C4B	5.50	130.06	121.38
6	E	184	CYC	C2A-C1A-NA	5.49	118.04	110.05
6	J	184	CYC	C2A-C1A-NA	5.48	118.02	110.05
6	K	184	CYC	CMB-C2B-C1B	5.46	130.98	124.17
6	T	184	CYC	CBD-CAD-C3D	5.44	121.91	112.62
7	D	255	BLA	C4B-C3B-C2B	-5.43	100.95	107.92
6	M	184	CYC	C2B-C1B-NB	5.43	114.94	106.99
6	T	184	CYC	CMA-C3A-C4A	5.41	133.40	125.06
6	V	184	CYC	C2A-C1A-NA	5.40	117.91	110.05
6	C	184	CYC	CHA-C1A-NA	-5.40	121.34	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	184	CYC	CHB-C4A-NA	-5.39	113.65	124.93
6	J	255	CYC	CHB-C4A-NA	-5.39	113.67	124.93
6	P	184	CYC	CHB-C1B-NB	-5.38	114.50	126.06
6	R	184	CYC	CAA-CBA-CGA	-5.38	102.03	113.60
6	E	184	CYC	C2B-C1B-NB	5.38	114.86	106.99
6	G	184	CYC	CHB-C1B-NB	-5.34	114.59	126.06
6	T	255	CYC	CMC-C2C-C1C	-5.34	100.90	112.40
6	H	184	CYC	C2B-C1B-NB	5.33	114.79	106.99
6	O	184	CYC	CHB-C4A-NA	-5.32	113.79	124.93
6	N	255	CYC	C1B-NB-C4B	-5.31	103.90	110.67
7	B	184	BLA	CHD-C1D-ND	-5.31	113.82	124.93
6	X	184	CYC	C1A-C2A-C3A	-5.31	100.91	106.78
6	N	255	CYC	C4D-CHA-C1A	5.29	135.13	128.81
6	O	184	CYC	C2A-C1A-NA	5.29	117.74	110.05
6	I	184	CYC	OC-C1C-C2C	-5.27	121.98	126.17
6	M	184	CYC	CAC-C3C-C4C	5.25	126.16	112.67
6	R	255	CYC	C2C-C1C-NC	5.25	112.80	108.27
6	P	184	CYC	C2A-C1A-NA	5.24	117.67	110.05
6	R	184	CYC	CHB-C4A-NA	-5.23	113.99	124.93
6	W	184	CYC	C2B-C1B-NB	5.22	114.63	106.99
6	V	184	CYC	C2C-C1C-NC	5.21	112.77	108.27
6	T	184	CYC	CHB-C1B-C2B	5.19	137.23	126.95
6	K	184	CYC	OB-C4B-C3B	-5.17	122.43	128.04
6	J	255	CYC	CHB-C1B-C2B	5.17	137.19	126.95
6	X	184	CYC	OB-C4B-C3B	-5.17	122.43	128.04
6	D	184	CYC	CHB-C1B-NB	-5.17	114.97	126.06
6	R	255	CYC	C4A-C3A-C2A	-5.16	100.58	106.51
6	U	184	CYC	CHB-C1B-NB	-5.16	114.98	126.06
6	L	184	CYC	CHB-C4A-NA	-5.16	114.14	124.93
7	B	184	BLA	CHB-C1B-NB	-5.16	113.07	130.40
6	L	184	CYC	C2C-C1C-NC	5.16	112.72	108.27
6	T	184	CYC	CMB-C2B-C1B	5.12	130.57	124.17
6	N	184	CYC	CMB-C2B-C1B	5.12	130.56	124.17
6	H	184	CYC	CHB-C4A-NA	-5.12	114.22	124.93
6	E	184	CYC	CHB-C1B-NB	-5.12	115.07	126.06
6	M	184	CYC	C2A-C1A-NA	5.11	117.49	110.05
7	B	255	BLA	CHA-C4D-ND	-5.11	121.73	128.83
6	Q	184	CYC	CAC-C3C-C4C	5.11	125.78	112.67
6	F	184	CYC	CMC-C2C-C1C	-5.10	101.40	112.40
6	L	184	CYC	C2A-C1A-NA	5.09	117.45	110.05
6	X	184	CYC	CHB-C4A-C3A	5.06	137.92	124.90
7	B	255	BLA	CHD-C1D-ND	-5.05	114.36	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	255	CYC	CAB-C3B-C2B	5.04	136.15	127.53
6	X	184	CYC	CMB-C2B-C1B	5.03	130.44	124.17
6	I	184	CYC	C2C-C1C-NC	5.02	112.60	108.27
7	B	255	BLA	OB-C4B-C3B	-5.02	118.08	129.46
6	A	184	CYC	C1B-NB-C4B	-4.99	104.31	110.67
6	T	184	CYC	OB-C4B-C3B	-4.98	122.63	128.04
6	F	255	CYC	C2C-C3C-C4C	4.97	108.78	101.34
6	L	255	CYC	CAB-C3B-C4B	4.96	129.22	121.38
6	T	255	CYC	CHB-C4A-NA	-4.96	114.55	124.93
6	F	184	CYC	C2A-C1A-NA	4.93	117.22	110.05
6	H	255	CYC	CHD-C4C-NC	4.93	131.06	125.20
6	C	184	CYC	CAD-CBD-CGD	-4.92	99.98	113.76
6	X	184	CYC	CBB-CAB-C3B	-4.91	98.90	112.43
6	N	255	CYC	CAB-C3B-C4B	4.88	129.09	121.38
6	G	184	CYC	CAA-C2A-C1A	-4.87	116.38	125.01
6	S	184	CYC	OB-C4B-C3B	-4.87	122.75	128.04
6	X	184	CYC	CMA-C3A-C4A	4.87	132.56	125.06
6	K	184	CYC	C2C-C1C-NC	4.85	112.45	108.27
7	B	184	BLA	CAD-C3D-C2D	4.85	136.91	127.88
6	R	184	CYC	CHB-C1B-C2B	4.84	136.54	126.95
6	T	255	CYC	OC-C1C-C2C	-4.82	122.34	126.17
6	X	255	CYC	CHB-C4A-NA	-4.81	114.86	124.93
6	U	184	CYC	C2A-C1A-NA	4.81	117.05	110.05
6	J	184	CYC	OB-C4B-C3B	-4.81	122.82	128.04
6	P	255	CYC	C2C-C3C-C4C	4.81	108.54	101.34
6	W	184	CYC	CAB-C3B-C4B	4.81	128.97	121.38
6	R	184	CYC	CBD-CAD-C3D	4.80	120.82	112.62
6	P	255	CYC	CAC-C3C-C4C	-4.80	100.34	112.67
6	A	184	CYC	CBB-CAB-C3B	-4.80	99.20	112.43
6	R	255	CYC	C2A-C1A-NA	4.79	117.02	110.05
6	G	184	CYC	C2A-C1A-NA	4.78	117.01	110.05
6	F	184	CYC	CMB-C2B-C1B	4.76	130.11	124.17
6	J	184	CYC	CMC-C2C-C1C	-4.75	102.16	112.40
6	F	184	CYC	CHB-C4A-NA	-4.75	115.00	124.93
6	R	184	CYC	C2B-C1B-NB	4.73	113.91	106.99
6	H	184	CYC	CBB-CAB-C3B	-4.72	99.41	112.43
6	L	255	CYC	CMC-C2C-C1C	-4.71	102.25	112.40
6	D	184	CYC	C2B-C1B-NB	4.71	113.88	106.99
6	L	255	CYC	C2B-C1B-NB	4.71	113.88	106.99
6	H	184	CYC	C2A-C1A-NA	4.71	116.90	110.05
6	C	184	CYC	CAC-C3C-C4C	4.70	124.75	112.67
6	A	184	CYC	CAD-C3D-C2D	4.70	140.74	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	P	255	CYC	CAA-CBA-CGA	4.69	123.71	113.60
6	F	184	CYC	C2B-C1B-NB	4.69	113.85	106.99
6	X	255	CYC	C2B-C1B-NB	4.68	113.84	106.99
6	N	184	CYC	C2A-C1A-NA	4.68	116.86	110.05
6	G	184	CYC	CBB-CAB-C3B	-4.68	99.53	112.43
6	Q	184	CYC	C2A-C1A-NA	4.68	116.86	110.05
6	H	255	CYC	CMC-C2C-C1C	-4.68	102.32	112.40
6	N	184	CYC	CHB-C4A-NA	-4.67	115.16	124.93
6	W	184	CYC	C4D-CHA-C1A	4.67	134.39	128.81
6	T	184	CYC	CMC-C2C-C1C	-4.67	102.34	112.40
6	G	184	CYC	CAC-C3C-C4C	4.67	124.66	112.67
6	W	184	CYC	CAD-CBD-CGD	-4.65	100.72	113.76
6	R	184	CYC	CBA-CAA-C2A	4.65	125.54	112.63
6	V	184	CYC	CMC-C2C-C1C	-4.65	102.39	112.40
6	N	255	CYC	CMA-C3A-C4A	4.64	132.22	125.06
6	V	184	CYC	CHB-C4A-NA	-4.64	115.22	124.93
6	J	255	CYC	C4D-CHA-C1A	4.64	134.35	128.81
6	P	184	CYC	OC-C1C-C2C	-4.61	122.51	126.17
6	P	255	CYC	CAC-C3C-C2C	-4.61	102.74	114.26
6	F	255	CYC	CAC-C3C-C4C	-4.60	100.86	112.67
6	J	184	CYC	CMB-C2B-C1B	4.59	129.90	124.17
6	D	184	CYC	C2A-C1A-NA	4.59	116.73	110.05
6	W	184	CYC	CMB-C2B-C1B	4.58	129.89	124.17
6	G	184	CYC	C2B-C1B-NB	4.58	113.69	106.99
6	S	184	CYC	CAB-C3B-C4B	4.58	128.61	121.38
6	J	184	CYC	CHB-C4A-NA	-4.57	115.37	124.93
6	I	184	CYC	CBB-CAB-C3B	-4.56	99.86	112.43
6	N	184	CYC	CBB-CAB-C3B	-4.54	99.91	112.43
6	Q	184	CYC	CHB-C4A-NA	-4.53	115.46	124.93
6	H	184	CYC	C4A-C3A-C2A	-4.53	101.31	106.51
6	I	184	CYC	C2B-C1B-NB	4.52	113.60	106.99
6	G	184	CYC	CAB-C3B-C4B	4.52	128.51	121.38
6	S	184	CYC	CAC-C3C-C4C	4.51	124.24	112.67
6	L	255	CYC	C4A-C3A-C2A	-4.50	101.34	106.51
6	L	255	CYC	CMB-C2B-C1B	4.47	129.74	124.17
6	S	184	CYC	CMB-C2B-C1B	4.46	129.73	124.17
6	I	184	CYC	CHB-C1B-NB	-4.45	116.51	126.06
6	W	184	CYC	CHB-C1B-NB	-4.44	116.52	126.06
6	G	184	CYC	C2C-C1C-NC	4.44	112.10	108.27
6	D	184	CYC	CAA-C2A-C3A	4.44	136.14	127.88
6	O	184	CYC	CAC-C3C-C4C	4.43	124.05	112.67
6	M	184	CYC	C2C-C1C-NC	4.43	112.09	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	184	CYC	CHB-C4A-C3A	4.42	136.26	124.90
6	L	184	CYC	C2B-C1B-NB	4.42	113.46	106.99
6	L	255	CYC	O2A-CGA-O1A	-4.42	112.29	123.30
6	V	255	CYC	CAB-C3B-C4B	4.41	128.34	121.38
6	U	184	CYC	CMA-C3A-C4A	4.41	131.85	125.06
6	L	255	CYC	CHB-C4A-NA	-4.41	115.71	124.93
6	P	255	CYC	CBD-CAD-C3D	-4.40	105.11	112.62
6	S	184	CYC	CBB-CAB-C3B	-4.40	100.31	112.43
7	D	255	BLA	CMB-C2B-C1B	4.40	129.66	124.17
6	L	255	CYC	C2C-C3C-C4C	4.39	107.91	101.34
7	B	184	BLA	C1A-CHA-C4D	4.38	134.04	128.81
6	M	184	CYC	C1B-C2B-C3B	-4.38	103.31	107.87
7	B	184	BLA	C2B-C1B-NB	4.37	113.39	106.99
6	F	255	CYC	CAC-C3C-C2C	-4.37	103.34	114.26
6	U	184	CYC	CHB-C4A-NA	-4.37	115.80	124.93
6	T	255	CYC	CMA-C3A-C4A	4.36	131.78	125.06
6	T	184	CYC	C2B-C1B-NB	4.36	113.37	106.99
6	S	184	CYC	CAD-CBD-CGD	-4.35	101.56	113.76
6	K	184	CYC	CAB-C3B-C4B	4.35	128.25	121.38
6	E	184	CYC	CHB-C4A-NA	-4.34	115.86	124.93
6	E	184	CYC	CAC-C3C-C4C	4.34	123.81	112.67
6	T	255	CYC	C2A-C1A-NA	4.33	116.35	110.05
6	E	184	CYC	OC-C1C-NC	4.33	130.19	124.94
6	G	184	CYC	CHA-C1A-NA	-4.33	122.82	128.83
6	N	184	CYC	CAD-C3D-C2D	4.31	139.64	127.25
6	A	184	CYC	CBD-CAD-C3D	4.31	119.98	112.62
6	H	184	CYC	CAD-C3D-C2D	4.30	139.61	127.25
6	H	184	CYC	OC-C1C-NC	-4.30	119.74	124.94
6	T	255	CYC	C2B-C1B-NB	4.29	113.27	106.99
6	J	255	CYC	O2A-CGA-CBA	4.29	127.80	114.03
7	B	184	BLA	C4B-C3B-C2B	-4.28	102.43	107.92
6	H	184	CYC	CAC-C3C-C2C	-4.28	103.56	114.26
6	L	255	CYC	CAA-CBA-CGA	4.28	122.81	113.60
6	C	184	CYC	CMC-C2C-C1C	4.28	121.62	112.40
6	J	255	CYC	CHA-C1A-NA	-4.27	122.90	128.83
6	U	184	CYC	C2B-C1B-NB	4.27	113.23	106.99
6	N	184	CYC	CAB-C3B-C4B	4.26	128.11	121.38
6	L	184	CYC	CAB-C3B-C4B	4.25	128.10	121.38
6	V	184	CYC	CHB-C1B-NB	-4.25	116.92	126.06
6	A	184	CYC	CAB-C3B-C4B	4.25	128.10	121.38
6	X	255	CYC	OC-C1C-NC	4.25	130.08	124.94
6	N	184	CYC	CMA-C3A-C4A	4.24	131.60	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	255	CYC	CHA-C1A-NA	-4.24	122.95	128.83
6	T	255	CYC	C4A-C3A-C2A	-4.23	101.65	106.51
6	P	255	CYC	CAB-C3B-C4B	4.23	128.06	121.38
6	G	184	CYC	CHB-C4A-NA	-4.22	116.11	124.93
6	R	184	CYC	C2A-C1A-NA	4.22	116.19	110.05
6	V	184	CYC	OB-C4B-C3B	-4.22	123.46	128.04
7	B	255	BLA	C2B-C1B-NB	4.22	113.16	106.99
7	B	255	BLA	C4B-C3B-C2B	-4.21	102.52	107.92
6	F	255	CYC	OC-C1C-C2C	-4.21	122.83	126.17
6	W	184	CYC	CAD-C3D-C2D	4.21	139.34	127.25
6	C	184	CYC	CBD-CAD-C3D	4.21	119.80	112.62
6	O	184	CYC	CBD-CAD-C3D	4.21	119.80	112.62
6	P	255	CYC	C2B-C1B-NB	4.19	113.12	106.99
6	P	255	CYC	CHA-C1A-NA	-4.19	123.02	128.83
6	F	184	CYC	CHB-C1B-C2B	4.17	135.22	126.95
6	N	255	CYC	CHB-C1B-NB	-4.16	117.13	126.06
6	R	184	CYC	CHB-C4A-C3A	4.15	135.58	124.90
6	H	255	CYC	CAB-C3B-C4B	4.15	127.93	121.38
6	S	184	CYC	CHB-C4A-NA	-4.14	116.27	124.93
6	J	184	CYC	CMA-C3A-C4A	4.14	131.44	125.06
6	K	184	CYC	C2A-C1A-NA	4.13	116.05	110.05
6	U	184	CYC	OB-C4B-C3B	-4.12	123.57	128.04
6	P	184	CYC	CHB-C4A-NA	-4.12	116.31	124.93
6	O	184	CYC	C2B-C1B-NB	4.12	113.02	106.99
6	M	184	CYC	CHB-C4A-C3A	4.12	135.49	124.90
6	T	255	CYC	CHB-C1B-NB	-4.11	117.23	126.06
6	F	255	CYC	CAB-C3B-C4B	4.11	127.88	121.38
6	F	184	CYC	CAB-C3B-C2B	4.11	134.56	127.53
6	F	255	CYC	C2C-C1C-NC	4.11	111.81	108.27
6	E	184	CYC	C4A-C3A-C2A	-4.09	101.81	106.51
6	K	184	CYC	C4A-C3A-C2A	-4.09	101.81	106.51
6	X	184	CYC	CHD-C4C-NC	-4.09	120.35	125.20
6	P	255	CYC	CHB-C1B-NB	-4.08	117.29	126.06
6	O	184	CYC	C4A-C3A-C2A	-4.08	101.82	106.51
6	N	184	CYC	CBD-CAD-C3D	4.08	119.58	112.62
6	L	184	CYC	CMA-C3A-C4A	4.07	131.33	125.06
6	D	184	CYC	CHA-C1A-NA	-4.06	123.19	128.83
6	I	184	CYC	O2A-CGA-CBA	4.06	127.08	114.03
6	H	255	CYC	C2C-C3C-C4C	4.06	107.42	101.34
6	L	184	CYC	OB-C4B-C3B	-4.05	123.65	128.04
6	X	255	CYC	C2A-C1A-NA	4.03	115.91	110.05
7	D	255	BLA	CHD-C1D-ND	-4.03	116.51	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	184	CYC	CMC-C2C-C1C	4.02	121.07	112.40
6	K	184	CYC	CHB-C4A-C3A	4.02	135.24	124.90
6	F	184	CYC	CMA-C3A-C4A	4.01	131.25	125.06
6	O	184	CYC	CAD-CBD-CGD	-4.01	102.51	113.76
6	I	184	CYC	CAD-C3D-C2D	4.01	138.77	127.25
7	D	255	BLA	CHB-C1B-NB	-3.99	116.98	130.40
6	E	184	CYC	CMC-C2C-C1C	-3.99	103.80	112.40
6	H	255	CYC	C2C-C1C-NC	3.99	111.71	108.27
6	O	184	CYC	C2C-C3C-C4C	3.98	107.30	101.34
6	R	255	CYC	C2C-C3C-C4C	3.97	107.28	101.34
6	H	184	CYC	CHD-C4C-NC	-3.97	120.49	125.20
6	X	255	CYC	C4A-C3A-C2A	-3.97	101.95	106.51
6	H	184	CYC	OC-C1C-C2C	-3.95	123.03	126.17
6	S	184	CYC	C2B-C1B-NB	3.95	112.77	106.99
6	T	184	CYC	C1B-CHB-C4A	-3.94	118.45	128.08
6	W	184	CYC	C4A-C3A-C2A	-3.94	101.99	106.51
6	M	184	CYC	OB-C4B-C3B	-3.93	123.78	128.04
6	X	255	CYC	CMA-C3A-C4A	3.92	131.10	125.06
6	W	184	CYC	CHB-C4A-C3A	3.91	134.97	124.90
6	F	255	CYC	C2B-C1B-NB	3.91	112.71	106.99
6	Q	184	CYC	OC-C1C-C2C	-3.91	123.07	126.17
6	X	255	CYC	C2C-C3C-C4C	3.89	107.17	101.34
6	N	255	CYC	CHB-C4A-NA	-3.89	116.79	124.93
6	E	184	CYC	C2C-C1C-NC	3.89	111.63	108.27
6	R	184	CYC	OB-C4B-C3B	-3.89	123.82	128.04
6	C	184	CYC	CBC-CAC-C3C	-3.88	104.83	113.47
6	P	184	CYC	CMC-C2C-C1C	-3.88	104.05	112.40
6	M	184	CYC	C4A-C3A-C2A	-3.88	102.06	106.51
6	P	255	CYC	C4A-C3A-C2A	-3.87	102.06	106.51
7	B	255	BLA	C1A-CHA-C4D	3.87	133.43	128.81
6	Q	184	CYC	C4D-CHA-C1A	3.87	133.43	128.81
6	W	184	CYC	OB-C4B-C3B	-3.86	123.85	128.04
6	M	184	CYC	CHB-C1B-C2B	3.86	134.59	126.95
6	I	184	CYC	CHB-C4A-NA	-3.86	116.86	124.93
6	R	255	CYC	O2A-CGA-O1A	-3.86	113.69	123.30
7	B	255	BLA	CAC-C3C-C4C	-3.86	112.36	123.54
6	T	184	CYC	CAD-C3D-C2D	3.85	138.32	127.25
6	H	255	CYC	CHA-C1A-NA	-3.85	123.49	128.83
6	X	184	CYC	CHB-C1B-C2B	3.84	134.56	126.95
6	X	255	CYC	O2A-CGA-O1A	-3.84	113.72	123.30
7	B	184	BLA	CAC-C3C-C4C	-3.83	112.43	123.54
6	F	255	CYC	C4A-C3A-C2A	-3.82	102.12	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	U	184	CYC	C4A-C3A-C2A	-3.82	102.13	106.51
6	V	184	CYC	C2B-C1B-NB	3.81	112.57	106.99
6	W	184	CYC	C1A-NA-C4A	-3.81	99.34	106.51
6	D	184	CYC	CAA-C2A-C1A	-3.80	118.28	125.01
6	D	184	CYC	CHB-C4A-NA	-3.80	116.99	124.93
6	E	184	CYC	CMB-C2B-C1B	3.79	128.90	124.17
6	J	255	CYC	CAA-C2A-C3A	-3.78	120.83	127.88
6	T	255	CYC	CBD-CAD-C3D	-3.78	106.17	112.62
6	W	184	CYC	CMA-C3A-C4A	3.77	130.87	125.06
6	J	184	CYC	CAD-C3D-C2D	3.77	138.08	127.25
6	V	184	CYC	CMA-C3A-C4A	3.77	130.87	125.06
6	L	255	CYC	CHB-C1B-NB	-3.76	117.99	126.06
6	R	255	CYC	O2A-CGA-CBA	3.75	126.09	114.03
6	R	184	CYC	C2C-C1C-NC	3.75	111.50	108.27
6	X	184	CYC	C1A-NA-C4A	-3.74	99.46	106.51
6	X	255	CYC	C2C-C1C-NC	3.74	111.49	108.27
6	A	184	CYC	C1A-C2A-C3A	-3.73	102.65	106.78
6	P	184	CYC	C2B-C1B-NB	3.73	112.44	106.99
6	C	184	CYC	CHB-C4A-NA	-3.72	117.15	124.93
6	V	255	CYC	C2C-C3C-C4C	3.71	106.89	101.34
6	J	255	CYC	C2C-C3C-C4C	3.70	106.88	101.34
6	A	184	CYC	C2B-C1B-NB	3.70	112.40	106.99
6	V	255	CYC	CBA-CAA-C2A	-3.67	102.42	112.63
6	X	255	CYC	CAB-C3B-C4B	3.67	127.18	121.38
6	L	184	CYC	CHB-C4A-C3A	3.67	134.33	124.90
7	B	184	BLA	CBB-CAB-C3B	-3.67	109.38	127.62
6	M	184	CYC	CBB-CAB-C3B	-3.65	102.37	112.43
6	J	255	CYC	CMB-C2B-C1B	3.65	128.72	124.17
6	X	184	CYC	CBA-CAA-C2A	3.64	122.75	112.63
6	C	184	CYC	C2B-C1B-NB	3.64	112.32	106.99
6	I	184	CYC	O1A-CGA-CBA	-3.64	111.39	123.08
6	I	184	CYC	CAC-C3C-C4C	3.64	122.02	112.67
6	J	255	CYC	C4A-C3A-C2A	-3.63	102.34	106.51
7	D	255	BLA	CAD-C3D-C4D	3.63	131.43	125.01
6	N	184	CYC	O1A-CGA-CBA	-3.62	111.44	123.08
7	D	255	BLA	CAD-CBD-CGD	-3.61	105.83	113.60
6	L	255	CYC	C2A-C1A-NA	3.60	115.29	110.05
6	J	255	CYC	CMC-C2C-C1C	-3.60	104.64	112.40
6	K	184	CYC	CAA-C2A-C3A	3.59	134.56	127.88
6	J	184	CYC	O1A-CGA-CBA	-3.58	111.57	123.08
6	S	184	CYC	C2A-C1A-NA	3.58	115.25	110.05
6	J	255	CYC	C2B-C1B-NB	3.57	112.21	106.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	184	CYC	OB-C4B-C3B	-3.57	124.17	128.04
6	I	184	CYC	CBC-CAC-C3C	-3.56	105.53	113.47
6	O	184	CYC	OC-C1C-NC	3.56	129.26	124.94
6	C	184	CYC	OB-C4B-C3B	-3.56	124.17	128.04
6	N	255	CYC	OB-C4B-C3B	-3.56	124.18	128.04
6	H	184	CYC	C1B-C2B-C3B	-3.56	104.16	107.87
6	L	184	CYC	CMB-C2B-C1B	3.56	128.61	124.17
6	Q	184	CYC	C2B-C1B-NB	3.55	112.19	106.99
6	E	184	CYC	CAD-CBD-CGD	-3.55	103.80	113.76
6	V	255	CYC	C2B-C1B-NB	3.54	112.17	106.99
7	B	184	BLA	CHD-C1D-C2D	3.54	134.01	124.90
7	D	255	BLA	C2B-C1B-NB	3.54	112.17	106.99
6	T	255	CYC	CMB-C2B-C1B	3.54	128.59	124.17
6	D	184	CYC	CBA-CAA-C2A	3.54	122.45	112.63
6	C	184	CYC	CBB-CAB-C3B	-3.53	102.70	112.43
6	U	184	CYC	CBC-CAC-C3C	-3.52	105.62	113.47
6	X	255	CYC	CBB-CAB-C3B	-3.52	102.72	112.43
6	M	184	CYC	CMA-C3A-C4A	3.52	130.48	125.06
7	B	184	BLA	CMB-C2B-C1B	3.51	128.55	124.17
6	G	184	CYC	CBC-CAC-C3C	-3.51	105.65	113.47
6	T	184	CYC	C2C-C1C-NC	3.51	111.30	108.27
6	X	255	CYC	CAC-C3C-C4C	-3.51	103.67	112.67
6	O	184	CYC	CAA-C2A-C3A	3.49	134.38	127.88
6	V	255	CYC	CBC-CAC-C3C	3.49	121.23	113.47
6	E	184	CYC	OB-C4B-NB	-3.48	116.99	125.08
6	C	184	CYC	OC-C1C-NC	-3.47	120.73	124.94
6	H	255	CYC	CMA-C3A-C4A	3.47	130.41	125.06
6	H	255	CYC	OC-C1C-NC	3.47	129.15	124.94
7	D	255	BLA	CBB-CAB-C3B	-3.47	110.36	127.62
7	D	255	BLA	C4D-C3D-C2D	-3.46	102.95	106.78
7	B	255	BLA	CHD-C1D-C2D	3.46	133.80	124.90
6	A	184	CYC	CAC-C3C-C4C	3.46	121.56	112.67
6	R	184	CYC	CAC-C3C-C2C	-3.45	105.65	114.26
6	C	184	CYC	C1A-C2A-C3A	-3.44	102.97	106.78
6	T	184	CYC	C1A-C2A-C3A	-3.44	102.97	106.78
6	J	184	CYC	CBA-CAA-C2A	3.44	122.19	112.63
7	D	255	BLA	CBA-CAA-C2A	-3.44	106.75	112.62
6	H	255	CYC	CAC-C3C-C2C	-3.43	105.69	114.26
6	S	184	CYC	C4A-C3A-C2A	-3.43	102.57	106.51
7	B	255	BLA	C2C-C1C-NC	3.43	115.62	106.45
6	G	184	CYC	C1B-C2B-C3B	-3.43	104.30	107.87
6	V	255	CYC	C4A-C3A-C2A	-3.43	102.57	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	255	CYC	CHB-C4A-C3A	3.42	133.71	124.90
6	H	255	CYC	CHB-C1B-NB	-3.42	118.71	126.06
6	F	255	CYC	CHA-C1A-C2A	-3.42	117.42	125.32
7	B	184	BLA	C3D-C4D-ND	3.42	115.02	110.05
6	U	184	CYC	O1D-CGD-CBD	-3.41	112.13	123.08
6	W	184	CYC	C1B-C2B-C3B	-3.41	104.32	107.87
7	B	184	BLA	CAD-C3D-C4D	-3.40	118.98	125.01
6	F	184	CYC	C1B-C2B-C3B	-3.40	104.32	107.87
6	V	184	CYC	CAB-C3B-C4B	3.40	126.75	121.38
6	K	184	CYC	O2A-CGA-O1A	3.39	131.75	123.30
6	G	184	CYC	CHB-C4A-C3A	3.39	133.61	124.90
6	A	184	CYC	CHB-C4A-C3A	3.38	133.59	124.90
6	L	184	CYC	C1A-C2A-C3A	-3.38	103.04	106.78
6	J	255	CYC	C1B-CHB-C4A	3.38	136.34	128.08
6	V	255	CYC	C4D-CHA-C1A	3.38	132.84	128.81
6	O	184	CYC	C2C-C1C-NC	3.37	111.18	108.27
6	F	255	CYC	CBA-CAA-C2A	-3.36	103.30	112.63
6	A	184	CYC	C4D-CHA-C1A	3.35	132.82	128.81
6	H	184	CYC	CAB-C3B-C4B	3.35	126.67	121.38
6	J	184	CYC	C1B-C2B-C3B	-3.34	104.38	107.87
6	P	184	CYC	CAC-C3C-C2C	-3.34	105.91	114.26
6	L	255	CYC	CAC-C3C-C2C	-3.34	105.92	114.26
6	H	184	CYC	CMB-C2B-C1B	3.34	128.33	124.17
7	B	184	BLA	CHB-C1B-C2B	3.33	133.55	126.97
6	F	255	CYC	CAD-C3D-C2D	3.32	136.79	127.25
6	L	184	CYC	CHB-C1B-C2B	3.32	133.53	126.95
7	B	255	BLA	CMD-C2D-C1D	3.32	130.18	125.06
6	T	255	CYC	CHB-C4A-C3A	3.32	133.43	124.90
6	P	255	CYC	CMB-C2B-C1B	3.32	128.31	124.17
6	A	184	CYC	C1A-NA-C4A	-3.31	100.27	106.51
6	N	184	CYC	C1B-CHB-C4A	-3.31	119.99	128.08
6	R	255	CYC	C1B-C2B-C3B	-3.31	104.42	107.87
6	L	184	CYC	CAA-C2A-C1A	3.30	130.84	125.01
6	G	184	CYC	CHD-C4C-NC	-3.29	121.29	125.20
6	F	184	CYC	CHB-C4A-C3A	3.29	133.36	124.90
6	N	184	CYC	CMC-C2C-C1C	-3.28	105.33	112.40
6	T	184	CYC	C1B-C2B-C3B	-3.28	104.45	107.87
6	N	184	CYC	C1B-C2B-C3B	-3.28	104.45	107.87
6	E	184	CYC	C2C-C3C-C4C	3.28	106.25	101.34
6	T	255	CYC	CAB-C3B-C2B	3.27	133.12	127.53
6	M	184	CYC	O1D-CGD-CBD	-3.26	112.60	123.08
6	O	184	CYC	CHB-C4A-C3A	3.26	133.29	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	255	CYC	CAA-C2A-C1A	3.26	130.77	125.01
6	Q	184	CYC	CBD-CAD-C3D	3.26	118.18	112.62
6	H	255	CYC	C2B-C1B-NB	3.25	111.75	106.99
6	T	255	CYC	CHD-C4C-NC	-3.25	121.34	125.20
6	T	255	CYC	C2C-C1C-NC	3.25	111.07	108.27
6	X	255	CYC	CBA-CAA-C2A	-3.25	103.61	112.63
6	K	184	CYC	CAA-C2A-C1A	-3.24	119.27	125.01
6	X	255	CYC	CMC-C2C-C1C	-3.24	105.42	112.40
7	B	184	BLA	CHA-C4D-C3D	-3.23	117.85	125.32
6	U	184	CYC	CAC-C3C-C4C	3.23	120.97	112.67
7	B	184	BLA	CBD-CAD-C3D	3.23	121.60	112.63
6	M	184	CYC	O2D-CGD-CBD	3.23	124.41	114.03
6	T	184	CYC	CAB-C3B-C2B	3.23	133.05	127.53
6	V	184	CYC	CHB-C4A-C3A	3.22	133.19	124.90
6	W	184	CYC	CAA-C2A-C3A	3.22	133.87	127.88
6	E	184	CYC	CAA-C2A-C3A	3.22	133.87	127.88
6	M	184	CYC	CAA-C2A-C3A	3.21	133.86	127.88
6	T	184	CYC	CAC-C3C-C2C	-3.21	106.24	114.26
6	S	184	CYC	CHD-C4C-NC	-3.20	121.40	125.20
6	C	184	CYC	C1A-NA-C4A	-3.19	100.50	106.51
6	G	184	CYC	OC-C1C-C2C	-3.19	123.64	126.17
6	T	184	CYC	OC-C1C-NC	3.19	128.80	124.94
6	D	184	CYC	OC-C1C-C2C	-3.18	123.65	126.17
6	J	184	CYC	CAC-C3C-C2C	-3.17	106.33	114.26
6	L	255	CYC	CBB-CAB-C3B	-3.17	103.69	112.43
6	A	184	CYC	OB-C4B-C3B	-3.17	124.60	128.04
6	F	255	CYC	C1A-NA-C4A	-3.14	100.59	106.51
6	H	184	CYC	C1A-NA-C4A	-3.14	100.59	106.51
6	D	184	CYC	C4A-C3A-C2A	-3.14	102.91	106.51
6	J	184	CYC	CAB-C3B-C4B	3.14	126.33	121.38
6	D	184	CYC	CAB-C3B-C4B	3.13	126.32	121.38
6	P	255	CYC	O1D-CGD-CBD	-3.12	113.04	123.08
7	D	255	BLA	C3D-C4D-ND	3.12	114.59	110.05
6	N	255	CYC	CHB-C4A-C3A	3.12	132.93	124.90
6	U	184	CYC	CBD-CAD-C3D	-3.11	107.31	112.62
6	N	255	CYC	CMB-C2B-C1B	3.11	128.04	124.17
6	A	184	CYC	CMA-C3A-C4A	3.10	129.84	125.06
6	J	255	CYC	O2A-CGA-O1A	-3.09	115.60	123.30
6	I	184	CYC	C1A-C2A-C3A	-3.09	103.37	106.78
6	P	184	CYC	CHB-C1B-C2B	3.08	133.05	126.95
6	W	184	CYC	C2C-C3C-C4C	3.07	105.94	101.34
6	J	255	CYC	OC-C1C-NC	3.07	128.66	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	J	184	CYC	C2C-C3C-C4C	3.07	105.94	101.34
6	A	184	CYC	CBC-CAC-C3C	-3.07	106.64	113.47
6	G	184	CYC	CBD-CAD-C3D	3.06	117.85	112.62
6	N	184	CYC	OB-C4B-C3B	-3.06	124.72	128.04
6	D	184	CYC	CBD-CAD-C3D	3.06	117.84	112.62
6	J	184	CYC	C4A-C3A-C2A	-3.06	103.00	106.51
6	Q	184	CYC	CHB-C4A-C3A	3.05	132.75	124.90
6	N	184	CYC	CBA-CAA-C2A	-3.05	104.16	112.63
6	L	184	CYC	C1B-CHB-C4A	-3.04	120.64	128.08
6	J	184	CYC	C1A-NA-C4A	-3.04	100.78	106.51
6	H	255	CYC	CBC-CAC-C3C	3.04	120.24	113.47
6	G	184	CYC	C2C-C3C-C4C	3.04	105.89	101.34
6	R	184	CYC	CAB-C3B-C4B	3.04	126.17	121.38
6	A	184	CYC	CAD-CBD-CGD	-3.04	105.25	113.76
6	R	255	CYC	CHB-C1B-C2B	-3.03	120.95	126.95
6	K	184	CYC	C1B-C2B-C3B	-3.03	104.71	107.87
6	R	184	CYC	C1B-C2B-C3B	-3.02	104.72	107.87
6	V	255	CYC	CMA-C3A-C4A	3.02	129.72	125.06
7	B	255	BLA	CHB-C1B-NB	-3.02	120.26	130.40
6	P	255	CYC	O2A-CGA-CBA	3.02	123.72	114.03
6	A	184	CYC	O1A-CGA-CBA	-3.01	113.42	123.08
6	T	184	CYC	O2D-CGD-CBD	3.01	123.69	114.03
6	R	184	CYC	OB-C4B-NB	-3.00	118.11	125.08
6	H	184	CYC	CAA-C2A-C1A	3.00	130.31	125.01
6	R	184	CYC	C1A-C2A-C3A	-3.00	103.47	106.78
6	H	255	CYC	CMB-C2B-C1B	2.99	127.90	124.17
6	N	184	CYC	C4A-C3A-C2A	-2.99	103.08	106.51
6	P	184	CYC	CHD-C4C-NC	-2.98	121.66	125.20
6	N	255	CYC	C2A-C1A-NA	2.98	114.39	110.05
6	R	255	CYC	OC-C1C-C2C	-2.98	123.80	126.17
6	H	255	CYC	C2A-C1A-NA	2.97	114.37	110.05
6	X	255	CYC	CBD-CAD-C3D	-2.97	107.55	112.62
6	V	184	CYC	CHD-C4C-NC	-2.97	121.67	125.20
6	P	255	CYC	CHA-C1A-C2A	-2.96	118.48	125.32
6	V	255	CYC	CAC-C3C-C2C	-2.96	106.87	114.26
6	X	184	CYC	CBD-CAD-C3D	2.96	117.66	112.62
6	T	255	CYC	CHA-C1A-NA	-2.95	124.73	128.83
6	J	255	CYC	C2A-C1A-NA	2.95	114.34	110.05
6	H	255	CYC	CBA-CAA-C2A	-2.95	104.44	112.63
6	C	184	CYC	CHB-C1B-NB	-2.94	119.74	126.06
6	X	255	CYC	CHD-C4C-NC	2.93	128.69	125.20
6	P	184	CYC	CHB-C4A-C3A	2.93	132.43	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	184	CYC	CBB-CAB-C3B	-2.92	104.39	112.43
6	I	184	CYC	CMA-C3A-C4A	2.91	129.55	125.06
6	N	184	CYC	CHB-C4A-C3A	2.90	132.37	124.90
6	S	184	CYC	C2C-C3C-C4C	2.90	105.69	101.34
6	O	184	CYC	CBC-CAC-C3C	-2.90	107.02	113.47
6	V	184	CYC	CAC-C3C-C2C	-2.89	107.04	114.26
6	N	184	CYC	CHB-C1B-C2B	2.88	132.66	126.95
6	H	255	CYC	CHB-C4A-NA	-2.87	118.92	124.93
6	P	255	CYC	OC-C1C-NC	2.87	128.41	124.94
6	Q	184	CYC	C2C-C1C-NC	2.86	110.74	108.27
6	Q	184	CYC	C2C-C3C-C4C	2.86	105.62	101.34
7	B	184	BLA	CMD-C2D-C1D	2.85	129.46	125.06
7	D	255	BLA	O2A-CGA-CBA	2.85	123.18	114.03
6	R	184	CYC	CAD-C3D-C2D	2.84	135.41	127.25
6	N	184	CYC	O1D-CGD-CBD	-2.84	113.95	123.08
6	R	184	CYC	C2C-C3C-C4C	2.84	105.59	101.34
6	K	184	CYC	CHB-C1B-C2B	2.84	132.57	126.95
6	I	184	CYC	CAB-C3B-C4B	2.84	125.86	121.38
6	F	255	CYC	O2A-CGA-O1A	-2.83	116.26	123.30
6	X	184	CYC	CAB-C3B-C4B	2.83	125.84	121.38
6	R	184	CYC	O1A-CGA-CBA	-2.82	114.02	123.08
7	B	184	BLA	CBC-CAC-C3C	-2.82	113.61	127.62
6	N	255	CYC	CHB-C1B-C2B	2.82	132.53	126.95
6	G	184	CYC	CAC-C3C-C2C	-2.81	107.23	114.26
7	D	255	BLA	CHD-C1D-C2D	2.81	132.13	124.90
6	N	184	CYC	C2C-C3C-C4C	2.81	105.55	101.34
6	K	184	CYC	CAD-CBD-CGD	-2.80	105.90	113.76
6	N	255	CYC	O1D-CGD-CBD	-2.80	114.08	123.08
7	B	255	BLA	CMB-C2B-C1B	2.80	127.66	124.17
6	W	184	CYC	C1A-C2A-C3A	-2.80	103.69	106.78
6	O	184	CYC	CAB-C3B-C4B	2.79	125.79	121.38
6	L	255	CYC	C1A-NA-C4A	-2.79	101.26	106.51
6	I	184	CYC	O1D-CGD-CBD	-2.78	114.14	123.08
6	U	184	CYC	CHB-C4A-C3A	2.78	132.05	124.90
6	T	255	CYC	CHA-C1A-C2A	-2.78	118.90	125.32
6	J	184	CYC	CHB-C1B-C2B	2.78	132.45	126.95
6	H	184	CYC	CAA-C2A-C3A	-2.77	122.71	127.88
6	F	184	CYC	OC-C1C-C2C	-2.77	123.97	126.17
6	E	184	CYC	C1B-C2B-C3B	-2.77	104.98	107.87
6	C	184	CYC	C2C-C3C-C4C	2.76	105.48	101.34
6	E	184	CYC	CBC-CAC-C3C	-2.76	107.32	113.47
6	A	184	CYC	CMD-C2D-C3D	2.76	130.14	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	255	CYC	C1A-NA-C4A	-2.75	101.32	106.51
6	L	184	CYC	O2A-CGA-CBA	2.75	122.86	114.03
6	A	184	CYC	CHB-C1B-NB	-2.75	120.16	126.06
6	P	184	CYC	CMA-C3A-C4A	2.74	129.29	125.06
6	J	255	CYC	CBC-CAC-C3C	2.74	119.56	113.47
6	I	184	CYC	C2C-C3C-C4C	2.73	105.43	101.34
6	S	184	CYC	O2A-CGA-O1A	2.73	130.10	123.30
6	N	255	CYC	O2A-CGA-CBA	2.72	122.78	114.03
6	X	255	CYC	CHB-C4A-C3A	2.72	131.88	124.90
6	C	184	CYC	CHA-C1A-C2A	-2.72	119.05	125.32
6	O	184	CYC	CHD-C4C-NC	2.71	128.43	125.20
6	K	184	CYC	C2C-C3C-C4C	2.71	105.39	101.34
6	H	184	CYC	OB-C4B-NB	-2.70	118.79	125.08
6	T	255	CYC	O1D-CGD-CBD	-2.70	114.41	123.08
6	S	184	CYC	CMA-C3A-C4A	2.70	129.22	125.06
6	P	184	CYC	O1D-CGD-CBD	-2.69	114.42	123.08
6	F	255	CYC	O1D-CGD-CBD	-2.69	114.45	123.08
6	H	184	CYC	C1B-CHB-C4A	-2.68	121.52	128.08
6	I	184	CYC	C1B-C2B-C3B	-2.68	105.07	107.87
6	H	255	CYC	C4A-C3A-C2A	-2.68	103.43	106.51
6	O	184	CYC	CAB-C3B-C2B	2.68	132.11	127.53
6	V	184	CYC	CBA-CAA-C2A	2.65	120.00	112.63
6	O	184	CYC	CBB-CAB-C3B	-2.65	105.13	112.43
6	A	184	CYC	CAA-C2A-C3A	2.64	132.80	127.88
6	L	184	CYC	OB-C4B-NB	-2.64	118.94	125.08
6	L	255	CYC	CHA-C1A-C2A	-2.64	119.22	125.32
6	S	184	CYC	OC-C1C-C2C	-2.64	124.08	126.17
6	G	184	CYC	O2D-CGD-CBD	2.63	122.49	114.03
6	F	184	CYC	CHD-C4C-NC	-2.63	122.07	125.20
6	V	184	CYC	CAC-C3C-C4C	2.63	119.43	112.67
6	D	184	CYC	CAD-CBD-CGD	-2.62	106.42	113.76
6	L	255	CYC	O2A-CGA-CBA	2.62	122.44	114.03
6	N	184	CYC	C4D-CHA-C1A	-2.61	125.69	128.81
6	V	255	CYC	CHB-C1B-NB	-2.61	120.46	126.06
6	F	184	CYC	C1A-C2A-C3A	-2.60	103.90	106.78
6	H	184	CYC	OB-C4B-C3B	-2.60	125.22	128.04
7	B	184	BLA	C4D-C3D-C2D	-2.59	103.91	106.78
6	Q	184	CYC	CHB-C1B-NB	-2.59	120.50	126.06
7	B	184	BLA	CBA-CAA-C2A	2.59	117.04	112.62
6	H	184	CYC	C2C-C3C-C4C	2.58	105.20	101.34
6	N	255	CYC	C2C-C3C-C4C	2.58	105.20	101.34
6	T	184	CYC	CBC-CAC-C3C	-2.58	107.73	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	184	CYC	CMA-C3A-C4A	2.58	129.03	125.06
6	X	184	CYC	CAB-C3B-C2B	2.57	131.93	127.53
6	T	184	CYC	O1D-CGD-CBD	-2.57	114.82	123.08
6	P	184	CYC	CAB-C3B-C4B	2.57	125.44	121.38
6	I	184	CYC	CAC-C3C-C2C	2.57	120.67	114.26
6	R	255	CYC	CHB-C4A-C3A	2.57	131.50	124.90
6	I	184	CYC	CHB-C4A-C3A	2.56	131.49	124.90
6	M	184	CYC	C2C-C3C-C4C	2.56	105.17	101.34
6	C	184	CYC	CAB-C3B-C4B	2.55	125.41	121.38
6	H	184	CYC	CHB-C4A-C3A	2.55	131.46	124.90
6	P	184	CYC	CBB-CAB-C3B	-2.55	105.41	112.43
6	J	184	CYC	O2A-CGA-CBA	2.55	122.21	114.03
6	P	184	CYC	C1B-C2B-C3B	-2.54	105.22	107.87
6	L	184	CYC	C2C-C3C-C4C	2.54	105.14	101.34
7	B	255	BLA	CHD-C4C-NC	-2.54	120.61	126.06
6	N	255	CYC	C4A-C3A-C2A	-2.53	103.60	106.51
6	X	255	CYC	CAA-CBA-CGA	2.53	119.04	113.60
6	Q	184	CYC	C4A-C3A-C2A	-2.52	103.61	106.51
6	D	184	CYC	OC-C1C-NC	-2.52	121.89	124.94
6	P	184	CYC	O2D-CGD-CBD	2.52	122.13	114.03
6	I	184	CYC	CAA-C2A-C1A	2.52	129.46	125.01
6	E	184	CYC	CBD-CAD-C3D	2.51	116.91	112.62
6	S	184	CYC	CHB-C1B-NB	-2.51	120.68	126.06
6	K	184	CYC	CBD-CAD-C3D	2.51	116.90	112.62
6	V	184	CYC	CAD-C3D-C2D	2.50	134.44	127.25
7	B	255	BLA	O2A-CGA-O1A	-2.50	117.07	123.30
7	B	255	BLA	CBB-CAB-C3B	-2.50	115.18	127.62
6	N	255	CYC	O2D-CGD-CBD	2.49	122.04	114.03
6	M	184	CYC	CAA-C2A-C1A	-2.49	120.60	125.01
6	N	255	CYC	CHA-C1A-NA	-2.49	125.37	128.83
6	E	184	CYC	CHB-C4A-C3A	2.49	131.29	124.90
6	G	184	CYC	OB-C4B-NB	-2.49	119.30	125.08
6	I	184	CYC	C1A-NA-C4A	-2.48	101.83	106.51
6	J	184	CYC	C1A-C2A-C3A	-2.48	104.03	106.78
7	D	255	BLA	O1A-CGA-CBA	-2.48	115.10	123.08
6	V	184	CYC	C1A-C2A-C3A	-2.48	104.04	106.78
7	B	255	BLA	C3D-C4D-ND	2.48	113.66	110.05
6	D	184	CYC	CAB-C3B-C2B	2.48	131.76	127.53
6	L	184	CYC	OC-C1C-C2C	-2.48	124.20	126.17
7	D	255	BLA	CMD-C2D-C1D	2.47	128.87	125.06
6	N	255	CYC	CBC-CAC-C3C	2.47	118.97	113.47
6	W	184	CYC	OB-C4B-NB	-2.47	119.34	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	184	CYC	CAB-C3B-C2B	2.47	131.75	127.53
6	F	184	CYC	O1A-CGA-CBA	-2.47	115.16	123.08
6	G	184	CYC	C4A-C3A-C2A	-2.46	103.68	106.51
6	O	184	CYC	CAA-C2A-C1A	-2.45	120.67	125.01
6	P	184	CYC	CMC-C2C-C3C	-2.44	103.98	113.83
6	I	184	CYC	CBD-CAD-C3D	2.44	116.78	112.62
6	R	255	CYC	CAC-C3C-C2C	-2.44	108.17	114.26
6	U	184	CYC	CHB-C1B-C2B	2.43	131.76	126.95
6	X	255	CYC	C1A-NA-C4A	-2.42	101.94	106.51
6	T	184	CYC	CAA-CBA-CGA	-2.42	108.39	113.60
6	L	184	CYC	O1A-CGA-CBA	-2.42	115.32	123.08
6	P	255	CYC	C1A-NA-C4A	-2.41	101.96	106.51
6	D	184	CYC	CHB-C4A-C3A	2.41	131.10	124.90
6	G	184	CYC	CHB-C1B-C2B	2.41	131.72	126.95
6	L	255	CYC	CHA-C1A-NA	-2.41	125.49	128.83
6	J	184	CYC	C1B-CHB-C4A	-2.41	122.20	128.08
6	C	184	CYC	CAA-C2A-C3A	2.40	132.35	127.88
6	G	184	CYC	O1D-CGD-CBD	-2.40	115.37	123.08
6	X	255	CYC	O2A-CGA-CBA	2.39	121.72	114.03
6	J	184	CYC	CAA-C2A-C1A	2.39	129.24	125.01
7	D	255	BLA	C2C-C1C-NC	2.39	112.84	106.45
6	D	184	CYC	CHD-C4C-NC	-2.38	122.37	125.20
6	F	184	CYC	CBA-CAA-C2A	2.38	119.25	112.63
6	P	255	CYC	CAA-C2A-C3A	2.38	132.31	127.88
6	Q	184	CYC	OB-C4B-NB	-2.38	119.55	125.08
7	B	255	BLA	C4D-C3D-C2D	-2.38	104.15	106.78
6	G	184	CYC	CMC-C2C-C1C	2.38	117.52	112.40
6	G	184	CYC	O2A-CGA-O1A	2.37	129.21	123.30
6	M	184	CYC	OC-C1C-NC	2.37	127.81	124.94
6	L	255	CYC	CAC-C3C-C4C	-2.37	106.59	112.67
6	E	184	CYC	C1A-NA-C4A	-2.37	102.05	106.51
6	E	184	CYC	CAA-C2A-C1A	-2.36	120.82	125.01
6	N	184	CYC	O2A-CGA-CBA	2.36	121.61	114.03
6	A	184	CYC	C1B-CHB-C4A	-2.36	122.32	128.08
6	X	255	CYC	O1D-CGD-CBD	-2.36	115.51	123.08
6	J	184	CYC	CBC-CAC-C3C	-2.34	108.25	113.47
6	T	255	CYC	CAB-C3B-C4B	2.34	125.07	121.38
7	D	255	BLA	CBC-CAC-C3C	-2.34	115.98	127.62
7	B	255	BLA	C3C-C4C-NC	2.33	110.45	106.80
6	F	255	CYC	C1A-C2A-C3A	-2.33	104.20	106.78
6	N	255	CYC	OB-C4B-NB	-2.33	119.67	125.08
6	S	184	CYC	CHB-C4A-C3A	2.32	130.87	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	Q	184	CYC	O1D-CGD-CBD	-2.32	115.64	123.08
6	V	184	CYC	C4A-C3A-C2A	-2.31	103.85	106.51
7	B	255	BLA	CAD-C3D-C4D	2.31	129.09	125.01
6	T	184	CYC	C1A-NA-C4A	-2.31	102.17	106.51
6	K	184	CYC	OB-C4B-NB	-2.30	119.73	125.08
6	H	255	CYC	O2A-CGA-O1A	-2.30	117.57	123.30
6	L	184	CYC	CAD-CBD-CGD	-2.30	107.32	113.76
6	X	255	CYC	C4D-CHA-C1A	-2.29	126.07	128.81
6	H	184	CYC	CHB-C1B-C2B	2.29	131.48	126.95
6	W	184	CYC	CBB-CAB-C3B	-2.29	106.13	112.43
6	X	184	CYC	CMC-C2C-C3C	-2.29	104.61	113.83
6	X	184	CYC	C1B-C2B-C3B	-2.29	105.49	107.87
6	Q	184	CYC	C1A-C2A-C3A	-2.28	104.26	106.78
6	P	184	CYC	CAA-C2A-C3A	2.27	132.11	127.88
6	D	184	CYC	CHA-C1A-C2A	-2.27	120.08	125.32
6	N	255	CYC	C2B-C1B-NB	2.27	110.31	106.99
6	T	255	CYC	CAA-C2A-C1A	-2.27	120.99	125.01
6	J	184	CYC	OB-C4B-NB	-2.26	119.81	125.08
6	K	184	CYC	CMD-C2D-C3D	2.26	129.21	124.94
6	U	184	CYC	CMC-C2C-C1C	2.26	117.28	112.40
6	V	184	CYC	C4D-CHA-C1A	2.26	131.51	128.81
6	C	184	CYC	C4A-C3A-C2A	-2.25	103.92	106.51
6	I	184	CYC	O2D-CGD-CBD	2.24	121.24	114.03
6	T	184	CYC	CAA-C2A-C3A	2.24	132.05	127.88
6	S	184	CYC	OC-C1C-NC	-2.24	122.23	124.94
6	F	184	CYC	CBB-CAB-C3B	-2.24	106.26	112.43
6	J	255	CYC	CAC-C3C-C4C	2.24	118.42	112.67
6	F	184	CYC	O2A-CGA-CBA	2.24	121.21	114.03
6	G	184	CYC	CHA-C1A-C2A	-2.23	120.17	125.32
6	J	255	CYC	C1B-C2B-C3B	-2.23	105.55	107.87
7	D	255	BLA	CAA-CBA-CGA	2.23	120.00	113.76
7	B	184	BLA	OB-C4B-C3B	-2.22	124.43	129.46
6	R	255	CYC	OB-C4B-NB	2.22	130.24	125.08
6	C	184	CYC	CMA-C3A-C4A	2.22	128.48	125.06
6	M	184	CYC	CAB-C3B-C4B	2.22	124.88	121.38
6	P	184	CYC	C4A-C3A-C2A	-2.22	103.96	106.51
7	B	184	BLA	O1A-CGA-CBA	-2.21	115.98	123.08
6	R	255	CYC	C3A-C4A-NA	2.21	115.24	110.53
7	B	255	BLA	CAA-C2A-C3A	2.20	133.57	127.25
6	A	184	CYC	C2C-C3C-C4C	2.20	104.64	101.34
6	N	255	CYC	CHA-C1A-C2A	-2.20	120.24	125.32
7	D	255	BLA	OC-C1C-C2C	-2.19	118.52	128.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	255	BLA	CMB-C2B-C3B	-2.19	122.94	128.30
6	U	184	CYC	C1A-NA-C4A	-2.19	102.39	106.51
6	T	184	CYC	OB-C4B-NB	-2.19	120.00	125.08
7	B	255	BLA	C4C-CHD-C1D	2.18	133.40	128.08
6	V	255	CYC	CHA-C1A-NA	-2.17	125.81	128.83
6	L	255	CYC	O1D-CGD-CBD	-2.17	116.12	123.08
6	L	184	CYC	CBA-CAA-C2A	2.16	118.64	112.63
6	A	184	CYC	C4A-C3A-C2A	-2.16	104.03	106.51
6	J	184	CYC	C4D-CHA-C1A	2.16	131.39	128.81
6	J	184	CYC	CHB-C4A-C3A	2.15	130.44	124.90
6	W	184	CYC	CHA-C1A-C2A	-2.14	120.37	125.32
6	Q	184	CYC	CMD-C2D-C3D	2.14	128.98	124.94
6	P	184	CYC	C1A-C2A-C3A	-2.14	104.42	106.78
6	X	255	CYC	CHB-C1B-NB	-2.14	121.47	126.06
6	V	184	CYC	CAA-C2A-C3A	2.13	131.84	127.88
6	V	255	CYC	CMC-C2C-C3C	-2.13	105.25	113.83
6	N	184	CYC	OB-C4B-NB	-2.13	120.14	125.08
6	J	255	CYC	CAD-C3D-C2D	2.13	133.35	127.25
6	V	184	CYC	CAA-CBA-CGA	-2.12	109.03	113.60
6	D	184	CYC	CHB-C1B-C2B	2.12	131.15	126.95
6	T	255	CYC	CAA-C2A-C3A	2.12	131.82	127.88
6	K	184	CYC	CMA-C3A-C4A	2.11	128.32	125.06
6	R	255	CYC	CMA-C3A-C2A	2.10	131.83	126.12
6	R	184	CYC	CBB-CAB-C3B	-2.10	106.64	112.43
6	M	184	CYC	C1B-CHB-C4A	-2.10	122.95	128.08
6	F	184	CYC	C1A-NA-C4A	-2.09	102.56	106.51
6	N	184	CYC	CAC-C3C-C2C	-2.09	109.03	114.26
6	N	184	CYC	C1A-NA-C4A	-2.08	102.60	106.51
6	S	184	CYC	C1B-C2B-C3B	-2.07	105.71	107.87
6	V	184	CYC	C1A-NA-C4A	-2.07	102.61	106.51
6	O	184	CYC	C1A-NA-C4A	-2.07	102.61	106.51
7	B	184	BLA	C3C-C4C-NC	2.07	110.03	106.80
6	E	184	CYC	CHD-C4C-NC	2.07	127.66	125.20
6	N	184	CYC	CAD-CBD-CGD	-2.06	107.97	113.76
6	J	255	CYC	C1A-NA-C4A	-2.06	102.62	106.51
6	V	184	CYC	CMB-C2B-C1B	2.06	126.74	124.17
6	V	255	CYC	C2A-C1A-NA	2.06	113.05	110.05
6	Q	184	CYC	OB-C4B-C3B	-2.06	125.81	128.04
6	O	184	CYC	O1A-CGA-CBA	-2.06	116.47	123.08
6	H	255	CYC	CHB-C4A-C3A	2.06	130.19	124.90
6	F	255	CYC	CAB-C3B-C2B	2.05	131.03	127.53
6	Q	184	CYC	CMA-C3A-C4A	2.04	128.21	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	V	255	CYC	CMB-C2B-C1B	2.04	126.71	124.17
6	J	184	CYC	CAD-CBD-CGD	-2.03	108.05	113.76
6	S	184	CYC	O1A-CGA-CBA	-2.03	116.56	123.08
6	R	255	CYC	CAA-C2A-C3A	2.03	131.66	127.88
6	P	184	CYC	C1A-NA-C4A	-2.03	102.69	106.51
6	U	184	CYC	CMC-C2C-C3C	2.03	122.00	113.83
6	X	184	CYC	C4A-C3A-C2A	-2.02	104.18	106.51
6	J	255	CYC	O1A-CGA-CBA	-2.02	116.58	123.08
6	T	255	CYC	CAD-C3D-C2D	2.02	133.06	127.25
6	X	184	CYC	O1D-CGD-CBD	-2.01	116.63	123.08
6	P	255	CYC	CAB-C3B-C2B	2.01	130.96	127.53
6	R	255	CYC	CMB-C2B-C3B	2.00	131.56	126.12
6	F	255	CYC	CMB-C2B-C1B	2.00	126.67	124.17
6	R	255	CYC	CBB-CAB-C3B	-2.00	106.91	112.43

There are no chirality outliers.

All (427) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	184	CYC	C1A-C2A-CAA-CBA
6	A	184	CYC	C3A-C2A-CAA-CBA
6	A	184	CYC	NA-C4A-CHB-C1B
6	A	184	CYC	C3A-C4A-CHB-C1B
6	A	184	CYC	C2C-C3C-CAC-CBC
6	A	184	CYC	C4C-C3C-CAC-CBC
6	A	184	CYC	ND-C1D-CHD-C4C
6	A	184	CYC	C2D-C1D-CHD-C4C
6	A	184	CYC	C2D-C3D-CAD-CBD
6	A	184	CYC	C4D-C3D-CAD-CBD
6	C	184	CYC	C3A-C2A-CAA-CBA
6	C	184	CYC	C3A-C4A-CHB-C1B
6	C	184	CYC	C2C-C3C-CAC-CBC
6	C	184	CYC	C4C-C3C-CAC-CBC
6	C	184	CYC	ND-C1D-CHD-C4C
6	C	184	CYC	C2D-C1D-CHD-C4C
6	C	184	CYC	C2D-C3D-CAD-CBD
6	C	184	CYC	C4D-C3D-CAD-CBD
6	D	184	CYC	C1A-C2A-CAA-CBA
6	D	184	CYC	NA-C4A-CHB-C1B
6	D	184	CYC	C3A-C4A-CHB-C1B
6	D	184	CYC	ND-C1D-CHD-C4C
6	D	184	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	D	184	CYC	C2D-C3D-CAD-CBD
6	D	184	CYC	C4D-C3D-CAD-CBD
6	E	184	CYC	C3A-C2A-CAA-CBA
6	E	184	CYC	NA-C4A-CHB-C1B
6	E	184	CYC	C3A-C4A-CHB-C1B
6	E	184	CYC	ND-C1D-CHD-C4C
6	E	184	CYC	C2D-C1D-CHD-C4C
6	E	184	CYC	C2D-C3D-CAD-CBD
6	E	184	CYC	C4D-C3D-CAD-CBD
6	F	184	CYC	NA-C4A-CHB-C1B
6	F	184	CYC	C3A-C4A-CHB-C1B
6	F	184	CYC	ND-C1D-CHD-C4C
6	F	184	CYC	C2D-C1D-CHD-C4C
6	F	255	CYC	NA-C4A-CHB-C1B
6	F	255	CYC	C3A-C4A-CHB-C1B
6	F	255	CYC	C2B-C3B-CAB-CBB
6	F	255	CYC	ND-C1D-CHD-C4C
6	F	255	CYC	C2D-C1D-CHD-C4C
6	G	184	CYC	C3A-C2A-CAA-CBA
6	G	184	CYC	C3A-C4A-CHB-C1B
6	G	184	CYC	C4C-C3C-CAC-CBC
6	G	184	CYC	ND-C1D-CHD-C4C
6	G	184	CYC	C2D-C1D-CHD-C4C
6	H	184	CYC	NA-C4A-CHB-C1B
6	H	184	CYC	C3A-C4A-CHB-C1B
6	H	184	CYC	ND-C1D-CHD-C4C
6	H	184	CYC	C2D-C1D-CHD-C4C
6	H	184	CYC	C2D-C3D-CAD-CBD
6	H	184	CYC	C4D-C3D-CAD-CBD
6	H	255	CYC	NA-C4A-CHB-C1B
6	H	255	CYC	C3A-C4A-CHB-C1B
6	H	255	CYC	ND-C1D-CHD-C4C
6	H	255	CYC	C2D-C1D-CHD-C4C
6	I	184	CYC	NA-C4A-CHB-C1B
6	I	184	CYC	C3A-C4A-CHB-C1B
6	I	184	CYC	C2C-C3C-CAC-CBC
6	I	184	CYC	ND-C1D-CHD-C4C
6	I	184	CYC	C2D-C1D-CHD-C4C
6	I	184	CYC	C2D-C3D-CAD-CBD
6	I	184	CYC	C4D-C3D-CAD-CBD
6	J	184	CYC	NA-C4A-CHB-C1B
6	J	184	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
6	J	184	CYC	ND-C1D-CHD-C4C
6	J	184	CYC	C2D-C1D-CHD-C4C
6	J	184	CYC	C2D-C3D-CAD-CBD
6	J	184	CYC	C4D-C3D-CAD-CBD
6	J	255	CYC	NA-C4A-CHB-C1B
6	J	255	CYC	C3A-C4A-CHB-C1B
6	J	255	CYC	C2B-C1B-CHB-C4A
6	J	255	CYC	C2C-C3C-CAC-CBC
6	J	255	CYC	C4C-C3C-CAC-CBC
6	J	255	CYC	ND-C1D-CHD-C4C
6	J	255	CYC	C2D-C1D-CHD-C4C
6	K	184	CYC	C1A-C2A-CAA-CBA
6	K	184	CYC	C3A-C2A-CAA-CBA
6	K	184	CYC	NA-C4A-CHB-C1B
6	K	184	CYC	C3A-C4A-CHB-C1B
6	K	184	CYC	C4C-C3C-CAC-CBC
6	K	184	CYC	ND-C1D-CHD-C4C
6	K	184	CYC	C2D-C1D-CHD-C4C
6	K	184	CYC	C2D-C3D-CAD-CBD
6	K	184	CYC	C4D-C3D-CAD-CBD
6	L	184	CYC	NA-C4A-CHB-C1B
6	L	184	CYC	C3A-C4A-CHB-C1B
6	L	184	CYC	ND-C1D-CHD-C4C
6	L	184	CYC	C2D-C1D-CHD-C4C
6	L	184	CYC	C2D-C3D-CAD-CBD
6	L	184	CYC	C4D-C3D-CAD-CBD
6	L	255	CYC	NA-C4A-CHB-C1B
6	L	255	CYC	C3A-C4A-CHB-C1B
6	L	255	CYC	C2A-CAA-CBA-CGA
6	L	255	CYC	C4C-C3C-CAC-CBC
6	L	255	CYC	ND-C1D-CHD-C4C
6	L	255	CYC	C2D-C1D-CHD-C4C
6	M	184	CYC	C3A-C2A-CAA-CBA
6	M	184	CYC	NA-C4A-CHB-C1B
6	M	184	CYC	C3A-C4A-CHB-C1B
6	M	184	CYC	ND-C1D-CHD-C4C
6	M	184	CYC	C2D-C1D-CHD-C4C
6	N	184	CYC	NA-C4A-CHB-C1B
6	N	184	CYC	C3A-C4A-CHB-C1B
6	N	184	CYC	ND-C1D-CHD-C4C
6	N	184	CYC	C2D-C1D-CHD-C4C
6	N	184	CYC	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
6	N	184	CYC	C4D-C3D-CAD-CBD
6	N	255	CYC	NA-C4A-CHB-C1B
6	N	255	CYC	C3A-C4A-CHB-C1B
6	N	255	CYC	C2C-C3C-CAC-CBC
6	N	255	CYC	C4C-C3C-CAC-CBC
6	N	255	CYC	ND-C1D-CHD-C4C
6	N	255	CYC	C2D-C1D-CHD-C4C
6	N	255	CYC	C2D-C3D-CAD-CBD
6	N	255	CYC	C4D-C3D-CAD-CBD
6	O	184	CYC	C1A-C2A-CAA-CBA
6	O	184	CYC	C3A-C2A-CAA-CBA
6	O	184	CYC	NA-C4A-CHB-C1B
6	O	184	CYC	C3A-C4A-CHB-C1B
6	O	184	CYC	C4C-C3C-CAC-CBC
6	O	184	CYC	ND-C1D-CHD-C4C
6	O	184	CYC	C2D-C1D-CHD-C4C
6	O	184	CYC	C2D-C3D-CAD-CBD
6	O	184	CYC	C4D-C3D-CAD-CBD
6	P	184	CYC	C3A-C2A-CAA-CBA
6	P	184	CYC	NA-C4A-CHB-C1B
6	P	184	CYC	C3A-C4A-CHB-C1B
6	P	184	CYC	ND-C1D-CHD-C4C
6	P	184	CYC	C2D-C1D-CHD-C4C
6	P	184	CYC	C2D-C3D-CAD-CBD
6	P	184	CYC	C4D-C3D-CAD-CBD
6	P	255	CYC	NA-C4A-CHB-C1B
6	P	255	CYC	C3A-C4A-CHB-C1B
6	P	255	CYC	C2C-C3C-CAC-CBC
6	P	255	CYC	C4C-C3C-CAC-CBC
6	P	255	CYC	ND-C1D-CHD-C4C
6	P	255	CYC	C2D-C1D-CHD-C4C
6	Q	184	CYC	C3A-C2A-CAA-CBA
6	Q	184	CYC	NA-C4A-CHB-C1B
6	Q	184	CYC	C3A-C4A-CHB-C1B
6	Q	184	CYC	ND-C1D-CHD-C4C
6	Q	184	CYC	C2D-C1D-CHD-C4C
6	Q	184	CYC	C2D-C3D-CAD-CBD
6	Q	184	CYC	C4D-C3D-CAD-CBD
6	R	184	CYC	NA-C4A-CHB-C1B
6	R	184	CYC	C3A-C4A-CHB-C1B
6	R	184	CYC	C2A-CAA-CBA-CGA
6	R	184	CYC	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	R	184	CYC	C2D-C1D-CHD-C4C
6	R	184	CYC	C2D-C3D-CAD-CBD
6	R	184	CYC	C4D-C3D-CAD-CBD
6	R	255	CYC	NA-C4A-CHB-C1B
6	R	255	CYC	C3A-C4A-CHB-C1B
6	R	255	CYC	C4C-C3C-CAC-CBC
6	R	255	CYC	ND-C1D-CHD-C4C
6	R	255	CYC	C2D-C1D-CHD-C4C
6	S	184	CYC	C1A-C2A-CAA-CBA
6	S	184	CYC	C3A-C2A-CAA-CBA
6	S	184	CYC	NA-C4A-CHB-C1B
6	S	184	CYC	C3A-C4A-CHB-C1B
6	S	184	CYC	C4C-C3C-CAC-CBC
6	S	184	CYC	ND-C1D-CHD-C4C
6	S	184	CYC	C2D-C1D-CHD-C4C
6	S	184	CYC	C2D-C3D-CAD-CBD
6	S	184	CYC	C4D-C3D-CAD-CBD
6	T	184	CYC	NA-C4A-CHB-C1B
6	T	184	CYC	C3A-C4A-CHB-C1B
6	T	184	CYC	ND-C1D-CHD-C4C
6	T	184	CYC	C2D-C1D-CHD-C4C
6	T	184	CYC	C2D-C3D-CAD-CBD
6	T	184	CYC	C4D-C3D-CAD-CBD
6	T	255	CYC	NA-C4A-CHB-C1B
6	T	255	CYC	C3A-C4A-CHB-C1B
6	T	255	CYC	C4C-C3C-CAC-CBC
6	T	255	CYC	ND-C1D-CHD-C4C
6	T	255	CYC	C2D-C1D-CHD-C4C
6	U	184	CYC	C3A-C2A-CAA-CBA
6	U	184	CYC	NA-C4A-CHB-C1B
6	U	184	CYC	C3A-C4A-CHB-C1B
6	U	184	CYC	C4C-C3C-CAC-CBC
6	U	184	CYC	ND-C1D-CHD-C4C
6	U	184	CYC	C2D-C1D-CHD-C4C
6	U	184	CYC	C2D-C3D-CAD-CBD
6	U	184	CYC	C4D-C3D-CAD-CBD
6	V	184	CYC	C1A-C2A-CAA-CBA
6	V	184	CYC	C3A-C2A-CAA-CBA
6	V	184	CYC	NA-C4A-CHB-C1B
6	V	184	CYC	C3A-C4A-CHB-C1B
6	V	184	CYC	ND-C1D-CHD-C4C
6	V	184	CYC	C2D-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
6	V	255	CYC	NA-C4A-CHB-C1B
6	V	255	CYC	C3A-C4A-CHB-C1B
6	V	255	CYC	C4C-C3C-CAC-CBC
6	V	255	CYC	ND-C1D-CHD-C4C
6	V	255	CYC	C2D-C1D-CHD-C4C
6	W	184	CYC	C1A-C2A-CAA-CBA
6	W	184	CYC	C3A-C2A-CAA-CBA
6	W	184	CYC	NA-C4A-CHB-C1B
6	W	184	CYC	C3A-C4A-CHB-C1B
6	W	184	CYC	C2C-C3C-CAC-CBC
6	W	184	CYC	C4C-C3C-CAC-CBC
6	W	184	CYC	ND-C1D-CHD-C4C
6	W	184	CYC	C2D-C1D-CHD-C4C
6	W	184	CYC	C2D-C3D-CAD-CBD
6	W	184	CYC	C4D-C3D-CAD-CBD
6	X	184	CYC	NA-C4A-CHB-C1B
6	X	184	CYC	C3A-C4A-CHB-C1B
6	X	184	CYC	ND-C1D-CHD-C4C
6	X	184	CYC	C2D-C1D-CHD-C4C
6	X	255	CYC	NA-C4A-CHB-C1B
6	X	255	CYC	C3A-C4A-CHB-C1B
6	X	255	CYC	ND-C1D-CHD-C4C
6	X	255	CYC	C2D-C1D-CHD-C4C
7	B	184	BLA	C1A-C2A-CAA-CBA
7	B	184	BLA	C3A-C2A-CAA-CBA
7	B	184	BLA	NA-C4A-CHB-C1B
7	B	184	BLA	C3A-C4A-CHB-C1B
7	B	184	BLA	ND-C1D-CHD-C4C
7	B	184	BLA	C2D-C1D-CHD-C4C
7	B	184	BLA	C4D-C3D-CAD-CBD
7	B	255	BLA	NA-C4A-CHB-C1B
7	B	255	BLA	C3A-C4A-CHB-C1B
7	B	255	BLA	C2A-CAA-CBA-CGA
7	B	255	BLA	C4C-C3C-CAC-CBC
7	B	255	BLA	ND-C1D-CHD-C4C
7	B	255	BLA	C2D-C1D-CHD-C4C
7	B	255	BLA	C2D-C3D-CAD-CBD
7	D	255	BLA	NA-C4A-CHB-C1B
7	D	255	BLA	C3A-C4A-CHB-C1B
7	D	255	BLA	C2B-C3B-CAB-CBB
7	D	255	BLA	C4B-C3B-CAB-CBB
7	D	255	BLA	ND-C1D-CHD-C4C

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Mol	Chain	Res	Type	Atoms
7	D	255	BLA	C2D-C1D-CHD-C4C
7	D	255	BLA	C2D-C3D-CAD-CBD
7	D	255	BLA	C4D-C3D-CAD-CBD
6	J	255	CYC	C2B-C3B-CAB-CBB
6	D	184	CYC	C3A-C2A-CAA-CBA
6	C	184	CYC	C1A-C2A-CAA-CBA
6	E	184	CYC	C1A-C2A-CAA-CBA
6	G	184	CYC	C1A-C2A-CAA-CBA
6	M	184	CYC	C1A-C2A-CAA-CBA
6	P	184	CYC	C1A-C2A-CAA-CBA
6	Q	184	CYC	C1A-C2A-CAA-CBA
6	U	184	CYC	C1A-C2A-CAA-CBA
7	B	255	BLA	C4D-C3D-CAD-CBD
6	F	184	CYC	C2B-C3B-CAB-CBB
6	H	184	CYC	C2A-CAA-CBA-CGA
6	N	184	CYC	C2A-CAA-CBA-CGA
6	P	255	CYC	C2A-CAA-CBA-CGA
6	R	255	CYC	C2A-CAA-CBA-CGA
6	D	184	CYC	C2B-C3B-CAB-CBB
6	T	184	CYC	C1A-C2A-CAA-CBA
7	B	184	BLA	C2D-C3D-CAD-CBD
6	P	255	CYC	C3D-CAD-CBD-CGD
6	F	184	CYC	C4B-C3B-CAB-CBB
6	F	255	CYC	C4B-C3B-CAB-CBB
6	J	255	CYC	C4B-C3B-CAB-CBB
6	R	255	CYC	C4B-C3B-CAB-CBB
6	V	255	CYC	C4B-C3B-CAB-CBB
6	V	255	CYC	C2B-C3B-CAB-CBB
6	C	184	CYC	NA-C4A-CHB-C1B
6	N	255	CYC	C2A-CAA-CBA-CGA
6	T	255	CYC	C2A-CAA-CBA-CGA
6	X	184	CYC	C2A-CAA-CBA-CGA
6	T	255	CYC	C2B-C3B-CAB-CBB
6	T	184	CYC	C3A-C2A-CAA-CBA
6	R	255	CYC	C2B-C3B-CAB-CBB
6	T	184	CYC	C2B-C3B-CAB-CBB
6	G	184	CYC	NA-C4A-CHB-C1B
6	J	255	CYC	NB-C1B-CHB-C4A
7	B	184	BLA	C4B-C3B-CAB-CBB
6	I	184	CYC	C2A-CAA-CBA-CGA
6	T	184	CYC	C2A-CAA-CBA-CGA
7	B	184	BLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
7	B	184	BLA	C2C-C3C-CAC-CBC
6	N	255	CYC	C1A-C2A-CAA-CBA
6	A	184	CYC	C3D-CAD-CBD-CGD
6	I	184	CYC	C3D-CAD-CBD-CGD
6	L	255	CYC	C2C-C3C-CAC-CBC
6	T	255	CYC	C2C-C3C-CAC-CBC
6	D	184	CYC	C4B-C3B-CAB-CBB
6	F	184	CYC	C1A-C2A-CAA-CBA
6	W	184	CYC	C3D-CAD-CBD-CGD
6	D	184	CYC	C2A-CAA-CBA-CGA
6	H	255	CYC	C4B-C3B-CAB-CBB
6	L	184	CYC	C2B-C3B-CAB-CBB
6	X	255	CYC	C4C-C3C-CAC-CBC
6	P	184	CYC	C3D-CAD-CBD-CGD
6	W	184	CYC	C2B-C3B-CAB-CBB
6	T	255	CYC	C1A-C2A-CAA-CBA
6	N	255	CYC	C3A-C2A-CAA-CBA
6	H	255	CYC	C2B-C3B-CAB-CBB
6	R	255	CYC	C2C-C3C-CAC-CBC
6	U	184	CYC	C2C-C3C-CAC-CBC
6	V	255	CYC	C2C-C3C-CAC-CBC
6	I	184	CYC	C2B-C3B-CAB-CBB
6	F	184	CYC	C2D-C3D-CAD-CBD
6	F	184	CYC	C4D-C3D-CAD-CBD
6	J	255	CYC	C4D-C3D-CAD-CBD
6	K	184	CYC	C2B-C3B-CAB-CBB
6	F	184	CYC	C3A-C2A-CAA-CBA
6	X	255	CYC	C2A-CAA-CBA-CGA
6	T	255	CYC	CAA-CBA-CGA-O1A
6	J	184	CYC	CAA-CBA-CGA-O2A
7	B	184	BLA	CAD-CBD-CGD-O2D
6	I	184	CYC	CAA-CBA-CGA-O1A
6	Q	184	CYC	CAD-CBD-CGD-O1D
6	R	184	CYC	C2B-C3B-CAB-CBB
6	D	184	CYC	CAD-CBD-CGD-O1D
6	W	184	CYC	CAA-CBA-CGA-O1A
6	W	184	CYC	CAA-CBA-CGA-O2A
6	C	184	CYC	CAA-CBA-CGA-O1A
6	M	184	CYC	CAA-CBA-CGA-O2A
6	U	184	CYC	CAD-CBD-CGD-O2D
7	B	255	BLA	CAA-CBA-CGA-O1A
7	D	255	BLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	V	184	CYC	C2B-C3B-CAB-CBB
6	E	184	CYC	C3D-CAD-CBD-CGD
6	I	184	CYC	CAA-CBA-CGA-O2A
6	M	184	CYC	CAA-CBA-CGA-O1A
6	Q	184	CYC	CAA-CBA-CGA-O1A
6	S	184	CYC	CAA-CBA-CGA-O1A
6	V	184	CYC	CAA-CBA-CGA-O2A
6	J	184	CYC	CAA-CBA-CGA-O1A
6	K	184	CYC	CAA-CBA-CGA-O2A
6	L	184	CYC	CAA-CBA-CGA-O1A
6	N	184	CYC	CAA-CBA-CGA-O1A
6	C	184	CYC	CAA-CBA-CGA-O2A
6	C	184	CYC	CAD-CBD-CGD-O2D
6	U	184	CYC	CAD-CBD-CGD-O1D
7	B	184	BLA	CAA-CBA-CGA-O1A
6	H	255	CYC	CAA-CBA-CGA-O1A
7	B	184	BLA	CAA-CBA-CGA-O2A
6	C	184	CYC	CAD-CBD-CGD-O1D
6	Q	184	CYC	CAD-CBD-CGD-O2D
7	B	255	BLA	CAA-CBA-CGA-O2A
6	I	184	CYC	CAD-CBD-CGD-O2D
6	R	184	CYC	CAA-CBA-CGA-O2A
6	U	184	CYC	CAA-CBA-CGA-O1A
6	V	184	CYC	CAA-CBA-CGA-O1A
6	Q	184	CYC	CAA-CBA-CGA-O2A
6	W	184	CYC	CAD-CBD-CGD-O2D
6	E	184	CYC	CAA-CBA-CGA-O2A
6	I	184	CYC	CAD-CBD-CGD-O1D
6	J	255	CYC	CAA-CBA-CGA-O1A
6	J	255	CYC	CAA-CBA-CGA-O2A
6	S	184	CYC	CAA-CBA-CGA-O2A
6	X	255	CYC	CAA-CBA-CGA-O1A
6	K	184	CYC	CAA-CBA-CGA-O1A
6	L	184	CYC	CAA-CBA-CGA-O2A
6	D	184	CYC	CAD-CBD-CGD-O2D
6	G	184	CYC	CAA-CBA-CGA-O1A
7	B	184	BLA	CAD-CBD-CGD-O1D
6	A	184	CYC	CAD-CBD-CGD-O2D
6	P	184	CYC	CAA-CBA-CGA-O2A
6	W	184	CYC	CAD-CBD-CGD-O1D
6	A	184	CYC	CAD-CBD-CGD-O1D
6	T	255	CYC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
6	X	184	CYC	CAA-CBA-CGA-O1A
6	N	184	CYC	CAD-CBD-CGD-O2D
6	R	184	CYC	CAA-CBA-CGA-O1A
7	D	255	BLA	CAA-CBA-CGA-O2A
6	H	255	CYC	CAA-CBA-CGA-O2A
6	U	184	CYC	CAA-CBA-CGA-O2A
6	V	184	CYC	CAD-CBD-CGD-O2D
6	O	184	CYC	C2C-C3C-CAC-CBC
7	D	255	BLA	C2A-CAA-CBA-CGA
6	E	184	CYC	CAD-CBD-CGD-O2D
6	X	184	CYC	CAA-CBA-CGA-O2A
6	O	184	CYC	CAD-CBD-CGD-O2D
6	X	255	CYC	CAA-CBA-CGA-O2A
6	G	184	CYC	CAA-CBA-CGA-O2A
6	G	184	CYC	C2A-CAA-CBA-CGA
6	N	184	CYC	CAD-CBD-CGD-O1D
6	R	255	CYC	CAD-CBD-CGD-O2D
6	S	184	CYC	CAD-CBD-CGD-O2D
6	V	184	CYC	CAD-CBD-CGD-O1D
6	D	184	CYC	CAA-CBA-CGA-O2A
6	G	184	CYC	CAD-CBD-CGD-O1D
6	L	184	CYC	CAD-CBD-CGD-O2D
6	N	255	CYC	CAA-CBA-CGA-O1A
6	A	184	CYC	CAA-CBA-CGA-O2A
6	S	184	CYC	CAD-CBD-CGD-O1D
6	L	255	CYC	CAA-CBA-CGA-O2A
6	E	184	CYC	CAA-CBA-CGA-O1A
6	F	184	CYC	CAA-CBA-CGA-O1A
6	P	255	CYC	CAA-CBA-CGA-O2A
6	N	184	CYC	CAA-CBA-CGA-O2A
6	J	184	CYC	CAD-CBD-CGD-O2D
6	G	184	CYC	CAD-CBD-CGD-O2D
6	N	255	CYC	CAD-CBD-CGD-O1D
6	O	184	CYC	CAA-CBA-CGA-O2A
6	F	255	CYC	CAA-CBA-CGA-O1A
6	P	184	CYC	CAA-CBA-CGA-O1A
6	V	255	CYC	CAA-CBA-CGA-O2A
6	F	184	CYC	CAA-CBA-CGA-O2A
6	L	255	CYC	CAA-CBA-CGA-O1A
6	R	255	CYC	CAA-CBA-CGA-O1A
6	R	255	CYC	CAD-CBD-CGD-O1D
6	A	184	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	E	184	CYC	CAD-CBD-CGD-O1D
6	F	255	CYC	CAA-CBA-CGA-O2A
6	L	184	CYC	CAD-CBD-CGD-O1D
6	N	255	CYC	CAD-CBD-CGD-O2D
6	O	184	CYC	CAA-CBA-CGA-O1A
6	O	184	CYC	CAD-CBD-CGD-O1D
6	P	255	CYC	CAA-CBA-CGA-O1A
6	H	184	CYC	CAD-CBD-CGD-O2D
6	J	184	CYC	CAD-CBD-CGD-O1D
6	D	184	CYC	CAA-CBA-CGA-O1A
6	P	184	CYC	CAD-CBD-CGD-O1D
6	R	255	CYC	CAA-CBA-CGA-O2A
6	P	184	CYC	CAD-CBD-CGD-O2D
6	N	255	CYC	CAA-CBA-CGA-O2A
6	E	184	CYC	C2B-C3B-CAB-CBB
7	D	255	BLA	CAD-CBD-CGD-O2D
6	R	255	CYC	C1A-C2A-CAA-CBA
6	V	255	CYC	CAA-CBA-CGA-O1A
6	J	255	CYC	CAD-CBD-CGD-O2D
6	P	255	CYC	C2B-C3B-CAB-CBB
6	H	184	CYC	CAA-CBA-CGA-O2A
6	S	184	CYC	C2C-C3C-CAC-CBC
6	R	184	CYC	CAD-CBD-CGD-O2D
7	D	255	BLA	CAD-CBD-CGD-O1D
6	K	184	CYC	CAD-CBD-CGD-O1D
6	R	184	CYC	CAD-CBD-CGD-O1D

There are no ring outliers.

36 monomers are involved in 586 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	O	184	CYC	19	0
6	S	184	CYC	15	0
6	N	255	CYC	17	0
6	X	184	CYC	12	0
6	E	184	CYC	19	0
6	C	184	CYC	16	0
6	X	255	CYC	16	0
6	D	184	CYC	15	0
6	A	184	CYC	14	0
6	Q	184	CYC	23	0
6	W	184	CYC	13	0

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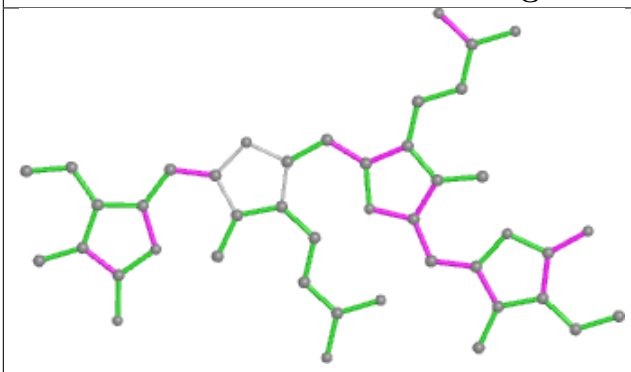
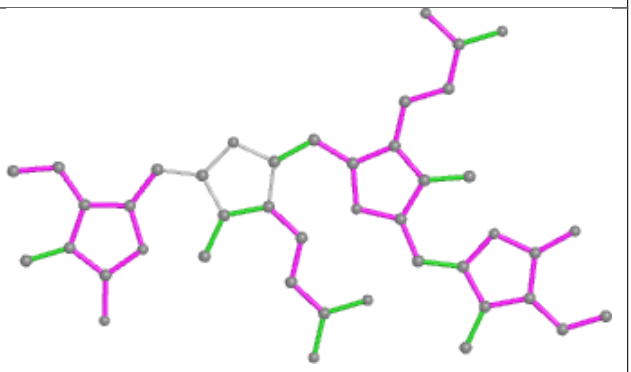
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	255	CYC	14	0
6	J	184	CYC	14	0
6	K	184	CYC	18	0
6	N	184	CYC	24	0
6	R	184	CYC	15	0
6	P	184	CYC	19	0
6	L	184	CYC	24	0
7	B	184	BLA	14	0
6	P	255	CYC	15	0
7	B	255	BLA	12	0
6	I	184	CYC	12	0
6	R	255	CYC	13	0
6	M	184	CYC	16	0
6	L	255	CYC	21	0
6	T	255	CYC	23	0
6	V	184	CYC	11	0
6	F	184	CYC	14	0
6	H	255	CYC	13	0
6	H	184	CYC	11	0
7	D	255	BLA	17	0
6	J	255	CYC	22	0
6	G	184	CYC	13	0
6	U	184	CYC	20	0
6	F	255	CYC	15	0
6	T	184	CYC	17	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.

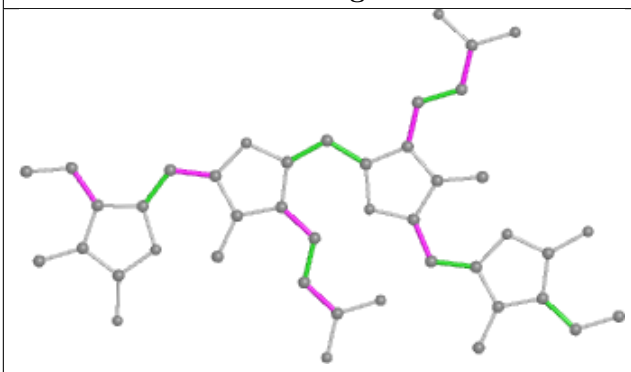
Ligand CYC O 184



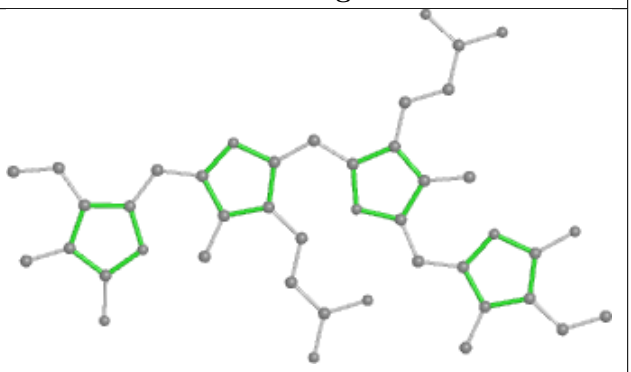
Bond lengths



Bond angles

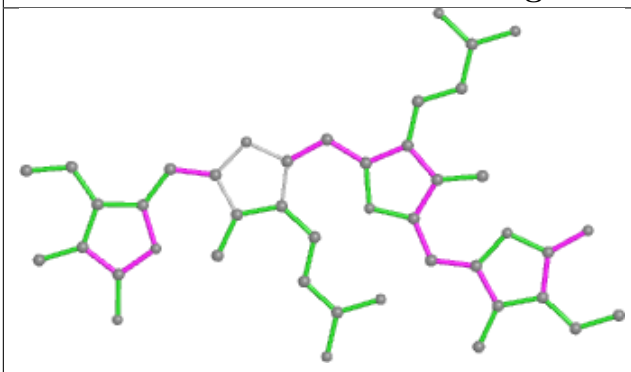


Torsions

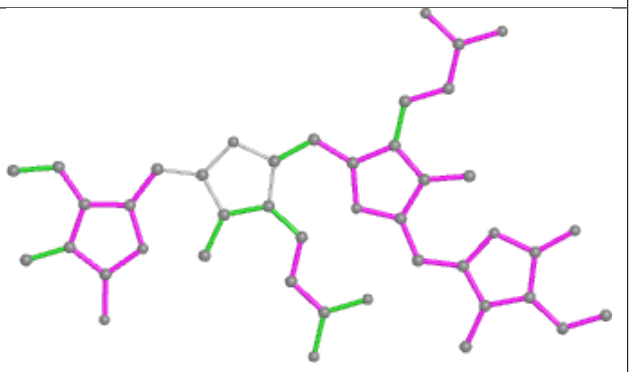


Rings

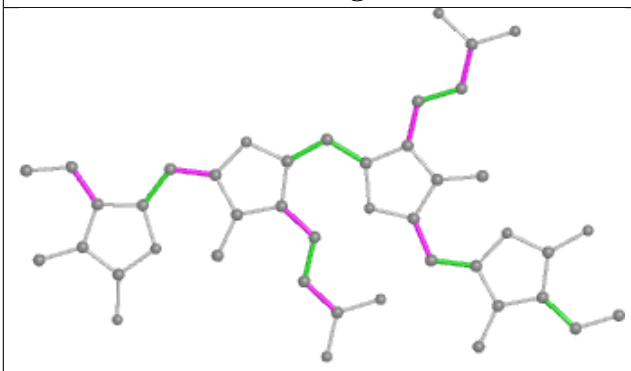
Ligand CYC S 184



Bond lengths



Bond angles



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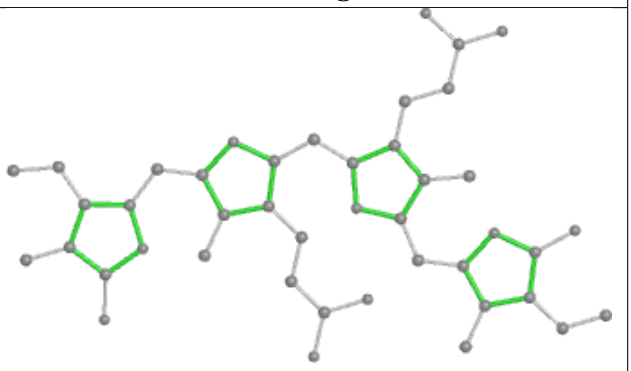
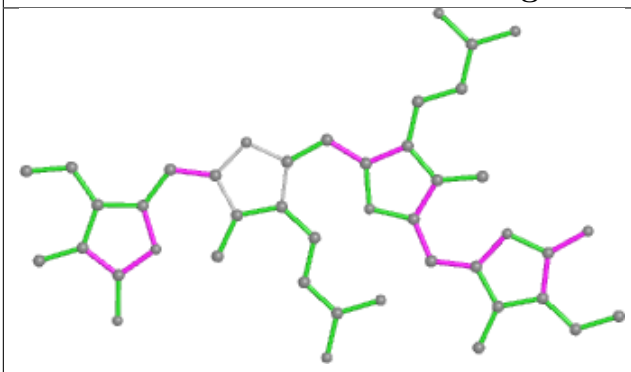
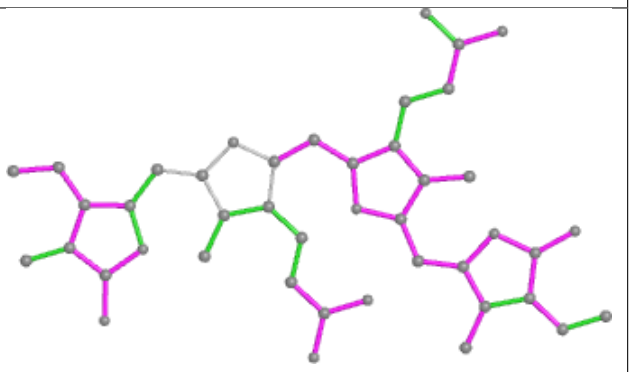


Rings

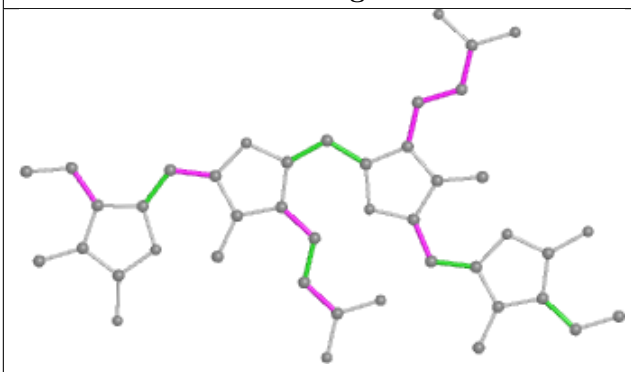
Ligand CYC N 255



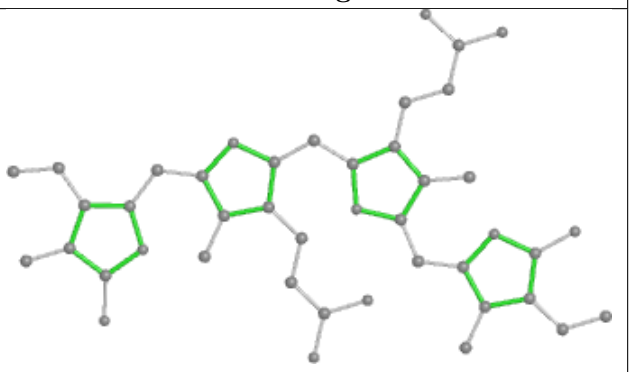
Bond lengths



Bond angles

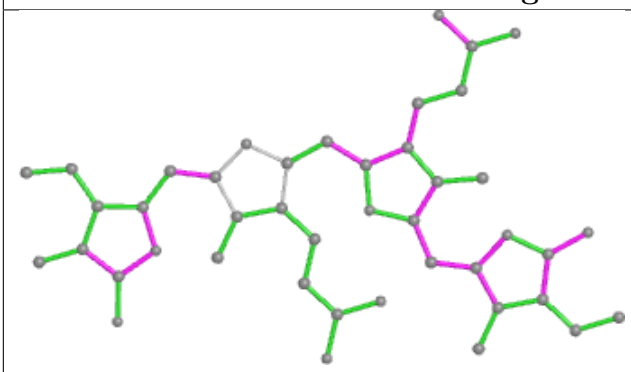


Torsions

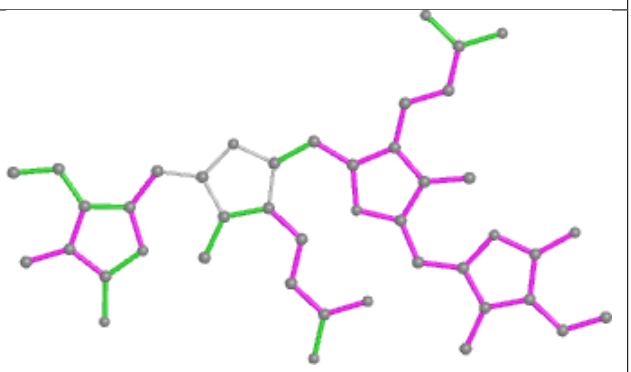


Rings

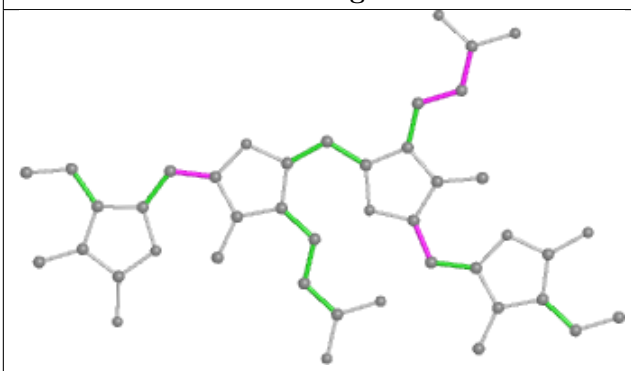
Ligand CYC X 184



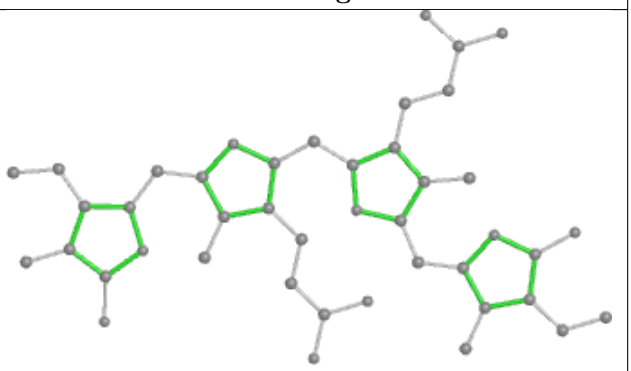
Bond lengths



Bond angles

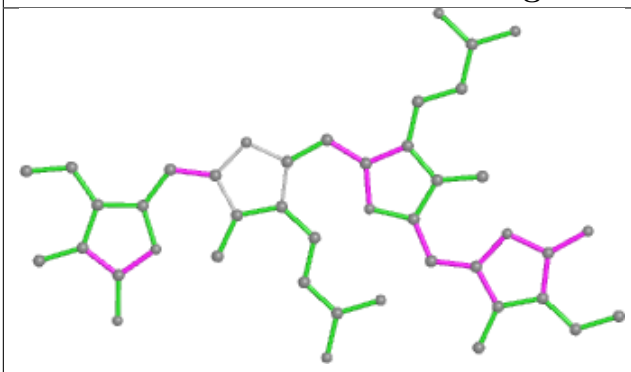


Torsions



Rings

Ligand CYC E 184



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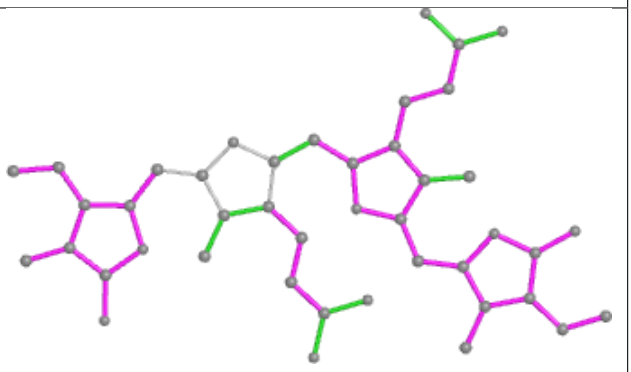
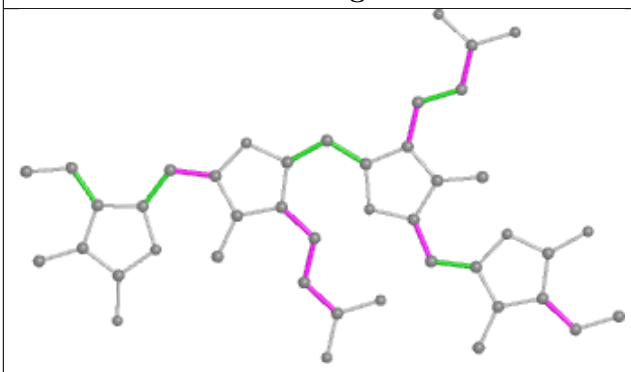
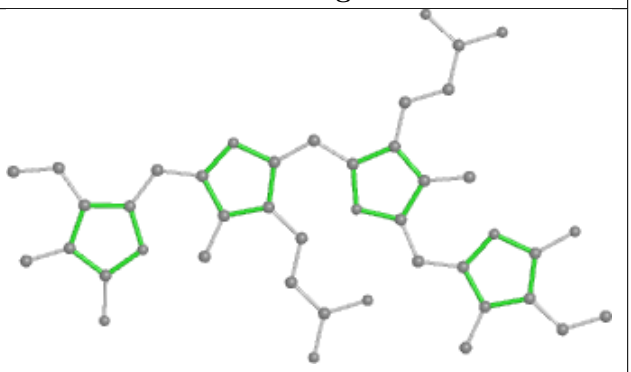


Bond angles

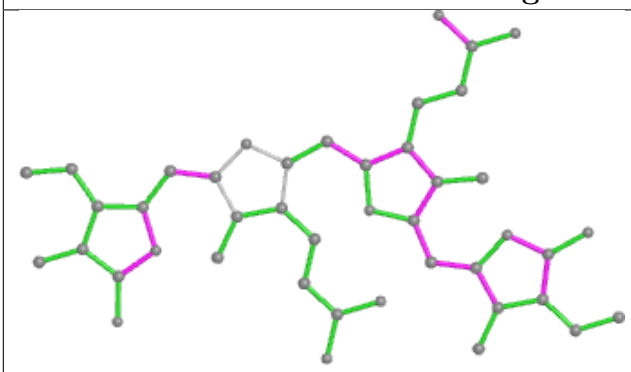


Torsions



Rings

Ligand CYC C 184



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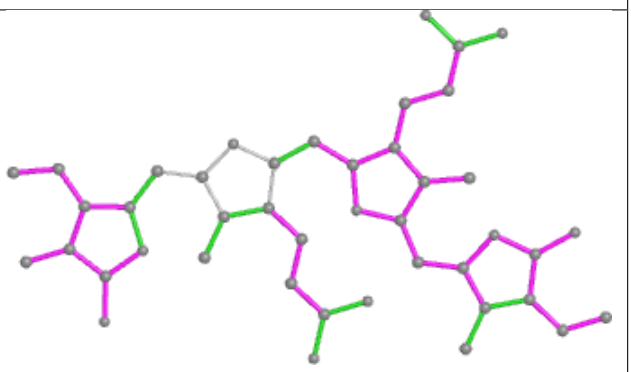
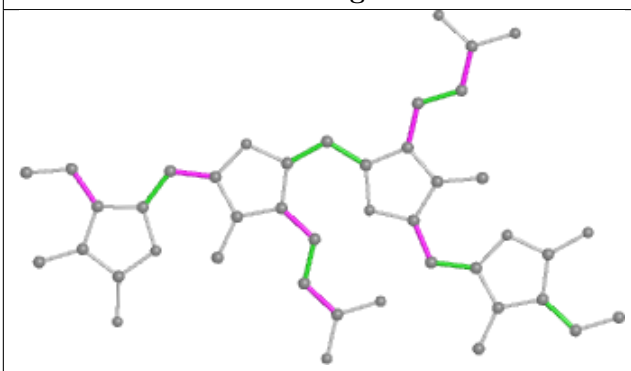
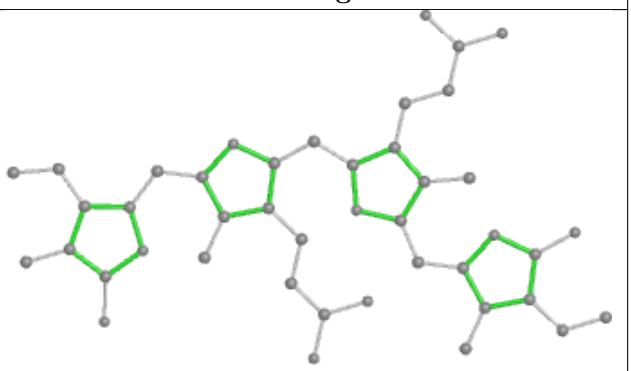


Bond angles

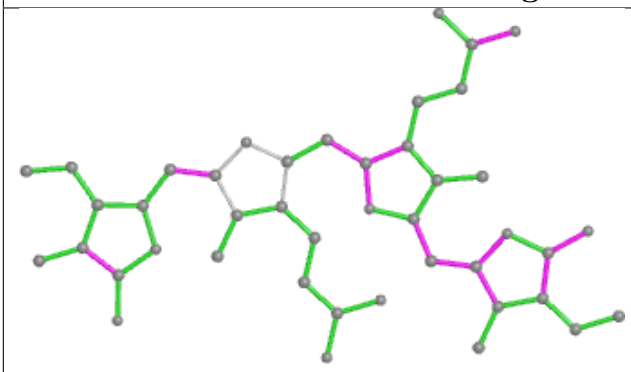


Torsions

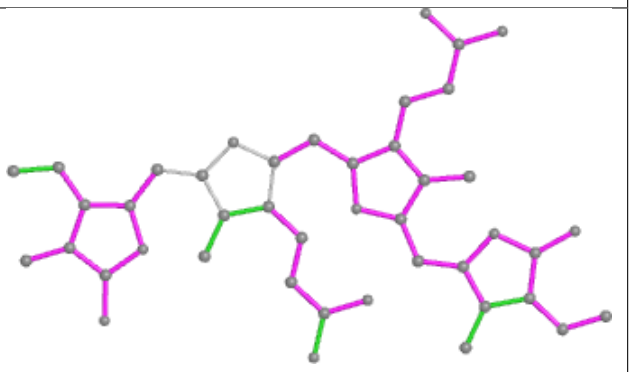


Rings

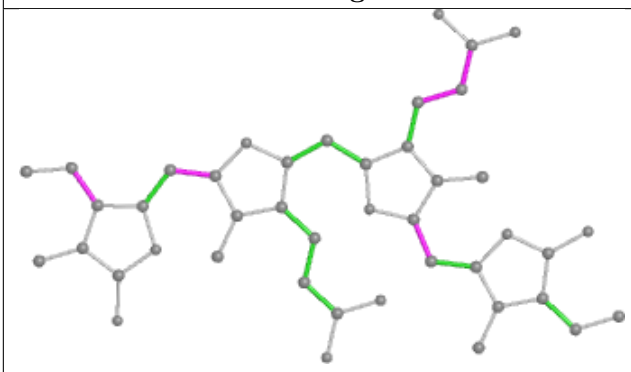
Ligand CYC X 255



Bond lengths



Bond angles



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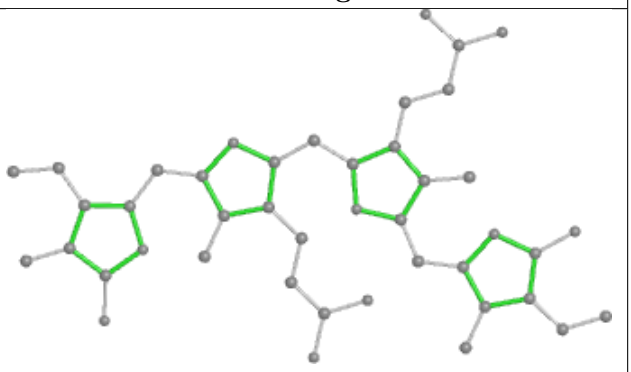
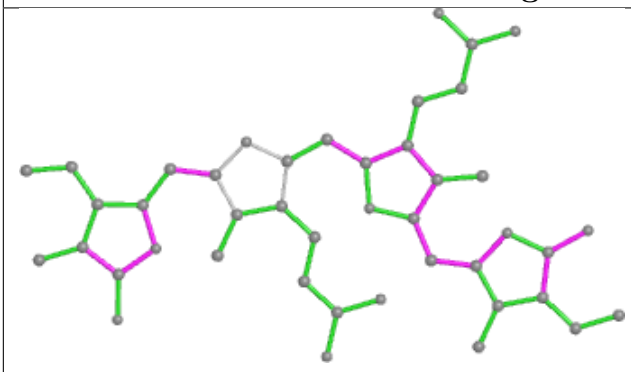
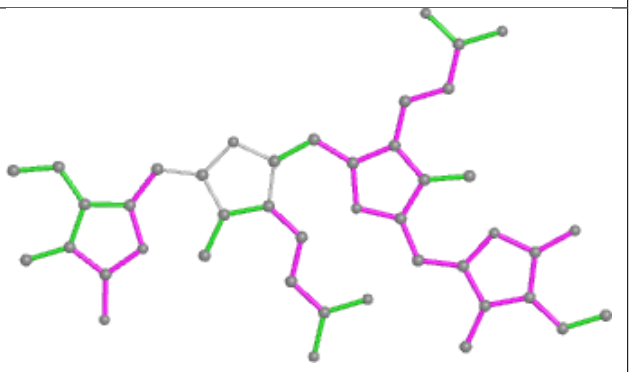


Rings

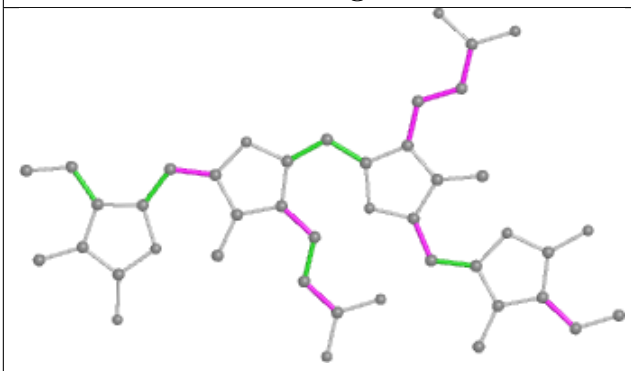
Ligand CYC D 184



Bond lengths



Bond angles



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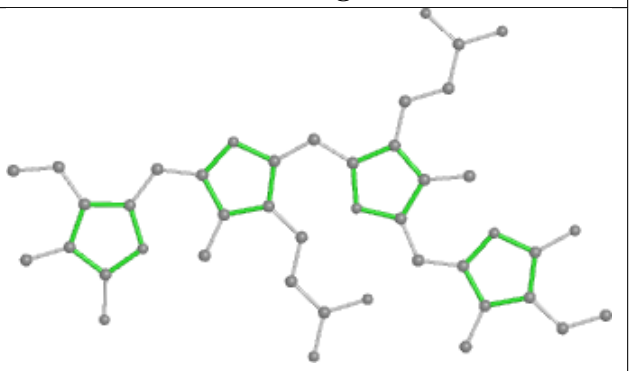
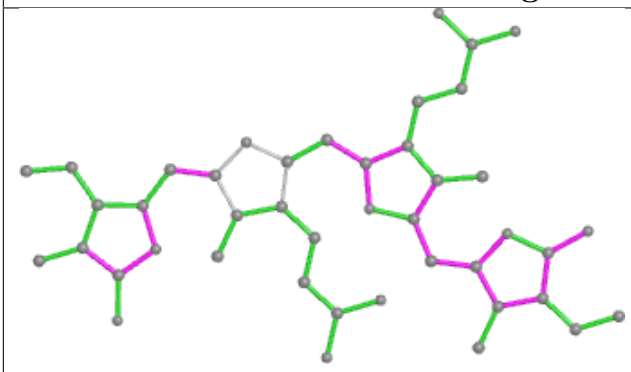
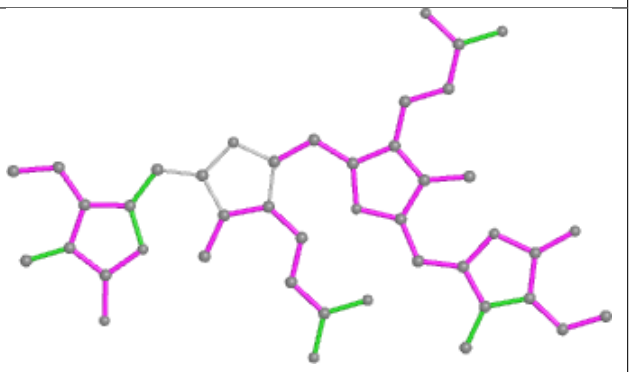


Rings

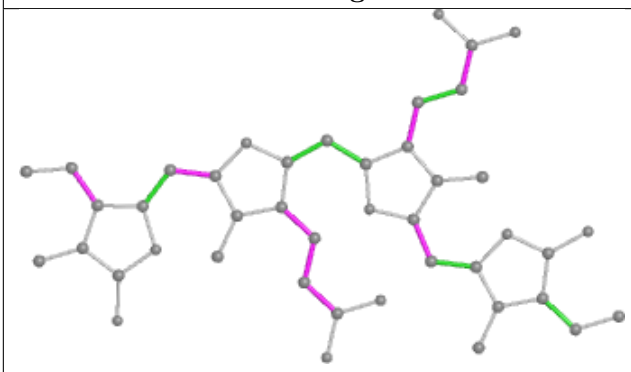
Ligand CYC A 184



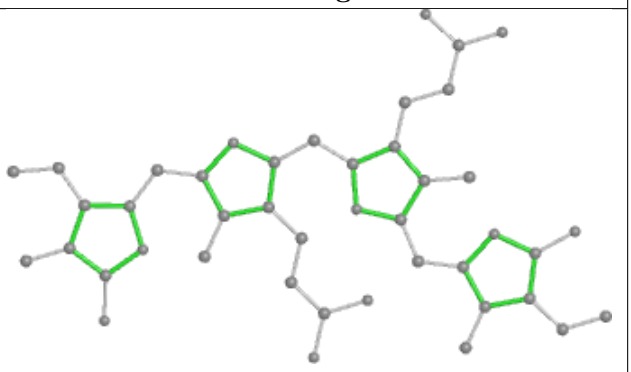
Bond lengths



Bond angles

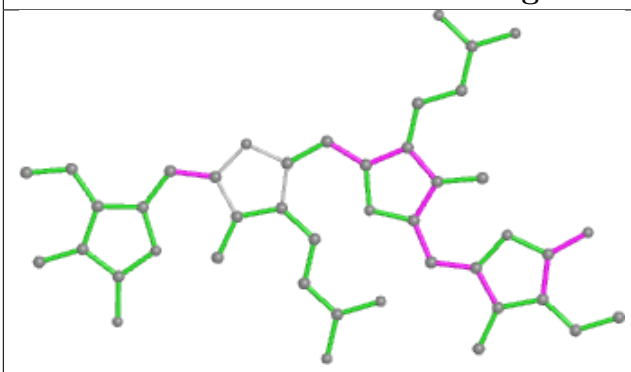


Torsions

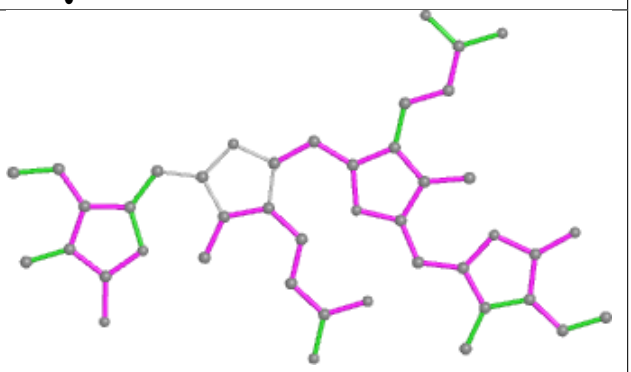


Rings

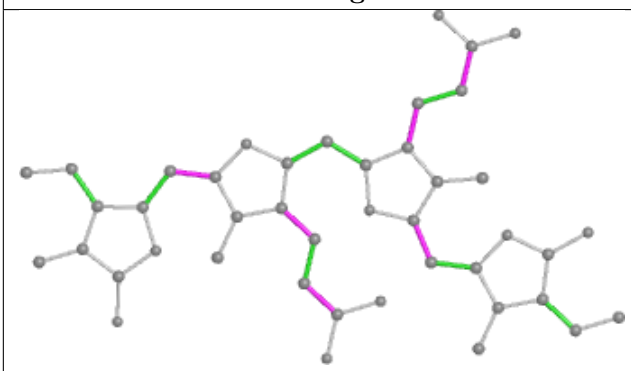
Ligand CYC Q 184



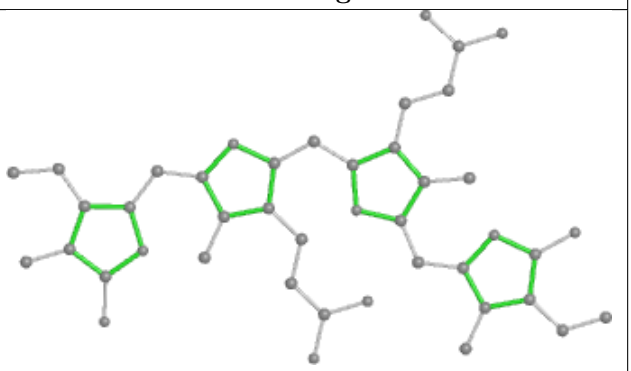
Bond lengths



Bond angles

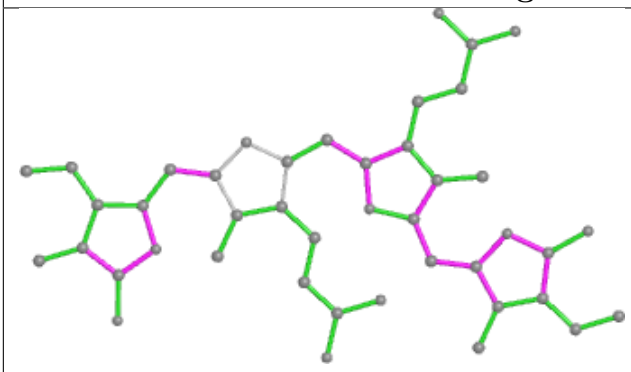


Torsions

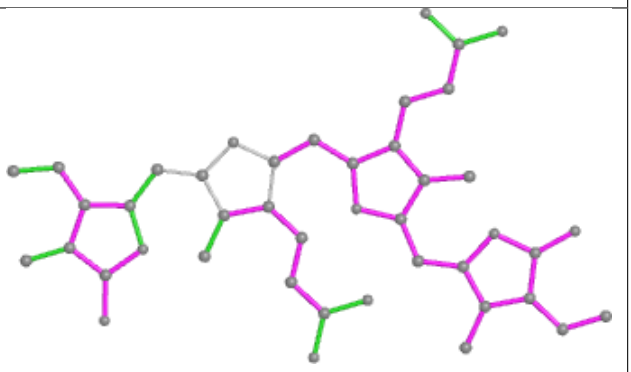


Rings

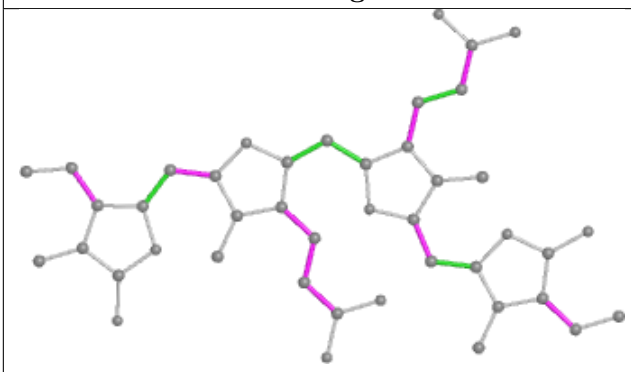
Ligand CYC W 184



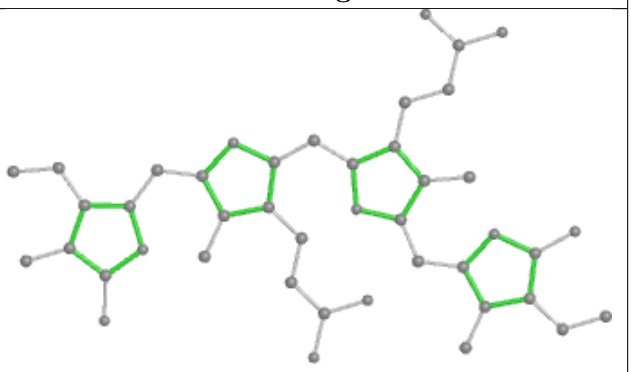
Bond lengths



Bond angles

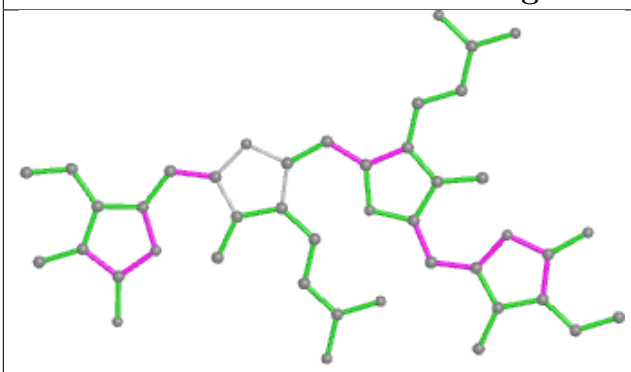


Torsions



Rings

Ligand CYC V 255



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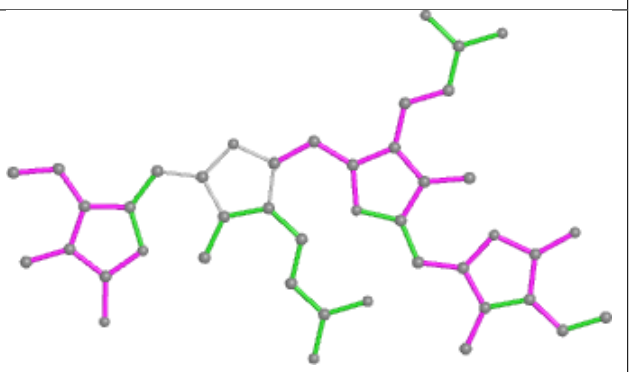
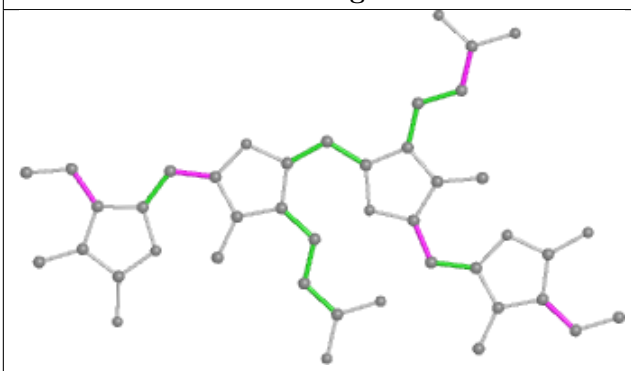


Bond angles



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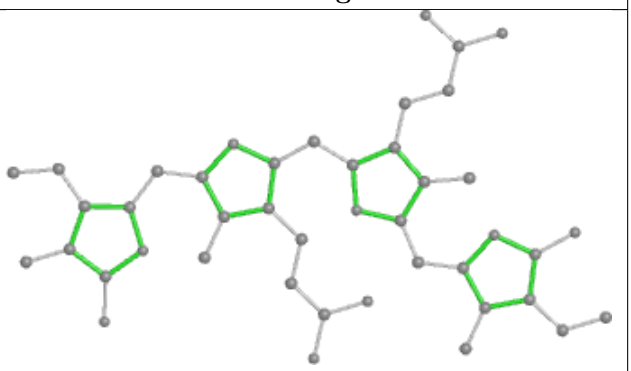
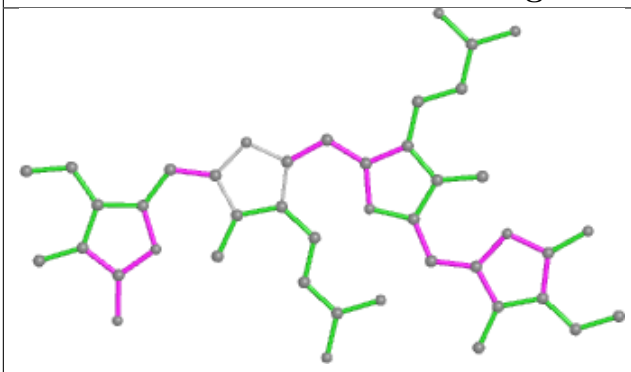


Rings

Ligand CYC J 184



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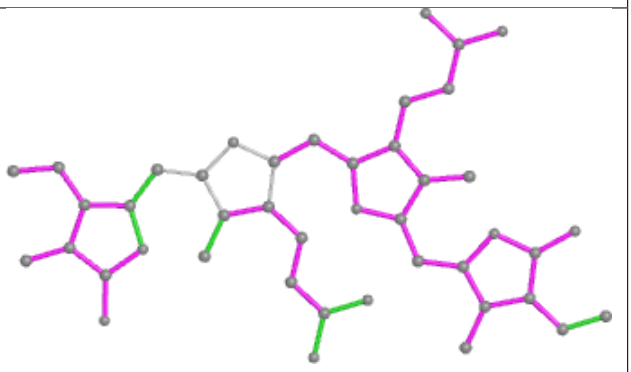

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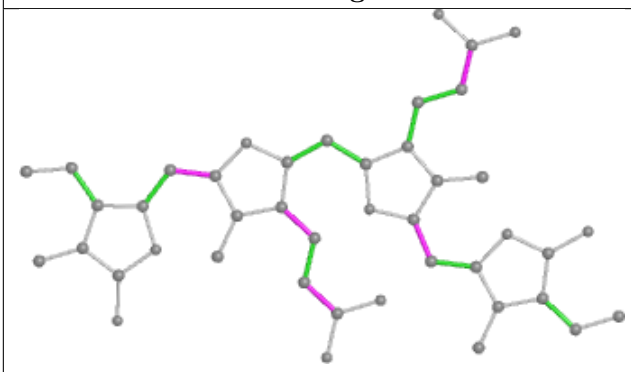

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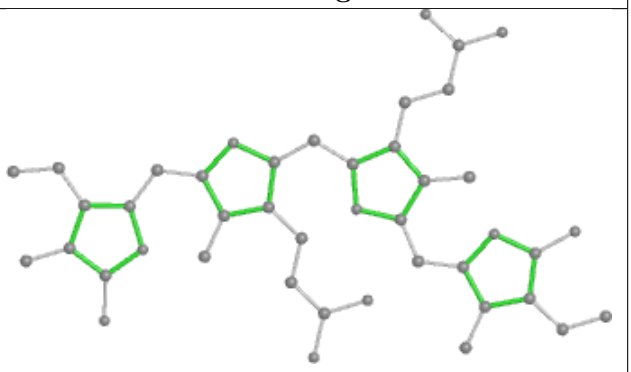
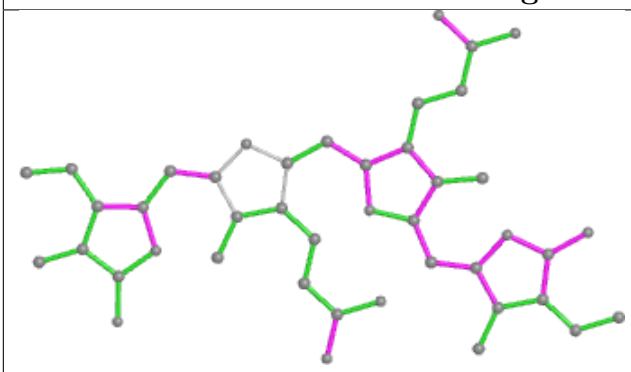


Rings

Ligand CYC K 184



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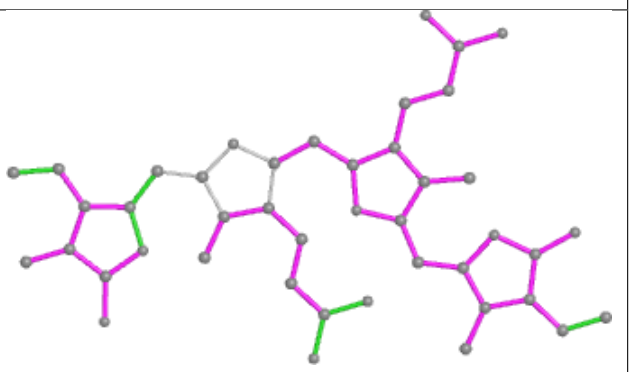

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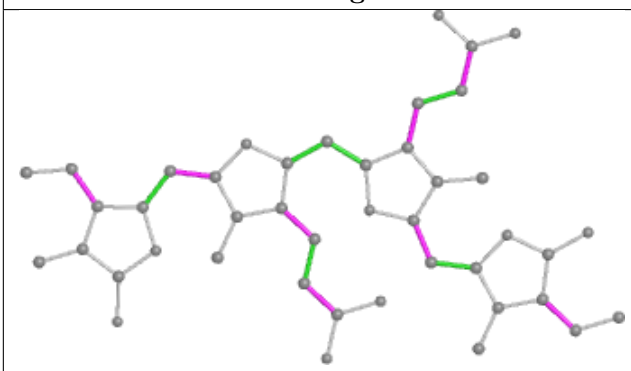

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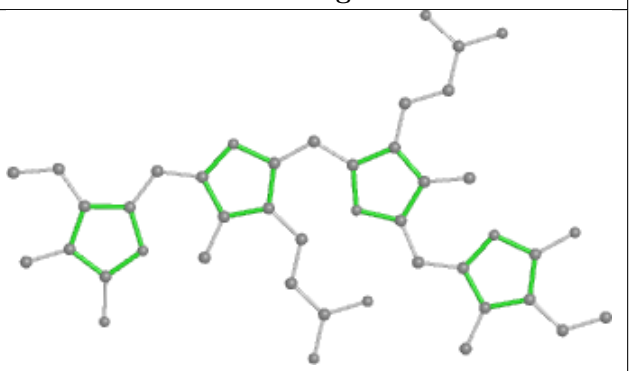
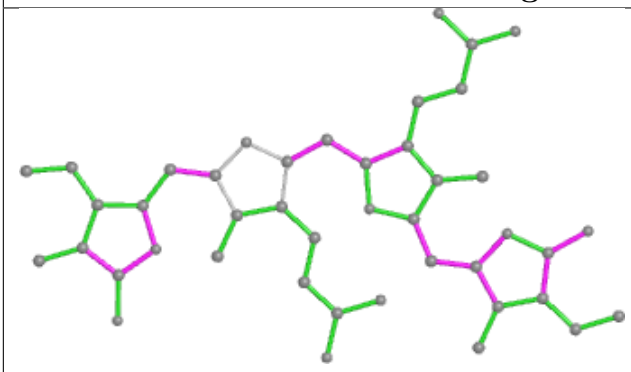


Rings

Ligand CYC N 184



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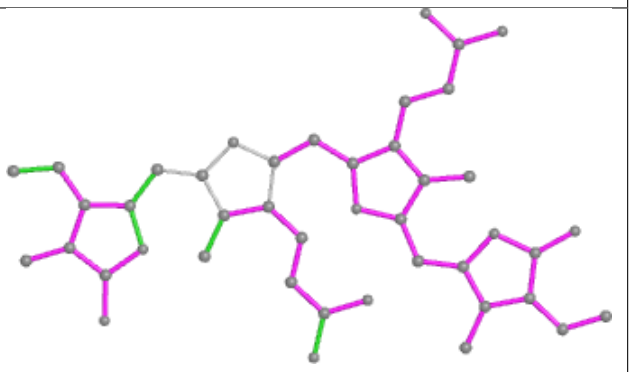
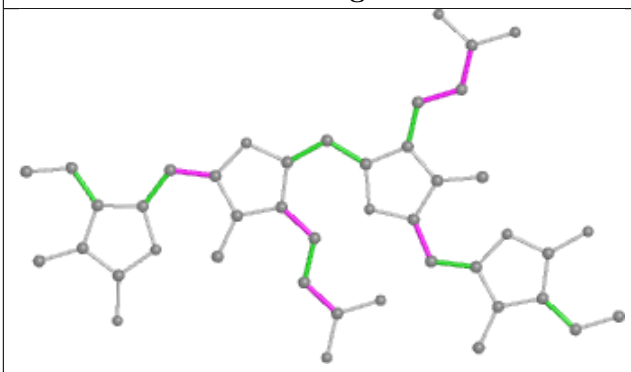


Bond angles



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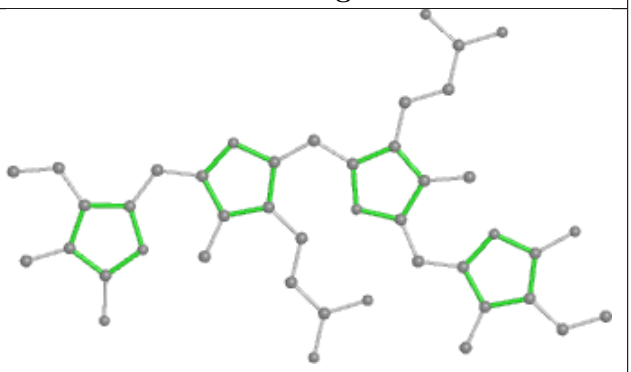
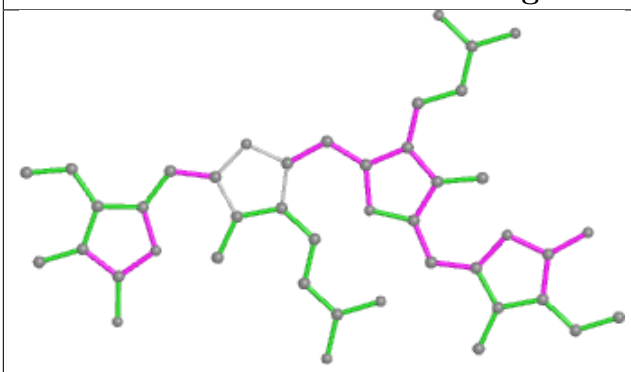


Rings

Ligand CYC R 184



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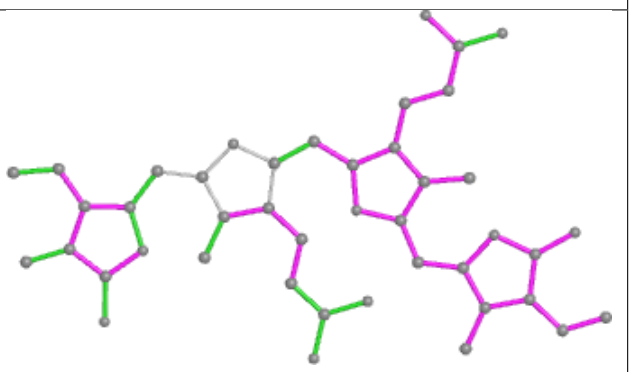

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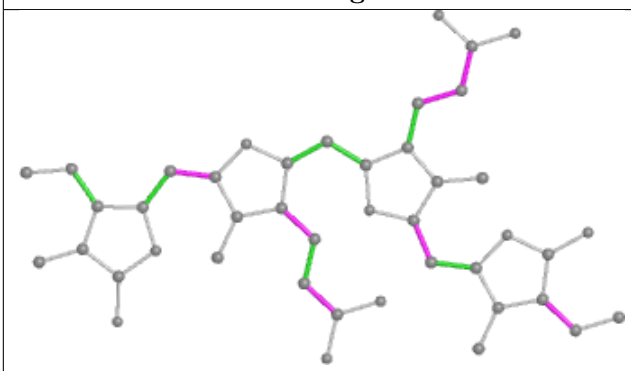

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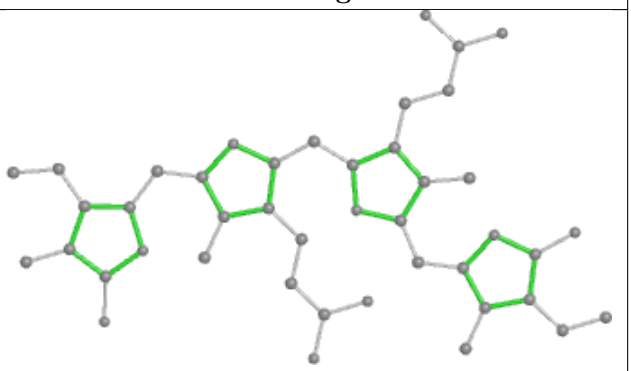
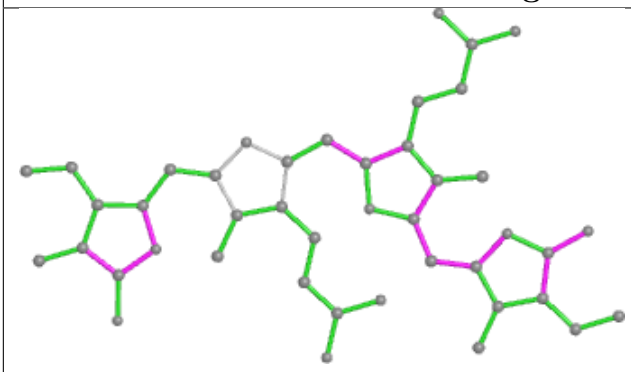


Rings

Ligand CYC P 184



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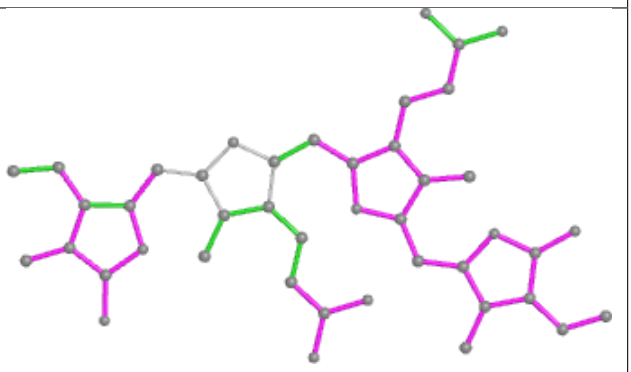

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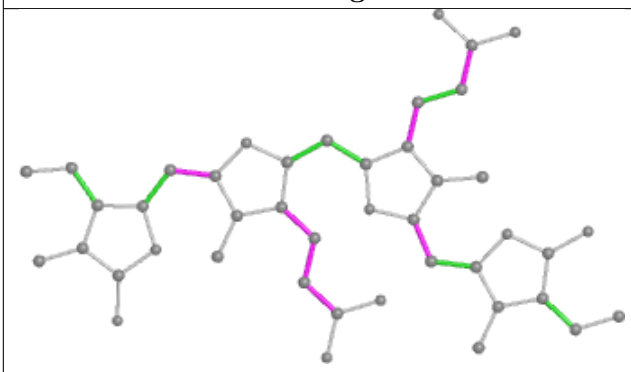

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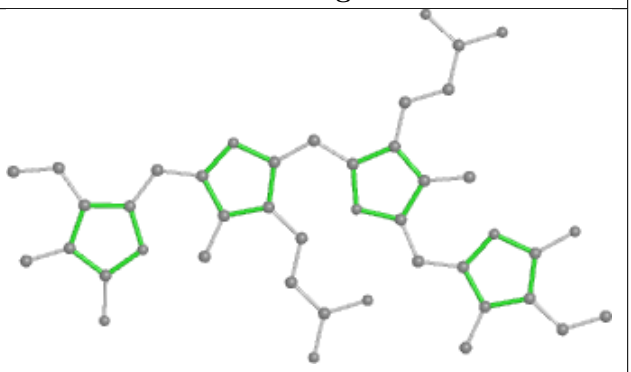
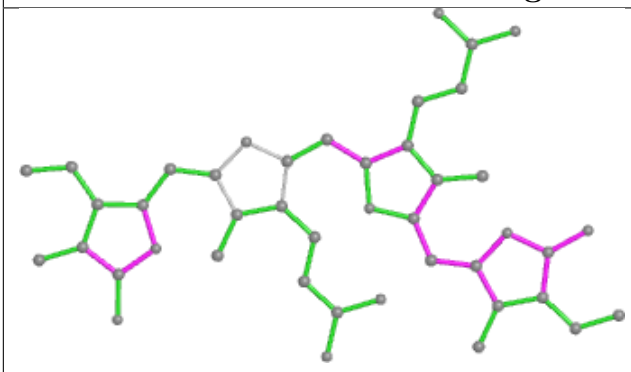


Rings

Ligand CYC L 184



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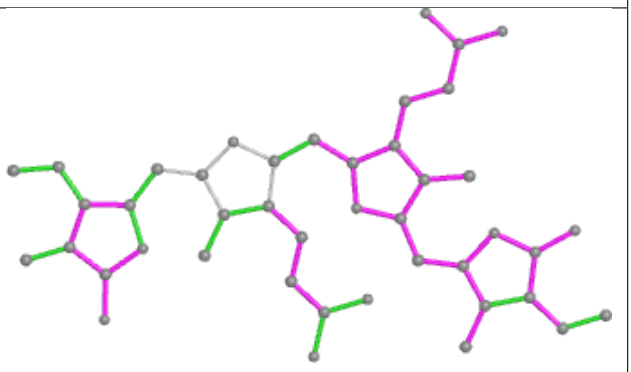
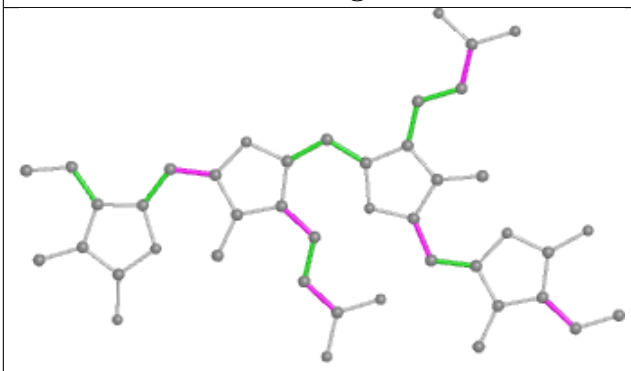


Bond angles



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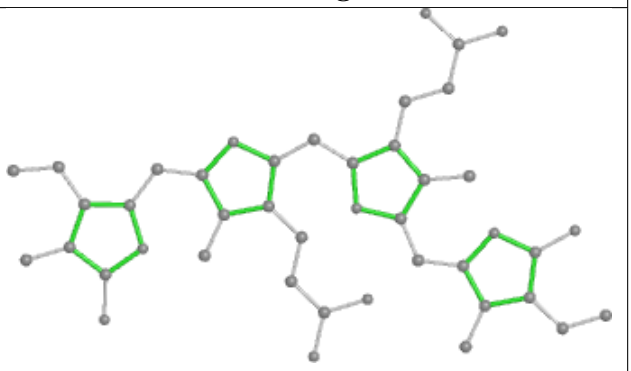
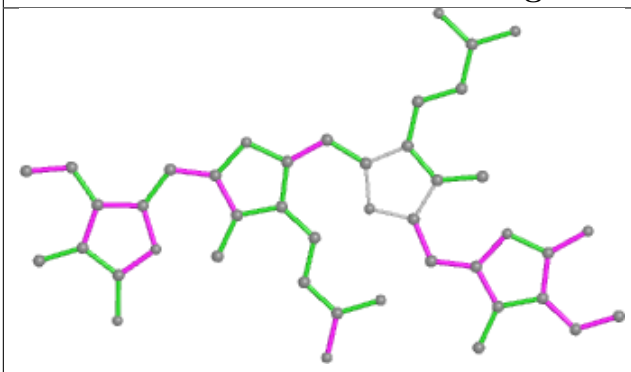


Rings

Ligand BLA B 184



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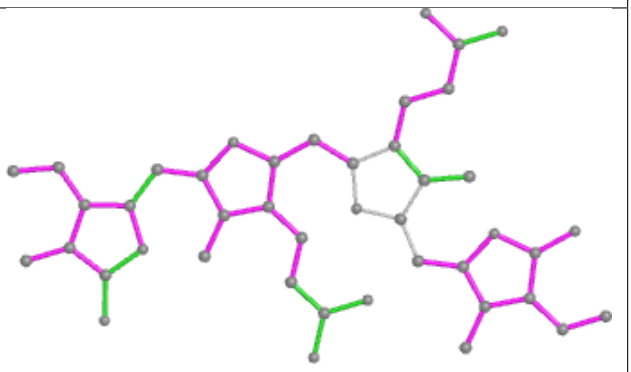
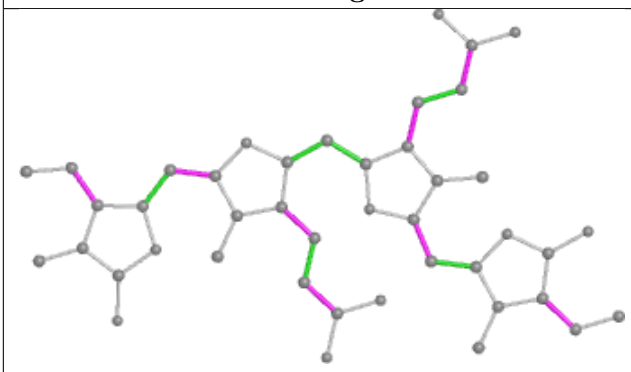


Bond angles



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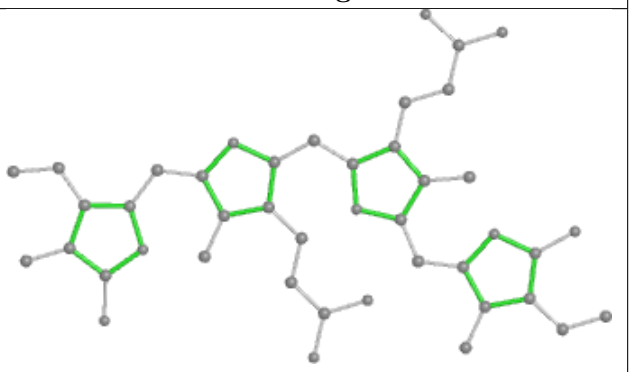
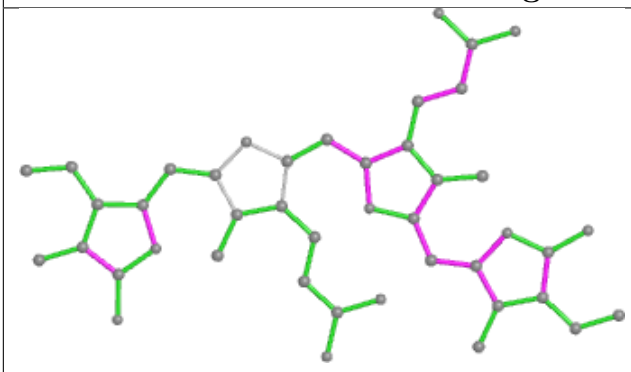


Rings

Ligand CYC P 255



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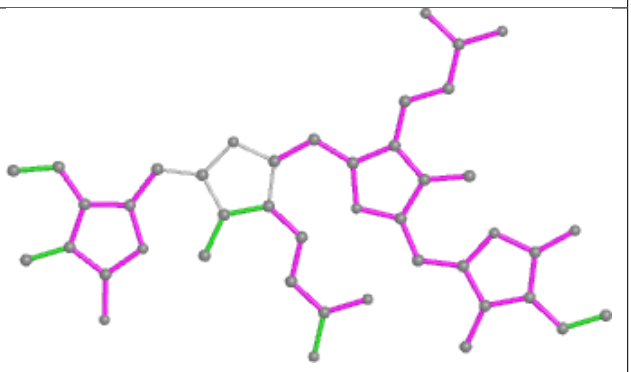
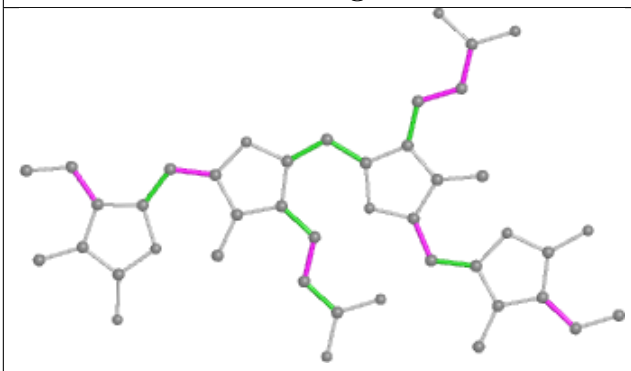


Bond angles



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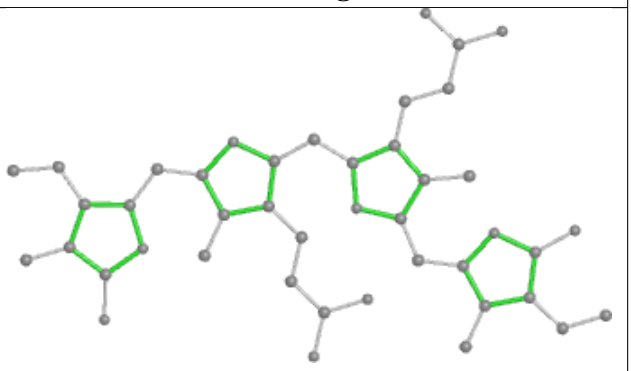
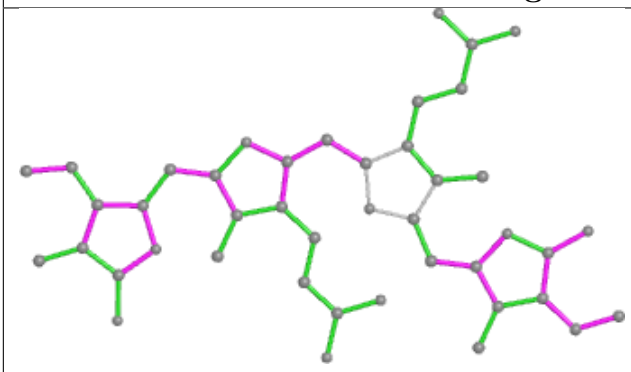


Rings

Ligand BLA B 255



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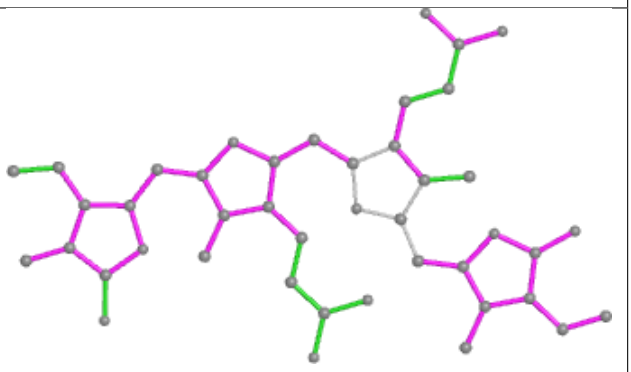
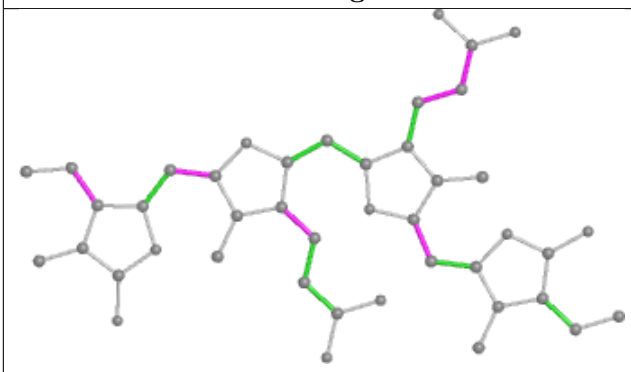


Bond angles



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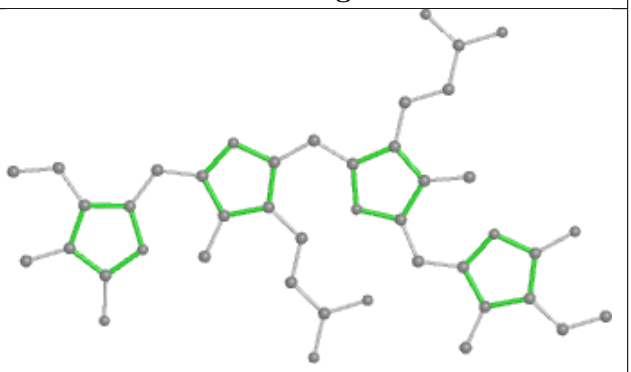
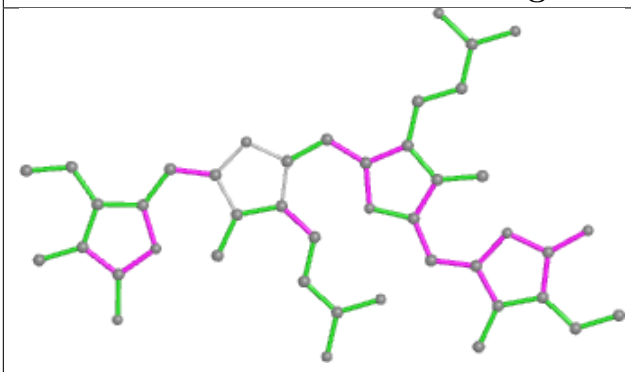


Rings

Ligand CYC I 184



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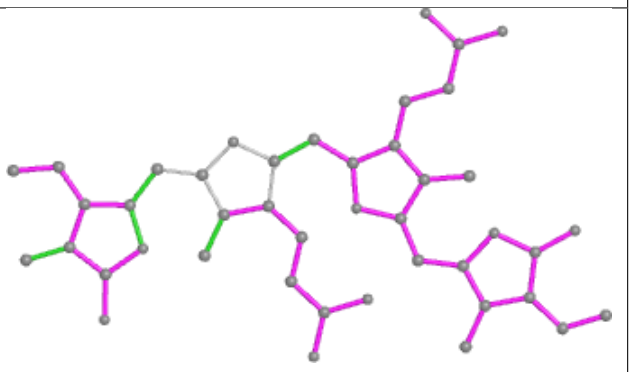
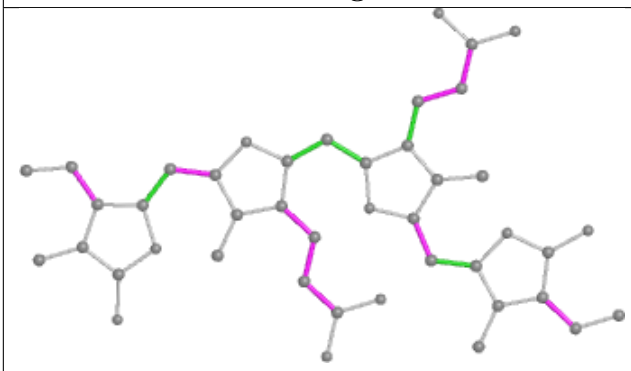


Bond angles



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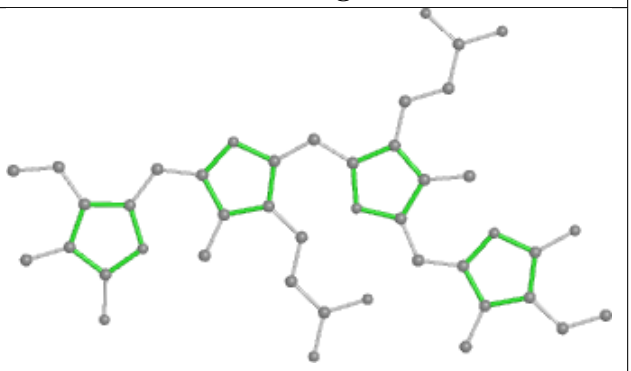
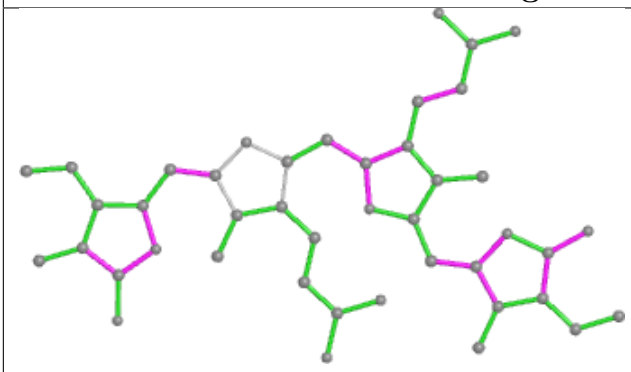


Rings

Ligand CYC R 255



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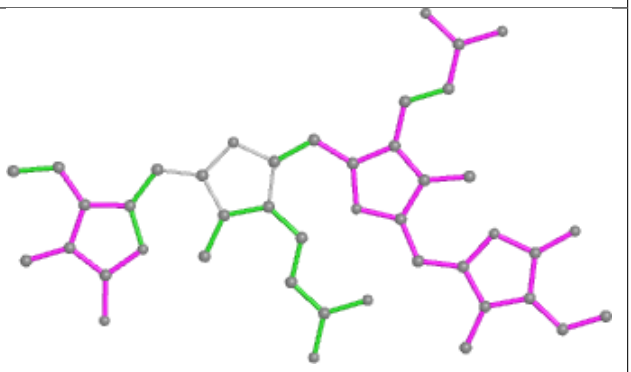
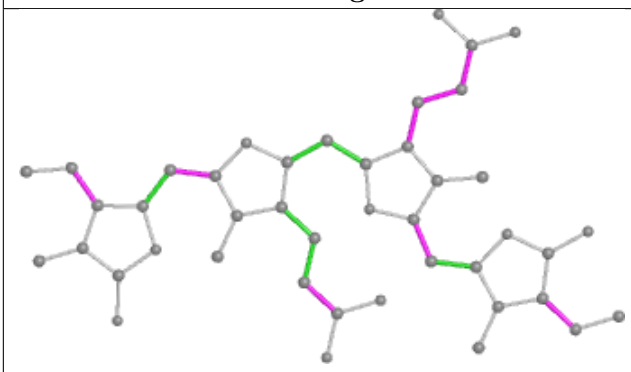


Bond angles



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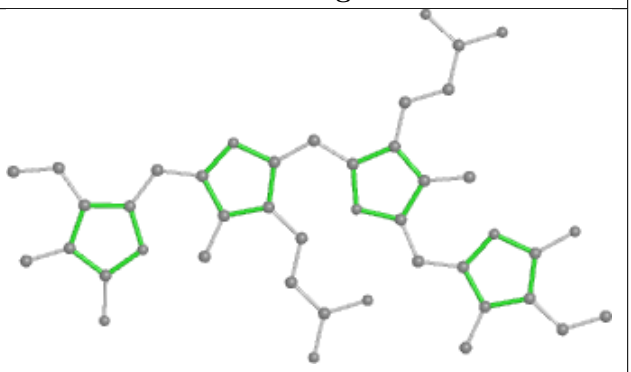
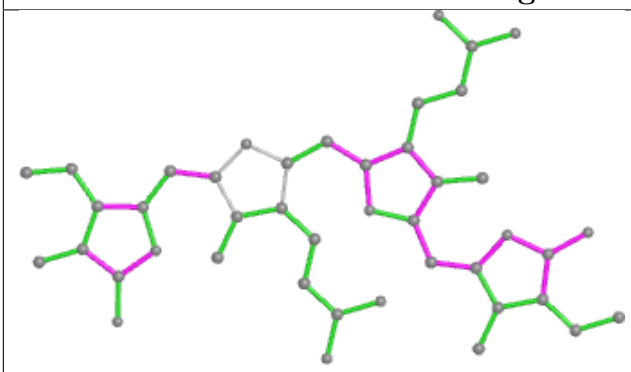


Rings

Ligand CYC M 184



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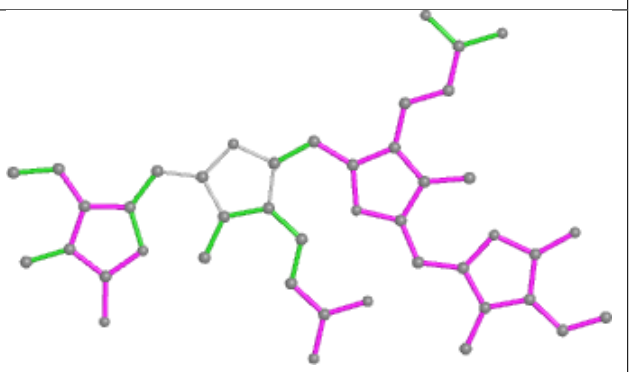

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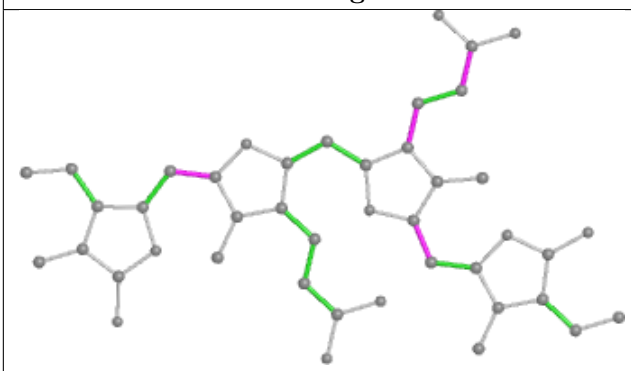
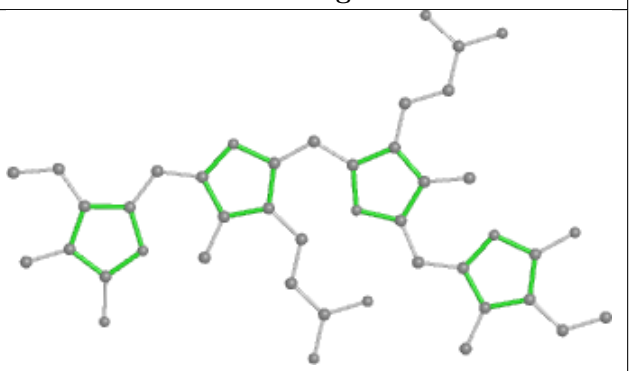
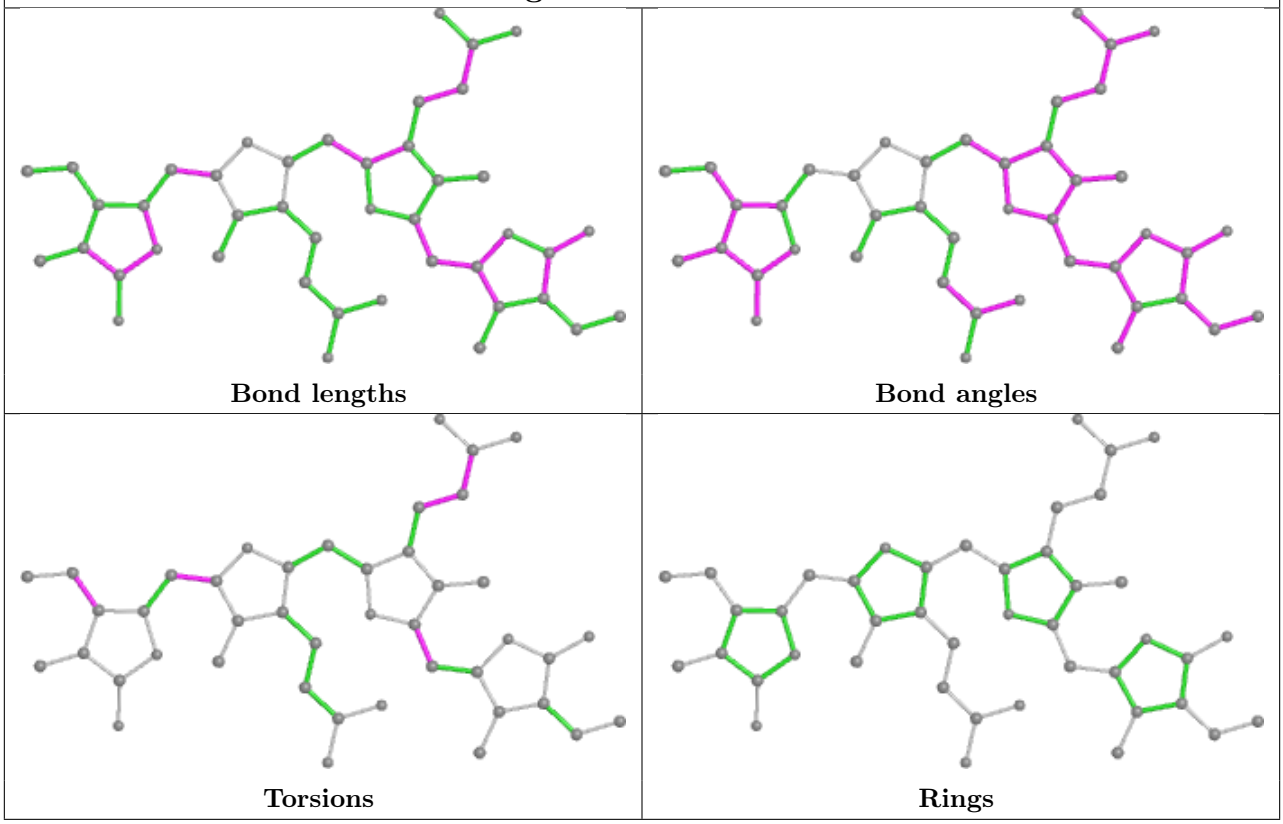


Torsions

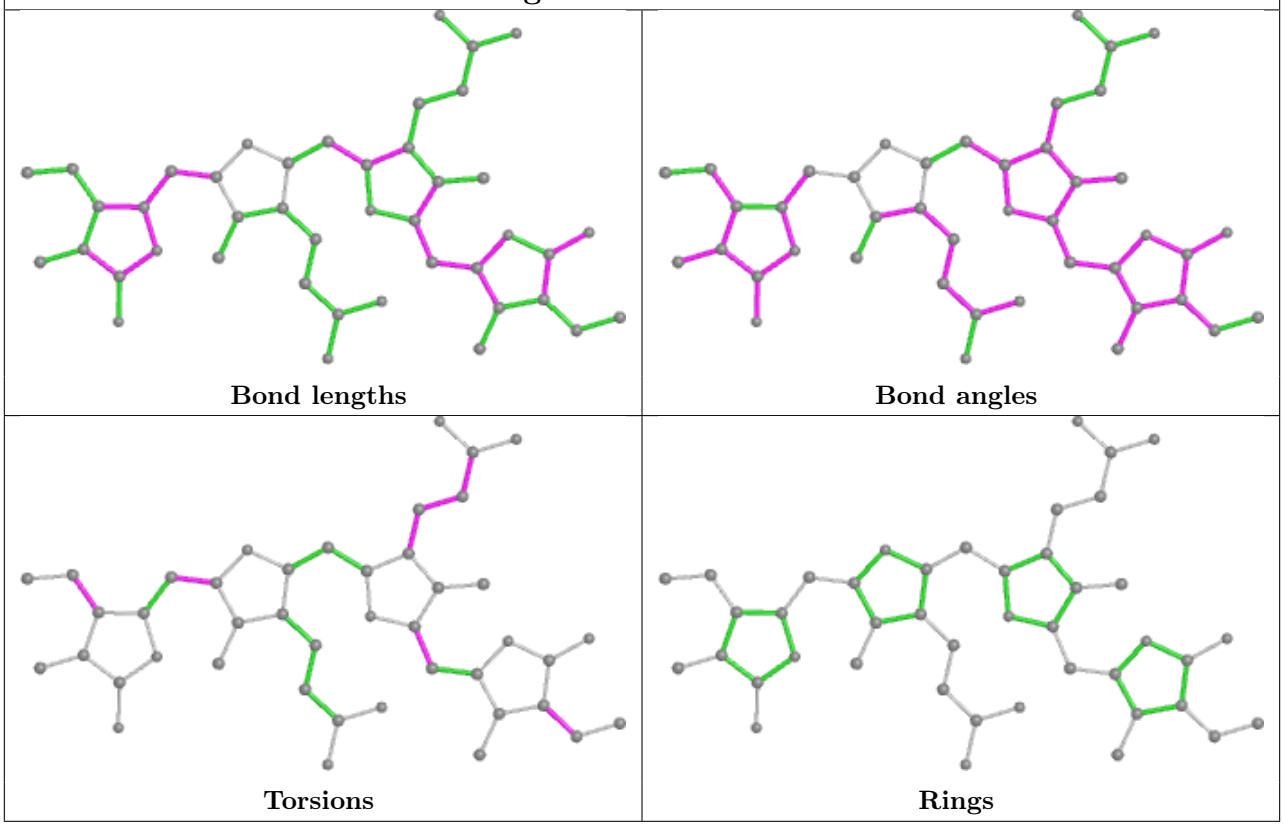


Rings

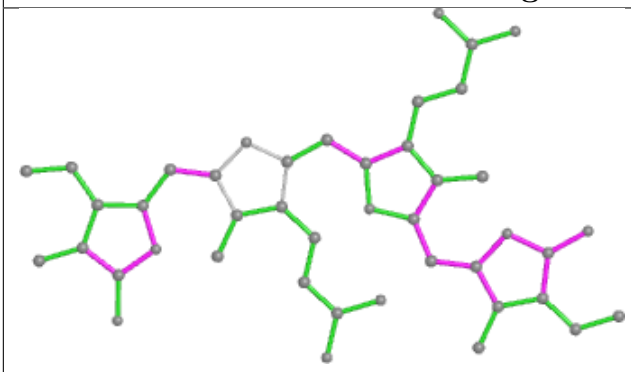
Ligand CYC L 255



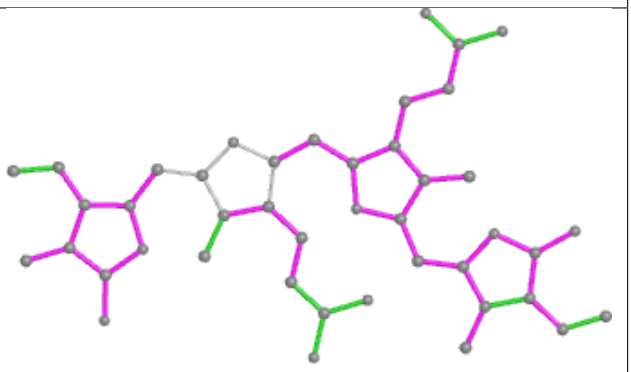
Ligand CYC T 255



Ligand CYC V 184



Bond lengths



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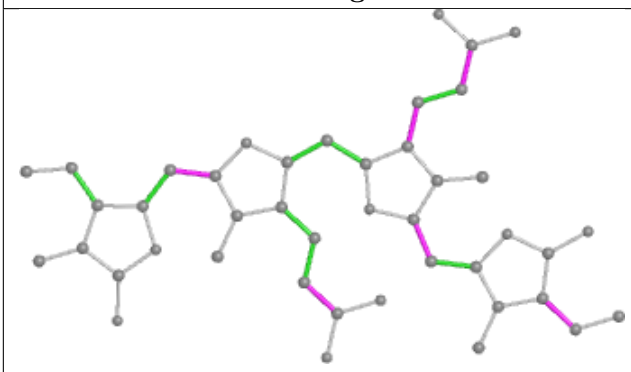
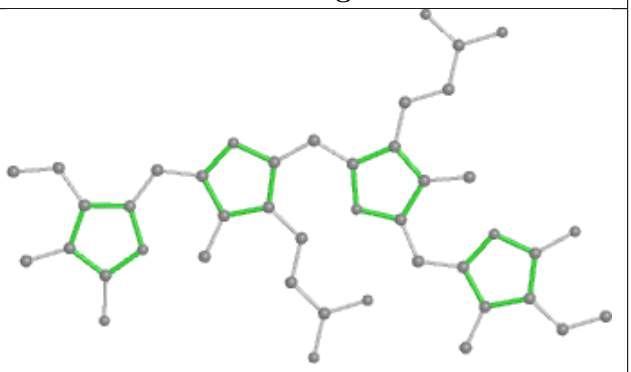
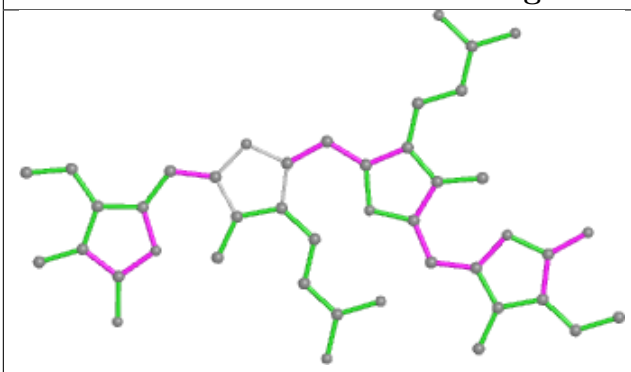


Torsions

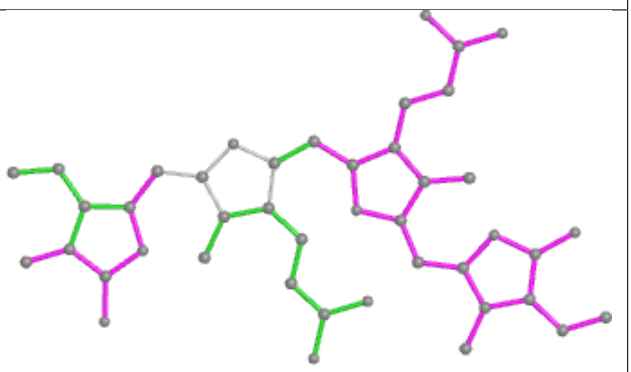


Rings

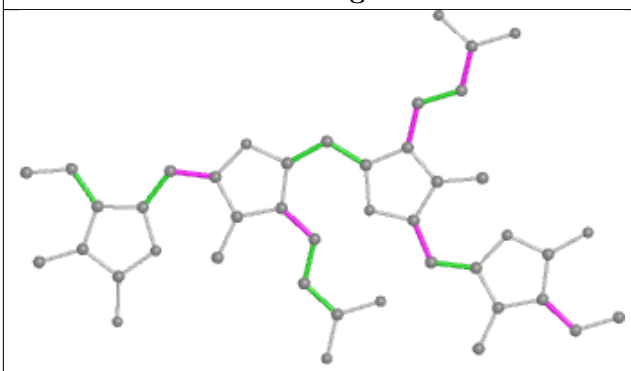
Ligand CYC F 184



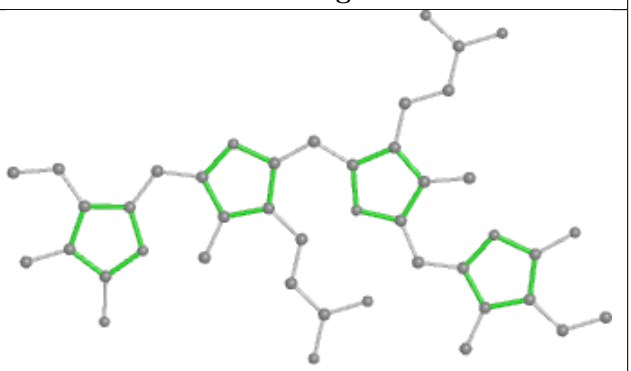
Bond lengths



Bond angles

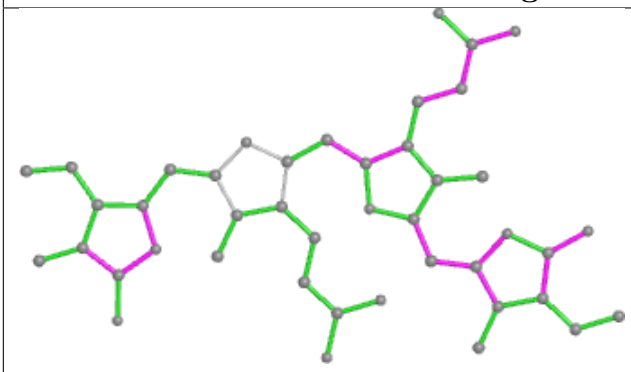


Torsions

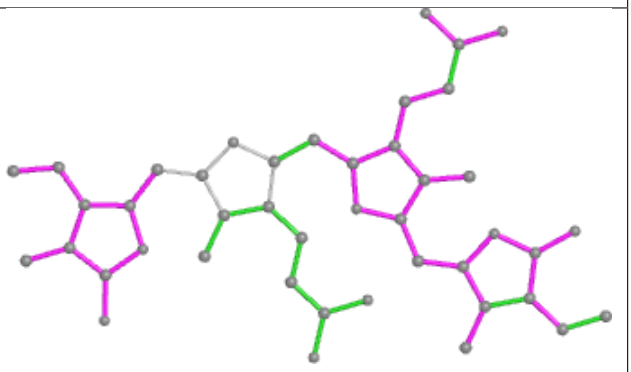


Rings

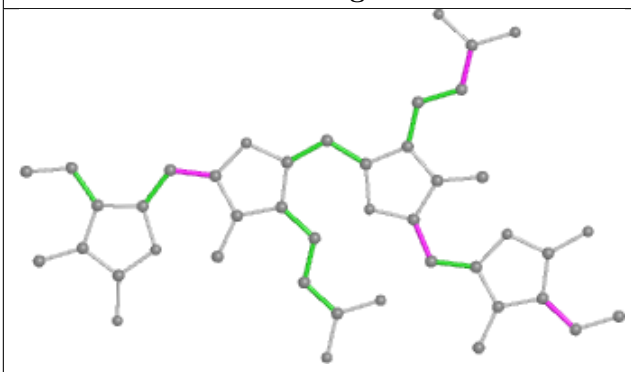
Ligand CYC H 255



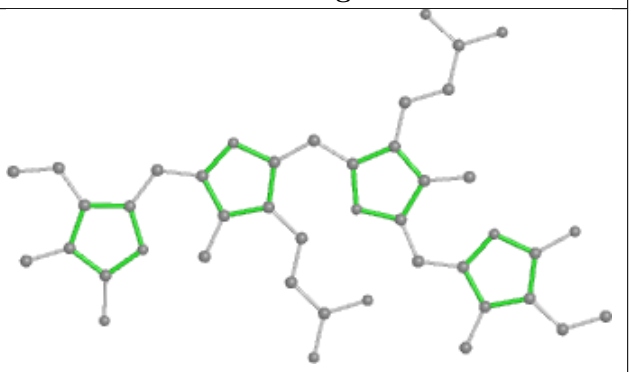
Bond lengths



Bond angles

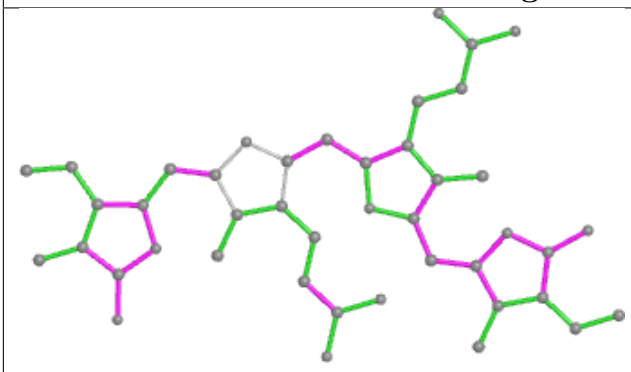


Torsions

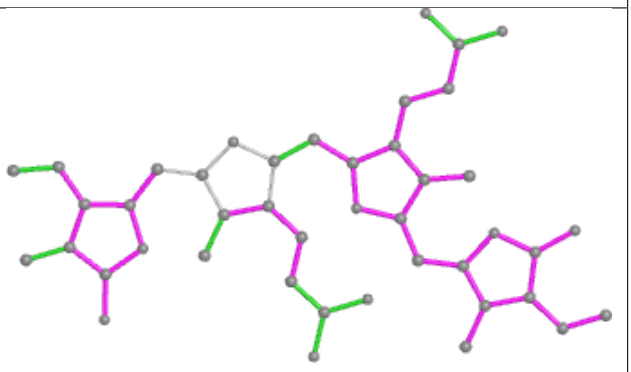


Rings

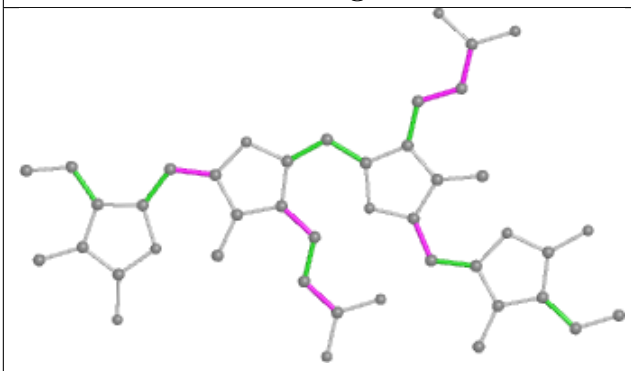
Ligand CYC H 184



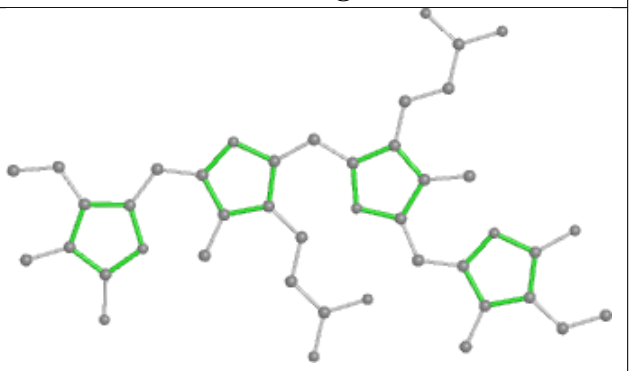
Bond lengths



Bond angles

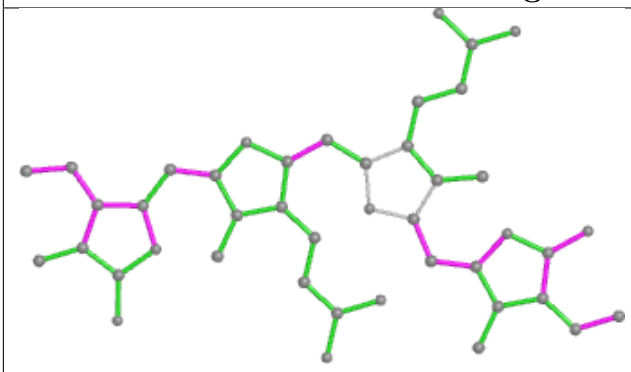


Torsions

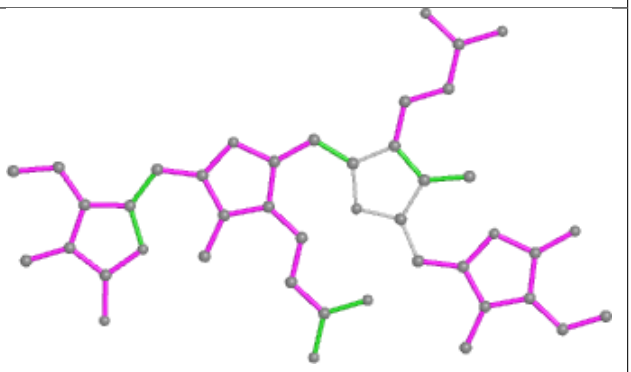


Rings

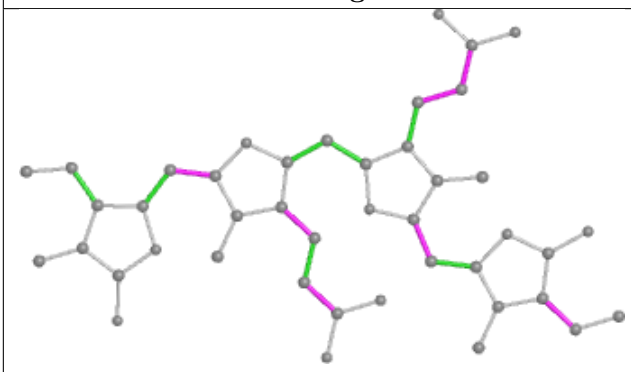
Ligand BLA D 255



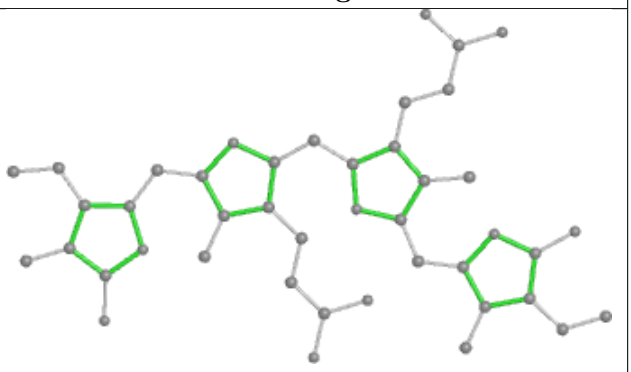
Bond lengths



Bond angles

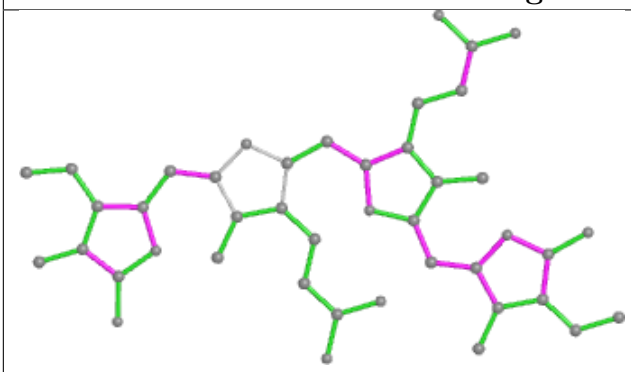


Torsions

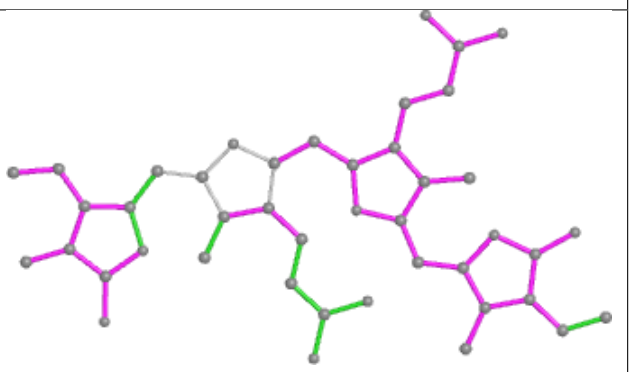


Rings

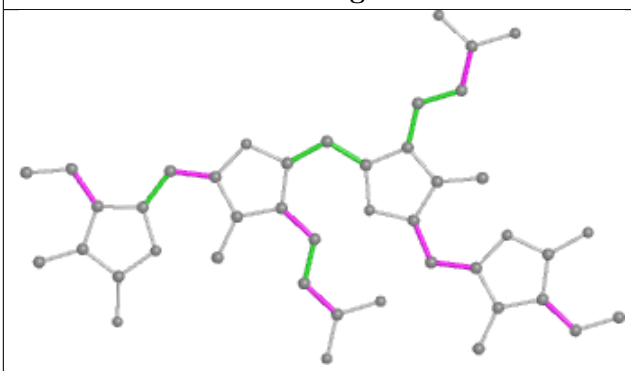
Ligand CYC J 255



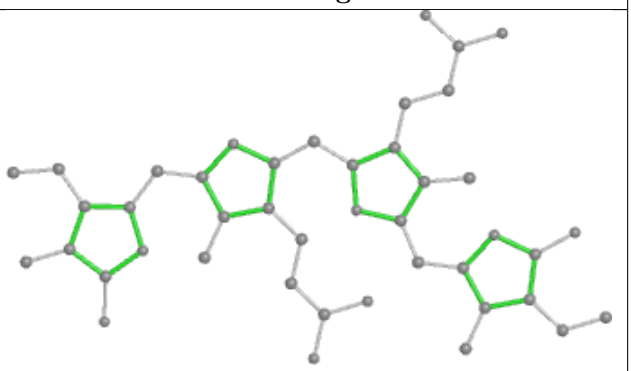
Bond lengths



Bond angles

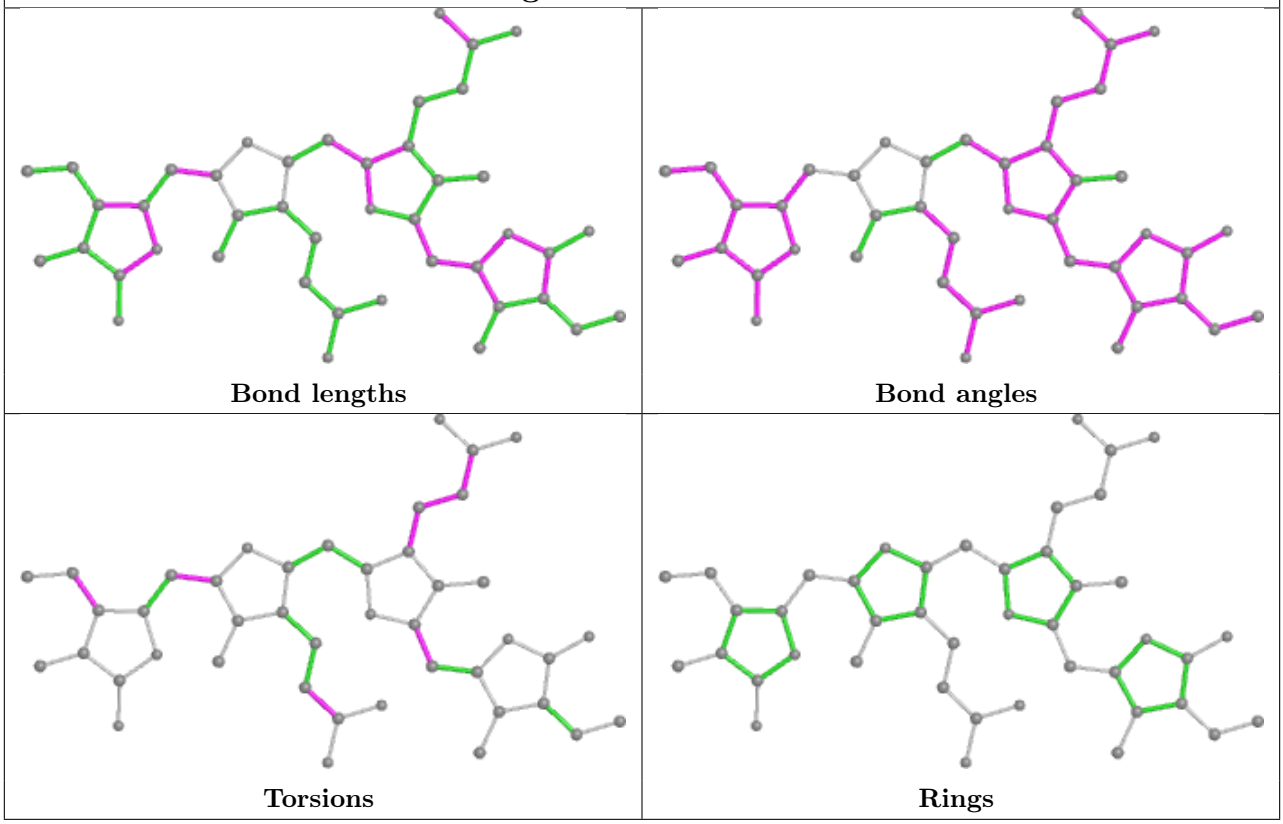


Torsions

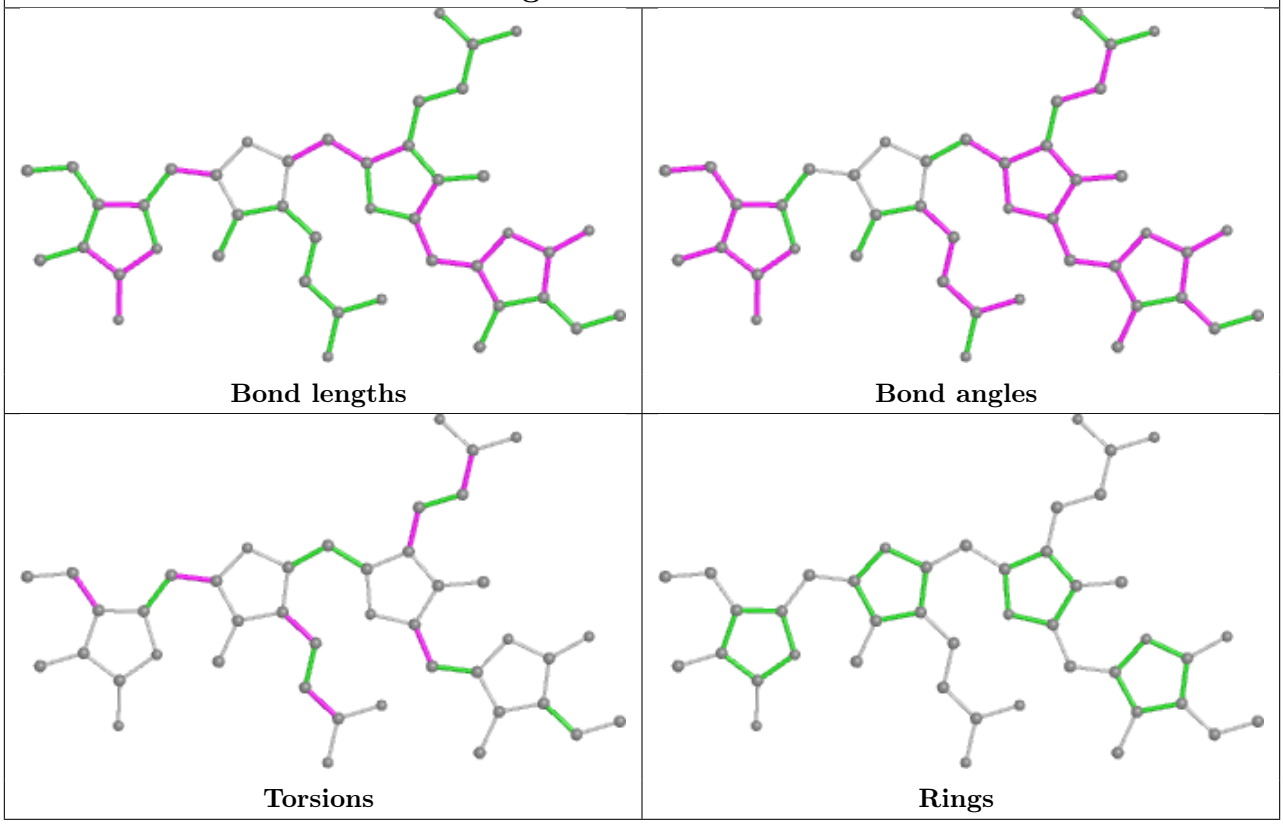


Rings

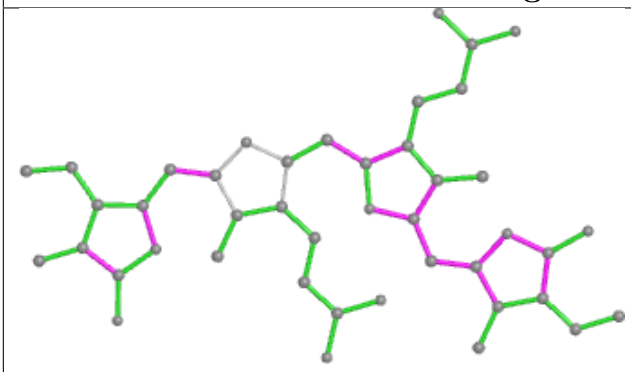
Ligand CYC G 184



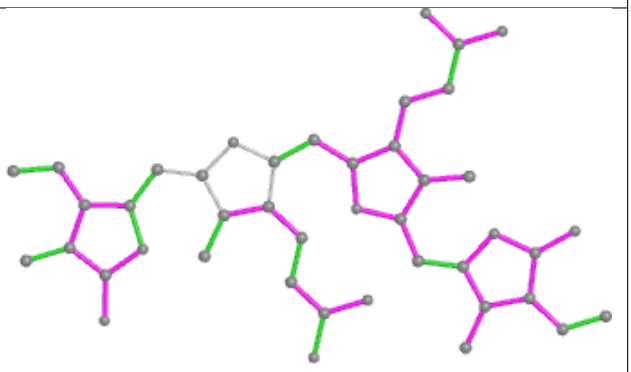
Ligand CYC U 184



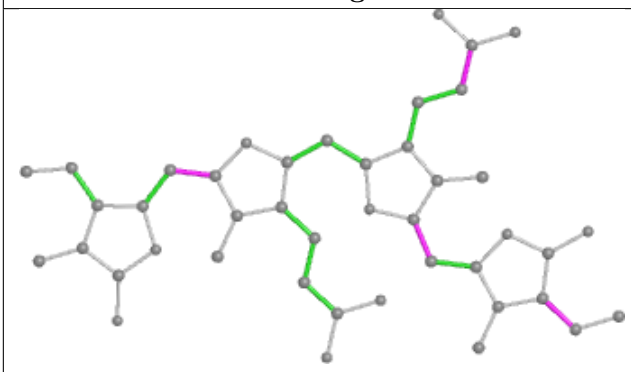
Ligand CYC F 255



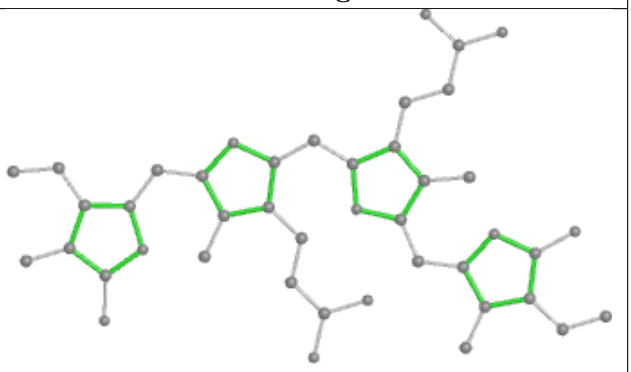
Bond lengths



Bond angles

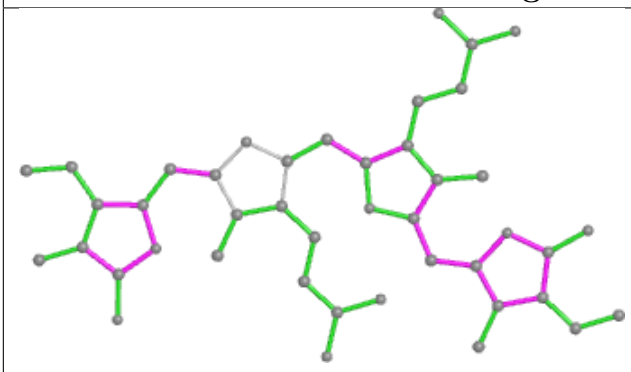


Torsions

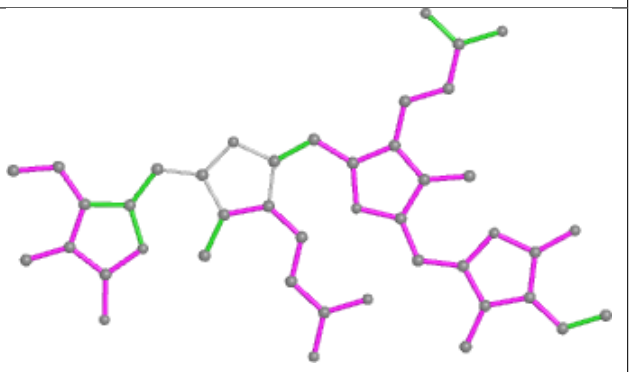


Rings

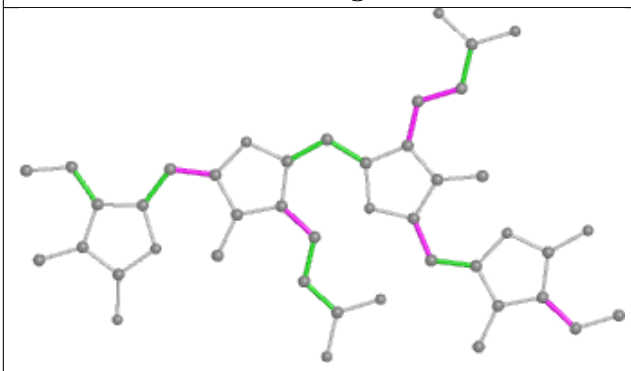
Ligand CYC T 184



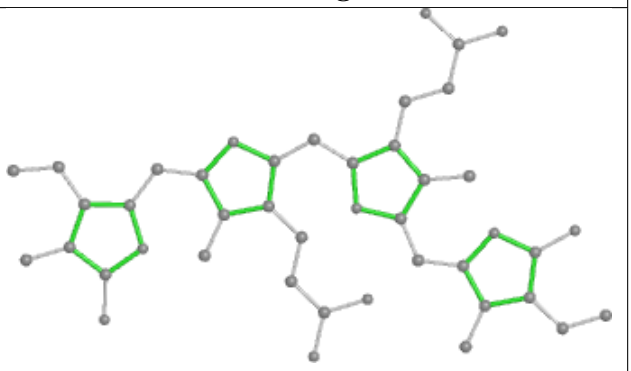
Bond lengths



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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.59	0	100	100	3, 12, 21, 29	0
1	E	162/162 (100%)	-0.65	0	100	100	3, 12, 21, 29	0
1	G	162/162 (100%)	-0.61	1 (0%)	89	78	3, 12, 22, 29	0
1	I	162/162 (100%)	-0.66	0	100	100	3, 12, 21, 29	0
1	K	162/162 (100%)	-0.61	0	100	100	3, 12, 22, 29	0
1	M	162/162 (100%)	-0.60	0	100	100	3, 12, 22, 29	0
1	O	162/162 (100%)	-0.61	0	100	100	3, 12, 21, 29	0
1	Q	162/162 (100%)	-0.51	1 (0%)	89	78	3, 12, 22, 29	0
1	S	162/162 (100%)	-0.44	1 (0%)	89	78	3, 12, 22, 29	0
1	U	162/162 (100%)	-0.61	0	100	100	3, 12, 22, 29	0
1	W	162/162 (100%)	-0.67	0	100	100	3, 12, 21, 29	0
2	B	172/172 (100%)	-0.42	0	100	100	3, 15, 24, 33	0
2	F	172/172 (100%)	-0.51	0	100	100	3, 15, 24, 33	0
2	J	172/172 (100%)	-0.46	0	100	100	3, 15, 24, 33	0
2	L	172/172 (100%)	-0.55	0	100	100	3, 15, 24, 33	0
2	N	172/172 (100%)	-0.42	0	100	100	3, 15, 24, 33	0
2	P	172/172 (100%)	-0.49	0	100	100	3, 15, 24, 33	0
2	R	172/172 (100%)	-0.45	0	100	100	3, 15, 24, 33	0
2	T	172/172 (100%)	-0.46	0	100	100	3, 15, 24, 33	0
2	V	172/172 (100%)	-0.29	0	100	100	3, 15, 24, 33	0
2	X	172/172 (100%)	-0.49	0	100	100	3, 15, 24, 33	0
3	C	162/162 (100%)	-0.63	0	100	100	3, 12, 22, 29	0
4	D	172/172 (100%)	-0.46	0	100	100	3, 15, 24, 33	0
5	H	172/172 (100%)	-0.53	0	100	100	3, 15, 24, 33	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
All	All	4008/4008 (100%)	-0.53	3 (0%)	95 92	3, 14, 24, 33	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	68	CYS	2.6
1	S	68	CYS	2.2
1	G	70	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no 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
6	CYC	V	184	43/43	0.85	0.26	44,49,54,58	0
7	BLA	B	184	43/43	0.87	0.25	18,24,29,35	0
6	CYC	D	184	43/43	0.88	0.23	19,28,29,33	0
6	CYC	L	184	43/43	0.88	0.25	12,20,27,36	0
6	CYC	H	184	43/43	0.89	0.22	13,19,31,38	0
6	CYC	X	184	43/43	0.89	0.24	5,15,27,30	0
6	CYC	T	184	43/43	0.89	0.24	16,23,27,30	0
7	BLA	D	255	43/43	0.89	0.27	27,31,33,35	0
6	CYC	J	255	43/43	0.90	0.28	11,23,24,26	0
6	CYC	F	184	43/43	0.90	0.22	16,25,29,32	0
6	CYC	V	255	43/43	0.90	0.25	22,33,34,37	0
6	CYC	N	184	43/43	0.90	0.21	24,29,32,34	0
6	CYC	N	255	43/43	0.90	0.30	32,38,40,42	0
7	BLA	B	255	43/43	0.90	0.27	26,33,33,34	0

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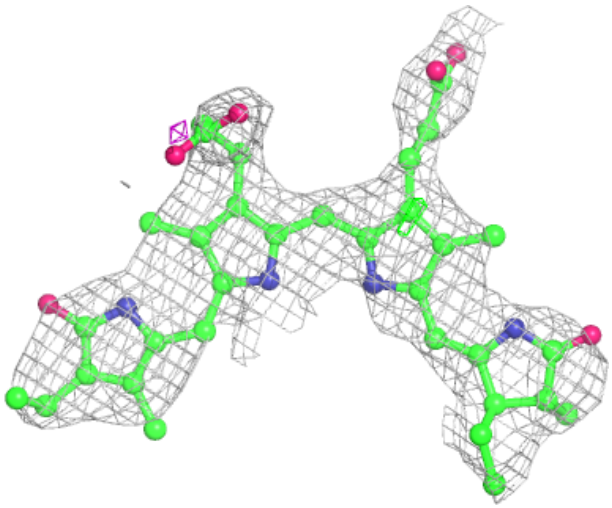
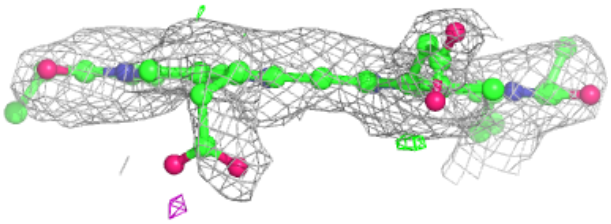
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CYC	R	184	43/43	0.90	0.24	5,18,23,27	0
6	CYC	P	184	43/43	0.91	0.21	25,31,38,41	0
6	CYC	T	255	43/43	0.91	0.25	19,26,27,27	0
6	CYC	P	255	43/43	0.91	0.24	20,29,29,30	0
6	CYC	J	184	43/43	0.91	0.23	15,20,30,32	0
6	CYC	I	184	43/43	0.92	0.21	13,15,19,27	0
6	CYC	F	255	43/43	0.92	0.23	7,17,21,22	0
6	CYC	E	184	43/43	0.92	0.21	9,13,17,23	0
6	CYC	H	255	43/43	0.92	0.24	6,23,24,26	0
6	CYC	X	255	43/43	0.92	0.22	11,27,28,28	0
6	CYC	L	255	43/43	0.92	0.25	7,22,23,24	0
6	CYC	R	255	43/43	0.92	0.24	6,13,15,18	0
6	CYC	M	184	43/43	0.92	0.22	22,25,27,30	0
6	CYC	Q	184	43/43	0.93	0.19	18,22,23,23	0
6	CYC	G	184	43/43	0.93	0.20	6,13,14,16	0
6	CYC	O	184	43/43	0.93	0.20	5,12,13,15	0
6	CYC	W	184	43/43	0.94	0.18	11,18,18,19	0
6	CYC	K	184	43/43	0.94	0.19	9,16,17,19	0
6	CYC	A	184	43/43	0.94	0.18	9,16,17,18	0
6	CYC	U	184	43/43	0.94	0.19	2,11,12,13	0
6	CYC	C	184	43/43	0.94	0.18	14,17,21,22	0
6	CYC	S	184	43/43	0.94	0.19	22,25,25,26	0

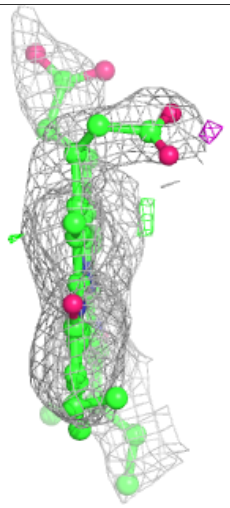
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC V 184:

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

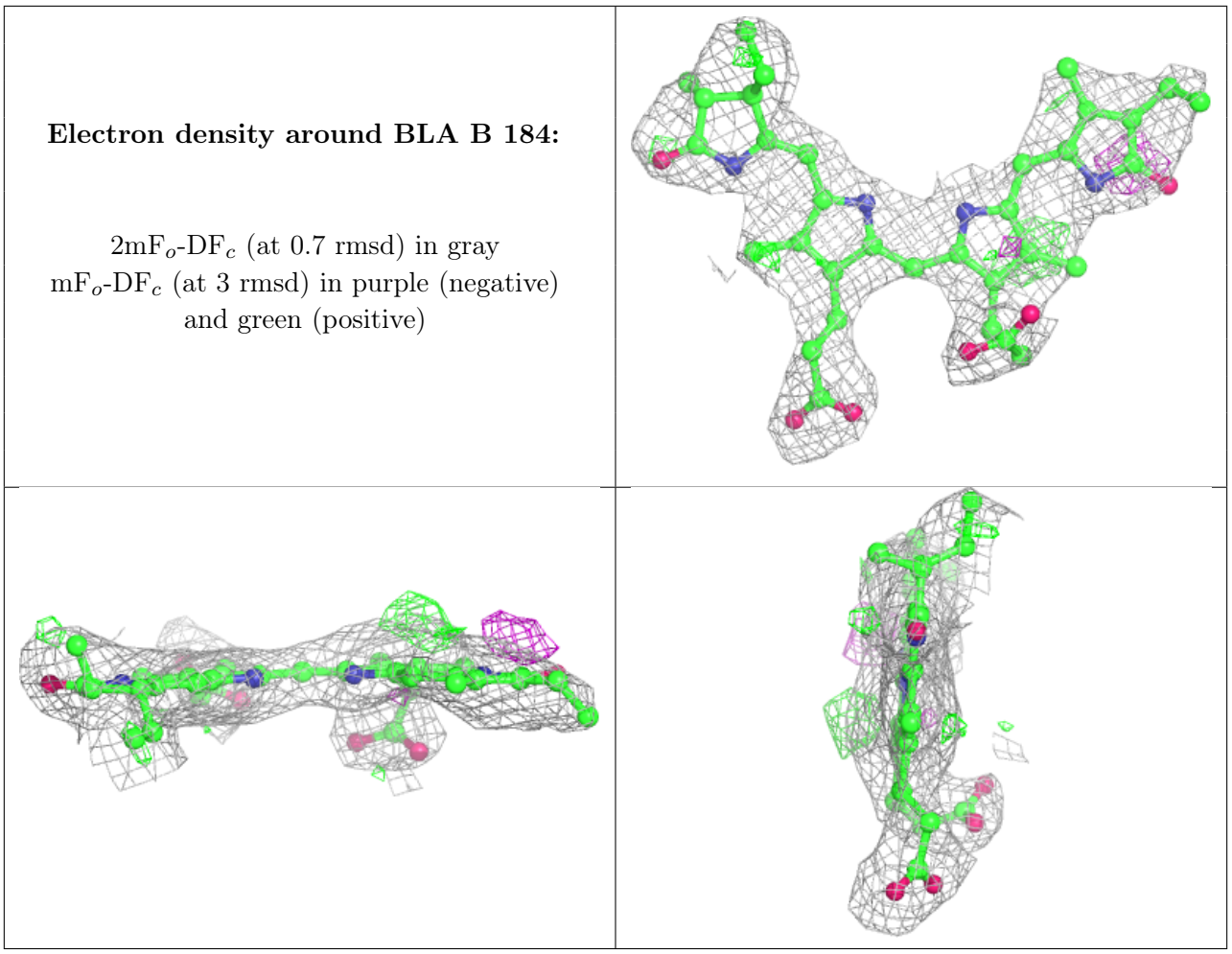






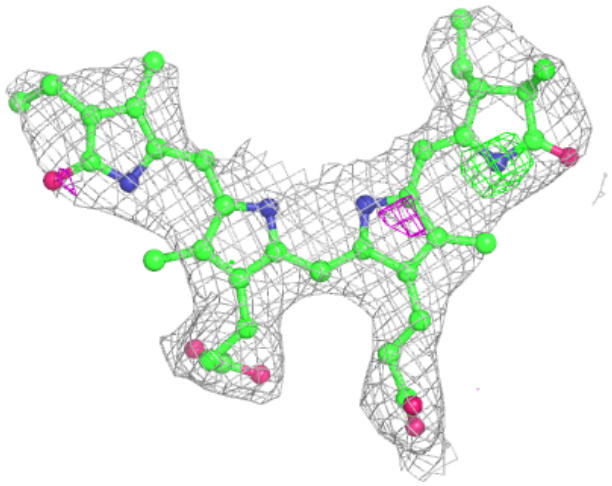
Electron density around BLA B 184:

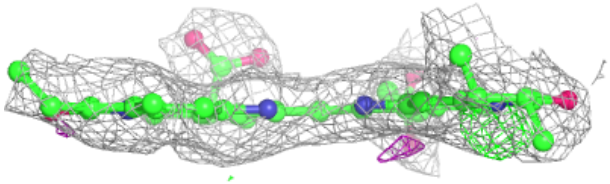
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

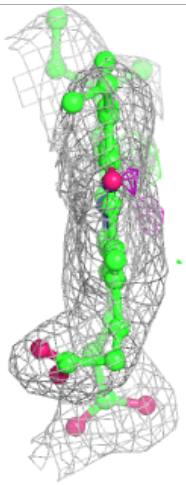


Electron density around CYC D 184:

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

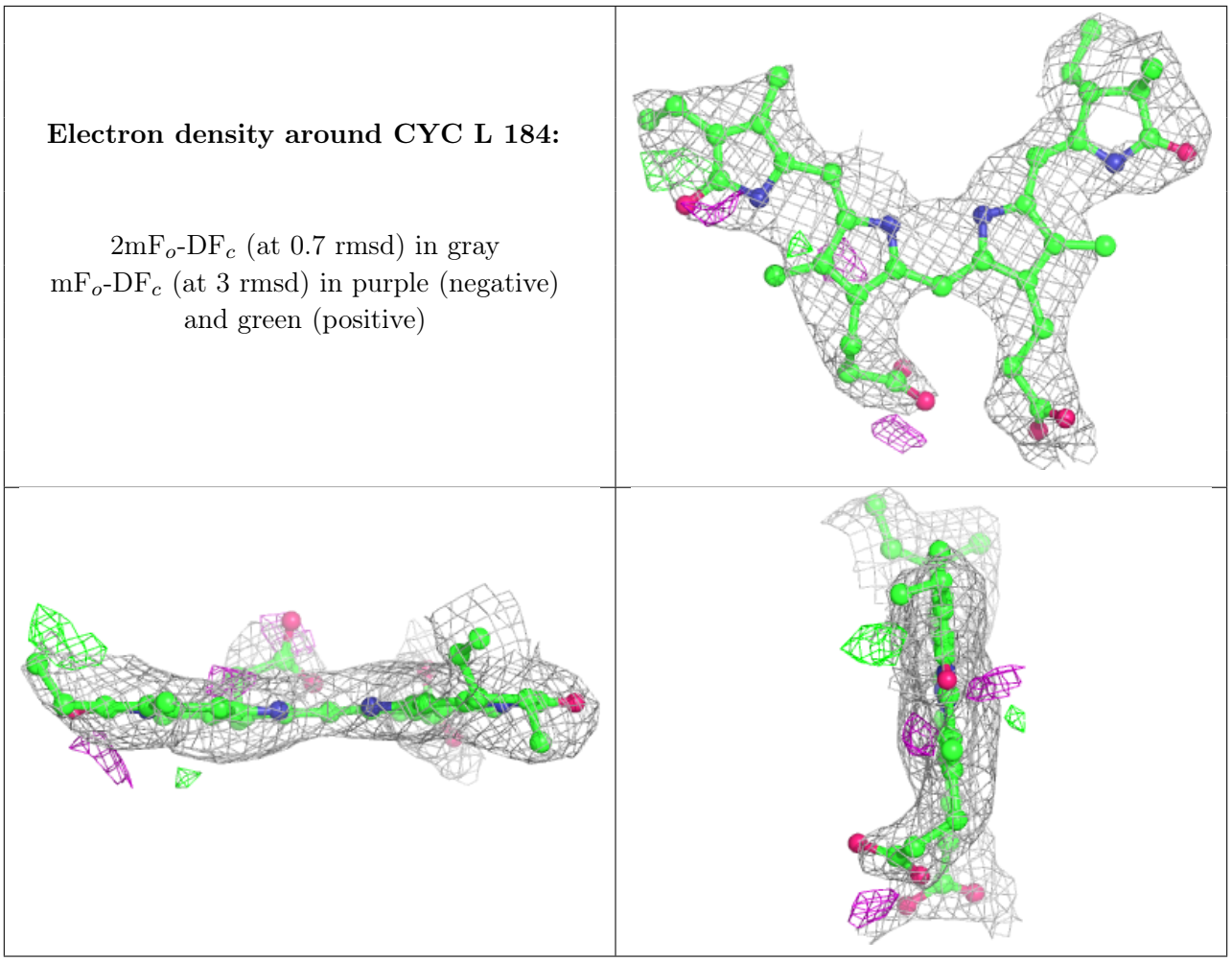






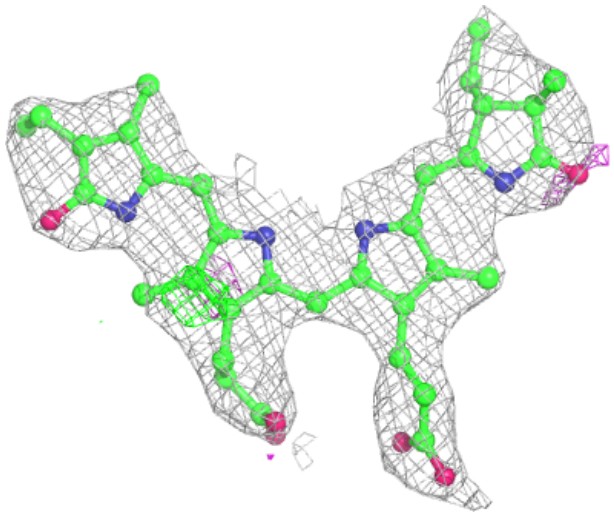
Electron density around CYC L 184:

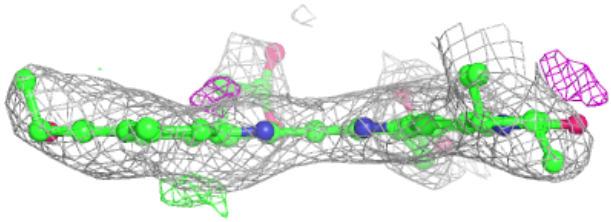
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

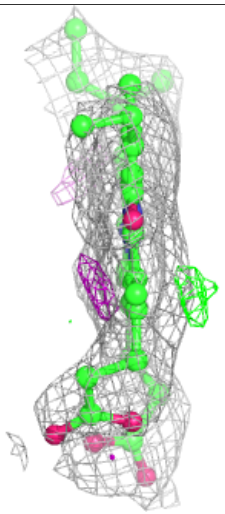


Electron density around CYC H 184:

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

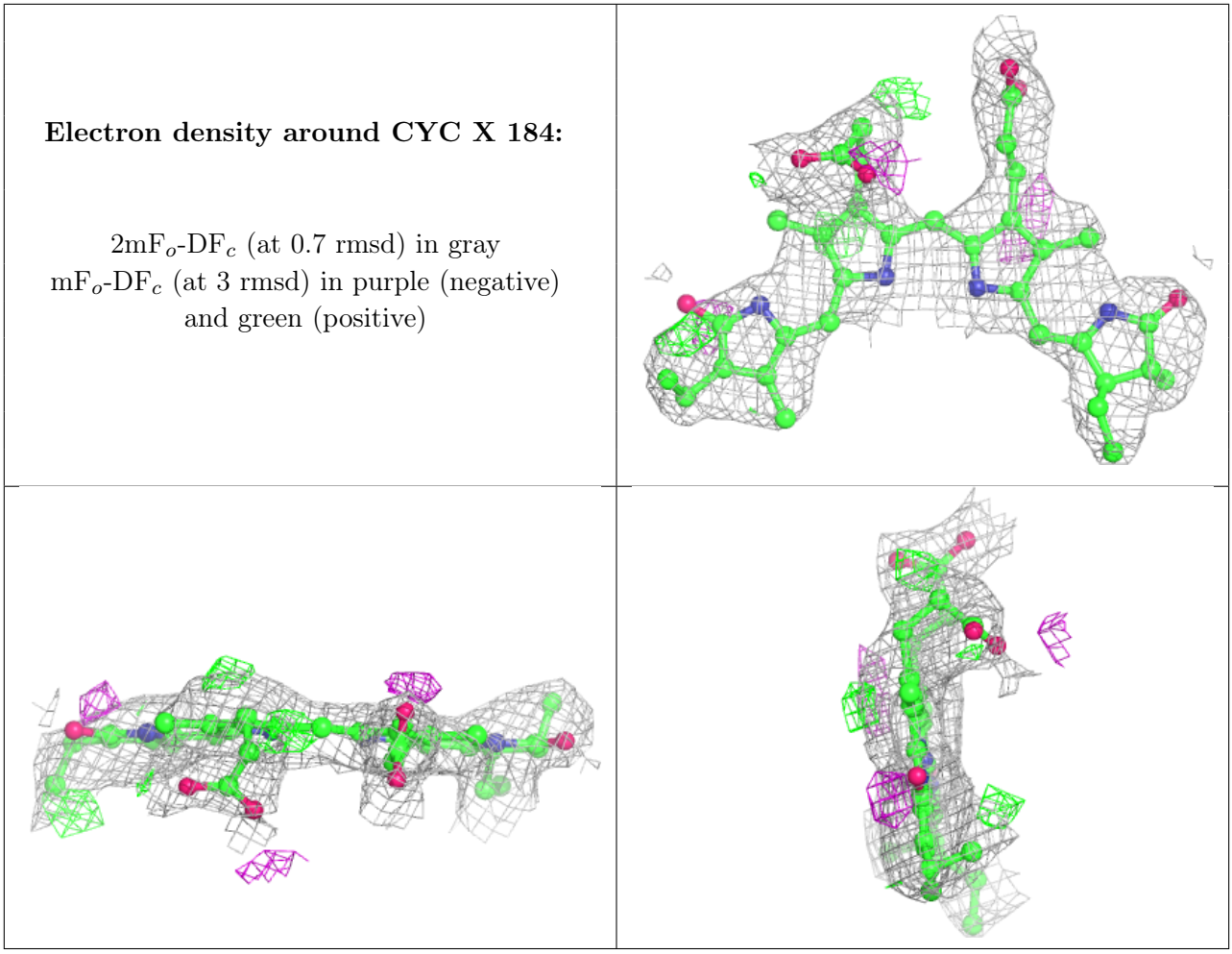






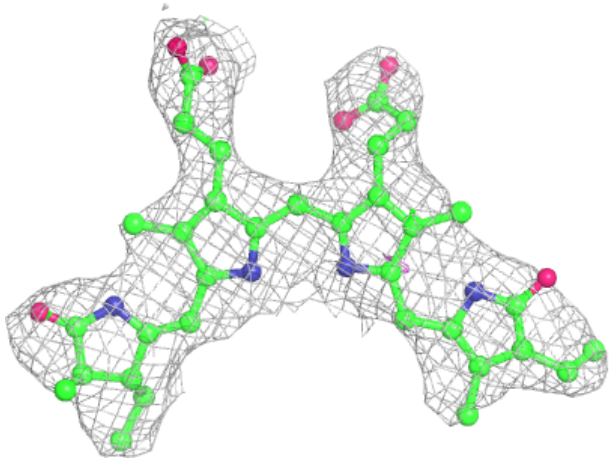
Electron density around CYC X 184:

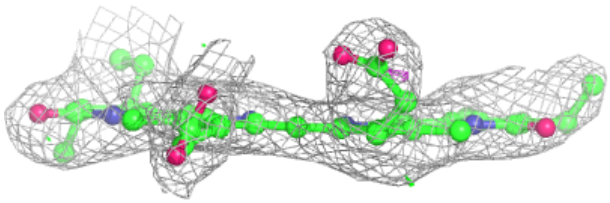
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

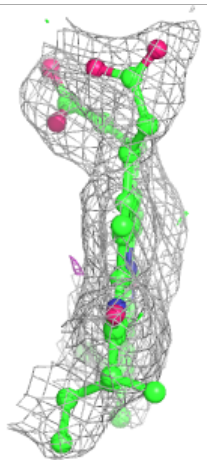


Electron density around CYC T 184:

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

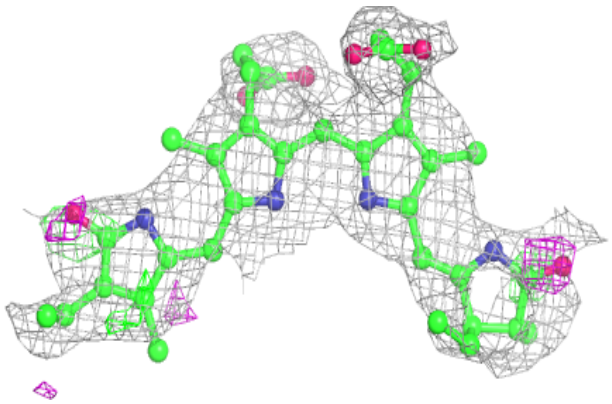


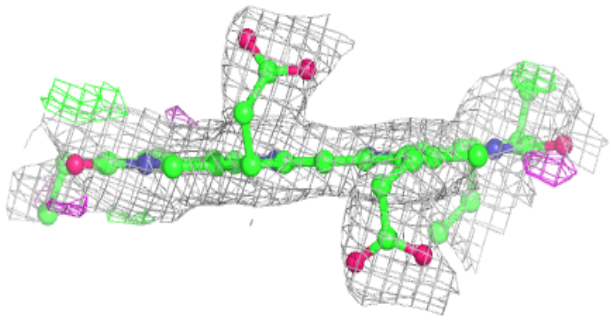


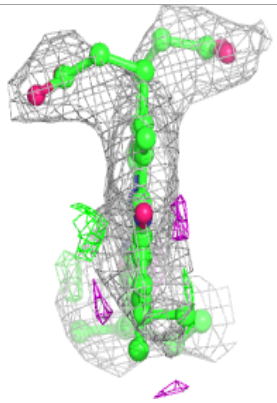


Electron density around BLA D 255:

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

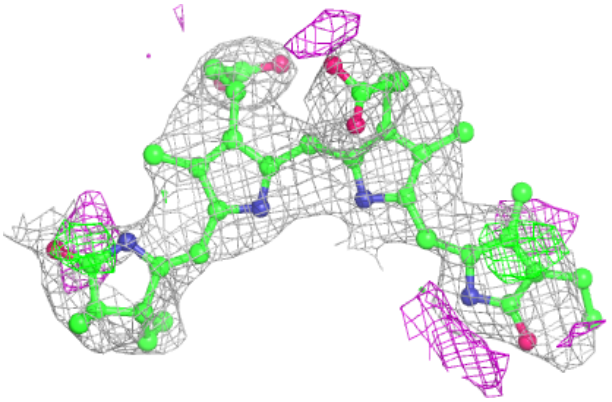


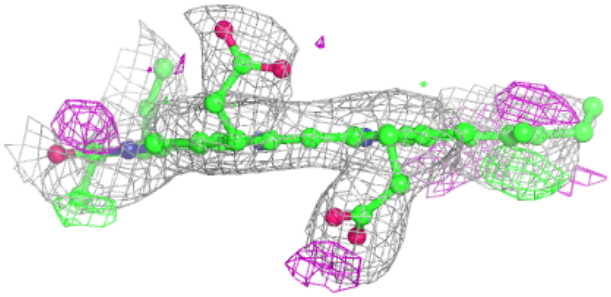


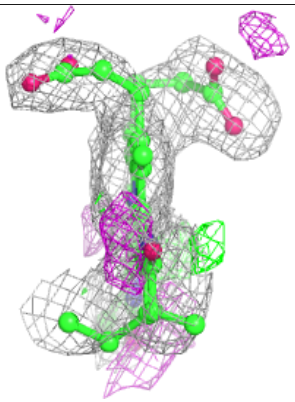


Electron density around CYC J 255:

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

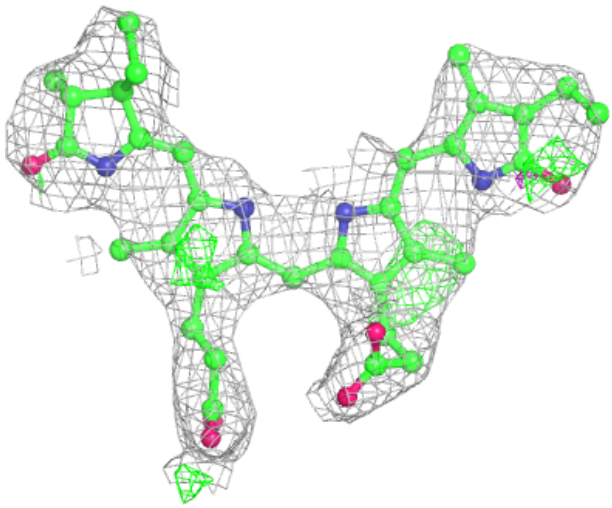


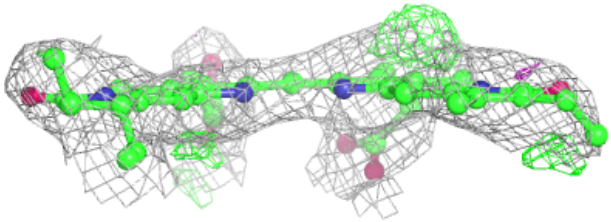


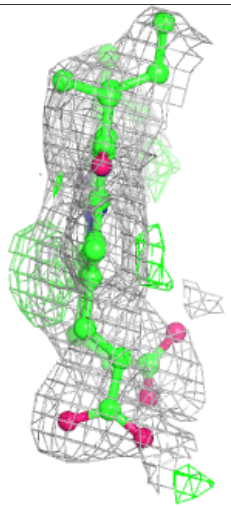


Electron density around CYC F 184:

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

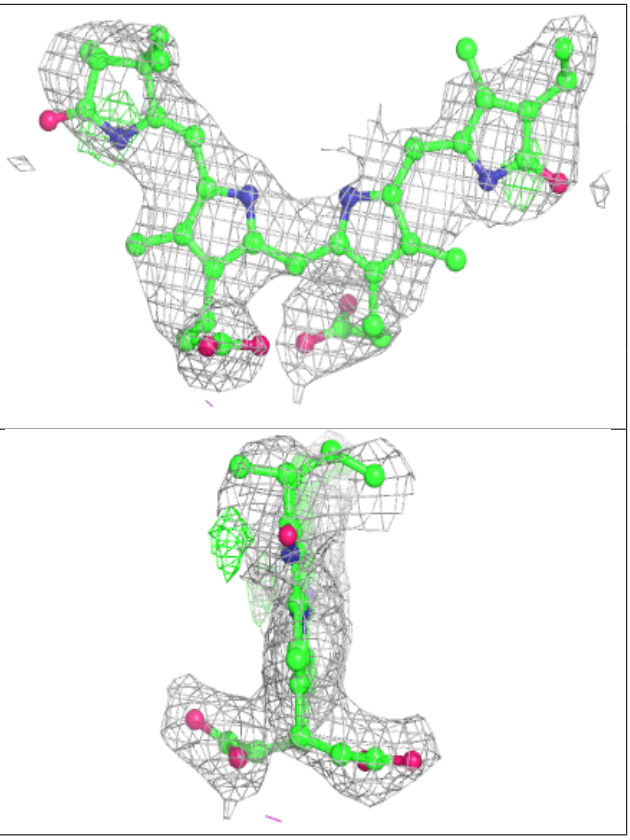


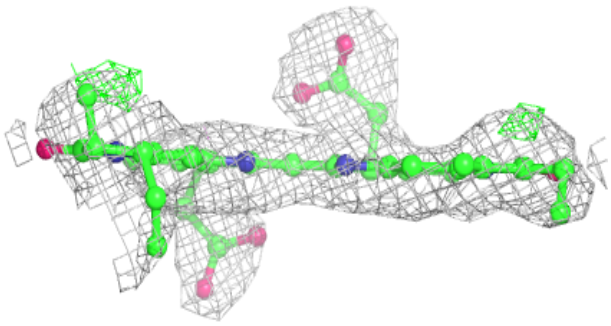




Electron density around CYC V 255:

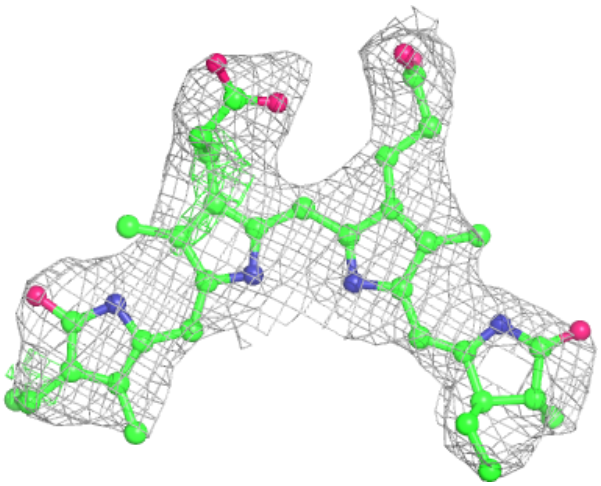
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

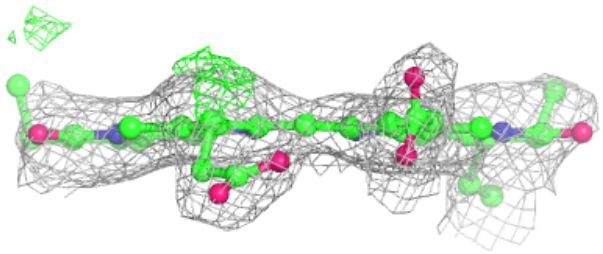


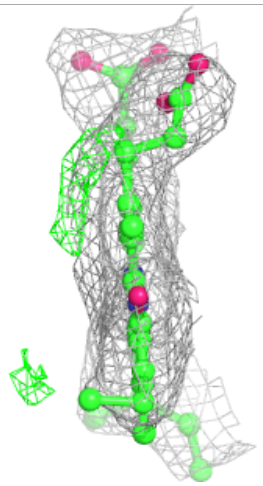


Electron density around CYC N 184:

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

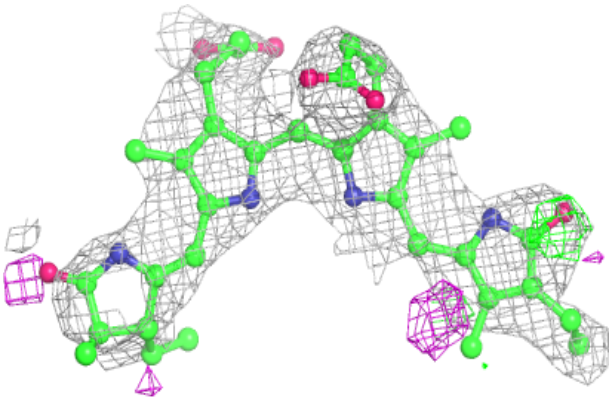


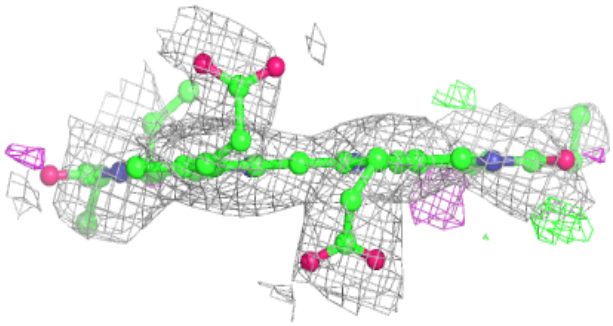


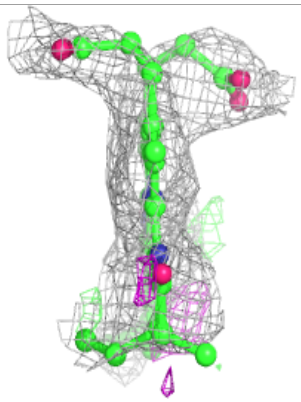


Electron density around CYC N 255:

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

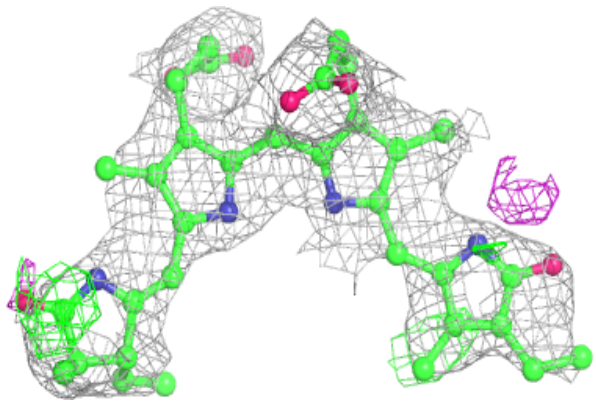


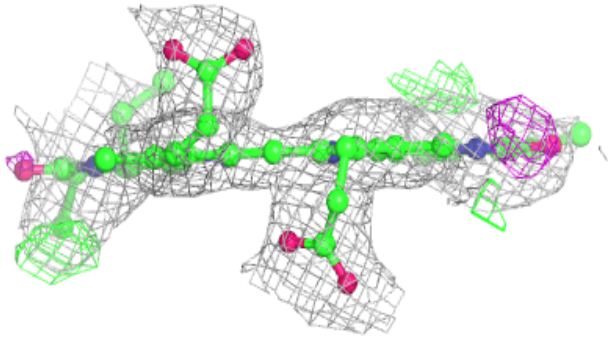


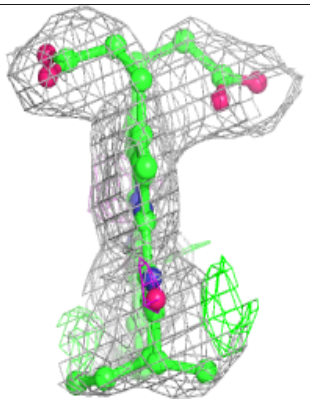


Electron density around BLA B 255:

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

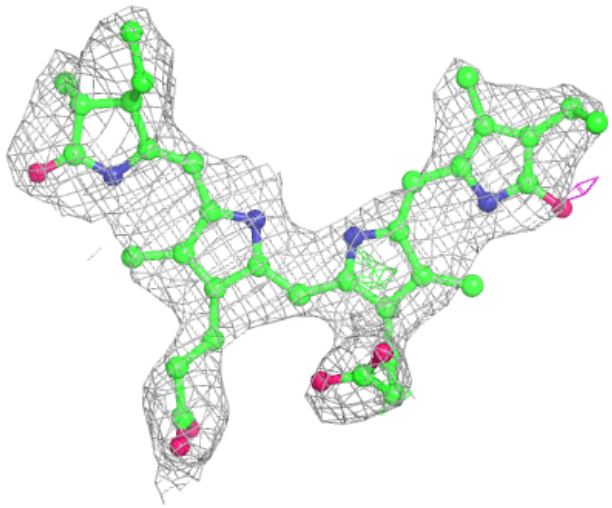


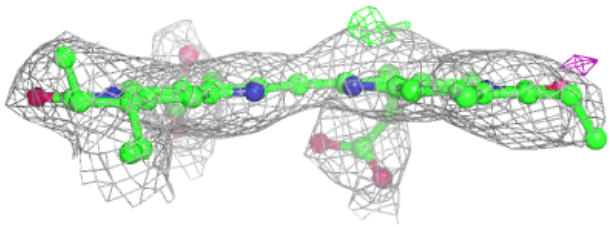


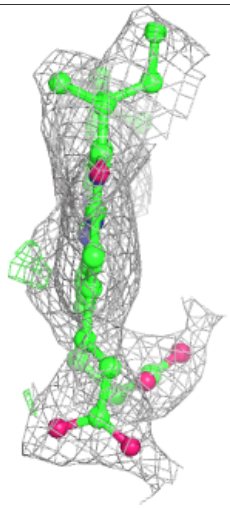


Electron density around CYC R 184:

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

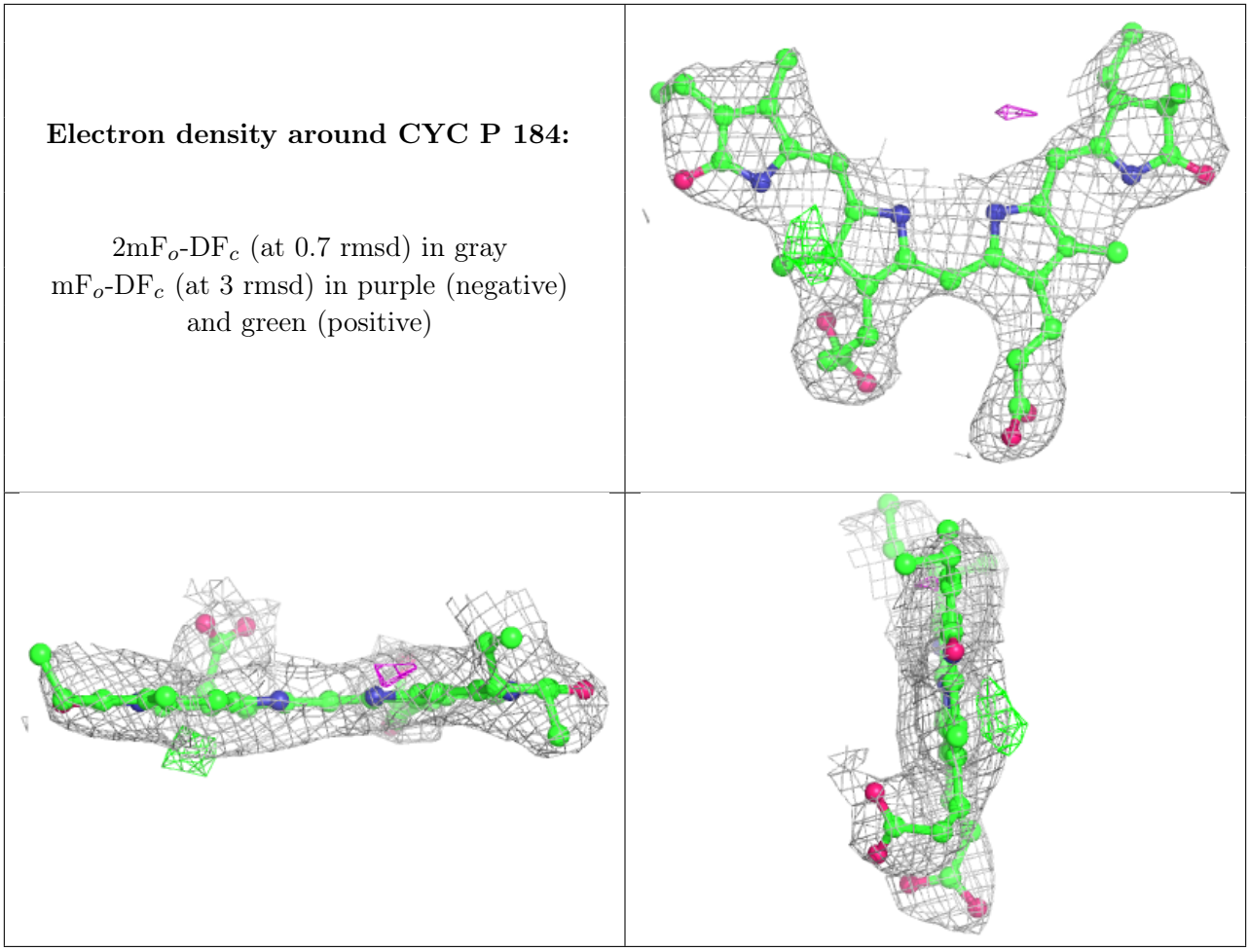






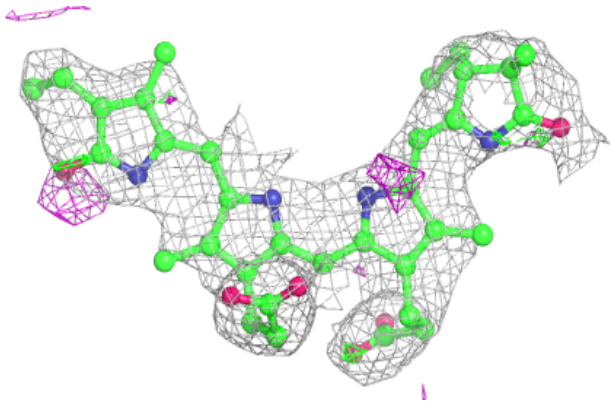
Electron density around CYC P 184:

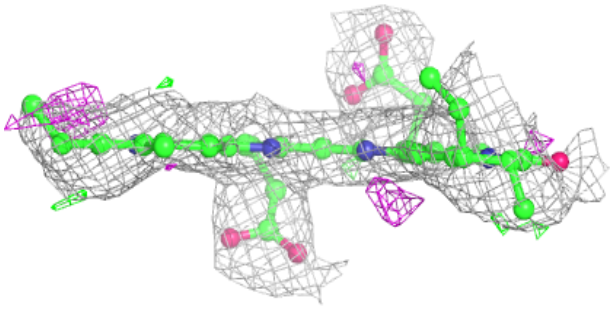
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

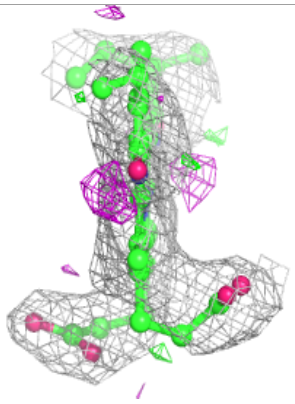


Electron density around CYC T 255:

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

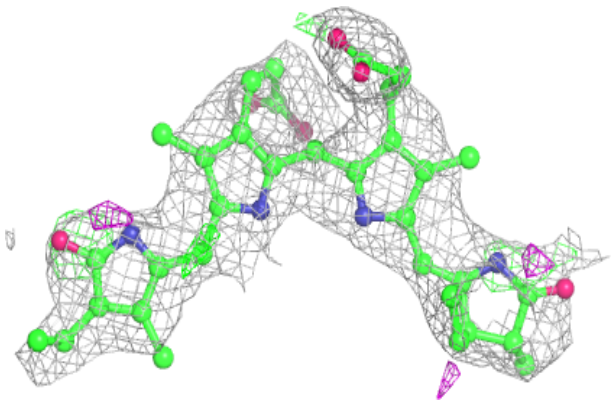


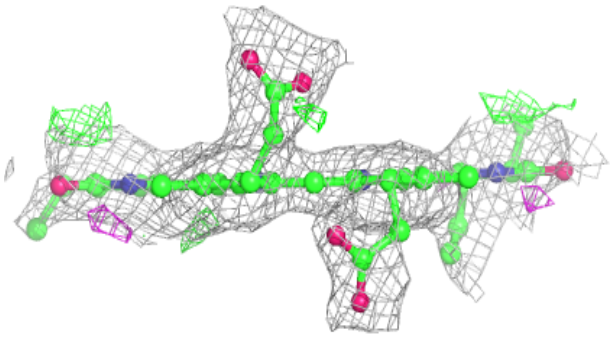


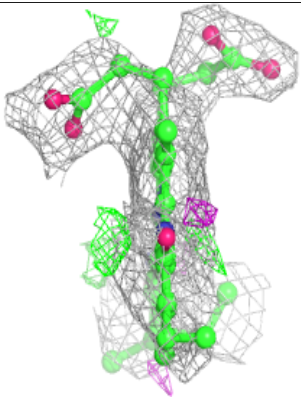


Electron density around CYC P 255:

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

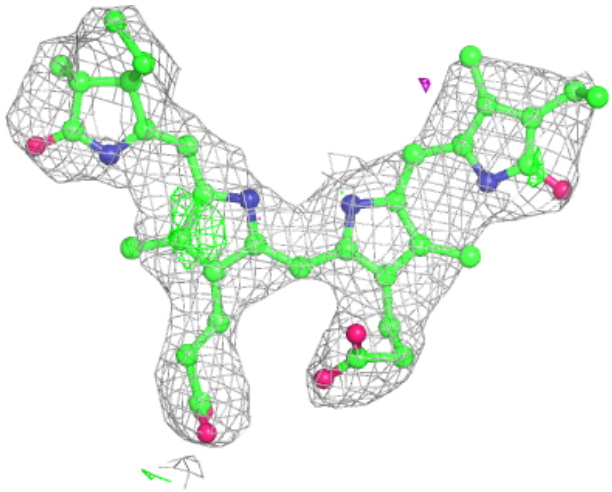


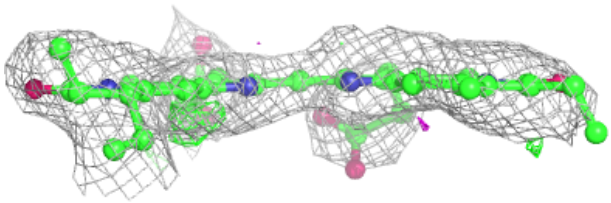


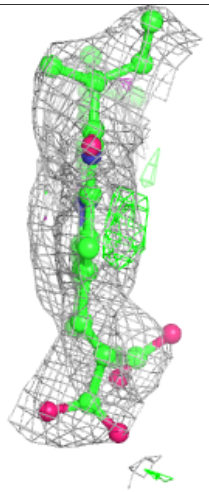


Electron density around CYC J 184:

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

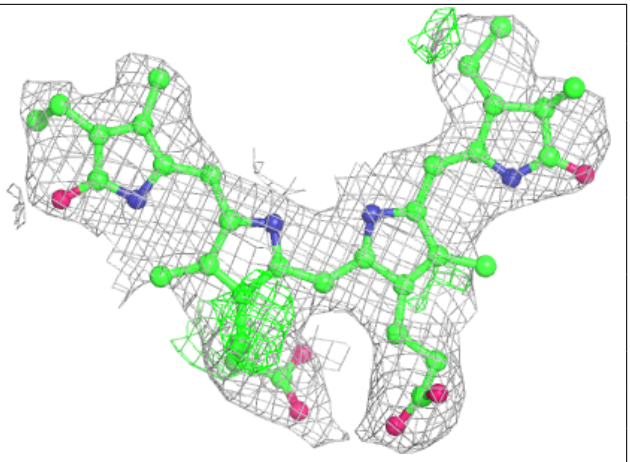


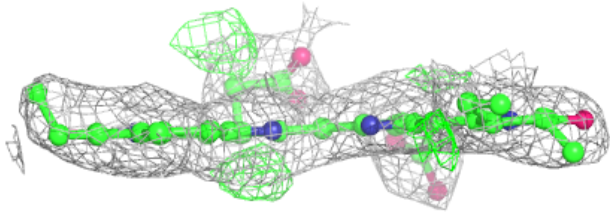


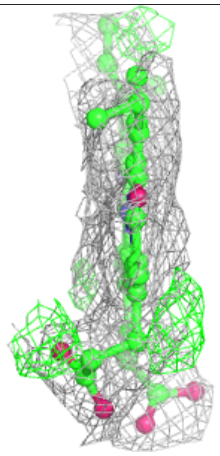


Electron density around CYC I 184:

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

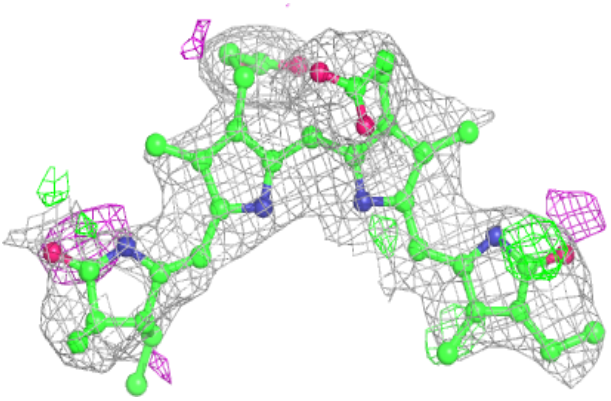


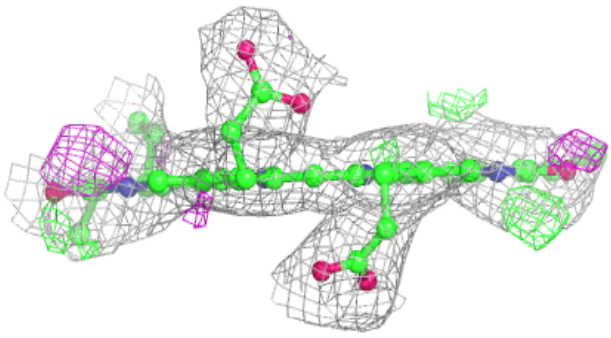


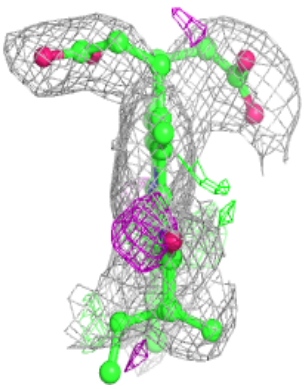


Electron density around CYC F 255:

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

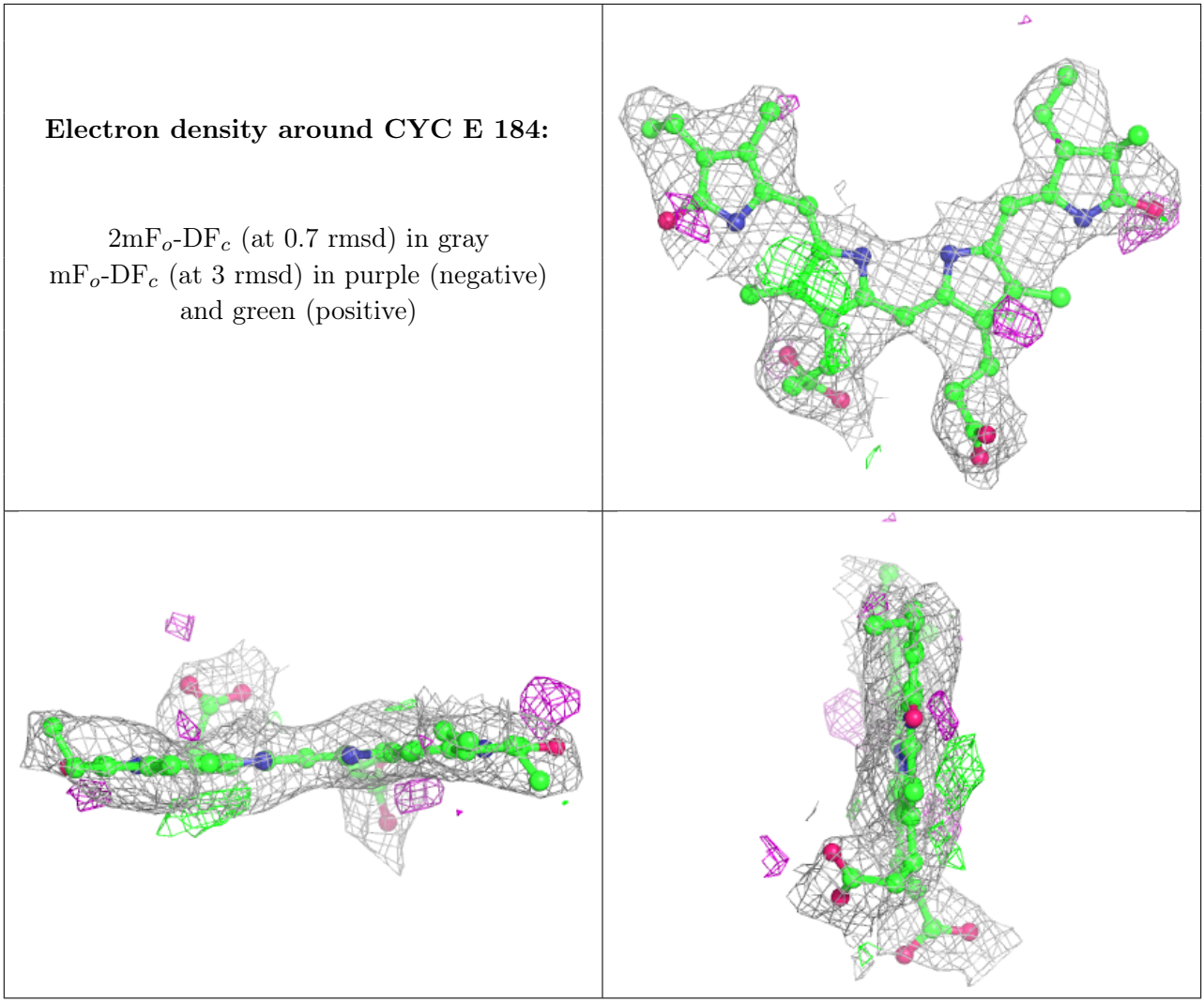






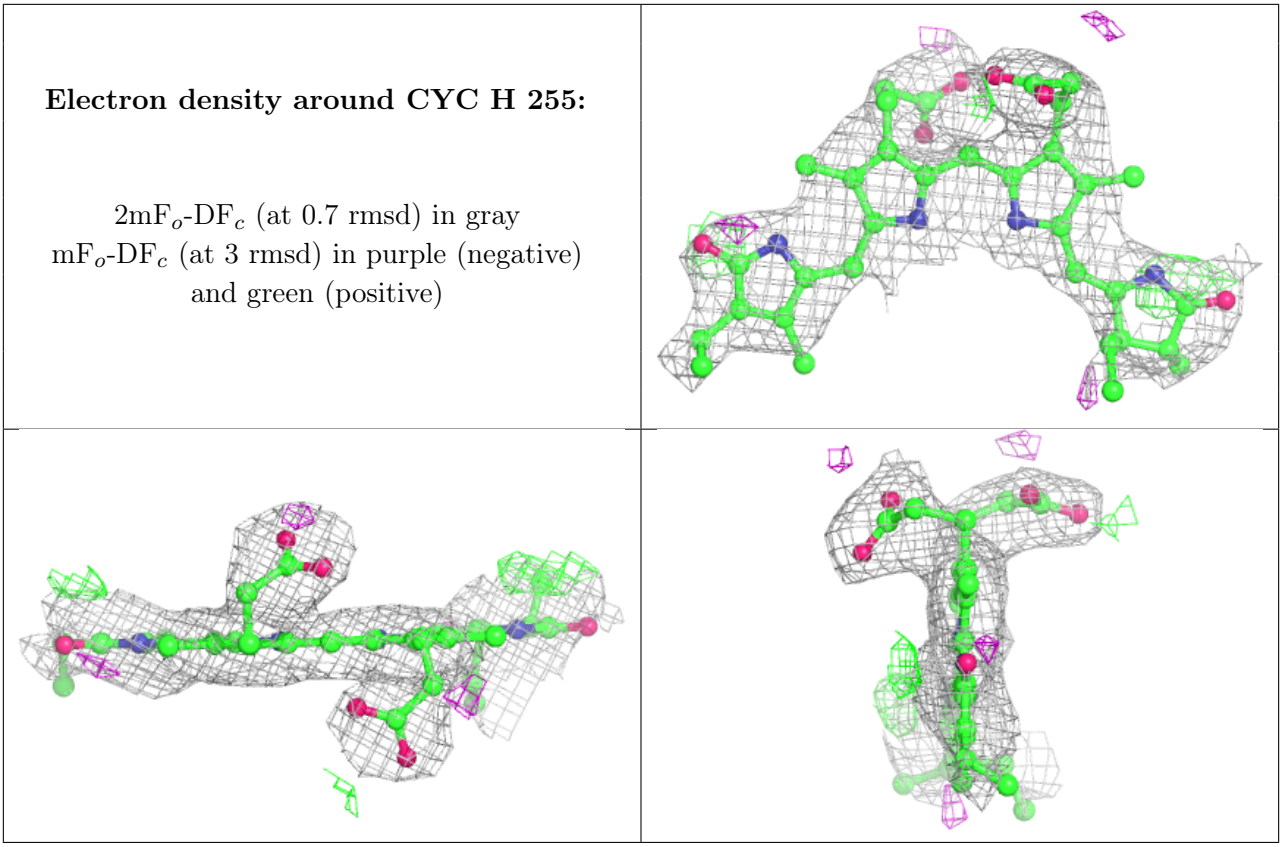
Electron density around CYC E 184:

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



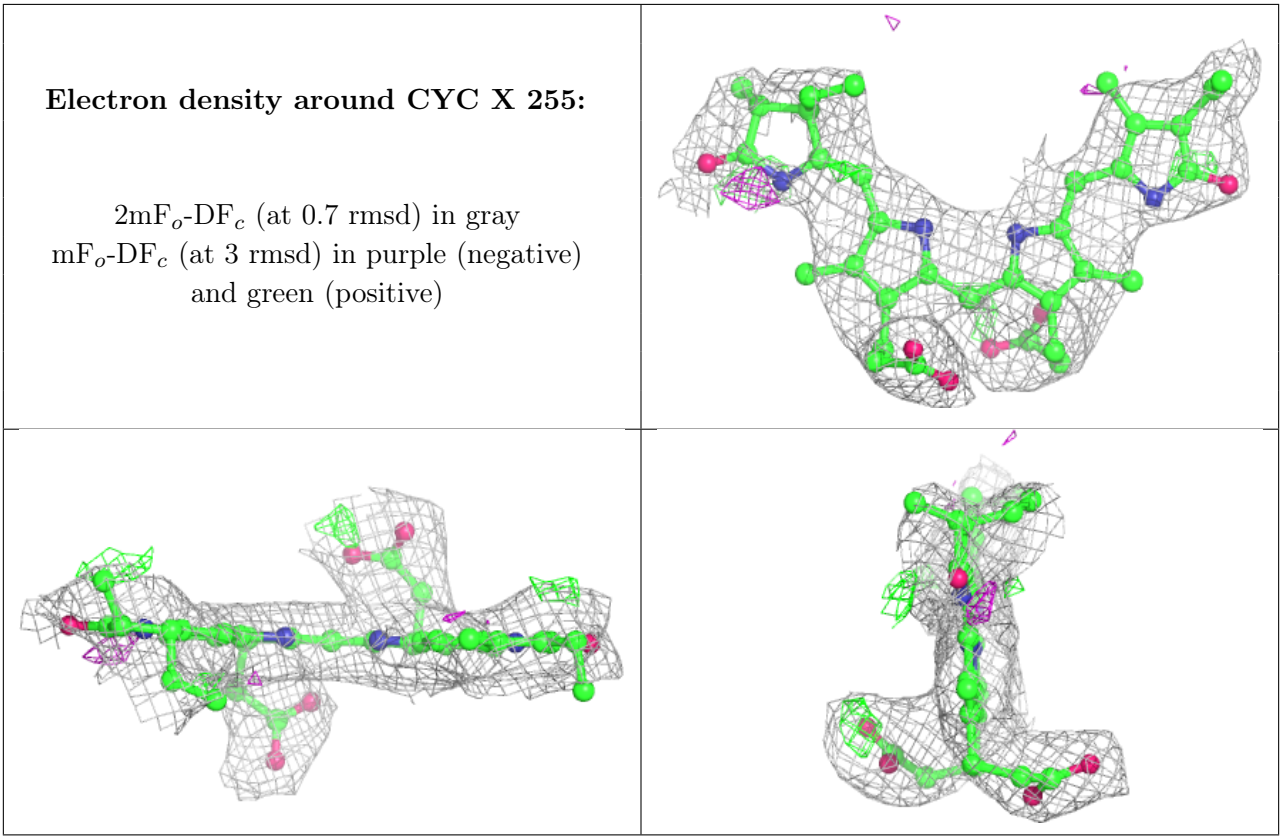
Electron density around CYC H 255:

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



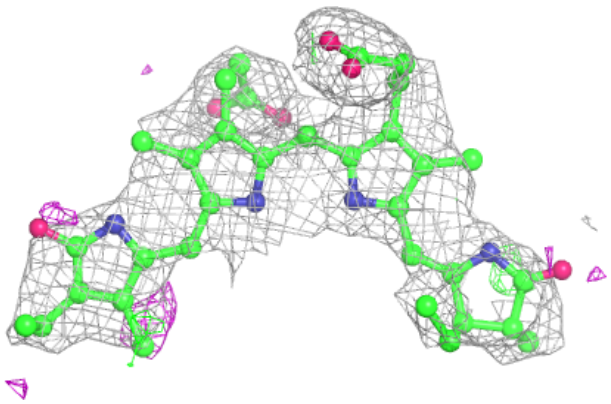
Electron density around CYC X 255:

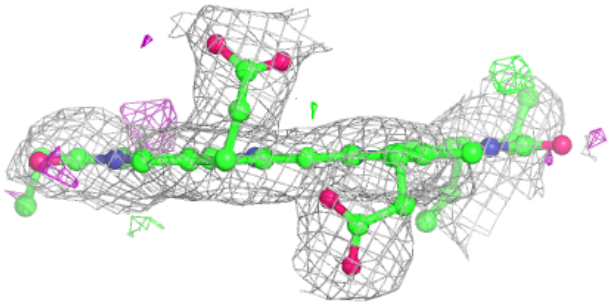
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

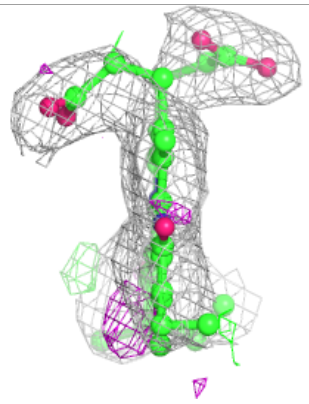


Electron density around CYC L 255:

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

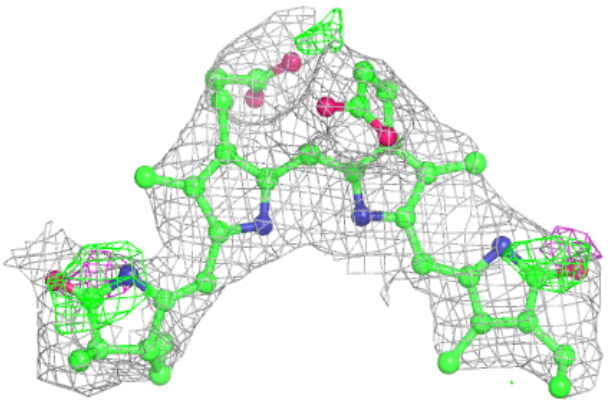


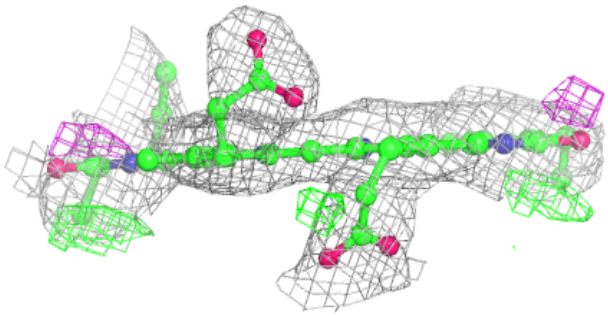


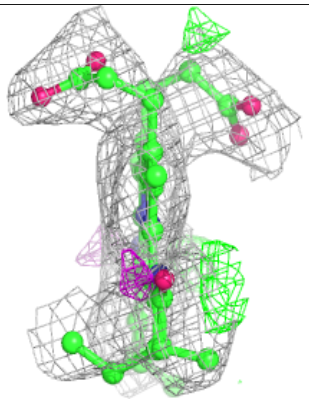


Electron density around CYC R 255:

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

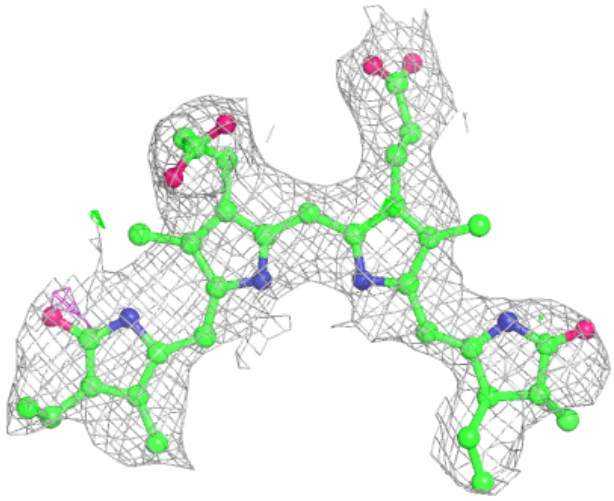


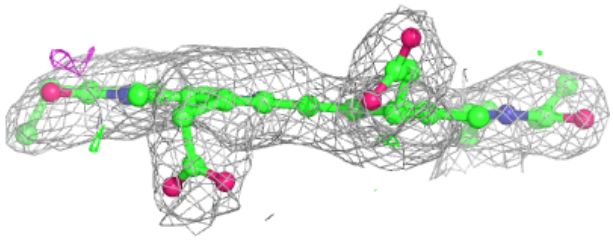


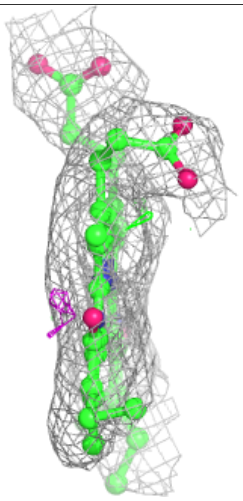


Electron density around CYC M 184:

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

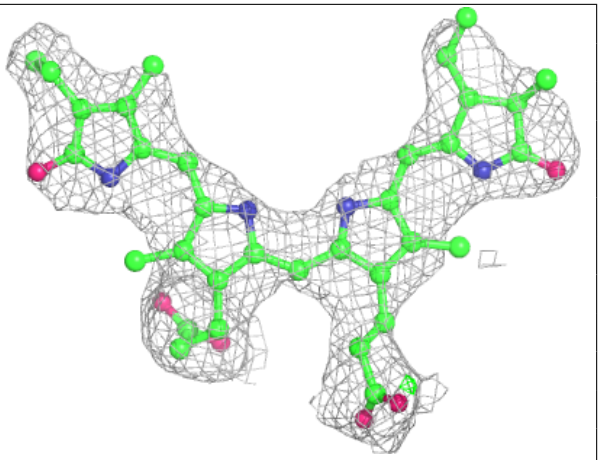


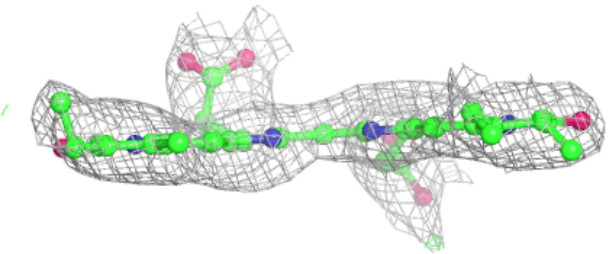


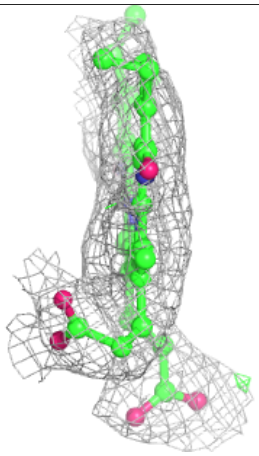


Electron density around CYC Q 184:

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

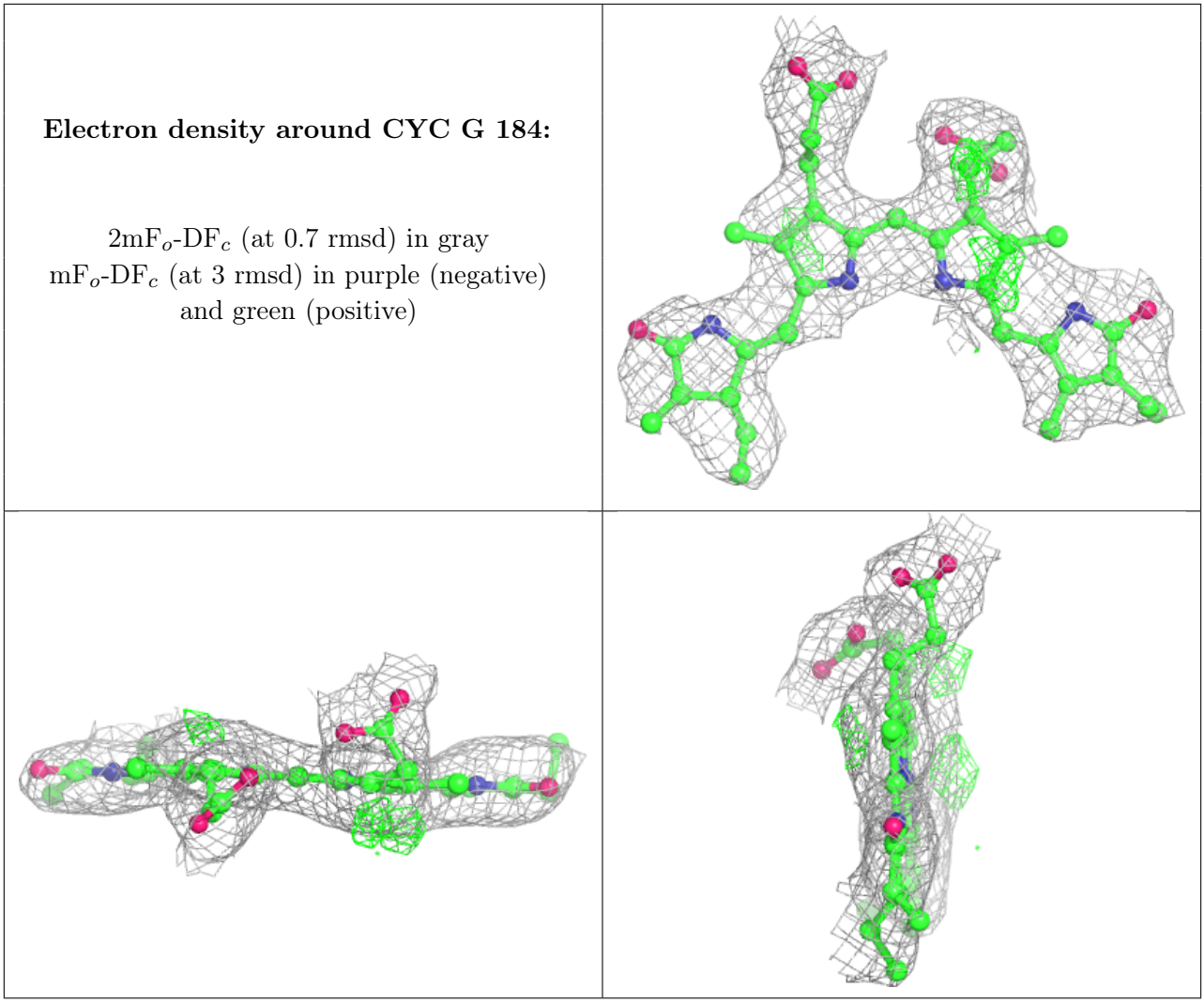






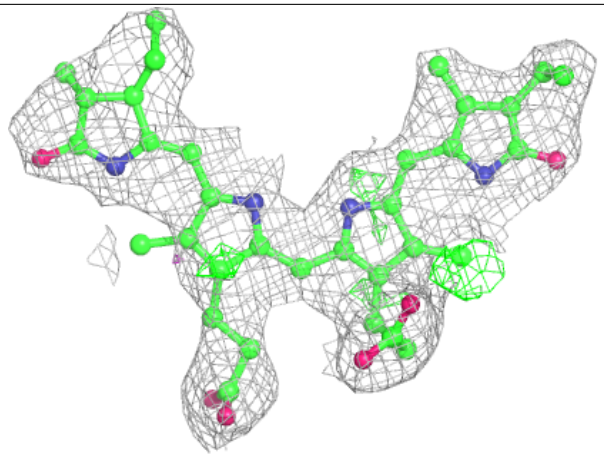
Electron density around CYC G 184:

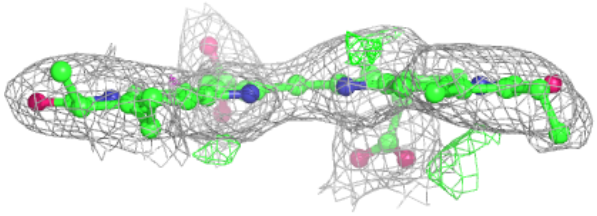
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

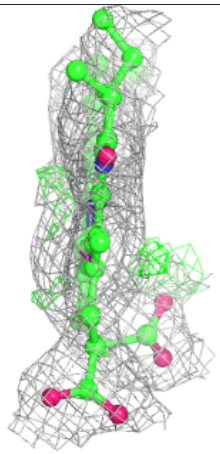


Electron density around CYC O 184:

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

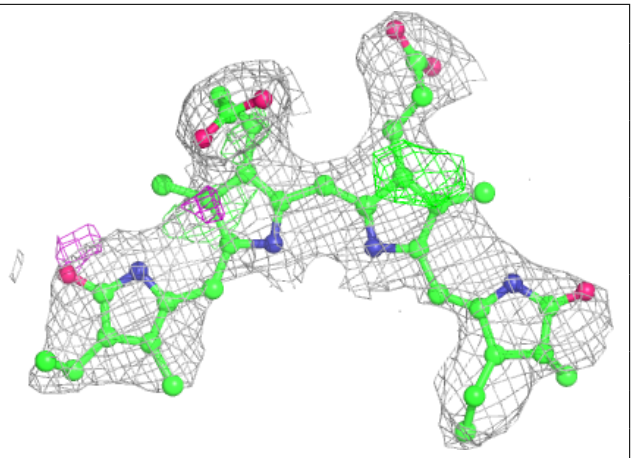


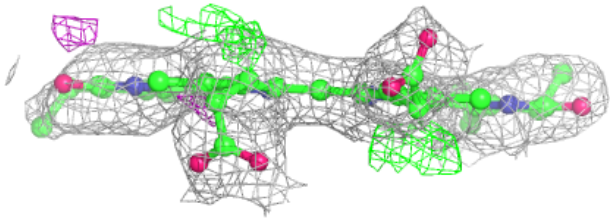




Electron density around CYC W 184:

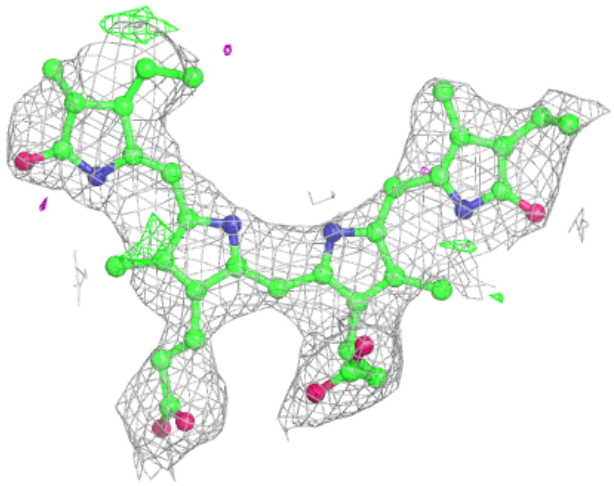
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

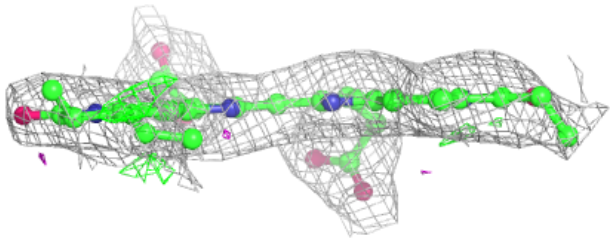


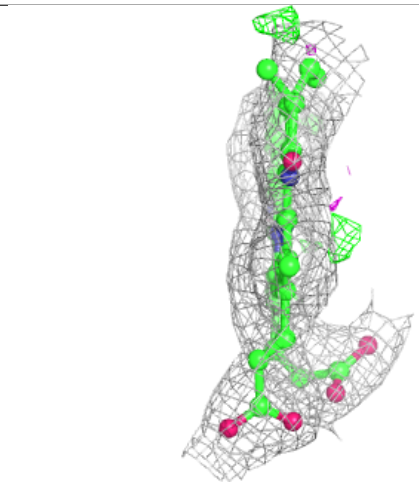


Electron density around CYC K 184:

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

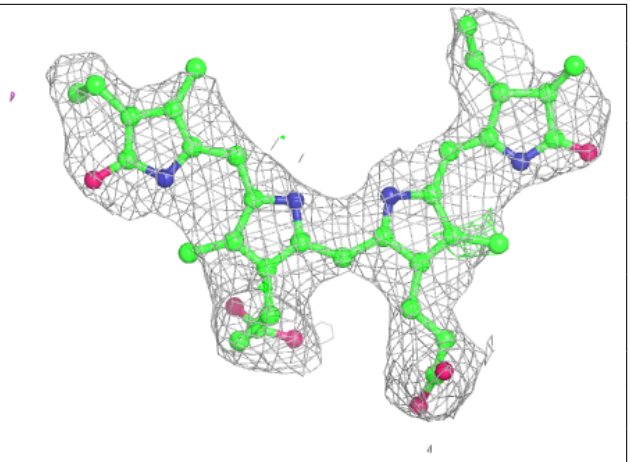


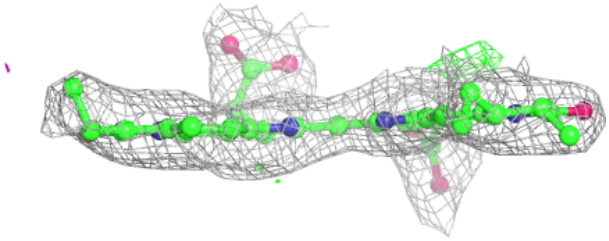


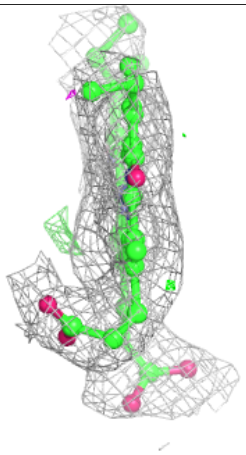


Electron density around CYC A 184:

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

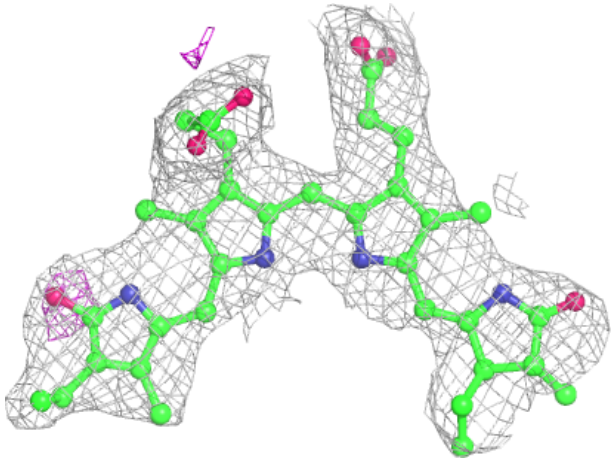


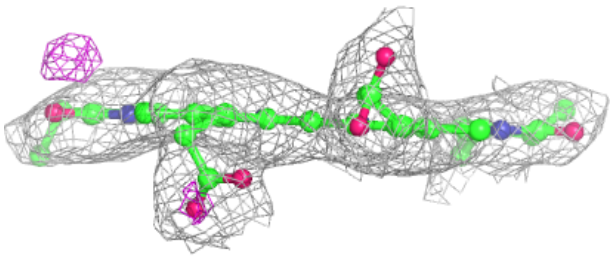


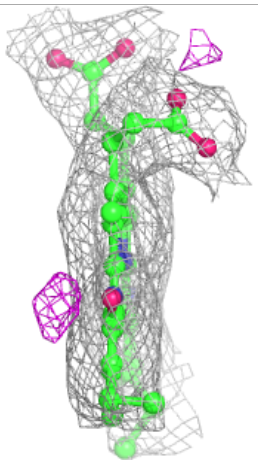


Electron density around CYC U 184:

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

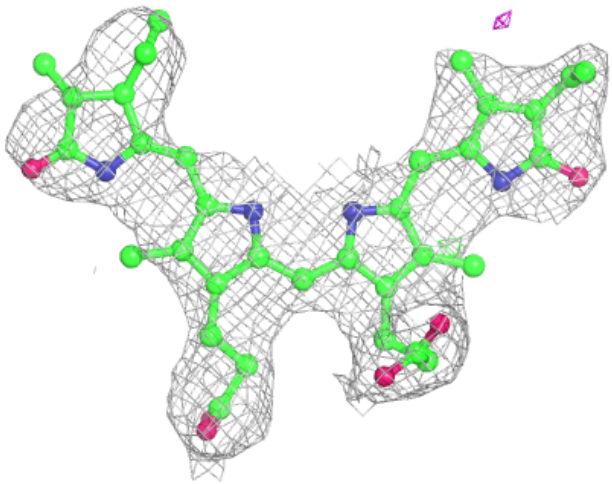


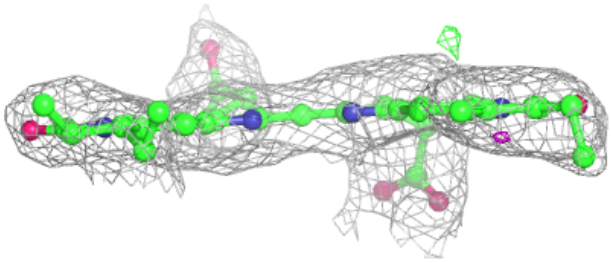


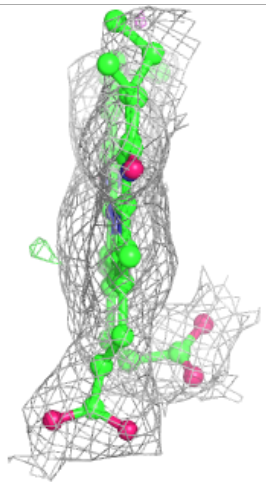


Electron density around CYC C 184:

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

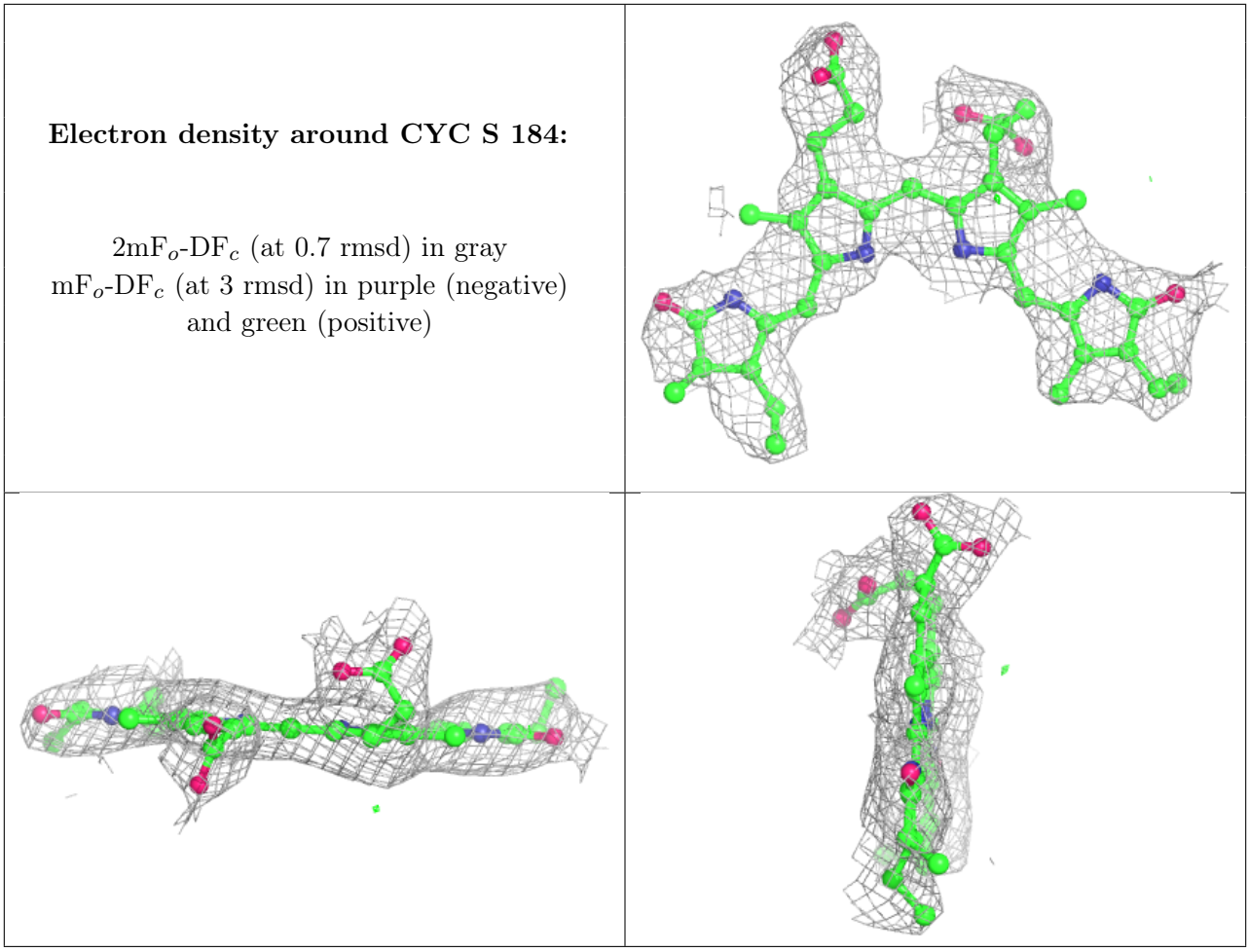






Electron density around CYC S 184:

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



6.5 Other polymers (i)

There are no such residues in this entry.