



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 01:07 AM EDT

PDB ID : 1PYH  
Title : Crystal structure of RC-LH1 core complex from Rhodopseudomonas palustris  
Authors : Roszak, A.W.; Howard, T.D.; Southall, J.; Gardiner, A.T.; Law, C.J.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2003-07-08  
Resolution : 4.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

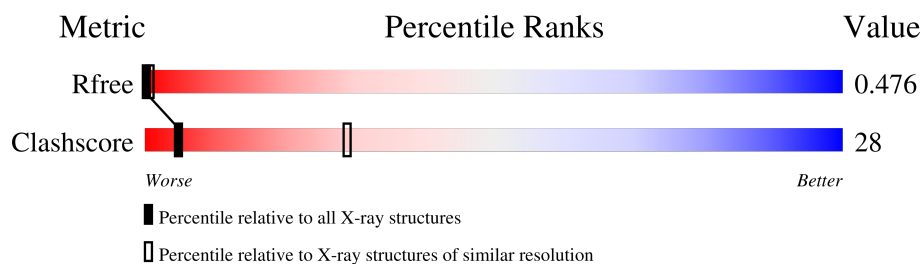
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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.



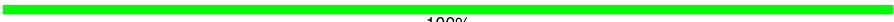













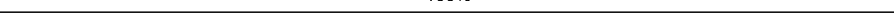

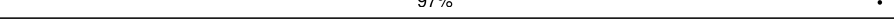
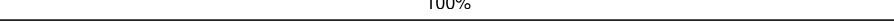
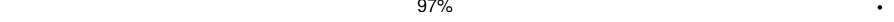
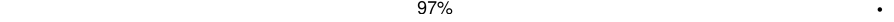
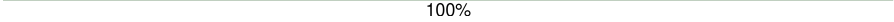
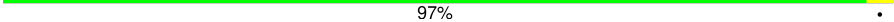
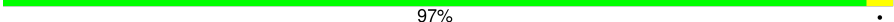

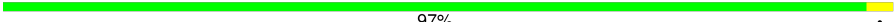
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	281	99% .
2	B	302	99% .
3	C	241	96% .
4	1	26	96% .
4	3	26	96% .
4	5	26	96% .
4	7	26	96% .
4	D	26	100%
4	F	26	92% 8%

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Mol	Chain	Length	Quality of chain
4	H	26	 100%
4	J	26	 88% 12%
4	L	26	 92% 8%
4	N	26	 100%
4	P	26	 100%
4	R	26	 96% .
4	T	26	 96% .
4	V	26	 85% 15%
4	X	26	 100%
4	Z	26	 92% 8%
5	2	30	 100%
5	4	30	 100%
5	6	30	 100%
5	8	30	 100%
5	E	30	 87% 13%
5	G	30	 97% .
5	I	30	 100%
5	K	30	 97% .
5	M	30	 97% .
5	O	30	 100%
5	Q	30	 97% .
5	S	30	 97% .
5	U	30	 100%
5	W	30	 97% .
5	Y	30	 93% 7%

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	BCL	1	38	-	-	-	X
6	BCL	5	38	-	-	-	X
6	BCL	6	36	-	-	-	X
6	BCL	7	38	-	-	-	X
6	BCL	8	36	-	-	-	X
6	BCL	A	301	-	-	-	X
6	BCL	A	302	-	-	-	X
6	BCL	B	303	-	-	-	X
6	BCL	B	304	-	-	-	X
6	BCL	D	2	-	-	-	X
6	BCL	E	1	-	-	-	X
6	BCL	F	4	-	-	-	X
6	BCL	I	5	-	-	-	X
6	BCL	J	8	-	-	X	-
6	BCL	L	10	-	-	X	-
6	BCL	N	38	-	-	X	-
6	BCL	P	38	-	-	X	-
6	BCL	P	39	-	-	X	-
6	BCL	S	36	-	-	-	X
6	BCL	U	36	-	-	-	X
6	BCL	V	38	-	-	-	X
6	BCL	W	36	-	-	-	X
6	BCL	Y	37	-	-	-	X
7	BPH	A	401	-	-	-	X
7	BPH	B	402	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	0	0	0
			1373	811	281	281			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	0	0	0
			1474	870	302	302			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	0	0	0
			1182	700	241	241			

- Molecule 4 is a protein called Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	F	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	H	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	J	26	Total	C	N	O	0	0	0
			127	75	26	26			
4	L	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	N	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	P	26	Total	C	N	O	0	0	0
			128	76	26	26			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	26	Total 128	C 76	N 26	O 26	0	0	0
4	T	26	Total 128	C 76	N 26	O 26	0	0	0
4	V	26	Total 128	C 76	N 26	O 26	0	0	0
4	X	26	Total 127	C 75	N 26	O 26	0	0	0
4	Z	26	Total 128	C 76	N 26	O 26	0	0	0
4	1	26	Total 128	C 76	N 26	O 26	0	0	0
4	3	26	Total 128	C 76	N 26	O 26	0	0	0
4	5	26	Total 128	C 76	N 26	O 26	0	0	0
4	7	26	Total 128	C 76	N 26	O 26	0	0	0

- Molecule 5 is a protein called Light-harvesting protein B-800/850, beta chain.

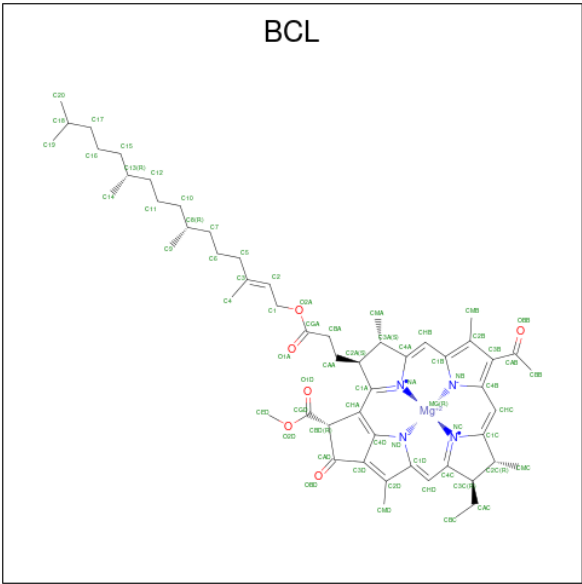
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	30	Total 148	C 88	N 30	O 30	0	0	0
5	G	30	Total 148	C 88	N 30	O 30	0	0	0
5	I	30	Total 148	C 88	N 30	O 30	0	0	0
5	K	30	Total 148	C 88	N 30	O 30	0	0	0
5	M	30	Total 148	C 88	N 30	O 30	0	0	0
5	O	30	Total 148	C 88	N 30	O 30	0	0	0
5	Q	30	Total 148	C 88	N 30	O 30	0	0	0
5	S	30	Total 148	C 88	N 30	O 30	0	0	0
5	U	30	Total 148	C 88	N 30	O 30	0	0	0
5	W	30	Total 148	C 88	N 30	O 30	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	2	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	4	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	6	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	8	30	Total	C	N	O	0	0	0
			148	88	30	30			

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
6	D	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
6	E	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	G	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	H	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	I	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	J	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	K	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	R	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	S	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	T	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	U	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	V	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	W	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

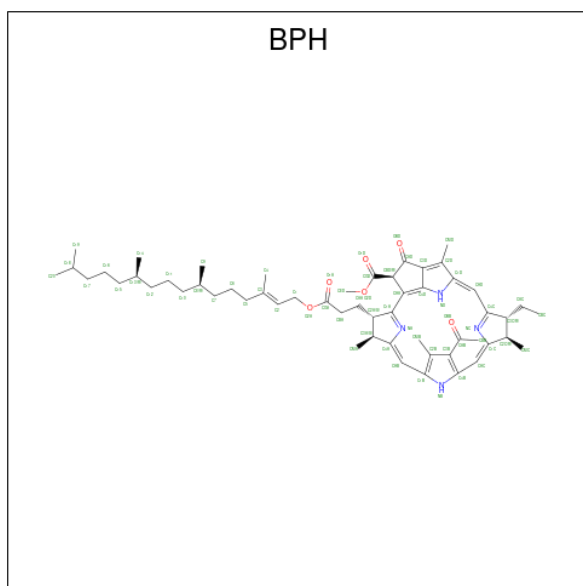
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
6	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			65	55	4	6		
7	B	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

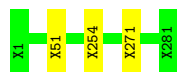
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Fe 1	0	0

### 3 Residue-property plots

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.

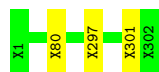
- Molecule 1: Reaction center protein L chain

Chain A:  99% .



- Molecule 2: Reaction center protein M chain

Chain B:  99% .



- Molecule 3: Reaction center protein H chain

Chain C:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain F:  92% 8%




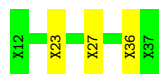
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain H:  100%

There are no outlier residues recorded for this chain.

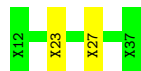
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain J:  88% 12%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain L:  92% 8%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain N:  100%

There are no outlier residues recorded for this chain.

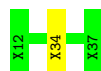
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain R:  96% .




- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain T:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain V:  85% 15%



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain Z:  92% 8%



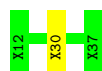
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 1:  96% .



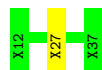
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 3:  96% .



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 5:  96% .




- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 7:  96% .



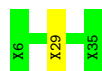
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain E:  87% 13%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain G:  97% .



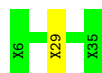
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain K:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain M:  97%



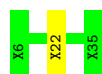
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain O:  100%

There are no outlier residues recorded for this chain.

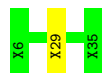
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Q:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain S:  97%



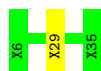
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain U:  100%

There are no outlier residues recorded for this chain.

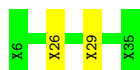
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain W:  97%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Y:  93% 7%



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 2:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 4:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 6:  100%

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 8:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.04Å 119.02Å 130.43Å 69.32° 72.69° 66.52°	Depositor
Resolution (Å)	60.00 – 4.80 59.99 – 4.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (60.00-4.80) 97.3 (59.99-4.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 4.86Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.467 , 0.491 0.454 , 0.476	Depositor DCC
$R_{free}$ test set	944 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	202.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.03 , 999.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, BCL, FE

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	257	10	0
2	B	1474	0	274	2	0
3	C	1182	0	230	13	0
4	1	128	0	26	2	0
4	3	128	0	26	1	0
4	5	128	0	26	1	0
4	7	128	0	26	2	0
4	D	128	0	26	0	0
4	F	128	0	26	7	0
4	H	128	0	26	0	0
4	J	127	0	25	7	0
4	L	128	0	26	3	0
4	N	128	0	26	0	0
4	P	128	0	26	0	0
4	R	128	0	26	1	0
4	T	128	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	128	0	26	5	0
4	X	127	0	25	0	0
4	Z	128	0	26	4	0
5	2	148	0	30	0	0
5	4	148	0	30	0	0
5	6	148	0	30	0	0
5	8	148	0	30	0	0
5	E	148	0	30	11	0
5	G	148	0	30	3	0
5	I	148	0	30	0	0
5	K	148	0	30	4	0
5	M	148	0	30	1	0
5	O	148	0	30	0	0
5	Q	148	0	30	5	0
5	S	148	0	30	1	0
5	U	148	0	30	0	0
5	W	148	0	30	2	0
5	Y	148	0	30	4	0
6	1	47	0	34	18	0
6	2	47	0	34	10	0
6	3	94	0	68	15	0
6	5	47	0	33	12	0
6	6	47	0	34	3	0
6	7	47	0	34	8	0
6	8	47	0	34	5	0
6	A	132	0	148	9	0
6	B	132	0	148	6	0
6	D	47	0	34	14	0
6	E	47	0	34	14	0
6	F	47	0	34	7	0
6	G	47	0	34	11	0
6	H	47	0	33	11	0
6	I	47	0	34	6	0
6	J	47	0	33	32	0
6	K	47	0	34	18	0
6	L	47	0	34	25	0
6	M	47	0	34	13	0
6	N	94	0	68	39	0
6	P	94	0	68	51	0
6	R	47	0	34	16	0
6	S	47	0	34	10	0
6	T	47	0	34	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	47	0	34	8	0
6	V	47	0	34	8	0
6	W	47	0	34	6	0
6	Y	94	0	68	23	0
7	A	65	0	76	5	0
7	B	65	0	76	0	0
8	B	1	0	0	0	0
All	All	10100	0	3090	367	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (367) 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)
6:N:38:BCL:HMC3	6:P:38:BCL:CBB	1.44	1.47
6:H:6:BCL:C1	6:H:6:BCL:O2A	1.63	1.46
6:R:38:BCL:C1	6:R:38:BCL:O2A	1.63	1.42
6:P:38:BCL:CBC	6:P:39:BCL:HMD2	1.56	1.33
6:L:10:BCL:CMB	6:N:11:BCL:HMA1	1.64	1.26
6:N:38:BCL:CMC	6:P:38:BCL:HBB2	1.63	1.25
5:G:29:UNK:CB	6:G:3:BCL:HMD3	1.67	1.22
1:A:271:UNK:HA	4:V:37:UNK:CB	1.68	1.21
6:T:38:BCL:CBB	6:T:38:BCL:HHC	1.71	1.18
6:R:38:BCL:CBB	6:R:38:BCL:HHC	1.70	1.18
6:N:11:BCL:HBC1	6:N:38:BCL:HAC2	1.26	1.18
6:L:10:BCL:HMB3	6:N:11:BCL:CMA	1.74	1.17
6:3:39:BCL:CBB	6:3:39:BCL:HHC	1.70	1.17
6:P:39:BCL:CBB	6:P:39:BCL:HHC	1.70	1.17
6:D:2:BCL:CBB	6:D:2:BCL:HHC	1.71	1.16
6:5:38:BCL:CBB	6:5:38:BCL:HHC	1.70	1.16
6:J:8:BCL:HMA1	6:M:36:BCL:HMA1	1.27	1.14
6:P:38:BCL:HBC2	6:P:39:BCL:CMD	1.76	1.14
6:L:10:BCL:H2A	6:L:10:BCL:HED3	1.27	1.14
6:Y:37:BCL:CBB	6:Y:37:BCL:HHC	1.71	1.13
6:F:4:BCL:CBB	6:F:4:BCL:HHC	1.71	1.13
6:W:36:BCL:CBB	6:W:36:BCL:HHC	1.71	1.12
6:R:38:BCL:HHC	6:R:38:BCL:HBB2	1.13	1.12
6:D:2:BCL:HHC	6:D:2:BCL:HBB2	1.14	1.12
6:T:38:BCL:HHC	6:T:38:BCL:HBB2	1.14	1.12
6:L:10:BCL:HBB2	6:L:10:BCL:HHC	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:8:BCL:CBB	6:J:8:BCL:HHC	1.70	1.11
1:A:254:UNK:HA	4:Z:37:UNK:CB	1.79	1.11
6:P:38:BCL:CBC	6:P:39:BCL:CMD	2.28	1.11
6:7:38:BCL:HHC	6:7:38:BCL:HBB2	1.14	1.11
6:L:10:BCL:HHC	6:L:10:BCL:CBB	1.70	1.11
6:7:38:BCL:HHC	6:7:38:BCL:CBB	1.71	1.11
6:1:38:BCL:CBB	6:1:38:BCL:HHC	1.70	1.11
6:J:8:BCL:C1	6:J:8:BCL:CED	2.28	1.10
6:N:38:BCL:CBB	6:N:38:BCL:HHC	1.71	1.10
6:F:4:BCL:HHC	6:F:4:BCL:HBB2	1.14	1.10
6:N:38:BCL:HMA1	6:P:38:BCL:HMA1	1.32	1.09
6:W:36:BCL:HHC	6:W:36:BCL:HBB2	1.13	1.09
6:1:38:BCL:HHC	6:1:38:BCL:HBB2	1.12	1.09
6:P:39:BCL:HHC	6:P:39:BCL:HBB2	1.14	1.09
6:J:8:BCL:HHC	6:J:8:BCL:HBB2	1.13	1.09
6:H:6:BCL:HHC	6:H:6:BCL:HBB2	1.14	1.08
6:Y:36:BCL:HBA1	6:Y:36:BCL:CED	1.81	1.08
6:5:38:BCL:HHC	6:5:38:BCL:HBB2	1.13	1.08
6:H:6:BCL:HHC	6:H:6:BCL:CBB	1.71	1.08
6:3:39:BCL:HHC	6:3:39:BCL:HBB2	1.12	1.08
6:J:8:BCL:CBC	6:K:36:BCL:CBC	2.31	1.07
6:Y:37:BCL:HHC	6:Y:37:BCL:HBB2	1.14	1.07
6:N:38:BCL:HHC	6:N:38:BCL:HBB2	1.13	1.07
6:H:6:BCL:HBB2	6:H:6:BCL:CHC	1.86	1.06
6:T:38:BCL:HBB2	6:T:38:BCL:CHC	1.85	1.06
6:W:36:BCL:HBB2	6:W:36:BCL:CHC	1.85	1.05
6:1:38:BCL:HBB2	6:1:38:BCL:CHC	1.84	1.05
6:5:38:BCL:HBB2	6:5:38:BCL:CHC	1.84	1.05
6:7:38:BCL:HBB2	6:7:38:BCL:CHC	1.85	1.05
6:R:38:BCL:HBB2	6:R:38:BCL:CHC	1.85	1.05
6:J:8:BCL:HBB2	6:J:8:BCL:CHC	1.85	1.05
6:L:10:BCL:HBB2	6:L:10:BCL:CHC	1.85	1.05
6:D:2:BCL:HBB2	6:D:2:BCL:CHC	1.86	1.05
6:Y:37:BCL:HBB2	6:Y:37:BCL:CHC	1.85	1.05
6:F:4:BCL:HBB2	6:F:4:BCL:CHC	1.86	1.05
6:3:39:BCL:HBB2	6:3:39:BCL:CHC	1.84	1.05
6:J:8:BCL:HBC2	6:K:36:BCL:HBC2	1.36	1.04
6:P:39:BCL:HBB2	6:P:39:BCL:CHC	1.85	1.04
6:J:8:BCL:HMA1	6:M:36:BCL:CMA	1.87	1.04
6:P:38:BCL:HBC1	6:P:39:BCL:HHH	1.36	1.04
6:J:8:BCL:HBC1	6:K:36:BCL:CBC	1.84	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:38:BCL:HMB3	6:P:38:BCL:HMA3	1.39	1.04
6:N:38:BCL:HBB2	6:N:38:BCL:CHC	1.85	1.03
6:L:10:BCL:CMB	6:N:11:BCL:CMA	2.33	1.03
6:J:8:BCL:C1	6:J:8:BCL:HED1	1.87	1.03
6:Y:36:BCL:HBA1	6:Y:36:BCL:HED2	1.38	1.02
6:P:38:BCL:HBC2	6:P:39:BCL:HMD2	1.04	1.02
6:L:10:BCL:HMB3	6:N:11:BCL:HMA1	1.04	1.01
5:G:29:UNK:CB	6:G:3:BCL:CMD	2.39	1.00
7:A:401:BPH:H141	7:A:401:BPH:H171	1.44	0.99
6:R:38:BCL:H3A	6:R:38:BCL:O1A	1.62	0.98
6:R:38:BCL:C1	6:R:38:BCL:CGA	2.41	0.98
6:L:10:BCL:CHD	6:M:36:BCL:HMD2	1.94	0.98
6:H:6:BCL:C1	6:H:6:BCL:CGA	2.41	0.97
6:P:38:BCL:CBC	6:P:39:BCL:HHH	1.96	0.96
6:6:36:BCL:HHC	6:6:36:BCL:HBB3	1.47	0.96
6:3:38:BCL:HBB3	6:3:38:BCL:HHC	1.48	0.95
6:Y:36:BCL:HED2	6:Y:36:BCL:CBA	1.94	0.95
6:3:39:BCL:CBB	6:3:39:BCL:CHC	2.42	0.95
6:7:38:BCL:CBB	6:7:38:BCL:CHC	2.43	0.95
6:D:2:BCL:HMC3	6:G:3:BCL:HBB2	1.47	0.95
6:2:36:BCL:HBB3	6:2:36:BCL:HHC	1.49	0.94
6:V:38:BCL:HHC	6:V:38:BCL:HBB3	1.50	0.94
6:8:36:BCL:HHC	6:8:36:BCL:HBB3	1.48	0.94
6:K:36:BCL:HBB3	6:K:36:BCL:HHC	1.48	0.93
6:U:36:BCL:HBB3	6:U:36:BCL:HHC	1.49	0.93
6:N:11:BCL:HHC	6:N:11:BCL:HBB3	1.48	0.93
6:I:5:BCL:HBB3	6:I:5:BCL:HHC	1.49	0.92
6:E:1:BCL:HHC	6:E:1:BCL:HBB3	1.49	0.92
6:G:3:BCL:HHC	6:G:3:BCL:HBB3	1.50	0.92
6:J:8:BCL:CMA	6:M:36:BCL:HMA1	1.98	0.92
5:E:26:UNK:N	6:E:1:BCL:HED2	1.84	0.92
6:Y:37:BCL:CBB	6:Y:37:BCL:CHC	2.43	0.92
6:M:36:BCL:HBB3	6:M:36:BCL:HHC	1.48	0.92
6:P:38:BCL:HED2	5:Q:22:UNK:HA	1.51	0.92
6:R:38:BCL:CBB	6:R:38:BCL:CHC	2.43	0.91
3:C:52:UNK:HA	4:F:13:UNK:CB	2.00	0.91
6:U:36:BCL:CGD	6:U:36:BCL:HBA1	2.00	0.91
6:Y:36:BCL:HHC	6:Y:36:BCL:HBB3	1.50	0.91
6:N:38:BCL:HMA1	6:P:38:BCL:CMA	2.00	0.91
6:S:36:BCL:HHC	6:S:36:BCL:HBB3	1.49	0.91
6:P:38:BCL:HBC3	6:P:39:BCL:HMD2	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:2:BCL:CBB	6:D:2:BCL:CHC	2.44	0.89
6:P:38:BCL:HBB3	6:P:38:BCL:HHC	1.50	0.89
6:N:38:BCL:HMC3	6:P:38:BCL:HBB1	1.53	0.88
6:J:8:BCL:CBC	6:K:36:BCL:HBC2	1.99	0.88
6:T:38:BCL:CBB	6:T:38:BCL:CHC	2.43	0.88
5:E:22:UNK:O	6:E:1:BCL:HED1	1.73	0.87
6:Y:36:BCL:HBA1	6:Y:36:BCL:O2D	1.74	0.87
1:A:51:UNK:CB	4:7:36:UNK:CB	2.54	0.86
6:J:8:BCL:HBC1	6:K:36:BCL:CAC	2.05	0.85
6:N:38:BCL:CMA	6:P:38:BCL:HMA1	2.06	0.85
5:E:22:UNK:O	6:E:1:BCL:CED	2.25	0.85
3:C:51:UNK:O	4:F:13:UNK:CB	2.25	0.85
1:A:271:UNK:CA	4:V:37:UNK:CB	2.54	0.84
6:J:8:BCL:CBC	6:K:36:BCL:HBC1	2.07	0.84
6:P:38:BCL:HAC2	6:P:39:BCL:HBC2	1.59	0.83
6:1:38:BCL:CBB	6:1:38:BCL:CHC	2.42	0.83
3:C:10:UNK:O	4:J:36:UNK:CB	2.26	0.82
6:N:38:BCL:HMC3	6:P:38:BCL:HBB2	0.83	0.82
6:U:36:BCL:HBA1	6:U:36:BCL:O2D	1.78	0.82
6:J:8:BCL:HBC1	6:K:36:BCL:HAC2	1.59	0.81
6:N:38:BCL:CMC	6:P:38:BCL:CBB	2.40	0.81
6:N:38:BCL:CBB	6:N:38:BCL:CHC	2.43	0.81
6:J:8:BCL:HBC1	6:K:36:BCL:HBC1	1.60	0.81
6:Y:36:BCL:HBA1	6:Y:36:BCL:CGD	2.10	0.80
6:1:38:BCL:HMC3	6:3:38:BCL:HBB1	1.62	0.80
6:W:36:BCL:CBB	6:W:36:BCL:CHC	2.43	0.79
6:H:6:BCL:CBB	6:H:6:BCL:CHC	2.43	0.78
6:P:39:BCL:HHC	6:P:39:BCL:HBB3	1.66	0.77
6:P:38:BCL:CBB	6:P:38:BCL:HHC	2.11	0.77
6:1:38:BCL:HHC	6:1:38:BCL:HBB3	1.67	0.77
6:I:5:BCL:HBA2	6:I:5:BCL:CGD	2.15	0.76
6:W:36:BCL:HHC	6:W:36:BCL:HBB3	1.68	0.76
3:C:51:UNK:C	4:F:13:UNK:CB	2.63	0.76
6:L:10:BCL:CBB	6:L:10:BCL:CHC	2.43	0.76
6:5:38:BCL:CBB	6:5:38:BCL:CHC	2.42	0.76
6:L:10:BCL:HMB1	6:N:11:BCL:CMA	2.15	0.75
5:Y:29:UNK:CB	6:Y:36:BCL:CMD	2.64	0.75
6:L:10:BCL:HHC	6:L:10:BCL:HBB3	1.67	0.75
6:3:39:BCL:HHC	6:3:39:BCL:HBB3	1.66	0.75
4:J:27:UNK:CB	6:J:8:BCL:OBD	2.35	0.75
6:J:8:BCL:HHC	6:J:8:BCL:HBB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:10:BCL:HMB1	6:N:11:BCL:HMA1	1.68	0.75
6:Y:37:BCL:HHC	6:Y:37:BCL:HBB3	1.68	0.75
6:H:6:BCL:HHC	6:H:6:BCL:HBB3	1.67	0.74
6:T:38:BCL:HHC	6:T:38:BCL:HBB3	1.67	0.74
6:R:38:BCL:HHC	6:R:38:BCL:HBB3	1.67	0.74
6:D:2:BCL:HHC	6:D:2:BCL:HBB3	1.68	0.74
3:C:52:UNK:CA	4:F:13:UNK:CB	2.66	0.73
6:7:38:BCL:HHC	6:7:38:BCL:HBB3	1.67	0.73
6:Y:36:BCL:HED2	6:Y:36:BCL:CGA	2.18	0.73
4:L:23:UNK:CB	6:L:10:BCL:HED2	2.19	0.72
6:L:10:BCL:HED3	6:L:10:BCL:C2A	2.15	0.71
6:5:38:BCL:HHC	6:5:38:BCL:HBB3	1.66	0.71
5:Y:29:UNK:CB	6:Y:36:BCL:HMD3	2.20	0.71
6:F:4:BCL:HHC	6:F:4:BCL:HBB3	1.68	0.71
6:P:39:BCL:CBB	6:P:39:BCL:CHC	2.43	0.70
6:I:5:BCL:HBA2	6:I:5:BCL:O2D	1.91	0.70
6:J:8:BCL:CBB	6:J:8:BCL:CHC	2.43	0.70
6:N:38:BCL:HHC	6:N:38:BCL:HBB3	1.67	0.70
6:R:38:BCL:H3A	6:R:38:BCL:CGA	2.17	0.70
6:R:38:BCL:HBC2	6:S:36:BCL:HBC1	1.74	0.70
6:P:39:BCL:O2D	6:P:39:BCL:HBA2	1.92	0.70
6:R:38:BCL:O1A	6:R:38:BCL:C3A	2.37	0.70
6:N:38:BCL:CMB	6:P:38:BCL:HMA3	2.20	0.69
1:A:254:UNK:CB	4:Z:36:UNK:CB	2.71	0.68
6:P:38:BCL:HED1	5:Q:22:UNK:CB	2.23	0.68
6:U:36:BCL:CGD	6:U:36:BCL:CBA	2.71	0.68
6:5:38:BCL:C3A	6:5:38:BCL:O1A	2.42	0.68
6:P:38:BCL:HBC3	6:P:39:BCL:CMD	2.14	0.67
7:A:401:BPH:H141	7:A:401:BPH:C17	2.20	0.67
2:B:297:UNK:O	2:B:301:UNK:N	2.27	0.67
6:5:38:BCL:O1A	6:5:38:BCL:HMA2	1.95	0.67
3:C:54:UNK:O	4:F:14:UNK:CB	2.43	0.67
6:P:38:BCL:HAC2	6:P:39:BCL:CBC	2.25	0.67
6:M:36:BCL:HHC	6:M:36:BCL:CBB	2.24	0.66
6:T:38:BCL:HMA2	6:T:38:BCL:C1	2.25	0.66
3:C:54:UNK:C	4:F:14:UNK:CB	2.73	0.66
6:F:4:BCL:CBB	6:F:4:BCL:CHC	2.44	0.66
6:J:8:BCL:HBC2	6:K:36:BCL:CBC	2.04	0.66
6:E:1:BCL:HHC	6:E:1:BCL:CBB	2.24	0.66
6:U:36:BCL:HBA1	6:U:36:BCL:CBD	2.26	0.66
6:8:36:BCL:HHC	6:8:36:BCL:CBB	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:25:UNK:CB	6:E:1:BCL:HED2	2.25	0.65
6:N:11:BCL:HBC1	6:N:38:BCL:CAC	2.17	0.65
4:1:23:UNK:CB	6:1:38:BCL:CED	2.74	0.65
6:G:3:BCL:HHC	6:G:3:BCL:CBB	2.25	0.65
6:J:8:BCL:C1	6:J:8:BCL:O2D	2.44	0.65
6:1:38:BCL:CMD	6:2:36:BCL:HBC2	2.27	0.64
3:C:10:UNK:O	4:J:36:UNK:CA	2.46	0.64
6:P:38:BCL:HBC2	6:P:39:BCL:C2D	2.25	0.64
6:P:38:BCL:CBC	6:P:39:BCL:CHD	2.75	0.64
6:P:38:BCL:CAC	6:P:39:BCL:HBC2	2.26	0.64
6:2:36:BCL:HHC	6:2:36:BCL:CBB	2.24	0.63
3:C:10:UNK:O	4:J:36:UNK:HA	1.97	0.63
6:U:36:BCL:HBA1	6:U:36:BCL:HBD	1.79	0.63
6:Y:36:BCL:HHC	6:Y:36:BCL:CBB	2.25	0.63
6:D:2:BCL:HMA3	6:G:3:BCL:CMA	2.29	0.63
6:D:2:BCL:O2D	6:D:2:BCL:HBA2	2.00	0.62
6:N:38:BCL:HMB3	6:P:38:BCL:CMA	2.22	0.62
6:S:36:BCL:HHC	6:S:36:BCL:CBB	2.23	0.62
4:R:34:UNK:CB	6:R:38:BCL:HMD3	2.30	0.62
6:1:38:BCL:HMC3	6:3:38:BCL:CBB	2.30	0.62
5:Y:29:UNK:CB	6:Y:36:BCL:HMD1	2.29	0.61
6:V:38:BCL:HHC	6:V:38:BCL:CBB	2.25	0.61
6:5:38:BCL:O1A	6:5:38:BCL:H3A	1.99	0.61
6:Y:36:BCL:CED	6:Y:36:BCL:CBA	2.60	0.61
5:E:22:UNK:O	6:E:1:BCL:HED2	2.00	0.61
6:P:38:BCL:CED	5:Q:22:UNK:CB	2.79	0.61
5:E:25:UNK:CB	6:E:1:BCL:CED	2.78	0.60
6:R:38:BCL:C1	6:R:38:BCL:O1A	2.48	0.60
6:3:38:BCL:HHC	6:3:38:BCL:CBB	2.23	0.60
6:N:38:BCL:CHB	6:P:38:BCL:HMA1	2.31	0.60
6:1:38:BCL:HMD2	6:2:36:BCL:CHD	2.32	0.60
6:H:6:BCL:C1	6:H:6:BCL:O1A	2.49	0.60
5:K:29:UNK:CB	6:K:36:BCL:C2D	2.80	0.60
6:P:39:BCL:HBA2	6:P:39:BCL:CGD	2.32	0.59
6:Y:36:BCL:CED	6:Y:36:BCL:CGA	2.78	0.59
6:1:38:BCL:C1D	6:2:36:BCL:HMD2	2.32	0.59
6:K:36:BCL:HHC	6:K:36:BCL:CBB	2.23	0.59
6:B:303:BCL:CBB	6:B:303:BCL:HMB1	2.33	0.59
7:A:401:BPH:H7C2	7:A:401:BPH:H142	1.85	0.59
1:A:254:UNK:CA	4:Z:37:UNK:CB	2.69	0.59
5:E:29:UNK:CB	6:E:1:BCL:C3D	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:301:BCL:H102	6:B:303:BCL:H171	1.85	0.58
6:N:11:BCL:HHC	6:N:11:BCL:CBB	2.23	0.58
6:B:304:BCL:HMB1	6:B:304:BCL:HBB2	1.85	0.58
6:1:38:BCL:CHC	6:3:38:BCL:HBB2	2.34	0.58
6:I:5:BCL:HHC	6:I:5:BCL:CBB	2.24	0.58
6:U:36:BCL:O2D	6:U:36:BCL:CBA	2.50	0.58
6:U:36:BCL:HHC	6:U:36:BCL:CBB	2.24	0.58
6:1:38:BCL:HMB3	6:3:38:BCL:CHB	2.34	0.58
6:P:38:BCL:HED2	5:Q:22:UNK:CA	2.31	0.57
6:J:8:BCL:C1	6:J:8:BCL:HED3	2.31	0.57
7:A:401:BPH:HBC3	7:A:401:BPH:HHH	1.85	0.57
6:D:2:BCL:HMA3	6:G:3:BCL:HMA1	1.85	0.57
6:P:38:BCL:CBC	6:P:39:BCL:HMD3	2.31	0.57
6:5:38:BCL:O1A	6:5:38:BCL:CMA	2.53	0.57
6:L:10:BCL:HMD2	6:M:36:BCL:C1D	2.35	0.56
6:R:38:BCL:HBC2	6:S:36:BCL:CBC	2.35	0.56
6:7:38:BCL:O1A	6:7:38:BCL:H2A	2.05	0.56
6:Y:37:BCL:O1A	6:Y:37:BCL:HMA2	2.05	0.56
5:E:26:UNK:HA	6:E:1:BCL:OBD	2.06	0.56
4:L:23:UNK:CB	6:L:10:BCL:CED	2.84	0.56
6:N:11:BCL:HBA1	6:N:11:BCL:O2D	2.05	0.56
6:N:38:BCL:HHB	6:P:38:BCL:HMA1	1.89	0.55
6:8:36:BCL:HAA2	6:8:36:BCL:HBD	1.88	0.55
4:J:23:UNK:CB	6:J:8:BCL:HED1	2.36	0.55
6:P:39:BCL:CMA	6:S:36:BCL:HMA1	2.38	0.54
6:2:36:BCL:HAA2	6:2:36:BCL:HBD	1.90	0.54
6:5:38:BCL:H3A	6:5:38:BCL:CGA	2.38	0.54
4:J:23:UNK:CB	6:J:8:BCL:CED	2.85	0.54
5:E:25:UNK:C	6:E:1:BCL:HED2	2.37	0.54
6:6:36:BCL:HHC	6:6:36:BCL:CBB	2.23	0.54
6:P:39:BCL:HMA1	6:S:36:BCL:HMA1	1.89	0.53
3:C:249:UNK:O	3:C:250:UNK:C	2.55	0.53
6:Y:36:BCL:HBD	6:Y:37:BCL:OBD	2.08	0.53
6:T:38:BCL:HMA3	6:V:38:BCL:HMA3	1.91	0.53
6:A:301:BCL:C4	6:A:301:BCL:C7	2.84	0.53
2:B:80:UNK:O	4:T:36:UNK:O	2.27	0.53
4:1:23:UNK:O	6:1:38:BCL:HED2	2.09	0.52
5:E:26:UNK:HA	6:E:1:BCL:CGD	2.38	0.52
6:J:8:BCL:HMA1	6:M:36:BCL:HMA2	1.86	0.52
6:P:38:BCL:HBC2	6:P:39:BCL:HHH	1.89	0.52
6:A:302:BCL:HBB3	6:A:302:BCL:HMB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:10:BCL:C4C	6:M:36:BCL:HMD2	2.40	0.52
6:Y:36:BCL:HAA2	6:Y:37:BCL:OBD	2.10	0.51
6:J:8:BCL:HBB2	6:M:36:BCL:HBB2	1.92	0.51
6:P:38:BCL:HBC2	6:P:39:BCL:CHD	2.38	0.51
6:1:38:BCL:HMD2	6:2:36:BCL:HBC2	1.92	0.51
6:R:38:BCL:CBC	6:S:36:BCL:HBC1	2.41	0.50
6:1:38:BCL:HMD3	6:2:36:BCL:HBC2	1.92	0.50
6:B:303:BCL:HMB1	6:B:303:BCL:HBB3	1.94	0.50
6:S:36:BCL:HAA2	6:S:36:BCL:HBD	1.93	0.50
5:G:29:UNK:CB	6:G:3:BCL:HMD1	2.40	0.49
6:J:8:BCL:HED3	6:J:8:BCL:O1A	2.13	0.49
6:6:36:BCL:HAA2	6:6:36:BCL:HBD	1.94	0.49
6:A:302:BCL:HMB1	6:A:302:BCL:CBB	2.42	0.49
6:J:8:BCL:CMA	6:M:36:BCL:CMA	2.71	0.49
6:D:2:BCL:HMC3	6:G:3:BCL:CBB	2.32	0.49
6:N:11:BCL:HAC2	6:N:38:BCL:HBC2	1.94	0.49
6:T:38:BCL:CMA	6:V:38:BCL:HMA3	2.43	0.49
5:K:29:UNK:C	6:K:36:BCL:HMD3	2.42	0.48
4:3:30:UNK:CB	6:3:39:BCL:HMD3	2.43	0.48
6:D:2:BCL:HBA2	6:D:2:BCL:CGD	2.42	0.48
5:E:22:UNK:C	6:E:1:BCL:HED1	2.43	0.48
6:F:4:BCL:CAB	6:I:5:BCL:HBB2	2.44	0.48
3:C:75:UNK:HA	3:C:76:UNK:C	2.44	0.48
6:G:3:BCL:HAA2	6:G:3:BCL:HBD	1.96	0.48
6:H:6:BCL:O2D	6:H:6:BCL:HBA2	2.14	0.48
6:L:10:BCL:HMB1	6:N:11:BCL:HMA3	1.94	0.48
6:A:301:BCL:H8	6:B:303:BCL:H192	1.96	0.47
1:A:271:UNK:O	4:V:36:UNK:C	2.63	0.47
6:P:38:BCL:HBC2	6:P:39:BCL:C1D	2.45	0.47
6:T:38:BCL:HMA3	6:V:38:BCL:CMA	2.45	0.47
6:8:36:BCL:HAA2	6:8:36:BCL:CBD	2.44	0.47
6:L:10:BCL:HMB3	6:N:11:BCL:HMA2	1.85	0.46
6:L:10:BCL:HBC2	6:M:36:BCL:HHH	1.97	0.46
6:1:38:BCL:CMC	6:3:38:BCL:CBB	2.93	0.46
6:P:38:BCL:CED	5:Q:22:UNK:HA	2.34	0.46
6:7:38:BCL:O1A	6:7:38:BCL:C2A	2.64	0.45
6:F:4:BCL:H3A	6:F:4:BCL:HBA1	1.73	0.45
5:K:29:UNK:CB	6:K:36:BCL:CMD	2.94	0.45
6:A:301:BCL:CBB	6:A:301:BCL:HMB1	2.47	0.45
3:C:40:UNK:HA	3:C:41:UNK:C	2.46	0.45
6:2:36:BCL:HAA2	6:2:36:BCL:CBD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:8:BCL:CBC	6:K:36:BCL:CAC	2.85	0.45
7:A:401:BPH:C17	7:A:401:BPH:C14	2.93	0.45
6:E:1:BCL:HBA1	6:E:1:BCL:H3A	1.39	0.44
6:D:2:BCL:H2A	6:D:2:BCL:O1A	2.17	0.44
5:S:29:UNK:CB	6:S:36:BCL:HMD3	2.47	0.44
6:I:5:BCL:HBA2	6:I:5:BCL:CED	2.48	0.44
6:3:38:BCL:HAA2	6:3:38:BCL:HBD	1.99	0.43
4:5:27:UNK:CB	6:5:38:BCL:OBD	2.67	0.43
6:W:36:BCL:HBA1	6:W:36:BCL:H3A	1.71	0.43
6:T:38:BCL:C3A	6:T:38:BCL:CGA	2.96	0.43
6:N:11:BCL:CBC	6:N:38:BCL:HHH	2.48	0.43
6:V:38:BCL:HMD3	5:W:29:UNK:CB	2.49	0.43
6:1:38:BCL:C2D	6:2:36:BCL:HMD2	2.49	0.43
6:V:38:BCL:CMD	5:W:29:UNK:CB	2.97	0.42
6:J:8:BCL:CAC	6:K:36:BCL:HBC1	2.48	0.42
6:P:38:BCL:CBB	6:P:38:BCL:CHC	2.83	0.42
1:A:51:UNK:CA	4:7:36:UNK:CB	2.96	0.42
6:L:10:BCL:H2A	6:L:10:BCL:CED	2.20	0.42
6:N:38:BCL:HHB	6:P:38:BCL:CMA	2.49	0.42
6:G:3:BCL:HAA2	6:G:3:BCL:CBD	2.49	0.42
6:H:6:BCL:O1A	6:H:6:BCL:H2A	2.19	0.42
6:L:10:BCL:C1D	6:M:36:BCL:HMD2	2.46	0.42
6:P:38:BCL:HBD	6:P:38:BCL:HAA2	2.01	0.42
6:P:39:BCL:CHC	6:P:39:BCL:HBB3	2.37	0.42
6:3:39:BCL:CHC	6:3:39:BCL:HBB3	2.37	0.42
6:A:301:BCL:C4	6:A:301:BCL:H71	2.49	0.42
4:V:34:UNK:O	4:V:35:UNK:C	2.68	0.42
6:V:38:BCL:HBA1	6:V:38:BCL:H3A	1.33	0.42
6:7:38:BCL:CHC	6:7:38:BCL:HBB3	2.37	0.42
6:A:301:BCL:HMB1	6:A:301:BCL:HBB2	2.01	0.42
6:H:6:BCL:O1A	6:H:6:BCL:C2A	2.67	0.42
6:J:8:BCL:CBC	6:K:36:BCL:HAC2	2.40	0.42
6:B:304:BCL:HMB1	6:B:304:BCL:CBB	2.49	0.42
1:A:271:UNK:CB	4:V:37:UNK:CB	2.97	0.42
4:J:23:UNK:CB	6:J:8:BCL:HED2	2.50	0.42
6:N:38:BCL:CHC	6:N:38:BCL:HBB3	2.38	0.41
6:R:38:BCL:CGA	6:R:38:BCL:C3A	2.88	0.41
3:C:52:UNK:N	4:F:13:UNK:CB	2.83	0.41
6:N:11:BCL:HBC2	6:N:38:BCL:HHH	2.02	0.41
6:Y:36:BCL:C1D	6:Y:37:BCL:HMD2	2.50	0.41
6:N:38:BCL:HBA1	6:N:38:BCL:H3A	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:26:UNK:HA	6:Y:36:BCL:OBD	2.21	0.41
6:5:38:BCL:O1A	6:5:38:BCL:C2A	2.68	0.41
6:D:2:BCL:CHC	6:D:2:BCL:HBB3	2.38	0.41
5:K:29:UNK:CB	6:K:36:BCL:HMD3	2.51	0.41
4:L:27:UNK:CB	6:L:10:BCL:OBD	2.69	0.41
6:N:11:BCL:HBD	6:N:11:BCL:HAA2	2.02	0.41
6:N:38:BCL:HMB3	6:P:38:BCL:C4A	2.51	0.41
6:8:36:BCL:HBA1	6:8:36:BCL:CED	2.50	0.41
6:L:10:BCL:HBC1	5:M:33:UNK:CB	2.51	0.40
6:S:36:BCL:HAA2	6:S:36:BCL:CBD	2.50	0.40
6:A:301:BCL:H91	6:A:301:BCL:H111	1.75	0.40
1:A:254:UNK:O	4:Z:36:UNK:O	2.39	0.40
6:D:2:BCL:O1A	6:D:2:BCL:C2A	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

There are no protein backbone outliers to report in this entry.

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

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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	BCL	B	304	-	64,74,74	1.76	7 (10%)	74,115,115	1.39	13 (17%)
6	BCL	Y	36	-	45,55,74	4.14	20 (44%)	51,92,115	2.73	20 (39%)
6	BCL	B	303	-	64,74,74	1.79	9 (14%)	74,115,115	1.57	14 (18%)
7	BPH	A	401	-	51,70,70	1.07	4 (7%)	52,101,101	1.59	11 (21%)
7	BPH	B	402	-	51,70,70	1.10	6 (11%)	52,101,101	1.33	5 (9%)
6	BCL	I	5	-	45,55,74	4.24	20 (44%)	51,92,115	2.92	24 (47%)
6	BCL	N	38	-	45,55,74	3.78	30 (66%)	51,92,115	3.73	21 (41%)
6	BCL	H	6	-	45,55,74	4.12	30 (66%)	51,92,115	3.71	21 (41%)
6	BCL	F	4	-	45,55,74	3.89	29 (64%)	51,92,115	3.69	21 (41%)
6	BCL	K	36	-	45,55,74	4.17	21 (46%)	51,92,115	2.78	20 (39%)
6	BCL	R	38	-	45,55,74	4.00	31 (68%)	51,92,115	3.73	21 (41%)
6	BCL	6	36	-	45,55,74	3.96	19 (42%)	51,92,115	2.71	21 (41%)
6	BCL	N	11	-	45,55,74	3.98	20 (44%)	51,92,115	3.09	23 (45%)
6	BCL	5	38	-	45,55,74	3.74	29 (64%)	51,92,115	3.77	22 (43%)
6	BCL	G	3	-	45,55,74	4.12	18 (40%)	51,92,115	2.81	23 (45%)
6	BCL	E	1	-	45,55,74	4.23	19 (42%)	51,92,115	2.79	23 (45%)
6	BCL	Y	37	-	45,55,74	3.85	30 (66%)	51,92,115	3.75	21 (41%)
6	BCL	2	36	-	45,55,74	4.10	19 (42%)	51,92,115	2.78	20 (39%)
6	BCL	A	301	-	64,74,74	1.75	5 (7%)	74,115,115	1.88	21 (28%)
6	BCL	W	36	-	45,55,74	3.84	31 (68%)	51,92,115	3.73	21 (41%)
6	BCL	1	38	-	45,55,74	3.82	32 (71%)	51,92,115	3.80	21 (41%)
6	BCL	V	38	-	45,55,74	4.12	20 (44%)	51,92,115	2.97	23 (45%)
6	BCL	D	2	-	45,55,74	3.87	31 (68%)	51,92,115	3.69	21 (41%)
6	BCL	T	38	-	45,55,74	4.05	31 (68%)	51,92,115	3.71	21 (41%)
6	BCL	3	39	-	45,55,74	3.83	30 (66%)	51,92,115	3.76	21 (41%)
6	BCL	3	38	-	45,55,74	4.01	20 (44%)	51,92,115	2.72	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BCL	M	36	-	45,55,74	4.14	20 (44%)	51,92,115	2.88	22 (43%)
6	BCL	U	36	-	45,55,74	4.17	20 (44%)	51,92,115	2.73	20 (39%)
6	BCL	P	38	-	45,55,74	4.10	20 (44%)	51,92,115	2.85	20 (39%)
6	BCL	8	36	-	45,55,74	4.02	20 (44%)	51,92,115	2.81	24 (47%)
6	BCL	J	8	-	45,55,74	3.87	29 (64%)	51,92,115	3.71	21 (41%)
6	BCL	S	36	-	45,55,74	4.20	21 (46%)	51,92,115	2.79	23 (45%)
6	BCL	A	302	-	64,74,74	1.54	6 (9%)	74,115,115	1.59	16 (21%)
6	BCL	P	39	-	45,55,74	3.95	30 (66%)	51,92,115	3.73	21 (41%)
6	BCL	7	38	-	45,55,74	3.77	29 (64%)	51,92,115	3.72	21 (41%)
6	BCL	L	10	-	45,55,74	3.87	29 (64%)	51,92,115	3.75	21 (41%)

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	BCL	B	304	-	-	4/37/137/137	-
6	BCL	Y	36	-	-	4/15/115/137	-
6	BCL	B	303	-	-	0/37/137/137	-
7	BPH	A	401	-	-	7/37/105/105	0/5/6/6
7	BPH	B	402	-	-	3/37/105/105	0/5/6/6
6	BCL	I	5	-	-	2/15/115/137	-
6	BCL	N	38	-	-	2/15/115/137	-
6	BCL	H	6	-	-	4/15/115/137	-
6	BCL	F	4	-	-	4/15/115/137	-
6	BCL	K	36	-	-	0/15/115/137	-
6	BCL	R	38	-	-	5/15/115/137	-
6	BCL	6	36	-	-	2/15/115/137	-
6	BCL	N	11	-	-	2/15/115/137	-
6	BCL	5	38	-	-	4/15/115/137	-
6	BCL	G	3	-	-	1/15/115/137	-
6	BCL	E	1	-	-	3/15/115/137	-
6	BCL	Y	37	-	-	3/15/115/137	-
6	BCL	2	36	-	-	1/15/115/137	-
6	BCL	A	301	-	-	7/37/137/137	-
6	BCL	W	36	-	-	6/15/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	1	38	-	-	4/15/115/137	-
6	BCL	V	38	-	-	5/15/115/137	-
6	BCL	D	2	-	-	4/15/115/137	-
6	BCL	T	38	-	-	5/15/115/137	-
6	BCL	3	39	-	-	5/15/115/137	-
6	BCL	3	38	-	-	0/15/115/137	-
6	BCL	M	36	-	-	2/15/115/137	-
6	BCL	U	36	-	-	3/15/115/137	-
6	BCL	P	38	-	-	1/15/115/137	-
6	BCL	8	36	-	-	1/15/115/137	-
6	BCL	J	8	-	-	4/15/115/137	-
6	BCL	S	36	-	-	4/15/115/137	-
6	BCL	A	302	-	-	6/37/137/137	-
6	BCL	P	39	-	-	4/15/115/137	-
6	BCL	7	38	-	-	2/15/115/137	-
6	BCL	L	10	-	-	6/15/115/137	-

All (785) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	36	BCL	CHB-C4A	14.00	1.46	1.33
6	I	5	BCL	CHB-C4A	13.98	1.46	1.33
6	G	3	BCL	CHB-C4A	13.94	1.46	1.33
6	U	36	BCL	CHB-C4A	13.94	1.46	1.33
6	2	36	BCL	CHB-C4A	13.94	1.46	1.33
6	V	38	BCL	CHB-C4A	13.90	1.46	1.33
6	K	36	BCL	CHB-C4A	13.81	1.46	1.33
6	M	36	BCL	CHB-C4A	13.81	1.46	1.33
6	E	1	BCL	CHB-C4A	13.77	1.45	1.33
6	8	36	BCL	CHB-C4A	13.61	1.45	1.33
6	S	36	BCL	CHB-C4A	13.58	1.45	1.33
6	3	38	BCL	CHB-C4A	13.53	1.45	1.33
6	6	36	BCL	CHB-C4A	13.43	1.45	1.33
6	P	38	BCL	CHB-C4A	13.30	1.45	1.33
6	N	11	BCL	CHB-C4A	13.10	1.45	1.33
6	I	5	BCL	CHC-C1C	12.55	1.44	1.33
6	K	36	BCL	CHC-C1C	12.47	1.44	1.33
6	G	3	BCL	CHC-C1C	12.33	1.44	1.33
6	Y	36	BCL	CHC-C1C	12.25	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	36	BCL	CHC-C1C	12.14	1.44	1.33
6	E	1	BCL	CHC-C1C	12.06	1.44	1.33
6	U	36	BCL	CHC-C1C	11.97	1.44	1.33
6	S	36	BCL	CHC-C1C	11.94	1.44	1.33
6	M	36	BCL	CHC-C1C	11.90	1.44	1.33
6	V	38	BCL	CHC-C1C	11.88	1.44	1.33
6	P	38	BCL	CHC-C1C	11.86	1.44	1.33
6	8	36	BCL	CHC-C1C	11.58	1.43	1.33
6	3	38	BCL	CHC-C1C	11.29	1.43	1.33
6	N	11	BCL	CHC-C1C	11.23	1.43	1.33
6	F	4	BCL	CHC-C1C	11.04	1.43	1.33
6	W	36	BCL	CHC-C1C	11.02	1.43	1.33
6	T	38	BCL	CHC-C1C	10.98	1.43	1.33
6	L	10	BCL	CHC-C1C	10.89	1.43	1.33
6	3	39	BCL	CHC-C1C	10.88	1.43	1.33
6	6	36	BCL	CHC-C1C	10.86	1.43	1.33
6	D	2	BCL	CHC-C1C	10.63	1.43	1.33
6	Y	37	BCL	CHC-C1C	10.61	1.43	1.33
6	R	38	BCL	CHC-C1C	10.58	1.42	1.33
6	H	6	BCL	CHC-C1C	10.50	1.42	1.33
6	7	38	BCL	CHC-C1C	10.43	1.42	1.33
6	J	8	BCL	CHC-C1C	10.36	1.42	1.33
6	1	38	BCL	CHC-C1C	10.24	1.42	1.33
6	P	39	BCL	CHC-C1C	10.22	1.42	1.33
6	N	38	BCL	CHC-C1C	10.13	1.42	1.33
6	5	38	BCL	CHC-C1C	9.75	1.42	1.33
6	Y	36	BCL	OBB-CAB	9.40	1.50	1.22
6	I	5	BCL	OBB-CAB	9.36	1.50	1.22
6	K	36	BCL	OBB-CAB	9.30	1.50	1.22
6	M	36	BCL	OBB-CAB	9.23	1.49	1.22
6	G	3	BCL	OBB-CAB	9.23	1.49	1.22
6	2	36	BCL	OBB-CAB	9.22	1.49	1.22
6	V	38	BCL	OBB-CAB	9.20	1.49	1.22
6	U	36	BCL	OBB-CAB	9.13	1.49	1.22
6	P	38	BCL	OBB-CAB	9.13	1.49	1.22
6	S	36	BCL	OBB-CAB	9.08	1.49	1.22
6	N	11	BCL	OBB-CAB	9.03	1.49	1.22
6	3	38	BCL	OBB-CAB	9.02	1.49	1.22
6	E	1	BCL	OBB-CAB	9.02	1.49	1.22
6	6	36	BCL	OBB-CAB	8.87	1.48	1.22
6	8	36	BCL	OBB-CAB	8.79	1.48	1.22
6	A	301	BCL	CHB-C4A	8.54	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	6	BCL	O2A-C1	8.35	1.63	1.45
6	B	304	BCL	CHC-C1C	8.27	1.40	1.33
6	R	38	BCL	O2A-C1	8.26	1.63	1.45
6	B	303	BCL	CHC-C1C	8.18	1.40	1.33
6	8	36	BCL	CBB-CAB	-8.13	1.26	1.49
6	T	38	BCL	O2A-C1	8.11	1.63	1.45
6	3	38	BCL	CBB-CAB	-8.04	1.26	1.49
6	Y	36	BCL	CBB-CAB	-8.03	1.26	1.49
6	G	3	BCL	CBB-CAB	-8.01	1.26	1.49
6	6	36	BCL	CBB-CAB	-8.00	1.26	1.49
6	2	36	BCL	CBB-CAB	-8.00	1.26	1.49
6	E	1	BCL	CBB-CAB	-8.00	1.26	1.49
6	I	5	BCL	CBB-CAB	-7.98	1.26	1.49
6	K	36	BCL	CBB-CAB	-7.96	1.26	1.49
6	M	36	BCL	CBB-CAB	-7.96	1.26	1.49
6	P	38	BCL	CBB-CAB	-7.95	1.26	1.49
6	N	11	BCL	CBB-CAB	-7.95	1.26	1.49
6	E	1	BCL	O2D-CED	-7.95	1.27	1.45
6	B	303	BCL	CHB-C4A	7.91	1.40	1.33
6	V	38	BCL	CBB-CAB	-7.90	1.27	1.49
6	S	36	BCL	CBB-CAB	-7.88	1.27	1.49
6	U	36	BCL	CBB-CAB	-7.86	1.27	1.49
6	P	39	BCL	O2A-C1	7.83	1.62	1.45
6	F	4	BCL	CHB-C4A	7.63	1.40	1.33
6	A	301	BCL	CHC-C1C	7.60	1.40	1.33
6	B	304	BCL	CHB-C4A	7.43	1.40	1.33
6	H	6	BCL	CHB-C4A	7.42	1.40	1.33
6	F	4	BCL	MG-ND	7.37	2.20	2.05
6	I	5	BCL	CMB-C2B	7.27	1.66	1.51
6	T	38	BCL	CHB-C4A	7.26	1.39	1.33
6	K	36	BCL	CMB-C2B	7.18	1.65	1.51
6	L	10	BCL	CHB-C4A	7.13	1.39	1.33
6	W	36	BCL	MG-ND	7.13	2.19	2.05
6	M	36	BCL	CMB-C2B	7.11	1.65	1.51
6	Y	37	BCL	CHB-C4A	7.11	1.39	1.33
6	G	3	BCL	CMB-C2B	7.09	1.65	1.51
6	T	38	BCL	MG-ND	7.09	2.19	2.05
6	H	6	BCL	MG-ND	7.06	2.19	2.05
6	J	8	BCL	MG-ND	7.05	2.19	2.05
6	R	38	BCL	CHB-C4A	7.02	1.39	1.33
6	W	36	BCL	CHB-C4A	7.02	1.39	1.33
6	Y	37	BCL	MG-ND	7.01	2.19	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Y	36	BCL	CMB-C2B	6.99	1.65	1.51
6	R	38	BCL	MG-ND	6.94	2.19	2.05
6	2	36	BCL	CMB-C2B	6.93	1.65	1.51
6	D	2	BCL	CHB-C4A	6.91	1.39	1.33
6	N	38	BCL	CHB-C4A	6.90	1.39	1.33
6	U	36	BCL	CMB-C2B	6.89	1.65	1.51
6	D	2	BCL	MG-ND	6.89	2.19	2.05
6	J	8	BCL	CHB-C4A	6.89	1.39	1.33
6	E	1	BCL	CMB-C2B	6.81	1.65	1.51
6	3	39	BCL	CHB-C4A	6.81	1.39	1.33
6	P	38	BCL	CMB-C2B	6.81	1.65	1.51
6	1	38	BCL	MG-ND	6.80	2.19	2.05
6	S	36	BCL	CMB-C2B	6.79	1.65	1.51
6	3	39	BCL	MG-ND	6.77	2.19	2.05
6	V	38	BCL	CMB-C2B	6.76	1.65	1.51
6	L	10	BCL	MG-ND	6.76	2.19	2.05
6	P	39	BCL	CHB-C4A	6.76	1.39	1.33
6	N	38	BCL	MG-ND	6.74	2.19	2.05
6	N	11	BCL	CMB-C2B	6.68	1.65	1.51
6	P	39	BCL	MG-ND	6.63	2.18	2.05
6	A	302	BCL	CHB-C4A	6.56	1.39	1.33
6	7	38	BCL	CHB-C4A	6.54	1.39	1.33
6	3	38	BCL	CMB-C2B	6.51	1.64	1.51
6	6	36	BCL	CMB-C2B	6.49	1.64	1.51
6	7	38	BCL	MG-ND	6.49	2.18	2.05
6	8	36	BCL	CMB-C2B	6.42	1.64	1.51
6	5	38	BCL	MG-ND	6.36	2.18	2.05
6	L	10	BCL	C3B-C2B	-6.20	1.29	1.39
6	F	4	BCL	C3B-C2B	-6.17	1.29	1.39
6	J	8	BCL	C3B-C2B	-6.13	1.29	1.39
6	7	38	BCL	C3B-C2B	-6.12	1.29	1.39
6	5	38	BCL	CHB-C4A	6.06	1.38	1.33
6	N	38	BCL	C3B-C2B	-6.05	1.29	1.39
6	3	39	BCL	C3B-C2B	-6.05	1.29	1.39
6	H	6	BCL	C3B-C2B	-6.01	1.29	1.39
6	W	36	BCL	C3B-C2B	-6.00	1.29	1.39
6	D	2	BCL	C3B-C2B	-5.99	1.29	1.39
6	1	38	BCL	CHB-C4A	5.99	1.38	1.33
6	A	302	BCL	CHC-C1C	5.96	1.38	1.33
6	1	38	BCL	C3B-C2B	-5.94	1.29	1.39
6	Y	37	BCL	C3B-C2B	-5.93	1.29	1.39
6	T	38	BCL	C3B-C2B	-5.91	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	38	BCL	C3B-C2B	-5.90	1.29	1.39
6	5	38	BCL	C3B-C2B	-5.87	1.29	1.39
6	Y	37	BCL	C1D-ND	5.86	1.45	1.37
6	1	38	BCL	C1D-ND	5.85	1.45	1.37
6	P	39	BCL	C3B-C2B	-5.83	1.29	1.39
6	3	39	BCL	C1D-ND	5.70	1.45	1.37
6	5	38	BCL	C2C-C3C	-5.69	1.39	1.54
6	W	36	BCL	C1D-ND	5.67	1.45	1.37
6	T	38	BCL	C1D-ND	5.66	1.45	1.37
6	1	38	BCL	C2C-C3C	-5.58	1.39	1.54
6	R	38	BCL	C2C-C3C	-5.54	1.39	1.54
6	P	39	BCL	CHD-C1D	5.50	1.49	1.38
6	3	39	BCL	C2C-C3C	-5.50	1.39	1.54
6	F	4	BCL	C1D-ND	5.49	1.45	1.37
6	P	39	BCL	C2C-C3C	-5.49	1.39	1.54
6	H	6	BCL	C1D-ND	5.49	1.45	1.37
6	L	10	BCL	C2C-C3C	-5.47	1.39	1.54
6	7	38	BCL	C2C-C3C	-5.47	1.39	1.54
6	J	8	BCL	C1D-ND	5.45	1.45	1.37
6	R	38	BCL	CHD-C1D	5.45	1.49	1.38
6	L	10	BCL	CHD-C1D	5.44	1.49	1.38
6	J	8	BCL	CHD-C1D	5.44	1.49	1.38
6	D	2	BCL	CHD-C1D	5.43	1.49	1.38
6	D	2	BCL	C2C-C3C	-5.42	1.39	1.54
6	H	6	BCL	CHD-C1D	5.42	1.49	1.38
6	D	2	BCL	C1D-ND	5.41	1.45	1.37
6	T	38	BCL	CHD-C1D	5.39	1.49	1.38
6	N	38	BCL	C2C-C3C	-5.38	1.39	1.54
6	7	38	BCL	CHD-C1D	5.38	1.48	1.38
6	5	38	BCL	CHD-C1D	5.33	1.48	1.38
6	J	8	BCL	CMA-C3A	-5.33	1.41	1.53
6	W	36	BCL	C2C-C3C	-5.33	1.40	1.54
6	H	6	BCL	CMA-C3A	-5.32	1.42	1.53
6	J	8	BCL	CMB-C2B	-5.31	1.41	1.51
6	H	6	BCL	CBB-CAB	-5.31	1.34	1.49
6	Y	37	BCL	C2C-C3C	-5.31	1.40	1.54
6	J	8	BCL	C2C-C3C	-5.31	1.40	1.54
6	F	4	BCL	CHD-C1D	5.31	1.48	1.38
6	J	8	BCL	CBB-CAB	-5.31	1.34	1.49
6	7	38	BCL	C1D-ND	5.30	1.44	1.37
6	F	4	BCL	CMA-C3A	-5.29	1.42	1.53
6	H	6	BCL	C2C-C3C	-5.29	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	38	BCL	CHD-C1D	5.29	1.48	1.38
6	P	39	BCL	C1D-ND	5.28	1.44	1.37
6	L	10	BCL	CMB-C2B	-5.28	1.41	1.51
6	Y	37	BCL	CHD-C1D	5.27	1.48	1.38
6	K	36	BCL	C1D-ND	5.27	1.44	1.37
6	H	6	BCL	CMB-C2B	-5.27	1.41	1.51
6	3	39	BCL	CHD-C1D	5.26	1.48	1.38
6	5	38	BCL	C1D-ND	5.26	1.44	1.37
6	7	38	BCL	CBB-CAB	-5.25	1.34	1.49
6	N	38	BCL	CMB-C2B	-5.25	1.41	1.51
6	W	36	BCL	CHD-C1D	5.24	1.48	1.38
6	T	38	BCL	C2C-C3C	-5.24	1.40	1.54
6	R	38	BCL	C1D-ND	5.24	1.44	1.37
6	5	38	BCL	CMB-C2B	-5.24	1.41	1.51
6	I	5	BCL	C1D-ND	5.24	1.44	1.37
6	5	38	BCL	C1D-C2D	-5.23	1.35	1.45
6	R	38	BCL	CMB-C2B	-5.23	1.41	1.51
6	5	38	BCL	CBB-CAB	-5.21	1.34	1.49
6	P	39	BCL	CMB-C2B	-5.20	1.41	1.51
6	D	2	BCL	CBB-CAB	-5.20	1.34	1.49
6	F	4	BCL	C2C-C3C	-5.19	1.40	1.54
6	S	36	BCL	C1D-ND	5.15	1.44	1.37
6	7	38	BCL	CMB-C2B	-5.15	1.41	1.51
6	N	38	BCL	CBB-CAB	-5.13	1.35	1.49
6	L	10	BCL	CBB-CAB	-5.13	1.35	1.49
6	G	3	BCL	C3B-C2B	5.13	1.48	1.39
6	N	38	BCL	C1D-ND	5.12	1.44	1.37
6	L	10	BCL	C1D-ND	5.12	1.44	1.37
6	1	38	BCL	CHD-C1D	5.12	1.48	1.38
6	H	6	BCL	O2D-CED	-5.11	1.33	1.45
6	P	38	BCL	C3B-C2B	5.11	1.48	1.39
6	1	38	BCL	CMA-C3A	-5.11	1.42	1.53
6	Y	37	BCL	CBB-CAB	-5.10	1.35	1.49
6	7	38	BCL	C1D-C2D	-5.10	1.35	1.45
6	F	4	BCL	CBB-CAB	-5.10	1.35	1.49
6	P	39	BCL	CBB-CAB	-5.09	1.35	1.49
6	Y	37	BCL	CMA-C3A	-5.09	1.42	1.53
6	I	5	BCL	O2A-C1	5.08	1.56	1.45
6	E	1	BCL	C1D-ND	5.08	1.44	1.37
6	U	36	BCL	C1D-ND	5.07	1.44	1.37
6	S	36	BCL	O2A-C1	5.07	1.56	1.45
6	1	38	BCL	CBB-CAB	-5.06	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3	BCL	C1D-ND	5.04	1.44	1.37
6	3	39	BCL	CMB-C2B	-5.04	1.41	1.51
6	W	36	BCL	CMA-C3A	-5.04	1.42	1.53
6	N	11	BCL	C3B-C2B	5.04	1.48	1.39
6	E	1	BCL	C3B-C2B	5.04	1.48	1.39
6	S	36	BCL	C3B-C2B	5.03	1.48	1.39
6	P	39	BCL	MG-NC	5.03	2.18	2.06
6	T	38	BCL	CMB-C2B	-5.03	1.41	1.51
6	D	2	BCL	CMB-C2B	-5.02	1.41	1.51
6	5	38	BCL	CMA-C3A	-5.02	1.42	1.53
6	Y	36	BCL	C1D-ND	5.01	1.44	1.37
6	3	39	BCL	CBB-CAB	-5.00	1.35	1.49
6	T	38	BCL	MG-NC	5.00	2.18	2.06
6	V	38	BCL	C3B-C2B	5.00	1.48	1.39
6	W	36	BCL	MG-NC	5.00	2.18	2.06
6	1	38	BCL	C1D-C2D	-4.99	1.35	1.45
6	Y	37	BCL	MG-NC	4.99	2.18	2.06
6	L	10	BCL	CMA-C3A	-4.99	1.42	1.53
6	M	36	BCL	C1D-ND	4.98	1.44	1.37
6	D	2	BCL	CMA-C3A	-4.98	1.42	1.53
6	V	38	BCL	C1D-ND	4.98	1.44	1.37
6	P	38	BCL	C1D-ND	4.97	1.44	1.37
6	R	38	BCL	MG-NC	4.97	2.18	2.06
6	T	38	BCL	CBB-CAB	-4.97	1.35	1.49
6	8	36	BCL	C3B-C2B	4.97	1.48	1.39
6	K	36	BCL	C3B-C2B	4.96	1.48	1.39
6	R	38	BCL	CBB-CAB	-4.96	1.35	1.49
6	W	36	BCL	CBB-CAB	-4.95	1.35	1.49
6	F	4	BCL	CMB-C2B	-4.94	1.41	1.51
6	5	38	BCL	MG-NC	4.94	2.18	2.06
6	3	38	BCL	C3B-C2B	4.94	1.48	1.39
6	M	36	BCL	C3B-C2B	4.94	1.48	1.39
6	3	39	BCL	MG-NC	4.93	2.18	2.06
6	U	36	BCL	O2A-C1	4.93	1.56	1.45
6	D	2	BCL	C1D-C2D	-4.93	1.35	1.45
6	3	39	BCL	CMA-C3A	-4.93	1.42	1.53
6	J	8	BCL	MG-NC	4.93	2.18	2.06
6	N	38	BCL	CMA-C3A	-4.92	1.42	1.53
6	U	36	BCL	C3B-C2B	4.91	1.48	1.39
6	7	38	BCL	MG-NC	4.91	2.17	2.06
6	1	38	BCL	MG-NC	4.91	2.17	2.06
6	D	2	BCL	MG-NC	4.91	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	302	BCL	MG-NA	4.90	2.17	2.06
6	N	38	BCL	MG-NC	4.90	2.17	2.06
6	Y	37	BCL	CMB-C2B	-4.90	1.41	1.51
6	L	10	BCL	MG-NC	4.90	2.17	2.06
6	2	36	BCL	C3B-C2B	4.90	1.48	1.39
6	7	38	BCL	CMA-C3A	-4.90	1.42	1.53
6	F	4	BCL	MG-NC	4.90	2.17	2.06
6	3	39	BCL	C1D-C2D	-4.90	1.35	1.45
6	H	6	BCL	MG-NC	4.89	2.17	2.06
6	T	38	BCL	CMA-C3A	-4.88	1.42	1.53
6	1	38	BCL	CMB-C2B	-4.87	1.41	1.51
6	P	39	BCL	C1D-C2D	-4.86	1.35	1.45
6	T	38	BCL	C1D-C2D	-4.85	1.35	1.45
6	I	5	BCL	C3B-C2B	4.85	1.47	1.39
6	8	36	BCL	C1D-ND	4.84	1.44	1.37
6	D	2	BCL	O2D-CED	-4.84	1.34	1.45
6	R	38	BCL	C1D-C2D	-4.83	1.35	1.45
6	W	36	BCL	CMB-C2B	-4.83	1.42	1.51
6	R	38	BCL	CMA-C3A	-4.79	1.43	1.53
6	K	36	BCL	O2D-CGD	-4.78	1.21	1.33
6	Y	36	BCL	C3B-C2B	4.78	1.47	1.39
6	N	11	BCL	C1D-ND	4.76	1.44	1.37
6	J	8	BCL	C1D-C2D	-4.76	1.35	1.45
6	6	36	BCL	C3B-C2B	4.75	1.47	1.39
6	J	8	BCL	CAC-C3C	-4.75	1.44	1.54
6	2	36	BCL	C1D-ND	4.75	1.44	1.37
6	S	36	BCL	O1D-CGD	4.74	1.33	1.21
6	L	10	BCL	C1D-C2D	-4.73	1.36	1.45
6	M	36	BCL	O2D-CGD	-4.73	1.21	1.33
6	S	36	BCL	O2D-CGD	-4.72	1.21	1.33
6	1	38	BCL	CBA-CGA	-4.72	1.37	1.50
6	P	39	BCL	CMA-C3A	-4.72	1.43	1.53
6	F	4	BCL	CBA-CGA	-4.71	1.37	1.50
6	8	36	BCL	O2D-CGD	-4.70	1.21	1.33
6	R	38	BCL	CBA-CGA	-4.70	1.37	1.50
6	P	38	BCL	O2D-CGD	-4.69	1.21	1.33
6	I	5	BCL	O2D-CGD	-4.68	1.21	1.33
6	7	38	BCL	CBA-CGA	-4.67	1.37	1.50
6	Y	37	BCL	C1D-C2D	-4.67	1.36	1.45
6	L	10	BCL	CBA-CGA	-4.67	1.37	1.50
6	J	8	BCL	CBA-CGA	-4.65	1.37	1.50
6	D	2	BCL	CBA-CGA	-4.64	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1	BCL	O2D-CGD	-4.64	1.21	1.33
6	U	36	BCL	O2D-CGD	-4.63	1.21	1.33
6	Y	37	BCL	C4B-CHC	4.63	1.53	1.41
6	N	38	BCL	C1D-C2D	-4.62	1.36	1.45
6	P	38	BCL	O1D-CGD	4.62	1.32	1.21
6	N	11	BCL	O1D-CGD	4.62	1.32	1.21
6	6	36	BCL	O2D-CGD	-4.61	1.21	1.33
6	3	38	BCL	C1D-ND	4.61	1.43	1.37
6	G	3	BCL	O2D-CGD	-4.61	1.21	1.33
6	H	6	BCL	CBA-CGA	-4.60	1.37	1.50
6	U	36	BCL	O1D-CGD	4.60	1.32	1.21
6	1	38	BCL	C4B-CHC	4.60	1.53	1.41
6	V	38	BCL	O2D-CGD	-4.59	1.21	1.33
6	V	38	BCL	O1D-CGD	4.58	1.32	1.21
6	8	36	BCL	O1D-CGD	4.57	1.32	1.21
6	K	36	BCL	CAC-C3C	-4.56	1.45	1.54
6	T	38	BCL	C4B-CHC	4.56	1.53	1.41
6	5	38	BCL	CBA-CGA	-4.55	1.37	1.50
6	3	39	BCL	CBA-CGA	-4.54	1.37	1.50
6	W	36	BCL	C4B-CHC	4.53	1.53	1.41
6	F	4	BCL	C1D-C2D	-4.52	1.36	1.45
6	2	36	BCL	O2D-CGD	-4.52	1.22	1.33
6	6	36	BCL	C1D-ND	4.51	1.43	1.37
6	N	38	BCL	C4B-CHC	4.51	1.53	1.41
6	P	39	BCL	C4B-CHC	4.51	1.53	1.41
6	3	39	BCL	C4B-CHC	4.51	1.53	1.41
6	W	36	BCL	C1D-C2D	-4.50	1.36	1.45
6	H	6	BCL	C4B-CHC	4.50	1.53	1.41
6	N	11	BCL	O2D-CGD	-4.50	1.22	1.33
6	3	38	BCL	CAC-C3C	-4.50	1.45	1.54
6	6	36	BCL	C1D-C2D	-4.49	1.36	1.45
6	D	2	BCL	C4B-CHC	4.49	1.53	1.41
6	M	36	BCL	O1D-CGD	4.49	1.32	1.21
6	T	38	BCL	CBA-CGA	-4.49	1.37	1.50
6	H	6	BCL	CAC-C3C	-4.49	1.45	1.54
6	Y	36	BCL	O2D-CGD	-4.49	1.22	1.33
6	7	38	BCL	C4B-CHC	4.47	1.53	1.41
6	F	4	BCL	C4B-CHC	4.47	1.53	1.41
6	Y	37	BCL	CBA-CGA	-4.46	1.37	1.50
6	3	38	BCL	O1D-CGD	4.46	1.32	1.21
6	L	10	BCL	C4B-CHC	4.46	1.53	1.41
6	W	36	BCL	CBA-CGA	-4.46	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	38	BCL	C4B-CHC	4.46	1.53	1.41
6	6	36	BCL	O1D-CGD	4.46	1.32	1.21
6	H	6	BCL	C1D-C2D	-4.45	1.36	1.45
6	P	39	BCL	CBA-CGA	-4.45	1.37	1.50
6	3	38	BCL	O2D-CGD	-4.44	1.22	1.33
6	N	11	BCL	CAC-C3C	-4.44	1.45	1.54
6	I	5	BCL	O1D-CGD	4.43	1.32	1.21
6	R	38	BCL	C4B-CHC	4.43	1.53	1.41
6	N	11	BCL	C1D-C2D	-4.42	1.36	1.45
6	N	38	BCL	CBA-CGA	-4.42	1.37	1.50
6	I	5	BCL	CAC-C3C	-4.41	1.45	1.54
6	Y	36	BCL	O1D-CGD	4.40	1.32	1.21
6	V	38	BCL	O2D-CED	-4.38	1.35	1.45
6	2	36	BCL	O1D-CGD	4.37	1.32	1.21
6	F	4	BCL	CAC-C3C	-4.36	1.45	1.54
6	P	38	BCL	C1D-C2D	-4.36	1.36	1.45
6	2	36	BCL	CAC-C3C	-4.34	1.45	1.54
6	1	38	BCL	O2D-CED	-4.34	1.35	1.45
6	K	36	BCL	C1D-C2D	-4.33	1.36	1.45
6	J	8	BCL	C4B-CHC	4.33	1.53	1.41
6	G	3	BCL	O1D-CGD	4.32	1.32	1.21
6	E	1	BCL	O1D-CGD	4.32	1.32	1.21
6	S	36	BCL	O2D-CED	-4.31	1.35	1.45
6	M	36	BCL	C1D-C2D	-4.31	1.36	1.45
6	L	10	BCL	CAC-C3C	-4.29	1.45	1.54
6	8	36	BCL	C1D-C2D	-4.28	1.36	1.45
6	N	38	BCL	CAC-C3C	-4.28	1.45	1.54
6	P	38	BCL	CAC-C3C	-4.27	1.45	1.54
6	7	38	BCL	C3B-CAB	4.27	1.60	1.49
6	N	38	BCL	O2D-CGD	-4.27	1.22	1.33
6	R	38	BCL	O2D-CGD	-4.26	1.22	1.33
6	5	38	BCL	O2D-CGD	-4.25	1.22	1.33
6	S	36	BCL	C1D-C2D	-4.25	1.36	1.45
6	W	36	BCL	O2D-CGD	-4.24	1.22	1.33
6	U	36	BCL	CAC-C3C	-4.23	1.45	1.54
6	U	36	BCL	C1D-C2D	-4.23	1.37	1.45
6	H	6	BCL	C3B-CAB	4.22	1.60	1.49
6	1	38	BCL	O2D-CGD	-4.22	1.22	1.33
6	Y	36	BCL	CAC-C3C	-4.22	1.46	1.54
6	Y	37	BCL	O2D-CGD	-4.20	1.22	1.33
6	F	4	BCL	C3B-CAB	4.20	1.60	1.49
6	1	38	BCL	CAC-C3C	-4.19	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	7	38	BCL	CAC-C3C	-4.19	1.46	1.54
6	L	10	BCL	O2D-CGD	-4.18	1.22	1.33
6	K	36	BCL	O1D-CGD	4.18	1.31	1.21
6	M	36	BCL	CAC-C3C	-4.17	1.46	1.54
6	J	8	BCL	O2D-CGD	-4.16	1.23	1.33
6	E	1	BCL	C1D-C2D	-4.16	1.37	1.45
6	I	5	BCL	C1D-C2D	-4.15	1.37	1.45
6	P	39	BCL	O2D-CGD	-4.15	1.23	1.33
6	3	38	BCL	C1D-C2D	-4.14	1.37	1.45
6	7	38	BCL	O2D-CGD	-4.13	1.23	1.33
6	2	36	BCL	C1D-C2D	-4.13	1.37	1.45
6	F	4	BCL	O2D-CGD	-4.12	1.23	1.33
6	L	10	BCL	C3B-CAB	4.12	1.60	1.49
6	5	38	BCL	CAC-C3C	-4.12	1.46	1.54
6	T	38	BCL	O2D-CGD	-4.11	1.23	1.33
6	D	2	BCL	C3B-CAB	4.11	1.60	1.49
6	6	36	BCL	C3D-C4D	-4.11	1.34	1.44
6	3	39	BCL	O2D-CGD	-4.10	1.23	1.33
6	V	38	BCL	CAC-C3C	-4.09	1.46	1.54
6	Y	37	BCL	CAC-C3C	-4.09	1.46	1.54
6	6	36	BCL	CAC-C3C	-4.09	1.46	1.54
6	3	39	BCL	CAC-C3C	-4.09	1.46	1.54
6	Y	36	BCL	C1D-C2D	-4.08	1.37	1.45
6	V	38	BCL	C1D-C2D	-4.07	1.37	1.45
6	S	36	BCL	CAC-C3C	-4.07	1.46	1.54
6	G	3	BCL	C1D-C2D	-4.06	1.37	1.45
6	A	301	BCL	MG-NA	4.06	2.15	2.06
6	B	304	BCL	MG-NA	4.06	2.15	2.06
6	N	38	BCL	C3B-CAB	4.05	1.59	1.49
6	L	10	BCL	C3C-C4C	4.04	1.56	1.51
6	H	6	BCL	O2D-CGD	-4.04	1.23	1.33
6	D	2	BCL	O2D-CGD	-4.02	1.23	1.33
6	W	36	BCL	C3B-CAB	4.01	1.59	1.49
6	J	8	BCL	C3B-CAB	4.00	1.59	1.49
6	P	39	BCL	C3B-CAB	3.99	1.59	1.49
6	T	38	BCL	CAC-C3C	-3.99	1.46	1.54
6	B	303	BCL	MG-NA	3.98	2.15	2.06
6	P	38	BCL	O2D-CED	-3.98	1.36	1.45
6	N	11	BCL	C3D-C4D	-3.98	1.35	1.44
6	T	38	BCL	C3B-CAB	3.97	1.59	1.49
6	R	38	BCL	CAC-C3C	-3.96	1.46	1.54
6	P	39	BCL	CAC-C3C	-3.95	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	38	BCL	C3B-CAB	3.93	1.59	1.49
6	3	39	BCL	C3B-CAB	3.92	1.59	1.49
6	G	3	BCL	CAC-C3C	-3.92	1.46	1.54
6	Y	37	BCL	C3B-CAB	3.92	1.59	1.49
6	3	38	BCL	C3D-C4D	-3.91	1.35	1.44
6	K	36	BCL	O2A-CGA	-3.91	1.20	1.33
6	8	36	BCL	C3D-C4D	-3.90	1.35	1.44
6	H	6	BCL	C3C-C4C	3.89	1.56	1.51
6	5	38	BCL	C3B-CAB	3.85	1.59	1.49
6	D	2	BCL	CAC-C3C	-3.85	1.46	1.54
6	2	36	BCL	C3D-C4D	-3.84	1.35	1.44
6	8	36	BCL	CAC-C3C	-3.83	1.46	1.54
6	W	36	BCL	CAC-C3C	-3.80	1.46	1.54
6	S	36	BCL	O2A-CGA	-3.80	1.21	1.33
6	E	1	BCL	CAC-C3C	-3.79	1.46	1.54
6	K	36	BCL	C3D-C4D	-3.79	1.35	1.44
6	M	36	BCL	C3D-C4D	-3.76	1.35	1.44
6	P	38	BCL	C3D-C4D	-3.76	1.35	1.44
6	U	36	BCL	O2A-CGA	-3.74	1.21	1.33
6	M	36	BCL	O2A-CGA	-3.74	1.21	1.33
6	J	8	BCL	C3C-C4C	3.70	1.56	1.51
6	3	38	BCL	O2A-CGA	-3.68	1.21	1.33
6	T	38	BCL	O2D-CED	-3.67	1.37	1.45
6	U	36	BCL	C3D-C4D	-3.66	1.35	1.44
6	S	36	BCL	C3D-C4D	-3.66	1.36	1.44
6	I	5	BCL	O2A-CGA	-3.66	1.21	1.33
6	P	39	BCL	C3C-C4C	3.65	1.56	1.51
6	M	36	BCL	O2D-CED	-3.65	1.37	1.45
6	E	1	BCL	C3D-C4D	-3.64	1.36	1.44
6	Y	36	BCL	C3D-C4D	-3.62	1.36	1.44
6	1	38	BCL	C3B-CAB	3.61	1.58	1.49
6	N	38	BCL	C3C-C4C	3.61	1.56	1.51
6	F	4	BCL	C3C-C4C	3.59	1.56	1.51
6	R	38	BCL	C3C-C4C	3.59	1.56	1.51
6	T	38	BCL	C3C-C4C	3.57	1.56	1.51
6	Y	37	BCL	O2D-CED	-3.57	1.37	1.45
6	G	3	BCL	C3D-C4D	-3.55	1.36	1.44
6	3	39	BCL	C3C-C4C	3.53	1.56	1.51
6	Y	36	BCL	O2A-C1	-3.50	1.37	1.45
6	V	38	BCL	C3D-C4D	-3.49	1.36	1.44
6	I	5	BCL	C3D-C4D	-3.47	1.36	1.44
6	1	38	BCL	C3C-C4C	3.46	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3	BCL	O2A-C1	-3.46	1.37	1.45
6	Y	37	BCL	C3C-C4C	3.42	1.55	1.51
6	W	36	BCL	C3C-C4C	3.41	1.55	1.51
7	B	402	BPH	C3A-C2A	-3.38	1.51	1.54
6	D	2	BCL	C3C-C4C	3.38	1.55	1.51
6	D	2	BCL	CBD-CGD	-3.38	1.42	1.52
6	5	38	BCL	C3C-C4C	3.37	1.55	1.51
6	7	38	BCL	CBD-CGD	-3.36	1.42	1.52
7	A	401	BPH	C2C-C3C	-3.36	1.51	1.54
6	H	6	BCL	CBD-CGD	-3.33	1.42	1.52
6	6	36	BCL	CMA-C3A	3.33	1.60	1.53
6	F	4	BCL	CBD-CGD	-3.32	1.42	1.52
6	1	38	BCL	CBD-CGD	-3.32	1.42	1.52
6	3	39	BCL	CBD-CGD	-3.31	1.42	1.52
6	Y	37	BCL	CBD-CGD	-3.27	1.42	1.52
6	5	38	BCL	CBD-CGD	-3.27	1.42	1.52
6	J	8	BCL	O2D-CED	-3.25	1.38	1.45
6	7	38	BCL	C3C-C4C	3.24	1.55	1.51
6	5	38	BCL	O2D-CED	-3.24	1.38	1.45
6	P	38	BCL	O2A-C1	-3.23	1.38	1.45
6	L	10	BCL	CBD-CGD	-3.23	1.42	1.52
6	J	8	BCL	CBD-CGD	-3.22	1.42	1.52
6	W	36	BCL	CBD-CGD	-3.17	1.42	1.52
7	A	401	BPH	C3A-C2A	-3.15	1.52	1.54
6	S	36	BCL	CMA-C3A	3.15	1.59	1.53
6	T	38	BCL	CBD-CGD	-3.15	1.42	1.52
6	8	36	BCL	CMA-C3A	3.14	1.59	1.53
6	W	36	BCL	O2A-CGA	-3.14	1.23	1.33
6	N	38	BCL	CBD-CGD	-3.14	1.43	1.52
6	J	8	BCL	O2A-CGA	-3.11	1.23	1.33
6	8	36	BCL	O2A-C1	-3.11	1.38	1.45
6	P	39	BCL	CBD-CGD	-3.10	1.43	1.52
6	E	1	BCL	CMA-C3A	3.10	1.59	1.53
6	P	38	BCL	CMA-C3A	3.09	1.59	1.53
6	G	3	BCL	CMA-C3A	3.08	1.59	1.53
6	R	38	BCL	CBD-CGD	-3.08	1.43	1.52
7	A	401	BPH	C3B-C2B	-3.07	1.34	1.39
6	G	3	BCL	CHD-C4C	3.07	1.47	1.39
6	V	38	BCL	CHD-C4C	3.07	1.47	1.39
6	V	38	BCL	O2A-C1	-3.06	1.38	1.45
6	5	38	BCL	C3A-C2A	-3.06	1.46	1.54
6	Y	36	BCL	CHD-C4C	3.04	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	36	BCL	CHD-C4C	3.03	1.47	1.39
6	3	38	BCL	CHD-C4C	3.00	1.47	1.39
6	M	36	BCL	CMA-C3A	3.00	1.59	1.53
6	U	36	BCL	CMA-C3A	2.99	1.59	1.53
6	N	11	BCL	CMA-C3A	2.97	1.59	1.53
6	P	39	BCL	O2A-CGA	-2.96	1.23	1.33
6	2	36	BCL	CMA-C3A	2.95	1.59	1.53
6	P	39	BCL	O2D-CED	-2.94	1.38	1.45
6	1	38	BCL	O2A-CGA	-2.94	1.23	1.33
6	F	4	BCL	CHD-C4C	2.93	1.47	1.39
6	3	38	BCL	CMA-C3A	2.92	1.59	1.53
6	5	38	BCL	CAA-C2A	2.92	1.59	1.54
6	H	6	BCL	CHD-C4C	2.91	1.47	1.39
6	U	36	BCL	CHD-C4C	2.91	1.47	1.39
6	E	1	BCL	CHD-C4C	2.91	1.47	1.39
6	P	38	BCL	CHD-C4C	2.90	1.47	1.39
6	B	303	BCL	MG-NC	2.90	2.13	2.06
6	V	38	BCL	CMA-C3A	2.89	1.59	1.53
6	M	36	BCL	CHD-C4C	2.89	1.47	1.39
6	1	38	BCL	C2C-C1C	2.89	1.61	1.51
6	Y	37	BCL	C2C-C1C	2.87	1.61	1.51
6	I	5	BCL	CHD-C4C	2.86	1.47	1.39
6	W	36	BCL	C2C-C1C	2.86	1.61	1.51
6	I	5	BCL	CMA-C3A	2.86	1.59	1.53
6	B	304	BCL	MG-ND	-2.85	2.00	2.05
6	E	1	BCL	O2A-CGA	2.84	1.41	1.33
6	N	38	BCL	O2A-CGA	-2.83	1.24	1.33
6	7	38	BCL	CAA-C2A	2.83	1.59	1.54
6	5	38	BCL	C2C-C1C	2.82	1.61	1.51
7	B	402	BPH	CBD-CGD	-2.82	1.48	1.52
6	R	38	BCL	C2C-C1C	2.81	1.61	1.51
6	S	36	BCL	CHD-C4C	2.81	1.47	1.39
6	T	38	BCL	O2A-CGA	-2.81	1.24	1.33
6	Y	37	BCL	O2A-CGA	-2.80	1.24	1.33
6	1	38	BCL	C3A-C2A	-2.80	1.46	1.54
6	Y	37	BCL	CHD-C4C	2.80	1.47	1.39
6	N	11	BCL	CHD-C4C	2.80	1.47	1.39
6	T	38	BCL	C2C-C1C	2.80	1.61	1.51
6	J	8	BCL	CHD-C4C	2.79	1.47	1.39
6	P	39	BCL	C2C-C1C	2.79	1.61	1.51
6	H	6	BCL	O2A-CGA	-2.79	1.24	1.33
6	3	39	BCL	C2C-C1C	2.78	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	36	BCL	CHD-C4C	2.78	1.47	1.39
6	K	36	BCL	CMA-C3A	2.78	1.59	1.53
6	6	36	BCL	CHD-C4C	2.77	1.47	1.39
6	8	36	BCL	CHD-C4C	2.77	1.47	1.39
6	K	36	BCL	CHD-C4C	2.77	1.47	1.39
6	H	6	BCL	C2C-C1C	2.77	1.61	1.51
6	3	39	BCL	O2A-CGA	-2.77	1.24	1.33
6	L	10	BCL	C2C-C1C	2.77	1.61	1.51
6	Y	36	BCL	CMA-C3A	2.76	1.59	1.53
6	D	2	BCL	C2C-C1C	2.75	1.60	1.51
6	P	39	BCL	C3A-C2A	-2.73	1.47	1.54
6	R	38	BCL	O2A-CGA	-2.73	1.24	1.33
6	3	39	BCL	C3A-C2A	-2.73	1.47	1.54
6	F	4	BCL	O2A-CGA	-2.72	1.24	1.33
6	N	38	BCL	C2C-C1C	2.70	1.60	1.51
6	T	38	BCL	CHD-C4C	2.69	1.46	1.39
6	R	38	BCL	C3A-C2A	-2.68	1.47	1.54
6	F	4	BCL	C2C-C1C	2.68	1.60	1.51
6	7	38	BCL	C2C-C1C	2.67	1.60	1.51
6	N	38	BCL	CHD-C4C	2.67	1.46	1.39
6	R	38	BCL	CHD-C4C	2.67	1.46	1.39
6	L	10	BCL	O2A-CGA	-2.67	1.24	1.33
6	J	8	BCL	C2C-C1C	2.66	1.60	1.51
6	D	2	BCL	CAA-C2A	2.65	1.58	1.54
6	N	38	BCL	C3A-C2A	-2.63	1.47	1.54
6	7	38	BCL	C3A-C2A	-2.63	1.47	1.54
6	D	2	BCL	C3A-C2A	-2.62	1.47	1.54
6	1	38	BCL	O2A-C1	-2.62	1.39	1.45
6	L	10	BCL	CHD-C4C	2.59	1.46	1.39
6	P	38	BCL	C3B-CAB	-2.59	1.42	1.49
6	L	10	BCL	C3A-C2A	-2.59	1.47	1.54
6	P	39	BCL	CHD-C4C	2.59	1.46	1.39
6	5	38	BCL	CMD-C2D	-2.59	1.45	1.50
6	6	36	BCL	C3B-CAB	-2.59	1.42	1.49
6	H	6	BCL	C3D-CAD	2.58	1.54	1.45
6	J	8	BCL	C3A-C2A	-2.57	1.47	1.54
6	D	2	BCL	CHD-C4C	2.57	1.46	1.39
6	P	39	BCL	CAA-C2A	2.57	1.58	1.54
6	N	38	BCL	CAA-C2A	2.57	1.58	1.54
7	B	402	BPH	C3B-C2B	-2.57	1.35	1.39
6	A	301	BCL	MG-NC	2.56	2.12	2.06
6	K	36	BCL	C3B-CAB	-2.56	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	10	BCL	CMD-C2D	-2.55	1.45	1.50
6	H	6	BCL	C3A-C2A	-2.55	1.47	1.54
6	D	2	BCL	O2A-CGA	-2.55	1.25	1.33
6	1	38	BCL	CHD-C4C	2.54	1.46	1.39
6	R	38	BCL	CMD-C2D	-2.54	1.45	1.50
6	W	36	BCL	O2D-CED	-2.53	1.39	1.45
6	J	8	BCL	CMD-C2D	-2.52	1.45	1.50
6	3	39	BCL	CHD-C4C	2.52	1.46	1.39
6	7	38	BCL	O1D-CGD	2.51	1.27	1.21
6	5	38	BCL	O1D-CGD	2.51	1.27	1.21
6	Y	37	BCL	C3A-C2A	-2.51	1.47	1.54
6	N	38	BCL	CMD-C2D	-2.50	1.45	1.50
6	T	38	BCL	C3A-C2A	-2.50	1.47	1.54
6	N	11	BCL	C3B-CAB	-2.50	1.42	1.49
6	R	38	BCL	CAA-C2A	2.50	1.58	1.54
6	L	10	BCL	C3D-CAD	2.50	1.53	1.45
6	8	36	BCL	C3B-CAB	-2.49	1.42	1.49
6	Y	37	BCL	C3D-CAD	2.48	1.53	1.45
6	F	4	BCL	CAA-C2A	2.47	1.58	1.54
6	R	38	BCL	C3D-CAD	2.47	1.53	1.45
6	Y	37	BCL	CAA-C2A	2.47	1.58	1.54
6	T	38	BCL	CAA-C2A	2.47	1.58	1.54
6	G	3	BCL	C3B-CAB	-2.47	1.42	1.49
6	3	39	BCL	O2A-C1	-2.47	1.39	1.45
6	E	1	BCL	C3B-CAB	-2.46	1.42	1.49
6	3	39	BCL	C3D-CAD	2.45	1.53	1.45
6	7	38	BCL	C3D-CAD	2.45	1.53	1.45
6	W	36	BCL	C3A-C2A	-2.44	1.47	1.54
6	N	38	BCL	C3D-CAD	2.44	1.53	1.45
6	P	39	BCL	C3D-CAD	2.44	1.53	1.45
6	L	10	BCL	CAA-C2A	2.44	1.58	1.54
6	F	4	BCL	O2D-CED	-2.44	1.39	1.45
6	B	304	BCL	C3B-C2B	-2.43	1.35	1.39
6	M	36	BCL	C3B-CAB	-2.43	1.42	1.49
7	B	402	BPH	C1A-C2A	-2.43	1.47	1.51
6	7	38	BCL	CHD-C4C	2.43	1.46	1.39
6	S	36	BCL	C3B-CAB	-2.42	1.42	1.49
6	D	2	BCL	CMD-C2D	-2.42	1.45	1.50
6	R	38	BCL	O1D-CGD	2.42	1.27	1.21
6	W	36	BCL	C3D-CAD	2.42	1.53	1.45
6	F	4	BCL	C3D-CAD	2.41	1.53	1.45
6	I	5	BCL	C3B-CAB	-2.41	1.42	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	8	BCL	C3D-CAD	2.41	1.53	1.45
6	V	38	BCL	C3B-CAB	-2.41	1.42	1.49
6	U	36	BCL	C3B-CAB	-2.40	1.42	1.49
6	5	38	BCL	CHD-C4C	2.39	1.45	1.39
6	3	38	BCL	C3B-CAB	-2.39	1.42	1.49
6	P	39	BCL	CMD-C2D	-2.39	1.45	1.50
6	H	6	BCL	CMD-C2D	-2.38	1.45	1.50
6	G	3	BCL	C2C-C1C	2.37	1.59	1.51
6	7	38	BCL	CMD-C2D	-2.37	1.45	1.50
6	D	2	BCL	O1D-CGD	2.37	1.27	1.21
6	M	36	BCL	C2C-C1C	2.37	1.59	1.51
6	3	39	BCL	CMD-C2D	-2.37	1.45	1.50
6	W	36	BCL	CAA-C2A	2.36	1.58	1.54
6	1	38	BCL	C3D-CAD	2.36	1.53	1.45
6	A	302	BCL	C1A-CHA	-2.36	1.33	1.43
6	N	11	BCL	C1A-CHA	-2.36	1.33	1.43
6	D	2	BCL	C3D-CAD	2.36	1.53	1.45
6	3	39	BCL	CAA-C2A	2.36	1.58	1.54
6	L	10	BCL	O1D-CGD	2.36	1.27	1.21
6	N	38	BCL	O1D-CGD	2.35	1.27	1.21
6	T	38	BCL	C3D-CAD	2.35	1.53	1.45
6	3	39	BCL	C4D-CHA	2.33	1.46	1.38
6	6	36	BCL	C1A-CHA	-2.33	1.33	1.43
6	U	36	BCL	C2C-C1C	2.32	1.59	1.51
6	F	4	BCL	O1D-CGD	2.31	1.27	1.21
6	V	38	BCL	C2C-C1C	2.31	1.59	1.51
6	F	4	BCL	CMD-C2D	-2.30	1.46	1.50
6	8	36	BCL	C2C-C1C	2.30	1.59	1.51
6	B	303	BCL	C3B-C2B	-2.30	1.35	1.39
6	P	39	BCL	O1D-CGD	2.30	1.27	1.21
6	I	5	BCL	C2C-C1C	2.30	1.59	1.51
6	T	38	BCL	CMD-C2D	-2.29	1.46	1.50
6	K	36	BCL	C2C-C1C	2.29	1.59	1.51
6	5	38	BCL	C3D-CAD	2.29	1.53	1.45
6	F	4	BCL	C3A-C2A	-2.29	1.48	1.54
6	Y	36	BCL	C3B-CAB	-2.28	1.43	1.49
6	B	304	BCL	C2C-C3C	-2.28	1.48	1.54
6	S	36	BCL	C2C-C1C	2.27	1.59	1.51
6	W	36	BCL	O1D-CGD	2.27	1.27	1.21
6	P	38	BCL	C2C-C1C	2.26	1.59	1.51
6	D	2	BCL	C4D-CHA	2.26	1.46	1.38
6	3	38	BCL	C1A-CHA	-2.26	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	2	36	BCL	C3B-CAB	-2.26	1.43	1.49
6	T	38	BCL	O1D-CGD	2.25	1.26	1.21
6	Y	36	BCL	O2D-CED	-2.24	1.40	1.45
6	E	1	BCL	C2C-C1C	2.24	1.59	1.51
6	Y	36	BCL	C2C-C1C	2.22	1.59	1.51
6	H	6	BCL	CAA-C2A	2.22	1.58	1.54
6	A	302	BCL	C3B-C2B	-2.21	1.35	1.39
6	B	304	BCL	O2D-CED	-2.21	1.40	1.45
6	3	39	BCL	O1D-CGD	2.21	1.26	1.21
6	Y	37	BCL	C4D-CHA	2.21	1.46	1.38
6	N	38	BCL	O2D-CED	-2.21	1.40	1.45
6	N	11	BCL	C2C-C1C	2.21	1.59	1.51
6	2	36	BCL	C2C-C1C	2.20	1.59	1.51
7	B	402	BPH	C4A-C3A	-2.20	1.47	1.51
6	T	38	BCL	C4D-CHA	2.19	1.45	1.38
6	1	38	BCL	O1D-CGD	2.19	1.26	1.21
6	I	5	BCL	O2D-CED	-2.19	1.40	1.45
6	5	38	BCL	C3D-C4D	-2.18	1.39	1.44
7	A	401	BPH	O2D-CED	-2.18	1.40	1.45
6	1	38	BCL	C4D-CHA	2.18	1.45	1.38
6	L	10	BCL	O2A-C1	-2.17	1.40	1.45
6	2	36	BCL	O2D-CED	-2.17	1.40	1.45
6	1	38	BCL	CAA-C2A	2.17	1.58	1.54
6	7	38	BCL	C4D-CHA	2.16	1.45	1.38
6	K	36	BCL	O2A-C1	-2.16	1.40	1.45
6	Y	37	BCL	CMD-C2D	-2.16	1.46	1.50
6	M	36	BCL	C1A-CHA	-2.16	1.34	1.43
6	Y	37	BCL	O1D-CGD	2.16	1.26	1.21
6	F	4	BCL	C4D-CHA	2.16	1.45	1.38
6	6	36	BCL	C3A-C2A	-2.15	1.48	1.54
6	W	36	BCL	C4D-CHA	2.15	1.45	1.38
6	P	39	BCL	C4D-CHA	2.14	1.45	1.38
6	8	36	BCL	C1A-CHA	-2.13	1.34	1.43
6	W	36	BCL	CMD-C2D	-2.13	1.46	1.50
6	3	38	BCL	C2C-C1C	2.13	1.58	1.51
6	S	36	BCL	C1A-CHA	-2.13	1.34	1.43
6	N	38	BCL	C4D-CHA	2.12	1.45	1.38
6	D	2	BCL	C3D-C4D	-2.12	1.39	1.44
6	7	38	BCL	C3D-C4D	-2.11	1.39	1.44
6	H	6	BCL	C4D-CHA	2.11	1.45	1.38
6	R	38	BCL	C4D-CHA	2.11	1.45	1.38
6	8	36	BCL	C4B-CHC	-2.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	BCL	C1A-CHA	-2.11	1.34	1.43
6	6	36	BCL	C2C-C1C	2.11	1.58	1.51
6	J	8	BCL	CAA-C2A	2.11	1.57	1.54
6	K	36	BCL	O2D-CED	-2.11	1.40	1.45
6	R	38	BCL	C3D-C4D	-2.10	1.39	1.44
6	L	10	BCL	C4D-CHA	2.10	1.45	1.38
6	S	36	BCL	C4B-CHC	-2.10	1.35	1.41
6	3	38	BCL	O2A-C1	-2.09	1.40	1.45
6	J	8	BCL	C4D-CHA	2.09	1.45	1.38
6	2	36	BCL	C1A-CHA	-2.09	1.34	1.43
6	1	38	BCL	CMD-C2D	-2.09	1.46	1.50
6	5	38	BCL	C4D-CHA	2.09	1.45	1.38
6	U	36	BCL	C1A-CHA	-2.09	1.34	1.43
6	1	38	BCL	C2A-C1A	2.09	1.56	1.52
6	1	38	BCL	CBC-CAC	-2.08	1.39	1.51
6	E	1	BCL	C1A-CHA	-2.08	1.34	1.43
6	P	38	BCL	C1A-CHA	-2.08	1.34	1.43
6	J	8	BCL	O1D-CGD	2.07	1.26	1.21
6	Y	36	BCL	CHD-C1D	2.07	1.42	1.38
6	K	36	BCL	C1A-CHA	-2.07	1.34	1.43
6	W	36	BCL	O2A-C1	-2.07	1.40	1.45
6	3	38	BCL	C4B-CHC	-2.07	1.35	1.41
6	B	303	BCL	C3D-C4D	-2.07	1.39	1.44
6	2	36	BCL	C4B-CHC	-2.07	1.35	1.41
6	N	11	BCL	C4B-CHC	-2.06	1.35	1.41
6	N	11	BCL	C3A-C2A	-2.06	1.48	1.54
6	H	6	BCL	CBC-CAC	-2.05	1.39	1.51
6	7	38	BCL	CAA-CBA	-2.05	1.46	1.52
6	A	302	BCL	C1D-C2D	-2.04	1.41	1.45
6	B	303	BCL	C1B-CHB	-2.04	1.35	1.41
6	B	303	BCL	CBA-CGA	-2.04	1.44	1.50
6	I	5	BCL	C1A-CHA	-2.04	1.34	1.43
6	D	2	BCL	O2A-C1	-2.04	1.40	1.45
6	N	11	BCL	O2D-CED	-2.03	1.40	1.45
6	W	36	BCL	CBC-CAC	-2.03	1.39	1.51
6	8	36	BCL	C3A-C2A	-2.03	1.49	1.54
6	6	36	BCL	C4B-CHC	-2.03	1.35	1.41
6	Y	36	BCL	C4B-CHC	-2.02	1.35	1.41
6	U	36	BCL	CHD-C1D	2.02	1.42	1.38
6	V	38	BCL	C1A-CHA	-2.02	1.34	1.43
6	R	38	BCL	CBC-CAC	-2.01	1.39	1.51
6	M	36	BCL	CHD-C1D	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	3	BCL	C1A-CHA	-2.01	1.34	1.43
6	T	38	BCL	CAA-CBA	-2.01	1.46	1.52
6	N	38	BCL	C3D-C4D	-2.01	1.39	1.44
6	P	38	BCL	C4B-CHC	-2.01	1.35	1.41
6	V	38	BCL	C4B-CHC	-2.01	1.35	1.41
6	Y	37	BCL	CBC-CAC	-2.01	1.39	1.51
7	B	402	BPH	C3D-C2D	-2.00	1.36	1.39
6	B	303	BCL	O2D-CED	-2.00	1.40	1.45
6	3	39	BCL	CBC-CAC	-2.00	1.39	1.51
6	K	36	BCL	C4B-CHC	-2.00	1.35	1.41

All (721) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	38	BCL	C4D-C3D-CAD	-14.35	92.52	108.11
6	5	38	BCL	C4D-C3D-CAD	-14.13	92.76	108.11
6	3	39	BCL	C4D-C3D-CAD	-14.06	92.83	108.11
6	Y	37	BCL	C4D-C3D-CAD	-14.06	92.83	108.11
6	W	36	BCL	C4D-C3D-CAD	-13.93	92.98	108.11
6	R	38	BCL	C4D-C3D-CAD	-13.85	93.06	108.11
6	P	39	BCL	C4D-C3D-CAD	-13.83	93.09	108.11
6	N	38	BCL	C4D-C3D-CAD	-13.82	93.09	108.11
6	7	38	BCL	C4D-C3D-CAD	-13.82	93.10	108.11
6	T	38	BCL	C4D-C3D-CAD	-13.79	93.13	108.11
6	L	10	BCL	C4D-C3D-CAD	-13.77	93.15	108.11
6	D	2	BCL	C4D-C3D-CAD	-13.72	93.21	108.11
6	F	4	BCL	C4D-C3D-CAD	-13.71	93.21	108.11
6	H	6	BCL	C4D-C3D-CAD	-13.56	93.38	108.11
6	J	8	BCL	C4D-C3D-CAD	-13.48	93.47	108.11
6	P	38	BCL	C4D-C3D-CAD	-11.37	95.76	108.11
6	K	36	BCL	C4D-C3D-CAD	-11.35	95.77	108.11
6	M	36	BCL	C4D-C3D-CAD	-11.23	95.90	108.11
6	I	5	BCL	C4D-C3D-CAD	-11.20	95.95	108.11
6	S	36	BCL	C4D-C3D-CAD	-11.16	95.98	108.11
6	G	3	BCL	C4D-C3D-CAD	-11.15	96.00	108.11
6	E	1	BCL	C4D-C3D-CAD	-11.14	96.01	108.11
6	V	38	BCL	C4D-C3D-CAD	-11.12	96.02	108.11
6	U	36	BCL	C4D-C3D-CAD	-11.07	96.08	108.11
6	8	36	BCL	C4D-C3D-CAD	-11.05	96.10	108.11
6	2	36	BCL	C4D-C3D-CAD	-11.03	96.13	108.11
6	N	11	BCL	C4D-C3D-CAD	-11.01	96.15	108.11
6	6	36	BCL	C4D-C3D-CAD	-11.00	96.15	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3	38	BCL	C4D-C3D-CAD	-10.95	96.22	108.11
6	Y	36	BCL	C4D-C3D-CAD	-10.90	96.27	108.11
6	1	38	BCL	O2D-CGD-CBD	8.05	125.31	111.23
6	H	6	BCL	O2D-CGD-CBD	8.05	125.30	111.23
6	J	8	BCL	O2D-CGD-CBD	8.04	125.28	111.23
6	W	36	BCL	O2D-CGD-CBD	8.03	125.27	111.23
6	N	38	BCL	O2D-CGD-CBD	8.00	125.21	111.23
6	L	10	BCL	O2D-CGD-CBD	7.97	125.16	111.23
6	R	38	BCL	O2D-CGD-CBD	7.95	125.12	111.23
6	3	39	BCL	O2D-CGD-CBD	7.94	125.12	111.23
6	Y	37	BCL	O2D-CGD-CBD	7.91	125.05	111.23
6	F	4	BCL	O2D-CGD-CBD	7.91	125.05	111.23
6	7	38	BCL	O2D-CGD-CBD	7.91	125.05	111.23
6	D	2	BCL	O2D-CGD-CBD	7.89	125.02	111.23
6	P	39	BCL	O2D-CGD-CBD	7.83	124.91	111.23
6	T	38	BCL	O2D-CGD-CBD	7.80	124.87	111.23
6	3	39	BCL	C4B-C3B-CAB	-7.80	112.24	127.08
6	1	38	BCL	C4B-C3B-CAB	-7.77	112.31	127.08
6	5	38	BCL	O2D-CGD-CBD	7.76	124.79	111.23
6	5	38	BCL	C4B-C3B-CAB	-7.74	112.36	127.08
6	W	36	BCL	C4B-C3B-CAB	-7.72	112.40	127.08
6	L	10	BCL	C4B-C3B-CAB	-7.71	112.40	127.08
6	R	38	BCL	C4B-C3B-CAB	-7.70	112.44	127.08
6	N	38	BCL	C4B-C3B-CAB	-7.69	112.44	127.08
6	7	38	BCL	C4B-C3B-CAB	-7.69	112.44	127.08
6	Y	37	BCL	C4B-C3B-CAB	-7.68	112.47	127.08
6	P	39	BCL	C4B-C3B-CAB	-7.65	112.52	127.08
6	D	2	BCL	C4B-C3B-CAB	-7.65	112.53	127.08
6	J	8	BCL	C4B-C3B-CAB	-7.63	112.57	127.08
6	H	6	BCL	C4B-C3B-CAB	-7.57	112.67	127.08
6	T	38	BCL	C4B-C3B-CAB	-7.56	112.70	127.08
6	F	4	BCL	C4B-C3B-CAB	-7.54	112.74	127.08
6	J	8	BCL	C1D-ND-C4D	-7.48	101.06	106.31
6	H	6	BCL	C1D-ND-C4D	-7.33	101.17	106.31
6	W	36	BCL	C1D-ND-C4D	-7.28	101.20	106.31
6	F	4	BCL	C1D-ND-C4D	-7.25	101.23	106.31
6	Y	37	BCL	C1D-ND-C4D	-7.23	101.24	106.31
6	D	2	BCL	C1D-ND-C4D	-7.20	101.26	106.31
6	J	8	BCL	CMB-C2B-C1B	-7.18	117.93	128.46
6	L	10	BCL	C1D-ND-C4D	-7.13	101.31	106.31
6	N	38	BCL	CMB-C2B-C1B	-7.10	118.06	128.46
6	1	38	BCL	CMB-C2B-C1B	-7.10	118.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3	39	BCL	CMB-C2B-C1B	-7.09	118.07	128.46
6	T	38	BCL	C1D-ND-C4D	-7.08	101.34	106.31
6	7	38	BCL	C1D-ND-C4D	-7.05	101.36	106.31
6	L	10	BCL	CMB-C2B-C1B	-7.05	118.12	128.46
6	H	6	BCL	CMB-C2B-C1B	-7.04	118.14	128.46
6	5	38	BCL	CMB-C2B-C1B	-7.03	118.16	128.46
6	N	38	BCL	C1D-ND-C4D	-7.01	101.39	106.31
6	7	38	BCL	CMB-C2B-C1B	-6.99	118.22	128.46
6	P	39	BCL	CMB-C2B-C1B	-6.98	118.22	128.46
6	P	39	BCL	C1D-ND-C4D	-6.98	101.42	106.31
6	1	38	BCL	C1D-ND-C4D	-6.98	101.42	106.31
6	F	4	BCL	CMB-C2B-C1B	-6.95	118.27	128.46
6	R	38	BCL	CMB-C2B-C1B	-6.95	118.27	128.46
6	R	38	BCL	C1D-ND-C4D	-6.95	101.44	106.31
6	Y	37	BCL	CMB-C2B-C1B	-6.93	118.31	128.46
6	T	38	BCL	CMB-C2B-C1B	-6.91	118.33	128.46
6	3	39	BCL	C1D-ND-C4D	-6.87	101.49	106.31
6	D	2	BCL	CMB-C2B-C1B	-6.84	118.43	128.46
6	W	36	BCL	CMB-C2B-C1B	-6.80	118.50	128.46
6	5	38	BCL	C4A-NA-C1A	-6.77	103.59	106.68
6	P	39	BCL	C4A-NA-C1A	-6.66	103.64	106.68
6	5	38	BCL	C1D-ND-C4D	-6.56	101.71	106.31
6	L	10	BCL	C4A-NA-C1A	-6.50	103.72	106.68
6	R	38	BCL	C4A-NA-C1A	-6.48	103.72	106.68
6	3	39	BCL	C4A-NA-C1A	-6.46	103.73	106.68
6	1	38	BCL	C4A-NA-C1A	-6.44	103.74	106.68
6	N	11	BCL	C1-O2A-CGA	6.29	136.21	116.07
6	N	38	BCL	C4A-NA-C1A	-6.27	103.82	106.68
6	Y	36	BCL	O2D-CGD-CBD	6.26	122.17	111.23
6	K	36	BCL	O2D-CGD-CBD	6.24	122.13	111.23
6	G	3	BCL	O2D-CGD-CBD	6.23	122.13	111.23
6	I	5	BCL	O2D-CGD-CBD	6.21	122.09	111.23
6	8	36	BCL	O2D-CGD-CBD	6.21	122.08	111.23
6	3	38	BCL	O2D-CGD-CBD	6.19	122.05	111.23
6	V	38	BCL	O2D-CGD-CBD	6.17	122.01	111.23
6	Y	37	BCL	C4A-NA-C1A	-6.15	103.87	106.68
6	2	36	BCL	O2D-CGD-CBD	6.13	121.95	111.23
6	M	36	BCL	O2D-CGD-CBD	6.12	121.93	111.23
6	T	38	BCL	C4A-NA-C1A	-6.12	103.89	106.68
6	6	36	BCL	O2D-CGD-CBD	6.11	121.91	111.23
6	S	36	BCL	O2D-CGD-CBD	6.08	121.85	111.23
6	E	1	BCL	O2D-CGD-CBD	6.06	121.83	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	11	BCL	O2A-CGA-CBA	6.04	134.96	112.14
6	P	38	BCL	O2D-CGD-CBD	6.03	121.78	111.23
6	U	36	BCL	O2D-CGD-CBD	6.03	121.77	111.23
6	N	11	BCL	O2A-CGA-O1A	-5.96	105.40	123.20
6	H	6	BCL	C4A-NA-C1A	-5.95	103.96	106.68
6	N	11	BCL	O2D-CGD-CBD	5.93	121.59	111.23
6	1	38	BCL	CMB-C2B-C3B	5.90	136.47	124.68
6	7	38	BCL	C4A-NA-C1A	-5.89	103.99	106.68
6	3	39	BCL	CMB-C2B-C3B	5.88	136.43	124.68
6	W	36	BCL	C4A-NA-C1A	-5.80	104.03	106.68
6	Y	37	BCL	CMB-C2B-C3B	5.80	136.28	124.68
6	D	2	BCL	C4A-NA-C1A	-5.79	104.04	106.68
6	R	38	BCL	CMB-C2B-C3B	5.79	136.24	124.68
6	7	38	BCL	CMB-C2B-C3B	5.78	136.23	124.68
6	N	38	BCL	CMB-C2B-C3B	5.76	136.20	124.68
6	L	10	BCL	CMB-C2B-C3B	5.76	136.19	124.68
6	J	8	BCL	CMB-C2B-C3B	5.74	136.16	124.68
6	F	4	BCL	CMB-C2B-C3B	5.72	136.12	124.68
6	5	38	BCL	CMB-C2B-C3B	5.72	136.11	124.68
6	W	36	BCL	CMB-C2B-C3B	5.70	136.08	124.68
6	F	4	BCL	C4A-NA-C1A	-5.69	104.08	106.68
6	H	6	BCL	CMB-C2B-C3B	5.69	136.05	124.68
6	P	39	BCL	CMB-C2B-C3B	5.67	136.02	124.68
6	T	38	BCL	CMB-C2B-C3B	5.66	136.00	124.68
6	D	2	BCL	CMB-C2B-C3B	5.65	135.98	124.68
6	J	8	BCL	C4A-NA-C1A	-5.53	104.16	106.68
6	P	38	BCL	CED-O2D-CGD	5.42	128.22	115.92
6	A	301	BCL	CED-O2D-CGD	-5.41	103.63	115.92
6	3	39	BCL	CAC-C3C-C4C	5.29	124.32	112.58
6	Y	37	BCL	CAC-C3C-C4C	5.28	124.31	112.58
6	L	10	BCL	C2C-C3C-C4C	5.27	109.24	101.34
6	1	38	BCL	CAC-C3C-C4C	5.27	124.27	112.58
6	T	38	BCL	CAC-C3C-C4C	5.25	124.23	112.58
6	J	8	BCL	CAC-C3C-C4C	5.23	124.20	112.58
6	5	38	BCL	CAC-C3C-C4C	5.23	124.20	112.58
6	I	5	BCL	O2A-CGA-O1A	-5.23	107.58	123.20
6	P	39	BCL	CAC-C3C-C4C	5.23	124.19	112.58
6	J	8	BCL	C2C-C3C-C4C	5.23	109.17	101.34
6	H	6	BCL	CAC-C3C-C4C	5.23	124.19	112.58
6	N	38	BCL	CAC-C3C-C4C	5.23	124.18	112.58
6	H	6	BCL	C2C-C3C-C4C	5.17	109.09	101.34
6	L	10	BCL	CAC-C3C-C4C	5.17	124.06	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	36	BCL	CAC-C3C-C4C	5.17	124.06	112.58
6	F	4	BCL	CAC-C3C-C4C	5.16	124.04	112.58
6	A	301	BCL	CMB-C2B-C1B	-5.16	120.90	128.46
6	R	38	BCL	CAC-C3C-C4C	5.15	124.02	112.58
6	7	38	BCL	CAC-C3C-C4C	5.15	124.01	112.58
6	D	2	BCL	C2C-C3C-C4C	5.12	109.01	101.34
6	N	38	BCL	C2C-C3C-C4C	5.08	108.95	101.34
6	D	2	BCL	CAC-C3C-C4C	5.05	123.79	112.58
6	P	39	BCL	C2C-C3C-C4C	5.05	108.90	101.34
6	R	38	BCL	C2C-C3C-C4C	5.05	108.90	101.34
6	W	36	BCL	C2C-C3C-C4C	5.03	108.88	101.34
6	7	38	BCL	C2C-C3C-C4C	4.99	108.82	101.34
6	F	4	BCL	C2C-C3C-C4C	4.95	108.76	101.34
6	T	38	BCL	C2C-C3C-C4C	4.94	108.74	101.34
6	Y	37	BCL	C2C-C3C-C4C	4.94	108.74	101.34
6	3	39	BCL	C2C-C3C-C4C	4.90	108.68	101.34
6	5	38	BCL	C2C-C3C-C4C	4.87	108.63	101.34
6	M	36	BCL	O2A-CGA-O1A	-4.79	108.91	123.20
6	V	38	BCL	O2A-CGA-CBA	4.77	130.16	112.14
6	1	38	BCL	C2C-C3C-C4C	4.75	108.46	101.34
6	5	38	BCL	C1C-NC-C4C	-4.61	104.58	106.68
6	A	301	BCL	C4D-CHA-C1A	4.60	126.73	121.24
6	7	38	BCL	C1C-NC-C4C	-4.53	104.61	106.68
6	J	8	BCL	CHD-C1D-ND	-4.42	118.58	124.80
6	V	38	BCL	O2A-CGA-O1A	-4.42	110.00	123.20
6	W	36	BCL	CHA-C4D-ND	-4.41	123.45	132.55
6	1	38	BCL	O2D-CGD-O1D	-4.38	115.32	123.85
6	A	301	BCL	C1-O2A-CGA	4.38	127.25	116.65
6	F	4	BCL	CHA-C4D-ND	-4.37	123.54	132.55
6	B	303	BCL	CMB-C2B-C1B	-4.36	122.07	128.46
6	D	2	BCL	CHA-C4D-ND	-4.35	123.57	132.55
6	1	38	BCL	C1C-NC-C4C	-4.35	104.70	106.68
6	Y	37	BCL	CHA-C4D-ND	-4.34	123.59	132.55
6	6	36	BCL	CMB-C2B-C1B	-4.34	122.10	128.46
6	3	39	BCL	O2D-CGD-O1D	-4.33	115.42	123.85
6	H	6	BCL	CHD-C1D-ND	-4.31	118.73	124.80
6	W	36	BCL	O2D-CGD-O1D	-4.31	115.46	123.85
6	7	38	BCL	CHA-C4D-ND	-4.31	123.66	132.55
6	L	10	BCL	O2D-CGD-O1D	-4.29	115.49	123.85
6	3	39	BCL	CHA-C4D-ND	-4.28	123.71	132.55
6	L	10	BCL	CHD-C1D-ND	-4.28	118.78	124.80
6	T	38	BCL	CHA-C4D-ND	-4.28	123.72	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	8	BCL	CHA-C4D-ND	-4.28	123.72	132.55
6	R	38	BCL	O2D-CGD-O1D	-4.28	115.52	123.85
6	1	38	BCL	CHA-C4D-ND	-4.28	123.72	132.55
6	H	6	BCL	CHA-C4D-ND	-4.27	123.73	132.55
6	3	38	BCL	CMB-C2B-C1B	-4.26	122.21	128.46
6	N	38	BCL	CHA-C4D-ND	-4.26	123.76	132.55
6	N	11	BCL	CMB-C2B-C1B	-4.25	122.23	128.46
6	R	38	BCL	CHA-C4D-ND	-4.24	123.79	132.55
7	A	401	BPH	C3D-CAD-CBD	-4.24	102.02	107.61
6	3	39	BCL	C1C-NC-C4C	-4.23	104.75	106.68
6	P	39	BCL	O2D-CGD-O1D	-4.21	115.64	123.85
6	F	4	BCL	CHD-C1D-ND	-4.21	118.88	124.80
6	L	10	BCL	CHA-C4D-ND	-4.21	123.86	132.55
6	P	39	BCL	CHD-C1D-ND	-4.21	118.88	124.80
6	2	36	BCL	CMB-C2B-C1B	-4.20	122.30	128.46
6	N	38	BCL	O2D-CGD-O1D	-4.20	115.67	123.85
6	Y	36	BCL	CMB-C2B-C1B	-4.20	122.30	128.46
6	8	36	BCL	CBC-CAC-C3C	4.20	122.32	113.41
6	J	8	BCL	O2D-CGD-O1D	-4.20	115.68	123.85
6	Y	37	BCL	CHD-C1D-ND	-4.19	118.90	124.80
6	T	38	BCL	O2D-CGD-O1D	-4.19	115.69	123.85
6	M	36	BCL	CMB-C2B-C1B	-4.19	122.32	128.46
6	Y	37	BCL	O2D-CGD-O1D	-4.18	115.70	123.85
6	S	36	BCL	CMB-C2B-C1B	-4.18	122.33	128.46
6	I	5	BCL	CMB-C2B-C1B	-4.17	122.34	128.46
6	5	38	BCL	CHA-C4D-ND	-4.17	123.94	132.55
6	U	36	BCL	CMB-C2B-C1B	-4.17	122.35	128.46
6	K	36	BCL	CMB-C2B-C1B	-4.17	122.35	128.46
6	T	38	BCL	CHD-C1D-ND	-4.17	118.94	124.80
6	P	39	BCL	CHA-C4D-ND	-4.17	123.95	132.55
6	W	36	BCL	CHD-C1D-ND	-4.16	118.95	124.80
6	P	38	BCL	CMB-C2B-C1B	-4.14	122.40	128.46
6	H	6	BCL	O2D-CGD-O1D	-4.13	115.81	123.85
6	N	38	BCL	CHD-C1D-ND	-4.13	118.99	124.80
6	R	38	BCL	CHD-C1D-ND	-4.13	119.00	124.80
6	8	36	BCL	O2A-CGA-CBA	4.12	127.72	112.14
6	1	38	BCL	CHD-C1D-ND	-4.12	119.00	124.80
6	7	38	BCL	O2D-CGD-O1D	-4.12	115.82	123.85
6	6	36	BCL	CBC-CAC-C3C	4.11	122.12	113.41
6	3	39	BCL	CHD-C1D-ND	-4.11	119.02	124.80
6	8	36	BCL	CMB-C2B-C1B	-4.10	122.45	128.46
6	E	1	BCL	CMB-C2B-C1B	-4.10	122.45	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2	BCL	CHD-C1D-ND	-4.09	119.04	124.80
6	G	3	BCL	CMB-C2B-C1B	-4.09	122.46	128.46
6	A	302	BCL	C1C-NC-C4C	4.09	108.55	106.68
6	V	38	BCL	C1-O2A-CGA	4.08	129.15	116.07
6	V	38	BCL	CMB-C2B-C1B	-4.08	122.47	128.46
6	5	38	BCL	O2D-CGD-O1D	-4.07	115.94	123.85
6	D	2	BCL	O2D-CGD-O1D	-4.06	115.94	123.85
6	P	38	BCL	CBC-CAC-C3C	4.05	122.00	113.41
6	F	4	BCL	O2D-CGD-O1D	-4.04	115.98	123.85
6	N	38	BCL	C1C-NC-C4C	-4.04	104.84	106.68
6	7	38	BCL	CHD-C1D-ND	-4.02	119.15	124.80
6	P	39	BCL	C1C-NC-C4C	-4.00	104.85	106.68
6	Y	37	BCL	C1C-NC-C4C	-4.00	104.86	106.68
6	E	1	BCL	C4D-CHA-C1A	4.00	126.01	121.24
6	G	3	BCL	CBC-CAC-C3C	3.99	121.89	113.41
6	5	38	BCL	CGD-CBD-CAD	3.98	123.74	110.85
6	3	38	BCL	CAC-C3C-C4C	3.98	121.42	112.58
6	K	36	BCL	CAC-C3C-C4C	3.98	121.42	112.58
6	E	1	BCL	CAC-C3C-C4C	3.97	121.40	112.58
6	I	5	BCL	CAC-C3C-C4C	3.97	121.39	112.58
6	U	36	BCL	CBC-CAC-C3C	3.97	121.83	113.41
6	M	36	BCL	CAC-C3C-C4C	3.97	121.39	112.58
6	E	1	BCL	CBC-CAC-C3C	3.95	121.80	113.41
6	N	11	BCL	CBC-CAC-C3C	3.95	121.80	113.41
6	3	38	BCL	CBC-CAC-C3C	3.95	121.79	113.41
6	S	36	BCL	CBC-CAC-C3C	3.95	121.79	113.41
6	7	38	BCL	CGD-CBD-CAD	3.94	123.62	110.85
6	5	38	BCL	CHD-C1D-ND	-3.94	119.25	124.80
6	W	36	BCL	CGD-CBD-CAD	3.94	123.60	110.85
6	2	36	BCL	CBC-CAC-C3C	3.93	121.76	113.41
6	N	11	BCL	CAC-C3C-C4C	3.93	121.31	112.58
6	6	36	BCL	CAC-C3C-C4C	3.93	121.31	112.58
6	V	38	BCL	CBC-CAC-C3C	3.92	121.72	113.41
6	R	38	BCL	C1C-NC-C4C	-3.92	104.89	106.68
6	T	38	BCL	CGD-CBD-CAD	3.91	123.52	110.85
6	P	38	BCL	CAC-C3C-C4C	3.91	121.27	112.58
6	P	39	BCL	CGD-CBD-CAD	3.91	123.50	110.85
6	D	2	BCL	CGD-CBD-CAD	3.90	123.49	110.85
6	I	5	BCL	C4D-CHA-C1A	3.90	125.89	121.24
6	Y	36	BCL	CAC-C3C-C4C	3.88	121.20	112.58
6	R	38	BCL	CGD-CBD-CAD	3.88	123.42	110.85
6	D	2	BCL	C1C-NC-C4C	-3.88	104.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	4	BCL	CGD-CBD-CAD	3.88	123.39	110.85
6	W	36	BCL	C1C-NC-C4C	-3.86	104.92	106.68
6	G	3	BCL	CAC-C3C-C4C	3.86	121.15	112.58
6	Y	37	BCL	CGD-CBD-CAD	3.86	123.33	110.85
6	S	36	BCL	CAC-C3C-C4C	3.86	121.14	112.58
6	2	36	BCL	CHA-C4D-ND	-3.85	124.60	132.55
6	K	36	BCL	OBD-CAD-C3D	-3.85	119.42	128.42
6	3	39	BCL	CGD-CBD-CAD	3.85	123.30	110.85
6	1	38	BCL	CGD-CBD-CAD	3.85	123.30	110.85
6	K	36	BCL	CBC-CAC-C3C	3.84	121.57	113.41
6	M	36	BCL	C4D-CHA-C1A	3.84	125.83	121.24
6	I	5	BCL	CBC-CAC-C3C	3.84	121.56	113.41
6	N	38	BCL	CGD-CBD-CAD	3.84	123.28	110.85
6	H	6	BCL	CGD-CBD-CAD	3.84	123.27	110.85
6	U	36	BCL	CAC-C3C-C4C	3.84	121.10	112.58
6	E	1	BCL	CHA-C4D-ND	-3.83	124.64	132.55
6	T	38	BCL	C1C-NC-C4C	-3.83	104.93	106.68
7	A	401	BPH	C1-C2-C3	-3.83	119.93	126.20
6	2	36	BCL	CAC-C3C-C4C	3.82	121.07	112.58
6	M	36	BCL	CHA-C4D-ND	-3.82	124.66	132.55
6	8	36	BCL	CAC-C3C-C4C	3.82	121.06	112.58
6	K	36	BCL	C4D-CHA-C1A	3.82	125.80	121.24
6	V	38	BCL	CAC-C3C-C4C	3.81	121.05	112.58
6	M	36	BCL	CBC-CAC-C3C	3.81	121.49	113.41
6	L	10	BCL	C4B-CHC-C1C	-3.80	122.79	130.04
6	Y	36	BCL	CHA-C4D-ND	-3.80	124.70	132.55
6	Y	36	BCL	CBC-CAC-C3C	3.79	121.46	113.41
6	V	38	BCL	O1D-CGD-CBD	-3.78	117.06	124.52
6	K	36	BCL	O1D-CGD-CBD	-3.78	117.06	124.52
6	K	36	BCL	CHA-C4D-ND	-3.78	124.76	132.55
6	S	36	BCL	CHA-C4D-ND	-3.76	124.78	132.55
6	J	8	BCL	C4B-CHC-C1C	-3.76	122.86	130.04
6	G	3	BCL	CHA-C4D-ND	-3.76	124.79	132.55
6	U	36	BCL	CHA-C4D-ND	-3.76	124.80	132.55
6	V	38	BCL	CHA-C4D-ND	-3.76	124.80	132.55
6	L	10	BCL	CGD-CBD-CAD	3.75	123.00	110.85
6	M	36	BCL	OBD-CAD-C3D	-3.75	119.65	128.42
6	H	6	BCL	C4B-CHC-C1C	-3.75	122.89	130.04
6	I	5	BCL	CHA-C4D-ND	-3.75	124.82	132.55
6	P	38	BCL	OBD-CAD-C3D	-3.73	119.69	128.42
6	U	36	BCL	OBD-CAD-C3D	-3.73	119.69	128.42
6	S	36	BCL	OBD-CAD-C3D	-3.72	119.73	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	4	BCL	C1C-NC-C4C	-3.72	104.98	106.68
6	S	36	BCL	O1D-CGD-CBD	-3.71	117.19	124.52
6	V	38	BCL	OBD-CAD-C3D	-3.71	119.74	128.42
6	8	36	BCL	O1D-CGD-CBD	-3.71	117.20	124.52
6	M	36	BCL	O1D-CGD-CBD	-3.71	117.21	124.52
6	P	38	BCL	C4D-CHA-C1A	3.71	125.67	121.24
6	N	11	BCL	CHA-C4D-ND	-3.70	124.90	132.55
6	G	3	BCL	C4D-CHA-C1A	3.70	125.66	121.24
6	G	3	BCL	O1D-CGD-CBD	-3.70	117.23	124.52
6	G	3	BCL	OBD-CAD-C3D	-3.70	119.78	128.42
6	8	36	BCL	CHA-C4D-ND	-3.69	124.94	132.55
6	P	39	BCL	C4B-CHC-C1C	-3.68	123.02	130.04
6	Y	36	BCL	C4A-NA-C1A	3.68	108.36	106.68
6	I	5	BCL	O1D-CGD-CBD	-3.67	117.28	124.52
6	P	38	BCL	CHA-C4D-ND	-3.67	124.98	132.55
6	S	36	BCL	C4D-CHA-C1A	3.66	125.61	121.24
6	J	8	BCL	CGD-CBD-CAD	3.66	122.69	110.85
6	H	6	BCL	C1C-NC-C4C	-3.66	105.01	106.68
6	E	1	BCL	O1D-CGD-CBD	-3.65	117.32	124.52
6	R	38	BCL	C4B-CHC-C1C	-3.65	123.08	130.04
6	T	38	BCL	C4B-CHC-C1C	-3.65	123.08	130.04
6	I	5	BCL	OBD-CAD-C3D	-3.65	119.89	128.42
6	P	38	BCL	O1D-CGD-CBD	-3.65	117.33	124.52
6	B	303	BCL	C4A-NA-C1A	3.64	108.34	106.68
6	2	36	BCL	O1D-CGD-CBD	-3.64	117.34	124.52
6	U	36	BCL	O1D-CGD-CBD	-3.64	117.35	124.52
6	Y	36	BCL	C4D-CHA-C1A	3.64	125.58	121.24
6	N	11	BCL	O1D-CGD-CBD	-3.63	117.35	124.52
6	E	1	BCL	OBD-CAD-C3D	-3.63	119.93	128.42
6	N	11	BCL	OBD-CAD-C3D	-3.63	119.93	128.42
6	Y	36	BCL	O1D-CGD-CBD	-3.63	117.36	124.52
6	U	36	BCL	C4D-CHA-C1A	3.63	125.57	121.24
6	S	36	BCL	O2A-CGA-O1A	-3.62	112.39	123.20
6	N	38	BCL	C4B-CHC-C1C	-3.62	123.14	130.04
6	6	36	BCL	O1D-CGD-CBD	-3.62	117.39	124.52
6	6	36	BCL	CHA-C4D-ND	-3.61	125.10	132.55
6	Y	36	BCL	OBD-CAD-C3D	-3.61	119.98	128.42
6	8	36	BCL	C4D-CHA-C1A	3.60	125.53	121.24
6	5	38	BCL	C4B-CHC-C1C	-3.59	123.19	130.04
6	G	3	BCL	C1-O2A-CGA	3.58	127.54	116.07
6	2	36	BCL	C4D-CHA-C1A	3.57	125.51	121.24
6	2	36	BCL	OBD-CAD-C3D	-3.57	120.07	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	3	39	BCL	C4B-CHC-C1C	-3.57	123.23	130.04
6	3	38	BCL	CHA-C4D-ND	-3.56	125.20	132.55
6	D	2	BCL	C4B-CHC-C1C	-3.56	123.25	130.04
6	V	38	BCL	C4D-CHA-C1A	3.55	125.48	121.24
6	3	38	BCL	OBD-CAD-C3D	-3.55	120.12	128.42
6	3	38	BCL	O1D-CGD-CBD	-3.54	117.53	124.52
6	8	36	BCL	O2A-CGA-O1A	-3.54	112.64	123.20
6	8	36	BCL	OBD-CAD-C3D	-3.54	120.15	128.42
6	F	4	BCL	C4B-CHC-C1C	-3.54	123.30	130.04
6	B	304	BCL	CMB-C2B-C1B	-3.52	123.30	128.46
6	V	38	BCL	CED-O2D-CGD	3.51	123.88	115.92
6	6	36	BCL	OBD-CAD-C3D	-3.50	120.24	128.42
6	N	11	BCL	C4D-CHA-C1A	3.48	125.40	121.24
6	W	36	BCL	C4B-CHC-C1C	-3.48	123.40	130.04
6	L	10	BCL	C1C-NC-C4C	-3.47	105.09	106.68
6	7	38	BCL	C4B-CHC-C1C	-3.47	123.42	130.04
6	1	38	BCL	C4B-CHC-C1C	-3.47	123.43	130.04
6	Y	37	BCL	C4B-CHC-C1C	-3.45	123.45	130.04
6	I	5	BCL	O1A-CGA-CBA	3.43	137.20	123.78
6	2	36	BCL	C4A-NA-C1A	3.42	108.24	106.68
6	B	303	BCL	C4D-CHA-C1A	3.40	125.30	121.24
6	K	36	BCL	CMD-C2D-C3D	3.39	135.46	127.69
6	G	3	BCL	CMD-C2D-C3D	3.38	135.44	127.69
6	J	8	BCL	C2A-C1A-CHA	-3.36	118.03	123.87
6	6	36	BCL	C4D-CHA-C1A	3.36	125.25	121.24
7	A	401	BPH	O1D-CGD-CBD	3.35	129.81	124.72
6	B	303	BCL	C1C-NC-C4C	3.34	108.20	106.68
6	P	38	BCL	CMD-C2D-C3D	3.32	135.30	127.69
6	I	5	BCL	CMD-C2D-C3D	3.31	135.29	127.69
6	B	304	BCL	CAA-C2A-C3A	-3.31	104.05	113.00
6	3	38	BCL	CMD-C2D-C3D	3.31	135.28	127.69
7	B	402	BPH	CMA-C3A-C4A	-3.31	107.48	114.61
6	3	38	BCL	C4D-CHA-C1A	3.31	125.19	121.24
6	L	10	BCL	C2A-C1A-CHA	-3.30	118.14	123.87
6	N	38	BCL	C2A-C1A-CHA	-3.30	118.14	123.87
6	5	38	BCL	C1-O2A-CGA	-3.30	105.51	116.07
6	P	39	BCL	C2A-C1A-CHA	-3.29	118.16	123.87
6	H	6	BCL	C2A-C1A-CHA	-3.29	118.16	123.87
6	8	36	BCL	CMD-C2D-C3D	3.27	135.19	127.69
6	S	36	BCL	CMD-C2D-C3D	3.27	135.18	127.69
6	M	36	BCL	CMD-C2D-C3D	3.26	135.17	127.69
6	M	36	BCL	O1A-CGA-CBA	3.26	136.52	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	36	BCL	CED-O2D-CGD	3.26	123.30	115.92
6	E	1	BCL	CMD-C2D-C3D	3.25	135.14	127.69
6	J	8	BCL	C1C-NC-C4C	-3.25	105.20	106.68
6	N	11	BCL	CMD-C2D-C3D	3.24	135.13	127.69
6	7	38	BCL	C2A-C1A-CHA	-3.24	118.24	123.87
6	V	38	BCL	C4A-NA-C1A	3.24	108.16	106.68
6	A	301	BCL	OBB-CAB-CBB	-3.24	113.29	120.19
6	U	36	BCL	CMD-C2D-C3D	3.24	135.11	127.69
6	A	302	BCL	CHA-C1A-NA	-3.21	119.12	126.39
6	6	36	BCL	CMD-C2D-C3D	3.19	135.02	127.69
6	3	39	BCL	C2A-C1A-CHA	-3.19	118.33	123.87
6	A	302	BCL	CMB-C2B-C1B	-3.18	123.79	128.46
6	V	38	BCL	CMD-C2D-C3D	3.18	134.98	127.69
6	R	38	BCL	C2A-C1A-CHA	-3.18	118.35	123.87
6	A	302	BCL	C4D-CHA-C1A	3.16	125.02	121.24
6	Y	37	BCL	C2A-C1A-CHA	-3.16	118.38	123.87
6	D	2	BCL	C2A-C1A-CHA	-3.16	118.38	123.87
6	F	4	BCL	C2A-C1A-CHA	-3.16	118.38	123.87
6	T	38	BCL	C2A-C1A-CHA	-3.16	118.39	123.87
6	I	5	BCL	C4A-NA-C1A	3.15	108.12	106.68
6	K	36	BCL	CED-O2D-CGD	3.15	123.07	115.92
6	M	36	BCL	C4A-NA-C1A	3.14	108.11	106.68
6	2	36	BCL	CMD-C2D-C3D	3.14	134.88	127.69
6	Y	36	BCL	CMD-C2D-C3D	3.13	134.87	127.69
7	A	401	BPH	CMA-C3A-C4A	-3.12	107.89	114.61
6	5	38	BCL	C2A-C1A-CHA	-3.11	118.48	123.87
6	W	36	BCL	C2A-C1A-CHA	-3.09	118.51	123.87
6	1	38	BCL	C2A-C1A-CHA	-3.09	118.51	123.87
6	A	301	BCL	CAA-C2A-C3A	-3.08	104.69	113.00
6	A	301	BCL	CMB-C2B-C3B	3.06	130.79	124.68
6	W	36	BCL	C4D-CHA-C1A	3.05	124.89	121.24
6	A	301	BCL	OBB-CAB-C3B	3.04	125.07	119.99
7	B	402	BPH	O2A-CGA-O1A	-3.03	116.05	123.63
6	V	38	BCL	CMA-C3A-C4A	-3.01	103.69	111.77
6	1	38	BCL	C4D-CHA-C1A	3.00	124.83	121.24
6	S	36	BCL	CMA-C3A-C4A	-2.99	103.74	111.77
6	G	3	BCL	C4A-NA-C1A	2.97	108.03	106.68
6	U	36	BCL	CMA-C3A-C4A	-2.96	103.83	111.77
6	B	304	BCL	CHA-C1A-NA	-2.95	119.72	126.39
6	P	38	BCL	CMA-C3A-C4A	-2.93	103.90	111.77
6	Y	37	BCL	C4D-CHA-C1A	2.93	124.74	121.24
6	N	11	BCL	CMA-C3A-C4A	-2.92	103.91	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	36	BCL	CMA-C3A-C4A	-2.92	103.93	111.77
6	A	302	BCL	OBB-CAB-CBB	-2.91	113.98	120.19
6	5	38	BCL	C4D-CHA-C1A	2.90	124.70	121.24
6	P	38	BCL	C4A-NA-C1A	2.90	108.00	106.68
6	Y	36	BCL	CMA-C3A-C4A	-2.90	103.98	111.77
6	U	36	BCL	C4A-NA-C1A	2.90	108.00	106.68
7	A	401	BPH	O2D-CGD-CBD	-2.89	107.77	110.95
6	I	5	BCL	CHB-C4A-NA	2.88	128.56	124.40
6	E	1	BCL	C4A-NA-C1A	2.88	107.99	106.68
6	G	3	BCL	CMA-C3A-C4A	-2.88	104.05	111.77
6	F	4	BCL	C4D-CHA-C1A	2.87	124.67	121.24
6	D	2	BCL	C4D-CHA-C1A	2.86	124.66	121.24
6	E	1	BCL	CMA-C3A-C4A	-2.86	104.08	111.77
6	A	302	BCL	CAA-C2A-C3A	-2.86	105.28	113.00
6	M	36	BCL	CED-O2D-CGD	2.85	122.39	115.92
6	H	6	BCL	O1D-CGD-CBD	-2.85	118.89	124.52
6	M	36	BCL	CMA-C3A-C4A	-2.85	104.11	111.77
6	A	301	BCL	CHA-C1A-NA	-2.85	119.94	126.39
6	6	36	BCL	CMA-C3A-C4A	-2.84	104.13	111.77
6	3	39	BCL	C4D-CHA-C1A	2.84	124.63	121.24
6	A	301	BCL	C5-C3-C2	2.84	127.54	121.17
6	S	36	BCL	CMB-C2B-C3B	2.84	130.36	124.68
6	N	11	BCL	CAA-CBA-CGA	2.84	121.26	113.21
6	A	302	BCL	CMA-C3A-C2A	-2.83	103.04	113.98
6	T	38	BCL	C4D-CHA-C1A	2.83	124.61	121.24
6	K	36	BCL	CMA-C3A-C4A	-2.82	104.18	111.77
6	Y	36	BCL	CHB-C4A-NA	2.82	128.47	124.40
6	K	36	BCL	CAA-CBA-CGA	2.82	121.21	113.21
6	F	4	BCL	O1D-CGD-CBD	-2.81	118.97	124.52
6	U	36	BCL	CMB-C2B-C3B	2.81	130.29	124.68
6	8	36	BCL	CMA-C3A-C4A	-2.81	104.23	111.77
6	I	5	BCL	CMB-C2B-C3B	2.80	130.28	124.68
6	3	38	BCL	CMA-C3A-C4A	-2.80	104.25	111.77
6	A	302	BCL	C15-C13-C12	-2.79	97.92	112.07
6	I	5	BCL	CMA-C3A-C4A	-2.79	104.27	111.77
6	S	36	BCL	C4A-NA-C1A	2.79	107.95	106.68
6	D	2	BCL	O1D-CGD-CBD	-2.78	119.03	124.52
6	J	8	BCL	O1D-CGD-CBD	-2.78	119.03	124.52
6	Y	36	BCL	CAA-CBA-CGA	2.78	121.10	113.21
7	A	401	BPH	C7-C6-C5	-2.78	105.86	113.26
6	R	38	BCL	C4D-CHA-C1A	2.78	124.56	121.24
6	E	1	BCL	O2A-CGA-CBA	2.77	122.61	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	BCL	C1C-NC-C4C	2.77	107.94	106.68
6	M	36	BCL	CAA-CBA-CGA	2.77	121.06	113.21
7	B	402	BPH	CAA-C2A-C3A	-2.77	105.53	113.00
6	G	3	BCL	CAA-CBA-CGA	2.76	121.06	113.21
6	G	3	BCL	CHB-C4A-NA	2.76	128.39	124.40
6	K	36	BCL	CMB-C2B-C3B	2.76	130.20	124.68
6	7	38	BCL	C4D-CHA-C1A	2.76	124.53	121.24
6	M	36	BCL	CHB-C4A-NA	2.76	128.38	124.40
6	N	11	BCL	CMB-C2B-C3B	2.76	130.19	124.68
6	V	38	BCL	CHB-C4A-NA	2.76	128.38	124.40
6	E	1	BCL	CAA-CBA-CGA	2.75	121.03	113.21
6	P	38	BCL	CAA-CBA-CGA	2.75	121.02	113.21
6	E	1	BCL	CMB-C2B-C3B	2.74	130.17	124.68
6	2	36	BCL	CAA-CBA-CGA	2.74	121.00	113.21
6	P	38	BCL	CMB-C2B-C3B	2.74	130.16	124.68
6	A	302	BCL	O2D-CGD-CBD	2.74	116.02	111.23
6	U	36	BCL	CHB-C4A-NA	2.74	128.35	124.40
6	N	38	BCL	O1D-CGD-CBD	-2.74	119.12	124.52
6	M	36	BCL	CMB-C2B-C3B	2.73	130.14	124.68
6	7	38	BCL	O1D-CGD-CBD	-2.73	119.13	124.52
6	2	36	BCL	CHB-C4A-NA	2.73	128.34	124.40
6	E	1	BCL	CED-O2D-CGD	2.73	122.11	115.92
6	B	303	BCL	CHA-C1A-NA	-2.72	120.22	126.39
6	B	304	BCL	C4D-CHA-C1A	2.72	124.48	121.24
6	L	10	BCL	C4D-CHA-C1A	2.72	124.48	121.24
6	U	36	BCL	CAA-CBA-CGA	2.71	120.91	113.21
6	V	38	BCL	CMB-C2B-C3B	2.71	130.10	124.68
6	G	3	BCL	CMB-C2B-C3B	2.71	130.09	124.68
6	B	304	BCL	C4-C3-C5	2.71	119.92	115.23
6	P	38	BCL	CHB-C4A-NA	2.70	128.30	124.40
6	B	303	BCL	O2D-CGD-O1D	-2.70	118.59	123.85
6	S	36	BCL	CAA-CBA-CGA	2.70	120.87	113.21
6	8	36	BCL	CMB-C2B-C3B	2.69	130.06	124.68
6	V	38	BCL	CAA-CBA-CGA	2.69	120.85	113.21
6	Y	36	BCL	CMB-C2B-C3B	2.69	130.05	124.68
6	6	36	BCL	CAA-CBA-CGA	2.69	120.83	113.21
6	N	11	BCL	CED-O2D-CGD	2.68	122.00	115.92
6	N	38	BCL	C4D-CHA-C1A	2.68	124.44	121.24
6	A	302	BCL	O1D-CGD-CBD	-2.68	119.23	124.52
6	I	5	BCL	CAA-CBA-CGA	2.68	120.82	113.21
6	S	36	BCL	CHB-C4A-NA	2.68	128.27	124.40
6	3	38	BCL	CAA-CBA-CGA	2.68	120.81	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	37	BCL	O1D-CGD-CBD	-2.67	119.24	124.52
6	I	5	BCL	CED-O2D-CGD	2.67	121.98	115.92
6	8	36	BCL	CAA-CBA-CGA	2.67	120.79	113.21
6	3	38	BCL	CMB-C2B-C3B	2.66	130.01	124.68
6	W	36	BCL	O1D-CGD-CBD	-2.66	119.28	124.52
6	5	38	BCL	O1D-CGD-CBD	-2.66	119.28	124.52
6	6	36	BCL	CMB-C2B-C3B	2.65	129.98	124.68
6	B	303	BCL	CHD-C1D-ND	-2.65	121.08	124.80
6	G	3	BCL	CED-O2D-CGD	2.65	121.92	115.92
6	3	38	BCL	O2A-CGA-O1A	-2.63	115.35	123.20
6	3	38	BCL	CHB-C4A-NA	2.62	128.18	124.40
6	A	301	BCL	C4-C3-C2	-2.62	116.90	123.63
6	R	38	BCL	O1D-CGD-CBD	-2.62	119.35	124.52
6	L	10	BCL	O1D-CGD-CBD	-2.62	119.36	124.52
6	B	304	BCL	C4B-C3B-CAB	-2.61	122.11	127.08
6	1	38	BCL	O1D-CGD-CBD	-2.61	119.37	124.52
6	E	1	BCL	CHB-C4A-NA	2.61	128.16	124.40
6	2	36	BCL	O2A-CGA-CBA	2.61	121.98	112.14
6	6	36	BCL	C4A-NA-C1A	2.60	107.87	106.68
6	2	36	BCL	CMB-C2B-C3B	2.60	129.88	124.68
6	5	38	BCL	CHB-C4A-NA	-2.59	120.66	124.40
6	N	11	BCL	CHB-C4A-NA	2.59	128.13	124.40
6	A	302	BCL	C2C-C3C-C4C	2.59	105.21	101.34
6	T	38	BCL	O1D-CGD-CBD	-2.58	119.44	124.52
6	P	39	BCL	O1D-CGD-CBD	-2.57	119.44	124.52
6	H	6	BCL	C4D-CHA-C1A	2.57	124.31	121.24
6	L	10	BCL	CHB-C4A-NA	-2.57	120.69	124.40
6	P	39	BCL	C4D-CHA-C1A	2.56	124.30	121.24
6	3	39	BCL	O1D-CGD-CBD	-2.56	119.46	124.52
6	A	302	BCL	CHD-C1D-ND	-2.55	121.21	124.80
6	R	38	BCL	CHB-C4A-NA	-2.55	120.72	124.40
6	A	301	BCL	O2A-CGA-O1A	-2.54	117.28	123.63
6	A	302	BCL	C17-C16-C15	-2.54	101.91	113.28
6	K	36	BCL	CHB-C4A-NA	2.53	128.06	124.40
6	J	8	BCL	C4D-CHA-C1A	2.52	124.25	121.24
6	P	39	BCL	CHB-C4A-NA	-2.52	120.76	124.40
6	Y	37	BCL	CHB-C4A-NA	-2.52	120.76	124.40
6	6	36	BCL	CHB-C4A-NA	2.52	128.03	124.40
6	N	11	BCL	C4A-NA-C1A	2.51	107.83	106.68
6	3	38	BCL	C4A-NA-C1A	2.51	107.82	106.68
6	3	39	BCL	CHB-C4A-NA	-2.51	120.78	124.40
6	Y	37	BCL	C2D-C1D-ND	2.49	112.59	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	401	BPH	CAA-C2A-C3A	-2.49	106.28	113.00
6	A	301	BCL	C6-C5-C3	-2.48	107.42	113.47
6	1	38	BCL	CHB-C4A-NA	-2.48	120.82	124.40
6	T	38	BCL	CHB-C4A-NA	-2.48	120.82	124.40
6	B	303	BCL	CAC-C3C-C4C	-2.47	107.09	112.58
6	W	36	BCL	CAA-C2A-C1A	-2.47	103.89	111.97
6	A	301	BCL	CMA-C3A-C2A	-2.46	104.46	113.98
6	L	10	BCL	C2D-C1D-ND	2.46	112.56	110.13
6	8	36	BCL	CHB-C4A-NA	2.46	127.95	124.40
6	6	36	BCL	CHC-C1C-NC	-2.45	120.86	124.40
6	B	303	BCL	C1-C2-C3	-2.45	122.18	126.20
6	N	38	BCL	CHB-C4A-NA	-2.45	120.87	124.40
6	B	303	BCL	CMB-C2B-C3B	2.44	129.56	124.68
6	T	38	BCL	CAA-C2A-C1A	-2.44	103.98	111.97
6	R	38	BCL	CAA-C2A-C1A	-2.42	104.05	111.97
6	B	303	BCL	CMD-C2D-C1D	2.41	128.96	124.73
6	Y	37	BCL	CAA-C2A-C1A	-2.40	104.10	111.97
6	B	304	BCL	O2D-CGD-CBD	2.40	115.42	111.23
6	F	4	BCL	C2D-C1D-ND	2.40	112.50	110.13
6	W	36	BCL	C2D-C1D-ND	2.40	112.50	110.13
6	K	36	BCL	CMA-C3A-C2A	-2.40	104.72	113.98
6	D	2	BCL	C2D-C1D-ND	2.39	112.49	110.13
6	Y	36	BCL	C2A-C3A-C4A	2.39	105.73	101.87
6	A	302	BCL	C4B-C3B-CAB	-2.39	122.53	127.08
6	P	39	BCL	CAA-C2A-C1A	-2.38	104.16	111.97
6	5	38	BCL	CAA-C2A-C1A	-2.38	104.16	111.97
6	1	38	BCL	CAA-C2A-C1A	-2.38	104.17	111.97
6	B	303	BCL	CHD-C1D-C2D	2.36	130.40	125.49
6	D	2	BCL	CAA-C2A-C1A	-2.36	104.23	111.97
7	A	401	BPH	CHA-C4D-C3D	2.36	115.91	111.19
6	A	301	BCL	CHD-C1D-ND	-2.36	121.48	124.80
6	H	6	BCL	CHB-C4A-NA	-2.36	120.99	124.40
6	2	36	BCL	CMA-C3A-C2A	-2.35	104.89	113.98
6	3	38	BCL	CMA-C3A-C2A	-2.35	104.90	113.98
6	A	301	BCL	C4B-C3B-CAB	-2.35	122.61	127.08
6	J	8	BCL	CHB-C4A-NA	-2.35	121.01	124.40
6	B	304	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
6	1	38	BCL	C2D-C1D-ND	2.34	112.44	110.13
6	7	38	BCL	CHB-C4A-NA	-2.34	121.02	124.40
6	N	11	BCL	CHC-C1C-NC	-2.34	121.02	124.40
6	W	36	BCL	CHB-C4A-NA	-2.34	121.03	124.40
6	N	38	BCL	CAA-C2A-C1A	-2.33	104.33	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	10	BCL	CAA-C2A-C1A	-2.33	104.35	111.97
6	3	39	BCL	CAA-C2A-C1A	-2.33	104.35	111.97
6	2	36	BCL	C2A-C3A-C4A	2.32	105.62	101.87
7	A	401	BPH	CMB-C2B-C3B	2.32	129.33	124.68
6	B	304	BCL	OBB-CAB-CBB	-2.32	115.24	120.19
6	N	11	BCL	C2A-C3A-C4A	2.32	105.62	101.87
6	3	38	BCL	C2A-C3A-C4A	2.32	105.62	101.87
6	D	2	BCL	CHB-C4A-NA	-2.32	121.05	124.40
6	N	11	BCL	CMA-C3A-C2A	-2.32	105.02	113.98
6	F	4	BCL	CHB-C4A-NA	-2.32	121.05	124.40
6	3	39	BCL	C2D-C1D-ND	2.32	112.42	110.13
6	Y	36	BCL	CMA-C3A-C2A	-2.31	105.04	113.98
6	F	4	BCL	CAA-C2A-C1A	-2.31	104.41	111.97
6	A	302	BCL	C14-C13-C15	2.31	119.50	111.27
6	6	36	BCL	C2A-C3A-C4A	2.30	105.59	101.87
6	P	38	BCL	CHC-C1C-NC	-2.30	121.07	124.40
6	I	5	BCL	CMA-C3A-C2A	-2.30	105.08	113.98
6	7	38	BCL	CAA-C2A-C1A	-2.30	104.44	111.97
6	J	8	BCL	C2D-C1D-ND	2.29	112.39	110.13
6	H	6	BCL	CAA-C2A-C1A	-2.29	104.48	111.97
7	A	401	BPH	C1-O2A-CGA	2.29	122.19	116.65
6	6	36	BCL	CMA-C3A-C2A	-2.28	105.16	113.98
6	S	36	BCL	O1A-CGA-CBA	2.28	132.70	123.78
6	S	36	BCL	C2A-C3A-C4A	2.28	105.55	101.87
6	6	36	BCL	O2A-CGA-CBA	2.28	120.75	112.14
6	M	36	BCL	CMA-C3A-C2A	-2.27	105.20	113.98
6	H	6	BCL	C2D-C1D-ND	2.26	112.37	110.13
6	K	36	BCL	CHC-C1C-NC	-2.26	121.14	124.40
6	I	5	BCL	C1B-CHB-C4A	-2.26	125.74	130.04
6	T	38	BCL	C2D-C1D-ND	2.25	112.36	110.13
6	A	301	BCL	CHD-C1D-C2D	2.25	130.16	125.49
6	P	38	BCL	CMA-C3A-C2A	-2.25	105.30	113.98
6	8	36	BCL	CHC-C1C-NC	-2.24	121.17	124.40
6	G	3	BCL	CMA-C3A-C2A	-2.23	105.35	113.98
6	S	36	BCL	CHC-C1C-NC	-2.22	121.19	124.40
6	J	8	BCL	CAA-C2A-C1A	-2.22	104.71	111.97
6	V	38	BCL	C2A-C3A-C4A	2.22	105.45	101.87
7	A	401	BPH	C4B-NB-C1B	2.21	111.63	107.09
6	A	302	BCL	O2A-CGA-O1A	-2.21	118.11	123.63
6	U	36	BCL	CMA-C3A-C2A	-2.21	105.46	113.98
6	8	36	BCL	C4A-NA-C1A	2.20	107.68	106.68
6	V	38	BCL	CMA-C3A-C2A	-2.20	105.48	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	36	BCL	C1B-CHB-C4A	-2.20	125.85	130.04
6	7	38	BCL	C2D-C1D-ND	2.19	112.30	110.13
6	U	36	BCL	C2A-C3A-C4A	2.19	105.41	101.87
6	K	36	BCL	C4A-NA-C1A	2.18	107.67	106.68
6	A	301	BCL	OBD-CAD-C3D	2.17	133.49	128.42
6	S	36	BCL	CMA-C3A-C2A	-2.17	105.61	113.98
6	3	38	BCL	CHC-C1C-NC	-2.16	121.28	124.40
6	I	5	BCL	CHC-C1C-NC	-2.16	121.28	124.40
6	8	36	BCL	C2A-C3A-C4A	2.16	105.35	101.87
6	M	36	BCL	C2A-C3A-C4A	2.15	105.35	101.87
6	B	304	BCL	CMA-C3A-C2A	-2.15	105.66	113.98
6	M	36	BCL	CHC-C1C-NC	-2.15	121.29	124.40
6	P	39	BCL	C2D-C1D-ND	2.15	112.25	110.13
7	B	402	BPH	CMB-C2B-C3B	2.15	128.98	124.68
6	5	38	BCL	C2D-C1D-ND	2.15	112.25	110.13
6	U	36	BCL	C1B-CHB-C4A	-2.14	125.95	130.04
6	R	38	BCL	C2D-C1D-ND	2.14	112.25	110.13
6	N	38	BCL	C2D-C1D-ND	2.14	112.24	110.13
6	E	1	BCL	CMA-C3A-C2A	-2.14	105.71	113.98
6	K	36	BCL	C1B-CHB-C4A	-2.14	125.96	130.04
6	8	36	BCL	CAA-C2A-C3A	2.14	118.78	113.00
6	8	36	BCL	C1B-CHB-C4A	-2.14	125.97	130.04
6	G	3	BCL	C1B-CHB-C4A	-2.13	125.97	130.04
6	I	5	BCL	C2A-C3A-C4A	2.13	105.31	101.87
6	G	3	BCL	C2A-C3A-C4A	2.13	105.31	101.87
6	E	1	BCL	C1B-CHB-C4A	-2.13	125.98	130.04
6	8	36	BCL	CMA-C3A-C2A	-2.13	105.76	113.98
6	2	36	BCL	CHC-C1C-NC	-2.12	121.33	124.40
6	K	36	BCL	C3D-C2D-C1D	-2.12	102.94	105.83
6	V	38	BCL	CHC-C1C-NC	-2.12	121.34	124.40
6	Y	36	BCL	CHC-C1C-NC	-2.11	121.35	124.40
6	P	38	BCL	C2A-C3A-C4A	2.11	105.28	101.87
6	G	3	BCL	CHC-C1C-NC	-2.11	121.36	124.40
6	N	11	BCL	C1B-CHB-C4A	-2.11	126.02	130.04
6	E	1	BCL	CHC-C1C-NC	-2.11	121.36	124.40
6	P	38	BCL	C1B-CHB-C4A	-2.10	126.03	130.04
6	B	304	BCL	C5-C3-C2	-2.10	116.44	121.17
6	U	36	BCL	CHC-C1C-NC	-2.10	121.36	124.40
6	E	1	BCL	C2A-C3A-C4A	2.10	105.26	101.87
6	S	36	BCL	C1B-CHB-C4A	-2.10	126.04	130.04
6	8	36	BCL	CBA-CAA-C2A	-2.10	107.56	113.79
6	B	304	BCL	CMB-C2B-C3B	2.09	128.86	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	303	BCL	O2A-C1-C2	2.08	116.13	108.11
6	8	36	BCL	CED-O2D-CGD	2.07	120.62	115.92
6	G	3	BCL	C3D-C2D-C1D	-2.07	103.00	105.83
6	I	5	BCL	CBA-CAA-C2A	-2.06	107.67	113.79
6	S	36	BCL	CBA-CAA-C2A	-2.06	107.67	113.79
6	A	301	BCL	C2C-C3C-C4C	2.06	104.42	101.34
6	S	36	BCL	CAA-C2A-C3A	2.05	118.55	113.00
6	V	38	BCL	C1B-CHB-C4A	-2.05	126.12	130.04
6	B	304	BCL	C1C-NC-C4C	-2.04	105.75	106.68
6	E	1	BCL	CBA-CAA-C2A	-2.04	107.72	113.79
7	B	402	BPH	C4B-NB-C1B	2.04	111.28	107.09
6	I	5	BCL	C3D-C2D-C1D	-2.04	103.05	105.83
6	B	303	BCL	O2D-CGD-CBD	2.03	114.78	111.23
6	E	1	BCL	CAA-C2A-C3A	2.03	118.48	113.00
6	6	36	BCL	CBA-CAA-C2A	-2.03	107.76	113.79
6	Y	36	BCL	CBA-CAA-C2A	-2.02	107.78	113.79
6	6	36	BCL	C1B-CHB-C4A	-2.02	126.19	130.04
6	U	36	BCL	CBA-CAA-C2A	-2.01	107.81	113.79
6	Y	36	BCL	C1B-CHB-C4A	-2.01	126.21	130.04
6	G	3	BCL	CBA-CAA-C2A	-2.01	107.83	113.79
6	A	301	BCL	CMA-C3A-C4A	-2.00	106.39	111.77

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	302	BCL	C14-C13-C15-C16
6	D	2	BCL	C4C-C3C-CAC-CBC
6	E	1	BCL	C1A-C2A-CAA-CBA
6	E	1	BCL	C3A-C2A-CAA-CBA
6	F	4	BCL	C3A-C2A-CAA-CBA
6	F	4	BCL	C4C-C3C-CAC-CBC
6	H	6	BCL	C1A-C2A-CAA-CBA
6	H	6	BCL	C4C-C3C-CAC-CBC
6	J	8	BCL	C4C-C3C-CAC-CBC
6	L	10	BCL	C1A-C2A-CAA-CBA
6	L	10	BCL	C3A-C2A-CAA-CBA
6	L	10	BCL	C4C-C3C-CAC-CBC
6	L	10	BCL	CBD-CGD-O2D-CED
6	M	36	BCL	C3A-C2A-CAA-CBA
6	N	11	BCL	C3A-C2A-CAA-CBA
6	N	38	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	P	39	BCL	C4C-C3C-CAC-CBC
6	R	38	BCL	C3A-C2A-CAA-CBA
6	R	38	BCL	C4C-C3C-CAC-CBC
6	S	36	BCL	C1A-C2A-CAA-CBA
6	T	38	BCL	C4C-C3C-CAC-CBC
6	U	36	BCL	C1A-C2A-CAA-CBA
6	U	36	BCL	C3A-C2A-CAA-CBA
6	V	38	BCL	C3A-C2A-CAA-CBA
6	W	36	BCL	C3A-C2A-CAA-CBA
6	W	36	BCL	C4C-C3C-CAC-CBC
6	Y	36	BCL	CBD-CGD-O2D-CED
6	Y	36	BCL	O1D-CGD-O2D-CED
6	Y	37	BCL	C4C-C3C-CAC-CBC
6	1	38	BCL	C3A-C2A-CAA-CBA
6	1	38	BCL	C4C-C3C-CAC-CBC
6	3	39	BCL	C4C-C3C-CAC-CBC
6	5	38	BCL	C3A-C2A-CAA-CBA
6	5	38	BCL	C4C-C3C-CAC-CBC
6	6	36	BCL	C1A-C2A-CAA-CBA
6	7	38	BCL	C4C-C3C-CAC-CBC
6	V	38	BCL	O1D-CGD-O2D-CED
6	V	38	BCL	CBD-CGD-O2D-CED
6	L	10	BCL	O1D-CGD-O2D-CED
6	T	38	BCL	C2A-CAA-CBA-CGA
6	V	38	BCL	C2A-CAA-CBA-CGA
6	A	301	BCL	C3-C5-C6-C7
6	A	301	BCL	C11-C10-C8-C9
6	E	1	BCL	C2A-CAA-CBA-CGA
6	G	3	BCL	C2A-CAA-CBA-CGA
6	A	302	BCL	C15-C16-C17-C18
6	B	304	BCL	C13-C15-C16-C17
6	A	301	BCL	C13-C15-C16-C17
6	A	301	BCL	C16-C17-C18-C19
6	A	301	BCL	C8-C10-C11-C12
6	A	302	BCL	C13-C15-C16-C17
6	D	2	BCL	C3A-C2A-CAA-CBA
6	H	6	BCL	C3A-C2A-CAA-CBA
6	I	5	BCL	C3A-C2A-CAA-CBA
6	P	39	BCL	C3A-C2A-CAA-CBA
6	Y	36	BCL	C3A-C2A-CAA-CBA
6	6	36	BCL	C3A-C2A-CAA-CBA
7	A	401	BPH	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
6	Y	37	BCL	C2A-CAA-CBA-CGA
6	D	2	BCL	C1A-C2A-CAA-CBA
6	F	4	BCL	C1A-C2A-CAA-CBA
6	I	5	BCL	C1A-C2A-CAA-CBA
6	N	11	BCL	C1A-C2A-CAA-CBA
6	P	39	BCL	C1A-C2A-CAA-CBA
6	R	38	BCL	C1A-C2A-CAA-CBA
6	V	38	BCL	C1A-C2A-CAA-CBA
6	W	36	BCL	C1A-C2A-CAA-CBA
6	Y	36	BCL	C1A-C2A-CAA-CBA
6	1	38	BCL	C1A-C2A-CAA-CBA
6	5	38	BCL	C1A-C2A-CAA-CBA
6	A	302	BCL	C12-C13-C15-C16
6	B	304	BCL	C12-C13-C15-C16
6	D	2	BCL	C2C-C3C-CAC-CBC
6	F	4	BCL	C2C-C3C-CAC-CBC
6	H	6	BCL	C2C-C3C-CAC-CBC
6	J	8	BCL	C2C-C3C-CAC-CBC
6	L	10	BCL	C2C-C3C-CAC-CBC
6	P	39	BCL	C2C-C3C-CAC-CBC
6	R	38	BCL	C2C-C3C-CAC-CBC
6	T	38	BCL	C2C-C3C-CAC-CBC
6	W	36	BCL	C2C-C3C-CAC-CBC
6	Y	37	BCL	C2C-C3C-CAC-CBC
6	1	38	BCL	C2C-C3C-CAC-CBC
6	3	39	BCL	C2C-C3C-CAC-CBC
6	5	38	BCL	C2C-C3C-CAC-CBC
6	7	38	BCL	C2C-C3C-CAC-CBC
7	A	401	BPH	C2-C3-C5-C6
7	B	402	BPH	C8-C10-C11-C12
7	B	402	BPH	C4-C3-C5-C6
7	A	401	BPH	C8-C10-C11-C12
6	N	38	BCL	C3A-C2A-CAA-CBA
6	A	301	BCL	C5-C6-C7-C8
6	A	301	BCL	C16-C17-C18-C20
7	B	402	BPH	C2-C3-C5-C6
7	A	401	BPH	C11-C12-C13-C15
7	A	401	BPH	C11-C12-C13-C14
6	M	36	BCL	C1A-C2A-CAA-CBA
6	2	36	BCL	C1A-C2A-CAA-CBA
6	S	36	BCL	C3A-C2A-CAA-CBA
6	B	304	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
6	A	302	BCL	C16-C17-C18-C20
6	3	39	BCL	C1A-C2A-CAA-CBA
6	8	36	BCL	C1A-C2A-CAA-CBA
6	A	302	BCL	C11-C12-C13-C15
6	3	39	BCL	C3A-C2A-CAA-CBA
7	A	401	BPH	C10-C11-C12-C13
6	S	36	BCL	CAA-CBA-CGA-O2A
6	T	38	BCL	CAA-CBA-CGA-O2A
6	3	39	BCL	CAA-CBA-CGA-O2A
6	J	8	BCL	CAA-CBA-CGA-O2A
6	R	38	BCL	CAA-CBA-CGA-O2A
6	J	8	BCL	CAA-CBA-CGA-O1A
6	W	36	BCL	CAA-CBA-CGA-O2A
6	U	36	BCL	CAA-CBA-CGA-O2A
6	S	36	BCL	CAA-CBA-CGA-O1A
6	T	38	BCL	CAA-CBA-CGA-O1A
6	B	304	BCL	CAD-CBD-CGD-O2D
7	A	401	BPH	CAD-CBD-CGD-O2D
6	P	38	BCL	CAA-CBA-CGA-O2A
6	W	36	BCL	CAA-CBA-CGA-O1A

There are no ring outliers.

35 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	304	BCL	2	0
6	Y	36	BCL	17	0
6	B	303	BCL	4	0
7	A	401	BPH	5	0
6	I	5	BCL	6	0
6	N	38	BCL	27	0
6	H	6	BCL	11	0
6	F	4	BCL	7	0
6	K	36	BCL	18	0
6	R	38	BCL	16	0
6	6	36	BCL	3	0
6	N	11	BCL	17	0
6	5	38	BCL	12	0
6	G	3	BCL	11	0
6	E	1	BCL	14	0
6	Y	37	BCL	9	0
6	2	36	BCL	10	0

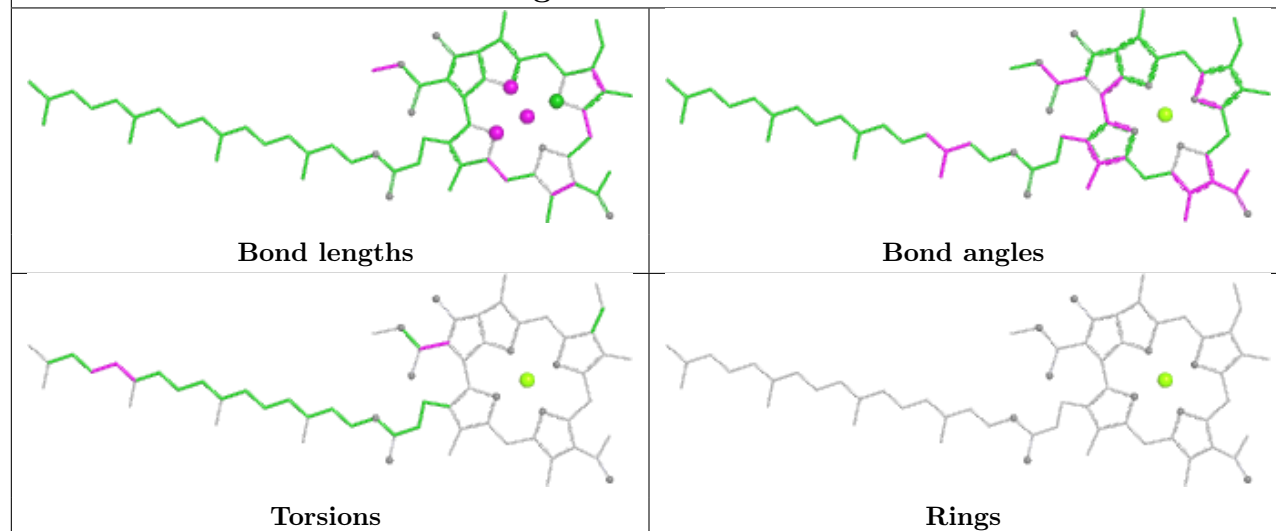
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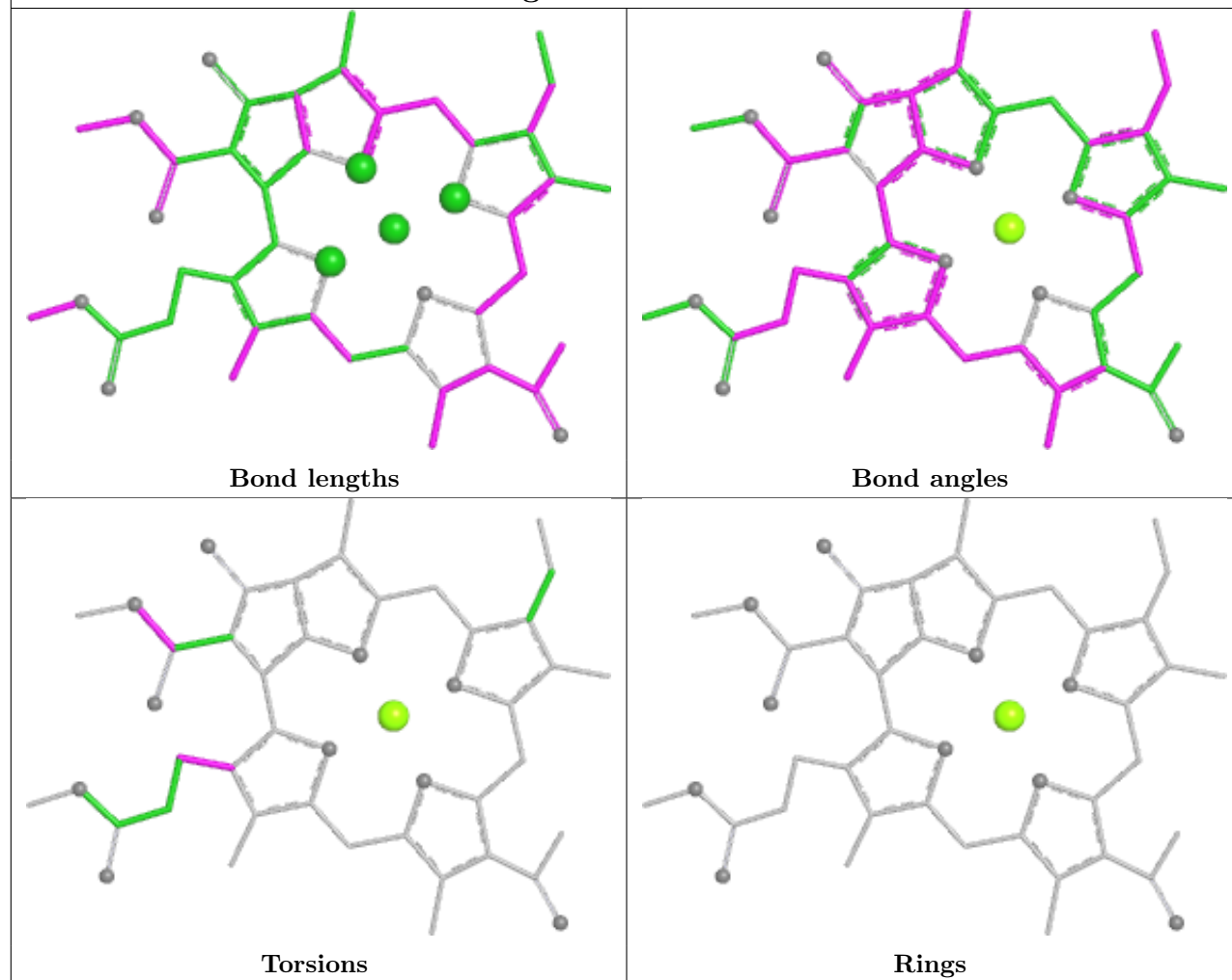
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	301	BCL	7	0
6	W	36	BCL	6	0
6	1	38	BCL	18	0
6	V	38	BCL	8	0
6	D	2	BCL	14	0
6	T	38	BCL	10	0
6	3	39	BCL	7	0
6	3	38	BCL	8	0
6	M	36	BCL	13	0
6	U	36	BCL	8	0
6	P	38	BCL	41	0
6	8	36	BCL	5	0
6	J	8	BCL	32	0
6	S	36	BCL	10	0
6	A	302	BCL	2	0
6	P	39	BCL	27	0
6	7	38	BCL	8	0
6	L	10	BCL	25	0

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

## Ligand BCL B 304

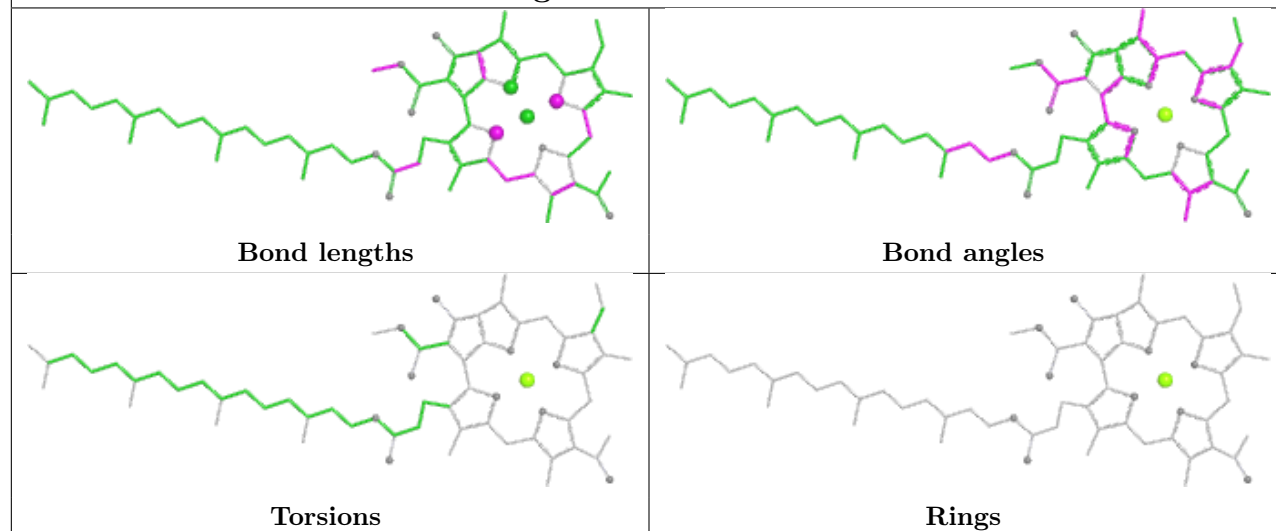


## Ligand BCL Y 36

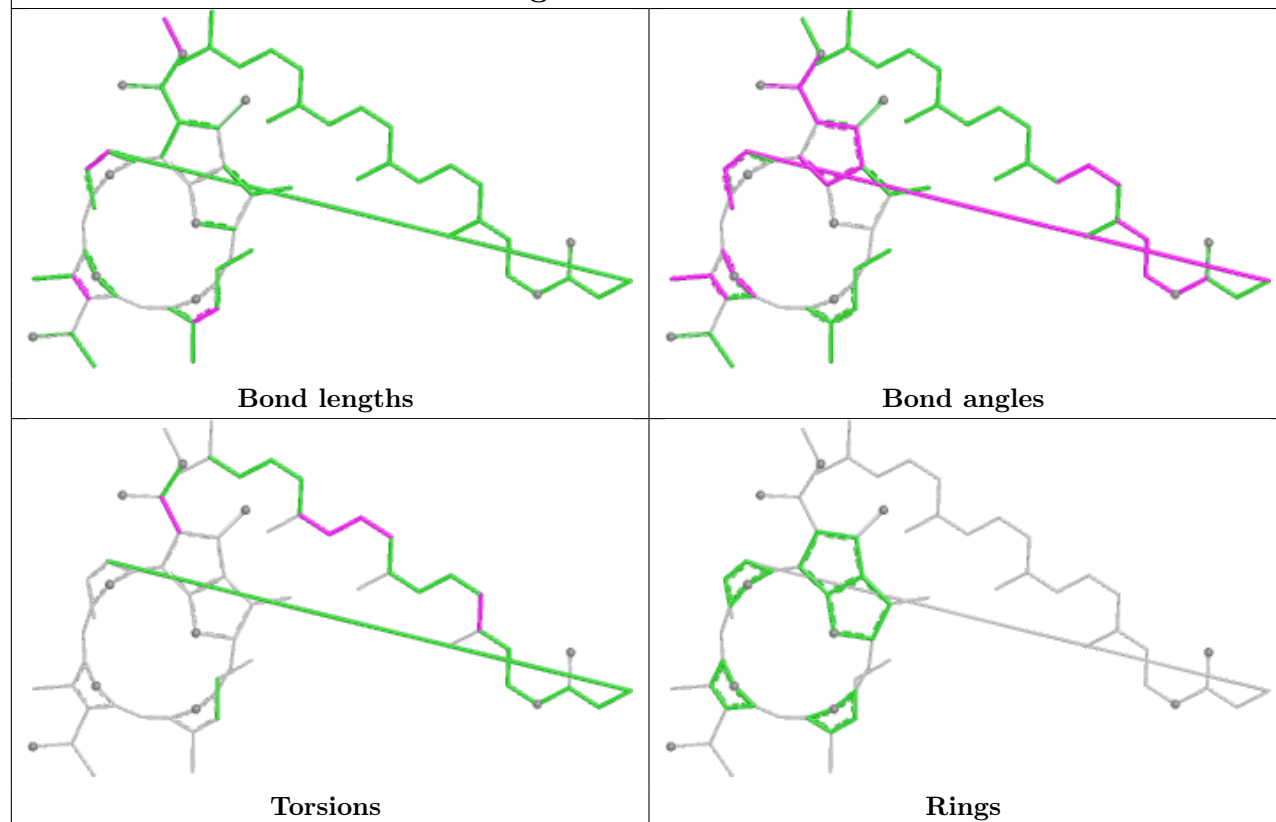


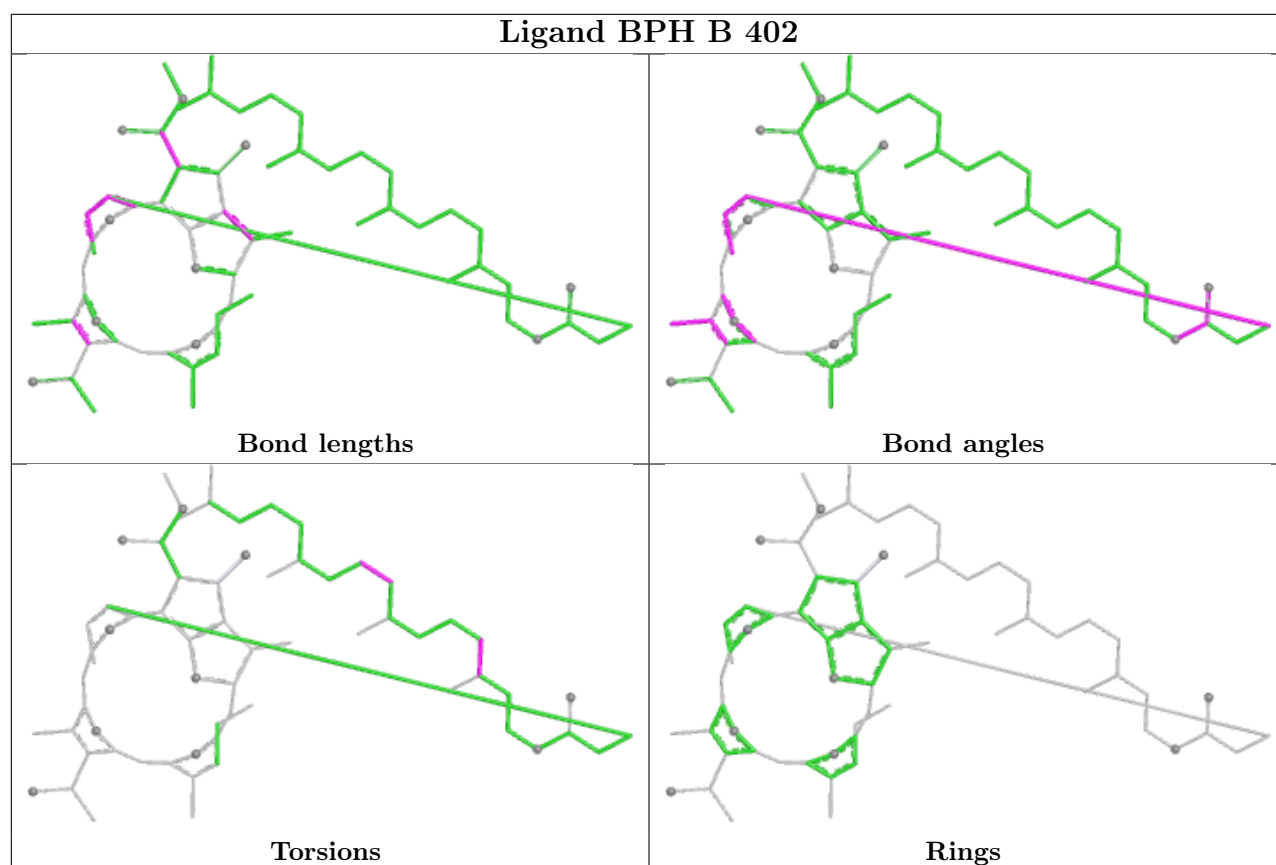


## Ligand BCL B 303

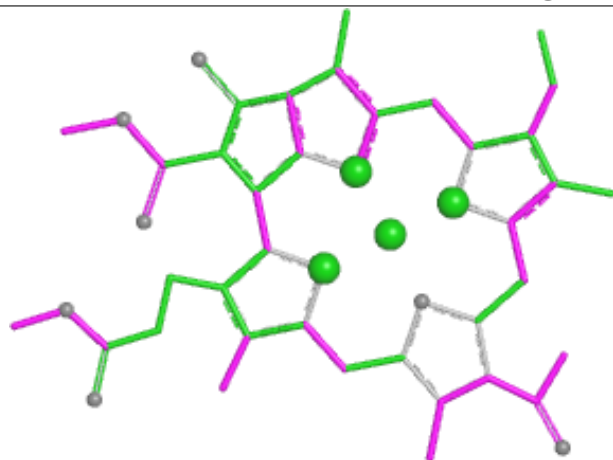


## Ligand BPH A 401

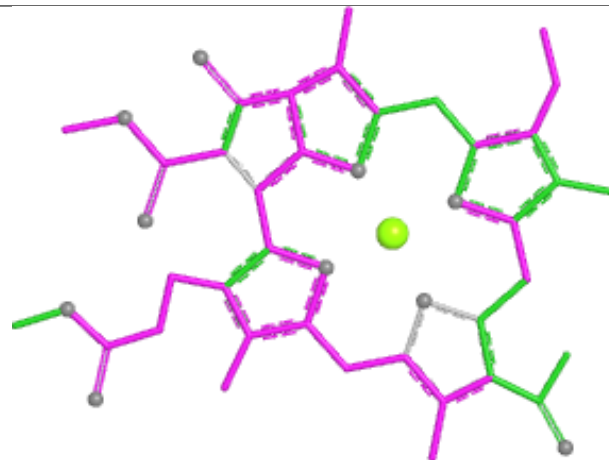




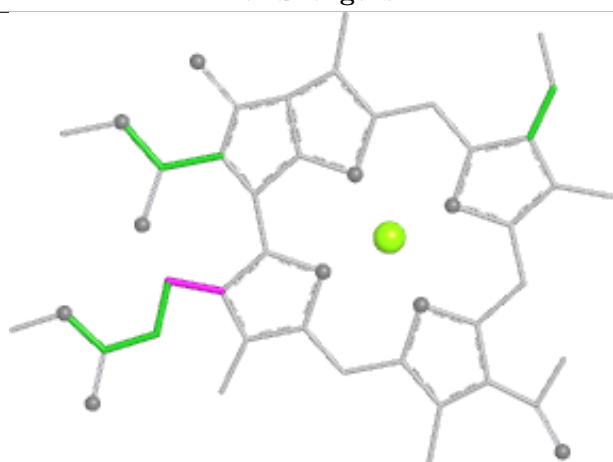
## Ligand BCL I 5



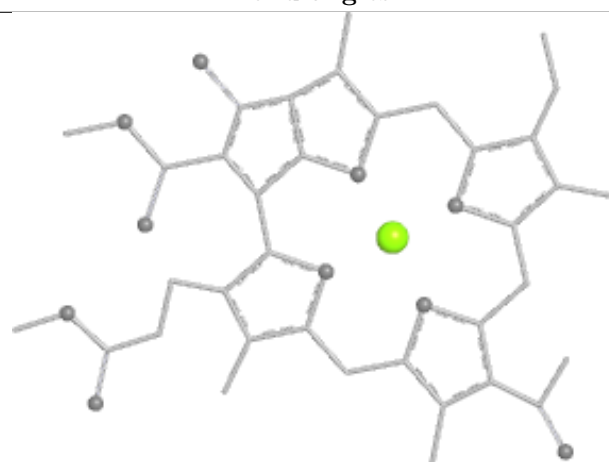
Bond lengths



Bond angles

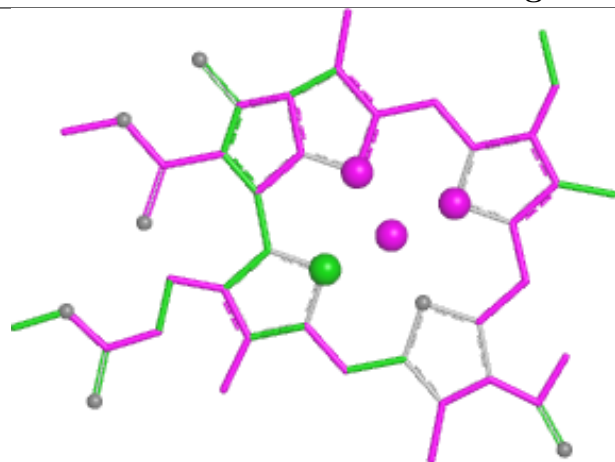


Torsions

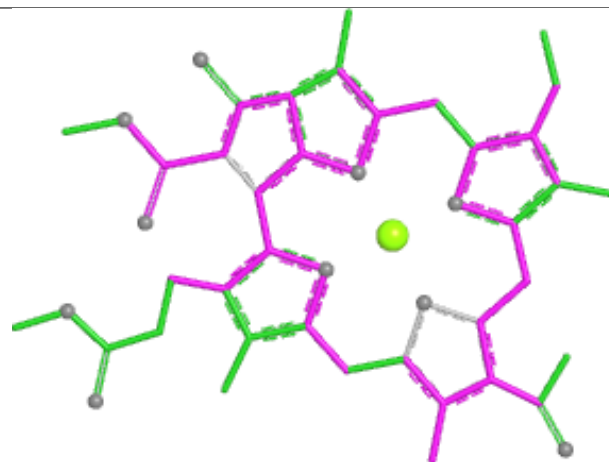


Rings

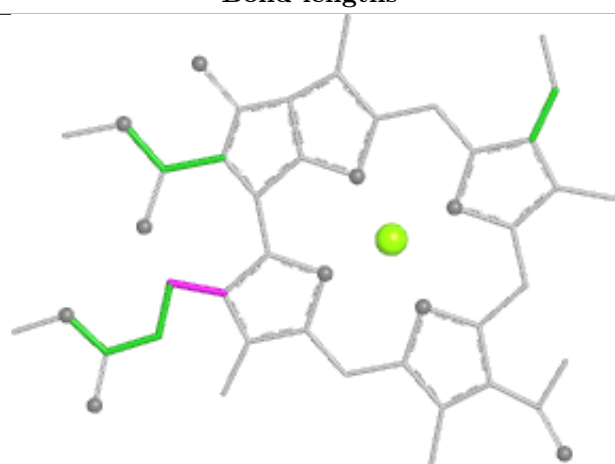
## Ligand BCL N 38



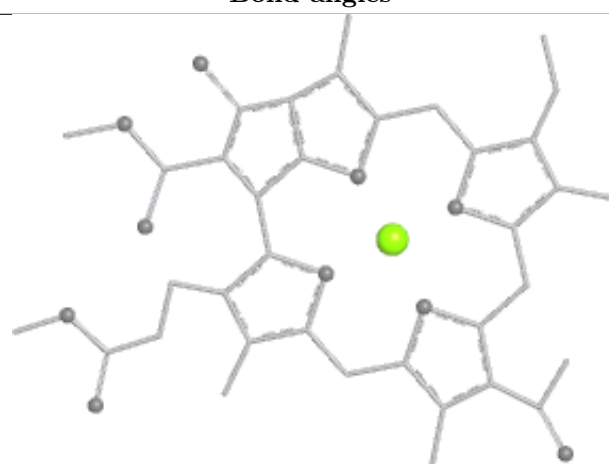
Bond lengths



Bond angles

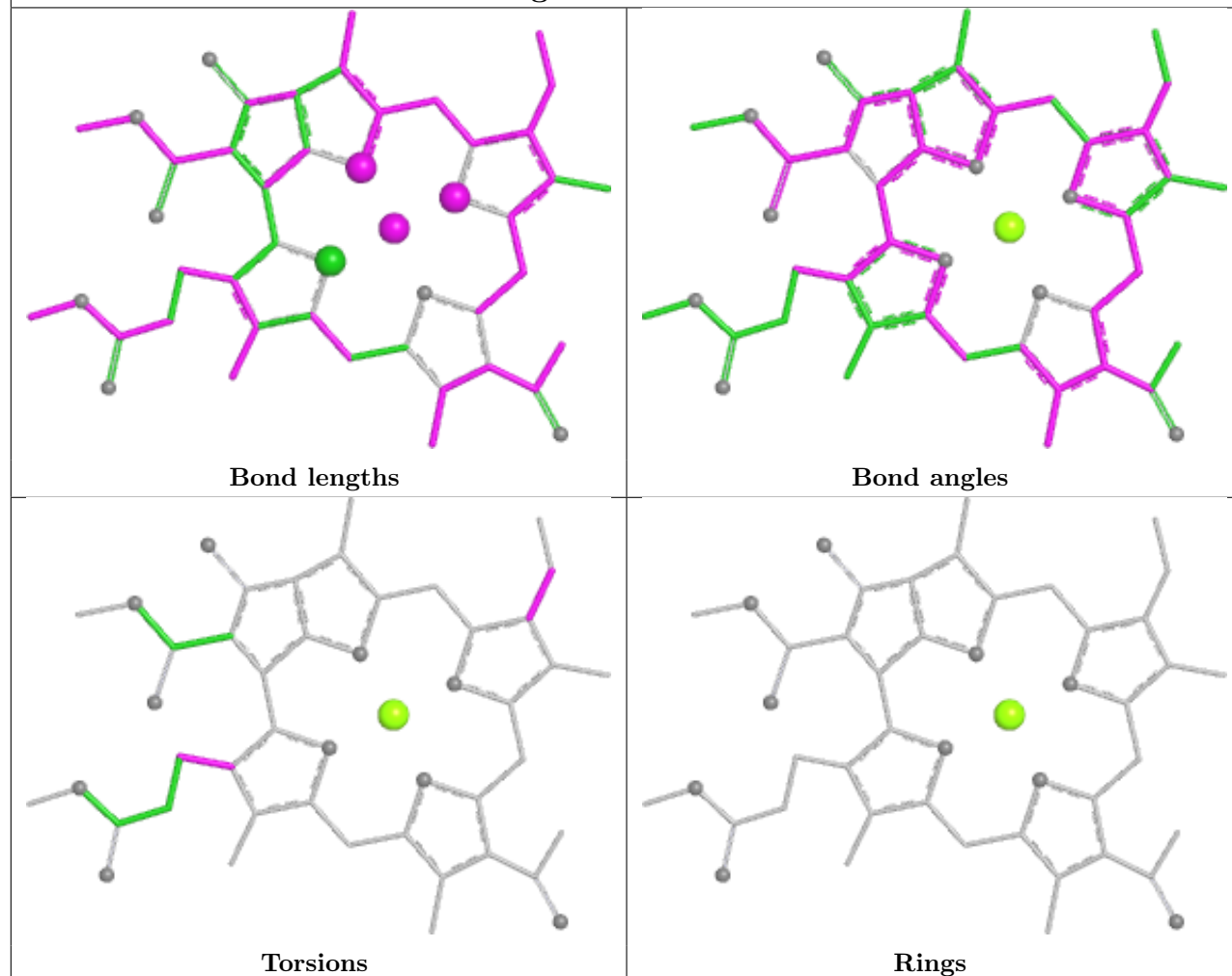


Torsions

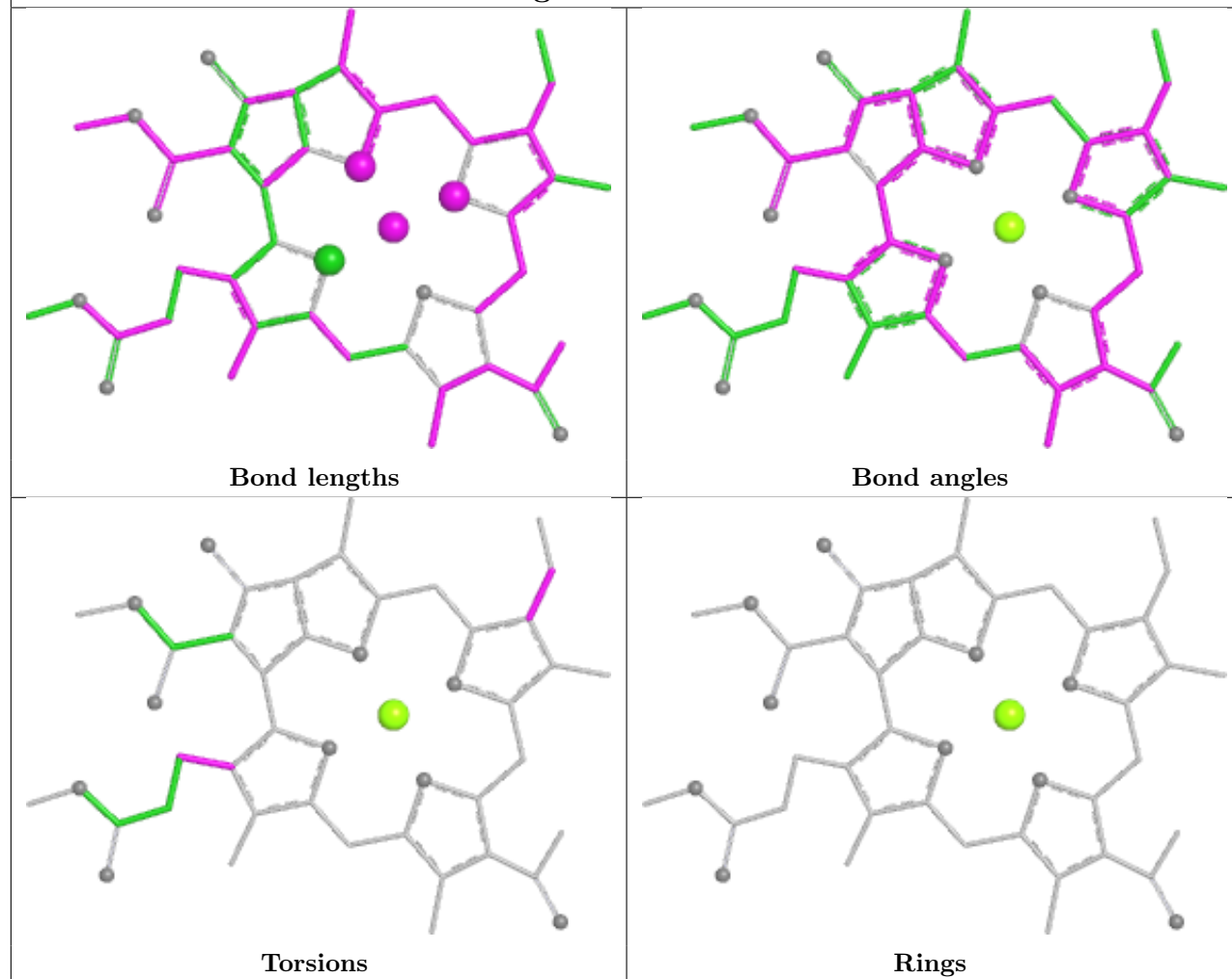


Rings

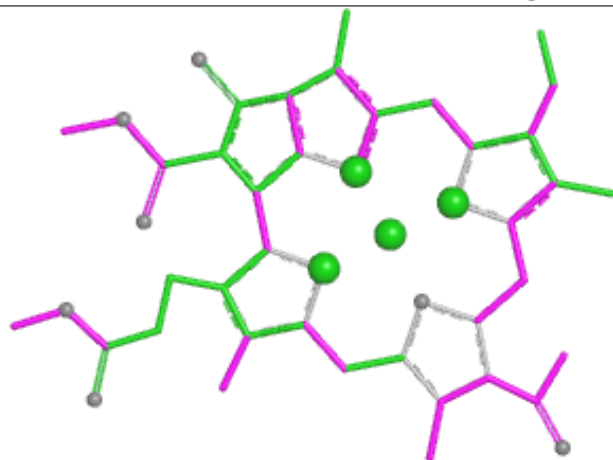
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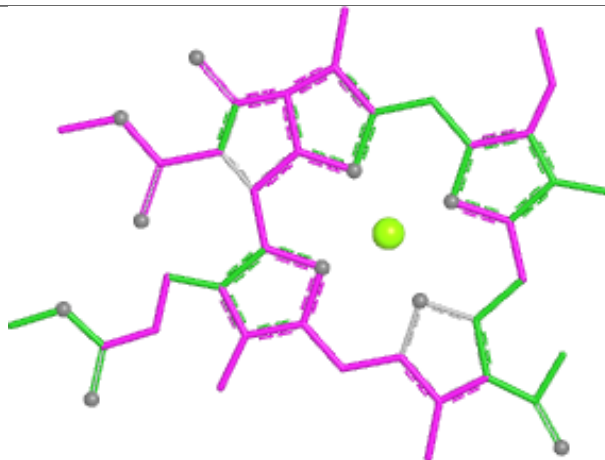
## Ligand BCL F 4



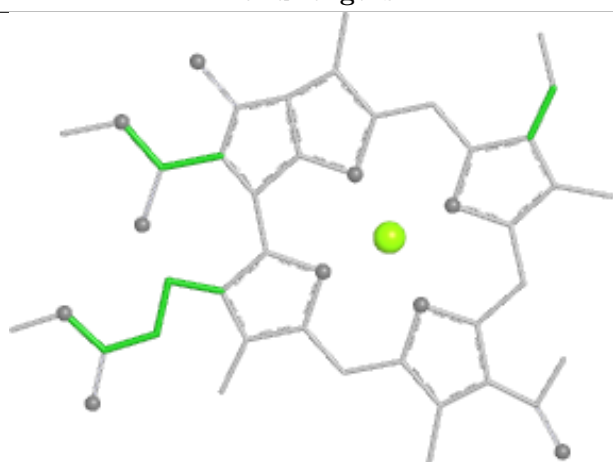
## Ligand BCL K 36



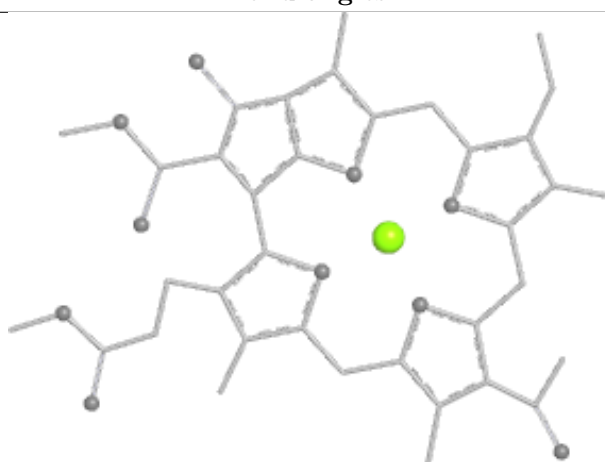
Bond lengths



Bond angles

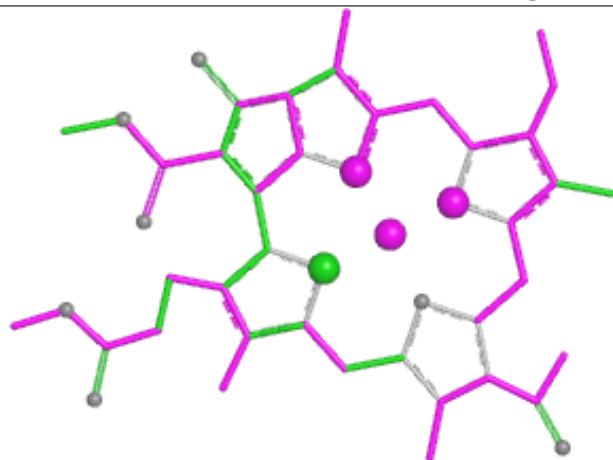


Torsions

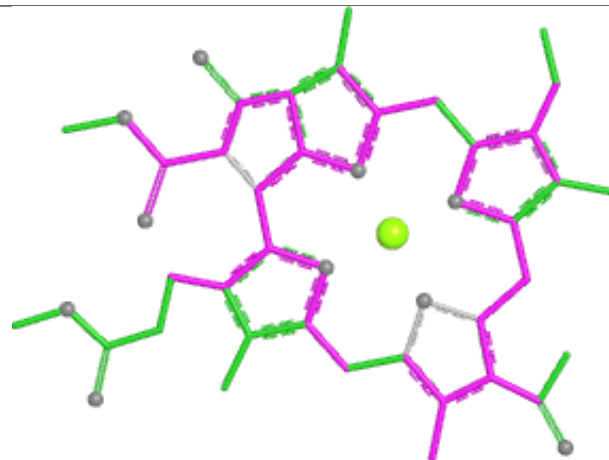


Rings

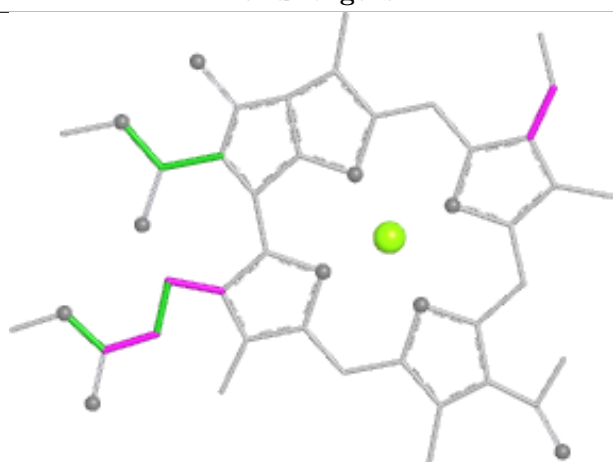
## Ligand BCL R 38



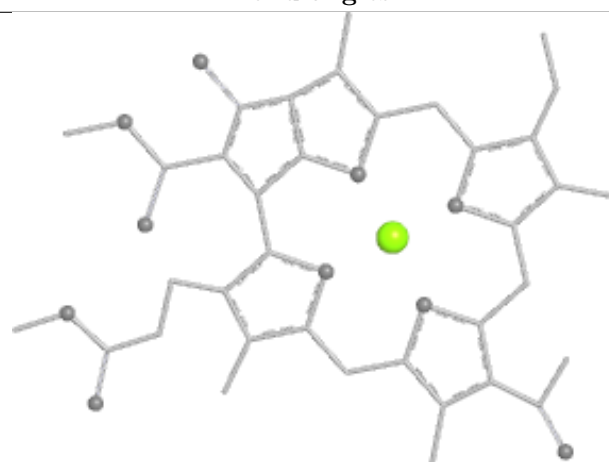
Bond lengths



Bond angles



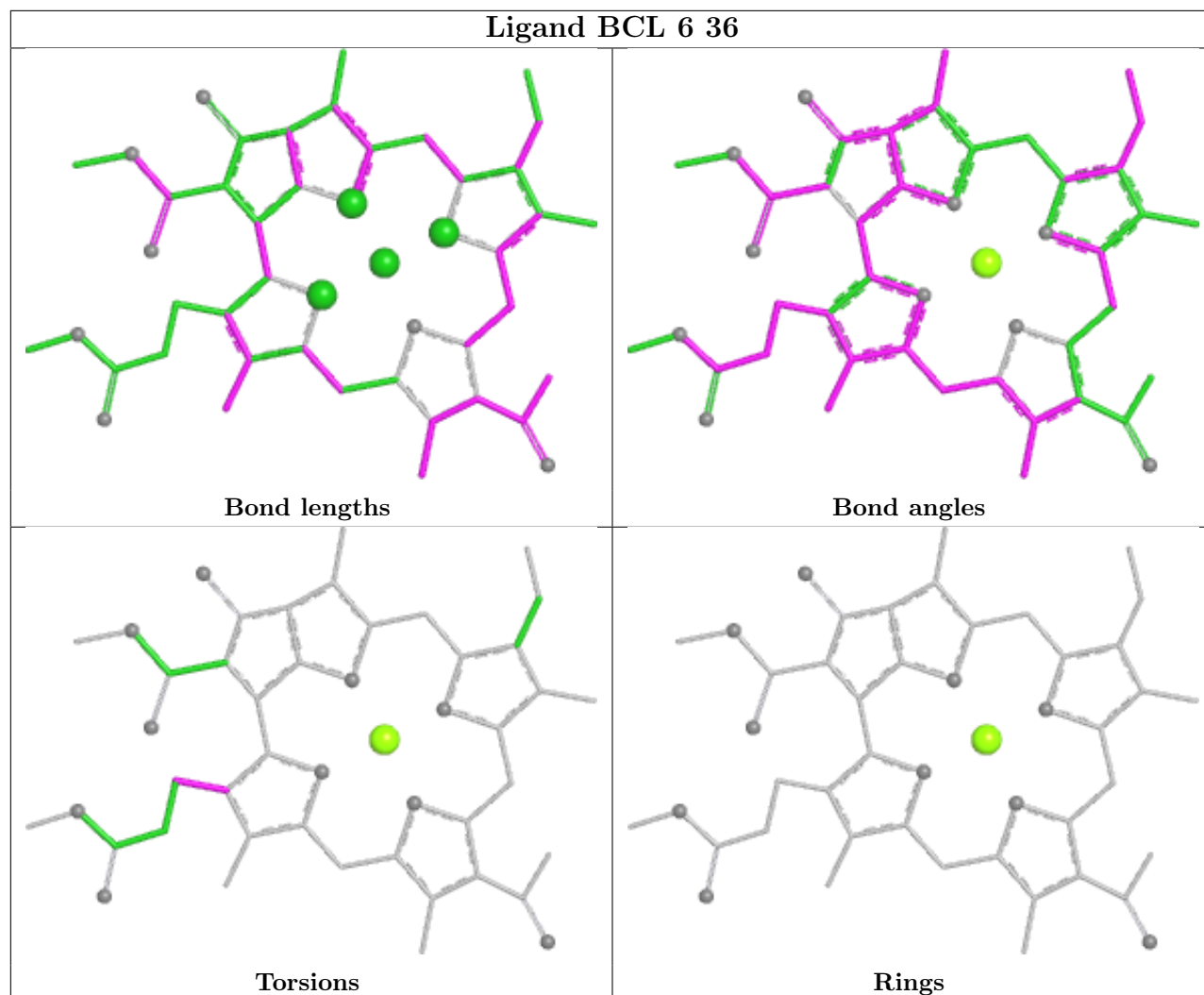
Torsions



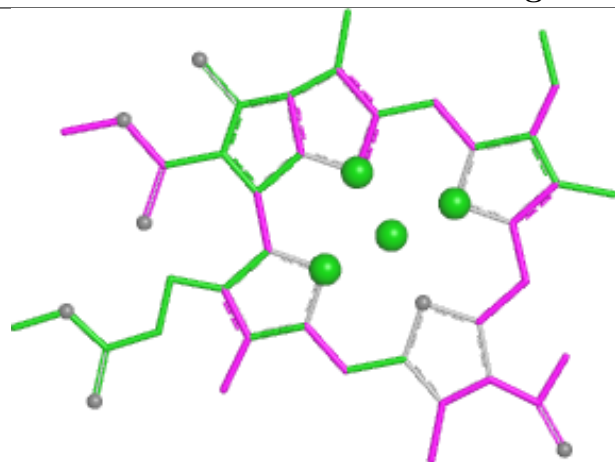
Rings



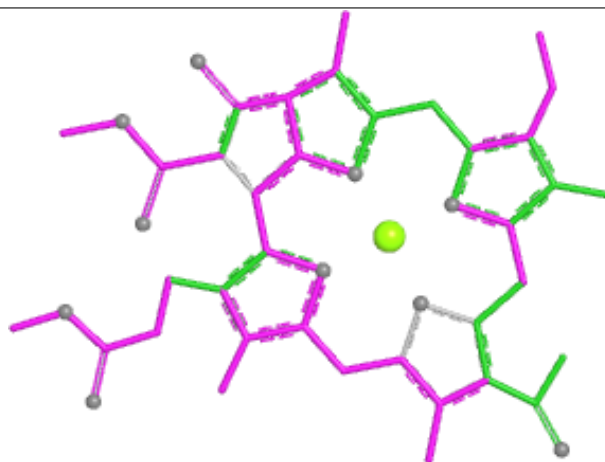
## Ligand BCL 6 36



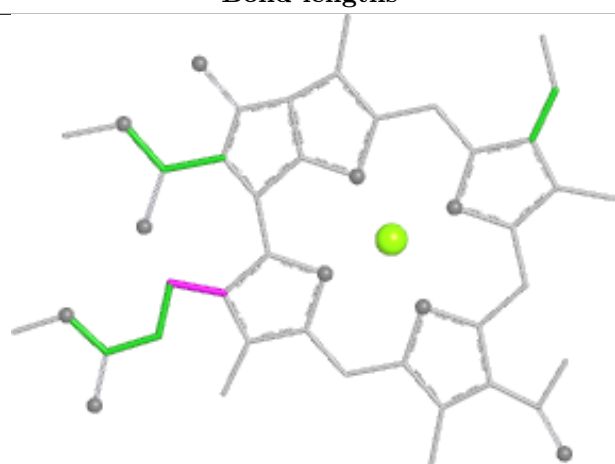
## Ligand BCL N 11



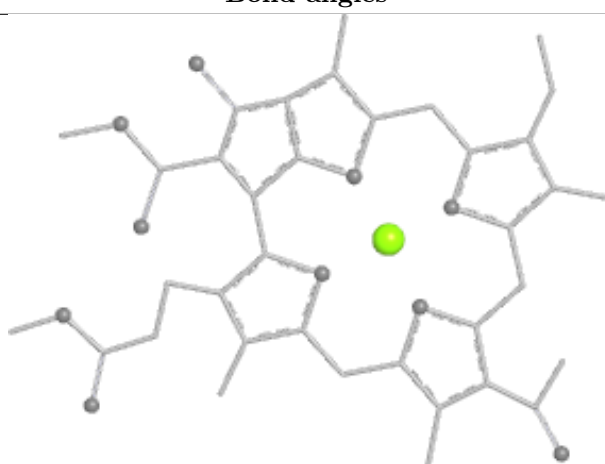
Bond lengths



Bond angles

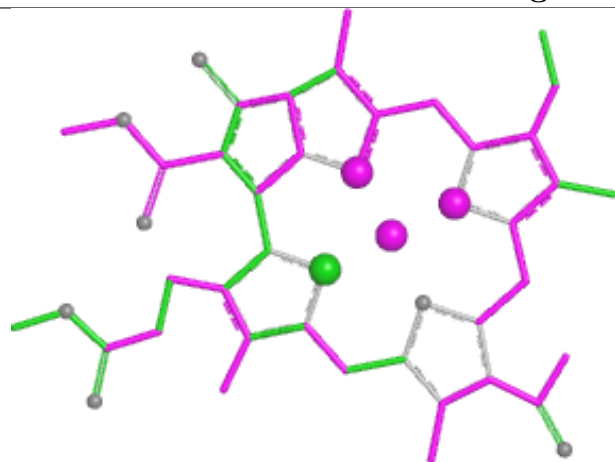


Torsions

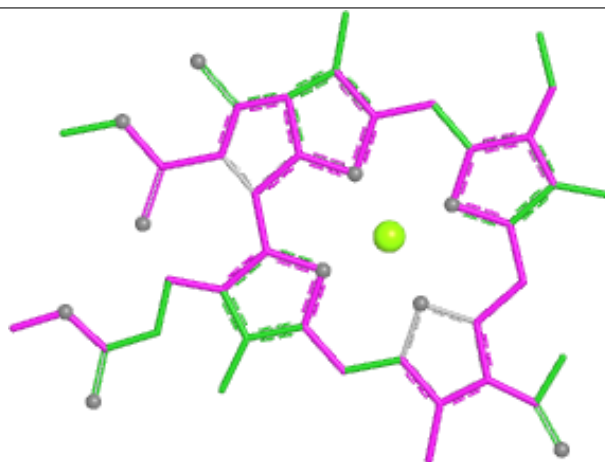


Rings

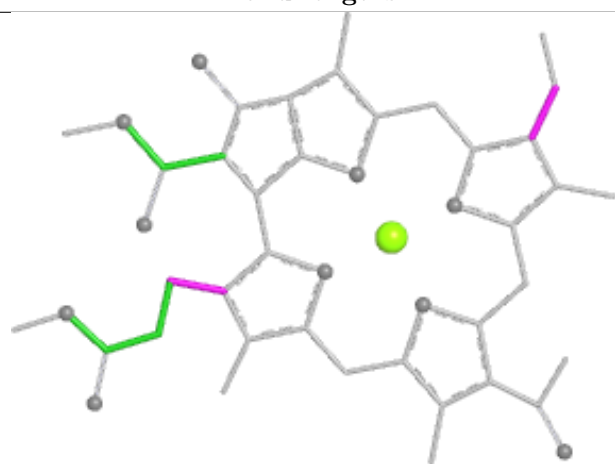
## Ligand BCL 5 38



Bond lengths



Bond angles

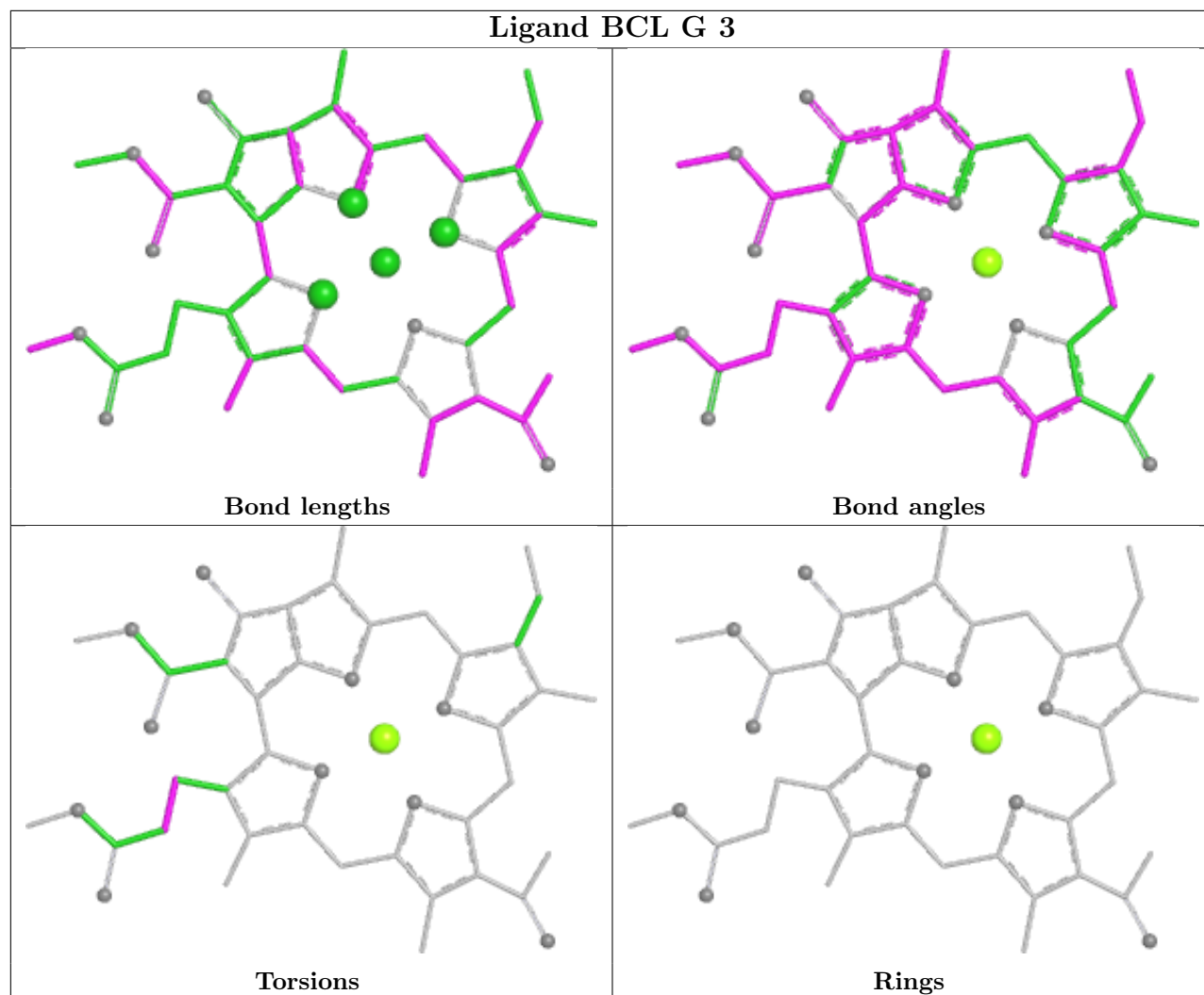


Torsions

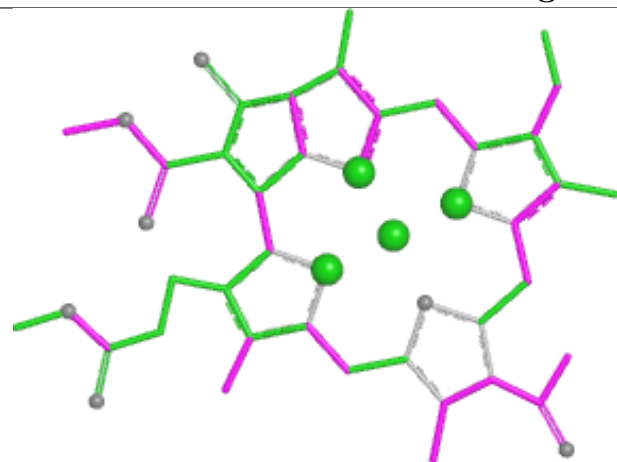


Rings

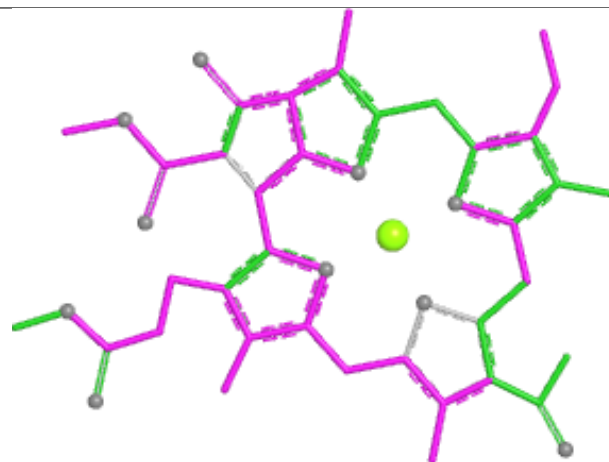
## Ligand BCL G 3



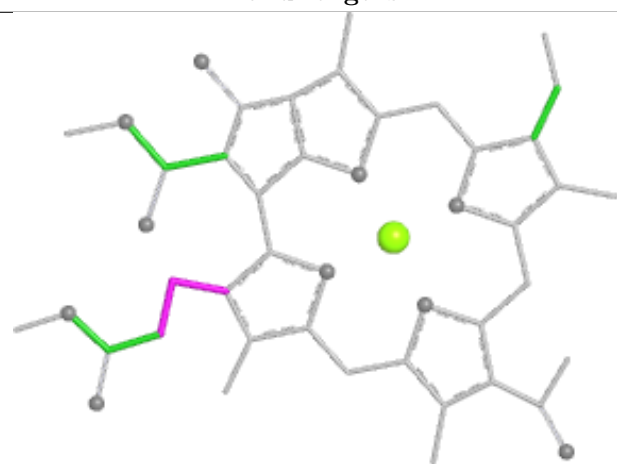
## Ligand BCL E 1



Bond lengths



Bond angles

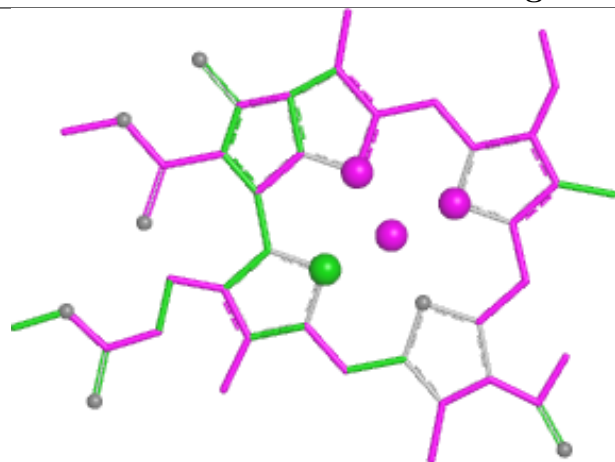


Torsions

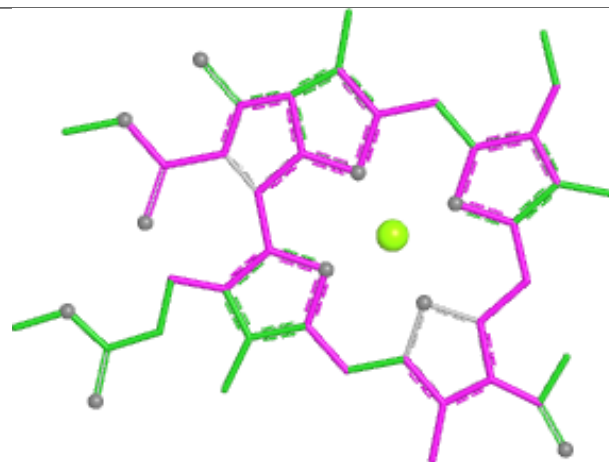


Rings

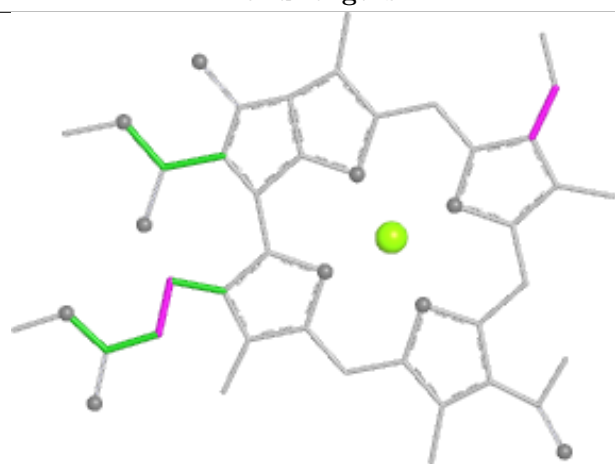
## Ligand BCL Y 37



Bond lengths



Bond angles

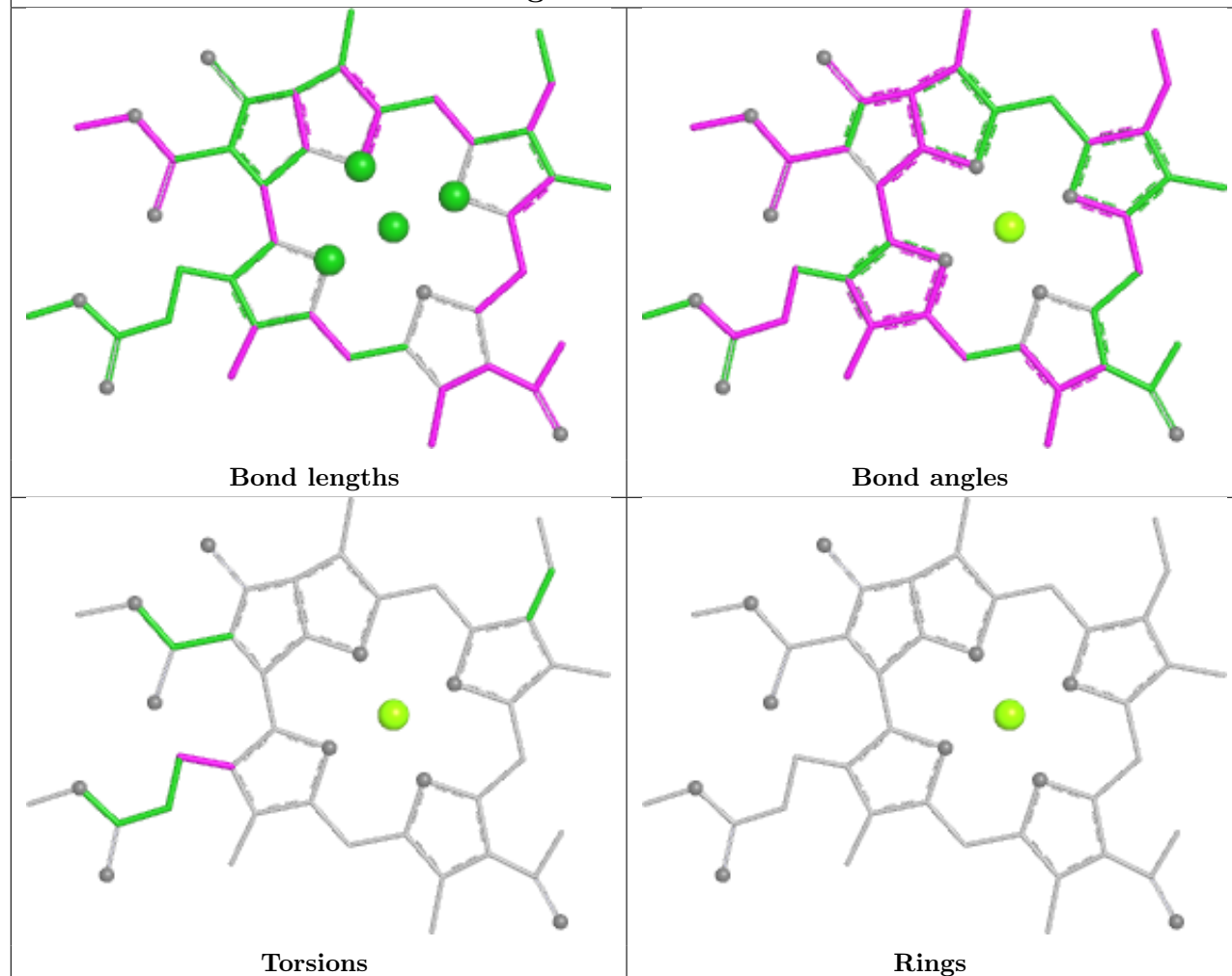


Torsions

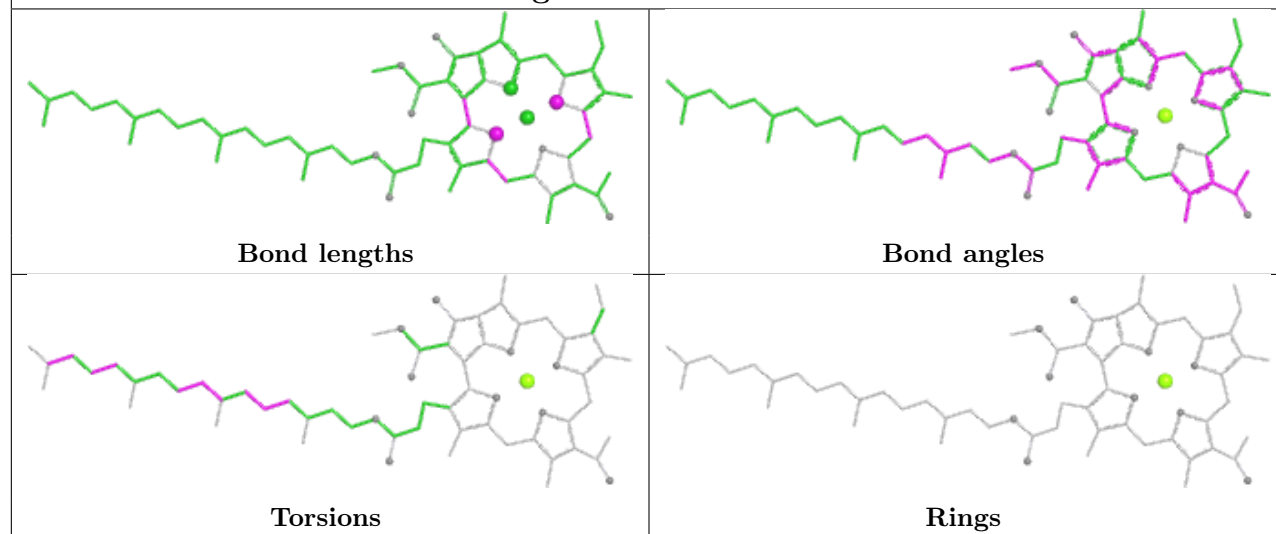


Rings

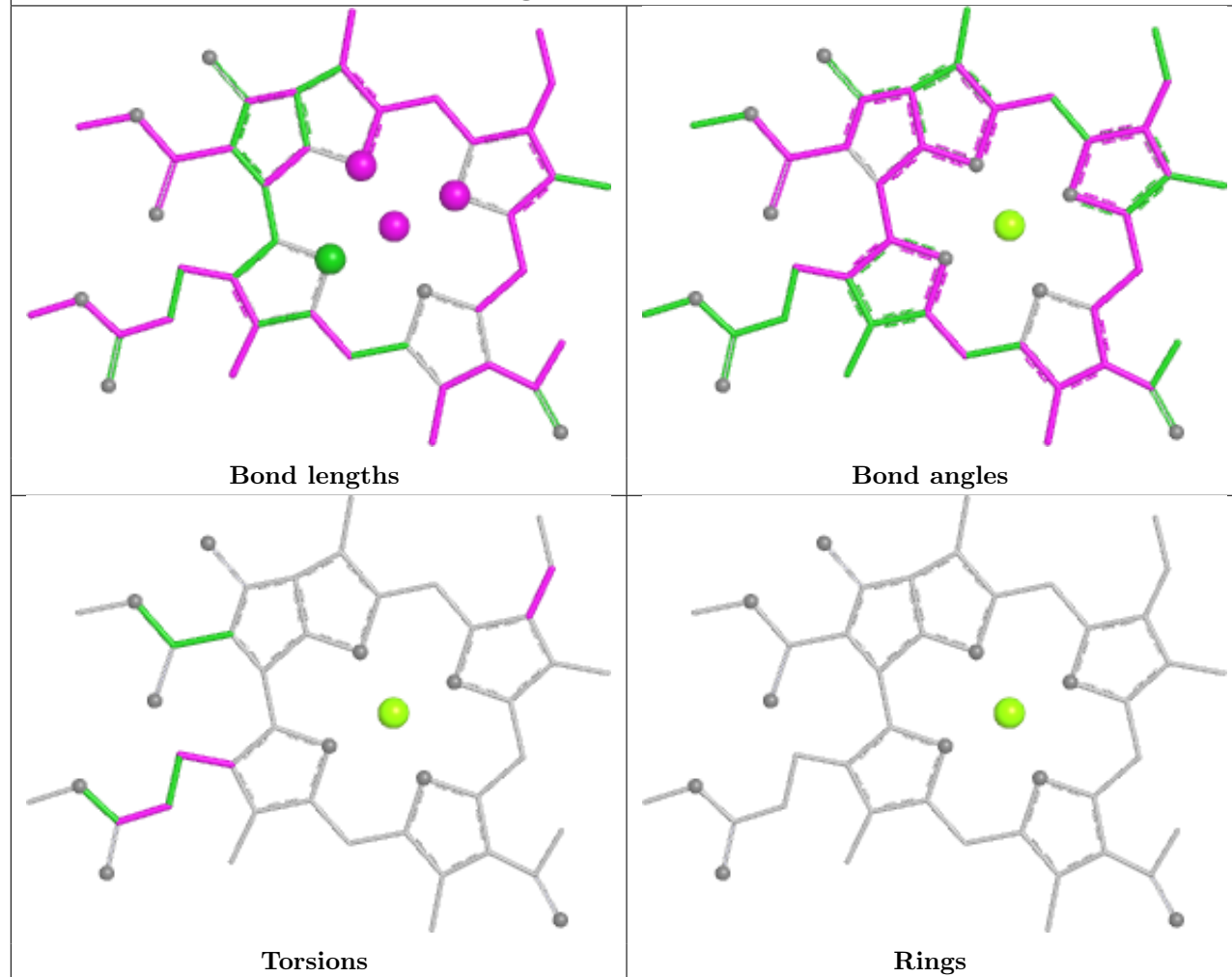
## Ligand BCL 2 36



## Ligand BCL A 301

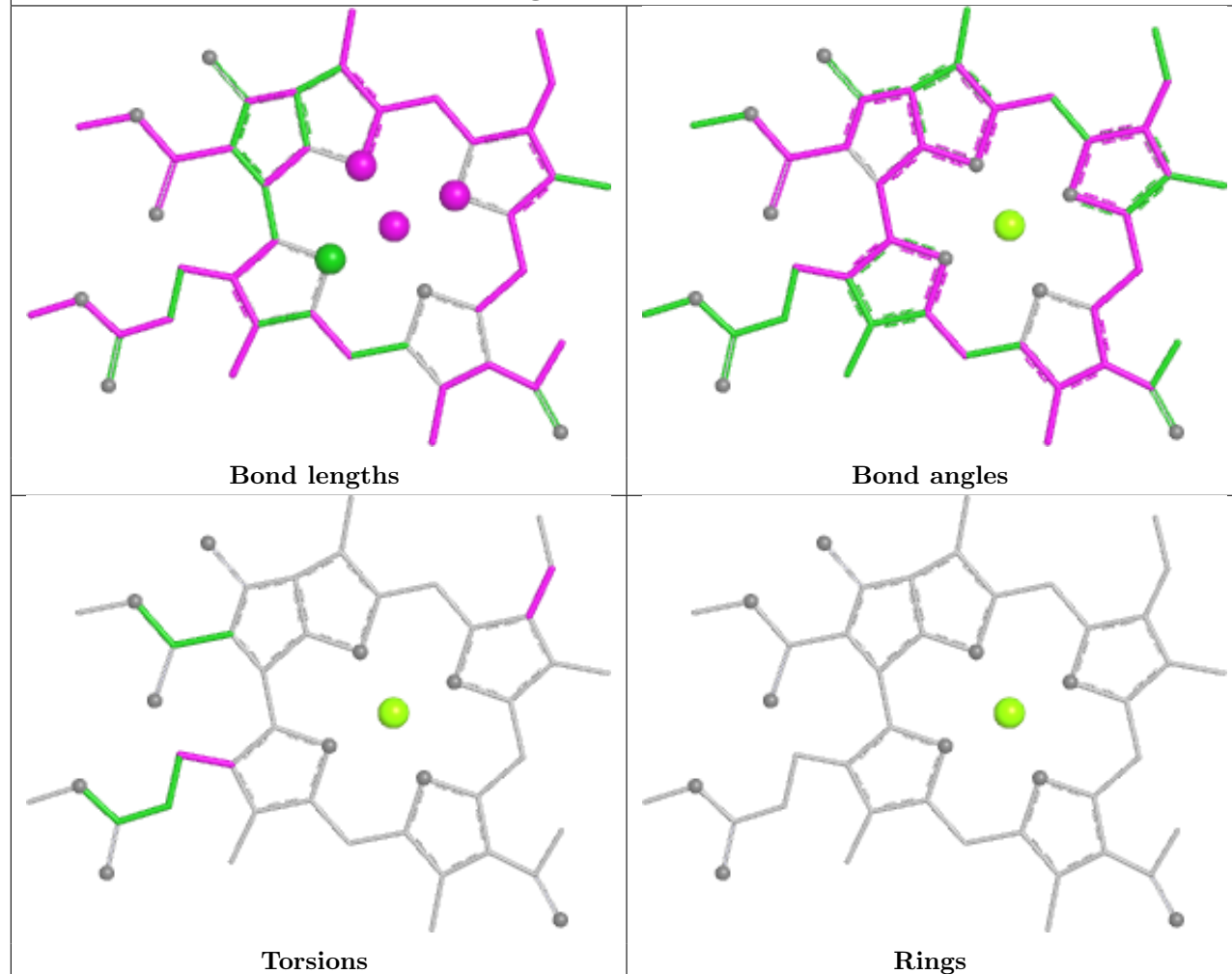


## Ligand BCL W 36

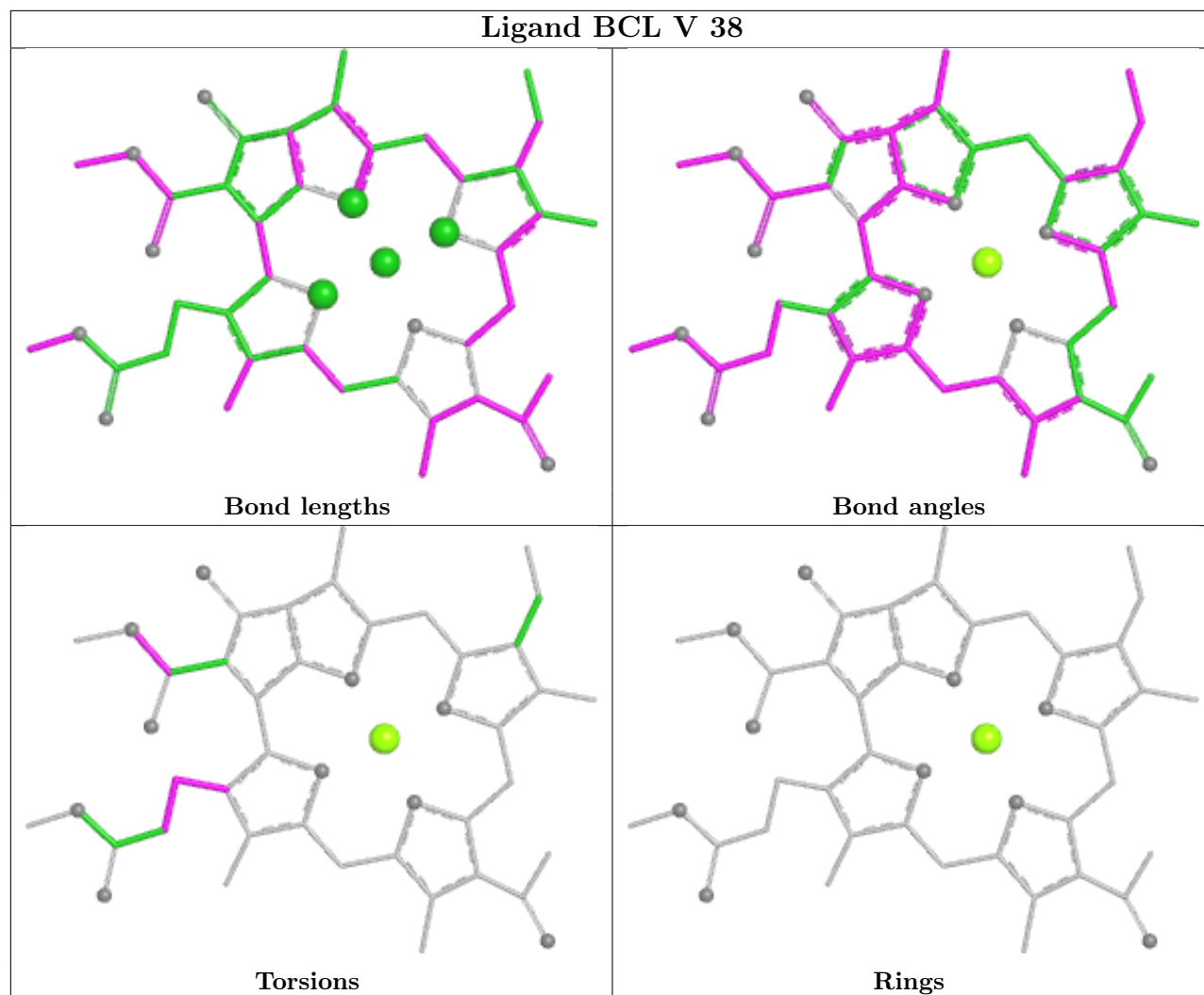




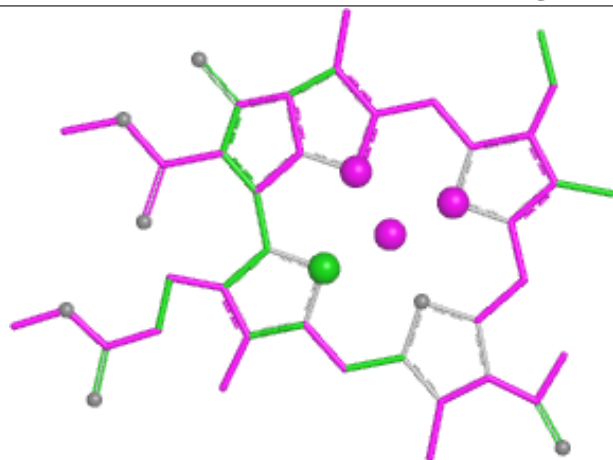
## Ligand BCL 1 38



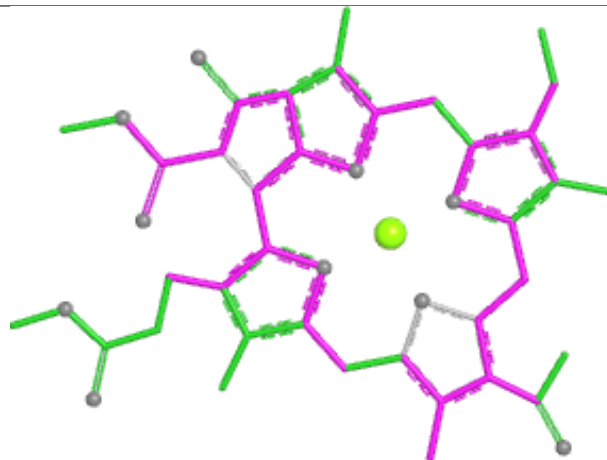
## Ligand BCL V 38



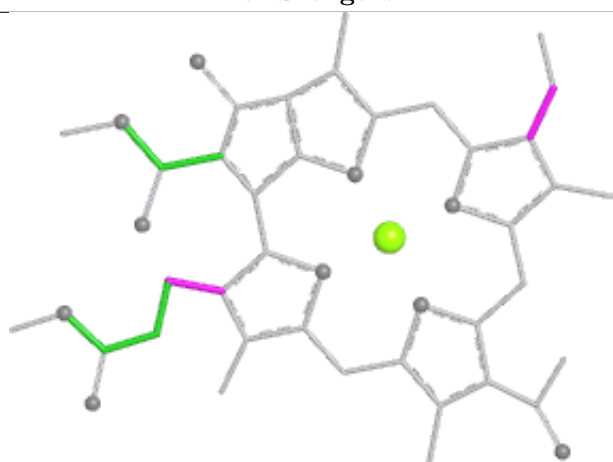
## Ligand BCL D 2



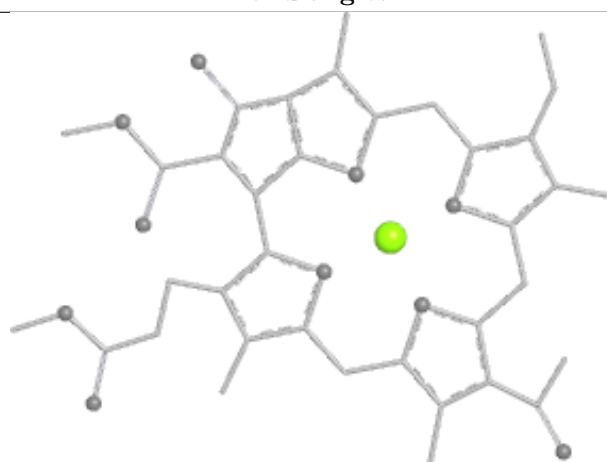
Bond lengths



Bond angles

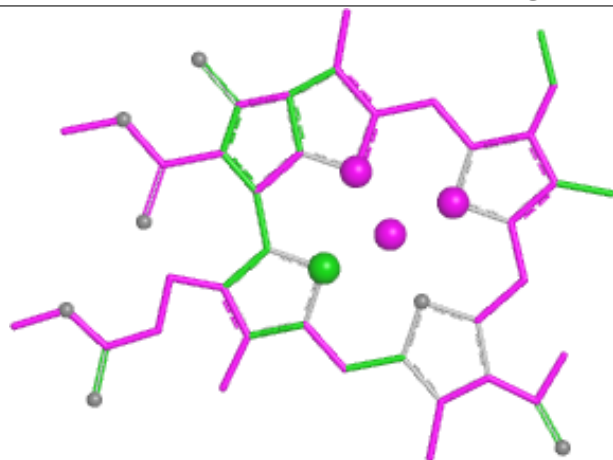


Torsions

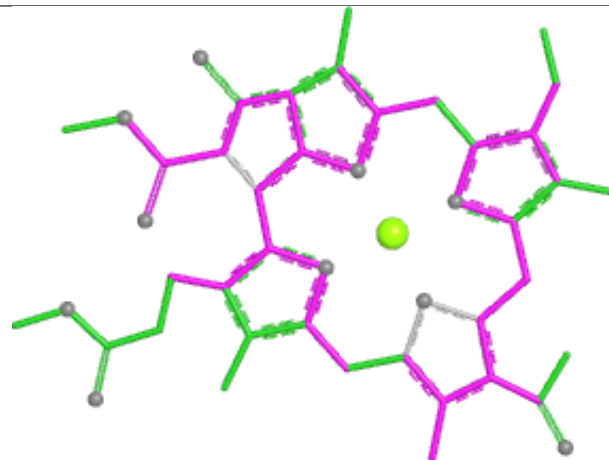


Rings

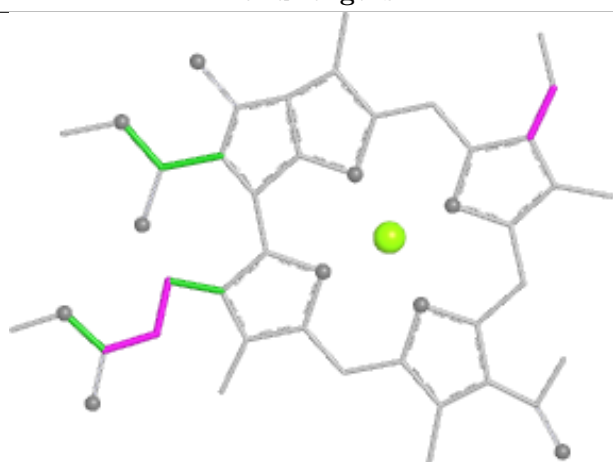
## Ligand BCL T 38



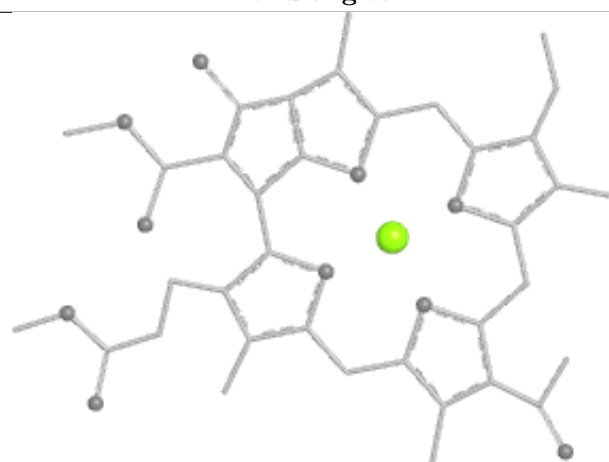
Bond lengths



Bond angles

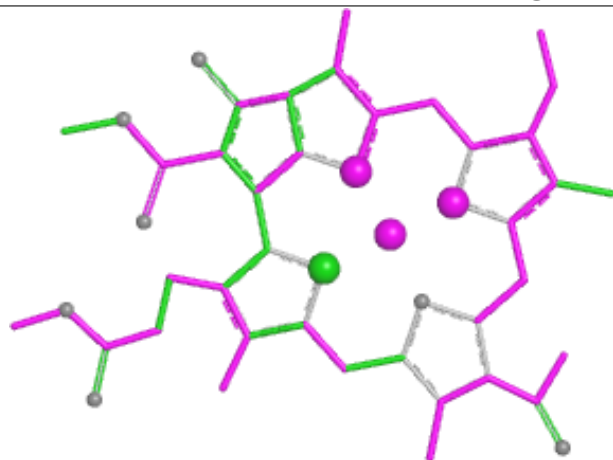


Torsions

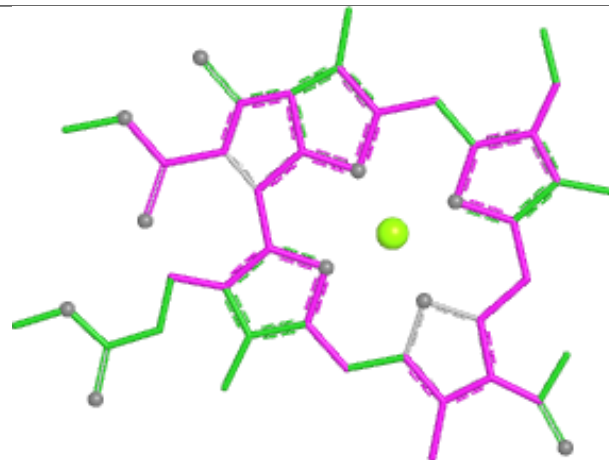


Rings

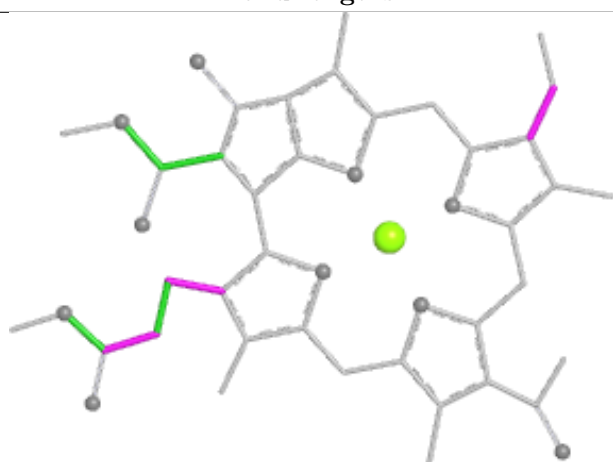
## Ligand BCL 3 39



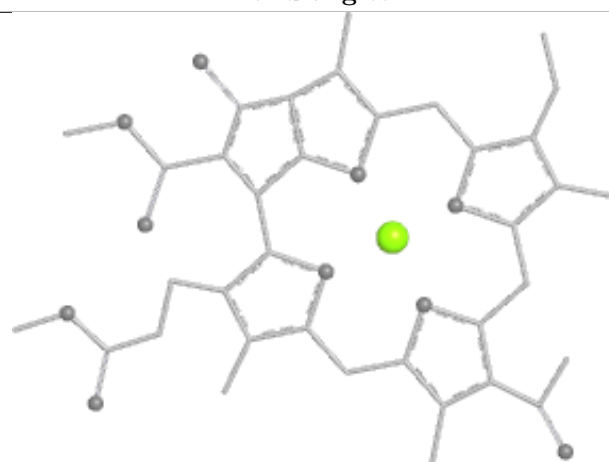
Bond lengths



Bond angles

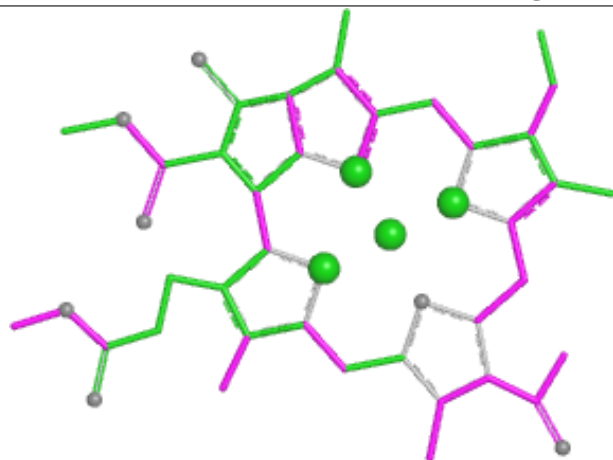


Torsions

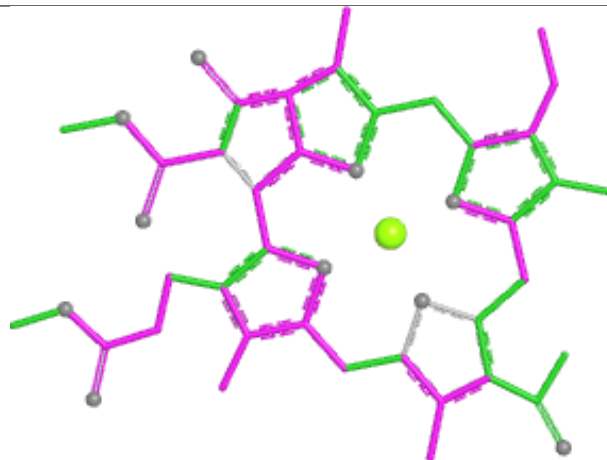


Rings

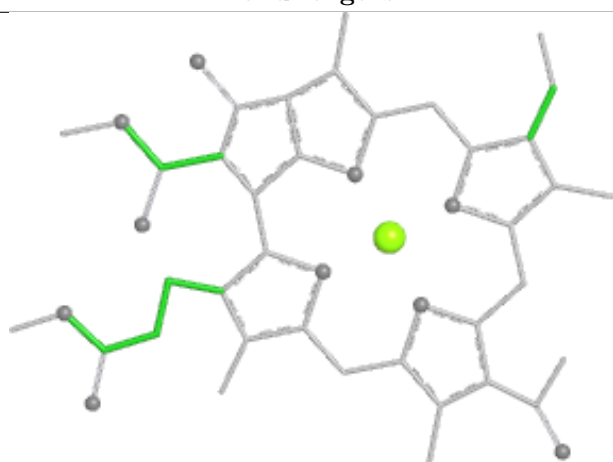
## Ligand BCL 3 38



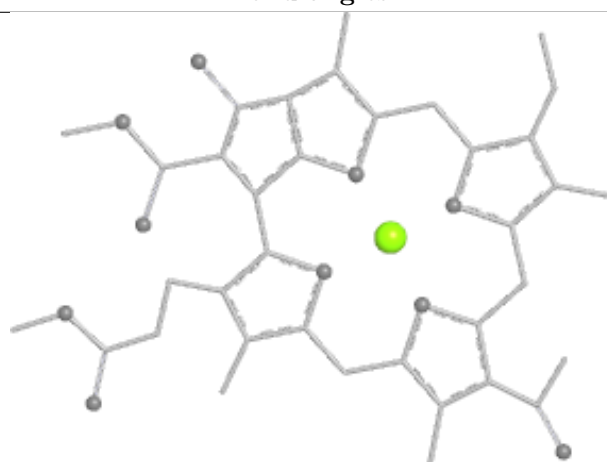
Bond lengths



Bond angles

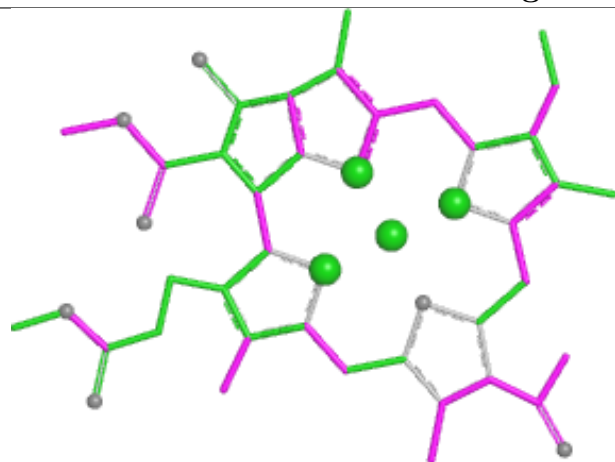


Torsions

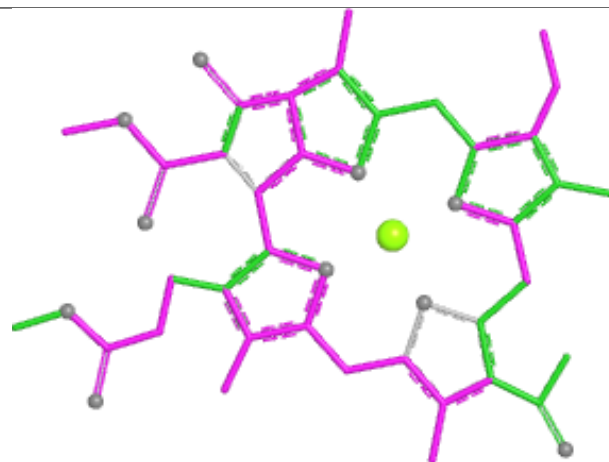


Rings

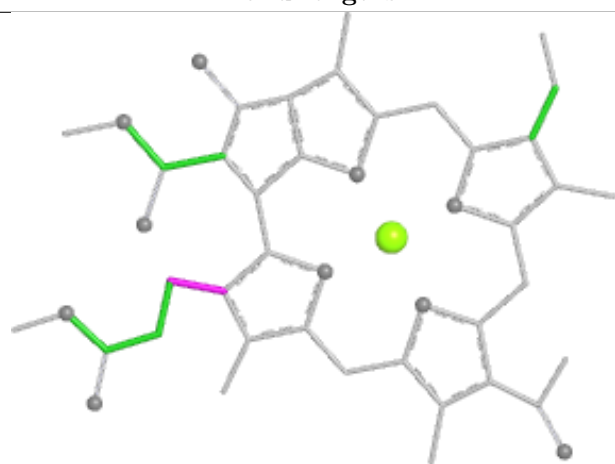
## Ligand BCL M 36



Bond lengths



Bond angles

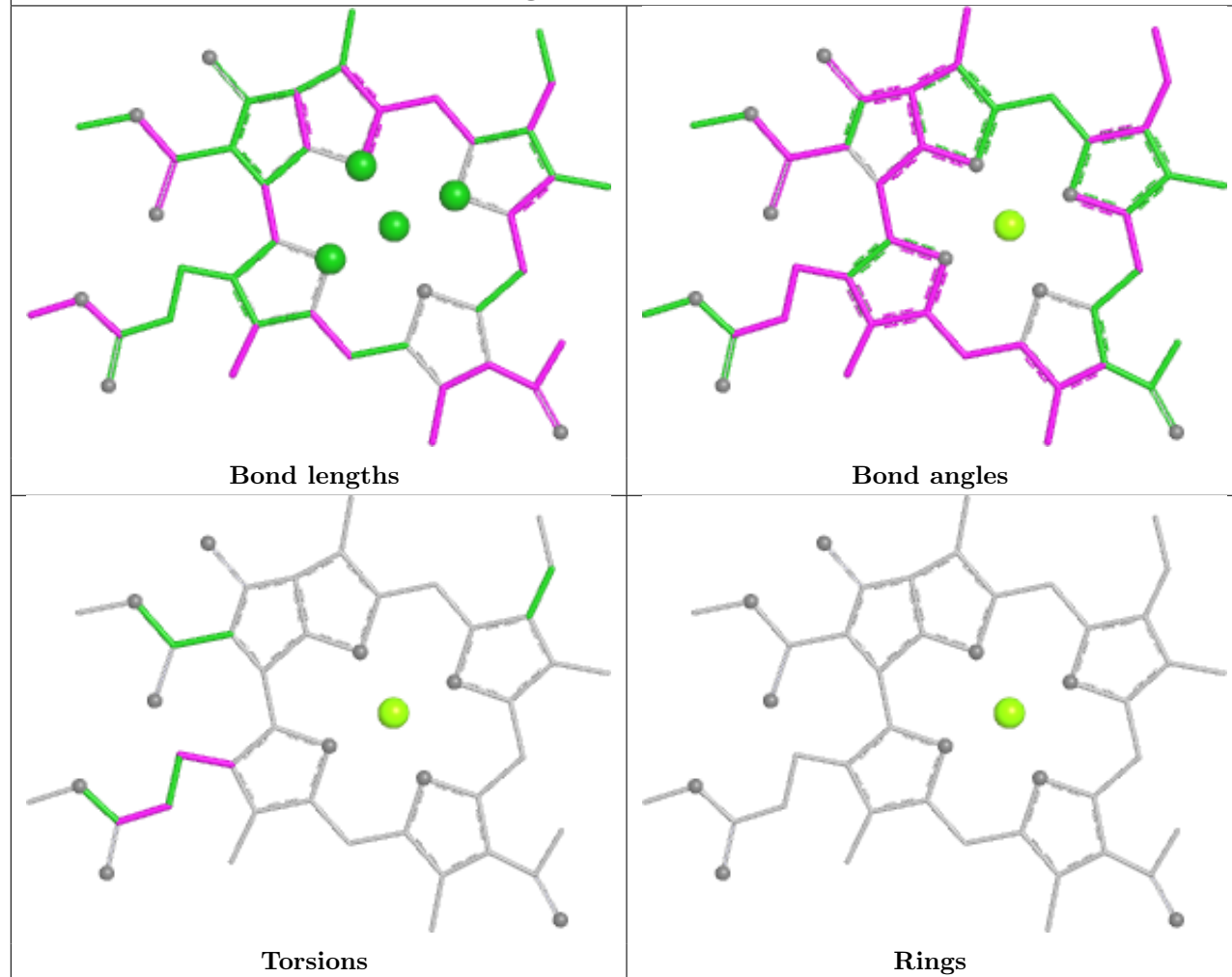


Torsions



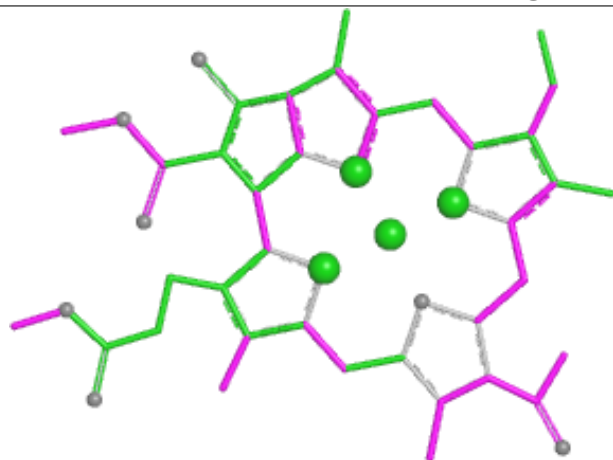
Rings

## Ligand BCL U 36

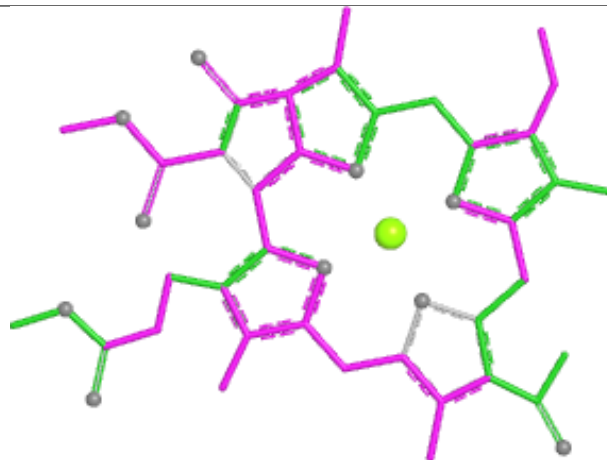




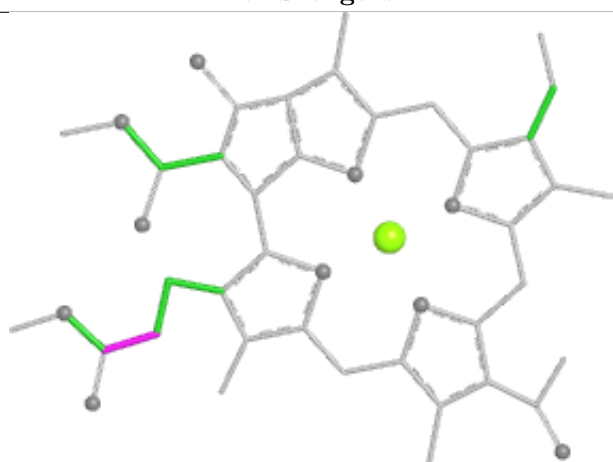
## Ligand BCL P 38



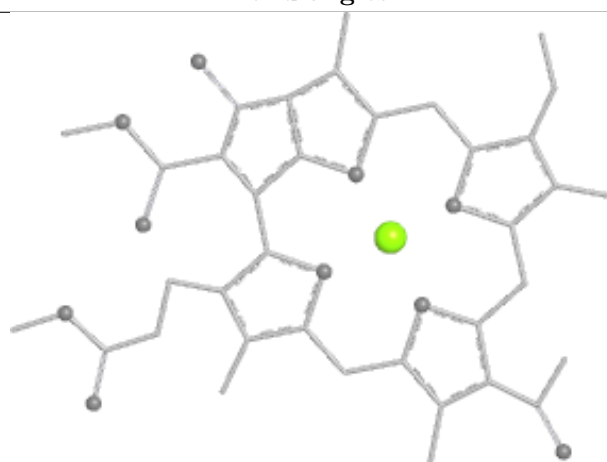
Bond lengths



Bond angles

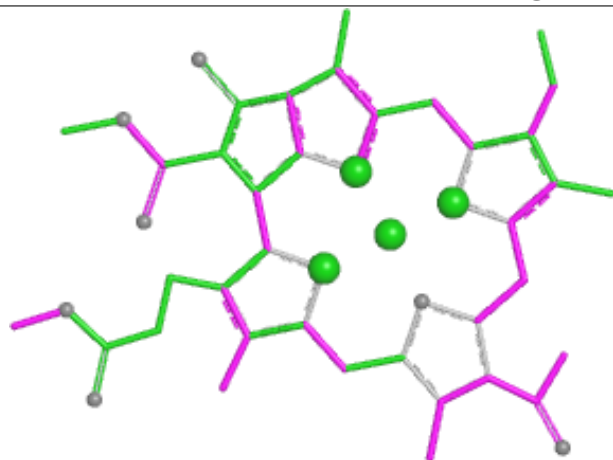


Torsions

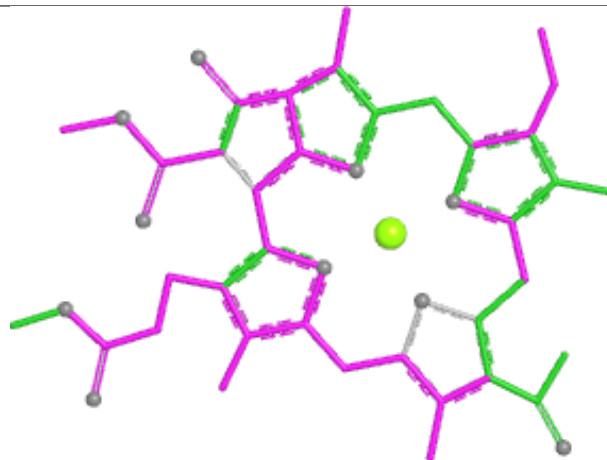


Rings

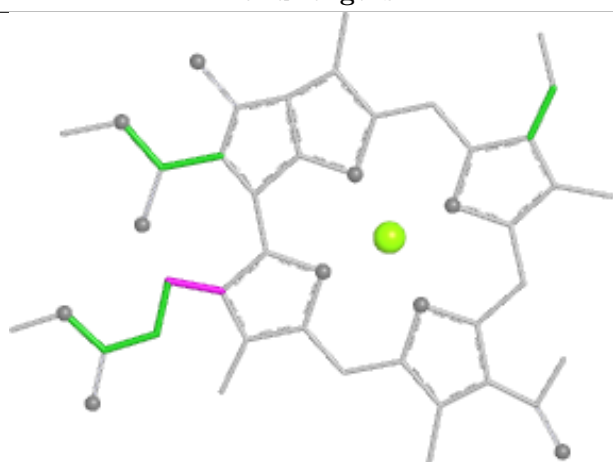
## Ligand BCL 8 36



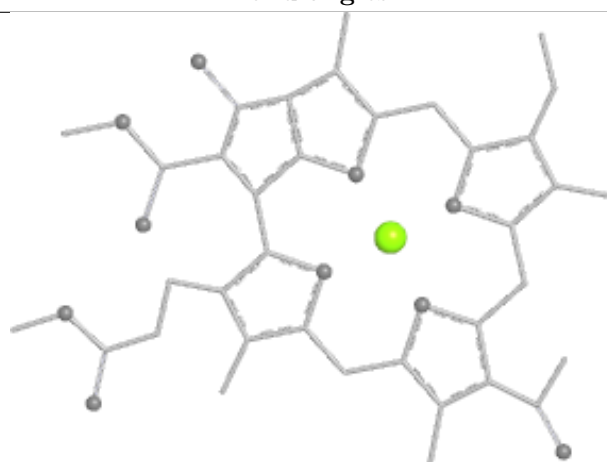
Bond lengths



Bond angles

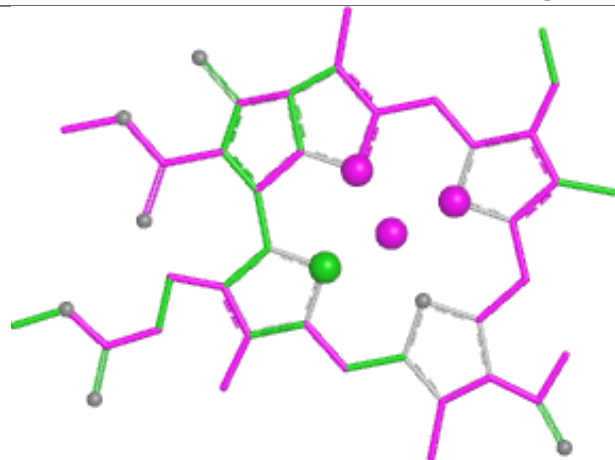


Torsions

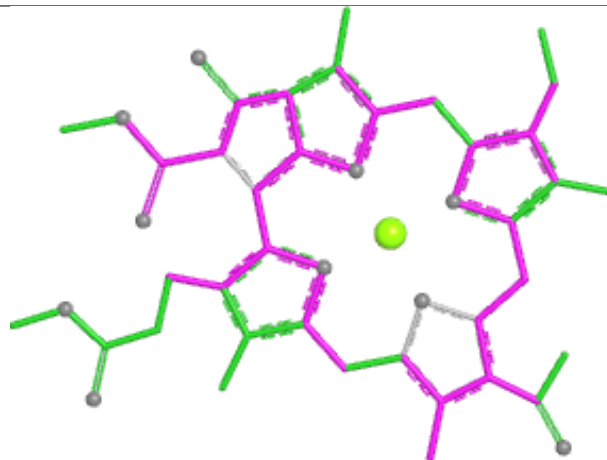


Rings

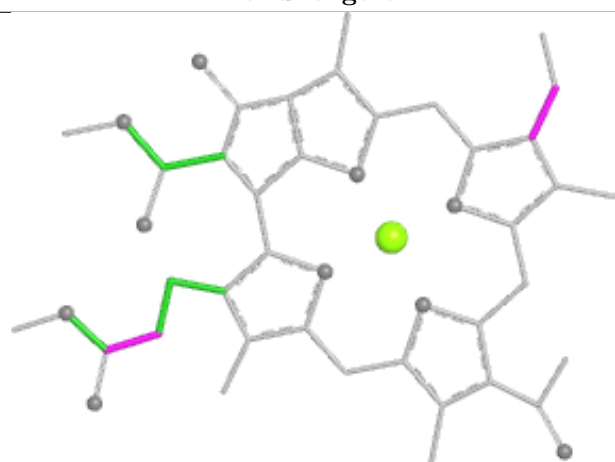
## Ligand BCL J 8



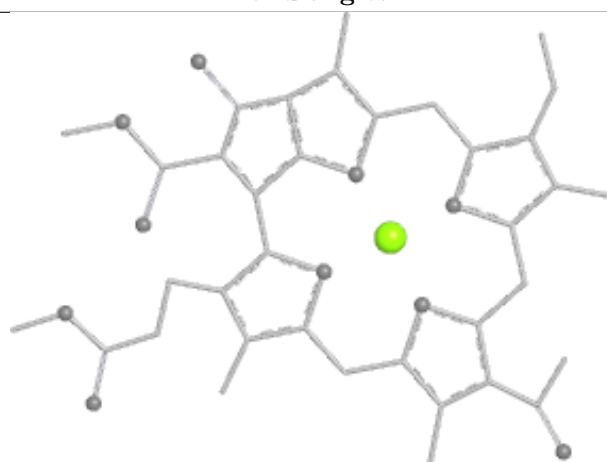
Bond lengths



Bond angles

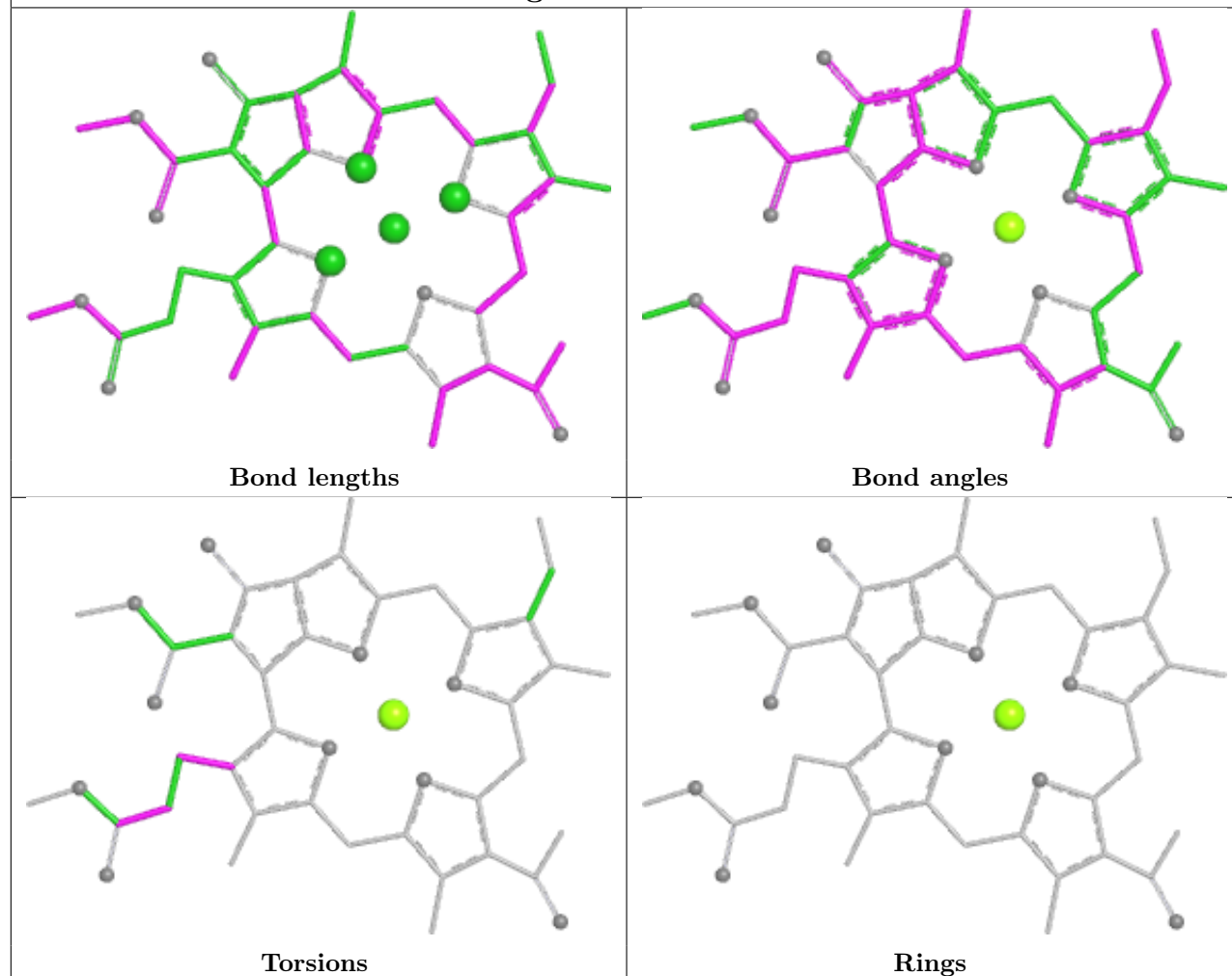


Torsions

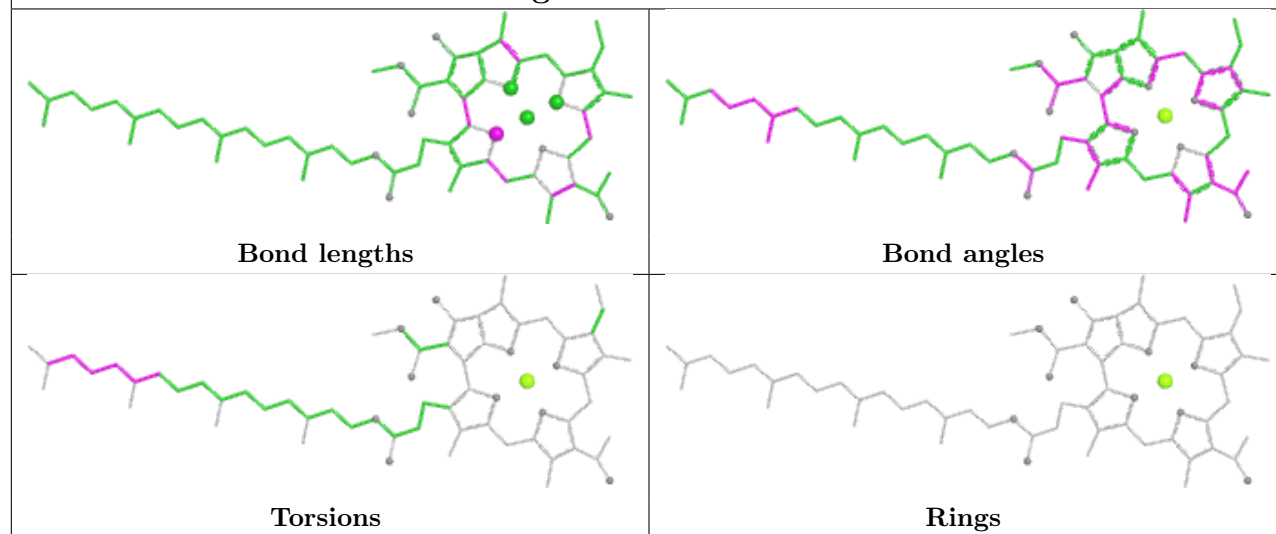


Rings

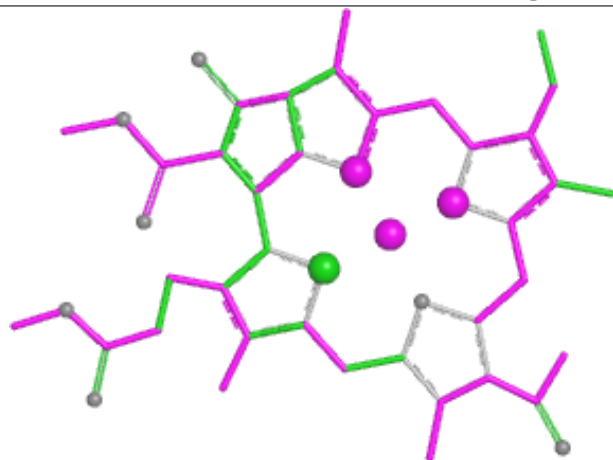
## Ligand BCL S 36



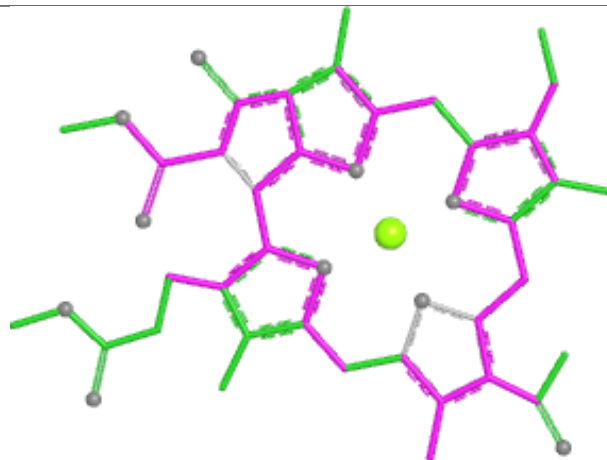
## Ligand BCL A 302



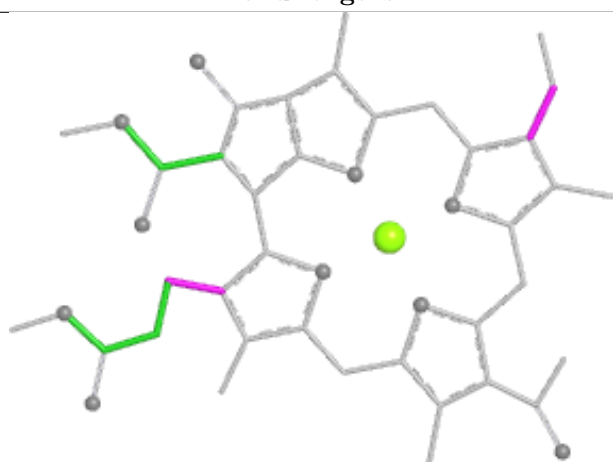
## Ligand BCL P 39



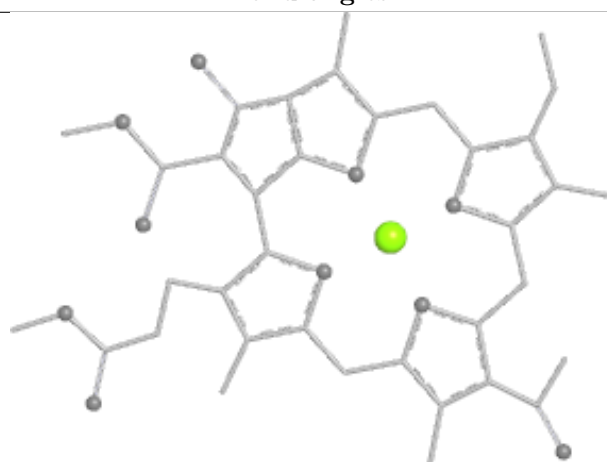
Bond lengths



Bond angles

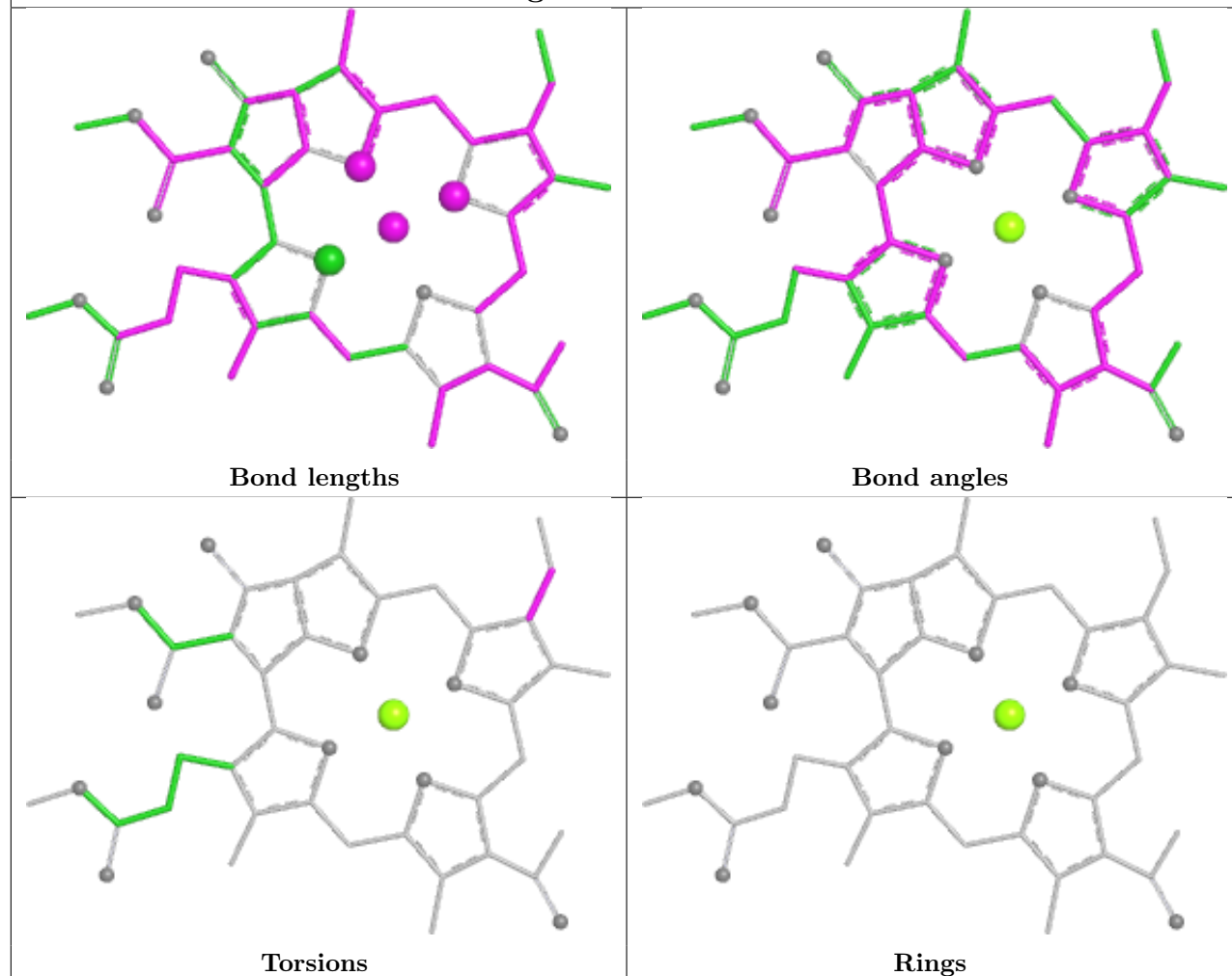


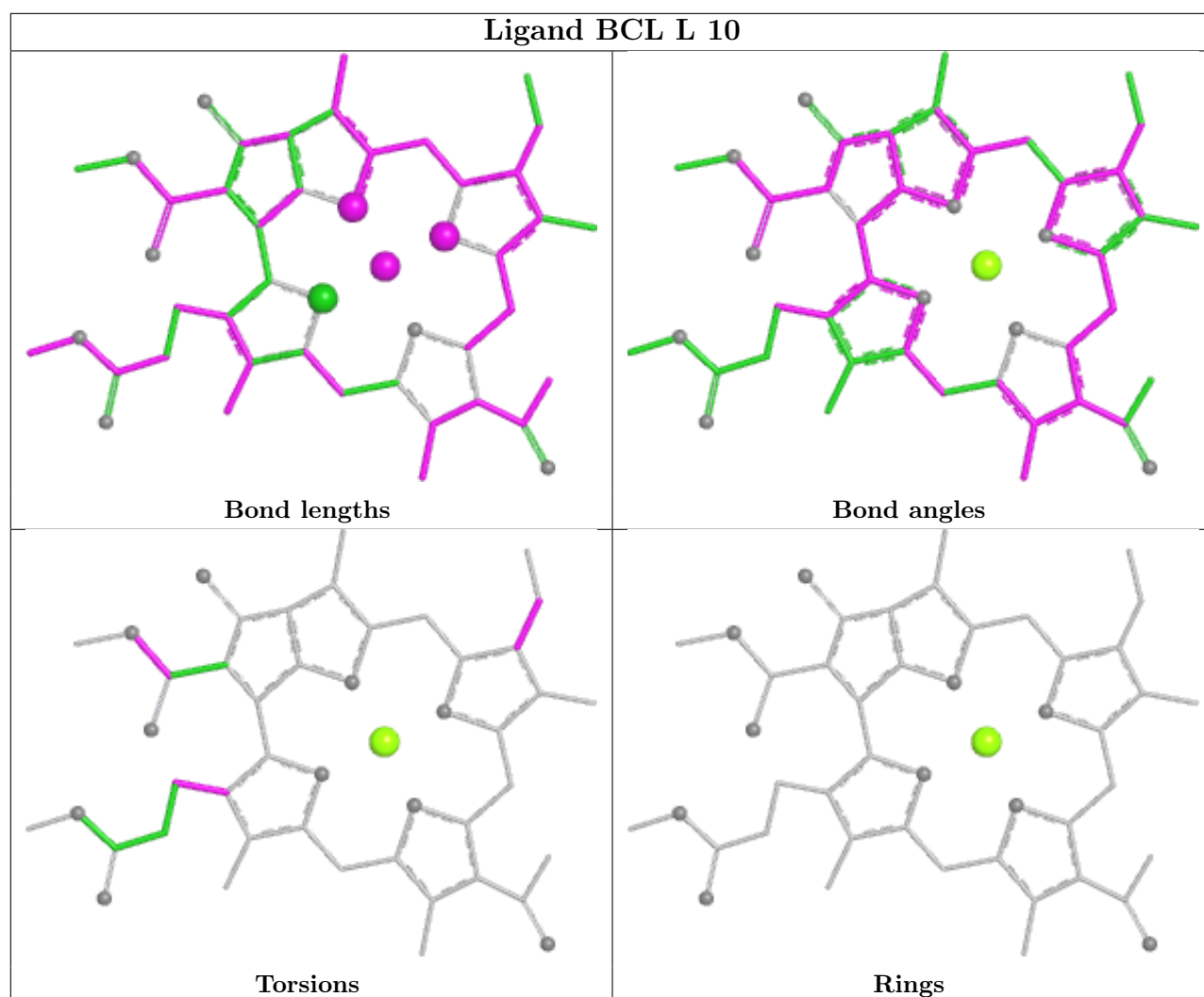
Torsions



Rings

## Ligand BCL 7 38





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	0/281	-	-	-	-
2	B	0/302	-	-	-	-
3	C	0/241	-	-	-	-
4	1	0/26	-	-	-	-
4	3	0/26	-	-	-	-
4	5	0/26	-	-	-	-
4	7	0/26	-	-	-	-
4	D	0/26	-	-	-	-
4	F	0/26	-	-	-	-
4	H	0/26	-	-	-	-
4	J	0/26	-	-	-	-
4	L	0/26	-	-	-	-
4	N	0/26	-	-	-	-
4	P	0/26	-	-	-	-
4	R	0/26	-	-	-	-
4	T	0/26	-	-	-	-
4	V	0/26	-	-	-	-
4	X	0/26	-	-	-	-
4	Z	0/26	-	-	-	-
5	2	0/30	-	-	-	-
5	4	0/30	-	-	-	-
5	6	0/30	-	-	-	-
5	8	0/30	-	-	-	-
5	E	0/30	-	-	-	-
5	G	0/30	-	-	-	-
5	I	0/30	-	-	-	-
5	K	0/30	-	-	-	-
5	M	0/30	-	-	-	-
5	O	0/30	-	-	-	-
5	Q	0/30	-	-	-	-
5	S	0/30	-	-	-	-
5	U	0/30	-	-	-	-

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	W	0/30	-	-	-	-
5	Y	0/30	-	-	-	-
All	All	0/1690	-	-	-	-

There are no RSRZ outliers to report.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	BCL	5	38	47/66	0.52	0.75	198,198,198,198	0
7	BPH	A	401	65/65	0.52	0.69	198,198,198,198	0
6	BCL	U	36	47/66	0.57	0.42	198,198,198,198	0
7	BPH	B	402	65/65	0.57	0.74	198,198,198,198	0
6	BCL	S	36	47/66	0.60	0.58	198,198,198,198	0
6	BCL	P	39	47/66	0.62	0.35	198,198,198,198	0
6	BCL	Y	37	47/66	0.63	0.57	198,198,198,198	0
6	BCL	A	302	66/66	0.64	0.78	198,198,198,198	0
6	BCL	B	304	66/66	0.65	0.67	198,198,198,198	0
6	BCL	F	4	47/66	0.66	0.89	198,198,198,198	0
6	BCL	8	36	47/66	0.66	0.81	198,198,198,198	0
6	BCL	V	38	47/66	0.66	0.56	198,198,198,198	0
6	BCL	M	36	47/66	0.66	0.40	198,198,198,198	0
6	BCL	7	38	47/66	0.67	0.44	198,198,198,198	0
6	BCL	J	8	47/66	0.67	0.30	198,198,198,198	0
6	BCL	T	38	47/66	0.67	0.34	198,198,198,198	0
6	BCL	R	38	47/66	0.67	0.36	198,198,198,198	0

*Continued on next page...*

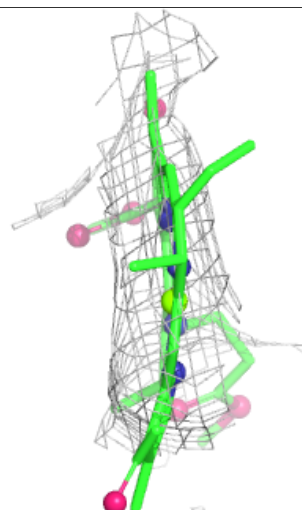
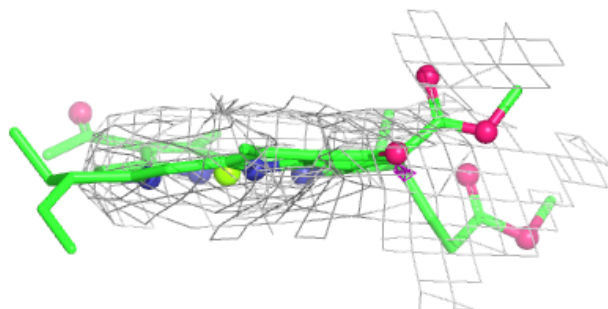
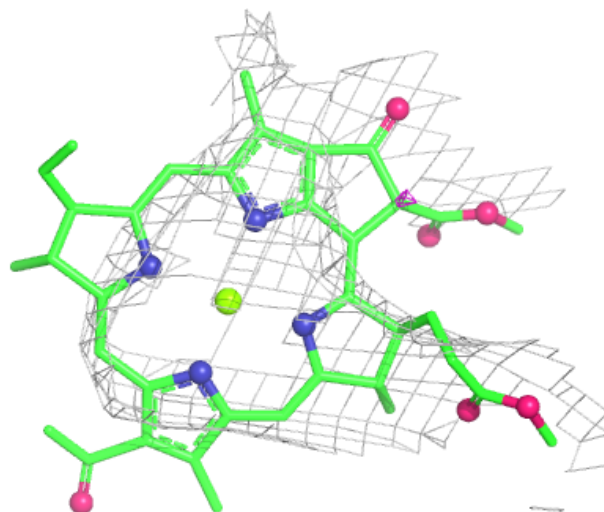
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	BCL	E	1	47/66	0.68	0.40	198,198,198,198	0
6	BCL	D	2	47/66	0.68	0.50	198,198,198,198	0
6	BCL	I	5	47/66	0.70	0.46	198,198,198,198	0
6	BCL	P	38	47/66	0.70	0.27	198,198,198,198	0
6	BCL	1	38	47/66	0.71	0.44	198,198,198,198	0
6	BCL	K	36	47/66	0.71	0.37	198,198,198,198	0
6	BCL	3	39	47/66	0.72	0.33	198,198,198,198	0
6	BCL	A	301	66/66	0.72	0.54	198,198,198,198	0
6	BCL	L	10	47/66	0.73	0.37	198,198,198,198	0
6	BCL	6	36	47/66	0.73	0.42	198,198,198,198	0
6	BCL	B	303	66/66	0.73	0.70	198,198,198,198	0
6	BCL	H	6	47/66	0.76	0.27	198,198,198,198	0
6	BCL	W	36	47/66	0.78	0.67	198,198,198,198	0
6	BCL	Y	36	47/66	0.79	0.32	198,198,198,198	0
6	BCL	N	38	47/66	0.79	0.22	198,198,198,198	0
6	BCL	3	38	47/66	0.80	0.24	198,198,198,198	0
6	BCL	N	11	47/66	0.81	0.22	198,198,198,198	0
6	BCL	G	3	47/66	0.82	0.43	198,198,198,198	0
6	BCL	2	36	47/66	0.83	0.52	198,198,198,198	0
8	FE	B	500	1/1	0.94	0.63	198,198,198,198	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.

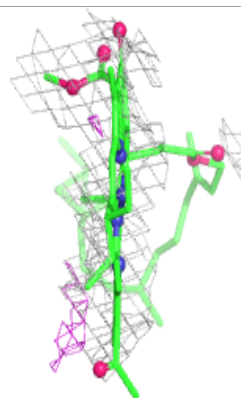
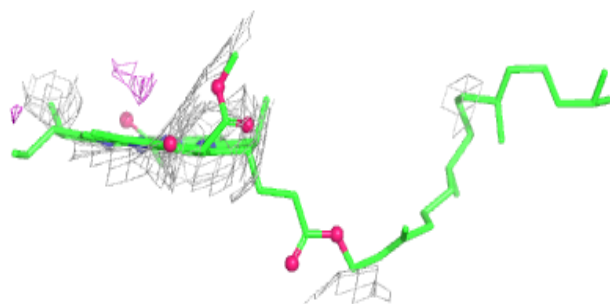
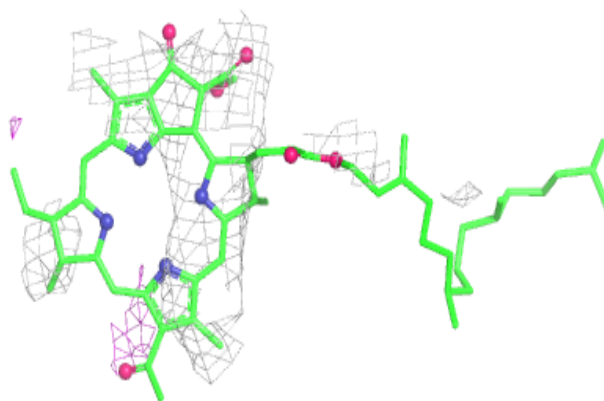
**Electron density around BCL 5 38:**

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



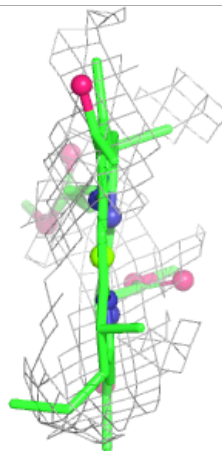
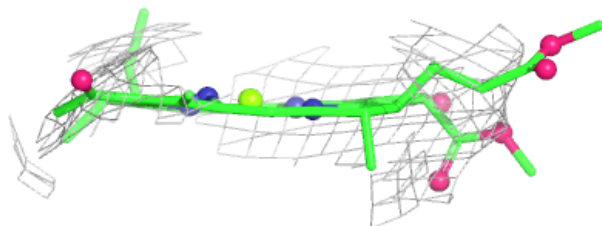
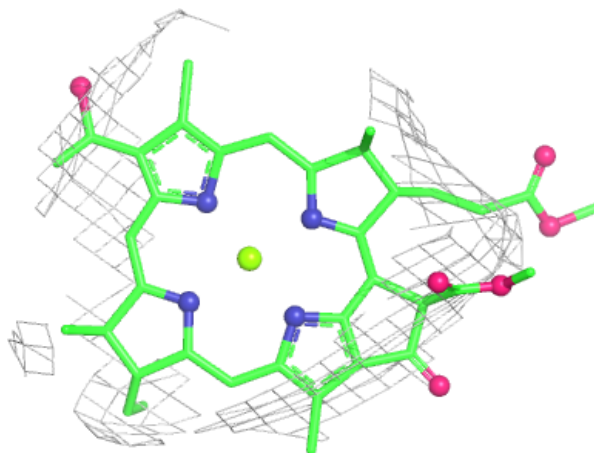
**Electron density around BPH A 401:**

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



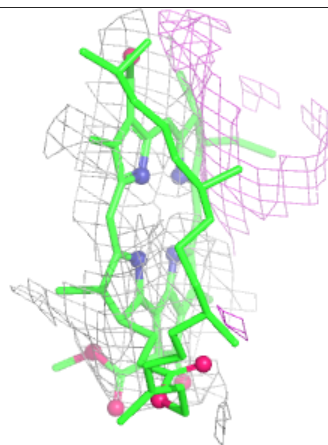
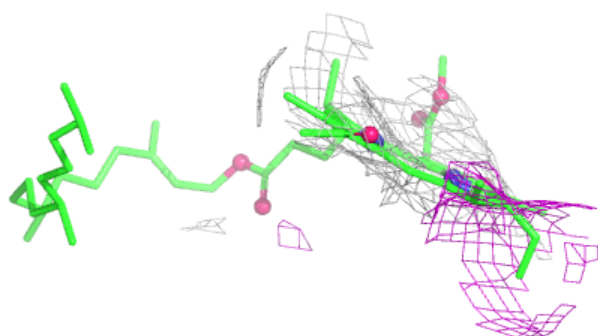
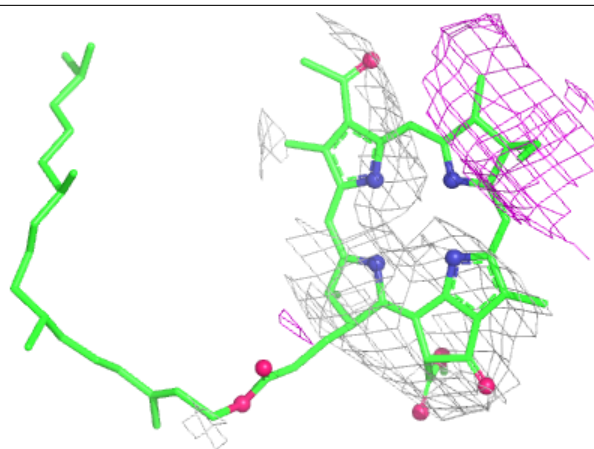
**Electron density around BCL U 36:**

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



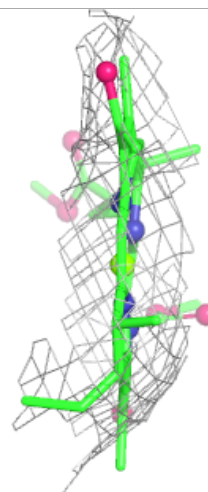
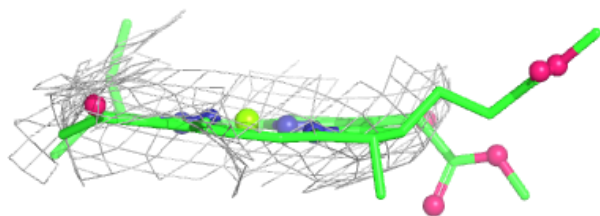
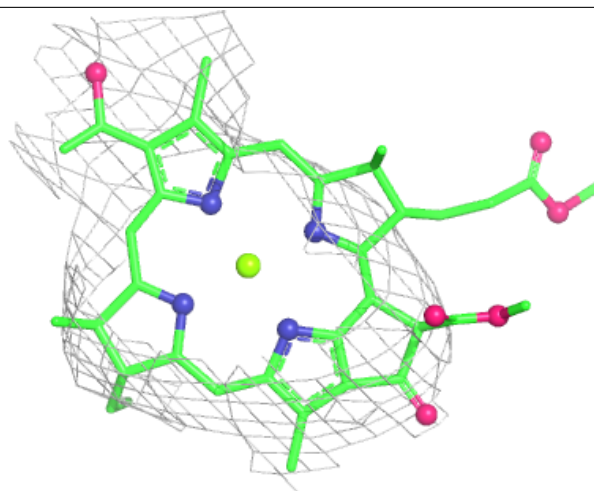
**Electron density around BPH B 402:**

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



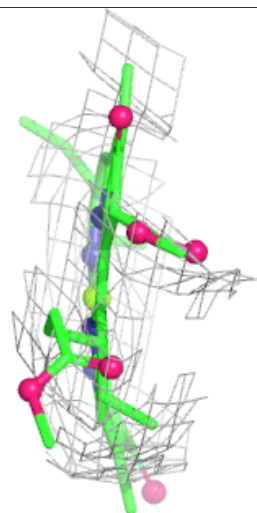
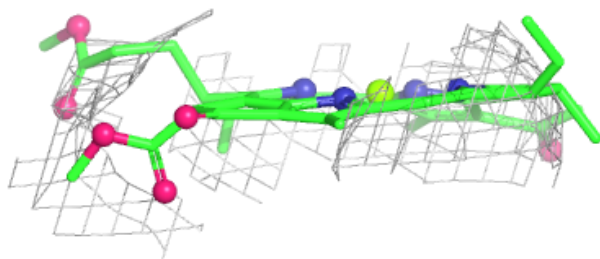
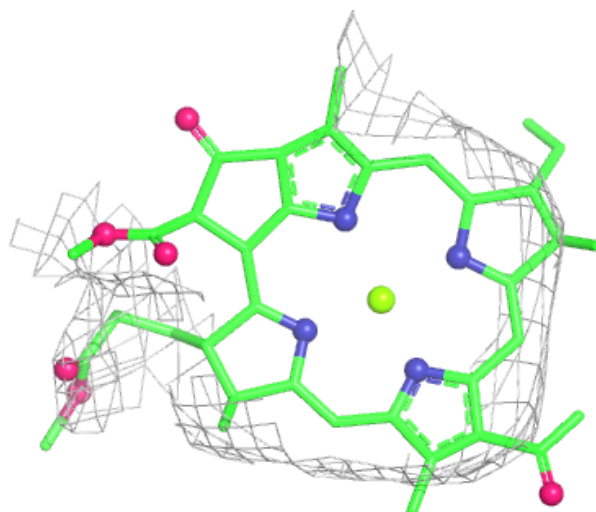
**Electron density around BCL S 36:**

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



**Electron density around BCL P 39:**

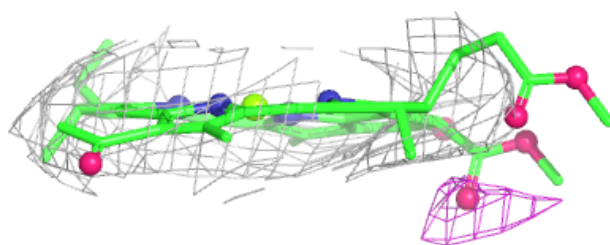
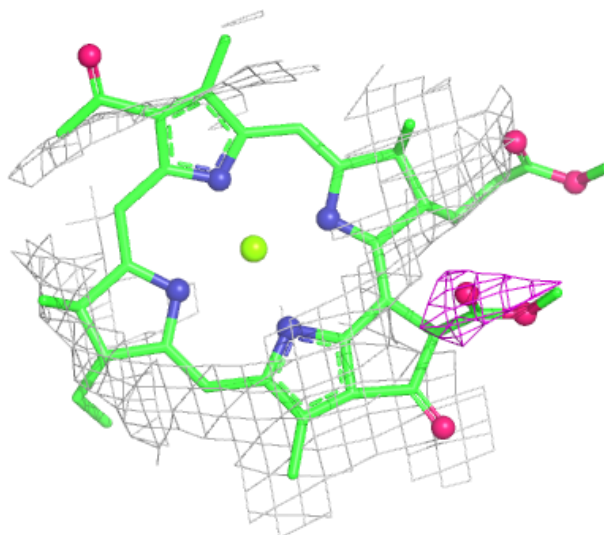
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





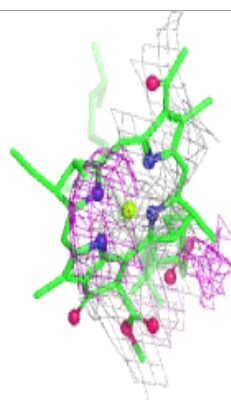
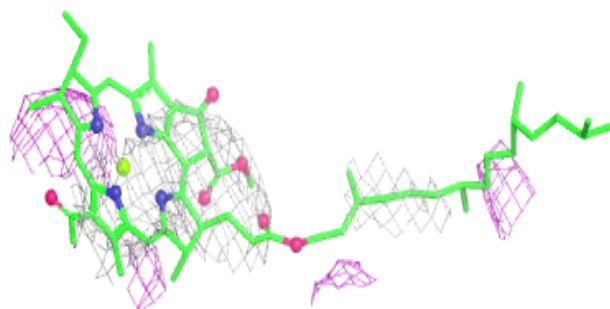
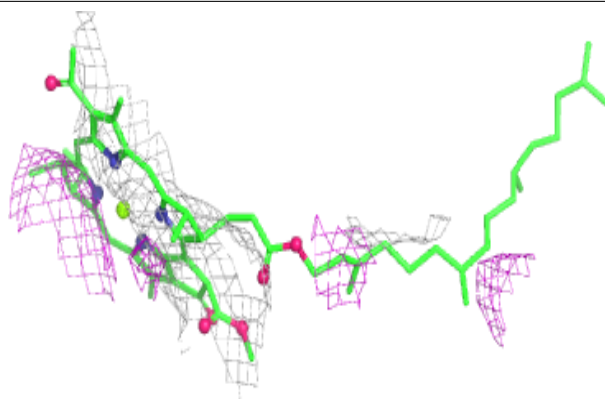
**Electron density around BCL Y 37:**

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

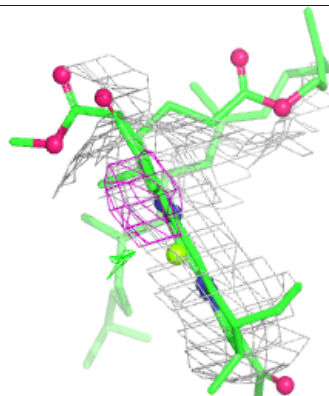
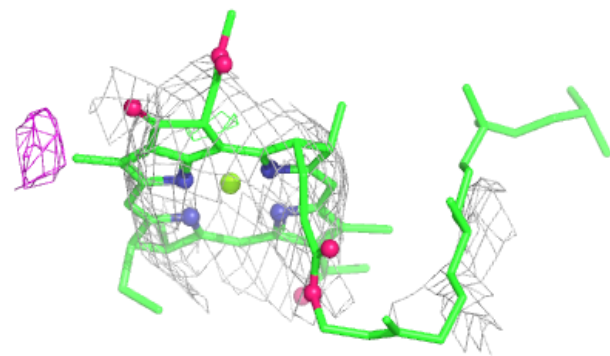
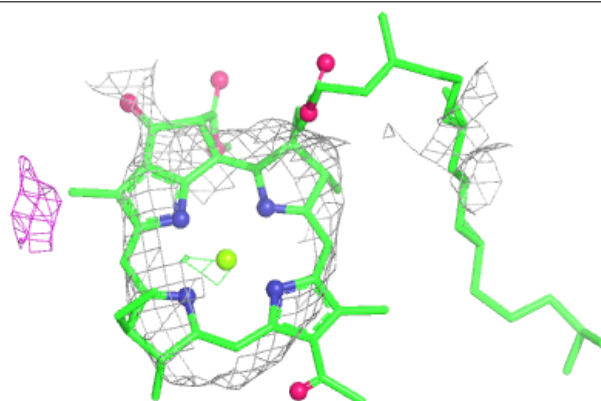


**Electron density around BCL A 302:**

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

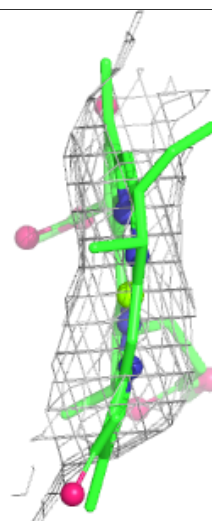
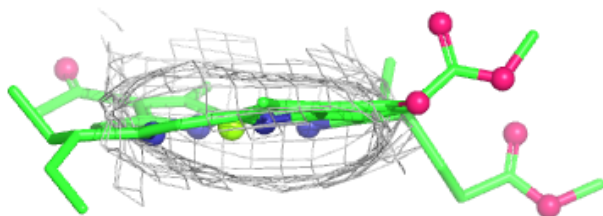
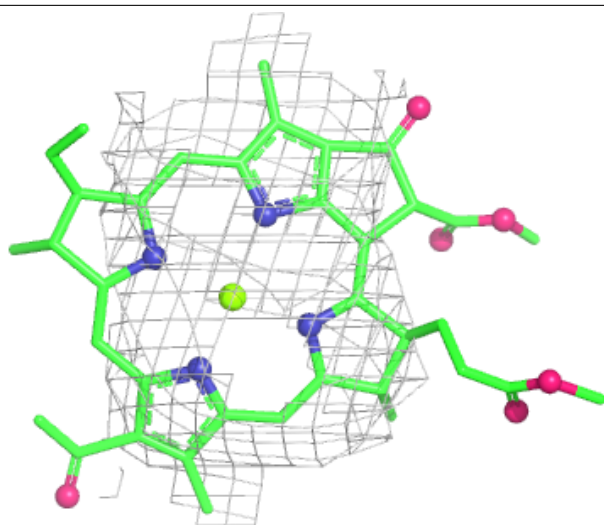
**Electron density around BCL B 304:**

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



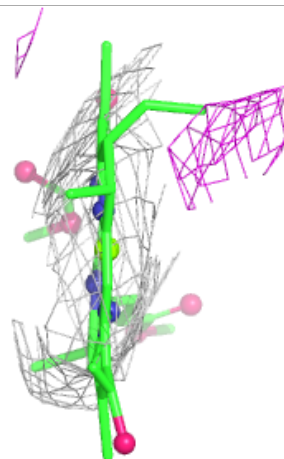
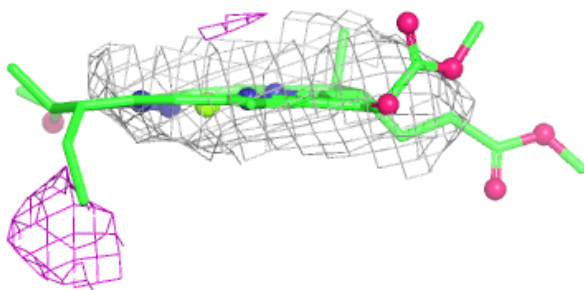
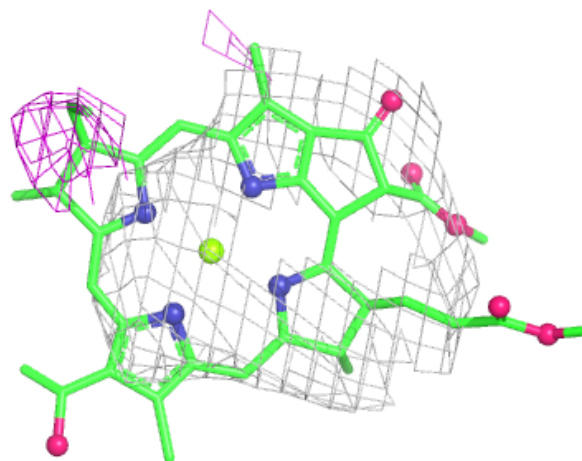
**Electron density around BCL F 4:**

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



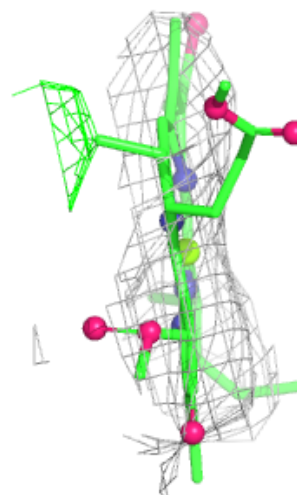
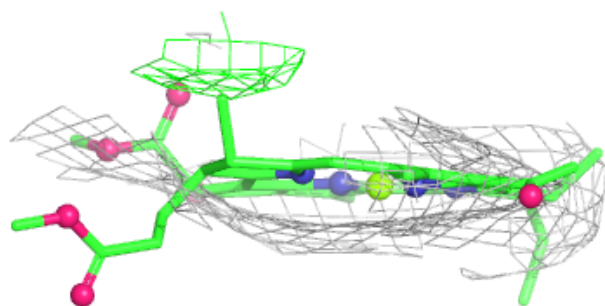
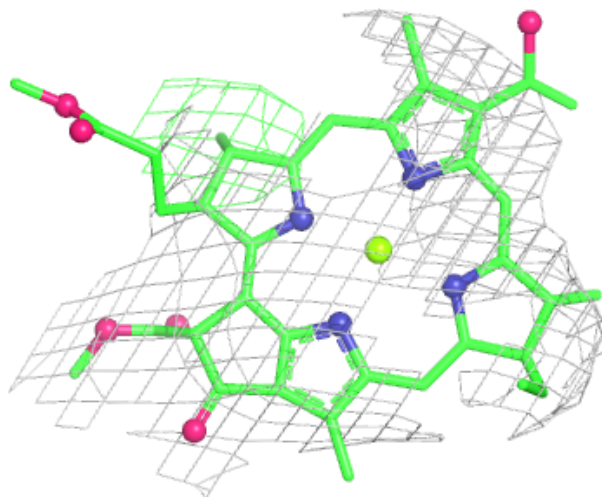
**Electron density around BCL 8 36:**

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



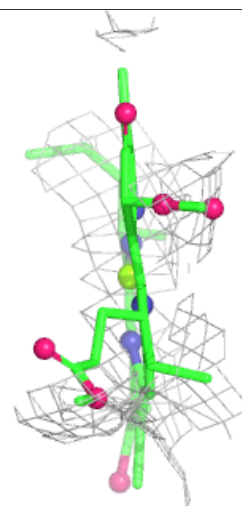
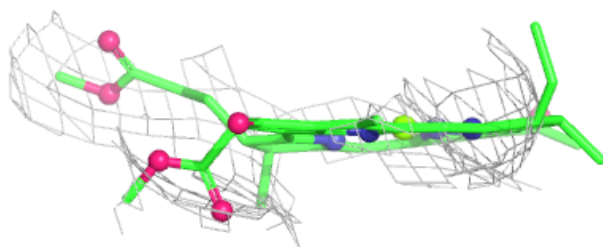
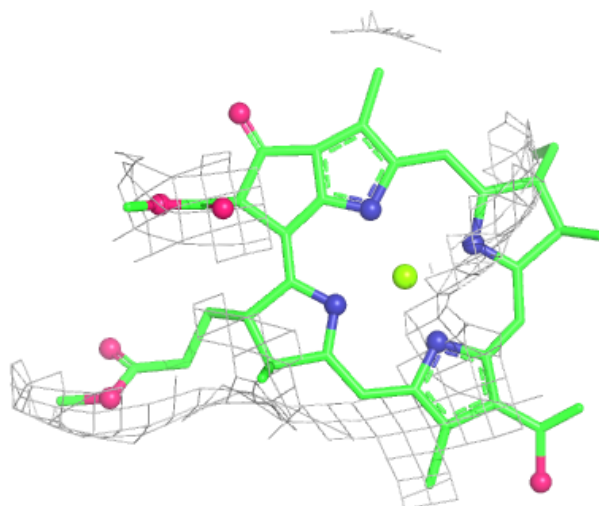
**Electron density around BCL V 38:**

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



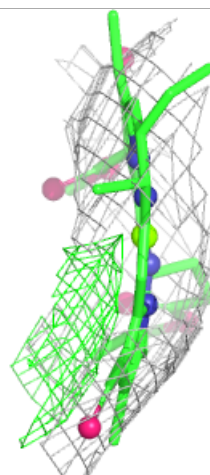
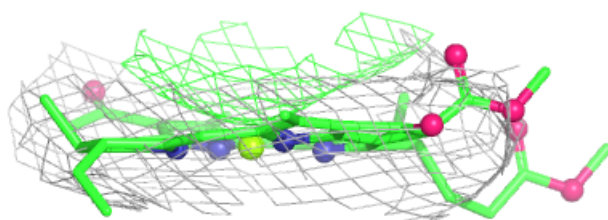
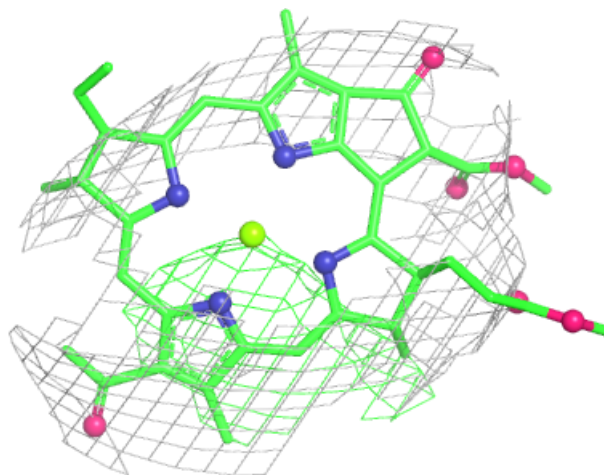
**Electron density around BCL M 36:**

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



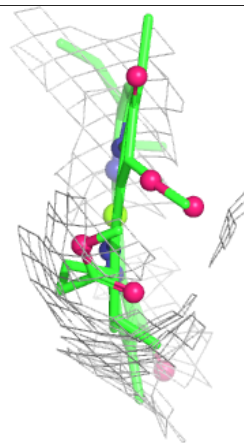
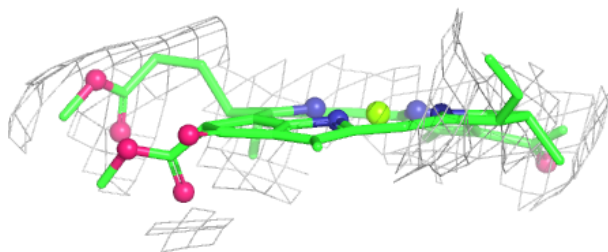
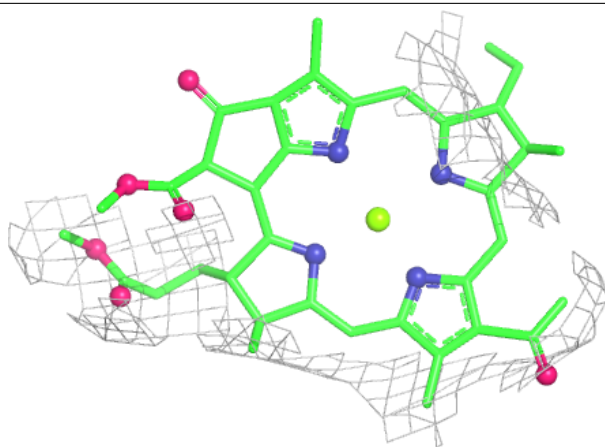
**Electron density around BCL 7 38:**

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



**Electron density around BCL J 8:**

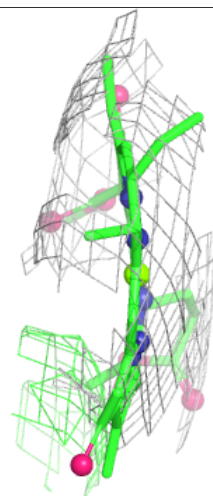
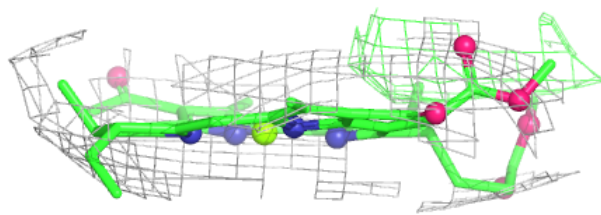
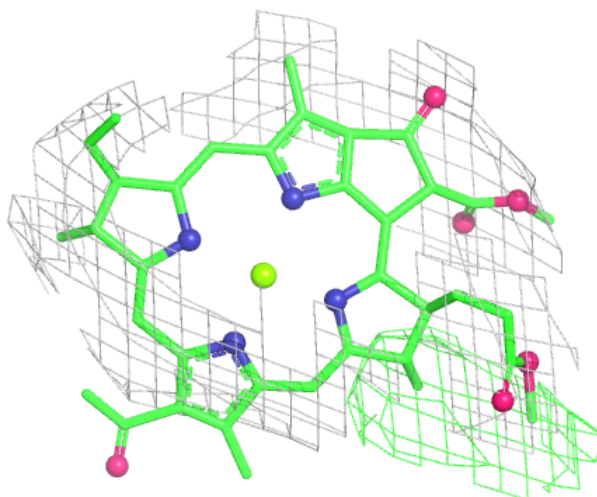
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





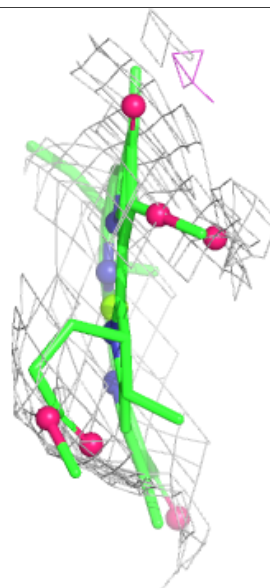
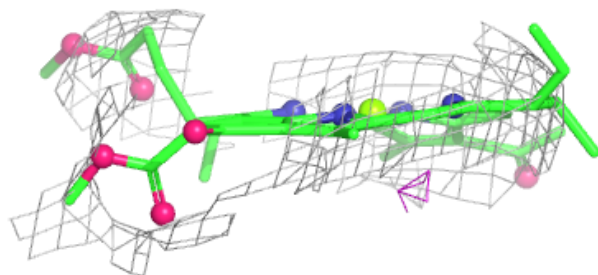
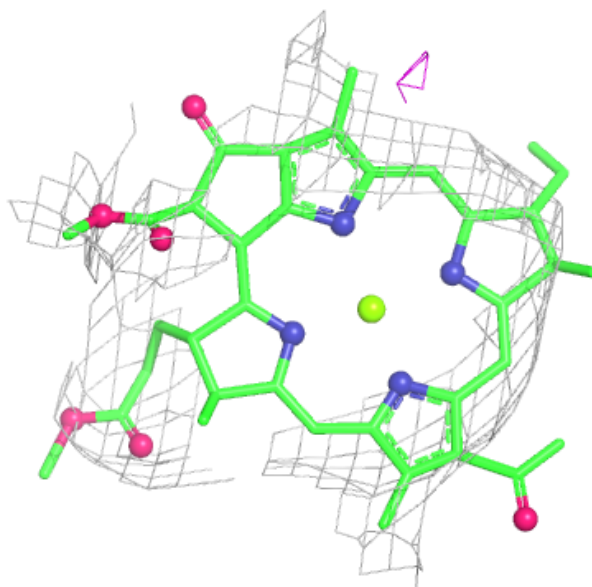
**Electron density around BCL T 38:**

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



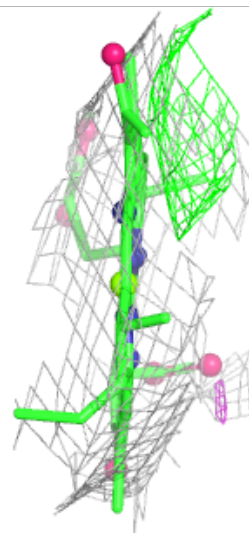
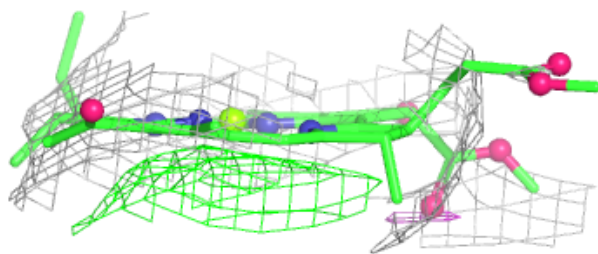
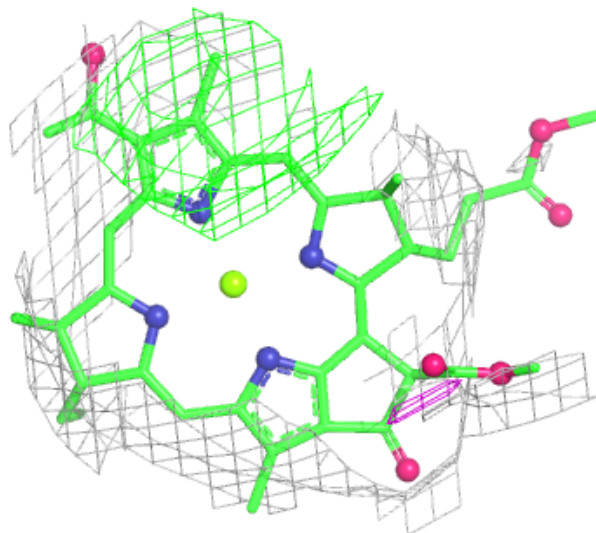
**Electron density around BCL R 38:**

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



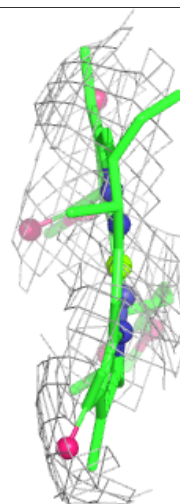
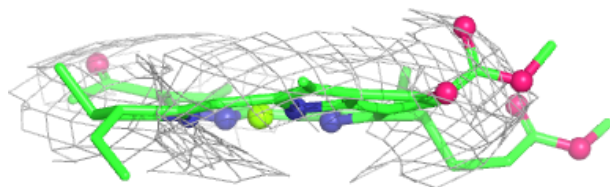
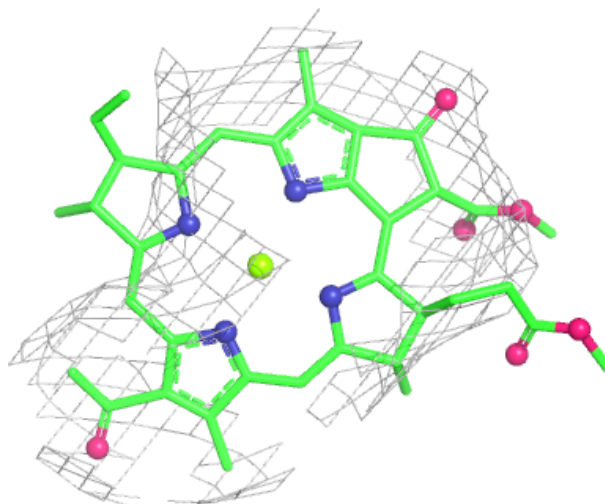
**Electron density around BCL E 1:**

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



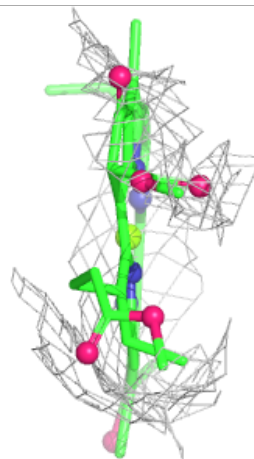
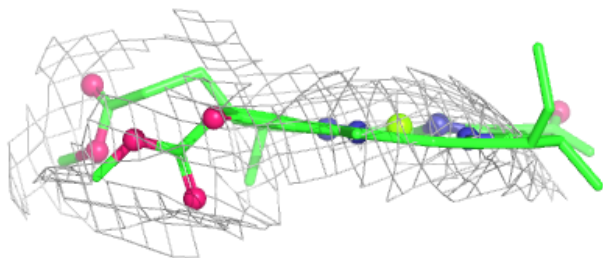
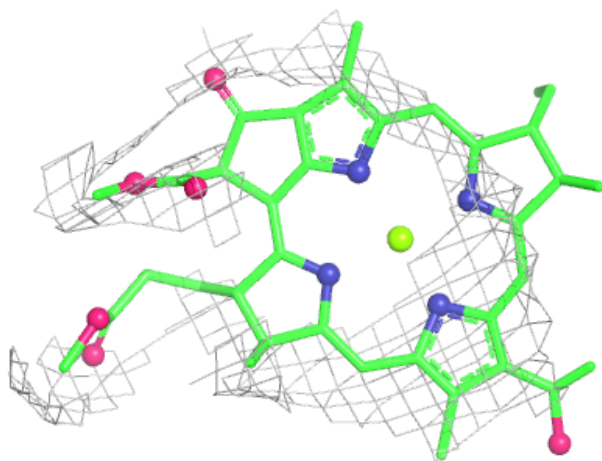
**Electron density around BCL D 2:**

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



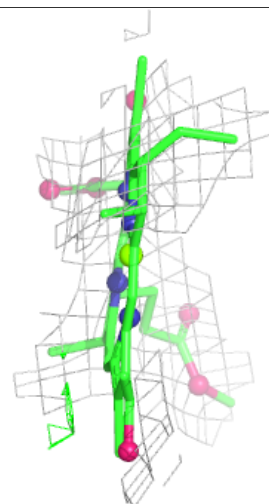
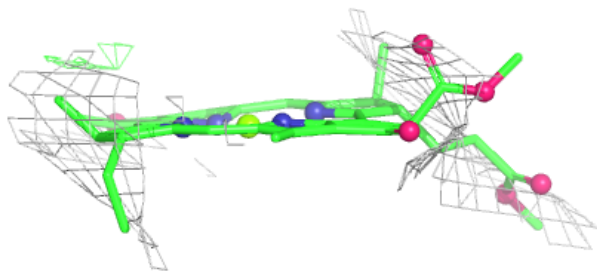
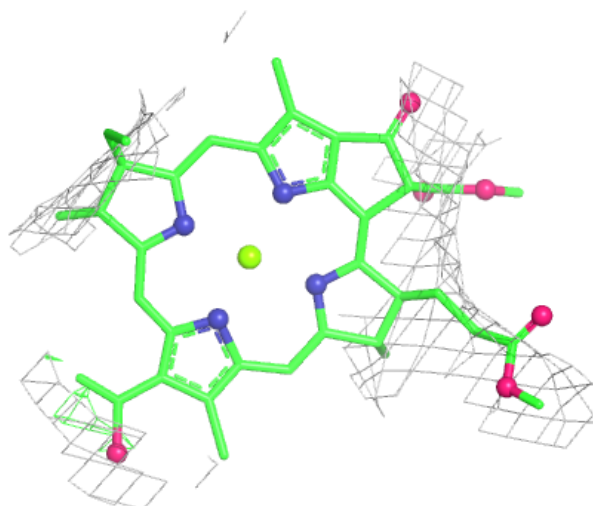
**Electron density around BCL I 5:**

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



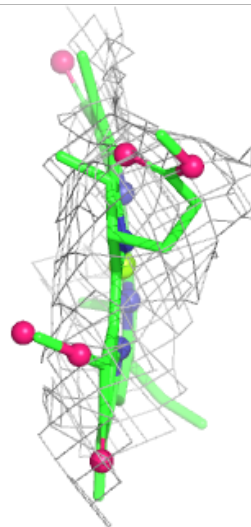
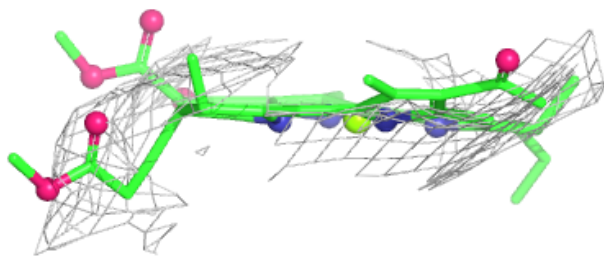
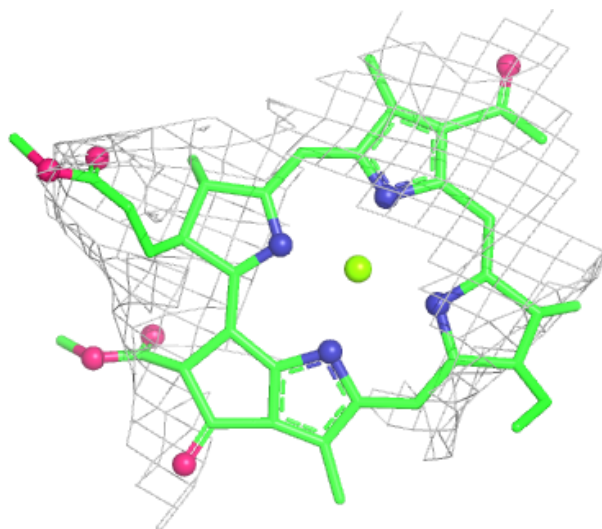
**Electron density around BCL P 38:**

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



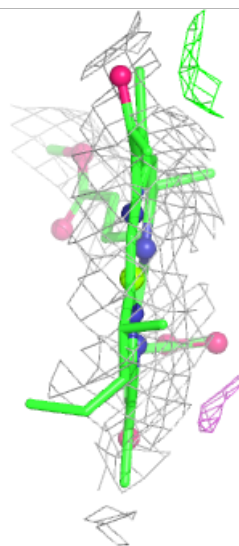
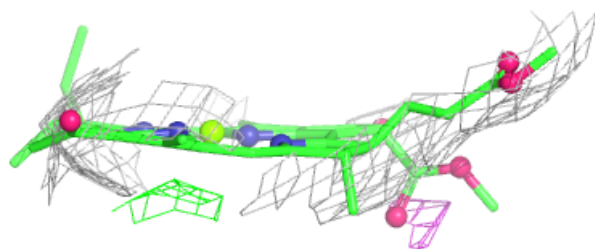
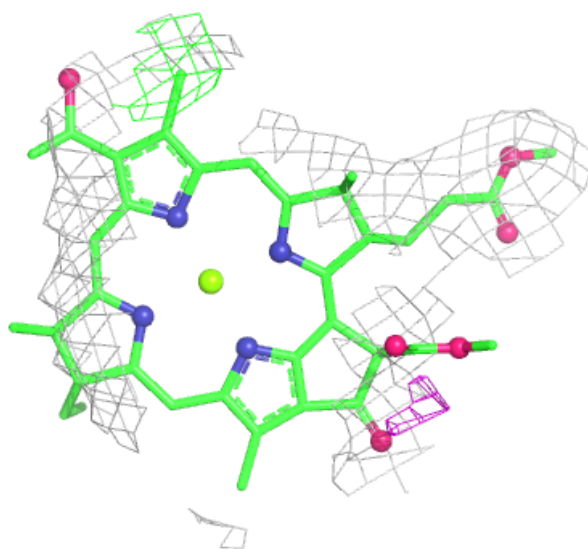
**Electron density around BCL 1 38:**

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



**Electron density around BCL K 36:**

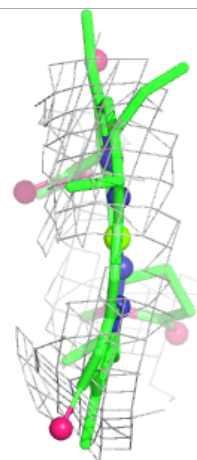
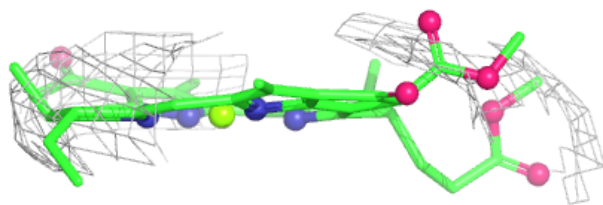
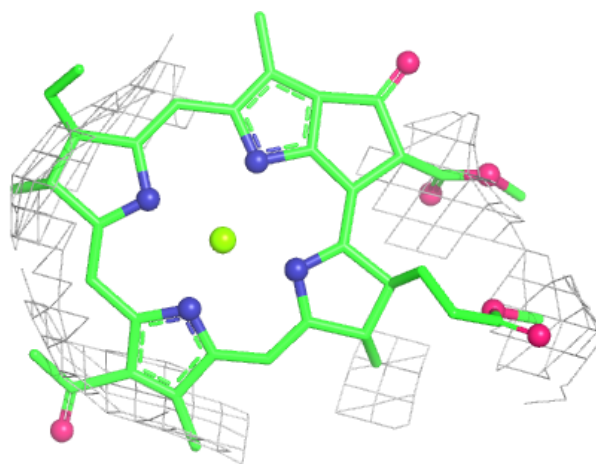
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





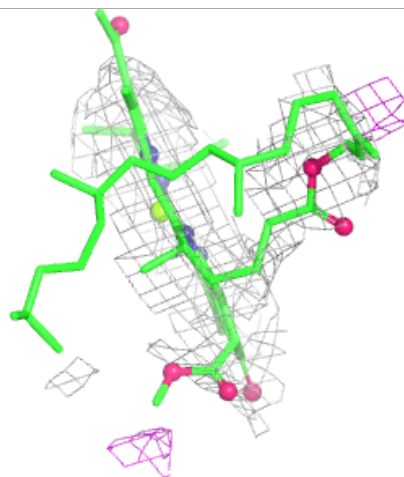
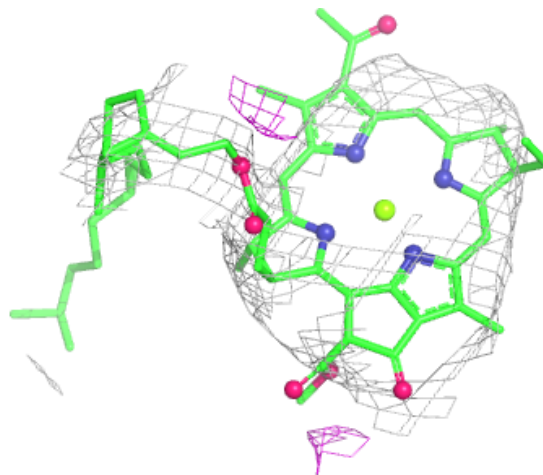
**Electron density around BCL 3 39:**

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



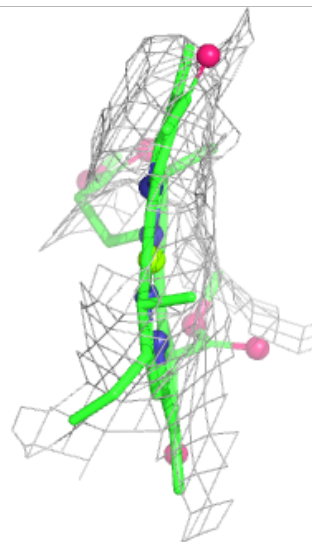
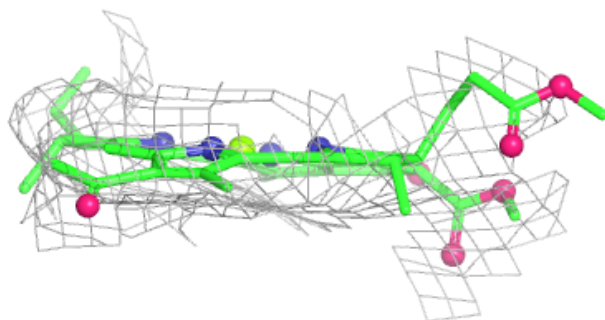
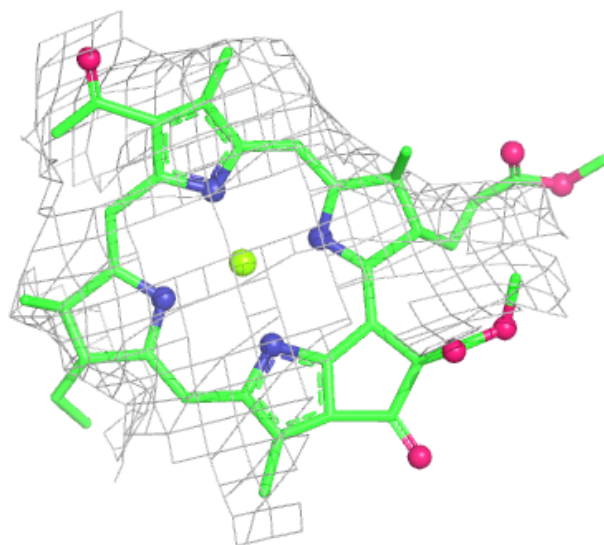
**Electron density around BCL A 301:**

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



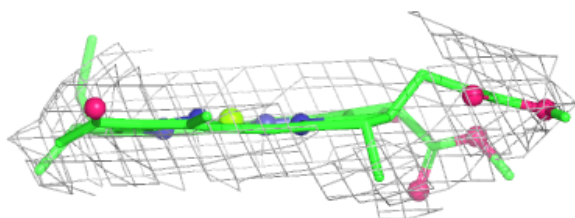
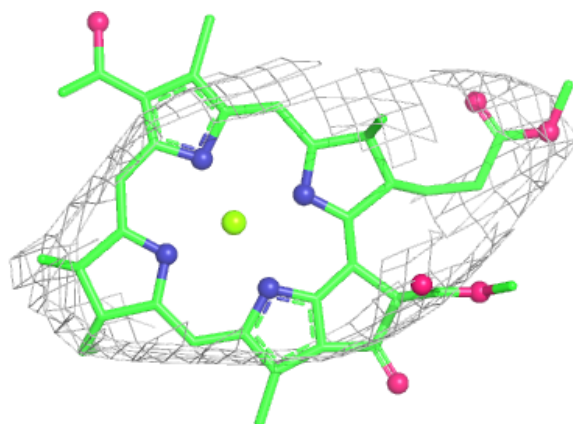
**Electron density around BCL L 10:**

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

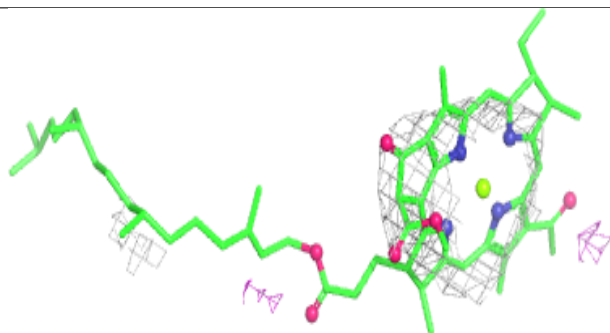
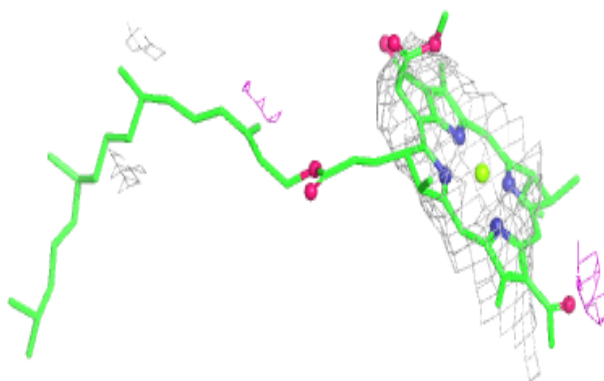


**Electron density around BCL 6 36:**

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

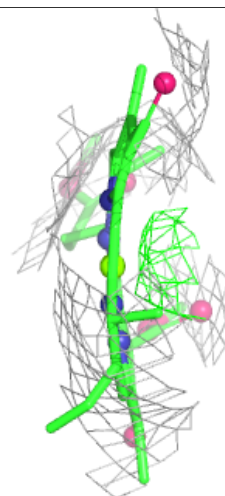
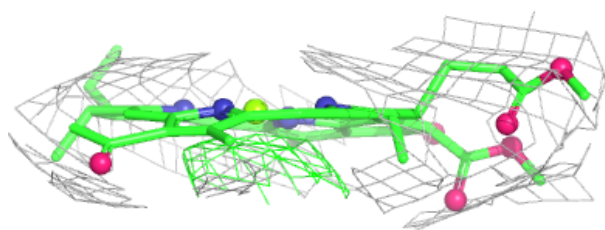
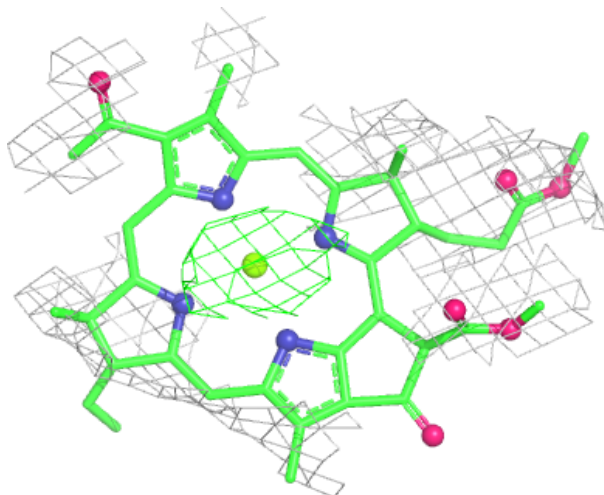
**Electron density around BCL B 303:**

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



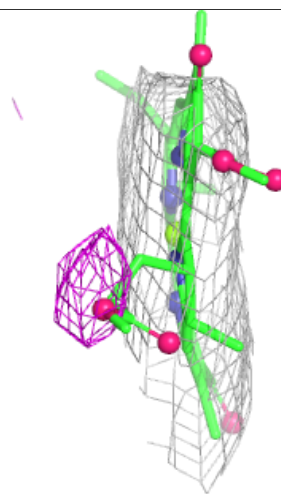
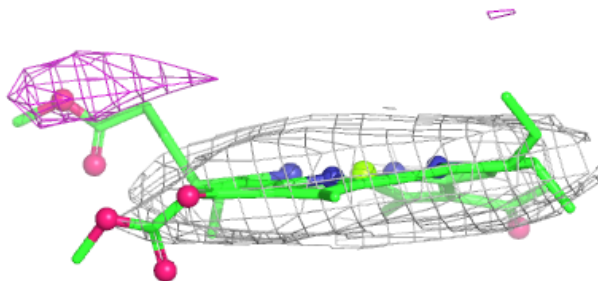
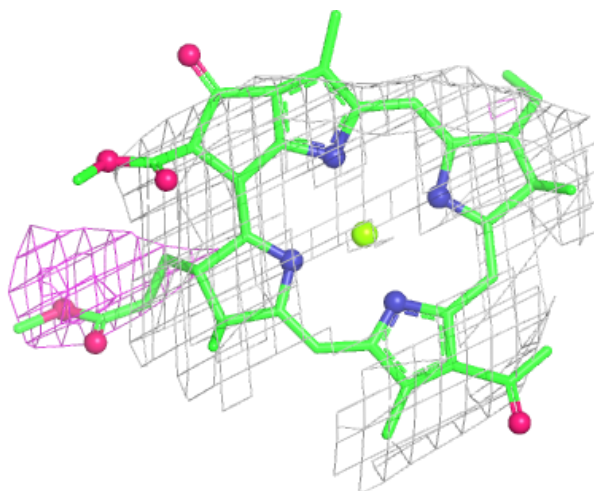
**Electron density around BCL H 6:**

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



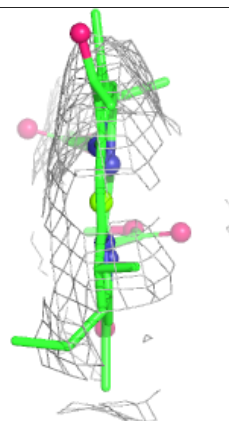
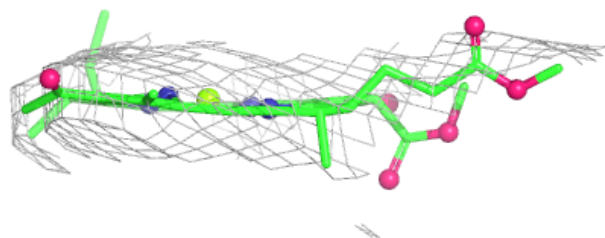
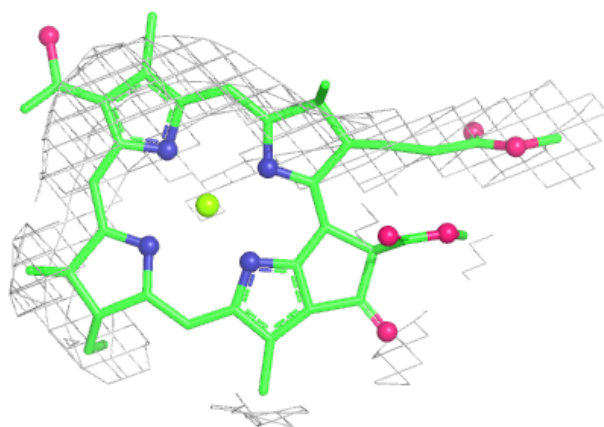
**Electron density around BCL W 36:**

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



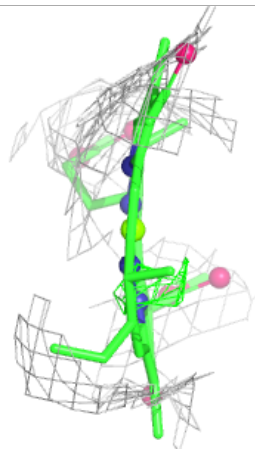
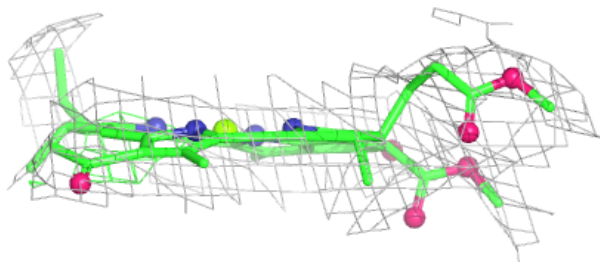
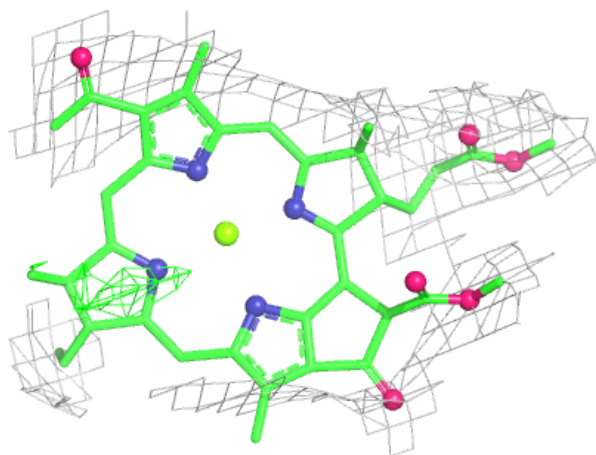
**Electron density around BCL Y 36:**

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



**Electron density around BCL N 38:**

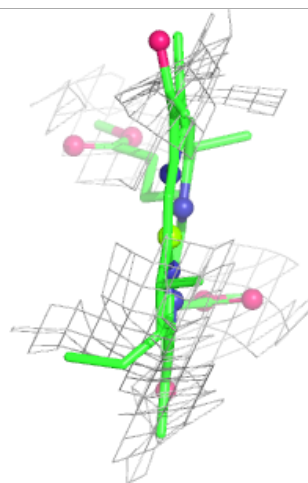
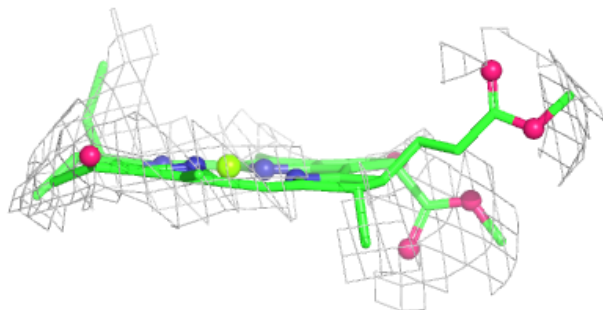
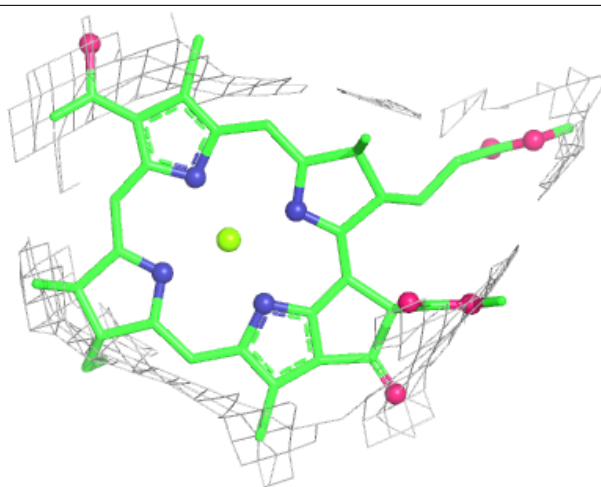
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





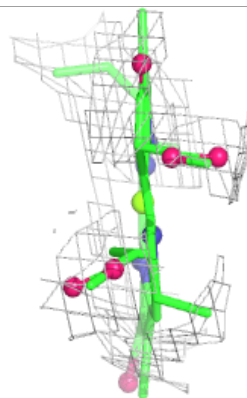
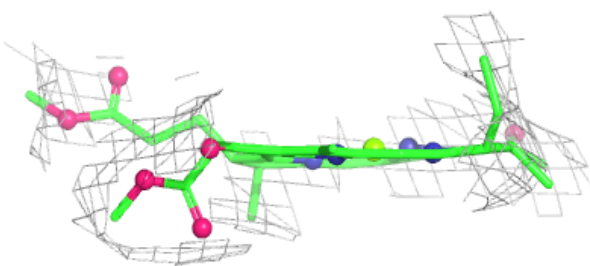
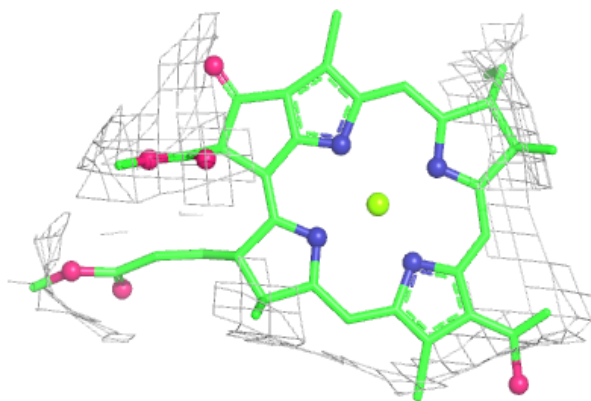
**Electron density around BCL 3 38:**

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

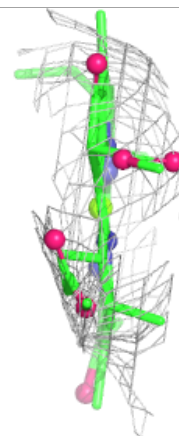
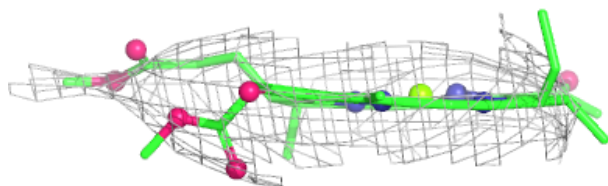
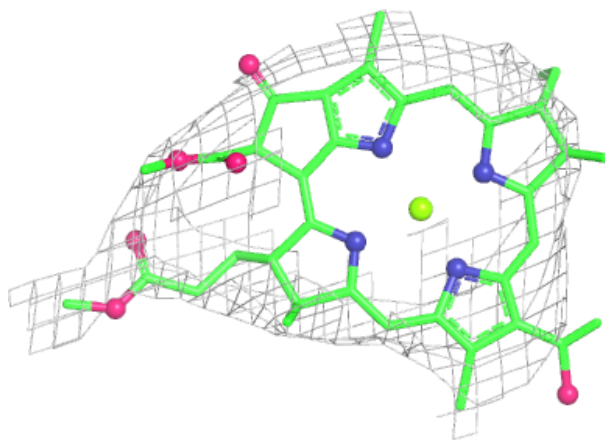


**Electron density around BCL N 11:**

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

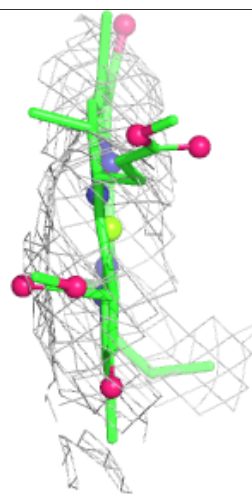
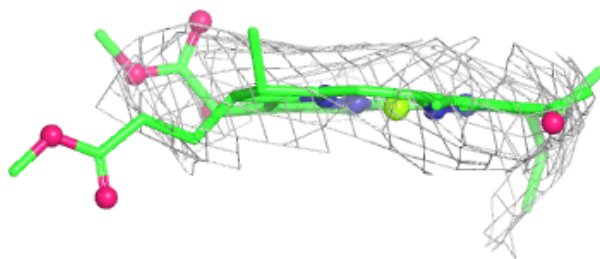
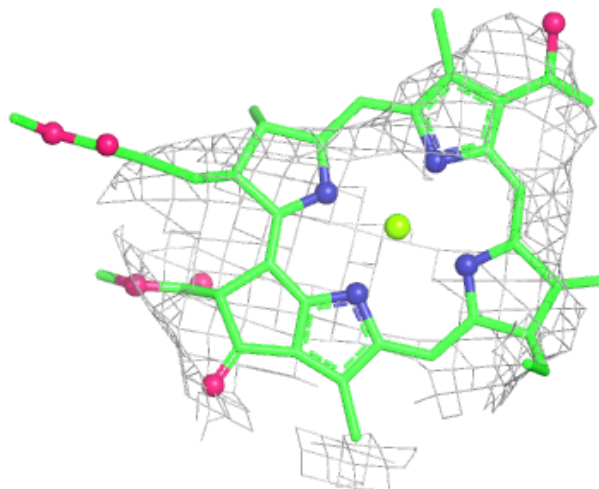
**Electron density around BCL G 3:**

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



**Electron density around BCL 2 36:**

$2mF_o-DF_c$  (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.