



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:31 AM UTC

PDB ID : 9DWZ / pdb_00009dwz
EMDB ID : EMD-47275
Title : Light Harvesting complex 3 (LH3), B800-B820, of Rhodoblastus (Rbl.) acidophilus strain 7750
Authors : Harris, D.; Schlau-Cohen, G.S.
Deposited on : 2024-10-10
Resolution : 2.35 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

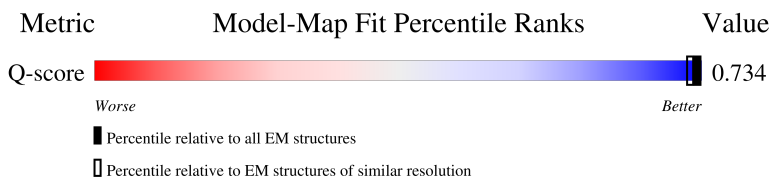
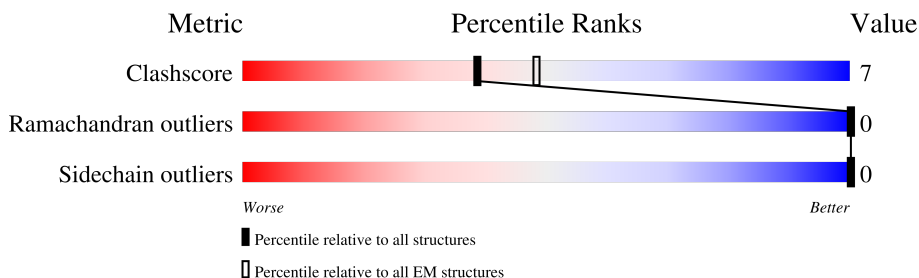
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 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.








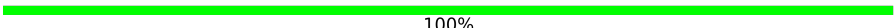
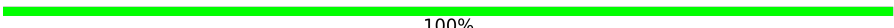
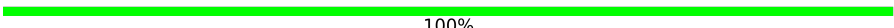
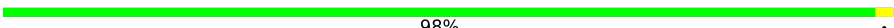
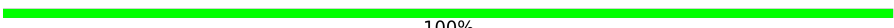
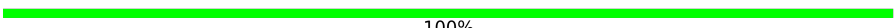
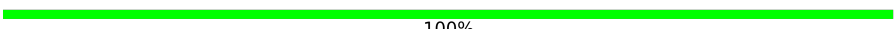
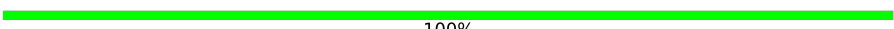
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4607 (1.85 - 2.85)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	48	 90% 10%
1	C	48	 92% 8%
1	E	48	 88% 12%
1	G	48	 90% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	48	 92% 8%
1	K	48	 92% 8%
1	M	48	 90% 10%
1	O	48	 92% 8%
1	Q	48	 92% 8%
2	B	41	 100%
2	D	41	 100%
2	F	41	 100%
2	H	41	 100%
2	J	41	 98% .
2	L	41	 100%
2	N	41	 100%
2	P	41	 100%
2	R	41	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8766 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Light-harvesting protein B-800/820 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	C	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	E	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	G	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	I	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	K	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	M	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	O	48	Total	C	N	O	S	0	0
			361	240	60	60	1		
1	Q	48	Total	C	N	O	S	0	0
			361	240	60	60	1		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	GLN	THR	conflict	UNP P35090
C	45	GLN	THR	conflict	UNP P35090
E	45	GLN	THR	conflict	UNP P35090
G	45	GLN	THR	conflict	UNP P35090
I	45	GLN	THR	conflict	UNP P35090
K	45	GLN	THR	conflict	UNP P35090
M	45	GLN	THR	conflict	UNP P35090
O	45	GLN	THR	conflict	UNP P35090
Q	45	GLN	THR	conflict	UNP P35090

- Molecule 2 is a protein called Light-harvesting protein B-800/820 beta-2 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	41	Total	C	N	O	0	0
			323	215	53	55		
2	D	41	Total	C	N	O	0	0
			323	215	53	55		
2	F	41	Total	C	N	O	0	0
			323	215	53	55		
2	H	41	Total	C	N	O	0	0
			323	215	53	55		
2	J	41	Total	C	N	O	0	0
			323	215	53	55		
2	L	41	Total	C	N	O	0	0
			323	215	53	55		
2	N	41	Total	C	N	O	0	0
			323	215	53	55		
2	P	41	Total	C	N	O	0	0
			323	215	53	55		
2	R	41	Total	C	N	O	0	0
			323	215	53	55		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	LEU	ALA	conflict	UNP P35096
D	37	LEU	ALA	conflict	UNP P35096
F	37	LEU	ALA	conflict	UNP P35096
H	37	LEU	ALA	conflict	UNP P35096
J	37	LEU	ALA	conflict	UNP P35096
L	37	LEU	ALA	conflict	UNP P35096
N	37	LEU	ALA	conflict	UNP P35096
P	37	LEU	ALA	conflict	UNP P35096
R	37	LEU	ALA	conflict	UNP P35096

- Molecule 3 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

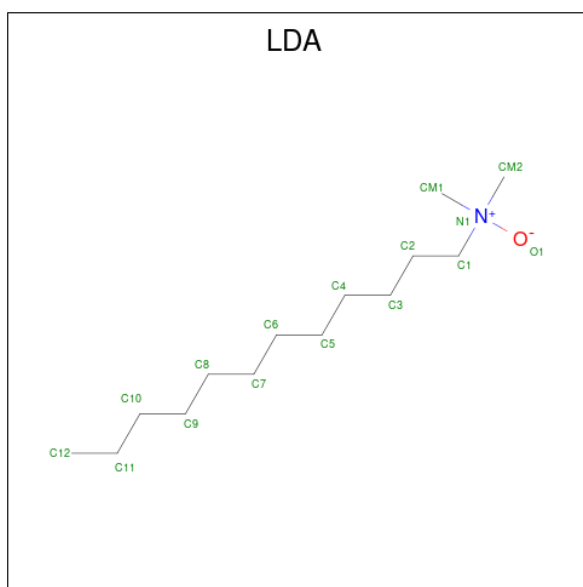


Continued on next page...

Continued from previous page...

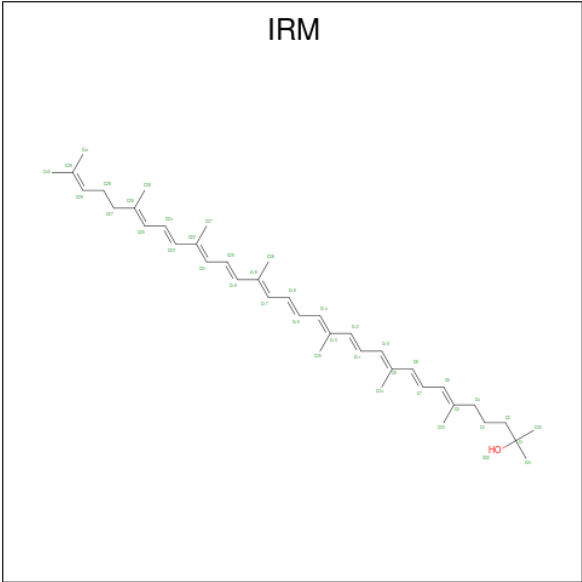
Mol	Chain	Residues	Atoms					AltConf
3	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



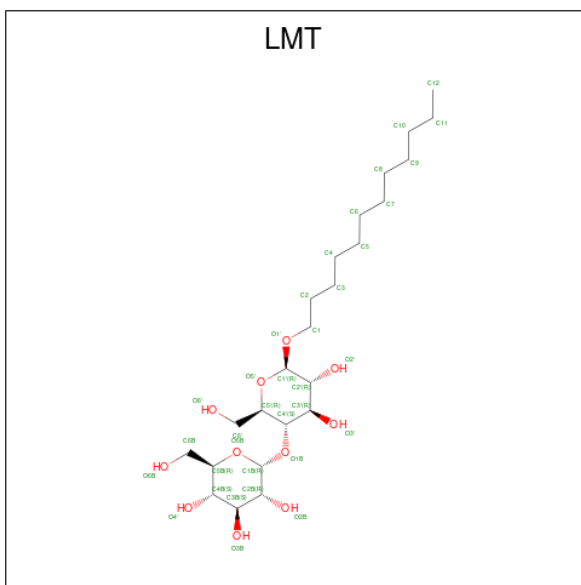
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			16	14	1	1	
4	C	1	Total	C	N	O	0
			16	14	1	1	
4	E	1	Total	C	N	O	0
			16	14	1	1	
4	G	1	Total	C	N	O	0
			16	14	1	1	
4	I	1	Total	C	N	O	0
			16	14	1	1	
4	K	1	Total	C	N	O	0
			16	14	1	1	
4	M	1	Total	C	N	O	0
			16	14	1	1	
4	O	1	Total	C	N	O	0
			16	14	1	1	
4	Q	1	Total	C	N	O	0
			16	14	1	1	

- Molecule 5 is 1,2-Dihydro-psi,psi-caroten-1-ol (CCD ID: IRM) (formula: C₄₀H₅₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			41	40	1	
5	C	1	Total	C	O	0
			41	40	1	
5	E	1	Total	C	O	0
			41	40	1	
5	G	1	Total	C	O	0
			41	40	1	
5	I	1	Total	C	O	0
			41	40	1	
5	K	1	Total	C	O	0
			41	40	1	
5	M	1	Total	C	O	0
			41	40	1	
5	O	1	Total	C	O	0
			41	40	1	
5	Q	1	Total	C	O	0
			41	40	1	

- Molecule 6 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



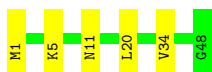
Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total 35	C 24	O 11	0
6	D	1	Total 35	C 24	O 11	0
6	F	1	Total 35	C 24	O 11	0
6	H	1	Total 35	C 24	O 11	0
6	J	1	Total 35	C 24	O 11	0
6	L	1	Total 35	C 24	O 11	0
6	N	1	Total 35	C 24	O 11	0
6	P	1	Total 35	C 24	O 11	0
6	R	1	Total 35	C 24	O 11	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: Light-harvesting protein B-800/820 alpha chain

Chain A: 




- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain C: 




- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain E: 




- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain G: 



- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain I: 



- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain K:  92% 8%



- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain M:  90% 10%



- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain O:  92% 8%



- Molecule 1: Light-harvesting protein B-800/820 alpha chain

Chain Q:  92% 8%



- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain D:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain F:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain J:  98% .



- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain P:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: Light-harvesting protein B-800/820 beta-2 chain

Chain R:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49453	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.37	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	21.294	Depositor
Minimum map value	-0.206	Depositor
Average map value	-0.041	Depositor
Map value standard deviation	0.576	Depositor
Recommended contour level	7.06	Depositor
Map size (Å)	248.51999, 248.51999, 248.51999	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.654, 0.654, 0.654	Depositor

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: LDA, LMT, IRM, BCL, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	0/361	1.20	0/498
1	C	0.66	0/361	1.21	0/498
1	E	0.66	0/361	1.21	0/498
1	G	0.65	0/361	1.20	0/498
1	I	0.66	0/361	1.21	0/498
1	K	0.65	0/361	1.21	0/498
1	M	0.66	0/361	1.21	0/498
1	O	0.66	0/361	1.21	0/498
1	Q	0.66	0/361	1.21	0/498
2	B	0.69	0/333	1.23	0/454
2	D	0.69	0/333	1.23	0/454
2	F	0.68	0/333	1.23	0/454
2	H	0.69	0/333	1.23	0/454
2	J	0.69	0/333	1.23	0/454
2	L	0.69	0/333	1.23	0/454
2	N	0.69	0/333	1.23	0/454
2	P	0.69	0/333	1.23	0/454
2	R	0.69	0/333	1.23	0/454
All	All	0.67	0/6246	1.22	0/8568

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	361	0	376	4	0
1	C	361	0	376	4	0
1	E	361	0	376	5	0
1	G	361	0	376	4	0
1	I	361	0	376	4	0
1	K	361	0	376	4	0
1	M	361	0	376	4	0
1	O	361	0	376	4	0
1	Q	361	0	376	4	0
2	B	323	0	320	0	0
2	D	323	0	320	0	0
2	F	323	0	320	0	0
2	H	323	0	320	0	0
2	J	323	0	320	1	0
2	L	323	0	320	0	0
2	N	323	0	320	0	0
2	P	323	0	320	0	0
2	R	323	0	320	0	0
3	A	132	0	148	11	0
3	B	66	0	74	4	0
3	C	132	0	147	8	0
3	D	66	0	74	5	0
3	E	132	0	148	11	0
3	F	66	0	74	4	0
3	G	132	0	147	8	0
3	H	66	0	74	4	0
3	I	132	0	148	7	0
3	J	66	0	74	4	0
3	K	132	0	147	8	0
3	L	66	0	74	4	0
3	M	132	0	148	10	0
3	N	66	0	74	4	0
3	O	132	0	147	6	0
3	P	66	0	74	5	0
3	Q	132	0	148	10	0
3	R	66	0	74	4	0
4	A	16	0	31	1	0
4	C	16	0	31	1	0
4	E	16	0	31	1	0
4	G	16	0	31	1	0
4	I	16	0	31	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	16	0	31	1	0
4	M	16	0	31	1	0
4	O	16	0	31	1	0
4	Q	16	0	31	1	0
5	A	41	0	0	7	0
5	C	41	0	0	7	0
5	E	41	0	0	6	0
5	G	41	0	0	7	0
5	I	41	0	0	7	0
5	K	41	0	0	6	0
5	M	41	0	0	6	0
5	O	41	0	0	6	0
5	Q	41	0	0	6	0
6	B	35	0	46	0	0
6	D	35	0	46	0	0
6	F	35	0	46	0	0
6	H	35	0	46	0	0
6	J	35	0	46	0	0
6	L	35	0	46	0	0
6	N	35	0	46	0	0
6	P	35	0	46	0	0
6	R	35	0	46	0	0
All	All	8766	0	8951	130	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 7.

All (130) 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)
3:G:101:BCL:HMB2	5:O:102:IRM:C27	1.83	1.08
3:A:101:BCL:HMB2	5:I:102:IRM:C27	1.84	1.07
5:A:104:IRM:C27	3:Q:103:BCL:HMB2	1.83	1.07
5:C:104:IRM:C27	3:M:101:BCL:HMB2	1.84	1.06
3:K:103:BCL:HMB2	5:M:104:IRM:C27	1.86	1.06
3:E:103:BCL:HMB2	5:G:104:IRM:C27	1.87	1.05
3:O:103:BCL:HMB2	5:Q:102:IRM:C27	1.88	1.02
3:I:103:BCL:HMB2	5:K:102:IRM:C27	1.92	0.99
3:C:101:BCL:HMB2	5:E:102:IRM:C27	1.93	0.97
5:C:104:IRM:C37	3:M:101:BCL:H52	1.99	0.93
3:K:103:BCL:H52	5:M:104:IRM:C37	2.06	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:LYS:HB3	5:G:104:IRM:C30	2.09	0.82
1:M:5:LYS:HB3	5:M:104:IRM:C30	2.09	0.82
1:A:5:LYS:HB3	5:A:104:IRM:C30	2.09	0.82
3:O:103:BCL:H52	5:Q:102:IRM:C37	2.13	0.79
1:C:5:LYS:HB3	5:C:104:IRM:C30	2.13	0.79
5:A:104:IRM:C37	3:Q:103:BCL:H52	2.15	0.77
3:E:103:BCL:H52	5:G:104:IRM:C37	2.16	0.76
1:O:5:LYS:HB3	5:O:102:IRM:C30	2.17	0.74
1:I:5:LYS:HB3	5:I:102:IRM:C30	2.18	0.73
1:Q:5:LYS:HB3	5:Q:102:IRM:C30	2.19	0.73
1:K:5:LYS:HB3	5:K:102:IRM:C30	2.19	0.72
1:E:5:LYS:HB3	5:E:102:IRM:C30	2.19	0.72
5:A:104:IRM:C35	3:B:101:BCL:H192	2.22	0.70
5:G:104:IRM:C35	3:H:101:BCL:H192	2.22	0.69
5:M:104:IRM:C35	3:N:101:BCL:H192	2.22	0.69
3:I:103:BCL:H52	5:K:102:IRM:C37	2.23	0.69
5:C:104:IRM:C35	3:D:101:BCL:H192	2.26	0.66
3:H:101:BCL:H193	1:I:20:LEU:HD22	1.81	0.63
3:B:101:BCL:H193	1:C:20:LEU:HD22	1.81	0.62
3:N:101:BCL:H193	1:O:20:LEU:HD22	1.81	0.62
5:O:102:IRM:C35	3:P:101:BCL:H192	2.29	0.62
5:I:102:IRM:C35	3:J:101:BCL:H192	2.29	0.62
3:A:101:BCL:H52	5:I:102:IRM:C37	2.30	0.60
3:A:102:BCL:HHC	3:A:102:BCL:HBB2	1.84	0.60
3:C:102:BCL:HBB2	3:C:102:BCL:HHC	1.84	0.59
3:E:104:BCL:HBB2	3:E:104:BCL:HHC	1.84	0.59
3:K:103:BCL:C5	5:M:104:IRM:C37	2.80	0.59
5:E:102:IRM:C35	3:F:101:BCL:H192	2.33	0.59
3:Q:104:BCL:HBB2	3:Q:104:BCL:HHC	1.84	0.59
3:M:102:BCL:HHC	3:M:102:BCL:HBB2	1.84	0.59
3:O:104:BCL:HHC	3:O:104:BCL:HBB2	1.84	0.59
3:I:104:BCL:HBB2	3:I:104:BCL:HHC	1.84	0.59
5:K:102:IRM:C35	3:L:101:BCL:H192	2.33	0.59
5:Q:102:IRM:C35	3:R:101:BCL:H192	2.33	0.59
3:K:104:BCL:HHC	3:K:104:BCL:HBB2	1.84	0.59
5:C:104:IRM:C37	3:M:101:BCL:C5	2.78	0.58
3:G:102:BCL:HBB2	3:G:102:BCL:HHC	1.84	0.58
3:D:101:BCL:H193	1:Q:20:LEU:HD22	1.86	0.58
3:O:103:BCL:C5	5:Q:102:IRM:C37	2.82	0.57
3:C:101:BCL:H52	5:E:102:IRM:C37	2.35	0.57
3:E:103:BCL:C5	5:G:104:IRM:C37	2.83	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:101:BCL:H11	3:R:101:BCL:H203	1.87	0.56
1:Q:11:ASN:HD22	4:Q:101:LDA:HM21	1.71	0.55
1:K:11:ASN:HD22	4:K:101:LDA:HM21	1.71	0.55
1:K:20:LEU:HD22	3:P:101:BCL:H193	1.88	0.55
1:E:11:ASN:HD22	4:E:101:LDA:HM21	1.71	0.55
3:A:101:BCL:CMB	5:I:102:IRM:C27	2.75	0.55
3:I:103:BCL:C5	5:K:102:IRM:C37	2.85	0.55
5:A:104:IRM:C37	3:Q:103:BCL:C5	2.84	0.54
3:G:101:BCL:H11	3:L:101:BCL:H203	1.87	0.54
1:E:20:LEU:HD22	3:J:101:BCL:H193	1.91	0.53
1:I:11:ASN:HD22	4:I:101:LDA:HM21	1.74	0.53
3:L:101:BCL:HMB3	3:L:101:BCL:HBB2	1.92	0.52
5:C:104:IRM:C27	3:M:101:BCL:CMB	2.75	0.52
1:C:11:ASN:HD22	4:C:103:LDA:HM21	1.73	0.52
3:F:101:BCL:HBB2	3:F:101:BCL:HMB3	1.92	0.52
3:N:101:BCL:HBB2	3:N:101:BCL:HMB3	1.92	0.52
3:P:101:BCL:HMB3	3:P:101:BCL:HBB2	1.92	0.52
3:R:101:BCL:HBB2	3:R:101:BCL:HMB3	1.92	0.52
3:B:101:BCL:HBB2	3:B:101:BCL:HMB3	1.92	0.52
3:J:101:BCL:HBB2	3:J:101:BCL:HMB3	1.92	0.52
3:H:101:BCL:C19	1:I:20:LEU:HD22	2.41	0.51
3:N:101:BCL:C19	1:O:20:LEU:HD22	2.41	0.51
1:O:11:ASN:HD22	4:O:101:LDA:HM21	1.74	0.51
3:B:101:BCL:C19	1:C:20:LEU:HD22	2.41	0.51
5:A:104:IRM:C27	3:Q:103:BCL:CMB	2.73	0.51
3:D:101:BCL:HMB3	3:D:101:BCL:HBB2	1.92	0.50
1:G:11:ASN:HD22	4:G:103:LDA:HM21	1.76	0.50
3:H:101:BCL:HMB3	3:H:101:BCL:HBB2	1.92	0.50
1:A:11:ASN:HD22	4:A:103:LDA:HM21	1.76	0.50
3:A:101:BCL:C5	5:I:102:IRM:C37	2.90	0.50
3:E:103:BCL:CMB	5:G:104:IRM:C27	2.76	0.50
3:G:101:BCL:C3	5:O:102:IRM:C37	2.91	0.49
3:M:101:BCL:HMB1	3:M:101:BCL:HBB3	1.93	0.49
1:M:11:ASN:HD22	4:M:103:LDA:HM21	1.76	0.49
3:C:101:BCL:C5	5:E:102:IRM:C37	2.90	0.49
1:A:20:LEU:HD22	3:F:101:BCL:H193	1.95	0.48
3:E:103:BCL:C3	5:G:104:IRM:C37	2.91	0.48
1:G:20:LEU:HD22	3:L:101:BCL:H193	1.95	0.48
1:M:20:LEU:HD22	3:R:101:BCL:H193	1.96	0.48
3:O:103:BCL:C3	5:Q:102:IRM:C37	2.92	0.48
3:C:101:BCL:H41	3:C:101:BCL:H62	1.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:104:IRM:C37	3:M:101:BCL:C3	2.92	0.47
3:A:101:BCL:H62	3:A:101:BCL:H41	1.34	0.47
3:A:101:BCL:C3	5:I:102:IRM:C37	2.92	0.46
3:E:103:BCL:H8	3:E:103:BCL:H51	1.57	0.46
3:K:103:BCL:CMB	5:M:104:IRM:C27	2.76	0.46
3:C:101:BCL:H51	3:C:101:BCL:H8	1.68	0.45
3:K:103:BCL:H11	3:P:101:BCL:H203	1.97	0.45
3:O:103:BCL:H41	3:O:103:BCL:H62	1.56	0.45
3:D:101:BCL:C19	1:Q:20:LEU:HD22	2.46	0.45
3:C:101:BCL:C3	5:E:102:IRM:C37	2.95	0.45
3:Q:103:BCL:H41	3:Q:103:BCL:H62	1.47	0.45
3:G:101:BCL:C5	5:O:102:IRM:C37	2.95	0.45
3:D:101:BCL:H203	3:Q:103:BCL:H11	1.99	0.44
1:G:34:VAL:HG11	3:G:101:BCL:HBC1	1.98	0.44
3:I:103:BCL:H41	3:I:103:BCL:H62	1.52	0.44
3:K:103:BCL:HBB3	3:K:103:BCL:HMB1	2.00	0.43
3:I:103:BCL:C3	5:K:102:IRM:C37	2.96	0.43
1:K:20:LEU:HD22	3:P:101:BCL:C19	2.49	0.43
3:M:101:BCL:HBA2	3:M:101:BCL:H3A	1.60	0.43
3:E:103:BCL:H161	3:E:103:BCL:H192	1.57	0.43
1:A:34:VAL:HG11	3:A:101:BCL:HBC1	2.01	0.43
5:A:104:IRM:C37	3:Q:103:BCL:C3	2.98	0.42
3:Q:103:BCL:HBB3	3:Q:103:BCL:HMB1	2.02	0.42
1:M:34:VAL:HG11	3:M:101:BCL:HBC1	2.01	0.42
3:G:101:BCL:CMB	5:O:102:IRM:C27	2.75	0.42
3:I:103:BCL:HBA2	3:I:103:BCL:H3A	1.79	0.42
3:K:103:BCL:H41	3:K:103:BCL:H62	1.64	0.41
3:Q:103:BCL:H8	3:Q:103:BCL:H51	1.69	0.41
3:G:101:BCL:HBA2	3:G:101:BCL:H3A	1.83	0.41
3:E:103:BCL:H41	3:E:103:BCL:H62	1.35	0.41
3:A:101:BCL:H11	3:F:101:BCL:H203	2.01	0.41
3:A:101:BCL:H51	3:A:101:BCL:H8	1.54	0.41
3:A:101:BCL:H192	3:A:101:BCL:H161	1.73	0.41
3:E:103:BCL:H11	3:J:101:BCL:H203	2.03	0.41
1:E:34:VAL:HG11	3:E:103:BCL:HBC1	2.02	0.41
3:C:101:BCL:HBA2	3:C:101:BCL:H3A	1.75	0.40
1:E:47:GLY:HA3	2:J:39:PRO:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	46/48 (96%)	46 (100%)	0	0	100	100
1	C	46/48 (96%)	46 (100%)	0	0	100	100
1	E	46/48 (96%)	46 (100%)	0	0	100	100
1	G	46/48 (96%)	46 (100%)	0	0	100	100
1	I	46/48 (96%)	46 (100%)	0	0	100	100
1	K	46/48 (96%)	46 (100%)	0	0	100	100
1	M	46/48 (96%)	46 (100%)	0	0	100	100
1	O	46/48 (96%)	46 (100%)	0	0	100	100
1	Q	46/48 (96%)	46 (100%)	0	0	100	100
2	B	39/41 (95%)	39 (100%)	0	0	100	100
2	D	39/41 (95%)	39 (100%)	0	0	100	100
2	F	39/41 (95%)	39 (100%)	0	0	100	100
2	H	39/41 (95%)	39 (100%)	0	0	100	100
2	J	39/41 (95%)	39 (100%)	0	0	100	100
2	L	39/41 (95%)	39 (100%)	0	0	100	100
2	N	39/41 (95%)	39 (100%)	0	0	100	100
2	P	39/41 (95%)	39 (100%)	0	0	100	100
2	R	39/41 (95%)	39 (100%)	0	0	100	100
All	All	765/801 (96%)	765 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	37/37 (100%)	37 (100%)	0	100	100
1	C	37/37 (100%)	37 (100%)	0	100	100
1	E	37/37 (100%)	37 (100%)	0	100	100
1	G	37/37 (100%)	37 (100%)	0	100	100
1	I	37/37 (100%)	37 (100%)	0	100	100
1	K	37/37 (100%)	37 (100%)	0	100	100
1	M	37/37 (100%)	37 (100%)	0	100	100
1	O	37/37 (100%)	37 (100%)	0	100	100
1	Q	37/37 (100%)	37 (100%)	0	100	100
2	B	33/33 (100%)	33 (100%)	0	100	100
2	D	33/33 (100%)	33 (100%)	0	100	100
2	F	33/33 (100%)	33 (100%)	0	100	100
2	H	33/33 (100%)	33 (100%)	0	100	100
2	J	33/33 (100%)	33 (100%)	0	100	100
2	L	33/33 (100%)	33 (100%)	0	100	100
2	N	33/33 (100%)	33 (100%)	0	100	100
2	P	33/33 (100%)	33 (100%)	0	100	100
2	R	33/33 (100%)	33 (100%)	0	100	100
All	All	630/630 (100%)	630 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	ASN
1	C	3	GLN
1	C	11	ASN
1	C	37	HIS
1	E	3	GLN
1	E	11	ASN
1	E	37	HIS
1	G	3	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	11	ASN
1	I	3	GLN
1	I	11	ASN
1	I	37	HIS
1	K	3	GLN
1	K	11	ASN
1	K	37	HIS
1	M	3	GLN
1	M	11	ASN
1	O	3	GLN
1	O	11	ASN
1	O	37	HIS
1	Q	3	GLN
1	Q	11	ASN
1	Q	37	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	Q	1	1,3	8,9,10	0.63	0	8,9,11	1.25	2 (25%)
1	FME	G	1	1,3	8,9,10	0.63	0	8,9,11	1.26	2 (25%)
1	FME	O	1	1,3	8,9,10	0.64	0	8,9,11	1.24	2 (25%)
1	FME	A	1	1,3	8,9,10	0.62	0	8,9,11	1.24	1 (12%)
1	FME	I	1	1,3	8,9,10	0.63	0	8,9,11	1.26	2 (25%)
1	FME	C	1	1,3	8,9,10	0.62	0	8,9,11	1.26	1 (12%)
1	FME	K	1	1,3	8,9,10	0.64	0	8,9,11	1.25	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	E	1	1,3	8,9,10	0.62	0	8,9,11	1.24	1 (12%)
1	FME	M	1	1,3	8,9,10	0.63	0	8,9,11	1.24	2 (25%)

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
1	FME	Q	1	1,3	-	2/7/9/11	-
1	FME	G	1	1,3	-	2/7/9/11	-
1	FME	O	1	1,3	-	2/7/9/11	-
1	FME	A	1	1,3	-	2/7/9/11	-
1	FME	I	1	1,3	-	2/7/9/11	-
1	FME	C	1	1,3	-	2/7/9/11	-
1	FME	K	1	1,3	-	2/7/9/11	-
1	FME	E	1	1,3	-	2/7/9/11	-
1	FME	M	1	1,3	-	2/7/9/11	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	FME	C-CA-N	2.61	114.53	109.50
1	G	1	FME	C-CA-N	2.60	114.51	109.50
1	E	1	FME	C-CA-N	2.59	114.50	109.50
1	I	1	FME	C-CA-N	2.58	114.48	109.50
1	A	1	FME	C-CA-N	2.57	114.46	109.50
1	Q	1	FME	C-CA-N	2.55	114.43	109.50
1	M	1	FME	C-CA-N	2.55	114.42	109.50
1	K	1	FME	C-CA-N	2.55	114.42	109.50
1	O	1	FME	C-CA-N	2.54	114.41	109.50
1	K	1	FME	O-C-CA	-2.04	119.53	124.77
1	O	1	FME	O-C-CA	-2.03	119.55	124.77
1	Q	1	FME	O-C-CA	-2.03	119.55	124.77
1	I	1	FME	O-C-CA	-2.01	119.60	124.77
1	M	1	FME	O-C-CA	-2.01	119.61	124.77
1	G	1	FME	O-C-CA	-2.01	119.61	124.77

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	C	1	FME	O1-CN-N-CA
1	E	1	FME	O1-CN-N-CA
1	G	1	FME	O1-CN-N-CA
1	I	1	FME	O1-CN-N-CA
1	K	1	FME	O1-CN-N-CA
1	M	1	FME	O1-CN-N-CA
1	O	1	FME	O1-CN-N-CA
1	Q	1	FME	O1-CN-N-CA
1	A	1	FME	CB-CA-N-CN
1	C	1	FME	CB-CA-N-CN
1	E	1	FME	CB-CA-N-CN
1	G	1	FME	CB-CA-N-CN
1	I	1	FME	CB-CA-N-CN
1	K	1	FME	CB-CA-N-CN
1	M	1	FME	CB-CA-N-CN
1	O	1	FME	CB-CA-N-CN
1	Q	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

54 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LMT	B	102	-	36,36,36	0.79	0	47,47,47	0.63	0
5	IRM	G	104	-	40,40,40	2.67	14 (35%)	49,49,49	1.53	4 (8%)
3	BCL	K	104	1	69,74,74	1.91	8 (11%)	79,115,115	1.94	9 (11%)
3	BCL	Q	103	1	69,74,74	3.43	37 (53%)	79,115,115	3.59	41 (51%)
3	BCL	G	101	1	69,74,74	3.39	36 (52%)	79,115,115	4.19	45 (56%)
4	LDA	K	101	-	13,15,15	0.96	1 (7%)	14,17,17	0.54	0
6	LMT	R	102	-	36,36,36	0.78	0	47,47,47	0.63	0
6	LMT	J	102	-	36,36,36	0.77	0	47,47,47	0.63	0
6	LMT	L	102	-	36,36,36	0.78	0	47,47,47	0.63	0
3	BCL	B	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.10	11 (13%)
6	LMT	N	102	-	36,36,36	0.77	0	47,47,47	0.63	0
5	IRM	A	104	-	40,40,40	2.67	14 (35%)	49,49,49	1.52	4 (8%)
3	BCL	N	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.11	11 (13%)
3	BCL	I	104	1	69,74,74	1.91	8 (11%)	79,115,115	1.95	9 (11%)
3	BCL	O	103	1	69,74,74	3.54	36 (52%)	79,115,115	3.71	43 (54%)
3	BCL	L	101	2	69,74,74	2.00	8 (11%)	79,115,115	2.11	11 (13%)
3	BCL	Q	104	1	69,74,74	1.91	8 (11%)	79,115,115	1.94	9 (11%)
4	LDA	C	103	-	13,15,15	0.97	1 (7%)	14,17,17	0.54	0
5	IRM	M	104	-	40,40,40	2.67	14 (35%)	49,49,49	1.52	4 (8%)
6	LMT	P	102	-	36,36,36	0.78	0	47,47,47	0.63	0
5	IRM	E	102	-	40,40,40	2.67	14 (35%)	49,49,49	1.52	4 (8%)
4	LDA	O	101	-	13,15,15	0.95	1 (7%)	14,17,17	0.54	0
4	LDA	M	103	-	13,15,15	0.99	2 (15%)	14,17,17	0.54	0
5	IRM	O	102	-	40,40,40	2.66	14 (35%)	49,49,49	1.53	4 (8%)
3	BCL	M	102	1	69,74,74	1.90	8 (11%)	79,115,115	1.94	9 (11%)
3	BCL	R	101	2	69,74,74	2.00	8 (11%)	79,115,115	2.11	11 (13%)
6	LMT	H	102	-	36,36,36	0.78	0	47,47,47	0.63	0
5	IRM	C	104	-	40,40,40	2.67	14 (35%)	49,49,49	1.53	4 (8%)
6	LMT	D	102	-	36,36,36	0.78	0	47,47,47	0.63	0
6	LMT	F	102	-	36,36,36	0.78	0	47,47,47	0.63	0
3	BCL	O	104	1	69,74,74	1.91	8 (11%)	79,115,115	1.93	9 (11%)
3	BCL	A	101	1	69,74,74	3.41	37 (53%)	79,115,115	3.48	42 (53%)
4	LDA	G	103	-	13,15,15	0.97	1 (7%)	14,17,17	0.54	0
3	BCL	H	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.09	11 (13%)
5	IRM	K	102	-	40,40,40	2.67	14 (35%)	49,49,49	1.52	4 (8%)
4	LDA	A	103	-	13,15,15	0.95	1 (7%)	14,17,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BCL	C	101	1	69,74,74	3.32	39 (56%)	79,115,115	3.22	39 (49%)
3	BCL	C	102	1	69,74,74	1.91	8 (11%)	79,115,115	1.93	9 (11%)
3	BCL	K	103	1	69,74,74	3.43	37 (53%)	79,115,115	3.61	39 (49%)
5	IRM	I	102	-	40,40,40	2.67	14 (35%)	49,49,49	1.52	4 (8%)
3	BCL	I	103	1	69,74,74	3.49	40 (57%)	79,115,115	3.64	42 (53%)
3	BCL	M	101	1	69,74,74	3.27	35 (50%)	79,115,115	3.93	46 (58%)
3	BCL	P	101	2	69,74,74	2.00	8 (11%)	79,115,115	2.11	11 (13%)
4	LDA	I	101	-	13,15,15	0.99	2 (15%)	14,17,17	0.54	0
3	BCL	E	104	1	69,74,74	1.91	8 (11%)	79,115,115	1.93	8 (10%)
3	BCL	F	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.12	11 (13%)
3	BCL	J	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.10	11 (13%)
5	IRM	Q	102	-	40,40,40	2.67	14 (35%)	49,49,49	1.53	4 (8%)
3	BCL	G	102	1	69,74,74	1.91	8 (11%)	79,115,115	1.94	9 (11%)
4	LDA	Q	101	-	13,15,15	0.96	1 (7%)	14,17,17	0.54	0
3	BCL	D	101	2	69,74,74	1.99	8 (11%)	79,115,115	2.10	11 (13%)
3	BCL	A	102	1	69,74,74	1.90	8 (11%)	79,115,115	1.94	8 (10%)
4	LDA	E	101	-	13,15,15	0.97	1 (7%)	14,17,17	0.54	0
3	BCL	E	103	1	69,74,74	3.30	39 (56%)	79,115,115	3.57	42 (53%)

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	LMT	B	102	-	-	4/21/61/61	0/2/2/2
5	IRM	G	104	-	-	3/44/44/44	-
3	BCL	K	104	1	-	5/41/137/137	-
3	BCL	Q	103	1	-	14/41/137/137	-
3	BCL	G	101	1	-	8/41/137/137	-
4	LDA	K	101	-	-	0/13/13/13	-
6	LMT	R	102	-	-	4/21/61/61	0/2/2/2
6	LMT	J	102	-	-	4/21/61/61	0/2/2/2
6	LMT	L	102	-	-	4/21/61/61	0/2/2/2
3	BCL	B	101	2	-	1/41/137/137	-
6	LMT	N	102	-	-	4/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	IRM	A	104	-	-	3/44/44/44	-
3	BCL	N	101	2	-	1/41/137/137	-
3	BCL	I	104	1	-	5/41/137/137	-
3	BCL	O	103	1	-	9/41/137/137	-
3	BCL	L	101	2	-	1/41/137/137	-
3	BCL	Q	104	1	-	5/41/137/137	-
4	LDA	C	103	-	-	0/13/13/13	-
5	IRM	M	104	-	-	3/44/44/44	-
6	LMT	P	102	-	-	4/21/61/61	0/2/2/2
5	IRM	E	102	-	-	3/44/44/44	-
4	LDA	O	101	-	-	0/13/13/13	-
4	LDA	M	103	-	-	0/13/13/13	-
5	IRM	O	102	-	-	3/44/44/44	-
3	BCL	M	102	1	-	5/41/137/137	-
3	BCL	R	101	2	-	1/41/137/137	-
6	LMT	H	102	-	-	4/21/61/61	0/2/2/2
5	IRM	C	104	-	-	3/44/44/44	-
6	LMT	D	102	-	-	4/21/61/61	0/2/2/2
6	LMT	F	102	-	-	4/21/61/61	0/2/2/2
3	BCL	O	104	1	-	5/41/137/137	-
3	BCL	A	101	1	-	10/41/137/137	-
4	LDA	G	103	-	-	0/13/13/13	-
3	BCL	H	101	2	-	1/41/137/137	-
5	IRM	K	102	-	-	3/44/44/44	-
4	LDA	A	103	-	-	0/13/13/13	-
3	BCL	C	101	1	-	14/41/137/137	-
3	BCL	C	102	1	-	5/41/137/137	-
3	BCL	K	103	1	-	13/41/137/137	-
5	IRM	I	102	-	-	3/44/44/44	-
3	BCL	I	103	1	-	11/41/137/137	-
3	BCL	M	101	1	-	10/41/137/137	-
3	BCL	P	101	2	-	1/41/137/137	-
4	LDA	I	101	-	-	0/13/13/13	-
3	BCL	E	104	1	-	5/41/137/137	-
3	BCL	F	101	2	-	1/41/137/137	-
3	BCL	J	101	2	-	1/41/137/137	-
5	IRM	Q	102	-	-	3/44/44/44	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	G	102	1	-	5/41/137/137	-
4	LDA	Q	101	-	-	0/13/13/13	-
3	BCL	D	101	2	-	1/41/137/137	-
3	BCL	A	102	1	-	5/41/137/137	-
4	LDA	E	101	-	-	0/13/13/13	-
3	BCL	E	103	1	-	13/41/137/137	-

All (617) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	101	BCL	MG-NC	12.16	2.35	2.06
3	J	101	BCL	MG-NC	12.15	2.35	2.06
3	F	101	BCL	MG-NC	12.15	2.35	2.06
3	R	101	BCL	MG-NC	12.14	2.35	2.06
3	D	101	BCL	MG-NC	12.14	2.35	2.06
3	L	101	BCL	MG-NC	12.14	2.35	2.06
3	N	101	BCL	MG-NC	12.13	2.35	2.06
3	B	101	BCL	MG-NC	12.11	2.35	2.06
3	H	101	BCL	MG-NC	12.10	2.35	2.06
3	E	104	BCL	MG-NC	10.96	2.32	2.06
3	O	104	BCL	MG-NC	10.93	2.32	2.06
3	C	102	BCL	MG-NC	10.92	2.32	2.06
3	M	102	BCL	MG-NC	10.92	2.32	2.06
3	K	104	BCL	MG-NC	10.91	2.32	2.06
3	Q	104	BCL	MG-NC	10.90	2.32	2.06
3	I	104	BCL	MG-NC	10.88	2.32	2.06
3	G	102	BCL	MG-NC	10.88	2.32	2.06
3	A	102	BCL	MG-NC	10.88	2.32	2.06
3	O	103	BCL	C3D-C4D	-9.18	1.23	1.44
3	A	101	BCL	C3D-C4D	-8.94	1.24	1.44
3	E	103	BCL	C3D-C4D	-8.53	1.25	1.44
3	Q	103	BCL	C3D-C4D	-8.50	1.25	1.44
3	G	101	BCL	C4B-NB	-8.43	1.26	1.37
3	Q	103	BCL	OBB-CAB	-8.39	1.04	1.23
3	Q	103	BCL	C1D-ND	-8.28	1.27	1.37
3	K	103	BCL	OBB-CAB	-8.22	1.04	1.23
3	I	103	BCL	C3D-C4D	-8.21	1.25	1.44
3	C	101	BCL	C3D-C4D	-8.14	1.25	1.44
3	A	101	BCL	OBB-CAB	-8.00	1.05	1.23
3	I	103	BCL	OBB-CAB	-7.96	1.05	1.23
3	G	101	BCL	C3D-C4D	-7.95	1.26	1.44
3	K	103	BCL	C3D-C4D	-7.93	1.26	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	103	BCL	OBB-CAB	-7.83	1.05	1.23
3	Q	103	BCL	C4B-NB	-7.79	1.27	1.37
3	C	101	BCL	C1D-ND	-7.78	1.27	1.37
3	C	101	BCL	OBB-CAB	-7.77	1.05	1.23
3	M	101	BCL	C3D-C4D	-7.76	1.26	1.44
3	O	103	BCL	OBB-CAB	-7.67	1.05	1.23
3	O	103	BCL	C4B-NB	-7.67	1.27	1.37
3	M	101	BCL	O1A-CGA	-7.65	0.99	1.22
3	K	103	BCL	O1A-CGA	-7.65	0.99	1.22
3	O	103	BCL	C1B-NB	-7.64	1.27	1.37
3	G	101	BCL	OBB-CAB	-7.55	1.06	1.23
3	O	103	BCL	C1D-ND	-7.45	1.28	1.37
3	K	103	BCL	OBD-CAD	-7.44	1.09	1.22
5	Q	102	IRM	C27-C26	-7.39	1.36	1.51
5	G	104	IRM	C27-C26	-7.38	1.36	1.51
5	C	104	IRM	C27-C26	-7.38	1.36	1.51
3	A	101	BCL	C1D-ND	-7.37	1.28	1.37
5	E	102	IRM	C27-C26	-7.37	1.36	1.51
5	O	102	IRM	C27-C26	-7.35	1.36	1.51
5	M	104	IRM	C27-C26	-7.35	1.36	1.51
5	I	102	IRM	C27-C26	-7.34	1.36	1.51
5	K	102	IRM	C27-C26	-7.34	1.36	1.51
5	A	104	IRM	C27-C26	-7.33	1.36	1.51
3	I	103	BCL	C1D-ND	-7.19	1.28	1.37
3	K	103	BCL	C4B-NB	-7.16	1.28	1.37
3	I	103	BCL	C1B-NB	-7.10	1.28	1.37
3	M	101	BCL	C4B-NB	-7.04	1.28	1.37
3	I	103	BCL	C4B-NB	-6.94	1.28	1.37
3	M	101	BCL	OBB-CAB	-6.92	1.07	1.23
3	A	101	BCL	C1B-NB	-6.90	1.28	1.37
3	A	101	BCL	C4B-NB	-6.89	1.28	1.37
3	I	103	BCL	O1A-CGA	-6.88	1.02	1.22
3	I	103	BCL	OBD-CAD	-6.85	1.10	1.22
3	K	103	BCL	C1B-NB	-6.85	1.28	1.37
3	Q	103	BCL	O1A-CGA	-6.85	1.02	1.22
3	E	103	BCL	O1A-CGA	-6.75	1.02	1.22
3	C	101	BCL	O2A-C1	-6.71	1.28	1.46
3	K	103	BCL	C1D-ND	-6.64	1.29	1.37
3	G	101	BCL	C1B-NB	-6.57	1.29	1.37
3	C	101	BCL	C4B-NB	-6.55	1.29	1.37
3	O	103	BCL	O2D-CED	-6.54	1.30	1.45
3	G	101	BCL	C1D-ND	-6.53	1.29	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	101	BCL	O1A-CGA	-6.50	1.03	1.22
3	G	101	BCL	OBD-CAD	-6.46	1.11	1.22
3	O	103	BCL	O1D-CGD	-6.38	1.05	1.21
3	M	101	BCL	C1B-NB	-6.36	1.29	1.37
3	O	103	BCL	O1A-CGA	-6.26	1.03	1.22
3	E	103	BCL	O2D-CED	-6.22	1.31	1.45
3	G	101	BCL	CMB-C2B	-6.20	1.38	1.50
3	G	101	BCL	O1A-CGA	-6.15	1.04	1.22
3	Q	103	BCL	C1B-NB	-6.08	1.29	1.37
3	E	103	BCL	OBD-CAD	-6.07	1.12	1.22
3	E	103	BCL	O2A-C1	-6.06	1.29	1.46
3	O	103	BCL	OBD-CAD	-6.00	1.12	1.22
3	E	103	BCL	C4B-NB	-5.98	1.30	1.37
3	M	101	BCL	O2D-CED	-5.92	1.32	1.45
3	M	101	BCL	C1D-ND	-5.88	1.30	1.37
3	E	103	BCL	C1B-NB	-5.87	1.30	1.37
3	I	103	BCL	O2D-CED	-5.84	1.32	1.45
3	I	103	BCL	O2A-C1	-5.78	1.30	1.46
3	E	103	BCL	C1D-ND	-5.78	1.30	1.37
3	I	103	BCL	CAA-C2A	-5.75	1.43	1.54
3	O	103	BCL	CMB-C2B	-5.73	1.39	1.50
3	G	101	BCL	O1D-CGD	-5.72	1.06	1.21
3	E	103	BCL	O1D-CGD	-5.70	1.06	1.21
3	Q	103	BCL	O2A-C1	-5.69	1.30	1.46
5	E	102	IRM	C27-C28	-5.64	1.35	1.53
5	O	102	IRM	C27-C28	-5.63	1.35	1.53
3	I	103	BCL	CMB-C2B	-5.62	1.39	1.50
5	I	102	IRM	C27-C28	-5.62	1.35	1.53
3	C	101	BCL	O2D-CED	-5.62	1.32	1.45
5	C	104	IRM	C27-C28	-5.61	1.35	1.53
5	A	104	IRM	C27-C28	-5.61	1.35	1.53
5	M	104	IRM	C27-C28	-5.60	1.35	1.53
5	Q	102	IRM	C27-C28	-5.60	1.35	1.53
5	G	104	IRM	C27-C28	-5.60	1.35	1.53
5	K	102	IRM	C27-C28	-5.60	1.35	1.53
3	K	103	BCL	O1D-CGD	-5.60	1.07	1.21
3	G	101	BCL	O2D-CED	-5.56	1.32	1.45
3	M	101	BCL	O2A-C1	-5.56	1.31	1.46
3	A	101	BCL	CMB-C2B	-5.55	1.39	1.50
3	A	101	BCL	O1A-CGA	-5.52	1.06	1.22
3	C	101	BCL	OBD-CAD	-5.51	1.13	1.22
3	A	101	BCL	O2D-CED	-5.50	1.33	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	103	BCL	O2D-CED	-5.50	1.33	1.45
3	A	101	BCL	O1D-CGD	-5.48	1.07	1.21
3	M	101	BCL	CMB-C2B	-5.43	1.39	1.50
3	K	103	BCL	CMB-C2B	-5.42	1.39	1.50
3	O	103	BCL	O2A-C1	-5.39	1.31	1.46
3	A	101	BCL	C3C-C4C	-5.37	1.44	1.51
3	I	104	BCL	C3D-C4D	-5.30	1.32	1.44
3	I	103	BCL	CHB-C4A	-5.30	1.24	1.37
3	A	102	BCL	C3D-C4D	-5.29	1.32	1.44
3	K	103	BCL	O2A-C1	-5.29	1.31	1.46
3	E	104	BCL	C3D-C4D	-5.29	1.32	1.44
3	K	104	BCL	C3D-C4D	-5.29	1.32	1.44
3	Q	104	BCL	C3D-C4D	-5.28	1.32	1.44
3	O	104	BCL	C3D-C4D	-5.28	1.32	1.44
3	C	102	BCL	C3D-C4D	-5.27	1.32	1.44
3	I	103	BCL	CHC-C1C	-5.27	1.24	1.37
5	C	104	IRM	C28-C29	-5.26	1.34	1.50
3	L	101	BCL	C3D-C4D	-5.25	1.32	1.44
3	M	101	BCL	O1D-CGD	-5.25	1.08	1.21
3	A	101	BCL	O2A-C1	-5.25	1.32	1.46
3	K	103	BCL	O2D-CED	-5.24	1.33	1.45
5	K	102	IRM	C28-C29	-5.24	1.34	1.50
3	G	102	BCL	C3D-C4D	-5.24	1.32	1.44
5	I	102	IRM	C28-C29	-5.22	1.34	1.50
5	E	102	IRM	C28-C29	-5.22	1.34	1.50
5	Q	102	IRM	C28-C29	-5.22	1.34	1.50
5	M	104	IRM	C28-C29	-5.22	1.34	1.50
3	M	102	BCL	C3D-C4D	-5.21	1.32	1.44
3	K	103	BCL	CHB-C4A	-5.21	1.24	1.37
5	A	104	IRM	C28-C29	-5.21	1.34	1.50
5	G	104	IRM	C28-C29	-5.20	1.34	1.50
3	N	101	BCL	C3D-C4D	-5.20	1.32	1.44
3	P	101	BCL	C3D-C4D	-5.20	1.32	1.44
3	C	101	BCL	O1D-CGD	-5.20	1.08	1.21
5	O	102	IRM	C28-C29	-5.19	1.34	1.50
3	R	101	BCL	C3D-C4D	-5.18	1.32	1.44
3	J	101	BCL	C3D-C4D	-5.18	1.32	1.44
3	G	101	BCL	CHC-C1C	-5.18	1.24	1.37
3	F	101	BCL	C3D-C4D	-5.17	1.32	1.44
3	B	101	BCL	C3D-C4D	-5.17	1.32	1.44
3	D	101	BCL	C3D-C4D	-5.12	1.32	1.44
3	M	101	BCL	OBD-CAD	-5.12	1.13	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	101	BCL	C3D-C4D	-5.11	1.32	1.44
5	I	102	IRM	C23-C22	-5.01	1.35	1.46
5	K	102	IRM	C23-C22	-5.01	1.35	1.46
5	M	104	IRM	C23-C22	-4.98	1.35	1.46
5	O	102	IRM	C23-C22	-4.97	1.35	1.46
5	G	104	IRM	C23-C22	-4.97	1.35	1.46
5	C	104	IRM	C23-C22	-4.97	1.35	1.46
5	Q	102	IRM	C23-C22	-4.97	1.35	1.46
5	E	102	IRM	O32-C1	-4.97	1.32	1.44
5	E	102	IRM	C23-C22	-4.96	1.35	1.46
3	I	103	BCL	O1D-CGD	-4.96	1.08	1.21
3	G	101	BCL	CHB-C4A	-4.96	1.25	1.37
5	A	104	IRM	C23-C22	-4.96	1.35	1.46
3	O	103	BCL	CHB-C4A	-4.95	1.25	1.37
5	G	104	IRM	O32-C1	-4.94	1.32	1.44
3	E	103	BCL	CMB-C2B	-4.93	1.40	1.50
5	A	104	IRM	O32-C1	-4.93	1.32	1.44
5	O	102	IRM	O32-C1	-4.93	1.32	1.44
5	M	104	IRM	O32-C1	-4.93	1.32	1.44
5	K	102	IRM	O32-C1	-4.91	1.32	1.44
5	Q	102	IRM	O32-C1	-4.90	1.32	1.44
5	C	104	IRM	O32-C1	-4.89	1.32	1.44
3	O	103	BCL	CHC-C1C	-4.88	1.25	1.37
3	M	101	BCL	CHC-C1C	-4.87	1.25	1.37
3	E	103	BCL	CHC-C1C	-4.87	1.25	1.37
5	I	102	IRM	O32-C1	-4.85	1.32	1.44
3	Q	103	BCL	CMB-C2B	-4.85	1.40	1.50
3	M	101	BCL	CHB-C4A	-4.85	1.25	1.37
3	Q	103	BCL	CAA-C2A	-4.84	1.45	1.54
3	Q	103	BCL	OBD-CAD	-4.81	1.14	1.22
3	G	101	BCL	CBB-CAB	-4.81	1.40	1.50
3	Q	103	BCL	CBB-CAB	-4.80	1.40	1.50
3	Q	103	BCL	O1D-CGD	-4.77	1.09	1.21
5	M	104	IRM	C19-C18	-4.76	1.35	1.46
3	A	101	BCL	OBD-CAD	-4.75	1.14	1.22
3	Q	103	BCL	CHC-C1C	-4.74	1.25	1.37
3	A	101	BCL	CHB-C4A	-4.73	1.25	1.37
5	G	104	IRM	C19-C18	-4.73	1.35	1.46
5	K	102	IRM	C19-C18	-4.72	1.35	1.46
5	I	102	IRM	C19-C18	-4.72	1.35	1.46
5	E	102	IRM	C19-C18	-4.72	1.35	1.46
5	Q	102	IRM	C19-C18	-4.71	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	104	IRM	C19-C18	-4.71	1.35	1.46
5	C	104	IRM	C19-C18	-4.71	1.35	1.46
5	A	104	IRM	C8-C9	-4.69	1.35	1.46
5	O	102	IRM	C19-C18	-4.67	1.35	1.46
3	C	101	BCL	CAA-C2A	-4.67	1.45	1.54
5	M	104	IRM	C8-C9	-4.65	1.36	1.46
5	Q	102	IRM	C8-C9	-4.65	1.36	1.46
5	K	102	IRM	C8-C9	-4.64	1.36	1.46
5	E	102	IRM	C8-C9	-4.64	1.36	1.46
5	G	104	IRM	C8-C9	-4.64	1.36	1.46
5	O	102	IRM	C8-C9	-4.63	1.36	1.46
5	I	102	IRM	C8-C9	-4.62	1.36	1.46
3	C	101	BCL	CMD-C2D	-4.62	1.41	1.50
5	C	104	IRM	C12-C13	-4.62	1.36	1.46
5	E	102	IRM	C12-C13	-4.62	1.36	1.46
5	Q	102	IRM	C12-C13	-4.62	1.36	1.46
3	O	103	BCL	CAA-C2A	-4.62	1.45	1.54
5	A	104	IRM	C12-C13	-4.62	1.36	1.46
5	G	104	IRM	C12-C13	-4.62	1.36	1.46
5	M	104	IRM	C12-C13	-4.62	1.36	1.46
5	I	102	IRM	C12-C13	-4.62	1.36	1.46
5	O	102	IRM	C12-C13	-4.61	1.36	1.46
5	K	102	IRM	C12-C13	-4.61	1.36	1.46
5	C	104	IRM	C8-C9	-4.59	1.36	1.46
3	Q	103	BCL	CHB-C4A	-4.59	1.26	1.37
3	C	101	BCL	C1B-NB	-4.52	1.31	1.37
3	C	101	BCL	CMB-C2B	-4.42	1.41	1.50
3	A	101	BCL	CHC-C1C	-4.41	1.26	1.37
3	E	103	BCL	CAA-C2A	-4.40	1.46	1.54
3	G	101	BCL	C2A-C1A	-4.36	1.42	1.52
3	C	101	BCL	C2A-C1A	-4.32	1.42	1.52
3	K	103	BCL	CMD-C2D	-4.30	1.41	1.50
3	A	101	BCL	CAA-C2A	-4.29	1.46	1.54
3	E	103	BCL	C3C-C4C	-4.27	1.46	1.51
3	A	101	BCL	C2A-C1A	-4.21	1.42	1.52
3	A	101	BCL	CBB-CAB	-4.20	1.42	1.50
3	G	101	BCL	O2A-C1	-4.08	1.35	1.46
3	C	101	BCL	CHB-C4A	-4.06	1.27	1.37
3	O	103	BCL	C3B-C4B	4.02	1.49	1.41
3	Q	103	BCL	C9-C8	-4.02	1.40	1.52
3	K	103	BCL	C2A-C1A	-4.01	1.43	1.52
3	K	103	BCL	CHC-C1C	-4.00	1.27	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	103	BCL	CMD-C2D	-3.99	1.42	1.50
3	C	101	BCL	CHC-C1C	-3.98	1.27	1.37
3	I	103	BCL	C4-C3	-3.97	1.41	1.50
3	E	103	BCL	CHB-C4A	-3.95	1.27	1.37
3	O	103	BCL	C2A-C1A	-3.95	1.43	1.52
3	E	103	BCL	C2A-C1A	-3.93	1.43	1.52
3	C	101	BCL	C3C-C4C	-3.91	1.46	1.51
3	G	101	BCL	C3C-C4C	-3.88	1.46	1.51
3	K	104	BCL	MG-ND	3.86	2.13	2.05
3	I	104	BCL	MG-ND	3.85	2.13	2.05
3	O	103	BCL	C3C-C4C	-3.83	1.46	1.51
3	G	102	BCL	MG-ND	3.83	2.13	2.05
3	K	103	BCL	CAA-CBA	-3.82	1.41	1.52
3	G	101	BCL	CMD-C2D	-3.82	1.42	1.50
3	E	104	BCL	MG-ND	3.80	2.13	2.05
3	M	102	BCL	MG-ND	3.78	2.13	2.05
3	Q	104	BCL	MG-ND	3.78	2.13	2.05
3	K	103	BCL	CBB-CAB	-3.78	1.42	1.50
3	O	104	BCL	MG-ND	3.78	2.13	2.05
3	C	102	BCL	MG-ND	3.77	2.13	2.05
3	K	103	BCL	C3C-C4C	-3.77	1.46	1.51
3	Q	103	BCL	CMD-C2D	-3.77	1.43	1.50
3	O	103	BCL	CBB-CAB	-3.77	1.42	1.50
3	N	101	BCL	CHD-C1D	3.76	1.45	1.38
3	H	101	BCL	CHD-C1D	3.76	1.45	1.38
3	M	101	BCL	C2A-C1A	-3.76	1.43	1.52
3	C	101	BCL	CBA-CGA	-3.75	1.39	1.50
3	A	101	BCL	CBA-CGA	-3.75	1.39	1.50
3	P	101	BCL	CHD-C1D	3.75	1.45	1.38
3	A	102	BCL	MG-ND	3.75	2.13	2.05
3	L	101	BCL	CHD-C1D	3.75	1.45	1.38
3	D	101	BCL	CHD-C1D	3.75	1.45	1.38
3	F	101	BCL	CHD-C1D	3.75	1.45	1.38
3	R	101	BCL	CHD-C1D	3.74	1.45	1.38
3	J	101	BCL	CHD-C1D	3.74	1.45	1.38
3	B	101	BCL	CHD-C1D	3.74	1.45	1.38
3	N	101	BCL	C1D-C2D	-3.70	1.38	1.45
3	K	104	BCL	CHD-C1D	3.70	1.45	1.38
3	H	101	BCL	C1D-C2D	-3.70	1.38	1.45
3	E	103	BCL	CAA-CBA	-3.69	1.41	1.52
3	L	101	BCL	C1D-C2D	-3.67	1.38	1.45
3	I	103	BCL	C9-C8	-3.66	1.41	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	BCL	C1D-C2D	-3.66	1.38	1.45
3	M	101	BCL	C4-C3	-3.65	1.41	1.50
3	M	101	BCL	CAA-C2A	-3.65	1.47	1.54
3	P	101	BCL	C1D-C2D	-3.64	1.38	1.45
3	I	103	BCL	C2A-C1A	-3.64	1.44	1.52
3	B	101	BCL	C1D-C2D	-3.64	1.38	1.45
3	G	102	BCL	CHD-C1D	3.63	1.45	1.38
3	C	102	BCL	CHD-C1D	3.63	1.45	1.38
3	G	101	BCL	CAA-C2A	-3.63	1.47	1.54
3	R	101	BCL	C1D-C2D	-3.62	1.38	1.45
3	F	101	BCL	C1D-C2D	-3.62	1.38	1.45
3	I	104	BCL	CHD-C1D	3.62	1.45	1.38
3	O	104	BCL	CHD-C1D	3.62	1.45	1.38
3	P	101	BCL	CHC-C1C	3.62	1.46	1.37
3	J	101	BCL	C1D-C2D	-3.61	1.38	1.45
3	H	101	BCL	CHC-C1C	3.61	1.46	1.37
3	I	103	BCL	C3C-C4C	-3.61	1.47	1.51
3	I	104	BCL	CHC-C1C	3.61	1.46	1.37
3	E	104	BCL	CHD-C1D	3.61	1.45	1.38
3	R	101	BCL	CHC-C1C	3.61	1.46	1.37
3	G	102	BCL	CHC-C1C	3.60	1.46	1.37
3	M	102	BCL	CHD-C1D	3.60	1.45	1.38
3	M	102	BCL	CHC-C1C	3.60	1.46	1.37
3	A	102	BCL	CHD-C1D	3.60	1.45	1.38
3	O	104	BCL	CHC-C1C	3.59	1.46	1.37
3	Q	104	BCL	CHC-C1C	3.58	1.46	1.37
3	A	101	BCL	CMD-C2D	-3.58	1.43	1.50
3	A	101	BCL	C5-C3	-3.58	1.43	1.51
3	L	101	BCL	CHC-C1C	3.58	1.46	1.37
3	D	101	BCL	CHC-C1C	3.58	1.46	1.37
3	N	101	BCL	CHC-C1C	3.58	1.46	1.37
3	K	104	BCL	CHC-C1C	3.57	1.46	1.37
3	E	104	BCL	CHC-C1C	3.57	1.46	1.37
3	B	101	BCL	CHC-C1C	3.57	1.46	1.37
3	C	102	BCL	CHC-C1C	3.57	1.46	1.37
3	A	102	BCL	CHC-C1C	3.56	1.46	1.37
3	Q	103	BCL	C2A-C1A	-3.56	1.44	1.52
3	E	103	BCL	CBA-CGA	-3.56	1.40	1.50
3	J	101	BCL	CHC-C1C	3.56	1.46	1.37
3	F	101	BCL	CHC-C1C	3.56	1.46	1.37
3	Q	104	BCL	CHD-C1D	3.54	1.45	1.38
3	M	101	BCL	MG-NB	-3.53	1.98	2.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	103	BCL	C9-C8	-3.49	1.41	1.52
3	Q	104	BCL	CHB-C4A	3.48	1.46	1.37
3	E	103	BCL	CBB-CAB	-3.46	1.43	1.50
3	G	101	BCL	CAA-CBA	-3.45	1.42	1.52
3	O	104	BCL	CHB-C4A	3.44	1.46	1.37
3	K	103	BCL	C4-C3	-3.43	1.42	1.50
3	I	104	BCL	CHB-C4A	3.43	1.46	1.37
3	E	104	BCL	CHB-C4A	3.41	1.46	1.37
3	G	102	BCL	CHB-C4A	3.41	1.46	1.37
3	D	101	BCL	CHB-C4A	3.40	1.46	1.37
3	A	102	BCL	CHB-C4A	3.40	1.46	1.37
3	C	102	BCL	CHB-C4A	3.40	1.46	1.37
3	M	101	BCL	MG-NA	-3.39	1.98	2.06
3	O	103	BCL	C4-C3	-3.39	1.42	1.50
3	B	101	BCL	CHB-C4A	3.39	1.46	1.37
3	M	102	BCL	CHB-C4A	3.39	1.46	1.37
3	K	103	BCL	CAA-C2A	-3.39	1.47	1.54
3	P	101	BCL	CHB-C4A	3.39	1.46	1.37
3	R	101	BCL	CHB-C4A	3.39	1.46	1.37
3	F	101	BCL	CHB-C4A	3.39	1.46	1.37
3	K	104	BCL	CHB-C4A	3.38	1.46	1.37
3	L	101	BCL	CHB-C4A	3.38	1.46	1.37
3	A	101	BCL	CAA-CBA	-3.38	1.42	1.52
3	Q	103	BCL	C5-C3	-3.37	1.44	1.51
3	J	101	BCL	CHB-C4A	3.37	1.46	1.37
3	O	103	BCL	C3A-C2A	-3.37	1.45	1.54
3	I	103	BCL	C5-C3	-3.37	1.44	1.51
3	H	101	BCL	CHB-C4A	3.36	1.46	1.37
3	O	103	BCL	C9-C8	-3.35	1.42	1.52
3	M	101	BCL	C9-C8	-3.35	1.42	1.52
3	C	102	BCL	C1D-C2D	-3.34	1.38	1.45
3	M	102	BCL	C1D-C2D	-3.34	1.38	1.45
3	N	101	BCL	CHB-C4A	3.33	1.46	1.37
3	M	101	BCL	CAA-CBA	-3.33	1.42	1.52
3	G	101	BCL	C4-C3	-3.33	1.42	1.50
3	I	104	BCL	C1D-C2D	-3.32	1.38	1.45
3	E	104	BCL	C1D-C2D	-3.32	1.38	1.45
3	A	102	BCL	C1D-C2D	-3.32	1.38	1.45
3	G	102	BCL	C1D-C2D	-3.32	1.38	1.45
3	K	104	BCL	C1D-C2D	-3.32	1.38	1.45
3	Q	103	BCL	CAA-CBA	-3.31	1.43	1.52
3	O	104	BCL	C1D-C2D	-3.31	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	101	BCL	CAA-CBA	-3.30	1.43	1.52
3	E	103	BCL	C4-C3	-3.27	1.42	1.50
3	K	103	BCL	C5-C3	-3.27	1.44	1.51
3	I	103	BCL	CMD-C2D	-3.27	1.44	1.50
3	A	101	BCL	C4-C3	-3.27	1.42	1.50
3	Q	104	BCL	C1D-C2D	-3.27	1.38	1.45
3	O	103	BCL	CBA-CGA	-3.26	1.41	1.50
3	M	101	BCL	CMD-C2D	-3.25	1.44	1.50
3	I	103	BCL	CAA-CBA	-3.25	1.43	1.52
3	O	103	BCL	C5-C3	-3.25	1.44	1.51
3	K	103	BCL	C3A-C2A	-3.23	1.45	1.54
3	O	103	BCL	CAA-CBA	-3.23	1.43	1.52
3	I	103	BCL	CBA-CGA	-3.22	1.41	1.50
3	G	101	BCL	C9-C8	-3.20	1.42	1.52
3	K	103	BCL	C9-C8	-3.19	1.42	1.52
3	C	101	BCL	C3B-C4B	3.18	1.47	1.41
3	A	101	BCL	CMA-C3A	-3.18	1.46	1.53
3	O	103	BCL	CBD-CAD	-3.18	1.42	1.56
3	I	103	BCL	CMA-C3A	-3.18	1.46	1.53
3	Q	103	BCL	CBA-CGA	-3.17	1.41	1.50
3	K	103	BCL	CBA-CGA	-3.12	1.41	1.50
3	C	101	BCL	O2D-CGD	3.12	1.40	1.33
3	M	101	BCL	C3A-C2A	-3.11	1.46	1.54
3	E	103	BCL	C5-C3	-3.11	1.44	1.51
3	C	101	BCL	MG-ND	-3.10	1.99	2.05
3	Q	103	BCL	C3C-C4C	-3.10	1.47	1.51
3	G	101	BCL	CBA-CGA	-3.08	1.41	1.50
3	Q	103	BCL	C4-C3	-3.05	1.43	1.50
3	C	101	BCL	C9-C8	-3.05	1.43	1.52
3	A	101	BCL	C3A-C2A	-3.03	1.46	1.54
3	I	103	BCL	CBB-CAB	-2.99	1.44	1.50
3	M	101	BCL	C3C-C4C	-2.99	1.47	1.51
3	I	103	BCL	CBD-CAD	-2.98	1.43	1.56
3	Q	103	BCL	C3A-C2A	-2.95	1.46	1.54
3	E	103	BCL	CMD-C2D	-2.95	1.44	1.50
3	C	101	BCL	C3A-C2A	-2.94	1.46	1.54
3	I	103	BCL	CAC-C3C	-2.92	1.48	1.54
3	A	101	BCL	C4D-CHA	2.90	1.48	1.38
3	E	103	BCL	C3A-C2A	-2.90	1.46	1.54
3	K	103	BCL	CBD-CAD	-2.89	1.43	1.56
3	M	101	BCL	CMA-C3A	-2.86	1.47	1.53
3	M	101	BCL	C2C-C3C	-2.84	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	101	BCL	CBB-CAB	-2.84	1.44	1.50
3	L	101	BCL	MG-NB	2.84	2.11	2.05
3	G	101	BCL	CBD-CAD	-2.84	1.43	1.56
3	C	101	BCL	C2C-C3C	-2.84	1.46	1.54
3	R	101	BCL	MG-NB	2.83	2.11	2.05
3	P	101	BCL	MG-NB	2.82	2.11	2.05
3	G	101	BCL	C3A-C2A	-2.81	1.46	1.54
3	F	101	BCL	MG-NB	2.80	2.11	2.05
3	G	101	BCL	CAC-C3C	-2.79	1.48	1.54
3	N	101	BCL	MG-NB	2.79	2.11	2.05
3	I	103	BCL	C3A-C2A	-2.77	1.47	1.54
3	C	101	BCL	CBB-CAB	-2.76	1.44	1.50
3	Q	103	BCL	MG-ND	-2.76	2.00	2.05
3	J	101	BCL	MG-NB	2.75	2.11	2.05
3	H	101	BCL	MG-NB	2.74	2.11	2.05
3	D	101	BCL	MG-NB	2.74	2.11	2.05
3	A	101	BCL	MG-NA	-2.73	1.99	2.06
3	Q	103	BCL	C1-C2	-2.73	1.41	1.49
3	B	101	BCL	MG-NB	2.73	2.11	2.05
3	O	103	BCL	C11-C12	-2.72	1.40	1.52
3	Q	103	BCL	C3B-C4B	2.72	1.46	1.41
3	A	101	BCL	C9-C8	-2.72	1.44	1.52
3	C	101	BCL	CMA-C3A	-2.72	1.47	1.53
5	G	104	IRM	C24-C25	-2.70	1.34	1.43
3	I	103	BCL	C2C-C3C	-2.69	1.47	1.54
5	Q	102	IRM	C20-C21	-2.69	1.34	1.43
3	K	103	BCL	MG-NA	-2.69	1.99	2.06
3	G	101	BCL	CMA-C3A	-2.68	1.47	1.53
5	I	102	IRM	C20-C21	-2.68	1.34	1.43
5	Q	102	IRM	C24-C25	-2.68	1.34	1.43
3	C	101	BCL	C11-C12	-2.67	1.41	1.52
5	M	104	IRM	C24-C25	-2.67	1.34	1.43
3	A	101	BCL	C2C-C3C	-2.67	1.47	1.54
5	G	104	IRM	C20-C21	-2.67	1.34	1.43
5	E	102	IRM	C20-C21	-2.67	1.34	1.43
5	A	104	IRM	C20-C21	-2.66	1.34	1.43
5	K	102	IRM	C24-C25	-2.66	1.34	1.43
3	A	101	BCL	O2D-CGD	2.66	1.39	1.33
5	I	102	IRM	C24-C25	-2.66	1.34	1.43
5	M	104	IRM	C20-C21	-2.66	1.34	1.43
5	Q	102	IRM	C7-C6	-2.66	1.34	1.43
5	A	104	IRM	C24-C25	-2.66	1.34	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	102	IRM	C24-C25	-2.66	1.34	1.43
5	O	102	IRM	C20-C21	-2.66	1.34	1.43
5	E	102	IRM	C24-C25	-2.66	1.34	1.43
5	M	104	IRM	C7-C6	-2.65	1.35	1.43
5	A	104	IRM	C7-C6	-2.65	1.35	1.43
5	C	104	IRM	C20-C21	-2.65	1.35	1.43
5	K	102	IRM	C7-C6	-2.65	1.35	1.43
5	C	104	IRM	C7-C6	-2.65	1.35	1.43
5	E	102	IRM	C7-C6	-2.65	1.35	1.43
5	G	104	IRM	C7-C6	-2.65	1.35	1.43
3	G	101	BCL	C11-C12	-2.64	1.41	1.52
3	E	103	BCL	CMC-C2C	-2.64	1.47	1.53
5	K	102	IRM	C20-C21	-2.64	1.35	1.43
5	O	102	IRM	C7-C6	-2.64	1.35	1.43
5	C	104	IRM	C24-C25	-2.64	1.35	1.43
5	I	102	IRM	C7-C6	-2.63	1.35	1.43
3	A	101	BCL	C20-C18	-2.62	1.38	1.51
3	M	101	BCL	CAC-C3C	-2.61	1.49	1.54
3	K	103	BCL	C2C-C3C	-2.61	1.47	1.54
5	Q	102	IRM	C16-C17	-2.59	1.35	1.43
5	G	104	IRM	C16-C17	-2.58	1.35	1.43
5	I	102	IRM	C16-C17	-2.58	1.35	1.43
3	G	101	BCL	C16-C15	-2.57	1.41	1.52
3	I	103	BCL	C4D-CHA	2.57	1.47	1.38
3	C	101	BCL	C1-C2	-2.57	1.42	1.49
5	C	104	IRM	C15-C14	-2.57	1.35	1.43
3	M	101	BCL	CBA-CGA	-2.57	1.43	1.50
5	C	104	IRM	C16-C17	-2.57	1.35	1.43
5	E	102	IRM	C16-C17	-2.56	1.35	1.43
5	O	102	IRM	C16-C17	-2.56	1.35	1.43
5	Q	102	IRM	C11-C10	-2.56	1.35	1.43
5	A	104	IRM	C16-C17	-2.56	1.35	1.43
5	I	102	IRM	C11-C10	-2.56	1.35	1.43
5	E	102	IRM	C11-C10	-2.56	1.35	1.43
5	A	104	IRM	C11-C10	-2.55	1.35	1.43
5	K	102	IRM	C11-C10	-2.55	1.35	1.43
3	I	103	BCL	C2-C3	-2.55	1.27	1.33
5	M	104	IRM	C11-C10	-2.55	1.35	1.43
5	M	104	IRM	C16-C17	-2.55	1.35	1.43
5	C	104	IRM	C11-C10	-2.55	1.35	1.43
5	O	102	IRM	C11-C10	-2.55	1.35	1.43
5	G	104	IRM	C11-C10	-2.55	1.35	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	103	BCL	CBD-CAD	-2.55	1.45	1.56
3	E	103	BCL	CMA-C3A	-2.55	1.47	1.53
5	I	102	IRM	C15-C14	-2.54	1.35	1.43
5	K	102	IRM	C15-C14	-2.54	1.35	1.43
3	M	101	BCL	CBD-CAD	-2.54	1.45	1.56
5	M	104	IRM	C15-C14	-2.53	1.35	1.43
5	K	102	IRM	C16-C17	-2.53	1.35	1.43
5	A	104	IRM	C15-C14	-2.53	1.35	1.43
3	C	101	BCL	C16-C15	-2.53	1.41	1.52
5	G	104	IRM	C15-C14	-2.53	1.35	1.43
5	Q	102	IRM	C15-C14	-2.53	1.35	1.43
3	M	101	BCL	C20-C18	-2.52	1.38	1.51
3	K	103	BCL	CAC-C3C	-2.51	1.49	1.54
3	G	101	BCL	C14-C13	-2.51	1.45	1.52
5	E	102	IRM	C15-C14	-2.51	1.35	1.43
5	O	102	IRM	C15-C14	-2.50	1.35	1.43
3	A	101	BCL	C3D-C2D	2.50	1.45	1.39
3	K	103	BCL	C1-C2	-2.49	1.42	1.49
3	K	103	BCL	CMA-C3A	-2.49	1.47	1.53
3	A	101	BCL	CMC-C2C	-2.49	1.47	1.53
3	I	103	BCL	C3A-C4A	-2.48	1.43	1.51
3	Q	103	BCL	MG-NA	-2.47	2.00	2.06
3	E	103	BCL	C11-C12	-2.46	1.41	1.52
3	Q	103	BCL	C2-C3	-2.46	1.27	1.33
3	K	103	BCL	C2-C3	-2.45	1.27	1.33
3	C	101	BCL	CHB-C1B	2.45	1.44	1.39
3	C	101	BCL	CBD-CAD	-2.44	1.45	1.56
3	Q	103	BCL	C20-C18	-2.44	1.39	1.51
3	C	101	BCL	C20-C18	-2.42	1.39	1.51
3	G	101	BCL	O2D-CGD	2.41	1.39	1.33
3	Q	103	BCL	C4D-CHA	2.41	1.46	1.38
3	C	101	BCL	C4D-CHA	2.41	1.46	1.38
3	O	103	BCL	CMA-C3A	-2.41	1.48	1.53
3	Q	103	BCL	C19-C18	-2.39	1.39	1.51
3	O	103	BCL	C3D-C2D	2.39	1.45	1.39
3	K	103	BCL	CHC-C4B	2.38	1.44	1.39
3	K	103	BCL	C4D-CHA	2.38	1.46	1.38
3	E	103	BCL	C20-C18	-2.38	1.39	1.51
3	M	101	BCL	CMC-C2C	-2.37	1.48	1.53
3	E	103	BCL	CAC-C3C	-2.37	1.49	1.54
3	I	103	BCL	C1-C2	-2.37	1.42	1.49
3	Q	104	BCL	C3B-C4B	2.36	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	103	BCL	C16-C15	-2.36	1.42	1.52
3	K	103	BCL	C3A-C4A	-2.36	1.44	1.51
3	E	103	BCL	C2C-C3C	-2.34	1.48	1.54
3	Q	103	BCL	C11-C10	-2.33	1.42	1.52
3	E	104	BCL	C3B-C4B	2.31	1.45	1.41
3	C	102	BCL	C3B-C4B	2.31	1.45	1.41
3	I	104	BCL	C3B-C4B	2.30	1.45	1.41
3	O	103	BCL	C16-C15	-2.29	1.42	1.52
3	A	102	BCL	C3B-C4B	2.29	1.45	1.41
3	O	103	BCL	C2C-C3C	-2.28	1.48	1.54
3	G	102	BCL	C3B-C4B	2.28	1.45	1.41
3	I	103	BCL	MG-NA	-2.27	2.00	2.06
3	O	104	BCL	C3B-C4B	2.27	1.45	1.41
3	M	101	BCL	C14-C13	-2.27	1.45	1.52
3	K	104	BCL	C3B-C4B	2.26	1.45	1.41
3	C	101	BCL	C5-C3	-2.25	1.46	1.51
3	I	103	BCL	C19-C18	-2.25	1.40	1.51
3	I	103	BCL	C11-C12	-2.25	1.42	1.52
3	C	101	BCL	C14-C13	-2.25	1.45	1.52
3	C	101	BCL	C3D-C2D	2.24	1.45	1.39
3	K	103	BCL	C14-C13	-2.24	1.45	1.52
3	A	101	BCL	C2-C3	-2.24	1.27	1.33
3	Q	103	BCL	C2C-C3C	-2.23	1.48	1.54
3	H	101	BCL	C3B-C4B	2.23	1.45	1.41
3	M	102	BCL	C3B-C4B	2.22	1.45	1.41
3	G	101	BCL	C2C-C3C	-2.22	1.48	1.54
3	M	101	BCL	C16-C15	-2.22	1.42	1.52
3	E	103	BCL	C4D-CHA	2.21	1.46	1.38
4	I	101	LDA	C1-N1	2.21	1.53	1.51
3	A	101	BCL	CHB-C1B	2.21	1.44	1.39
3	B	101	BCL	C3B-C4B	2.21	1.45	1.41
3	L	101	BCL	C3B-C4B	2.21	1.45	1.41
3	E	103	BCL	C16-C15	-2.21	1.42	1.52
3	A	101	BCL	CBD-CAD	-2.21	1.46	1.56
3	K	103	BCL	C20-C18	-2.20	1.40	1.51
4	M	103	LDA	C1-N1	2.19	1.53	1.51
3	I	103	BCL	C3D-C2D	2.19	1.45	1.39
3	R	101	BCL	C3B-C4B	2.19	1.45	1.41
3	E	103	BCL	CHB-C1B	2.18	1.44	1.39
3	M	101	BCL	O2D-CGD	2.18	1.38	1.33
4	E	101	LDA	C1-N1	2.18	1.53	1.51
3	J	101	BCL	C3B-C4B	2.18	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	101	BCL	C20-C18	-2.17	1.40	1.51
3	I	103	BCL	C20-C18	-2.17	1.40	1.51
3	E	103	BCL	O2D-CGD	2.16	1.38	1.33
3	C	101	BCL	CMC-C2C	-2.16	1.48	1.53
3	D	101	BCL	C3B-C4B	2.15	1.45	1.41
4	G	103	LDA	C1-N1	2.15	1.53	1.51
3	E	103	BCL	C14-C13	-2.15	1.46	1.52
3	G	101	BCL	MG-NA	-2.14	2.01	2.06
4	K	101	LDA	C1-N1	2.14	1.53	1.51
3	P	101	BCL	C3B-C4B	2.14	1.45	1.41
3	Q	103	BCL	CMA-C3A	-2.13	1.48	1.53
3	N	101	BCL	C3B-C4B	2.13	1.45	1.41
3	E	103	BCL	C3A-C4A	-2.13	1.44	1.51
3	G	101	BCL	C3B-C4B	2.12	1.45	1.41
3	O	103	BCL	C19-C18	-2.12	1.40	1.51
4	Q	101	LDA	C1-N1	2.12	1.53	1.51
3	F	101	BCL	C3B-C4B	2.12	1.45	1.41
3	O	103	BCL	CAC-C3C	-2.11	1.50	1.54
3	O	103	BCL	C20-C18	-2.11	1.40	1.51
3	O	103	BCL	C16-C17	-2.11	1.43	1.52
4	C	103	LDA	C1-N1	2.10	1.53	1.51
3	C	101	BCL	C4-C3	-2.10	1.45	1.50
3	O	103	BCL	C2-C3	-2.09	1.28	1.33
4	A	103	LDA	C1-N1	2.08	1.53	1.51
3	A	101	BCL	C3B-C4B	2.08	1.45	1.41
3	G	101	BCL	C16-C17	-2.07	1.43	1.52
4	O	101	LDA	C1-N1	2.06	1.53	1.51
3	E	103	BCL	C19-C18	-2.06	1.41	1.51
3	M	101	BCL	C11-C12	-2.06	1.43	1.52
3	G	101	BCL	O2A-CGA	2.05	1.39	1.33
3	Q	103	BCL	CMC-C2C	-2.05	1.48	1.53
4	M	103	LDA	O1-N1	-2.03	1.37	1.42
3	E	103	BCL	C1-C2	-2.03	1.43	1.49
3	K	103	BCL	C3B-C4B	2.02	1.45	1.41
3	I	103	BCL	C16-C17	-2.02	1.43	1.52
3	Q	103	BCL	C3D-C2D	2.02	1.44	1.39
3	A	101	BCL	C16-C15	-2.02	1.43	1.52
4	I	101	LDA	O1-N1	-2.00	1.37	1.42
3	I	103	BCL	C3B-C4B	2.00	1.45	1.41

All (593) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	103	BCL	C4A-NA-C1A	12.81	112.53	106.68
3	O	103	BCL	O2D-CGD-CBD	12.20	132.55	111.23
3	G	101	BCL	O2D-CGD-CBD	11.74	131.76	111.23
3	K	103	BCL	O2A-CGA-CBA	11.65	147.36	111.83
3	M	101	BCL	O2D-CGD-CBD	11.52	131.37	111.23
3	M	101	BCL	O2A-CGA-CBA	11.32	146.35	111.83
3	O	103	BCL	C4A-NA-C1A	11.22	111.80	106.68
3	Q	103	BCL	O2A-CGA-CBA	11.16	145.86	111.83
3	M	101	BCL	C4A-NA-C1A	10.92	111.66	106.68
3	I	103	BCL	C4A-NA-C1A	10.87	111.64	106.68
3	K	103	BCL	O2D-CGD-CBD	10.67	129.89	111.23
3	O	103	BCL	O2D-CGD-O1D	-10.52	103.36	123.85
3	F	101	BCL	C4A-NA-C1A	10.42	111.43	106.68
3	I	103	BCL	O2A-CGA-CBA	10.41	143.56	111.83
3	N	101	BCL	C4A-NA-C1A	10.40	111.42	106.68
3	G	101	BCL	C4A-NA-C1A	10.37	111.41	106.68
3	P	101	BCL	C4A-NA-C1A	10.37	111.41	106.68
3	J	101	BCL	C4A-NA-C1A	10.36	111.41	106.68
3	R	101	BCL	C4A-NA-C1A	10.36	111.41	106.68
3	L	101	BCL	C4A-NA-C1A	10.33	111.39	106.68
3	B	101	BCL	C4A-NA-C1A	10.30	111.38	106.68
3	D	101	BCL	C4A-NA-C1A	10.27	111.36	106.68
3	A	101	BCL	O2D-CGD-CBD	10.20	129.07	111.23
3	H	101	BCL	C4A-NA-C1A	10.20	111.33	106.68
3	E	103	BCL	O2D-CGD-CBD	9.93	128.60	111.23
3	O	103	BCL	O2A-CGA-CBA	9.93	142.10	111.83
3	C	101	BCL	O2D-CGD-CBD	9.91	128.56	111.23
3	E	103	BCL	O2A-CGA-CBA	9.88	141.96	111.83
3	A	101	BCL	O2A-CGA-CBA	9.83	141.80	111.83
3	M	101	BCL	O2D-CGD-O1D	-9.82	104.72	123.85
3	G	101	BCL	C9-C8-C7	-9.59	77.08	111.27
3	Q	103	BCL	C4A-NA-C1A	9.44	110.99	106.68
3	G	101	BCL	O2A-CGA-CBA	9.43	140.58	111.83
3	K	103	BCL	O2D-CGD-O1D	-9.33	105.68	123.85
3	G	101	BCL	C4-C3-C2	-9.32	99.70	123.63
3	C	101	BCL	O2A-CGA-CBA	9.27	140.11	111.83
3	K	103	BCL	C4A-NA-C1A	9.14	110.85	106.68
3	G	101	BCL	O2D-CGD-O1D	-9.12	106.09	123.85
3	I	104	BCL	C4A-NA-C1A	8.99	110.78	106.68
3	A	102	BCL	C4A-NA-C1A	8.94	110.76	106.68
3	G	102	BCL	C4A-NA-C1A	8.92	110.75	106.68
3	Q	104	BCL	C4A-NA-C1A	8.92	110.75	106.68
3	K	104	BCL	C4A-NA-C1A	8.91	110.74	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	104	BCL	C4A-NA-C1A	8.89	110.73	106.68
3	A	101	BCL	CED-O2D-CGD	8.82	135.93	115.92
3	E	104	BCL	C4A-NA-C1A	8.82	110.70	106.68
3	I	103	BCL	O2D-CGD-O1D	-8.81	106.71	123.85
3	M	102	BCL	C4A-NA-C1A	8.80	110.69	106.68
3	C	102	BCL	C4A-NA-C1A	8.79	110.69	106.68
3	A	101	BCL	O2D-CGD-O1D	-8.61	107.08	123.85
3	G	101	BCL	C5-C3-C2	8.61	140.49	121.17
3	G	101	BCL	CED-O2D-CGD	8.36	134.87	115.92
3	E	103	BCL	O2D-CGD-O1D	-8.34	107.62	123.85
3	Q	103	BCL	O2D-CGD-O1D	-8.32	107.66	123.85
3	Q	103	BCL	O2D-CGD-CBD	8.31	125.76	111.23
3	I	103	BCL	O2D-CGD-CBD	8.31	125.75	111.23
3	F	101	BCL	C1C-NC-C4C	8.22	110.43	106.68
3	R	101	BCL	C1C-NC-C4C	8.18	110.41	106.68
3	L	101	BCL	C1C-NC-C4C	8.16	110.40	106.68
3	P	101	BCL	C1C-NC-C4C	8.16	110.40	106.68
3	A	101	BCL	C4A-NA-C1A	8.15	110.40	106.68
3	D	101	BCL	C1C-NC-C4C	8.12	110.38	106.68
3	J	101	BCL	C1C-NC-C4C	8.11	110.38	106.68
3	N	101	BCL	C1C-NC-C4C	8.11	110.38	106.68
3	Q	103	BCL	CED-O2D-CGD	8.10	134.30	115.92
3	B	101	BCL	C1C-NC-C4C	8.06	110.36	106.68
3	H	101	BCL	C1C-NC-C4C	7.97	110.31	106.68
3	K	103	BCL	CED-O2D-CGD	7.84	133.69	115.92
3	M	101	BCL	CED-O2D-CGD	7.73	133.44	115.92
3	C	101	BCL	O2D-CGD-O1D	-7.58	109.10	123.85
3	M	101	BCL	C9-C8-C7	-7.15	85.78	111.27
3	I	104	BCL	C1C-NC-C4C	7.15	109.94	106.68
3	E	104	BCL	C1C-NC-C4C	7.13	109.93	106.68
3	C	102	BCL	C1C-NC-C4C	7.12	109.93	106.68
3	M	102	BCL	C1C-NC-C4C	7.11	109.92	106.68
3	Q	104	BCL	C1C-NC-C4C	7.10	109.92	106.68
3	A	102	BCL	C1C-NC-C4C	7.07	109.90	106.68
3	G	102	BCL	C1C-NC-C4C	7.04	109.89	106.68
3	K	104	BCL	C1C-NC-C4C	7.03	109.89	106.68
3	O	104	BCL	C1C-NC-C4C	7.02	109.88	106.68
3	G	101	BCL	C1-C2-C3	6.86	137.44	126.20
3	O	103	BCL	CED-O2D-CGD	6.85	131.46	115.92
3	E	103	BCL	CED-O2D-CGD	6.84	131.44	115.92
3	K	103	BCL	CMD-C2D-C1D	6.74	136.59	124.73
3	I	103	BCL	C3D-C2D-C1D	-6.73	96.65	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	101	BCL	C3D-C2D-C1D	-6.72	96.66	105.83
3	E	103	BCL	CMD-C2D-C1D	6.71	136.54	124.73
3	G	101	BCL	CHD-C1D-ND	-6.64	115.46	124.80
3	I	103	BCL	CBB-CAB-C3B	6.55	134.22	120.40
3	M	101	BCL	O2A-CGA-O1A	-6.52	107.32	123.63
3	K	103	BCL	CBB-CAB-C3B	6.46	134.01	120.40
3	I	103	BCL	CED-O2D-CGD	6.29	130.18	115.92
3	G	101	BCL	CHC-C4B-NB	-6.27	114.64	124.05
3	A	101	BCL	CMD-C2D-C1D	6.25	135.73	124.73
3	O	103	BCL	CBB-CAB-C3B	6.12	133.29	120.40
3	K	103	BCL	O1A-CGA-CBA	-6.06	100.09	123.78
3	O	103	BCL	CMD-C2D-C1D	6.00	135.30	124.73
3	C	101	BCL	C4A-NA-C1A	5.98	109.41	106.68
3	G	101	BCL	OBD-CAD-C3D	-5.93	114.56	128.42
3	C	101	BCL	CBB-CAB-C3B	5.91	132.87	120.40
3	E	103	BCL	C14-C13-C15	-5.85	90.41	111.27
3	Q	103	BCL	C14-C13-C15	-5.84	90.44	111.27
3	A	101	BCL	O1A-CGA-CBA	-5.84	100.94	123.78
3	F	101	BCL	C1D-ND-C4D	5.83	110.41	106.31
3	G	101	BCL	C2B-C1B-NB	5.83	116.37	110.33
3	E	103	BCL	C3D-C2D-C1D	-5.81	97.90	105.83
3	B	101	BCL	C1D-ND-C4D	5.79	110.38	106.31
3	M	101	BCL	C3D-C2D-C1D	-5.78	97.94	105.83
3	M	101	BCL	CBB-CAB-C3B	5.78	132.58	120.40
3	C	101	BCL	CED-O2D-CGD	5.78	129.02	115.92
3	H	101	BCL	C1D-ND-C4D	5.77	110.36	106.31
3	P	101	BCL	C1D-ND-C4D	5.76	110.35	106.31
3	R	101	BCL	C1D-ND-C4D	5.74	110.34	106.31
3	D	101	BCL	C1D-ND-C4D	5.74	110.34	106.31
3	G	101	BCL	C12-C11-C10	-5.71	87.70	113.28
3	J	101	BCL	C1D-ND-C4D	5.70	110.31	106.31
3	L	101	BCL	C1D-ND-C4D	5.70	110.31	106.31
3	O	103	BCL	CHC-C4B-NB	-5.70	115.49	124.05
5	M	104	IRM	C28-C27-C26	5.67	131.97	113.19
5	E	102	IRM	C28-C27-C26	5.66	131.95	113.19
5	G	104	IRM	C28-C27-C26	5.66	131.94	113.19
5	I	102	IRM	C28-C27-C26	5.65	131.92	113.19
3	G	102	BCL	C4D-CHA-C1A	5.65	127.98	121.24
5	Q	102	IRM	C28-C27-C26	5.65	131.91	113.19
5	C	104	IRM	C28-C27-C26	5.65	131.90	113.19
3	N	101	BCL	C1D-ND-C4D	5.65	110.27	106.31
5	A	104	IRM	C28-C27-C26	5.64	131.88	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	102	BCL	C4D-CHA-C1A	5.64	127.97	121.24
3	Q	104	BCL	C4D-CHA-C1A	5.63	127.96	121.24
5	O	102	IRM	C28-C27-C26	5.63	131.85	113.19
3	A	102	BCL	C4D-CHA-C1A	5.63	127.95	121.24
3	K	104	BCL	C4D-CHA-C1A	5.63	127.95	121.24
5	K	102	IRM	C28-C27-C26	5.62	131.82	113.19
3	E	104	BCL	C4D-CHA-C1A	5.61	127.94	121.24
3	M	102	BCL	C1D-ND-C4D	5.60	110.24	106.31
3	O	104	BCL	C4D-CHA-C1A	5.60	127.92	121.24
3	Q	103	BCL	CMD-C2D-C1D	5.59	134.58	124.73
3	I	104	BCL	C1D-ND-C4D	5.59	110.24	106.31
3	I	104	BCL	C4D-CHA-C1A	5.59	127.91	121.24
3	G	101	BCL	CMD-C2D-C1D	5.59	134.57	124.73
3	Q	103	BCL	C2B-C1B-NB	5.59	116.12	110.33
3	I	103	BCL	CMD-C2D-C1D	5.59	134.57	124.73
3	I	103	BCL	C14-C13-C15	-5.58	91.37	111.27
3	Q	104	BCL	C1D-ND-C4D	5.57	110.22	106.31
3	G	102	BCL	C1D-ND-C4D	5.57	110.22	106.31
3	M	102	BCL	C4D-CHA-C1A	5.56	127.87	121.24
3	K	104	BCL	C1D-ND-C4D	5.56	110.21	106.31
3	C	101	BCL	O1A-CGA-CBA	-5.53	102.13	123.78
3	E	104	BCL	C1D-ND-C4D	5.52	110.18	106.31
3	Q	103	BCL	CBB-CAB-C3B	5.52	132.03	120.40
3	O	103	BCL	C1D-ND-C4D	5.51	110.18	106.31
3	A	102	BCL	C1D-ND-C4D	5.50	110.17	106.31
3	A	101	BCL	CBB-CAB-C3B	5.50	131.99	120.40
3	O	104	BCL	C1D-ND-C4D	5.48	110.16	106.31
3	C	102	BCL	C1D-ND-C4D	5.44	110.13	106.31
3	I	103	BCL	C4D-C3D-CAD	-5.42	102.22	108.11
3	K	103	BCL	C3D-C2D-C1D	-5.42	98.44	105.83
3	C	101	BCL	C3D-C2D-C1D	-5.41	98.45	105.83
3	Q	103	BCL	O2A-CGA-O1A	-5.39	110.14	123.63
3	I	103	BCL	O1A-CGA-CBA	-5.38	102.73	123.78
3	K	103	BCL	C3C-C4C-CHD	-5.38	112.05	123.39
3	K	103	BCL	C14-C13-C15	-5.38	92.11	111.27
3	G	101	BCL	O1A-CGA-CBA	-5.37	102.79	123.78
3	M	101	BCL	CMD-C2D-C1D	5.35	134.14	124.73
3	A	101	BCL	C3D-C2D-C1D	-5.34	98.55	105.83
3	O	103	BCL	C14-C13-C15	-5.32	92.32	111.27
3	C	101	BCL	OBD-CAD-C3D	-5.31	116.02	128.42
3	M	101	BCL	C9-C8-C10	-5.30	92.37	111.27
3	I	103	BCL	C9-C8-C7	-5.27	92.47	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	103	BCL	CBB-CAB-C3B	5.27	131.52	120.40
3	A	101	BCL	C3C-C4C-CHD	-5.25	112.31	123.39
3	O	103	BCL	C3D-C2D-C1D	-5.24	98.67	105.83
3	I	103	BCL	OB B-CAB-C3B	-5.22	111.20	120.43
3	Q	103	BCL	C3D-C2D-C1D	-5.19	98.75	105.83
3	O	103	BCL	O2A-CGA-O1A	-5.18	110.67	123.63
3	Q	103	BCL	O1A-CGA-CBA	-5.17	103.56	123.78
3	E	103	BCL	O1A-CGA-CBA	-5.10	103.84	123.78
3	D	101	BCL	C2D-C1D-ND	-5.06	105.12	110.13
3	O	103	BCL	C2B-C1B-NB	5.04	115.55	110.33
3	P	101	BCL	C2D-C1D-ND	-5.02	105.16	110.13
3	C	101	BCL	C14-C13-C15	-5.01	93.42	111.27
3	F	101	BCL	C2D-C1D-ND	-5.01	105.17	110.13
3	N	101	BCL	C4D-CHA-C1A	5.01	127.22	121.24
3	L	101	BCL	C2D-C1D-ND	-5.00	105.18	110.13
3	B	101	BCL	C2D-C1D-ND	-4.99	105.18	110.13
3	R	101	BCL	C2D-C1D-ND	-4.99	105.19	110.13
3	J	101	BCL	C4D-CHA-C1A	4.98	127.19	121.24
3	O	103	BCL	C1-O2A-CGA	4.97	128.69	116.65
3	J	101	BCL	C2D-C1D-ND	-4.96	105.22	110.13
3	H	101	BCL	C2D-C1D-ND	-4.96	105.22	110.13
3	R	101	BCL	C4D-CHA-C1A	4.95	127.14	121.24
3	L	101	BCL	C4D-CHA-C1A	4.94	127.14	121.24
3	C	101	BCL	CMD-C2D-C1D	4.94	133.43	124.73
3	H	101	BCL	C4D-CHA-C1A	4.94	127.14	121.24
3	B	101	BCL	C4D-CHA-C1A	4.93	127.12	121.24
3	D	101	BCL	C4D-CHA-C1A	4.93	127.12	121.24
3	P	101	BCL	C4D-CHA-C1A	4.92	127.11	121.24
3	N	101	BCL	C2D-C1D-ND	-4.92	105.26	110.13
3	F	101	BCL	C4D-CHA-C1A	4.89	127.08	121.24
3	Q	103	BCL	CHC-C4B-NB	-4.89	116.71	124.05
3	M	102	BCL	C2D-C1D-ND	-4.89	105.29	110.13
3	A	101	BCL	OBD-CAD-C3D	-4.86	117.05	128.42
3	I	104	BCL	C2D-C1D-ND	-4.86	105.31	110.13
3	K	103	BCL	CMB-C2B-C1B	4.86	132.82	125.42
3	Q	104	BCL	C2D-C1D-ND	-4.85	105.33	110.13
3	E	104	BCL	C2D-C1D-ND	-4.85	105.33	110.13
3	K	104	BCL	C2D-C1D-ND	-4.83	105.34	110.13
3	A	102	BCL	C2D-C1D-ND	-4.83	105.35	110.13
3	A	101	BCL	C14-C13-C15	-4.81	94.11	111.27
3	O	104	BCL	C2D-C1D-ND	-4.81	105.36	110.13
3	M	101	BCL	C4-C3-C2	-4.80	111.29	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	102	BCL	C2D-C1D-ND	-4.78	105.39	110.13
3	C	102	BCL	C2D-C1D-ND	-4.78	105.40	110.13
3	M	101	BCL	OBD-CAD-C3D	-4.74	117.33	128.42
3	E	103	BCL	C3C-C4C-CHD	-4.73	113.43	123.39
5	O	102	IRM	C38-C26-C27	4.72	123.42	115.23
5	A	104	IRM	C38-C26-C27	4.71	123.40	115.23
5	K	102	IRM	C38-C26-C27	4.70	123.38	115.23
5	C	104	IRM	C38-C26-C27	4.69	123.36	115.23
5	Q	102	IRM	C38-C26-C27	4.68	123.35	115.23
5	G	104	IRM	C38-C26-C27	4.66	123.32	115.23
5	M	104	IRM	C38-C26-C27	4.66	123.31	115.23
5	I	102	IRM	C38-C26-C27	4.66	123.31	115.23
5	E	102	IRM	C38-C26-C27	4.65	123.30	115.23
3	M	101	BCL	C20-C18-C19	-4.63	89.88	110.53
3	I	103	BCL	C9-C8-C10	-4.60	94.88	111.27
3	I	103	BCL	C3C-C4C-CHD	-4.57	113.75	123.39
3	M	101	BCL	CMB-C2B-C1B	4.54	132.33	125.42
3	Q	103	BCL	CMB-C2B-C1B	4.54	132.32	125.42
3	Q	103	BCL	C20-C18-C19	-4.52	90.37	110.53
3	A	101	BCL	C2B-C1B-NB	4.50	115.00	110.33
3	M	101	BCL	O1A-CGA-CBA	-4.50	106.17	123.78
3	M	101	BCL	C11-C12-C13	4.50	130.92	115.97
3	M	101	BCL	CBC-CAC-C3C	4.49	122.94	113.41
3	A	101	BCL	C1D-ND-C4D	4.49	109.46	106.31
3	Q	103	BCL	C9-C8-C10	-4.48	95.29	111.27
3	G	101	BCL	C4D-C3D-CAD	-4.46	103.26	108.11
3	K	103	BCL	O2A-CGA-O1A	-4.44	112.52	123.63
3	G	101	BCL	CBB-CAB-C3B	4.41	129.70	120.40
3	O	103	BCL	O1A-CGA-CBA	-4.40	106.57	123.78
3	M	102	BCL	C2B-C1B-NB	-4.37	105.79	110.33
3	A	101	BCL	C1-O2A-CGA	4.37	127.23	116.65
3	O	104	BCL	C2B-C1B-NB	-4.36	105.81	110.33
3	I	104	BCL	C2B-C1B-NB	-4.35	105.81	110.33
3	A	101	BCL	OBB-CAB-C3B	-4.35	112.74	120.43
3	C	102	BCL	C2B-C1B-NB	-4.35	105.82	110.33
3	A	102	BCL	C2B-C1B-NB	-4.33	105.83	110.33
3	I	103	BCL	OBD-CAD-C3D	-4.33	118.28	128.42
3	C	101	BCL	C1D-ND-C4D	4.33	109.35	106.31
3	K	104	BCL	C2B-C1B-NB	-4.33	105.84	110.33
3	Q	103	BCL	OBD-CAD-C3D	-4.32	118.32	128.42
3	E	103	BCL	C2B-C1B-NB	4.32	114.80	110.33
3	C	101	BCL	OBB-CAB-CBB	-4.29	110.16	119.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	103	BCL	CAA-CBA-CGA	-4.29	101.04	113.21
3	E	103	BCL	CHC-C4B-NB	-4.27	117.64	124.05
3	Q	103	BCL	C9-C8-C7	-4.27	96.05	111.27
3	C	101	BCL	C2B-C1B-NB	4.27	114.75	110.33
3	Q	104	BCL	C2B-C1B-NB	-4.27	105.90	110.33
3	G	102	BCL	C2B-C1B-NB	-4.26	105.91	110.33
3	I	103	BCL	CHD-C1D-ND	-4.25	118.82	124.80
3	I	103	BCL	C1D-ND-C4D	4.23	109.28	106.31
3	E	103	BCL	C9-C8-C10	-4.20	96.28	111.27
3	E	104	BCL	C2B-C1B-NB	-4.20	105.97	110.33
3	A	101	BCL	CHC-C4B-NB	-4.20	117.75	124.05
3	Q	103	BCL	OB B-CAB-CBB	-4.18	110.41	119.77
3	E	103	BCL	C1-O2A-CGA	4.15	126.69	116.65
3	K	103	BCL	C2B-C1B-NB	4.14	114.61	110.33
3	C	101	BCL	C9-C8-C7	-4.12	96.60	111.27
3	I	103	BCL	C2B-C1B-NB	4.11	114.59	110.33
3	I	103	BCL	CHC-C4B-NB	-4.10	117.89	124.05
3	I	103	BCL	O2A-CGA-O1A	-4.04	113.52	123.63
3	Q	103	BCL	C1D-ND-C4D	4.04	109.14	106.31
3	O	103	BCL	C20-C18-C19	-4.03	92.53	110.53
3	C	101	BCL	CHC-C4B-NB	-4.01	118.03	124.05
3	E	103	BCL	CHD-C1D-ND	-4.00	119.17	124.80
3	Q	103	BCL	C3B-C4B-NB	3.99	115.03	109.76
3	M	101	BCL	C3C-C4C-CHD	-3.98	115.01	123.39
3	C	101	BCL	C9-C8-C10	-3.97	97.11	111.27
3	E	103	BCL	OB D-CAD-C3D	-3.97	119.13	128.42
3	M	101	BCL	CHD-C1D-ND	-3.96	119.23	124.80
3	A	101	BCL	C9-C8-C10	-3.91	97.33	111.27
3	G	101	BCL	C3C-C4C-CHD	-3.88	115.21	123.39
3	K	103	BCL	CHD-C1D-ND	-3.88	119.34	124.80
3	O	103	BCL	C7-C6-C5	-3.86	102.97	113.26
3	E	103	BCL	O2A-CGA-O1A	-3.83	114.06	123.63
3	H	101	BCL	C2B-C1B-NB	-3.82	106.36	110.33
3	N	101	BCL	C2B-C1B-NB	-3.82	106.37	110.33
3	M	101	BCL	CHC-C4B-NB	-3.81	118.33	124.05
3	L	101	BCL	C2B-C1B-NB	-3.81	106.38	110.33
3	F	101	BCL	C2B-C1B-NB	-3.80	106.39	110.33
3	C	101	BCL	CAA-CBA-CGA	-3.80	102.42	113.21
3	M	101	BCL	C6-C5-C3	3.80	122.72	113.47
3	K	103	BCL	OB B-CAB-CBB	-3.79	111.28	119.77
3	J	101	BCL	C2B-C1B-NB	-3.79	106.40	110.33
3	G	101	BCL	C20-C18-C19	-3.76	93.73	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	101	BCL	C2B-C1B-NB	-3.75	106.43	110.33
3	D	101	BCL	C2B-C1B-NB	-3.75	106.44	110.33
3	P	101	BCL	C2B-C1B-NB	-3.74	106.45	110.33
3	O	103	BCL	C9-C8-C7	-3.74	97.94	111.27
3	I	103	BCL	C6-C7-C8	3.73	128.37	115.97
3	R	101	BCL	C2B-C1B-NB	-3.73	106.46	110.33
3	A	101	BCL	CAA-CBA-CGA	-3.72	102.66	113.21
3	M	101	BCL	C2B-C1B-NB	3.71	114.17	110.33
3	Q	103	BCL	CBA-CAA-C2A	-3.70	102.78	113.79
3	E	103	BCL	C9-C8-C7	-3.69	98.13	111.27
3	E	103	BCL	OBB-CAB-CBB	-3.69	111.51	119.77
3	G	101	BCL	C3B-C4B-NB	3.67	114.60	109.76
3	M	101	BCL	C4D-C3D-CAD	-3.66	104.13	108.11
3	K	103	BCL	C20-C18-C19	-3.65	94.26	110.53
3	K	103	BCL	C9-C8-C10	-3.61	98.42	111.27
3	G	101	BCL	CMC-C2C-C1C	3.60	121.44	111.77
3	M	101	BCL	C5-C3-C2	3.58	129.21	121.17
3	E	103	BCL	CAA-CBA-CGA	-3.57	103.08	113.21
3	K	103	BCL	OBD-CAD-C3D	-3.56	120.09	128.42
3	K	103	BCL	CHC-C4B-NB	-3.54	118.74	124.05
3	C	101	BCL	C4D-CHA-C1A	-3.54	117.03	121.24
3	A	101	BCL	C11-C12-C13	3.53	127.69	115.97
3	I	103	BCL	C20-C18-C19	-3.50	94.92	110.53
3	O	103	BCL	OBB-CAB-C3B	-3.49	114.25	120.43
3	M	101	BCL	C1-O2A-CGA	3.49	125.11	116.65
3	M	101	BCL	C1C-NC-C4C	-3.49	105.09	106.68
3	K	103	BCL	C4-C3-C5	3.49	121.29	115.23
3	A	101	BCL	C9-C8-C7	-3.48	98.86	111.27
3	G	101	BCL	C1-O2A-CGA	3.44	124.97	116.65
3	G	101	BCL	C9-C8-C10	-3.42	99.09	111.27
3	Q	103	BCL	CHB-C1B-NB	-3.41	118.94	124.05
3	M	101	BCL	OBB-CAB-C3B	-3.39	114.44	120.43
3	K	103	BCL	OBB-CAB-C3B	-3.38	114.46	120.43
3	M	102	BCL	CHD-C1D-C2D	3.37	132.49	125.49
3	K	104	BCL	CHD-C1D-C2D	3.35	132.46	125.49
3	I	104	BCL	CHD-C1D-C2D	3.35	132.46	125.49
3	I	103	BCL	C11-C12-C13	3.35	127.10	115.97
3	G	101	BCL	C1C-NC-C4C	3.35	108.21	106.68
3	Q	104	BCL	CHD-C1D-C2D	3.34	132.44	125.49
3	E	104	BCL	CHD-C1D-C2D	3.34	132.43	125.49
3	C	102	BCL	CHD-C1D-C2D	3.33	132.42	125.49
3	G	102	BCL	CHD-C1D-C2D	3.33	132.42	125.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	104	BCL	CHD-C1D-C2D	3.33	132.41	125.49
3	C	101	BCL	C3C-C4C-CHD	-3.32	116.39	123.39
3	A	102	BCL	CHD-C1D-C2D	3.32	132.39	125.49
3	G	101	BCL	OBB-CAB-C3B	-3.31	114.57	120.43
3	Q	103	BCL	CHD-C1D-ND	-3.29	120.17	124.80
3	C	101	BCL	CBC-CAC-C3C	3.29	120.40	113.41
3	O	103	BCL	OBB-CAB-CBB	-3.28	112.42	119.77
3	M	101	BCL	CMC-C2C-C1C	3.28	120.58	111.77
3	C	101	BCL	C16-C17-C18	-3.27	101.33	115.94
3	K	103	BCL	C4D-C3D-CAD	-3.27	104.56	108.11
3	G	101	BCL	CBC-CAC-C3C	3.26	120.33	113.41
3	C	101	BCL	O2A-C1-C2	-3.26	95.57	108.11
3	M	101	BCL	C14-C13-C15	-3.24	99.72	111.27
3	E	103	BCL	CHB-C4A-NA	3.24	129.07	124.40
5	K	102	IRM	C27-C28-C29	3.22	127.97	112.02
5	I	102	IRM	C27-C28-C29	3.22	127.96	112.02
3	Q	103	BCL	C1-C2-C3	-3.22	120.92	126.20
3	C	101	BCL	C4D-C3D-CAD	-3.22	104.61	108.11
5	C	104	IRM	C27-C28-C29	3.22	127.94	112.02
5	O	102	IRM	C27-C28-C29	3.22	127.94	112.02
5	E	102	IRM	C27-C28-C29	3.22	127.93	112.02
5	A	104	IRM	C27-C28-C29	3.22	127.93	112.02
5	Q	102	IRM	C27-C28-C29	3.21	127.92	112.02
3	G	101	BCL	C6-C5-C3	3.21	121.30	113.47
3	Q	103	BCL	C1-O2A-CGA	3.21	124.43	116.65
5	M	104	IRM	C27-C28-C29	3.21	127.88	112.02
3	O	103	BCL	C3C-C4C-CHD	-3.20	116.64	123.39
5	G	104	IRM	C27-C28-C29	3.20	127.84	112.02
3	E	103	BCL	C20-C18-C19	-3.19	96.31	110.53
3	M	101	BCL	OBB-CAB-CBB	-3.19	112.64	119.77
3	A	101	BCL	C4D-CHA-C1A	-3.15	117.49	121.24
3	M	101	BCL	CAC-C3C-C4C	3.13	119.54	112.58
3	G	101	BCL	C14-C13-C15	-3.12	100.14	111.27
3	E	103	BCL	CBC-CAC-C3C	3.11	120.02	113.41
3	A	101	BCL	C4D-C3D-CAD	-3.11	104.73	108.11
3	C	101	BCL	CMB-C2B-C1B	3.10	130.15	125.42
3	A	101	BCL	CHD-C1D-ND	-3.08	120.46	124.80
3	O	103	BCL	CHA-C4D-ND	3.08	138.91	132.55
3	A	101	BCL	C20-C18-C19	-3.07	96.83	110.53
3	E	103	BCL	C1D-ND-C4D	3.05	108.45	106.31
3	E	103	BCL	C4D-C3D-CAD	-3.05	104.79	108.11
3	O	103	BCL	C3B-C4B-NB	3.04	113.77	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	101	BCL	CBA-CAA-C2A	-3.01	104.83	113.79
3	K	103	BCL	C16-C17-C18	-2.99	102.58	115.94
3	K	103	BCL	CMC-C2C-C1C	2.99	119.81	111.77
3	I	103	BCL	C11-C10-C8	2.99	125.89	115.97
3	Q	103	BCL	C1C-NC-C4C	2.98	108.04	106.68
3	O	103	BCL	C4-C3-C5	2.97	120.38	115.23
3	Q	103	BCL	C15-C13-C12	2.96	127.07	112.07
3	G	101	BCL	C4D-CHA-C1A	-2.96	117.72	121.24
3	O	103	BCL	CMB-C2B-C1B	2.95	129.91	125.42
3	O	103	BCL	C1C-NC-C4C	2.95	108.03	106.68
3	K	103	BCL	C7-C6-C5	-2.95	105.40	113.26
3	K	103	BCL	C4-C3-C2	-2.94	116.06	123.63
3	D	101	BCL	CHD-C1D-C2D	2.93	131.58	125.49
3	I	103	BCL	C3A-C2A-C1A	2.91	105.69	101.34
3	N	101	BCL	CHD-C1D-C2D	2.90	131.52	125.49
3	H	101	BCL	CHD-C1D-C2D	2.90	131.52	125.49
3	A	101	BCL	C11-C10-C8	2.90	125.59	115.97
3	F	101	BCL	CHD-C1D-C2D	2.89	131.51	125.49
3	L	101	BCL	CHD-C1D-C2D	2.89	131.50	125.49
3	Q	103	BCL	C11-C12-C13	2.88	125.55	115.97
3	R	101	BCL	CHD-C1D-C2D	2.88	131.48	125.49
3	O	103	BCL	C1D-CHD-C4C	-2.87	119.69	126.62
3	B	101	BCL	CHD-C1D-C2D	2.87	131.45	125.49
3	P	101	BCL	CHD-C1D-C2D	2.87	131.45	125.49
3	Q	103	BCL	C4D-C3D-CAD	-2.86	105.00	108.11
3	Q	103	BCL	C3A-C2A-C1A	2.85	105.61	101.34
3	G	101	BCL	O2A-CGA-O1A	-2.85	116.50	123.63
3	Q	103	BCL	C6-C7-C8	2.85	125.42	115.97
3	O	103	BCL	OBD-CAD-C3D	-2.84	121.77	128.42
3	J	101	BCL	CHD-C1D-C2D	2.84	131.40	125.49
3	I	103	BCL	CBC-CAC-C3C	2.84	119.44	113.41
3	Q	103	BCL	CMC-C2C-C1C	2.84	119.41	111.77
3	C	101	BCL	C11-C10-C8	2.84	125.40	115.97
3	E	103	BCL	CAC-C3C-C4C	2.84	118.89	112.58
3	G	101	BCL	CHD-C1D-C2D	2.83	131.37	125.49
3	I	103	BCL	C14-C13-C12	2.82	121.33	111.27
3	G	101	BCL	C2D-C1D-ND	2.82	112.92	110.13
3	M	101	BCL	C10-C8-C7	2.81	126.32	112.07
3	C	101	BCL	CBA-CAA-C2A	-2.81	105.44	113.79
3	I	103	BCL	C10-C8-C7	2.78	126.17	112.07
3	I	103	BCL	C1-O2A-CGA	2.77	123.36	116.65
3	K	103	BCL	C1D-CHD-C4C	-2.76	119.95	126.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	103	BCL	CAA-CBA-CGA	-2.76	105.38	113.21
3	I	103	BCL	C4-C3-C2	-2.74	116.60	123.63
3	M	101	BCL	C15-C13-C12	-2.73	98.22	112.07
3	K	103	BCL	CBA-CAA-C2A	-2.70	105.75	113.79
3	C	101	BCL	C20-C18-C19	-2.70	98.49	110.53
3	C	101	BCL	CHB-C4A-NA	2.69	128.28	124.40
3	O	103	BCL	C16-C17-C18	-2.69	103.93	115.94
3	C	101	BCL	CHA-C4D-ND	2.68	138.09	132.55
3	C	101	BCL	CHD-C1D-ND	-2.68	121.03	124.80
3	A	101	BCL	CHA-C4D-ND	2.67	138.06	132.55
3	A	101	BCL	C1D-CHD-C4C	-2.66	120.19	126.62
3	A	101	BCL	O2A-CGA-O1A	-2.66	116.96	123.63
3	O	103	BCL	C4-C3-C2	-2.66	116.80	123.63
3	M	101	BCL	C1-C2-C3	2.65	130.53	126.20
3	G	101	BCL	C4-C3-C5	2.64	119.80	115.23
3	K	103	BCL	CHB-C4A-NA	2.62	128.19	124.40
3	Q	103	BCL	CBC-CAC-C3C	2.62	118.96	113.41
3	K	103	BCL	CMA-C3A-C2A	-2.61	103.88	113.98
3	G	101	BCL	C11-C12-C13	2.61	124.65	115.97
3	E	103	BCL	C11-C12-C13	2.61	124.65	115.97
3	A	101	BCL	CHB-C1B-NB	-2.60	120.15	124.05
3	E	103	BCL	C4-C3-C2	-2.60	116.95	123.63
3	E	103	BCL	C4D-CHA-C1A	-2.60	118.14	121.24
3	K	103	BCL	C3A-C2A-C1A	2.59	105.21	101.34
3	A	101	BCL	CBA-CAA-C2A	-2.59	106.10	113.79
3	E	103	BCL	C3A-C2A-C1A	2.58	105.21	101.34
3	K	103	BCL	CBC-CAC-C3C	2.58	118.88	113.41
3	Q	103	BCL	C11-C10-C8	2.57	124.52	115.97
3	K	103	BCL	C9-C8-C7	-2.57	102.11	111.27
3	E	103	BCL	C6-C7-C8	2.56	124.48	115.97
3	O	103	BCL	C6-C7-C8	2.55	124.45	115.97
3	O	103	BCL	CAA-CBA-CGA	-2.54	105.98	113.21
3	O	103	BCL	C14-C13-C12	2.54	120.34	111.27
3	J	101	BCL	CAA-C2A-C1A	2.54	120.29	111.97
3	I	103	BCL	CAC-C3C-C4C	2.53	118.21	112.58
3	O	103	BCL	C3A-C2A-C1A	2.53	105.12	101.34
3	H	101	BCL	CAA-C2A-C1A	2.52	120.24	111.97
3	N	101	BCL	CAA-C2A-C1A	2.52	120.23	111.97
3	I	103	BCL	CMB-C2B-C1B	2.51	129.25	125.42
3	R	101	BCL	CAA-C2A-C1A	2.51	120.21	111.97
3	D	101	BCL	CAA-C2A-C1A	2.51	120.21	111.97
3	B	101	BCL	CAA-C2A-C1A	2.51	120.21	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	101	BCL	CAA-C2A-C1A	2.51	120.21	111.97
3	O	103	BCL	CBC-CAC-C3C	2.51	118.73	113.41
3	P	101	BCL	CAA-C2A-C1A	2.51	120.19	111.97
3	O	103	BCL	C9-C8-C10	-2.50	102.36	111.27
3	M	101	BCL	C3A-C2A-C1A	2.50	105.08	101.34
3	M	101	BCL	C11-C10-C8	2.50	124.27	115.97
3	F	101	BCL	CAA-C2A-C1A	2.50	120.16	111.97
3	C	101	BCL	C1-O2A-CGA	2.49	122.69	116.65
3	I	103	BCL	CHA-C4D-ND	2.49	137.69	132.55
3	M	101	BCL	C16-C17-C18	-2.49	104.83	115.94
3	G	101	BCL	C7-C6-C5	-2.49	106.64	113.26
3	E	103	BCL	CBA-CAA-C2A	-2.48	106.41	113.79
3	E	103	BCL	C5-C3-C2	2.48	126.73	121.17
3	D	101	BCL	CMB-C2B-C1B	-2.46	121.67	125.42
3	C	101	BCL	CAC-C3C-C4C	2.46	118.05	112.58
3	M	101	BCL	C4-C3-C5	2.46	119.50	115.23
3	H	101	BCL	CMB-C2B-C1B	-2.45	121.69	125.42
3	A	101	BCL	CHC-C1C-NC	2.44	127.92	124.40
3	L	101	BCL	CMB-C2B-C1B	-2.44	121.70	125.42
3	N	101	BCL	CMB-C2B-C1B	-2.44	121.70	125.42
3	M	101	BCL	C3B-C4B-NB	2.44	112.97	109.76
3	C	101	BCL	CHC-C1C-NC	2.44	127.91	124.40
3	C	101	BCL	O2A-CGA-O1A	-2.43	117.55	123.63
3	C	101	BCL	C10-C8-C7	2.43	124.39	112.07
3	B	101	BCL	CMB-C2B-C1B	-2.43	121.72	125.42
3	O	103	BCL	CAA-C2A-C3A	-2.43	106.44	113.00
3	A	101	BCL	C3A-C2A-C1A	2.43	104.98	101.34
3	I	103	BCL	CMC-C2C-C1C	2.43	118.30	111.77
3	C	101	BCL	C6-C7-C8	2.42	124.00	115.97
3	A	101	BCL	C7-C6-C5	-2.41	106.84	113.26
3	F	101	BCL	CMB-C2B-C1B	-2.40	121.77	125.42
3	J	101	BCL	CMB-C2B-C1B	-2.39	121.78	125.42
3	A	101	BCL	C10-C8-C7	2.39	124.17	112.07
3	R	101	BCL	CMB-C2B-C1B	-2.38	121.79	125.42
3	O	103	BCL	CHD-C1D-ND	-2.38	121.45	124.80
3	P	101	BCL	CMB-C2B-C1B	-2.38	121.80	125.42
3	I	103	BCL	C1C-NC-C4C	-2.37	105.60	106.68
3	Q	103	BCL	CHC-C1C-NC	2.36	127.80	124.40
5	G	104	IRM	C16-C17-C18	-2.35	123.98	127.28
5	C	104	IRM	C16-C17-C18	-2.35	123.99	127.28
3	I	103	BCL	OBB-CAB-CBB	-2.34	114.54	119.77
3	O	103	BCL	CHC-C1C-NC	2.33	127.76	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	102	IRM	C16-C17-C18	-2.32	124.03	127.28
5	E	102	IRM	C16-C17-C18	-2.31	124.03	127.28
5	Q	102	IRM	C16-C17-C18	-2.31	124.03	127.28
5	O	102	IRM	C16-C17-C18	-2.31	124.04	127.28
5	I	102	IRM	C16-C17-C18	-2.31	124.04	127.28
3	G	101	BCL	C16-C17-C18	-2.30	105.65	115.94
3	A	101	BCL	C16-C17-C18	-2.30	105.66	115.94
3	E	103	BCL	C7-C6-C5	-2.30	107.13	113.26
3	Q	103	BCL	C4D-CHA-C1A	-2.30	118.50	121.24
3	G	101	BCL	CBA-CAA-C2A	-2.30	106.95	113.79
3	O	103	BCL	C4D-CHA-C1A	-2.30	118.50	121.24
3	Q	103	BCL	C7-C6-C5	-2.30	107.14	113.26
3	M	101	BCL	C1D-ND-C4D	2.29	107.92	106.31
3	G	101	BCL	CMA-C3A-C2A	-2.29	105.14	113.98
3	Q	103	BCL	CHB-C4A-NA	2.28	127.70	124.40
3	G	101	BCL	C14-C13-C12	2.28	119.39	111.27
3	G	101	BCL	CHA-C4D-ND	2.27	137.23	132.55
5	A	104	IRM	C16-C17-C18	-2.27	124.10	127.28
3	D	101	BCL	CHA-C1A-NA	-2.26	121.27	126.39
3	E	103	BCL	C3B-C4B-NB	2.26	112.75	109.76
3	H	101	BCL	CHA-C1A-NA	-2.26	121.27	126.39
3	J	101	BCL	CHA-C1A-NA	-2.26	121.27	126.39
3	N	101	BCL	CHA-C1A-NA	-2.25	121.29	126.39
3	C	101	BCL	C12-C11-C10	-2.25	103.21	113.28
3	K	103	BCL	C11-C10-C8	2.25	123.43	115.97
3	B	101	BCL	CHA-C1A-NA	-2.24	121.31	126.39
3	E	103	BCL	CMC-C2C-C1C	2.24	117.80	111.77
3	I	103	BCL	CMA-C3A-C2A	-2.24	105.31	113.98
3	E	103	BCL	CMB-C2B-C1B	2.24	128.83	125.42
3	L	101	BCL	CHA-C1A-NA	-2.24	121.33	126.39
3	R	101	BCL	CHA-C1A-NA	-2.24	121.33	126.39
3	P	101	BCL	CHA-C1A-NA	-2.23	121.33	126.39
3	F	101	BCL	CHA-C1A-NA	-2.22	121.36	126.39
5	M	104	IRM	C16-C17-C18	-2.22	124.17	127.28
3	A	101	BCL	CAA-C2A-C3A	-2.22	107.01	113.00
3	M	101	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
3	I	103	BCL	CBA-CAA-C2A	-2.19	107.28	113.79
3	F	101	BCL	CHB-C1B-NB	2.19	127.33	124.05
3	A	101	BCL	C6-C7-C8	2.18	123.22	115.97
3	M	101	BCL	CAA-CBA-CGA	-2.17	107.04	113.21
3	K	103	BCL	C1-C2-C3	-2.17	122.64	126.20
3	J	101	BCL	CHB-C1B-NB	2.16	127.29	124.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	103	BCL	CHA-C4D-ND	2.14	136.96	132.55
3	R	101	BCL	CHB-C1B-NB	2.13	127.24	124.05
3	E	103	BCL	OB B-CAB-C3B	-2.12	116.68	120.43
3	L	101	BCL	CHB-C1B-NB	2.12	127.23	124.05
3	K	103	BCL	C10-C8-C7	2.12	122.80	112.07
3	P	101	BCL	CHB-C1B-NB	2.10	127.20	124.05
3	Q	104	BCL	C3B-C4B-NB	-2.09	107.00	109.76
3	A	101	BCL	CMA-C3A-C2A	-2.09	105.89	113.98
3	C	101	BCL	C3B-C4B-NB	2.09	112.52	109.76
3	O	103	BCL	C1-C2-C3	-2.09	122.78	126.20
3	G	101	BCL	CAA-CBA-CGA	-2.09	107.28	113.21
3	M	101	BCL	C14-C13-C12	2.09	118.71	111.27
3	N	101	BCL	CHB-C1B-NB	2.09	127.18	124.05
3	H	101	BCL	CHB-C1B-NB	2.08	127.17	124.05
3	I	104	BCL	CHB-C1B-NB	2.08	127.17	124.05
3	A	101	BCL	CMB-C2B-C1B	2.08	128.58	125.42
3	B	101	BCL	CHB-C1B-NB	2.08	127.16	124.05
3	D	101	BCL	CHB-C1B-NB	2.07	127.16	124.05
3	E	103	BCL	CHA-C4D-ND	2.07	136.82	132.55
3	K	103	BCL	CAA-CBA-CGA	-2.07	107.34	113.21
3	M	102	BCL	CHB-C1B-NB	2.07	127.15	124.05
3	G	102	BCL	C3B-C4B-NB	-2.07	107.03	109.76
3	O	104	BCL	CHB-C1B-NB	2.06	127.14	124.05
3	O	103	BCL	CMC-C2C-C1C	2.06	117.31	111.77
3	I	104	BCL	C3B-C4B-NB	-2.05	107.05	109.76
3	K	104	BCL	CHB-C1B-NB	2.04	127.12	124.05
3	O	104	BCL	C3B-C4B-NB	-2.04	107.06	109.76
3	M	102	BCL	C3B-C4B-NB	-2.04	107.06	109.76
3	I	103	BCL	CHC-C1C-NC	2.03	127.33	124.40
3	C	102	BCL	CHB-C1B-NB	2.03	127.10	124.05
3	G	101	BCL	C10-C8-C7	2.03	122.36	112.07
3	M	101	BCL	CHB-C1B-NB	-2.03	121.00	124.05
3	K	104	BCL	C3B-C4B-NB	-2.03	107.08	109.76
3	E	104	BCL	C3B-C4B-NB	-2.03	107.08	109.76
3	A	102	BCL	CHB-C1B-NB	2.03	127.09	124.05
3	A	101	BCL	CMC-C2C-C3C	-2.03	106.15	113.98
3	E	103	BCL	CMA-C3A-C2A	-2.02	106.16	113.98
3	E	103	BCL	CHD-C1D-C2D	2.02	129.69	125.49
3	Q	103	BCL	C3C-C4C-CHD	-2.02	119.13	123.39
3	G	102	BCL	CHB-C1B-NB	2.02	127.08	124.05
3	O	103	BCL	CMA-C3A-C2A	-2.02	106.18	113.98
3	C	102	BCL	C3B-C4B-NB	-2.02	107.10	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	103	BCL	C4-C3-C5	2.01	118.72	115.23
3	A	101	BCL	OBB-CAB-CBB	-2.01	115.26	119.77
3	Q	104	BCL	CHB-C1B-NB	2.01	127.06	124.05
3	G	101	BCL	CMB-C2B-C1B	2.00	128.47	125.42

There are no chirality outliers.

All (219) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	101	BCL	C4C-C3C-CAC-CBC
3	A	101	BCL	O1A-CGA-O2A-C1
3	O	103	BCL	O1A-CGA-O2A-C1
3	A	101	BCL	C5-C6-C7-C8
3	C	101	BCL	C5-C6-C7-C8
3	E	103	BCL	C5-C6-C7-C8
3	I	103	BCL	C5-C6-C7-C8
3	A	101	BCL	CBA-CGA-O2A-C1
3	C	101	BCL	O1A-CGA-O2A-C1
3	E	103	BCL	O1A-CGA-O2A-C1
3	G	101	BCL	O1A-CGA-O2A-C1
3	I	103	BCL	O1A-CGA-O2A-C1
3	K	103	BCL	O1A-CGA-O2A-C1
3	M	101	BCL	O1A-CGA-O2A-C1
3	Q	103	BCL	O1A-CGA-O2A-C1
3	Q	103	BCL	C5-C6-C7-C8
3	K	103	BCL	C3-C5-C6-C7
3	E	103	BCL	CBA-CGA-O2A-C1
3	G	101	BCL	CBA-CGA-O2A-C1
3	I	103	BCL	CBA-CGA-O2A-C1
3	K	103	BCL	CBA-CGA-O2A-C1
3	M	101	BCL	CBA-CGA-O2A-C1
3	O	103	BCL	CBA-CGA-O2A-C1
3	Q	103	BCL	CBA-CGA-O2A-C1
3	M	101	BCL	C4-C3-C5-C6
5	A	104	IRM	C38-C26-C27-C28
5	C	104	IRM	C38-C26-C27-C28
5	E	102	IRM	C38-C26-C27-C28
5	G	104	IRM	C38-C26-C27-C28
5	I	102	IRM	C38-C26-C27-C28
5	K	102	IRM	C38-C26-C27-C28
5	M	104	IRM	C38-C26-C27-C28
5	O	102	IRM	C38-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	Q	102	IRM	C38-C26-C27-C28
3	M	101	BCL	C2-C3-C5-C6
5	A	104	IRM	C25-C26-C27-C28
5	C	104	IRM	C25-C26-C27-C28
5	E	102	IRM	C25-C26-C27-C28
5	G	104	IRM	C25-C26-C27-C28
5	I	102	IRM	C25-C26-C27-C28
5	K	102	IRM	C25-C26-C27-C28
5	M	104	IRM	C25-C26-C27-C28
5	O	102	IRM	C25-C26-C27-C28
5	Q	102	IRM	C25-C26-C27-C28
3	O	103	BCL	C3-C5-C6-C7
3	C	101	BCL	CBA-CGA-O2A-C1
3	G	101	BCL	C3-C5-C6-C7
3	A	102	BCL	C3-C5-C6-C7
3	C	102	BCL	C3-C5-C6-C7
3	E	104	BCL	C3-C5-C6-C7
3	G	102	BCL	C3-C5-C6-C7
3	I	104	BCL	C3-C5-C6-C7
3	K	104	BCL	C3-C5-C6-C7
3	M	102	BCL	C3-C5-C6-C7
3	O	104	BCL	C3-C5-C6-C7
3	Q	104	BCL	C3-C5-C6-C7
3	C	101	BCL	C4-C3-C5-C6
3	E	103	BCL	C4-C3-C5-C6
3	O	103	BCL	C4-C3-C5-C6
3	Q	103	BCL	C4-C3-C5-C6
3	A	101	BCL	C2-C3-C5-C6
3	C	101	BCL	C2-C3-C5-C6
3	E	103	BCL	C2-C3-C5-C6
3	I	103	BCL	C2-C3-C5-C6
3	K	103	BCL	C2-C3-C5-C6
3	O	103	BCL	C2-C3-C5-C6
3	Q	103	BCL	C2-C3-C5-C6
3	A	101	BCL	C4-C3-C5-C6
3	I	103	BCL	C4-C3-C5-C6
3	K	103	BCL	C4-C3-C5-C6
3	A	102	BCL	C6-C7-C8-C9
3	C	102	BCL	C6-C7-C8-C9
3	E	104	BCL	C6-C7-C8-C9
3	G	102	BCL	C6-C7-C8-C9
3	I	104	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	104	BCL	C6-C7-C8-C9
3	M	102	BCL	C6-C7-C8-C9
3	O	104	BCL	C6-C7-C8-C9
3	Q	104	BCL	C6-C7-C8-C9
3	M	101	BCL	C10-C11-C12-C13
3	G	101	BCL	C5-C6-C7-C8
3	K	103	BCL	C10-C11-C12-C13
3	O	103	BCL	C10-C11-C12-C13
3	Q	103	BCL	C15-C16-C17-C18
3	C	101	BCL	C10-C11-C12-C13
3	I	103	BCL	C10-C11-C12-C13
3	G	101	BCL	C10-C11-C12-C13
3	E	103	BCL	C3-C5-C6-C7
3	B	101	BCL	C2A-CAA-CBA-CGA
3	D	101	BCL	C2A-CAA-CBA-CGA
3	F	101	BCL	C2A-CAA-CBA-CGA
3	H	101	BCL	C2A-CAA-CBA-CGA
3	J	101	BCL	C2A-CAA-CBA-CGA
3	L	101	BCL	C2A-CAA-CBA-CGA
3	N	101	BCL	C2A-CAA-CBA-CGA
3	P	101	BCL	C2A-CAA-CBA-CGA
3	R	101	BCL	C2A-CAA-CBA-CGA
3	G	101	BCL	C15-C16-C17-C18
3	I	103	BCL	C15-C16-C17-C18
3	A	101	BCL	C10-C11-C12-C13
3	E	103	BCL	C15-C16-C17-C18
3	E	103	BCL	C10-C11-C12-C13
5	A	104	IRM	C26-C27-C28-C29
5	C	104	IRM	C26-C27-C28-C29
5	E	102	IRM	C26-C27-C28-C29
5	G	104	IRM	C26-C27-C28-C29
5	I	102	IRM	C26-C27-C28-C29
5	K	102	IRM	C26-C27-C28-C29
5	M	104	IRM	C26-C27-C28-C29
5	O	102	IRM	C26-C27-C28-C29
5	Q	102	IRM	C26-C27-C28-C29
3	K	103	BCL	C11-C10-C8-C7
3	A	101	BCL	C15-C16-C17-C18
3	C	101	BCL	C15-C16-C17-C18
3	Q	103	BCL	C12-C13-C15-C16
3	Q	103	BCL	C10-C11-C12-C13
3	I	103	BCL	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	O	103	BCL	C15-C16-C17-C18
3	M	101	BCL	C15-C16-C17-C18
3	A	101	BCL	C6-C7-C8-C9
3	C	101	BCL	C6-C7-C8-C9
3	M	101	BCL	C6-C7-C8-C10
3	M	101	BCL	C11-C10-C8-C7
3	Q	103	BCL	C6-C7-C8-C10
3	C	101	BCL	C3A-C2A-CAA-CBA
3	E	103	BCL	C3A-C2A-CAA-CBA
3	I	103	BCL	C3-C5-C6-C7
3	C	101	BCL	C4C-C3C-CAC-CBC
3	E	103	BCL	C4C-C3C-CAC-CBC
3	G	101	BCL	C4C-C3C-CAC-CBC
3	I	103	BCL	C4C-C3C-CAC-CBC
3	O	103	BCL	C4C-C3C-CAC-CBC
3	K	103	BCL	C15-C16-C17-C18
3	M	101	BCL	C3-C5-C6-C7
3	A	101	BCL	C6-C7-C8-C10
3	C	101	BCL	C6-C7-C8-C10
3	I	103	BCL	C6-C7-C8-C10
3	K	103	BCL	C5-C6-C7-C8
3	E	103	BCL	C6-C7-C8-C9
3	Q	103	BCL	C11-C10-C8-C9
6	B	102	LMT	C1-C2-C3-C4
6	J	102	LMT	C1-C2-C3-C4
6	P	102	LMT	C1-C2-C3-C4
6	N	102	LMT	C1-C2-C3-C4
6	R	102	LMT	C1-C2-C3-C4
6	D	102	LMT	C1-C2-C3-C4
6	F	102	LMT	C1-C2-C3-C4
6	L	102	LMT	C1-C2-C3-C4
6	H	102	LMT	C1-C2-C3-C4
6	F	102	LMT	C5'-C4'-O1B-C1B
6	J	102	LMT	C5'-C4'-O1B-C1B
6	L	102	LMT	C5'-C4'-O1B-C1B
6	N	102	LMT	C5'-C4'-O1B-C1B
6	B	102	LMT	C5'-C4'-O1B-C1B
6	D	102	LMT	C5'-C4'-O1B-C1B
6	F	102	LMT	C3'-C4'-O1B-C1B
6	P	102	LMT	C5'-C4'-O1B-C1B
6	R	102	LMT	C5'-C4'-O1B-C1B
6	N	102	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	R	102	LMT	C3'-C4'-O1B-C1B
6	H	102	LMT	C5'-C4'-O1B-C1B
3	Q	103	BCL	C6-C7-C8-C9
6	B	102	LMT	C3'-C4'-O1B-C1B
6	L	102	LMT	C3'-C4'-O1B-C1B
6	D	102	LMT	C3'-C4'-O1B-C1B
6	P	102	LMT	C3'-C4'-O1B-C1B
6	H	102	LMT	C3'-C4'-O1B-C1B
6	J	102	LMT	C3'-C4'-O1B-C1B
3	Q	103	BCL	C8-C10-C11-C12
3	G	101	BCL	C11-C10-C8-C7
3	K	103	BCL	C3A-C2A-CAA-CBA
3	Q	103	BCL	C14-C13-C15-C16
6	J	102	LMT	C5-C6-C7-C8
6	P	102	LMT	C5-C6-C7-C8
6	R	102	LMT	C5-C6-C7-C8
3	A	102	BCL	C2B-C3B-CAB-CBB
3	C	102	BCL	C2B-C3B-CAB-CBB
3	E	104	BCL	C2B-C3B-CAB-CBB
3	G	102	BCL	C2B-C3B-CAB-CBB
3	I	104	BCL	C2B-C3B-CAB-CBB
3	K	104	BCL	C2B-C3B-CAB-CBB
3	M	102	BCL	C2B-C3B-CAB-CBB
3	O	104	BCL	C2B-C3B-CAB-CBB
3	Q	104	BCL	C2B-C3B-CAB-CBB
6	D	102	LMT	C5-C6-C7-C8
6	L	102	LMT	C5-C6-C7-C8
6	B	102	LMT	C5-C6-C7-C8
6	F	102	LMT	C5-C6-C7-C8
6	H	102	LMT	C5-C6-C7-C8
6	N	102	LMT	C5-C6-C7-C8
3	C	101	BCL	C1A-C2A-CAA-CBA
3	A	101	BCL	C3-C5-C6-C7
3	C	101	BCL	C2A-CAA-CBA-CGA
3	Q	103	BCL	C4C-C3C-CAC-CBC
3	K	103	BCL	C11-C10-C8-C9
3	C	101	BCL	C3-C5-C6-C7
3	A	102	BCL	C2B-C3B-CAB-OBB
3	C	102	BCL	C2B-C3B-CAB-OBB
3	E	104	BCL	C2B-C3B-CAB-OBB
3	G	102	BCL	C2B-C3B-CAB-OBB
3	I	104	BCL	C2B-C3B-CAB-OBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	104	BCL	C2B-C3B-CAB-OBB
3	M	102	BCL	C2B-C3B-CAB-OBB
3	O	104	BCL	C2B-C3B-CAB-OBB
3	Q	104	BCL	C2B-C3B-CAB-OBB
3	A	102	BCL	C6-C7-C8-C10
3	E	103	BCL	C12-C13-C15-C16
3	E	104	BCL	C6-C7-C8-C10
3	I	104	BCL	C6-C7-C8-C10
3	K	104	BCL	C6-C7-C8-C10
3	M	102	BCL	C6-C7-C8-C10
3	K	103	BCL	C11-C12-C13-C14
3	E	103	BCL	C1A-C2A-CAA-CBA
3	C	102	BCL	C6-C7-C8-C10
3	G	102	BCL	C6-C7-C8-C10
3	O	104	BCL	C6-C7-C8-C10
3	Q	104	BCL	C6-C7-C8-C10
3	O	103	BCL	C5-C6-C7-C8
3	K	103	BCL	C6-C7-C8-C9

There are no ring outliers.

45 monomers are involved in 129 short contacts:

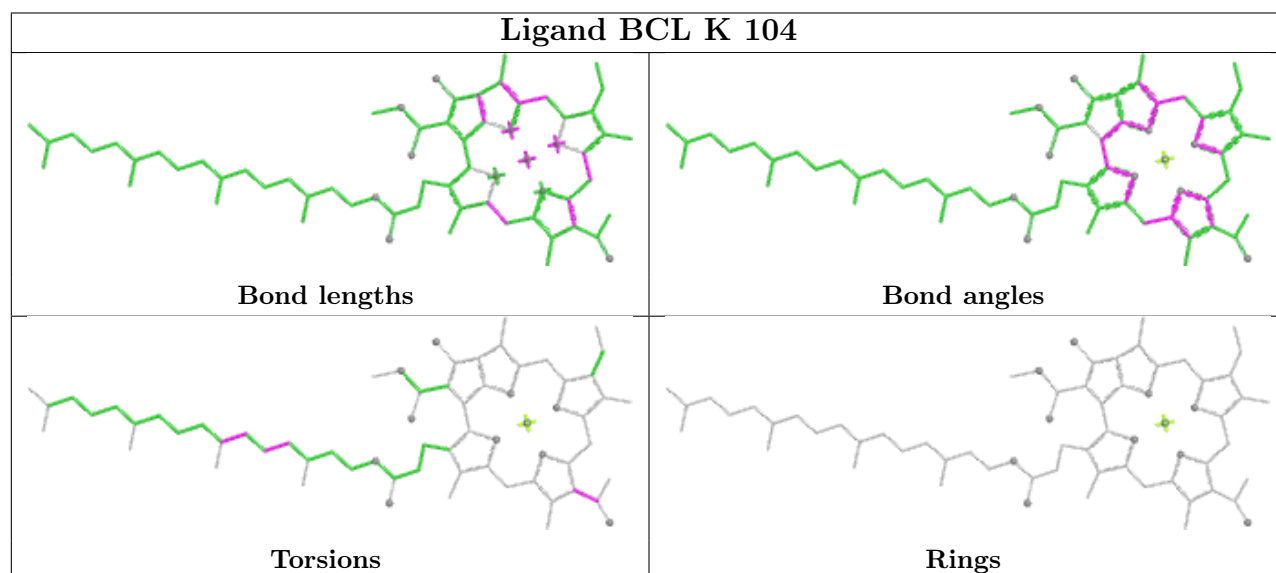
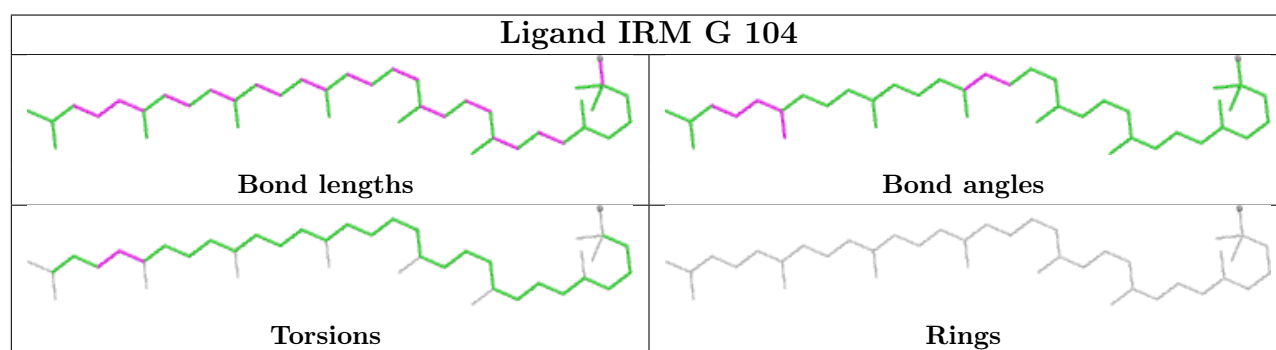
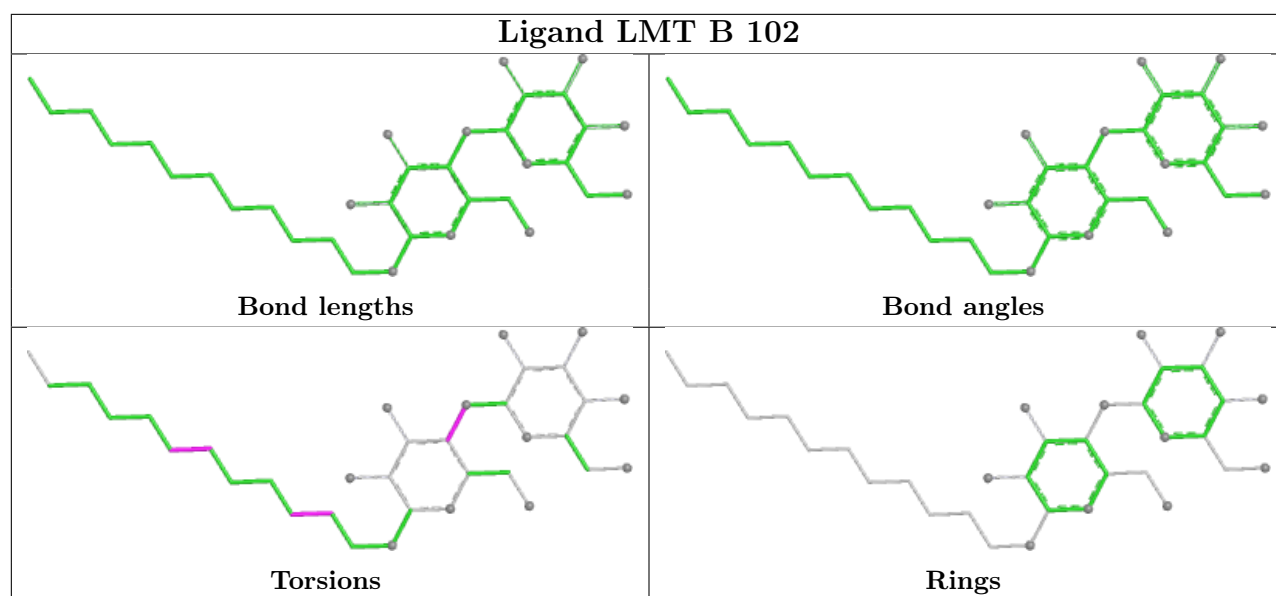
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	104	IRM	7	0
3	K	104	BCL	1	0
3	Q	103	BCL	9	0
3	G	101	BCL	7	0
4	K	101	LDA	1	0
3	B	101	BCL	4	0
5	A	104	IRM	7	0
3	N	101	BCL	4	0
3	I	104	BCL	1	0
3	O	103	BCL	5	0
3	L	101	BCL	4	0
3	Q	104	BCL	1	0
4	C	103	LDA	1	0
5	M	104	IRM	6	0
5	E	102	IRM	6	0
4	O	101	LDA	1	0
4	M	103	LDA	1	0
5	O	102	IRM	6	0
3	M	102	BCL	1	0

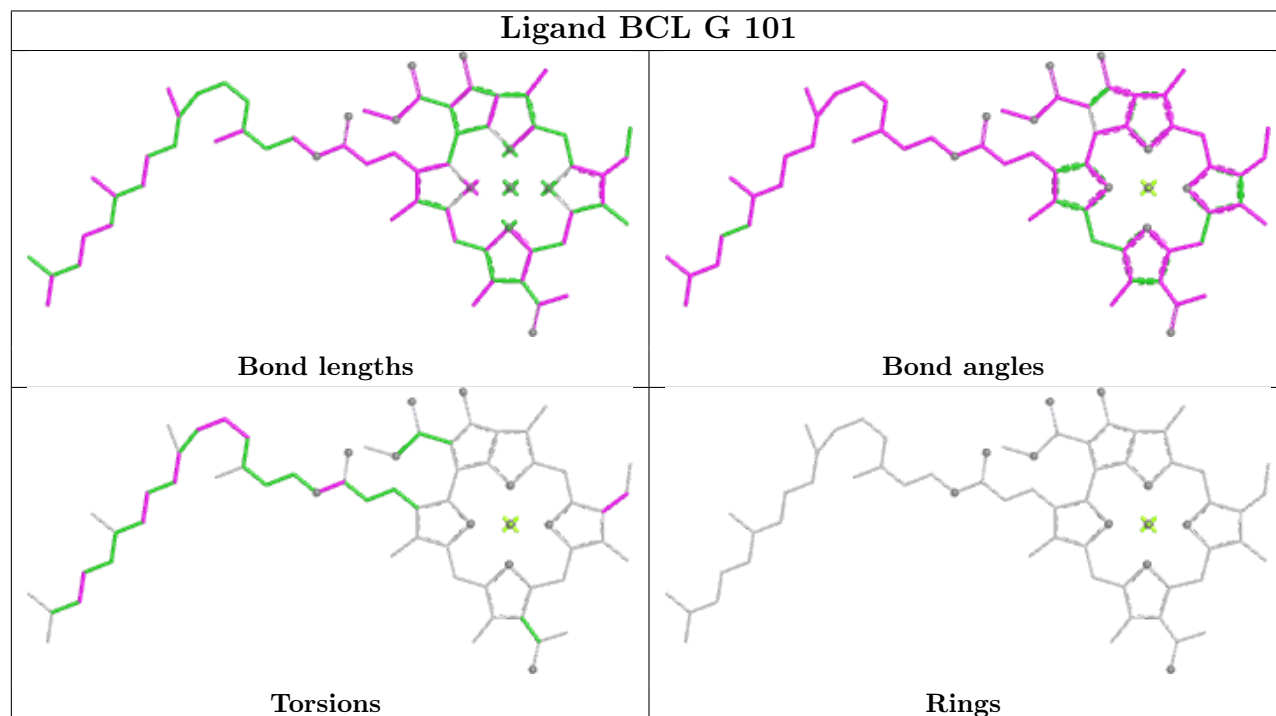
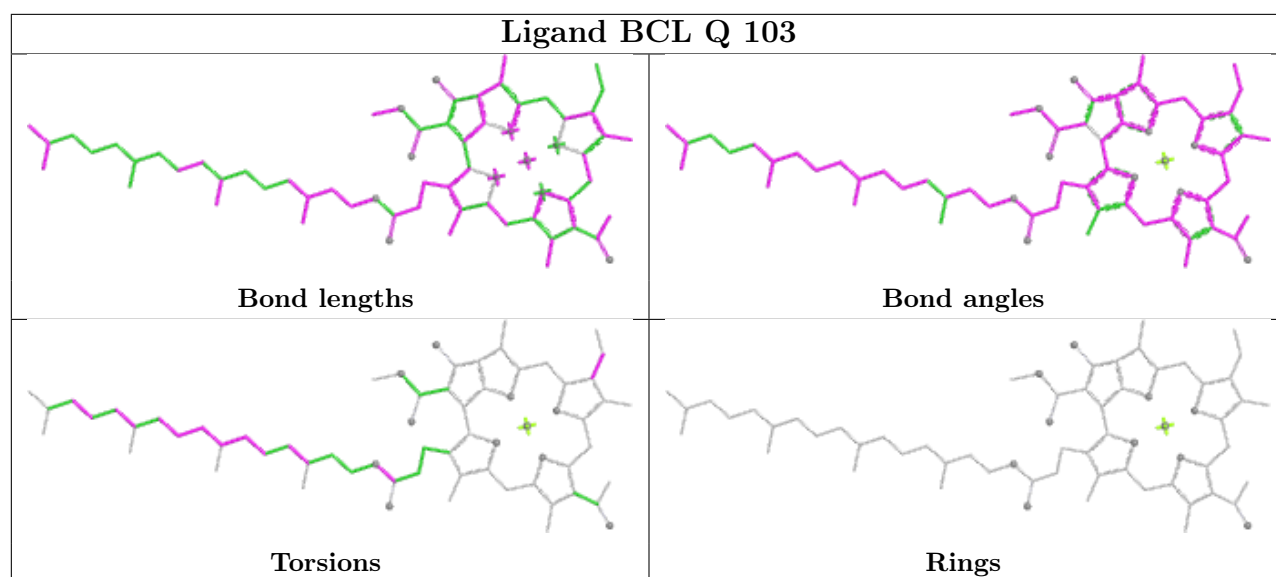
Continued on next page...

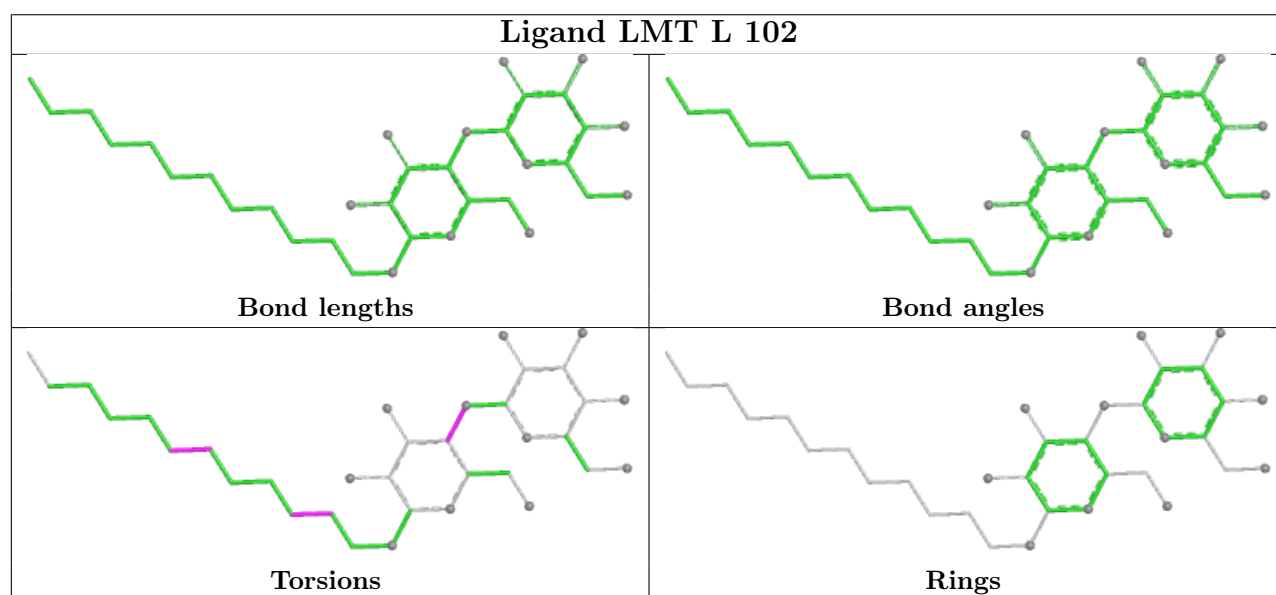
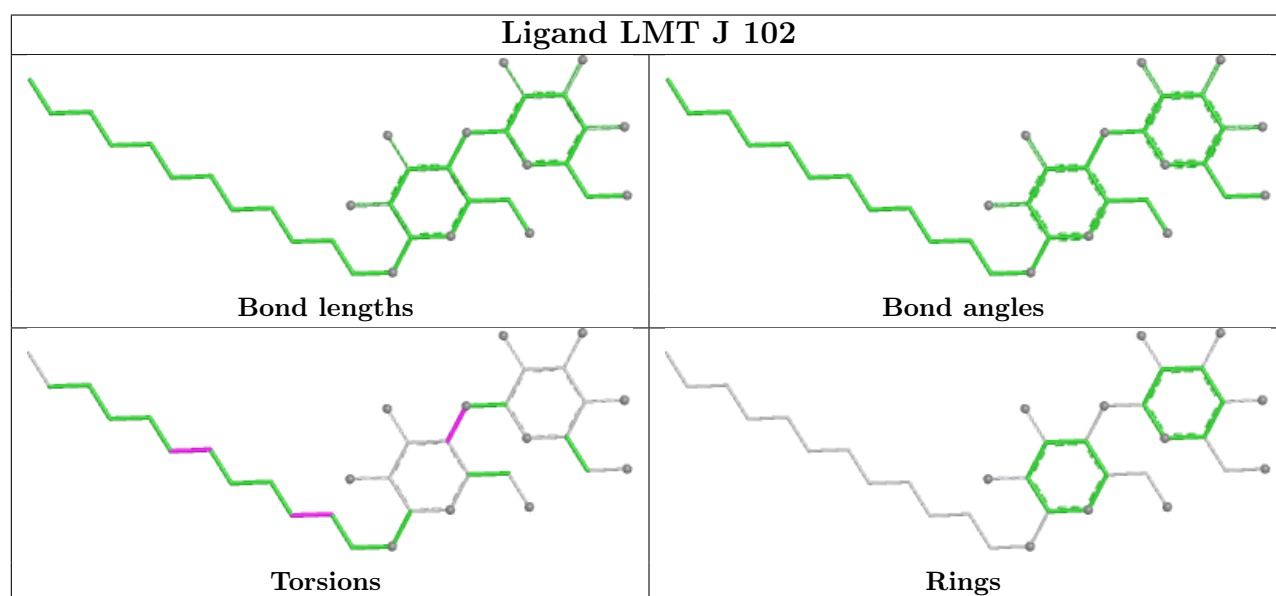
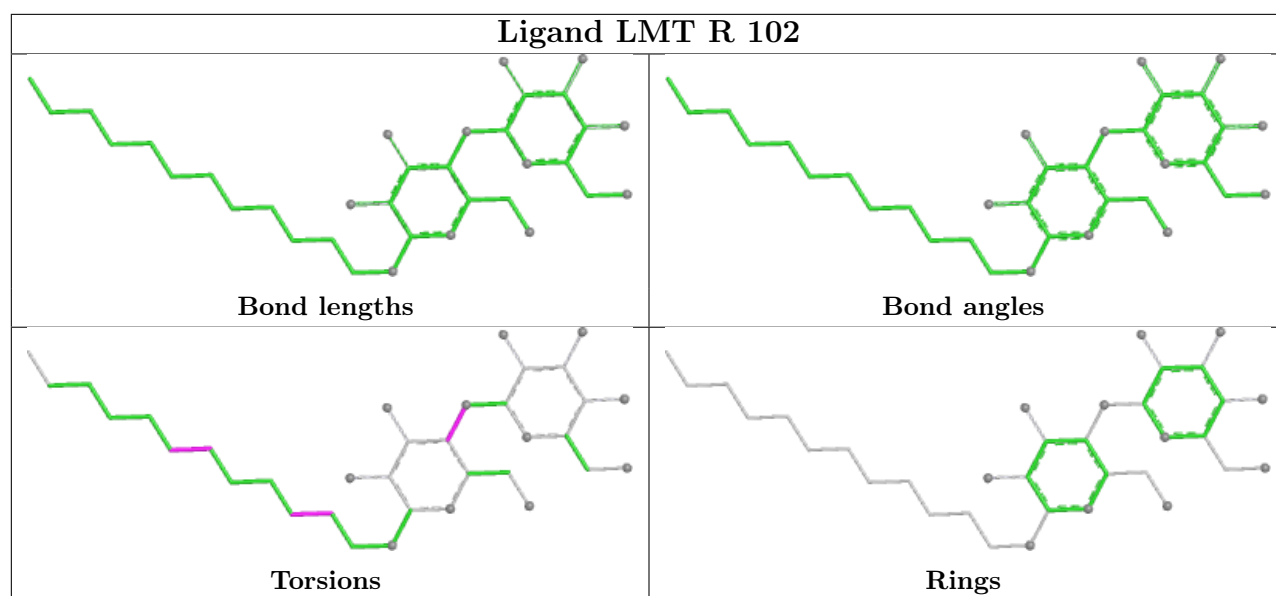
Continued from previous page...

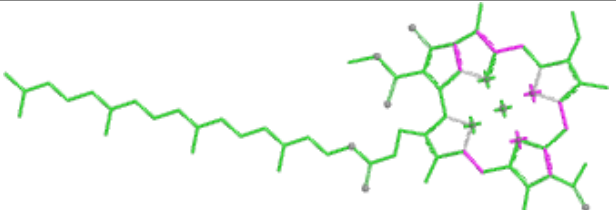
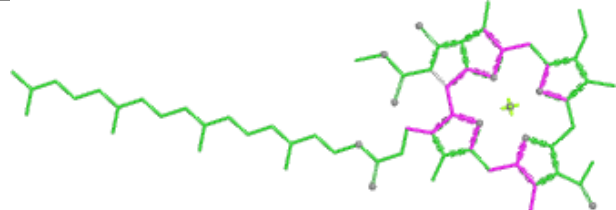
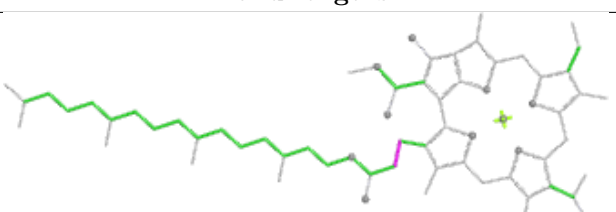
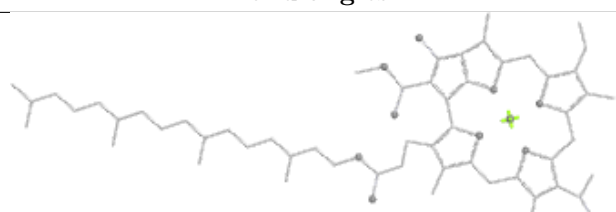
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	101	BCL	4	0
5	C	104	IRM	7	0
3	O	104	BCL	1	0
3	A	101	BCL	10	0
4	G	103	LDA	1	0
3	H	101	BCL	4	0
5	K	102	IRM	6	0
4	A	103	LDA	1	0
3	C	101	BCL	7	0
3	C	102	BCL	1	0
3	K	103	BCL	7	0
5	I	102	IRM	7	0
3	I	103	BCL	6	0
3	M	101	BCL	9	0
3	P	101	BCL	5	0
4	I	101	LDA	1	0
3	E	104	BCL	1	0
3	F	101	BCL	4	0
3	J	101	BCL	4	0
5	Q	102	IRM	6	0
3	G	102	BCL	1	0
4	Q	101	LDA	1	0
3	D	101	BCL	5	0
3	A	102	BCL	1	0
4	E	101	LDA	1	0
3	E	103	BCL	10	0

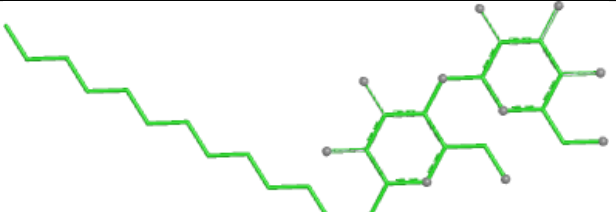
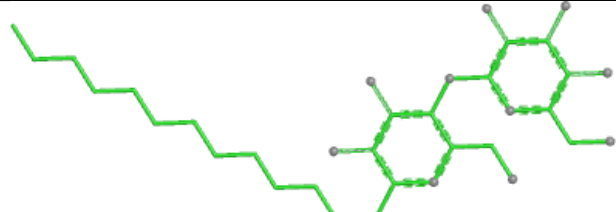
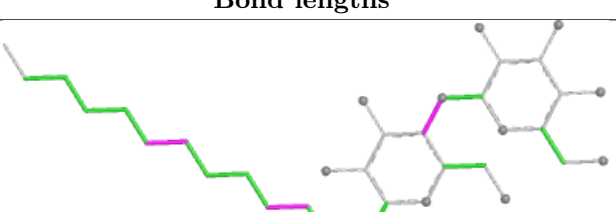
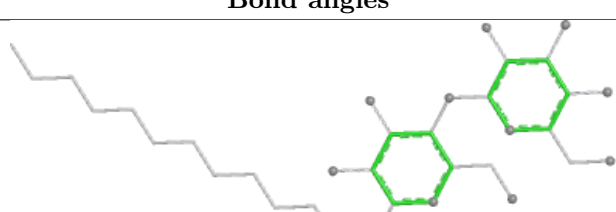
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

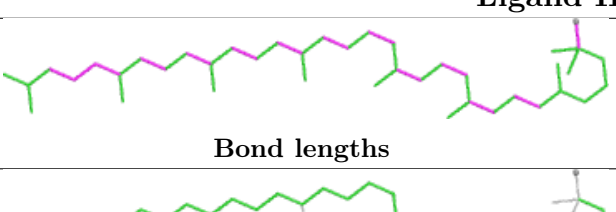
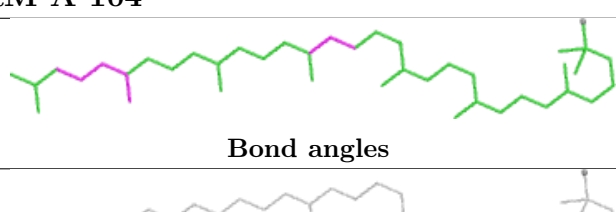




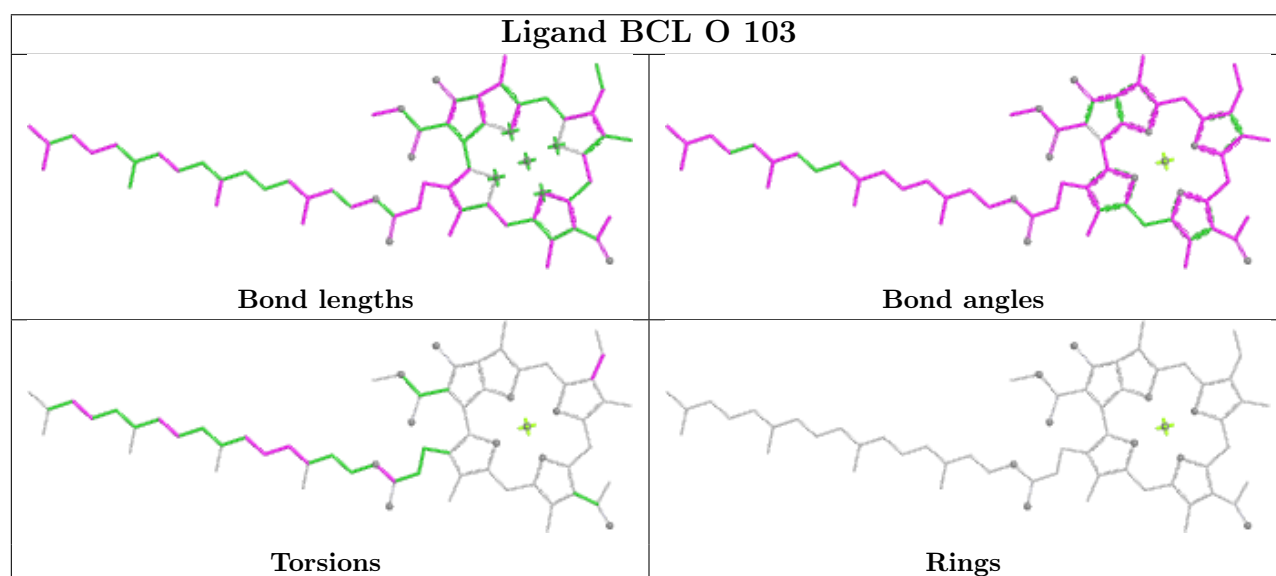
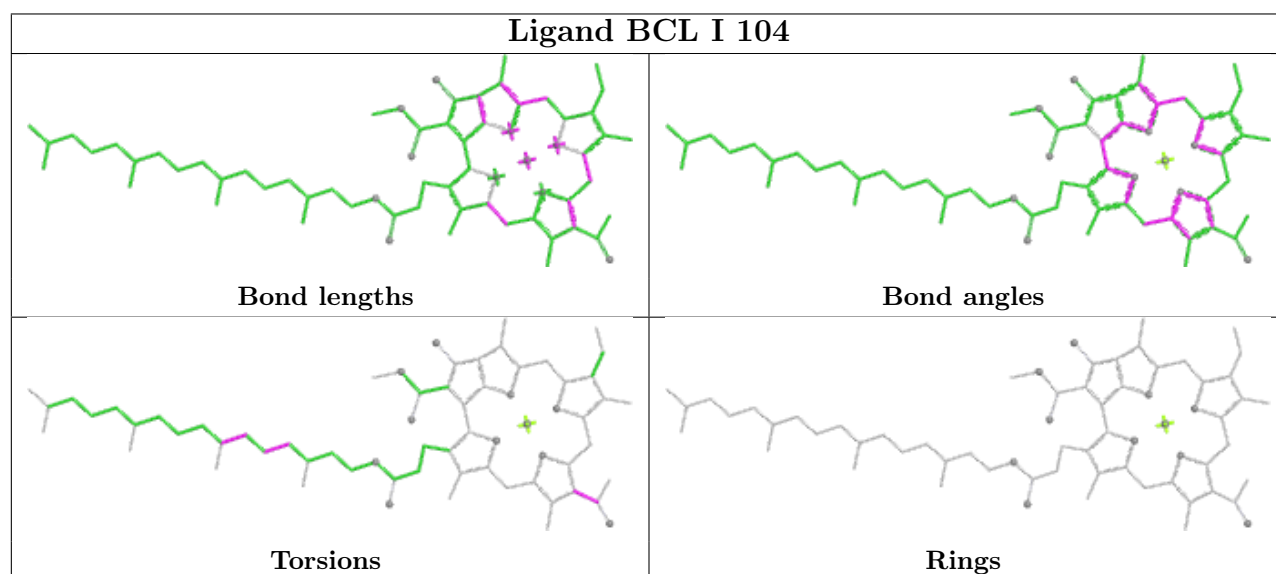
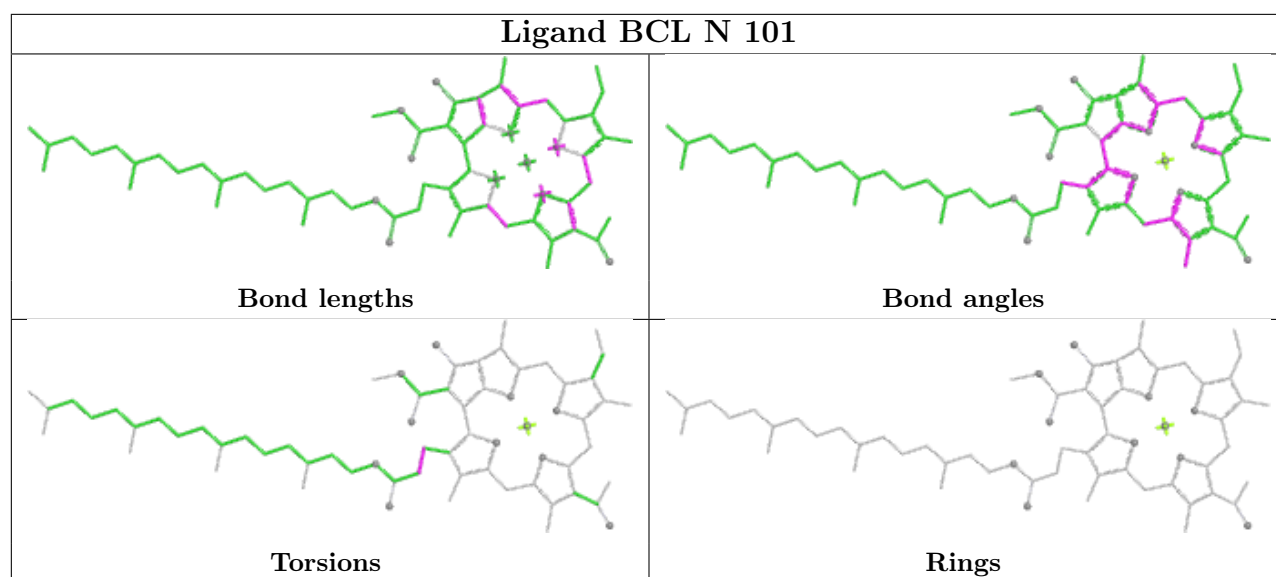


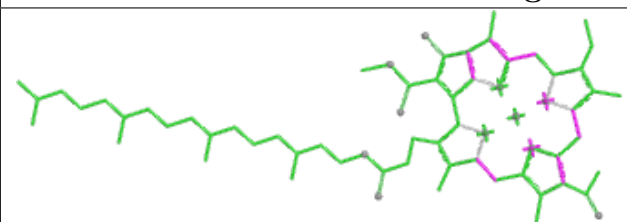
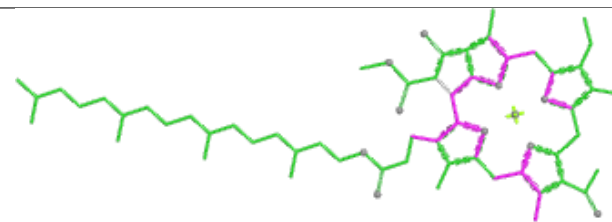
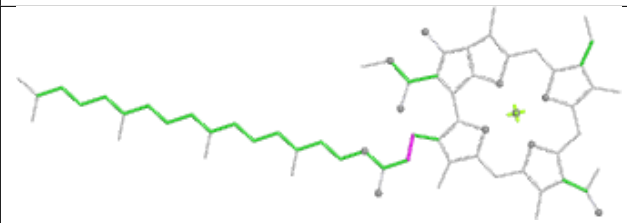
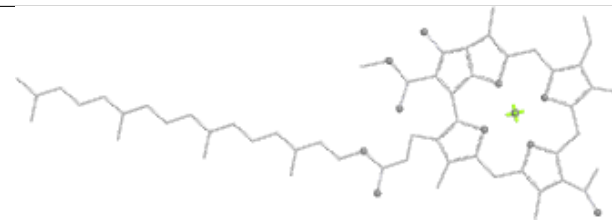


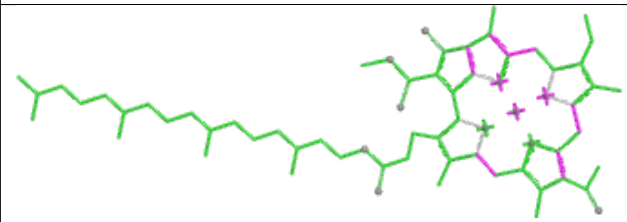
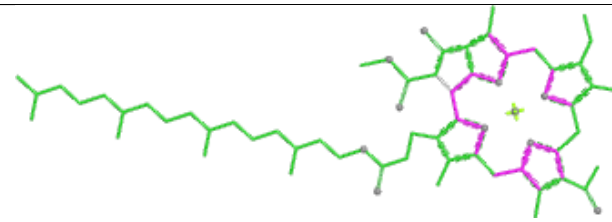
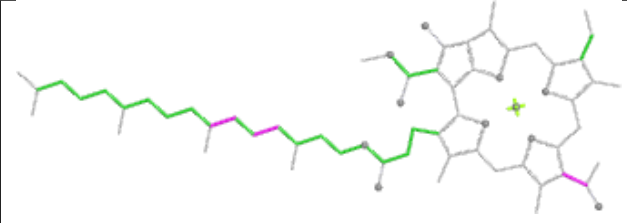
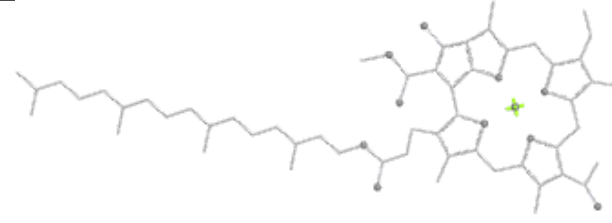
Ligand BCL B 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

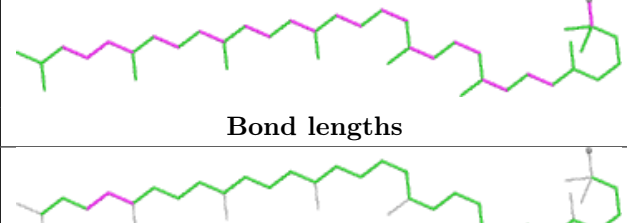
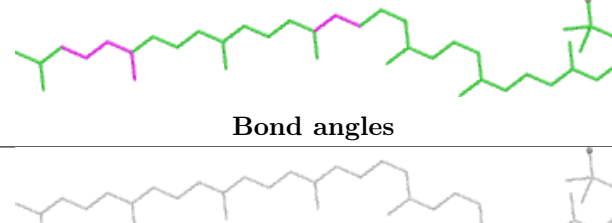


Ligand LMT N 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

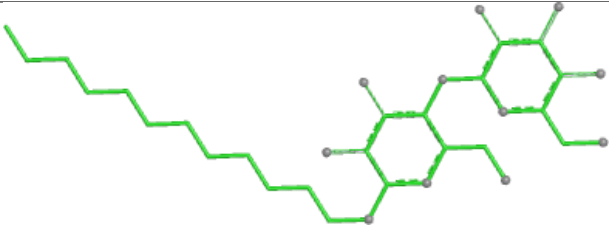
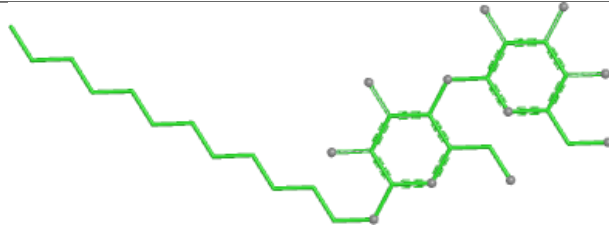
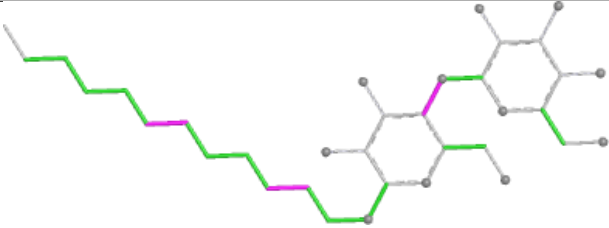
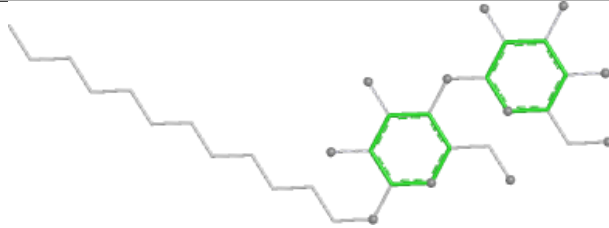
Ligand IRM A 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

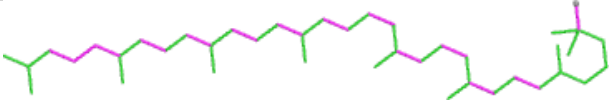
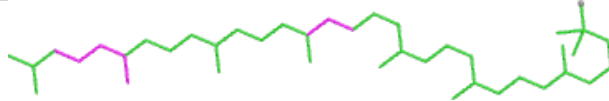
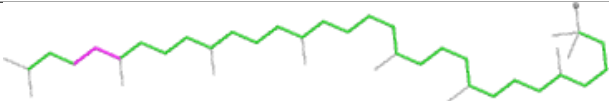
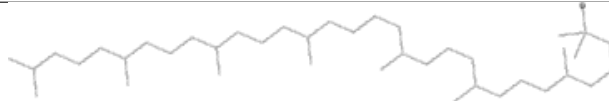


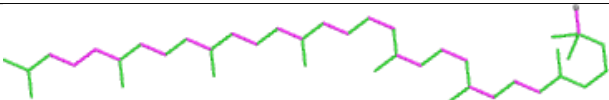
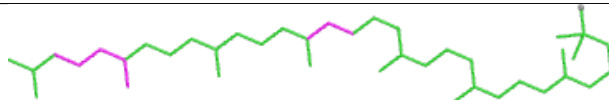
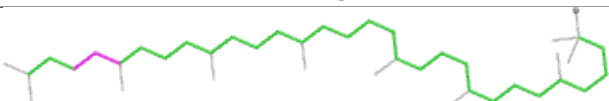

Ligand BCL L 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

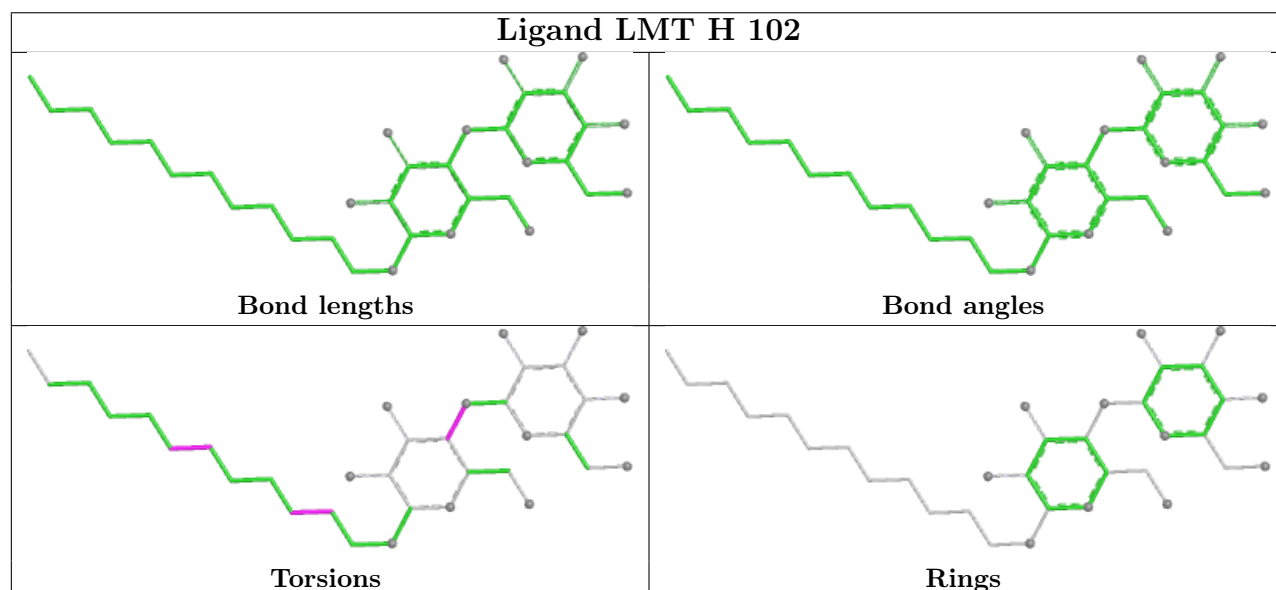
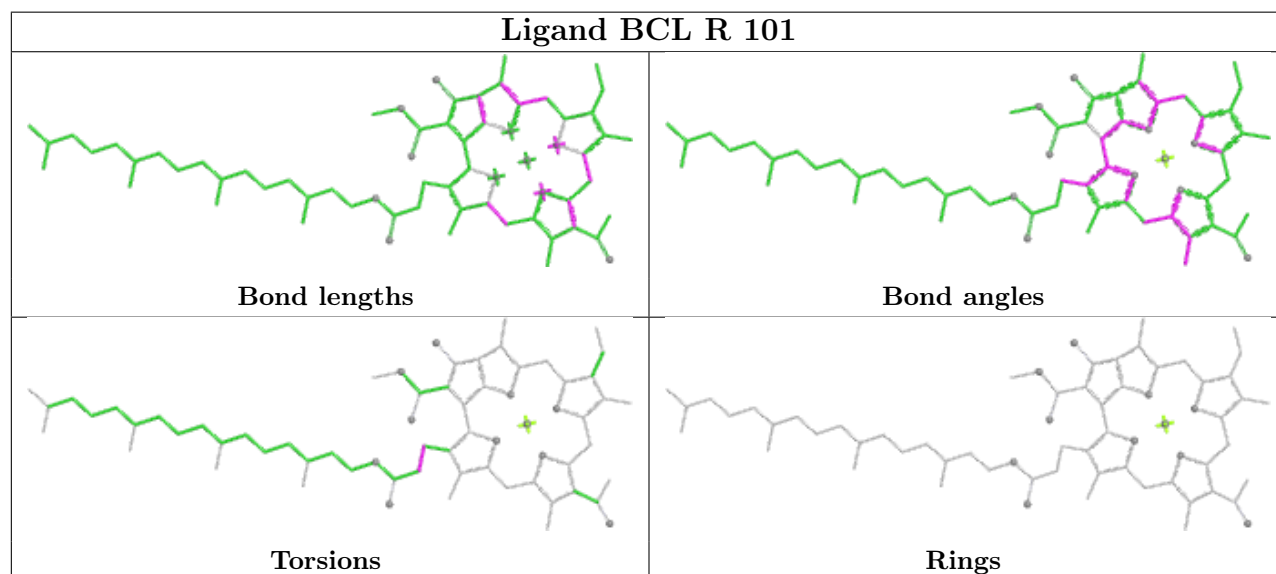
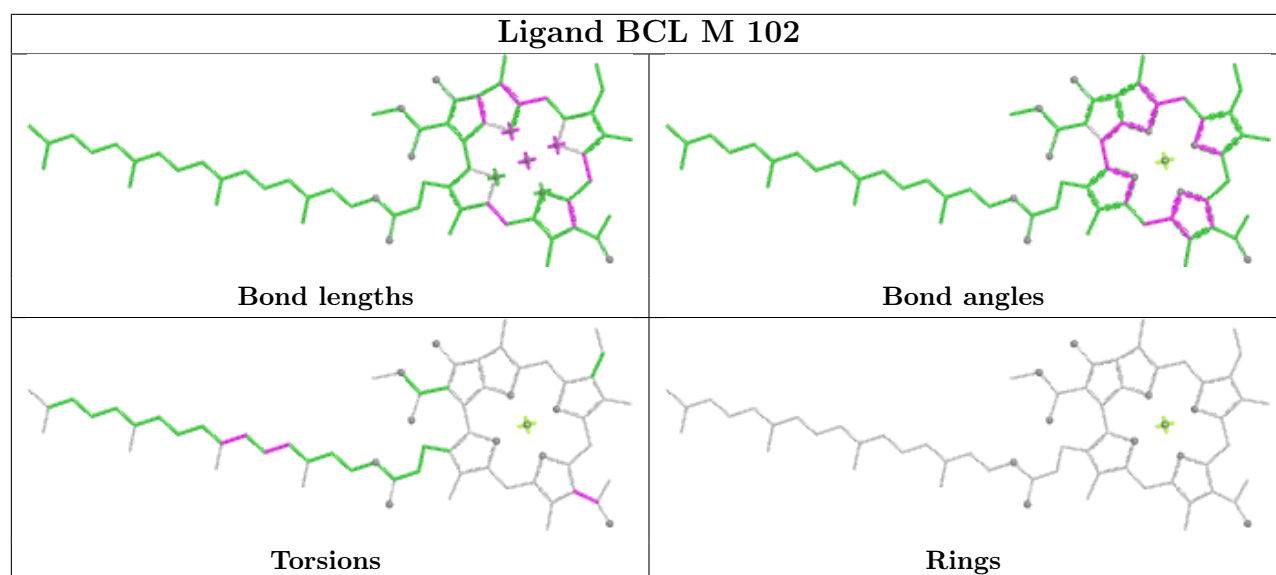
Ligand BCL Q 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

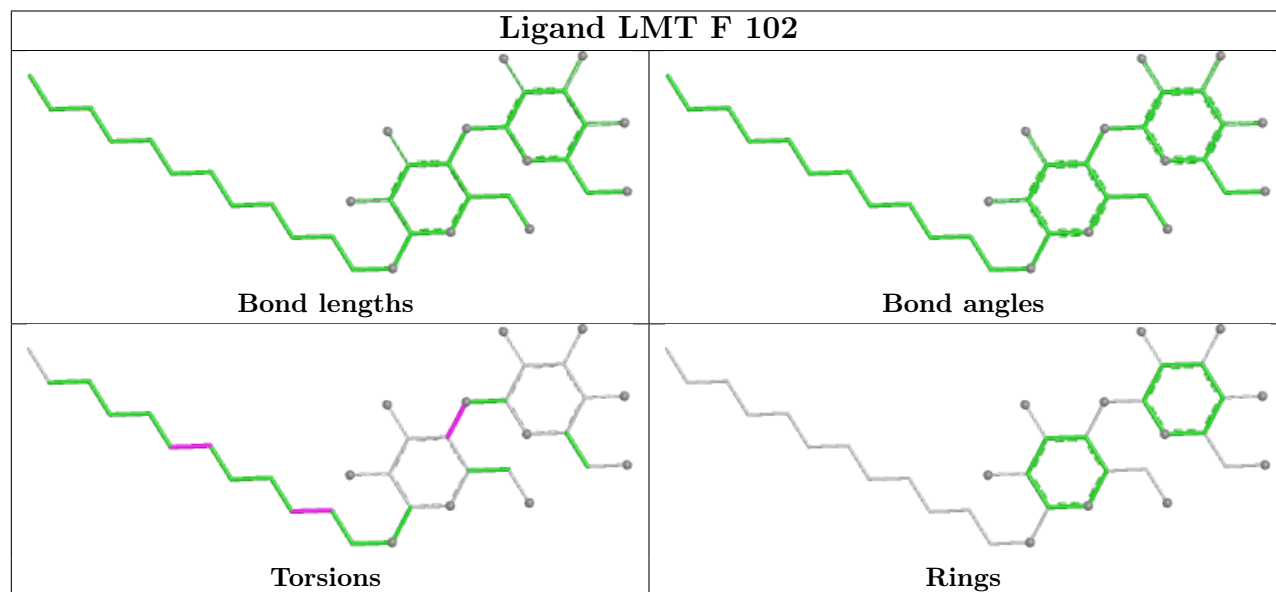
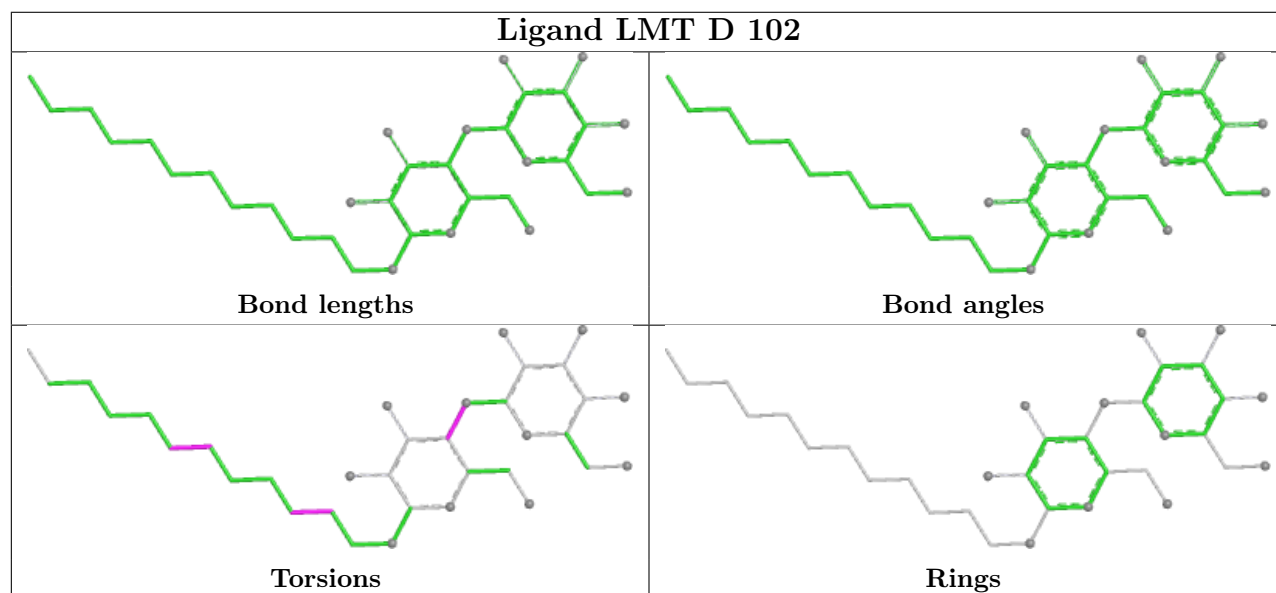
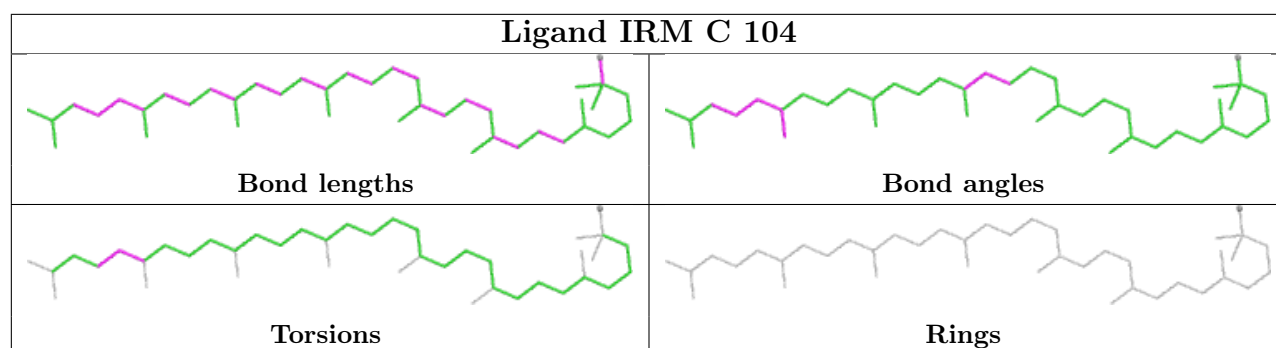
Ligand IRM M 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

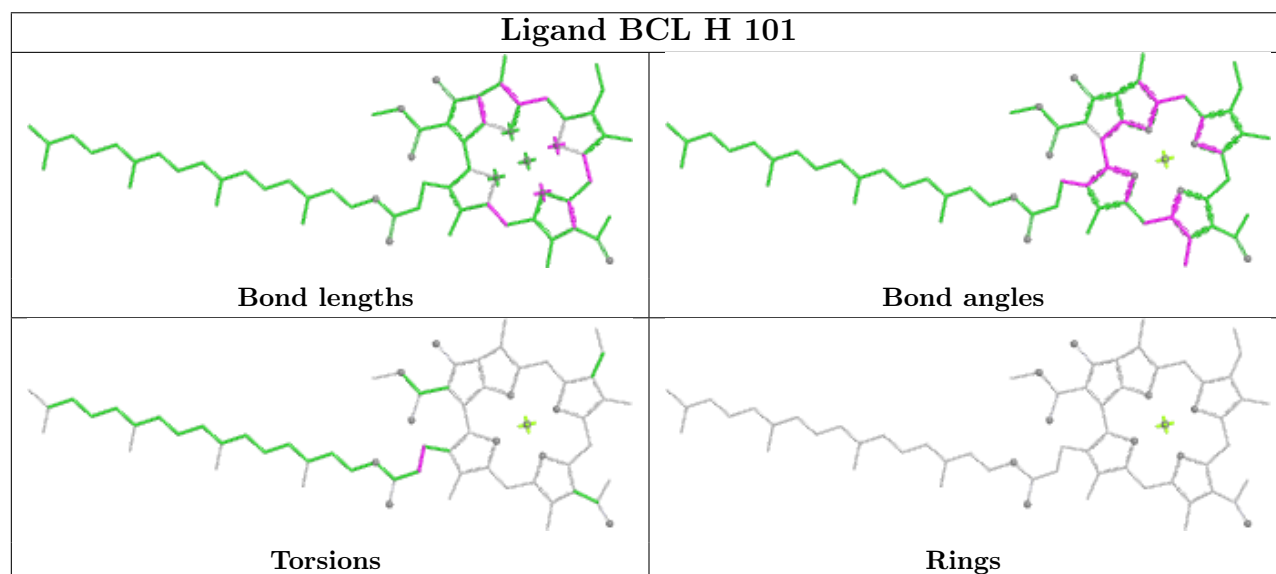
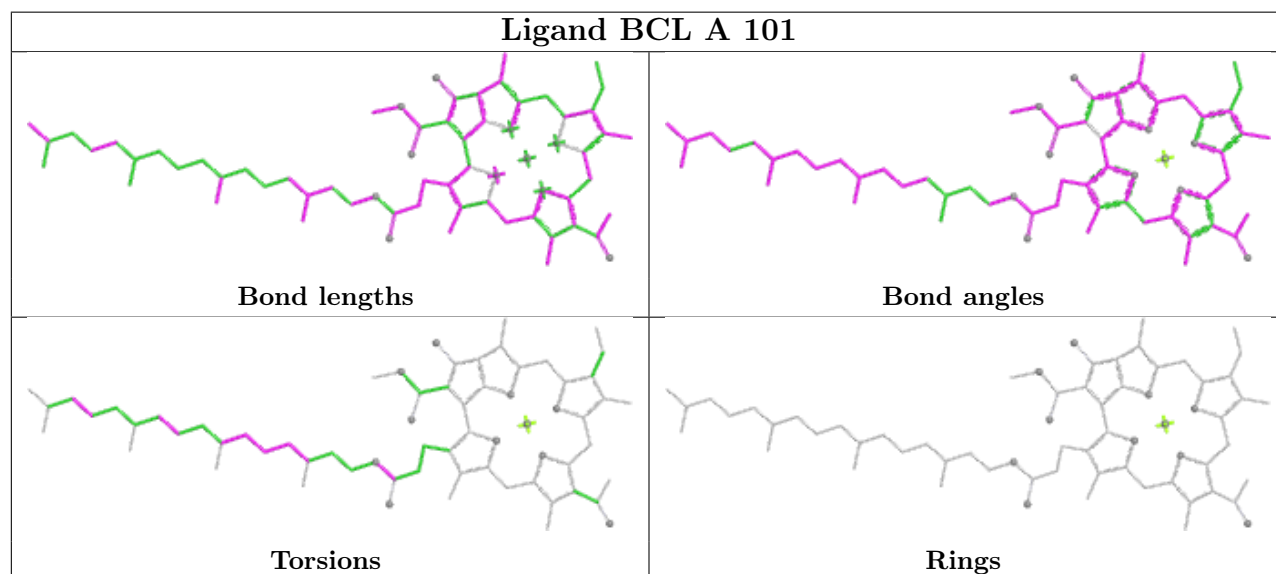
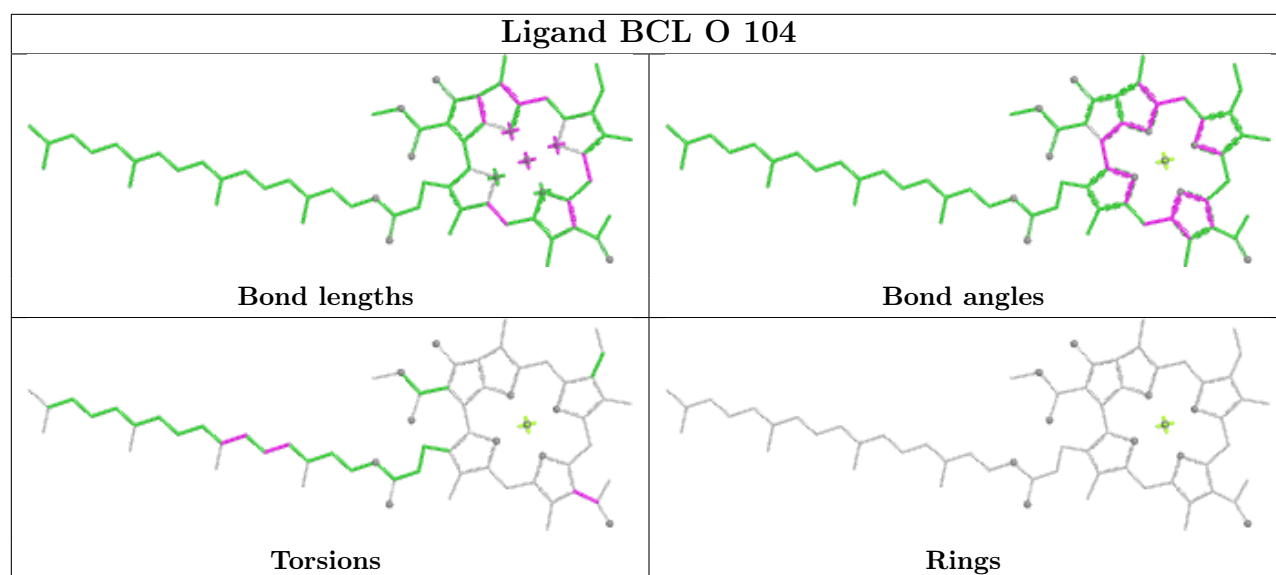
Ligand LMT P 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

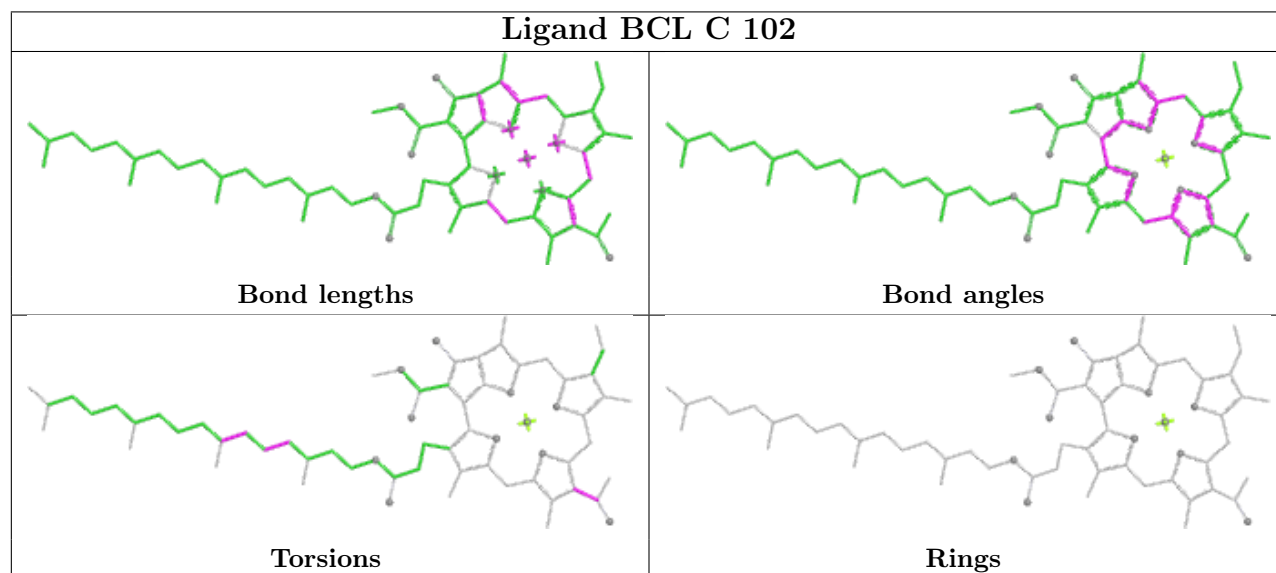
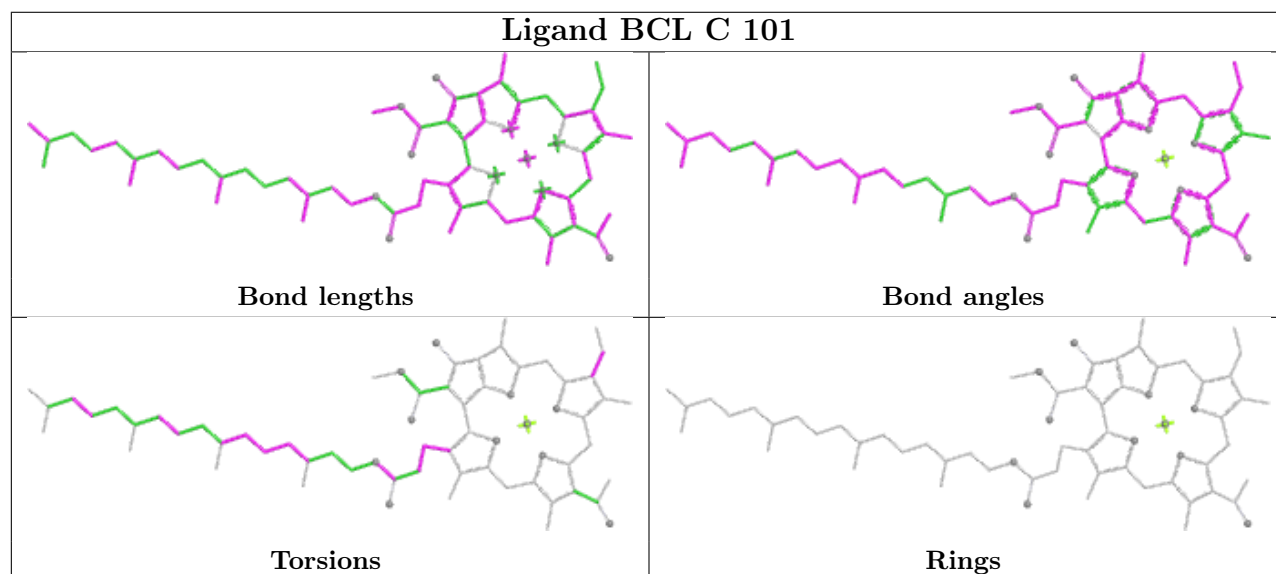
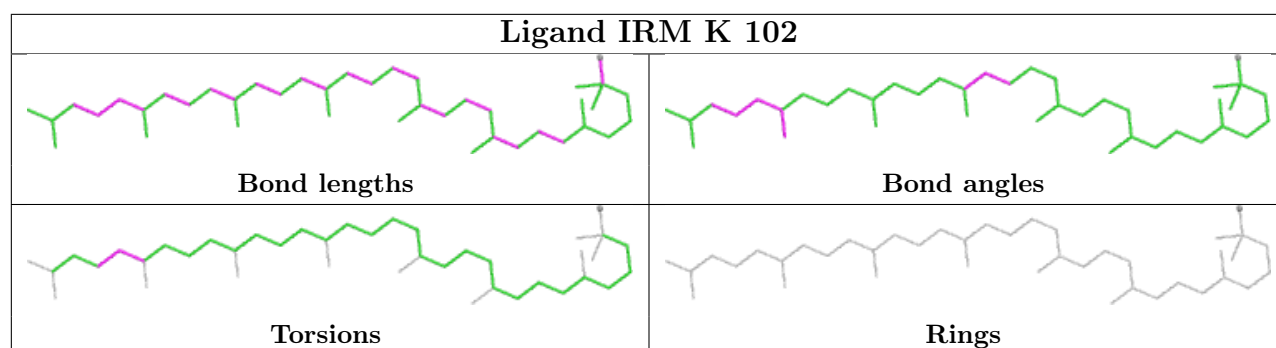
Ligand IRM E 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

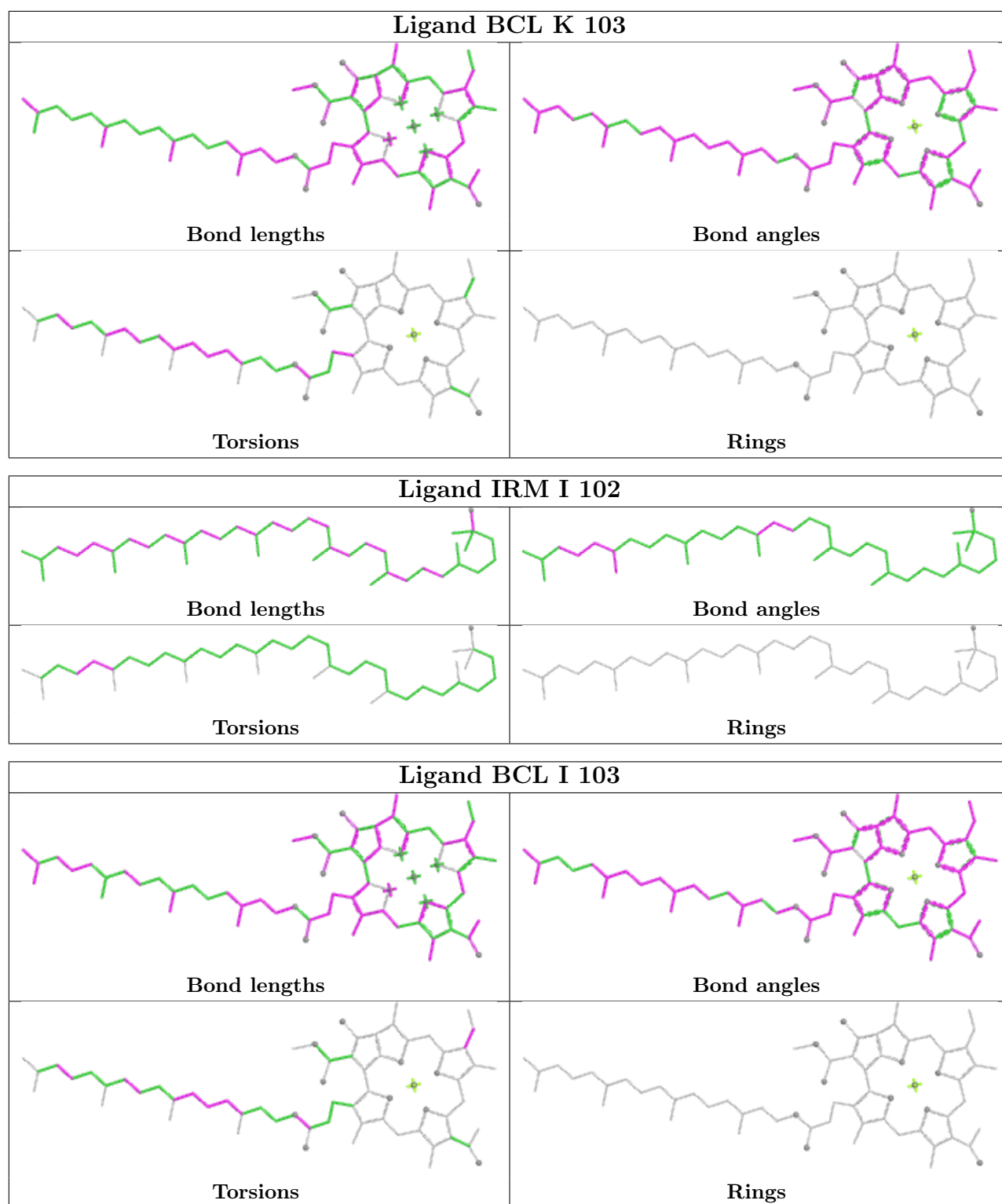
Ligand IRM O 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

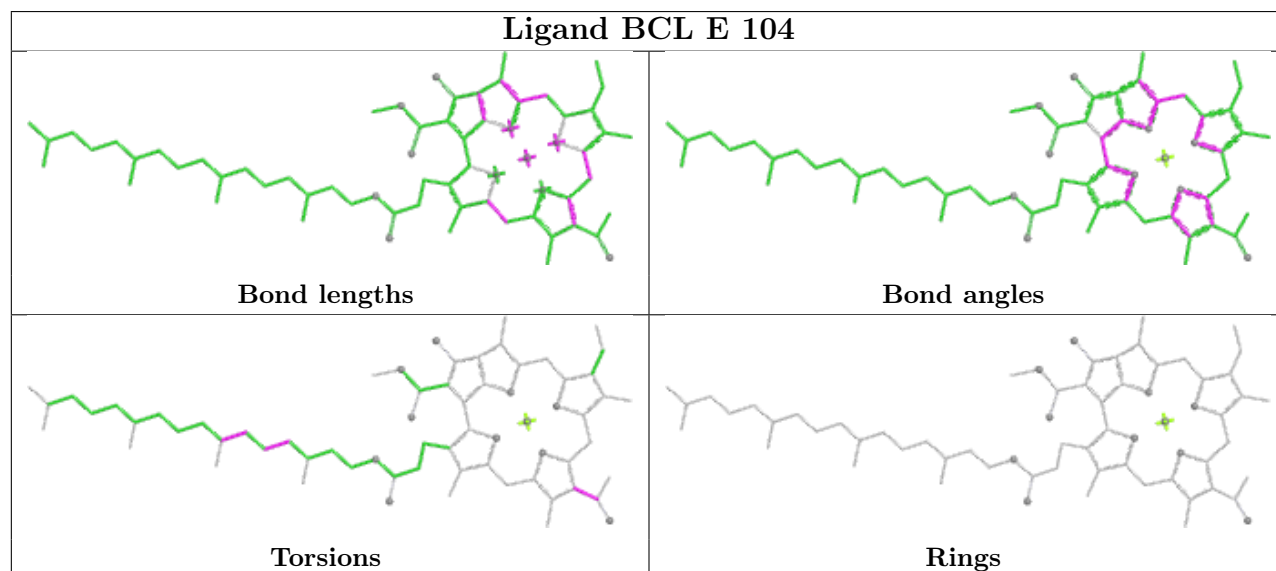
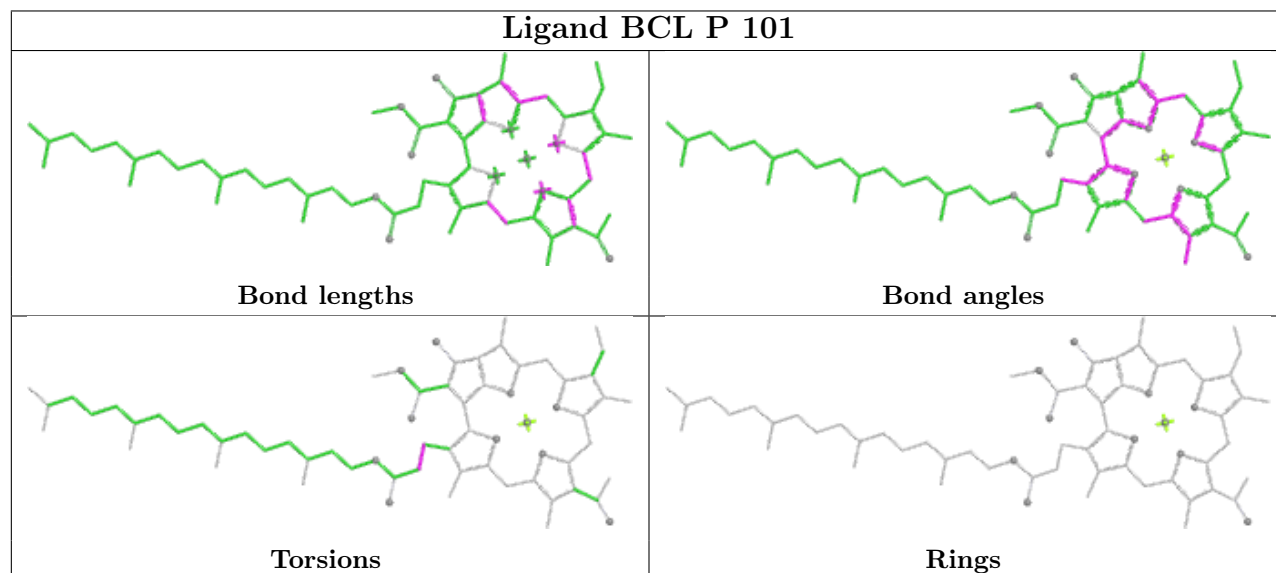
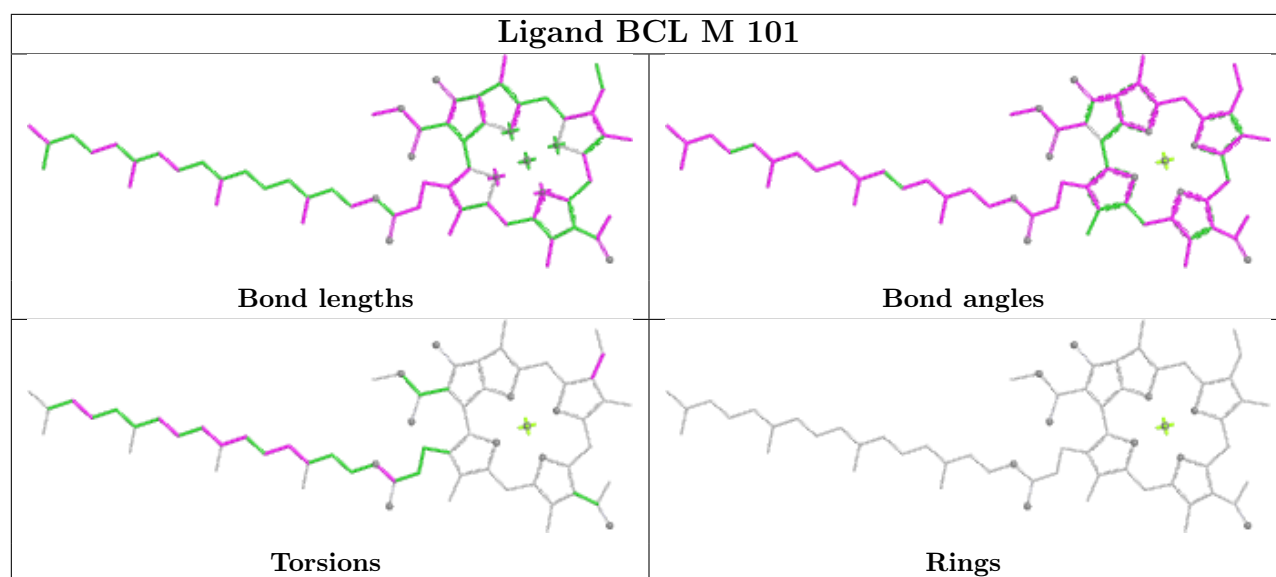


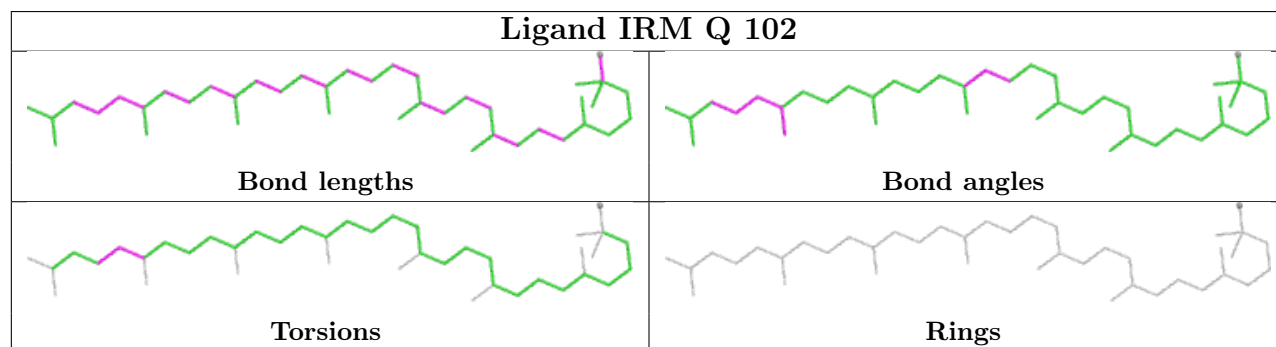
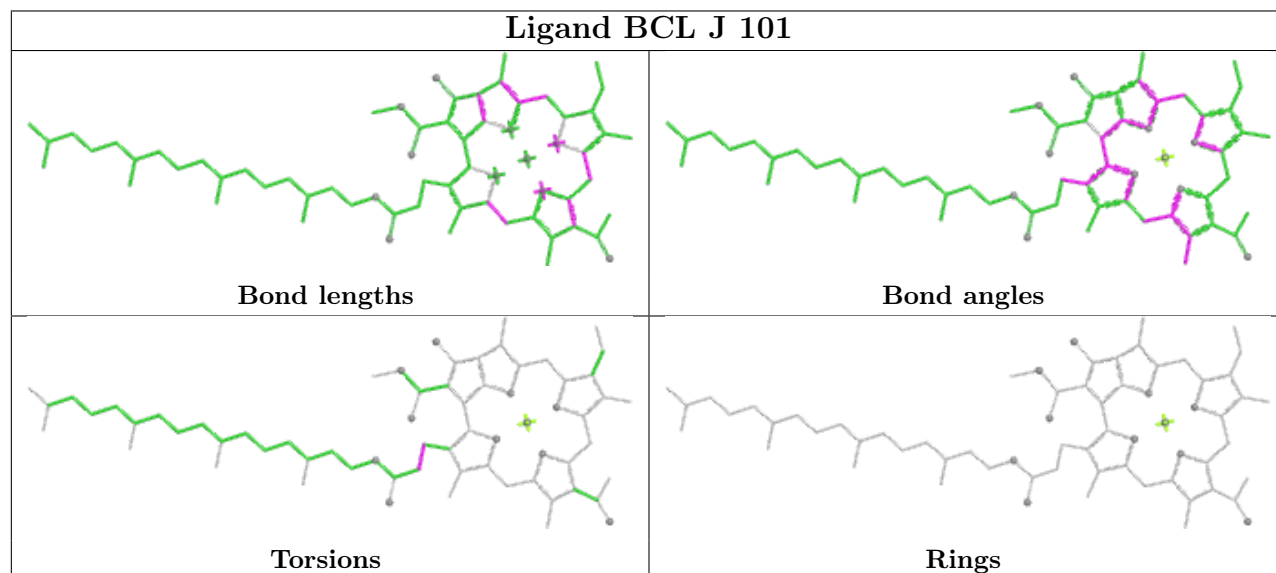
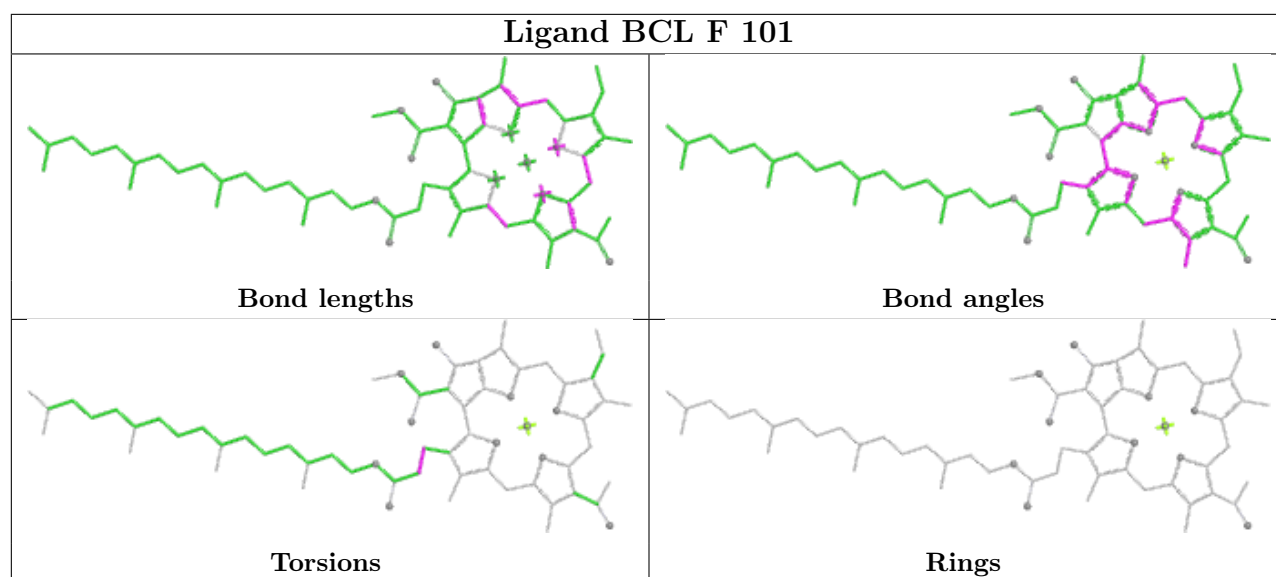


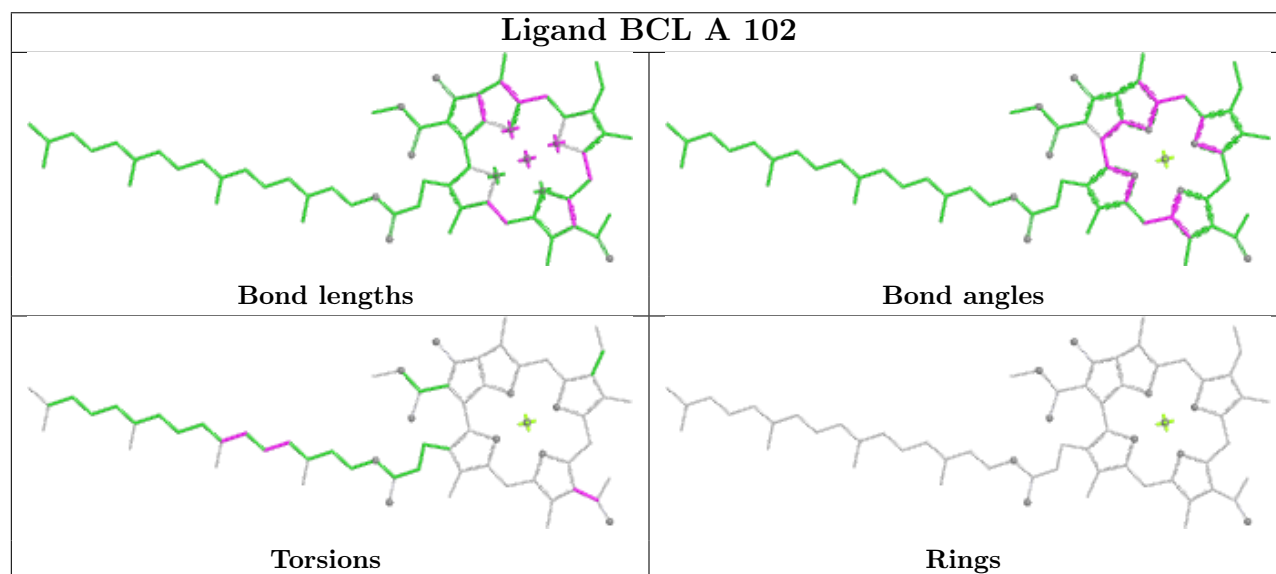
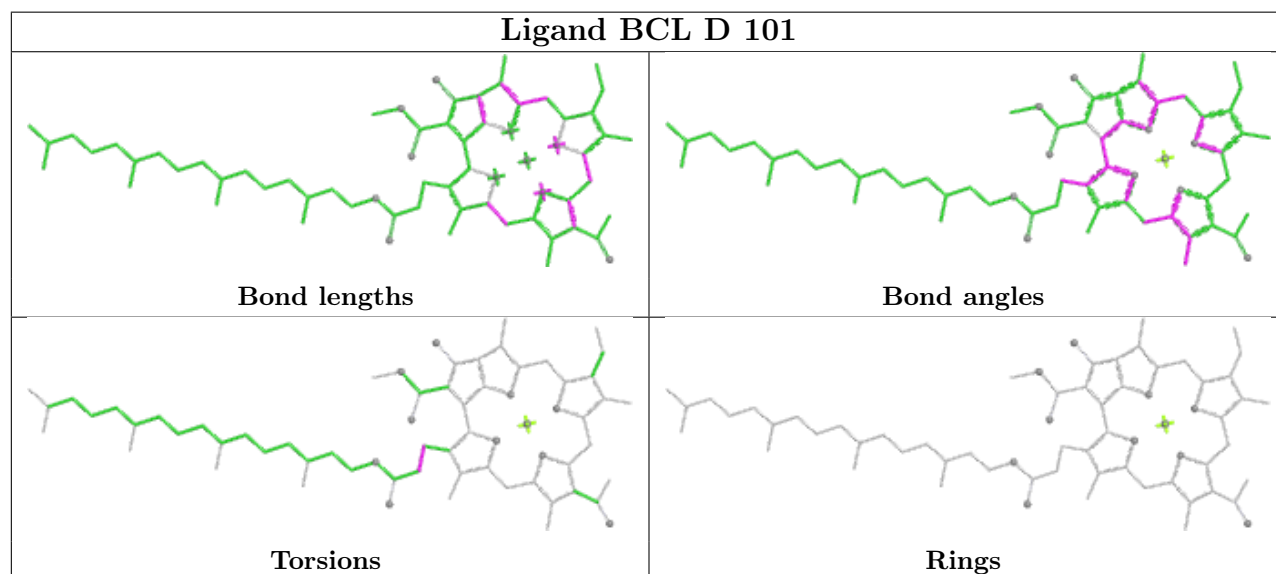
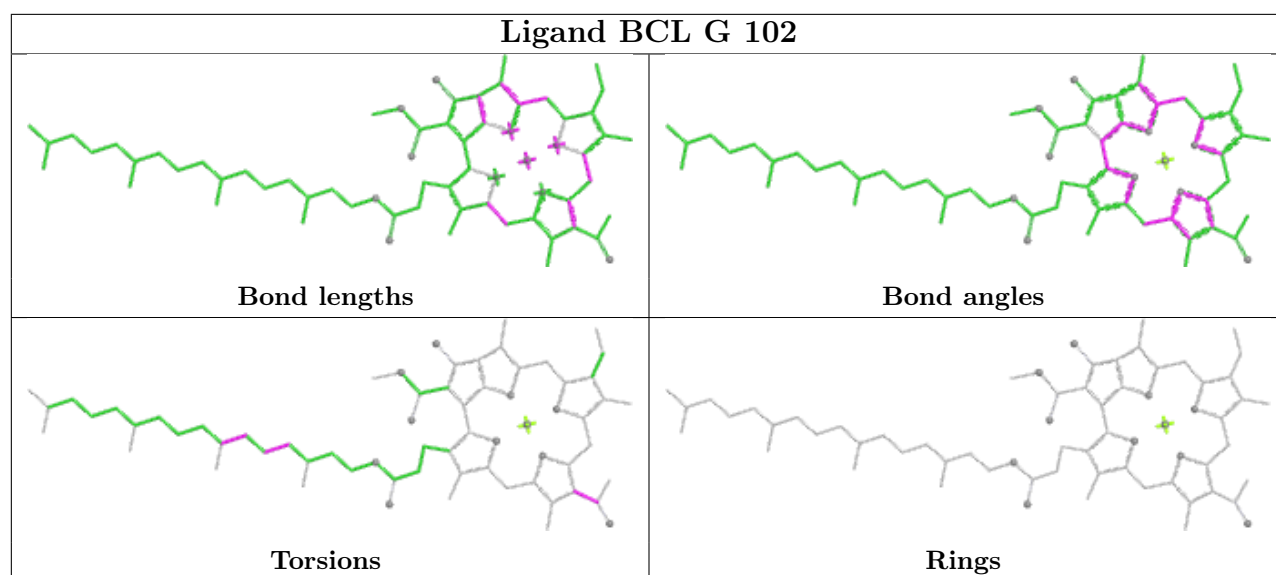


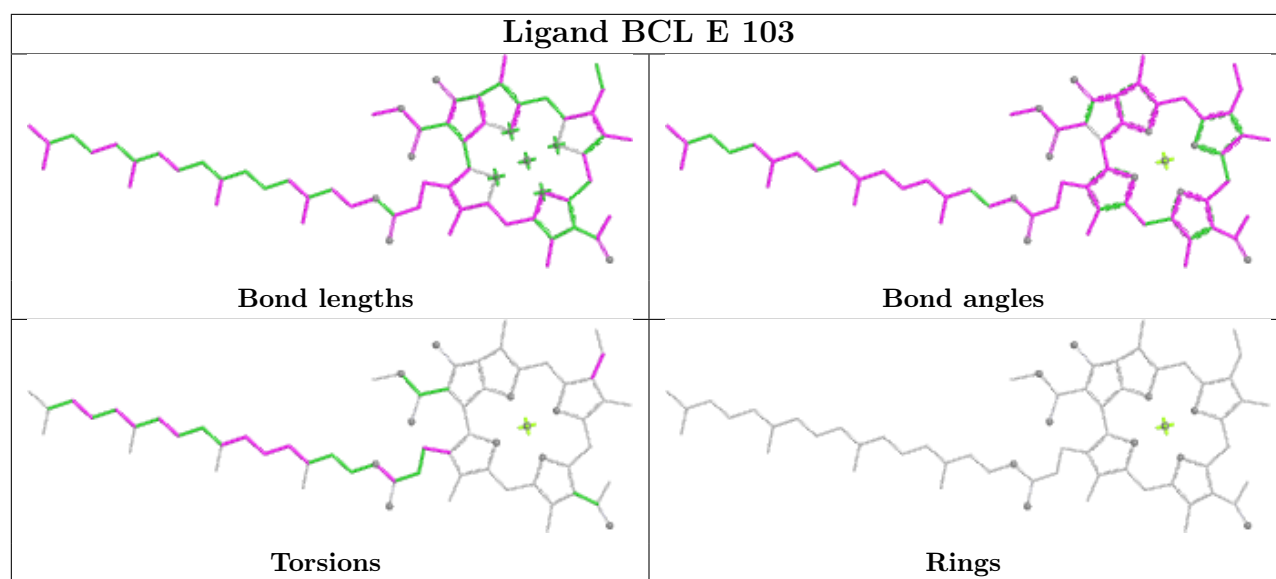












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

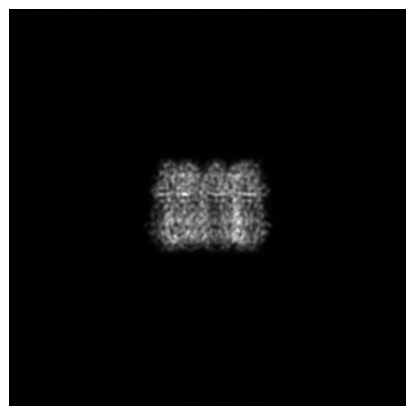
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47275. These allow visual inspection of the internal detail of the map and identification of artifacts.

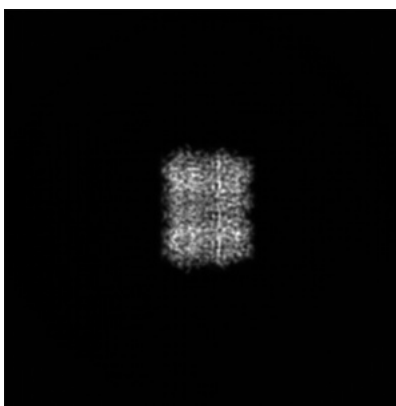
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

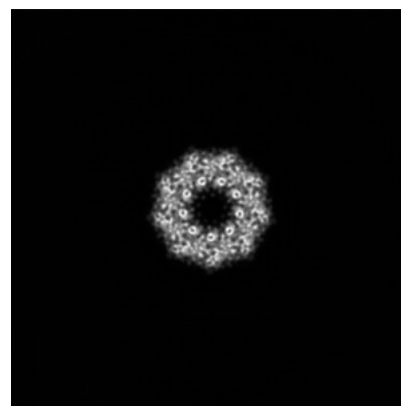
6.1.1 Primary map



X

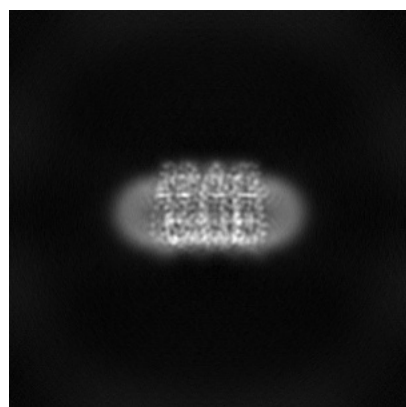


Y

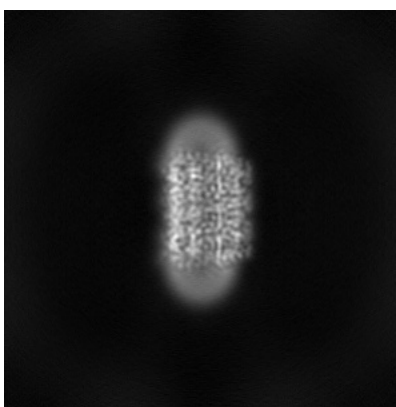


Z

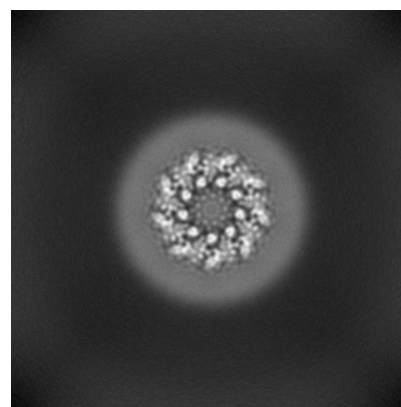
6.1.2 Raw map



X



Y

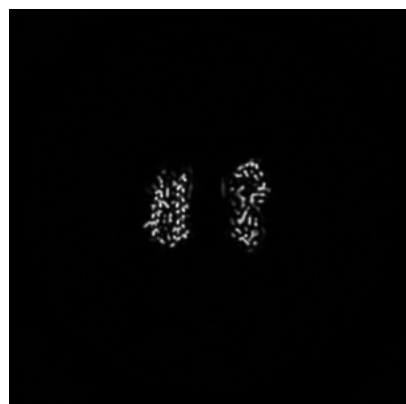


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

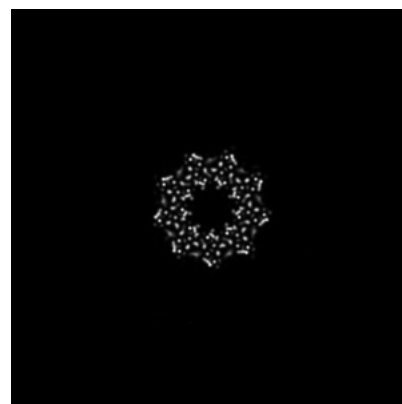
6.2.1 Primary map



X Index: 190

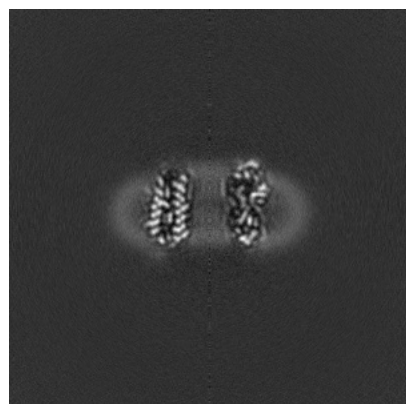


Y Index: 190

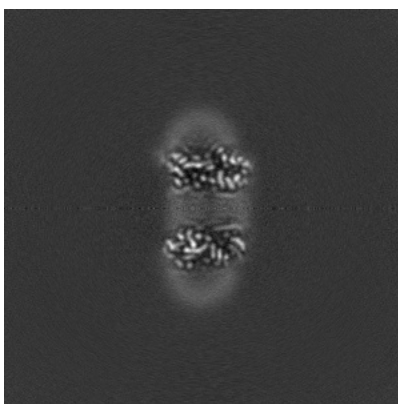


Z Index: 190

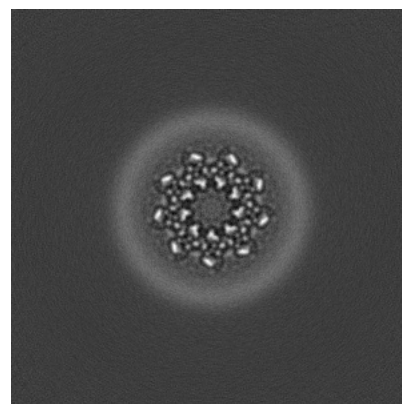
6.2.2 Raw map



X Index: 190



Y Index: 190

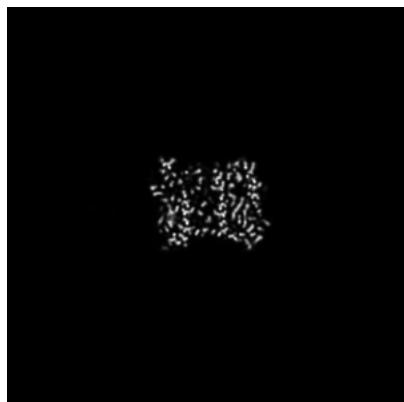


Z Index: 190

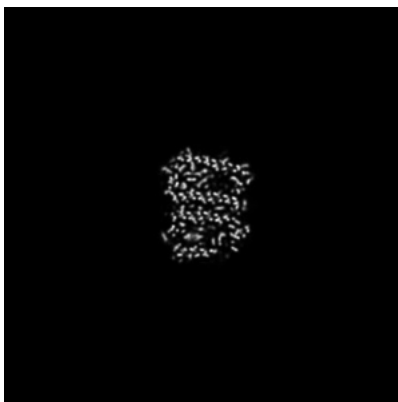
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

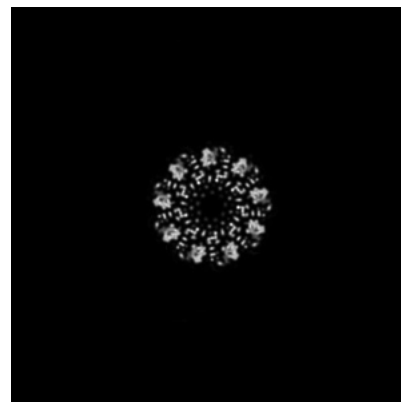
6.3.1 Primary map



X Index: 169

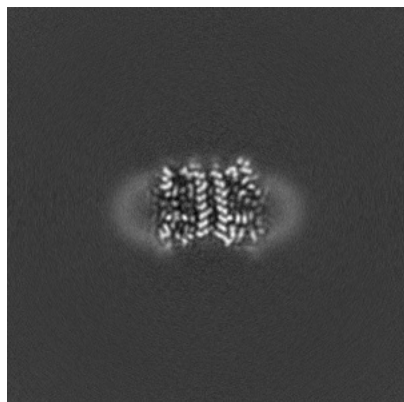


Y Index: 217

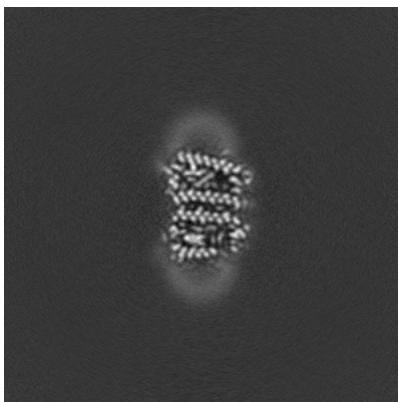


Z Index: 204

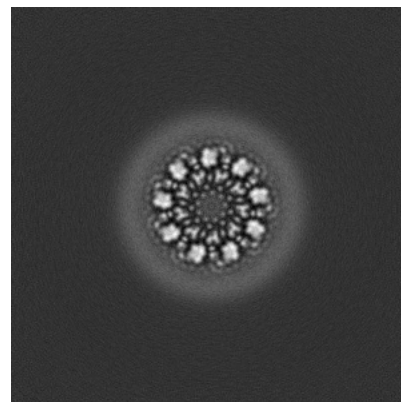
6.3.2 Raw map



X Index: 165



Y Index: 216

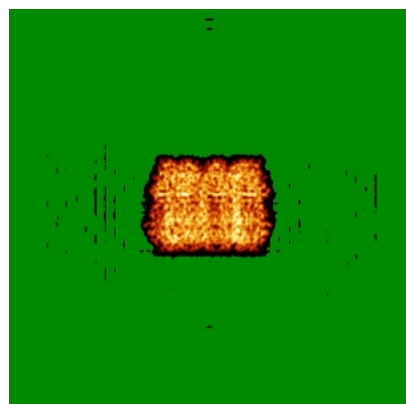


Z Index: 204

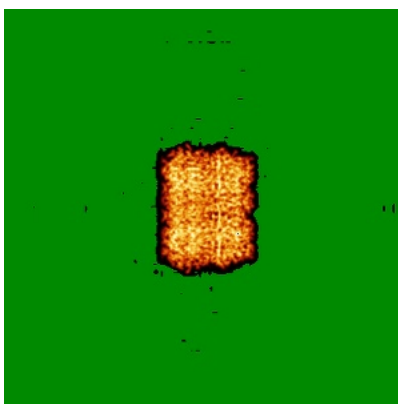
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

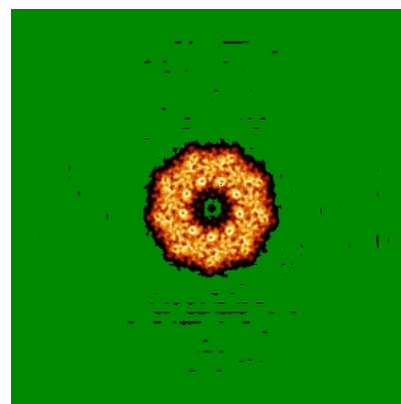
6.4.1 Primary map



X

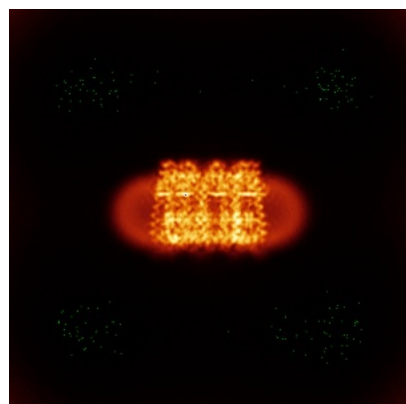


Y

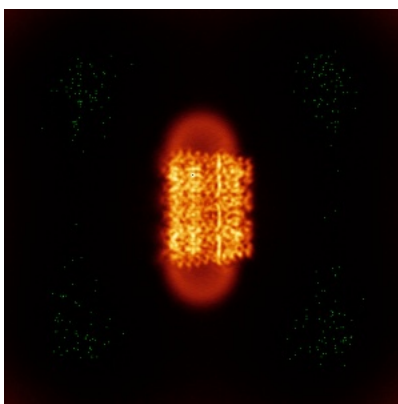


Z

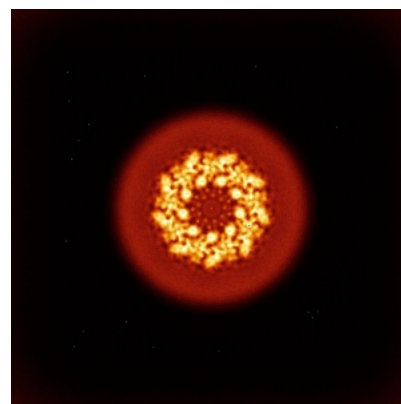
6.4.2 Raw map



X



Y

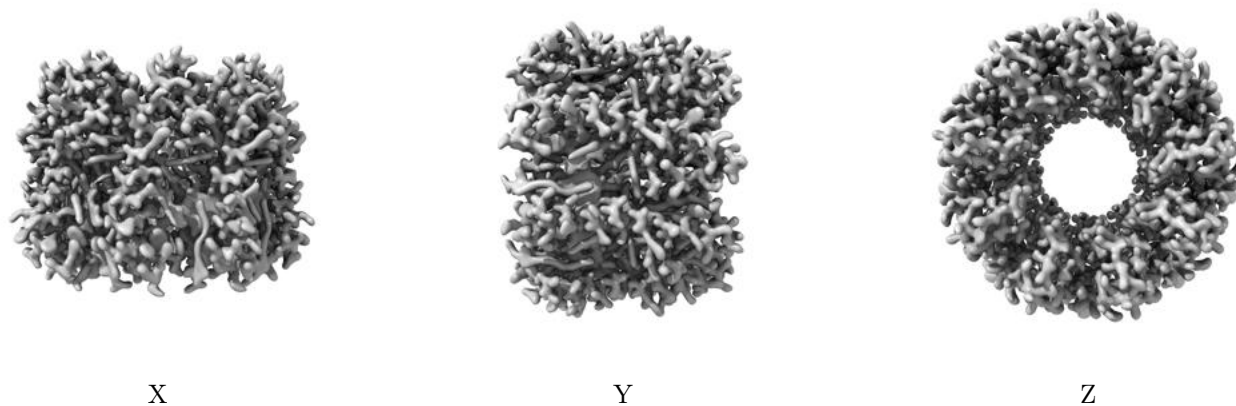


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

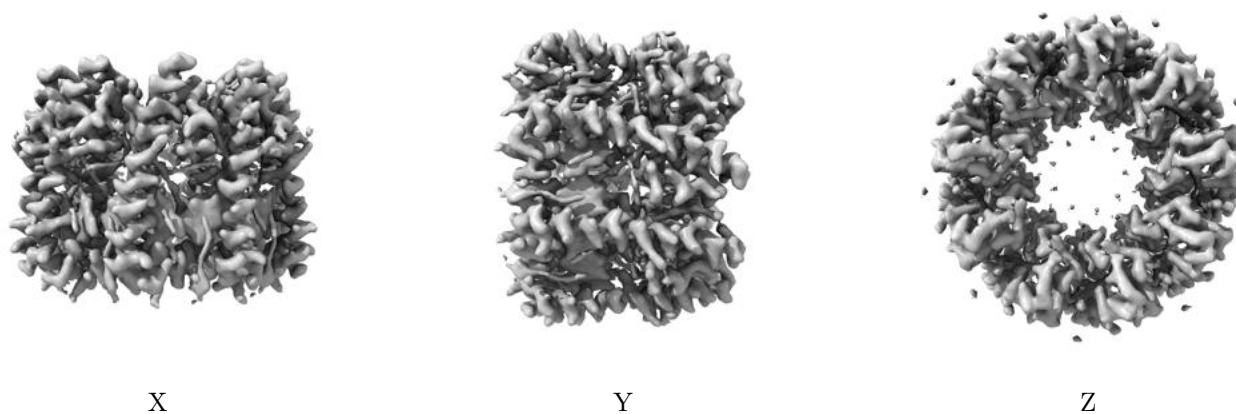
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 7.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

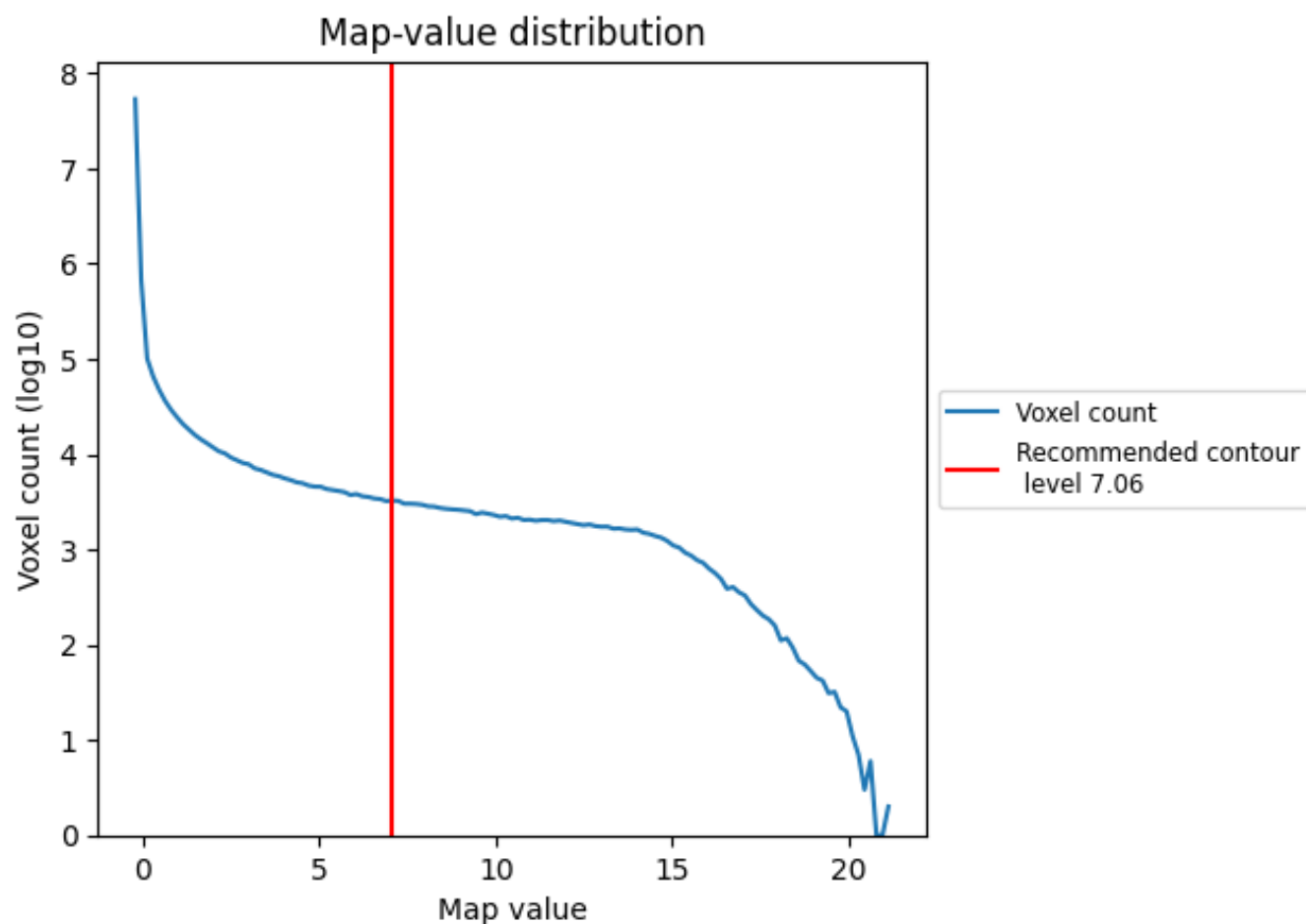
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

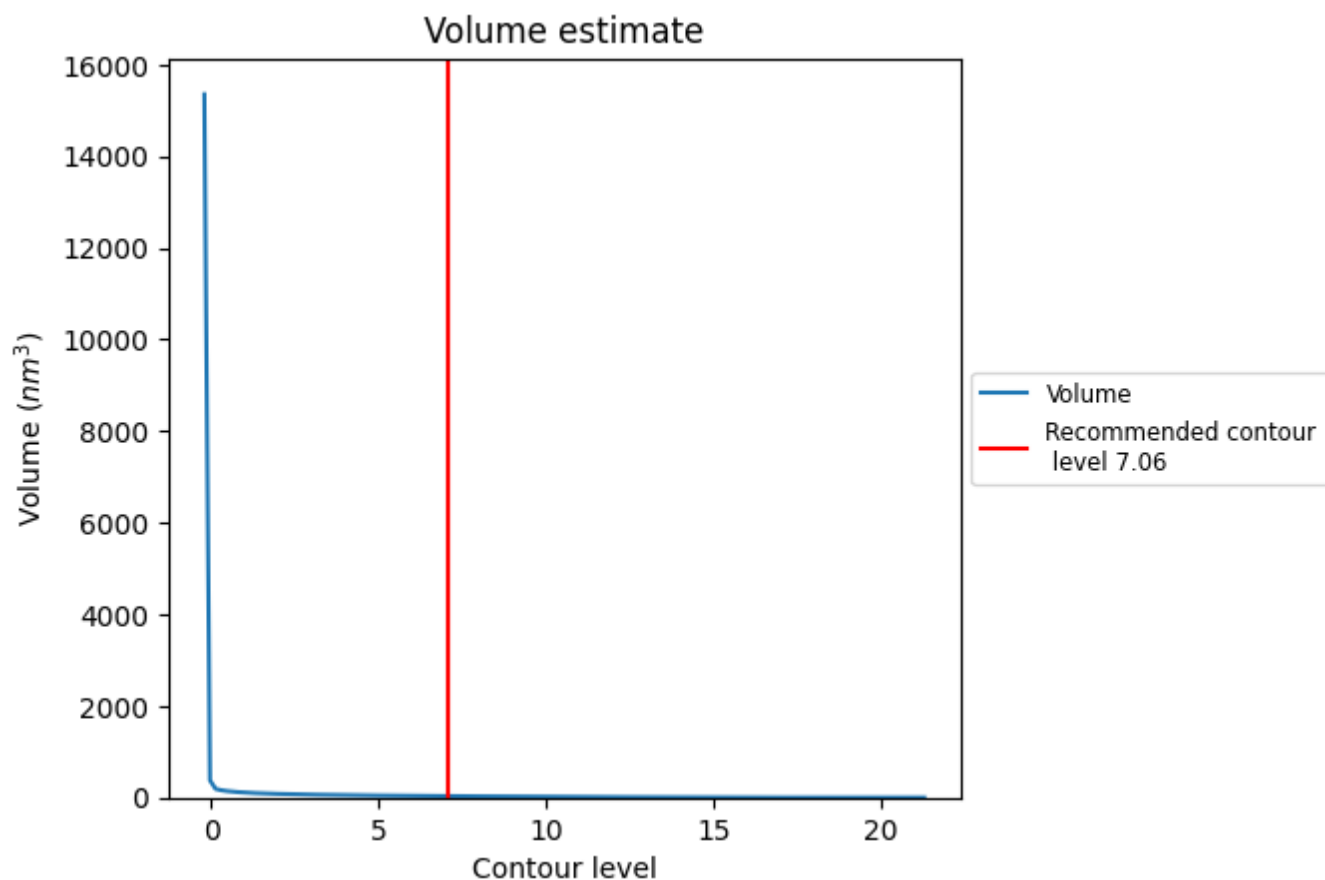
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

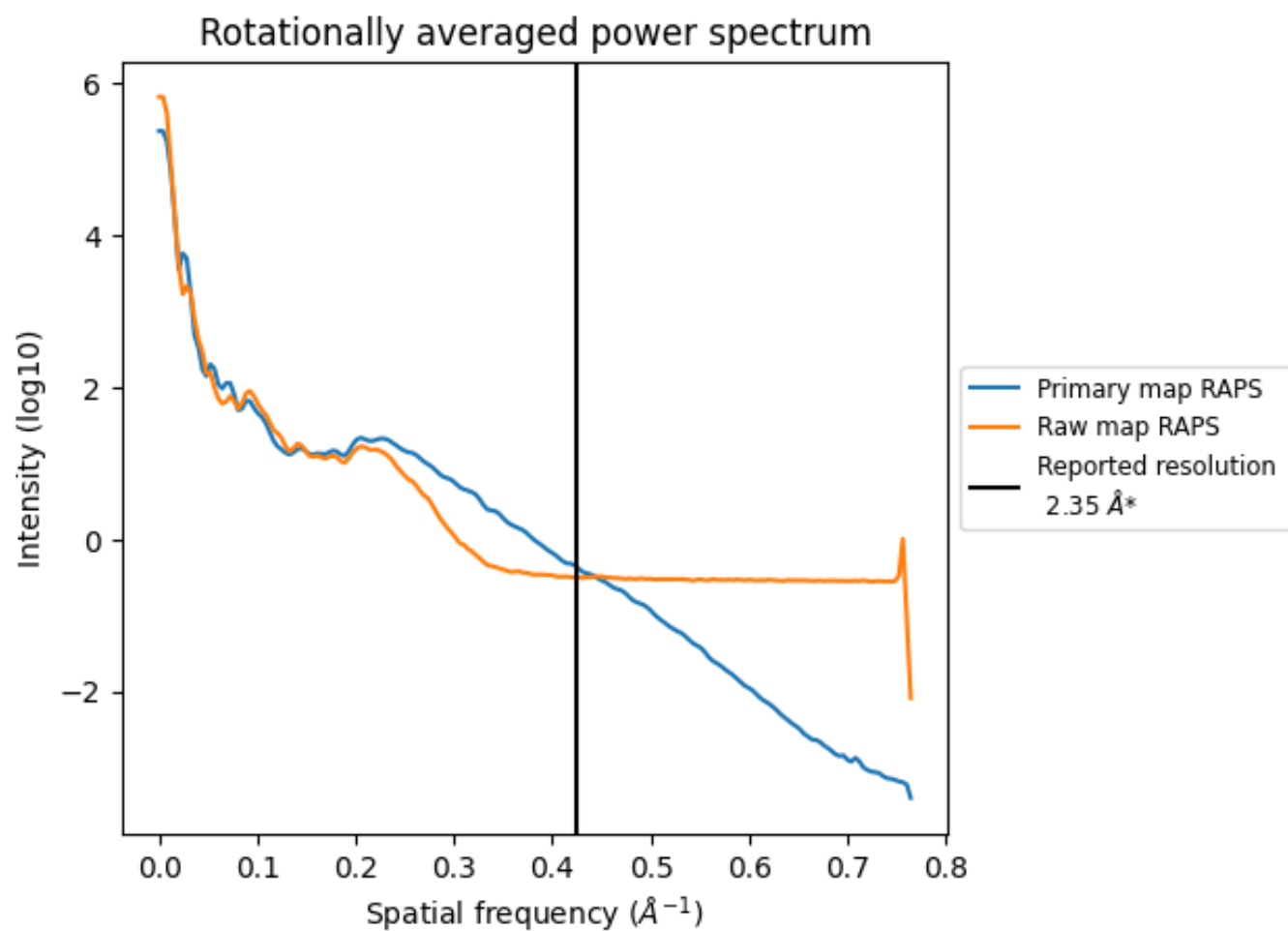
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 31 nm^3 ; this corresponds to an approximate mass of 28 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

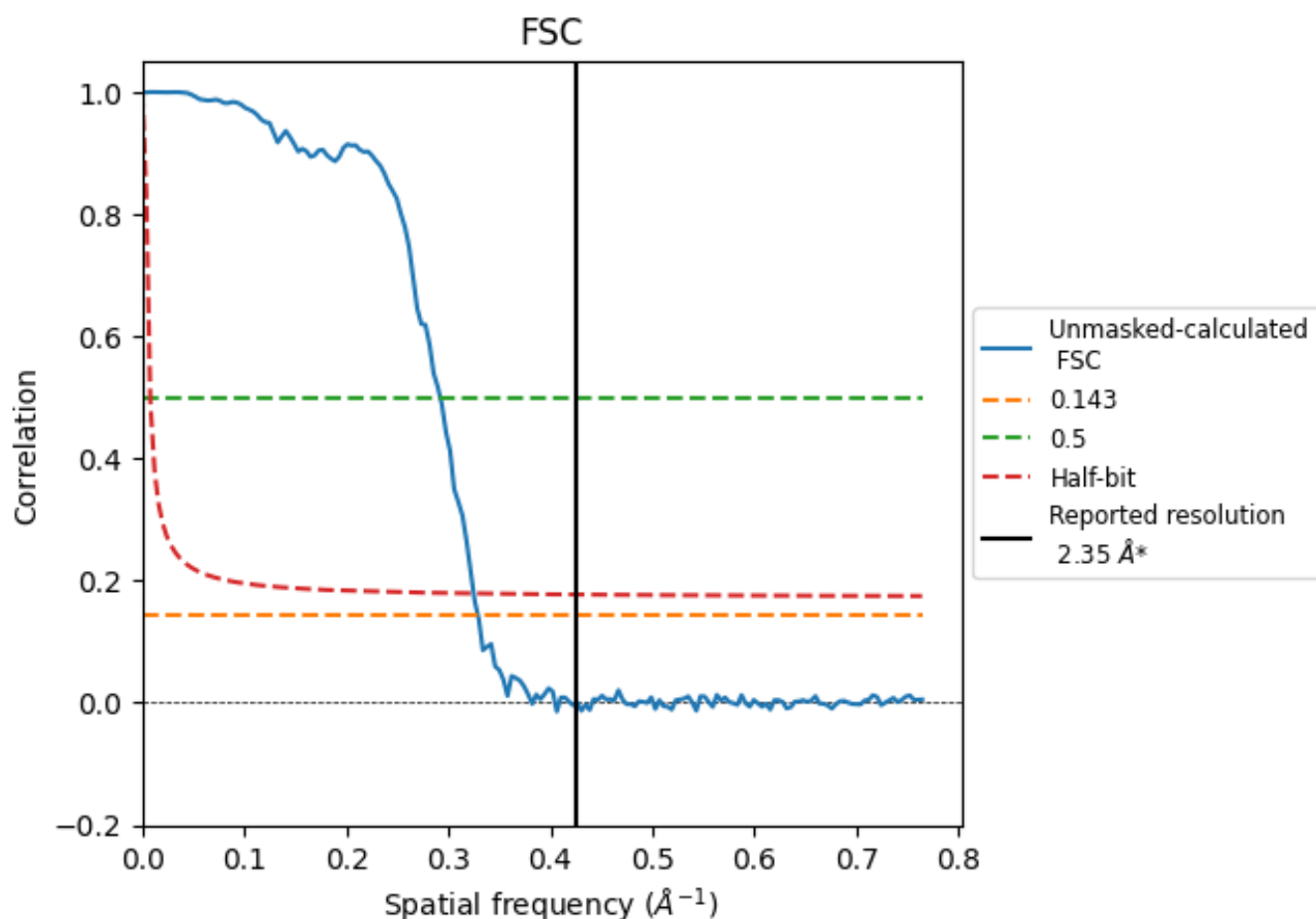


*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 \AA^{-1}

8.2 Resolution estimates [i](#)

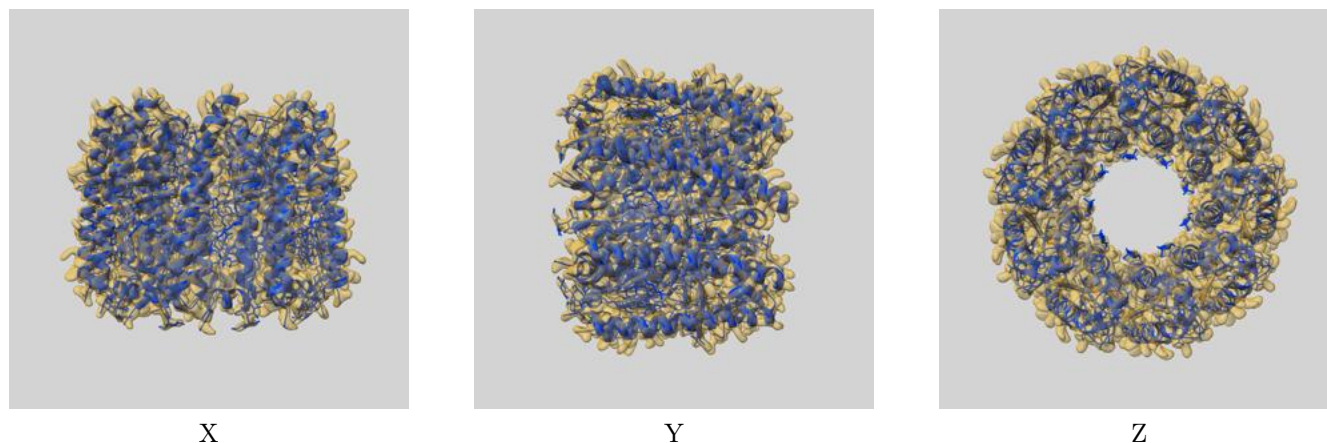
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.04	3.42	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.04 differs from the reported value 2.35 by more than 10 %

9 Map-model fit [i](#)

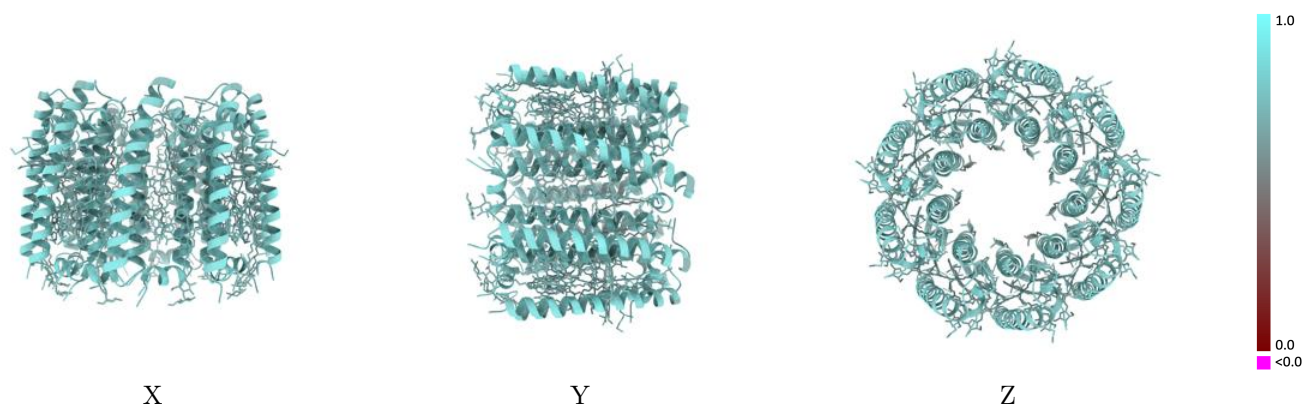
This section contains information regarding the fit between EMDB map EMD-47275 and PDB model 9DWZ. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



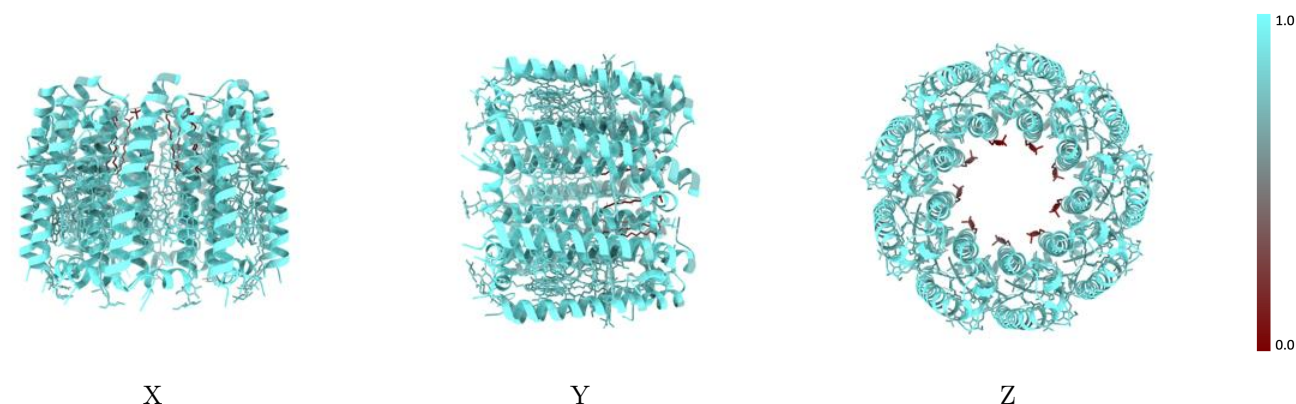
The images above show the 3D surface view of the map at the recommended contour level 7.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



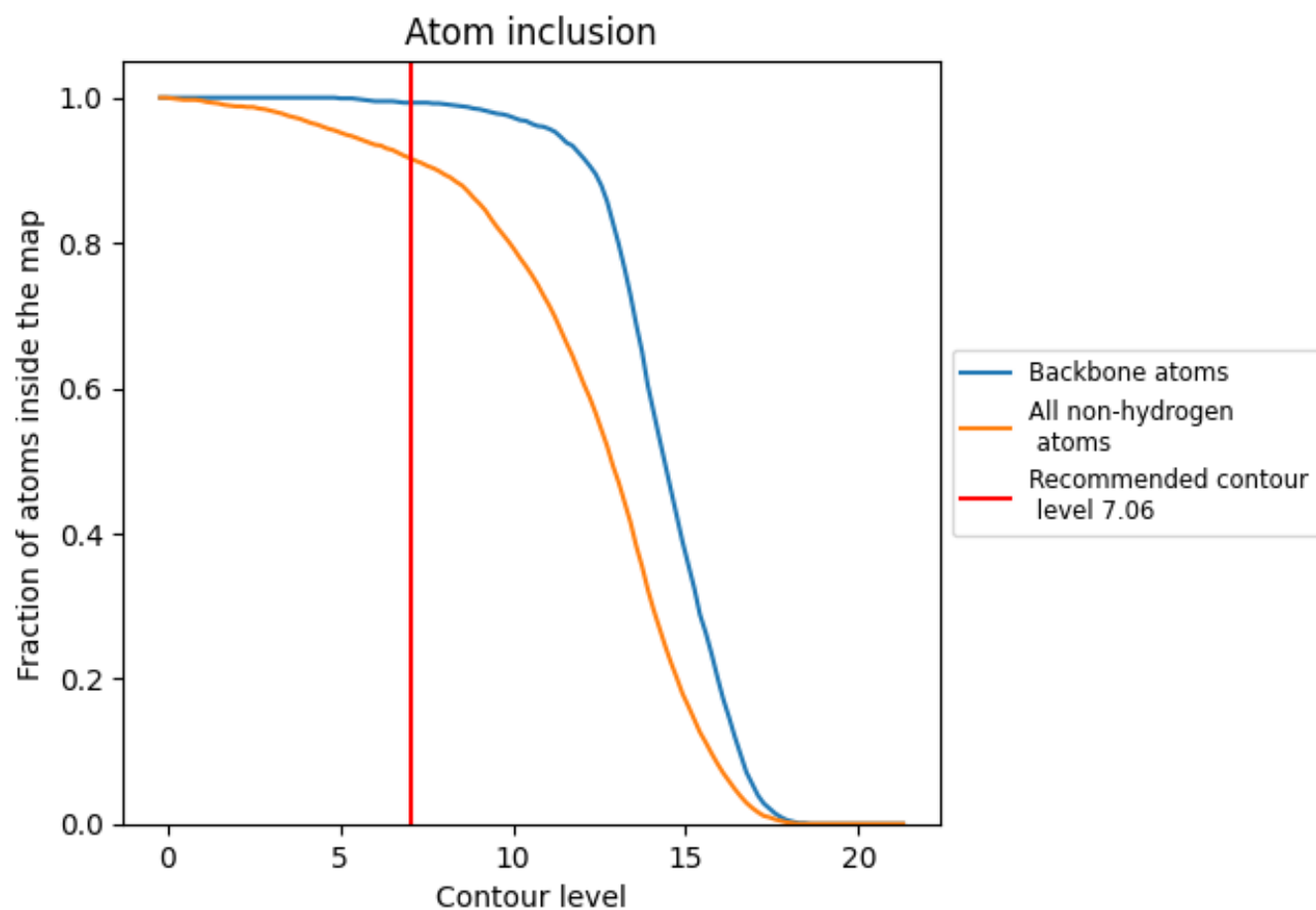
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (7.06).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (7.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.7340
A	 0.9180	 0.7380
B	 0.9130	 0.7320
C	 0.9220	 0.7380
D	 0.9160	 0.7290
E	 0.9200	 0.7360
F	 0.9110	 0.7290
G	 0.9170	 0.7360
H	 0.9090	 0.7320
I	 0.9240	 0.7360
J	 0.9130	 0.7330
K	 0.9130	 0.7370
L	 0.9110	 0.7320
M	 0.9170	 0.7400
N	 0.9160	 0.7310
O	 0.9150	 0.7380
P	 0.9180	 0.7320
Q	 0.9180	 0.7340
R	 0.9110	 0.7270

