



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:59 am BST

PDB ID : 2FKW
Title : Structure of LH2 from Rps. acidophila crystallized in lipidic mesophases
Authors : Papiz, M.Z.; Cherezov, V.; Clogston, J.; Caffrey, M.
Deposited on : 2006-01-05
Resolution : 2.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

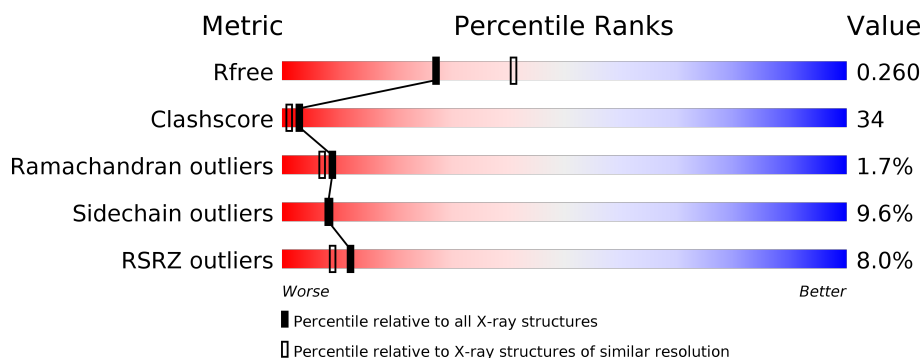
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



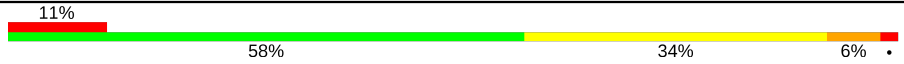


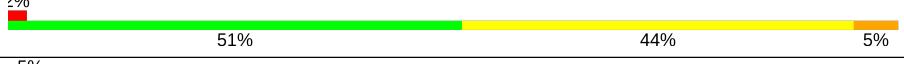


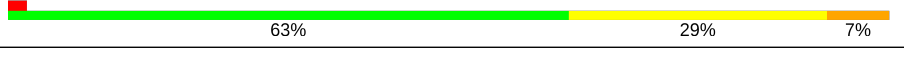

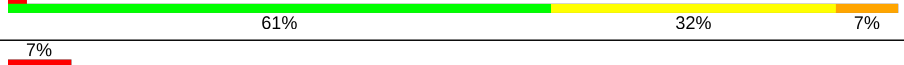


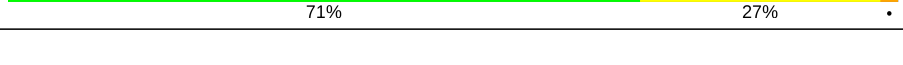
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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

Mol	Chain	Length	Quality of chain
1	A	53	<div> <div>11%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>9%</div> </div> </div>
1	C	53	<div> <div>13%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> </div> </div>
1	E	53	<div> <div>13%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>9%</div> </div> </div>
1	G	53	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>8%</div> </div> </div>
1	I	53	<div> <div>11%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
1	K	53	<div> <div>11%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>• •</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	53	
1	O	53	
1	R	53	
2	B	41	
2	D	41	
2	F	41	
2	H	41	
2	J	41	
2	L	41	
2	N	41	
2	P	41	
2	S	41	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BCL	A	1501	X	-	-	-
3	BCL	A	1701	X	-	-	-
3	BCL	B	1601	X	-	-	-
3	BCL	C	1502	X	-	-	-
3	BCL	C	1702	X	-	-	-
3	BCL	G	1704	X	-	X	-
3	BCL	H	1604	X	-	-	-
3	BCL	I	1705	-	-	X	-
3	BCL	J	1605	X	-	-	-
3	BCL	K	1506	X	-	-	-
3	BCL	K	1706	X	-	-	-
3	BCL	L	1606	X	-	X	-
3	BCL	M	1707	X	-	X	-
3	BCL	N	1607	X	-	-	-
3	BCL	O	1508	X	-	-	-
3	BCL	O	1708	X	-	-	-
3	BCL	P	1608	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BCL	R	1509	X	-	-	-
3	BCL	R	1709	X	-	X	-
3	BCL	S	1609	X	-	-	-
4	LDA	A	1816	-	-	-	X
4	LDA	C	1815	-	-	-	X
4	LDA	E	1823	-	-	-	X
4	LDA	G	1824	-	-	X	-
4	LDA	I	1812	-	-	-	X
4	LDA	I	1825	-	-	-	X
4	LDA	K	1810	-	-	-	X
4	LDA	M	1827	-	-	-	X
4	LDA	R	1818	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9829 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	G	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	I	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	K	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	M	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	O	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	R	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

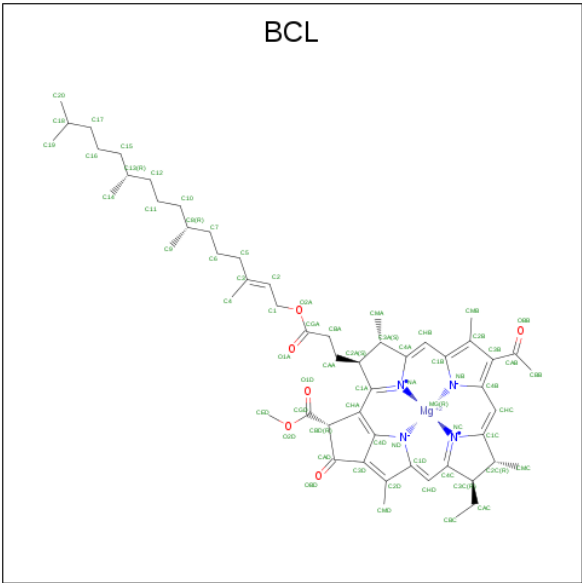
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
C	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
E	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
G	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
I	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
K	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
M	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
O	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
R	1	CXM	MET	MODIFIED RESIDUE	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	H	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	J	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	L	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	N	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	P	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	S	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
3	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

Continued on next page...

Continued from previous page...

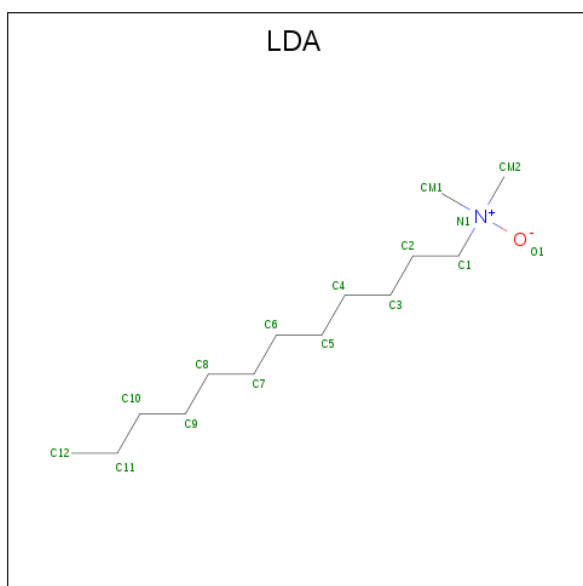
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	H	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	J	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	N	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



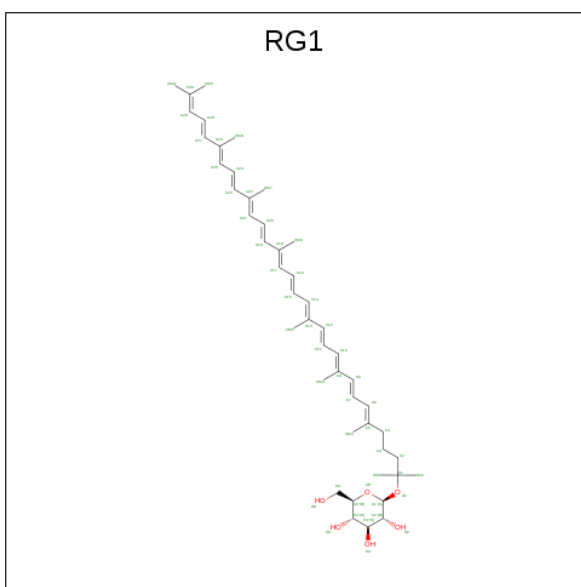
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	D	1	Total	C	N	O	0	0
			16	14	1	1		
4	E	1	Total	C	N	O	0	0
			16	14	1	1		
4	E	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	F	1	Total 16	C 14	N 1	O 1	0	0
4	G	1	Total 16	C 14	N 1	O 1	0	0
4	G	1	Total 16	C 14	N 1	O 1	0	0
4	H	1	Total 16	C 14	N 1	O 1	0	0
4	I	1	Total 16	C 14	N 1	O 1	0	0
4	I	1	Total 16	C 14	N 1	O 1	0	0
4	I	1	Total 16	C 14	N 1	O 1	0	0
4	J	1	Total 16	C 14	N 1	O 1	0	0
4	K	1	Total 16	C 14	N 1	O 1	0	0
4	K	1	Total 16	C 14	N 1	O 1	0	0
4	L	1	Total 16	C 14	N 1	O 1	0	0
4	M	1	Total 16	C 14	N 1	O 1	0	0
4	M	1	Total 16	C 14	N 1	O 1	0	0
4	N	1	Total 16	C 14	N 1	O 1	0	0
4	O	1	Total 16	C 14	N 1	O 1	0	0
4	P	1	Total 16	C 14	N 1	O 1	0	0
4	R	1	Total 16	C 14	N 1	O 1	0	0
4	R	1	Total 16	C 14	N 1	O 1	0	0
4	R	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 5 is Rhodopin b-D-glucoside (three-letter code: RG1) (formula: $C_{46}H_{66}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			52	46	6		
5	F	1	Total	C	O	0	0
			52	46	6		
5	H	1	Total	C	O	0	0
			52	46	6		
5	J	1	Total	C	O	0	0
			52	46	6		
5	L	1	Total	C	O	0	0
			52	46	6		
5	N	1	Total	C	O	0	0
			52	46	6		
5	P	1	Total	C	O	0	0
			52	46	6		
5	R	1	Total	C	O	0	0
			52	46	6		
5	S	1	Total	C	O	0	0
			52	46	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	O	0	0
			33	33		
6	B	26	Total	O	0	0
			26	26		
6	C	24	Total	O	0	0
			24	24		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	27	Total 27	O 27	0	0
6	E	40	Total 40	O 40	0	0
6	F	28	Total 28	O 28	0	0
6	G	41	Total 41	O 41	0	0
6	H	37	Total 37	O 37	2	0
6	I	38	Total 38	O 38	0	0
6	J	39	Total 39	O 39	1	0
6	K	47	Total 47	O 47	0	0
6	L	29	Total 29	O 29	0	0
6	M	36	Total 36	O 36	0	0
6	N	30	Total 30	O 30	0	0
6	O	33	Total 33	O 33	1	0
6	P	32	Total 32	O 32	0	0
6	R	39	Total 39	O 39	0	0
6	S	34	Total 34	O 34	0	0

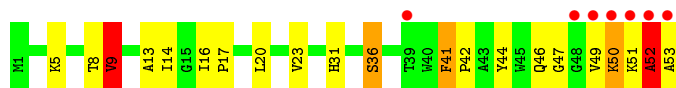
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Light-harvesting protein B-800/850, alpha chain



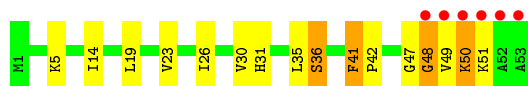
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



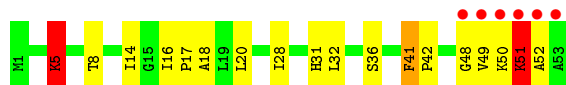
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



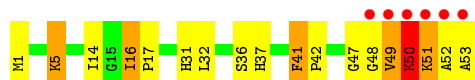
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



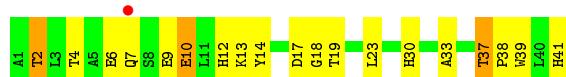
- Molecule 2: Light-harvesting protein B-800/850, beta chain



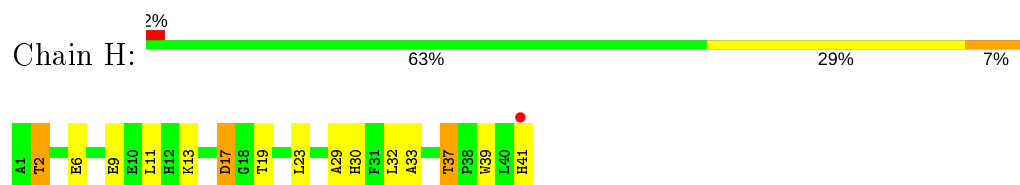
- Molecule 2: Light-harvesting protein B-800/850, beta chain



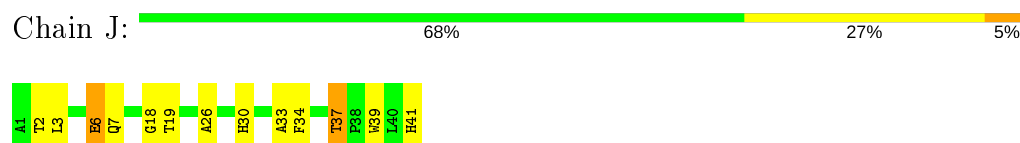
- Molecule 2: Light-harvesting protein B-800/850, beta chain



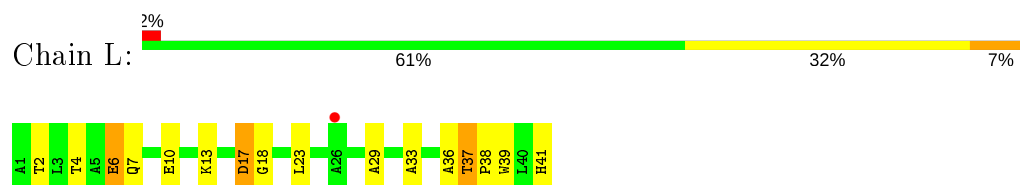
- Molecule 2: Light-harvesting protein B-800/850, beta chain



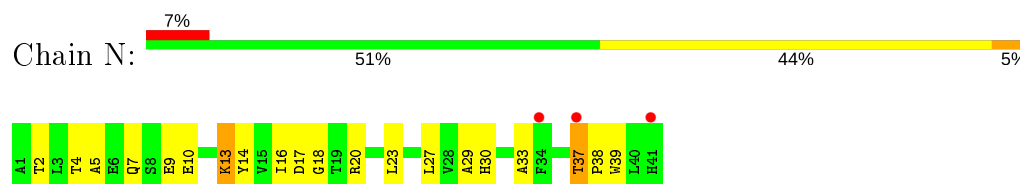
- Molecule 2: Light-harvesting protein B-800/850, beta chain



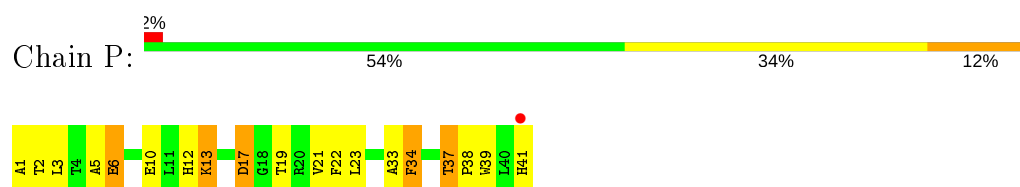
- Molecule 2: Light-harvesting protein B-800/850, beta chain



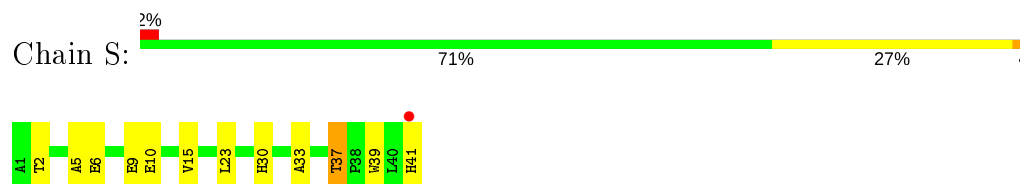
- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 126.38Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 38.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.45) 99.7 (38.85-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.254 0.203 , 0.260	Depositor DCC
R_{free} test set	2531 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9829	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, RG1, LDA, CXM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.27	1/404 (0.2%)	0.51	0/556
1	C	1.51	4/404 (1.0%)	0.51	0/556
1	E	1.35	1/404 (0.2%)	0.53	0/556
1	G	1.34	2/404 (0.5%)	0.50	0/556
1	I	1.38	1/404 (0.2%)	0.53	0/556
1	K	1.47	2/404 (0.5%)	0.55	0/556
1	M	1.35	1/404 (0.2%)	0.57	0/556
1	O	1.36	2/404 (0.5%)	0.51	0/556
1	R	1.35	3/404 (0.7%)	0.53	0/556
2	B	1.40	1/332 (0.3%)	0.49	0/453
2	D	1.25	1/332 (0.3%)	0.45	0/453
2	F	1.48	2/332 (0.6%)	0.42	0/453
2	H	1.40	2/332 (0.6%)	0.45	0/453
2	J	1.29	2/332 (0.6%)	0.44	0/453
2	L	1.62	5/332 (1.5%)	0.47	0/453
2	N	1.38	2/332 (0.6%)	0.44	0/453
2	P	1.60	3/332 (0.9%)	0.49	0/453
2	S	1.21	1/332 (0.3%)	0.45	0/453
All	All	1.39	36/6624 (0.5%)	0.50	0/9081

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	2	1
1	E	1	0
1	G	1	0
1	I	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	1
1	M	3	1
1	O	0	1
1	R	2	0
All	All	12	7

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	GLU	CG-CD	11.70	1.69	1.51
2	L	10	GLU	CG-CD	11.28	1.68	1.51
2	F	10	GLU	CG-CD	9.26	1.65	1.51
2	L	17	ASP	CB-CG	7.49	1.67	1.51
1	A	49	VAL	CA-CB	7.42	1.70	1.54
1	I	5	LYS	CD-CE	7.06	1.68	1.51
1	C	9	VAL	CB-CG1	-6.83	1.38	1.52
2	F	6	GLU	CG-CD	6.81	1.62	1.51
2	P	6	GLU	CB-CG	6.80	1.65	1.52
2	P	1	ALA	CA-CB	6.73	1.66	1.52
1	M	9	VAL	CB-CG2	-6.58	1.39	1.52
1	G	36	SER	C-O	-6.41	1.11	1.23
2	L	17	ASP	CG-OD1	6.39	1.40	1.25
2	H	17	ASP	CB-CG	-6.35	1.38	1.51
2	H	6	GLU	CG-CD	6.29	1.61	1.51
2	B	13	LYS	CD-CE	6.16	1.66	1.51
1	O	9	VAL	CB-CG2	-5.97	1.40	1.52
1	O	44	TYR	CD2-CE2	5.95	1.48	1.39
1	K	23	VAL	CB-CG2	-5.95	1.40	1.52
2	N	10	GLU	CG-CD	5.89	1.60	1.51
1	R	5	LYS	CD-CE	5.88	1.66	1.51
1	C	52	ALA	CA-CB	-5.75	1.40	1.52
1	C	53	ALA	CA-CB	-5.70	1.40	1.52
2	D	31	PHE	CE2-CZ	5.57	1.48	1.37
2	J	34	PHE	CE1-CZ	5.56	1.48	1.37
2	J	6	GLU	CD-OE2	5.42	1.31	1.25
2	N	14	TYR	CD1-CE1	-5.39	1.31	1.39
1	R	53	ALA	CA-CB	-5.34	1.41	1.52
1	K	9	VAL	CB-CG2	-5.31	1.41	1.52
1	E	49	VAL	N-CA	5.26	1.56	1.46
2	L	29	ALA	CA-CB	5.18	1.63	1.52
2	L	6	GLU	CG-CD	5.17	1.59	1.51
1	R	49	VAL	CA-CB	5.14	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	48	GLY	CA-C	5.07	1.59	1.51
1	C	36	SER	CB-OG	-5.06	1.35	1.42
2	S	15	VAL	CB-CG2	-5.04	1.42	1.52

There are no bond angle outliers.

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	52	ALA	CA
1	C	53	ALA	CA
1	E	51	LYS	CA
1	G	50	LYS	CA
1	I	49	VAL	CA
1	I	50	LYS	CA
1	K	51	LYS	CA
1	M	49	VAL	CA
1	M	51	LYS	CA
1	M	52	ALA	CA
1	R	50	LYS	CA
1	R	53	ALA	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	LYS	Peptide
1	A	51	LYS	Peptide
1	C	52	ALA	Peptide
1	I	51	LYS	Peptide
1	K	50	LYS	Peptide
1	M	51	LYS	Peptide
1	O	50	LYS	Peptide

5.2 Too-close contacts

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	403	0	422	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	403	0	422	27	0
1	E	403	0	422	27	0
1	G	403	0	422	21	0
1	I	403	0	422	21	0
1	K	403	0	422	27	0
1	M	403	0	422	32	0
1	O	403	0	422	17	0
1	R	403	0	422	22	0
2	B	323	0	321	25	0
2	D	323	0	321	22	0
2	F	323	0	321	24	0
2	H	323	0	321	19	0
2	J	323	0	321	23	0
2	L	323	0	321	22	0
2	N	323	0	321	29	0
2	P	323	0	321	30	0
2	S	323	0	321	11	0
3	A	132	0	146	25	0
3	B	66	0	74	11	0
3	C	132	0	148	15	0
3	D	66	0	74	8	0
3	E	132	0	147	12	0
3	F	66	0	74	12	0
3	G	132	0	147	27	0
3	H	66	0	73	12	0
3	I	132	0	148	33	0
3	J	66	0	73	17	0
3	K	132	0	146	14	0
3	L	66	0	74	25	0
3	M	132	0	147	28	0
3	N	66	0	74	16	0
3	O	132	0	147	21	0
3	P	66	0	73	10	0
3	R	132	0	147	28	0
3	S	66	0	74	13	0
4	A	32	0	62	11	0
4	B	16	0	31	2	0
4	C	32	0	62	6	0
4	D	16	0	31	3	0
4	E	32	0	62	14	0
4	F	16	0	31	7	0
4	G	32	0	62	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	16	0	31	3	0
4	I	48	0	93	15	0
4	J	16	0	31	1	0
4	K	32	0	62	12	0
4	L	16	0	31	5	0
4	M	32	0	62	6	0
4	N	16	0	31	2	0
4	O	16	0	31	7	0
4	P	16	0	31	3	0
4	R	48	0	93	12	0
5	D	52	0	66	5	0
5	F	52	0	66	5	0
5	H	52	0	66	5	0
5	J	52	0	66	1	0
5	L	52	0	66	4	0
5	N	52	0	66	4	0
5	P	52	0	66	4	0
5	R	52	0	66	4	0
5	S	52	0	66	5	0
6	A	33	0	0	9	0
6	B	26	0	0	6	0
6	C	24	0	0	3	0
6	D	27	0	0	8	0
6	E	40	0	0	20	0
6	F	28	0	0	7	0
6	G	41	0	0	22	0
6	H	37	0	0	5	0
6	I	38	0	0	11	0
6	J	39	0	0	14	0
6	K	47	0	0	28	0
6	L	29	0	0	2	0
6	M	36	0	0	10	0
6	N	30	0	0	8	0
6	O	33	0	0	11	0
6	P	32	0	0	8	0
6	R	39	0	0	24	0
6	S	34	0	0	4	0
All	All	9829	0	10104	659	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 34.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1:CXM:CE	1:M:1:CXM:SD	2.21	1.28
1:G:48:GLY:HA2	6:G:1839:HOH:O	1.32	1.24
4:I:1825:LDA:HM22	6:I:1845:HOH:O	1.06	1.24
4:H:1804:LDA:H92	6:H:1825:HOH:O	1.38	1.22
1:E:49:VAL:HG11	6:E:1850:HOH:O	1.45	1.15
3:I:1705:BCL:H41	3:I:1705:BCL:H8	1.25	1.15
6:A:1831:HOH:O	2:D:21:VAL:HG11	1.53	1.08
3:R:1709:BCL:H2	6:R:1831:HOH:O	1.54	1.07
3:G:1504:BCL:H143	6:G:1853:HOH:O	1.54	1.05
3:O:1708:BCL:H2	6:O:1833:HOH:O	1.59	1.02
2:P:33:ALA:O	2:P:37:THR:HB	1.58	1.02
3:O:1708:BCL:C2	6:O:1833:HOH:O	2.08	1.01
4:I:1812:LDA:HM23	6:I:1829:HOH:O	1.59	1.01
2:D:6:GLU:HB3	6:D:1825:HOH:O	1.61	1.01
3:J:1605:BCL:O2D	6:J:1813:HOH:O	1.79	1.01
4:G:1824:LDA:CM1	6:G:1828:HOH:O	2.08	1.00
4:E:1822:LDA:CM2	6:E:1859:HOH:O	2.09	0.99
1:G:48:GLY:O	6:G:1832:HOH:O	1.79	0.98
1:I:48:GLY:HA2	6:I:1836:HOH:O	1.63	0.98
1:I:48:GLY:CA	6:I:1836:HOH:O	2.10	0.97
3:A:1501:BCL:H191	3:R:1709:BCL:HED1	1.41	0.97
3:A:1501:BCL:O1D	3:A:1501:BCL:CAA	2.14	0.96
1:E:14:ILE:HG22	6:E:1835:HOH:O	1.65	0.96
2:L:39:TRP:CE2	3:L:1606:BCL:CMC	2.49	0.95
3:J:1605:BCL:CBD	6:J:1813:HOH:O	2.12	0.95
2:P:23:LEU:HB2	3:P:1608:BCL:H2	1.46	0.95
4:G:1824:LDA:HM11	6:G:1828:HOH:O	1.66	0.94
3:M:1707:BCL:O2D	6:M:1859:HOH:O	1.86	0.94
1:E:44:TYR:CZ	6:E:1862:HOH:O	2.19	0.94
1:K:31:HIS:CE1	3:L:1606:BCL:HMD1	2.03	0.93
3:A:1501:BCL:HAA2	3:A:1501:BCL:O1D	1.68	0.93
1:C:13:ALA:HB2	6:D:1826:HOH:O	1.67	0.92
1:M:51:LYS:HG2	1:M:52:ALA:O	1.69	0.92
2:F:33:ALA:O	2:F:37:THR:HB	1.68	0.92
2:N:33:ALA:O	2:N:37:THR:HB	1.68	0.92
4:O:1820:LDA:HM12	6:O:1823:HOH:O	1.70	0.91
2:H:33:ALA:O	2:H:37:THR:HB	1.70	0.91
4:R:1818:LDA:H92	6:R:1852:HOH:O	1.70	0.90
1:C:14:ILE:HG21	4:C:1815:LDA:H21	1.53	0.90
3:M:1707:BCL:CBD	6:M:1859:HOH:O	2.20	0.89
1:M:51:LYS:HA	1:M:52:ALA:HB2	1.52	0.89
1:C:36:SER:OG	4:E:1822:LDA:HM21	1.72	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:ALA:O	2:D:37:THR:HB	1.74	0.87
2:S:33:ALA:O	2:S:37:THR:HG22	1.74	0.87
2:D:9:GLU:OE1	6:D:1809:HOH:O	1.91	0.87
6:K:1864:HOH:O	4:L:1806:LDA:H82	1.75	0.86
2:P:33:ALA:HB1	6:P:1837:HOH:O	1.76	0.86
1:A:31:HIS:CE1	3:B:1601:BCL:HMD1	2.10	0.86
1:R:5:LYS:HD3	6:R:1835:HOH:O	1.75	0.85
2:L:33:ALA:O	2:L:37:THR:HB	1.77	0.85
2:J:33:ALA:O	2:J:37:THR:HB	1.76	0.85
3:R:1709:BCL:H41	3:R:1709:BCL:H92	1.59	0.84
1:I:48:GLY:N	6:I:1836:HOH:O	2.10	0.84
2:J:41:HIS:NE2	1:K:49:VAL:HG12	1.92	0.84
1:I:5:LYS:HG3	6:J:1823:HOH:O	1.78	0.83
4:K:1810:LDA:HM22	1:M:14:ILE:HD11	1.58	0.83
4:O:1820:LDA:HM23	6:O:1823:HOH:O	1.76	0.83
3:I:1705:BCL:H41	3:I:1705:BCL:C8	2.06	0.82
6:K:1848:HOH:O	1:M:13:ALA:HB2	1.79	0.82
3:A:1501:BCL:C19	3:R:1709:BCL:HED1	2.08	0.82
4:O:1820:LDA:H122	6:O:1850:HOH:O	1.80	0.81
3:P:1608:BCL:HMB1	3:P:1608:BCL:HBB2	1.63	0.81
2:P:37:THR:HG22	2:P:39:TRP:H	1.45	0.81
3:A:1501:BCL:H62	3:R:1709:BCL:HED2	1.59	0.81
3:J:1605:BCL:CBB	6:K:1864:HOH:O	2.28	0.81
6:R:1835:HOH:O	2:S:5:ALA:HB1	1.81	0.81
3:N:1607:BCL:HBB2	3:N:1607:BCL:HMB1	1.62	0.81
2:L:39:TRP:CE2	3:L:1606:BCL:HMC3	2.14	0.80
3:R:1709:BCL:CAD	3:S:1609:BCL:H203	2.10	0.80
4:I:1825:LDA:H92	6:K:1842:HOH:O	1.80	0.80
4:A:1816:LDA:H31	1:C:14:ILE:HD13	1.64	0.80
1:A:14:ILE:HG21	4:A:1816:LDA:H42	1.62	0.80
2:B:4:THR:OG1	2:B:7:GLN:HG3	1.81	0.80
1:C:31:HIS:CE1	3:D:1602:BCL:HMD1	2.17	0.80
6:A:1850:HOH:O	2:B:8:SER:HB2	1.82	0.80
2:P:41:HIS:NE2	1:R:49:VAL:CG1	2.46	0.79
3:M:1707:BCL:H8	3:M:1707:BCL:H41	1.65	0.78
2:B:37:THR:HG23	2:B:39:TRP:H	1.47	0.78
3:G:1704:BCL:CED	3:I:1505:BCL:H191	2.14	0.78
1:M:31:HIS:CE1	3:N:1607:BCL:HMD1	2.19	0.77
3:R:1709:BCL:H102	6:S:419:HOH:O	1.85	0.77
4:K:1810:LDA:H21	1:M:14:ILE:HD13	1.68	0.76
3:R:1709:BCL:C9	3:R:1709:BCL:H41	2.16	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:LYS:CG	6:J:1823:HOH:O	2.32	0.75
4:O:1820:LDA:HM22	1:R:32:LEU:HD22	1.67	0.75
2:S:37:THR:HG23	2:S:39:TRP:H	1.49	0.75
2:P:33:ALA:CB	6:P:1837:HOH:O	2.31	0.75
1:M:48:GLY:HA2	6:M:1829:HOH:O	1.86	0.75
4:I:1812:LDA:H121	6:K:1856:HOH:O	1.85	0.75
4:G:1824:LDA:CM2	6:G:1828:HOH:O	2.35	0.75
2:S:23:LEU:HB2	3:S:1609:BCL:H2	1.67	0.74
2:F:10:GLU:OE1	5:F:1403:RG1:O2'	2.03	0.74
4:R:1818:LDA:C11	6:R:1856:HOH:O	2.35	0.74
1:A:14:ILE:HD13	4:A:1816:LDA:H22	1.68	0.74
4:A:1816:LDA:C3	1:C:14:ILE:HD13	2.18	0.74
2:L:39:TRP:CD2	3:L:1606:BCL:CMC	2.71	0.74
4:R:1818:LDA:H122	6:R:1856:HOH:O	1.88	0.74
1:E:18:ALA:O	6:E:1860:HOH:O	2.05	0.74
2:H:32:LEU:HD12	4:H:1804:LDA:H122	1.70	0.73
1:M:41:PHE:HB3	1:M:42:PRO:HD3	1.69	0.73
3:I:1705:BCL:C4	3:I:1705:BCL:H8	2.15	0.73
2:N:39:TRP:CE2	3:N:1607:BCL:CMC	2.72	0.73
2:P:39:TRP:CE2	3:P:1608:BCL:HMC2	2.24	0.73
4:G:1824:LDA:HM21	6:G:1843:HOH:O	1.89	0.72
1:O:31:HIS:CE1	3:P:1608:BCL:HMD1	2.24	0.72
4:G:1824:LDA:H31	6:G:1844:HOH:O	1.86	0.72
3:P:1608:BCL:CBB	3:P:1608:BCL:HMB1	2.19	0.72
4:R:1818:LDA:C9	6:R:1852:HOH:O	2.30	0.72
4:A:1817:LDA:H11	6:A:1820:HOH:O	1.90	0.72
2:D:37:THR:HG22	2:D:39:TRP:H	1.54	0.71
1:M:33:ALA:HA	4:M:1827:LDA:HM11	1.70	0.71
3:P:1608:BCL:HBC1	6:P:1837:HOH:O	1.90	0.71
4:G:1824:LDA:HM23	6:I:1859:HOH:O	1.89	0.71
4:E:1822:LDA:HM22	6:E:1859:HOH:O	1.83	0.71
2:H:23:LEU:HB2	3:H:1604:BCL:H2	1.72	0.71
1:E:14:ILE:CG2	6:E:1835:HOH:O	2.30	0.70
1:A:20:LEU:HD13	3:R:1709:BCL:HED3	1.73	0.70
2:N:39:TRP:CD2	3:N:1607:BCL:HMC2	2.26	0.70
3:O:1508:BCL:HHC	3:O:1508:BCL:OBB	1.89	0.70
4:R:1818:LDA:C9	6:R:1856:HOH:O	2.39	0.70
2:B:1:ALA:N	6:B:278:HOH:O	2.23	0.70
2:H:39:TRP:CE3	3:H:1604:BCL:CBC	2.75	0.70
1:M:49:VAL:HG12	6:M:1843:HOH:O	1.91	0.70
4:N:1807:LDA:HM12	6:N:1810:HOH:O	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1824:LDA:C6	6:G:1865:HOH:O	2.38	0.70
1:K:48:GLY:HA2	6:K:1829:HOH:O	1.90	0.70
4:R:1818:LDA:C10	6:R:1856:HOH:O	2.40	0.70
3:K:1506:BCL:HMC3	4:L:1806:LDA:H51	1.71	0.70
4:K:1810:LDA:H101	6:K:1856:HOH:O	1.92	0.70
2:P:41:HIS:NE2	1:R:49:VAL:HG13	2.06	0.70
3:F:1603:BCL:HMB1	3:F:1603:BCL:HBB2	1.72	0.69
3:R:1509:BCL:O1D	3:R:1509:BCL:H2A	1.92	0.69
3:M:1707:BCL:C7	3:M:1707:BCL:H41	2.22	0.69
1:E:44:TYR:CE1	6:E:1862:HOH:O	2.44	0.69
1:E:49:VAL:CG1	6:E:1850:HOH:O	2.16	0.69
2:J:26:ALA:HB1	6:J:1825:HOH:O	1.92	0.69
2:F:2:THR:HG22	6:F:1823:HOH:O	1.92	0.69
3:K:1706:BCL:HBB2	3:K:1706:BCL:HHC	1.73	0.69
2:P:41:HIS:NE2	1:R:49:VAL:HG12	2.07	0.69
1:G:41:PHE:HB3	1:G:42:PRO:HD3	1.75	0.68
2:N:39:TRP:CE2	3:N:1607:BCL:HMC2	2.27	0.68
4:R:1818:LDA:H71	6:R:1852:HOH:O	1.93	0.68
3:I:1705:BCL:HHB	2:J:19:THR:HG21	1.76	0.68
1:R:48:GLY:HA2	6:R:1823:HOH:O	1.92	0.68
6:A:1850:HOH:O	2:B:3:LEU:HB2	1.94	0.68
1:K:30:VAL:CG2	5:L:1406:RG1:HM03	2.24	0.68
1:R:37:HIS:ND1	6:R:1845:HOH:O	2.27	0.68
3:J:1605:BCL:CGD	6:J:1813:HOH:O	2.27	0.68
3:G:1704:BCL:C10	6:H:1808:HOH:O	2.40	0.67
3:A:1501:BCL:O1D	3:A:1501:BCL:C2A	2.42	0.67
3:O:1508:BCL:O1D	3:O:1508:BCL:HAA2	1.95	0.67
6:E:1862:HOH:O	4:F:1803:LDA:C3	2.42	0.67
2:F:41:HIS:CE1	1:G:49:VAL:H	2.12	0.67
3:L:1606:BCL:CHB	3:M:1507:BCL:HMB3	2.24	0.67
1:A:35:LEU:HD21	1:R:37:HIS:CD2	2.30	0.67
1:I:31:HIS:CE1	3:J:1605:BCL:HMD1	2.30	0.66
3:R:1709:BCL:C10	6:S:419:HOH:O	2.41	0.66
4:I:1825:LDA:HM11	6:I:1859:HOH:O	1.95	0.66
1:I:41:PHE:HB3	1:I:42:PRO:HD3	1.78	0.66
2:J:41:HIS:NE2	1:K:49:VAL:CG1	2.58	0.66
3:F:1603:BCL:H62	3:F:1603:BCL:H112	1.76	0.66
4:K:1810:LDA:H21	1:M:14:ILE:CD1	2.25	0.66
3:G:1704:BCL:H101	6:H:1808:HOH:O	1.96	0.65
1:A:14:ILE:HG21	4:A:1816:LDA:C4	2.26	0.65
2:B:41:HIS:O	6:B:186:HOH:O	2.13	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1403:RG1:O1'	6:F:1827:HOH:O	2.13	0.65
1:I:51:LYS:HB2	1:I:52:ALA:HA	1.77	0.65
3:F:1603:BCL:H142	3:F:1603:BCL:C10	2.26	0.65
4:E:1823:LDA:H11	6:E:1854:HOH:O	1.97	0.65
1:R:1:CXM:HE2	6:R:1842:HOH:O	1.96	0.65
3:G:1704:BCL:CB D	6:G:1854:HOH:O	2.44	0.64
1:O:41:PHE:HB3	1:O:42:PRO:HD3	1.77	0.64
4:E:1823:LDA:HM21	6:E:1853:HOH:O	1.96	0.64
1:G:50:LYS:NZ	6:G:1840:HOH:O	2.29	0.64
4:I:1825:LDA:C9	6:K:1842:HOH:O	2.41	0.64
1:R:5:LYS:CD	6:R:1835:HOH:O	2.37	0.64
1:C:36:SER:OG	4:E:1822:LDA:CM2	2.43	0.64
1:K:14:ILE:HG21	4:K:1810:LDA:H31	1.79	0.64
1:K:30:VAL:HG22	5:L:1406:RG1:HM03	1.80	0.64
2:B:41:HIS:NE2	1:C:49:VAL:HG12	2.13	0.64
1:E:49:VAL:HG21	6:E:1849:HOH:O	1.96	0.63
2:D:37:THR:CG2	2:D:39:TRP:H	2.11	0.63
4:F:1803:LDA:C8	6:F:1809:HOH:O	2.44	0.63
2:B:19:THR:CG2	3:B:1601:BCL:H42	2.27	0.63
3:M:1707:BCL:C8	3:M:1707:BCL:H41	2.27	0.63
3:M:1707:BCL:H141	2:N:30:HIS:ND1	2.12	0.63
4:G:1824:LDA:H52	6:G:1865:HOH:O	1.98	0.63
2:N:23:LEU:HD22	3:N:1607:BCL:H61	1.79	0.63
3:H:1604:BCL:HMB1	3:H:1604:BCL:HBB2	1.79	0.63
1:A:48:GLY:HA2	6:A:1843:HOH:O	1.98	0.63
3:G:1704:BCL:HAA1	3:G:1704:BCL:O1D	1.98	0.63
2:H:39:TRP:CE2	3:H:1604:BCL:HMC2	2.34	0.63
2:J:30:HIS:CE1	6:J:1825:HOH:O	2.50	0.63
2:N:17:ASP:CG	6:N:1829:HOH:O	2.35	0.63
2:P:37:THR:CG2	2:P:39:TRP:H	2.12	0.63
2:D:41:HIS:NE2	1:E:49:VAL:HG23	2.14	0.62
3:J:1605:BCL:HBB2	3:J:1605:BCL:HMB1	1.81	0.62
4:O:1820:LDA:C12	6:O:1850:HOH:O	2.42	0.62
2:D:38:PRO:O	1:E:47:GLY:HA3	1.99	0.62
4:G:1824:LDA:C5	6:G:1865:HOH:O	2.46	0.62
3:I:1705:BCL:H2	3:J:1605:BCL:H192	1.82	0.62
3:S:1609:BCL:HBB2	3:S:1609:BCL:HMB1	1.80	0.62
2:B:4:THR:H	2:B:7:GLN:HE21	1.47	0.62
3:A:1701:BCL:HBB2	3:A:1701:BCL:HHC	1.82	0.62
4:G:1824:LDA:H61	6:G:1865:HOH:O	1.99	0.62
3:R:1709:BCL:C2	6:R:1831:HOH:O	2.28	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:16:ILE:HB	1:R:17:PRO:HD3	1.82	0.62
4:E:1822:LDA:HM23	6:E:1859:HOH:O	1.82	0.62
2:H:37:THR:HG22	2:H:39:TRP:H	1.65	0.62
2:J:7:GLN:NE2	6:J:1812:HOH:O	2.31	0.62
4:I:1812:LDA:C2	6:K:1860:HOH:O	2.47	0.61
3:G:1704:BCL:HED2	3:I:1505:BCL:H191	1.81	0.61
3:R:1709:BCL:H41	3:R:1709:BCL:C8	2.31	0.61
3:B:1601:BCL:CHB	3:C:1502:BCL:HMB3	2.31	0.61
2:P:41:HIS:CD2	1:R:49:VAL:N	2.69	0.61
2:F:37:THR:CG2	2:F:39:TRP:H	2.14	0.60
1:E:31:HIS:CE1	3:F:1603:BCL:HMD1	2.37	0.60
3:G:1704:BCL:O1D	3:I:1505:BCL:C5	2.49	0.60
3:G:1704:BCL:HBB	2:H:19:THR:HG21	1.83	0.60
3:N:1607:BCL:CBB	3:N:1607:BCL:HMB1	2.30	0.60
3:A:1501:BCL:HMB1	3:A:1501:BCL:CBB	2.32	0.60
2:F:9:GLU:OE1	6:F:1804:HOH:O	2.15	0.60
2:J:37:THR:HG23	2:J:39:TRP:H	1.67	0.60
3:C:1702:BCL:HBB2	3:C:1702:BCL:HHC	1.84	0.60
3:M:1707:BCL:O1D	3:O:1508:BCL:C5	2.50	0.60
2:P:34:PHE:CG	6:P:1817:HOH:O	2.51	0.60
3:F:1603:BCL:C6	3:F:1603:BCL:H112	2.31	0.60
3:A:1501:BCL:O1D	3:A:1501:BCL:CBA	2.49	0.60
4:G:1824:LDA:HM21	6:G:1828:HOH:O	1.99	0.60
2:H:33:ALA:N	6:H:1825:HOH:O	2.35	0.60
3:K:1506:BCL:HBB1	6:K:1851:HOH:O	2.02	0.59
2:L:39:TRP:HA	6:M:1862:HOH:O	2.01	0.59
3:O:1708:BCL:H91	3:P:1608:BCL:HBB	1.84	0.59
1:A:41:PHE:HB3	1:A:42:PRO:HD3	1.84	0.59
1:R:31:HIS:CE1	3:S:1609:BCL:HMD1	2.37	0.59
3:A:1701:BCL:C1D	6:A:1831:HOH:O	2.49	0.59
2:J:37:THR:CG2	2:J:39:TRP:H	2.15	0.59
1:R:48:GLY:CA	6:R:1823:HOH:O	2.49	0.59
3:M:1707:BCL:H143	2:N:27:LEU:HD23	1.83	0.59
3:M:1707:BCL:CED	3:O:1508:BCL:H191	2.33	0.59
2:D:33:ALA:HB2	6:D:1806:HOH:O	2.00	0.59
1:M:5:LYS:HE3	6:M:1856:HOH:O	2.01	0.59
6:E:1862:HOH:O	4:F:1803:LDA:H42	2.02	0.59
1:A:14:ILE:CD1	4:A:1816:LDA:H22	2.33	0.58
1:G:14:ILE:HD13	4:G:1814:LDA:C4	2.33	0.58
5:N:1407:RG1:HM82	3:O:1508:BCL:HAA1	1.84	0.58
2:J:41:HIS:HB3	1:K:50:LYS:NZ	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:34:PHE:CD2	2:P:34:PHE:C	2.77	0.58
2:B:41:HIS:NE2	1:C:49:VAL:CG1	2.66	0.58
3:A:1701:BCL:CHD	6:A:1831:HOH:O	2.51	0.58
2:P:34:PHE:CD1	6:P:1817:HOH:O	2.55	0.58
3:G:1704:BCL:C7	6:G:1863:HOH:O	2.52	0.58
3:M:1707:BCL:O1D	3:M:1707:BCL:HAA1	2.04	0.58
4:R:1818:LDA:H92	6:R:1856:HOH:O	2.02	0.58
6:E:1862:HOH:O	4:F:1803:LDA:C4	2.51	0.57
3:P:1608:BCL:CAC	6:P:1837:HOH:O	2.51	0.57
3:K:1706:BCL:H191	6:M:1849:HOH:O	2.04	0.57
3:R:1509:BCL:HBB3	3:R:1509:BCL:HMB1	1.86	0.57
1:G:31:HIS:CE1	3:H:1604:BCL:HMD1	2.40	0.57
6:K:1861:HOH:O	1:M:12:PRO:C	2.43	0.57
3:M:1707:BCL:H71	6:N:1831:HOH:O	2.04	0.57
5:P:1408:RG1:HM82	3:R:1509:BCL:HAA1	1.87	0.57
2:S:33:ALA:O	2:S:37:THR:CG2	2.50	0.57
4:M:1827:LDA:HM22	1:O:32:LEU:HD22	1.85	0.57
5:P:1408:RG1:HM82	3:R:1509:BCL:CAA	2.35	0.57
1:C:8:THR:HG22	2:D:3:LEU:O	2.05	0.57
2:H:37:THR:CG2	2:H:39:TRP:H	2.18	0.57
3:C:1702:BCL:H42	3:E:1503:BCL:CMA	2.35	0.57
2:L:37:THR:CG2	2:L:39:TRP:H	2.18	0.57
2:L:39:TRP:CZ2	3:L:1606:BCL:CMC	2.88	0.57
4:R:1818:LDA:C12	6:R:1856:HOH:O	2.48	0.56
1:C:5:LYS:NZ	2:D:9:GLU:OE2	2.34	0.56
2:J:6:GLU:CD	6:J:1821:HOH:O	2.42	0.56
2:L:39:TRP:CD2	3:L:1606:BCL:HMC1	2.40	0.56
2:J:41:HIS:CD2	1:K:49:VAL:N	2.74	0.56
2:D:41:HIS:NE2	1:E:49:VAL:CG2	2.69	0.56
1:C:9:VAL:CG2	1:E:12:PRO:HB2	2.36	0.56
3:C:1502:BCL:CBB	3:C:1502:BCL:HMB1	2.36	0.55
1:E:37:HIS:CD2	1:G:35:LEU:HD21	2.41	0.55
4:K:1810:LDA:HM22	1:M:14:ILE:CD1	2.31	0.55
1:R:5:LYS:CE	6:R:1835:HOH:O	2.54	0.55
1:A:44:TYR:HB2	4:B:1801:LDA:HM22	1.88	0.55
2:D:23:LEU:HD13	3:D:1602:BCL:H2	1.87	0.55
3:G:1504:BCL:HMB1	3:G:1504:BCL:CBB	2.37	0.55
3:I:1705:BCL:C9	3:I:1705:BCL:C4	2.84	0.55
1:K:14:ILE:HG21	4:K:1810:LDA:C5	2.36	0.55
2:B:33:ALA:O	2:B:37:THR:HB	2.07	0.55
3:R:1709:BCL:C4	3:R:1709:BCL:H92	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1501:BCL:H191	3:R:1709:BCL:CED	2.26	0.55
2:L:41:HIS:NE2	1:M:49:VAL:N	2.54	0.55
3:C:1702:BCL:CAD	3:D:1602:BCL:H192	2.36	0.55
2:F:37:THR:HG22	2:F:39:TRP:H	1.71	0.55
4:I:1812:LDA:H21	6:K:1860:HOH:O	2.05	0.55
2:P:39:TRP:HB2	6:R:1857:HOH:O	2.07	0.55
2:D:41:HIS:CD2	1:E:49:VAL:N	2.75	0.55
4:F:1803:LDA:C7	6:F:1809:HOH:O	2.54	0.55
3:A:1501:BCL:C1D	3:B:1601:BCL:HMD2	2.37	0.54
1:C:41:PHE:HB3	1:C:42:PRO:HD3	1.88	0.54
1:A:5:LYS:HG2	5:D:1402:RG1:HM12	1.90	0.54
1:K:41:PHE:HB3	1:K:42:PRO:HD3	1.88	0.54
2:L:39:TRP:CE2	3:L:1606:BCL:HMC2	2.37	0.54
3:B:1601:BCL:HMB1	3:B:1601:BCL:HBB2	1.87	0.54
1:M:14:ILE:HG13	4:M:1811:LDA:H12	1.90	0.54
3:R:1709:BCL:H122	3:R:1709:BCL:H91	1.88	0.54
2:H:2:THR:CG2	6:H:1822:HOH:O	2.55	0.54
3:M:1707:BCL:HED3	3:O:1508:BCL:H62	1.90	0.54
2:N:38:PRO:O	1:O:47:GLY:HA3	2.07	0.54
3:C:1702:BCL:H42	3:E:1503:BCL:HMA2	1.90	0.54
3:L:1606:BCL:HMA3	3:L:1606:BCL:HBA2	1.89	0.54
5:H:1404:RG1:HM01	1:I:32:LEU:HD21	1.89	0.54
2:B:18:GLY:HA2	3:R:1709:BCL:CMD	2.38	0.53
1:G:48:GLY:CA	6:G:1839:HOH:O	2.15	0.53
3:L:1606:BCL:HBC2	3:L:1606:BCL:HMC1	1.89	0.53
3:N:1607:BCL:HBC3	3:N:1607:BCL:HMC2	1.90	0.53
1:A:28:ILE:HG22	1:A:32:LEU:HD12	1.88	0.53
3:G:1704:BCL:HHC	3:G:1704:BCL:HBB2	1.90	0.53
3:K:1506:BCL:CBB	3:K:1506:BCL:HMB1	2.39	0.53
3:M:1707:BCL:HBB2	3:M:1707:BCL:HHC	1.89	0.53
1:A:39:THR:OG1	1:C:46:GLN:NE2	2.33	0.53
1:C:16:ILE:HB	1:C:17:PRO:HD3	1.89	0.53
3:E:1703:BCL:H11	3:F:1603:BCL:H192	1.90	0.53
2:J:7:GLN:NE2	6:J:1818:HOH:O	2.41	0.53
3:I:1705:BCL:H92	3:I:1705:BCL:H43	1.90	0.53
1:E:41:PHE:HB3	1:E:42:PRO:HD3	1.91	0.53
2:N:37:THR:CG2	2:N:39:TRP:H	2.22	0.53
3:R:1709:BCL:H41	3:R:1709:BCL:H8	1.91	0.53
1:A:16:ILE:HB	1:A:17:PRO:HD3	1.91	0.52
3:G:1704:BCL:O1D	3:I:1505:BCL:H62	2.09	0.52
4:G:1824:LDA:H11	6:G:1843:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:LYS:N	6:G:1832:HOH:O	2.29	0.52
1:K:4:GLY:N	6:K:1840:HOH:O	2.41	0.52
3:C:1502:BCL:HMB1	3:C:1502:BCL:HBB3	1.91	0.52
4:C:1815:LDA:HM21	1:E:14:ILE:HD13	1.91	0.52
2:N:39:TRP:CD2	3:N:1607:BCL:CMC	2.90	0.52
3:E:1503:BCL:OBB	3:E:1503:BCL:HHC	2.10	0.52
3:M:1707:BCL:CGD	6:M:1859:HOH:O	2.35	0.52
2:S:33:ALA:HB2	6:S:296:HOH:O	2.08	0.52
3:I:1705:BCL:C2	3:J:1605:BCL:H192	2.39	0.52
6:C:1838:HOH:O	3:D:1602:BCL:H121	2.10	0.52
3:E:1703:BCL:H2	3:F:1603:BCL:H162	1.92	0.52
3:A:1701:BCL:CMD	2:D:18:GLY:HA2	2.40	0.52
1:C:9:VAL:HG21	1:E:12:PRO:HB2	1.92	0.52
3:J:1605:BCL:C19	6:K:1854:HOH:O	2.57	0.52
3:L:1606:BCL:CMA	6:L:1835:HOH:O	2.58	0.52
1:K:9:VAL:HB	6:K:1861:HOH:O	2.09	0.52
6:K:1864:HOH:O	4:L:1806:LDA:C8	2.47	0.52
1:K:31:HIS:ND1	3:L:1606:BCL:HMD1	2.26	0.51
1:M:47:GLY:N	6:M:1862:HOH:O	2.43	0.51
3:A:1501:BCL:O1D	3:A:1501:BCL:H2A	2.10	0.51
1:G:14:ILE:HD13	4:G:1814:LDA:H42	1.91	0.51
1:E:1:CXM:HG2	3:E:1703:BCL:CHC	2.41	0.51
1:O:44:TYR:CE1	4:P:1808:LDA:H11	2.45	0.51
2:L:39:TRP:CD2	3:L:1606:BCL:HMC2	2.44	0.51
3:D:1602:BCL:HMB1	3:D:1602:BCL:HBB2	1.92	0.51
3:I:1705:BCL:H92	3:I:1705:BCL:C4	2.40	0.51
1:M:6:ILE:N	5:P:1408:RG1:HM32	2.25	0.51
1:O:1:CXM:HG2	3:O:1708:BCL:CHC	2.40	0.51
4:A:1816:LDA:C3	1:C:14:ILE:CD1	2.88	0.51
3:E:1703:BCL:HBB2	3:E:1703:BCL:HHC	1.93	0.51
3:I:1505:BCL:HMC3	4:J:1805:LDA:H51	1.93	0.51
1:K:1:CXM:C	6:K:1840:HOH:O	2.59	0.51
3:L:1606:BCL:HBB2	3:L:1606:BCL:HMB1	1.93	0.51
4:O:1820:LDA:CM1	6:O:1823:HOH:O	2.45	0.51
1:I:18:ALA:HA	4:I:1813:LDA:H91	1.93	0.51
2:L:37:THR:HG22	2:L:39:TRP:H	1.75	0.51
2:P:38:PRO:O	1:R:47:GLY:HA3	2.11	0.51
2:F:41:HIS:CE1	1:G:49:VAL:N	2.79	0.51
1:M:30:VAL:HG22	5:N:1407:RG1:HM03	1.93	0.51
1:R:49:VAL:O	1:R:49:VAL:HG22	2.10	0.51
4:C:1815:LDA:HM11	1:E:14:ILE:CD1	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1705:BCL:C4	3:I:1705:BCL:C8	2.83	0.50
2:J:41:HIS:NE2	1:K:49:VAL:N	2.59	0.50
3:K:1706:BCL:CMD	2:N:18:GLY:HA2	2.40	0.50
3:A:1501:BCL:O1D	3:A:1501:BCL:HBA1	2.11	0.50
3:I:1705:BCL:H141	6:J:1825:HOH:O	2.11	0.50
3:F:1603:BCL:CHB	3:G:1504:BCL:HMB3	2.42	0.50
3:L:1606:BCL:HMA2	6:L:1835:HOH:O	2.11	0.50
1:A:20:LEU:HD13	3:R:1709:BCL:CED	2.41	0.50
2:F:41:HIS:HB3	1:G:50:LYS:HE2	1.92	0.50
2:N:39:TRP:CE2	3:N:1607:BCL:HMC3	2.45	0.50
1:K:30:VAL:HG23	5:L:1406:RG1:HM03	1.93	0.50
1:G:19:LEU:O	1:G:23:VAL:HG23	2.11	0.50
2:D:7:GLN:HB3	6:D:1829:HOH:O	2.10	0.50
2:N:20:ARG:NH1	6:N:1812:HOH:O	2.45	0.49
3:O:1708:BCL:HED3	5:S:1409:RG1:HM42	1.92	0.49
1:E:25:VAL:HG11	4:E:1823:LDA:C12	2.43	0.49
4:I:1812:LDA:H111	6:K:1863:HOH:O	2.11	0.49
1:C:14:ILE:HG21	4:C:1815:LDA:C2	2.36	0.49
3:G:1504:BCL:HMD1	2:H:30:HIS:CE1	2.47	0.49
3:J:1605:BCL:HMC3	6:K:1851:HOH:O	2.12	0.49
3:M:1707:BCL:H101	6:N:1831:HOH:O	2.13	0.49
4:R:1818:LDA:C7	6:R:1852:HOH:O	2.57	0.49
3:H:1604:BCL:CHB	3:I:1505:BCL:HMB3	2.43	0.49
1:M:51:LYS:HA	1:M:52:ALA:CB	2.29	0.49
2:N:17:ASP:CB	6:N:1829:HOH:O	2.60	0.49
3:R:1509:BCL:HMB1	3:R:1509:BCL:CBB	2.42	0.49
4:E:1823:LDA:CM2	6:E:1853:HOH:O	2.57	0.49
2:H:37:THR:HG22	2:H:39:TRP:HB3	1.94	0.49
1:K:51:LYS:HD3	1:K:52:ALA:O	2.12	0.49
3:G:1704:BCL:H91	3:G:1704:BCL:H122	1.94	0.49
3:R:1509:BCL:HMD1	2:S:30:HIS:CE1	2.48	0.49
2:B:34:PHE:CD1	2:B:40:LEU:HD12	2.48	0.48
2:L:39:TRP:CZ2	3:L:1606:BCL:HMC3	2.46	0.48
2:J:41:HIS:HB3	1:K:50:LYS:HZ1	1.77	0.48
3:M:1707:BCL:HED1	3:O:1508:BCL:H191	1.94	0.48
3:M:1707:BCL:HBC3	3:N:1607:BCL:H143	1.95	0.48
1:A:49:VAL:HG12	2:S:41:HIS:NE2	2.28	0.48
3:B:1601:BCL:CBB	3:B:1601:BCL:HMB1	2.43	0.48
3:K:1706:BCL:CBB	3:K:1706:BCL:HHC	2.42	0.48
2:B:6:GLU:CG	6:B:597:HOH:O	2.62	0.48
3:F:1603:BCL:H142	3:F:1603:BCL:H101	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:LYS:NZ	2:S:9:GLU:OE2	2.46	0.48
3:E:1503:BCL:HMB1	3:E:1503:BCL:CBB	2.44	0.48
3:O:1508:BCL:HAA2	3:O:1508:BCL:CGD	2.44	0.48
3:O:1708:BCL:H3C	6:O:1822:HOH:O	2.14	0.48
1:C:14:ILE:HG13	4:C:1815:LDA:O1	2.13	0.48
1:I:5:LYS:HG2	6:J:1823:HOH:O	2.09	0.47
3:J:1605:BCL:CHB	3:K:1506:BCL:HMB3	2.44	0.47
6:C:1843:HOH:O	4:E:1822:LDA:C3	2.62	0.47
3:G:1704:BCL:C6	6:G:1863:HOH:O	2.62	0.47
3:I:1705:BCL:H2	3:J:1605:BCL:H161	1.95	0.47
1:O:5:LYS:CE	2:P:5:ALA:HB1	2.44	0.47
2:P:39:TRP:CD2	3:P:1608:BCL:HMC2	2.49	0.47
3:R:1709:BCL:C3D	3:S:1609:BCL:H203	2.44	0.47
3:S:1609:BCL:HHC	3:S:1609:BCL:OBB	2.14	0.47
2:H:39:TRP:CE3	3:H:1604:BCL:HBC2	2.47	0.47
3:G:1704:BCL:HED1	3:I:1505:BCL:H191	1.92	0.47
1:O:4:GLY:HA2	2:P:12:HIS:CD2	2.49	0.47
3:D:1602:BCL:HMB1	3:D:1602:BCL:CBB	2.44	0.47
1:M:14:ILE:HG13	4:M:1811:LDA:C1	2.44	0.47
4:M:1811:LDA:H41	1:O:14:ILE:HD12	1.95	0.47
3:M:1707:BCL:C4D	3:N:1607:BCL:H172	2.45	0.47
3:L:1606:BCL:C4A	3:M:1507:BCL:HMB3	2.45	0.47
4:O:1820:LDA:CM2	6:O:1823:HOH:O	2.49	0.47
2:F:37:THR:HG22	2:F:39:TRP:HB3	1.96	0.47
1:I:8:THR:HG22	2:J:3:LEU:O	2.15	0.47
2:L:39:TRP:CZ2	3:L:1606:BCL:HMC2	2.50	0.47
1:M:1:CXM:CN	2:N:16:ILE:HD11	2.44	0.47
1:R:50:LYS:O	1:R:51:LYS:HB2	2.14	0.47
4:A:1816:LDA:H32	1:C:14:ILE:CD1	2.44	0.47
3:F:1603:BCL:HMB1	3:F:1603:BCL:CBB	2.40	0.47
6:C:1843:HOH:O	4:E:1822:LDA:C2	2.63	0.47
2:N:37:THR:HG22	2:N:39:TRP:HB3	1.96	0.47
6:E:1862:HOH:O	4:F:1803:LDA:H31	2.08	0.47
3:B:1601:BCL:OBB	3:B:1601:BCL:HHC	2.14	0.47
1:I:31:HIS:ND1	3:J:1605:BCL:HMD1	2.30	0.47
1:M:1:CXM:HG2	3:M:1707:BCL:CHC	2.45	0.47
2:D:37:THR:HG22	2:D:39:TRP:HB3	1.97	0.46
4:G:1824:LDA:HM12	6:G:1828:HOH:O	1.94	0.46
1:O:5:LYS:HE2	2:P:5:ALA:HB1	1.96	0.46
3:B:1601:BCL:H62	3:B:1601:BCL:H112	1.97	0.46
1:R:14:ILE:HD11	4:R:1818:LDA:H11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1502:BCL:CHD	6:D:1806:HOH:O	2.62	0.46
4:E:1823:LDA:HM11	6:E:1853:HOH:O	2.14	0.46
3:I:1705:BCL:C9	3:I:1705:BCL:H41	2.46	0.46
1:K:14:ILE:HG21	4:K:1810:LDA:H52	1.95	0.46
3:L:1606:BCL:CGD	3:L:1606:BCL:H2A	2.45	0.46
2:L:4:THR:OG1	2:L:7:GLN:HG3	2.14	0.46
3:S:1609:BCL:H43	6:S:515:HOH:O	2.14	0.46
6:R:1831:HOH:O	3:S:1609:BCL:C19	2.62	0.46
3:J:1605:BCL:HAA1	6:J:1825:HOH:O	2.14	0.46
1:M:30:VAL:CG2	5:N:1407:RG1:HM03	2.46	0.46
2:H:39:TRP:CD2	3:H:1604:BCL:HBC3	2.51	0.46
3:I:1705:BCL:HMB1	3:I:1705:BCL:OBB	2.16	0.46
1:M:1:CXM:SD	2:N:20:ARG:NH2	2.88	0.46
3:J:1605:BCL:HBB3	6:K:1864:HOH:O	2.03	0.46
3:C:1702:BCL:CMD	2:F:18:GLY:HA2	2.45	0.46
2:J:37:THR:HG22	2:J:39:TRP:HB3	1.97	0.46
3:A:1501:BCL:HMB1	3:A:1501:BCL:HBB3	1.98	0.46
3:O:1708:BCL:HBC3	6:O:1822:HOH:O	2.16	0.46
2:F:38:PRO:O	1:G:47:GLY:HA3	2.16	0.45
2:H:11:LEU:CD1	5:H:1404:RG1:H41	2.47	0.45
4:K:1826:LDA:C12	6:K:1863:HOH:O	2.64	0.45
3:K:1506:BCL:CMC	4:L:1806:LDA:H51	2.45	0.45
4:I:1825:LDA:HM12	6:I:1840:HOH:O	2.16	0.45
4:K:1826:LDA:H121	6:K:1847:HOH:O	2.17	0.45
2:P:37:THR:HG22	2:P:39:TRP:N	2.23	0.45
1:I:51:LYS:HB2	1:I:52:ALA:CA	2.45	0.45
1:I:14:ILE:HD11	6:I:1862:HOH:O	2.15	0.45
2:J:37:THR:CG2	2:J:39:TRP:HB3	2.47	0.45
3:M:1507:BCL:HMD2	3:N:1607:BCL:CHD	2.46	0.45
2:P:3:LEU:HD21	6:P:1824:HOH:O	2.16	0.45
2:B:4:THR:HG23	2:B:7:GLN:NE2	2.32	0.45
2:D:1:ALA:N	6:D:1826:HOH:O	2.49	0.45
3:G:1704:BCL:CED	1:I:20:LEU:HD13	2.47	0.45
5:H:1404:RG1:H7	5:H:1404:RG1:HM31	1.83	0.45
3:G:1704:BCL:HMB2	3:H:1604:BCL:H61	1.98	0.45
2:N:17:ASP:HB3	6:N:1829:HOH:O	2.15	0.45
1:O:4:GLY:HA2	2:P:12:HIS:CG	2.52	0.45
2:B:19:THR:HG21	3:B:1601:BCL:H42	1.99	0.45
2:B:37:THR:CG2	2:B:39:TRP:H	2.25	0.45
2:F:2:THR:HG21	6:F:1825:HOH:O	2.17	0.45
3:G:1704:BCL:C4D	3:H:1604:BCL:H172	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:1708:BCL:HMB1	3:O:1708:BCL:OBB	2.16	0.45
5:H:1404:RG1:HM41	5:H:1404:RG1:H11	1.87	0.45
3:I:1705:BCL:C9	3:I:1705:BCL:H43	2.47	0.45
3:G:1704:BCL:CMD	2:J:18:GLY:HA2	2.46	0.45
1:A:21:GLY:HA3	4:A:1817:LDA:H101	1.99	0.45
1:A:49:VAL:CG1	2:S:41:HIS:NE2	2.80	0.45
3:B:1601:BCL:H2	6:B:282:HOH:O	2.15	0.45
2:H:29:ALA:HA	4:H:1804:LDA:H112	1.99	0.45
3:A:1701:BCL:H92	3:B:1601:BCL:H92	1.99	0.44
3:I:1705:BCL:HBB2	3:I:1705:BCL:HHC	1.99	0.44
1:C:5:LYS:HZ1	2:D:9:GLU:HG3	1.81	0.44
1:E:51:LYS:O	1:E:52:ALA:HB2	2.18	0.44
3:I:1505:BCL:HMD1	2:J:30:HIS:CE1	2.53	0.44
3:I:1705:BCL:C14	6:J:1825:HOH:O	2.65	0.44
2:L:36:ALA:HB1	4:L:1806:LDA:H32	1.99	0.44
3:M:1507:BCL:HMD1	2:N:30:HIS:CE1	2.52	0.44
3:E:1703:BCL:HHB	2:F:19:THR:HG21	1.98	0.44
3:G:1504:BCL:HBB3	3:G:1504:BCL:HMB1	1.98	0.44
2:P:19:THR:CG2	3:P:1608:BCL:H42	2.47	0.44
3:J:1605:BCL:HBB1	6:K:1864:HOH:O	2.06	0.44
1:K:9:VAL:HG12	6:K:1853:HOH:O	2.17	0.44
1:C:23:VAL:HG13	3:D:1602:BCL:HED1	1.98	0.44
2:J:39:TRP:CD2	3:J:1605:BCL:HBC2	2.53	0.44
5:L:1406:RG1:H11	5:L:1406:RG1:HM41	1.86	0.44
2:F:4:THR:HG1	2:F:7:GLN:CD	2.21	0.44
4:M:1811:LDA:H21	1:O:14:ILE:CD1	2.47	0.44
2:B:38:PRO:O	1:C:47:GLY:HA3	2.18	0.44
5:D:1402:RG1:HM31	5:D:1402:RG1:H7	1.82	0.44
1:E:25:VAL:HG11	4:E:1823:LDA:H111	1.99	0.44
3:I:1505:BCL:HMB1	3:I:1505:BCL:CBB	2.48	0.44
1:M:39:THR:OG1	1:O:46:GLN:NE2	2.37	0.44
3:A:1701:BCL:HMB1	3:A:1701:BCL:OBB	2.18	0.44
3:E:1503:BCL:HMD1	2:F:30:HIS:CE1	2.52	0.44
1:A:43:ALA:HA	6:A:1825:HOH:O	2.17	0.43
2:B:37:THR:CG2	2:B:39:TRP:HB3	2.48	0.43
1:R:41:PHE:HB3	1:R:42:PRO:CD	2.48	0.43
2:D:6:GLU:CB	6:D:1825:HOH:O	2.41	0.43
2:L:39:TRP:CE3	3:L:1606:BCL:HMC2	2.53	0.43
3:O:1708:BCL:HHC	3:O:1708:BCL:HBB2	2.00	0.43
4:K:1826:LDA:H121	6:K:1863:HOH:O	2.17	0.43
2:N:37:THR:HG23	2:N:39:TRP:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1822:LDA:O1	6:E:1859:HOH:O	2.20	0.43
1:K:16:ILE:HB	1:K:17:PRO:HD3	1.99	0.43
5:R:1401:RG1:H20	5:R:1401:RG1:HM61	1.85	0.43
2:B:6:GLU:HG2	6:B:597:HOH:O	2.18	0.43
5:J:1405:RG1:H7	5:J:1405:RG1:HM31	1.84	0.43
3:L:1606:BCL:CMA	3:L:1606:BCL:HBA2	2.49	0.43
3:M:1507:BCL:HBD	3:M:1507:BCL:HAA2	2.00	0.43
3:M:1707:BCL:H91	3:M:1707:BCL:H112	1.77	0.43
2:N:33:ALA:CB	3:N:1607:BCL:HBC1	2.48	0.43
3:A:1501:BCL:H3C	4:B:1801:LDA:H71	2.01	0.43
1:A:8:THR:HG22	2:B:3:LEU:O	2.19	0.43
2:F:41:HIS:HB3	1:G:50:LYS:CG	2.49	0.43
3:G:1704:BCL:CGD	6:G:1854:HOH:O	2.64	0.43
1:E:14:ILE:HG13	4:G:1814:LDA:H12	2.00	0.43
3:I:1705:BCL:C4	3:K:1506:BCL:HMA2	2.47	0.43
3:C:1502:BCL:C1D	3:D:1602:BCL:HMD2	2.49	0.43
1:E:4:GLY:HA2	2:F:12:HIS:CD2	2.54	0.43
2:F:41:HIS:HE1	1:G:49:VAL:H	1.60	0.43
3:I:1705:BCL:O1A	3:K:1506:BCL:H2	2.19	0.43
2:F:14:TYR:CE1	5:F:1403:RG1:HM11	2.53	0.43
3:F:1603:BCL:C14	3:F:1603:BCL:C10	2.97	0.43
5:H:1404:RG1:HM22	5:H:1404:RG1:H1'	1.73	0.43
1:A:49:VAL:N	2:S:41:HIS:CD2	2.87	0.42
1:A:50:LYS:HG3	6:A:1833:HOH:O	2.18	0.42
3:I:1705:BCL:C2	6:K:1854:HOH:O	2.67	0.42
5:S:1409:RG1:H7	5:S:1409:RG1:HM31	1.77	0.42
2:N:29:ALA:HB1	4:N:1807:LDA:H112	2.01	0.42
4:R:1818:LDA:C8	6:R:1852:HOH:O	2.64	0.42
4:K:1826:LDA:H22	4:K:1826:LDA:HM22	1.87	0.42
1:M:14:ILE:HG22	6:M:1852:HOH:O	2.19	0.42
1:G:26:ILE:HG12	1:I:28:ILE:HD11	2.01	0.42
1:K:40:TRP:HH2	3:K:1506:BCL:CBC	2.32	0.42
2:J:41:HIS:CE1	1:K:49:VAL:HG12	2.53	0.42
5:N:1407:RG1:H7	5:N:1407:RG1:HM31	1.85	0.42
2:F:4:THR:OG1	2:F:7:GLN:CD	2.58	0.42
2:P:13:LYS:NZ	6:P:1835:HOH:O	2.52	0.42
5:R:1401:RG1:HM31	5:R:1401:RG1:H7	1.80	0.42
3:C:1702:BCL:OBD	5:F:1403:RG1:H11	2.19	0.42
2:F:23:LEU:HB2	3:F:1603:BCL:H2	2.01	0.42
3:R:1509:BCL:HMD2	3:S:1609:BCL:CHD	2.50	0.42
3:A:1701:BCL:OBD	5:D:1402:RG1:H11	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1847:HOH:O	2:J:6:GLU:HA	2.20	0.42
3:M:1507:BCL:CBB	3:M:1507:BCL:HMB1	2.50	0.42
2:N:4:THR:H	2:N:7:GLN:HE21	1.67	0.42
1:O:44:TYR:HB2	4:P:1808:LDA:HM11	2.02	0.42
3:A:1501:BCL:HED3	2:B:22:PHE:CE1	2.55	0.42
2:L:39:TRP:CG	3:L:1606:BCL:HMC1	2.54	0.42
2:N:37:THR:HG22	2:N:39:TRP:H	1.85	0.42
2:P:17:ASP:O	2:P:21:VAL:HG23	2.20	0.42
3:S:1609:BCL:CBB	3:S:1609:BCL:HMB1	2.48	0.42
3:A:1501:BCL:OBB	3:A:1501:BCL:HHC	2.20	0.42
5:P:1408:RG1:H7	5:P:1408:RG1:HM31	1.91	0.42
1:A:13:ALA:HB1	4:A:1817:LDA:HM11	2.02	0.42
3:A:1701:BCL:HMB3	2:B:16:ILE:HG23	2.01	0.42
5:D:1402:RG1:HM51	5:D:1402:RG1:H15	1.92	0.42
5:S:1409:RG1:C17	3:S:1609:BCL:H12	2.50	0.42
1:C:44:TYR:CD1	4:D:1802:LDA:HM21	2.55	0.41
2:F:37:THR:HG23	2:F:39:TRP:H	1.84	0.41
1:I:14:ILE:HD13	4:I:1812:LDA:HM12	2.02	0.41
2:N:9:GLU:O	2:N:13:LYS:HD2	2.19	0.41
3:O:1508:BCL:H12	2:P:22:PHE:HE1	1.85	0.41
5:S:1409:RG1:H15	5:S:1409:RG1:HM51	1.91	0.41
5:F:1403:RG1:HM13	5:F:1403:RG1:H1'	1.79	0.41
1:G:5:LYS:HE2	2:H:9:GLU:OE2	2.20	0.41
3:M:1507:BCL:H102	3:M:1507:BCL:H61	1.93	0.41
1:O:43:ALA:HB2	6:O:1830:HOH:O	2.20	0.41
3:C:1702:BCL:H41	3:C:1702:BCL:C8	2.49	0.41
3:I:1705:BCL:CMD	2:L:18:GLY:HA2	2.50	0.41
4:I:1812:LDA:H22	6:K:1860:HOH:O	2.13	0.41
4:I:1825:LDA:CM1	6:I:1859:HOH:O	2.60	0.41
3:M:1707:BCL:OBB	3:M:1707:BCL:HMB1	2.19	0.41
1:M:41:PHE:O	1:M:44:TYR:HB3	2.19	0.41
1:O:49:VAL:O	1:O:49:VAL:HG13	2.21	0.41
3:C:1702:BCL:H192	2:D:39:TRP:HZ2	1.85	0.41
3:G:1504:BCL:HHC	3:G:1504:BCL:OBB	2.20	0.41
1:I:18:ALA:HA	4:I:1813:LDA:C9	2.50	0.41
1:M:16:ILE:HB	1:M:17:PRO:HD3	2.02	0.41
5:R:1401:RG1:CM1	5:R:1401:RG1:O5'	2.68	0.41
1:I:16:ILE:HB	1:I:17:PRO:HD3	2.02	0.41
3:K:1706:BCL:H2C	3:K:1706:BCL:HBC3	1.87	0.41
3:O:1508:BCL:H3C	4:P:1808:LDA:H51	2.02	0.41
1:O:32:LEU:HD23	1:O:32:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:O	1:A:8:THR:OG1	2.31	0.41
1:C:44:TYR:CD1	4:D:1802:LDA:H11	2.55	0.41
1:K:48:GLY:CA	6:K:1829:HOH:O	2.60	0.41
1:C:16:ILE:O	1:C:20:LEU:HG	2.21	0.41
3:E:1703:BCL:H161	3:E:1703:BCL:H202	1.74	0.41
3:I:1505:BCL:HMB1	3:I:1505:BCL:HBB3	2.03	0.41
1:K:1:CXM:C	1:K:1:CXM:ON1	2.69	0.41
3:L:1606:BCL:HMA1	3:L:1606:BCL:HHB	1.93	0.41
4:C:1815:LDA:HM11	1:E:14:ILE:HD13	2.03	0.41
1:E:1:CXM:HG2	3:E:1703:BCL:HHC	2.03	0.41
4:F:1803:LDA:H82	6:F:1809:HOH:O	2.17	0.41
1:K:50:LYS:O	1:K:51:LYS:CB	2.69	0.41
2:L:38:PRO:O	1:M:47:GLY:HA3	2.21	0.41
3:O:1708:BCL:HHC	3:O:1708:BCL:CBB	2.51	0.41
2:P:6:GLU:HG2	2:P:10:GLU:OE2	2.21	0.41
1:A:5:LYS:HE3	2:B:5:ALA:HB1	2.01	0.41
3:C:1502:BCL:HMD1	2:D:30:HIS:CE1	2.56	0.41
2:L:37:THR:HG22	2:L:39:TRP:HB3	2.02	0.41
1:M:31:HIS:ND1	3:N:1607:BCL:HMD1	2.35	0.41
2:N:4:THR:H	2:N:7:GLN:NE2	2.19	0.41
5:D:1402:RG1:H11	5:D:1402:RG1:HM41	1.98	0.40
2:F:41:HIS:HB3	1:G:50:LYS:CE	2.51	0.40
4:G:1824:LDA:HM22	4:G:1824:LDA:H22	1.78	0.40
1:G:30:VAL:HG12	3:H:1604:BCL:HMD3	2.03	0.40
3:O:1508:BCL:CHD	3:O:1508:BCL:HBC2	2.50	0.40
6:B:517:HOH:O	1:R:5:LYS:HE2	2.21	0.40
1:C:44:TYR:CE1	4:D:1802:LDA:H11	2.56	0.40
3:G:1704:BCL:O1D	3:I:1505:BCL:C6	2.69	0.40
2:N:5:ALA:HB3	6:N:1826:HOH:O	2.20	0.40
3:R:1709:BCL:H92	3:S:1609:BCL:H51	2.03	0.40
3:C:1502:BCL:HHC	3:C:1502:BCL:OBB	2.21	0.40
2:H:39:TRP:NE1	3:H:1604:BCL:HMC2	2.35	0.40
3:R:1709:BCL:C4D	3:S:1609:BCL:H172	2.52	0.40
3:A:1501:BCL:HED3	2:B:22:PHE:CZ	2.56	0.40
2:L:23:LEU:HB2	3:L:1606:BCL:H2	2.04	0.40
2:N:39:TRP:CZ3	3:N:1607:BCL:HBC3	2.57	0.40
2:P:41:HIS:HA	6:R:1823:HOH:O	2.22	0.40
3:G:1704:BCL:O1D	3:I:1505:BCL:H52	2.22	0.40
2:H:41:HIS:CD2	1:I:49:VAL:C	2.95	0.40
3:K:1506:BCL:HBC1	3:L:1606:BCL:CBC	2.51	0.40
2:P:37:THR:HG23	2:P:38:PRO:HD2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:1401:RG1:HM41	5:R:1401:RG1:H11	1.87	0.40
5:S:1409:RG1:HM61	5:S:1409:RG1:H20	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
1	C	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	1	0
1	E	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	0
1	G	51/53 (96%)	51 (100%)	0	0	100	100
1	I	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	K	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	7	5
1	M	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	1	0
1	O	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	7	5
1	R	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	1	0
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%)	38 (97%)	1 (3%)	0	100	100
2	S	39/41 (95%)	39 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	810/846 (96%)	775 (96%)	21 (3%)	14 (2%)	9	7

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	LYS
1	E	51	LYS
1	E	52	ALA
1	K	50	LYS
1	M	50	LYS
1	M	51	LYS
1	M	52	ALA
1	R	51	LYS
1	C	51	LYS
1	R	50	LYS
1	R	52	ALA
1	C	52	ALA
1	E	50	LYS
1	O	50	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	40/40 (100%)	37 (92%)	3 (8%)	13	16
1	C	40/40 (100%)	37 (92%)	3 (8%)	13	16
1	E	40/40 (100%)	34 (85%)	6 (15%)	3	2
1	G	40/40 (100%)	36 (90%)	4 (10%)	7	7
1	I	40/40 (100%)	35 (88%)	5 (12%)	4	3
1	K	40/40 (100%)	39 (98%)	1 (2%)	47	60
1	M	40/40 (100%)	38 (95%)	2 (5%)	24	32
1	O	40/40 (100%)	38 (95%)	2 (5%)	24	32
1	R	40/40 (100%)	36 (90%)	4 (10%)	7	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	D	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	F	33/33 (100%)	29 (88%)	4 (12%)	5	4
2	H	33/33 (100%)	29 (88%)	4 (12%)	5	4
2	J	33/33 (100%)	31 (94%)	2 (6%)	18	24
2	L	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	N	33/33 (100%)	30 (91%)	3 (9%)	9	10
2	P	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	S	33/33 (100%)	29 (88%)	4 (12%)	5	4
All	All	657/657 (100%)	594 (90%)	63 (10%)	8	8

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	41	PHE
1	A	51	LYS
2	B	2	THR
2	B	6	GLU
2	B	37	THR
1	C	9	VAL
1	C	41	PHE
1	C	50	LYS
2	D	2	THR
2	D	35	SER
2	D	37	THR
1	E	5	LYS
1	E	9	VAL
1	E	14	ILE
1	E	41	PHE
1	E	49	VAL
1	E	50	LYS
2	F	2	THR
2	F	13	LYS
2	F	17	ASP
2	F	37	THR
1	G	36	SER
1	G	41	PHE
1	G	50	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	51	LYS
2	H	2	THR
2	H	13	LYS
2	H	17	ASP
2	H	37	THR
1	I	5	LYS
1	I	36	SER
1	I	41	PHE
1	I	50	LYS
1	I	51	LYS
2	J	2	THR
2	J	37	THR
1	K	50	LYS
2	L	2	THR
2	L	6	GLU
2	L	13	LYS
2	L	17	ASP
2	L	37	THR
1	M	9	VAL
1	M	41	PHE
2	N	2	THR
2	N	13	LYS
2	N	37	THR
1	O	5	LYS
1	O	41	PHE
2	P	2	THR
2	P	13	LYS
2	P	17	ASP
2	P	34	PHE
2	P	37	THR
1	R	16	ILE
1	R	36	SER
1	R	41	PHE
1	R	50	LYS
2	S	2	THR
2	S	6	GLU
2	S	10	GLU
2	S	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	7	GLN
2	D	7	GLN
1	E	37	HIS
2	H	7	GLN
1	I	37	HIS
1	K	37	HIS
2	L	7	GLN
2	N	7	GLN
1	R	37	HIS
2	S	7	GLN

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	CXM	M	1	1,3	6,10,11	2.99	1 (16%)	5,11,13	1.19	1 (20%)
1	CXM	I	1	1,3	6,10,11	1.22	1 (16%)	5,11,13	1.03	0
1	CXM	O	1	1,3	6,10,11	1.29	1 (16%)	5,11,13	0.86	0
1	CXM	E	1	1,3	6,10,11	1.31	1 (16%)	5,11,13	1.28	0
1	CXM	K	1	1,3	6,10,11	1.62	2 (33%)	5,11,13	1.15	0
1	CXM	A	1	1,3	6,10,11	1.64	1 (16%)	5,11,13	1.28	1 (20%)
1	CXM	G	1	1,3	6,10,11	1.64	1 (16%)	5,11,13	1.02	1 (20%)
1	CXM	R	1	1,3	6,10,11	1.16	0	5,11,13	0.68	0
1	CXM	C	1	1,3	6,10,11	1.70	1 (16%)	5,11,13	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	M	1	1,3	-	1/7/10/12	-
1	CXM	I	1	1,3	-	0/7/10/12	-
1	CXM	O	1	1,3	-	1/7/10/12	-
1	CXM	E	1	1,3	-	1/7/10/12	-
1	CXM	K	1	1,3	-	2/7/10/12	-
1	CXM	A	1	1,3	-	2/7/10/12	-
1	CXM	G	1	1,3	-	2/7/10/12	-
1	CXM	R	1	1,3	-	2/7/10/12	-
1	CXM	C	1	1,3	-	0/7/10/12	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	1	CXM	CE-SD	7.14	2.21	1.78
1	G	1	CXM	CE-SD	3.60	2.00	1.78
1	C	1	CXM	CE-SD	3.06	1.97	1.78
1	A	1	CXM	CA-N	2.79	1.50	1.46
1	O	1	CXM	CB-CA	-2.66	1.48	1.53
1	E	1	CXM	CE-SD	2.38	1.93	1.78
1	K	1	CXM	CB-CA	-2.28	1.49	1.53
1	K	1	CXM	CA-N	2.26	1.49	1.46
1	I	1	CXM	CA-N	2.22	1.49	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1	CXM	C-CA-N	2.12	113.56	109.73
1	G	1	CXM	O-C-CA	-2.11	119.26	124.78
1	A	1	CXM	C-CA-N	2.06	113.45	109.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	K	1	CXM	O-C-CA-CB
1	A	1	CXM	C-CA-CB-CG
1	G	1	CXM	O-C-CA-CB
1	R	1	CXM	O-C-CA-CB
1	O	1	CXM	CB-CG-SD-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	G	1	CXM	C-CA-CB-CG
1	M	1	CXM	C-CA-N-CN
1	E	1	CXM	C-CA-N-CN
1	K	1	CXM	C-CA-N-CN
1	A	1	CXM	C-CA-N-CN
1	R	1	CXM	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	M	1	CXM	4	0
1	O	1	CXM	1	0
1	E	1	CXM	2	0
1	K	1	CXM	2	0
1	R	1	CXM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

63 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	BCL	M	1507	1	58,74,74	2.21	14 (24%)	69,115,115	2.58	22 (31%)
3	BCL	G	1504	1	58,74,74	2.36	12 (20%)	69,115,115	2.25	25 (36%)
5	RG1	N	1407	-	52,52,52	1.22	4 (7%)	64,67,67	1.55	13 (20%)
3	BCL	A	1501	1	58,74,74	2.32	16 (27%)	69,115,115	2.44	23 (33%)
4	LDA	L	1806	-	12,15,15	2.08	1 (8%)	14,17,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LDA	K	1810	-	12,15,15	2.15	1 (8%)	14,17,17	0.49	0
4	LDA	M	1827	-	12,15,15	2.01	1 (8%)	14,17,17	0.42	0
3	BCL	C	1502	1	58,74,74	1.95	16 (27%)	69,115,115	2.36	23 (33%)
3	BCL	N	1607	2	58,74,74	2.15	14 (24%)	69,115,115	2.52	21 (30%)
3	BCL	R	1509	1	58,74,74	2.39	15 (25%)	69,115,115	2.60	25 (36%)
3	BCL	D	1602	2	58,74,74	2.37	19 (32%)	69,115,115	2.49	22 (31%)
3	BCL	P	1608	2	58,74,74	2.27	19 (32%)	69,115,115	2.47	23 (33%)
3	BCL	E	1703	1	58,74,74	2.12	10 (17%)	69,115,115	2.13	21 (30%)
4	LDA	D	1802	-	12,15,15	2.08	1 (8%)	14,17,17	0.61	0
3	BCL	K	1706	1	58,74,74	2.17	14 (24%)	69,115,115	2.37	19 (27%)
3	BCL	M	1707	1	58,74,74	2.33	15 (25%)	69,115,115	2.13	18 (26%)
3	BCL	G	1704	1	58,74,74	2.23	16 (27%)	69,115,115	2.43	24 (34%)
3	BCL	O	1708	1	58,74,74	2.35	15 (25%)	69,115,115	2.21	20 (28%)
4	LDA	E	1823	-	12,15,15	1.87	1 (8%)	14,17,17	0.46	0
5	RG1	P	1408	-	52,52,52	1.38	10 (19%)	64,67,67	1.60	12 (18%)
3	BCL	L	1606	2	58,74,74	2.37	20 (34%)	69,115,115	3.04	24 (34%)
3	BCL	A	1701	1	58,74,74	2.78	22 (37%)	69,115,115	2.46	23 (33%)
4	LDA	N	1807	-	12,15,15	1.92	1 (8%)	14,17,17	0.38	0
4	LDA	P	1808	-	12,15,15	1.94	1 (8%)	14,17,17	0.58	0
3	BCL	I	1505	1	58,74,74	2.03	15 (25%)	69,115,115	2.20	19 (27%)
4	LDA	G	1814	-	12,15,15	2.08	1 (8%)	14,17,17	0.44	0
4	LDA	J	1805	-	12,15,15	1.90	1 (8%)	14,17,17	0.31	0
5	RG1	D	1402	-	52,52,52	1.29	7 (13%)	64,67,67	1.63	16 (25%)
3	BCL	K	1506	1	58,74,74	2.54	18 (31%)	69,115,115	2.54	25 (36%)
4	LDA	A	1816	-	12,15,15	2.00	1 (8%)	14,17,17	0.36	0
4	LDA	R	1819	-	12,15,15	1.92	1 (8%)	14,17,17	0.42	0
3	BCL	J	1605	2	58,74,74	2.26	18 (31%)	69,115,115	2.64	23 (33%)
3	BCL	O	1508	1	58,74,74	2.18	13 (22%)	69,115,115	2.39	25 (36%)
4	LDA	K	1826	-	12,15,15	1.89	1 (8%)	14,17,17	0.53	0
4	LDA	A	1817	-	12,15,15	2.01	1 (8%)	14,17,17	0.44	0
3	BCL	S	1609	2	58,74,74	2.06	13 (22%)	69,115,115	2.47	23 (33%)
3	BCL	C	1702	1	58,74,74	2.37	15 (25%)	69,115,115	2.27	21 (30%)
4	LDA	I	1825	-	12,15,15	2.06	1 (8%)	14,17,17	0.51	0
3	BCL	I	1705	1	58,74,74	2.20	18 (31%)	69,115,115	2.29	16 (23%)
4	LDA	C	1815	-	12,15,15	2.11	1 (8%)	14,17,17	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	RG1	S	1409	-	52,52,52	1.38	8 (15%)	64,67,67	1.57	16 (25%)
3	BCL	F	1603	2	58,74,74	2.10	14 (24%)	69,115,115	2.31	22 (31%)
4	LDA	G	1824	-	12,15,15	2.08	1 (8%)	14,17,17	0.35	0
4	LDA	F	1803	-	12,15,15	2.25	1 (8%)	14,17,17	0.57	0
3	BCL	R	1709	1	58,74,74	2.52	22 (37%)	69,115,115	2.28	22 (31%)
5	RG1	H	1404	-	52,52,52	1.34	5 (9%)	64,67,67	1.66	13 (20%)
3	BCL	B	1601	2	58,74,74	2.05	15 (25%)	69,115,115	2.70	21 (30%)
5	RG1	J	1405	-	52,52,52	1.28	6 (11%)	64,67,67	1.61	14 (21%)
4	LDA	I	1812	-	12,15,15	2.39	1 (8%)	14,17,17	0.37	0
4	LDA	R	1818	-	12,15,15	2.00	1 (8%)	14,17,17	0.46	0
4	LDA	H	1804	-	12,15,15	1.90	1 (8%)	14,17,17	0.57	0
5	RG1	R	1401	-	52,52,52	1.26	5 (9%)	64,67,67	1.69	12 (18%)
4	LDA	E	1822	-	12,15,15	1.89	1 (8%)	14,17,17	0.51	0
5	RG1	F	1403	-	52,52,52	1.34	5 (9%)	64,67,67	1.64	17 (26%)
4	LDA	B	1801	-	12,15,15	2.13	1 (8%)	14,17,17	0.43	0
4	LDA	I	1813	-	12,15,15	2.05	1 (8%)	14,17,17	0.40	0
5	RG1	L	1406	-	52,52,52	1.37	7 (13%)	64,67,67	1.50	13 (20%)
4	LDA	O	1820	-	12,15,15	2.14	1 (8%)	14,17,17	0.43	0
4	LDA	C	1821	-	12,15,15	1.92	1 (8%)	14,17,17	0.41	0
4	LDA	R	1809	-	12,15,15	1.97	1 (8%)	14,17,17	0.52	0
3	BCL	E	1503	1	58,74,74	2.07	13 (22%)	69,115,115	2.42	21 (30%)
3	BCL	H	1604	2	58,74,74	2.12	18 (31%)	69,115,115	2.52	29 (42%)
4	LDA	M	1811	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BCL	M	1507	1	-	5/37/137/137	-
3	BCL	G	1504	1	-	7/37/137/137	-
5	RG1	N	1407	-	-	3/51/71/71	0/1/1/1
3	BCL	A	1501	1	1/1/21/25	5/37/137/137	-
4	LDA	L	1806	-	-	10/13/13/13	-
4	LDA	K	1810	-	-	7/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	M	1827	-	-	4/13/13/13	-
3	BCL	C	1502	1	1/1/21/25	6/37/137/137	-
3	BCL	N	1607	2	1/1/21/25	18/37/137/137	-
3	BCL	R	1509	1	1/1/21/25	10/37/137/137	-
3	BCL	D	1602	2	-	9/37/137/137	-
3	BCL	P	1608	2	2/2/21/25	16/37/137/137	-
3	BCL	E	1703	1	-	14/37/137/137	-
4	LDA	D	1802	-	-	8/13/13/13	-
3	BCL	K	1706	1	1/1/21/25	6/37/137/137	-
3	BCL	M	1707	1	1/1/21/25	13/37/137/137	-
3	BCL	G	1704	1	1/1/21/25	8/37/137/137	-
3	BCL	O	1708	1	1/1/21/25	11/37/137/137	-
4	LDA	E	1823	-	-	5/13/13/13	-
5	RG1	P	1408	-	-	7/51/71/71	0/1/1/1
3	BCL	L	1606	2	3/3/21/25	9/37/137/137	-
3	BCL	A	1701	1	1/1/21/25	11/37/137/137	-
4	LDA	N	1807	-	-	6/13/13/13	-
4	LDA	P	1808	-	-	8/13/13/13	-
3	BCL	I	1505	1	-	6/37/137/137	-
4	LDA	G	1814	-	-	8/13/13/13	-
4	LDA	J	1805	-	-	9/13/13/13	-
5	RG1	D	1402	-	-	4/51/71/71	0/1/1/1
3	BCL	K	1506	1	1/1/21/25	8/37/137/137	-
4	LDA	A	1816	-	-	6/13/13/13	-
4	LDA	R	1819	-	-	8/13/13/13	-
3	BCL	J	1605	2	1/1/21/25	11/37/137/137	-
3	BCL	O	1508	1	2/2/21/25	11/37/137/137	-
4	LDA	K	1826	-	-	6/13/13/13	-
4	LDA	A	1817	-	-	9/13/13/13	-
3	BCL	R	1709	1	1/1/21/25	16/37/137/137	-
3	BCL	C	1702	1	1/1/21/25	16/37/137/137	-
4	LDA	I	1825	-	-	8/13/13/13	-
3	BCL	I	1705	1	-	8/37/137/137	-
4	LDA	C	1815	-	-	6/13/13/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RG1	S	1409	-	-	3/51/71/71	0/1/1/1
3	BCL	F	1603	2	-	12/37/137/137	-
4	LDA	G	1824	-	-	4/13/13/13	-
4	LDA	F	1803	-	-	9/13/13/13	-
3	BCL	S	1609	2	1/1/21/25	15/37/137/137	-
5	RG1	H	1404	-	-	9/51/71/71	0/1/1/1
3	BCL	B	1601	2	1/1/21/25	10/37/137/137	-
5	RG1	J	1405	-	-	6/51/71/71	0/1/1/1
4	LDA	I	1812	-	-	7/13/13/13	-
4	LDA	R	1818	-	-	5/13/13/13	-
4	LDA	H	1804	-	-	6/13/13/13	-
5	RG1	R	1401	-	-	3/51/71/71	0/1/1/1
4	LDA	E	1822	-	-	7/13/13/13	-
5	RG1	F	1403	-	-	4/51/71/71	0/1/1/1
4	LDA	B	1801	-	-	8/13/13/13	-
4	LDA	I	1813	-	-	5/13/13/13	-
5	RG1	L	1406	-	-	5/51/71/71	0/1/1/1
4	LDA	O	1820	-	-	5/13/13/13	-
4	LDA	C	1821	-	-	5/13/13/13	-
4	LDA	R	1809	-	-	10/13/13/13	-
3	BCL	E	1503	1	-	7/37/137/137	-
3	BCL	H	1604	2	1/1/21/25	15/37/137/137	-
4	LDA	M	1811	-	-	7/13/13/13	-

All (513) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1702	BCL	C2-C3	8.30	1.52	1.33
3	K	1506	BCL	CAC-C3C	-7.93	1.38	1.54
3	G	1504	BCL	C4B-NB	7.91	1.42	1.35
4	I	1812	LDA	O1-N1	-7.79	1.23	1.42
3	R	1509	BCL	C4B-NB	7.41	1.41	1.35
3	A	1701	BCL	C2-C3	7.40	1.50	1.33
3	S	1609	BCL	C2-C3	7.39	1.50	1.33
3	J	1605	BCL	C2-C3	7.23	1.50	1.33
3	A	1701	BCL	C3C-C4C	-7.23	1.42	1.51
3	O	1708	BCL	C2-C3	7.16	1.50	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1803	LDA	O1-N1	-7.14	1.25	1.42
4	K	1810	LDA	O1-N1	-7.09	1.25	1.42
4	O	1820	LDA	O1-N1	-7.09	1.25	1.42
4	D	1802	LDA	O1-N1	-7.08	1.25	1.42
3	G	1704	BCL	C2-C3	7.07	1.49	1.33
3	M	1707	BCL	CBD-CGD	-7.00	1.30	1.52
4	G	1824	LDA	O1-N1	-6.99	1.25	1.42
4	I	1813	LDA	O1-N1	-6.90	1.26	1.42
4	I	1825	LDA	O1-N1	-6.89	1.26	1.42
3	R	1709	BCL	C1B-NB	6.88	1.41	1.35
3	O	1508	BCL	C3B-C2B	6.87	1.51	1.39
3	M	1507	BCL	C3B-C2B	6.86	1.51	1.39
3	E	1503	BCL	C2-C3	6.85	1.49	1.33
3	M	1507	BCL	C3D-C2D	6.84	1.51	1.39
3	G	1504	BCL	C3B-C2B	6.82	1.51	1.39
4	A	1817	LDA	O1-N1	-6.80	1.26	1.42
4	L	1806	LDA	O1-N1	-6.79	1.26	1.42
4	C	1815	LDA	O1-N1	-6.78	1.26	1.42
3	K	1506	BCL	C3B-C2B	6.74	1.51	1.39
3	L	1606	BCL	C3B-C2B	6.74	1.51	1.39
3	R	1709	BCL	C2-C3	6.69	1.49	1.33
3	N	1607	BCL	C2-C3	6.69	1.49	1.33
4	M	1827	LDA	O1-N1	-6.68	1.26	1.42
3	G	1704	BCL	C4B-NB	6.67	1.41	1.35
3	A	1501	BCL	C2-C3	6.63	1.48	1.33
3	A	1701	BCL	C1B-NB	6.63	1.41	1.35
3	E	1503	BCL	C3B-C2B	6.60	1.51	1.39
4	G	1814	LDA	O1-N1	-6.59	1.26	1.42
3	F	1603	BCL	C3D-C2D	6.57	1.51	1.39
3	M	1707	BCL	C2-C3	6.56	1.48	1.33
4	B	1801	LDA	O1-N1	-6.55	1.26	1.42
3	I	1505	BCL	C4B-NB	6.53	1.41	1.35
4	H	1804	LDA	O1-N1	-6.49	1.27	1.42
3	M	1507	BCL	C2-C3	6.48	1.48	1.33
3	O	1708	BCL	C4B-NB	6.48	1.41	1.35
3	K	1506	BCL	C2-C3	6.46	1.48	1.33
4	A	1816	LDA	O1-N1	-6.46	1.27	1.42
4	R	1819	LDA	O1-N1	-6.45	1.27	1.42
4	R	1818	LDA	O1-N1	-6.45	1.27	1.42
4	K	1826	LDA	O1-N1	-6.45	1.27	1.42
3	B	1601	BCL	C2-C3	6.43	1.48	1.33
3	D	1602	BCL	C2-C3	6.42	1.48	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1602	BCL	C3B-C2B	6.40	1.50	1.39
4	C	1821	LDA	O1-N1	-6.37	1.27	1.42
4	E	1822	LDA	O1-N1	-6.37	1.27	1.42
4	P	1808	LDA	O1-N1	-6.37	1.27	1.42
3	R	1709	BCL	C3B-C2B	6.34	1.50	1.39
3	I	1705	BCL	C4B-NB	6.34	1.40	1.35
3	C	1702	BCL	C3B-C2B	6.32	1.50	1.39
4	R	1809	LDA	O1-N1	-6.29	1.27	1.42
3	K	1706	BCL	C4B-NB	6.27	1.40	1.35
4	E	1823	LDA	O1-N1	-6.27	1.27	1.42
3	C	1702	BCL	C3D-C2D	6.23	1.50	1.39
3	P	1608	BCL	C2-C3	6.23	1.47	1.33
3	E	1703	BCL	C3B-C2B	6.23	1.50	1.39
3	R	1509	BCL	OBD-CAD	6.21	1.31	1.22
3	F	1603	BCL	C2-C3	6.20	1.47	1.33
4	M	1811	LDA	O1-N1	-6.20	1.27	1.42
3	M	1707	BCL	C1B-NB	6.19	1.40	1.35
3	H	1604	BCL	C2-C3	6.19	1.47	1.33
3	E	1703	BCL	C2-C3	6.10	1.47	1.33
3	C	1502	BCL	C2-C3	6.04	1.47	1.33
3	R	1709	BCL	C4B-NB	6.04	1.40	1.35
3	E	1703	BCL	C3D-C2D	6.04	1.50	1.39
3	E	1503	BCL	C3D-C2D	5.95	1.50	1.39
3	G	1504	BCL	C2-C3	5.95	1.47	1.33
3	K	1706	BCL	C2-C3	5.92	1.47	1.33
3	A	1501	BCL	OBD-CAD	5.87	1.30	1.22
3	R	1509	BCL	C2-C3	5.86	1.47	1.33
3	E	1703	BCL	O1D-CGD	5.86	1.35	1.21
4	N	1807	LDA	O1-N1	-5.84	1.28	1.42
3	J	1605	BCL	C3B-C2B	5.78	1.49	1.39
4	J	1805	LDA	O1-N1	-5.77	1.28	1.42
3	A	1501	BCL	C4B-NB	5.77	1.40	1.35
3	J	1605	BCL	C1D-C2D	5.75	1.55	1.42
3	O	1708	BCL	C3D-C2D	5.75	1.49	1.39
3	F	1603	BCL	C3B-C2B	5.75	1.49	1.39
3	D	1602	BCL	C1B-NB	5.75	1.40	1.35
3	B	1601	BCL	C3B-C2B	5.71	1.49	1.39
3	P	1608	BCL	OBD-CAD	5.70	1.30	1.22
3	D	1602	BCL	C3D-C2D	5.68	1.49	1.39
3	O	1708	BCL	C3B-C2B	5.66	1.49	1.39
3	S	1609	BCL	C3D-C2D	5.63	1.49	1.39
3	R	1709	BCL	C3D-C2D	5.62	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1708	BCL	C1B-NB	5.57	1.40	1.35
3	O	1508	BCL	OBD-CAD	5.57	1.30	1.22
3	N	1607	BCL	C3D-C2D	5.55	1.49	1.39
3	K	1706	BCL	C3D-C2D	5.47	1.49	1.39
3	O	1508	BCL	C2-C3	5.47	1.46	1.33
3	P	1608	BCL	O1D-CGD	5.47	1.34	1.21
3	L	1606	BCL	C2C-C3C	-5.47	1.39	1.54
3	K	1706	BCL	C1D-C2D	5.46	1.54	1.42
3	N	1607	BCL	CMC-C2C	-5.41	1.41	1.53
3	A	1701	BCL	C3D-C2D	5.41	1.49	1.39
3	M	1707	BCL	C1D-C2D	5.38	1.54	1.42
3	A	1701	BCL	OBD-CAD	5.38	1.29	1.22
3	S	1609	BCL	C3B-C2B	5.37	1.49	1.39
3	L	1606	BCL	C2-C3	5.33	1.45	1.33
3	I	1705	BCL	C1D-C2D	5.32	1.54	1.42
3	C	1702	BCL	C1B-NB	5.29	1.39	1.35
3	G	1504	BCL	C1D-C2D	5.28	1.54	1.42
3	M	1707	BCL	OBD-CAD	5.27	1.29	1.22
3	A	1701	BCL	C1D-C2D	5.25	1.54	1.42
3	R	1509	BCL	C3A-C2A	-5.19	1.40	1.54
3	G	1704	BCL	C3B-C2B	5.19	1.48	1.39
3	I	1505	BCL	C3B-C2B	5.18	1.48	1.39
3	H	1604	BCL	C3C-C4C	-5.15	1.45	1.51
3	I	1705	BCL	C3D-C2D	5.14	1.48	1.39
3	H	1604	BCL	C3B-C2B	5.14	1.48	1.39
3	I	1705	BCL	C2-C3	5.10	1.45	1.33
3	R	1509	BCL	C3B-C2B	5.08	1.48	1.39
3	R	1509	BCL	C3D-C2D	5.07	1.48	1.39
3	K	1506	BCL	CAA-C2A	5.06	1.63	1.54
3	C	1702	BCL	O1D-CGD	5.00	1.33	1.21
3	G	1704	BCL	C3D-C2D	4.93	1.48	1.39
3	P	1608	BCL	C1B-NB	4.93	1.39	1.35
3	P	1608	BCL	C3D-C2D	4.93	1.48	1.39
3	J	1605	BCL	CBD-CGD	-4.91	1.37	1.52
3	A	1701	BCL	C3B-C2B	4.91	1.48	1.39
3	E	1703	BCL	C1D-C2D	4.88	1.53	1.42
3	G	1504	BCL	O1D-CGD	4.87	1.33	1.21
3	H	1604	BCL	C3D-C2D	4.86	1.48	1.39
3	K	1506	BCL	O1D-CGD	4.84	1.33	1.21
3	B	1601	BCL	C1D-C2D	4.81	1.53	1.42
3	O	1508	BCL	C4B-NB	4.81	1.39	1.35
3	A	1501	BCL	C3D-C2D	4.80	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1702	BCL	C1D-C2D	4.78	1.53	1.42
5	F	1403	RG1	C19-C18	4.77	1.56	1.45
3	C	1502	BCL	C1B-NB	4.76	1.39	1.35
3	F	1603	BCL	C1B-NB	4.70	1.39	1.35
3	I	1505	BCL	C1D-C2D	4.70	1.53	1.42
3	M	1507	BCL	C1B-NB	4.68	1.39	1.35
3	K	1506	BCL	C3D-C2D	4.66	1.47	1.39
3	A	1701	BCL	CAC-C3C	-4.61	1.44	1.54
3	O	1508	BCL	C1D-C2D	4.61	1.53	1.42
3	G	1704	BCL	CBD-CGD	-4.59	1.38	1.52
3	C	1502	BCL	C3B-C2B	4.58	1.47	1.39
3	B	1601	BCL	C3D-C2D	4.53	1.47	1.39
3	O	1708	BCL	O1D-CGD	4.50	1.32	1.21
3	A	1501	BCL	C3B-C2B	4.50	1.47	1.39
3	D	1602	BCL	C4B-NB	4.49	1.39	1.35
3	R	1709	BCL	C1D-C2D	4.49	1.52	1.42
3	G	1504	BCL	MG-NA	4.47	2.16	2.06
3	G	1504	BCL	OBD-CAD	4.46	1.28	1.22
3	S	1609	BCL	C1B-NB	4.44	1.39	1.35
3	N	1607	BCL	C2C-C3C	-4.43	1.42	1.54
3	R	1509	BCL	C1D-C2D	4.43	1.52	1.42
3	D	1602	BCL	MG-NA	4.42	2.16	2.06
3	K	1506	BCL	O2D-CGD	4.41	1.44	1.33
3	L	1606	BCL	MG-NC	4.39	2.16	2.06
3	M	1707	BCL	MG-NA	4.37	2.16	2.06
3	A	1701	BCL	MG-NA	4.34	2.16	2.06
3	B	1601	BCL	OBD-CAD	4.32	1.28	1.22
3	O	1708	BCL	C1D-C2D	4.31	1.52	1.42
5	N	1407	RG1	O1'-C1	-4.30	1.40	1.46
3	K	1506	BCL	C1B-NB	4.30	1.39	1.35
3	K	1706	BCL	O1D-CGD	4.26	1.31	1.21
3	J	1605	BCL	MG-NA	4.24	2.16	2.06
3	I	1505	BCL	C2-C3	4.23	1.43	1.33
3	K	1706	BCL	C3B-C2B	4.21	1.47	1.39
3	G	1504	BCL	C3D-C2D	4.18	1.46	1.39
3	C	1702	BCL	C4B-NB	4.16	1.38	1.35
3	H	1604	BCL	O1D-CGD	4.15	1.31	1.21
3	K	1506	BCL	C4B-NB	4.14	1.38	1.35
3	A	1501	BCL	MG-NA	4.12	2.16	2.06
3	C	1502	BCL	C3D-C2D	4.12	1.46	1.39
3	O	1508	BCL	C1B-NB	4.11	1.38	1.35
3	E	1503	BCL	C1B-NB	4.10	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	BCL	C1B-NB	4.10	1.38	1.35
3	R	1509	BCL	O1D-CGD	4.10	1.31	1.21
3	L	1606	BCL	O1D-CGD	4.09	1.31	1.21
3	E	1703	BCL	C4B-NB	4.06	1.38	1.35
3	O	1508	BCL	C14-C13	-4.05	1.40	1.52
3	S	1609	BCL	OBD-CAD	4.05	1.28	1.22
3	N	1607	BCL	C1B-NB	4.04	1.38	1.35
3	L	1606	BCL	CMC-C2C	-4.03	1.44	1.53
3	C	1502	BCL	OBD-CAD	4.02	1.27	1.22
3	A	1701	BCL	O1D-CGD	4.00	1.31	1.21
3	J	1605	BCL	C3D-C2D	4.00	1.46	1.39
3	I	1705	BCL	OBD-CAD	3.97	1.27	1.22
3	A	1501	BCL	O1A-CGA	3.95	1.34	1.22
3	A	1701	BCL	O1A-CGA	3.93	1.34	1.22
3	L	1606	BCL	C3D-C2D	3.90	1.46	1.39
3	O	1508	BCL	CBD-CGD	-3.90	1.40	1.52
3	N	1607	BCL	MG-NA	3.88	2.15	2.06
3	E	1503	BCL	OBD-CAD	3.85	1.27	1.22
3	F	1603	BCL	OBD-CAD	3.81	1.27	1.22
3	G	1704	BCL	C1D-C2D	3.80	1.51	1.42
3	N	1607	BCL	OBD-CAD	3.80	1.27	1.22
3	F	1603	BCL	C4B-NB	3.79	1.38	1.35
3	L	1606	BCL	OBD-CAD	3.79	1.27	1.22
3	M	1507	BCL	O1D-CGD	3.79	1.30	1.21
3	J	1605	BCL	C1B-NB	3.74	1.38	1.35
5	R	1401	RG1	C6-C5	3.74	1.38	1.34
3	A	1701	BCL	C4B-NB	3.73	1.38	1.35
3	I	1505	BCL	O2D-CGD	3.71	1.42	1.33
3	R	1709	BCL	MG-NA	3.70	2.15	2.06
3	A	1501	BCL	O1D-CGD	3.70	1.30	1.21
3	I	1705	BCL	C3B-C2B	3.70	1.46	1.39
3	O	1508	BCL	O1A-CGA	3.70	1.33	1.22
3	I	1705	BCL	O1A-CGA	3.70	1.33	1.22
3	P	1608	BCL	C2C-C3C	-3.69	1.44	1.54
3	M	1507	BCL	C1D-C2D	3.69	1.50	1.42
3	D	1602	BCL	C2A-C1A	-3.69	1.43	1.52
3	D	1602	BCL	OBD-CAD	3.68	1.27	1.22
3	F	1603	BCL	C1D-C2D	3.65	1.50	1.42
3	I	1505	BCL	MG-NC	3.65	2.14	2.06
3	I	1705	BCL	O2D-CGD	3.65	1.42	1.33
3	A	1701	BCL	O2D-CGD	3.62	1.42	1.33
3	K	1706	BCL	OBD-CAD	3.62	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1405	RG1	C6-C5	-3.58	1.30	1.34
3	P	1608	BCL	C3B-C2B	3.57	1.45	1.39
3	N	1607	BCL	C3B-C2B	3.57	1.45	1.39
3	L	1606	BCL	C4B-NB	3.54	1.38	1.35
3	M	1507	BCL	C4B-NB	3.52	1.38	1.35
3	G	1704	BCL	MG-NC	3.52	2.14	2.06
3	D	1602	BCL	O1A-CGA	3.51	1.33	1.22
3	M	1507	BCL	O2D-CGD	3.51	1.41	1.33
3	R	1709	BCL	C1B-CHB	3.48	1.50	1.41
3	I	1505	BCL	C4B-CHC	3.47	1.50	1.41
5	S	1409	RG1	C2-C1	3.46	1.58	1.53
3	R	1509	BCL	O1A-CGA	3.45	1.32	1.22
3	D	1602	BCL	O2A-CGA	3.44	1.43	1.33
3	M	1707	BCL	C3B-C2B	3.43	1.45	1.39
3	B	1601	BCL	O1D-CGD	3.43	1.29	1.21
3	P	1608	BCL	MG-NC	3.43	2.14	2.06
3	E	1703	BCL	MG-NC	3.41	2.14	2.06
3	H	1604	BCL	O1A-CGA	3.41	1.32	1.22
3	L	1606	BCL	C3A-C4A	-3.40	1.40	1.51
3	I	1505	BCL	O1A-CGA	3.39	1.32	1.22
3	H	1604	BCL	C1D-C2D	3.38	1.50	1.42
3	I	1705	BCL	CAA-C2A	3.37	1.60	1.54
5	H	1404	RG1	C2-C1	3.37	1.58	1.53
3	K	1706	BCL	OBB-CAB	3.36	1.33	1.22
3	K	1506	BCL	C2C-C3C	-3.35	1.45	1.54
3	N	1607	BCL	C1D-C2D	3.34	1.50	1.42
3	L	1606	BCL	C1B-NB	3.33	1.38	1.35
3	B	1601	BCL	C1B-NB	3.30	1.38	1.35
3	G	1704	BCL	C3C-C4C	-3.30	1.47	1.51
3	M	1707	BCL	C3C-C4C	-3.29	1.47	1.51
3	A	1501	BCL	C3C-C4C	3.29	1.55	1.51
3	D	1602	BCL	C1B-CHB	3.29	1.50	1.41
3	C	1502	BCL	C1D-C2D	3.27	1.50	1.42
3	J	1605	BCL	O1A-CGA	3.26	1.32	1.22
3	P	1608	BCL	CMC-C2C	-3.26	1.46	1.53
5	D	1402	RG1	C6-C5	3.24	1.37	1.34
3	P	1608	BCL	MG-NA	3.24	2.14	2.06
3	M	1707	BCL	C1B-CHB	3.24	1.50	1.41
5	L	1406	RG1	C17-C18	3.24	1.40	1.35
3	K	1506	BCL	C1D-C2D	3.24	1.49	1.42
3	I	1505	BCL	C1B-CHB	3.23	1.50	1.41
3	O	1508	BCL	C3D-C2D	3.23	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1409	RG1	O1'-C1	-3.23	1.42	1.46
3	G	1704	BCL	MG-NA	3.22	2.13	2.06
3	R	1709	BCL	MG-NC	3.22	2.13	2.06
3	A	1501	BCL	C1D-C2D	3.21	1.49	1.42
3	L	1606	BCL	CMA-C3A	-3.20	1.46	1.53
3	O	1708	BCL	MG-NA	3.20	2.13	2.06
3	F	1603	BCL	C5-C3	3.19	1.57	1.51
3	S	1609	BCL	O1D-CGD	3.19	1.29	1.21
3	N	1607	BCL	C4B-NB	3.19	1.38	1.35
3	R	1509	BCL	C3C-C4C	-3.19	1.47	1.51
3	L	1606	BCL	C4B-CHC	3.19	1.49	1.41
5	L	1406	RG1	C16-C15	3.17	1.44	1.36
3	G	1504	BCL	C1B-NB	3.17	1.38	1.35
3	L	1606	BCL	C3A-C2A	-3.16	1.45	1.54
3	A	1501	BCL	CBD-CGD	-3.16	1.42	1.52
3	E	1503	BCL	C4B-NB	3.13	1.38	1.35
3	M	1707	BCL	MG-NC	3.11	2.13	2.06
3	A	1501	BCL	O2D-CGD	3.11	1.40	1.33
3	K	1506	BCL	O2A-CGA	3.10	1.42	1.33
3	H	1604	BCL	C1B-CHB	3.10	1.49	1.41
3	I	1705	BCL	C3D-CAD	3.10	1.53	1.46
3	A	1701	BCL	C1B-CHB	3.10	1.49	1.41
5	N	1407	RG1	C21-C22	3.10	1.39	1.35
3	K	1706	BCL	O1A-CGA	3.10	1.31	1.22
3	R	1709	BCL	O1D-CGD	3.09	1.29	1.21
5	J	1405	RG1	O1'-C1	-3.08	1.42	1.46
3	E	1503	BCL	O1A-CGA	3.07	1.31	1.22
3	H	1604	BCL	C4B-CHC	3.07	1.49	1.41
3	R	1709	BCL	C5-C3	3.04	1.57	1.51
3	L	1606	BCL	C1D-C2D	3.03	1.49	1.42
5	H	1404	RG1	C23-C22	3.02	1.52	1.45
5	L	1406	RG1	C16-C17	3.01	1.52	1.43
3	D	1602	BCL	MG-NC	3.01	2.13	2.06
3	S	1609	BCL	O2A-CGA	3.00	1.42	1.33
5	P	1408	RG1	C17-C18	2.99	1.39	1.35
3	A	1701	BCL	C2C-C3C	-2.99	1.46	1.54
5	S	1409	RG1	C14-C13	-2.98	1.31	1.35
3	F	1603	BCL	O2D-CGD	2.98	1.40	1.33
3	P	1608	BCL	C1D-C2D	2.98	1.49	1.42
3	J	1605	BCL	O2A-CGA	2.98	1.42	1.33
3	E	1503	BCL	O1D-CGD	2.98	1.28	1.21
3	C	1502	BCL	MG-NC	2.97	2.13	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1503	BCL	MG-NC	2.97	2.13	2.06
3	O	1508	BCL	OBB-CAB	2.96	1.32	1.22
3	H	1604	BCL	OBD-CAD	2.96	1.26	1.22
3	N	1607	BCL	CBD-CGD	-2.95	1.43	1.52
3	S	1609	BCL	MG-NC	2.95	2.13	2.06
3	R	1709	BCL	O1A-CGA	2.94	1.31	1.22
3	B	1601	BCL	O2D-CGD	2.94	1.40	1.33
5	P	1408	RG1	C23-C22	2.93	1.52	1.45
3	G	1704	BCL	CBD-CHA	-2.92	1.38	1.52
3	C	1702	BCL	O1A-CGA	2.92	1.31	1.22
3	K	1706	BCL	MG-NC	2.92	2.13	2.06
3	D	1602	BCL	O1D-CGD	2.91	1.28	1.21
3	C	1502	BCL	C1B-CHB	2.89	1.49	1.41
5	S	1409	RG1	C24-C25	2.89	1.52	1.43
3	A	1701	BCL	O2A-CGA	2.89	1.41	1.33
3	N	1607	BCL	O1A-CGA	2.89	1.31	1.22
5	H	1404	RG1	C27-C26	2.88	1.52	1.45
3	K	1506	BCL	C3B-CAB	2.87	1.56	1.49
3	K	1706	BCL	MG-NA	2.87	2.13	2.06
3	J	1605	BCL	MG-NC	2.87	2.13	2.06
5	F	1403	RG1	C24-C25	2.87	1.52	1.43
3	O	1708	BCL	MG-NC	2.86	2.13	2.06
3	J	1605	BCL	CBA-CGA	-2.86	1.42	1.50
3	G	1704	BCL	C1B-CHB	2.85	1.48	1.41
3	J	1605	BCL	O1D-CGD	2.85	1.28	1.21
3	P	1608	BCL	O2D-CGD	2.85	1.40	1.33
3	C	1702	BCL	OBD-CAD	2.85	1.26	1.22
3	S	1609	BCL	C1B-CHB	2.85	1.48	1.41
3	P	1608	BCL	C1B-CHB	2.84	1.48	1.41
3	L	1606	BCL	O1A-CGA	2.84	1.31	1.22
3	M	1507	BCL	MG-NC	2.83	2.13	2.06
3	R	1709	BCL	C2A-C1A	-2.83	1.45	1.52
5	F	1403	RG1	C11-C10	2.83	1.52	1.43
3	M	1707	BCL	O1A-CGA	2.82	1.30	1.22
3	C	1502	BCL	MG-NA	2.82	2.13	2.06
3	O	1708	BCL	OBD-CAD	2.80	1.26	1.22
3	P	1608	BCL	C4B-CHC	2.80	1.48	1.41
3	G	1504	BCL	C1B-CHB	2.80	1.48	1.41
3	S	1609	BCL	MG-NA	2.79	2.12	2.06
3	R	1709	BCL	OBD-CAD	2.79	1.26	1.22
3	J	1605	BCL	C1B-CHB	2.79	1.48	1.41
5	R	1401	RG1	CM1-C1	2.78	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1606	BCL	O2A-CGA	2.78	1.41	1.33
3	K	1706	BCL	C1B-CHB	2.78	1.48	1.41
3	O	1508	BCL	MG-NA	2.78	2.12	2.06
3	D	1602	BCL	O2D-CGD	2.76	1.39	1.33
3	A	1701	BCL	OBB-CAB	2.76	1.31	1.22
3	G	1504	BCL	CBD-CGD	-2.76	1.43	1.52
3	I	1505	BCL	C3D-C2D	2.75	1.44	1.39
3	N	1607	BCL	C1B-CHB	2.75	1.48	1.41
3	R	1509	BCL	OBB-CAB	2.75	1.31	1.22
3	I	1505	BCL	O1D-CGD	2.75	1.28	1.21
3	I	1705	BCL	MG-NA	2.75	2.12	2.06
3	H	1604	BCL	OBB-CAB	2.74	1.31	1.22
5	L	1406	RG1	C11-C10	2.74	1.51	1.43
5	D	1402	RG1	C2-C1	2.73	1.57	1.53
3	I	1705	BCL	C3B-CAB	2.73	1.56	1.49
3	M	1507	BCL	C2A-C1A	-2.73	1.46	1.52
3	H	1604	BCL	O2D-CGD	2.72	1.39	1.33
3	K	1506	BCL	O1A-CGA	2.70	1.30	1.22
5	D	1402	RG1	C11-C10	2.70	1.51	1.43
3	E	1503	BCL	O2A-CGA	2.70	1.41	1.33
3	C	1502	BCL	O1A-CGA	2.69	1.30	1.22
3	S	1609	BCL	C1D-C2D	2.69	1.48	1.42
3	G	1704	BCL	O1A-CGA	2.69	1.30	1.22
3	B	1601	BCL	O2A-CGA	2.69	1.41	1.33
3	O	1508	BCL	O1D-CGD	2.68	1.28	1.21
3	D	1602	BCL	CBD-CGD	-2.68	1.44	1.52
3	A	1501	BCL	C1B-CHB	2.68	1.48	1.41
3	R	1509	BCL	C4B-CHC	2.68	1.48	1.41
5	L	1406	RG1	C19-C18	2.66	1.51	1.45
3	R	1709	BCL	CBD-CGD	-2.66	1.44	1.52
3	C	1502	BCL	O1D-CGD	2.66	1.27	1.21
3	C	1502	BCL	C2A-C1A	-2.65	1.46	1.52
3	I	1505	BCL	C2A-C1A	-2.65	1.46	1.52
3	M	1707	BCL	C3D-C2D	2.65	1.44	1.39
3	P	1608	BCL	O1A-CGA	2.65	1.30	1.22
5	D	1402	RG1	C7-C6	2.64	1.51	1.43
3	R	1509	BCL	MG-NC	2.64	2.12	2.06
5	R	1401	RG1	C8-C9	2.64	1.51	1.45
3	A	1701	BCL	CBD-CGD	-2.63	1.44	1.52
3	H	1604	BCL	C2A-C1A	-2.62	1.46	1.52
3	K	1706	BCL	C9-C8	2.62	1.61	1.52
3	H	1604	BCL	C2C-C1C	-2.61	1.43	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	1401	RG1	C25-C26	-2.61	1.32	1.35
3	B	1601	BCL	MG-NA	2.61	2.12	2.06
5	P	1408	RG1	C24-C25	2.60	1.51	1.43
5	N	1407	RG1	C27-C26	2.60	1.51	1.45
3	F	1603	BCL	CMC-C2C	-2.58	1.47	1.53
3	R	1709	BCL	C3C-C4C	-2.58	1.48	1.51
3	A	1501	BCL	O2A-CGA	2.56	1.40	1.33
3	A	1701	BCL	C5-C3	2.56	1.56	1.51
3	L	1606	BCL	C1B-CHB	2.56	1.48	1.41
3	I	1705	BCL	CBD-CGD	-2.56	1.44	1.52
3	I	1705	BCL	CMB-C2B	-2.55	1.46	1.51
3	S	1609	BCL	O2D-CGD	2.55	1.39	1.33
3	I	1705	BCL	O1D-CGD	2.55	1.27	1.21
5	J	1405	RG1	C8-C9	2.54	1.51	1.45
3	F	1603	BCL	O1A-CGA	2.54	1.30	1.22
3	A	1701	BCL	MG-NC	2.54	2.12	2.06
3	I	1505	BCL	CBD-CGD	-2.53	1.44	1.52
5	P	1408	RG1	C6-C5	2.52	1.36	1.34
3	D	1602	BCL	C3C-C4C	-2.51	1.48	1.51
3	P	1608	BCL	CBA-CGA	-2.50	1.43	1.50
3	K	1506	BCL	MG-NC	2.49	2.12	2.06
3	B	1601	BCL	C4B-CHC	2.48	1.47	1.41
3	E	1503	BCL	C1D-C2D	2.48	1.48	1.42
3	J	1605	BCL	C3A-C2A	-2.48	1.47	1.54
3	M	1507	BCL	C2C-C3C	-2.47	1.47	1.54
3	K	1506	BCL	CBD-CGD	-2.47	1.44	1.52
5	H	1404	RG1	CM5-C13	-2.47	1.45	1.50
3	N	1607	BCL	C3C-C4C	-2.46	1.48	1.51
3	J	1605	BCL	CAA-C2A	-2.46	1.49	1.54
3	A	1701	BCL	CHD-C4C	2.46	1.48	1.41
3	I	1705	BCL	MG-NC	2.46	2.12	2.06
5	N	1407	RG1	C15-C14	2.46	1.51	1.43
3	C	1502	BCL	C4B-CHC	2.45	1.47	1.41
5	P	1408	RG1	CM7-C22	-2.45	1.45	1.50
5	D	1402	RG1	C28-C27	-2.45	1.28	1.34
3	M	1707	BCL	C5-C3	2.45	1.56	1.51
3	B	1601	BCL	O1A-CGA	2.44	1.29	1.22
3	H	1604	BCL	O2A-CGA	2.44	1.40	1.33
5	F	1403	RG1	C6-C5	2.44	1.36	1.34
3	I	1705	BCL	C1B-NB	2.43	1.37	1.35
3	M	1707	BCL	CBD-CHA	-2.42	1.40	1.52
3	O	1708	BCL	O1A-CGA	2.41	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1403	RG1	C25-C26	-2.41	1.32	1.35
3	E	1703	BCL	C3B-CAB	2.40	1.55	1.49
3	M	1507	BCL	OBB-CAB	2.40	1.30	1.22
5	D	1402	RG1	C8-C9	2.40	1.51	1.45
3	D	1602	BCL	CMD-C2D	-2.39	1.45	1.51
5	S	1409	RG1	C25-C26	2.38	1.38	1.35
3	S	1609	BCL	C2A-C1A	-2.38	1.46	1.52
3	J	1605	BCL	O2D-CED	-2.38	1.39	1.45
5	D	1402	RG1	O5'-C1'	2.37	1.47	1.41
3	I	1505	BCL	OBD-CAD	2.37	1.25	1.22
5	S	1409	RG1	C12-C13	2.35	1.51	1.45
3	A	1501	BCL	C3D-CAD	2.35	1.52	1.46
3	K	1706	BCL	O2D-CGD	2.34	1.38	1.33
5	P	1408	RG1	C19-C18	2.34	1.51	1.45
5	R	1401	RG1	C11-C10	2.34	1.50	1.43
3	F	1603	BCL	C3C-C4C	-2.34	1.48	1.51
3	I	1505	BCL	OBB-CAB	2.34	1.30	1.22
3	F	1603	BCL	O2D-CED	-2.34	1.39	1.45
3	B	1601	BCL	MG-NC	2.34	2.11	2.06
3	F	1603	BCL	O1D-CGD	2.33	1.27	1.21
3	O	1708	BCL	CMD-C2D	-2.33	1.46	1.51
3	O	1708	BCL	OBB-CAB	2.32	1.30	1.22
5	P	1408	RG1	CM5-C13	-2.32	1.46	1.50
5	P	1408	RG1	C28-C29	2.32	1.50	1.43
3	R	1709	BCL	O2A-CGA	2.32	1.40	1.33
3	H	1604	BCL	MG-NA	2.31	2.11	2.06
3	M	1507	BCL	OBD-CAD	2.30	1.25	1.22
3	B	1601	BCL	C1B-CHB	2.30	1.47	1.41
3	C	1502	BCL	O2D-CGD	2.30	1.38	1.33
3	K	1506	BCL	MG-NA	2.29	2.11	2.06
3	G	1504	BCL	CMD-C2D	-2.29	1.46	1.51
3	R	1509	BCL	C3B-CAB	2.29	1.55	1.49
3	C	1702	BCL	MG-NC	2.28	2.11	2.06
5	S	1409	RG1	O5'-C1'	2.28	1.47	1.41
3	R	1709	BCL	OBB-CAB	2.28	1.29	1.22
3	O	1708	BCL	C1B-CHB	2.28	1.47	1.41
3	P	1608	BCL	C4B-NB	2.27	1.37	1.35
3	C	1502	BCL	CAC-C3C	-2.26	1.49	1.54
3	B	1601	BCL	C3A-C2A	-2.25	1.48	1.54
3	E	1703	BCL	O1A-CGA	2.24	1.29	1.22
3	C	1702	BCL	O2A-CGA	2.23	1.39	1.33
3	K	1506	BCL	C3D-CAD	2.23	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1704	BCL	CMB-C2B	-2.22	1.47	1.51
3	P	1608	BCL	OBB-CAB	2.22	1.29	1.22
3	C	1502	BCL	C4B-NB	2.22	1.37	1.35
3	D	1602	BCL	C1D-C2D	2.21	1.47	1.42
5	L	1406	RG1	O2'-C2'	2.21	1.48	1.43
3	R	1709	BCL	CMD-C2D	-2.20	1.46	1.51
3	C	1702	BCL	C3C-C4C	-2.19	1.48	1.51
3	J	1605	BCL	CBD-CHA	-2.18	1.41	1.52
5	S	1409	RG1	CM6-C18	-2.17	1.46	1.50
3	C	1702	BCL	C2A-C1A	-2.17	1.47	1.52
5	J	1405	RG1	C12-C13	2.14	1.50	1.45
5	P	1408	RG1	O5'-C1'	2.13	1.47	1.41
3	A	1701	BCL	C4B-CHC	2.13	1.46	1.41
3	R	1709	BCL	C4B-CHC	2.12	1.46	1.41
3	G	1704	BCL	CMC-C2C	2.12	1.57	1.53
3	O	1708	BCL	CBD-CGD	-2.12	1.45	1.52
3	H	1604	BCL	CMD-C2D	-2.10	1.46	1.51
3	C	1702	BCL	C5-C3	2.09	1.55	1.51
3	I	1705	BCL	OBB-CAB	2.09	1.29	1.22
3	L	1606	BCL	O2D-CED	-2.09	1.40	1.45
3	E	1703	BCL	OBB-CAB	2.09	1.29	1.22
3	H	1604	BCL	C5-C3	2.09	1.55	1.51
3	J	1605	BCL	C1A-CHA	2.08	1.51	1.43
3	R	1709	BCL	CHD-C4C	2.08	1.47	1.41
3	M	1707	BCL	O1D-CGD	2.08	1.26	1.21
3	P	1608	BCL	C3C-C4C	-2.08	1.49	1.51
3	L	1606	BCL	MG-NA	2.06	2.11	2.06
3	G	1704	BCL	C1B-NB	2.06	1.37	1.35
5	J	1405	RG1	C11-C10	2.06	1.49	1.43
5	J	1405	RG1	C15-C14	2.06	1.49	1.43
3	G	1704	BCL	C1A-CHA	2.05	1.51	1.43
3	R	1709	BCL	C1-C2	2.05	1.55	1.49
3	E	1503	BCL	O2D-CGD	2.05	1.38	1.33
3	C	1702	BCL	MG-NA	2.04	2.11	2.06
3	R	1509	BCL	CAA-CBA	-2.03	1.46	1.52
3	M	1507	BCL	MG-NA	2.03	2.11	2.06
5	L	1406	RG1	C20-C21	2.02	1.49	1.43
5	H	1404	RG1	C11-C10	2.02	1.49	1.43
3	D	1602	BCL	OBB-CAB	2.01	1.29	1.22
3	E	1503	BCL	C2A-C1A	-2.01	1.47	1.52
5	P	1408	RG1	C11-C10	2.01	1.49	1.43

All (726) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1606	BCL	C4A-NA-C1A	-14.72	100.09	106.71
3	B	1601	BCL	C4A-NA-C1A	-13.70	100.55	106.71
3	R	1509	BCL	C4A-NA-C1A	-12.45	101.11	106.71
3	M	1507	BCL	C4A-NA-C1A	-12.02	101.30	106.71
3	D	1602	BCL	C4A-NA-C1A	-11.87	101.37	106.71
3	J	1605	BCL	C4A-NA-C1A	-10.72	101.89	106.71
3	E	1503	BCL	C4A-NA-C1A	-10.68	101.90	106.71
3	N	1607	BCL	C4A-NA-C1A	-10.30	102.08	106.71
3	F	1603	BCL	C4A-NA-C1A	-10.02	102.20	106.71
3	C	1502	BCL	C4A-NA-C1A	-9.65	102.37	106.71
3	J	1605	BCL	C1C-NC-C4C	-9.48	102.44	106.71
3	A	1701	BCL	C4A-NA-C1A	-9.42	102.47	106.71
3	K	1506	BCL	C4A-NA-C1A	-9.37	102.50	106.71
3	P	1608	BCL	C1C-NC-C4C	-9.26	102.54	106.71
3	A	1501	BCL	C4A-NA-C1A	-9.12	102.61	106.71
3	L	1606	BCL	C1C-NC-C4C	-9.05	102.64	106.71
3	S	1609	BCL	C4A-NA-C1A	-9.04	102.64	106.71
3	K	1706	BCL	C4A-NA-C1A	-8.93	102.69	106.71
3	I	1505	BCL	C4A-NA-C1A	-8.91	102.70	106.71
3	S	1609	BCL	C1C-NC-C4C	-8.66	102.81	106.71
3	O	1508	BCL	C4A-NA-C1A	-8.55	102.86	106.71
3	C	1702	BCL	C4A-NA-C1A	-8.53	102.87	106.71
3	G	1504	BCL	C4A-NA-C1A	-8.33	102.96	106.71
3	P	1608	BCL	C4A-NA-C1A	-8.29	102.98	106.71
3	O	1708	BCL	C4A-NA-C1A	-8.16	103.04	106.71
3	R	1709	BCL	C4A-NA-C1A	-8.02	103.10	106.71
3	H	1604	BCL	C4A-NA-C1A	-7.81	103.20	106.71
3	I	1705	BCL	C4A-NA-C1A	-7.75	103.22	106.71
3	G	1704	BCL	C4D-C3D-CAD	-7.71	104.17	108.47
3	G	1704	BCL	C1-C2-C3	-7.67	112.78	126.04
3	K	1706	BCL	C1-C2-C3	-7.37	113.31	126.04
3	B	1601	BCL	C1C-NC-C4C	-7.24	103.45	106.71
3	M	1707	BCL	C1-C2-C3	-7.20	113.58	126.04
3	K	1506	BCL	C1-C2-C3	-7.14	113.69	126.04
3	I	1705	BCL	C1-C2-C3	-7.11	113.75	126.04
3	N	1607	BCL	C1C-NC-C4C	-7.09	103.52	106.71
3	M	1507	BCL	C1C-NC-C4C	-6.87	103.62	106.71
3	A	1701	BCL	C1-C2-C3	-6.85	114.20	126.04
3	J	1605	BCL	C4D-C3D-CAD	-6.78	104.69	108.47
3	H	1604	BCL	C1C-NC-C4C	-6.70	103.69	106.71
3	O	1708	BCL	C1-C2-C3	-6.68	114.49	126.04
3	G	1704	BCL	C4A-NA-C1A	-6.58	103.75	106.71
3	E	1703	BCL	C4A-NA-C1A	-6.55	103.76	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1703	BCL	C1-C2-C3	-6.41	114.96	126.04
3	I	1505	BCL	C1-C2-C3	-6.41	114.97	126.04
3	R	1709	BCL	C1-C2-C3	-6.33	115.09	126.04
3	N	1607	BCL	C1B-CHB-C4A	-6.30	117.65	130.12
3	R	1509	BCL	C1B-CHB-C4A	-6.24	117.76	130.12
3	C	1702	BCL	C1-C2-C3	-6.20	115.32	126.04
3	A	1501	BCL	C1-C2-C3	-6.18	115.36	126.04
3	E	1503	BCL	C1B-CHB-C4A	-6.11	118.02	130.12
3	A	1501	BCL	C1C-NC-C4C	-6.09	103.97	106.71
3	D	1602	BCL	C1-C2-C3	-6.07	115.54	126.04
3	M	1707	BCL	C4D-C3D-CAD	-6.03	105.11	108.47
3	C	1702	BCL	C1B-CHB-C4A	-6.02	118.20	130.12
3	R	1709	BCL	C1B-CHB-C4A	-5.94	118.36	130.12
3	N	1607	BCL	C1-C2-C3	-5.84	115.93	126.04
3	K	1706	BCL	C1C-NC-C4C	-5.84	104.08	106.71
3	A	1701	BCL	C1B-CHB-C4A	-5.81	118.62	130.12
3	M	1507	BCL	C1B-CHB-C4A	-5.80	118.62	130.12
3	R	1509	BCL	C1-C2-C3	-5.74	116.12	126.04
3	O	1508	BCL	C1B-CHB-C4A	-5.73	118.77	130.12
5	H	1404	RG1	C16-C17-C18	-5.73	119.14	127.31
3	E	1503	BCL	C1C-NC-C4C	-5.72	104.13	106.71
3	L	1606	BCL	C1B-CHB-C4A	-5.71	118.81	130.12
3	K	1506	BCL	C1C-NC-C4C	-5.68	104.15	106.71
5	J	1405	RG1	C16-C17-C18	-5.65	119.25	127.31
3	E	1503	BCL	C1-C2-C3	-5.59	116.38	126.04
3	P	1608	BCL	C1B-CHB-C4A	-5.58	119.08	130.12
3	G	1504	BCL	C1-C2-C3	-5.58	116.40	126.04
5	R	1401	RG1	C16-C17-C18	-5.56	119.38	127.31
3	M	1707	BCL	C4A-NA-C1A	-5.52	104.22	106.71
5	D	1402	RG1	C16-C17-C18	-5.46	119.52	127.31
3	S	1609	BCL	C1B-CHB-C4A	-5.44	119.34	130.12
3	I	1505	BCL	C1B-CHB-C4A	-5.39	119.44	130.12
3	A	1701	BCL	C1C-NC-C4C	-5.38	104.29	106.71
3	K	1506	BCL	C2C-C3C-C4C	5.38	109.40	101.34
3	L	1606	BCL	C1-C2-C3	-5.37	116.75	126.04
3	C	1502	BCL	C1B-CHB-C4A	-5.35	119.52	130.12
3	F	1603	BCL	C1B-CHB-C4A	-5.32	119.58	130.12
3	P	1608	BCL	C1-C2-C3	-5.30	116.87	126.04
3	O	1708	BCL	C1B-CHB-C4A	-5.30	119.62	130.12
3	G	1704	BCL	C1B-CHB-C4A	-5.30	119.63	130.12
3	A	1501	BCL	C1B-CHB-C4A	-5.27	119.69	130.12
3	D	1602	BCL	C1B-CHB-C4A	-5.24	119.73	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1502	BCL	C1-C2-C3	-5.23	117.00	126.04
3	I	1705	BCL	C1B-CHB-C4A	-5.20	119.82	130.12
3	B	1601	BCL	C1B-CHB-C4A	-5.20	119.82	130.12
3	J	1605	BCL	C1B-CHB-C4A	-5.19	119.85	130.12
3	E	1703	BCL	C1B-CHB-C4A	-5.08	120.05	130.12
3	G	1704	BCL	C1C-NC-C4C	-5.06	104.43	106.71
3	O	1508	BCL	C1C-NC-C4C	-5.05	104.44	106.71
3	B	1601	BCL	C1-C2-C3	-5.02	117.36	126.04
3	D	1602	BCL	C1C-NC-C4C	-5.02	104.45	106.71
5	N	1407	RG1	C16-C17-C18	-5.02	120.14	127.31
3	M	1707	BCL	C1B-CHB-C4A	-5.00	120.22	130.12
3	R	1509	BCL	O2D-CGD-CBD	4.98	120.12	111.27
3	K	1706	BCL	C1B-CHB-C4A	-4.97	120.27	130.12
3	R	1709	BCL	O2D-CGD-CBD	4.96	120.08	111.27
3	F	1603	BCL	C1-C2-C3	-4.95	117.47	126.04
3	H	1604	BCL	C1-C2-C3	-4.95	117.49	126.04
3	G	1504	BCL	C1B-CHB-C4A	-4.92	120.37	130.12
3	E	1703	BCL	C1C-NC-C4C	-4.92	104.49	106.71
3	H	1604	BCL	C1B-CHB-C4A	-4.91	120.40	130.12
3	L	1606	BCL	C4D-C3D-CAD	-4.88	105.75	108.47
3	K	1506	BCL	C1D-CHD-C4C	-4.87	118.70	125.88
3	J	1605	BCL	C1-C2-C3	-4.86	117.63	126.04
3	M	1507	BCL	C1-C2-C3	-4.81	117.73	126.04
3	C	1502	BCL	C1C-NC-C4C	-4.77	104.56	106.71
5	P	1408	RG1	C16-C17-C18	-4.74	120.54	127.31
3	I	1705	BCL	C1C-NC-C4C	-4.72	104.59	106.71
5	R	1401	RG1	C28-C29-C30	-4.71	120.54	127.30
3	K	1506	BCL	C1B-CHB-C4A	-4.71	120.79	130.12
3	A	1701	BCL	C1D-CHD-C4C	-4.71	118.93	125.88
3	H	1604	BCL	C4B-CHC-C1C	-4.71	120.79	130.12
3	O	1508	BCL	C1-C2-C3	-4.67	117.97	126.04
5	S	1409	RG1	C16-C17-C18	-4.65	120.67	127.31
3	L	1606	BCL	O2D-CGD-O1D	-4.63	114.78	123.84
3	I	1705	BCL	C4D-C3D-CAD	-4.58	105.91	108.47
3	I	1705	BCL	OBB-CAB-C3B	-4.56	111.90	119.99
3	O	1508	BCL	OBB-CAB-C3B	-4.56	111.91	119.99
3	G	1504	BCL	C1C-NC-C4C	-4.54	104.66	106.71
3	O	1508	BCL	O2A-C1-C2	-4.51	96.79	108.64
3	C	1702	BCL	C4D-C3D-CAD	-4.48	105.97	108.47
3	M	1707	BCL	C1C-NC-C4C	-4.46	104.70	106.71
3	A	1501	BCL	O2D-CGD-CBD	4.43	119.14	111.27
5	F	1403	RG1	C11-C10-C9	-4.43	120.99	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1708	BCL	O2A-CGA-O1A	-4.42	112.44	123.59
3	C	1502	BCL	OBB-CAB-C3B	-4.37	112.24	119.99
3	L	1606	BCL	OBB-CAB-C3B	-4.36	112.26	119.99
3	A	1501	BCL	C4D-C3D-CAD	-4.35	106.04	108.47
3	G	1504	BCL	O2A-C1-C2	-4.35	97.21	108.64
3	C	1502	BCL	C6-C5-C3	-4.33	102.09	113.45
3	A	1701	BCL	OBB-CAB-C3B	-4.31	112.35	119.99
3	R	1509	BCL	C3A-C2A-C1A	-4.29	94.91	101.34
3	J	1605	BCL	OBB-CAB-C3B	-4.27	112.42	119.99
3	O	1708	BCL	OBB-CAB-C3B	-4.24	112.47	119.99
3	N	1607	BCL	O2D-CGD-CBD	4.22	118.76	111.27
3	S	1609	BCL	OBD-CAD-C3D	-4.21	120.99	127.98
3	S	1609	BCL	O2D-CGD-CBD	4.18	118.70	111.27
3	L	1606	BCL	CMD-C2D-C3D	4.17	132.49	124.68
3	C	1702	BCL	OBB-CAB-C3B	-4.16	112.60	119.99
3	H	1604	BCL	CAC-C3C-C2C	4.15	124.63	114.26
3	N	1607	BCL	C1D-CHD-C4C	-4.12	119.80	125.88
3	G	1504	BCL	O2A-CGA-O1A	-4.12	113.20	123.59
3	K	1706	BCL	C4D-C3D-CAD	-4.11	106.18	108.47
3	B	1601	BCL	O2D-CGD-CBD	4.08	118.52	111.27
5	F	1403	RG1	C16-C17-C18	-4.08	121.49	127.31
3	B	1601	BCL	OBB-CAB-C3B	-4.04	112.82	119.99
3	M	1507	BCL	C4D-C3D-CAD	-4.01	106.23	108.47
3	S	1609	BCL	C1-C2-C3	-4.01	119.12	126.04
3	L	1606	BCL	O2D-CGD-CBD	4.00	118.37	111.27
3	R	1509	BCL	O2A-C1-C2	-4.00	98.13	108.64
3	S	1609	BCL	CMD-C2D-C3D	3.99	132.14	124.68
3	O	1508	BCL	O2D-CGD-CBD	3.99	118.35	111.27
3	M	1707	BCL	O2A-CGA-O1A	-3.99	113.53	123.59
3	K	1706	BCL	O2A-CGA-O1A	-3.98	113.55	123.59
3	J	1605	BCL	CBA-CAA-C2A	-3.96	102.19	113.86
3	E	1703	BCL	OBD-CAD-C3D	-3.94	121.43	127.98
3	A	1501	BCL	OBB-CAB-C3B	-3.94	113.00	119.99
3	M	1707	BCL	OBB-CAB-C3B	-3.94	113.00	119.99
3	K	1706	BCL	O2D-CGD-CBD	3.93	118.26	111.27
5	L	1406	RG1	C11-C10-C9	-3.93	121.70	127.31
3	H	1604	BCL	O2D-CGD-CBD	3.93	118.25	111.27
3	P	1608	BCL	C4D-C3D-CAD	-3.93	106.28	108.47
3	E	1703	BCL	O2A-C1-C2	-3.92	98.33	108.64
5	R	1401	RG1	C16-C15-C14	-3.92	115.45	123.47
3	N	1607	BCL	OBB-CAB-C3B	-3.91	113.05	119.99
3	F	1603	BCL	C1C-NC-C4C	-3.89	104.96	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1705	BCL	O2A-CGA-O1A	-3.88	113.79	123.59
3	N	1607	BCL	O2A-CGA-O1A	-3.87	113.82	123.59
3	P	1608	BCL	CMC-C2C-C1C	3.87	122.17	111.77
3	M	1507	BCL	O2A-C1-C2	-3.87	98.46	108.64
3	M	1507	BCL	CMD-C2D-C3D	3.86	131.90	124.68
3	C	1502	BCL	O2D-CGD-CBD	3.86	118.12	111.27
3	I	1505	BCL	O2A-C1-C2	-3.85	98.51	108.64
3	G	1704	BCL	O2A-CGA-O1A	-3.84	113.90	123.59
3	E	1703	BCL	O2A-CGA-O1A	-3.84	113.91	123.59
3	C	1502	BCL	O2A-CGA-O1A	-3.84	113.91	123.59
3	F	1603	BCL	CMD-C2D-C3D	3.81	131.80	124.68
3	B	1601	BCL	C4D-C3D-CAD	-3.80	106.35	108.47
3	D	1602	BCL	OBG-CAB-C3B	-3.79	113.27	119.99
3	M	1507	BCL	O2A-CGA-O1A	-3.78	114.05	123.59
3	S	1609	BCL	OBG-CAB-C3B	-3.78	113.29	119.99
3	E	1503	BCL	CMD-C2D-C3D	3.77	131.74	124.68
3	R	1509	BCL	O2A-CGA-O1A	-3.77	114.08	123.59
3	P	1608	BCL	CMD-C2D-C3D	3.77	131.73	124.68
3	L	1606	BCL	CMB-C2B-C3B	3.76	131.71	124.68
3	L	1606	BCL	OBD-CAD-C3D	-3.76	121.74	127.98
3	O	1708	BCL	C1D-CHD-C4C	-3.75	120.35	125.88
3	H	1604	BCL	CMB-C2B-C3B	3.74	131.68	124.68
3	B	1601	BCL	CMD-C2D-C3D	3.74	131.68	124.68
3	R	1709	BCL	C1D-CHD-C4C	-3.74	120.36	125.88
3	A	1701	BCL	C4D-C3D-CAD	-3.74	106.39	108.47
3	R	1709	BCL	O2A-CGA-O1A	-3.74	114.16	123.59
3	A	1701	BCL	O2A-CGA-O1A	-3.72	114.19	123.59
3	O	1508	BCL	O2A-CGA-O1A	-3.72	114.19	123.59
3	F	1603	BCL	O2D-CGD-CBD	3.72	117.87	111.27
3	R	1709	BCL	OBD-CAD-C3D	-3.72	121.81	127.98
5	P	1408	RG1	C24-C25-C26	-3.71	122.02	127.31
3	J	1605	BCL	O2D-CGD-CBD	3.70	117.84	111.27
3	N	1607	BCL	CMD-C2D-C3D	3.70	131.59	124.68
5	L	1406	RG1	C16-C15-C14	-3.70	115.90	123.47
3	O	1508	BCL	C4D-C3D-CAD	-3.69	106.41	108.47
3	I	1705	BCL	O2D-CGD-CBD	3.69	117.82	111.27
3	I	1705	BCL	C4-C3-C5	3.69	121.47	115.27
3	E	1503	BCL	O2A-CGA-O1A	-3.68	114.32	123.59
3	E	1503	BCL	O2D-CGD-CBD	3.67	117.79	111.27
5	S	1409	RG1	CM7-C22-C23	3.66	123.84	118.08
3	I	1505	BCL	OBG-CAB-C3B	-3.66	113.50	119.99
3	H	1604	BCL	CMC-C2C-C1C	3.65	121.59	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1704	BCL	OBB-CAB-C3B	-3.65	113.51	119.99
5	H	1404	RG1	CM3-C5-C4	3.64	121.40	115.27
3	K	1506	BCL	CMD-C2D-C3D	3.64	131.50	124.68
3	F	1603	BCL	C4D-C3D-CAD	-3.63	106.44	108.47
5	P	1408	RG1	C16-C15-C14	-3.63	116.03	123.47
3	K	1706	BCL	OBB-CAB-C3B	-3.63	113.55	119.99
3	B	1601	BCL	O2A-CGA-O1A	-3.63	114.44	123.59
3	H	1604	BCL	C3C-C2C-C1C	3.61	107.70	101.87
3	H	1604	BCL	CBA-CAA-C2A	-3.60	103.24	113.86
3	G	1704	BCL	CMD-C2D-C3D	3.60	131.41	124.68
3	C	1702	BCL	CMD-C2D-C3D	3.59	131.40	124.68
3	J	1605	BCL	CMD-C2D-C3D	3.59	131.40	124.68
3	H	1604	BCL	CMD-C2D-C3D	3.59	131.39	124.68
3	K	1706	BCL	C1D-CHD-C4C	-3.58	120.60	125.88
3	O	1508	BCL	O2D-CGD-O1D	-3.58	116.84	123.84
3	P	1608	BCL	CBA-CAA-C2A	-3.58	103.31	113.86
3	D	1602	BCL	CMD-C2D-C3D	3.57	131.36	124.68
3	F	1603	BCL	O2A-CGA-O1A	-3.56	114.61	123.59
3	L	1606	BCL	C1D-CHD-C4C	-3.56	120.63	125.88
3	M	1507	BCL	OBB-CAB-C3B	-3.55	113.69	119.99
3	N	1607	BCL	OBD-CAD-C3D	-3.55	122.09	127.98
3	L	1606	BCL	C2A-C3A-C4A	3.55	107.60	101.87
3	I	1505	BCL	O2A-CGA-O1A	-3.55	114.64	123.59
3	M	1507	BCL	O2D-CGD-CBD	3.54	117.56	111.27
3	K	1706	BCL	C4B-CHC-C1C	-3.53	123.12	130.12
3	C	1702	BCL	O2A-CGA-O1A	-3.53	114.67	123.59
3	R	1709	BCL	OBB-CAB-C3B	-3.53	113.72	119.99
3	K	1506	BCL	O2A-C1-C2	-3.52	99.38	108.64
3	I	1705	BCL	C4B-CHC-C1C	-3.52	123.15	130.12
3	E	1703	BCL	CMB-C2B-C3B	3.52	131.26	124.68
3	L	1606	BCL	C3C-C2C-C1C	3.52	107.55	101.87
3	C	1502	BCL	OBD-CAD-C3D	-3.51	122.15	127.98
3	G	1704	BCL	O2D-CGD-CBD	3.51	117.51	111.27
3	A	1701	BCL	C4B-CHC-C1C	-3.50	123.18	130.12
3	S	1609	BCL	CBA-CAA-C2A	-3.48	103.59	113.86
3	C	1502	BCL	O2D-CGD-O1D	-3.48	117.03	123.84
3	O	1508	BCL	OBD-CAD-CBD	3.47	130.86	125.89
3	D	1602	BCL	C1D-CHD-C4C	-3.46	120.77	125.88
5	P	1408	RG1	C11-C10-C9	-3.46	122.38	127.31
5	J	1405	RG1	C20-C21-C22	-3.46	122.38	127.31
3	S	1609	BCL	C14-C13-C12	3.45	123.79	111.29
3	P	1608	BCL	OBB-CAB-C3B	-3.45	113.88	119.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1505	BCL	C1D-CHD-C4C	-3.44	120.81	125.88
3	R	1709	BCL	C4D-C3D-CAD	-3.43	106.56	108.47
3	F	1603	BCL	C6-C5-C3	-3.43	104.46	113.45
3	G	1704	BCL	C6-C5-C3	-3.42	104.48	113.45
3	S	1609	BCL	O2D-CGD-O1D	-3.42	117.15	123.84
3	F	1603	BCL	OBB-CAB-C3B	-3.42	113.92	119.99
3	G	1704	BCL	CHA-C1A-NA	-3.41	118.58	126.40
5	D	1402	RG1	C28-C29-C30	-3.41	122.41	127.30
3	R	1509	BCL	C1D-CHD-C4C	-3.41	120.85	125.88
3	E	1703	BCL	C4-C3-C5	3.40	121.00	115.27
3	L	1606	BCL	O2A-CGA-O1A	-3.39	115.03	123.59
3	D	1602	BCL	O2D-CGD-CBD	3.39	117.30	111.27
3	A	1501	BCL	O2D-CGD-O1D	-3.38	117.22	123.84
3	G	1504	BCL	C4B-CHC-C1C	-3.38	123.42	130.12
3	P	1608	BCL	C4B-CHC-C1C	-3.36	123.47	130.12
5	N	1407	RG1	C11-C10-C9	-3.35	122.53	127.31
3	H	1604	BCL	C4D-C3D-CAD	-3.35	106.60	108.47
3	H	1604	BCL	OBB-CAB-C3B	-3.34	114.06	119.99
5	N	1407	RG1	C16-C15-C14	-3.34	116.63	123.47
3	E	1503	BCL	OBB-CAB-C3B	-3.34	114.06	119.99
3	G	1504	BCL	C6-C5-C3	-3.34	104.71	113.45
3	H	1604	BCL	OBD-CAD-C3D	-3.33	122.46	127.98
3	K	1506	BCL	CBC-CAC-C3C	-3.32	106.07	113.47
3	A	1701	BCL	C2C-C3C-C4C	3.30	106.29	101.34
3	R	1709	BCL	O2A-CGA-CBA	3.30	122.27	111.91
3	R	1509	BCL	C4B-CHC-C1C	-3.30	123.58	130.12
3	O	1708	BCL	OBD-CAD-C3D	-3.30	122.50	127.98
3	M	1507	BCL	CMB-C2B-C3B	3.30	130.84	124.68
3	D	1602	BCL	CMB-C2B-C3B	3.30	130.84	124.68
3	C	1702	BCL	CMB-C2B-C3B	3.29	130.84	124.68
3	N	1607	BCL	C4D-C3D-CAD	-3.29	106.63	108.47
3	D	1602	BCL	O2A-CGA-O1A	-3.29	115.30	123.59
3	K	1506	BCL	CBA-CAA-C2A	-3.28	104.17	113.86
5	S	1409	RG1	C16-C15-C14	-3.28	116.76	123.47
3	F	1603	BCL	C4B-CHC-C1C	-3.28	123.63	130.12
3	A	1501	BCL	CMD-C2D-C3D	3.27	130.80	124.68
5	R	1401	RG1	C11-C10-C9	-3.27	122.65	127.31
3	O	1708	BCL	O2A-CGA-CBA	3.26	122.12	111.91
3	A	1501	BCL	CBA-CAA-C2A	-3.25	104.26	113.86
3	H	1604	BCL	CMC-C2C-C3C	3.25	126.95	113.83
3	K	1706	BCL	O2D-CGD-O1D	-3.25	117.48	123.84
3	M	1507	BCL	C1D-CHD-C4C	-3.24	121.10	125.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1708	BCL	C4B-CHC-C1C	-3.24	123.70	130.12
3	E	1503	BCL	CMB-C2B-C3B	3.24	130.74	124.68
3	A	1501	BCL	C1D-CHD-C4C	-3.24	121.10	125.88
3	K	1506	BCL	C6-C5-C3	-3.23	104.98	113.45
3	R	1709	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
3	E	1503	BCL	OBD-CAD-C3D	-3.23	122.61	127.98
3	B	1601	BCL	OBD-CAD-C3D	-3.23	122.63	127.98
3	A	1501	BCL	O2A-C1-C2	-3.21	100.20	108.64
3	G	1704	BCL	C1D-CHD-C4C	-3.21	121.14	125.88
3	B	1601	BCL	CMB-C2B-C3B	3.20	130.67	124.68
3	A	1501	BCL	O2A-CGA-O1A	-3.20	115.52	123.59
3	O	1508	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
3	A	1501	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
3	R	1709	BCL	C1C-NC-C4C	-3.19	105.27	106.71
3	K	1506	BCL	O2A-CGA-O1A	-3.18	115.57	123.59
3	D	1602	BCL	C4D-C3D-CAD	-3.17	106.70	108.47
3	R	1509	BCL	O2D-CGD-O1D	-3.17	117.64	123.84
3	D	1602	BCL	OBD-CAD-C3D	-3.15	122.74	127.98
3	G	1504	BCL	C1D-CHD-C4C	-3.14	121.24	125.88
5	F	1403	RG1	CM3-C5-C4	3.14	120.56	115.27
3	E	1503	BCL	CBA-CAA-C2A	-3.13	104.63	113.86
3	R	1709	BCL	CMB-C2B-C3B	3.13	130.53	124.68
3	I	1705	BCL	C1D-CHD-C4C	-3.12	121.28	125.88
3	B	1601	BCL	O2D-CGD-O1D	-3.12	117.75	123.84
5	F	1403	RG1	C12-C13-C14	-3.11	114.17	118.94
3	I	1705	BCL	O2A-C1-C2	-3.10	100.49	108.64
3	G	1704	BCL	C4B-CHC-C1C	-3.10	123.98	130.12
5	H	1404	RG1	C16-C15-C14	-3.10	117.13	123.47
5	R	1401	RG1	C20-C21-C22	-3.09	122.90	127.31
3	C	1502	BCL	C1D-CHD-C4C	-3.08	121.33	125.88
3	H	1604	BCL	C1D-CHD-C4C	-3.08	121.33	125.88
3	K	1506	BCL	CAC-C3C-C4C	3.08	119.43	112.58
5	S	1409	RG1	C20-C21-C22	-3.08	122.91	127.31
5	D	1402	RG1	C15-C14-C13	-3.07	122.92	127.31
3	N	1607	BCL	O2D-CGD-O1D	-3.05	117.87	123.84
3	I	1505	BCL	CBA-CAA-C2A	-3.05	104.86	113.86
5	S	1409	RG1	CM3-C5-C4	3.04	120.39	115.27
3	C	1502	BCL	O2A-C1-C2	-3.04	100.64	108.64
3	M	1707	BCL	C4-C3-C5	3.04	120.38	115.27
3	E	1703	BCL	C4B-CHC-C1C	-3.03	124.11	130.12
3	P	1608	BCL	O2D-CGD-CBD	3.02	116.64	111.27
3	C	1702	BCL	C4B-CHC-C1C	-3.02	124.14	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1504	BCL	CMB-C2B-C3B	3.02	130.32	124.68
3	C	1702	BCL	O2A-C1-C2	-3.02	100.71	108.64
3	I	1705	BCL	CMD-C2D-C3D	3.01	130.31	124.68
3	K	1506	BCL	C4D-C3D-CAD	-3.00	106.80	108.47
3	G	1704	BCL	O2A-C1-C2	-3.00	100.76	108.64
3	G	1504	BCL	OBB-CAB-C3B	-2.99	114.68	119.99
3	F	1603	BCL	CMB-C2B-C3B	2.99	130.27	124.68
3	K	1706	BCL	O2A-C1-C2	-2.99	100.78	108.64
3	R	1509	BCL	OBD-CAD-C3D	-2.99	123.02	127.98
3	E	1703	BCL	C1D-CHD-C4C	-2.98	121.48	125.88
3	M	1707	BCL	O2A-CGA-CBA	2.98	121.27	111.91
5	J	1405	RG1	C25-C24-C23	-2.98	113.91	123.22
3	E	1503	BCL	C6-C5-C3	-2.98	105.64	113.45
5	D	1402	RG1	C16-C15-C14	-2.98	117.37	123.47
5	F	1403	RG1	C24-C25-C26	-2.98	123.06	127.31
3	O	1508	BCL	CMD-C2D-C3D	2.98	130.25	124.68
3	K	1506	BCL	CAC-C3C-C2C	2.98	121.70	114.26
3	A	1501	BCL	CGD-CBD-CAD	2.98	120.38	110.73
3	H	1604	BCL	C3C-C4C-CHD	-2.98	117.03	123.39
3	N	1607	BCL	CBA-CAA-C2A	-2.98	105.08	113.86
3	S	1609	BCL	O2A-CGA-O1A	-2.97	116.08	123.59
3	P	1608	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
3	E	1703	BCL	OBB-CAB-C3B	-2.97	114.72	119.99
3	H	1604	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
3	H	1604	BCL	C6-C5-C3	-2.97	105.67	113.45
3	S	1609	BCL	C4B-CHC-C1C	-2.97	124.24	130.12
3	D	1602	BCL	C6-C5-C3	-2.97	105.68	113.45
5	L	1406	RG1	C16-C17-C18	-2.96	123.08	127.31
3	D	1602	BCL	CBA-CAA-C2A	-2.96	105.14	113.86
3	B	1601	BCL	CBA-CAA-C2A	-2.95	105.15	113.86
3	M	1707	BCL	CHA-C1A-NA	-2.95	119.64	126.40
3	A	1701	BCL	CAC-C3C-C2C	2.95	121.62	114.26
3	F	1603	BCL	O2D-CGD-O1D	-2.95	118.08	123.84
3	I	1505	BCL	CMB-C2B-C3B	2.94	130.18	124.68
3	O	1508	BCL	CMB-C2B-C3B	2.94	130.17	124.68
3	S	1609	BCL	C1D-CHD-C4C	-2.94	121.55	125.88
3	R	1709	BCL	O2D-CGD-O1D	-2.93	118.11	123.84
5	J	1405	RG1	C16-C15-C14	-2.93	117.48	123.47
3	J	1605	BCL	C6-C5-C3	-2.92	105.80	113.45
3	M	1507	BCL	C4B-CHC-C1C	-2.92	124.34	130.12
3	P	1608	BCL	OBD-CAD-C3D	-2.91	123.14	127.98
3	C	1502	BCL	CMD-C2D-C3D	2.91	130.13	124.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1702	BCL	O2D-CGD-CBD	2.91	116.44	111.27
3	S	1609	BCL	C4D-C3D-CAD	-2.91	106.85	108.47
3	E	1503	BCL	O2D-CGD-O1D	-2.91	118.15	123.84
3	R	1509	BCL	C1C-NC-C4C	-2.91	105.40	106.71
3	M	1507	BCL	O2D-CGD-O1D	-2.91	118.15	123.84
5	F	1403	RG1	CM5-C13-C12	2.91	122.66	118.08
3	I	1505	BCL	OBD-CAD-C3D	-2.90	123.17	127.98
3	F	1603	BCL	C1-O2A-CGA	2.90	124.05	116.44
3	G	1504	BCL	O2D-CGD-CBD	2.90	116.41	111.27
3	C	1702	BCL	C1-O2A-CGA	2.89	124.04	116.44
3	A	1701	BCL	O2D-CGD-CBD	2.89	116.41	111.27
5	D	1402	RG1	CM0-C30-CM9	2.89	120.98	114.60
3	I	1705	BCL	O2A-CGA-CBA	2.89	120.97	111.91
3	R	1509	BCL	OBB-CAB-C3B	-2.89	114.87	119.99
3	J	1605	BCL	CMB-C2B-C3B	2.88	130.07	124.68
5	P	1408	RG1	CM3-C5-C4	2.88	120.12	115.27
3	B	1601	BCL	C6-C5-C3	-2.87	105.92	113.45
3	M	1707	BCL	C4B-CHC-C1C	-2.87	124.43	130.12
3	A	1701	BCL	C4-C3-C5	2.87	120.10	115.27
3	M	1507	BCL	C1-O2A-CGA	2.87	123.98	116.44
3	N	1607	BCL	C4B-CHC-C1C	-2.87	124.44	130.12
3	F	1603	BCL	C4-C3-C5	2.87	120.09	115.27
5	L	1406	RG1	C20-C21-C22	-2.86	123.23	127.31
3	G	1704	BCL	O2A-CGA-CBA	2.86	120.87	111.91
3	E	1503	BCL	C1D-CHD-C4C	-2.85	121.67	125.88
3	O	1708	BCL	C6-C5-C3	-2.85	105.98	113.45
3	I	1505	BCL	C4B-CHC-C1C	-2.84	124.48	130.12
3	O	1508	BCL	C6-C5-C3	-2.84	106.00	113.45
3	R	1509	BCL	CMA-C3A-C4A	2.83	119.37	111.77
3	G	1504	BCL	O2D-CGD-O1D	-2.83	118.31	123.84
3	R	1509	BCL	C6-C5-C3	-2.83	106.04	113.45
3	I	1705	BCL	C6-C5-C3	-2.82	106.05	113.45
3	A	1501	BCL	CHA-C1A-NA	-2.82	119.93	126.40
5	L	1406	RG1	C12-C13-C14	-2.82	114.61	118.94
3	K	1506	BCL	C4-C3-C5	2.82	120.01	115.27
3	B	1601	BCL	O2A-CGA-CBA	2.82	120.75	111.91
5	R	1401	RG1	CM7-C22-C23	2.81	122.50	118.08
3	B	1601	BCL	C1D-CHD-C4C	-2.81	121.74	125.88
5	F	1403	RG1	C16-C15-C14	-2.81	117.73	123.47
3	O	1708	BCL	C1C-NC-C4C	-2.80	105.45	106.71
3	G	1504	BCL	CMD-C2D-C3D	2.79	129.89	124.68
3	O	1708	BCL	O2D-CGD-O1D	-2.79	118.39	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1404	RG1	CM7-C22-C23	2.78	122.46	118.08
5	S	1409	RG1	CM5-C13-C12	2.78	122.46	118.08
3	C	1702	BCL	C1C-NC-C4C	-2.78	105.46	106.71
3	K	1706	BCL	CMD-C2D-C3D	2.78	129.88	124.68
3	G	1704	BCL	O2D-CGD-O1D	-2.77	118.42	123.84
3	R	1709	BCL	C4-C3-C5	2.77	119.93	115.27
3	B	1601	BCL	C4B-CHC-C1C	-2.77	124.63	130.12
3	R	1509	BCL	CMD-C2D-C3D	2.77	129.85	124.68
5	J	1405	RG1	CM6-C18-C17	-2.77	119.05	122.92
3	K	1706	BCL	C4-C3-C5	2.76	119.92	115.27
3	O	1508	BCL	OBD-CAD-C3D	-2.76	123.40	127.98
3	K	1506	BCL	CMB-C2B-C3B	2.75	129.83	124.68
3	J	1605	BCL	C1D-CHD-C4C	-2.75	121.83	125.88
3	A	1501	BCL	C4-C3-C5	2.74	119.88	115.27
3	A	1501	BCL	CMB-C2B-C3B	2.73	129.79	124.68
3	C	1502	BCL	C4-C3-C5	2.73	119.87	115.27
3	C	1702	BCL	OBD-CAD-C3D	-2.73	123.45	127.98
3	S	1609	BCL	C6-C5-C3	-2.73	106.30	113.45
3	O	1508	BCL	C1D-CHD-C4C	-2.72	121.86	125.88
5	L	1406	RG1	CM3-C5-C4	2.72	119.85	115.27
3	D	1602	BCL	C4-C3-C5	2.72	119.85	115.27
5	N	1407	RG1	CM3-C5-C4	2.72	119.85	115.27
5	H	1404	RG1	C11-C10-C9	-2.72	123.43	127.31
3	N	1607	BCL	C6-C5-C3	-2.72	106.33	113.45
5	P	1408	RG1	CM7-C22-C23	2.70	122.34	118.08
5	J	1405	RG1	C2-C3-C4	-2.70	105.82	112.33
3	F	1603	BCL	CBA-CAA-C2A	-2.70	105.89	113.86
5	H	1404	RG1	C25-C24-C23	-2.70	114.79	123.22
3	L	1606	BCL	C3A-C2A-C1A	-2.69	97.30	101.34
3	R	1509	BCL	CMB-C2B-C3B	2.69	129.72	124.68
5	D	1402	RG1	CM4-C9-C8	2.69	122.31	118.08
3	E	1503	BCL	O2A-C1-C2	-2.68	101.59	108.64
3	E	1503	BCL	C4D-C3D-CAD	-2.67	106.98	108.47
3	C	1502	BCL	C4B-CHC-C1C	-2.67	124.82	130.12
5	D	1402	RG1	C20-C21-C22	-2.67	123.50	127.31
3	A	1701	BCL	O2A-CGA-CBA	2.67	120.27	111.91
3	S	1609	BCL	C1-O2A-CGA	2.66	123.43	116.44
5	R	1401	RG1	C25-C24-C23	-2.66	114.91	123.22
3	A	1701	BCL	OBB-CAB-CBB	2.66	126.15	120.17
5	H	1404	RG1	C28-C29-C30	-2.65	123.50	127.30
5	J	1405	RG1	C28-C27-C26	-2.65	118.97	126.42
5	H	1404	RG1	C28-C27-C26	-2.65	118.97	126.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1701	BCL	CAC-C3C-C4C	2.65	118.46	112.58
5	J	1405	RG1	CM3-C5-C4	2.64	119.72	115.27
3	R	1509	BCL	C2A-C3A-C4A	2.64	106.14	101.87
3	E	1503	BCL	C4B-CHC-C1C	-2.64	124.89	130.12
3	I	1505	BCL	C1C-NC-C4C	-2.64	105.52	106.71
3	B	1601	BCL	O2A-C1-C2	-2.63	101.72	108.64
5	H	1404	RG1	CM2-C1-C2	-2.63	106.37	111.14
3	M	1707	BCL	O2D-CGD-CBD	2.63	115.94	111.27
3	M	1707	BCL	CMD-C2D-C3D	2.63	129.59	124.68
5	N	1407	RG1	C29-C28-C27	-2.62	115.04	123.22
3	R	1509	BCL	C4-C3-C5	2.62	119.68	115.27
3	G	1704	BCL	CBC-CAC-C3C	-2.62	107.64	113.47
5	H	1404	RG1	C20-C21-C22	-2.62	123.58	127.31
3	C	1702	BCL	O2D-CGD-O1D	-2.62	118.72	123.84
3	H	1604	BCL	CAC-C3C-C4C	-2.62	106.78	112.58
3	R	1709	BCL	CGD-CBD-CAD	-2.61	102.27	110.73
3	K	1706	BCL	OBBCAB-CBB	2.61	126.05	120.17
3	D	1602	BCL	O2A-C1-C2	-2.61	101.77	108.64
3	N	1607	BCL	O2A-CGA-CBA	2.61	120.11	111.91
3	A	1701	BCL	CMB-C2B-C3B	2.61	129.56	124.68
3	M	1507	BCL	C6-C5-C3	-2.61	106.61	113.45
3	C	1502	BCL	CBA-CAA-C2A	-2.61	106.16	113.86
3	L	1606	BCL	C4B-CHC-C1C	-2.61	124.96	130.12
3	C	1702	BCL	C1D-CHD-C4C	-2.60	122.04	125.88
5	S	1409	RG1	C28-C27-C26	-2.59	119.13	126.42
3	K	1706	BCL	OBDCAD-C3D	-2.59	123.68	127.98
3	F	1603	BCL	O2A-C1-C2	-2.59	101.83	108.64
5	N	1407	RG1	C24-C25-C26	-2.59	123.62	127.31
5	N	1407	RG1	CM6-C18-C17	-2.58	119.31	122.92
3	P	1608	BCL	O2A-C1-C2	-2.58	101.85	108.64
5	P	1408	RG1	C1'-O5'-C5'	2.58	118.75	113.69
3	O	1708	BCL	C4D-C3D-CAD	-2.58	107.03	108.47
3	I	1505	BCL	C4-C3-C5	2.57	119.60	115.27
5	L	1406	RG1	C28-C29-C30	-2.57	123.62	127.30
5	S	1409	RG1	C24-C25-C26	-2.57	123.65	127.31
3	K	1706	BCL	C6-C5-C3	-2.56	106.73	113.45
3	S	1609	BCL	CMB-C2B-C3B	2.56	129.46	124.68
3	J	1605	BCL	O2A-CGA-O1A	-2.56	117.14	123.59
3	A	1701	BCL	CBC-CAC-C3C	-2.55	107.78	113.47
3	C	1702	BCL	O2A-CGA-CBA	2.55	119.92	111.91
3	S	1609	BCL	C5-C3-C2	-2.55	115.95	121.12
3	H	1604	BCL	O2A-C1-C2	-2.54	101.95	108.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1405	RG1	C11-C10-C9	-2.54	123.69	127.31
3	C	1502	BCL	C14-C13-C12	2.54	120.49	111.29
3	P	1608	BCL	C1D-CHD-C4C	-2.54	122.14	125.88
3	L	1606	BCL	OBB-CAB-CBB	2.53	125.87	120.17
3	G	1504	BCL	CHA-C1A-NA	-2.53	120.60	126.40
3	J	1605	BCL	O2A-CGA-CBA	2.51	119.80	111.91
3	K	1506	BCL	OBD-CAD-C3D	-2.51	123.81	127.98
3	K	1506	BCL	O2D-CGD-CBD	2.51	115.73	111.27
3	O	1508	BCL	C5-C3-C2	-2.51	116.04	121.12
3	M	1707	BCL	C1D-CHD-C4C	-2.51	122.18	125.88
3	M	1707	BCL	C6-C5-C3	-2.50	106.89	113.45
5	F	1403	RG1	CM0-C30-CM9	2.50	120.13	114.60
3	M	1507	BCL	CBA-CAA-C2A	-2.50	106.47	113.86
3	I	1505	BCL	C4D-C3D-CAD	-2.49	107.08	108.47
3	K	1506	BCL	OBB-CAB-C3B	-2.49	115.57	119.99
3	E	1703	BCL	O2A-CGA-CBA	2.49	119.73	111.91
3	E	1503	BCL	O2A-CGA-CBA	2.49	119.73	111.91
3	O	1508	BCL	C4-C3-C5	2.49	119.45	115.27
3	K	1706	BCL	O2A-CGA-CBA	2.48	119.70	111.91
3	A	1501	BCL	OBD-CAD-C3D	-2.48	123.86	127.98
5	N	1407	RG1	C20-C21-C22	-2.48	123.77	127.31
3	F	1603	BCL	C1D-CHD-C4C	-2.47	122.23	125.88
3	G	1504	BCL	C4-C3-C5	2.47	119.43	115.27
3	G	1504	BCL	OBD-CAD-C3D	-2.46	123.89	127.98
5	D	1402	RG1	C28-C27-C26	-2.46	119.50	126.42
5	L	1406	RG1	O5'-C1'-C2'	2.46	115.56	110.35
3	C	1502	BCL	C5-C3-C2	-2.46	116.14	121.12
5	S	1409	RG1	CM0-C30-CM9	2.45	120.02	114.60
5	D	1402	RG1	C24-C25-C26	-2.45	123.81	127.31
3	A	1701	BCL	OBD-CAD-C3D	-2.45	123.91	127.98
5	F	1403	RG1	CM8-C26-C25	-2.45	119.50	122.92
3	G	1504	BCL	O2A-CGA-CBA	2.44	119.58	111.91
3	O	1708	BCL	CMB-C2B-C3B	2.43	129.23	124.68
3	D	1602	BCL	C4B-CHC-C1C	-2.43	125.30	130.12
3	L	1606	BCL	CBA-CAA-C2A	-2.43	106.69	113.86
3	N	1607	BCL	OBB-CAB-CBB	2.43	125.63	120.17
5	D	1402	RG1	CM5-C13-C12	2.43	121.90	118.08
3	M	1707	BCL	C3D-CAD-CBD	-2.42	104.42	107.61
3	O	1708	BCL	CBA-CAA-C2A	-2.42	106.71	113.86
3	B	1601	BCL	OBB-CAB-CBB	2.42	125.62	120.17
3	G	1504	BCL	CBA-CAA-C2A	-2.41	106.75	113.86
3	D	1602	BCL	C1-O2A-CGA	2.41	122.76	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1701	BCL	CMD-C2D-C3D	2.40	129.18	124.68
3	E	1703	BCL	C6-C5-C3	-2.40	107.16	113.45
5	P	1408	RG1	CM8-C26-C25	-2.40	119.56	122.92
3	S	1609	BCL	O2A-CGA-CBA	2.40	119.44	111.91
5	D	1402	RG1	C10-C11-C12	-2.40	115.74	123.22
3	O	1708	BCL	O2D-CGD-CBD	2.39	115.52	111.27
3	E	1703	BCL	CMD-C2D-C3D	2.39	129.15	124.68
5	J	1405	RG1	C24-C25-C26	-2.39	123.90	127.31
3	P	1608	BCL	OBB-CAB-CBB	2.39	125.54	120.17
3	R	1509	BCL	C4D-C3D-CAD	-2.39	107.14	108.47
3	F	1603	BCL	OBD-CAD-C3D	-2.38	124.02	127.98
3	O	1508	BCL	C14-C13-C12	2.38	119.92	111.29
5	R	1401	RG1	C23-C22-C21	-2.37	115.30	118.94
3	O	1708	BCL	CMD-C2D-C3D	2.37	129.10	124.68
3	B	1601	BCL	C1-O2A-CGA	2.37	122.65	116.44
5	N	1407	RG1	C15-C14-C13	-2.36	123.94	127.31
3	L	1606	BCL	O2A-CGA-CBA	2.36	119.32	111.91
3	R	1709	BCL	OBB-CAB-CBB	2.36	125.48	120.17
5	N	1407	RG1	C12-C13-C14	-2.36	115.32	118.94
3	O	1708	BCL	C4-C3-C5	2.36	119.24	115.27
3	H	1604	BCL	O2D-CGD-O1D	-2.35	119.24	123.84
3	H	1604	BCL	OBB-CAB-CBB	2.35	125.45	120.17
3	J	1605	BCL	CHA-C1A-NA	-2.34	121.03	126.40
5	F	1403	RG1	C28-C27-C26	-2.34	119.84	126.42
3	G	1504	BCL	C1-O2A-CGA	2.34	122.59	116.44
3	O	1508	BCL	CHA-C1A-NA	-2.34	121.05	126.40
3	G	1704	BCL	OBD-CAD-CBD	2.33	129.23	125.89
5	S	1409	RG1	C23-C22-C21	-2.33	115.36	118.94
3	K	1706	BCL	CBA-CAA-C2A	-2.33	106.98	113.86
3	H	1604	BCL	C2C-C3C-C4C	-2.33	97.85	101.34
3	J	1605	BCL	O2A-C1-C2	-2.33	102.52	108.64
3	L	1606	BCL	CMB-C2B-C1B	-2.32	124.89	128.46
3	G	1704	BCL	CBA-CAA-C2A	-2.32	107.00	113.86
5	D	1402	RG1	C1'-C2'-C3'	2.32	114.83	110.00
5	L	1406	RG1	CM4-C9-C10	-2.32	119.67	122.92
3	D	1602	BCL	O2D-CGD-O1D	-2.32	119.31	123.84
3	E	1703	BCL	CHA-C1A-NA	-2.32	121.09	126.40
3	G	1704	BCL	C4-C3-C5	2.31	119.16	115.27
3	R	1709	BCL	CMD-C2D-C3D	2.31	129.01	124.68
5	L	1406	RG1	CM5-C13-C12	2.31	121.71	118.08
3	C	1702	BCL	CBC-CAC-C3C	-2.31	108.33	113.47
3	G	1504	BCL	CBC-CAC-C3C	-2.30	108.34	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	1409	RG1	C25-C24-C23	-2.30	116.03	123.22
3	C	1502	BCL	O2A-CGA-CBA	2.30	119.12	111.91
3	N	1607	BCL	CMB-C2B-C3B	2.29	128.97	124.68
3	M	1707	BCL	CMB-C2B-C3B	2.29	128.97	124.68
3	M	1507	BCL	CHA-C1A-NA	-2.29	121.16	126.40
3	C	1702	BCL	C4-C3-C5	2.29	119.12	115.27
3	J	1605	BCL	CGD-CBD-CAD	2.29	118.14	110.73
5	F	1403	RG1	C29-C28-C27	-2.29	116.08	123.22
3	S	1609	BCL	OBD-CAD-CBD	2.28	129.15	125.89
3	A	1501	BCL	C6-C5-C3	-2.28	107.48	113.45
3	E	1503	BCL	C4-C3-C5	2.28	119.10	115.27
3	F	1603	BCL	O2A-CGA-CBA	2.28	119.06	111.91
3	P	1608	BCL	C4-C3-C5	2.28	119.10	115.27
3	M	1707	BCL	O2A-C1-C2	-2.27	102.67	108.64
3	A	1701	BCL	CHA-C1A-NA	-2.27	121.20	126.40
3	P	1608	BCL	CHA-C1A-NA	-2.27	121.20	126.40
3	F	1603	BCL	OBB-CAB-CBB	2.27	125.27	120.17
3	K	1506	BCL	CHA-C1A-NA	-2.26	121.21	126.40
5	F	1403	RG1	C28-C29-C30	-2.26	124.05	127.30
3	B	1601	BCL	C4-C3-C5	2.26	119.08	115.27
3	N	1607	BCL	CHA-C1A-NA	-2.26	121.22	126.40
5	R	1401	RG1	C28-C27-C26	-2.26	120.07	126.42
5	D	1402	RG1	C29-C28-C27	-2.26	116.17	123.22
5	R	1401	RG1	CM5-C13-C12	2.26	121.63	118.08
3	I	1505	BCL	C11-C10-C8	-2.26	108.63	115.92
3	I	1505	BCL	CMD-C2D-C3D	2.25	128.90	124.68
3	E	1703	BCL	C3D-CAD-CBD	2.25	110.57	107.61
3	I	1505	BCL	C6-C5-C3	-2.25	107.57	113.45
3	E	1703	BCL	CMB-C2B-C1B	-2.24	125.02	128.46
3	R	1509	BCL	CMA-C3A-C2A	2.24	122.86	113.83
5	D	1402	RG1	C25-C24-C23	-2.24	116.23	123.22
3	H	1604	BCL	CHA-C1A-NA	-2.24	121.28	126.40
5	L	1406	RG1	C29-C28-C27	-2.23	116.25	123.22
5	S	1409	RG1	C20-C19-C18	-2.23	120.14	126.42
5	J	1405	RG1	CM0-C30-CM9	2.23	119.53	114.60
3	J	1605	BCL	C4B-CHC-C1C	-2.23	125.70	130.12
3	P	1608	BCL	C3C-C2C-C1C	2.23	105.47	101.87
5	P	1408	RG1	C10-C11-C12	-2.23	116.26	123.22
3	H	1604	BCL	C4-C3-C5	2.23	119.02	115.27
3	A	1701	BCL	O2A-C1-C2	-2.23	102.78	108.64
3	L	1606	BCL	C6-C5-C3	-2.22	107.63	113.45
3	I	1705	BCL	O2D-CGD-O1D	-2.22	119.49	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1503	BCL	CHA-C1A-NA	-2.22	121.31	126.40
3	P	1608	BCL	O2A-CGA-CBA	2.22	118.88	111.91
3	A	1501	BCL	OBB-CAB-CBB	2.22	125.16	120.17
3	E	1503	BCL	C5-C3-C2	-2.22	116.63	121.12
5	S	1409	RG1	C29-C28-C27	-2.22	116.30	123.22
3	R	1709	BCL	CHA-C1A-NA	-2.21	121.33	126.40
5	F	1403	RG1	C25-C24-C23	-2.21	116.32	123.22
5	F	1403	RG1	C6-C7-C8	-2.20	116.34	123.22
3	J	1605	BCL	O2D-CGD-O1D	-2.20	119.53	123.84
3	S	1609	BCL	C4-C3-C5	2.20	118.97	115.27
5	N	1407	RG1	CM4-C9-C8	2.20	121.54	118.08
3	C	1502	BCL	CHA-C1A-NA	-2.20	121.37	126.40
3	M	1507	BCL	C2A-C1A-CHA	-2.20	120.02	123.86
5	S	1409	RG1	C7-C8-C9	-2.20	120.25	126.42
3	R	1709	BCL	CBC-CAC-C3C	-2.19	108.58	113.47
5	R	1401	RG1	C15-C14-C13	-2.19	124.18	127.31
3	O	1508	BCL	CGD-CBD-CAD	2.19	117.83	110.73
3	N	1607	BCL	O2A-C1-C2	-2.19	102.88	108.64
3	M	1507	BCL	O2A-CGA-CBA	2.19	118.78	111.91
3	G	1504	BCL	C14-C13-C15	-2.19	103.36	111.29
3	E	1703	BCL	O2D-CGD-CBD	2.19	115.16	111.27
3	L	1606	BCL	C1-O2A-CGA	2.19	122.18	116.44
5	P	1408	RG1	C2-C3-C4	-2.18	107.07	112.33
3	L	1606	BCL	C4-C3-C5	2.18	118.94	115.27
5	H	1404	RG1	CM6-C18-C17	-2.18	119.87	122.92
3	G	1504	BCL	C5-C3-C2	-2.18	116.71	121.12
3	C	1502	BCL	C2A-C1A-CHA	-2.17	120.06	123.86
3	I	1505	BCL	O2D-CGD-CBD	2.17	115.13	111.27
3	H	1604	BCL	O2A-CGA-CBA	2.17	118.72	111.91
3	O	1508	BCL	OBB-CAB-CBB	2.17	125.05	120.17
3	M	1507	BCL	CMB-C2B-C1B	-2.16	125.14	128.46
3	E	1703	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
3	J	1605	BCL	OBB-CAB-CBB	2.16	125.02	120.17
3	A	1701	BCL	C6-C5-C3	-2.15	107.81	113.45
5	N	1407	RG1	CM5-C13-C12	2.15	121.46	118.08
5	S	1409	RG1	C11-C10-C9	-2.14	124.25	127.31
3	K	1506	BCL	O2D-CGD-O1D	-2.14	119.66	123.84
3	R	1509	BCL	CHA-C1A-NA	-2.14	121.51	126.40
3	D	1602	BCL	O2A-CGA-CBA	2.13	118.60	111.91
5	H	1404	RG1	CM4-C9-C8	2.13	121.43	118.08
3	G	1504	BCL	CMB-C2B-C1B	-2.12	125.20	128.46
5	J	1405	RG1	C6-C7-C8	-2.12	116.59	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1602	BCL	OBB-CAB-CBB	2.12	124.95	120.17
3	K	1506	BCL	C1-O2A-CGA	2.12	122.01	116.44
3	O	1508	BCL	O2A-CGA-CBA	2.12	118.56	111.91
3	C	1702	BCL	OBB-CAB-CBB	2.12	124.94	120.17
5	D	1402	RG1	CM3-C5-C4	2.12	118.83	115.27
5	D	1402	RG1	CM7-C22-C23	2.12	121.41	118.08
3	O	1708	BCL	O2A-C1-C2	-2.12	103.07	108.64
5	L	1406	RG1	CM0-C30-CM9	2.12	119.28	114.60
3	G	1704	BCL	CGD-CBD-CAD	2.11	117.58	110.73
3	R	1509	BCL	O2A-CGA-CBA	2.11	118.52	111.91
5	N	1407	RG1	C25-C24-C23	-2.11	116.64	123.22
3	G	1704	BCL	CMB-C2B-C3B	2.10	128.61	124.68
3	E	1703	BCL	CBA-CAA-C2A	-2.10	107.67	113.86
3	K	1506	BCL	C4B-CHC-C1C	-2.10	125.96	130.12
3	R	1509	BCL	OBD-CAD-CBD	2.09	128.88	125.89
5	J	1405	RG1	C29-C28-C27	-2.08	116.71	123.22
3	J	1605	BCL	C16-C15-C13	-2.08	109.19	115.92
3	O	1508	BCL	C1-O2A-CGA	2.08	121.89	116.44
3	C	1502	BCL	C4D-C3D-CAD	-2.07	107.31	108.47
3	N	1607	BCL	C4-C3-C5	2.07	118.76	115.27
3	M	1507	BCL	C5-C3-C2	-2.07	116.92	121.12
3	C	1502	BCL	CMB-C2B-C3B	2.07	128.55	124.68
3	P	1608	BCL	C6-C5-C3	-2.07	108.03	113.45
3	G	1704	BCL	OBB-CAB-CBB	2.07	124.82	120.17
3	A	1501	BCL	CMB-C2B-C1B	-2.06	125.29	128.46
3	G	1504	BCL	C4D-C3D-CAD	-2.06	107.32	108.47
5	H	1404	RG1	C15-C14-C13	-2.06	124.37	127.31
5	F	1403	RG1	CM6-C18-C17	-2.06	120.03	122.92
3	R	1709	BCL	O2A-C1-C2	-2.06	103.22	108.64
3	R	1509	BCL	C5-C3-C2	-2.06	116.95	121.12
5	L	1406	RG1	C1'-O5'-C5'	2.06	117.73	113.69
3	H	1604	BCL	CMB-C2B-C1B	-2.05	125.31	128.46
3	K	1506	BCL	C3C-C2C-C1C	-2.05	98.55	101.87
3	F	1603	BCL	CHA-C1A-NA	-2.05	121.70	126.40
3	J	1605	BCL	C4-C3-C5	2.05	118.72	115.27
3	I	1505	BCL	C1-O2A-CGA	2.05	121.82	116.44
5	F	1403	RG1	O5'-C5'-C6'	2.05	111.53	106.44
3	G	1704	BCL	OBD-CAD-C3D	-2.05	124.58	127.98
3	D	1602	BCL	CHA-C1A-NA	-2.05	121.71	126.40
3	A	1501	BCL	C1-O2A-CGA	2.04	121.80	116.44
3	O	1708	BCL	CHA-C1A-NA	-2.04	121.73	126.40
3	R	1709	BCL	C6-C5-C3	-2.04	108.11	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1403	RG1	C20-C21-C22	-2.04	124.40	127.31
5	S	1409	RG1	C10-C11-C12	-2.03	116.88	123.22
5	R	1401	RG1	C20-C19-C18	-2.03	120.71	126.42
3	P	1608	BCL	C5-C3-C2	-2.03	117.02	121.12
3	S	1609	BCL	CHA-C1A-NA	-2.03	121.76	126.40
3	P	1608	BCL	CMB-C2B-C3B	2.02	128.47	124.68
3	C	1702	BCL	C6-C5-C3	-2.02	108.17	113.45
3	J	1605	BCL	C3C-C4C-CHD	-2.01	119.09	123.39
5	J	1405	RG1	C28-C29-C30	-2.01	124.42	127.30
5	P	1408	RG1	C29-C28-C27	-2.00	116.97	123.22
5	P	1408	RG1	C21-C20-C19	-2.00	116.97	123.22

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1501	BCL	CBD
3	C	1502	BCL	C13
3	N	1607	BCL	C2C
3	R	1509	BCL	C3A
3	P	1608	BCL	C2C
3	P	1608	BCL	C8
3	K	1706	BCL	C8
3	M	1707	BCL	CBD
3	G	1704	BCL	CBD
3	O	1708	BCL	C8
3	L	1606	BCL	C2C
3	L	1606	BCL	C8
3	L	1606	BCL	C3A
3	A	1701	BCL	C3C
3	K	1506	BCL	C3C
3	J	1605	BCL	CBD
3	O	1508	BCL	CBD
3	O	1508	BCL	C13
3	R	1709	BCL	C13
3	C	1702	BCL	C13
3	S	1609	BCL	C13
3	B	1601	BCL	C8
3	H	1604	BCL	C2C

All (513) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	1806	LDA	C2-C1-N1-O1
4	L	1806	LDA	C2-C1-N1-CM2
4	L	1806	LDA	N1-C1-C2-C3
4	K	1810	LDA	N1-C1-C2-C3
4	M	1827	LDA	N1-C1-C2-C3
3	N	1607	BCL	C1-C2-C3-C4
3	P	1608	BCL	C2C-C3C-CAC-CBC
3	P	1608	BCL	C4C-C3C-CAC-CBC
4	D	1802	LDA	C2-C1-N1-CM1
4	D	1802	LDA	N1-C1-C2-C3
3	M	1707	BCL	C2-C3-C5-C6
3	M	1707	BCL	C4-C3-C5-C6
5	P	1408	RG1	O1'-C1-C2-C3
5	P	1408	RG1	CM2-C1-C2-C3
5	P	1408	RG1	CM8-C26-C27-C28
3	A	1701	BCL	C4C-C3C-CAC-CBC
4	P	1808	LDA	N1-C1-C2-C3
4	J	1805	LDA	C2-C1-N1-O1
4	J	1805	LDA	N1-C1-C2-C3
3	K	1506	BCL	C4C-C3C-CAC-CBC
3	J	1605	BCL	CHA-CBD-CGD-O1D
4	A	1817	LDA	C2-C1-N1-CM1
4	A	1817	LDA	N1-C1-C2-C3
3	C	1702	BCL	C1-C2-C3-C4
3	C	1702	BCL	C1-C2-C3-C5
4	I	1825	LDA	C2-C1-N1-CM1
3	I	1705	BCL	C11-C10-C8-C9
4	C	1815	LDA	N1-C1-C2-C3
3	F	1603	BCL	C11-C10-C8-C7
4	F	1803	LDA	C2-C1-N1-O1
4	F	1803	LDA	C2-C1-N1-CM1
4	F	1803	LDA	C2-C1-N1-CM2
5	H	1404	RG1	O1'-C1-C2-C3
5	H	1404	RG1	CM1-C1-C2-C3
5	H	1404	RG1	CM2-C1-C2-C3
4	I	1812	LDA	N1-C1-C2-C3
4	G	1814	LDA	C2-C1-N1-CM1
4	G	1814	LDA	C2-C1-N1-CM2
4	E	1822	LDA	N1-C1-C2-C3
5	F	1403	RG1	C25-C26-C27-C28
5	F	1403	RG1	CM8-C26-C27-C28
4	B	1801	LDA	N1-C1-C2-C3
4	O	1820	LDA	N1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	R	1809	LDA	C2-C1-N1-O1
4	R	1809	LDA	C2-C1-N1-CM1
4	R	1809	LDA	C2-C1-N1-CM2
3	E	1503	BCL	C2C-C3C-CAC-CBC
3	H	1604	BCL	C2C-C3C-CAC-CBC
3	H	1604	BCL	C4C-C3C-CAC-CBC
3	H	1604	BCL	CHA-CBD-CGD-O1D
3	R	1709	BCL	O1D-CGD-O2D-CED
3	R	1709	BCL	CBD-CGD-O2D-CED
3	A	1501	BCL	CBD-CGD-O2D-CED
3	M	1707	BCL	CBD-CGD-O2D-CED
3	O	1708	BCL	CBD-CGD-O2D-CED
3	J	1605	BCL	C3-C5-C6-C7
3	R	1709	BCL	C3-C5-C6-C7
3	F	1603	BCL	C5-C6-C7-C8
3	H	1604	BCL	CBD-CGD-O2D-CED
3	O	1708	BCL	C3-C5-C6-C7
3	A	1701	BCL	C3-C5-C6-C7
3	S	1609	BCL	C3-C5-C6-C7
5	H	1404	RG1	C2-C3-C4-C5
3	G	1704	BCL	CBD-CGD-O2D-CED
5	P	1408	RG1	O5'-C5'-C6'-O6'
3	S	1609	BCL	CBD-CGD-O2D-CED
3	M	1707	BCL	O1D-CGD-O2D-CED
5	P	1408	RG1	C4'-C5'-C6'-O6'
3	D	1602	BCL	C5-C6-C7-C8
5	L	1406	RG1	O5'-C5'-C6'-O6'
3	O	1708	BCL	O1D-CGD-O2D-CED
5	L	1406	RG1	C4'-C5'-C6'-O6'
3	S	1609	BCL	C10-C11-C12-C13
3	M	1707	BCL	C10-C11-C12-C13
3	E	1703	BCL	C6-C7-C8-C9
3	R	1709	BCL	C11-C10-C8-C9
3	F	1603	BCL	C11-C12-C13-C14
3	S	1609	BCL	C11-C12-C13-C14
3	O	1508	BCL	CBD-CGD-O2D-CED
5	D	1402	RG1	CM8-C26-C27-C28
5	S	1409	RG1	CM8-C26-C27-C28
5	H	1404	RG1	CM8-C26-C27-C28
5	J	1405	RG1	CM8-C26-C27-C28
5	R	1401	RG1	CM8-C26-C27-C28
5	H	1404	RG1	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	R	1401	RG1	C25-C26-C27-C28
5	J	1405	RG1	O5'-C5'-C6'-O6'
3	P	1608	BCL	C3-C5-C6-C7
3	A	1501	BCL	C15-C16-C17-C18
3	A	1701	BCL	C10-C11-C12-C13
3	K	1506	BCL	C8-C10-C11-C12
3	C	1702	BCL	C5-C6-C7-C8
3	C	1702	BCL	C15-C16-C17-C18
3	M	1507	BCL	C15-C16-C17-C18
3	M	1707	BCL	C8-C10-C11-C12
3	F	1603	BCL	C8-C10-C11-C12
3	E	1503	BCL	C8-C10-C11-C12
5	J	1405	RG1	C4'-C5'-C6'-O6'
3	A	1501	BCL	O1D-CGD-O2D-CED
3	N	1607	BCL	C8-C10-C11-C12
3	G	1504	BCL	C12-C13-C15-C16
3	P	1608	BCL	C6-C7-C8-C10
3	C	1702	BCL	C11-C12-C13-C15
3	S	1609	BCL	C11-C10-C8-C7
3	B	1601	BCL	C6-C7-C8-C10
3	H	1604	BCL	O1D-CGD-O2D-CED
3	C	1502	BCL	C10-C11-C12-C13
3	D	1602	BCL	C13-C15-C16-C17
3	M	1507	BCL	C8-C10-C11-C12
3	G	1504	BCL	C8-C10-C11-C12
3	P	1608	BCL	C5-C6-C7-C8
4	R	1819	LDA	C3-C4-C5-C6
3	D	1602	BCL	C10-C11-C12-C13
3	O	1708	BCL	C10-C11-C12-C13
4	I	1813	LDA	C7-C8-C9-C10
4	R	1809	LDA	C6-C7-C8-C9
3	M	1707	BCL	C5-C6-C7-C8
4	P	1808	LDA	C2-C3-C4-C5
4	K	1826	LDA	C6-C7-C8-C9
3	G	1704	BCL	O1D-CGD-O2D-CED
3	N	1607	BCL	C16-C17-C18-C20
4	I	1813	LDA	C6-C7-C8-C9
4	O	1820	LDA	C6-C7-C8-C9
4	D	1802	LDA	C7-C8-C9-C10
4	P	1808	LDA	C11-C10-C9-C8
4	L	1806	LDA	C3-C4-C5-C6
4	J	1805	LDA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1816	LDA	C6-C7-C8-C9
4	E	1822	LDA	C5-C6-C7-C8
4	A	1816	LDA	C7-C8-C9-C10
4	F	1803	LDA	C6-C7-C8-C9
5	D	1402	RG1	O5'-C5'-C6'-O6'
4	D	1802	LDA	C11-C10-C9-C8
4	F	1803	LDA	C4-C5-C6-C7
3	J	1605	BCL	C16-C17-C18-C20
4	R	1819	LDA	C5-C6-C7-C8
3	G	1504	BCL	C14-C13-C15-C16
3	I	1505	BCL	C11-C12-C13-C14
3	J	1605	BCL	C11-C10-C8-C9
3	C	1702	BCL	C11-C10-C8-C9
3	F	1603	BCL	C14-C13-C15-C16
3	S	1609	BCL	C11-C10-C8-C9
3	E	1503	BCL	C14-C13-C15-C16
4	M	1827	LDA	C4-C5-C6-C7
4	M	1827	LDA	C7-C8-C9-C10
4	N	1807	LDA	C11-C10-C9-C8
4	K	1826	LDA	C2-C3-C4-C5
4	K	1826	LDA	C5-C6-C7-C8
4	C	1815	LDA	C5-C6-C7-C8
4	G	1824	LDA	C6-C7-C8-C9
4	G	1814	LDA	C5-C6-C7-C8
4	H	1804	LDA	C3-C4-C5-C6
4	O	1820	LDA	C11-C10-C9-C8
4	I	1825	LDA	C11-C10-C9-C8
5	P	1408	RG1	C25-C26-C27-C28
5	D	1402	RG1	C25-C26-C27-C28
5	S	1409	RG1	C25-C26-C27-C28
5	J	1405	RG1	C25-C26-C27-C28
3	C	1702	BCL	C3-C5-C6-C7
3	I	1705	BCL	C3-C5-C6-C7
4	L	1806	LDA	C5-C6-C7-C8
4	C	1815	LDA	C6-C7-C8-C9
4	E	1823	LDA	C5-C6-C7-C8
4	N	1807	LDA	C5-C6-C7-C8
4	J	1805	LDA	C2-C3-C4-C5
4	C	1815	LDA	C2-C3-C4-C5
4	I	1812	LDA	C2-C3-C4-C5
4	O	1820	LDA	C7-C8-C9-C10
4	C	1821	LDA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	M	1707	BCL	C16-C17-C18-C19
3	G	1704	BCL	C8-C10-C11-C12
3	A	1701	BCL	C8-C10-C11-C12
4	H	1804	LDA	C4-C5-C6-C7
3	G	1704	BCL	C5-C6-C7-C8
4	H	1804	LDA	C2-C3-C4-C5
4	I	1825	LDA	C3-C4-C5-C6
4	G	1824	LDA	C7-C8-C9-C10
3	O	1508	BCL	O1D-CGD-O2D-CED
3	S	1609	BCL	O1D-CGD-O2D-CED
3	R	1509	BCL	C3A-C2A-CAA-CBA
4	E	1823	LDA	C7-C8-C9-C10
4	A	1817	LDA	C3-C4-C5-C6
4	G	1824	LDA	C3-C4-C5-C6
4	R	1818	LDA	C7-C8-C9-C10
4	C	1821	LDA	C7-C8-C9-C10
4	K	1810	LDA	C1-C2-C3-C4
3	E	1503	BCL	C15-C16-C17-C18
4	B	1801	LDA	C2-C3-C4-C5
4	L	1806	LDA	C11-C10-C9-C8
3	E	1703	BCL	C3-C5-C6-C7
4	A	1817	LDA	C11-C10-C9-C8
4	I	1812	LDA	C7-C8-C9-C10
4	A	1817	LDA	C4-C5-C6-C7
3	N	1607	BCL	C2-C1-O2A-CGA
4	K	1810	LDA	C3-C4-C5-C6
4	E	1822	LDA	C11-C10-C9-C8
4	N	1807	LDA	C2-C3-C4-C5
4	A	1817	LDA	C1-C2-C3-C4
4	M	1811	LDA	C11-C10-C9-C8
3	R	1509	BCL	C8-C10-C11-C12
3	M	1707	BCL	C15-C16-C17-C18
4	I	1825	LDA	C7-C8-C9-C10
4	M	1811	LDA	C3-C4-C5-C6
3	C	1702	BCL	CBD-CGD-O2D-CED
3	C	1502	BCL	C12-C13-C15-C16
3	N	1607	BCL	C6-C7-C8-C10
3	D	1602	BCL	C6-C7-C8-C10
3	O	1708	BCL	C11-C10-C8-C7
3	I	1505	BCL	C11-C12-C13-C15
3	J	1605	BCL	C11-C10-C8-C7
3	F	1603	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	S	1609	BCL	C6-C7-C8-C10
3	E	1503	BCL	C12-C13-C15-C16
3	B	1601	BCL	C3-C5-C6-C7
4	L	1806	LDA	C1-C2-C3-C4
4	M	1811	LDA	C2-C3-C4-C5
4	A	1816	LDA	C1-C2-C3-C4
3	E	1703	BCL	C5-C6-C7-C8
3	E	1703	BCL	C15-C16-C17-C18
3	K	1506	BCL	C15-C16-C17-C18
4	O	1820	LDA	C3-C4-C5-C6
4	L	1806	LDA	C4-C5-C6-C7
4	D	1802	LDA	C5-C6-C7-C8
4	C	1821	LDA	C4-C5-C6-C7
4	B	1801	LDA	C11-C10-C9-C8
3	N	1607	BCL	CBD-CGD-O2D-CED
4	L	1806	LDA	C2-C3-C4-C5
4	E	1822	LDA	C1-C2-C3-C4
4	R	1809	LDA	C4-C5-C6-C7
3	M	1707	BCL	C16-C17-C18-C20
4	C	1821	LDA	C11-C10-C9-C8
3	E	1703	BCL	C13-C15-C16-C17
3	N	1607	BCL	C6-C7-C8-C9
3	N	1607	BCL	C14-C13-C15-C16
3	R	1509	BCL	C11-C12-C13-C14
3	D	1602	BCL	C6-C7-C8-C9
3	P	1608	BCL	C6-C7-C8-C9
3	P	1608	BCL	C11-C10-C8-C9
3	F	1603	BCL	C11-C10-C8-C9
3	M	1707	BCL	CBA-CGA-O2A-C1
5	L	1406	RG1	CM8-C26-C27-C28
4	K	1810	LDA	C6-C7-C8-C9
3	R	1509	BCL	C1A-C2A-CAA-CBA
4	N	1807	LDA	C7-C8-C9-C10
4	A	1816	LDA	C3-C4-C5-C6
4	E	1822	LDA	C4-C5-C6-C7
3	S	1609	BCL	C8-C10-C11-C12
4	C	1815	LDA	C4-C5-C6-C7
3	K	1706	BCL	C8-C10-C11-C12
3	O	1708	BCL	C8-C10-C11-C12
3	I	1505	BCL	C8-C10-C11-C12
3	R	1509	BCL	CBA-CGA-O2A-C1
3	A	1701	BCL	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	1506	BCL	C2C-C3C-CAC-CBC
4	F	1803	LDA	C2-C3-C4-C5
4	H	1804	LDA	C5-C6-C7-C8
3	M	1707	BCL	O1A-CGA-O2A-C1
4	A	1817	LDA	C7-C8-C9-C10
4	C	1815	LDA	C11-C10-C9-C8
4	M	1811	LDA	C7-C8-C9-C10
4	F	1803	LDA	C3-C4-C5-C6
4	I	1813	LDA	C5-C6-C7-C8
4	R	1819	LDA	C9-C10-C11-C12
3	L	1606	BCL	C3-C5-C6-C7
4	K	1810	LDA	C9-C10-C11-C12
4	G	1814	LDA	C6-C7-C8-C9
4	R	1818	LDA	C11-C10-C9-C8
4	E	1822	LDA	C3-C4-C5-C6
4	F	1803	LDA	C5-C6-C7-C8
3	A	1701	BCL	C16-C17-C18-C20
3	K	1706	BCL	C10-C11-C12-C13
4	R	1818	LDA	C5-C6-C7-C8
4	P	1808	LDA	C9-C10-C11-C12
3	K	1706	BCL	C5-C6-C7-C8
3	B	1601	BCL	C2-C1-O2A-CGA
4	H	1804	LDA	C6-C7-C8-C9
4	R	1818	LDA	C9-C10-C11-C12
3	A	1701	BCL	C16-C17-C18-C19
4	E	1823	LDA	C2-C3-C4-C5
4	M	1827	LDA	C3-C4-C5-C6
4	M	1811	LDA	C4-C5-C6-C7
4	G	1814	LDA	C3-C4-C5-C6
3	N	1607	BCL	C10-C11-C12-C13
4	J	1805	LDA	C9-C10-C11-C12
3	N	1607	BCL	C12-C13-C15-C16
3	E	1703	BCL	C6-C7-C8-C10
3	A	1701	BCL	C11-C10-C8-C7
3	I	1505	BCL	C12-C13-C15-C16
3	O	1508	BCL	C11-C12-C13-C15
3	R	1709	BCL	C11-C12-C13-C15
3	R	1709	BCL	C12-C13-C15-C16
3	R	1509	BCL	C14-C13-C15-C16
3	D	1602	BCL	C11-C12-C13-C14
3	P	1608	BCL	C11-C12-C13-C14
3	O	1708	BCL	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1701	BCL	C11-C10-C8-C9
3	O	1508	BCL	C11-C12-C13-C14
3	R	1709	BCL	C11-C12-C13-C14
3	S	1609	BCL	C6-C7-C8-C9
3	B	1601	BCL	C6-C7-C8-C9
3	E	1703	BCL	CBA-CGA-O2A-C1
3	R	1709	BCL	C13-C15-C16-C17
3	E	1703	BCL	O1A-CGA-O2A-C1
5	N	1407	RG1	CM8-C26-C27-C28
3	D	1602	BCL	C8-C10-C11-C12
3	H	1604	BCL	C16-C17-C18-C20
5	L	1406	RG1	C25-C26-C27-C28
4	R	1819	LDA	N1-C1-C2-C3
3	A	1501	BCL	C8-C10-C11-C12
3	N	1607	BCL	C1-C2-C3-C5
4	R	1818	LDA	C6-C7-C8-C9
4	I	1812	LDA	C6-C7-C8-C9
3	C	1702	BCL	CBA-CGA-O2A-C1
4	R	1819	LDA	C1-C2-C3-C4
5	P	1408	RG1	CM1-C1-C2-C3
3	P	1608	BCL	O2A-C1-C2-C3
4	J	1805	LDA	C5-C6-C7-C8
4	G	1814	LDA	C4-C5-C6-C7
4	I	1813	LDA	C3-C4-C5-C6
4	C	1821	LDA	C9-C10-C11-C12
3	G	1504	BCL	C15-C16-C17-C18
3	H	1604	BCL	C16-C17-C18-C19
3	R	1509	BCL	O1A-CGA-O2A-C1
4	I	1825	LDA	C1-C2-C3-C4
3	C	1702	BCL	O1D-CGD-O2D-CED
3	E	1703	BCL	C16-C17-C18-C20
3	K	1506	BCL	C16-C17-C18-C19
4	I	1825	LDA	C6-C7-C8-C9
5	H	1404	RG1	C4'-C5'-C6'-O6'
3	I	1705	BCL	C2-C1-O2A-CGA
3	E	1703	BCL	C11-C12-C13-C14
3	M	1507	BCL	C4C-C3C-CAC-CBC
3	N	1607	BCL	C16-C17-C18-C19
3	J	1605	BCL	C16-C17-C18-C19
4	I	1812	LDA	C4-C5-C6-C7
4	B	1801	LDA	C7-C8-C9-C10
4	R	1809	LDA	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	R	1509	BCL	C11-C12-C13-C15
3	R	1509	BCL	C12-C13-C15-C16
3	K	1706	BCL	C6-C7-C8-C10
3	C	1702	BCL	C6-C7-C8-C10
3	I	1705	BCL	C11-C10-C8-C7
3	S	1609	BCL	C12-C13-C15-C16
3	H	1604	BCL	C12-C13-C15-C16
5	N	1407	RG1	C27-C28-C29-C30
3	R	1709	BCL	C16-C17-C18-C20
4	R	1809	LDA	C5-C6-C7-C8
4	P	1808	LDA	C1-C2-C3-C4
3	A	1701	BCL	CAD-CBD-CGD-O2D
3	C	1702	BCL	CAD-CBD-CGD-O2D
3	I	1705	BCL	CAD-CBD-CGD-O2D
3	H	1604	BCL	C3-C5-C6-C7
4	B	1801	LDA	C6-C7-C8-C9
3	O	1508	BCL	C8-C10-C11-C12
3	E	1703	BCL	CBD-CGD-O2D-CED
4	L	1806	LDA	C2-C1-N1-CM1
4	D	1802	LDA	C2-C1-N1-CM2
4	J	1805	LDA	C2-C1-N1-CM2
4	A	1817	LDA	C2-C1-N1-CM2
3	R	1709	BCL	CHA-CBD-CGD-O1D
3	R	1709	BCL	CHA-CBD-CGD-O2D
3	H	1604	BCL	CHA-CBD-CGD-O2D
3	O	1508	BCL	O1A-CGA-O2A-C1
3	C	1702	BCL	O1A-CGA-O2A-C1
3	P	1608	BCL	CBD-CGD-O2D-CED
4	P	1808	LDA	C6-C7-C8-C9
4	R	1819	LDA	C6-C7-C8-C9
3	C	1502	BCL	C14-C13-C15-C16
3	H	1604	BCL	C14-C13-C15-C16
4	J	1805	LDA	C1-C2-C3-C4
3	O	1508	BCL	C10-C11-C12-C13
5	N	1407	RG1	C25-C26-C27-C28
3	M	1707	BCL	C1A-C2A-CAA-CBA
4	A	1816	LDA	C11-C10-C9-C8
4	P	1808	LDA	C7-C8-C9-C10
4	R	1809	LDA	C11-C10-C9-C8
3	G	1504	BCL	O1D-CGD-O2D-CED
5	S	1409	RG1	C2-C1-O1'-C1'
5	R	1401	RG1	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	F	1403	RG1	C2-C1-O1'-C1'
3	O	1708	BCL	C6-C7-C8-C10
3	R	1709	BCL	C11-C10-C8-C7
3	F	1603	BCL	C11-C12-C13-C15
4	G	1824	LDA	C5-C6-C7-C8
4	A	1816	LDA	C9-C10-C11-C12
3	C	1502	BCL	O1D-CGD-O2D-CED
4	J	1805	LDA	C7-C8-C9-C10
4	B	1801	LDA	C4-C5-C6-C7
5	H	1404	RG1	O5'-C5'-C6'-O6'
3	O	1508	BCL	CBA-CGA-O2A-C1
4	R	1819	LDA	C2-C3-C4-C5
3	I	1505	BCL	C14-C13-C15-C16
3	K	1506	BCL	C11-C12-C13-C14
3	C	1702	BCL	C6-C7-C8-C9
4	K	1826	LDA	C4-C5-C6-C7
3	N	1607	BCL	O1A-CGA-O2A-C1
4	D	1802	LDA	C6-C7-C8-C9
4	E	1822	LDA	C7-C8-C9-C10
3	R	1709	BCL	C16-C17-C18-C19
4	K	1826	LDA	C11-C10-C9-C8
4	G	1814	LDA	C11-C10-C9-C8
3	C	1502	BCL	C15-C16-C17-C18
4	B	1801	LDA	C1-C2-C3-C4
4	F	1803	LDA	C7-C8-C9-C10
3	P	1608	BCL	O1A-CGA-O2A-C1
4	G	1814	LDA	C7-C8-C9-C10
3	O	1708	BCL	C5-C6-C7-C8
3	G	1504	BCL	C11-C12-C13-C14
3	L	1606	BCL	C11-C10-C8-C9
3	E	1503	BCL	C11-C12-C13-C14
4	B	1801	LDA	C3-C4-C5-C6
3	N	1607	BCL	CBA-CGA-O2A-C1
3	L	1606	BCL	C13-C15-C16-C17
4	R	1819	LDA	C4-C5-C6-C7
3	L	1606	BCL	C10-C11-C12-C13
4	I	1813	LDA	N1-C1-C2-C3
3	P	1608	BCL	CBA-CGA-O2A-C1
4	I	1812	LDA	C11-C10-C9-C8
4	M	1811	LDA	C6-C7-C8-C9
3	A	1701	BCL	C15-C16-C17-C18
3	J	1605	BCL	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	N	1607	BCL	C11-C12-C13-C14
3	S	1609	BCL	O2A-C1-C2-C3
3	H	1604	BCL	O2A-C1-C2-C3
4	P	1808	LDA	C5-C6-C7-C8
4	K	1810	LDA	C4-C5-C6-C7
4	E	1823	LDA	C3-C4-C5-C6
3	G	1704	BCL	C11-C12-C13-C15
3	K	1506	BCL	C11-C12-C13-C15
3	J	1605	BCL	C12-C13-C15-C16
3	E	1503	BCL	C11-C12-C13-C15
3	C	1502	BCL	C8-C10-C11-C12
4	M	1811	LDA	C5-C6-C7-C8
4	H	1804	LDA	C9-C10-C11-C12
3	I	1705	BCL	C13-C15-C16-C17
4	D	1802	LDA	C4-C5-C6-C7
3	K	1706	BCL	O1A-CGA-O2A-C1
3	B	1601	BCL	O1A-CGA-O2A-C1
3	R	1709	BCL	C5-C6-C7-C8
3	N	1607	BCL	C4-C3-C5-C6
3	L	1606	BCL	C4-C3-C5-C6
3	F	1603	BCL	C4-C3-C5-C6
4	R	1809	LDA	C7-C8-C9-C10
4	K	1810	LDA	C11-C10-C9-C8
4	K	1826	LDA	C3-C4-C5-C6
3	R	1709	BCL	C8-C10-C11-C12
3	M	1507	BCL	C12-C13-C15-C16
3	A	1501	BCL	C1-C2-C3-C4
3	P	1608	BCL	C1-C2-C3-C4
3	E	1703	BCL	C1-C2-C3-C4
3	G	1704	BCL	C1-C2-C3-C4
3	I	1505	BCL	C1-C2-C3-C4
3	S	1609	BCL	C1-C2-C3-C4
3	B	1601	BCL	C1-C2-C3-C4
3	H	1604	BCL	C1-C2-C3-C4
4	R	1809	LDA	C2-C3-C4-C5
3	G	1504	BCL	C3-C5-C6-C7
3	M	1507	BCL	C14-C13-C15-C16
3	O	1508	BCL	C11-C10-C8-C9
3	H	1604	BCL	C11-C12-C13-C14
4	I	1825	LDA	C5-C6-C7-C8
3	R	1509	BCL	CAD-CBD-CGD-O2D
3	E	1703	BCL	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	O	1708	BCL	CAD-CBD-CGD-O2D
3	I	1705	BCL	O1A-CGA-O2A-C1
3	G	1704	BCL	C4-C3-C5-C6
5	H	1404	RG1	C17-C18-C19-C20
5	J	1405	RG1	C21-C22-C23-C24
3	G	1704	BCL	O2A-C1-C2-C3
3	L	1606	BCL	O2A-C1-C2-C3
3	F	1603	BCL	O2A-C1-C2-C3
3	B	1601	BCL	O1D-CGD-O2D-CED
3	N	1607	BCL	CHA-CBD-CGD-O2D
3	P	1608	BCL	CHA-CBD-CGD-O2D
3	J	1605	BCL	CHA-CBD-CGD-O2D
3	O	1508	BCL	CHA-CBD-CGD-O1D
3	O	1508	BCL	CHA-CBD-CGD-O2D
3	C	1702	BCL	CHA-CBD-CGD-O1D
4	I	1825	LDA	C2-C1-N1-CM2
3	F	1603	BCL	CHA-CBD-CGD-O2D
3	B	1601	BCL	CHA-CBD-CGD-O2D
4	I	1812	LDA	C2-C1-N1-CM1
5	L	1406	RG1	C27-C28-C29-C30
3	N	1607	BCL	C2-C3-C5-C6
4	N	1807	LDA	C6-C7-C8-C9
5	D	1402	RG1	C4'-C5'-C6'-O6'
3	K	1506	BCL	C12-C13-C15-C16
3	J	1605	BCL	C14-C13-C15-C16
3	B	1601	BCL	C11-C10-C8-C9
4	E	1823	LDA	C9-C10-C11-C12
3	K	1706	BCL	CBA-CGA-O2A-C1
3	S	1609	BCL	C1A-C2A-CAA-CBA
3	D	1602	BCL	C16-C17-C18-C19
3	R	1709	BCL	C2-C1-O2A-CGA
4	N	1807	LDA	C3-C4-C5-C6
3	O	1708	BCL	C15-C16-C17-C18
3	D	1602	BCL	CAD-CBD-CGD-O1D
3	P	1608	BCL	CAD-CBD-CGD-O1D
3	E	1703	BCL	CAD-CBD-CGD-O1D
3	L	1606	BCL	C14-C13-C15-C16
3	J	1605	BCL	C11-C12-C13-C14
3	B	1601	BCL	C5-C6-C7-C8
3	P	1608	BCL	C11-C12-C13-C15
3	L	1606	BCL	C11-C10-C8-C7
3	L	1606	BCL	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1702	BCL	C2C-C3C-CAC-CBC
3	H	1604	BCL	C6-C7-C8-C10
5	J	1405	RG1	C17-C18-C19-C20
5	F	1403	RG1	C17-C18-C19-C20
4	A	1817	LDA	C9-C10-C11-C12
3	F	1603	BCL	C15-C16-C17-C18
3	I	1705	BCL	CBA-CGA-O2A-C1
3	S	1609	BCL	C5-C6-C7-C8

There are no ring outliers.

60 monomers are involved in 432 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	1507	BCL	7	0
3	G	1504	BCL	6	0
5	N	1407	RG1	4	0
3	A	1501	BCL	17	0
4	L	1806	LDA	5	0
4	K	1810	LDA	8	0
4	M	1827	LDA	2	0
3	C	1502	BCL	7	0
3	N	1607	BCL	16	0
3	R	1509	BCL	7	0
3	D	1602	BCL	8	0
3	P	1608	BCL	10	0
3	E	1703	BCL	7	0
4	D	1802	LDA	3	0
3	K	1706	BCL	5	0
3	M	1707	BCL	21	0
3	G	1704	BCL	21	0
3	O	1708	BCL	10	0
4	E	1823	LDA	6	0
5	P	1408	RG1	4	0
3	L	1606	BCL	25	0
3	A	1701	BCL	8	0
4	N	1807	LDA	2	0
4	P	1808	LDA	3	0
3	I	1505	BCL	12	0
4	G	1814	LDA	3	0
4	J	1805	LDA	1	0
5	D	1402	RG1	5	0
3	K	1506	BCL	9	0

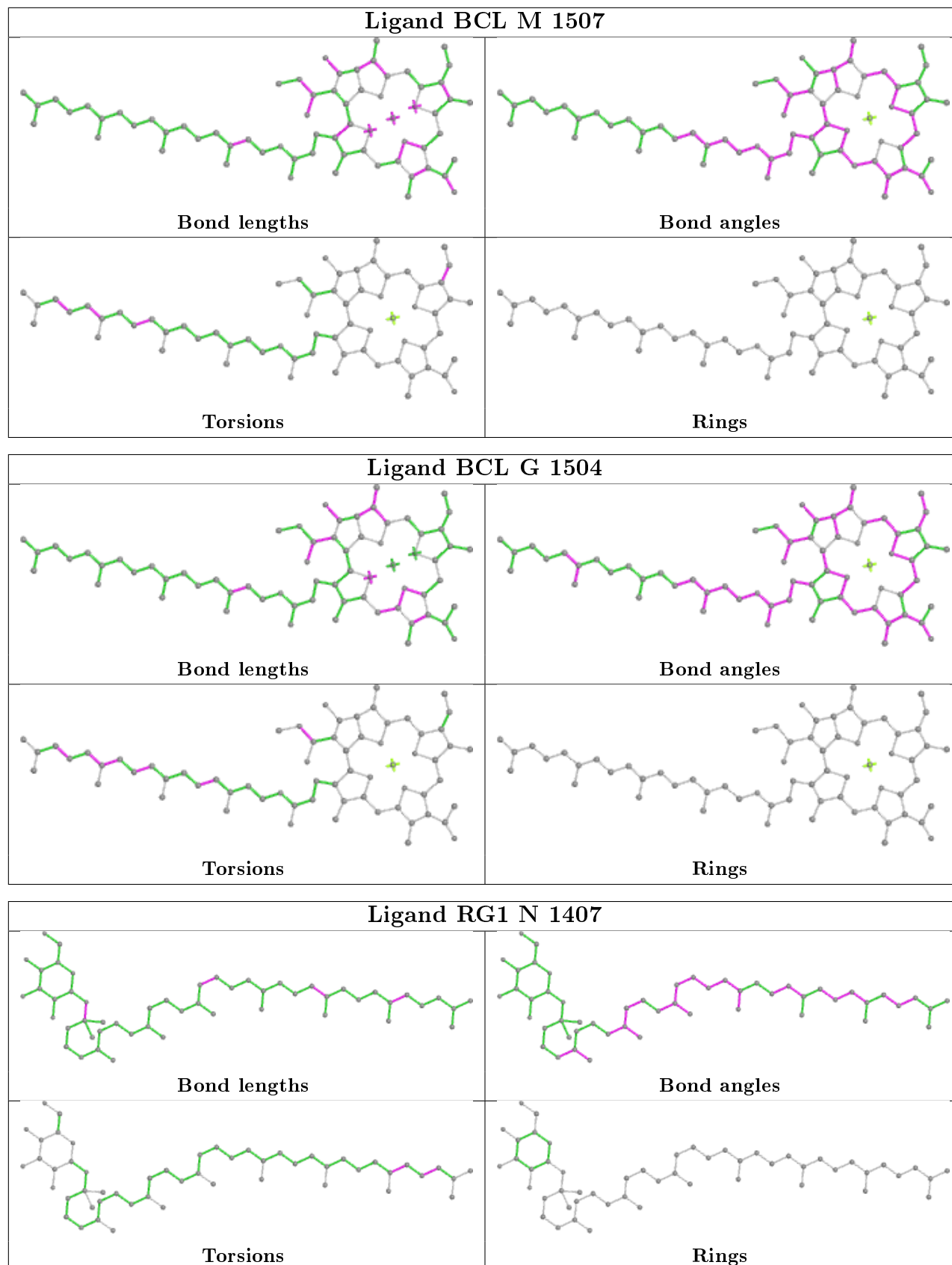
Continued on next page...

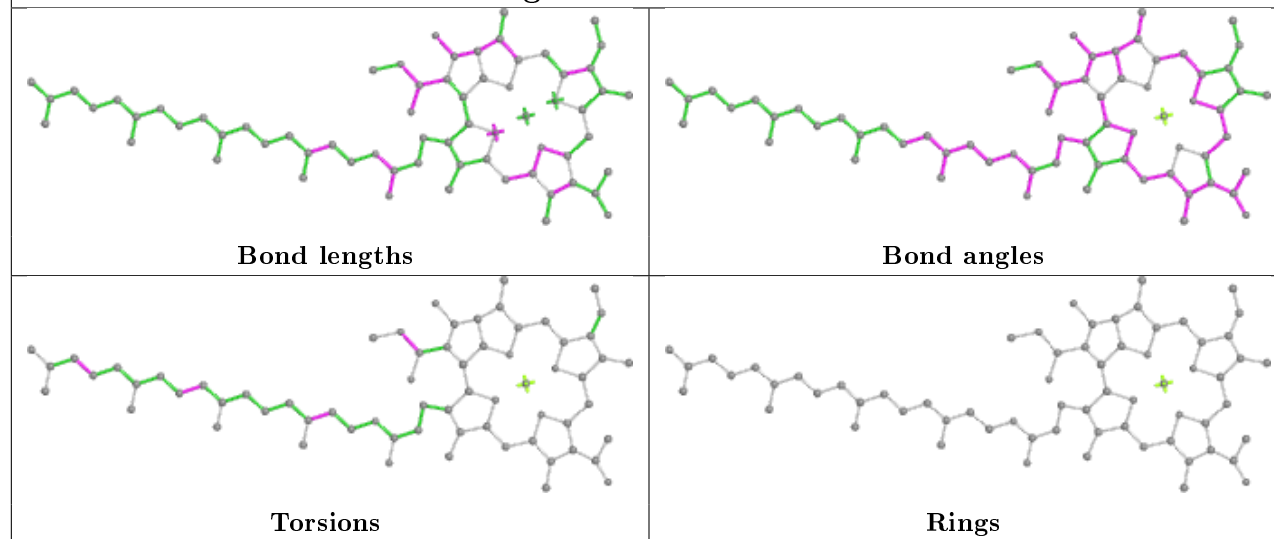
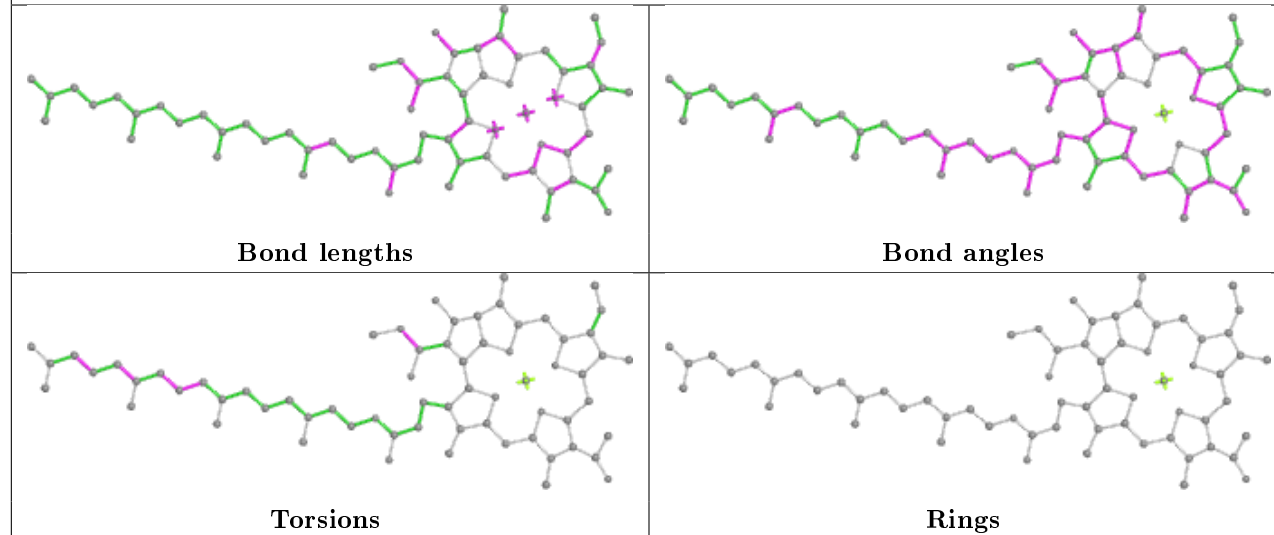
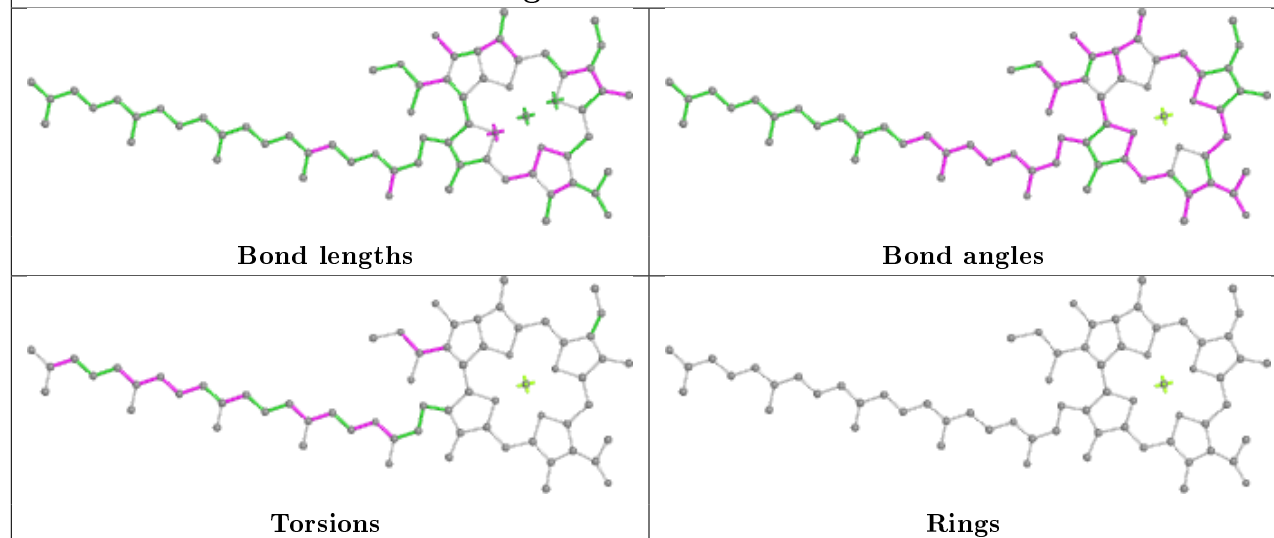
Continued from previous page...

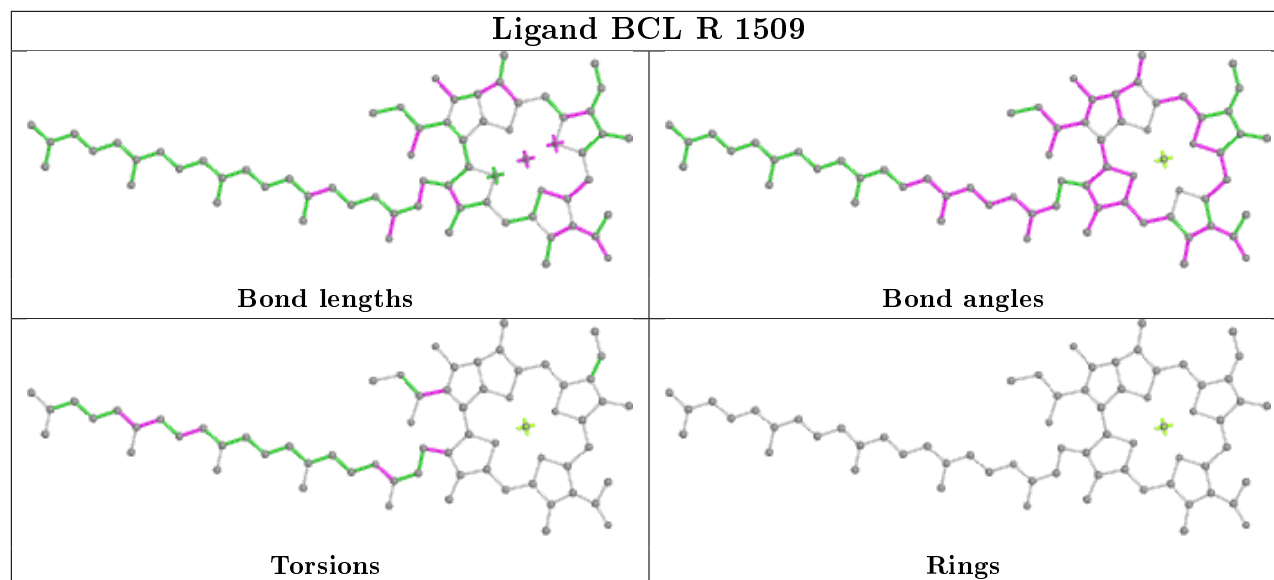
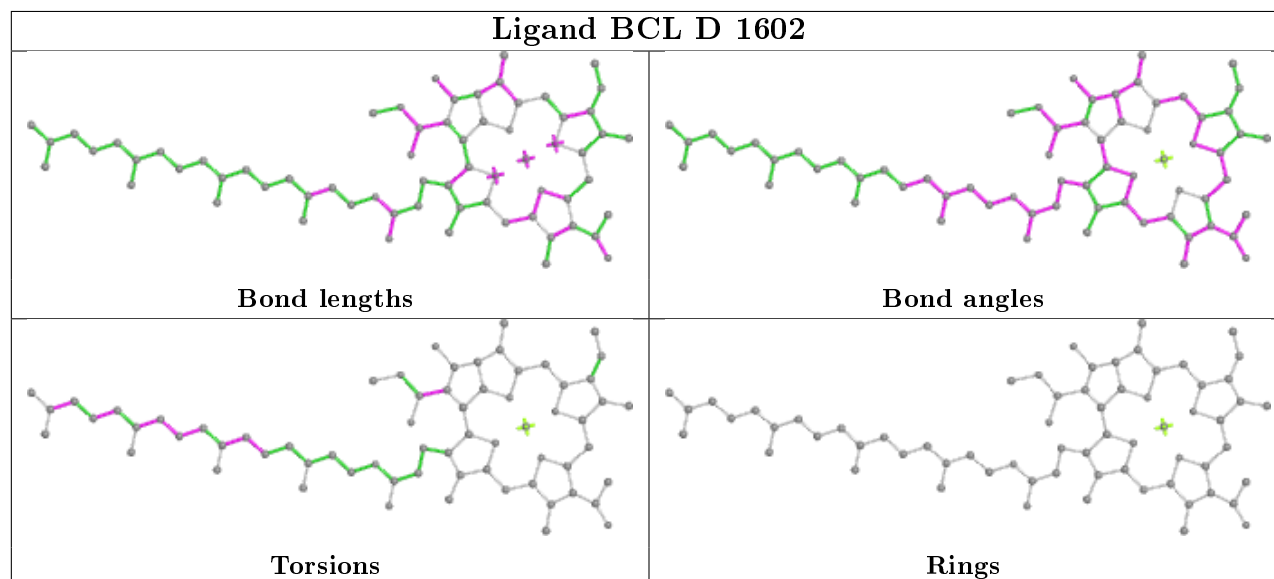
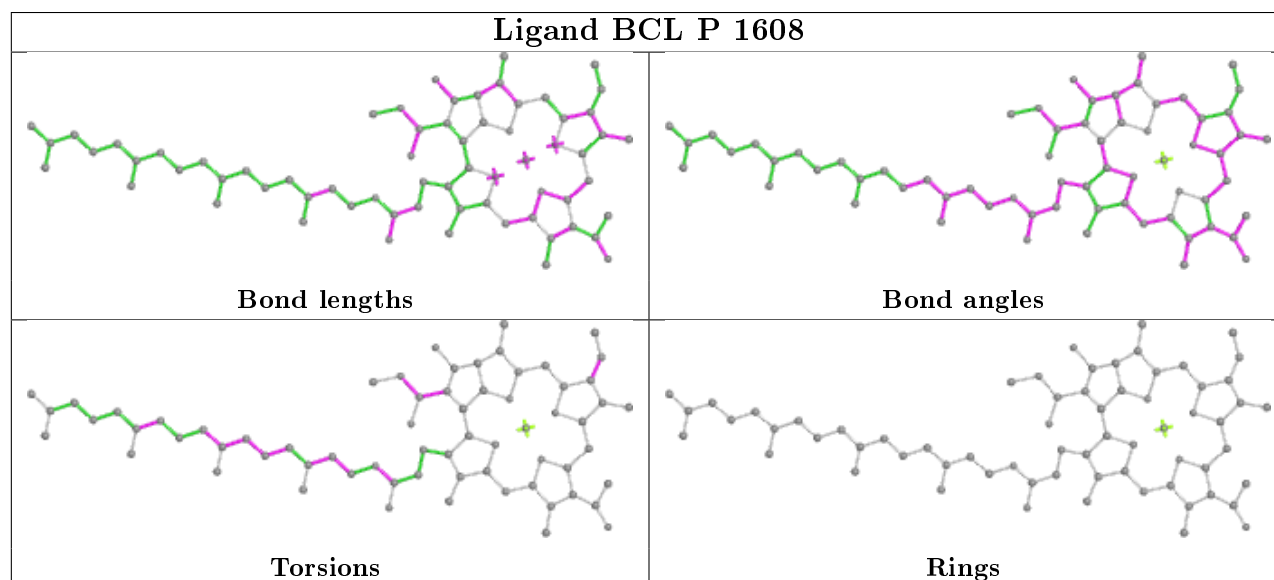
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1816	LDA	8	0
3	J	1605	BCL	17	0
3	O	1508	BCL	11	0
4	K	1826	LDA	4	0
4	A	1817	LDA	3	0
3	S	1609	BCL	13	0
3	C	1702	BCL	8	0
4	I	1825	LDA	6	0
3	I	1705	BCL	21	0
4	C	1815	LDA	6	0
5	S	1409	RG1	5	0
3	F	1603	BCL	12	0
4	G	1824	LDA	14	0
4	F	1803	LDA	7	0
3	R	1709	BCL	21	0
5	H	1404	RG1	5	0
3	B	1601	BCL	11	0
5	J	1405	RG1	1	0
4	I	1812	LDA	7	0
4	R	1818	LDA	12	0
4	H	1804	LDA	3	0
5	R	1401	RG1	4	0
4	E	1822	LDA	8	0
5	F	1403	RG1	5	0
4	B	1801	LDA	2	0
4	I	1813	LDA	2	0
5	L	1406	RG1	4	0
4	O	1820	LDA	7	0
3	E	1503	BCL	5	0
3	H	1604	BCL	12	0
4	M	1811	LDA	4	0

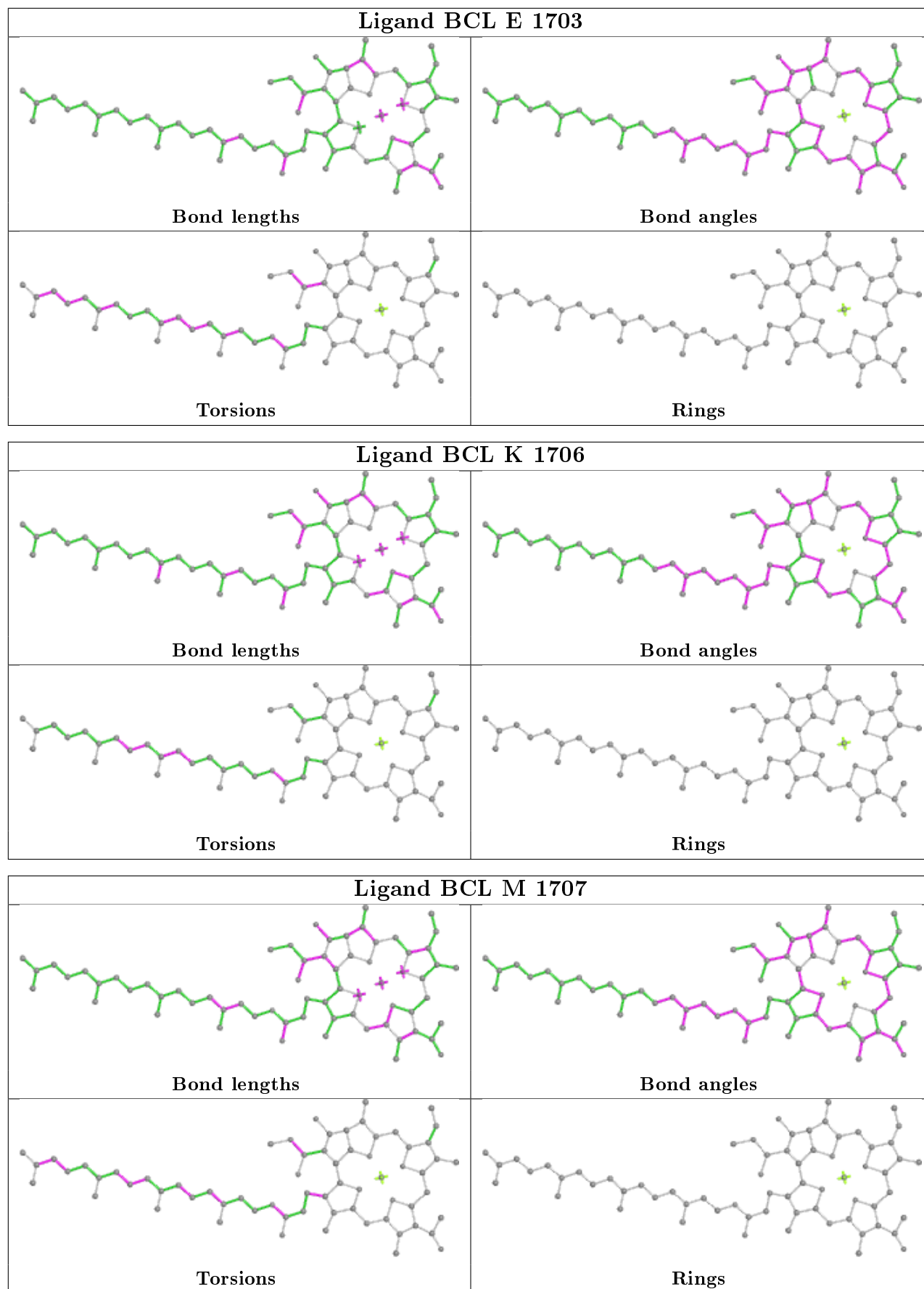
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

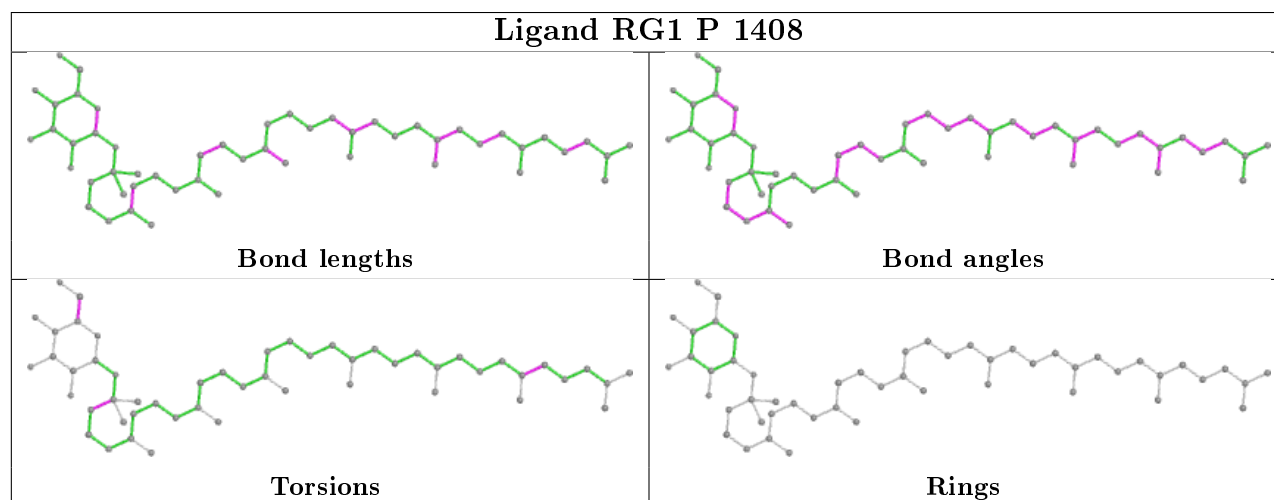
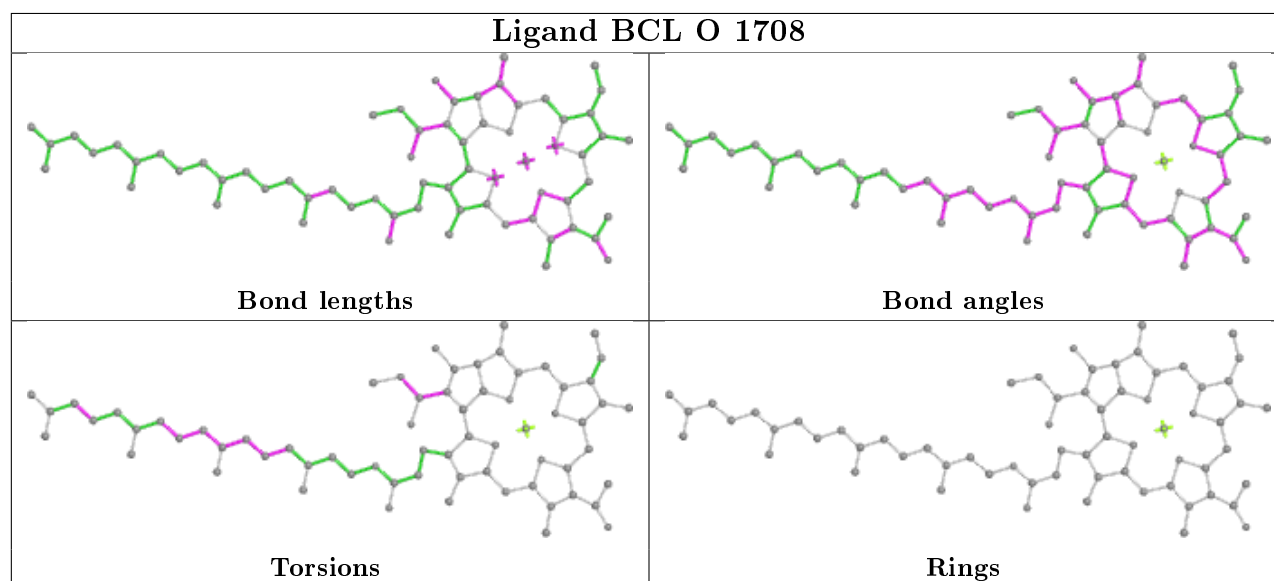
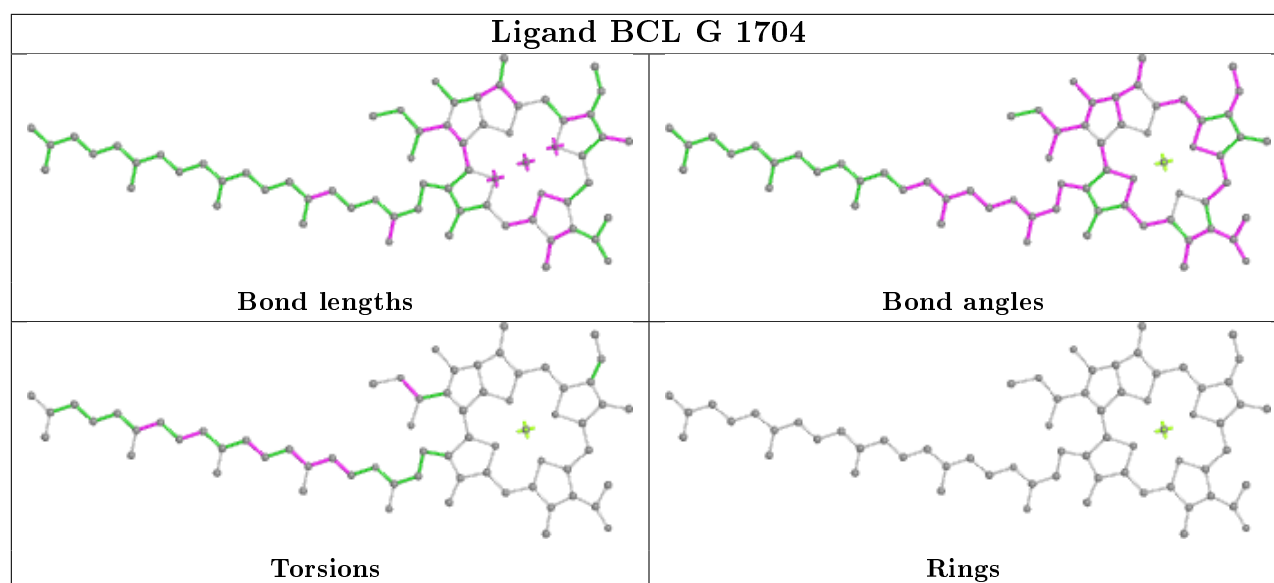
equivalents in the CSD to analyse the geometry.

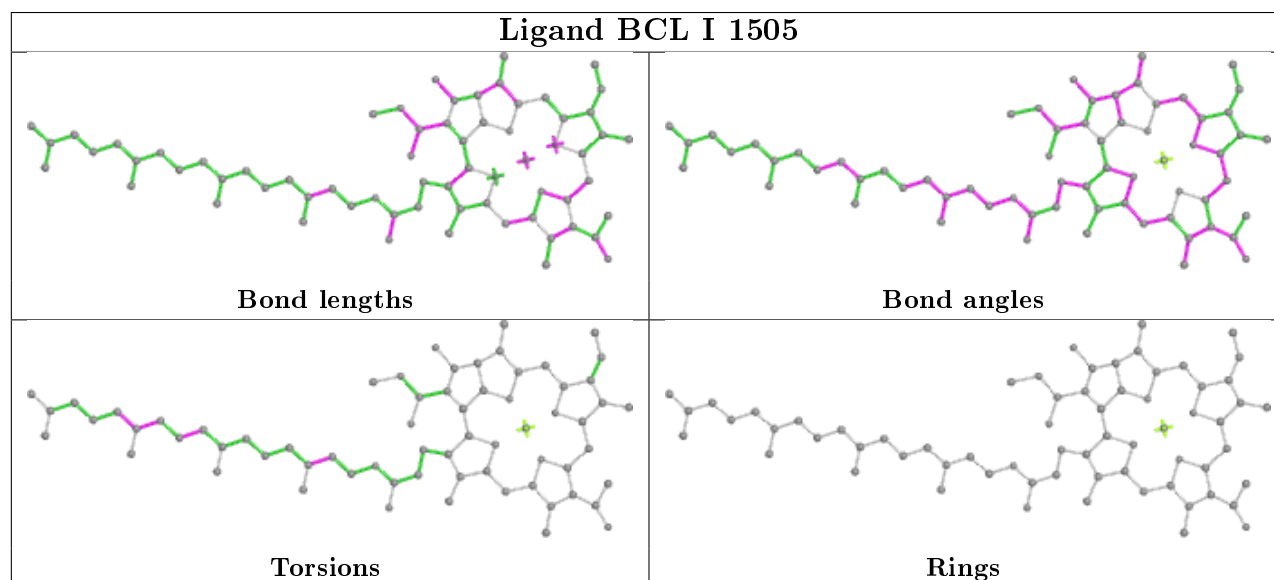
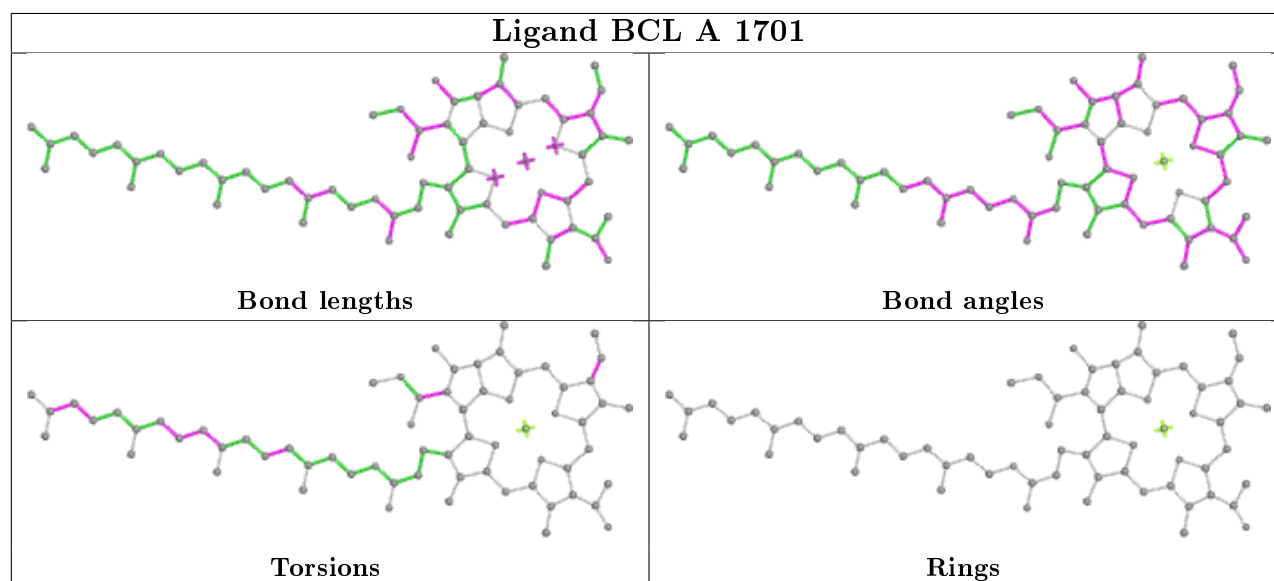
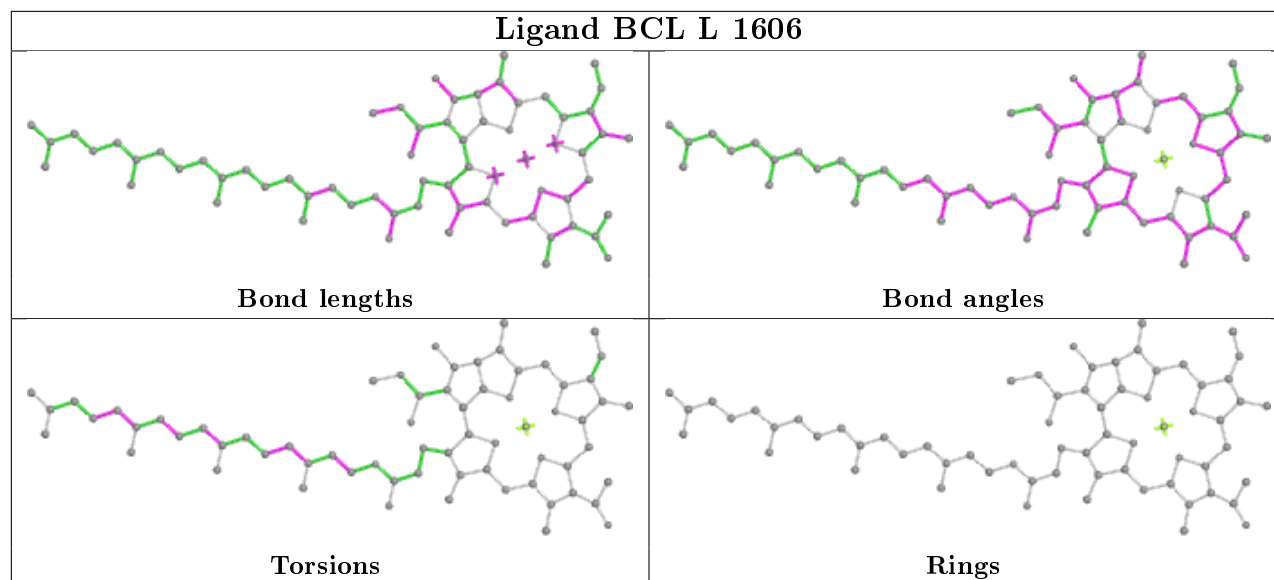


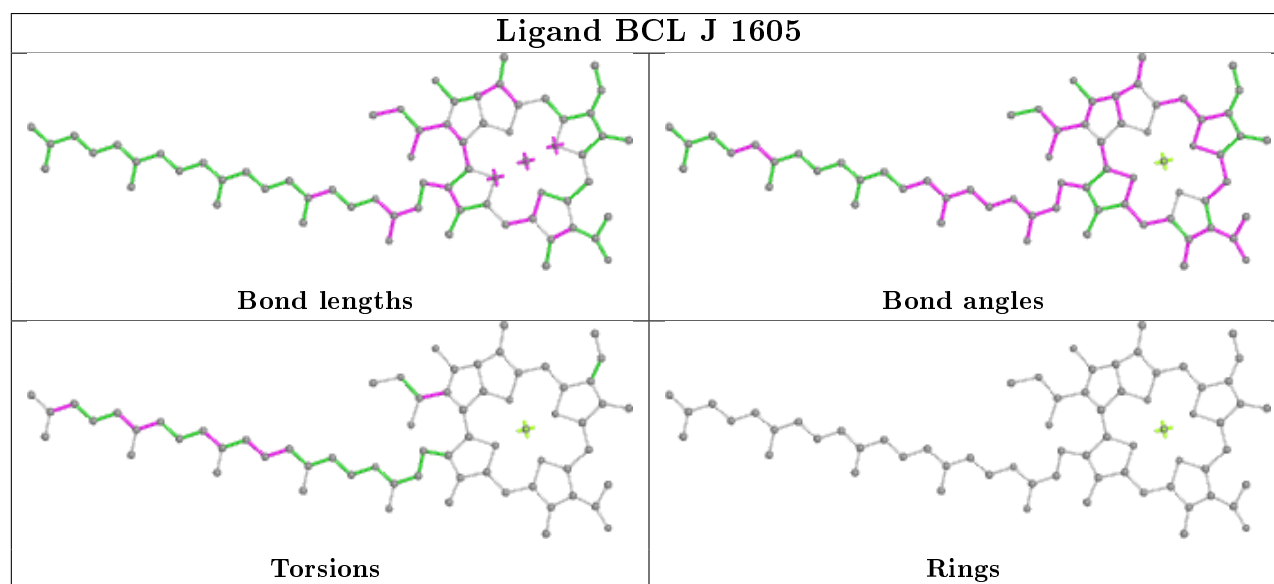
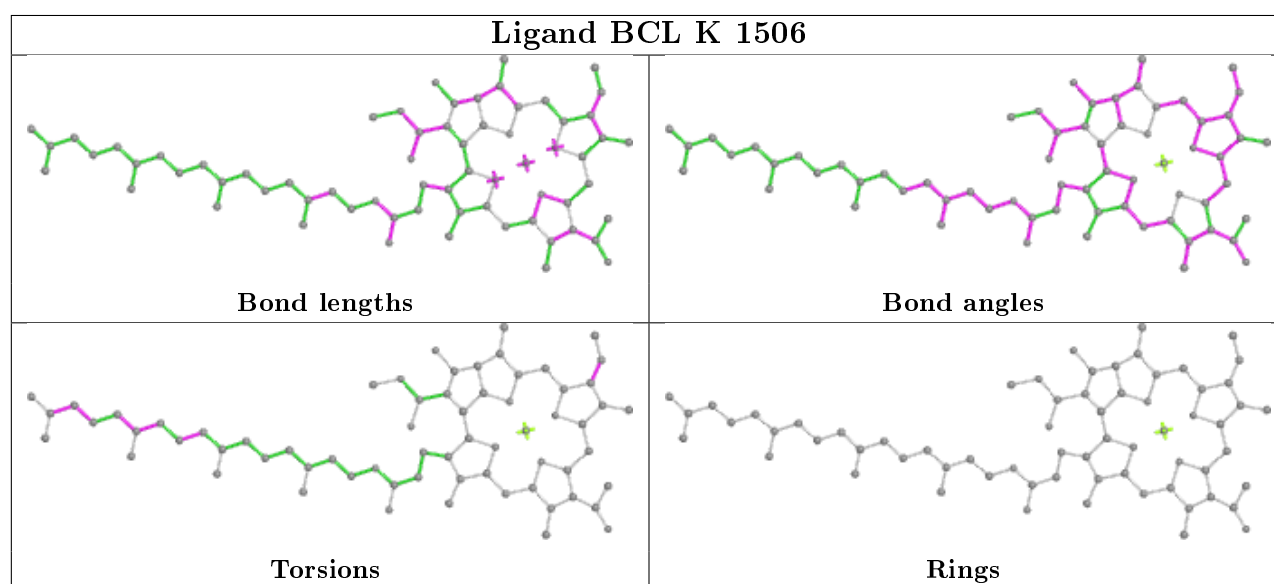
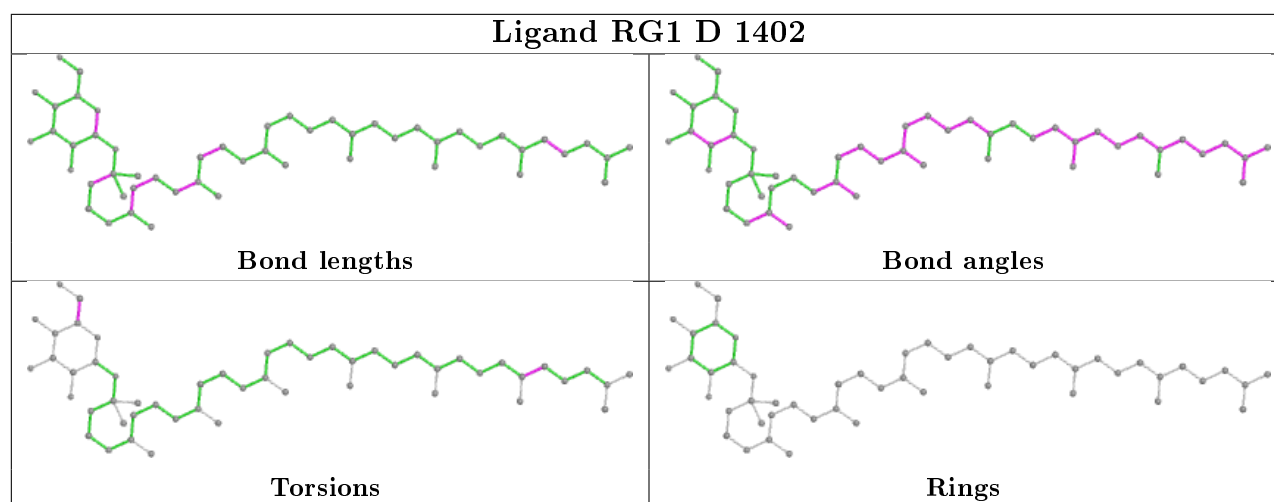
Ligand BCL A 1501**Ligand BCL C 1502****Ligand BCL N 1607**

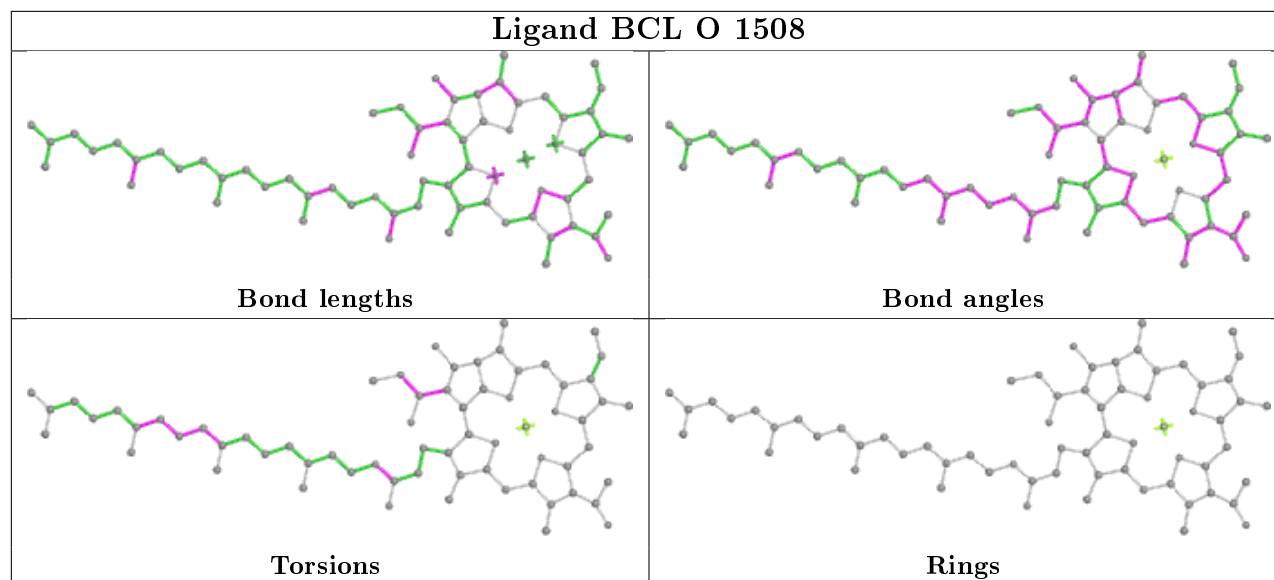
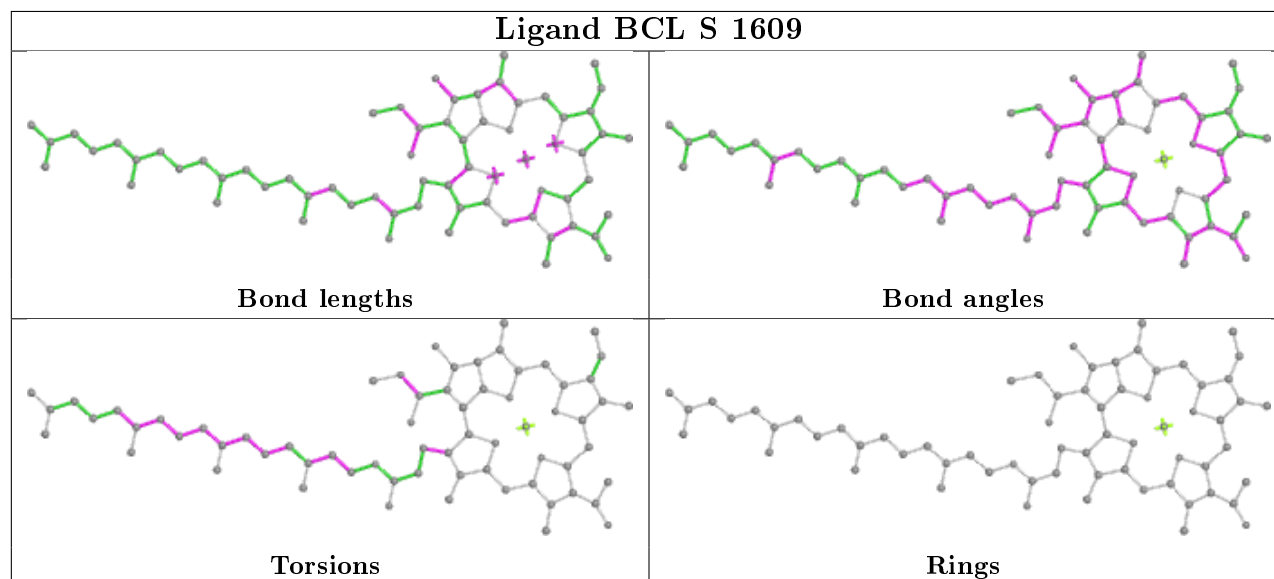
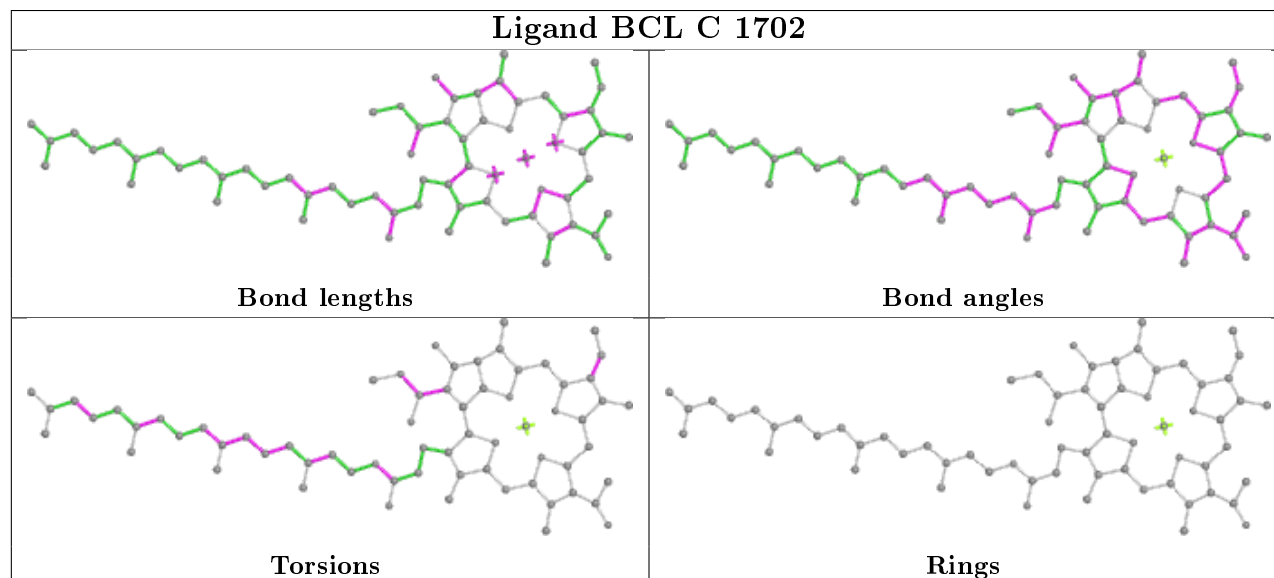
Ligand BCL R 1509**Ligand BCL D 1602****Ligand BCL P 1608**

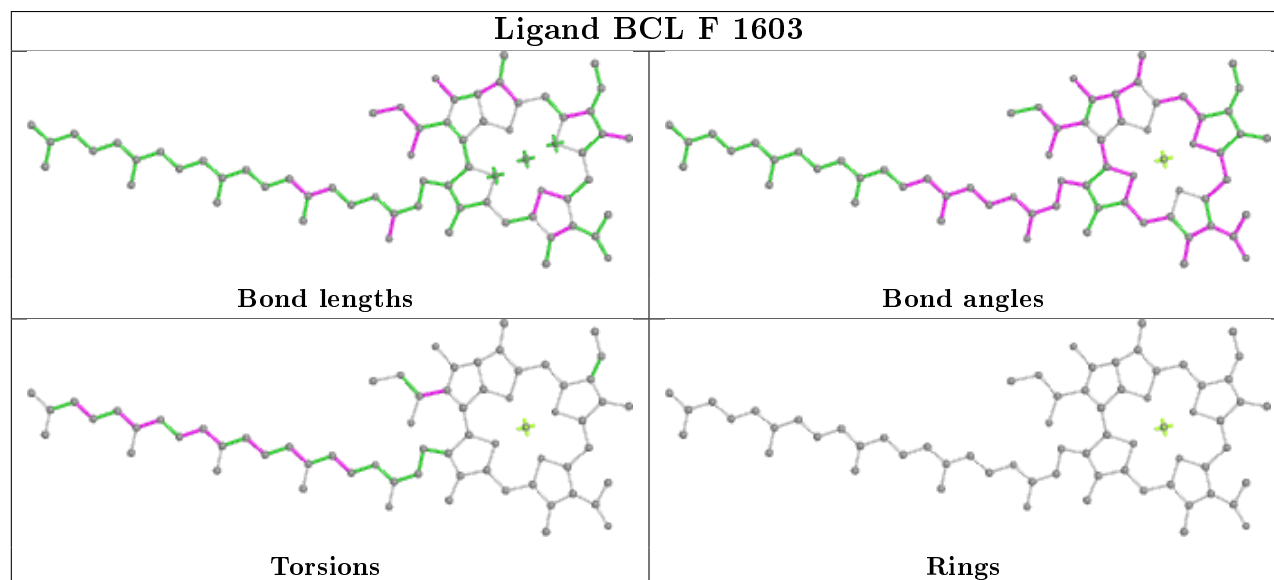
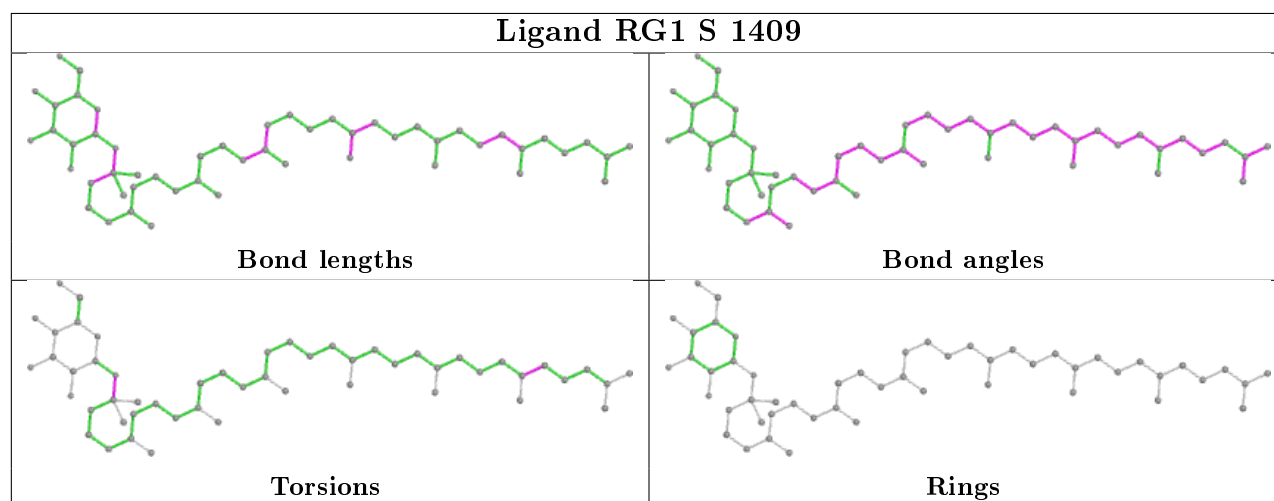
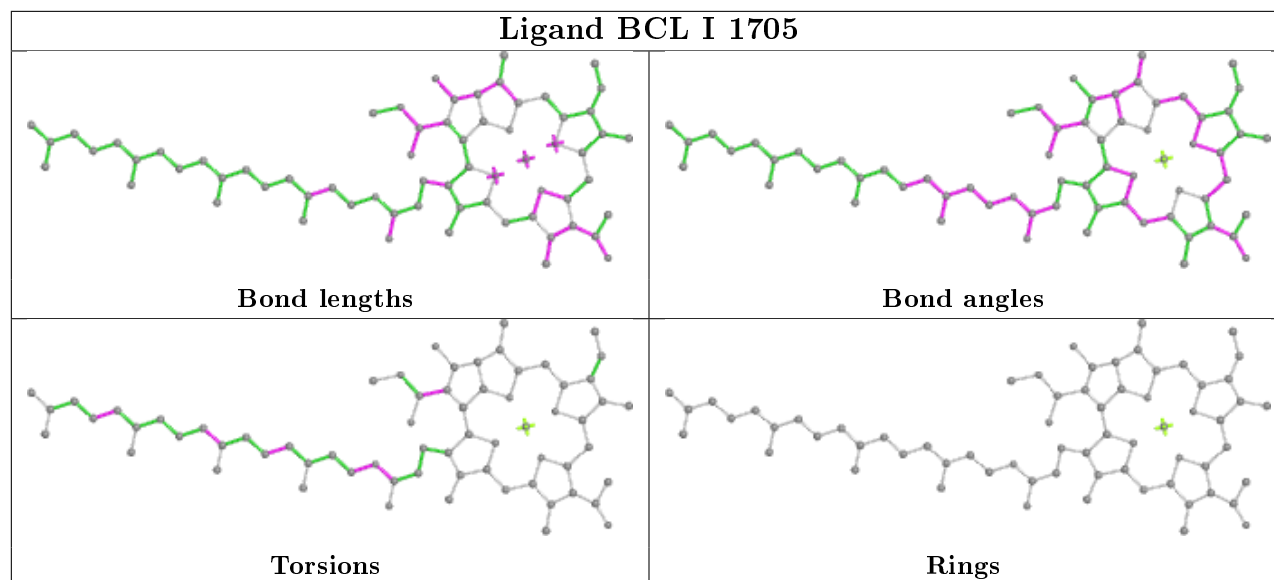


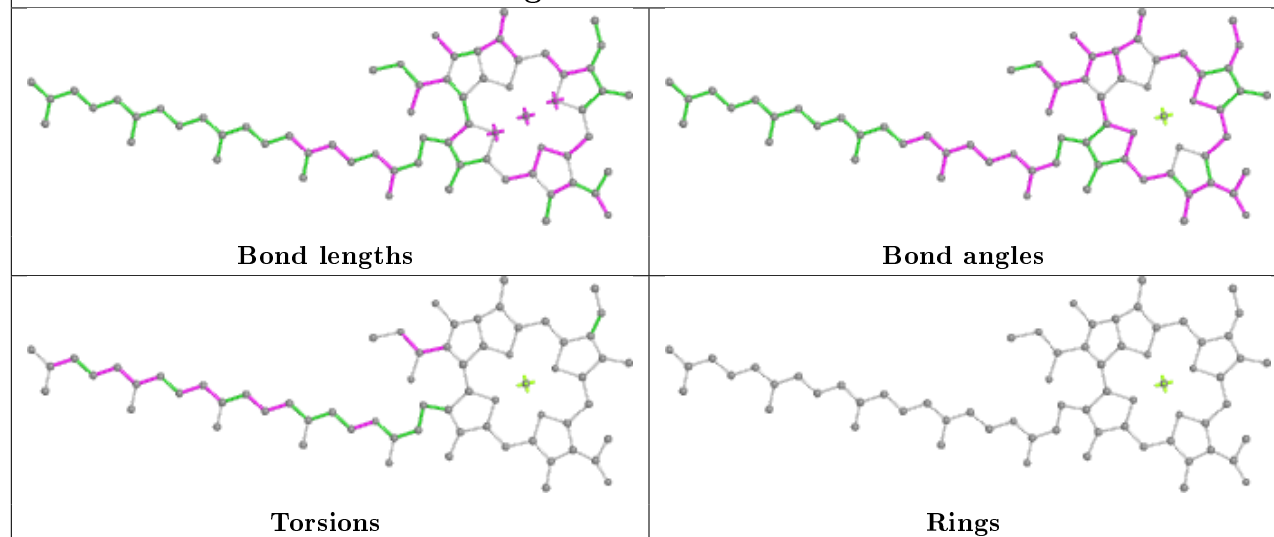
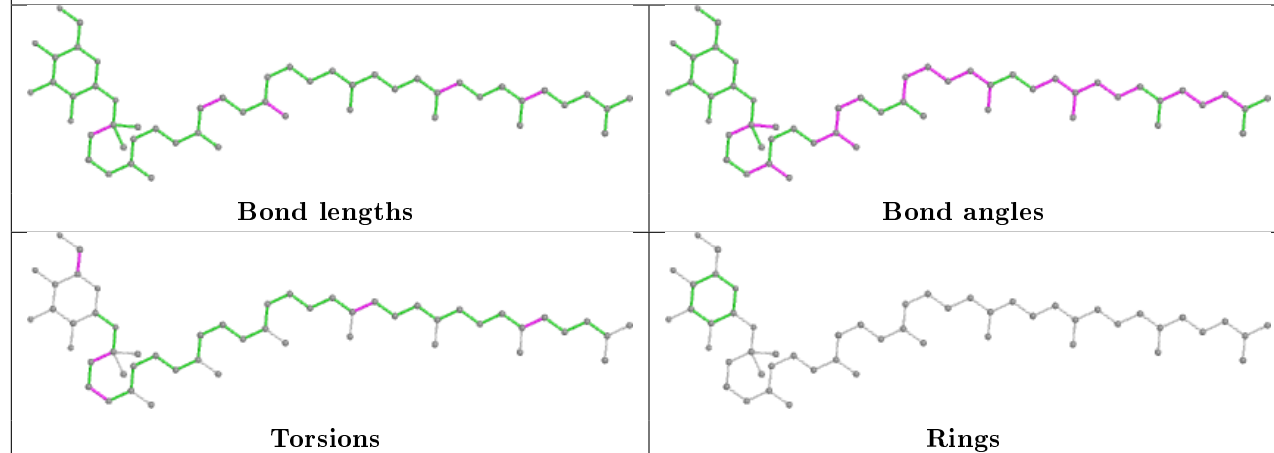
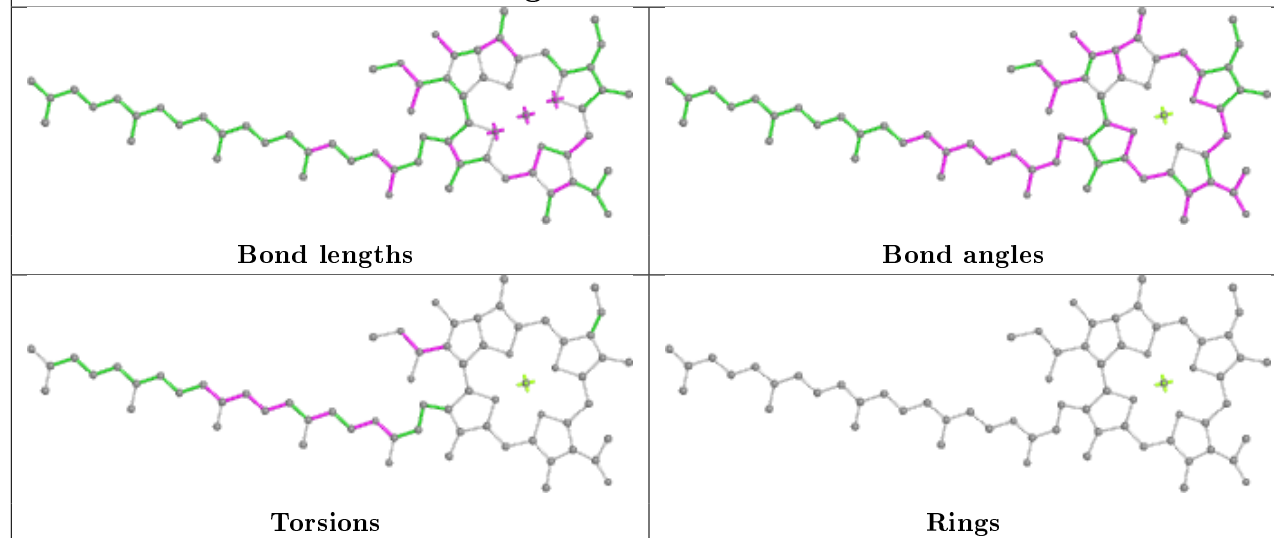


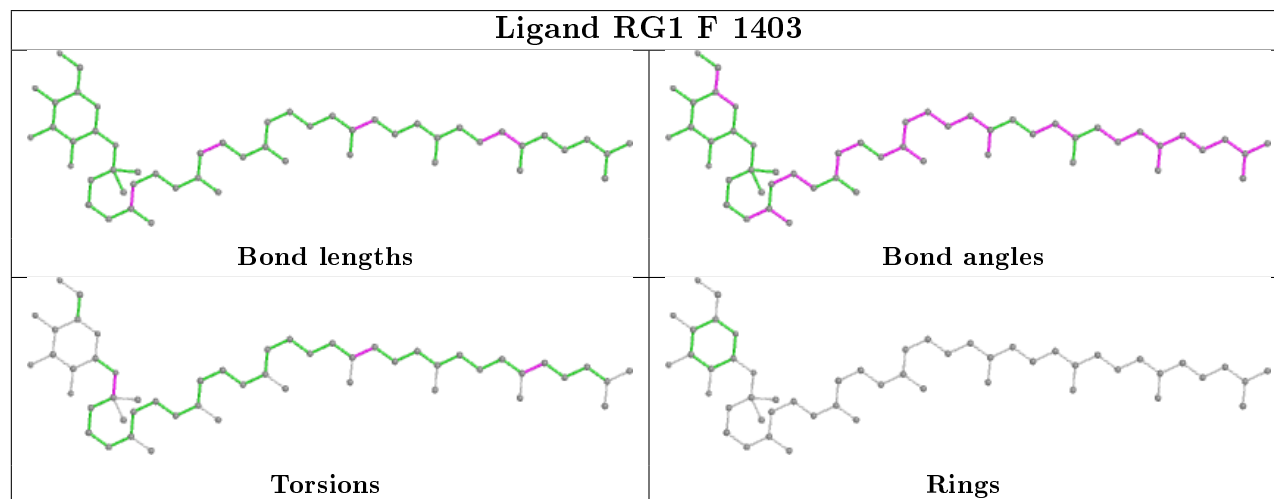
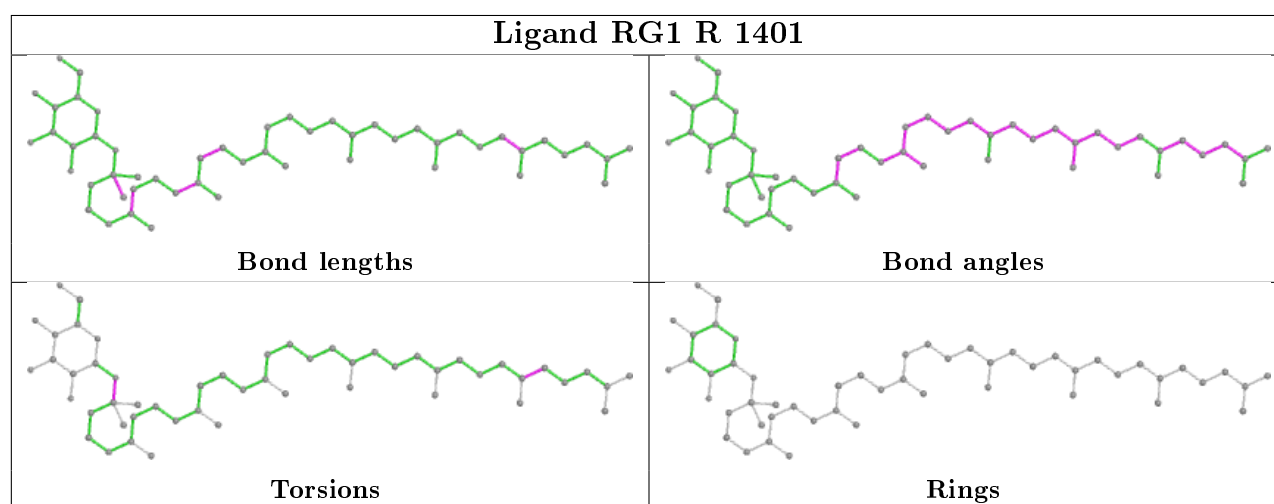
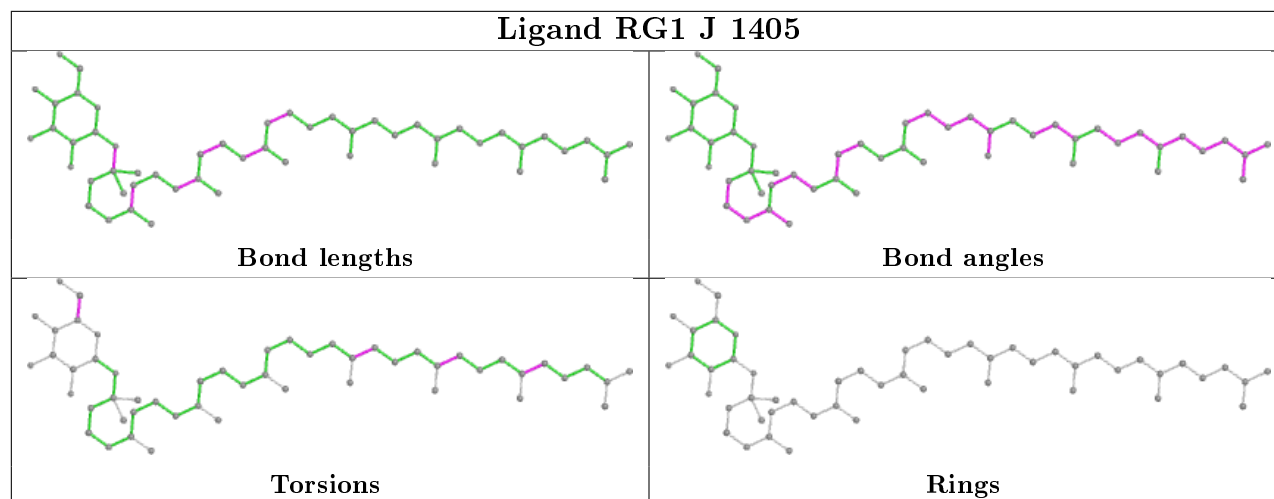


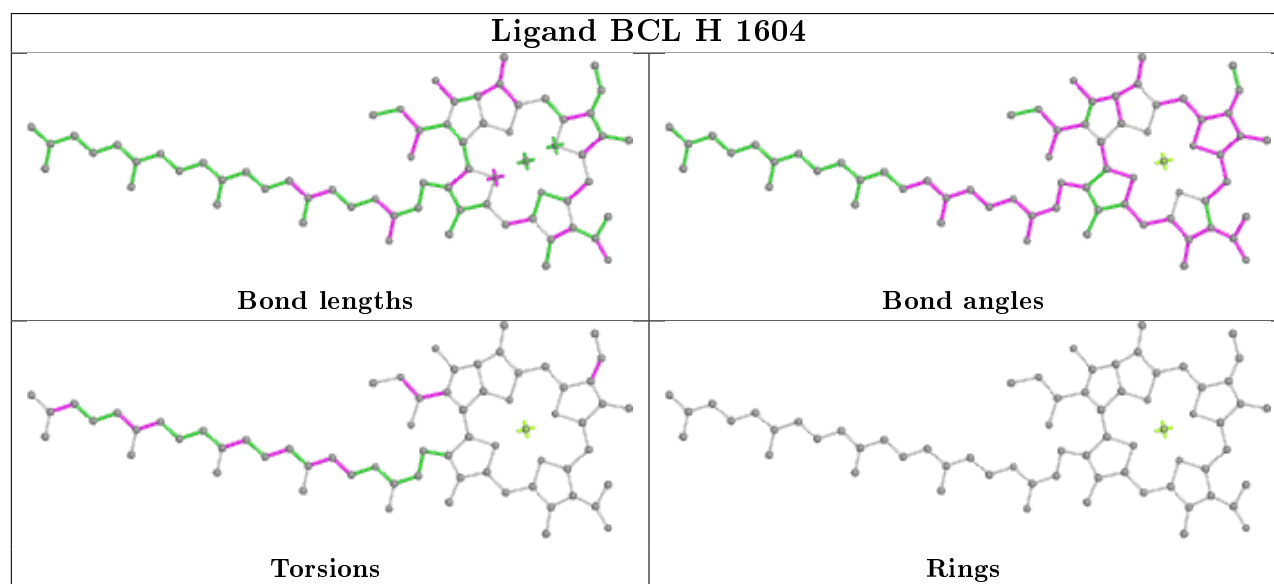
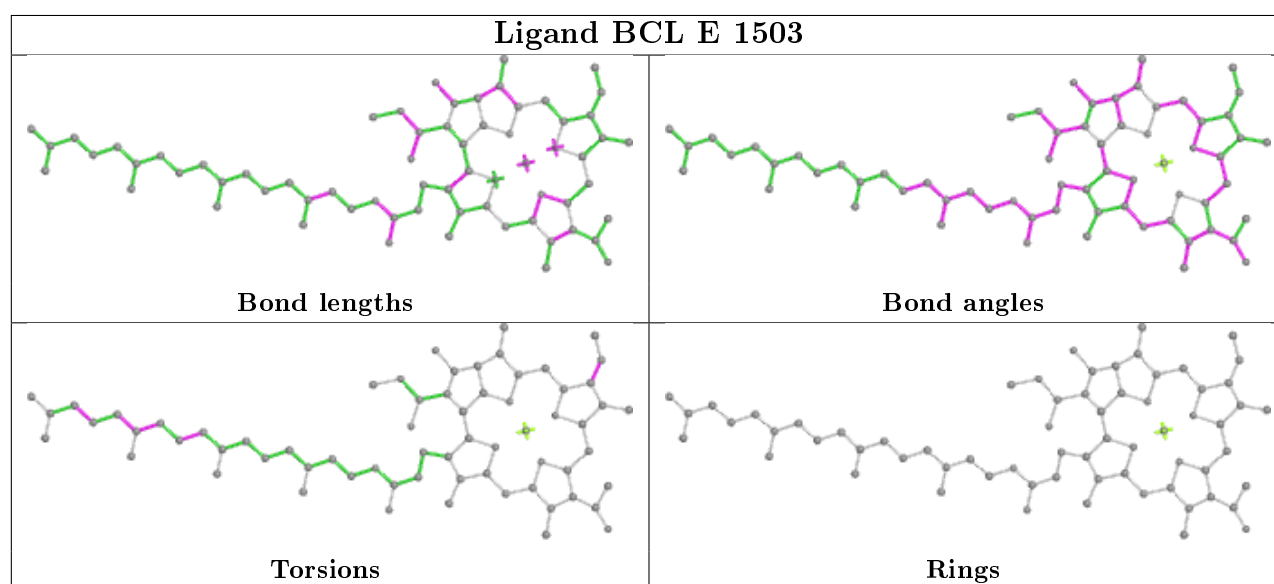
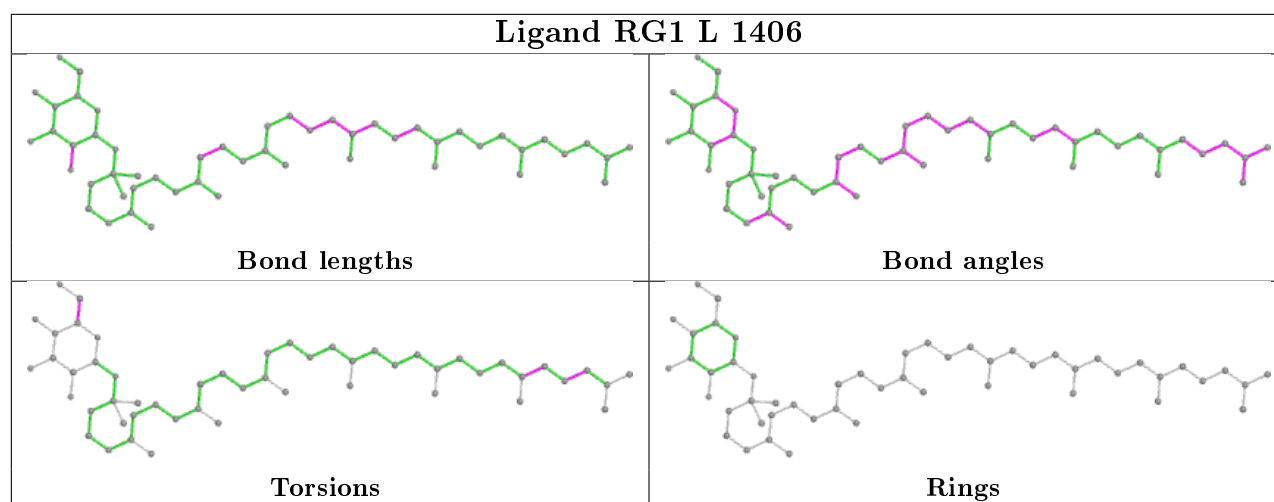


Ligand BCL O 1508**Ligand BCL S 1609****Ligand BCL C 1702**



Ligand BCL R 1709**Ligand RG1 H 1404****Ligand BCL B 1601**





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	52/53 (98%)	0.42	6 (11%) 4 3	35, 41, 88, 98	0
1	C	52/53 (98%)	0.99	7 (13%) 3 2	34, 41, 88, 102	0
1	E	52/53 (98%)	1.42	7 (13%) 3 2	35, 40, 88, 101	0
1	G	52/53 (98%)	0.77	6 (11%) 4 3	33, 40, 87, 99	0
1	I	52/53 (98%)	0.96	6 (11%) 4 3	34, 39, 88, 100	0
1	K	52/53 (98%)	0.68	6 (11%) 4 3	33, 40, 88, 100	0
1	M	52/53 (98%)	0.60	6 (11%) 4 3	35, 40, 88, 101	0
1	O	52/53 (98%)	0.91	6 (11%) 4 3	34, 41, 87, 100	0
1	R	52/53 (98%)	0.74	6 (11%) 4 3	35, 41, 87, 97	0
2	B	41/41 (100%)	-0.23	1 (2%) 59 54	42, 46, 54, 67	0
2	D	41/41 (100%)	0.02	2 (4%) 29 27	41, 46, 55, 64	0
2	F	41/41 (100%)	0.01	1 (2%) 59 54	38, 45, 52, 65	0
2	H	41/41 (100%)	-0.21	1 (2%) 59 54	37, 45, 52, 64	0
2	J	41/41 (100%)	-0.24	0 100 100	40, 45, 53, 65	0
2	L	41/41 (100%)	0.43	1 (2%) 59 54	39, 43, 52, 65	0
2	N	41/41 (100%)	0.21	3 (7%) 15 11	41, 45, 52, 69	0
2	P	41/41 (100%)	-0.02	1 (2%) 59 54	40, 46, 53, 68	0
2	S	41/41 (100%)	-0.35	1 (2%) 59 54	41, 46, 54, 67	0
All	All	837/846 (98%)	0.45	67 (8%) 12 9	33, 43, 79, 102	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	23.9
1	E	52	ALA	20.1
1	E	49	VAL	17.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	49	VAL	16.6
1	C	52	ALA	16.2
1	I	52	ALA	14.5
1	R	52	ALA	14.4
1	C	49	VAL	13.3
1	I	49	VAL	12.4
1	G	49	VAL	12.0
1	E	51	LYS	11.8
1	A	49	VAL	11.8
1	K	49	VAL	11.5
1	K	53	ALA	11.5
1	R	49	VAL	11.2
1	G	53	ALA	10.4
1	K	52	ALA	9.9
1	O	49	VAL	9.8
1	O	53	ALA	9.7
1	I	53	ALA	9.6
1	O	52	ALA	9.6
1	E	50	LYS	9.5
1	M	52	ALA	9.5
1	G	52	ALA	9.4
1	I	51	LYS	9.2
1	A	52	ALA	9.1
1	M	51	LYS	8.9
1	R	53	ALA	8.8
1	E	53	ALA	8.8
1	A	51	LYS	8.6
1	I	50	LYS	8.6
1	A	53	ALA	8.2
1	O	51	LYS	8.0
1	R	51	LYS	6.8
1	K	51	LYS	6.7
1	M	50	LYS	6.7
1	M	53	ALA	6.5
1	E	48	GLY	6.3
1	A	50	LYS	5.9
1	R	50	LYS	5.5
1	K	50	LYS	5.4
1	C	51	LYS	5.1
1	O	50	LYS	5.0
1	G	51	LYS	5.0
1	C	50	LYS	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	48	GLY	4.1
1	O	48	GLY	3.8
1	I	48	GLY	3.7
1	G	50	LYS	3.3
2	L	26	ALA	3.3
2	N	41	HIS	3.2
2	D	41	HIS	3.1
2	D	6	GLU	3.1
1	G	48	GLY	3.0
1	K	48	GLY	3.0
2	H	41	HIS	3.0
2	B	31	PHE	2.7
2	P	41	HIS	2.7
1	C	39	THR	2.6
1	M	48	GLY	2.5
2	N	37	THR	2.4
1	A	48	GLY	2.4
2	F	7	GLN	2.3
2	S	41	HIS	2.3
2	N	34	PHE	2.2
1	C	48	GLY	2.1
1	E	43	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CXM	K	1	11/12	0.94	0.12	40,46,54,54	0
1	CXM	I	1	11/12	0.95	0.15	38,45,51,52	0
1	CXM	A	1	11/12	0.95	0.12	45,48,60,62	0
1	CXM	R	1	11/12	0.95	0.21	45,48,54,59	0
1	CXM	C	1	11/12	0.95	0.28	45,47,55,58	0
1	CXM	O	1	11/12	0.96	0.14	45,47,54,58	0
1	CXM	G	1	11/12	0.96	0.16	45,46,52,58	0
1	CXM	E	1	11/12	0.96	0.15	41,46,48,50	0
1	CXM	M	1	11/12	0.96	0.13	40,45,51,52	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	LDA	E	1823	16/16	0.18	0.65	89,99,122,123	0
4	LDA	C	1815	16/16	0.46	0.53	79,96,103,103	0
4	LDA	M	1827	16/16	0.48	0.40	96,101,105,107	0
4	LDA	N	1807	16/16	0.52	0.32	61,66,76,78	0
4	LDA	I	1812	16/16	0.56	0.46	87,106,111,111	0
4	LDA	K	1810	16/16	0.57	0.56	107,110,116,116	0
4	LDA	E	1822	16/16	0.57	0.34	69,91,107,108	0
4	LDA	R	1818	16/16	0.58	0.41	85,90,95,96	0
4	LDA	M	1811	16/16	0.60	0.36	75,77,84,84	0
4	LDA	G	1824	16/16	0.61	0.37	89,105,120,121	0
4	LDA	A	1816	16/16	0.61	0.42	86,87,91,93	0
4	LDA	C	1821	16/16	0.63	0.34	82,90,101,103	0
4	LDA	G	1814	16/16	0.63	0.29	70,74,83,84	0
4	LDA	P	1808	16/16	0.64	0.38	53,61,84,86	0
4	LDA	I	1825	16/16	0.65	0.40	95,101,108,108	0
4	LDA	L	1806	16/16	0.70	0.30	44,52,74,75	0
4	LDA	B	1801	16/16	0.70	0.29	49,62,76,78	0
4	LDA	D	1802	16/16	0.71	0.34	53,57,75,77	0
4	LDA	R	1809	16/16	0.71	0.26	57,63,71,73	0
4	LDA	O	1820	16/16	0.71	0.29	71,80,92,95	0
4	LDA	F	1803	16/16	0.73	0.24	50,56,67,67	0
4	LDA	J	1805	16/16	0.75	0.21	44,54,67,68	0
4	LDA	R	1819	16/16	0.76	0.33	80,83,85,87	0
4	LDA	I	1813	16/16	0.76	0.19	50,54,76,76	0
5	RG1	F	1403	52/52	0.77	0.25	28,38,77,82	0
4	LDA	K	1826	16/16	0.80	0.24	83,88,103,104	0
5	RG1	J	1405	52/52	0.81	0.24	28,37,76,80	0
4	LDA	A	1817	16/16	0.82	0.21	67,69,87,87	0
5	RG1	D	1402	52/52	0.83	0.19	30,44,77,81	0
4	LDA	H	1804	16/16	0.84	0.26	49,57,66,67	0
5	RG1	N	1407	52/52	0.85	0.20	29,37,69,73	0
5	RG1	S	1409	52/52	0.85	0.20	29,40,77,78	0

Continued on next page...

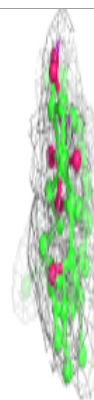
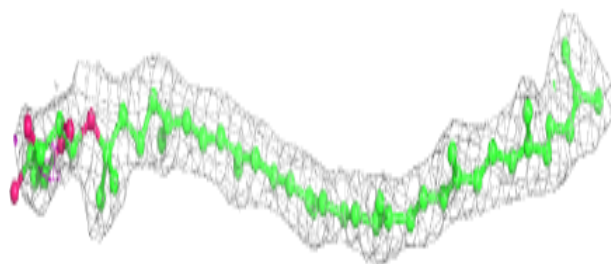
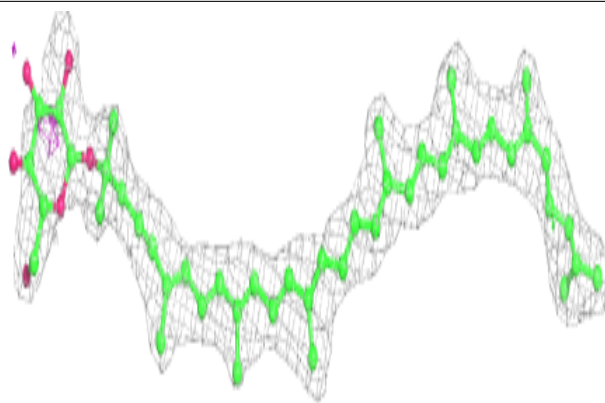
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	RG1	R	1401	52/52	0.87	0.23	30,40,74,77	0
5	RG1	P	1408	52/52	0.88	0.22	32,42,75,78	0
3	BCL	C	1702	66/66	0.88	0.19	41,48,78,80	0
3	BCL	R	1709	66/66	0.89	0.19	43,53,78,82	0
5	RG1	H	1404	52/52	0.89	0.21	27,37,78,80	0
3	BCL	N	1607	66/66	0.89	0.15	31,41,63,65	0
3	BCL	J	1605	66/66	0.90	0.16	31,39,64,66	0
3	BCL	G	1704	66/66	0.90	0.20	32,45,73,76	0
3	BCL	A	1701	66/66	0.91	0.17	42,49,80,83	0
5	RG1	L	1406	52/52	0.91	0.18	26,35,74,77	0
3	BCL	I	1705	66/66	0.92	0.17	34,41,73,75	0
3	BCL	M	1707	66/66	0.92	0.17	29,44,74,76	0
3	BCL	A	1501	66/66	0.92	0.17	33,42,51,65	0
3	BCL	O	1708	66/66	0.92	0.16	42,50,79,81	0
3	BCL	R	1509	66/66	0.93	0.17	31,38,49,57	0
3	BCL	O	1508	66/66	0.93	0.14	30,37,46,54	0
3	BCL	I	1505	66/66	0.93	0.15	28,36,42,48	0
3	BCL	E	1703	66/66	0.93	0.17	29,37,69,72	0
3	BCL	S	1609	66/66	0.93	0.15	31,41,69,72	0
3	BCL	K	1506	66/66	0.94	0.18	28,35,47,51	0
3	BCL	F	1603	66/66	0.94	0.17	26,35,62,64	0
3	BCL	K	1706	66/66	0.94	0.15	27,36,78,82	0
3	BCL	P	1608	66/66	0.94	0.16	34,42,66,68	0
3	BCL	H	1604	66/66	0.94	0.15	29,39,63,64	0
3	BCL	L	1606	66/66	0.94	0.16	27,36,66,69	0
3	BCL	G	1504	66/66	0.95	0.15	26,34,44,49	0
3	BCL	D	1602	66/66	0.95	0.13	30,37,64,67	0
3	BCL	B	1601	66/66	0.95	0.15	33,42,67,68	0
3	BCL	C	1502	66/66	0.96	0.12	33,38,50,57	0
3	BCL	M	1507	66/66	0.96	0.12	27,35,41,48	0
3	BCL	E	1503	66/66	0.97	0.11	28,35,46,49	0

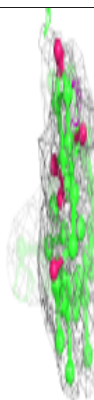
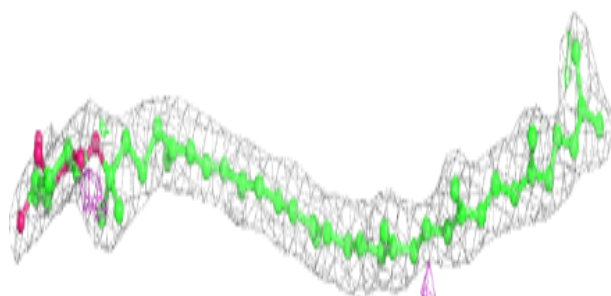
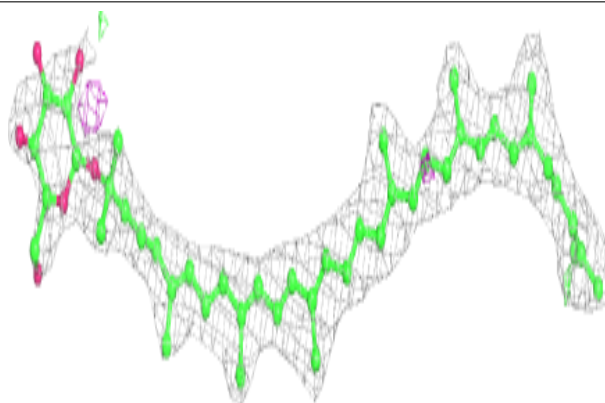
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RG1 F 1403:

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

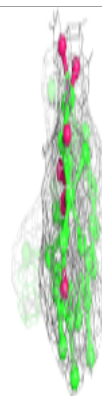
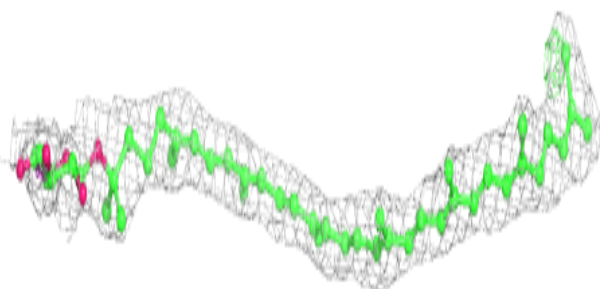
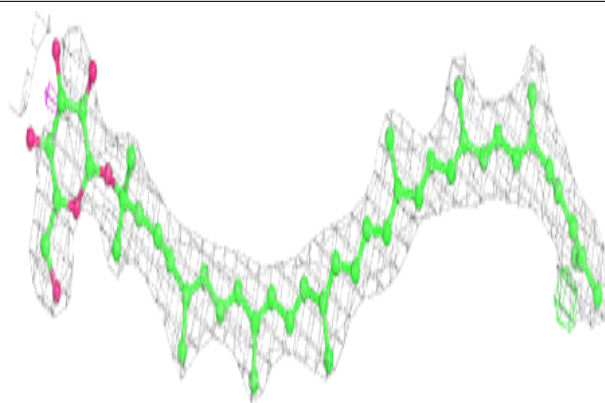
**Electron density around RG1 J 1405:**

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

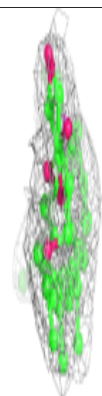
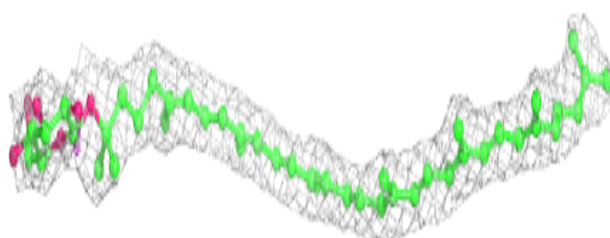
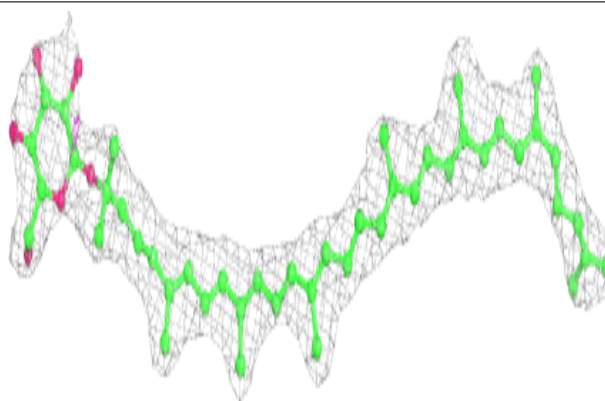


Electron density around RG1 D 1402:

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

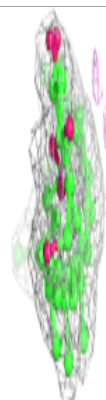
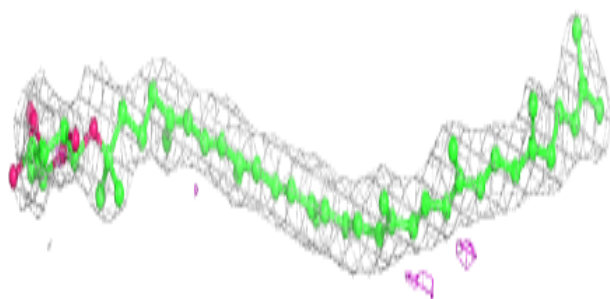
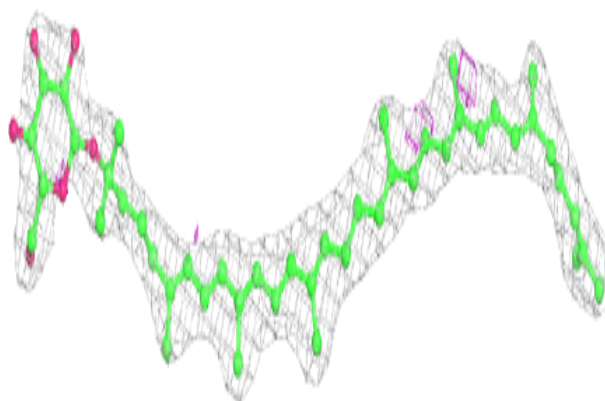
**Electron density around RG1 N 1407:**

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

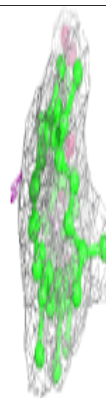
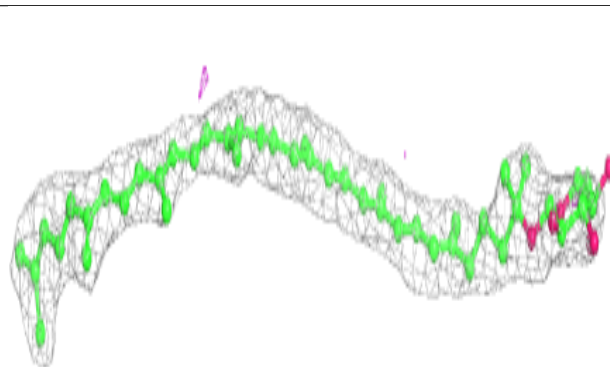
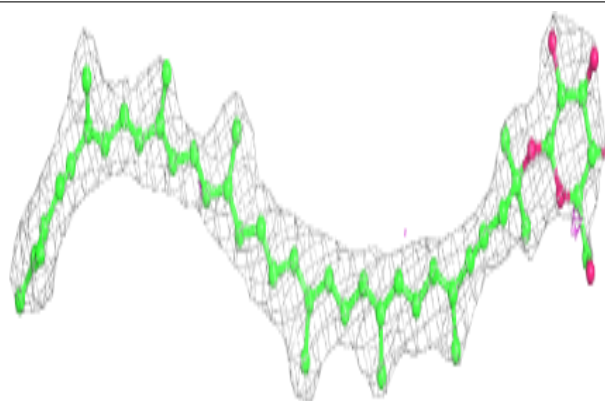


Electron density around RG1 S 1409:

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

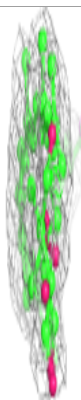
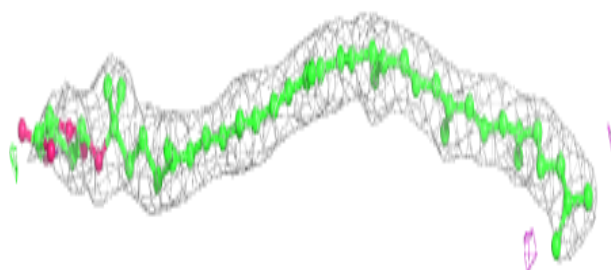
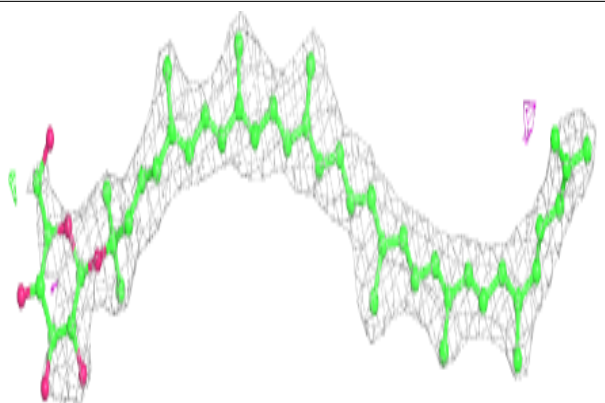
**Electron density around RG1 R 1401:**

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

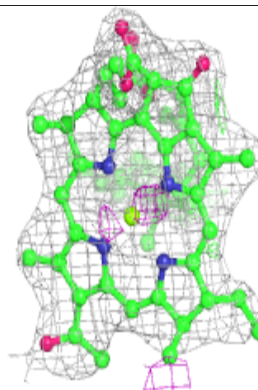
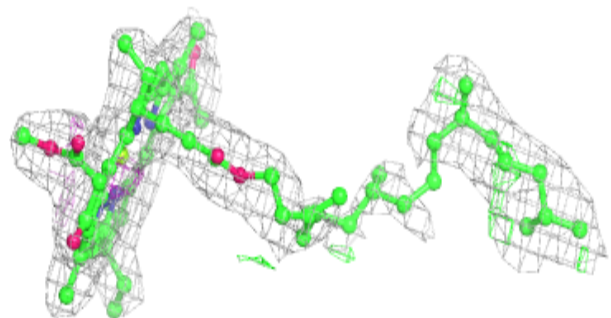
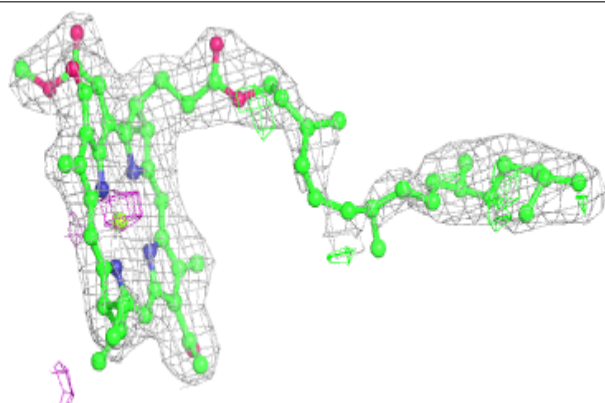


Electron density around RG1 P 1408:

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

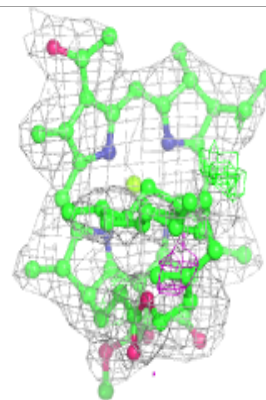
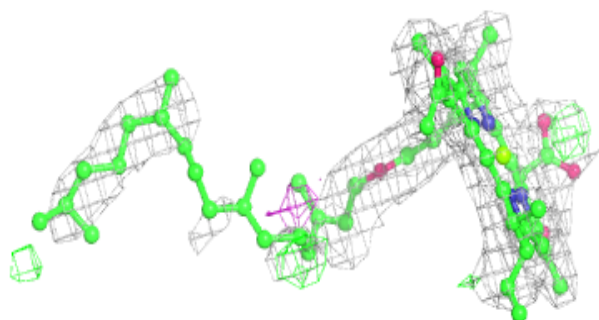
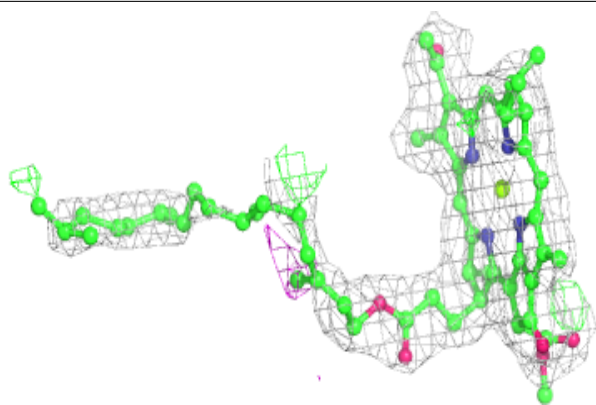
**Electron density around BCL C 1702:**

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

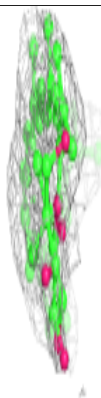
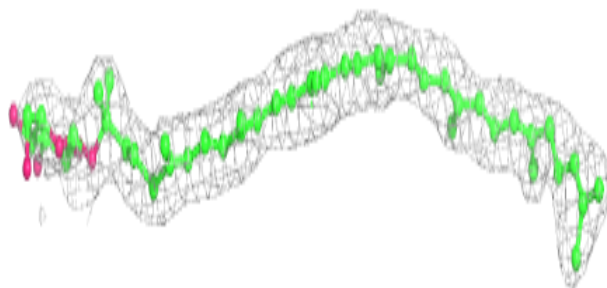
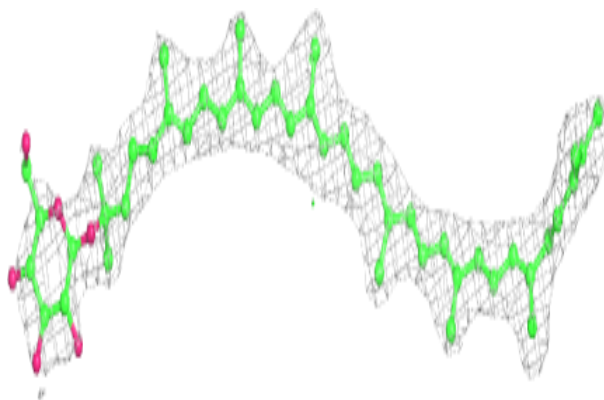


Electron density around BCL R 1709:

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

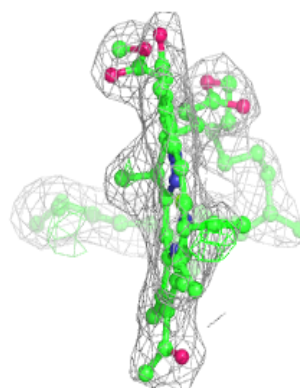
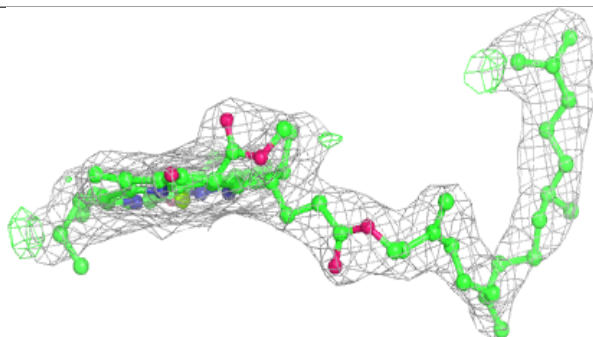
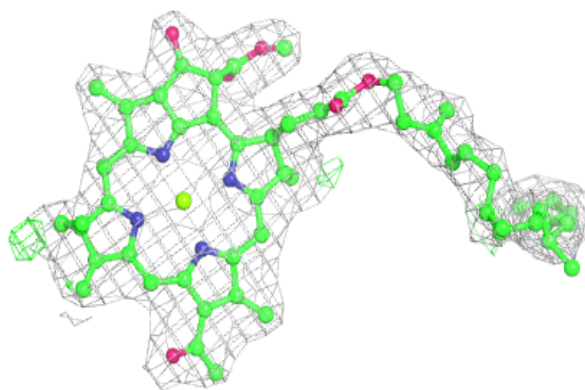
**Electron density around RG1 H 1404:**

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

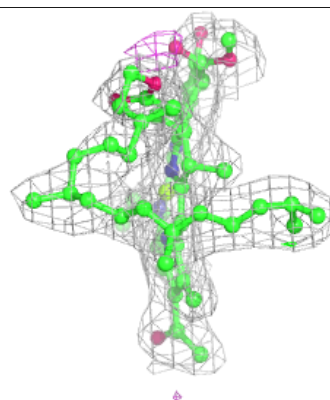
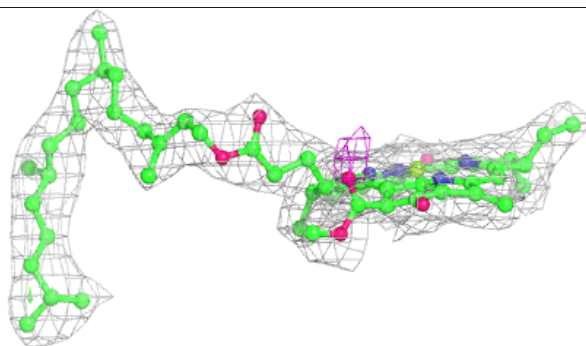
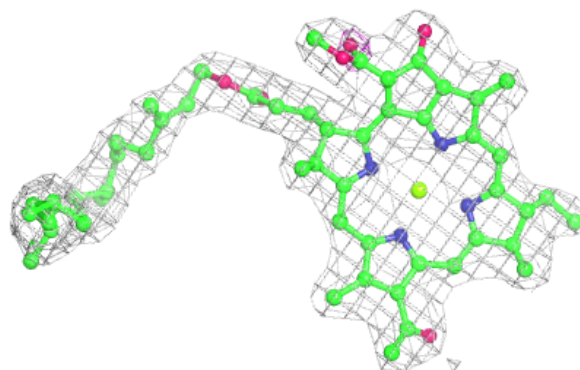


Electron density around BCL N 1607:

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

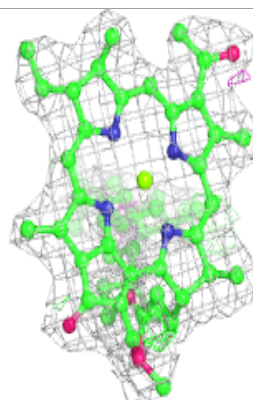
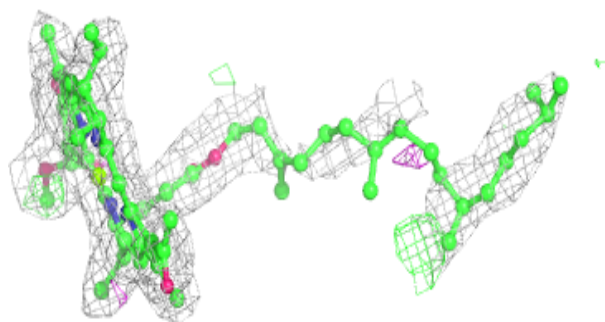
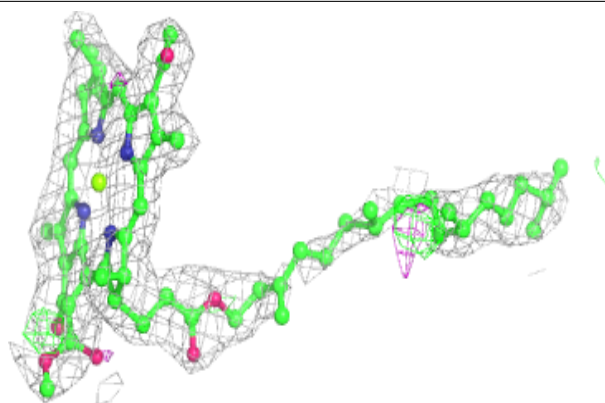
**Electron density around BCL J 1605:**

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

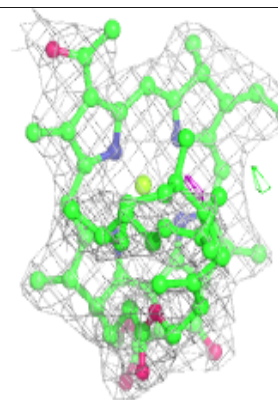
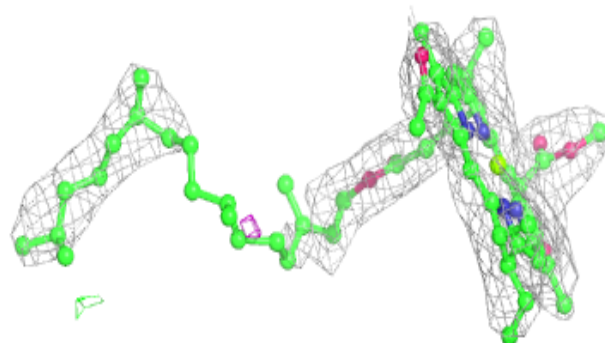
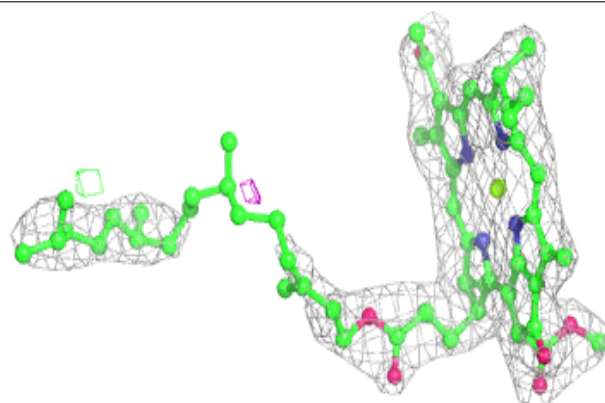


Electron density around BCL G 1704:

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

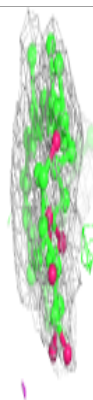
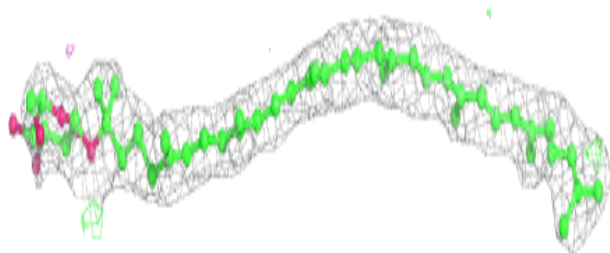
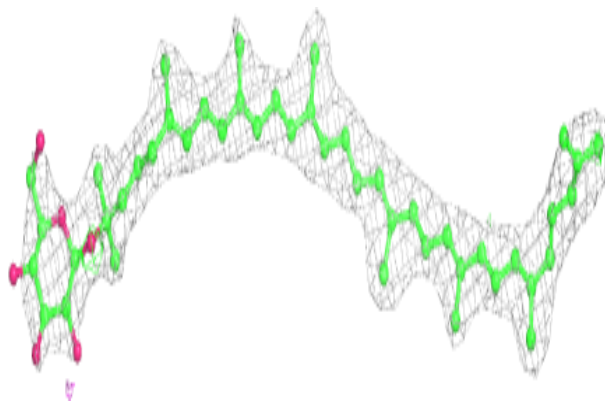
**Electron density around BCL A 1701:**

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

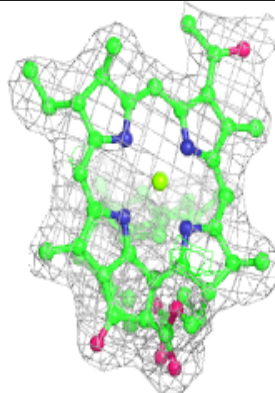
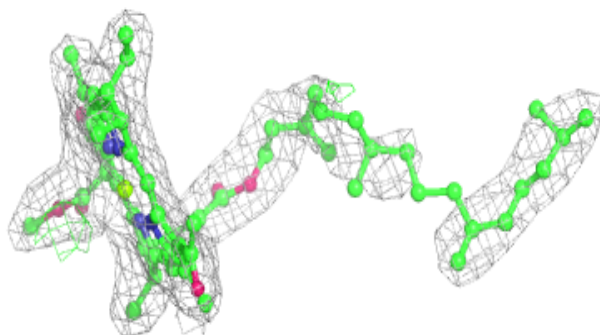
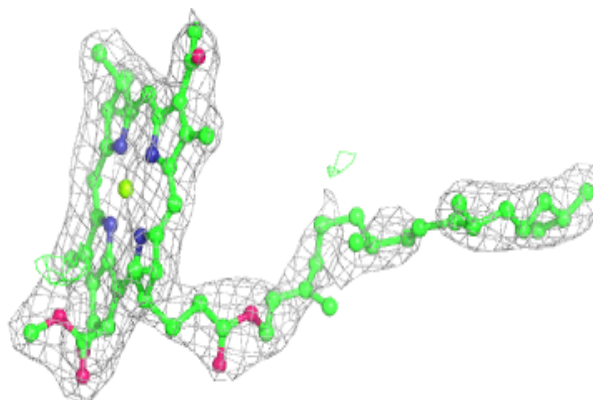


Electron density around RG1 L 1406:

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

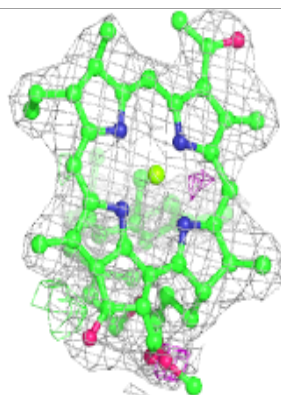
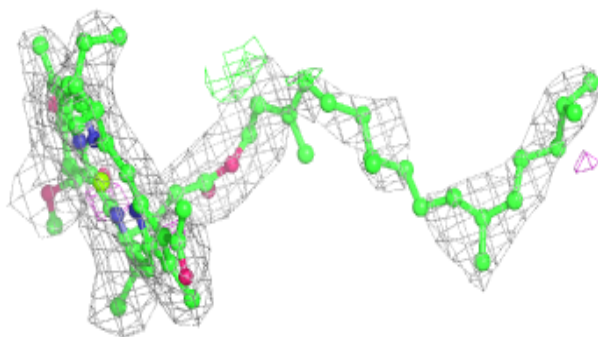
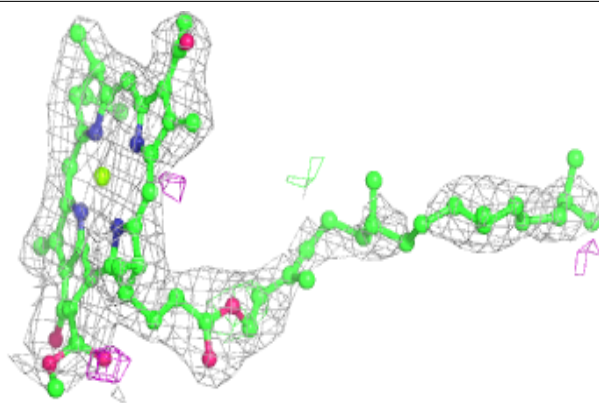
**Electron density around BCL I 1705:**

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

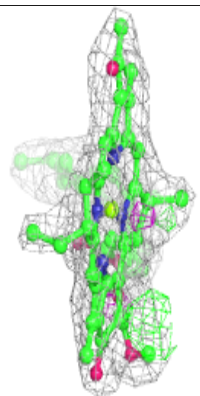
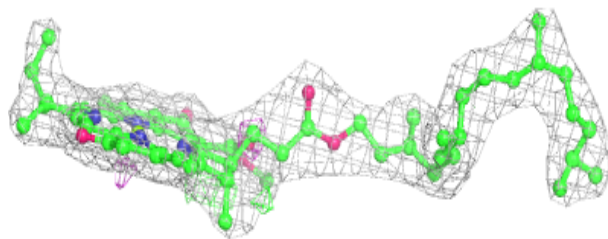
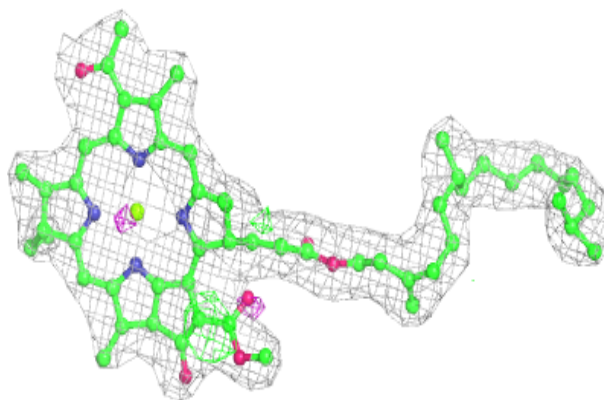


Electron density around BCL M 1707:

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

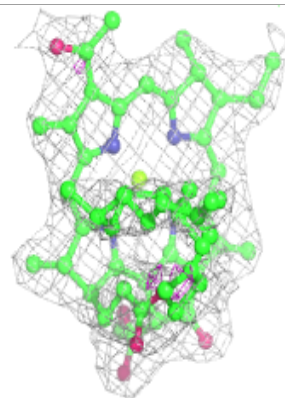
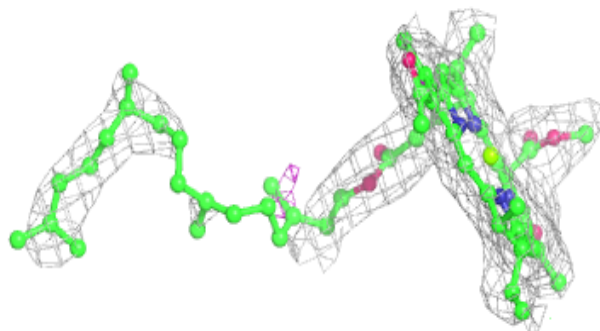
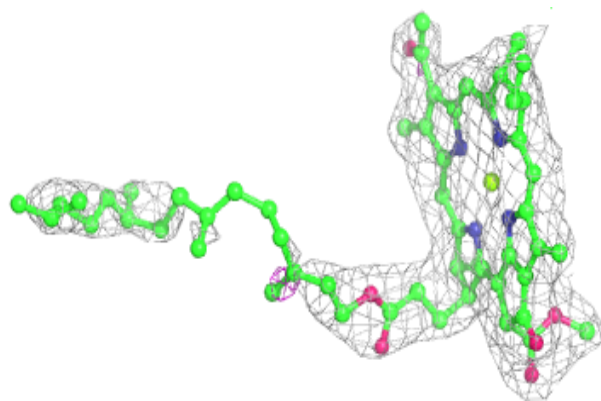
**Electron density around BCL A 1501:**

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

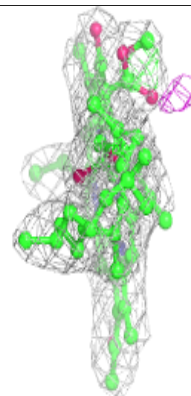
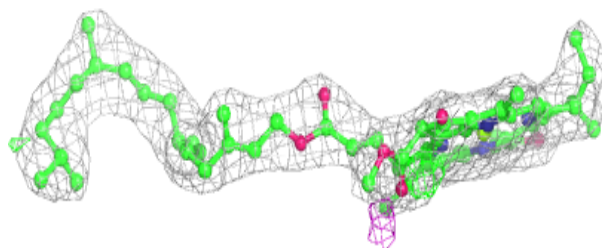
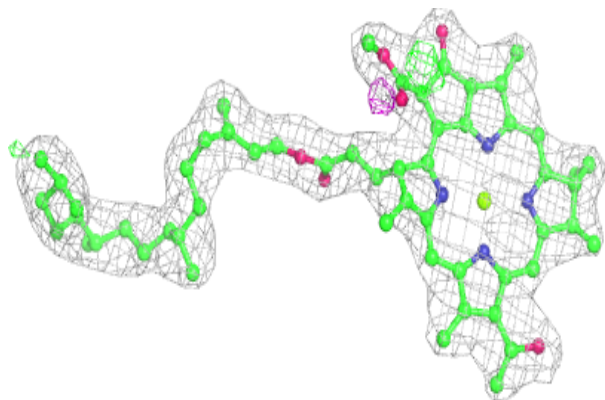


Electron density around BCL O 1708:

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

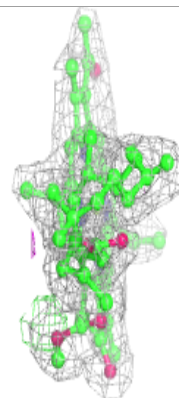
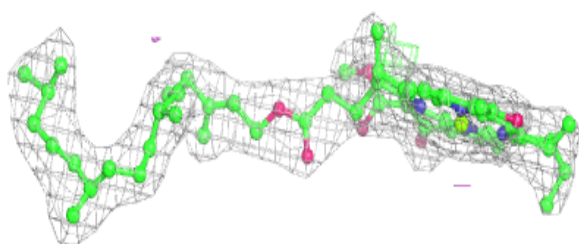
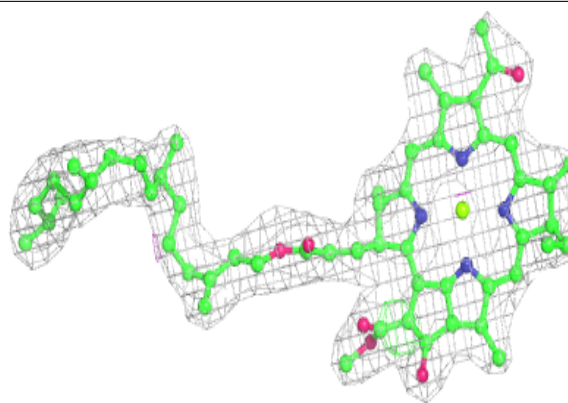
**Electron density around BCL R 1509:**

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

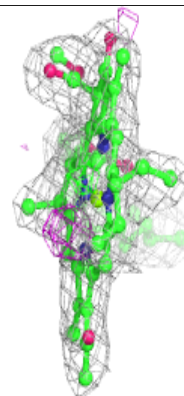
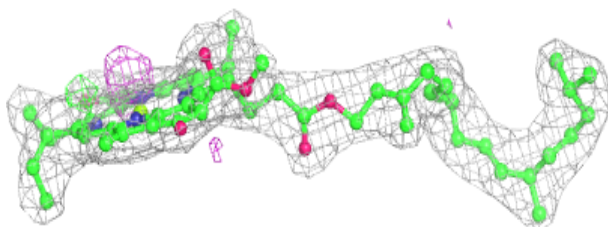
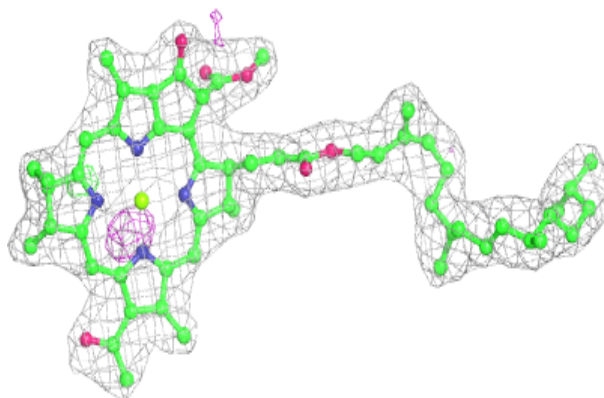


Electron density around BCL O 1508:

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

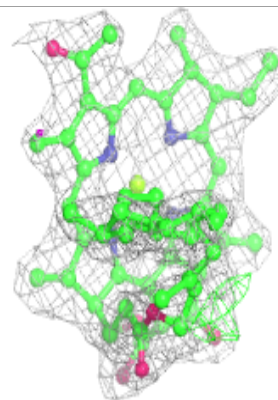
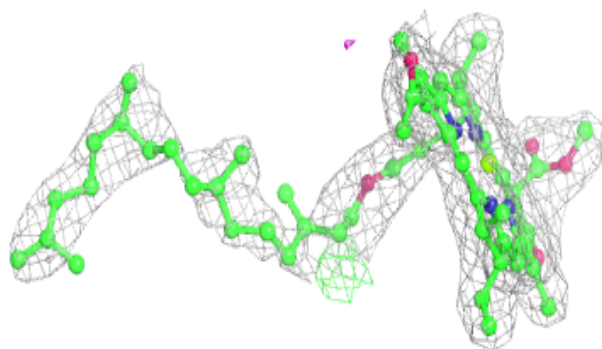
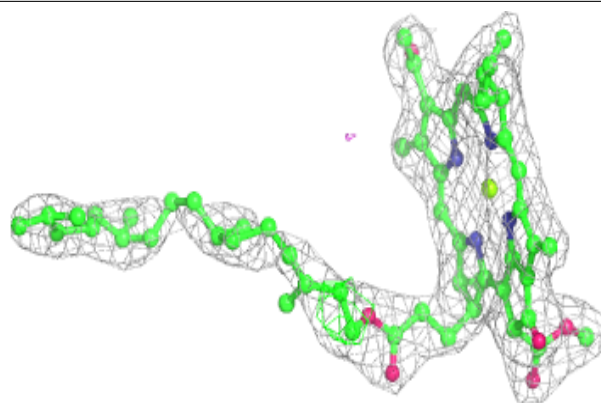
**Electron density around BCL I 1505:**

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

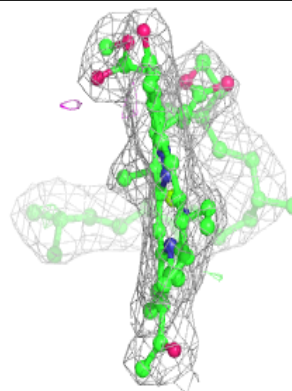
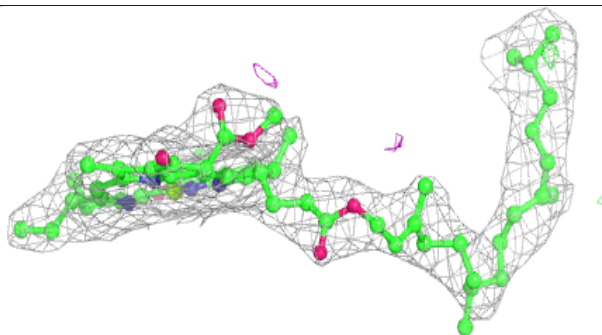
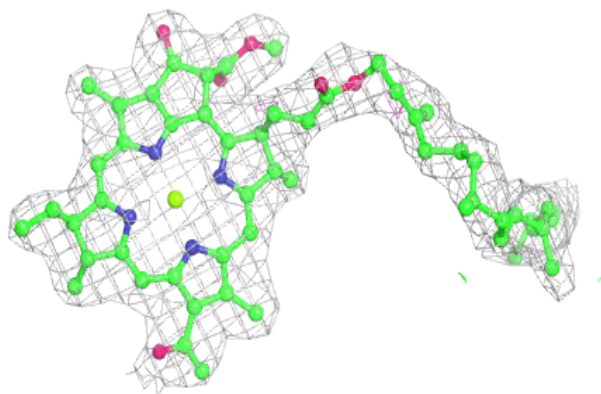


Electron density around BCL E 1703:

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

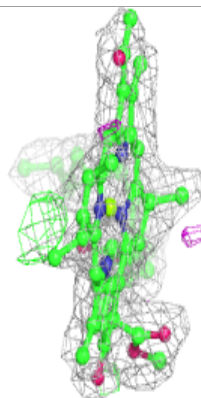
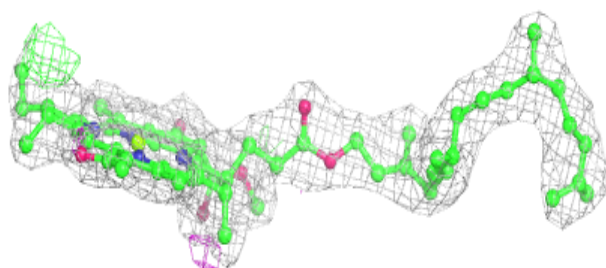
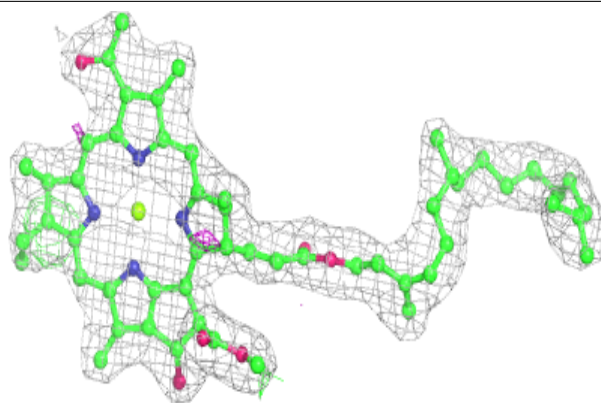
**Electron density around BCL S 1609:**

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

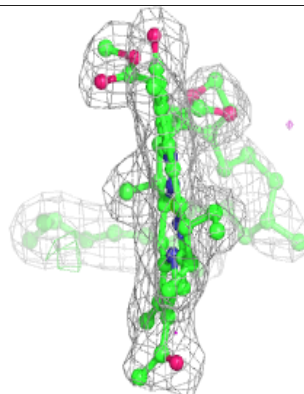
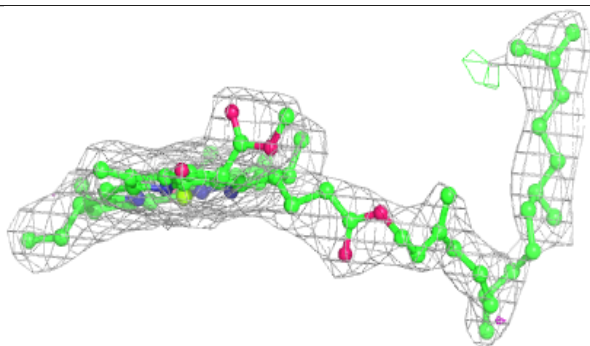
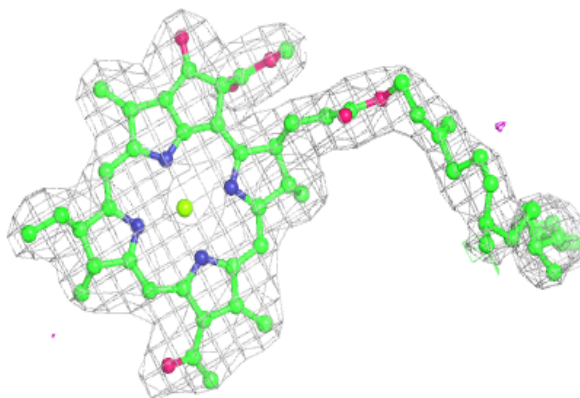


Electron density around BCL K 1506:

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

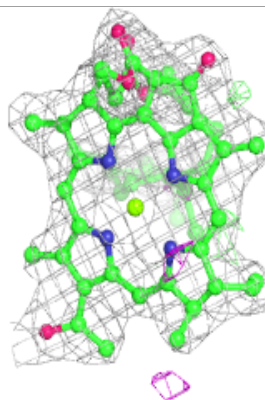
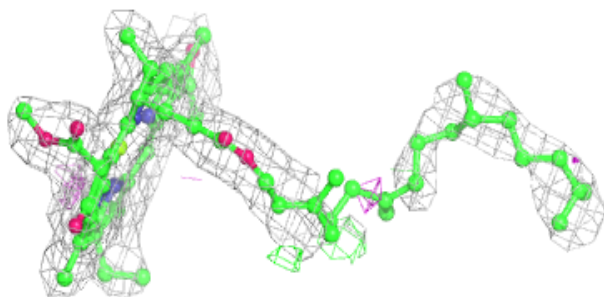
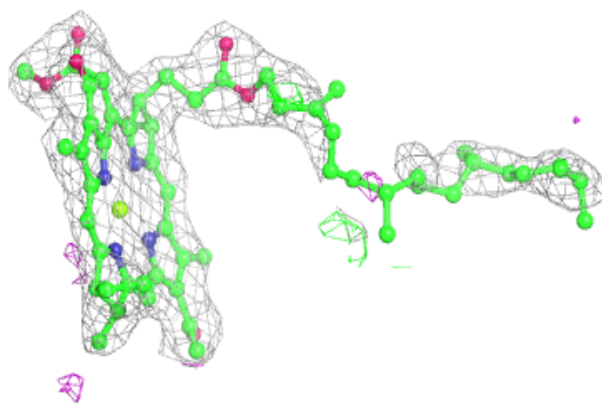
**Electron density around BCL F 1603:**

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

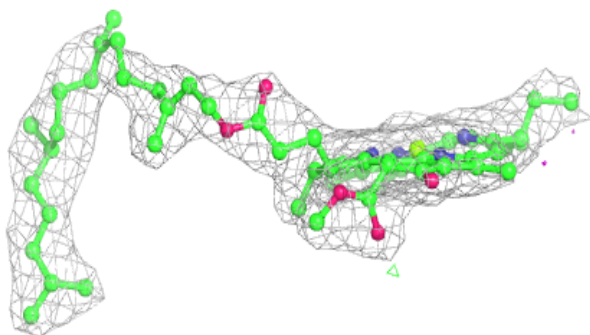
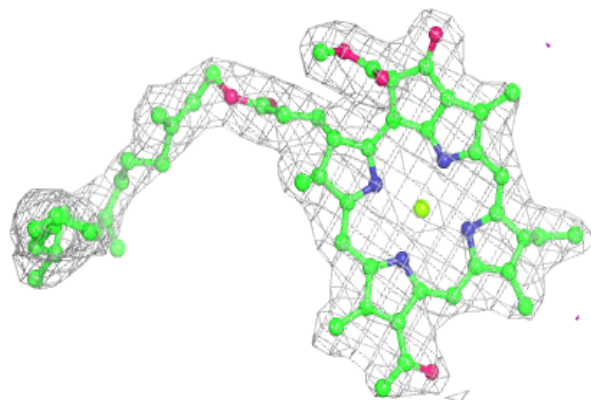


Electron density around BCL K 1706:

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

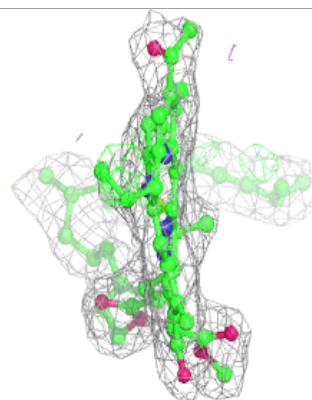
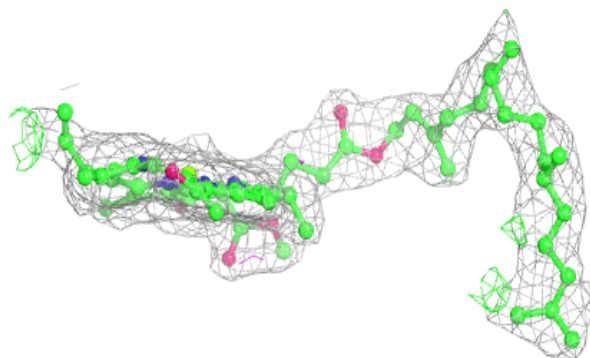
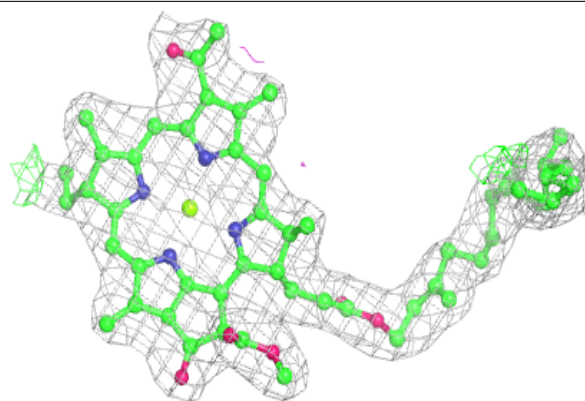
**Electron density around BCL P 1608:**

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

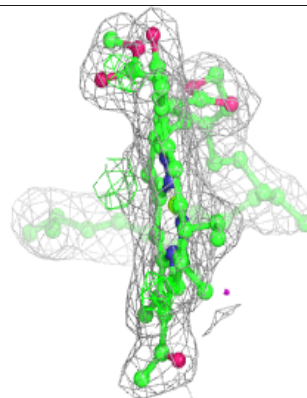
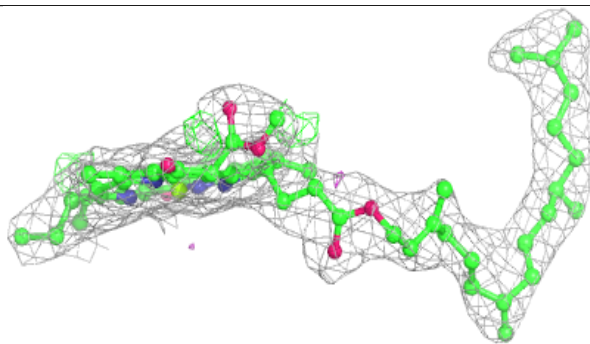
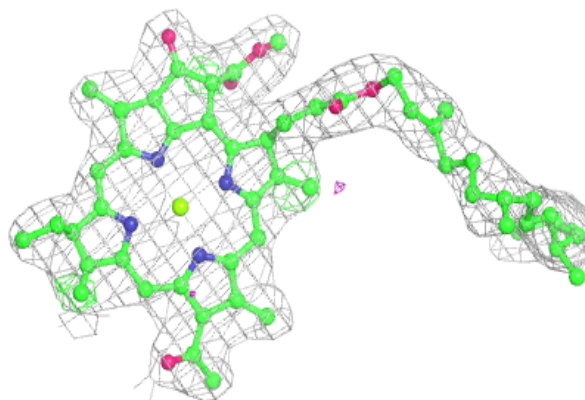


Electron density around BCL H 1604:

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

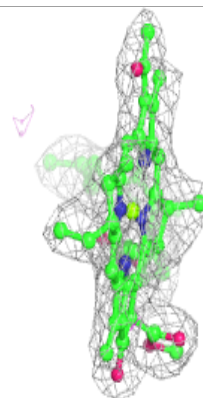
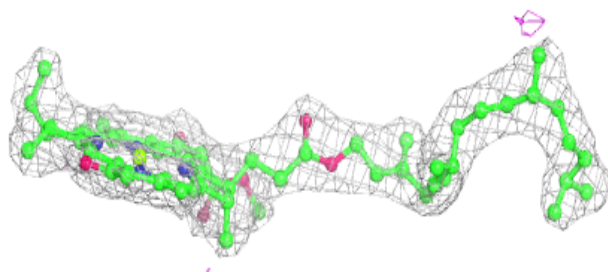
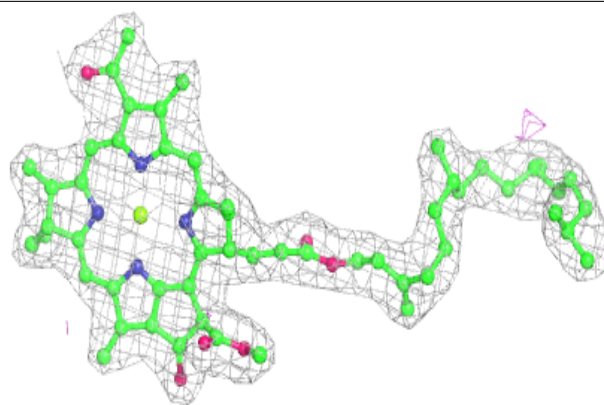
**Electron density around BCL L 1606:**

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

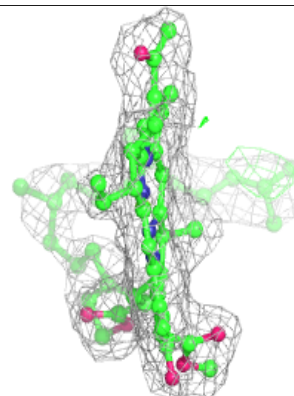
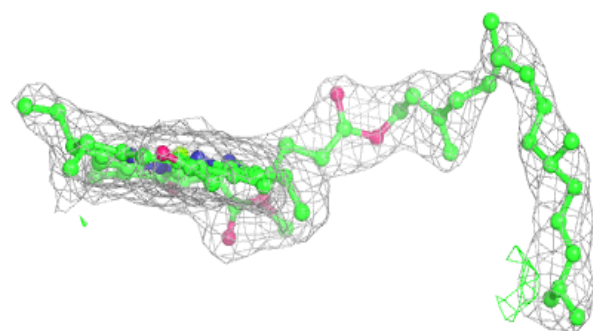
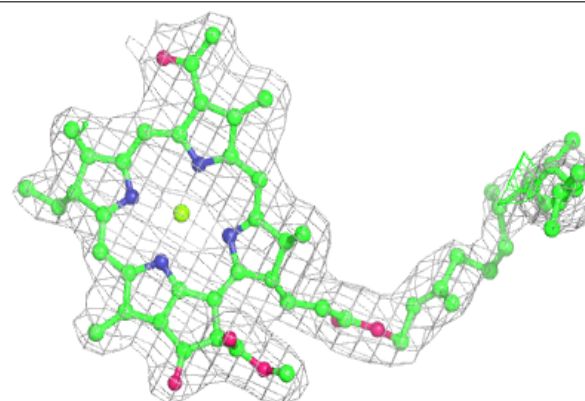


Electron density around BCL G 1504:

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

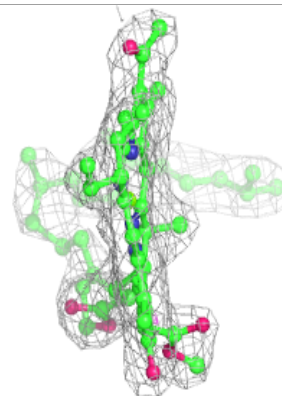
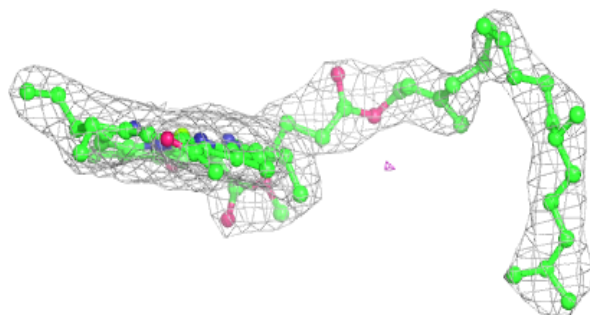
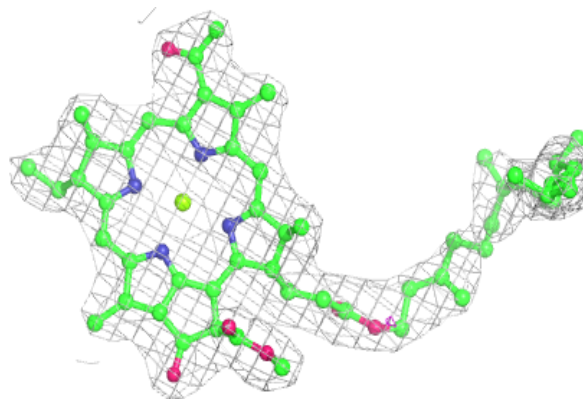
**Electron density around BCL D 1602:**

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

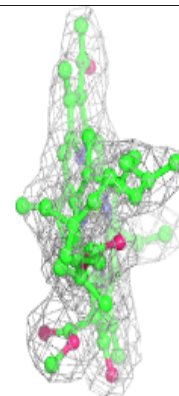
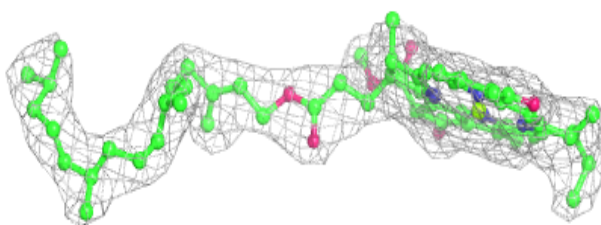
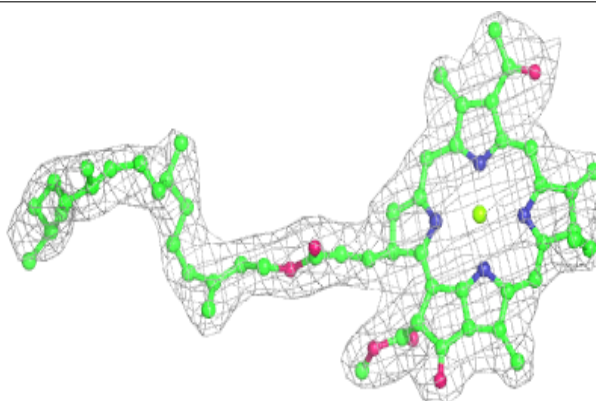


Electron density around BCL B 1601:

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

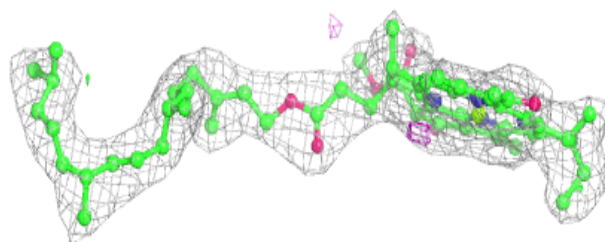
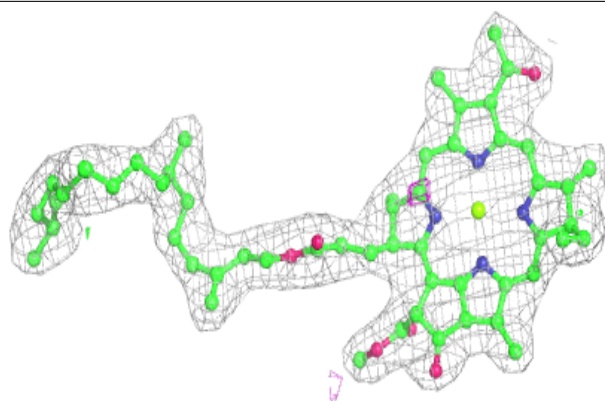
**Electron density around BCL C 1502:**

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

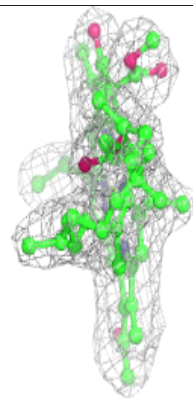
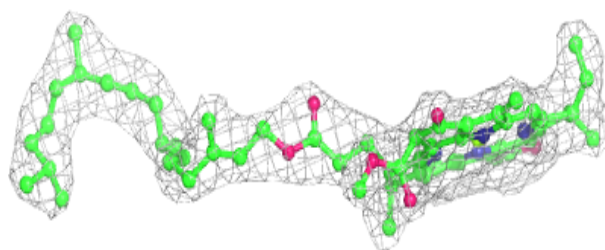
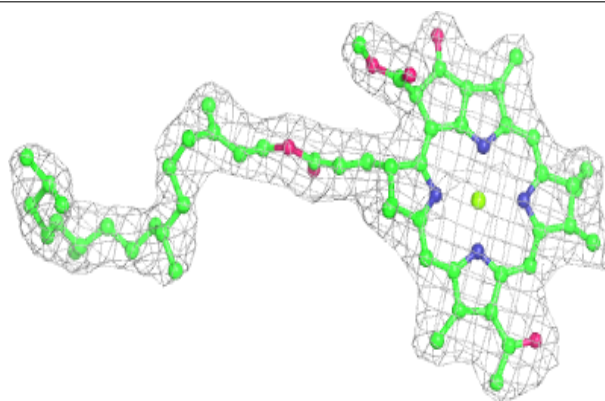


Electron density around BCL M 1507:

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

**Electron density around BCL E 1503:**

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



6.5 Other polymers

There are no such residues in this entry.