



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:32 PM UTC

PDB ID : 1NKZ / pdb_00001nkz
Title : Crystal structure of LH2 B800-850 from Rps. acidophila at 2.0 Angstrom resolution
Authors : Papiz, M.Z.; Prince, S.M.; Howard, T.; Cogdell, R.J.; Isaacs, N.W.
Deposited on : 2003-01-06
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

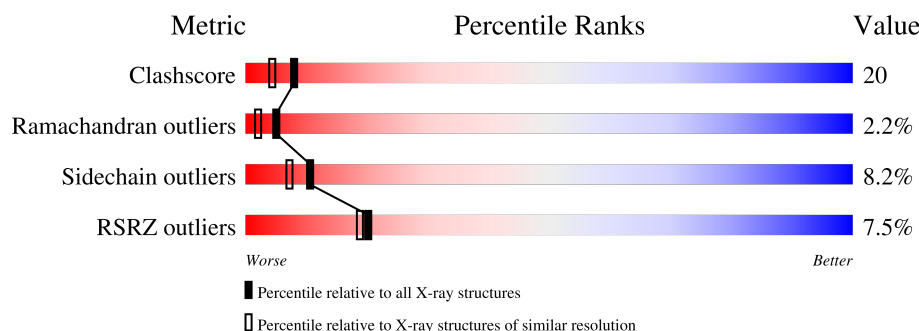
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	9% 72% 19% 8% .
1	C	53	11% 72% 21% 8%
1	E	53	13% 75% 15% 8% .
2	B	41	2% 83% 12% . .
2	D	41	2% 83% 12% . .
2	F	41	2% 83% 12% . .

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
4	BOG	A	507	X	X	-	-
4	BOG	C	504	X	X	-	-
4	BOG	C	508	X	X	-	-
4	BOG	E	505	X	X	-	-
4	BOG	E	506	X	X	-	-
4	BOG	E	509	X	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3461 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			

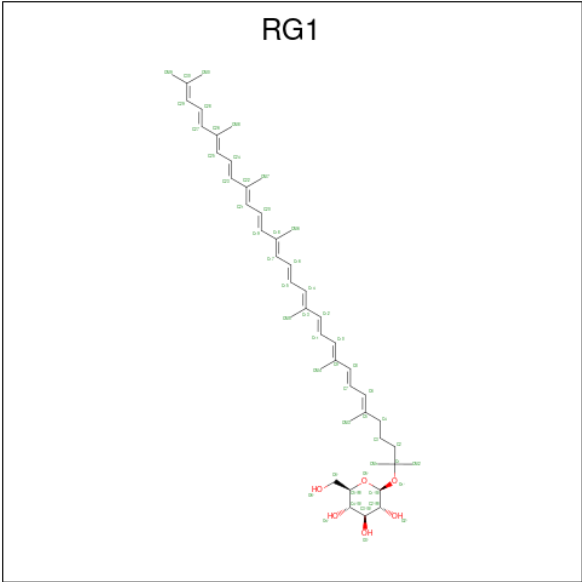
There are 3 discrepancies between the modelled and reference sequences:

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

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

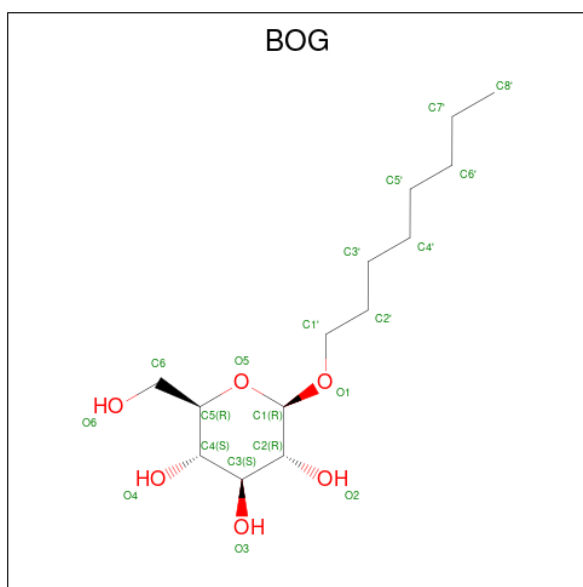
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is Rhodopin b-D-glucoside (CCD ID: RG1) (formula: $C_{46}H_{66}O_6$).



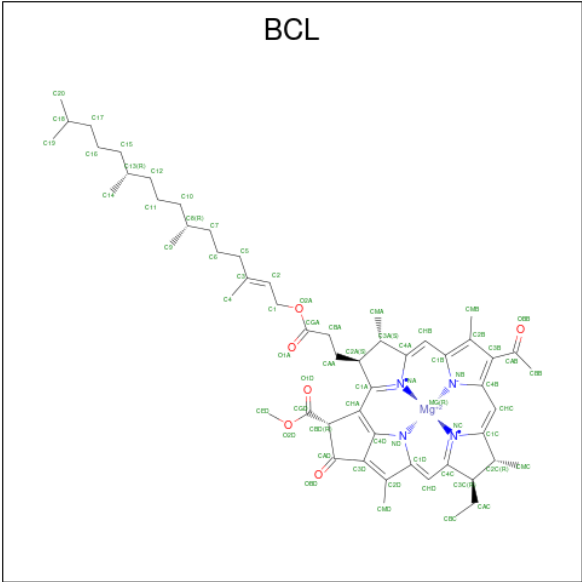
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	10	0
			52	46	6		
3	B	1	Total	C	O	0	0
			52	46	6		
3	C	1	Total	C	O	0	0
			52	46	6		
3	C	1	Total	C	O	10	0
			52	46	6		
3	D	1	Total	C	O	0	0
			52	46	6		
3	E	1	Total	C	O	10	0
			52	46	6		

- Molecule 4 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: C₁₄H₂₈O₆).



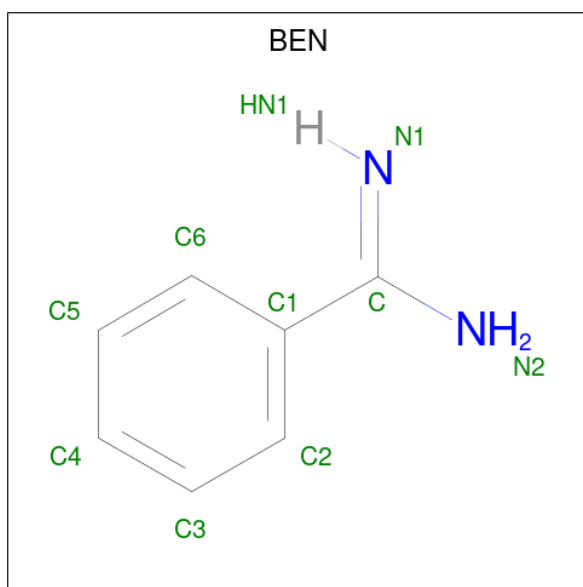
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		
4	E	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

- Molecule 6 is BENZAMIDINE (CCD ID: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	N	0	0
			9	7	2		
6	E	1	Total	C	N	0	0
			9	7	2		
6	E	1	Total	C	N	0	0
			9	7	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	41	Total	O	0	0
			41	41		
7	B	35	Total	O	0	0
			35	35		
7	C	43	Total	O	0	0
			43	43		
7	D	38	Total	O	0	0
			38	38		
7	E	49	Total	O	0	0
			49	49		
7	F	24	Total	O	0	0
			24	24		

3 Residue-property plots [i](#)

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

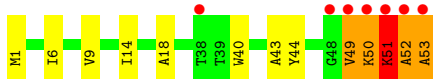
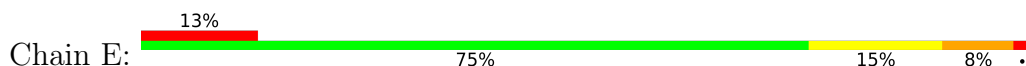
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



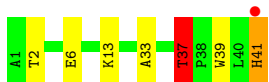
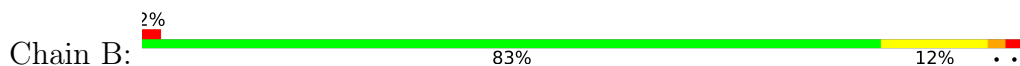
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



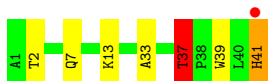
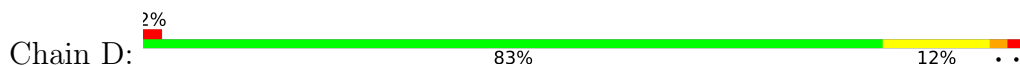
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



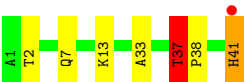
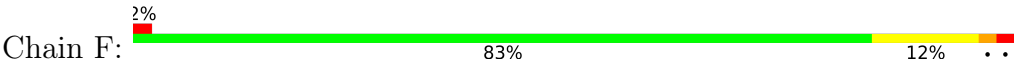
- Molecule 2: Light-harvesting protein B-800/850, beta chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.05Å 117.05Å 298.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.00) 96.1 (8.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.17 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.169 , 0.190 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.001 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.000 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3461	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: BEN, BCL, CXM, RG1, BOG

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	1.05	1/404 (0.2%)	0.91	0/556
1	C	0.64	0/404	0.87	1/556 (0.2%)
1	E	1.19	1/404 (0.2%)	0.95	0/556
2	B	0.62	0/332	0.91	1/453 (0.2%)
2	D	0.70	0/332	0.99	2/453 (0.4%)
2	F	0.67	0/332	0.99	2/453 (0.4%)
All	All	0.86	2/2208 (0.1%)	0.94	6/3027 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	53	ALA	C-O	20.19	1.64	1.23
1	A	53	ALA	C-O	14.93	1.53	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	GLN	N-CA-C	-7.96	102.58	111.82
2	F	7	GLN	N-CA-C	-7.69	102.90	111.82
2	B	37	THR	N-CA-CB	-6.31	99.09	110.39
2	F	37	THR	N-CA-CB	-6.01	99.63	110.39
1	C	4	GLY	N-CA-C	5.41	120.41	114.40
2	D	37	THR	N-CA-CB	-5.41	100.63	110.63

There are no chirality outliers.

There are no planarity outliers.

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	19	0
1	C	403	0	422	28	0
1	E	403	0	422	20	0
2	B	323	0	321	12	1
2	D	323	0	321	10	0
2	F	323	0	321	7	0
3	A	52	0	65	13	0
3	B	52	0	66	3	0
3	C	104	0	131	10	0
3	D	52	0	66	0	0
3	E	52	0	65	13	0
4	A	20	0	20	6	0
4	C	40	0	40	6	0
4	E	60	0	60	6	0
5	A	132	0	148	9	0
5	B	66	0	74	2	0
5	C	132	0	148	11	0
5	D	66	0	74	4	0
5	E	132	0	148	8	0
5	F	66	0	74	2	0
6	C	9	0	7	1	0
6	E	18	0	14	3	0
7	A	41	0	0	2	1
7	B	35	0	0	3	0
7	C	43	0	0	4	0
7	D	38	0	0	3	1
7	E	49	0	0	4	2
7	F	24	0	0	1	0
All	All	3461	0	3429	129	5

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 20.

All (129) 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:E:53:ALA:C	1:E:53:ALA:O	1.63	1.40
1:E:9:VAL:HB	7:E:554:HOH:O	1.36	1.24
3:E:406:RG1:CM5	5:E:305:BCL:HMA3	1.84	1.08
3:A:404:RG1:CM5	5:A:301:BCL:HMA3	1.84	1.08
3:C:405:RG1:CM5	5:C:303:BCL:HMA3	1.91	1.01
2:B:13:LYS:HE3	7:B:421:HOH:O	1.66	0.94
2:B:41:HIS:CE1	1:C:49:VAL:HG22	2.06	0.90
4:C:508:BOG:C1	7:C:525:HOH:O	2.20	0.90
4:A:507:BOG:H8'1	7:C:530:HOH:O	1.72	0.89
2:B:33:ALA:O	2:B:37:THR:HB	1.73	0.88
2:D:41:HIS:CE1	1:E:49:VAL:HG22	2.11	0.85
2:F:33:ALA:O	2:F:37:THR:HB	1.78	0.83
3:E:406:RG1:HM52	5:E:305:BCL:HMA3	1.58	0.83
1:A:31:HIS:CE1	5:B:302:BCL:HMD3	2.14	0.82
2:D:33:ALA:O	2:D:37:THR:HB	1.80	0.81
3:A:404:RG1:HM52	5:A:301:BCL:HMA3	1.60	0.80
3:C:405:RG1:HM52	5:C:303:BCL:HMA3	1.64	0.77
1:C:31:HIS:CE1	5:D:304:BCL:HMD1	2.23	0.73
1:A:49:VAL:HG11	3:A:404:RG1:O4'	1.91	0.70
2:D:41:HIS:NE2	1:E:49:VAL:HG13	2.06	0.69
1:A:44:TYR:HA	3:A:404:RG1:H2'	1.76	0.68
2:B:41:HIS:NE2	1:C:49:VAL:HG13	2.09	0.67
3:A:404:RG1:HM51	5:A:301:BCL:HMA3	1.73	0.66
1:E:51:LYS:O	1:E:52:ALA:HB2	1.95	0.66
1:C:41:PHE:HA	7:C:542:HOH:O	1.96	0.66
4:A:507:BOG:O6	1:C:32:LEU:CD2	2.43	0.66
1:C:51:LYS:O	1:C:52:ALA:HB3	1.96	0.66
3:C:405:RG1:HM51	5:C:303:BCL:HMA3	1.77	0.66
1:C:51:LYS:O	1:C:52:ALA:CB	2.44	0.65
2:B:41:HIS:ND1	1:C:49:VAL:HG22	2.09	0.65
3:C:405:RG1:HM32	7:D:420:HOH:O	1.95	0.65
1:C:44:TYR:HA	3:C:405:RG1:H2'	1.78	0.64
1:C:14:ILE:HD12	4:C:504:BOG:H6'1	1.80	0.64
2:D:13:LYS:HE2	7:D:413:HOH:O	1.97	0.63
1:A:51:LYS:O	1:A:52:ALA:CB	2.46	0.63
4:C:504:BOG:O3	6:E:511:BEN:N1	2.32	0.63
1:A:49:VAL:C	1:A:50:LYS:HG2	2.23	0.62
3:E:406:RG1:HM51	5:E:305:BCL:HMA3	1.76	0.61
2:B:41:HIS:CE1	1:C:49:VAL:HG13	2.35	0.61
4:A:507:BOG:H61	1:C:35:LEU:HD23	1.81	0.61
4:E:509:BOG:C1	7:E:547:HOH:O	2.48	0.60
2:D:41:HIS:ND1	1:E:49:VAL:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:C	1:E:50:LYS:HG2	2.28	0.59
1:E:49:VAL:O	1:E:50:LYS:NZ	2.32	0.59
2:D:41:HIS:CE1	1:E:49:VAL:HG13	2.38	0.58
4:E:506:BOG:C5	6:E:512:BEN:HN22	2.16	0.58
5:A:307:BCL:HBB2	5:A:307:BCL:HHC	1.85	0.58
1:A:49:VAL:HG11	3:A:404:RG1:C3'	2.34	0.58
5:E:309:BCL:HHC	5:E:309:BCL:HBB2	1.86	0.57
3:A:404:RG1:HM53	5:A:301:BCL:C1A	2.34	0.57
2:B:41:HIS:CE1	1:C:49:VAL:CG2	2.83	0.57
2:B:41:HIS:CD2	2:B:41:HIS:N	2.72	0.57
1:E:44:TYR:HA	3:E:406:RG1:H2'	1.85	0.57
3:E:406:RG1:HM21	2:F:37:THR:HA	1.87	0.56
1:C:49:VAL:HG11	3:C:405:RG1:O4'	2.04	0.56
5:C:308:BCL:HBB2	5:C:308:BCL:HHC	1.87	0.56
1:C:49:VAL:O	1:C:50:LYS:HG2	2.06	0.55
3:C:405:RG1:HM53	5:C:303:BCL:C1A	2.37	0.55
3:A:404:RG1:H6'2	7:A:535:HOH:O	2.07	0.55
2:D:41:HIS:N	2:D:41:HIS:CD2	2.74	0.55
1:E:49:VAL:HG11	3:E:406:RG1:O4'	2.07	0.55
1:E:51:LYS:O	1:E:52:ALA:CB	2.55	0.54
4:E:506:BOG:C5	6:E:512:BEN:N2	2.71	0.54
4:E:506:BOG:H7'1	7:E:559:HOH:O	2.07	0.54
1:E:14:ILE:CD1	4:E:505:BOG:H8'2	2.38	0.53
3:E:406:RG1:CM3	2:F:37:THR:OG1	2.57	0.53
4:A:507:BOG:O6	1:C:32:LEU:HD22	2.09	0.53
1:A:49:VAL:CG1	3:A:404:RG1:O4'	2.56	0.52
5:A:307:BCL:H72	5:A:307:BCL:H41	1.90	0.52
1:E:18:ALA:HB2	7:E:536:HOH:O	2.08	0.52
5:C:308:BCL:H92	5:C:308:BCL:C5	2.40	0.52
2:F:13:LYS:NZ	7:F:318:HOH:O	2.43	0.52
5:A:307:BCL:C5	5:A:307:BCL:H92	2.40	0.51
4:A:507:BOG:C6	1:C:35:LEU:HD23	2.41	0.50
3:E:406:RG1:HM53	5:E:305:BCL:C1A	2.42	0.50
1:C:50:LYS:NZ	1:C:50:LYS:HA	2.26	0.49
5:E:309:BCL:H92	5:E:309:BCL:C5	2.42	0.49
5:E:309:BCL:H72	5:E:309:BCL:H41	1.93	0.49
3:E:406:RG1:HM32	2:F:37:THR:OG1	2.12	0.49
5:F:306:BCL:HBB2	5:F:306:BCL:HMB3	1.94	0.49
1:C:37:HIS:HE2	4:C:508:BOG:C6	2.25	0.48
5:C:303:BCL:HMC1	7:D:420:HOH:O	2.13	0.48
5:C:308:BCL:H72	5:C:308:BCL:H41	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:41:HIS:CD2	2:F:41:HIS:N	2.80	0.47
1:A:51:LYS:O	1:A:52:ALA:HB3	2.12	0.47
1:A:49:VAL:O	1:A:50:LYS:HG2	2.15	0.47
1:A:50:LYS:HA	1:A:50:LYS:NZ	2.31	0.46
5:B:302:BCL:HBB2	5:B:302:BCL:HMB3	1.97	0.46
1:A:49:VAL:CG1	3:A:404:RG1:O3'	2.64	0.46
1:C:31:HIS:CE1	5:D:304:BCL:CMD	2.96	0.46
1:A:49:VAL:HG11	3:A:404:RG1:O3'	2.16	0.45
1:C:14:ILE:CD1	4:C:504:BOG:H8'2	2.46	0.45
1:A:41:PHE:HB3	1:A:42:PRO:HD3	1.99	0.45
2:D:41:HIS:HE1	1:E:49:VAL:HG22	1.73	0.45
1:E:14:ILE:HD11	4:E:505:BOG:H8'2	1.99	0.45
1:A:51:LYS:HB3	1:A:52:ALA:H	1.71	0.44
1:E:49:VAL:HG11	3:E:406:RG1:O3'	2.17	0.44
3:A:404:RG1:CM5	5:A:301:BCL:CMA	2.77	0.44
1:A:5:LYS:NZ	7:A:524:HOH:O	2.46	0.44
3:B:401:RG1:HM82	5:C:303:BCL:HAA1	2.01	0.43
3:B:401:RG1:H11	3:B:401:RG1:HM41	1.92	0.43
3:B:401:RG1:H24	3:B:401:RG1:HM71	1.90	0.43
1:C:53:ALA:C	7:C:553:HOH:O	2.61	0.43
3:E:406:RG1:HM23	2:F:38:PRO:HD3	2.01	0.43
5:F:306:BCL:H51	5:F:306:BCL:H8	1.90	0.43
1:C:50:LYS:HA	1:C:50:LYS:HZ2	1.82	0.43
1:C:49:VAL:CG1	3:C:405:RG1:O4'	2.67	0.42
1:E:6:ILE:O	1:E:9:VAL:HG22	2.19	0.42
1:A:49:VAL:O	1:A:50:LYS:NZ	2.26	0.42
1:E:40:TRP:CE3	3:E:406:RG1:HM22	2.55	0.42
3:C:405:RG1:HM21	2:D:37:THR:HA	2.02	0.42
1:C:14:ILE:CD1	4:C:504:BOG:H6'1	2.46	0.42
1:A:16:ILE:HB	1:A:17:PRO:HD3	2.02	0.42
1:E:43:ALA:HB1	3:E:406:RG1:H4'	2.01	0.41
2:B:13:LYS:CD	7:B:432:HOH:O	2.68	0.41
3:A:404:RG1:HM53	5:A:301:BCL:C2A	2.50	0.41
2:B:13:LYS:NZ	7:B:416:HOH:O	2.53	0.41
5:C:308:BCL:H161	5:C:308:BCL:H203	1.90	0.41
2:D:37:THR:CG2	2:D:39:TRP:H	2.34	0.41
1:A:37:HIS:CD2	4:A:507:BOG:H62	2.56	0.41
1:C:24:THR:CG2	6:C:510:BEN:H3	2.51	0.41
2:B:37:THR:CG2	2:B:39:TRP:H	2.34	0.41
1:A:14:ILE:HD13	1:A:14:ILE:N	2.36	0.41
1:C:49:VAL:HG11	3:C:405:RG1:C3'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:304:BCL:H51	5:D:304:BCL:H8	1.89	0.41
5:C:308:BCL:H143	5:C:308:BCL:H112	1.87	0.40
5:D:304:BCL:HBB2	5:D:304:BCL:HMB3	2.02	0.40
2:B:41:HIS:CE1	1:C:49:VAL:CG1	3.05	0.40
5:E:305:BCL:HMB1	5:E:305:BCL:HBB3	2.02	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:537:HOH:O	7:E:553:HOH:O[4_555]	1.95	0.25
7:A:542:HOH:O	7:A:542:HOH:O[12_555]	2.07	0.13
2:B:6:GLU:OE1	2:B:13:LYS:NZ[12_555]	2.12	0.08
7:D:426:HOH:O	7:D:436:HOH:O[12_555]	2.16	0.04
7:E:520:HOH:O	7:E:553:HOH:O[4_555]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	48 (94%)	1 (2%)	2 (4%)	2	1
1	C	51/53 (96%)	48 (94%)	1 (2%)	2 (4%)	2	1
1	E	51/53 (96%)	47 (92%)	2 (4%)	2 (4%)	2	1
2	B	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
2	D	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
2	F	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
All	All	270/282 (96%)	257 (95%)	7 (3%)	6 (2%)	5	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ALA
1	C	52	ALA
1	E	52	ALA
1	A	51	LYS
1	C	51	LYS
1	E	51	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%)	36 (90%)	4 (10%)	7	4
1	C	40/40 (100%)	38 (95%)	2 (5%)	22	20
1	E	40/40 (100%)	37 (92%)	3 (8%)	12	9
2	B	33/33 (100%)	30 (91%)	3 (9%)	9	6
2	D	33/33 (100%)	30 (91%)	3 (9%)	9	6
2	F	33/33 (100%)	30 (91%)	3 (9%)	9	6
All	All	219/219 (100%)	201 (92%)	18 (8%)	10	7

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	49	VAL
1	A	50	LYS
1	A	51	LYS
2	B	2	THR
2	B	37	THR
2	B	41	HIS
1	C	49	VAL
1	C	50	LYS
2	D	2	THR
2	D	37	THR
2	D	41	HIS
1	E	49	VAL

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Mol	Chain	Res	Type
1	E	50	LYS
1	E	51	LYS
2	F	2	THR
2	F	37	THR
2	F	41	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	C	3	GLN
2	D	7	GLN
1	E	3	GLN
2	F	7	GLN
2	F	41	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	C	1	5,1	9,10,11	0.97	1 (11%)	9,11,13	1.56	1 (11%)
1	CXM	E	1	5,1	9,10,11	0.92	1 (11%)	9,11,13	1.65	2 (22%)
1	CXM	A	1	5,1	9,10,11	0.96	1 (11%)	9,11,13	1.77	2 (22%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	C	1	5,1	-	3/9/10/12	-
1	CXM	E	1	5,1	-	3/9/10/12	-
1	CXM	A	1	5,1	-	2/9/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	CXM	ON1-CN	2.16	1.25	1.21
1	A	1	CXM	ON1-CN	2.07	1.25	1.21
1	E	1	CXM	ON1-CN	2.05	1.25	1.21

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	CXM	ON1-CN-N	-3.99	118.32	124.86
1	A	1	CXM	ON1-CN-N	-3.74	118.72	124.86
1	E	1	CXM	ON1-CN-N	-3.66	118.85	124.86
1	A	1	CXM	C-CA-N	2.96	115.22	109.50
1	E	1	CXM	C-CA-N	2.68	114.66	109.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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
4	BOG	E	509	-	20,20,20	5.48	15 (75%)	25,25,25	4.29	17 (68%)
5	BCL	C	308	1	69,74,74	2.01	20 (28%)	79,115,115	2.12	21 (26%)
4	BOG	C	504	-	20,20,20	5.50	14 (70%)	25,25,25	4.08	17 (68%)
4	BOG	E	505	-	20,20,20	5.49	14 (70%)	25,25,25	3.92	16 (64%)
5	BCL	A	307	1	69,74,74	2.01	21 (30%)	79,115,115	2.12	20 (25%)
5	BCL	F	306	2	69,74,74	1.94	19 (27%)	79,115,115	2.43	23 (29%)
4	BOG	C	508	-	20,20,20	5.48	14 (70%)	25,25,25	3.91	17 (68%)
3	RG1	C	403	-	52,52,52	1.27	3 (5%)	66,67,67	1.41	7 (10%)
3	RG1	A	404	-	52,52,52	1.55	7 (13%)	66,67,67	2.96	17 (25%)
3	RG1	D	402	-	52,52,52	1.32	5 (9%)	66,67,67	1.39	8 (12%)
5	BCL	E	309	1	69,74,74	2.07	21 (30%)	79,115,115	2.24	23 (29%)
4	BOG	A	507	-	20,20,20	5.51	14 (70%)	25,25,25	5.08	17 (68%)
6	BEN	E	511	-	9,9,9	1.31	1 (11%)	7,11,11	0.75	0
4	BOG	E	506	-	20,20,20	5.51	14 (70%)	25,25,25	4.04	17 (68%)
5	BCL	A	301	1	69,74,74	1.97	20 (28%)	79,115,115	2.25	23 (29%)
3	RG1	B	401	-	52,52,52	1.48	5 (9%)	66,67,67	1.69	11 (16%)
5	BCL	C	303	1	69,74,74	1.96	20 (28%)	79,115,115	2.19	23 (29%)
6	BEN	C	510	-	9,9,9	1.31	1 (11%)	7,11,11	0.82	0
3	RG1	E	406	-	52,52,52	1.54	8 (15%)	66,67,67	2.86	17 (25%)
6	BEN	E	512	-	9,9,9	1.36	1 (11%)	7,11,11	0.88	0
3	RG1	C	405	-	52,52,52	1.55	6 (11%)	66,67,67	2.97	16 (24%)
5	BCL	D	304	2	69,74,74	1.95	19 (27%)	79,115,115	2.33	25 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	B	302	2	69,74,74	1.97	18 (26%)	79,115,115	2.48	24 (30%)
5	BCL	E	305	1	69,74,74	1.97	18 (26%)	79,115,115	2.24	24 (30%)

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
4	BOG	E	509	-	4/4/5/5	7/11/31/31	0/1/1/1
5	BCL	C	308	1	-	10/41/137/137	-
4	BOG	C	504	-	4/4/5/5	7/11/31/31	0/1/1/1
4	BOG	E	505	-	4/4/5/5	9/11/31/31	0/1/1/1
5	BCL	A	307	1	-	11/41/137/137	-
5	BCL	F	306	2	-	7/41/137/137	-
4	BOG	C	508	-	4/4/5/5	9/11/31/31	0/1/1/1
3	RG1	C	403	-	-	4/51/71/71	0/1/1/1
3	RG1	A	404	-	-	24/51/71/71	0/1/1/1
3	RG1	D	402	-	-	4/51/71/71	0/1/1/1
5	BCL	E	309	1	-	11/41/137/137	-
4	BOG	A	507	-	4/4/5/5	6/11/31/31	0/1/1/1
6	BEN	E	511	-	-	2/4/4/4	0/1/1/1
4	BOG	E	506	-	4/4/5/5	6/11/31/31	0/1/1/1
5	BCL	A	301	1	-	6/41/137/137	-
3	RG1	B	401	-	-	4/51/71/71	0/1/1/1
5	BCL	C	303	1	-	6/41/137/137	-
6	BEN	C	510	-	-	4/4/4/4	0/1/1/1
3	RG1	E	406	-	-	25/51/71/71	0/1/1/1
6	BEN	E	512	-	-	2/4/4/4	0/1/1/1
3	RG1	C	405	-	-	24/51/71/71	0/1/1/1
5	BCL	D	304	2	-	8/41/137/137	-
5	BCL	B	302	2	-	7/41/137/137	-
5	BCL	E	305	1	-	6/41/137/137	-

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	506	BOG	O1-C1	-10.28	1.23	1.40
4	A	507	BOG	O1-C1	-10.22	1.23	1.40
4	C	504	BOG	O1-C1	-10.19	1.23	1.40
4	C	508	BOG	O1-C1	-10.18	1.23	1.40
4	E	505	BOG	O1-C1	-10.11	1.23	1.40
4	E	509	BOG	O1-C1	-10.05	1.23	1.40
4	A	507	BOG	C4-C5	-9.59	1.32	1.53
4	C	504	BOG	C4-C5	-9.45	1.32	1.53
4	E	509	BOG	C4-C5	-9.27	1.33	1.53
4	E	505	BOG	C4-C5	-9.27	1.33	1.53
4	C	508	BOG	C4-C5	-9.25	1.33	1.53
4	E	506	BOG	C4-C5	-9.24	1.33	1.53
4	C	504	BOG	O4-C4	-8.26	1.22	1.43
4	E	506	BOG	O4-C4	-8.25	1.22	1.43
4	E	509	BOG	O4-C4	-8.22	1.22	1.43
4	E	505	BOG	O4-C4	-8.16	1.22	1.43
4	A	507	BOG	O4-C4	-8.14	1.22	1.43
4	A	507	BOG	O3-C3	-8.14	1.22	1.43
4	C	504	BOG	O3-C3	-8.13	1.22	1.43
4	C	508	BOG	O4-C4	-8.12	1.22	1.43
4	E	505	BOG	O2-C2	-8.11	1.22	1.43
4	E	505	BOG	O3-C3	-8.11	1.22	1.43
4	E	506	BOG	O3-C3	-8.10	1.22	1.43
4	E	509	BOG	O3-C3	-8.09	1.22	1.43
4	E	506	BOG	O2-C2	-8.08	1.22	1.43
4	C	508	BOG	O2-C2	-8.06	1.23	1.43
4	A	507	BOG	O2-C2	-8.04	1.23	1.43
4	E	509	BOG	O2-C2	-8.02	1.23	1.43
4	C	504	BOG	O2-C2	-7.99	1.23	1.43
4	C	508	BOG	O3-C3	-7.98	1.23	1.43
4	E	505	BOG	C4-C3	-7.27	1.33	1.52
4	A	507	BOG	C4-C3	-7.26	1.33	1.52
4	E	509	BOG	C4-C3	-7.25	1.33	1.52
4	E	506	BOG	C4-C3	-7.21	1.33	1.52
4	C	508	BOG	C4-C3	-7.19	1.33	1.52
4	C	504	BOG	C4-C3	-7.11	1.33	1.52
4	E	509	BOG	C3-C2	-6.99	1.34	1.52
4	E	506	BOG	C3-C2	-6.97	1.34	1.52
4	C	508	BOG	C3-C2	-6.95	1.34	1.52
4	E	505	BOG	C3-C2	-6.95	1.34	1.52
4	A	507	BOG	C3-C2	-6.93	1.34	1.52
5	E	309	BCL	C2-C3	6.92	1.49	1.33
5	C	308	BCL	C2-C3	6.90	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	BOG	C3-C2	-6.85	1.34	1.52
5	A	307	BCL	C2-C3	6.81	1.48	1.33
5	A	301	BCL	C2-C3	6.62	1.48	1.33
5	F	306	BCL	C2-C3	6.57	1.48	1.33
5	B	302	BCL	C2-C3	6.47	1.47	1.33
5	D	304	BCL	C2-C3	6.46	1.47	1.33
5	E	305	BCL	C2-C3	6.42	1.47	1.33
4	C	508	BOG	C1-C2	-6.27	1.34	1.52
5	C	303	BCL	C2-C3	6.10	1.47	1.33
3	C	403	RG1	C28-C27	6.09	1.50	1.34
3	D	402	RG1	C28-C27	6.07	1.50	1.34
4	E	505	BOG	C1-C2	-6.06	1.34	1.52
4	E	509	BOG	C1-C2	-6.04	1.34	1.52
4	C	504	BOG	C1-C2	-6.01	1.34	1.52
3	B	401	RG1	C28-C27	5.96	1.50	1.34
4	E	506	BOG	C1-C2	-5.95	1.35	1.52
4	A	507	BOG	C1-C2	-5.92	1.35	1.52
3	E	406	RG1	C28-C27	5.30	1.48	1.34
5	C	308	BCL	C3B-C4B	5.23	1.51	1.41
5	A	307	BCL	C3B-C4B	5.18	1.51	1.41
5	C	303	BCL	C3B-C4B	5.15	1.51	1.41
3	C	405	RG1	C28-C27	5.08	1.47	1.34
3	A	404	RG1	C28-C27	5.07	1.47	1.34
5	E	309	BCL	C3B-C4B	5.03	1.51	1.41
5	A	301	BCL	C3B-C4B	4.84	1.50	1.41
5	B	302	BCL	C3B-C4B	4.83	1.50	1.41
5	E	305	BCL	C3B-C4B	4.70	1.50	1.41
5	F	306	BCL	C3B-C4B	4.65	1.50	1.41
5	D	304	BCL	C3B-C4B	4.61	1.50	1.41
3	E	406	RG1	C27-C26	4.43	1.55	1.46
3	A	404	RG1	C25-C26	4.41	1.46	1.35
3	C	405	RG1	C25-C26	4.40	1.46	1.35
3	A	404	RG1	C27-C26	4.34	1.55	1.46
3	C	405	RG1	C27-C26	4.33	1.55	1.46
5	B	302	BCL	O1D-CGD	4.31	1.32	1.21
3	E	406	RG1	C25-C26	4.29	1.45	1.35
5	A	301	BCL	MG-NA	4.25	2.16	2.06
5	D	304	BCL	MG-NC	4.18	2.16	2.06
3	C	405	RG1	C28-C29	4.16	1.56	1.43
3	A	404	RG1	C28-C29	4.14	1.56	1.43
5	B	302	BCL	MG-NC	4.14	2.16	2.06
5	E	305	BCL	C3D-C2D	4.12	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	309	BCL	O1D-CGD	4.11	1.31	1.21
3	E	406	RG1	C28-C29	4.05	1.55	1.43
5	E	305	BCL	O1D-CGD	4.03	1.31	1.21
5	A	307	BCL	C3D-C2D	4.03	1.50	1.39
5	E	309	BCL	C3D-C2D	4.00	1.49	1.39
5	C	303	BCL	C3D-C2D	3.99	1.49	1.39
5	C	308	BCL	C3D-C2D	3.99	1.49	1.39
5	F	306	BCL	C1D-C2D	3.97	1.53	1.45
5	F	306	BCL	O1D-CGD	3.92	1.31	1.21
5	C	303	BCL	OBD-CAD	3.89	1.29	1.22
5	A	301	BCL	CHB-C4A	3.89	1.47	1.37
5	A	307	BCL	O1D-CGD	3.88	1.31	1.21
5	B	302	BCL	CHB-C1B	3.85	1.48	1.39
5	E	309	BCL	C1D-C2D	3.85	1.53	1.45
4	E	506	BOG	O1-C1'	-3.84	1.32	1.43
5	E	305	BCL	CHB-C4A	3.82	1.47	1.37
5	C	308	BCL	C1D-C2D	3.81	1.52	1.45
4	C	504	BOG	O1-C1'	-3.80	1.32	1.43
5	C	303	BCL	CHB-C1B	3.79	1.47	1.39
6	E	512	BEN	C1-C	-3.78	1.40	1.47
4	E	505	BOG	O1-C1'	-3.77	1.32	1.43
5	A	307	BCL	CHB-C4A	3.77	1.47	1.37
5	E	305	BCL	C1D-C2D	3.76	1.52	1.45
5	C	303	BCL	MG-NA	3.74	2.15	2.06
3	B	401	RG1	O3'-C3'	3.73	1.52	1.43
5	A	301	BCL	C3D-C2D	3.73	1.49	1.39
5	E	305	BCL	CHB-C1B	3.72	1.47	1.39
4	A	507	BOG	O1-C1'	-3.72	1.32	1.43
5	E	309	BCL	CHB-C4A	3.71	1.47	1.37
5	A	307	BCL	C1D-C2D	3.71	1.52	1.45
5	E	309	BCL	MG-NA	3.71	2.15	2.06
4	E	506	BOG	C3'-C2'	-3.70	1.33	1.51
4	E	506	BOG	C5'-C4'	-3.68	1.33	1.51
5	D	304	BCL	C3D-C2D	3.67	1.49	1.39
5	D	304	BCL	CHC-C1C	3.67	1.46	1.37
4	E	506	BOG	C4'-C3'	-3.66	1.33	1.51
5	C	308	BCL	O1D-CGD	3.66	1.30	1.21
4	E	505	BOG	C3'-C2'	-3.66	1.33	1.51
4	E	509	BOG	C5'-C4'	-3.66	1.33	1.51
4	C	508	BOG	O1-C1'	-3.66	1.33	1.43
4	C	504	BOG	C5'-C4'	-3.66	1.33	1.51
5	D	304	BCL	CHC-C4B	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	BOG	C6'-C5'	-3.66	1.33	1.51
4	C	504	BOG	C4'-C3'	-3.66	1.33	1.51
5	D	304	BCL	O1D-CGD	3.65	1.30	1.21
4	C	508	BOG	C6'-C5'	-3.65	1.33	1.51
4	A	507	BOG	C5'-C4'	-3.65	1.33	1.51
4	E	509	BOG	C6'-C5'	-3.65	1.33	1.51
4	C	504	BOG	C3'-C2'	-3.64	1.33	1.51
6	E	511	BEN	C1-C	-3.64	1.40	1.47
4	C	508	BOG	C5'-C4'	-3.64	1.33	1.51
4	A	507	BOG	C6'-C5'	-3.63	1.33	1.51
4	A	507	BOG	C3'-C2'	-3.63	1.33	1.51
5	A	301	BCL	C1D-C2D	3.63	1.52	1.45
4	E	505	BOG	C5'-C4'	-3.63	1.33	1.51
4	C	508	BOG	C4'-C3'	-3.63	1.33	1.51
5	B	302	BCL	C3D-C2D	3.63	1.48	1.39
4	A	507	BOG	C4'-C3'	-3.63	1.33	1.51
4	E	505	BOG	C4'-C3'	-3.62	1.33	1.51
4	E	506	BOG	C6'-C5'	-3.62	1.33	1.51
4	C	508	BOG	C3'-C2'	-3.62	1.33	1.51
5	C	303	BCL	CHB-C4A	3.61	1.46	1.37
4	E	509	BOG	C4'-C3'	-3.61	1.33	1.51
4	E	505	BOG	C6'-C5'	-3.60	1.33	1.51
6	C	510	BEN	C1-C	-3.60	1.40	1.47
4	E	509	BOG	C3'-C2'	-3.58	1.34	1.51
4	E	509	BOG	O1-C1'	-3.57	1.33	1.43
5	A	301	BCL	CHB-C1B	3.56	1.47	1.39
5	E	305	BCL	OBD-CAD	3.53	1.28	1.22
5	E	309	BCL	CHB-C1B	3.52	1.47	1.39
5	C	303	BCL	O1D-CGD	3.51	1.30	1.21
5	F	306	BCL	C3D-C2D	3.47	1.48	1.39
3	D	402	RG1	C27-C26	3.47	1.53	1.46
5	C	308	BCL	CHB-C4A	3.46	1.46	1.37
5	F	306	BCL	CHB-C4A	3.46	1.46	1.37
5	A	301	BCL	O1D-CGD	3.46	1.30	1.21
5	C	308	BCL	CHB-C1B	3.43	1.47	1.39
5	D	304	BCL	CHB-C4A	3.43	1.46	1.37
5	C	303	BCL	CHC-C1C	3.40	1.46	1.37
5	D	304	BCL	C1D-C2D	3.40	1.52	1.45
5	E	309	BCL	CHD-C1D	3.40	1.45	1.38
5	E	305	BCL	C1D-ND	3.39	1.42	1.37
5	A	301	BCL	CHC-C4B	3.39	1.47	1.39
5	C	303	BCL	MG-NC	3.38	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	BCL	CHD-C1D	3.38	1.45	1.38
5	E	309	BCL	O1A-CGA	3.37	1.32	1.22
5	B	302	BCL	CHC-C4B	3.36	1.47	1.39
5	D	304	BCL	CHB-C1B	3.36	1.46	1.39
5	E	305	BCL	MG-NC	3.35	2.14	2.06
5	E	305	BCL	CHC-C4B	3.35	1.46	1.39
5	F	306	BCL	MG-NC	3.34	2.14	2.06
5	F	306	BCL	CHC-C4B	3.33	1.46	1.39
5	C	303	BCL	CHC-C4B	3.32	1.46	1.39
5	E	305	BCL	MG-NA	3.32	2.14	2.06
5	B	302	BCL	C1D-C2D	3.32	1.51	1.45
5	B	302	BCL	CHB-C4A	3.32	1.46	1.37
5	C	308	BCL	O1A-CGA	3.29	1.32	1.22
5	B	302	BCL	CHC-C1C	3.29	1.45	1.37
5	A	307	BCL	MG-NA	3.27	2.14	2.06
5	F	306	BCL	CHB-C1B	3.27	1.46	1.39
5	A	307	BCL	CHB-C1B	3.24	1.46	1.39
3	D	402	RG1	C28-C29	3.22	1.53	1.43
5	C	303	BCL	C1D-C2D	3.22	1.51	1.45
5	E	309	BCL	CHC-C4B	3.21	1.46	1.39
5	C	308	BCL	MG-NC	3.20	2.13	2.06
3	C	405	RG1	C24-C25	3.20	1.53	1.43
3	B	401	RG1	C28-C29	3.20	1.53	1.43
3	A	404	RG1	C24-C25	3.20	1.53	1.43
5	C	308	BCL	CHD-C1D	3.19	1.44	1.38
5	A	307	BCL	CHD-C1D	3.18	1.44	1.38
5	C	308	BCL	OBD-CAD	3.14	1.27	1.22
5	A	301	BCL	OBD-CAD	3.13	1.27	1.22
5	D	304	BCL	CHD-C1D	3.13	1.44	1.38
3	A	404	RG1	C29-C30	3.12	1.43	1.34
3	C	405	RG1	C29-C30	3.12	1.43	1.34
5	F	306	BCL	CHC-C1C	3.12	1.45	1.37
3	C	403	RG1	C28-C29	3.11	1.52	1.43
5	C	308	BCL	MG-NA	3.10	2.13	2.06
3	B	401	RG1	C27-C26	3.09	1.52	1.46
5	A	301	BCL	CHC-C1C	3.09	1.45	1.37
5	D	304	BCL	O2D-CGD	3.05	1.40	1.33
5	A	307	BCL	CHC-C4B	3.03	1.46	1.39
5	C	308	BCL	CHC-C4B	3.01	1.46	1.39
5	E	309	BCL	MG-NC	3.00	2.13	2.06
5	E	309	BCL	OBD-CAD	2.99	1.27	1.22
5	E	309	BCL	CHC-C1C	2.98	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	BCL	O2D-CGD	2.97	1.40	1.33
5	E	305	BCL	CHC-C1C	2.96	1.45	1.37
5	E	305	BCL	C4D-CHA	2.96	1.48	1.38
4	A	507	BOG	C7'-C6'	-2.94	1.33	1.51
4	E	505	BOG	C7'-C6'	-2.93	1.33	1.51
5	A	307	BCL	O1A-CGA	2.93	1.31	1.22
4	C	508	BOG	C7'-C6'	-2.93	1.33	1.51
4	C	504	BOG	C7'-C6'	-2.92	1.33	1.51
5	E	309	BCL	C4D-CHA	2.92	1.48	1.38
5	A	307	BCL	C4D-CHA	2.91	1.48	1.38
4	E	509	BOG	C7'-C6'	-2.91	1.33	1.51
5	F	306	BCL	C4D-CHA	2.91	1.48	1.38
5	C	308	BCL	C4D-CHA	2.91	1.48	1.38
4	E	506	BOG	C7'-C6'	-2.89	1.33	1.51
5	A	307	BCL	CHC-C1C	2.88	1.44	1.37
5	C	308	BCL	O2D-CGD	2.86	1.40	1.33
5	A	307	BCL	C1D-ND	2.86	1.41	1.37
5	A	301	BCL	MG-NC	2.85	2.13	2.06
5	D	304	BCL	O1A-CGA	2.84	1.31	1.22
5	F	306	BCL	CHD-C1D	2.84	1.43	1.38
5	A	301	BCL	CHD-C1D	2.84	1.43	1.38
5	B	302	BCL	O1A-CGA	2.83	1.30	1.22
5	F	306	BCL	O1A-CGA	2.82	1.30	1.22
5	A	301	BCL	C4D-CHA	2.82	1.48	1.38
5	C	308	BCL	CHC-C1C	2.82	1.44	1.37
5	D	304	BCL	MG-NA	2.81	2.12	2.06
5	B	302	BCL	MG-NA	2.81	2.12	2.06
5	D	304	BCL	C1D-ND	2.79	1.41	1.37
3	E	406	RG1	C29-C30	2.79	1.42	1.34
5	F	306	BCL	MG-NA	2.78	2.12	2.06
3	E	406	RG1	C24-C25	2.77	1.51	1.43
5	A	301	BCL	C1D-ND	2.77	1.41	1.37
5	C	303	BCL	C4D-CHA	2.77	1.47	1.38
5	A	307	BCL	MG-NC	2.77	2.12	2.06
5	F	306	BCL	O2D-CGD	2.76	1.40	1.33
5	B	302	BCL	C4D-CHA	2.75	1.47	1.38
5	C	303	BCL	C1B-C2B	2.75	1.49	1.43
5	B	302	BCL	OBD-CAD	2.74	1.27	1.22
5	F	306	BCL	OBD-CAD	2.72	1.27	1.22
5	D	304	BCL	OBD-CAD	2.70	1.27	1.22
5	A	307	BCL	C1B-C2B	2.70	1.49	1.43
5	A	307	BCL	O2D-CGD	2.69	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	308	BCL	C1B-C2B	2.68	1.49	1.43
5	B	302	BCL	C1B-C2B	2.68	1.49	1.43
5	D	304	BCL	C4D-CHA	2.66	1.47	1.38
5	E	309	BCL	C1B-C2B	2.64	1.49	1.43
5	A	307	BCL	OBD-CAD	2.62	1.27	1.22
5	C	303	BCL	O2D-CGD	2.56	1.39	1.33
5	C	303	BCL	O1A-CGA	2.55	1.30	1.22
5	E	309	BCL	O2D-CGD	2.55	1.39	1.33
3	B	401	RG1	O2'-C2'	2.54	1.49	1.43
5	C	303	BCL	CHD-C1D	2.54	1.43	1.38
5	A	301	BCL	O1A-CGA	2.52	1.30	1.22
5	F	306	BCL	C1B-C2B	2.52	1.49	1.43
5	A	301	BCL	C1B-C2B	2.50	1.49	1.43
5	C	303	BCL	C1D-ND	2.48	1.41	1.37
5	E	309	BCL	C1B-NB	2.47	1.41	1.37
5	E	305	BCL	O2D-CGD	2.45	1.39	1.33
3	C	403	RG1	C27-C26	2.44	1.51	1.46
5	D	304	BCL	C1B-C2B	2.41	1.48	1.43
5	E	305	BCL	C1B-C2B	2.41	1.48	1.43
5	E	309	BCL	C1D-ND	2.41	1.41	1.37
5	C	303	BCL	O2A-CGA	2.34	1.40	1.33
5	A	307	BCL	C1B-NB	2.32	1.40	1.37
5	E	305	BCL	CHD-C1D	2.29	1.42	1.38
5	F	306	BCL	O2A-CGA	2.28	1.40	1.33
5	E	309	BCL	O2A-CGA	2.27	1.40	1.33
3	D	402	RG1	C12-C13	2.26	1.50	1.46
5	C	303	BCL	C3B-C2B	2.26	1.50	1.42
3	D	402	RG1	O1'-C1	-2.25	1.43	1.46
5	D	304	BCL	C3B-C2B	2.24	1.50	1.42
5	A	307	BCL	O2A-CGA	2.23	1.39	1.33
5	A	307	BCL	OBb-CAB	2.23	1.28	1.23
5	C	308	BCL	O2A-CGA	2.23	1.39	1.33
5	A	301	BCL	O2D-CGD	2.22	1.38	1.33
5	E	305	BCL	O1A-CGA	2.19	1.29	1.22
5	A	301	BCL	O2A-CGA	2.17	1.39	1.33
4	E	509	BOG	O5-C1	2.15	1.47	1.41
3	E	406	RG1	CM9-C30	2.08	1.56	1.50
5	A	301	BCL	C3B-C2B	2.05	1.49	1.42
5	C	308	BCL	OBb-CAB	2.04	1.27	1.23
3	A	404	RG1	O1'-C1	-2.03	1.44	1.46
5	C	308	BCL	C3B-C2B	2.02	1.49	1.42
5	F	306	BCL	C3B-C2B	2.01	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	BCL	C3B-C2B	2.01	1.49	1.42
3	E	406	RG1	O1'-C1	-2.00	1.44	1.46
5	E	309	BCL	C3B-C2B	2.00	1.49	1.42

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	507	BOG	O1-C1'-C2'	16.69	166.00	109.37
3	C	405	RG1	C25-C24-C23	15.46	167.99	123.20
3	A	404	RG1	C25-C24-C23	15.33	167.61	123.20
3	E	406	RG1	C25-C24-C23	14.05	163.92	123.20
5	F	306	BCL	C4A-NA-C1A	-12.77	100.85	106.68
5	B	302	BCL	C4A-NA-C1A	-11.48	101.44	106.68
5	D	304	BCL	C4A-NA-C1A	-11.22	101.56	106.68
4	E	509	BOG	O1-C1'-C2'	10.12	143.70	109.37
5	A	301	BCL	C4A-NA-C1A	-10.10	102.07	106.68
5	E	309	BCL	C4A-NA-C1A	-10.06	102.09	106.68
3	C	405	RG1	C7-C6-C5	-9.87	113.80	127.69
3	A	404	RG1	C7-C6-C5	-9.73	114.01	127.69
5	E	305	BCL	C4A-NA-C1A	-9.62	102.29	106.68
3	E	406	RG1	C7-C6-C5	-9.53	114.29	127.69
5	B	302	BCL	C1C-NC-C4C	-9.48	102.35	106.68
5	A	307	BCL	C4A-NA-C1A	-9.12	102.52	106.68
4	E	505	BOG	O1-C1-C2	8.98	121.91	108.27
5	C	303	BCL	C4A-NA-C1A	-8.95	102.59	106.68
4	C	504	BOG	O1-C1-C2	8.75	121.57	108.27
4	A	507	BOG	O1-C1-C2	8.70	121.48	108.27
4	C	508	BOG	O1-C1-C2	8.53	121.23	108.27
4	E	506	BOG	O1-C1'-C2'	-8.37	80.98	109.37
5	C	308	BCL	C4A-NA-C1A	-8.00	103.03	106.68
4	C	504	BOG	O1-C1'-C2'	-7.63	83.49	109.37
4	E	509	BOG	O1-C1-C2	7.48	119.64	108.27
4	E	506	BOG	O1-C1-C2	7.42	119.54	108.27
3	C	405	RG1	C28-C29-C30	-7.12	116.61	127.48
3	A	404	RG1	C28-C29-C30	-7.10	116.63	127.48
5	F	306	BCL	C1C-NC-C4C	-7.05	103.46	106.68
3	E	406	RG1	C28-C29-C30	-6.91	116.93	127.48
4	A	507	BOG	O5-C5-C6	6.23	121.89	106.44
4	E	506	BOG	O5-C5-C6	6.10	121.56	106.44
5	C	308	BCL	C1-C2-C3	-6.08	116.24	126.20
4	C	508	BOG	C1'-O1-C1	6.03	123.98	113.68
5	E	309	BCL	C1-C2-C3	-6.02	116.34	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	BOG	O5-C5-C6	5.94	121.17	106.44
5	A	307	BCL	C1-C2-C3	-5.91	116.51	126.20
4	E	505	BOG	O5-C5-C6	5.86	120.96	106.44
4	E	505	BOG	O5-C5-C4	5.86	120.25	109.70
4	E	509	BOG	O5-C5-C6	5.77	120.73	106.44
4	E	506	BOG	C1-C2-C3	5.74	122.08	110.01
4	A	507	BOG	O4-C4-C3	5.73	123.87	110.38
4	E	509	BOG	C1'-O1-C1	5.53	123.13	113.68
4	E	505	BOG	C1'-O1-C1	5.50	123.07	113.68
3	B	401	RG1	C29-C28-C27	-5.40	107.56	123.20
4	A	507	BOG	C1-C2-C3	5.37	121.31	110.01
4	E	509	BOG	C1-C2-C3	5.37	121.31	110.01
4	C	508	BOG	O5-C5-C6	5.27	119.51	106.44
4	C	504	BOG	O4-C4-C3	5.25	122.75	110.38
3	C	403	RG1	C29-C28-C27	-5.25	108.00	123.20
5	E	309	BCL	OBB-CAB-C3B	-5.21	111.21	120.43
5	C	308	BCL	OBB-CAB-C3B	-5.19	111.25	120.43
4	A	507	BOG	O4-C4-C5	5.12	121.93	109.32
4	C	508	BOG	O4-C4-C5	5.08	121.83	109.32
5	D	304	BCL	C1C-NC-C4C	-5.05	104.37	106.68
4	E	506	BOG	O4-C4-C5	5.05	121.76	109.32
5	A	301	BCL	C3D-C2D-C1D	-4.99	99.02	105.83
5	A	301	BCL	OBB-CAB-C3B	-4.97	111.64	120.43
4	E	509	BOG	O4-C4-C5	4.96	121.55	109.32
4	E	509	BOG	O5-C5-C4	4.94	118.60	109.70
3	D	402	RG1	C29-C28-C27	-4.93	108.91	123.20
4	A	507	BOG	O5-C5-C4	4.92	118.57	109.70
5	E	305	BCL	C3D-C2D-C1D	-4.92	99.12	105.83
3	E	406	RG1	C29-C28-C27	-4.90	109.01	123.20
4	E	505	BOG	C1-C2-C3	4.90	120.31	110.01
4	E	506	BOG	O4-C4-C3	4.84	121.77	110.38
5	E	305	BCL	O2A-CGA-O1A	-4.82	111.56	123.63
5	C	303	BCL	C3D-C2D-C1D	-4.82	99.25	105.83
4	C	504	BOG	C1'-O1-C1	4.75	121.80	113.68
5	B	302	BCL	OBB-CAB-C3B	-4.73	112.07	120.43
4	C	508	BOG	O5-C5-C4	4.71	118.18	109.70
4	C	508	BOG	C1-C2-C3	4.70	119.90	110.01
3	C	405	RG1	C29-C28-C27	-4.67	109.67	123.20
3	A	404	RG1	C29-C28-C27	-4.66	109.69	123.20
5	F	306	BCL	OBB-CAB-C3B	-4.66	112.20	120.43
4	A	507	BOG	C1'-O1-C1	4.66	121.63	113.68
3	B	401	RG1	C28-C29-C30	-4.63	120.40	127.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	504	BOG	C1-C2-C3	4.61	119.72	110.01
4	E	506	BOG	C4-C3-C2	4.61	118.92	110.83
4	C	508	BOG	O3-C3-C2	4.61	121.24	110.38
3	D	402	RG1	C28-C29-C30	-4.60	120.45	127.48
5	D	304	BCL	OBB-CAB-C3B	-4.59	112.32	120.43
4	C	504	BOG	O4-C4-C5	4.59	120.62	109.32
4	E	505	BOG	C4-C3-C2	4.56	118.84	110.83
4	E	505	BOG	O4-C4-C3	4.56	121.12	110.38
4	A	507	BOG	O2-C2-C1	4.55	120.92	110.08
3	E	406	RG1	CM0-C30-CM9	4.53	125.01	114.59
5	C	308	BCL	C1C-NC-C4C	-4.52	104.62	106.68
4	E	505	BOG	O3-C3-C2	4.51	121.00	110.38
4	C	504	BOG	C4-C3-C2	4.48	118.70	110.83
5	D	304	BCL	CHB-C1B-NB	4.46	130.74	124.05
4	E	505	BOG	O4-C4-C5	4.46	120.31	109.32
3	C	405	RG1	CM0-C30-CM9	4.44	124.82	114.59
3	A	404	RG1	CM0-C30-CM9	4.44	124.82	114.59
4	E	509	BOG	C4-C3-C2	4.42	118.59	110.83
4	C	508	BOG	O4-C4-C3	4.40	120.76	110.38
4	C	504	BOG	O3-C3-C2	4.40	120.75	110.38
4	E	509	BOG	O3-C3-C2	4.36	120.65	110.38
4	E	509	BOG	O4-C4-C3	4.32	120.57	110.38
4	C	504	BOG	O2-C2-C1	4.32	120.38	110.08
4	E	506	BOG	O3-C3-C4	4.31	120.53	110.38
5	A	307	BCL	C3D-C2D-C1D	-4.30	99.96	105.83
4	C	504	BOG	O3-C3-C4	4.27	120.45	110.38
5	E	309	BCL	O2A-CGA-O1A	-4.27	112.94	123.63
5	C	303	BCL	OBB-CAB-C3B	-4.27	112.89	120.43
4	C	508	BOG	O2-C2-C3	4.27	120.44	110.38
4	E	505	BOG	O2-C2-C1	4.26	120.23	110.08
4	E	506	BOG	C1'-O1-C1	4.26	120.96	113.68
5	D	304	BCL	C3D-C2D-C1D	-4.24	100.04	105.83
5	A	307	BCL	O2A-CGA-O1A	-4.24	113.03	123.63
4	E	505	BOG	C3-C4-C5	4.24	117.91	110.23
5	E	305	BCL	OBB-CAB-C3B	-4.23	112.96	120.43
3	B	401	RG1	C28-C27-C26	-4.23	114.78	126.36
4	C	508	BOG	C4-C3-C2	4.21	118.22	110.83
5	E	305	BCL	C1-C2-C3	-4.21	119.30	126.20
3	C	403	RG1	C28-C29-C30	-4.21	121.05	127.48
4	A	507	BOG	O3-C3-C4	4.21	120.29	110.38
4	A	507	BOG	O3-C3-C2	4.19	120.24	110.38
5	A	301	BCL	O2A-CGA-O1A	-4.18	113.18	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	304	BCL	O2A-CGA-O1A	-4.15	113.23	123.63
3	D	402	RG1	C28-C27-C26	-4.15	114.98	126.36
4	E	506	BOG	O3-C3-C2	4.11	120.07	110.38
5	C	303	BCL	C2D-C1D-ND	4.09	114.17	110.13
5	E	309	BCL	C1C-NC-C4C	-4.09	104.81	106.68
4	C	508	BOG	O3-C3-C4	4.08	120.00	110.38
5	F	306	BCL	C3D-C2D-C1D	-4.06	100.28	105.83
4	E	509	BOG	O3-C3-C4	4.02	119.86	110.38
4	C	504	BOG	O5-C5-C4	4.01	116.92	109.70
5	B	302	BCL	CHB-C1B-NB	4.00	130.05	124.05
5	A	301	BCL	C1C-NC-C4C	-4.00	104.85	106.68
3	B	401	RG1	O2'-C2'-C3'	-4.00	100.95	110.38
5	B	302	BCL	C3D-C2D-C1D	-4.00	100.38	105.83
4	C	508	BOG	O5-C1-O1	3.99	119.48	110.04
3	B	401	RG1	O3'-C3'-C2'	3.98	119.75	110.38
4	E	506	BOG	O2-C2-C1	3.97	119.55	110.08
4	E	509	BOG	O5-C1-O1	3.97	119.42	110.04
5	C	303	BCL	CHB-C1B-NB	3.97	130.00	124.05
5	A	307	BCL	OBB-CAB-C3B	-3.96	113.43	120.43
4	E	509	BOG	C3-C4-C5	3.96	117.42	110.23
3	C	405	RG1	C11-C10-C9	-3.93	121.77	127.28
5	B	302	BCL	O2A-CGA-O1A	-3.91	113.84	123.63
5	C	308	BCL	C3D-C2D-C1D	-3.89	100.53	105.83
4	A	507	BOG	C4-C3-C2	3.89	117.65	110.83
5	A	301	BCL	O2D-CGD-O1D	-3.85	116.35	123.85
5	C	303	BCL	C1-C2-C3	-3.85	119.89	126.20
3	C	403	RG1	C28-C27-C26	-3.83	115.87	126.36
5	E	309	BCL	C3D-C2D-C1D	-3.81	100.63	105.83
4	E	506	BOG	O5-C5-C4	3.79	116.54	109.70
5	E	309	BCL	CHB-C1B-NB	3.79	129.74	124.05
4	E	509	BOG	O2-C2-C1	3.78	119.09	110.08
4	C	508	BOG	C6-C5-C4	3.78	122.31	113.02
5	C	303	BCL	O2A-CGA-O1A	-3.78	114.18	123.63
5	E	305	BCL	C2D-C1D-ND	3.77	113.86	110.13
3	A	404	RG1	C11-C10-C9	-3.77	122.00	127.28
5	F	306	BCL	O2A-CGA-O1A	-3.77	114.21	123.63
3	A	404	RG1	C15-C14-C13	-3.74	122.03	127.28
5	A	307	BCL	C6-C5-C3	-3.74	104.37	113.47
5	C	308	BCL	O2A-CGA-O1A	-3.73	114.29	123.63
5	F	306	BCL	CHB-C1B-NB	3.72	129.63	124.05
4	C	508	BOG	C3-C4-C5	3.69	116.93	110.23
3	C	405	RG1	C15-C14-C13	-3.69	122.11	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	308	BCL	C6-C5-C3	-3.68	104.49	113.47
3	A	404	RG1	C28-C27-C26	-3.68	116.27	126.36
3	C	405	RG1	C28-C27-C26	-3.68	116.28	126.36
5	A	307	BCL	CHB-C1B-NB	3.68	129.57	124.05
3	E	406	RG1	C11-C10-C9	-3.68	122.12	127.28
3	E	406	RG1	C28-C27-C26	-3.67	116.30	126.36
5	A	301	BCL	CHB-C1B-NB	3.67	129.55	124.05
5	E	305	BCL	CHC-C1C-NC	3.66	129.69	124.40
4	E	505	BOG	O3-C3-C4	3.66	119.00	110.38
3	E	406	RG1	C16-C17-C18	-3.64	122.17	127.28
4	E	505	BOG	O2-C2-C3	3.63	118.93	110.38
3	C	405	RG1	C16-C17-C18	-3.63	122.19	127.28
5	B	302	BCL	C1-C2-C3	-3.62	120.26	126.20
5	E	309	BCL	C6-C5-C3	-3.62	104.66	113.47
5	C	303	BCL	CHC-C1C-NC	3.61	129.61	124.40
4	C	504	BOG	O2-C2-C3	3.59	118.84	110.38
5	E	305	BCL	C1C-NC-C4C	-3.59	105.04	106.68
5	A	301	BCL	C1-C2-C3	-3.58	120.33	126.20
3	E	406	RG1	C15-C14-C13	-3.58	122.26	127.28
5	D	304	BCL	CHC-C1C-NC	3.58	129.56	124.40
4	C	508	BOG	O2-C2-C1	3.57	118.59	110.08
5	C	303	BCL	CHD-C1D-C2D	-3.55	118.10	125.49
3	A	404	RG1	C16-C17-C18	-3.52	122.34	127.28
4	E	506	BOG	O5-C1-O1	3.48	118.28	110.04
4	E	506	BOG	C6-C5-C4	3.47	121.53	113.02
4	C	504	BOG	O5-C1-O1	3.46	118.22	110.04
5	F	306	BCL	C1-C2-C3	-3.45	120.54	126.20
4	E	509	BOG	O2-C2-C3	3.45	118.52	110.38
5	C	303	BCL	C4-C3-C5	3.41	121.14	115.23
5	C	303	BCL	C1C-NC-C4C	-3.39	105.13	106.68
5	C	308	BCL	CHB-C1B-NB	3.38	129.12	124.05
3	E	406	RG1	C24-C25-C26	-3.38	122.54	127.28
5	E	305	BCL	O2D-CGD-O1D	-3.38	117.28	123.85
5	C	308	BCL	O2D-CGD-CBD	3.33	117.06	111.23
5	B	302	BCL	C1-O2A-CGA	3.30	124.65	116.65
3	E	406	RG1	C20-C21-C22	-3.28	122.67	127.28
5	D	304	BCL	CHD-C1D-C2D	-3.28	118.66	125.49
3	C	405	RG1	C20-C21-C22	-3.28	122.68	127.28
5	E	305	BCL	CBA-CAA-C2A	-3.25	104.13	113.79
3	A	404	RG1	C24-C25-C26	-3.25	122.72	127.28
5	A	307	BCL	CHB-C1B-C2B	-3.25	118.00	127.43
4	C	504	BOG	C6-C5-C4	3.22	120.92	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	405	RG1	C24-C25-C26	-3.22	122.77	127.28
5	C	303	BCL	CBA-CAA-C2A	-3.21	104.25	113.79
5	D	304	BCL	C1-C2-C3	-3.20	120.96	126.20
5	C	308	BCL	CHB-C1B-C2B	-3.18	118.20	127.43
5	A	301	BCL	O2D-CGD-CBD	3.17	116.77	111.23
5	E	305	BCL	CHD-C1D-C2D	-3.16	118.92	125.49
5	D	304	BCL	C1-O2A-CGA	3.15	124.28	116.65
4	E	509	BOG	C6-C5-C4	3.11	120.65	113.02
3	A	404	RG1	C20-C21-C22	-3.11	122.92	127.28
5	E	305	BCL	O2A-CGA-CBA	3.11	121.31	111.83
5	E	305	BCL	CHB-C1B-NB	3.10	128.71	124.05
5	F	306	BCL	OB B-CAB-CBB	3.10	126.72	119.77
5	A	301	BCL	C4-C3-C5	3.10	120.61	115.23
5	C	303	BCL	O2D-CGD-O1D	-3.09	117.82	123.85
5	B	302	BCL	C6-C5-C3	-3.09	105.93	113.47
5	D	304	BCL	C3B-C4B-NB	-3.09	105.68	109.76
5	A	301	BCL	C2D-C1D-ND	3.09	113.18	110.13
4	E	505	BOG	O5-C1-O1	3.09	117.34	110.04
5	B	302	BCL	CMD-C2D-C1D	3.08	130.16	124.73
5	C	303	BCL	O2D-CGD-CBD	3.07	116.59	111.23
4	A	507	BOG	O2-C2-C3	3.06	117.58	110.38
4	E	509	BOG	O5-C1-C2	3.05	116.63	110.37
4	E	506	BOG	O2-C2-C3	3.03	117.51	110.38
4	C	508	BOG	O1-C1'-C2'	3.03	119.63	109.37
3	B	401	RG1	C1'-C2'-C3'	3.03	116.38	110.01
5	D	304	BCL	C2D-C1D-ND	3.02	113.11	110.13
5	E	309	BCL	CHB-C1B-C2B	-3.01	118.69	127.43
5	D	304	BCL	CHB-C1B-C2B	-3.00	118.72	127.43
5	A	301	BCL	CHC-C1C-NC	3.00	128.73	124.40
4	E	506	BOG	C3-C4-C5	2.99	115.65	110.23
5	B	302	BCL	CBA-CAA-C2A	-2.98	104.92	113.79
5	A	307	BCL	C5-C3-C2	-2.97	114.51	121.17
5	F	306	BCL	CHB-C1B-C2B	-2.95	118.85	127.43
5	A	301	BCL	CHA-C1A-NA	-2.95	119.70	126.39
5	F	306	BCL	C1-O2A-CGA	2.95	123.80	116.65
4	A	507	BOG	C1-O5-C5	-2.93	107.99	113.72
5	A	307	BCL	C1C-NC-C4C	-2.92	105.35	106.68
5	A	301	BCL	CBA-CAA-C2A	-2.91	105.13	113.79
5	C	303	BCL	O2A-C1-C2	-2.89	96.98	108.11
5	C	308	BCL	O2D-CGD-O1D	-2.87	118.25	123.85
5	E	305	BCL	C4-C3-C5	2.85	120.18	115.23
3	B	401	RG1	O1'-C1'-C2'	2.84	116.33	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	305	BCL	O2A-C1-C2	-2.84	97.17	108.11
5	D	304	BCL	CMD-C2D-C1D	2.83	129.71	124.73
5	C	303	BCL	C3B-C4B-NB	-2.83	106.03	109.76
5	A	307	BCL	O2D-CGD-CBD	2.83	116.17	111.23
5	A	301	BCL	CHB-C1B-C2B	-2.82	119.24	127.43
5	E	309	BCL	O2D-CGD-CBD	2.80	116.13	111.23
5	B	302	BCL	CHB-C1B-C2B	-2.80	119.30	127.43
4	A	507	BOG	O5-C1-O1	2.79	116.63	110.04
5	F	306	BCL	O2D-CGD-O1D	-2.79	118.42	123.85
5	C	303	BCL	CHB-C1B-C2B	-2.78	119.34	127.43
5	A	301	BCL	O2A-C1-C2	-2.78	97.41	108.11
4	C	504	BOG	C3-C4-C5	2.78	115.27	110.23
5	D	304	BCL	O2D-CGD-CBD	2.75	116.04	111.23
5	F	306	BCL	CBA-CAA-C2A	-2.74	105.63	113.79
4	E	505	BOG	O1-C1'-C2'	2.74	118.66	109.37
5	B	302	BCL	C3B-C4B-NB	-2.72	106.17	109.76
5	C	308	BCL	C5-C3-C2	-2.70	115.11	121.17
5	D	304	BCL	CBA-CAA-C2A	-2.70	105.77	113.79
5	F	306	BCL	O2D-CGD-CBD	2.70	115.94	111.23
5	A	307	BCL	O2A-CGA-CBA	2.69	120.04	111.83
5	E	309	BCL	O2A-CGA-CBA	2.69	120.03	111.83
5	C	303	BCL	CMD-C2D-C1D	2.68	129.44	124.73
5	F	306	BCL	C6-C5-C3	-2.67	106.95	113.47
5	A	301	BCL	O2A-CGA-CBA	2.66	119.94	111.83
3	C	403	RG1	C1-O1'-C1'	-2.64	114.37	119.78
5	A	307	BCL	C2D-C1D-ND	2.64	112.74	110.13
4	E	506	BOG	O5-C1-C2	2.64	115.80	110.37
5	B	302	BCL	C2D-C1D-ND	2.64	112.74	110.13
5	B	302	BCL	O2D-CGD-O1D	-2.63	118.73	123.85
5	A	301	BCL	C5-C3-C2	-2.62	115.28	121.17
5	E	309	BCL	O2D-CGD-O1D	-2.61	118.78	123.85
3	E	406	RG1	C10-C11-C12	-2.60	115.67	123.20
5	D	304	BCL	C3D-C4D-ND	2.60	114.21	109.99
5	B	302	BCL	C5-C3-C2	-2.59	115.34	121.17
3	C	405	RG1	C10-C11-C12	-2.58	115.73	123.20
5	F	306	BCL	CHD-C1D-C2D	-2.57	120.14	125.49
5	E	305	BCL	CHB-C1B-C2B	-2.57	119.98	127.43
5	E	309	BCL	CHC-C4B-NB	2.56	127.89	124.05
5	E	305	BCL	CMD-C2D-C1D	2.55	129.23	124.73
5	E	309	BCL	OBBCAB-CBB	2.55	125.49	119.77
5	E	305	BCL	O2D-CGD-CBD	2.55	115.69	111.23
5	C	308	BCL	OBBCAB-CBB	2.54	125.45	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	404	RG1	CM5-C13-C12	2.53	121.96	118.09
5	C	303	BCL	C5-C3-C2	-2.53	115.48	121.17
5	C	303	BCL	O2A-CGA-CBA	2.53	119.55	111.83
5	B	302	BCL	CHC-C1C-NC	2.53	128.05	124.40
5	F	306	BCL	CMD-C2D-C1D	2.53	129.18	124.73
5	C	308	BCL	C3D-C4D-ND	2.52	114.09	109.99
4	C	504	BOG	C1-O5-C5	-2.52	108.79	113.72
5	D	304	BCL	C5-C3-C2	-2.52	115.50	121.17
5	E	309	BCL	C5-C3-C2	-2.52	115.51	121.17
5	E	309	BCL	C3D-C4D-ND	2.51	114.07	109.99
5	E	305	BCL	C5-C3-C2	-2.51	115.52	121.17
5	B	302	BCL	OBb-CAB-CBB	2.51	125.39	119.77
3	E	406	RG1	CM5-C13-C12	2.51	121.92	118.09
5	A	301	BCL	CHD-C1D-C2D	-2.50	120.30	125.49
3	A	404	RG1	C10-C11-C12	-2.49	115.98	123.20
5	D	304	BCL	C6-C5-C3	-2.49	107.40	113.47
5	E	305	BCL	C3D-C4D-ND	2.47	114.00	109.99
3	C	405	RG1	C6-C7-C8	2.46	130.34	123.20
5	A	307	BCL	C3D-C4D-ND	2.46	113.98	109.99
5	F	306	BCL	C3D-C4D-ND	2.45	113.98	109.99
5	B	302	BCL	CHD-C1D-C2D	-2.44	120.41	125.49
5	E	309	BCL	C1D-CHD-C4C	-2.44	120.75	126.62
5	B	302	BCL	C3D-C4D-ND	2.43	113.94	109.99
5	A	307	BCL	CMD-C2D-C1D	2.43	129.01	124.73
4	C	508	BOG	O5-C1-C2	2.43	115.36	110.37
5	A	301	BCL	OBd-CAD-C3D	-2.42	122.75	128.42
5	F	306	BCL	C3B-C4B-NB	-2.42	106.57	109.76
5	B	302	BCL	OBd-CAD-C3D	-2.41	122.77	128.42
3	B	401	RG1	C19-C18-C17	2.41	122.80	119.01
5	B	302	BCL	CHC-C4B-NB	2.40	127.64	124.05
3	C	405	RG1	O5'-C5'-C6'	2.39	112.36	106.44
5	B	302	BCL	C1D-CHD-C4C	-2.38	120.88	126.62
3	E	406	RG1	O5'-C5'-C6'	2.37	112.31	106.44
5	F	306	BCL	C1D-CHD-C4C	-2.36	120.92	126.62
5	A	301	BCL	CBB-CAB-C3B	2.36	125.38	120.40
5	D	304	BCL	OBb-CAB-CBB	2.36	125.05	119.77
3	D	402	RG1	CM5-C13-C12	2.36	121.69	118.09
5	A	307	BCL	C4-C3-C5	2.35	119.31	115.23
5	F	306	BCL	OBd-CAD-C3D	-2.35	122.93	128.42
5	A	307	BCL	O2D-CGD-O1D	-2.34	119.30	123.85
5	C	308	BCL	C1D-CHD-C4C	-2.33	120.99	126.62
5	C	303	BCL	C3D-C4D-ND	2.33	113.78	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	505	BOG	C6-C5-C4	2.33	118.73	113.02
5	F	306	BCL	CHC-C4B-NB	2.32	127.53	124.05
5	F	306	BCL	C5-C3-C2	-2.31	115.98	121.17
3	C	403	RG1	C19-C18-C17	2.31	122.64	119.01
3	C	405	RG1	CM5-C13-C12	2.31	121.62	118.09
5	D	304	BCL	C1D-CHD-C4C	-2.31	121.06	126.62
5	E	305	BCL	C3B-C4B-NB	-2.30	106.72	109.76
5	F	306	BCL	C2D-C1D-ND	2.27	112.37	110.13
5	E	309	BCL	C2D-C1D-ND	2.27	112.37	110.13
5	C	308	BCL	C4-C3-C5	2.26	119.16	115.23
3	D	402	RG1	C16-C17-C18	-2.26	124.11	127.28
5	A	307	BCL	OBD-CAD-C3D	-2.25	123.15	128.42
3	A	404	RG1	C6-C7-C8	2.25	129.72	123.20
5	E	305	BCL	C6-C5-C3	-2.25	107.99	113.47
3	B	401	RG1	CM5-C13-C12	2.25	121.52	118.09
5	C	308	BCL	C2B-C1B-NB	2.24	112.65	110.33
5	A	301	BCL	CMD-C2D-C3D	2.24	132.83	127.69
5	E	305	BCL	CHA-C1A-NA	-2.24	121.32	126.39
3	D	402	RG1	O3'-C3'-C2'	-2.23	105.12	110.38
5	D	304	BCL	O2D-CGD-O1D	-2.23	119.52	123.85
5	C	303	BCL	CHA-C1A-NA	-2.22	121.36	126.39
5	A	307	BCL	CBA-CAA-C2A	-2.21	107.22	113.79
5	B	302	BCL	O2D-CGD-CBD	2.19	115.06	111.23
4	A	507	BOG	C3-C4-C5	2.18	114.19	110.23
5	E	305	BCL	C1D-CHD-C4C	-2.18	121.36	126.62
5	C	308	BCL	O2A-CGA-CBA	2.18	118.48	111.83
3	E	406	RG1	C6-C7-C8	2.17	129.49	123.20
5	C	308	BCL	C2D-C1D-ND	2.17	112.27	110.13
3	A	404	RG1	O5'-C5'-C4'	-2.16	105.80	109.70
3	B	401	RG1	C16-C15-C14	-2.14	119.15	123.52
3	A	404	RG1	O5'-C5'-C6'	2.13	111.71	106.44
5	E	309	BCL	CHA-C1A-NA	-2.13	121.58	126.39
3	D	402	RG1	C16-C15-C14	-2.12	119.18	123.52
5	E	309	BCL	C2A-C1A-CHA	-2.12	120.19	123.87
5	E	309	BCL	CMD-C2D-C1D	2.12	128.45	124.73
5	C	308	BCL	CMD-C2D-C1D	2.11	128.44	124.73
5	E	309	BCL	C4-C3-C5	2.10	118.87	115.23
5	A	307	BCL	C1D-CHD-C4C	-2.10	121.56	126.62
5	E	309	BCL	CHA-C4D-ND	2.09	136.87	132.55
5	C	308	BCL	CHA-C1A-NA	-2.09	121.65	126.39
3	E	406	RG1	O5'-C5'-C4'	-2.08	105.96	109.70
4	A	507	BOG	O5-C1-C2	2.07	114.63	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	BCL	C1D-CHD-C4C	-2.07	121.63	126.62
5	D	304	BCL	CHD-C1D-ND	2.07	127.71	124.80
5	D	304	BCL	OBD-CAD-C3D	-2.06	123.61	128.42
3	A	404	RG1	CM4-C9-C8	2.04	121.21	118.09
3	E	406	RG1	CM4-C9-C8	2.04	121.20	118.09
3	C	403	RG1	C16-C15-C14	-2.04	119.36	123.52
5	A	301	BCL	CHA-C4D-ND	2.02	136.72	132.55
3	C	403	RG1	C7-C6-C5	-2.02	124.85	127.69
3	B	401	RG1	O3'-C3'-C4'	-2.02	105.62	110.38
3	C	405	RG1	C16-C15-C14	-2.01	119.41	123.52
3	D	402	RG1	C1-O1'-C1'	-2.01	115.67	119.78
5	D	304	BCL	C4-C3-C5	2.01	118.71	115.23

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	507	BOG	C5
4	A	507	BOG	C3
4	A	507	BOG	C4
4	A	507	BOG	C2
4	C	504	BOG	C5
4	C	504	BOG	C3
4	C	504	BOG	C4
4	C	504	BOG	C2
4	C	508	BOG	C5
4	C	508	BOG	C3
4	C	508	BOG	C4
4	C	508	BOG	C2
4	E	505	BOG	C5
4	E	505	BOG	C3
4	E	505	BOG	C4
4	E	505	BOG	C2
4	E	506	BOG	C5
4	E	506	BOG	C3
4	E	506	BOG	C4
4	E	506	BOG	C2
4	E	509	BOG	C5
4	E	509	BOG	C3
4	E	509	BOG	C4
4	E	509	BOG	C2

All (209) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	RG1	C2'-C1'-O1'-C1
3	A	404	RG1	O5'-C1'-O1'-C1
3	A	404	RG1	CM2-C1-O1'-C1'
3	A	404	RG1	C2-C1-O1'-C1'
3	A	404	RG1	C3-C4-C5-CM3
3	A	404	RG1	C11-C12-C13-CM5
3	A	404	RG1	C11-C12-C13-C14
3	B	401	RG1	C25-C26-C27-C28
3	B	401	RG1	CM8-C26-C27-C28
3	C	403	RG1	C25-C26-C27-C28
3	C	403	RG1	CM8-C26-C27-C28
3	C	405	RG1	C2'-C1'-O1'-C1
3	C	405	RG1	O5'-C1'-O1'-C1
3	C	405	RG1	CM2-C1-O1'-C1'
3	C	405	RG1	C2-C1-O1'-C1'
3	C	405	RG1	C11-C12-C13-CM5
3	C	405	RG1	C11-C12-C13-C14
3	D	402	RG1	C25-C26-C27-C28
3	D	402	RG1	CM8-C26-C27-C28
3	E	406	RG1	C2'-C1'-O1'-C1
3	E	406	RG1	O5'-C1'-O1'-C1
3	E	406	RG1	CM2-C1-O1'-C1'
3	E	406	RG1	C2-C1-O1'-C1'
3	E	406	RG1	C3-C4-C5-CM3
3	E	406	RG1	C7-C8-C9-C10
3	E	406	RG1	C11-C12-C13-CM5
3	E	406	RG1	C11-C12-C13-C14
3	E	406	RG1	C21-C22-C23-C24
3	E	406	RG1	CM7-C22-C23-C24
3	E	406	RG1	C22-C23-C24-C25
4	A	507	BOG	O5-C1-O1-C1'
4	A	507	BOG	C2'-C1'-O1-C1
4	E	505	BOG	O5-C1-O1-C1'
4	E	505	BOG	C2'-C1'-O1-C1
4	E	509	BOG	C2-C1-O1-C1'
6	E	512	BEN	N2-C-C1-C2
6	E	512	BEN	N2-C-C1-C6
5	B	302	BCL	C5-C6-C7-C8
5	D	304	BCL	C5-C6-C7-C8
5	F	306	BCL	C5-C6-C7-C8
3	A	404	RG1	C4'-C5'-C6'-O6'
3	C	405	RG1	C4'-C5'-C6'-O6'
3	E	406	RG1	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	A	404	RG1	C2-C3-C4-C5
3	C	405	RG1	C2-C3-C4-C5
3	E	406	RG1	C2-C3-C4-C5
3	C	405	RG1	C3-C4-C5-CM3
3	A	404	RG1	C3-C4-C5-C6
3	C	405	RG1	C3-C4-C5-C6
3	E	406	RG1	C3-C4-C5-C6
3	A	404	RG1	O5'-C5'-C6'-O6'
4	C	508	BOG	C4-C5-C6-O6
3	E	406	RG1	O5'-C5'-C6'-O6'
4	E	506	BOG	O5-C5-C6-O6
3	C	405	RG1	O5'-C5'-C6'-O6'
4	E	509	BOG	C4-C5-C6-O6
4	A	507	BOG	C4-C5-C6-O6
4	C	504	BOG	O5-C5-C6-O6
4	E	505	BOG	O5-C5-C6-O6
5	C	308	BCL	C3-C5-C6-C7
5	E	309	BCL	C3-C5-C6-C7
5	A	307	BCL	C11-C12-C13-C14
5	B	302	BCL	C11-C12-C13-C14
5	C	308	BCL	C11-C12-C13-C14
5	D	304	BCL	C11-C12-C13-C14
5	E	309	BCL	C11-C12-C13-C14
5	F	306	BCL	C11-C12-C13-C14
3	A	404	RG1	C7-C8-C9-CM4
3	C	405	RG1	C7-C8-C9-CM4
3	C	405	RG1	CM7-C22-C23-C24
3	E	406	RG1	C7-C8-C9-CM4
3	E	406	RG1	CM8-C26-C27-C28
5	A	307	BCL	C3-C5-C6-C7
5	E	305	BCL	C8-C10-C11-C12
3	A	404	RG1	C23-C24-C25-C26
5	A	301	BCL	C8-C10-C11-C12
5	C	303	BCL	C8-C10-C11-C12
4	E	506	BOG	O1-C1'-C2'-C3'
4	C	504	BOG	C2-C1-O1-C1'
4	C	508	BOG	C2-C1-O1-C1'
4	C	504	BOG	O1-C1'-C2'-C3'
3	A	404	RG1	C24-C25-C26-CM8
3	C	405	RG1	C24-C25-C26-CM8
3	E	406	RG1	C24-C25-C26-CM8
3	A	404	RG1	CM7-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	A	404	RG1	CM8-C26-C27-C28
3	C	405	RG1	CM8-C26-C27-C28
3	A	404	RG1	C21-C22-C23-C24
3	A	404	RG1	C25-C26-C27-C28
3	C	405	RG1	C7-C8-C9-C10
3	C	405	RG1	C21-C22-C23-C24
3	C	405	RG1	C25-C26-C27-C28
3	E	406	RG1	C25-C26-C27-C28
4	E	505	BOG	O1-C1'-C2'-C3'
3	A	404	RG1	C24-C25-C26-C27
3	C	405	RG1	C24-C25-C26-C27
3	E	406	RG1	C24-C25-C26-C27
4	E	505	BOG	C1'-C2'-C3'-C4'
3	C	405	RG1	C23-C24-C25-C26
4	E	506	BOG	C1'-C2'-C3'-C4'
4	C	508	BOG	C4'-C5'-C6'-C7'
3	A	404	RG1	C6-C7-C8-C9
3	C	405	RG1	C6-C7-C8-C9
3	E	406	RG1	C6-C7-C8-C9
5	F	306	BCL	C13-C15-C16-C17
5	D	304	BCL	C13-C15-C16-C17
4	C	504	BOG	C4'-C5'-C6'-C7'
4	E	509	BOG	C3'-C4'-C5'-C6'
5	F	306	BCL	C10-C11-C12-C13
4	C	508	BOG	C1'-C2'-C3'-C4'
5	B	302	BCL	C13-C15-C16-C17
4	C	508	BOG	C2'-C3'-C4'-C5'
4	E	509	BOG	C4'-C5'-C6'-C7'
4	E	509	BOG	O5-C5-C6-O6
4	C	504	BOG	C4-C5-C6-O6
3	C	403	RG1	O5'-C5'-C6'-O6'
5	B	302	BCL	C10-C11-C12-C13
4	E	505	BOG	C2'-C3'-C4'-C5'
5	D	304	BCL	C10-C11-C12-C13
3	C	403	RG1	C4'-C5'-C6'-O6'
4	C	508	BOG	O5-C5-C6-O6
4	E	505	BOG	C4'-C5'-C6'-C7'
5	A	307	BCL	C8-C10-C11-C12
5	C	308	BCL	C8-C10-C11-C12
4	C	508	BOG	C3'-C4'-C5'-C6'
3	A	404	RG1	C7-C8-C9-C10
5	E	309	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	E	509	BOG	O1-C1'-C2'-C3'
4	E	509	BOG	C2'-C3'-C4'-C5'
5	E	305	BCL	C15-C16-C17-C18
3	D	402	RG1	C4'-C5'-C6'-O6'
4	C	508	BOG	O1-C1'-C2'-C3'
5	A	301	BCL	C15-C16-C17-C18
4	A	507	BOG	C2-C1-O1-C1'
4	E	505	BOG	C2-C1-O1-C1'
4	E	506	BOG	C2-C1-O1-C1'
5	B	302	BCL	C6-C7-C8-C10
5	D	304	BCL	C6-C7-C8-C10
5	F	306	BCL	C6-C7-C8-C10
3	D	402	RG1	O5'-C5'-C6'-O6'
5	E	309	BCL	C10-C11-C12-C13
5	C	303	BCL	C15-C16-C17-C18
3	B	401	RG1	C4'-C5'-C6'-O6'
4	A	507	BOG	C4'-C5'-C6'-C7'
3	E	406	RG1	CM1-C1-O1'-C1'
5	E	309	BCL	C4B-C3B-CAB-CBB
5	B	302	BCL	C6-C7-C8-C9
5	C	303	BCL	C11-C12-C13-C14
5	D	304	BCL	C6-C7-C8-C9
5	E	305	BCL	C11-C12-C13-C14
5	F	306	BCL	C6-C7-C8-C9
5	C	308	BCL	C10-C11-C12-C13
5	C	308	BCL	C5-C6-C7-C8
5	A	307	BCL	C10-C11-C12-C13
5	E	305	BCL	C11-C12-C13-C15
5	A	307	BCL	C2B-C3B-CAB-OB
5	A	307	BCL	C2B-C3B-CAB-CBB
5	C	308	BCL	C2B-C3B-CAB-CBB
5	E	309	BCL	C2B-C3B-CAB-OB
5	E	309	BCL	C2B-C3B-CAB-CBB
3	B	401	RG1	O5'-C5'-C6'-O6'
4	E	506	BOG	C4'-C5'-C6'-C7'
5	A	307	BCL	C5-C6-C7-C8
5	E	309	BCL	C5-C6-C7-C8
4	C	504	BOG	C2'-C3'-C4'-C5'
5	A	301	BCL	C11-C12-C13-C15
5	B	302	BCL	C11-C12-C13-C15
5	C	303	BCL	C11-C12-C13-C15
5	D	304	BCL	C11-C12-C13-C15

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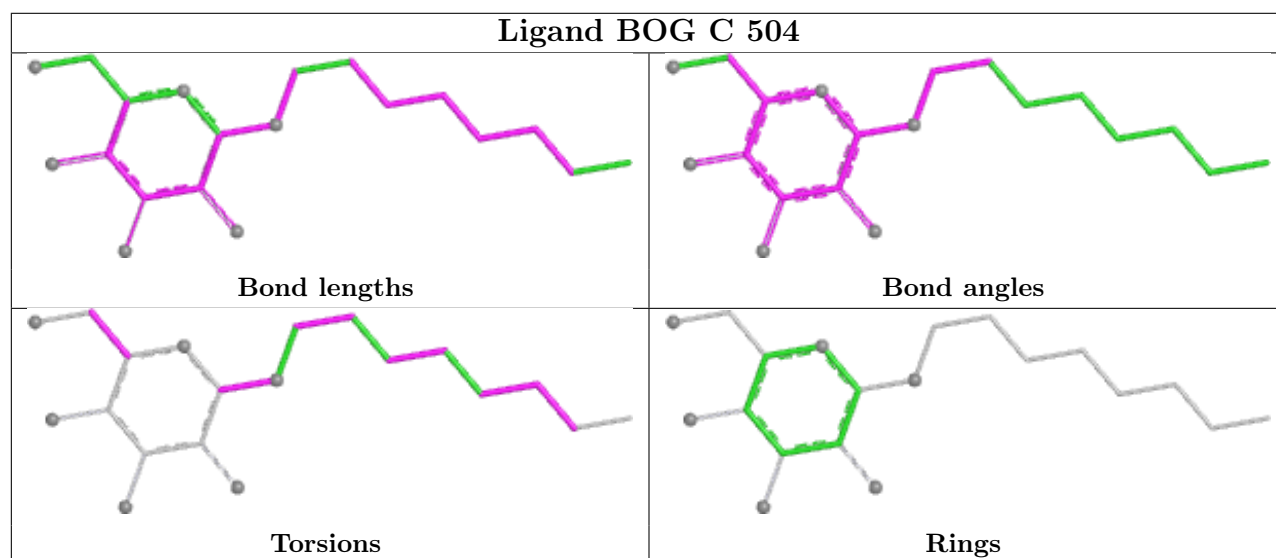
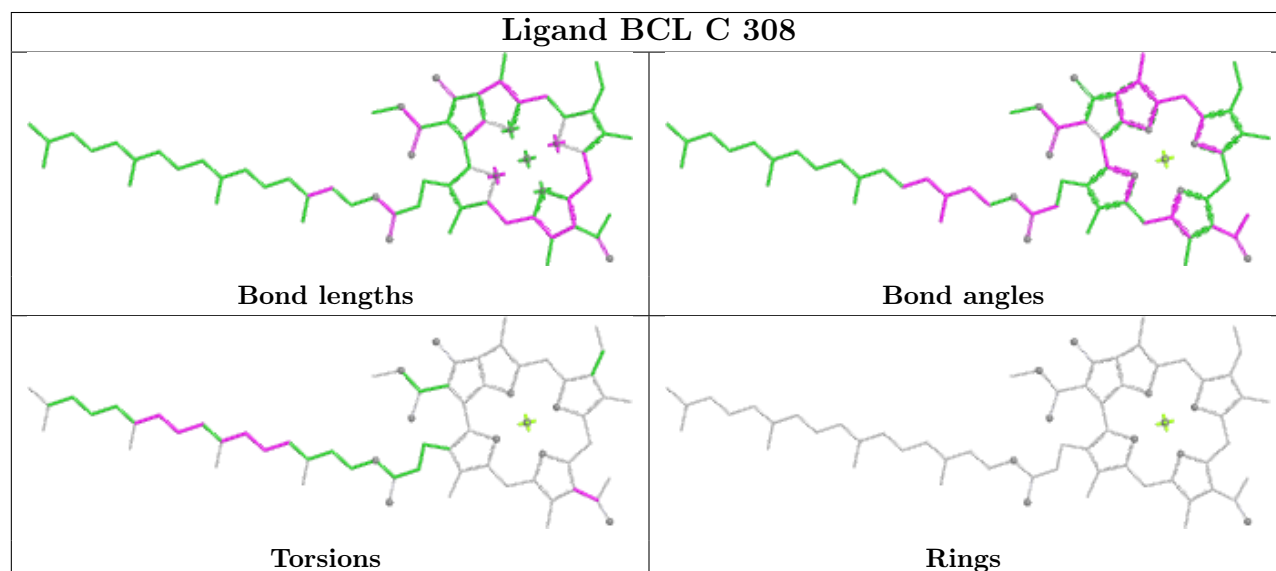
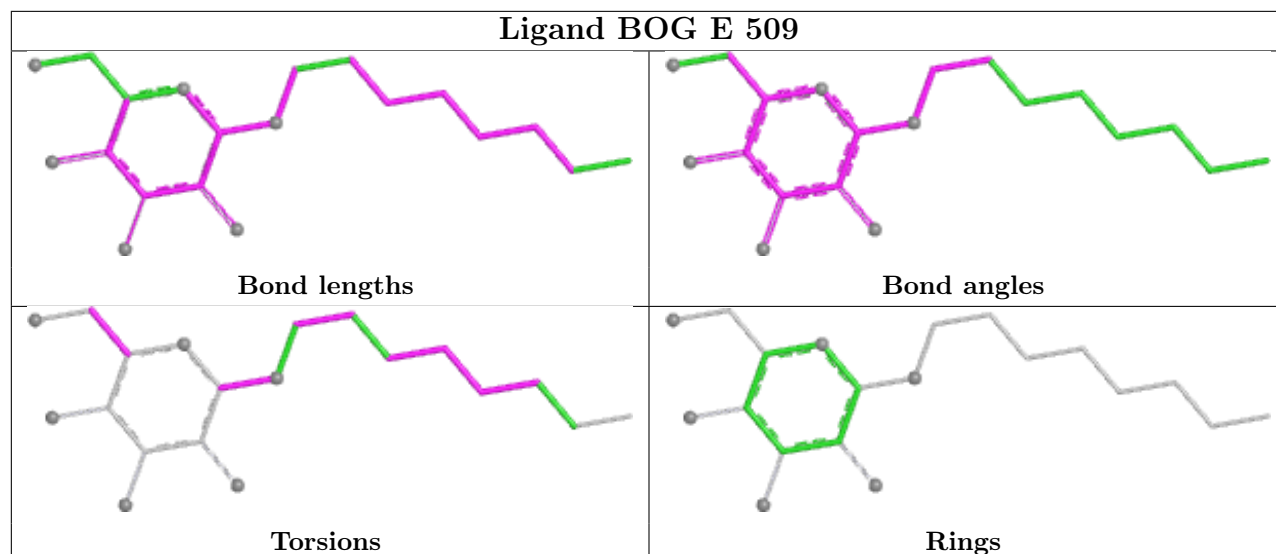
Mol	Chain	Res	Type	Atoms
5	A	301	BCL	C11-C12-C13-C14
4	E	506	BOG	C5'-C6'-C7'-C8'
3	A	404	RG1	C22-C23-C24-C25
3	C	405	RG1	C22-C23-C24-C25
4	A	507	BOG	O5-C5-C6-O6
5	A	307	BCL	C6-C7-C8-C9
5	E	309	BCL	C6-C7-C8-C9
5	F	306	BCL	C11-C12-C13-C15
3	A	404	RG1	C5-C6-C7-C8
5	E	309	BCL	C4B-C3B-CAB-OBB
3	E	406	RG1	C5-C6-C7-C8
3	C	405	RG1	C5-C6-C7-C8
5	C	308	BCL	C6-C7-C8-C9
6	C	510	BEN	N2-C-C1-C2
6	C	510	BEN	N2-C-C1-C6
6	E	511	BEN	N2-C-C1-C2
5	C	308	BCL	C2B-C3B-CAB-OBB
3	A	404	RG1	CM1-C1-O1'-C1'
3	C	405	RG1	CM1-C1-O1'-C1'
5	A	307	BCL	C4B-C3B-CAB-OBB
5	A	307	BCL	C4B-C3B-CAB-CBB
5	C	308	BCL	C4B-C3B-CAB-CBB
3	E	406	RG1	C27-C28-C29-C30
4	C	508	BOG	C5'-C6'-C7'-C8'
5	C	303	BCL	C12-C13-C15-C16
5	E	305	BCL	C12-C13-C15-C16
5	A	301	BCL	C14-C13-C15-C16
5	C	303	BCL	C14-C13-C15-C16
5	E	305	BCL	C14-C13-C15-C16
3	E	406	RG1	C9-C10-C11-C12
5	A	301	BCL	C12-C13-C15-C16
5	A	307	BCL	C11-C12-C13-C15
5	C	308	BCL	C11-C12-C13-C15
5	E	309	BCL	C11-C12-C13-C15
4	C	504	BOG	C5'-C6'-C7'-C8'
6	C	510	BEN	N1-C-C1-C2
6	C	510	BEN	N1-C-C1-C6
6	E	511	BEN	N2-C-C1-C6
4	E	505	BOG	C5'-C6'-C7'-C8'
5	D	304	BCL	C1-C2-C3-C4

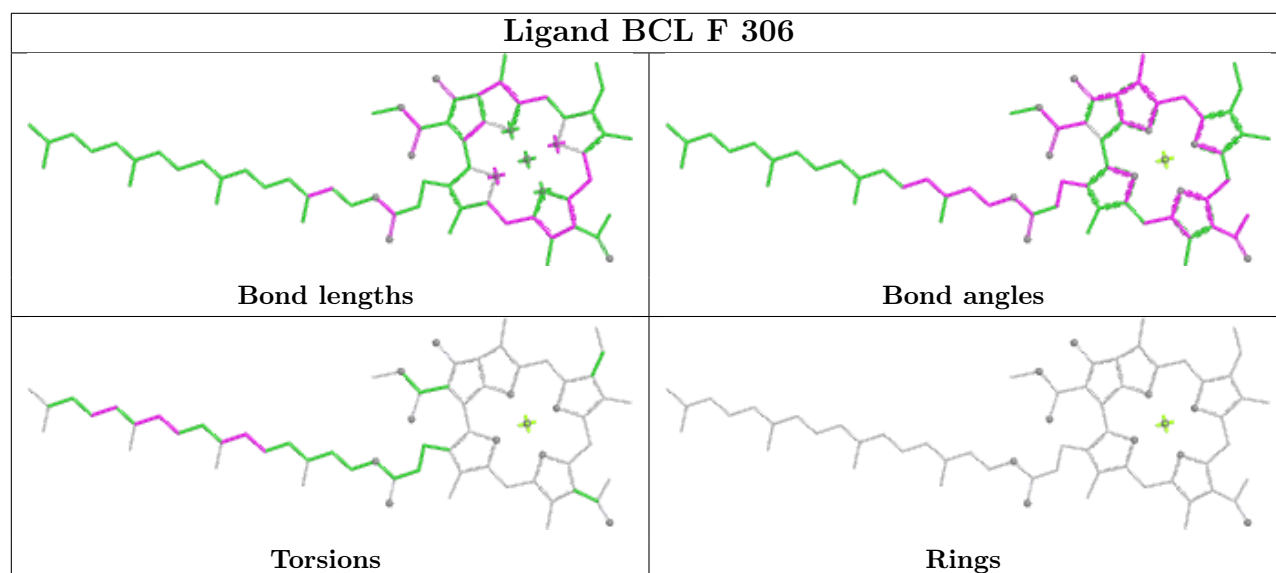
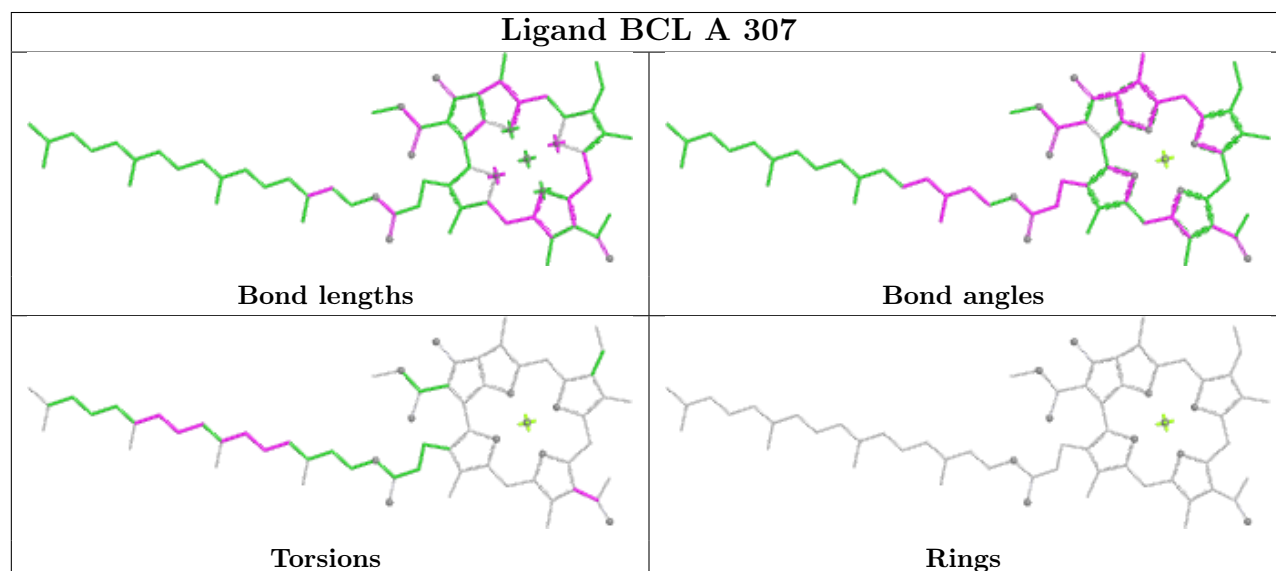
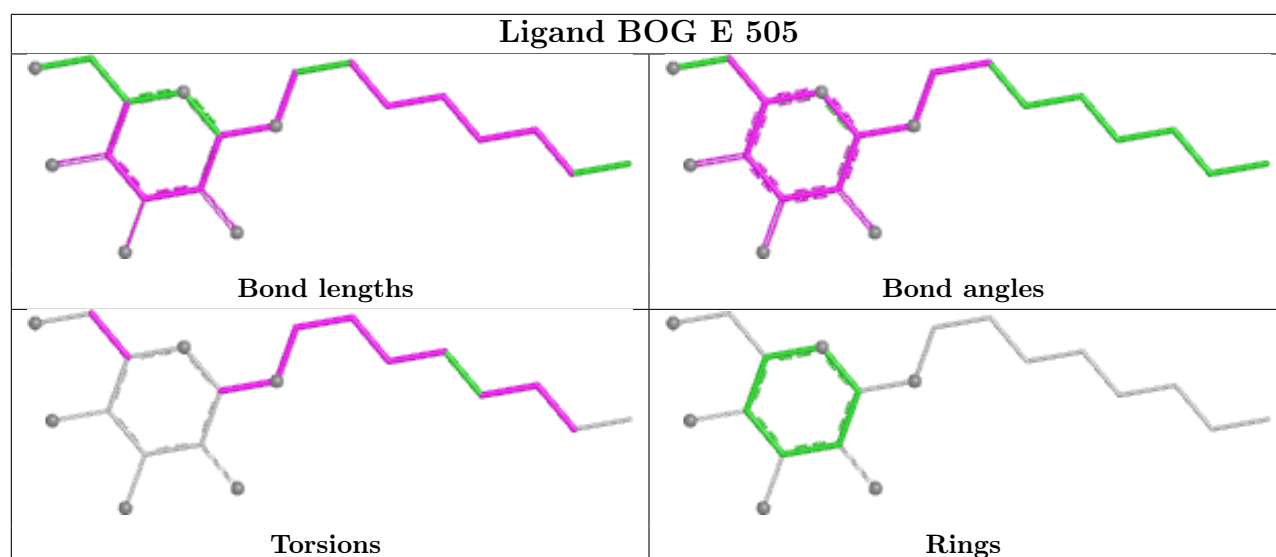
There are no ring outliers.

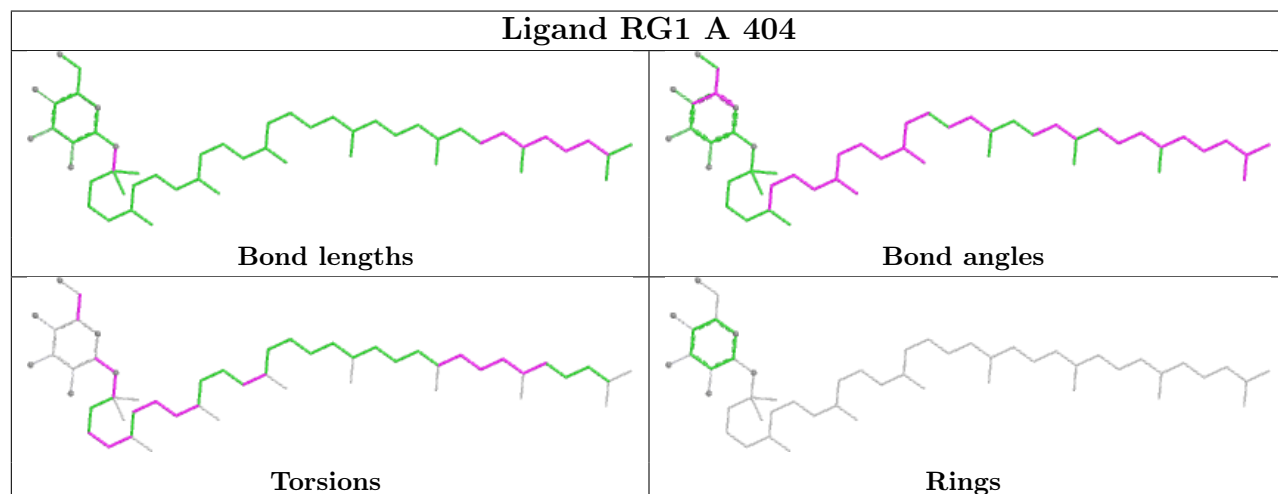
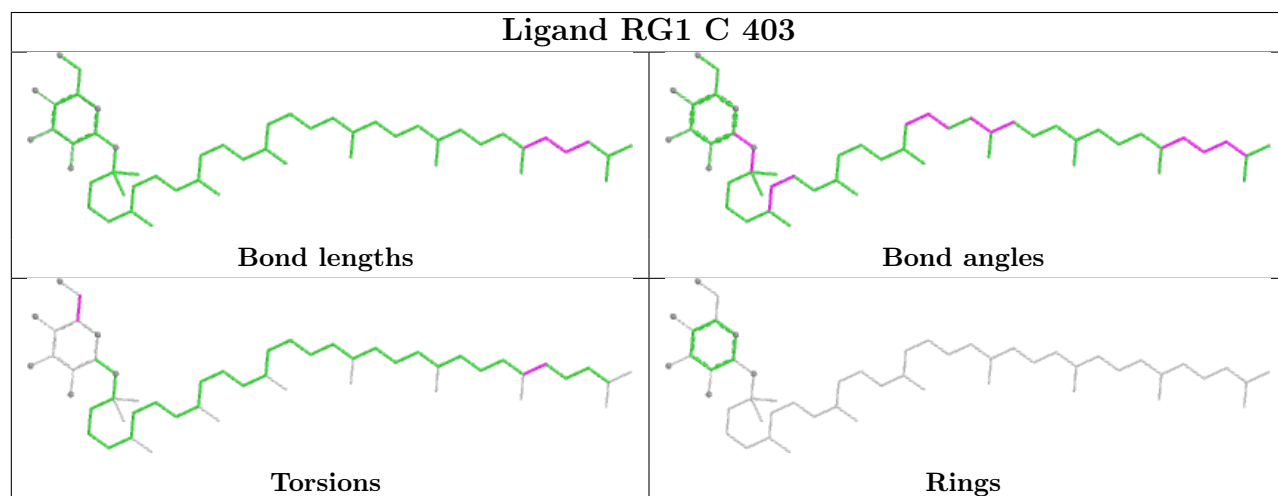
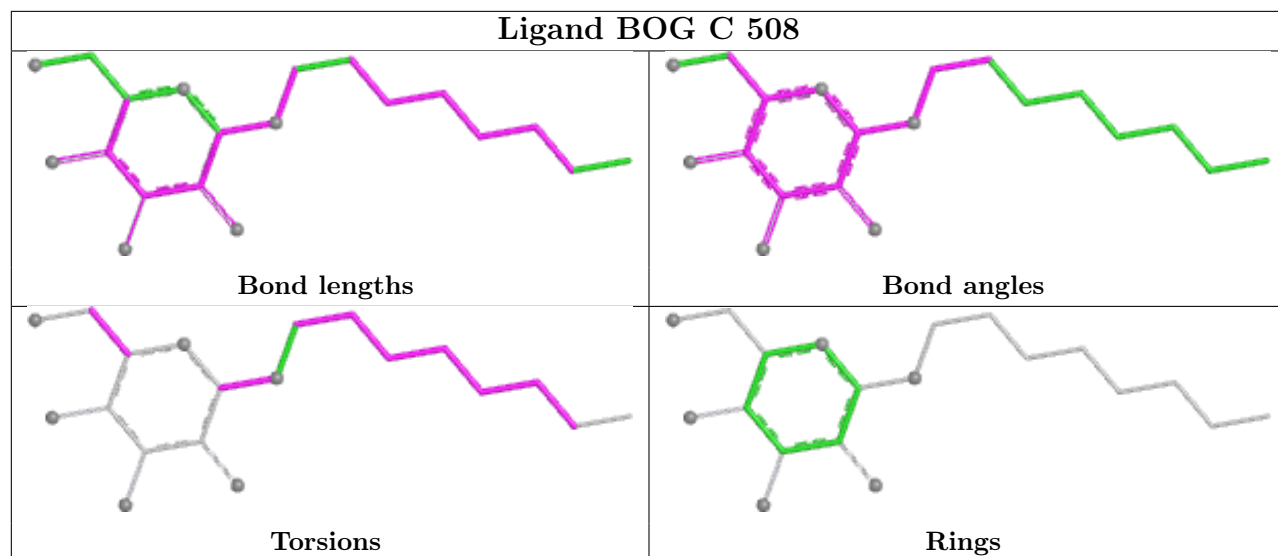
22 monomers are involved in 79 short contacts:

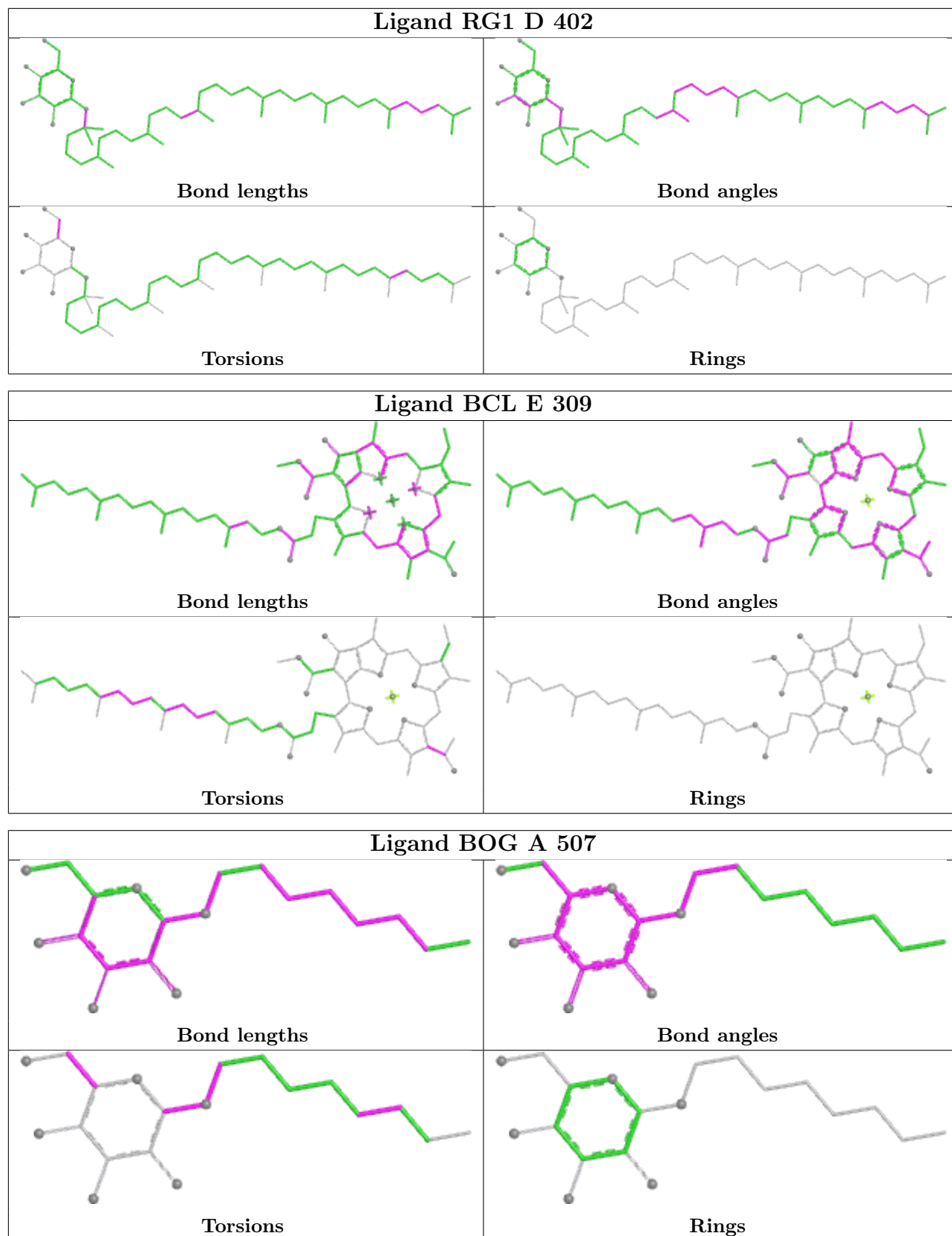
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	509	BOG	1	0
5	C	308	BCL	5	0
4	C	504	BOG	4	0
4	E	505	BOG	2	0
5	A	307	BCL	3	0
5	F	306	BCL	2	0
4	C	508	BOG	2	0
3	A	404	RG1	13	0
5	E	309	BCL	3	0
4	A	507	BOG	6	0
6	E	511	BEN	1	0
4	E	506	BOG	3	0
5	A	301	BCL	6	0
3	B	401	RG1	3	0
5	C	303	BCL	6	0
6	C	510	BEN	1	0
3	E	406	RG1	13	0
6	E	512	BEN	2	0
3	C	405	RG1	10	0
5	D	304	BCL	4	0
5	B	302	BCL	2	0
5	E	305	BCL	5	0

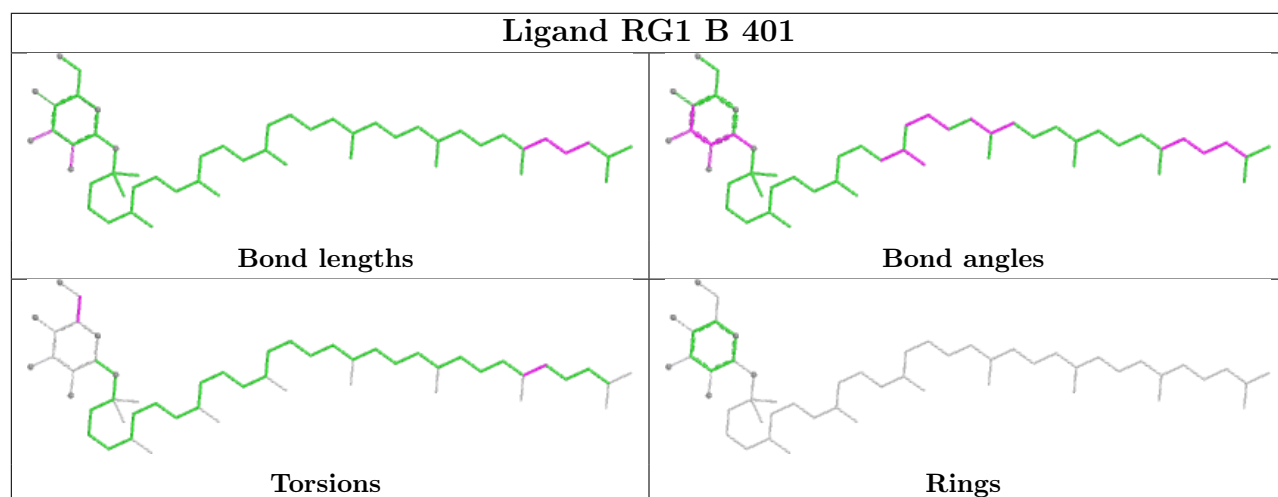
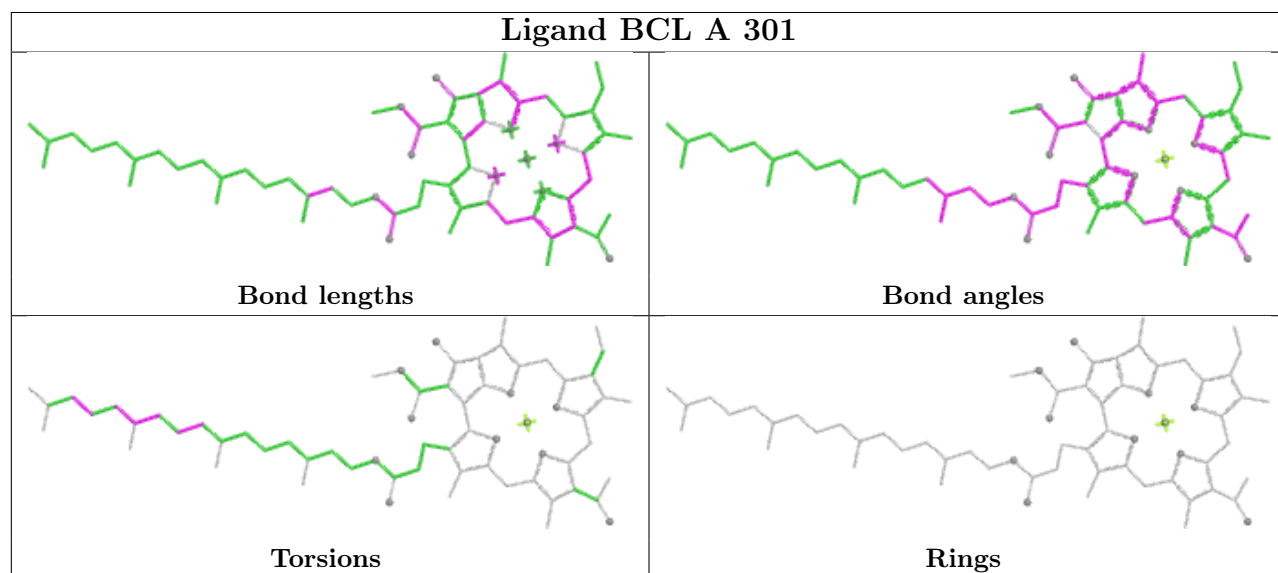
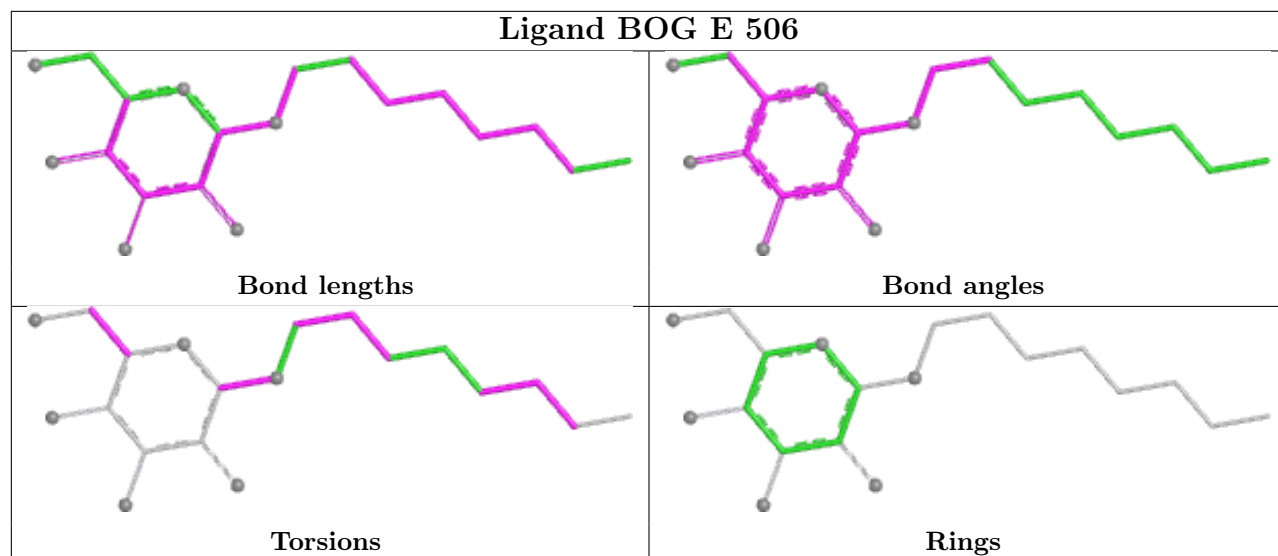
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

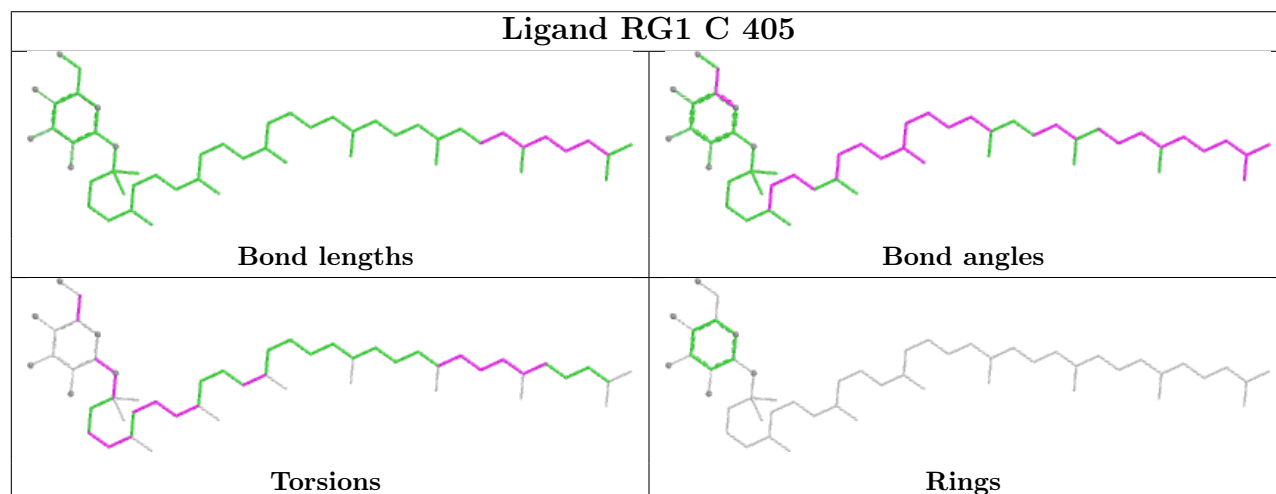
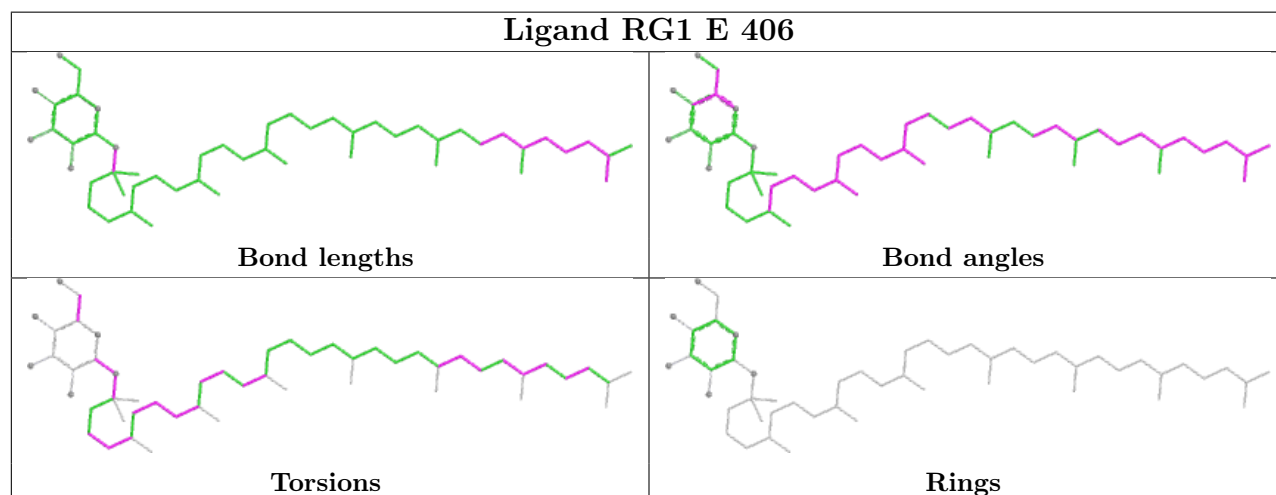
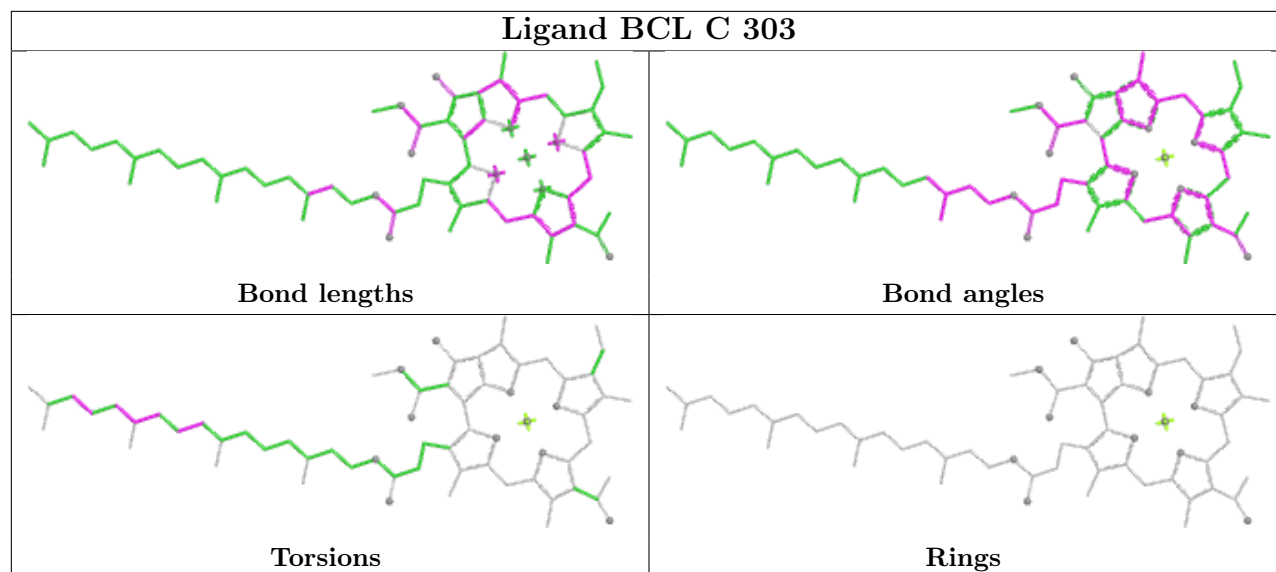


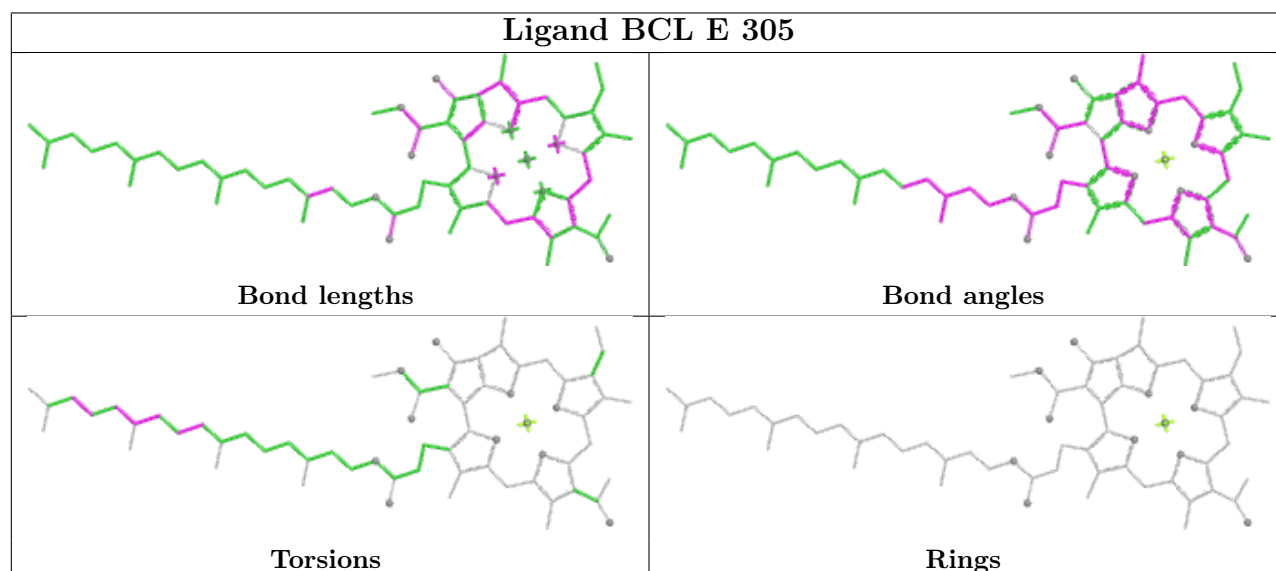
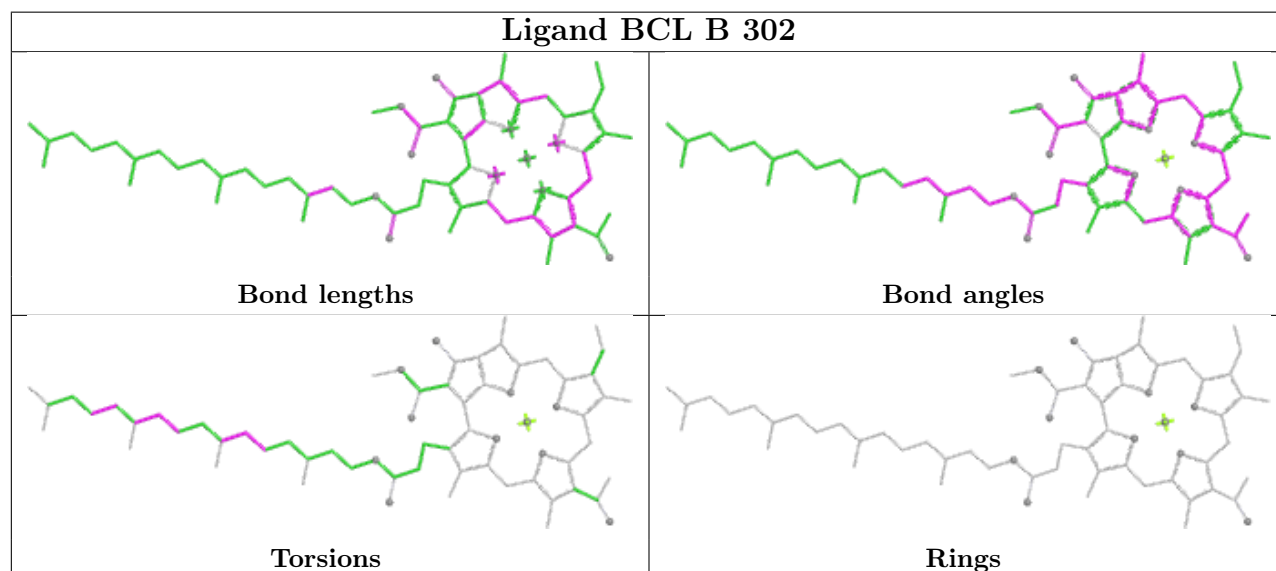
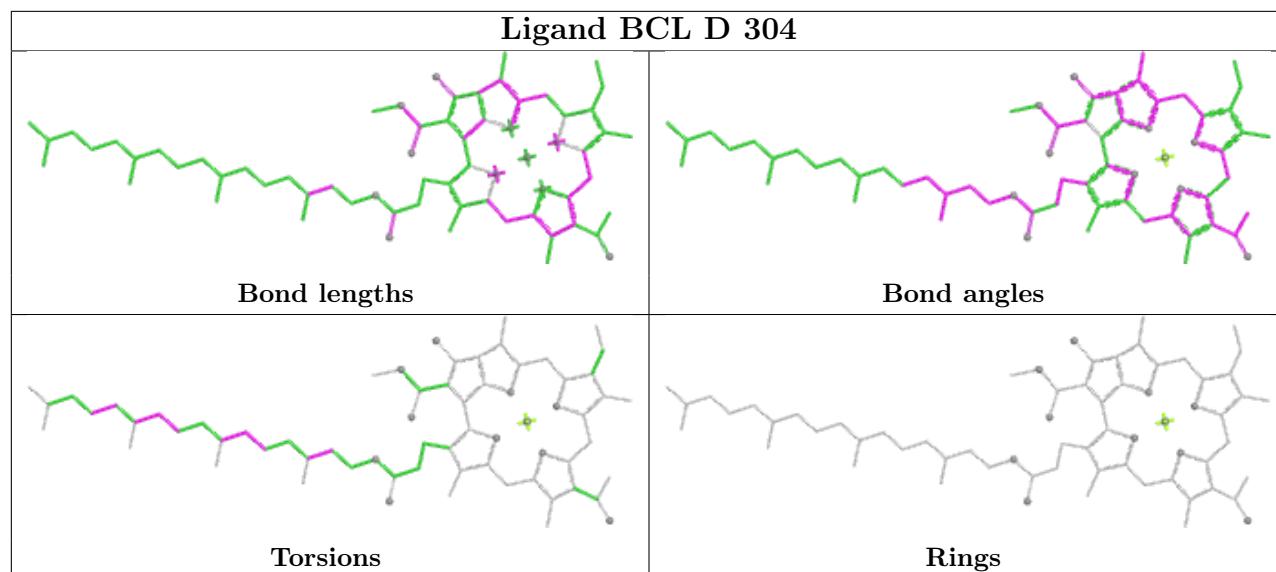












5.7 Other polymers [i](#)

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%)	0.20	5 (9%) 13 12	14, 18, 50, 51	0
1	C	52/53 (98%)	0.33	6 (11%) 9 8	14, 18, 50, 51	0
1	E	52/53 (98%)	0.29	7 (13%) 7 6	14, 18, 50, 51	0
2	B	41/41 (100%)	0.30	1 (2%) 59 59	16, 18, 22, 35	0
2	D	41/41 (100%)	0.29	1 (2%) 59 59	16, 18, 23, 35	0
2	F	41/41 (100%)	0.14	1 (2%) 59 59	16, 18, 23, 35	0
All	All	279/282 (98%)	0.26	21 (7%) 20 19	14, 18, 44, 51	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	VAL	7.2
1	A	49	VAL	7.2
1	E	50	LYS	6.8
1	A	50	LYS	6.7
1	E	49	VAL	6.4
1	C	50	LYS	6.3
1	C	51	LYS	4.3
1	E	51	LYS	4.3
2	B	41	HIS	4.1
1	A	51	LYS	3.7
2	D	41	HIS	3.6
1	E	53	ALA	3.3
1	C	48	GLY	3.2
2	F	41	HIS	3.1
1	E	52	ALA	3.0
1	C	52	ALA	2.8
1	E	48	GLY	2.7
1	A	53	ALA	2.5
1	C	53	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	48	GLY	2.2
1	E	38	THR	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CXM	E	1	11/12	0.91	0.11	13,16,20,20	0
1	CXM	C	1	11/12	0.92	0.09	14,17,20,20	0
1	CXM	A	1	11/12	0.93	0.07	15,17,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

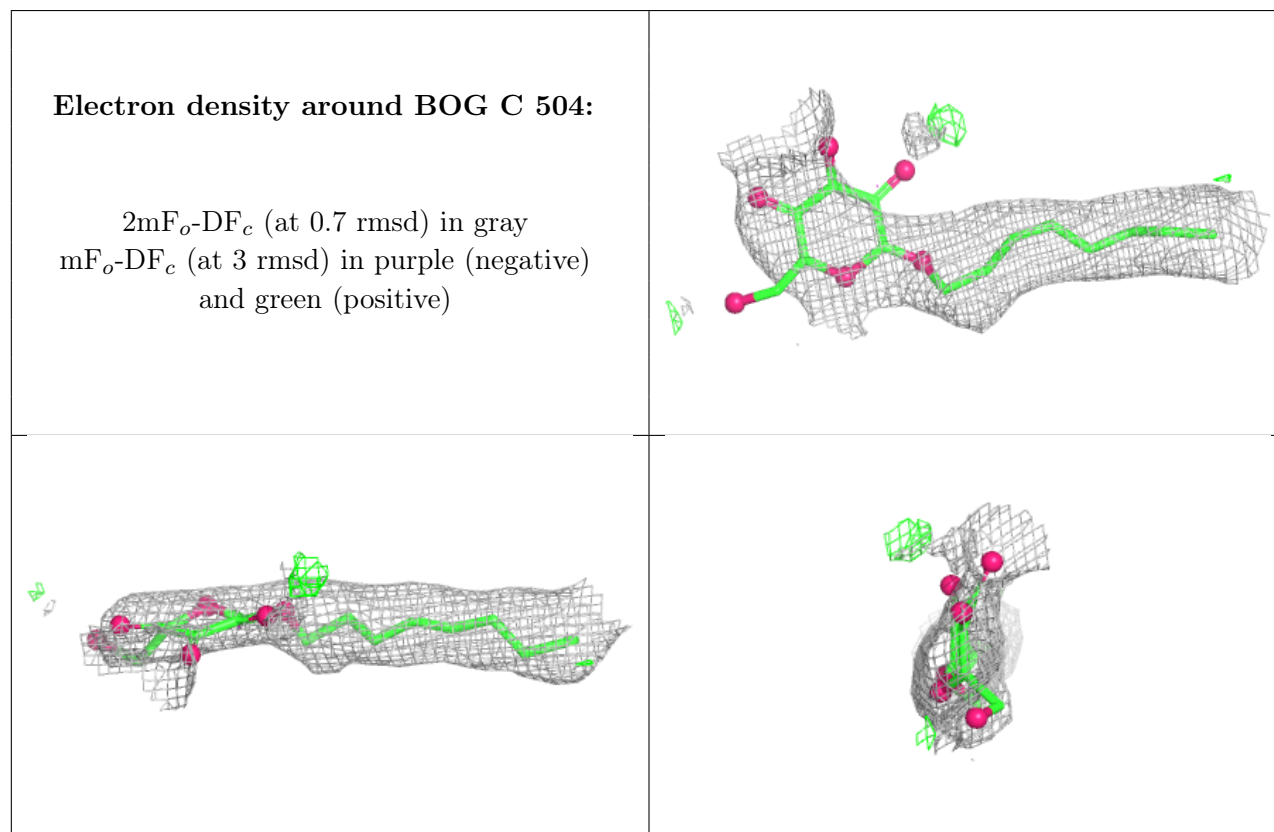
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BOG	C	504	20/20	0.63	0.16	86,101,103,104	0
4	BOG	E	505	20/20	0.64	0.19	99,111,116,116	0
4	BOG	E	509	20/20	0.64	0.17	81,100,105,106	0
4	BOG	A	507	20/20	0.66	0.16	88,104,108,108	0
4	BOG	C	508	20/20	0.69	0.16	79,96,102,104	0
4	BOG	E	506	20/20	0.71	0.15	89,102,105,105	0
3	RG1	C	405	52/52	0.71	0.22	39,57,63,63	52
3	RG1	A	404	52/52	0.74	0.20	40,57,63,63	52
3	RG1	E	406	52/52	0.75	0.22	40,57,63,64	52
6	BEN	E	512	9/9	0.85	0.10	76,79,80,80	0
5	BCL	A	307	66/66	0.86	0.10	11,17,38,43	0
3	RG1	C	403	52/52	0.86	0.09	13,16,29,31	0
3	RG1	D	402	52/52	0.87	0.09	13,16,28,31	0

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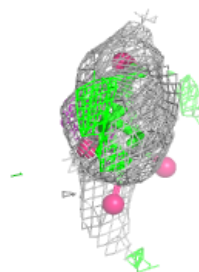
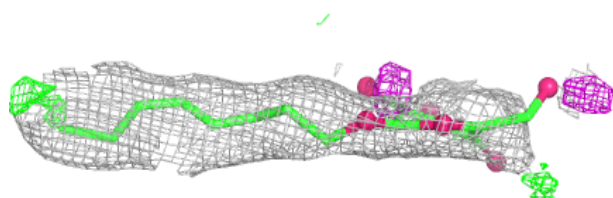
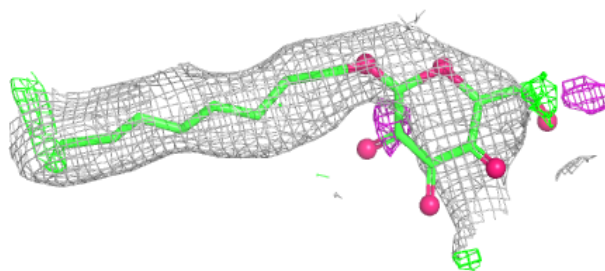
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BCL	B	302	66/66	0.89	0.08	12,16,29,36	0
5	BCL	E	309	66/66	0.89	0.08	11,16,37,43	0
6	BEN	C	510	9/9	0.89	0.10	73,76,78,79	0
3	RG1	B	401	52/52	0.89	0.09	13,16,29,31	0
5	BCL	C	308	66/66	0.91	0.08	11,16,38,43	0
5	BCL	D	304	66/66	0.92	0.07	13,16,29,36	0
6	BEN	E	511	9/9	0.92	0.07	77,80,83,83	0
5	BCL	F	306	66/66	0.92	0.07	13,16,29,36	0
5	BCL	C	303	66/66	0.94	0.05	13,16,22,23	0
5	BCL	A	301	66/66	0.94	0.05	13,16,22,24	0
5	BCL	E	305	66/66	0.95	0.05	13,17,21,24	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.

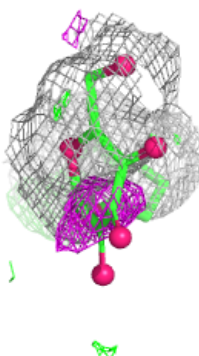
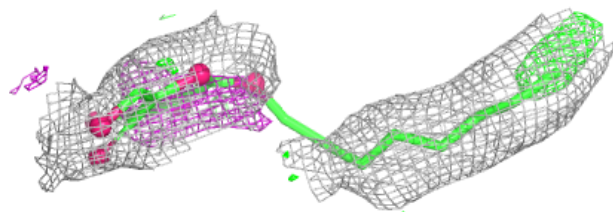
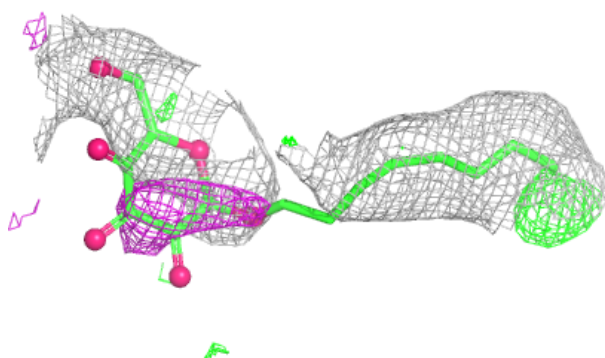


Electron density around BOG E 505:

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

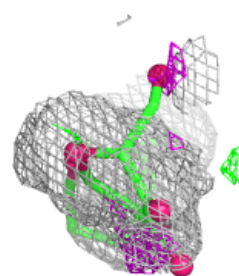
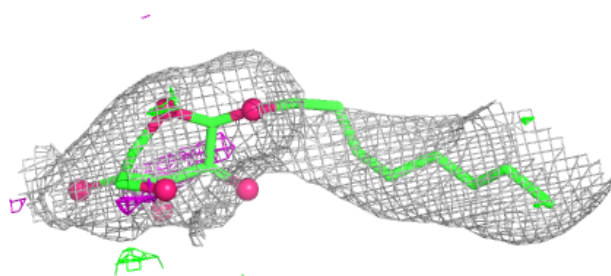
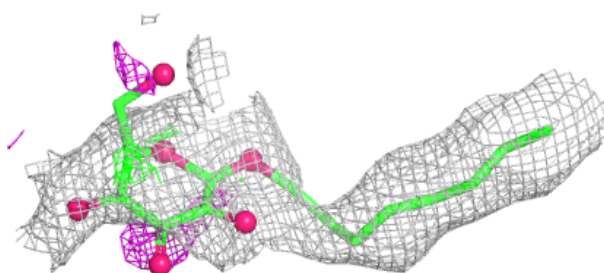
**Electron density around BOG E 509:**

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

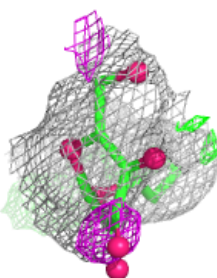
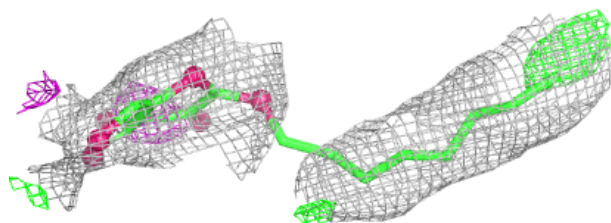
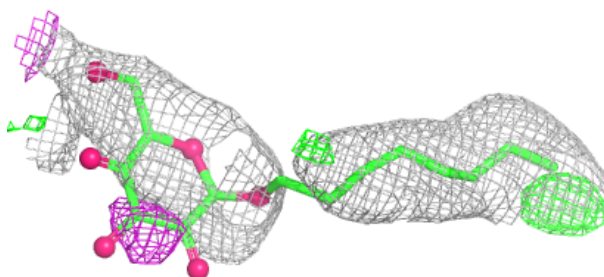


Electron density around BOG A 507:

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

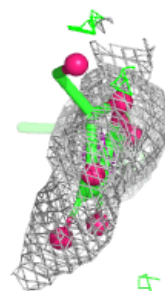
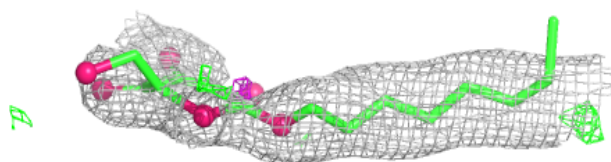
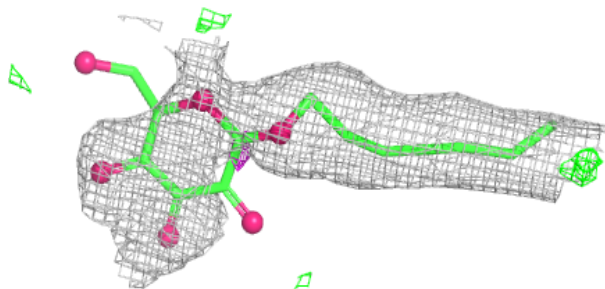
**Electron density around BOG C 508:**

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

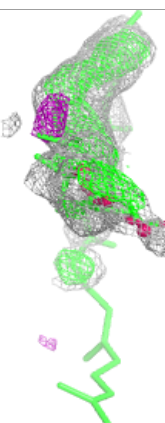
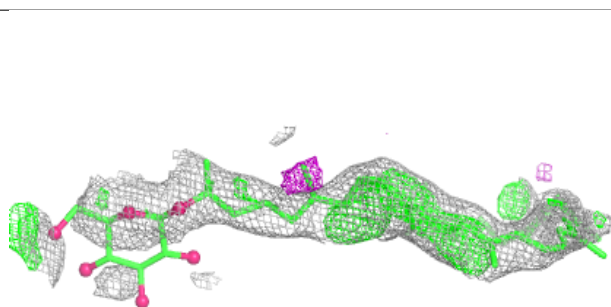
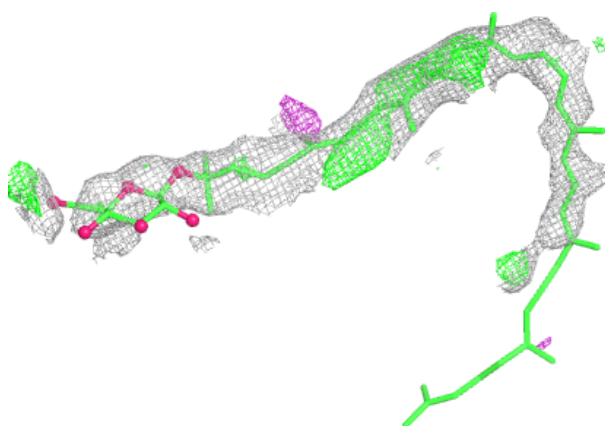


Electron density around BOG E 506:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

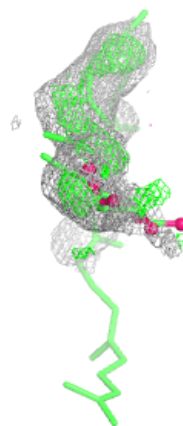
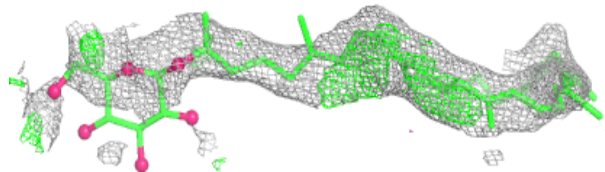
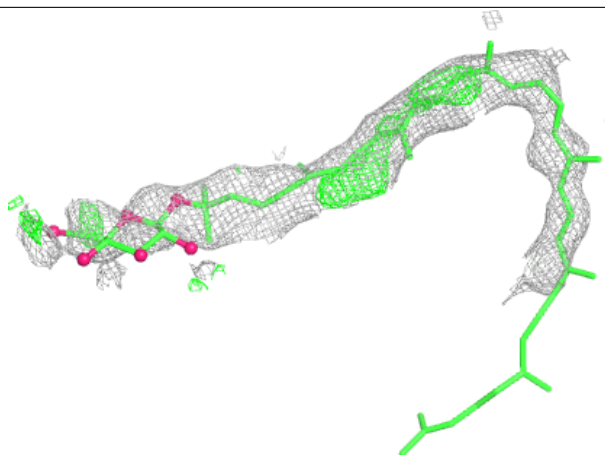
**Electron density around RG1 C 405:**

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



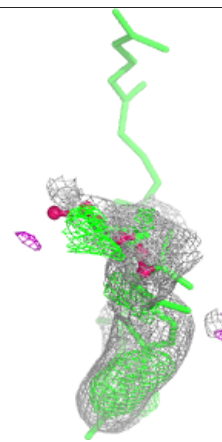
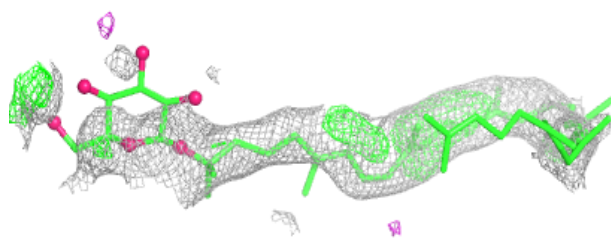
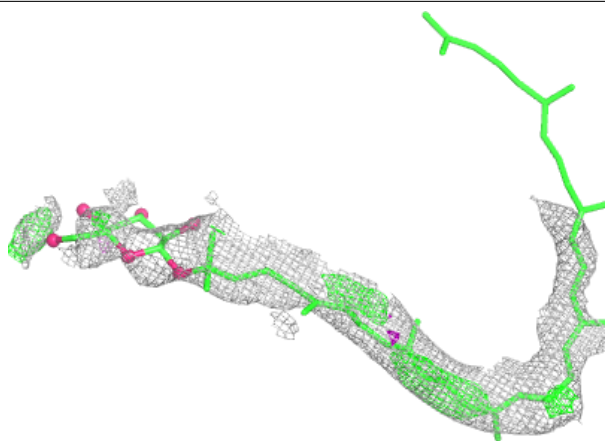
Electron density around RG1 A 404:

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



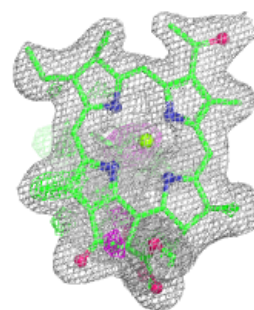
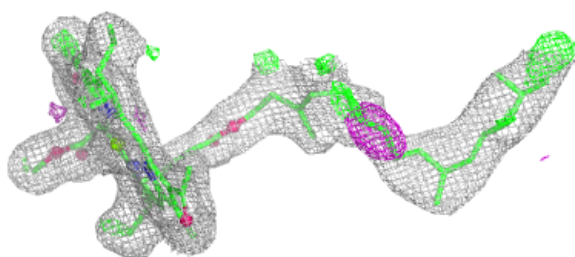
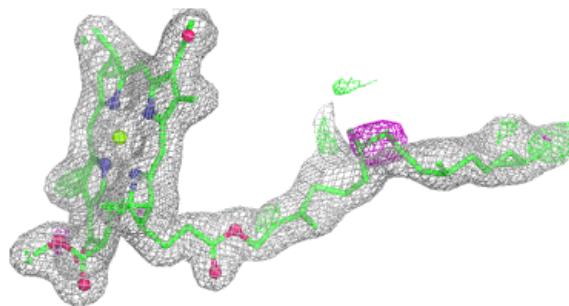
Electron density around RG1 E 406:

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

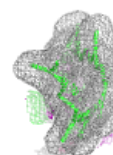
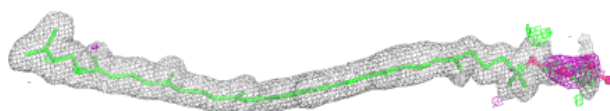
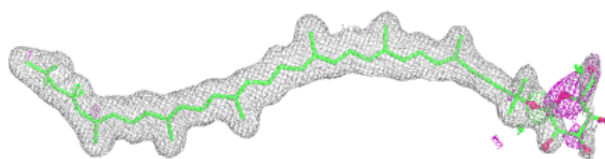


Electron density around BCL A 307:

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

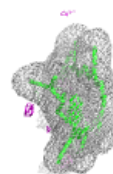
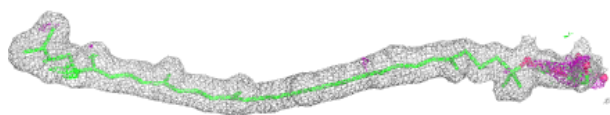
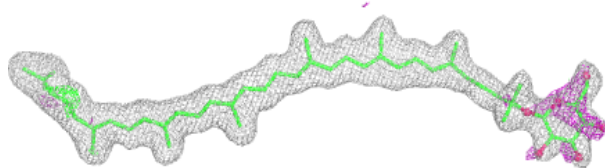
**Electron density around RG1 C 403:**

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

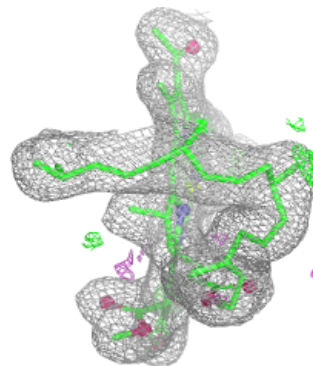
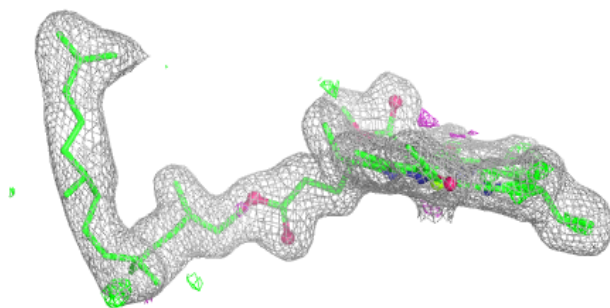
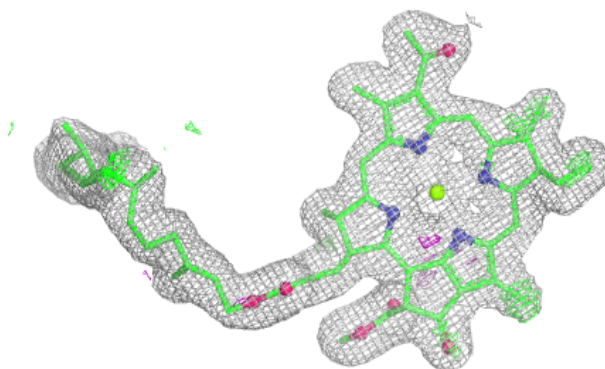


Electron density around RG1 D 402:

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

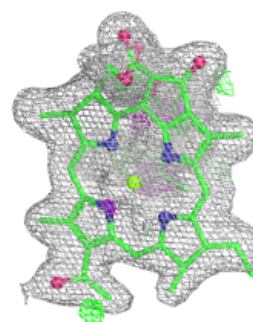
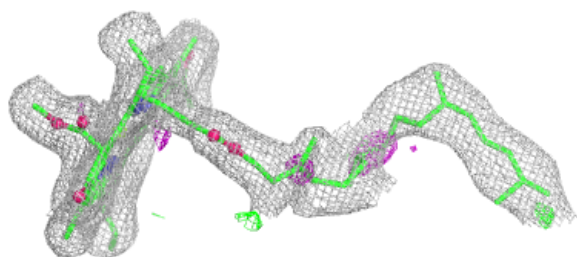
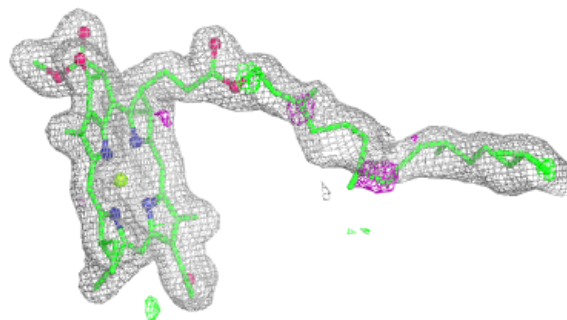
**Electron density around BCL B 302:**

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

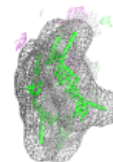
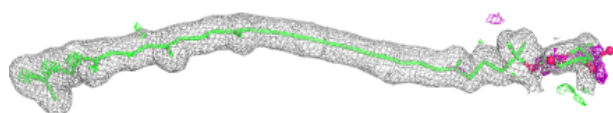
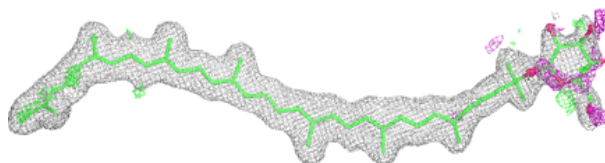


Electron density around BCL E 309:

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

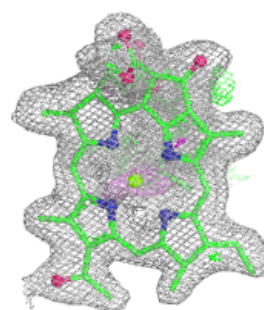
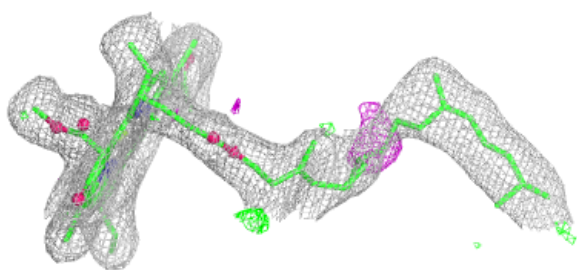
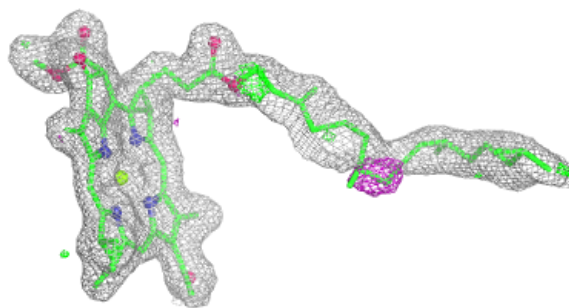
**Electron density around RG1 B 401:**

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

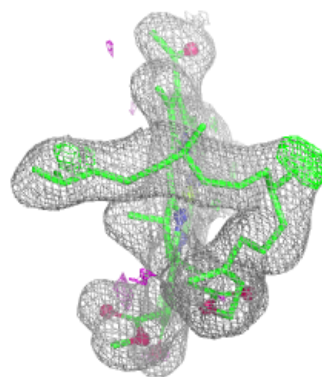
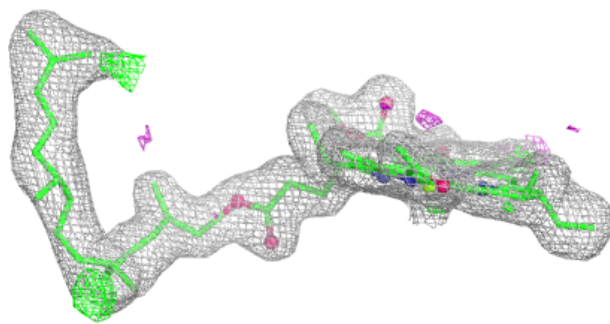
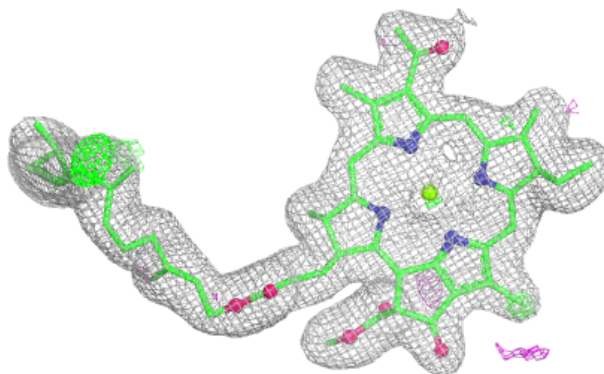


Electron density around BCL C 308:

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

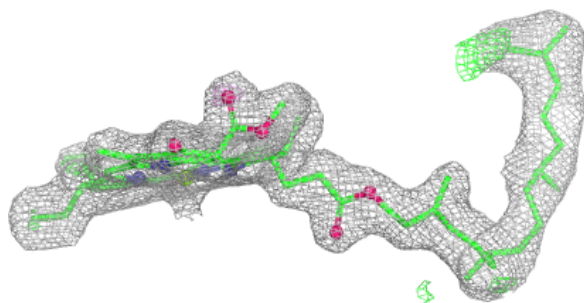
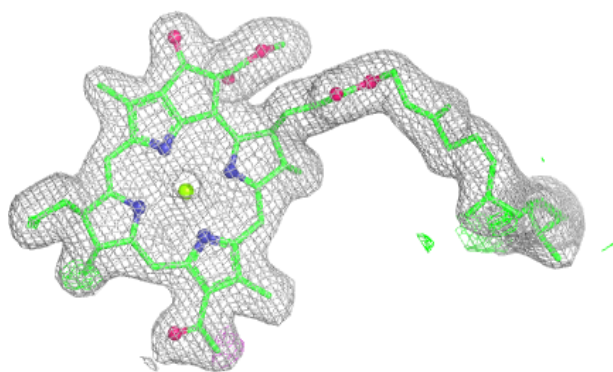
**Electron density around BCL D 304:**

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

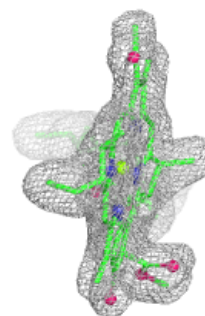
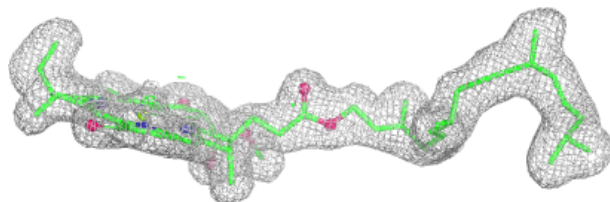
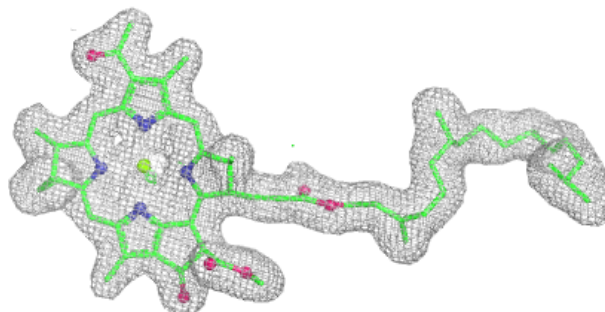


Electron density around BCL F 306:

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

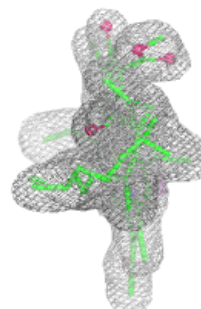
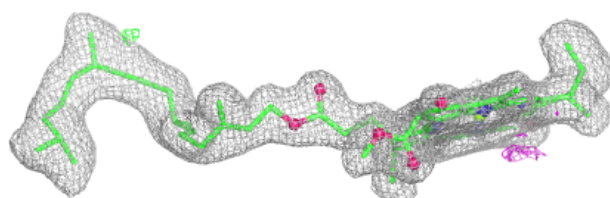
**Electron density around BCL C 303:**

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

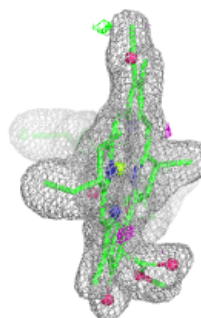
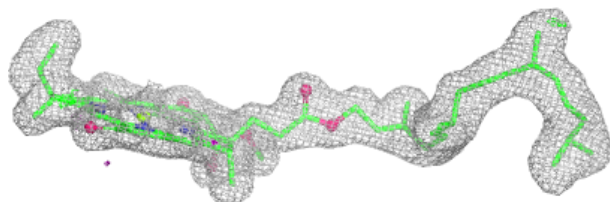
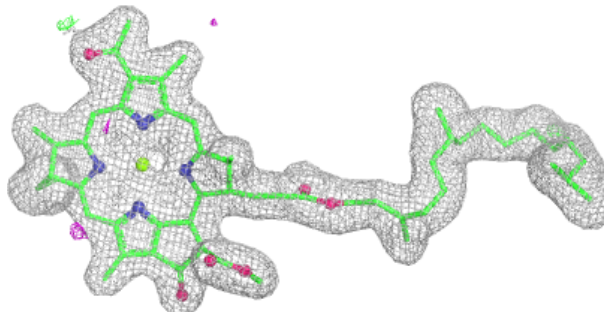


Electron density around BCL A 301:

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

**Electron density around BCL E 305:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.