



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:29 PM EDT

PDB ID : 2FKW / pdb_00002fkw
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 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

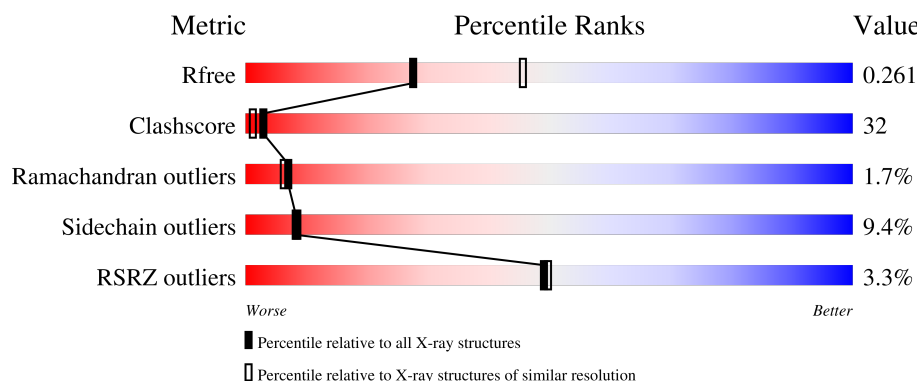
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	4% 53% 36% 11%
1	C	53	6% 58% 28% 11% .
1	E	53	6% 62% 25% 9% .
1	G	53	8% 64% 26% 9%
1	I	53	6% 60% 32% . .

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Mol	Chain	Length	Quality of chain
1	K	53	
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	-	-	-
3	BCL	H	1604	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	-	-	-
3	BCL	N	1607	X	-	-	-
3	BCL	O	1508	X	-	-	-
3	BCL	O	1708	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BCL	P	1608	X	-	-	-
3	BCL	R	1509	X	-	-	-
3	BCL	R	1709	X	-	X	-
3	BCL	S	1609	X	-	-	-
4	LDA	G	1824	-	-	X	-
4	LDA	R	1818	-	-	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			

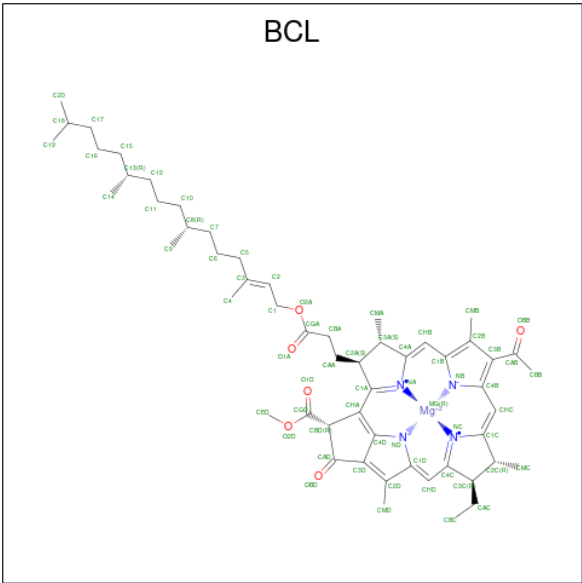
There are 9 discrepancies between the modelled and reference sequences:

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 (CCD ID: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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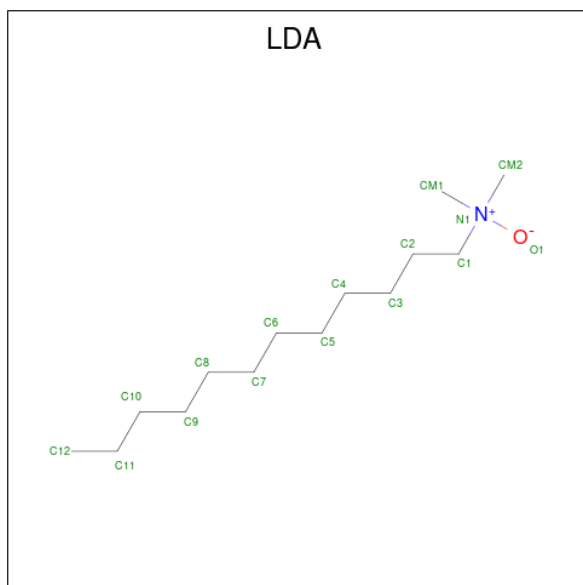
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
3	G	1	Total 66	C 55	Mg 1	N 4	O 6	0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

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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 (CCD ID: LDA) (formula: C₁₄H₃₁NO).



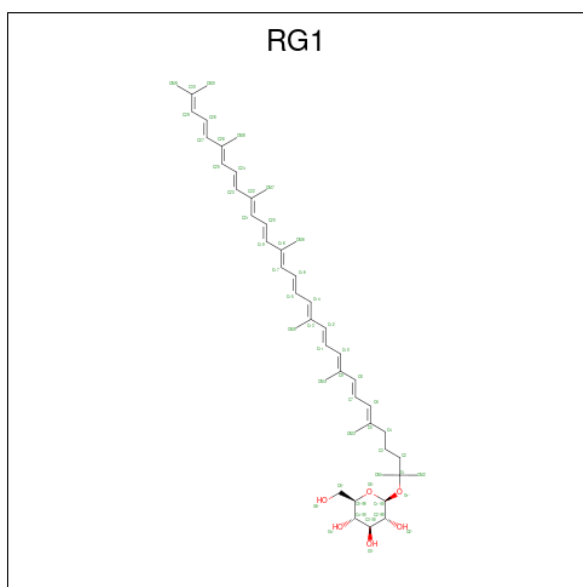
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	A	1	Total	C	N	O	0	0
			16	14	1	1		
4	B	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	C	1	Total	C	N	O	0	0
			16	14	1	1		
4	D	1	Total	C	N	O	0	0
			16	14	1	1		
4	E	1	Total	C	N	O	0	0
			16	14	1	1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

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

- Molecule 5 is Rhodopin b-D-glucoside (CCD ID: 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		

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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

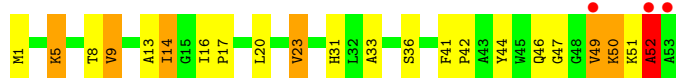
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

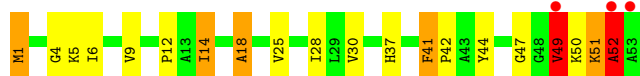
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



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



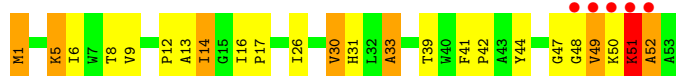
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- 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



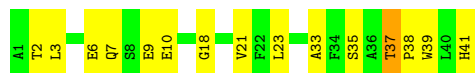
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



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



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

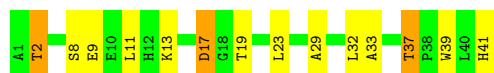


- Molecule 2: Light-harvesting protein B-800/850, beta chain



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

Chain H:  66% 27% 7%



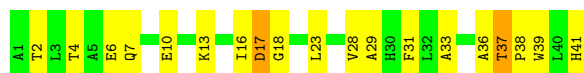
- Molecule 2: Light-harvesting protein B-800/850, beta chain

Chain J:  68% 27% 5%



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

Chain L:  54% 41% 5%



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

Chain N:  49% 46% 5%



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

Chain P:  54% 24% 22%



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

Chain S:  71% 27% 2%



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 10.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.45) 98.1 (10.00-2.45)	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 , 0.261	Depositor DCC
R_{free} test set	2531 reflections (5.06%)	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)	0.44 , 89.3	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	0.95	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: LDA, CXM, RG1, BCL

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	1.75	6/404 (1.5%)	0.71	0/556
1	C	1.94	7/404 (1.7%)	0.75	1/556 (0.2%)
1	E	1.89	9/404 (2.2%)	0.81	0/556
1	G	1.83	8/404 (2.0%)	0.86	1/556 (0.2%)
1	I	1.78	4/404 (1.0%)	0.77	0/556
1	K	1.99	14/404 (3.5%)	0.78	0/556
1	M	1.73	5/404 (1.2%)	0.82	1/556 (0.2%)
1	O	1.78	5/404 (1.2%)	0.76	0/556
1	R	1.79	5/404 (1.2%)	0.77	0/556
2	B	1.71	3/332 (0.9%)	0.71	0/453
2	D	1.53	0/332	0.65	0/453
2	F	1.75	5/332 (1.5%)	0.69	0/453
2	H	1.69	2/332 (0.6%)	0.71	0/453
2	J	1.57	3/332 (0.9%)	0.70	0/453
2	L	1.89	7/332 (2.1%)	0.67	0/453
2	N	1.56	3/332 (0.9%)	0.70	0/453
2	P	1.75	7/332 (2.1%)	0.69	0/453
2	S	1.56	1/332 (0.3%)	0.69	0/453
All	All	1.76	94/6624 (1.4%)	0.74	3/9081 (0.0%)

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

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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 (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	VAL	CA-CB	11.67	1.70	1.54
1	G	36	SER	C-O	-9.64	1.11	1.24
1	E	49	VAL	N-CA	8.41	1.56	1.46
1	C	52	ALA	CA-C	8.24	1.63	1.52
1	R	49	VAL	CA-CB	8.15	1.65	1.54
2	L	28	VAL	CA-CB	-7.91	1.45	1.54
1	A	14	ILE	C-O	7.76	1.31	1.23
1	C	52	ALA	CA-CB	-7.75	1.40	1.53
2	L	17	ASP	CG-OD1	7.74	1.40	1.25
1	G	49	VAL	CA-CB	7.70	1.64	1.53
1	R	49	VAL	N-CA	7.69	1.55	1.46
1	M	33	ALA	N-CA	-7.50	1.37	1.46
1	C	49	VAL	CA-CB	7.35	1.64	1.54
1	K	49	VAL	CA-CB	7.23	1.64	1.54
2	P	21	VAL	CA-CB	-7.11	1.45	1.54
2	P	6	GLU	CG-CD	6.98	1.69	1.52
1	E	6	ILE	CA-CB	6.93	1.63	1.54
1	G	49	VAL	CA-C	6.93	1.58	1.52
1	K	30	VAL	N-CA	-6.88	1.38	1.46
1	C	49	VAL	N-CA	6.88	1.54	1.46
2	F	26	ALA	CA-CB	-6.82	1.42	1.53
1	K	15	GLY	C-O	-6.76	1.15	1.23
2	L	10	GLU	CG-CD	6.73	1.68	1.52
1	G	30	VAL	CA-C	6.71	1.61	1.52
1	O	49	VAL	CA-C	6.71	1.61	1.52
1	E	49	VAL	CA-CB	6.64	1.63	1.54
1	O	49	VAL	N-CA	6.64	1.54	1.46
1	E	28	ILE	CA-CB	-6.57	1.46	1.54
1	R	24	THR	CA-CB	-6.54	1.43	1.53
1	K	11	ASN	CA-C	-6.54	1.45	1.52
2	L	29	ALA	CA-CB	6.42	1.63	1.53
2	J	2	THR	N-CA	-6.33	1.38	1.46
2	B	21	VAL	C-O	6.22	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	17	ASP	CB-CG	6.17	1.67	1.52
1	K	49	VAL	CA-C	6.16	1.60	1.52
2	N	22	PHE	C-O	-6.16	1.17	1.24
1	K	27	ALA	C-O	6.09	1.31	1.24
1	E	30	VAL	C-O	-6.04	1.17	1.24
1	A	49	VAL	N-CA	6.01	1.53	1.46
1	G	13	ALA	C-N	5.98	1.39	1.33
2	L	16	ILE	N-CA	-5.95	1.39	1.46
1	E	52	ALA	CA-C	5.92	1.60	1.52
1	K	45	TRP	C-O	-5.90	1.17	1.24
1	G	48	GLY	CA-C	5.89	1.59	1.51
1	K	10	VAL	CA-C	-5.85	1.45	1.52
1	M	26	ILE	C-O	5.84	1.30	1.24
1	K	27	ALA	CA-C	5.81	1.60	1.52
1	C	33	ALA	N-CA	-5.80	1.39	1.46
2	H	8	SER	C-O	-5.78	1.17	1.24
1	O	18	ALA	CA-CB	-5.75	1.44	1.53
1	G	6	ILE	CA-CB	5.74	1.62	1.54
1	A	33	ALA	CA-CB	-5.71	1.44	1.53
2	F	4	THR	CA-CB	5.70	1.62	1.53
2	F	15	VAL	C-O	-5.69	1.17	1.24
2	N	15	VAL	CA-CB	5.66	1.61	1.54
1	I	15	GLY	C-O	-5.57	1.17	1.23
1	R	51	LYS	N-CA	5.56	1.53	1.46
2	P	2	THR	N-CA	-5.56	1.39	1.46
2	N	3	LEU	C-O	-5.54	1.16	1.23
1	E	41	PHE	C-O	-5.54	1.19	1.24
1	K	16	ILE	CA-CB	-5.52	1.47	1.54
2	J	2	THR	CA-C	5.52	1.59	1.52
2	F	10	GLU	CG-CD	5.51	1.65	1.52
2	B	17	ASP	CA-C	-5.50	1.45	1.52
1	G	33	ALA	N-CA	-5.49	1.39	1.46
1	I	5	LYS	CD-CE	5.48	1.68	1.52
2	P	33	ALA	CA-CB	5.47	1.62	1.53
2	P	22	PHE	C-O	5.46	1.30	1.24
2	H	17	ASP	CB-CG	-5.45	1.38	1.52
1	K	6	ILE	CA-CB	5.44	1.61	1.54
2	J	28	VAL	CA-CB	-5.44	1.48	1.54
2	L	31	PHE	N-CA	-5.44	1.40	1.46
2	S	26	ALA	C-O	5.41	1.30	1.24
1	M	30	VAL	CA-CB	-5.40	1.48	1.54
1	O	41	PHE	CA-C	5.39	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	ALA	C-O	5.38	1.30	1.24
1	M	49	VAL	CA-C	5.34	1.59	1.52
1	K	33	ALA	CA-CB	-5.32	1.45	1.53
1	K	49	VAL	N-CA	5.31	1.52	1.46
1	R	48	GLY	CA-C	5.22	1.59	1.51
1	C	23	VAL	C-O	5.20	1.30	1.24
2	P	16	ILE	CA-CB	5.19	1.60	1.54
1	I	36	SER	C-O	-5.18	1.17	1.24
2	B	34	PHE	C-O	5.18	1.30	1.24
2	P	6	GLU	CA-CB	5.18	1.61	1.53
1	E	52	ALA	N-CA	5.18	1.52	1.46
1	O	33	ALA	CA-C	5.16	1.59	1.52
1	K	8	THR	CA-CB	5.10	1.62	1.53
2	F	37	THR	CA-CB	5.08	1.61	1.54
1	C	49	VAL	CA-C	5.07	1.59	1.52
1	I	43	ALA	CA-CB	5.02	1.61	1.53
1	A	28	ILE	CA-CB	-5.01	1.48	1.54
1	E	18	ALA	N-CA	-5.01	1.40	1.46
1	M	8	THR	C-O	-5.00	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	49	VAL	N-CA-C	6.01	112.64	106.21
1	M	14	ILE	CB-CA-C	-5.21	105.66	111.80
1	C	14	ILE	CB-CA-C	-5.20	105.67	111.80

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	403	0	422	25	0
1	C	403	0	422	27	0
1	E	403	0	422	28	0
1	G	403	0	422	19	0
1	I	403	0	422	20	0
1	K	403	0	422	26	0
1	M	403	0	422	32	0
1	O	403	0	422	17	0
1	R	403	0	422	20	0
2	B	323	0	321	25	0
2	D	323	0	321	19	0
2	F	323	0	321	23	0
2	H	323	0	321	18	0
2	J	323	0	321	22	0
2	L	323	0	321	22	0
2	N	323	0	321	28	0
2	P	323	0	321	30	0
2	S	323	0	321	11	0
3	A	132	0	146	22	0
3	B	66	0	74	7	0
3	C	132	0	148	11	0
3	D	66	0	74	5	0
3	E	132	0	147	10	0
3	F	66	0	74	9	0
3	G	132	0	147	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	66	0	73	8	0
3	I	132	0	148	29	0
3	J	66	0	73	15	0
3	K	132	0	146	14	0
3	L	66	0	74	21	0
3	M	132	0	147	22	0
3	N	66	0	74	14	0
3	O	132	0	147	20	0
3	P	66	0	73	11	0
3	R	132	0	147	27	0
3	S	66	0	74	10	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
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	10	0
6	B	26	0	0	6	0
6	C	24	0	0	3	0
6	D	27	0	0	7	0
6	E	40	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	28	0	0	8	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	23	0
6	S	34	0	0	4	0
All	All	9829	0	10104	622	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 32.

All (622) 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:SD	1:M:1:CXM:CE	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:H8	3:I:1705:BCL:H41	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
4:I:1812:LDA:HM23	6:I:1829:HOH:O	1.59	1.01
3:O:1708:BCL:C2	6:O:1833:HOH:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1501:BCL:H191	3:R:1709:BCL:HED1	1.41	0.97
3:A:1501:BCL:CAA	3:A:1501:BCL:O1D	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
3:A:1501:BCL:O1D	3:A:1501:BCL:HAA2	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
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: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:H92	3:R:1709:BCL:H41	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
1:K:31:HIS:CE1	3:L:1606:BCL:HMD3	2.13	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
2:P:37:THR:HG22	2:P:39:TRP:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:H41	3:M:1707:BCL:H8	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
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:H41	3:R:1709:BCL:C9	2.16	0.76
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
1:A:31:HIS:CE1	3:B:1601:BCL:HMD3	2.22	0.73
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:H8	3:I:1705:BCL:C4	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
4:G:1824:LDA:H31	6:G:1844:HOH:O	1.86	0.72
4:R:1818:LDA:C9	6:R:1852:HOH:O	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:1608:BCL:HBB2	3:P:1608:BCL:HMB3	1.70	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
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:R:1509:BCL:O1D	3:R:1509:BCL:H2A	1.92	0.69
3:M:1707:BCL:H41	3:M:1707:BCL:C7	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:17:ASP:CG	6:N:1829:HOH:O	2.35	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
1:A:35:LEU:HD21	1:R:37:HIS:CD2	2.30	0.67
3:R:1709:BCL:C10	6:S:419:HOH:O	2.41	0.66
1:I:41:PHE:HB3	1:I:42:PRO:HD3	1.78	0.66
4:I:1825:LDA:HM11	6:I:1859:HOH:O	1.95	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
5:F:1403:RG1:O1'	6:F:1827:HOH:O	2.13	0.65
3:N:1607:BCL:HBB2	3:N:1607:BCL:HMB3	1.78	0.65
1:I:51:LYS:HB2	1:I:52:ALA:HA	1.77	0.65
3:F:1603:BCL:C10	3:F:1603:BCL:H142	2.26	0.65
4:E:1823:LDA:H11	6:E:1854:HOH:O	1.97	0.65
3:G:1704:BCL:CBD	6:G:1854:HOH:O	2.44	0.64
1:O:41:PHE:HB3	1:O:42:PRO:HD3	1.77	0.64
1:C:31:HIS:CE1	3:D:1602:BCL:HMD3	2.32	0.64
4:E:1823:LDA:HM21	6:E:1853:HOH:O	1.96	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:H41	3:M:1707:BCL:C8	2.27	0.63
3:M:1707:BCL:H141	2:N:30:HIS:ND1	2.12	0.63
2:P:34:PHE:C	2:P:34:PHE:CD2	2.77	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
2:B:4:THR:H	2:B:7:GLN:HE21	1.47	0.62
3:A:1701:BCL:HHC	3:A:1701:BCL:HBB2	1.82	0.62
4:G:1824:LDA:H61	6:G:1865:HOH:O	1.99	0.62
1:R:16:ILE:HB	1:R:17:PRO:HD3	1.82	0.62
3:R:1709:BCL:C2	6:R:1831:HOH:O	2.28	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
6:K:1861:HOH:O	1:M:12:PRO:C	2.43	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
2:J:6:GLU:CD	6:J:1821:HOH:O	2.42	0.61
3:R:1709:BCL:H41	3:R:1709:BCL:C8	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
3:G:1704:BCL:O1D	3:I:1505:BCL:C5	2.49	0.60
3:G:1704:BCL:HHB	2:H:19:THR:HG21	1.83	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:HHC	3:C:1702:BCL:HBB2	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:H112	3:F:1603:BCL:C6	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:HHB	1.84	0.59
1:A:41:PHE:HB3	1:A:42:PRO:HD3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:4:THR:HG1	2:F:7:GLN:CD	2.11	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
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:LEU:HD13	3:D:1602:BCL:H2	1.87	0.55
3:I:1705:BCL:C4	3:I:1705:BCL:C9	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
1:G:50:LYS:NZ	6:G:1840:HOH:O	2.29	0.55
3:R:1709:BCL:H92	3:R:1709:BCL:C4	2.33	0.55
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
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
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:HBA2	3:L:1606:BCL:HMA3	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:HMC1	3:L:1606:BCL:HBC2	1.89	0.53
3:N:1607:BCL:HMC2	3:N:1607:BCL:HBC3	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:M:1707:BCL:HHC	3:M:1707:BCL:HBB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
3:R:1509:BCL:HMD3	2:S:30:HIS:CE1	2.46	0.51
1:E:1:CXM:HG2	3:E:1703:BCL:CHC	2.41	0.51
1:M:31:HIS:CE1	3:N:1607:BCL:HMD1	2.45	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:P:1608:BCL:HMB3	3:P:1608:BCL:CBB	2.39	0.51
3:I:1705:BCL:C4	3:I:1705:BCL:H92	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:HHC	3:E:1703:BCL:HBB2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:49:VAL:HG22	1:R:49:VAL:O	2.10	0.51
4:C:1815:LDA:HM11	1:E:14:ILE:CD1	2.42	0.50
3:I:1705:BCL:C8	3:I:1705:BCL:C4	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: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
1:O:31:HIS:CE1	3:P:1608:BCL:HMD1	2.47	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: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
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
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
1:A:49:VAL:HG12	2:S:41:HIS:NE2	2.28	0.48
3:M:1707:BCL:HBC3	3:N:1607:BCL:H143	1.95	0.48
3:K:1706:BCL:HHC	3:K:1706:BCL:CBB	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
1:R:5:LYS:NZ	2:S:9:GLU:OE2	2.46	0.48
3:O:1508:BCL:HAA2	3:O:1508:BCL:CGD	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:1603:BCL:HBB2	3:F:1603:BCL:HMB3	1.95	0.47
1:I:5:LYS:HG2	6:J:1823:HOH:O	2.09	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:OBB	3:S:1609:BCL:HHC	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
1:M:14:ILE:HG13	4:M:1811:LDA:C1	2.44	0.47
3:M:1707:BCL:C4D	3:N:1607:BCL:H172	2.45	0.47
4:M:1811:LDA:H41	1:O:14:ILE:HD12	1.95	0.47
4:O:1820:LDA:CM2	6:O:1823:HOH:O	2.49	0.47
4:A:1816:LDA:H32	1:C:14:ILE:CD1	2.44	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
6:C:1843:HOH:O	4:E:1822:LDA:C2	2.63	0.47
2:F:4:THR:OG1	2:F:7:GLN:CD	2.58	0.47
2:N:37:THR:HG22	2:N:39:TRP:HB3	1.96	0.47
3:S:1609:BCL:HBB2	3:S:1609:BCL:HMB3	1.96	0.47
6:E:1862:HOH:O	4:F:1803:LDA:H31	2.08	0.47
3:B:1601:BCL:HHC	3:B:1601:BCL:OBB	2.14	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
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:H41	3:I:1705:BCL:C9	2.46	0.46
1:K:14:ILE:HG21	4:K:1810:LDA:H52	1.95	0.46
2:L:4:THR:OG1	2:L:7:GLN:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1606:BCL:H2A	3:L:1606:BCL:CGD	2.45	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
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:G:1504:BCL:HMB1	3:G:1504:BCL:HBB3	1.99	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
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
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
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
2:H:41:HIS:CD2	1:I:49:VAL:C	2.95	0.45
3:G:1704:BCL:CMD	2:J:18:GLY:HA2	2.46	0.45
5:H:1404:RG1:H11	5:H:1404:RG1:HM41	1.87	0.45
3:I:1705:BCL:C9	3:I:1705:BCL:H43	2.47	0.45
1:A:7:TRP:C	6:A:1850:HOH:O	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HHC	3:I:1705:BCL:HBB2	1.99	0.44
1:E:51:LYS:O	1:E:52:ALA:HB2	2.18	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:E:1703:BCL:HHB	2:F:19:THR:HG21	1.98	0.44
2:P:19:THR:CG2	3:P:1608:BCL:H42	2.47	0.44
3:K:1506:BCL:HMB1	3:K:1506:BCL:HBB3	1.99	0.44
1:E:1:CXM:HE2	6:F:1820:HOH:O	2.17	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
4:M:1811:LDA:H21	1:O:14:ILE:CD1	2.47	0.44
2:B:27:LEU:O	2:B:28:VAL:C	2.57	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
1:M:39:THR:OG1	1:O:46:GLN:NE2	2.37	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
3:C:1502:BCL:HMB1	3:C:1502:BCL:HBB3	2.00	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
3:I:1505:BCL:HMB1	3:I:1505:BCL:HBB3	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
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:HBA2	3:L:1606:BCL:CMA	2.49	0.43
3:H:1604:BCL:HBB2	3:H:1604:BCL:HMB3	2.00	0.43
3:M:1507:BCL:HAA2	3:M:1507:BCL:HBD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:HG22	2:B:3:LEU:O	2.19	0.43
3:A:1501:BCL:H3C	4:B:1801:LDA:H71	2.01	0.43
1:E:14:ILE:HG13	4:G:1814:LDA:H12	2.00	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
3:I:1705:BCL:C4	3:K:1506:BCL:HMA2	2.47	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:C10	3:F:1603:BCL:C14	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
1:E:1:CXM:HE3	1:E:1:CXM:HB2	1.92	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
3:J:1605:BCL:HMB3	3:J:1605:BCL:HBB2	2.00	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:HM22	4:K:1826:LDA:H22	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
2:J:41:HIS:CE1	1:K:49:VAL:HG12	2.53	0.42
1:K:40:TRP:HH2	3:K:1506:BCL:CBC	2.32	0.42
5:N:1407:RG1:H7	5:N:1407:RG1:HM31	1.85	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:A:1701:BCL:OBD	5:D:1402:RG1:H11	2.19	0.42
6:I:1847:HOH:O	2:J:6:GLU:HA	2.20	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:P:1608:BCL:CBB	3:P:1608:BCL:CMB	2.97	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:A:1501:BCL:HHC	3:A:1501:BCL:OBB	2.20	0.42
5:P:1408:RG1:H7	5:P:1408:RG1:HM31	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ALA:HB1	4:A:1817:LDA:HM11	2.02	0.42
5:D:1402:RG1:H15	5:D:1402:RG1:HM51	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:H61	3:M:1507:BCL:H102	1.93	0.41
1:O:43:ALA:HB2	6:O:1830:HOH:O	2.20	0.41
1:C:5:LYS:O	1:C:8:THR:OG1	2.32	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
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:O5'	5:R:1401:RG1:CM1	2.68	0.41
1:I:16:ILE:HB	1:I:17:PRO:HD3	2.02	0.41
1:I:31:HIS:ND1	3:J:1605:BCL:HMD1	2.36	0.41
3:K:1706:BCL:HBC3	3:K:1706:BCL:H2C	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
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
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
3:E:1703:BCL:H161	3:E:1703:BCL:H202	1.74	0.41
4:F:1803:LDA:H82	6:F:1809:HOH:O	2.17	0.41
1:K:1:CXM:C	1:K:1:CXM:ON1	2.69	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:L:1606:BCL:HHB	3:L:1606:BCL:HMA1	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:31:HIS:ND1	3:N:1607:BCL:HMD1	2.36	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
2:L:37:THR:HG22	2:L:39:TRP:HB3	2.02	0.41
2:N:4:THR:H	2:N:7:GLN:NE2	2.19	0.41
6:B:517:HOH:O	1:R:5:LYS:HE2	2.21	0.40
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
3:O:1508:BCL:CHD	3:O:1508:BCL:HBC2	2.50	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
3:K:1506:BCL:HMB1	3:K:1506:BCL:CBB	2.51	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
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
5:R:1401:RG1:H11	5:R:1401:RG1:HM41	1.87	0.40
5:S:1409:RG1:H20	5:S:1409:RG1:HM61	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%)	6	4
1	M	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	1	0
1	O	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	6	4
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
All	All	810/846 (96%)	775 (96%)	21 (3%)	14 (2%)	7	6

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%)	38 (95%)	2 (5%)	22	32
1	C	40/40 (100%)	37 (92%)	3 (8%)	12	16
1	E	40/40 (100%)	36 (90%)	4 (10%)	7	7
1	G	40/40 (100%)	36 (90%)	4 (10%)	7	7
1	I	40/40 (100%)	35 (88%)	5 (12%)	4	4
1	K	40/40 (100%)	38 (95%)	2 (5%)	22	32
1	M	40/40 (100%)	38 (95%)	2 (5%)	22	32
1	O	40/40 (100%)	38 (95%)	2 (5%)	22	32
1	R	40/40 (100%)	37 (92%)	3 (8%)	12	16
2	B	33/33 (100%)	29 (88%)	4 (12%)	5	4
2	D	33/33 (100%)	29 (88%)	4 (12%)	5	4
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%)	17	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%)	595 (91%)	62 (9%)	8	8

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	51	LYS
2	B	2	THR
2	B	6	GLU
2	B	13	LYS
2	B	37	THR

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Mol	Chain	Res	Type
1	C	5	LYS
1	C	9	VAL
1	C	50	LYS
2	D	2	THR
2	D	10	GLU
2	D	35	SER
2	D	37	THR
1	E	5	LYS
1	E	9	VAL
1	E	14	ILE
1	E	49	VAL
2	F	2	THR
2	F	13	LYS
2	F	17	ASP
2	F	37	THR
1	G	14	ILE
1	G	36	SER
1	G	50	LYS
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	14	ILE
1	I	36	SER
1	I	50	LYS
1	I	51	LYS
2	J	2	THR
2	J	37	THR
1	K	14	ILE
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	5	LYS
1	M	9	VAL
2	N	2	THR
2	N	13	LYS
2	N	37	THR

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Mol	Chain	Res	Type
1	O	9	VAL
1	O	16	ILE
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	50	LYS
2	S	2	THR
2	S	6	GLU
2	S	10	GLU
2	S	37	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
2	B	7	GLN
1	C	3	GLN
1	C	37	HIS
2	D	7	GLN
1	E	37	HIS
2	H	7	GLN
1	I	37	HIS
1	K	37	HIS
2	L	7	GLN
1	M	3	GLN
2	N	7	GLN
1	O	3	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	G	1	3,1	9,10,11	1.77	2 (22%)	9,11,13	1.17	2 (22%)
1	CXM	C	1	3,1	9,10,11	2.27	2 (22%)	9,11,13	1.33	1 (11%)
1	CXM	M	1	3,1	9,10,11	2.88	2 (22%)	9,11,13	1.14	2 (22%)
1	CXM	R	1	3,1	9,10,11	1.63	1 (11%)	9,11,13	1.33	1 (11%)
1	CXM	A	1	3,1	9,10,11	1.50	2 (22%)	9,11,13	1.37	2 (22%)
1	CXM	O	1	3,1	9,10,11	1.49	1 (11%)	9,11,13	1.34	1 (11%)
1	CXM	I	1	3,1	9,10,11	1.36	1 (11%)	9,11,13	1.50	1 (11%)
1	CXM	E	1	3,1	9,10,11	1.38	2 (22%)	9,11,13	1.37	1 (11%)
1	CXM	K	1	3,1	9,10,11	1.49	2 (22%)	9,11,13	1.61	1 (11%)

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	G	1	3,1	-	3/9/10/12	-
1	CXM	C	1	3,1	-	1/9/10/12	-
1	CXM	M	1	3,1	-	2/9/10/12	-
1	CXM	R	1	3,1	-	4/9/10/12	-
1	CXM	A	1	3,1	-	3/9/10/12	-
1	CXM	O	1	3,1	-	4/9/10/12	-
1	CXM	I	1	3,1	-	2/9/10/12	-
1	CXM	E	1	3,1	-	2/9/10/12	-
1	CXM	K	1	3,1	-	3/9/10/12	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	1	CXM	CE-SD	7.04	2.21	1.78
1	C	1	CXM	ON1-CN	5.27	1.31	1.21
1	M	1	CXM	ON1-CN	4.56	1.30	1.21
1	R	1	CXM	ON1-CN	3.99	1.29	1.21
1	G	1	CXM	CE-SD	3.54	2.00	1.78
1	G	1	CXM	ON1-CN	3.45	1.28	1.21
1	O	1	CXM	ON1-CN	3.45	1.28	1.21
1	C	1	CXM	CE-SD	3.01	1.97	1.78
1	A	1	CXM	CA-N	2.55	1.50	1.46
1	E	1	CXM	CE-SD	2.33	1.93	1.78
1	K	1	CXM	ON1-CN	2.27	1.25	1.21
1	I	1	CXM	CN-N	-2.20	1.31	1.35
1	A	1	CXM	ON1-CN	2.16	1.25	1.21
1	E	1	CXM	ON1-CN	2.10	1.25	1.21
1	K	1	CXM	CA-N	2.02	1.49	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	1	CXM	ON1-CN-N	-3.92	118.42	124.86
1	I	1	CXM	ON1-CN-N	-3.75	118.70	124.86
1	R	1	CXM	ON1-CN-N	-3.65	118.86	124.86
1	C	1	CXM	ON1-CN-N	-3.52	119.09	124.86
1	O	1	CXM	ON1-CN-N	-3.47	119.16	124.86
1	E	1	CXM	ON1-CN-N	-2.93	120.05	124.86
1	A	1	CXM	ON1-CN-N	-2.82	120.23	124.86
1	G	1	CXM	ON1-CN-N	-2.66	120.50	124.86
1	G	1	CXM	O-C-CA	-2.14	119.26	124.77
1	M	1	CXM	ON1-CN-N	-2.14	121.35	124.86
1	M	1	CXM	C-CA-N	2.10	113.56	109.50
1	A	1	CXM	C-CA-N	2.05	113.45	109.50

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	CXM	C-CA-CB-CG
1	G	1	CXM	O-C-CA-CB
1	K	1	CXM	O-C-CA-CB
1	R	1	CXM	O-C-CA-CB
1	O	1	CXM	CB-CG-SD-CE
1	O	1	CXM	ON1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
1	G	1	CXM	C-CA-CB-CG
1	R	1	CXM	ON1-CN-N-CA
1	A	1	CXM	C-CA-N-CN
1	E	1	CXM	C-CA-N-CN
1	K	1	CXM	C-CA-N-CN
1	M	1	CXM	C-CA-N-CN
1	G	1	CXM	CB-CA-N-CN
1	I	1	CXM	CB-CA-N-CN
1	M	1	CXM	CB-CA-N-CN
1	O	1	CXM	CB-CA-N-CN
1	I	1	CXM	C-CA-N-CN
1	O	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	K	1	CXM	CB-CA-N-CN
1	R	1	CXM	CB-CA-N-CN
1	R	1	CXM	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 11 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	4	0
1	K	1	CXM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	LDA	F	1803	-	13,15,15	2.13	1 (7%)	14,17,17	0.57	0
4	LDA	M	1811	-	13,15,15	1.84	1 (7%)	14,17,17	0.49	0
4	LDA	R	1809	-	13,15,15	1.89	1 (7%)	14,17,17	0.52	0
3	BCL	E	1703	1	69,74,74	1.95	17 (24%)	79,115,115	2.03	23 (29%)
3	BCL	L	1606	2	69,74,74	2.26	26 (37%)	79,115,115	2.81	27 (34%)
4	LDA	E	1822	-	13,15,15	1.95	2 (15%)	14,17,17	0.51	0
3	BCL	G	1704	1	69,74,74	2.06	20 (28%)	79,115,115	2.23	26 (32%)
3	BCL	E	1503	1	69,74,74	1.90	16 (23%)	79,115,115	2.30	23 (29%)
4	LDA	D	1802	-	13,15,15	2.30	2 (15%)	14,17,17	0.61	0
4	LDA	L	1806	-	13,15,15	2.03	2 (15%)	14,17,17	0.58	0
4	LDA	M	1827	-	13,15,15	1.92	1 (7%)	14,17,17	0.42	0
3	BCL	D	1602	2	69,74,74	2.19	25 (36%)	79,115,115	2.37	23 (29%)
3	BCL	M	1707	1	69,74,74	2.34	20 (28%)	79,115,115	2.06	21 (26%)
5	RG1	F	1403	-	52,52,52	1.27	3 (5%)	66,67,67	1.66	18 (27%)
3	BCL	I	1705	1	69,74,74	2.13	27 (39%)	79,115,115	2.17	21 (26%)
3	BCL	C	1502	1	69,74,74	2.10	20 (28%)	79,115,115	2.30	27 (34%)
5	RG1	H	1404	-	52,52,52	1.31	7 (13%)	66,67,67	1.74	16 (24%)
3	BCL	N	1607	2	69,74,74	2.11	20 (28%)	79,115,115	2.37	23 (29%)
4	LDA	I	1813	-	13,15,15	1.92	1 (7%)	14,17,17	0.40	0
4	LDA	P	1808	-	13,15,15	1.91	2 (15%)	14,17,17	0.57	0
5	RG1	L	1406	-	52,52,52	1.27	6 (11%)	66,67,67	1.62	16 (24%)
5	RG1	R	1401	-	52,52,52	1.10	3 (5%)	66,67,67	1.81	16 (24%)
4	LDA	H	1804	-	13,15,15	2.45	2 (15%)	14,17,17	0.56	0
3	BCL	S	1609	2	69,74,74	1.99	18 (26%)	79,115,115	2.37	27 (34%)
3	BCL	J	1605	2	69,74,74	2.24	25 (36%)	79,115,115	2.47	25 (31%)
3	BCL	B	1601	2	69,74,74	1.97	21 (30%)	79,115,115	2.57	21 (26%)
3	BCL	R	1709	1	69,74,74	2.37	30 (43%)	79,115,115	2.18	22 (27%)
3	BCL	A	1501	1	69,74,74	2.18	19 (27%)	79,115,115	2.31	26 (32%)
4	LDA	C	1821	-	13,15,15	1.87	1 (7%)	14,17,17	0.40	0
5	RG1	D	1402	-	52,52,52	1.20	6 (11%)	66,67,67	1.71	17 (25%)
4	LDA	N	1807	-	13,15,15	1.82	1 (7%)	14,17,17	0.37	0
4	LDA	C	1815	-	13,15,15	2.08	2 (15%)	14,17,17	0.34	0
4	LDA	R	1819	-	13,15,15	2.14	2 (15%)	14,17,17	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BCL	K	1706	1	69,74,74	2.04	21 (30%)	79,115,115	2.27	22 (27%)
5	RG1	S	1409	-	52,52,52	1.34	7 (13%)	66,67,67	1.65	17 (25%)
4	LDA	I	1812	-	13,15,15	2.28	1 (7%)	14,17,17	0.37	0
3	BCL	I	1505	1	69,74,74	2.04	20 (28%)	79,115,115	2.07	23 (29%)
3	BCL	P	1608	2	69,74,74	2.23	22 (31%)	79,115,115	2.34	22 (27%)
4	LDA	A	1816	-	13,15,15	2.22	2 (15%)	14,17,17	0.35	0
4	LDA	B	1801	-	13,15,15	2.03	1 (7%)	14,17,17	0.43	0
4	LDA	G	1824	-	13,15,15	1.99	1 (7%)	14,17,17	0.34	0
4	LDA	R	1818	-	13,15,15	1.91	1 (7%)	14,17,17	0.45	0
4	LDA	O	1820	-	13,15,15	2.01	1 (7%)	14,17,17	0.42	0
3	BCL	A	1701	1	69,74,74	2.60	26 (37%)	79,115,115	2.31	23 (29%)
4	LDA	G	1814	-	13,15,15	2.02	1 (7%)	14,17,17	0.44	0
4	LDA	K	1810	-	13,15,15	2.06	1 (7%)	14,17,17	0.49	0
4	LDA	K	1826	-	13,15,15	1.94	2 (15%)	14,17,17	0.53	0
5	RG1	P	1408	-	52,52,52	1.30	8 (15%)	66,67,67	1.67	15 (22%)
4	LDA	J	1805	-	13,15,15	1.80	1 (7%)	14,17,17	0.30	0
4	LDA	A	1817	-	13,15,15	2.07	2 (15%)	14,17,17	0.43	0
3	BCL	G	1504	6,1	69,74,74	2.04	20 (28%)	79,115,115	2.15	24 (30%)
4	LDA	I	1825	-	13,15,15	1.95	1 (7%)	14,17,17	0.51	0
5	RG1	J	1405	-	52,52,52	1.19	5 (9%)	66,67,67	1.69	17 (25%)
5	RG1	N	1407	-	52,52,52	1.18	3 (5%)	66,67,67	1.68	15 (22%)
3	BCL	R	1509	1	69,74,74	2.21	22 (31%)	79,115,115	2.41	26 (32%)
3	BCL	F	1603	2	69,74,74	1.84	18 (26%)	79,115,115	2.23	21 (26%)
3	BCL	O	1508	1	69,74,74	1.85	18 (26%)	79,115,115	2.24	26 (32%)
4	LDA	E	1823	-	13,15,15	1.74	1 (7%)	14,17,17	0.45	0
3	BCL	H	1604	2	69,74,74	2.07	22 (31%)	79,115,115	2.30	29 (36%)
3	BCL	K	1506	1	69,74,74	2.46	26 (37%)	79,115,115	2.36	24 (30%)
3	BCL	O	1708	1	69,74,74	2.22	24 (34%)	79,115,115	2.13	22 (27%)
3	BCL	C	1702	1	69,74,74	2.10	20 (28%)	79,115,115	2.11	20 (25%)
3	BCL	M	1507	1	69,74,74	2.03	19 (27%)	79,115,115	2.41	23 (29%)

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	LDA	F	1803	-	-	9/13/13/13	-
4	LDA	M	1811	-	-	7/13/13/13	-
4	LDA	R	1809	-	-	10/13/13/13	-
3	BCL	E	1703	1	-	16/41/137/137	-
3	BCL	L	1606	2	3/3/21/25	6/41/137/137	-
4	LDA	E	1822	-	-	7/13/13/13	-
3	BCL	G	1704	1	1/1/21/25	10/41/137/137	-
3	BCL	E	1503	1	-	7/41/137/137	-
4	LDA	D	1802	-	-	8/13/13/13	-
4	LDA	L	1806	-	-	10/13/13/13	-
4	LDA	M	1827	-	-	4/13/13/13	-
3	BCL	D	1602	2	-	8/41/137/137	-
3	BCL	M	1707	1	1/1/21/25	15/41/137/137	-
5	RG1	F	1403	-	-	4/51/71/71	0/1/1/1
3	BCL	C	1502	1	1/1/21/25	6/41/137/137	-
3	BCL	I	1705	1	-	6/41/137/137	-
5	RG1	H	1404	-	-	9/51/71/71	0/1/1/1
3	BCL	N	1607	2	1/1/21/25	17/41/137/137	-
4	LDA	I	1813	-	-	4/13/13/13	-
4	LDA	P	1808	-	-	8/13/13/13	-
5	RG1	L	1406	-	-	5/51/71/71	0/1/1/1
5	RG1	R	1401	-	-	5/51/71/71	0/1/1/1
4	LDA	H	1804	-	-	6/13/13/13	-
3	BCL	S	1609	2	1/1/21/25	13/41/137/137	-
3	BCL	J	1605	2	1/1/21/25	8/41/137/137	-
3	BCL	B	1601	2	1/1/21/25	8/41/137/137	-
3	BCL	R	1709	1	1/1/21/25	17/41/137/137	-
3	BCL	A	1501	1	1/1/21/25	5/41/137/137	-
4	LDA	C	1821	-	-	5/13/13/13	-
5	RG1	D	1402	-	-	4/51/71/71	0/1/1/1
4	LDA	N	1807	-	-	6/13/13/13	-
4	LDA	C	1815	-	-	6/13/13/13	-
4	LDA	R	1819	-	-	8/13/13/13	-
3	BCL	K	1706	1	1/1/21/25	11/41/137/137	-
5	RG1	S	1409	-	-	3/51/71/71	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	I	1812	-	-	7/13/13/13	-
3	BCL	I	1505	1	-	5/41/137/137	-
3	BCL	P	1608	2	2/2/21/25	13/41/137/137	-
4	LDA	A	1816	-	-	6/13/13/13	-
4	LDA	B	1801	-	-	8/13/13/13	-
4	LDA	G	1824	-	-	4/13/13/13	-
4	LDA	R	1818	-	-	5/13/13/13	-
4	LDA	O	1820	-	-	5/13/13/13	-
3	BCL	A	1701	1	1/1/21/25	15/41/137/137	-
4	LDA	G	1814	-	-	8/13/13/13	-
4	LDA	K	1810	-	-	7/13/13/13	-
4	LDA	K	1826	-	-	6/13/13/13	-
5	RG1	P	1408	-	-	7/51/71/71	0/1/1/1
4	LDA	J	1805	-	-	9/13/13/13	-
4	LDA	A	1817	-	-	8/13/13/13	-
3	BCL	G	1504	6,1	-	7/41/137/137	-
4	LDA	I	1825	-	-	8/13/13/13	-
5	RG1	J	1405	-	-	5/51/71/71	0/1/1/1
5	RG1	N	1407	-	-	4/51/71/71	0/1/1/1
3	BCL	R	1509	1	1/1/21/25	9/41/137/137	-
3	BCL	F	1603	2	-	10/41/137/137	-
3	BCL	O	1508	1	2/2/21/25	9/41/137/137	-
4	LDA	E	1823	-	-	5/13/13/13	-
3	BCL	H	1604	2	1/1/21/25	10/41/137/137	-
3	BCL	K	1506	1	1/1/21/25	8/41/137/137	-
3	BCL	O	1708	1	1/1/21/25	10/41/137/137	-
3	BCL	C	1702	1	1/1/21/25	18/41/137/137	-
3	BCL	M	1507	1	-	3/41/137/137	-

All (667) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1702	BCL	C2-C3	8.61	1.52	1.33
3	K	1506	BCL	CAC-C3C	-8.21	1.38	1.54
3	A	1701	BCL	C2-C3	7.68	1.50	1.33
3	S	1609	BCL	C2-C3	7.66	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1605	BCL	C2-C3	7.50	1.50	1.33
4	I	1812	LDA	O1-N1	-7.43	1.23	1.42
3	O	1708	BCL	C2-C3	7.43	1.50	1.33
3	G	1704	BCL	C2-C3	7.33	1.49	1.33
3	M	1707	BCL	CBD-CGD	-7.27	1.30	1.52
3	A	1701	BCL	C3C-C4C	-7.23	1.42	1.51
3	E	1503	BCL	C2-C3	7.10	1.49	1.33
3	R	1709	BCL	C2-C3	6.94	1.49	1.33
3	N	1607	BCL	C2-C3	6.93	1.49	1.33
3	A	1501	BCL	C2-C3	6.88	1.48	1.33
4	F	1803	LDA	O1-N1	-6.81	1.25	1.42
3	M	1707	BCL	C2-C3	6.80	1.48	1.33
4	K	1810	LDA	O1-N1	-6.76	1.25	1.42
4	O	1820	LDA	O1-N1	-6.76	1.25	1.42
4	D	1802	LDA	O1-N1	-6.75	1.25	1.42
3	M	1507	BCL	C2-C3	6.72	1.48	1.33
3	K	1506	BCL	C2-C3	6.70	1.48	1.33
4	G	1824	LDA	O1-N1	-6.67	1.25	1.42
3	B	1601	BCL	C2-C3	6.66	1.48	1.33
3	D	1602	BCL	C2-C3	6.65	1.48	1.33
4	I	1813	LDA	O1-N1	-6.58	1.26	1.42
4	I	1825	LDA	O1-N1	-6.57	1.26	1.42
3	M	1707	BCL	C3B-C4B	6.50	1.54	1.41
4	A	1817	LDA	O1-N1	-6.48	1.26	1.42
4	L	1806	LDA	O1-N1	-6.47	1.26	1.42
4	C	1815	LDA	O1-N1	-6.47	1.26	1.42
3	P	1608	BCL	C2-C3	6.45	1.47	1.33
3	R	1709	BCL	C3B-C4B	6.45	1.53	1.41
3	F	1603	BCL	C2-C3	6.42	1.47	1.33
3	H	1604	BCL	C2-C3	6.41	1.47	1.33
4	M	1827	LDA	O1-N1	-6.37	1.26	1.42
3	E	1703	BCL	C2-C3	6.32	1.47	1.33
4	G	1814	LDA	O1-N1	-6.28	1.26	1.42
3	C	1502	BCL	C2-C3	6.26	1.47	1.33
4	B	1801	LDA	O1-N1	-6.24	1.26	1.42
4	H	1804	LDA	C1-N1	-6.19	1.45	1.51
4	H	1804	LDA	O1-N1	-6.18	1.27	1.42
3	G	1504	BCL	C2-C3	6.17	1.47	1.33
4	A	1816	LDA	O1-N1	-6.16	1.27	1.42
4	R	1819	LDA	O1-N1	-6.15	1.27	1.42
4	R	1818	LDA	O1-N1	-6.15	1.27	1.42
4	K	1826	LDA	O1-N1	-6.15	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1706	BCL	C2-C3	6.13	1.47	1.33
3	R	1509	BCL	C2-C3	6.07	1.47	1.33
4	C	1821	LDA	O1-N1	-6.07	1.27	1.42
4	E	1822	LDA	O1-N1	-6.07	1.27	1.42
4	P	1808	LDA	O1-N1	-6.07	1.27	1.42
3	C	1502	BCL	C3B-C4B	6.00	1.53	1.41
4	R	1809	LDA	O1-N1	-5.99	1.27	1.42
4	E	1823	LDA	O1-N1	-5.97	1.27	1.42
3	E	1503	BCL	MG-NB	-5.92	1.94	2.05
4	M	1811	LDA	O1-N1	-5.91	1.27	1.42
3	E	1703	BCL	O1D-CGD	5.82	1.35	1.21
3	K	1506	BCL	C3B-C4B	5.75	1.52	1.41
3	O	1508	BCL	C2-C3	5.67	1.46	1.33
3	I	1705	BCL	C3B-C4B	5.66	1.52	1.41
3	L	1606	BCL	C2C-C3C	-5.65	1.39	1.54
4	N	1807	LDA	O1-N1	-5.56	1.28	1.42
3	P	1608	BCL	C3B-C4B	5.53	1.52	1.41
3	N	1607	BCL	CMC-C2C	-5.52	1.41	1.53
3	L	1606	BCL	C2-C3	5.51	1.45	1.33
4	J	1805	LDA	O1-N1	-5.50	1.28	1.42
3	P	1608	BCL	O1D-CGD	5.43	1.34	1.21
3	O	1708	BCL	C3B-C4B	5.37	1.51	1.41
3	R	1509	BCL	C3A-C2A	-5.37	1.40	1.54
3	M	1507	BCL	MG-NB	-5.35	1.95	2.05
3	I	1705	BCL	C2-C3	5.28	1.45	1.33
3	A	1701	BCL	C3B-C4B	5.28	1.51	1.41
3	J	1605	BCL	C1D-C2D	5.18	1.55	1.45
3	K	1506	BCL	CAA-C2A	5.17	1.63	1.54
3	H	1604	BCL	C3C-C4C	-5.15	1.45	1.51
3	I	1505	BCL	C3B-C4B	5.15	1.51	1.41
3	D	1602	BCL	C3B-C4B	5.11	1.51	1.41
3	J	1605	BCL	CBD-CGD	-5.10	1.37	1.52
3	R	1709	BCL	CHB-C1B	5.02	1.50	1.39
3	C	1502	BCL	C1D-ND	5.01	1.44	1.37
3	I	1505	BCL	CHC-C4B	5.00	1.50	1.39
3	C	1702	BCL	O1D-CGD	4.96	1.33	1.21
3	R	1509	BCL	OBD-CAD	4.94	1.31	1.22
3	S	1609	BCL	MG-NB	-4.88	1.96	2.05
3	K	1706	BCL	C1D-C2D	4.85	1.54	1.45
3	G	1504	BCL	O1D-CGD	4.84	1.33	1.21
3	A	1501	BCL	C3B-C4B	4.82	1.50	1.41
5	N	1407	RG1	O1'-C1	-4.81	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1506	BCL	O1D-CGD	4.81	1.33	1.21
3	A	1701	BCL	CHD-C1D	4.80	1.47	1.38
3	M	1507	BCL	C3B-C4B	4.80	1.50	1.41
5	F	1403	RG1	C19-C18	4.78	1.56	1.46
3	A	1701	BCL	CAC-C3C	-4.78	1.44	1.54
3	D	1602	BCL	CHB-C1B	4.78	1.50	1.39
3	G	1704	BCL	CBD-CGD	-4.77	1.38	1.52
3	M	1707	BCL	C1D-C2D	4.76	1.54	1.45
3	M	1707	BCL	CHB-C1B	4.72	1.50	1.39
3	I	1505	BCL	CHB-C1B	4.71	1.50	1.39
3	A	1501	BCL	MG-NB	-4.69	1.96	2.05
3	I	1705	BCL	C1D-C2D	4.68	1.54	1.45
3	C	1502	BCL	CHB-C4A	4.68	1.49	1.37
3	A	1501	BCL	OBD-CAD	4.66	1.30	1.22
3	M	1507	BCL	C3D-C2D	4.66	1.51	1.39
3	L	1606	BCL	CHC-C4B	4.65	1.49	1.39
3	G	1504	BCL	C1D-C2D	4.64	1.54	1.45
3	R	1709	BCL	C1D-ND	4.63	1.43	1.37
3	A	1701	BCL	C1D-C2D	4.61	1.54	1.45
3	C	1702	BCL	C3B-C4B	4.60	1.50	1.41
3	N	1607	BCL	C2C-C3C	-4.58	1.42	1.54
4	D	1802	LDA	C1-N1	-4.57	1.46	1.51
3	H	1604	BCL	CHB-C1B	4.54	1.49	1.39
3	A	1701	BCL	CHB-C1B	4.54	1.49	1.39
3	P	1608	BCL	OBD-CAD	4.52	1.30	1.22
3	B	1601	BCL	MG-NB	-4.52	1.96	2.05
3	N	1607	BCL	C3B-C4B	4.51	1.50	1.41
3	H	1604	BCL	CHC-C4B	4.51	1.49	1.39
3	P	1608	BCL	CHB-C4A	4.50	1.49	1.37
3	O	1708	BCL	CHD-C1D	4.50	1.47	1.38
3	F	1603	BCL	C3D-C2D	4.48	1.51	1.39
3	O	1708	BCL	O1D-CGD	4.47	1.32	1.21
3	G	1504	BCL	MG-NA	4.47	2.16	2.06
3	D	1602	BCL	MG-NA	4.42	2.16	2.06
3	O	1508	BCL	OBD-CAD	4.42	1.30	1.22
3	J	1605	BCL	C3B-C4B	4.40	1.49	1.41
3	K	1706	BCL	OBB-CAB	4.39	1.33	1.23
3	L	1606	BCL	MG-NC	4.39	2.16	2.06
4	A	1816	LDA	C1-N1	-4.37	1.47	1.51
3	M	1707	BCL	MG-NA	4.37	2.16	2.06
3	I	1505	BCL	C2-C3	4.37	1.43	1.33
3	K	1506	BCL	O2D-CGD	4.37	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1708	BCL	CHB-C4A	4.36	1.48	1.37
3	A	1701	BCL	MG-NA	4.34	2.16	2.06
4	R	1819	LDA	C1-N1	-4.33	1.47	1.51
3	F	1603	BCL	C3B-C4B	4.31	1.49	1.41
3	C	1702	BCL	CHB-C4A	4.31	1.48	1.37
3	L	1606	BCL	MG-NB	-4.29	1.97	2.05
3	C	1502	BCL	CHB-C1B	4.29	1.49	1.39
3	L	1606	BCL	CHC-C1C	4.27	1.48	1.37
3	A	1701	BCL	OBD-CAD	4.26	1.29	1.22
3	C	1702	BCL	C3D-C2D	4.26	1.50	1.39
3	G	1704	BCL	CHB-C1B	4.24	1.48	1.39
3	J	1605	BCL	MG-NA	4.24	2.16	2.06
3	S	1609	BCL	CHB-C1B	4.23	1.48	1.39
3	K	1706	BCL	O1D-CGD	4.23	1.31	1.21
3	P	1608	BCL	CHB-C1B	4.22	1.48	1.39
3	E	1703	BCL	C1D-C2D	4.19	1.53	1.45
3	M	1707	BCL	CHB-C4A	4.18	1.48	1.37
3	M	1707	BCL	OBD-CAD	4.17	1.29	1.22
3	P	1608	BCL	CHC-C4B	4.17	1.48	1.39
3	G	1504	BCL	CHB-C1B	4.17	1.48	1.39
3	J	1605	BCL	CHB-C1B	4.16	1.48	1.39
3	R	1509	BCL	CHC-C1C	4.15	1.48	1.37
3	K	1706	BCL	CHB-C1B	4.15	1.48	1.39
3	E	1703	BCL	C3D-C2D	4.13	1.50	1.39
3	A	1501	BCL	MG-NA	4.12	2.16	2.06
3	I	1705	BCL	CHD-C1D	4.12	1.46	1.38
3	L	1606	BCL	CMC-C2C	-4.12	1.44	1.53
3	H	1604	BCL	O1D-CGD	4.12	1.31	1.21
3	N	1607	BCL	CHB-C1B	4.11	1.48	1.39
3	B	1601	BCL	C1D-C2D	4.11	1.53	1.45
3	O	1508	BCL	C14-C13	-4.10	1.40	1.52
3	C	1702	BCL	C1D-C2D	4.08	1.53	1.45
3	E	1503	BCL	C3D-C2D	4.07	1.50	1.39
3	K	1506	BCL	CHD-C1D	4.07	1.46	1.38
3	R	1509	BCL	O1D-CGD	4.07	1.31	1.21
3	L	1606	BCL	O1D-CGD	4.06	1.31	1.21
3	O	1508	BCL	CBD-CGD	-4.05	1.40	1.52
3	G	1704	BCL	CHB-C4A	4.04	1.47	1.37
3	A	1501	BCL	CHB-C1B	4.03	1.48	1.39
3	E	1703	BCL	C3B-C4B	4.02	1.49	1.41
3	R	1509	BCL	CHC-C4B	4.02	1.48	1.39
3	I	1505	BCL	C1B-C2B	4.02	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1505	BCL	C1D-C2D	3.98	1.53	1.45
3	A	1701	BCL	O1D-CGD	3.97	1.31	1.21
3	G	1704	BCL	C1B-C2B	3.96	1.52	1.43
3	A	1501	BCL	O1A-CGA	3.94	1.34	1.22
3	O	1708	BCL	C3D-C2D	3.94	1.49	1.39
3	A	1701	BCL	O1A-CGA	3.92	1.34	1.22
3	K	1706	BCL	C3B-C4B	3.92	1.48	1.41
3	D	1602	BCL	C3D-C2D	3.90	1.49	1.39
3	N	1607	BCL	MG-NA	3.88	2.15	2.06
3	J	1605	BCL	CHB-C4A	3.88	1.47	1.37
3	L	1606	BCL	CHB-C1B	3.87	1.48	1.39
3	O	1508	BCL	C1D-C2D	3.87	1.53	1.45
3	G	1504	BCL	CHB-C4A	3.87	1.47	1.37
3	S	1609	BCL	C3D-C2D	3.86	1.49	1.39
3	E	1503	BCL	C3B-C4B	3.85	1.48	1.41
3	R	1709	BCL	C3D-C2D	3.85	1.49	1.39
3	O	1508	BCL	OBB-CAB	3.85	1.32	1.23
3	H	1604	BCL	C3B-C4B	3.84	1.48	1.41
3	R	1509	BCL	C3B-C4B	3.84	1.48	1.41
3	E	1703	BCL	C1D-ND	3.83	1.42	1.37
3	P	1608	BCL	C2C-C3C	-3.81	1.44	1.54
3	N	1607	BCL	C3D-C2D	3.81	1.49	1.39
3	B	1601	BCL	CHC-C4B	3.78	1.47	1.39
3	K	1506	BCL	C1B-C2B	3.77	1.52	1.43
3	K	1706	BCL	C3D-C2D	3.76	1.49	1.39
3	M	1507	BCL	O1D-CGD	3.76	1.30	1.21
3	O	1708	BCL	C1D-ND	3.76	1.42	1.37
3	C	1502	BCL	CHC-C4B	3.74	1.47	1.39
3	R	1709	BCL	C1D-C2D	3.74	1.52	1.45
3	A	1501	BCL	CHB-C4A	3.72	1.47	1.37
3	A	1701	BCL	C3D-C2D	3.71	1.49	1.39
3	R	1709	BCL	MG-NA	3.70	2.15	2.06
3	O	1508	BCL	O1A-CGA	3.69	1.33	1.22
3	I	1705	BCL	O1A-CGA	3.69	1.33	1.22
3	D	1602	BCL	C2A-C1A	-3.69	1.43	1.52
3	A	1501	BCL	O1D-CGD	3.67	1.30	1.21
3	I	1505	BCL	O2D-CGD	3.67	1.42	1.33
3	D	1602	BCL	CHB-C4A	3.67	1.46	1.37
3	R	1509	BCL	C1D-C2D	3.66	1.52	1.45
3	I	1505	BCL	MG-NC	3.65	2.14	2.06
3	G	1704	BCL	C3B-C4B	3.64	1.48	1.41
5	S	1409	RG1	O1'-C1	-3.62	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1705	BCL	O2D-CGD	3.61	1.42	1.33
3	A	1701	BCL	O2D-CGD	3.58	1.42	1.33
3	A	1701	BCL	OBb-CAB	3.57	1.31	1.23
5	S	1409	RG1	C2-C1	3.56	1.58	1.53
3	R	1509	BCL	OBb-CAB	3.56	1.31	1.23
3	L	1606	BCL	C3B-C4B	3.55	1.48	1.41
3	D	1602	BCL	MG-NB	-3.55	1.98	2.05
3	B	1601	BCL	CHB-C1B	3.55	1.47	1.39
3	H	1604	BCL	OBb-CAB	3.55	1.31	1.23
3	I	1705	BCL	C3D-C2D	3.54	1.48	1.39
3	O	1708	BCL	C1D-C2D	3.54	1.52	1.45
3	F	1603	BCL	CHB-C4A	3.53	1.46	1.37
3	O	1708	BCL	CHB-C1B	3.52	1.47	1.39
3	G	1504	BCL	OBd-CAD	3.52	1.28	1.22
3	G	1704	BCL	MG-NC	3.52	2.14	2.06
3	K	1506	BCL	CHB-C4A	3.51	1.46	1.37
3	D	1602	BCL	O1A-CGA	3.50	1.33	1.22
3	R	1509	BCL	C3D-C2D	3.50	1.48	1.39
3	I	1505	BCL	CHC-C1C	3.48	1.46	1.37
3	M	1507	BCL	O2D-CGD	3.47	1.41	1.33
5	H	1404	RG1	C2-C1	3.47	1.58	1.53
3	K	1506	BCL	C2C-C3C	-3.46	1.45	1.54
3	S	1609	BCL	C3B-C4B	3.46	1.48	1.41
3	J	1605	BCL	MG-NB	-3.46	1.98	2.05
5	J	1405	RG1	O1'-C1	-3.45	1.42	1.46
3	N	1607	BCL	C1B-C2B	3.45	1.51	1.43
3	I	1705	BCL	CAA-C2A	3.44	1.60	1.54
3	D	1602	BCL	O2A-CGA	3.44	1.43	1.33
3	R	1509	BCL	O1A-CGA	3.44	1.32	1.22
3	A	1701	BCL	CHB-C4A	3.44	1.46	1.37
3	R	1509	BCL	MG-NB	-3.44	1.99	2.05
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	B	1601	BCL	OBd-CAD	3.40	1.28	1.22
3	G	1704	BCL	C3D-C2D	3.40	1.48	1.39
3	L	1606	BCL	C3A-C4A	-3.40	1.40	1.51
3	C	1502	BCL	C1B-C2B	3.40	1.51	1.43
3	B	1601	BCL	O1D-CGD	3.40	1.29	1.21
3	P	1608	BCL	C3D-C2D	3.40	1.48	1.39
3	I	1505	BCL	O1A-CGA	3.39	1.32	1.22
3	K	1706	BCL	CHC-C1C	3.39	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1509	BCL	CHB-C4A	3.36	1.46	1.37
3	H	1604	BCL	C3D-C2D	3.35	1.48	1.39
3	G	1504	BCL	C4B-NB	3.35	1.42	1.37
4	A	1817	LDA	C1-N1	-3.34	1.48	1.51
3	R	1709	BCL	CHB-C4A	3.34	1.46	1.37
3	I	1705	BCL	C4D-CHA	3.34	1.49	1.38
3	A	1701	BCL	CHC-C4B	3.34	1.46	1.39
3	R	1709	BCL	CHC-C4B	3.33	1.46	1.39
3	R	1709	BCL	CHD-C1D	3.33	1.44	1.38
3	P	1608	BCL	CMC-C2C	-3.32	1.46	1.53
3	A	1501	BCL	C3D-C2D	3.32	1.48	1.39
3	H	1604	BCL	CHB-C4A	3.31	1.46	1.37
3	I	1705	BCL	C1B-C2B	3.30	1.50	1.43
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	J	1605	BCL	C4D-CHA	3.28	1.49	1.38
3	A	1501	BCL	CBD-CGD	-3.28	1.42	1.52
3	M	1707	BCL	C1B-C2B	3.27	1.50	1.43
3	L	1606	BCL	C3A-C2A	-3.27	1.45	1.54
3	L	1606	BCL	CMA-C3A	-3.27	1.46	1.53
3	J	1605	BCL	O1A-CGA	3.26	1.32	1.22
3	P	1608	BCL	MG-NA	3.24	2.14	2.06
3	K	1506	BCL	C3B-CAB	3.23	1.56	1.46
3	A	1701	BCL	CHD-C4C	3.23	1.48	1.39
3	R	1709	BCL	CHC-C1C	3.23	1.45	1.37
3	K	1506	BCL	C3D-C2D	3.22	1.47	1.39
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	F	1603	BCL	C5-C3	3.22	1.57	1.51
3	O	1708	BCL	MG-NA	3.20	2.13	2.06
3	M	1507	BCL	CHC-C1C	3.19	1.45	1.37
3	R	1509	BCL	C3C-C4C	-3.19	1.47	1.51
3	S	1609	BCL	OBD-CAD	3.18	1.28	1.22
3	O	1708	BCL	C4D-CHA	3.18	1.49	1.38
3	O	1708	BCL	CHC-C1C	3.17	1.45	1.37
3	S	1609	BCL	O1D-CGD	3.17	1.29	1.21
4	K	1826	LDA	C1-N1	-3.16	1.48	1.51
3	F	1603	BCL	CHD-C1D	3.16	1.44	1.38
3	A	1501	BCL	CHC-C1C	3.16	1.45	1.37
3	C	1502	BCL	OBD-CAD	3.15	1.27	1.22
3	B	1601	BCL	C3D-C2D	3.14	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1822	LDA	C1-N1	-3.14	1.48	1.51
3	C	1702	BCL	CHB-C1B	3.13	1.46	1.39
3	C	1502	BCL	CHC-C1C	3.13	1.45	1.37
3	O	1508	BCL	CHB-C4A	3.13	1.45	1.37
3	C	1502	BCL	MG-NB	-3.13	1.99	2.05
3	D	1602	BCL	C4D-CHA	3.12	1.49	1.38
3	I	1705	BCL	OBD-CAD	3.12	1.27	1.22
3	N	1607	BCL	C4D-CHA	3.11	1.49	1.38
3	G	1504	BCL	CHC-C1C	3.11	1.45	1.37
3	M	1707	BCL	MG-NC	3.11	2.13	2.06
3	K	1506	BCL	O2A-CGA	3.10	1.42	1.33
3	I	1705	BCL	C3B-CAB	3.10	1.56	1.46
5	L	1406	RG1	C16-C17	3.09	1.52	1.43
3	K	1706	BCL	O1A-CGA	3.09	1.31	1.22
3	A	1701	BCL	C2C-C3C	-3.09	1.46	1.54
3	M	1507	BCL	OBB-CAB	3.08	1.30	1.23
3	A	1501	BCL	O2D-CGD	3.07	1.40	1.33
3	E	1503	BCL	O1A-CGA	3.07	1.31	1.22
3	R	1709	BCL	O1D-CGD	3.07	1.29	1.21
3	N	1607	BCL	CBD-CGD	-3.06	1.43	1.52
3	R	1709	BCL	C5-C3	3.06	1.57	1.51
3	L	1606	BCL	C4D-CHA	3.05	1.48	1.38
3	K	1506	BCL	C4D-CHA	3.05	1.48	1.38
3	B	1601	BCL	C3B-C4B	3.04	1.47	1.41
3	I	1705	BCL	CHB-C1B	3.03	1.46	1.39
3	S	1609	BCL	CHB-C4A	3.03	1.45	1.37
5	H	1404	RG1	C23-C22	3.03	1.52	1.46
3	M	1707	BCL	CBD-CAD	-3.03	1.43	1.56
3	E	1503	BCL	OBD-CAD	3.02	1.27	1.22
3	J	1605	BCL	CHC-C4B	3.02	1.46	1.39
3	R	1509	BCL	C4B-NB	3.02	1.41	1.37
3	G	1704	BCL	CBD-CAD	-3.01	1.43	1.56
3	D	1602	BCL	MG-NC	3.01	2.13	2.06
3	D	1602	BCL	C1B-C2B	3.00	1.50	1.43
3	S	1609	BCL	O2A-CGA	3.00	1.42	1.33
3	I	1505	BCL	OBB-CAB	3.00	1.30	1.23
3	O	1508	BCL	MG-NB	-2.99	1.99	2.05
3	A	1501	BCL	C4D-CHA	2.99	1.48	1.38
3	F	1603	BCL	OBD-CAD	2.98	1.27	1.22
3	A	1701	BCL	C4D-CHA	2.98	1.48	1.38
3	J	1605	BCL	O2A-CGA	2.98	1.42	1.33
3	N	1607	BCL	OBD-CAD	2.98	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	1409	RG1	C24-C25	2.97	1.52	1.43
3	O	1708	BCL	OBB-CAB	2.97	1.30	1.23
3	L	1606	BCL	OBD-CAD	2.97	1.27	1.22
3	C	1502	BCL	MG-NC	2.97	2.13	2.06
3	E	1503	BCL	MG-NC	2.97	2.13	2.06
3	E	1503	BCL	CHB-C4A	2.97	1.45	1.37
3	G	1704	BCL	C1D-C2D	2.95	1.51	1.45
3	E	1503	BCL	O1D-CGD	2.95	1.28	1.21
5	F	1403	RG1	C24-C25	2.95	1.52	1.43
3	F	1603	BCL	O2D-CGD	2.95	1.40	1.33
3	S	1609	BCL	MG-NC	2.95	2.13	2.06
3	O	1708	BCL	CHC-C4B	2.94	1.46	1.39
3	R	1709	BCL	O1A-CGA	2.94	1.31	1.22
5	P	1408	RG1	C23-C22	2.94	1.52	1.46
5	L	1406	RG1	C16-C15	2.93	1.44	1.36
3	L	1606	BCL	CHD-C1D	2.93	1.44	1.38
3	M	1707	BCL	CHD-C1D	2.92	1.44	1.38
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	K	1706	BCL	C1B-C2B	2.92	1.50	1.43
3	N	1607	BCL	C1D-ND	2.91	1.41	1.37
3	G	1504	BCL	C3D-C2D	2.91	1.46	1.39
5	F	1403	RG1	C11-C10	2.91	1.52	1.43
3	R	1709	BCL	OBB-CAB	2.91	1.29	1.23
3	B	1601	BCL	O2D-CGD	2.91	1.40	1.33
3	A	1701	BCL	O2A-CGA	2.89	1.41	1.33
3	K	1706	BCL	CHD-C1D	2.89	1.44	1.38
3	D	1602	BCL	O1D-CGD	2.89	1.28	1.21
3	N	1607	BCL	O1A-CGA	2.88	1.31	1.22
5	H	1404	RG1	C27-C26	2.88	1.52	1.46
3	B	1601	BCL	CHD-C1D	2.88	1.44	1.38
3	J	1605	BCL	CBA-CGA	-2.88	1.42	1.50
3	D	1602	BCL	OBD-CAD	2.88	1.27	1.22
3	G	1704	BCL	C4D-CHA	2.88	1.48	1.38
3	K	1706	BCL	MG-NA	2.87	2.13	2.06
3	I	1505	BCL	CHB-C4A	2.87	1.44	1.37
3	J	1605	BCL	MG-NC	2.87	2.13	2.06
3	C	1502	BCL	C3D-C2D	2.87	1.46	1.39
3	M	1507	BCL	CHB-C1B	2.87	1.45	1.39
3	O	1708	BCL	MG-NC	2.86	2.13	2.06
3	G	1504	BCL	CBD-CGD	-2.86	1.43	1.52
3	M	1507	BCL	CHB-C4A	2.86	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1509	BCL	CHB-C1B	2.85	1.45	1.39
3	P	1608	BCL	C4D-CHA	2.85	1.48	1.38
3	A	1501	BCL	CHC-C4B	2.85	1.45	1.39
3	R	1709	BCL	CHD-C4C	2.84	1.47	1.39
3	L	1606	BCL	O1A-CGA	2.84	1.31	1.22
3	P	1608	BCL	OBB-CAB	2.84	1.29	1.23
3	M	1507	BCL	MG-NC	2.83	2.13	2.06
3	K	1706	BCL	OBD-CAD	2.83	1.27	1.22
3	R	1709	BCL	C2A-C1A	-2.83	1.45	1.52
3	J	1605	BCL	O1D-CGD	2.82	1.28	1.21
5	L	1406	RG1	C11-C10	2.82	1.51	1.43
3	E	1703	BCL	C3B-CAB	2.82	1.55	1.46
3	M	1507	BCL	C1D-C2D	2.82	1.50	1.45
3	N	1607	BCL	CHD-C1D	2.82	1.43	1.38
3	M	1707	BCL	O1A-CGA	2.82	1.30	1.22
3	P	1608	BCL	O2D-CGD	2.82	1.40	1.33
3	R	1709	BCL	C1B-C2B	2.82	1.49	1.43
3	C	1502	BCL	MG-NA	2.82	2.13	2.06
3	N	1607	BCL	CHB-C4A	2.82	1.44	1.37
5	D	1402	RG1	C2-C1	2.81	1.57	1.53
3	S	1609	BCL	MG-NA	2.79	2.12	2.06
3	D	1602	BCL	CBD-CGD	-2.79	1.44	1.52
3	B	1601	BCL	C4B-NB	-2.79	1.34	1.37
3	P	1608	BCL	C1B-C2B	2.79	1.49	1.43
3	J	1605	BCL	C3D-C2D	2.79	1.46	1.39
3	R	1709	BCL	C4D-CHA	2.79	1.47	1.38
5	D	1402	RG1	C11-C10	2.78	1.51	1.43
3	L	1606	BCL	O2A-CGA	2.78	1.41	1.33
3	F	1603	BCL	C1D-C2D	2.78	1.50	1.45
3	O	1508	BCL	MG-NA	2.78	2.12	2.06
3	R	1509	BCL	C1B-C2B	2.78	1.49	1.43
5	R	1401	RG1	CM1-C1	2.77	1.58	1.52
3	S	1609	BCL	C4D-CHA	2.77	1.47	1.38
3	R	1709	BCL	CBD-CGD	-2.77	1.44	1.52
3	K	1506	BCL	C1D-ND	2.77	1.41	1.37
3	I	1705	BCL	MG-NA	2.75	2.12	2.06
3	D	1602	BCL	O2D-CGD	2.73	1.39	1.33
3	A	1701	BCL	CBD-CGD	-2.73	1.44	1.52
5	D	1402	RG1	C7-C6	2.73	1.51	1.43
3	M	1507	BCL	C2A-C1A	-2.73	1.46	1.52
3	L	1606	BCL	C3D-C2D	2.73	1.46	1.39
3	I	1505	BCL	O1D-CGD	2.72	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1509	BCL	C3B-CAB	2.72	1.55	1.46
3	C	1702	BCL	CHC-C1C	2.72	1.44	1.37
3	E	1703	BCL	CHB-C4A	2.72	1.44	1.37
3	K	1506	BCL	O1A-CGA	2.70	1.30	1.22
3	E	1503	BCL	O2A-CGA	2.70	1.41	1.33
3	G	1504	BCL	C3B-C4B	2.69	1.46	1.41
3	C	1502	BCL	O1A-CGA	2.69	1.30	1.22
3	B	1601	BCL	O2A-CGA	2.69	1.41	1.33
5	P	1408	RG1	C24-C25	2.69	1.51	1.43
3	G	1704	BCL	O1A-CGA	2.69	1.30	1.22
3	O	1508	BCL	C3B-C2B	2.69	1.51	1.42
3	H	1604	BCL	O2D-CGD	2.69	1.39	1.33
3	M	1507	BCL	C3B-C2B	2.68	1.51	1.42
3	C	1702	BCL	CHC-C4B	2.68	1.45	1.39
3	O	1708	BCL	CHD-C4C	2.67	1.46	1.39
5	L	1406	RG1	C19-C18	2.67	1.51	1.46
3	O	1508	BCL	O1D-CGD	2.66	1.28	1.21
3	D	1602	BCL	CHC-C1C	2.66	1.44	1.37
3	G	1504	BCL	C3B-C2B	2.66	1.51	1.42
3	I	1705	BCL	CBD-CGD	-2.66	1.44	1.52
3	R	1709	BCL	C1B-NB	2.65	1.41	1.37
3	C	1502	BCL	C2A-C1A	-2.65	1.46	1.52
3	I	1705	BCL	OBB-CAB	2.65	1.29	1.23
3	I	1505	BCL	C2A-C1A	-2.65	1.46	1.52
3	E	1703	BCL	OBB-CAB	2.65	1.29	1.23
3	P	1608	BCL	CHD-C1D	2.65	1.43	1.38
3	N	1607	BCL	MG-ND	-2.64	2.00	2.05
3	P	1608	BCL	O1A-CGA	2.64	1.30	1.22
5	R	1401	RG1	C8-C9	2.64	1.51	1.46
3	R	1509	BCL	MG-NC	2.64	2.12	2.06
3	L	1606	BCL	CHB-C4A	2.64	1.44	1.37
3	F	1603	BCL	CMC-C2C	-2.64	1.47	1.53
3	K	1706	BCL	C9-C8	2.64	1.61	1.52
3	K	1506	BCL	MG-NB	-2.64	2.00	2.05
3	I	1505	BCL	CBD-CGD	-2.63	1.44	1.52
3	K	1706	BCL	CHB-C4A	2.63	1.44	1.37
3	C	1502	BCL	O1D-CGD	2.63	1.27	1.21
3	H	1604	BCL	C2A-C1A	-2.62	1.46	1.52
3	A	1501	BCL	CBD-CAD	-2.62	1.44	1.56
3	K	1506	BCL	C3B-C2B	2.62	1.51	1.42
3	L	1606	BCL	C3B-C2B	2.62	1.51	1.42
3	H	1604	BCL	C2C-C1C	-2.61	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1601	BCL	MG-NA	2.61	2.12	2.06
5	N	1407	RG1	C27-C26	2.61	1.51	1.46
3	K	1706	BCL	C1D-ND	2.61	1.41	1.37
3	G	1504	BCL	MG-NB	-2.60	2.00	2.05
3	E	1703	BCL	MG-ND	-2.59	2.00	2.05
3	D	1602	BCL	CHD-C1D	2.59	1.43	1.38
3	R	1509	BCL	CHD-C1D	2.58	1.43	1.38
3	R	1709	BCL	C3C-C4C	-2.58	1.48	1.51
3	A	1701	BCL	C5-C3	2.58	1.56	1.51
3	H	1604	BCL	CHC-C1C	2.57	1.44	1.37
3	K	1506	BCL	CBD-CGD	-2.57	1.44	1.52
3	S	1609	BCL	CHD-C1D	2.57	1.43	1.38
3	S	1609	BCL	CBB-CAB	-2.57	1.45	1.50
3	J	1605	BCL	C3A-C2A	-2.56	1.47	1.54
3	A	1501	BCL	O2A-CGA	2.56	1.40	1.33
3	G	1504	BCL	MG-ND	-2.56	2.00	2.05
3	M	1507	BCL	C2C-C3C	-2.56	1.47	1.54
3	I	1705	BCL	C3D-CAD	2.56	1.53	1.45
3	I	1505	BCL	CHD-C1D	2.56	1.43	1.38
5	J	1405	RG1	C8-C9	2.55	1.51	1.46
3	D	1602	BCL	OBB-CAB	2.55	1.29	1.23
3	O	1508	BCL	CHB-C1B	2.55	1.45	1.39
3	F	1603	BCL	O1A-CGA	2.54	1.30	1.22
3	E	1503	BCL	C3B-C2B	2.54	1.51	1.42
5	N	1407	RG1	C15-C14	2.54	1.51	1.43
3	A	1701	BCL	MG-NC	2.54	2.12	2.06
3	M	1707	BCL	C4D-CHA	2.53	1.47	1.38
3	I	1705	BCL	O1D-CGD	2.52	1.27	1.21
3	S	1609	BCL	O2D-CGD	2.52	1.39	1.33
3	P	1608	BCL	CBA-CGA	-2.52	1.43	1.50
3	G	1704	BCL	C4B-NB	2.51	1.41	1.37
3	L	1606	BCL	OBB-CAB	2.51	1.28	1.23
3	D	1602	BCL	C3C-C4C	-2.51	1.48	1.51
5	H	1404	RG1	CM5-C13	-2.51	1.45	1.50
3	J	1605	BCL	CAA-C2A	-2.51	1.49	1.54
3	J	1605	BCL	O2D-CED	-2.50	1.39	1.45
3	M	1707	BCL	CHC-C4B	2.50	1.45	1.39
5	P	1408	RG1	CM7-C22	-2.49	1.45	1.50
3	M	1707	BCL	CHC-C1C	2.49	1.43	1.37
3	B	1601	BCL	CHC-C1C	2.49	1.43	1.37
3	K	1506	BCL	MG-NC	2.49	2.12	2.06
3	P	1608	BCL	CHC-C1C	2.48	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1506	BCL	CHB-C1B	2.48	1.45	1.39
3	E	1703	BCL	C1B-C2B	2.48	1.49	1.43
3	A	1701	BCL	C1B-NB	2.48	1.41	1.37
3	C	1702	BCL	C4D-CHA	2.48	1.46	1.38
3	A	1701	BCL	CHC-C1C	2.48	1.43	1.37
3	I	1705	BCL	CHB-C4A	2.47	1.43	1.37
3	H	1604	BCL	C1D-C2D	2.47	1.50	1.45
3	M	1707	BCL	C5-C3	2.47	1.56	1.51
3	N	1607	BCL	C3C-C4C	-2.46	1.48	1.51
3	I	1705	BCL	MG-NC	2.46	2.12	2.06
5	D	1402	RG1	C28-C27	-2.46	1.28	1.34
3	K	1506	BCL	CBD-CAD	-2.46	1.45	1.56
3	F	1603	BCL	O2D-CED	-2.45	1.39	1.45
3	G	1704	BCL	CBD-CHA	-2.45	1.38	1.51
3	B	1601	BCL	O1A-CGA	2.44	1.29	1.22
3	O	1508	BCL	C4D-CHA	2.44	1.46	1.38
3	D	1602	BCL	C3B-C2B	2.44	1.50	1.42
3	H	1604	BCL	O2A-CGA	2.44	1.40	1.33
3	K	1506	BCL	CHC-C1C	2.43	1.43	1.37
3	O	1708	BCL	C3B-CAB	2.43	1.54	1.46
5	R	1401	RG1	C11-C10	2.43	1.50	1.43
3	N	1607	BCL	C1D-C2D	2.42	1.50	1.45
3	M	1507	BCL	C1D-ND	2.42	1.41	1.37
3	I	1505	BCL	C4B-NB	2.42	1.41	1.37
3	G	1704	BCL	OBB-CAB	2.42	1.28	1.23
3	O	1708	BCL	O1A-CGA	2.41	1.29	1.22
3	R	1709	BCL	C3B-C2B	2.41	1.50	1.42
5	P	1408	RG1	C28-C29	2.40	1.50	1.43
5	D	1402	RG1	C8-C9	2.40	1.51	1.46
3	C	1702	BCL	C3B-C2B	2.40	1.50	1.42
3	D	1602	BCL	CMD-C2D	-2.39	1.45	1.50
3	K	1706	BCL	C4D-CHA	2.38	1.46	1.38
3	O	1708	BCL	C4B-NB	2.38	1.41	1.37
3	S	1609	BCL	C2A-C1A	-2.38	1.46	1.52
4	C	1815	LDA	C1-N1	-2.37	1.49	1.51
3	D	1602	BCL	C1D-ND	2.36	1.41	1.37
5	S	1409	RG1	C12-C13	2.36	1.51	1.46
5	P	1408	RG1	CM5-C13	-2.36	1.46	1.50
3	E	1503	BCL	CBB-CAB	-2.35	1.45	1.50
3	C	1502	BCL	CAC-C3C	-2.35	1.49	1.54
3	O	1708	BCL	C1B-C2B	2.35	1.48	1.43
5	D	1402	RG1	O5'-C1'	2.35	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	1408	RG1	C19-C18	2.35	1.51	1.46
3	E	1703	BCL	C3B-C2B	2.35	1.50	1.42
3	F	1603	BCL	C3C-C4C	-2.34	1.48	1.51
3	C	1502	BCL	C1D-C2D	2.34	1.50	1.45
3	E	1503	BCL	C1B-C2B	2.34	1.48	1.43
3	B	1601	BCL	MG-NC	2.34	2.11	2.06
3	B	1601	BCL	C3A-C2A	-2.33	1.48	1.54
3	M	1507	BCL	C3B-CAB	2.33	1.54	1.46
3	O	1708	BCL	CMD-C2D	-2.32	1.46	1.50
3	G	1504	BCL	CHD-C1D	2.32	1.42	1.38
3	K	1706	BCL	O2D-CGD	2.32	1.38	1.33
3	R	1709	BCL	O2A-CGA	2.32	1.40	1.33
3	F	1603	BCL	O1D-CGD	2.31	1.27	1.21
3	G	1504	BCL	C3B-CAB	2.31	1.54	1.46
3	H	1604	BCL	MG-NA	2.31	2.11	2.06
3	F	1603	BCL	MG-NB	-2.31	2.01	2.05
3	K	1506	BCL	C1D-C2D	2.30	1.49	1.45
3	H	1604	BCL	C4D-CHA	2.30	1.46	1.38
3	I	1505	BCL	CBD-CAD	-2.30	1.46	1.56
3	B	1601	BCL	C4D-CHA	2.30	1.46	1.38
3	H	1604	BCL	OBD-CAD	2.29	1.26	1.22
3	K	1506	BCL	MG-NA	2.29	2.11	2.06
3	O	1508	BCL	C3D-C2D	2.29	1.45	1.39
3	I	1705	BCL	C4B-NB	2.28	1.40	1.37
3	C	1702	BCL	MG-NC	2.28	2.11	2.06
3	K	1506	BCL	OBB-CAB	2.27	1.28	1.23
4	P	1808	LDA	C1-N1	-2.27	1.49	1.51
3	I	1705	BCL	CHD-C4C	2.27	1.45	1.39
3	G	1504	BCL	CMD-C2D	-2.27	1.46	1.50
3	C	1502	BCL	O2D-CGD	2.27	1.38	1.33
3	A	1501	BCL	C1D-C2D	2.27	1.49	1.45
5	S	1409	RG1	O5'-C1'	2.26	1.47	1.41
3	C	1502	BCL	C3B-CAB	2.26	1.53	1.46
3	E	1703	BCL	O1A-CGA	2.25	1.29	1.22
3	S	1609	BCL	C4B-NB	-2.24	1.34	1.37
3	N	1607	BCL	CHC-C1C	2.24	1.43	1.37
3	K	1706	BCL	C4B-NB	2.24	1.40	1.37
4	L	1806	LDA	C1-N1	2.24	1.53	1.51
3	I	1705	BCL	CHC-C4B	2.24	1.44	1.39
3	R	1709	BCL	C3B-CAB	2.24	1.53	1.46
3	C	1702	BCL	O2A-CGA	2.23	1.39	1.33
3	I	1505	BCL	C4D-CHA	2.23	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1704	BCL	C3B-CAB	2.21	1.53	1.46
3	I	1705	BCL	CHC-C1C	2.21	1.43	1.37
5	S	1409	RG1	CM6-C18	-2.20	1.46	1.50
3	C	1702	BCL	OBD-CAD	2.20	1.26	1.22
3	G	1504	BCL	C4D-CHA	2.20	1.46	1.38
3	O	1708	BCL	CBD-CGD	-2.20	1.45	1.52
3	J	1605	BCL	C1B-C2B	2.20	1.48	1.43
3	L	1606	BCL	O2D-CED	-2.19	1.40	1.45
3	F	1603	BCL	C1B-C2B	2.19	1.48	1.43
3	C	1702	BCL	C3C-C4C	-2.19	1.48	1.51
3	M	1707	BCL	C1B-NB	2.19	1.40	1.37
3	C	1702	BCL	CHD-C4C	2.19	1.45	1.39
3	C	1702	BCL	C2A-C1A	-2.17	1.47	1.52
3	H	1604	BCL	C1B-C2B	2.17	1.48	1.43
3	I	1505	BCL	C3B-CAB	2.17	1.53	1.46
3	R	1709	BCL	CMD-C2D	-2.17	1.46	1.50
3	I	1705	BCL	CMB-C2B	-2.16	1.46	1.50
3	O	1708	BCL	OBD-CAD	2.16	1.26	1.22
3	R	1509	BCL	CBB-CAB	-2.16	1.46	1.50
3	A	1701	BCL	C1B-C2B	2.16	1.48	1.43
3	R	1709	BCL	OBD-CAD	2.16	1.26	1.22
3	O	1508	BCL	CBD-CAD	-2.16	1.46	1.56
3	G	1704	BCL	CMC-C2C	2.16	1.57	1.53
3	J	1605	BCL	CBD-CAD	-2.15	1.46	1.56
3	R	1509	BCL	CAA-CBA	-2.15	1.46	1.52
5	J	1405	RG1	C12-C13	2.14	1.50	1.46
5	J	1405	RG1	C11-C10	2.14	1.49	1.43
5	J	1405	RG1	C15-C14	2.14	1.49	1.43
3	D	1602	BCL	CHC-C4B	2.13	1.44	1.39
3	F	1603	BCL	CHC-C1C	2.13	1.43	1.37
3	B	1601	BCL	CHB-C4A	2.13	1.43	1.37
3	R	1709	BCL	C1-C2	2.13	1.55	1.49
3	J	1605	BCL	C3B-C2B	2.11	1.49	1.42
5	L	1406	RG1	O2'-C2'	2.11	1.48	1.43
3	E	1703	BCL	CHB-C1B	2.11	1.44	1.39
3	I	1705	BCL	MG-NB	-2.11	2.01	2.05
3	C	1702	BCL	C5-C3	2.11	1.55	1.51
5	P	1408	RG1	O5'-C1'	2.11	1.47	1.41
5	L	1406	RG1	C20-C21	2.11	1.49	1.43
5	H	1404	RG1	C11-C10	2.11	1.49	1.43
3	J	1605	BCL	C1A-CHA	2.10	1.51	1.43
3	H	1604	BCL	C5-C3	2.10	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1603	BCL	C3B-C2B	2.10	1.49	1.42
5	P	1408	RG1	C11-C10	2.09	1.49	1.43
3	O	1508	BCL	C3B-C4B	2.09	1.45	1.41
3	R	1709	BCL	C4B-NB	2.08	1.40	1.37
3	I	1705	BCL	MG-ND	2.08	2.09	2.05
3	J	1605	BCL	C4B-NB	-2.08	1.35	1.37
3	P	1608	BCL	C3C-C4C	-2.08	1.49	1.51
3	L	1606	BCL	CAC-C3C	-2.07	1.50	1.54
3	B	1601	BCL	C3B-C2B	2.07	1.49	1.42
3	L	1606	BCL	C1D-C2D	2.07	1.49	1.45
3	G	1704	BCL	C1A-CHA	2.07	1.51	1.43
3	K	1706	BCL	CHD-C4C	2.07	1.45	1.39
3	E	1703	BCL	CHD-C1D	2.07	1.42	1.38
3	O	1508	BCL	C1B-C2B	2.06	1.48	1.43
3	L	1606	BCL	MG-NA	2.06	2.11	2.06
3	N	1607	BCL	MG-NB	-2.06	2.01	2.05
3	H	1604	BCL	CMD-C2D	-2.06	1.46	1.50
3	M	1707	BCL	O1D-CGD	2.06	1.26	1.21
3	E	1503	BCL	C1D-ND	2.06	1.40	1.37
3	O	1708	BCL	C3B-C2B	2.05	1.49	1.42
3	S	1609	BCL	C3B-CAB	2.05	1.53	1.46
3	C	1702	BCL	MG-NA	2.04	2.11	2.06
3	E	1703	BCL	C4D-CHA	2.04	1.45	1.38
3	M	1507	BCL	CHC-C4B	2.04	1.44	1.39
3	M	1507	BCL	MG-NA	2.03	2.11	2.06
5	H	1404	RG1	C7-C6	2.03	1.49	1.43
3	E	1503	BCL	O2D-CGD	2.02	1.38	1.33
3	G	1504	BCL	C1B-C2B	2.02	1.47	1.43
3	J	1605	BCL	CHC-C1C	2.01	1.42	1.37
3	E	1503	BCL	C2A-C1A	-2.01	1.47	1.52
5	H	1404	RG1	C4-C5	2.01	1.55	1.51
3	P	1608	BCL	C1D-C2D	2.01	1.49	1.45
5	S	1409	RG1	C19-C18	2.00	1.50	1.46

All (787) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1606	BCL	C4A-NA-C1A	-14.45	100.09	106.68
3	B	1601	BCL	C4A-NA-C1A	-13.44	100.55	106.68
3	R	1509	BCL	C4A-NA-C1A	-12.21	101.11	106.68
3	M	1507	BCL	C4A-NA-C1A	-11.78	101.30	106.68
3	D	1602	BCL	C4A-NA-C1A	-11.64	101.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1605	BCL	C4A-NA-C1A	-10.51	101.89	106.68
3	E	1503	BCL	C4A-NA-C1A	-10.47	101.90	106.68
3	N	1607	BCL	C4A-NA-C1A	-10.09	102.08	106.68
3	F	1603	BCL	C4A-NA-C1A	-9.82	102.20	106.68
3	C	1502	BCL	C4A-NA-C1A	-9.45	102.37	106.68
3	J	1605	BCL	C1C-NC-C4C	-9.28	102.44	106.68
3	A	1701	BCL	C4A-NA-C1A	-9.22	102.47	106.68
3	K	1506	BCL	C4A-NA-C1A	-9.17	102.50	106.68
3	P	1608	BCL	C1C-NC-C4C	-9.07	102.54	106.68
3	A	1501	BCL	C4A-NA-C1A	-8.93	102.61	106.68
3	L	1606	BCL	C1C-NC-C4C	-8.86	102.64	106.68
3	S	1609	BCL	C4A-NA-C1A	-8.85	102.64	106.68
3	K	1706	BCL	C4A-NA-C1A	-8.74	102.69	106.68
3	I	1505	BCL	C4A-NA-C1A	-8.72	102.70	106.68
3	S	1609	BCL	C1C-NC-C4C	-8.48	102.81	106.68
3	O	1508	BCL	C4A-NA-C1A	-8.36	102.86	106.68
3	C	1702	BCL	C4A-NA-C1A	-8.34	102.87	106.68
3	G	1704	BCL	C1-C2-C3	-8.19	112.78	126.20
3	G	1504	BCL	C4A-NA-C1A	-8.15	102.96	106.68
3	P	1608	BCL	C4A-NA-C1A	-8.11	102.98	106.68
3	O	1708	BCL	C4A-NA-C1A	-7.99	103.04	106.68
3	K	1706	BCL	C1-C2-C3	-7.87	113.31	126.20
3	R	1709	BCL	C4A-NA-C1A	-7.84	103.10	106.68
3	M	1707	BCL	C1-C2-C3	-7.70	113.58	126.20
3	H	1604	BCL	C4A-NA-C1A	-7.63	103.20	106.68
3	K	1506	BCL	C1-C2-C3	-7.63	113.69	126.20
3	I	1705	BCL	C1-C2-C3	-7.60	113.75	126.20
3	I	1705	BCL	C4A-NA-C1A	-7.58	103.22	106.68
3	A	1701	BCL	C1-C2-C3	-7.32	114.20	126.20
3	O	1708	BCL	C1-C2-C3	-7.14	114.49	126.20
3	B	1601	BCL	C1C-NC-C4C	-7.08	103.45	106.68
3	N	1607	BCL	C1C-NC-C4C	-6.93	103.52	106.68
3	E	1703	BCL	C1-C2-C3	-6.86	114.96	126.20
3	I	1505	BCL	C1-C2-C3	-6.86	114.97	126.20
3	R	1709	BCL	C1-C2-C3	-6.78	115.09	126.20
3	M	1507	BCL	C1C-NC-C4C	-6.71	103.62	106.68
3	C	1702	BCL	C1-C2-C3	-6.64	115.32	126.20
3	A	1501	BCL	C1-C2-C3	-6.62	115.36	126.20
3	H	1604	BCL	C1C-NC-C4C	-6.55	103.69	106.68
3	D	1602	BCL	C1-C2-C3	-6.50	115.54	126.20
3	G	1704	BCL	C4A-NA-C1A	-6.43	103.75	106.68
3	E	1703	BCL	C4A-NA-C1A	-6.39	103.76	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1607	BCL	C1-C2-C3	-6.26	115.93	126.20
3	R	1509	BCL	C1-C2-C3	-6.15	116.12	126.20
3	E	1503	BCL	C1-C2-C3	-5.99	116.38	126.20
3	G	1504	BCL	C1-C2-C3	-5.98	116.40	126.20
3	A	1501	BCL	C1C-NC-C4C	-5.95	103.97	106.68
5	H	1404	RG1	C16-C17-C18	-5.81	119.14	127.28
3	L	1606	BCL	C1-C2-C3	-5.77	116.75	126.20
5	J	1405	RG1	C16-C17-C18	-5.72	119.25	127.28
3	K	1706	BCL	C1C-NC-C4C	-5.69	104.08	106.68
3	P	1608	BCL	C1-C2-C3	-5.69	116.87	126.20
5	R	1401	RG1	C16-C17-C18	-5.64	119.38	127.28
3	C	1502	BCL	C1-C2-C3	-5.62	117.00	126.20
3	E	1503	BCL	C1C-NC-C4C	-5.58	104.13	106.68
3	K	1506	BCL	C1C-NC-C4C	-5.53	104.15	106.68
5	D	1402	RG1	C16-C17-C18	-5.53	119.52	127.28
3	B	1601	BCL	C1-C2-C3	-5.40	117.36	126.20
3	M	1707	BCL	C4A-NA-C1A	-5.38	104.22	106.68
3	K	1506	BCL	C2C-C3C-C4C	5.38	109.40	101.34
3	F	1603	BCL	C1-C2-C3	-5.32	117.47	126.20
3	H	1604	BCL	C1-C2-C3	-5.31	117.49	126.20
3	A	1701	BCL	C1C-NC-C4C	-5.24	104.29	106.68
3	J	1605	BCL	C1-C2-C3	-5.23	117.63	126.20
3	F	1603	BCL	CHB-C1B-NB	5.22	131.87	124.05
3	N	1607	BCL	CHB-C1B-NB	5.21	131.87	124.05
3	M	1507	BCL	C1-C2-C3	-5.17	117.73	126.20
3	B	1601	BCL	CHB-C1B-NB	5.16	131.79	124.05
3	A	1701	BCL	CHB-C1B-NB	5.09	131.68	124.05
5	N	1407	RG1	C16-C17-C18	-5.09	120.14	127.28
3	R	1509	BCL	O2D-CGD-CBD	5.08	120.12	111.23
3	S	1609	BCL	CHB-C1B-NB	5.07	131.66	124.05
3	M	1507	BCL	CHB-C1B-NB	5.07	131.66	124.05
3	R	1709	BCL	O2D-CGD-CBD	5.06	120.08	111.23
3	A	1501	BCL	CHB-C1B-NB	5.02	131.58	124.05
3	O	1508	BCL	C1-C2-C3	-5.02	117.97	126.20
3	D	1602	BCL	CHB-C1B-NB	5.02	131.57	124.05
3	J	1605	BCL	CHB-C1B-NB	4.98	131.52	124.05
3	L	1606	BCL	CHB-C1B-NB	4.97	131.50	124.05
3	G	1704	BCL	C3D-C2D-C1D	-4.95	99.07	105.83
3	G	1704	BCL	C1C-NC-C4C	-4.93	104.43	106.68
3	O	1508	BCL	C1C-NC-C4C	-4.92	104.44	106.68
3	D	1602	BCL	C1C-NC-C4C	-4.89	104.45	106.68
3	R	1709	BCL	CHB-C1B-NB	4.83	131.30	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1705	BCL	OBB-CAB-C3B	-4.83	111.90	120.43
3	G	1504	BCL	CHB-C1B-NB	4.83	131.29	124.05
3	O	1508	BCL	OBB-CAB-C3B	-4.82	111.91	120.43
3	I	1705	BCL	CHB-C1B-NB	4.82	131.28	124.05
5	P	1408	RG1	C16-C17-C18	-4.80	120.54	127.28
3	E	1703	BCL	C1C-NC-C4C	-4.79	104.49	106.68
3	E	1703	BCL	CHB-C1B-NB	4.77	131.21	124.05
5	S	1409	RG1	C16-C17-C18	-4.71	120.67	127.28
3	O	1708	BCL	CHB-C1B-NB	4.69	131.09	124.05
5	R	1401	RG1	C7-C6-C5	-4.69	121.10	127.69
3	O	1508	BCL	C3D-C2D-C1D	-4.67	99.45	105.83
3	O	1508	BCL	CHB-C1B-NB	4.67	131.06	124.05
3	C	1502	BCL	C6-C5-C3	-4.67	102.09	113.47
3	L	1606	BCL	O2D-CGD-O1D	-4.66	114.78	123.85
3	H	1604	BCL	CHB-C1B-NB	4.65	131.03	124.05
3	K	1706	BCL	CHB-C1B-NB	4.64	131.02	124.05
3	C	1502	BCL	C1C-NC-C4C	-4.64	104.56	106.68
3	C	1502	BCL	OBB-CAB-C3B	-4.63	112.24	120.43
3	L	1606	BCL	OBB-CAB-C3B	-4.62	112.26	120.43
5	D	1402	RG1	C7-C6-C5	-4.60	121.23	127.69
3	I	1705	BCL	C1C-NC-C4C	-4.59	104.59	106.68
3	E	1503	BCL	C3D-C2D-C1D	-4.57	99.59	105.83
3	A	1701	BCL	OBB-CAB-C3B	-4.57	112.35	120.43
3	F	1603	BCL	C3D-C2D-C1D	-4.57	99.60	105.83
3	C	1702	BCL	CHB-C1B-NB	4.56	130.89	124.05
3	P	1608	BCL	CHB-C1B-NB	4.55	130.88	124.05
5	R	1401	RG1	C28-C29-C30	-4.54	120.54	127.48
3	J	1605	BCL	OBB-CAB-C3B	-4.53	112.42	120.43
3	A	1501	BCL	O2D-CGD-CBD	4.52	119.14	111.23
3	G	1704	BCL	CHB-C1B-NB	4.52	130.82	124.05
3	O	1708	BCL	OBB-CAB-C3B	-4.51	112.47	120.43
3	C	1502	BCL	C3D-C2D-C1D	-4.50	99.68	105.83
3	E	1503	BCL	CHB-C1B-NB	4.49	130.78	124.05
5	F	1403	RG1	C11-C10-C9	-4.48	120.99	127.28
3	M	1507	BCL	C3D-C2D-C1D	-4.48	99.72	105.83
3	S	1609	BCL	C3D-C2D-C1D	-4.48	99.72	105.83
3	O	1708	BCL	O2A-CGA-O1A	-4.47	112.44	123.63
3	C	1702	BCL	OBB-CAB-C3B	-4.43	112.60	120.43
3	M	1707	BCL	C3D-C2D-C1D	-4.42	99.80	105.83
3	G	1504	BCL	C1C-NC-C4C	-4.42	104.66	106.68
3	L	1606	BCL	C3D-C2D-C1D	-4.40	99.83	105.83
3	M	1707	BCL	C1C-NC-C4C	-4.34	104.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1502	BCL	CHB-C1B-NB	4.33	130.55	124.05
3	M	1707	BCL	CHB-C1B-NB	4.33	130.54	124.05
3	S	1609	BCL	C1-C2-C3	-4.32	119.12	126.20
3	H	1604	BCL	C3D-C2D-C1D	-4.32	99.93	105.83
3	B	1601	BCL	C3D-C2D-C1D	-4.32	99.94	105.83
3	N	1607	BCL	O2D-CGD-CBD	4.31	118.76	111.23
3	B	1601	BCL	OBb-CAB-C3B	-4.31	112.82	120.43
3	R	1509	BCL	C3A-C2A-C1A	-4.29	94.91	101.34
5	N	1407	RG1	C7-C6-C5	-4.28	121.67	127.69
3	S	1609	BCL	O2D-CGD-CBD	4.28	118.70	111.23
3	K	1506	BCL	C3D-C2D-C1D	-4.27	100.01	105.83
3	N	1607	BCL	C3D-C2D-C1D	-4.23	100.05	105.83
5	S	1409	RG1	C7-C6-C5	-4.22	121.75	127.69
3	A	1501	BCL	OBb-CAB-C3B	-4.21	113.00	120.43
3	M	1707	BCL	OBb-CAB-C3B	-4.20	113.00	120.43
3	R	1709	BCL	C3D-C2D-C1D	-4.20	100.09	105.83
3	N	1607	BCL	OBb-CAB-C3B	-4.17	113.05	120.43
3	G	1504	BCL	O2A-CGA-O1A	-4.17	113.20	123.63
3	B	1601	BCL	O2D-CGD-CBD	4.17	118.52	111.23
5	F	1403	RG1	C16-C17-C18	-4.13	121.49	127.28
3	C	1702	BCL	C3D-C2D-C1D	-4.09	100.25	105.83
3	L	1606	BCL	O2D-CGD-CBD	4.09	118.37	111.23
3	O	1508	BCL	O2D-CGD-CBD	4.07	118.35	111.23
3	D	1602	BCL	OBb-CAB-C3B	-4.05	113.27	120.43
3	S	1609	BCL	OBb-CAB-C3B	-4.04	113.29	120.43
3	M	1707	BCL	O2A-CGA-O1A	-4.04	113.53	123.63
3	K	1706	BCL	O2A-CGA-O1A	-4.03	113.55	123.63
3	K	1706	BCL	O2D-CGD-CBD	4.02	118.26	111.23
3	G	1504	BCL	C3D-C2D-C1D	-4.02	100.34	105.83
5	L	1406	RG1	C7-C6-C5	-4.02	122.04	127.69
3	R	1509	BCL	CHB-C1B-NB	4.02	130.07	124.05
3	I	1505	BCL	CHB-C1B-NB	4.01	130.07	124.05
3	H	1604	BCL	O2D-CGD-CBD	4.01	118.25	111.23
3	J	1605	BCL	C3D-C2D-C1D	-4.00	100.38	105.83
3	R	1509	BCL	C3D-C2D-C1D	-3.98	100.40	105.83
5	L	1406	RG1	C11-C10-C9	-3.97	121.70	127.28
3	D	1602	BCL	C3D-C2D-C1D	-3.97	100.41	105.83
5	R	1401	RG1	C16-C15-C14	-3.95	115.45	123.52
5	P	1408	RG1	C7-C6-C5	-3.94	122.14	127.69
3	C	1502	BCL	O2D-CGD-CBD	3.94	118.12	111.23
3	I	1705	BCL	O2A-CGA-O1A	-3.93	113.79	123.63
3	I	1505	BCL	C3D-C2D-C1D	-3.93	100.47	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1608	BCL	C3D-C2D-C1D	-3.93	100.47	105.83
3	I	1505	BCL	OBB-CAB-C3B	-3.92	113.50	120.43
3	N	1607	BCL	O2A-CGA-O1A	-3.92	113.82	123.63
3	G	1704	BCL	OBB-CAB-C3B	-3.92	113.51	120.43
3	J	1605	BCL	CBA-CAA-C2A	-3.90	102.19	113.79
3	K	1706	BCL	OBB-CAB-C3B	-3.89	113.55	120.43
5	N	1407	RG1	C1-O1'-C1'	-3.89	111.82	119.78
3	G	1704	BCL	O2A-CGA-O1A	-3.89	113.90	123.63
3	E	1703	BCL	O2A-CGA-O1A	-3.89	113.91	123.63
3	C	1502	BCL	O2A-CGA-O1A	-3.89	113.91	123.63
3	P	1608	BCL	CMC-C2C-C1C	3.87	122.17	111.77
3	K	1506	BCL	CHB-C1B-NB	3.85	129.82	124.05
3	M	1507	BCL	O2A-CGA-O1A	-3.83	114.05	123.63
3	R	1509	BCL	O2A-CGA-O1A	-3.82	114.08	123.63
3	M	1507	BCL	OBB-CAB-C3B	-3.81	113.69	120.43
3	F	1603	BCL	O2D-CGD-CBD	3.80	117.87	111.23
3	R	1709	BCL	OBB-CAB-C3B	-3.79	113.72	120.43
3	R	1709	BCL	O2A-CGA-O1A	-3.78	114.16	123.63
3	J	1605	BCL	O2D-CGD-CBD	3.78	117.84	111.23
3	F	1603	BCL	C1C-NC-C4C	-3.77	104.96	106.68
3	A	1701	BCL	O2A-CGA-O1A	-3.77	114.19	123.63
3	O	1508	BCL	O2A-CGA-O1A	-3.77	114.19	123.63
3	I	1705	BCL	O2D-CGD-CBD	3.77	117.82	111.23
5	S	1409	RG1	CM7-C22-C23	3.77	123.84	118.09
3	K	1706	BCL	C3D-C2D-C1D	-3.76	100.70	105.83
3	E	1503	BCL	O2D-CGD-CBD	3.75	117.79	111.23
5	P	1408	RG1	C24-C25-C26	-3.75	122.02	127.28
5	H	1404	RG1	C7-C6-C5	-3.74	122.43	127.69
3	A	1701	BCL	C3D-C2D-C1D	-3.73	100.74	105.83
3	E	1503	BCL	O2A-CGA-O1A	-3.72	114.32	123.63
5	L	1406	RG1	C16-C15-C14	-3.72	115.90	123.52
3	A	1501	BCL	C3D-C2D-C1D	-3.71	100.77	105.83
3	P	1608	BCL	OBB-CAB-C3B	-3.71	113.88	120.43
3	E	1703	BCL	C3D-C2D-C1D	-3.71	100.77	105.83
3	F	1603	BCL	C6-C5-C3	-3.70	104.46	113.47
3	G	1704	BCL	C6-C5-C3	-3.69	104.48	113.47
3	F	1603	BCL	OBB-CAB-C3B	-3.68	113.92	120.43
3	B	1601	BCL	O2A-CGA-O1A	-3.68	114.44	123.63
5	P	1408	RG1	C16-C15-C14	-3.66	116.03	123.52
3	H	1604	BCL	CMC-C2C-C1C	3.65	121.59	111.77
3	G	1704	BCL	C4D-C3D-CAD	-3.62	104.17	108.11
3	M	1507	BCL	O2D-CGD-CBD	3.62	117.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1604	BCL	C3C-C2C-C1C	3.61	107.70	101.87
3	H	1604	BCL	OBB-CAB-C3B	-3.61	114.06	120.43
3	F	1603	BCL	O2A-CGA-O1A	-3.60	114.61	123.63
3	E	1503	BCL	OBB-CAB-C3B	-3.60	114.06	120.43
5	L	1406	RG1	C1-O1'-C1'	-3.60	112.41	119.78
3	O	1508	BCL	O2D-CGD-O1D	-3.60	116.84	123.85
3	I	1705	BCL	C4-C3-C5	3.60	121.47	115.23
3	G	1504	BCL	C6-C5-C3	-3.60	104.71	113.47
3	I	1505	BCL	O2A-CGA-O1A	-3.59	114.64	123.63
3	G	1704	BCL	O2D-CGD-CBD	3.59	117.51	111.23
3	A	1501	BCL	CHB-C1B-C2B	-3.58	117.02	127.43
3	C	1702	BCL	O2A-CGA-O1A	-3.58	114.67	123.63
3	A	1701	BCL	CHB-C1B-C2B	-3.57	117.08	127.43
5	H	1404	RG1	CM3-C5-C4	3.56	121.40	115.23
3	L	1606	BCL	C2A-C3A-C4A	3.55	107.60	101.87
3	H	1604	BCL	CBA-CAA-C2A	-3.55	103.24	113.79
5	J	1405	RG1	C1-O1'-C1'	-3.54	112.53	119.78
3	F	1603	BCL	CHB-C1B-C2B	-3.52	117.20	127.43
3	P	1608	BCL	CBA-CAA-C2A	-3.52	103.31	113.79
3	L	1606	BCL	C3C-C2C-C1C	3.52	107.55	101.87
3	S	1609	BCL	C14-C13-C12	3.51	123.79	111.27
3	E	1703	BCL	CHB-C1B-C2B	-3.50	117.26	127.43
3	C	1502	BCL	O2D-CGD-O1D	-3.50	117.03	123.85
5	P	1408	RG1	C11-C10-C9	-3.50	122.38	127.28
5	J	1405	RG1	C20-C21-C22	-3.49	122.38	127.28
3	K	1506	BCL	C6-C5-C3	-3.49	104.98	113.47
3	R	1709	BCL	CMD-C2D-C1D	3.48	130.86	124.73
3	L	1606	BCL	CHB-C1B-C2B	-3.48	117.32	127.43
3	D	1602	BCL	O2D-CGD-CBD	3.47	117.30	111.23
3	I	1705	BCL	C3D-C2D-C1D	-3.46	101.10	105.83
3	K	1506	BCL	CBC-CAC-C3C	-3.46	106.07	113.41
3	G	1704	BCL	CHA-C1A-NA	-3.45	118.58	126.39
3	S	1609	BCL	O2D-CGD-O1D	-3.44	117.15	123.85
3	L	1606	BCL	O2A-CGA-O1A	-3.44	115.03	123.63
3	M	1507	BCL	CHB-C1B-C2B	-3.44	117.45	127.43
3	S	1609	BCL	CBA-CAA-C2A	-3.43	103.59	113.79
3	O	1708	BCL	C3D-C2D-C1D	-3.43	101.16	105.83
3	R	1709	BCL	O2A-CGA-CBA	3.42	122.27	111.83
3	R	1709	BCL	CHB-C1B-C2B	-3.42	117.50	127.43
3	S	1609	BCL	CHC-C4B-NB	3.41	129.16	124.05
3	A	1501	BCL	O2D-CGD-O1D	-3.40	117.22	123.85
3	B	1601	BCL	CHB-C1B-C2B	-3.40	117.55	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1407	RG1	C11-C10-C9	-3.39	122.53	127.28
3	I	1705	BCL	CHB-C1B-C2B	-3.38	117.62	127.43
3	O	1708	BCL	O2A-CGA-CBA	3.37	122.12	111.83
3	O	1708	BCL	CHB-C1B-C2B	-3.37	117.63	127.43
3	D	1602	BCL	CHB-C1B-C2B	-3.37	117.63	127.43
5	N	1407	RG1	C16-C15-C14	-3.37	116.63	123.52
3	I	1505	BCL	CMD-C2D-C1D	3.35	130.63	124.73
3	H	1604	BCL	CMC-C2C-C3C	3.35	126.95	113.98
3	C	1702	BCL	CHB-C1B-C2B	-3.33	117.75	127.43
3	J	1605	BCL	CHB-C1B-C2B	-3.33	117.75	127.43
3	D	1602	BCL	O2A-CGA-O1A	-3.33	115.30	123.63
3	E	1703	BCL	C4-C3-C5	3.32	121.00	115.23
5	D	1402	RG1	C28-C29-C30	-3.32	122.41	127.48
3	M	1707	BCL	CHB-C1B-C2B	-3.31	117.82	127.43
3	A	1701	BCL	C2C-C3C-C4C	3.30	106.29	101.34
5	S	1409	RG1	C16-C15-C14	-3.30	116.76	123.52
5	R	1401	RG1	C11-C10-C9	-3.30	122.65	127.28
3	S	1609	BCL	CHB-C1B-C2B	-3.29	117.89	127.43
3	K	1506	BCL	C1D-CHD-C4C	-3.29	118.70	126.62
3	K	1706	BCL	O2D-CGD-O1D	-3.27	117.48	123.85
3	M	1707	BCL	CMD-C2D-C1D	3.27	130.48	124.73
3	G	1504	BCL	OBB-CAB-C3B	-3.25	114.68	120.43
3	A	1501	BCL	O2A-CGA-O1A	-3.24	115.52	123.63
3	K	1506	BCL	CBA-CAA-C2A	-3.23	104.17	113.79
3	E	1703	BCL	OBB-CAB-C3B	-3.23	114.72	120.43
3	N	1607	BCL	CHB-C1B-C2B	-3.22	118.08	127.43
3	K	1506	BCL	O2A-CGA-O1A	-3.22	115.57	123.63
3	E	1503	BCL	C6-C5-C3	-3.22	105.64	113.47
5	J	1405	RG1	C25-C24-C23	-3.21	113.91	123.20
3	A	1501	BCL	CBA-CAA-C2A	-3.20	104.26	113.79
3	K	1706	BCL	CHB-C1B-C2B	-3.20	118.14	127.43
3	H	1604	BCL	C6-C5-C3	-3.20	105.67	113.47
3	D	1602	BCL	C6-C5-C3	-3.20	105.68	113.47
3	A	1701	BCL	C1D-CHD-C4C	-3.19	118.93	126.62
3	R	1509	BCL	O2D-CGD-O1D	-3.19	117.64	123.85
3	S	1609	BCL	OBD-CAD-C3D	-3.18	120.99	128.42
3	H	1604	BCL	CHB-C1B-C2B	-3.16	118.25	127.43
3	J	1605	BCL	C6-C5-C3	-3.15	105.80	113.47
3	E	1503	BCL	CHB-C1B-C2B	-3.15	118.29	127.43
3	J	1605	BCL	C4D-C3D-CAD	-3.15	104.69	108.11
3	R	1509	BCL	OBB-CAB-C3B	-3.15	114.87	120.43
3	B	1601	BCL	O2D-CGD-O1D	-3.13	117.75	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	1401	RG1	C20-C21-C22	-3.12	122.90	127.28
5	H	1404	RG1	C16-C15-C14	-3.12	117.13	123.52
5	S	1409	RG1	C20-C21-C22	-3.11	122.91	127.28
3	O	1508	BCL	CMD-C2D-C1D	3.11	130.20	124.73
5	D	1402	RG1	C15-C14-C13	-3.10	122.92	127.28
3	B	1601	BCL	C6-C5-C3	-3.10	105.92	113.47
3	M	1707	BCL	O2A-CGA-CBA	3.10	121.27	111.83
3	P	1608	BCL	O2D-CGD-CBD	3.09	116.64	111.23
5	J	1405	RG1	C7-C6-C5	-3.08	123.35	127.69
3	K	1506	BCL	CAC-C3C-C4C	3.08	119.43	112.58
3	R	1709	BCL	C1C-NC-C4C	-3.08	105.27	106.68
3	G	1504	BCL	CHB-C1B-C2B	-3.08	118.48	127.43
3	E	1503	BCL	CBA-CAA-C2A	-3.08	104.63	113.79
5	F	1403	RG1	C12-C13-C14	-3.08	114.17	119.01
3	O	1708	BCL	C6-C5-C3	-3.07	105.98	113.47
3	O	1508	BCL	CHB-C1B-C2B	-3.07	118.50	127.43
3	N	1607	BCL	O2D-CGD-O1D	-3.07	117.87	123.85
5	F	1403	RG1	CM3-C5-C4	3.07	120.56	115.23
3	O	1508	BCL	C6-C5-C3	-3.06	106.00	113.47
3	F	1603	BCL	C1-O2A-CGA	3.06	124.05	116.65
3	C	1702	BCL	C1-O2A-CGA	3.05	124.04	116.65
3	E	1503	BCL	CHC-C4B-NB	3.05	128.63	124.05
3	R	1509	BCL	C6-C5-C3	-3.05	106.04	113.47
3	R	1509	BCL	CHB-C1B-C2B	-3.05	118.58	127.43
3	I	1705	BCL	C6-C5-C3	-3.04	106.05	113.47
3	P	1608	BCL	CHB-C1B-C2B	-3.04	118.60	127.43
3	O	1508	BCL	CHC-C4B-NB	3.04	128.61	124.05
3	E	1703	BCL	CMD-C2D-C1D	3.03	130.07	124.73
3	M	1507	BCL	C1-O2A-CGA	3.03	123.98	116.65
3	C	1502	BCL	CMD-C2D-C1D	3.02	130.05	124.73
3	H	1604	BCL	C3C-C4C-CHD	-3.02	117.03	123.39
3	S	1609	BCL	O2A-CGA-O1A	-3.02	116.08	123.63
3	P	1608	BCL	O2A-CGA-O1A	-3.01	116.09	123.63
3	H	1604	BCL	O2A-CGA-O1A	-3.01	116.10	123.63
5	F	1403	RG1	C24-C25-C26	-3.01	123.06	127.28
5	D	1402	RG1	C16-C15-C14	-3.01	117.37	123.52
3	I	1505	BCL	CBA-CAA-C2A	-3.00	104.86	113.79
5	R	1401	RG1	C1-O1'-C1'	-3.00	113.64	119.78
3	I	1705	BCL	O2A-CGA-CBA	3.00	120.97	111.83
5	L	1406	RG1	C16-C17-C18	-2.99	123.08	127.28
5	F	1403	RG1	CM5-C13-C12	2.99	122.66	118.09
3	E	1703	BCL	OBD-CAD-C3D	-2.99	121.43	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1604	BCL	C2D-C1D-ND	2.98	113.08	110.13
3	C	1702	BCL	O2D-CGD-CBD	2.98	116.44	111.23
3	M	1707	BCL	CHA-C1A-NA	-2.98	119.64	126.39
5	S	1409	RG1	CM3-C5-C4	2.97	120.39	115.23
3	A	1701	BCL	CMD-C2D-C1D	2.97	129.96	124.73
3	M	1707	BCL	C4-C3-C5	2.97	120.38	115.23
3	K	1706	BCL	CHC-C4B-NB	2.97	128.50	124.05
3	G	1504	BCL	O2D-CGD-CBD	2.97	116.41	111.23
3	F	1603	BCL	O2D-CGD-O1D	-2.97	118.08	123.85
3	G	1704	BCL	O2A-CGA-CBA	2.96	120.87	111.83
3	A	1701	BCL	O2D-CGD-CBD	2.96	116.41	111.23
3	B	1601	BCL	CHC-C4B-NB	2.96	128.49	124.05
5	J	1405	RG1	C16-C15-C14	-2.95	117.48	123.52
3	R	1709	BCL	O2D-CGD-O1D	-2.95	118.11	123.85
3	S	1609	BCL	C6-C5-C3	-2.94	106.30	113.47
3	A	1501	BCL	CGD-CBD-CAD	2.94	120.38	110.85
3	O	1508	BCL	O2A-C1-C2	-2.94	96.79	108.11
3	N	1607	BCL	C6-C5-C3	-2.93	106.33	113.47
3	N	1607	BCL	CBA-CAA-C2A	-2.93	105.08	113.79
3	E	1503	BCL	O2D-CGD-O1D	-2.93	118.15	123.85
3	M	1507	BCL	O2D-CGD-O1D	-2.93	118.15	123.85
3	B	1601	BCL	O2A-CGA-CBA	2.92	120.75	111.83
3	D	1602	BCL	CBA-CAA-C2A	-2.91	105.14	113.79
3	B	1601	BCL	CBA-CAA-C2A	-2.91	105.15	113.79
5	H	1404	RG1	C25-C24-C23	-2.90	114.79	123.20
3	A	1701	BCL	CHC-C4B-NB	2.89	128.39	124.05
5	R	1401	RG1	CM7-C22-C23	2.89	122.50	118.09
5	L	1406	RG1	C20-C21-C22	-2.89	123.23	127.28
3	C	1502	BCL	CHB-C1B-C2B	-2.88	119.06	127.43
3	K	1506	BCL	CHB-C1B-C2B	-2.87	119.10	127.43
5	H	1404	RG1	CM7-C22-C23	2.86	122.46	118.09
5	S	1409	RG1	CM5-C13-C12	2.86	122.46	118.09
5	R	1401	RG1	C25-C24-C23	-2.86	114.91	123.20
3	L	1606	BCL	OBD-CAD-C3D	-2.86	121.74	128.42
3	I	1505	BCL	CHB-C1B-C2B	-2.85	119.14	127.43
3	J	1605	BCL	CHC-C4B-NB	2.85	128.33	124.05
3	A	1501	BCL	CHA-C1A-NA	-2.85	119.93	126.39
3	A	1701	BCL	OBB-CAB-CBB	2.85	126.15	119.77
3	G	1504	BCL	O2D-CGD-O1D	-2.85	118.31	123.85
3	J	1605	BCL	C3D-C4D-ND	2.84	114.60	109.99
3	A	1501	BCL	CHC-C4B-NB	2.83	128.30	124.05
3	G	1504	BCL	O2A-C1-C2	-2.83	97.21	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1403	RG1	C16-C15-C14	-2.83	117.73	123.52
3	N	1607	BCL	C1D-CHD-C4C	-2.83	119.80	126.62
3	R	1509	BCL	CMA-C3A-C4A	2.83	119.37	111.77
3	R	1709	BCL	OBD-CAD-C3D	-2.83	121.81	128.42
5	P	1408	RG1	CM3-C5-C4	2.82	120.12	115.23
5	N	1407	RG1	C29-C28-C27	-2.82	115.04	123.20
3	M	1507	BCL	C6-C5-C3	-2.82	106.61	113.47
3	A	1701	BCL	C4-C3-C5	2.81	120.10	115.23
3	R	1509	BCL	C1C-NC-C4C	-2.81	105.40	106.68
3	O	1708	BCL	O2D-CGD-O1D	-2.80	118.39	123.85
3	K	1706	BCL	OBB-CAB-CBB	2.80	126.05	119.77
3	F	1603	BCL	C4-C3-C5	2.80	120.09	115.23
3	S	1609	BCL	C1-O2A-CGA	2.80	123.43	116.65
5	L	1406	RG1	C12-C13-C14	-2.80	114.61	119.01
3	G	1704	BCL	O2D-CGD-O1D	-2.79	118.42	123.85
3	G	1704	BCL	CHB-C1B-C2B	-2.79	119.33	127.43
5	P	1408	RG1	CM7-C22-C23	2.78	122.34	118.09
5	D	1402	RG1	CM0-C30-CM9	2.78	120.98	114.59
3	A	1701	BCL	O2A-CGA-CBA	2.77	120.27	111.83
3	K	1706	BCL	C6-C5-C3	-2.76	106.73	113.47
5	D	1402	RG1	CM4-C9-C8	2.76	122.31	118.09
5	H	1404	RG1	C1-O1'-C1'	-2.76	114.13	119.78
3	M	1707	BCL	C4D-C3D-CAD	-2.76	105.11	108.11
3	P	1608	BCL	CHC-C4B-NB	2.76	128.19	124.05
3	R	1509	BCL	CMD-C2D-C1D	2.76	129.58	124.73
3	K	1506	BCL	C4-C3-C5	2.76	120.01	115.23
3	K	1506	BCL	OBB-CAB-C3B	-2.75	115.57	120.43
3	A	1501	BCL	CHA-C4D-ND	2.75	138.22	132.55
5	H	1404	RG1	C11-C10-C9	-2.74	123.43	127.28
3	R	1509	BCL	CHC-C4B-NB	2.73	128.14	124.05
3	D	1602	BCL	CHC-C4B-NB	2.73	128.14	124.05
3	L	1606	BCL	OBB-CAB-CBB	2.72	125.87	119.77
3	G	1704	BCL	CBC-CAC-C3C	-2.72	107.64	113.41
3	N	1607	BCL	O2A-CGA-CBA	2.71	120.11	111.83
3	R	1709	BCL	C4-C3-C5	2.71	119.93	115.23
3	G	1504	BCL	CMD-C2D-C1D	2.71	129.50	124.73
3	N	1607	BCL	OBD-CAD-C3D	-2.71	122.09	128.42
5	J	1405	RG1	C2-C3-C4	-2.70	105.82	112.33
3	I	1705	BCL	CHC-C4B-NB	2.70	128.10	124.05
3	M	1707	BCL	C6-C5-C3	-2.70	106.89	113.47
3	K	1706	BCL	C4-C3-C5	2.70	119.92	115.23
3	O	1708	BCL	C1C-NC-C4C	-2.70	105.45	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1405	RG1	C28-C27-C26	-2.70	118.97	126.36
5	H	1404	RG1	C28-C27-C26	-2.70	118.97	126.36
3	L	1606	BCL	C3A-C2A-C1A	-2.69	97.30	101.34
3	M	1707	BCL	O2D-CGD-CBD	2.69	115.94	111.23
5	D	1402	RG1	C20-C21-C22	-2.69	123.50	127.28
3	C	1502	BCL	OBD-CAD-C3D	-2.68	122.15	128.42
3	A	1501	BCL	C4-C3-C5	2.68	119.88	115.23
3	C	1702	BCL	C1C-NC-C4C	-2.68	105.46	106.68
3	O	1708	BCL	CMD-C2D-C1D	2.68	129.44	124.73
5	H	1404	RG1	CM2-C1-C2	-2.67	106.37	111.12
3	C	1502	BCL	C4-C3-C5	2.67	119.87	115.23
5	F	1403	RG1	C1-O1'-C1'	-2.67	114.32	119.78
5	L	1406	RG1	CM3-C5-C4	2.66	119.85	115.23
3	D	1602	BCL	C4-C3-C5	2.66	119.85	115.23
5	N	1407	RG1	CM3-C5-C4	2.66	119.85	115.23
3	F	1603	BCL	CBA-CAA-C2A	-2.66	105.89	113.79
3	A	1701	BCL	CBC-CAC-C3C	-2.65	107.78	113.41
3	N	1607	BCL	CHC-C4B-NB	2.65	128.03	124.05
3	C	1702	BCL	O2A-CGA-CBA	2.65	119.92	111.83
3	R	1709	BCL	CGD-CBD-CAD	-2.65	102.27	110.85
3	A	1701	BCL	CAC-C3C-C4C	2.65	118.46	112.58
3	R	1509	BCL	C2A-C3A-C4A	2.64	106.14	101.87
3	M	1707	BCL	CHC-C4B-NB	2.64	128.01	124.05
5	H	1404	RG1	C20-C21-C22	-2.64	123.58	127.28
5	S	1409	RG1	C28-C27-C26	-2.64	119.13	126.36
3	K	1706	BCL	CMD-C2D-C1D	2.63	129.37	124.73
3	C	1702	BCL	O2D-CGD-O1D	-2.63	118.72	123.85
3	N	1607	BCL	OBb-CAB-CBB	2.62	125.63	119.77
3	H	1604	BCL	CAC-C3C-C4C	-2.62	106.78	112.58
3	B	1601	BCL	OBb-CAB-CBB	2.61	125.62	119.77
3	J	1605	BCL	O2A-CGA-CBA	2.61	119.80	111.83
5	N	1407	RG1	C24-C25-C26	-2.61	123.62	127.28
5	H	1404	RG1	C28-C29-C30	-2.61	123.50	127.48
3	D	1602	BCL	C2D-C1D-ND	2.60	112.70	110.13
3	C	1502	BCL	CHC-C4B-NB	2.60	127.95	124.05
3	O	1708	BCL	C1D-CHD-C4C	-2.60	120.35	126.62
3	L	1606	BCL	CHC-C4B-NB	2.60	127.95	124.05
3	G	1704	BCL	CMD-C2D-C1D	2.60	129.30	124.73
3	R	1709	BCL	C1D-CHD-C4C	-2.60	120.36	126.62
3	R	1509	BCL	O2A-C1-C2	-2.59	98.13	108.11
3	J	1605	BCL	O2A-CGA-O1A	-2.59	117.14	123.63
3	E	1703	BCL	C6-C5-C3	-2.59	107.16	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1703	BCL	O2A-CGA-CBA	2.59	119.73	111.83
5	S	1409	RG1	C24-C25-C26	-2.59	123.65	127.28
3	E	1503	BCL	O2A-CGA-CBA	2.59	119.73	111.83
5	J	1405	RG1	CM3-C5-C4	2.59	119.72	115.23
3	C	1502	BCL	C14-C13-C12	2.59	120.49	111.27
3	K	1706	BCL	O2A-CGA-CBA	2.58	119.70	111.83
5	P	1408	RG1	C1'-O5'-C5'	2.58	118.75	113.72
3	P	1608	BCL	OBB-CAB-CBB	2.58	125.54	119.77
5	D	1402	RG1	C10-C11-C12	-2.57	115.74	123.20
3	K	1506	BCL	O2D-CGD-CBD	2.57	115.73	111.23
3	C	1502	BCL	CBA-CAA-C2A	-2.56	106.16	113.79
3	R	1509	BCL	C4-C3-C5	2.56	119.68	115.23
5	J	1405	RG1	C11-C10-C9	-2.56	123.69	127.28
3	G	1504	BCL	CHA-C1A-NA	-2.56	120.60	126.39
3	J	1605	BCL	C2D-C1D-ND	2.55	112.65	110.13
3	R	1709	BCL	OBB-CAB-CBB	2.55	125.48	119.77
3	H	1604	BCL	OBD-CAD-C3D	-2.55	122.46	128.42
3	E	1703	BCL	O2A-C1-C2	-2.54	98.33	108.11
3	I	1505	BCL	C1C-NC-C4C	-2.54	105.52	106.68
3	G	1504	BCL	O2A-CGA-CBA	2.54	119.58	111.83
3	H	1604	BCL	OBB-CAB-CBB	2.53	125.45	119.77
3	I	1705	BCL	C3D-C4D-ND	2.53	114.10	109.99
3	O	1708	BCL	OBD-CAD-C3D	-2.53	122.50	128.42
5	L	1406	RG1	C28-C29-C30	-2.53	123.62	127.48
3	D	1602	BCL	C1-O2A-CGA	2.52	122.76	116.65
5	L	1406	RG1	O5'-C1'-C2'	2.52	115.56	110.37
3	O	1508	BCL	CHA-C4D-ND	2.52	137.75	132.55
3	I	1505	BCL	C4-C3-C5	2.52	119.60	115.23
3	R	1709	BCL	CHC-C4B-NB	2.52	127.82	124.05
3	O	1708	BCL	CHC-C4B-NB	2.51	127.82	124.05
3	G	1504	BCL	CHC-C4B-NB	2.51	127.81	124.05
3	K	1706	BCL	C3D-C4D-ND	2.51	114.06	109.99
3	M	1507	BCL	O2A-C1-C2	-2.51	98.46	108.11
5	D	1402	RG1	C28-C27-C26	-2.50	119.50	126.36
3	C	1702	BCL	CHC-C4B-NB	2.50	127.80	124.05
5	N	1407	RG1	C20-C21-C22	-2.50	123.77	127.28
3	K	1706	BCL	C1D-CHD-C4C	-2.50	120.60	126.62
3	S	1609	BCL	O2A-CGA-CBA	2.49	119.44	111.83
5	D	1402	RG1	CM5-C13-C12	2.49	121.90	118.09
3	I	1505	BCL	O2A-C1-C2	-2.49	98.51	108.11
3	O	1508	BCL	C2D-C1D-ND	2.48	112.58	110.13
3	C	1502	BCL	C2D-C1D-ND	2.48	112.58	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1606	BCL	C1D-CHD-C4C	-2.48	120.63	126.62
3	E	1503	BCL	OBD-CAD-C3D	-2.48	122.61	128.42
3	B	1601	BCL	C1-O2A-CGA	2.48	122.65	116.65
3	B	1601	BCL	OBD-CAD-C3D	-2.48	122.63	128.42
5	S	1409	RG1	C25-C24-C23	-2.47	116.03	123.20
3	M	1707	BCL	C3D-C4D-ND	2.47	114.01	109.99
5	D	1402	RG1	C24-C25-C26	-2.47	123.81	127.28
3	S	1609	BCL	C2D-C1D-ND	2.46	112.56	110.13
3	M	1507	BCL	CBA-CAA-C2A	-2.46	106.47	113.79
3	A	1501	BCL	C6-C5-C3	-2.46	107.48	113.47
3	D	1602	BCL	CHA-C4D-ND	2.46	137.62	132.55
3	F	1603	BCL	OBB-CAB-CBB	2.46	125.27	119.77
5	F	1403	RG1	C29-C28-C27	-2.46	116.08	123.20
3	F	1603	BCL	C1D-ND-C4D	2.46	108.03	106.31
3	O	1708	BCL	O2D-CGD-CBD	2.45	115.52	111.23
3	L	1606	BCL	O2A-CGA-CBA	2.45	119.32	111.83
3	G	1504	BCL	C1-O2A-CGA	2.45	122.59	116.65
3	P	1608	BCL	C2D-C1D-ND	2.45	112.55	110.13
3	K	1506	BCL	C3D-C4D-ND	2.44	113.95	109.99
3	S	1609	BCL	CHD-C1D-C2D	-2.44	120.42	125.49
3	O	1508	BCL	C4-C3-C5	2.43	119.45	115.23
3	E	1703	BCL	CHC-C4B-NB	2.43	127.69	124.05
3	D	1602	BCL	OBD-CAD-C3D	-2.43	122.74	128.42
3	D	1602	BCL	C1D-CHD-C4C	-2.43	120.77	126.62
5	D	1402	RG1	C29-C28-C27	-2.43	116.17	123.20
3	O	1508	BCL	C14-C13-C12	2.42	119.92	111.27
3	N	1607	BCL	C2D-C1D-ND	2.42	112.52	110.13
3	I	1505	BCL	C6-C5-C3	-2.42	107.57	113.47
3	G	1504	BCL	C4-C3-C5	2.42	119.43	115.23
3	I	1505	BCL	C1D-CHD-C4C	-2.41	120.81	126.62
5	J	1405	RG1	C24-C25-C26	-2.41	123.90	127.28
5	F	1403	RG1	CM0-C30-CM9	2.41	120.13	114.59
3	E	1503	BCL	CHD-C1D-C2D	-2.41	120.48	125.49
3	A	1501	BCL	OBB-CAB-CBB	2.41	125.16	119.77
3	M	1507	BCL	CHC-C4B-NB	2.41	127.66	124.05
5	D	1402	RG1	C25-C24-C23	-2.40	116.23	123.20
5	L	1406	RG1	C29-C28-C27	-2.40	116.25	123.20
3	L	1606	BCL	C6-C5-C3	-2.40	107.63	113.47
3	C	1702	BCL	CBC-CAC-C3C	-2.39	108.33	113.41
5	P	1408	RG1	C10-C11-C12	-2.39	116.26	123.20
3	G	1504	BCL	CBC-CAC-C3C	-2.39	108.34	113.41
3	C	1502	BCL	O2A-CGA-CBA	2.39	119.12	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	1509	BCL	C1D-CHD-C4C	-2.39	120.85	126.62
3	L	1606	BCL	CBA-CAA-C2A	-2.39	106.69	113.79
5	S	1409	RG1	C29-C28-C27	-2.38	116.30	123.20
5	N	1407	RG1	C15-C14-C13	-2.38	123.94	127.28
5	F	1403	RG1	C28-C27-C26	-2.38	119.84	126.36
3	O	1708	BCL	CBA-CAA-C2A	-2.38	106.71	113.79
3	F	1603	BCL	CHC-C4B-NB	2.38	127.62	124.05
3	E	1503	BCL	C2D-C1D-ND	2.38	112.48	110.13
5	F	1403	RG1	C25-C24-C23	-2.38	116.32	123.20
5	L	1406	RG1	CM5-C13-C12	2.37	121.71	118.09
3	H	1604	BCL	O2D-CGD-O1D	-2.37	119.24	123.85
3	F	1603	BCL	O2A-CGA-CBA	2.37	119.06	111.83
5	F	1403	RG1	C6-C7-C8	-2.37	116.34	123.20
3	J	1605	BCL	CHA-C1A-NA	-2.37	121.03	126.39
3	G	1504	BCL	CBA-CAA-C2A	-2.37	106.75	113.79
3	O	1508	BCL	CHA-C1A-NA	-2.36	121.05	126.39
5	S	1409	RG1	CM0-C30-CM9	2.36	120.02	114.59
5	R	1401	RG1	C23-C22-C21	-2.36	115.30	119.01
3	G	1704	BCL	CHC-C4B-NB	2.36	127.59	124.05
3	O	1508	BCL	OBB-CAB-CBB	2.36	125.05	119.77
3	D	1602	BCL	CHD-C1D-C2D	-2.35	120.60	125.49
3	R	1709	BCL	CHA-C4D-ND	2.35	137.39	132.55
3	I	1505	BCL	C3D-C4D-ND	2.35	113.80	109.99
5	N	1407	RG1	C12-C13-C14	-2.35	115.32	119.01
3	J	1605	BCL	OBB-CAB-CBB	2.34	125.02	119.77
3	E	1703	BCL	CHA-C1A-NA	-2.34	121.09	126.39
3	O	1708	BCL	CHA-C4D-ND	2.34	137.37	132.55
3	L	1606	BCL	C2D-C1D-ND	2.34	112.44	110.13
5	P	1408	RG1	C1-O1'-C1'	-2.33	115.00	119.78
3	D	1602	BCL	O2D-CGD-O1D	-2.33	119.31	123.85
3	O	1508	BCL	CHC-C4B-C3B	-2.33	122.46	131.72
3	L	1606	BCL	C3D-C4D-ND	2.33	113.77	109.99
3	H	1604	BCL	C2C-C3C-C4C	-2.33	97.85	101.34
3	G	1504	BCL	CHA-C4D-ND	2.33	137.35	132.55
5	J	1405	RG1	CM6-C18-C17	-2.33	119.05	122.82
3	A	1701	BCL	C6-C5-C3	-2.32	107.81	113.47
3	B	1601	BCL	C3D-C4D-ND	2.32	113.76	109.99
3	S	1609	BCL	C5-C3-C2	-2.32	115.95	121.17
5	R	1401	RG1	CM5-C13-C12	2.32	121.63	118.09
5	S	1409	RG1	C23-C22-C21	-2.32	115.36	119.01
3	M	1507	BCL	CHA-C1A-NA	-2.31	121.16	126.39
3	D	1602	BCL	OBB-CAB-CBB	2.31	124.95	119.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1708	BCL	C4-C3-C5	2.31	119.24	115.23
3	P	1608	BCL	O2A-CGA-CBA	2.31	118.88	111.83
3	C	1702	BCL	OBb-CAB-CBB	2.31	124.94	119.77
3	R	1509	BCL	OBD-CAD-C3D	-2.31	123.02	128.42
3	B	1601	BCL	C2D-C1D-ND	2.31	112.41	110.13
3	L	1606	BCL	CHD-C1D-C2D	-2.30	120.69	125.49
3	M	1507	BCL	C2D-C1D-ND	2.30	112.41	110.13
3	H	1604	BCL	CHD-C1D-C2D	-2.30	120.70	125.49
3	R	1509	BCL	CMA-C3A-C2A	2.30	122.86	113.98
5	R	1401	RG1	C28-C27-C26	-2.30	120.07	126.36
3	A	1501	BCL	C2D-C1D-ND	2.29	112.40	110.13
3	A	1701	BCL	CHA-C1A-NA	-2.29	121.20	126.39
3	P	1608	BCL	CHA-C1A-NA	-2.29	121.20	126.39
3	M	1507	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
5	D	1402	RG1	C1'-C2'-C3'	2.29	114.83	110.01
3	K	1706	BCL	CBA-CAA-C2A	-2.29	106.98	113.79
3	A	1501	BCL	C1D-CHD-C4C	-2.29	121.10	126.62
3	K	1506	BCL	CHA-C1A-NA	-2.29	121.21	126.39
3	L	1606	BCL	C1-O2A-CGA	2.28	122.18	116.65
3	O	1508	BCL	C5-C3-C2	-2.28	116.04	121.17
3	S	1609	BCL	CHC-C4B-C3B	-2.28	122.65	131.72
3	N	1607	BCL	CHA-C1A-NA	-2.28	121.22	126.39
5	J	1405	RG1	C6-C7-C8	-2.28	116.59	123.20
3	G	1704	BCL	CBA-CAA-C2A	-2.28	107.00	113.79
3	N	1607	BCL	CHA-C4D-ND	2.28	137.25	132.55
3	R	1709	BCL	CBC-CAC-C3C	-2.28	108.58	113.41
3	M	1507	BCL	O2A-CGA-CBA	2.28	118.78	111.83
3	C	1702	BCL	C3D-C4D-ND	2.27	113.68	109.99
3	G	1704	BCL	C1D-CHD-C4C	-2.27	121.14	126.62
5	S	1409	RG1	C20-C19-C18	-2.27	120.14	126.36
3	K	1506	BCL	O2A-C1-C2	-2.27	99.38	108.11
3	G	1704	BCL	C4-C3-C5	2.27	119.16	115.23
3	M	1707	BCL	CHA-C4D-ND	2.27	137.23	132.55
5	N	1407	RG1	C25-C24-C23	-2.26	116.64	123.20
3	H	1604	BCL	CHA-C1A-NA	-2.26	121.28	126.39
5	N	1407	RG1	CM4-C9-C8	2.26	121.54	118.09
3	H	1604	BCL	O2A-CGA-CBA	2.26	118.72	111.83
3	P	1608	BCL	OBD-CAD-C3D	-2.26	123.14	128.42
3	J	1605	BCL	CGD-CBD-CAD	2.25	118.14	110.85
3	G	1704	BCL	OBb-CAB-CBB	2.25	124.82	119.77
3	I	1505	BCL	OBD-CAD-C3D	-2.25	123.17	128.42
3	E	1703	BCL	O2D-CGD-CBD	2.25	115.16	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1503	BCL	CHA-C1A-NA	-2.24	121.31	126.39
5	F	1403	RG1	C28-C29-C30	-2.24	124.05	127.48
3	C	1702	BCL	C4-C3-C5	2.24	119.12	115.23
3	A	1701	BCL	C3D-C4D-ND	2.24	113.63	109.99
3	E	1703	BCL	CHC-C4B-C3B	-2.24	122.82	131.72
3	S	1609	BCL	CHA-C4D-ND	2.24	137.17	132.55
3	H	1604	BCL	CMD-C2D-C1D	2.24	128.67	124.73
3	E	1503	BCL	CMD-C2D-C1D	2.24	128.67	124.73
5	J	1405	RG1	C29-C28-C27	-2.24	116.71	123.20
3	C	1502	BCL	C5-C3-C2	-2.24	116.14	121.17
3	I	1705	BCL	O2D-CGD-O1D	-2.24	119.49	123.85
3	R	1709	BCL	CHA-C1A-NA	-2.24	121.33	126.39
3	E	1503	BCL	C4-C3-C5	2.23	119.10	115.23
3	P	1608	BCL	C6-C5-C3	-2.23	108.03	113.47
3	P	1608	BCL	C4-C3-C5	2.23	119.10	115.23
5	S	1409	RG1	C7-C8-C9	-2.23	120.25	126.36
3	G	1504	BCL	C1D-CHD-C4C	-2.23	121.24	126.62
3	P	1608	BCL	C3C-C2C-C1C	2.23	105.47	101.87
3	I	1505	BCL	O2D-CGD-CBD	2.23	115.13	111.23
3	G	1704	BCL	C3D-C4D-ND	2.22	113.60	109.99
3	C	1502	BCL	CHA-C1A-NA	-2.22	121.37	126.39
3	G	1504	BCL	C14-C13-C15	-2.22	103.36	111.27
3	J	1605	BCL	O2D-CGD-O1D	-2.22	119.53	123.85
3	D	1602	BCL	O2A-CGA-CBA	2.22	118.60	111.83
3	M	1507	BCL	C2A-C1A-CHA	-2.22	120.02	123.87
3	B	1601	BCL	C4-C3-C5	2.22	119.08	115.23
3	K	1506	BCL	C1-O2A-CGA	2.21	122.01	116.65
3	I	1705	BCL	C1D-CHD-C4C	-2.21	121.28	126.62
3	R	1509	BCL	C3D-C4D-ND	2.21	113.58	109.99
5	N	1407	RG1	CM5-C13-C12	2.21	121.46	118.09
5	R	1401	RG1	C15-C14-C13	-2.21	124.18	127.28
3	I	1505	BCL	C11-C10-C8	-2.21	108.63	115.97
3	O	1508	BCL	O2A-CGA-CBA	2.21	118.56	111.83
3	C	1502	BCL	CHD-C1D-C2D	-2.21	120.90	125.49
3	R	1709	BCL	C6-C5-C3	-2.20	108.11	113.47
3	C	1502	BCL	C2A-C1A-CHA	-2.19	120.06	123.87
3	C	1502	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
3	R	1509	BCL	O2A-CGA-CBA	2.19	118.52	111.83
3	H	1604	BCL	C1D-CHD-C4C	-2.19	121.33	126.62
3	P	1608	BCL	C3B-C4B-NB	-2.19	106.87	109.76
5	H	1404	RG1	CM4-C9-C8	2.19	121.43	118.09
5	P	1408	RG1	C2-C3-C4	-2.18	107.07	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1604	BCL	C4-C3-C5	2.18	119.02	115.23
5	S	1409	RG1	C10-C11-C12	-2.18	116.88	123.20
3	I	1505	BCL	CHC-C4B-NB	2.18	127.32	124.05
5	D	1402	RG1	CM7-C22-C23	2.18	121.41	118.09
3	C	1702	BCL	C6-C5-C3	-2.18	108.17	113.47
3	F	1603	BCL	C2D-C1D-ND	2.18	112.28	110.13
3	I	1705	BCL	CMD-C2D-C1D	2.17	128.55	124.73
3	E	1703	BCL	O2D-CGD-O1D	-2.17	119.62	123.85
3	L	1606	BCL	C4D-C3D-CAD	-2.17	105.75	108.11
3	P	1608	BCL	CAB-C3B-C2B	-2.17	123.24	127.74
3	E	1703	BCL	C3D-C4D-ND	2.17	113.51	109.99
5	N	1407	RG1	CM6-C18-C17	-2.17	119.31	122.82
3	I	1705	BCL	OBB-CAB-CBB	2.16	124.62	119.77
3	O	1508	BCL	C1-O2A-CGA	2.16	121.89	116.65
3	G	1704	BCL	CHC-C4B-C3B	-2.16	123.14	131.72
3	C	1502	BCL	C3D-C4D-ND	2.16	113.50	109.99
5	S	1409	RG1	C11-C10-C9	-2.16	124.25	127.28
3	O	1508	BCL	CGD-CBD-CAD	2.16	117.83	110.85
3	R	1509	BCL	CHA-C1A-NA	-2.16	121.51	126.39
3	M	1507	BCL	C3D-C4D-ND	2.16	113.49	109.99
3	S	1609	BCL	C4-C3-C5	2.16	118.97	115.23
3	F	1603	BCL	CMD-C2D-C1D	2.15	128.52	124.73
3	K	1506	BCL	O2D-CGD-O1D	-2.15	119.66	123.85
5	P	1408	RG1	C29-C28-C27	-2.15	116.97	123.20
5	P	1408	RG1	C21-C20-C19	-2.15	116.97	123.20
5	J	1405	RG1	CM0-C30-CM9	2.15	119.53	114.59
3	M	1707	BCL	CAB-C3B-C2B	-2.15	123.28	127.74
3	G	1704	BCL	C2D-C1D-ND	2.15	112.25	110.13
3	O	1508	BCL	OBD-CAD-C3D	-2.15	123.40	128.42
3	K	1706	BCL	CHC-C4B-C3B	-2.14	123.21	131.72
3	L	1606	BCL	C4-C3-C5	2.14	118.94	115.23
3	I	1505	BCL	C1-O2A-CGA	2.14	121.82	116.65
3	E	1703	BCL	C1D-CHD-C4C	-2.13	121.48	126.62
3	M	1707	BCL	OBB-CAB-CBB	2.13	124.54	119.77
5	J	1405	RG1	C10-C11-C12	-2.13	117.03	123.20
3	A	1501	BCL	C1-O2A-CGA	2.13	121.80	116.65
3	K	1506	BCL	CMD-C2D-C1D	2.13	128.48	124.73
3	A	1501	BCL	CHD-C1D-C2D	-2.13	121.06	125.49
3	C	1702	BCL	OBD-CAD-C3D	-2.13	123.45	128.42
5	R	1401	RG1	C10-C11-C12	-2.13	117.04	123.20
3	R	1509	BCL	CHC-C4B-C3B	-2.12	123.29	131.72
3	G	1504	BCL	C3D-C4D-ND	2.12	113.43	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1605	BCL	CHC-C4B-C3B	-2.12	123.31	131.72
3	O	1708	BCL	OBB-CAB-CBB	2.11	124.50	119.77
3	S	1609	BCL	OBB-CAB-CBB	2.11	124.50	119.77
3	C	1502	BCL	OBB-CAB-CBB	2.11	124.48	119.77
3	S	1609	BCL	C1D-CHD-C4C	-2.10	121.55	126.62
3	E	1503	BCL	CHC-C4B-C3B	-2.10	123.38	131.72
5	F	1403	RG1	C7-C6-C5	-2.09	124.75	127.69
3	L	1606	BCL	CMD-C2D-C3D	2.09	132.49	127.69
3	O	1708	BCL	C3D-C4D-ND	2.09	113.38	109.99
3	C	1502	BCL	CHA-C4D-ND	2.09	136.86	132.55
5	L	1406	RG1	C10-C11-C12	-2.08	117.17	123.20
3	G	1704	BCL	CGD-CBD-CAD	2.08	117.58	110.85
5	D	1402	RG1	CM3-C5-C4	2.08	118.83	115.23
3	E	1703	BCL	CHA-C4D-ND	2.08	136.84	132.55
5	H	1404	RG1	C6-C7-C8	-2.08	117.18	123.20
5	H	1404	RG1	C15-C14-C13	-2.08	124.37	127.28
3	I	1705	BCL	CHC-C4B-C3B	-2.08	123.47	131.72
3	A	1501	BCL	CMD-C2D-C1D	2.07	128.38	124.73
3	F	1603	BCL	CHA-C1A-NA	-2.07	121.70	126.39
3	D	1602	BCL	CHA-C1A-NA	-2.07	121.71	126.39
3	I	1505	BCL	OBB-CAB-CBB	2.06	124.39	119.77
3	H	1604	BCL	C1-O2A-CGA	2.06	121.64	116.65
5	R	1401	RG1	C20-C19-C18	-2.06	120.71	126.36
3	O	1708	BCL	CHA-C1A-NA	-2.06	121.73	126.39
3	E	1703	BCL	CBA-CAA-C2A	-2.06	107.67	113.79
3	M	1507	BCL	CHD-C1D-C2D	-2.06	121.21	125.49
5	H	1404	RG1	CM5-C13-C12	2.06	121.23	118.09
3	A	1501	BCL	O2A-C1-C2	-2.06	100.20	108.11
5	F	1403	RG1	O5'-C5'-C6'	2.05	111.53	106.44
3	K	1506	BCL	C3C-C2C-C1C	-2.05	98.55	101.87
5	L	1406	RG1	C1'-O5'-C5'	2.05	117.73	113.72
3	E	1503	BCL	C1D-CHD-C4C	-2.05	121.67	126.62
5	F	1403	RG1	C20-C21-C22	-2.05	124.40	127.28
3	C	1702	BCL	CMD-C2D-C1D	2.05	128.34	124.73
5	F	1403	RG1	CM8-C26-C25	-2.05	119.50	122.82
3	M	1707	BCL	CHC-C4B-C3B	-2.05	123.58	131.72
3	N	1607	BCL	CHC-C4B-C3B	-2.05	123.59	131.72
3	R	1509	BCL	C1-O2A-CGA	2.05	121.61	116.65
3	S	1609	BCL	CHA-C1A-NA	-2.05	121.76	126.39
3	I	1505	BCL	O2A-CGA-CBA	2.04	118.06	111.83
3	J	1605	BCL	C3C-C4C-CHD	-2.04	119.09	123.39
3	A	1701	BCL	CHA-C4D-ND	2.04	136.76	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1406	RG1	C25-C24-C23	-2.04	117.29	123.20
3	J	1605	BCL	C16-C15-C13	-2.04	109.19	115.97
5	P	1408	RG1	CM5-C13-C12	2.04	121.20	118.09
3	G	1704	BCL	CHA-C4D-ND	2.04	136.75	132.55
5	L	1406	RG1	CM0-C30-CM9	2.04	119.28	114.59
3	N	1607	BCL	C4-C3-C5	2.04	118.76	115.23
3	M	1507	BCL	CMD-C2D-C1D	2.03	128.30	124.73
3	K	1706	BCL	OBD-CAD-C3D	-2.03	123.68	128.42
3	J	1605	BCL	C1-O2A-CGA	2.03	121.56	116.65
5	R	1401	RG1	CM8-C26-C27	2.02	121.18	118.09
3	B	1601	BCL	C1D-CHD-C4C	-2.02	121.74	126.62
3	A	1701	BCL	CAB-C3B-C2B	-2.02	123.54	127.74
3	E	1503	BCL	C5-C3-C2	-2.02	116.63	121.17
3	I	1705	BCL	C4D-C3D-CAD	-2.02	105.91	108.11
3	K	1506	BCL	O2A-CGA-CBA	2.01	117.97	111.83
3	J	1605	BCL	C4-C3-C5	2.01	118.72	115.23
3	N	1607	BCL	CMD-C2D-C1D	2.01	128.27	124.73
3	I	1505	BCL	CHA-C4D-ND	2.01	136.70	132.55
3	H	1604	BCL	CHA-C4D-ND	2.01	136.70	132.55
5	P	1408	RG1	CM8-C26-C25	-2.01	119.56	122.82
3	A	1501	BCL	C3D-C4D-ND	2.01	113.25	109.99
3	A	1501	BCL	O2A-CGA-CBA	2.01	117.96	111.83
3	I	1705	BCL	CHA-C1A-NA	-2.01	121.84	126.39
3	S	1609	BCL	C3C-C4C-CHD	-2.01	119.16	123.39
5	J	1405	RG1	C28-C29-C30	-2.01	124.42	127.48
3	K	1706	BCL	CHA-C1A-NA	-2.00	121.85	126.39

All (23) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1501	BCL	CBD
3	A	1701	BCL	C3C
3	B	1601	BCL	C8
3	C	1502	BCL	C13
3	C	1702	BCL	C13
3	G	1704	BCL	CBD
3	H	1604	BCL	C2C
3	J	1605	BCL	CBD
3	K	1506	BCL	C3C
3	K	1706	BCL	C8
3	L	1606	BCL	C2C
3	L	1606	BCL	C3A

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Mol	Chain	Res	Type	Atom
3	L	1606	BCL	C8
3	M	1707	BCL	CBD
3	N	1607	BCL	C2C
3	O	1508	BCL	C13
3	O	1508	BCL	CBD
3	O	1708	BCL	C8
3	P	1608	BCL	C2C
3	P	1608	BCL	C8
3	R	1509	BCL	C3A
3	R	1709	BCL	C13
3	S	1609	BCL	C13

All (500) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1701	BCL	C4C-C3C-CAC-CBC
3	C	1702	BCL	C1-C2-C3-C5
3	E	1503	BCL	C2C-C3C-CAC-CBC
3	F	1603	BCL	C11-C10-C8-C7
3	H	1604	BCL	C2C-C3C-CAC-CBC
3	H	1604	BCL	C4C-C3C-CAC-CBC
3	I	1705	BCL	C11-C10-C8-C9
3	K	1506	BCL	C4C-C3C-CAC-CBC
3	P	1608	BCL	C2C-C3C-CAC-CBC
3	P	1608	BCL	C4C-C3C-CAC-CBC
3	R	1709	BCL	C2B-C3B-CAB-OBB
3	R	1709	BCL	C2B-C3B-CAB-CBB
3	R	1709	BCL	C4B-C3B-CAB-CBB
4	A	1817	LDA	C2-C1-N1-CM1
4	A	1817	LDA	N1-C1-C2-C3
4	B	1801	LDA	N1-C1-C2-C3
4	C	1815	LDA	N1-C1-C2-C3
4	D	1802	LDA	C2-C1-N1-CM1
4	D	1802	LDA	N1-C1-C2-C3
4	E	1822	LDA	N1-C1-C2-C3
4	F	1803	LDA	C2-C1-N1-O1
4	F	1803	LDA	C2-C1-N1-CM1
4	F	1803	LDA	C2-C1-N1-CM2
4	G	1814	LDA	C2-C1-N1-CM1
4	G	1814	LDA	C2-C1-N1-CM2
4	I	1812	LDA	N1-C1-C2-C3
4	I	1825	LDA	C2-C1-N1-CM1

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Mol	Chain	Res	Type	Atoms
4	J	1805	LDA	C2-C1-N1-O1
4	J	1805	LDA	N1-C1-C2-C3
4	K	1810	LDA	N1-C1-C2-C3
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	M	1827	LDA	N1-C1-C2-C3
4	O	1820	LDA	N1-C1-C2-C3
4	P	1808	LDA	N1-C1-C2-C3
4	R	1809	LDA	C2-C1-N1-O1
4	R	1809	LDA	C2-C1-N1-CM1
4	R	1809	LDA	C2-C1-N1-CM2
5	F	1403	RG1	C25-C26-C27-C28
5	F	1403	RG1	CM8-C26-C27-C28
5	H	1404	RG1	O1'-C1-C2-C3
5	H	1404	RG1	CM1-C1-C2-C3
5	H	1404	RG1	CM2-C1-C2-C3
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	R	1709	BCL	O1D-CGD-O2D-CED
3	R	1709	BCL	CBD-CGD-O2D-CED
3	J	1605	BCL	C3-C5-C6-C7
3	R	1709	BCL	C3-C5-C6-C7
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	M	1707	BCL	C4-C3-C5-C6
3	M	1707	BCL	C2-C3-C5-C6
3	A	1701	BCL	C3-C5-C6-C7
3	O	1708	BCL	C3-C5-C6-C7
3	S	1609	BCL	C3-C5-C6-C7
5	H	1404	RG1	C2-C3-C4-C5
3	F	1603	BCL	C5-C6-C7-C8
5	P	1408	RG1	O5'-C5'-C6'-O6'
3	H	1604	BCL	CBD-CGD-O2D-CED
3	M	1707	BCL	O1D-CGD-O2D-CED
3	G	1704	BCL	CBD-CGD-O2D-CED
5	P	1408	RG1	C4'-C5'-C6'-O6'
3	S	1609	BCL	CBD-CGD-O2D-CED
5	L	1406	RG1	O5'-C5'-C6'-O6'
3	D	1602	BCL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
5	L	1406	RG1	C4'-C5'-C6'-O6'
3	E	1703	BCL	C6-C7-C8-C9
3	F	1603	BCL	C11-C12-C13-C14
3	R	1709	BCL	C11-C10-C8-C9
3	S	1609	BCL	C11-C12-C13-C14
3	O	1708	BCL	O1D-CGD-O2D-CED
5	D	1402	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	S	1409	RG1	CM8-C26-C27-C28
5	H	1404	RG1	C25-C26-C27-C28
5	R	1401	RG1	C25-C26-C27-C28
5	J	1405	RG1	O5'-C5'-C6'-O6'
3	S	1609	BCL	C10-C11-C12-C13
3	M	1707	BCL	C10-C11-C12-C13
3	P	1608	BCL	C3-C5-C6-C7
5	J	1405	RG1	C4'-C5'-C6'-O6'
3	B	1601	BCL	C6-C7-C8-C10
3	C	1702	BCL	C11-C12-C13-C15
3	P	1608	BCL	C6-C7-C8-C10
3	A	1501	BCL	C15-C16-C17-C18
3	O	1508	BCL	CBD-CGD-O2D-CED
3	A	1701	BCL	C10-C11-C12-C13
3	C	1702	BCL	C15-C16-C17-C18
3	F	1603	BCL	C8-C10-C11-C12
3	C	1702	BCL	C5-C6-C7-C8
3	K	1506	BCL	C8-C10-C11-C12
3	M	1507	BCL	C15-C16-C17-C18
3	E	1503	BCL	C8-C10-C11-C12
3	M	1707	BCL	C8-C10-C11-C12
3	A	1501	BCL	O1D-CGD-O2D-CED
3	N	1607	BCL	C8-C10-C11-C12
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	G	1504	BCL	C8-C10-C11-C12
3	M	1507	BCL	C8-C10-C11-C12
3	P	1608	BCL	C5-C6-C7-C8
3	D	1602	BCL	C10-C11-C12-C13
3	O	1708	BCL	C10-C11-C12-C13
3	E	1703	BCL	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
3	E	1703	BCL	C4B-C3B-CAB-CBB
3	R	1709	BCL	C4B-C3B-CAB-OBB
5	D	1402	RG1	C25-C26-C27-C28
5	J	1405	RG1	C25-C26-C27-C28
5	P	1408	RG1	C25-C26-C27-C28
5	S	1409	RG1	C25-C26-C27-C28
4	R	1819	LDA	C3-C4-C5-C6
3	N	1607	BCL	C16-C17-C18-C20
3	G	1704	BCL	O1D-CGD-O2D-CED
3	C	1702	BCL	C3-C5-C6-C7
3	I	1705	BCL	C3-C5-C6-C7
3	M	1707	BCL	C5-C6-C7-C8
5	D	1402	RG1	O5'-C5'-C6'-O6'
3	N	1607	BCL	C2-C1-O2A-CGA
3	J	1605	BCL	C16-C17-C18-C20
4	I	1813	LDA	C7-C8-C9-C10
4	K	1826	LDA	C6-C7-C8-C9
4	P	1808	LDA	C2-C3-C4-C5
4	I	1813	LDA	C6-C7-C8-C9
4	R	1809	LDA	C6-C7-C8-C9
4	D	1802	LDA	C7-C8-C9-C10
4	F	1803	LDA	C6-C7-C8-C9
4	L	1806	LDA	C3-C4-C5-C6
4	O	1820	LDA	C6-C7-C8-C9
3	C	1502	BCL	C12-C13-C15-C16
4	A	1816	LDA	C6-C7-C8-C9
4	D	1802	LDA	C11-C10-C9-C8
4	F	1803	LDA	C4-C5-C6-C7
4	P	1808	LDA	C11-C10-C9-C8
3	G	1704	BCL	C5-C6-C7-C8
4	M	1827	LDA	C4-C5-C6-C7
3	R	1509	BCL	C3A-C2A-CAA-CBA
4	A	1816	LDA	C7-C8-C9-C10
4	J	1805	LDA	C3-C4-C5-C6
4	E	1822	LDA	C5-C6-C7-C8
3	A	1701	BCL	C8-C10-C11-C12
3	G	1704	BCL	C8-C10-C11-C12
3	M	1707	BCL	C16-C17-C18-C19
4	L	1806	LDA	C5-C6-C7-C8
4	R	1819	LDA	C5-C6-C7-C8
3	S	1609	BCL	O1D-CGD-O2D-CED
3	E	1703	BCL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	E	1503	BCL	C15-C16-C17-C18
4	G	1824	LDA	C3-C4-C5-C6
4	K	1826	LDA	C5-C6-C7-C8
3	O	1508	BCL	O1D-CGD-O2D-CED
4	K	1826	LDA	C2-C3-C4-C5
4	C	1821	LDA	C7-C8-C9-C10
4	H	1804	LDA	C3-C4-C5-C6
4	N	1807	LDA	C11-C10-C9-C8
4	C	1815	LDA	C5-C6-C7-C8
4	M	1827	LDA	C7-C8-C9-C10
4	I	1825	LDA	C11-C10-C9-C8
4	G	1824	LDA	C6-C7-C8-C9
4	B	1801	LDA	C2-C3-C4-C5
4	G	1814	LDA	C5-C6-C7-C8
4	J	1805	LDA	C2-C3-C4-C5
4	O	1820	LDA	C11-C10-C9-C8
4	R	1818	LDA	C7-C8-C9-C10
3	C	1702	BCL	C11-C10-C8-C9
4	A	1817	LDA	C1-C2-C3-C4
4	K	1810	LDA	C1-C2-C3-C4
4	A	1817	LDA	C11-C10-C9-C8
4	C	1815	LDA	C6-C7-C8-C9
4	C	1815	LDA	C2-C3-C4-C5
4	I	1812	LDA	C2-C3-C4-C5
4	O	1820	LDA	C7-C8-C9-C10
3	M	1707	BCL	C15-C16-C17-C18
4	E	1823	LDA	C5-C6-C7-C8
4	C	1821	LDA	C3-C4-C5-C6
4	I	1812	LDA	C7-C8-C9-C10
4	N	1807	LDA	C5-C6-C7-C8
3	M	1707	BCL	C16-C17-C18-C20
3	R	1509	BCL	C8-C10-C11-C12
3	C	1702	BCL	CBD-CGD-O2D-CED
5	L	1406	RG1	CM8-C26-C27-C28
4	N	1807	LDA	C2-C3-C4-C5
3	B	1601	BCL	C3-C5-C6-C7
4	H	1804	LDA	C2-C3-C4-C5
4	H	1804	LDA	C4-C5-C6-C7
4	I	1825	LDA	C7-C8-C9-C10
3	M	1707	BCL	CBA-CGA-O2A-C1
4	L	1806	LDA	C1-C2-C3-C4
4	G	1824	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
4	I	1825	LDA	C3-C4-C5-C6
3	E	1703	BCL	C15-C16-C17-C18
4	A	1816	LDA	C1-C2-C3-C4
4	A	1817	LDA	C3-C4-C5-C6
3	E	1703	BCL	C5-C6-C7-C8
3	K	1506	BCL	C15-C16-C17-C18
4	E	1823	LDA	C7-C8-C9-C10
3	R	1509	BCL	CBA-CGA-O2A-C1
4	L	1806	LDA	C11-C10-C9-C8
4	A	1817	LDA	C4-C5-C6-C7
4	C	1821	LDA	C4-C5-C6-C7
3	N	1607	BCL	CBD-CGD-O2D-CED
4	B	1801	LDA	C11-C10-C9-C8
4	E	1822	LDA	C11-C10-C9-C8
3	S	1609	BCL	C8-C10-C11-C12
4	K	1810	LDA	C3-C4-C5-C6
4	C	1821	LDA	C11-C10-C9-C8
4	M	1811	LDA	C11-C10-C9-C8
4	E	1822	LDA	C1-C2-C3-C4
3	M	1707	BCL	O1A-CGA-O2A-C1
3	R	1509	BCL	C1A-C2A-CAA-CBA
3	E	1703	BCL	C13-C15-C16-C17
4	M	1811	LDA	C3-C4-C5-C6
3	O	1708	BCL	C8-C10-C11-C12
3	A	1701	BCL	C11-C10-C8-C7
3	E	1703	BCL	C6-C7-C8-C10
3	N	1607	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	A	1701	BCL	C16-C17-C18-C20
3	A	1701	BCL	C2C-C3C-CAC-CBC
3	K	1506	BCL	C2C-C3C-CAC-CBC
4	K	1810	LDA	C6-C7-C8-C9
4	M	1811	LDA	C2-C3-C4-C5
3	I	1505	BCL	C8-C10-C11-C12
3	K	1706	BCL	C8-C10-C11-C12
3	A	1701	BCL	C11-C10-C8-C9
3	O	1508	BCL	C11-C12-C13-C14
3	R	1509	BCL	C11-C12-C13-C14
3	R	1509	BCL	C14-C13-C15-C16
3	R	1709	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
4	O	1820	LDA	C3-C4-C5-C6
4	C	1815	LDA	C11-C10-C9-C8
4	L	1806	LDA	C4-C5-C6-C7
4	A	1817	LDA	C7-C8-C9-C10
4	D	1802	LDA	C5-C6-C7-C8
3	L	1606	BCL	C3-C5-C6-C7
4	L	1806	LDA	C2-C3-C4-C5
5	N	1407	RG1	CM8-C26-C27-C28
3	A	1701	BCL	C16-C17-C18-C19
4	R	1809	LDA	C4-C5-C6-C7
5	L	1406	RG1	C25-C26-C27-C28
3	K	1706	BCL	C10-C11-C12-C13
3	K	1706	BCL	C5-C6-C7-C8
3	E	1703	BCL	CBA-CGA-O2A-C1
3	C	1702	BCL	C2B-C3B-CAB-CBB
3	E	1703	BCL	C2B-C3B-CAB-OB
3	E	1703	BCL	C2B-C3B-CAB-CBB
4	A	1816	LDA	C3-C4-C5-C6
4	E	1822	LDA	C4-C5-C6-C7
4	N	1807	LDA	C7-C8-C9-C10
3	E	1703	BCL	O1A-CGA-O2A-C1
4	C	1815	LDA	C4-C5-C6-C7
3	N	1607	BCL	C10-C11-C12-C13
3	H	1604	BCL	C16-C17-C18-C20
4	F	1803	LDA	C2-C3-C4-C5
4	H	1804	LDA	C5-C6-C7-C8
4	M	1811	LDA	C7-C8-C9-C10
4	R	1819	LDA	C9-C10-C11-C12
4	E	1823	LDA	C2-C3-C4-C5
4	F	1803	LDA	C3-C4-C5-C6
3	D	1602	BCL	C8-C10-C11-C12
4	I	1813	LDA	C5-C6-C7-C8
3	C	1702	BCL	CBA-CGA-O2A-C1
4	R	1818	LDA	C11-C10-C9-C8
4	E	1822	LDA	C3-C4-C5-C6
4	G	1814	LDA	C6-C7-C8-C9
4	K	1810	LDA	C9-C10-C11-C12
4	F	1803	LDA	C5-C6-C7-C8
3	A	1501	BCL	C8-C10-C11-C12
4	P	1808	LDA	C9-C10-C11-C12
4	R	1818	LDA	C5-C6-C7-C8
3	B	1601	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
3	D	1602	BCL	C11-C12-C13-C14
3	O	1708	BCL	C11-C10-C8-C9
3	P	1608	BCL	C11-C12-C13-C14
4	H	1804	LDA	C6-C7-C8-C9
4	R	1818	LDA	C9-C10-C11-C12
4	G	1814	LDA	C3-C4-C5-C6
4	M	1811	LDA	C4-C5-C6-C7
4	M	1827	LDA	C3-C4-C5-C6
5	P	1408	RG1	CM1-C1-C2-C3
4	J	1805	LDA	C9-C10-C11-C12
3	I	1505	BCL	C12-C13-C15-C16
3	I	1705	BCL	C11-C10-C8-C7
3	R	1509	BCL	C11-C12-C13-C15
3	R	1509	BCL	C12-C13-C15-C16
3	R	1709	BCL	C13-C15-C16-C17
5	N	1407	RG1	C27-C28-C29-C30
3	R	1509	BCL	O1A-CGA-O2A-C1
3	G	1504	BCL	C15-C16-C17-C18
3	C	1702	BCL	C1-C2-C3-C4
4	R	1818	LDA	C6-C7-C8-C9
5	H	1404	RG1	C4'-C5'-C6'-O6'
4	I	1812	LDA	C6-C7-C8-C9
4	J	1805	LDA	C5-C6-C7-C8
3	N	1607	BCL	C1-C2-C3-C5
4	G	1814	LDA	C4-C5-C6-C7
4	I	1813	LDA	C3-C4-C5-C6
3	G	1704	BCL	C4B-C3B-CAB-CBB
3	C	1502	BCL	C14-C13-C15-C16
3	N	1607	BCL	C14-C13-C15-C16
4	C	1821	LDA	C9-C10-C11-C12
3	H	1604	BCL	C16-C17-C18-C19
4	R	1819	LDA	C1-C2-C3-C4
3	M	1507	BCL	C4C-C3C-CAC-CBC
3	J	1605	BCL	C16-C17-C18-C19
3	N	1607	BCL	C16-C17-C18-C19
4	I	1825	LDA	C6-C7-C8-C9
3	C	1702	BCL	O1D-CGD-O2D-CED
3	E	1703	BCL	C16-C17-C18-C20
3	K	1506	BCL	C16-C17-C18-C19
3	C	1702	BCL	C6-C7-C8-C10
3	F	1603	BCL	C11-C12-C13-C15
3	K	1706	BCL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
3	R	1709	BCL	C11-C10-C8-C7
3	H	1604	BCL	C3-C5-C6-C7
3	O	1508	BCL	C8-C10-C11-C12
5	N	1407	RG1	C25-C26-C27-C28
3	O	1508	BCL	O1A-CGA-O2A-C1
3	C	1702	BCL	O1A-CGA-O2A-C1
4	I	1825	LDA	C1-C2-C3-C4
3	C	1702	BCL	C2B-C3B-CAB-OBB
3	G	1704	BCL	C2B-C3B-CAB-OBB
3	G	1704	BCL	C2B-C3B-CAB-CBB
3	K	1706	BCL	C2B-C3B-CAB-OBB
3	K	1706	BCL	C2B-C3B-CAB-CBB
3	P	1608	BCL	O2A-C1-C2-C3
4	I	1812	LDA	C4-C5-C6-C7
4	R	1809	LDA	C3-C4-C5-C6
4	B	1801	LDA	C7-C8-C9-C10
3	R	1709	BCL	C16-C17-C18-C20
4	R	1809	LDA	C5-C6-C7-C8
3	C	1702	BCL	C6-C7-C8-C9
3	E	1703	BCL	C11-C12-C13-C14
4	B	1801	LDA	C6-C7-C8-C9
3	O	1508	BCL	C10-C11-C12-C13
3	B	1601	BCL	C2-C1-O2A-CGA
4	A	1817	LDA	C2-C1-N1-CM2
4	D	1802	LDA	C2-C1-N1-CM2
4	J	1805	LDA	C2-C1-N1-CM2
4	L	1806	LDA	C2-C1-N1-CM1
4	P	1808	LDA	C1-C2-C3-C4
4	P	1808	LDA	C6-C7-C8-C9
4	R	1819	LDA	C6-C7-C8-C9
3	M	1707	BCL	C1A-C2A-CAA-CBA
3	E	1703	BCL	CBD-CGD-O2D-CED
3	O	1708	BCL	C6-C7-C8-C10
4	A	1816	LDA	C11-C10-C9-C8
4	P	1808	LDA	C7-C8-C9-C10
4	R	1809	LDA	C11-C10-C9-C8
5	F	1403	RG1	C2-C1-O1'-C1'
5	R	1401	RG1	C2-C1-O1'-C1'
5	S	1409	RG1	C2-C1-O1'-C1'
3	C	1702	BCL	C4B-C3B-CAB-CBB
3	G	1704	BCL	C4B-C3B-CAB-OBB
3	P	1608	BCL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
3	I	1505	BCL	C14-C13-C15-C16
3	K	1506	BCL	C11-C12-C13-C14
4	J	1805	LDA	C1-C2-C3-C4
3	G	1504	BCL	O1D-CGD-O2D-CED
3	O	1508	BCL	CBA-CGA-O2A-C1
3	R	1709	BCL	C16-C17-C18-C19
3	N	1607	BCL	O1A-CGA-O2A-C1
5	H	1404	RG1	O5'-C5'-C6'-O6'
4	G	1824	LDA	C5-C6-C7-C8
3	C	1502	BCL	C15-C16-C17-C18
4	B	1801	LDA	C4-C5-C6-C7
4	J	1805	LDA	C7-C8-C9-C10
4	A	1816	LDA	C9-C10-C11-C12
4	R	1819	LDA	C2-C3-C4-C5
4	K	1826	LDA	C4-C5-C6-C7
3	C	1502	BCL	O1D-CGD-O2D-CED
3	O	1708	BCL	C5-C6-C7-C8
4	E	1822	LDA	C7-C8-C9-C10
4	D	1802	LDA	C6-C7-C8-C9
3	P	1608	BCL	O1A-CGA-O2A-C1
4	R	1819	LDA	N1-C1-C2-C3
4	G	1814	LDA	C11-C10-C9-C8
4	K	1826	LDA	C11-C10-C9-C8
4	F	1803	LDA	C7-C8-C9-C10
4	B	1801	LDA	C1-C2-C3-C4
3	N	1607	BCL	CBA-CGA-O2A-C1
4	G	1814	LDA	C7-C8-C9-C10
3	E	1503	BCL	C11-C12-C13-C14
3	G	1504	BCL	C11-C12-C13-C14
3	L	1606	BCL	C11-C10-C8-C9
3	P	1608	BCL	CBA-CGA-O2A-C1
3	L	1606	BCL	C13-C15-C16-C17
3	J	1605	BCL	C5-C6-C7-C8
3	L	1606	BCL	C10-C11-C12-C13
3	G	1704	BCL	C11-C12-C13-C15
4	B	1801	LDA	C3-C4-C5-C6
4	R	1819	LDA	C4-C5-C6-C7
3	A	1701	BCL	C15-C16-C17-C18
3	C	1502	BCL	C8-C10-C11-C12
4	I	1812	LDA	C11-C10-C9-C8
4	M	1811	LDA	C6-C7-C8-C9
3	N	1607	BCL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
3	F	1603	BCL	C11-C10-C8-C9
3	N	1607	BCL	C6-C7-C8-C9
3	N	1607	BCL	C11-C12-C13-C14
3	P	1608	BCL	C11-C10-C8-C9
3	S	1609	BCL	C11-C10-C8-C9
3	A	1701	BCL	C2B-C3B-CAB-OBB
3	N	1607	BCL	C1-C2-C3-C4
3	F	1603	BCL	C4-C3-C5-C6
3	L	1606	BCL	C4-C3-C5-C6
3	D	1602	BCL	C6-C7-C8-C10
3	E	1503	BCL	C11-C12-C13-C15
3	I	1505	BCL	C11-C12-C13-C15
3	J	1605	BCL	C12-C13-C15-C16
3	K	1506	BCL	C11-C12-C13-C15
3	N	1607	BCL	C6-C7-C8-C10
3	S	1609	BCL	C11-C10-C8-C7
4	P	1808	LDA	C5-C6-C7-C8
4	E	1823	LDA	C3-C4-C5-C6
4	D	1802	LDA	C4-C5-C6-C7
4	K	1810	LDA	C4-C5-C6-C7
5	R	1401	RG1	CM1-C1-O1'-C1'
5	R	1401	RG1	CM2-C1-O1'-C1'
4	M	1811	LDA	C5-C6-C7-C8
3	R	1709	BCL	C5-C6-C7-C8
3	C	1702	BCL	C4B-C3B-CAB-OBB
3	K	1706	BCL	C4B-C3B-CAB-OBB
3	K	1706	BCL	C4B-C3B-CAB-CBB
3	G	1504	BCL	C3-C5-C6-C7
3	D	1602	BCL	C6-C7-C8-C9
3	I	1505	BCL	C11-C12-C13-C14
4	H	1804	LDA	C9-C10-C11-C12
3	I	1705	BCL	C13-C15-C16-C17
3	N	1607	BCL	C2-C3-C5-C6
3	K	1706	BCL	O1A-CGA-O2A-C1
3	G	1704	BCL	C4-C3-C5-C6
3	R	1709	BCL	C8-C10-C11-C12
3	B	1601	BCL	O1A-CGA-O2A-C1
3	G	1504	BCL	C12-C13-C15-C16
4	R	1809	LDA	C7-C8-C9-C10
3	E	1503	BCL	C14-C13-C15-C16
3	F	1603	BCL	C14-C13-C15-C16
3	G	1504	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
3	J	1605	BCL	C11-C10-C8-C9
3	P	1608	BCL	C6-C7-C8-C9
4	K	1810	LDA	C11-C10-C9-C8
3	I	1705	BCL	C2-C1-O2A-CGA
4	K	1826	LDA	C3-C4-C5-C6
3	A	1701	BCL	C2B-C3B-CAB-CBB
3	M	1707	BCL	C2B-C3B-CAB-CBB
5	L	1406	RG1	C27-C28-C29-C30
4	R	1809	LDA	C2-C3-C4-C5
4	I	1825	LDA	C5-C6-C7-C8
3	I	1705	BCL	O1A-CGA-O2A-C1
5	D	1402	RG1	C4'-C5'-C6'-O6'
3	A	1701	BCL	C4B-C3B-CAB-CBB
3	H	1604	BCL	C11-C12-C13-C14
3	O	1508	BCL	C11-C10-C8-C9
3	E	1503	BCL	C12-C13-C15-C16
3	F	1603	BCL	C12-C13-C15-C16
3	H	1604	BCL	C6-C7-C8-C10
3	J	1605	BCL	C11-C10-C8-C7
3	L	1606	BCL	C11-C10-C8-C7
3	O	1708	BCL	C11-C10-C8-C7
3	S	1609	BCL	C6-C7-C8-C10
4	I	1812	LDA	C2-C1-N1-CM1
4	I	1825	LDA	C2-C1-N1-CM2
4	N	1807	LDA	C6-C7-C8-C9
3	B	1601	BCL	O1D-CGD-O2D-CED
4	E	1823	LDA	C9-C10-C11-C12
5	H	1404	RG1	C17-C18-C19-C20
5	J	1405	RG1	C21-C22-C23-C24
3	O	1708	BCL	C15-C16-C17-C18
3	D	1602	BCL	C16-C17-C18-C19
5	F	1403	RG1	CM2-C1-C2-C3
5	N	1407	RG1	CM2-C1-C2-C3
3	E	1703	BCL	C12-C13-C15-C16
3	P	1608	BCL	C11-C12-C13-C15
3	M	1707	BCL	C2B-C3B-CAB-OBB
3	S	1609	BCL	O2A-C1-C2-C3
4	N	1807	LDA	C3-C4-C5-C6
3	C	1702	BCL	C2C-C3C-CAC-CBC
3	B	1601	BCL	C5-C6-C7-C8
3	K	1506	BCL	C3A-C2A-CAA-CBA
3	A	1701	BCL	C4B-C3B-CAB-OBB

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Mol	Chain	Res	Type	Atoms
3	J	1605	BCL	C14-C13-C15-C16
3	S	1609	BCL	C6-C7-C8-C9
3	K	1706	BCL	CBA-CGA-O2A-C1
3	A	1701	BCL	C2-C3-C5-C6
3	S	1609	BCL	C5-C6-C7-C8
3	K	1706	BCL	C4-C3-C5-C6
3	F	1603	BCL	C15-C16-C17-C18
3	A	1501	BCL	C1-C2-C3-C4
3	B	1601	BCL	C1-C2-C3-C4
3	H	1604	BCL	C1-C2-C3-C4
3	S	1609	BCL	C1-C2-C3-C4

There are no ring outliers.

60 monomers are involved in 394 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1803	LDA	7	0
4	M	1811	LDA	4	0
3	E	1703	BCL	7	0
3	L	1606	BCL	21	0
4	E	1822	LDA	8	0
3	G	1704	BCL	20	0
3	E	1503	BCL	3	0
4	D	1802	LDA	3	0
4	L	1806	LDA	5	0
4	M	1827	LDA	2	0
3	D	1602	BCL	5	0
3	M	1707	BCL	20	0
5	F	1403	RG1	5	0
3	I	1705	BCL	20	0
3	C	1502	BCL	3	0
5	H	1404	RG1	5	0
3	N	1607	BCL	14	0
4	I	1813	LDA	2	0
4	P	1808	LDA	3	0
5	L	1406	RG1	4	0
5	R	1401	RG1	4	0
4	H	1804	LDA	3	0
3	S	1609	BCL	10	0
3	J	1605	BCL	15	0
3	B	1601	BCL	7	0
3	R	1709	BCL	21	0

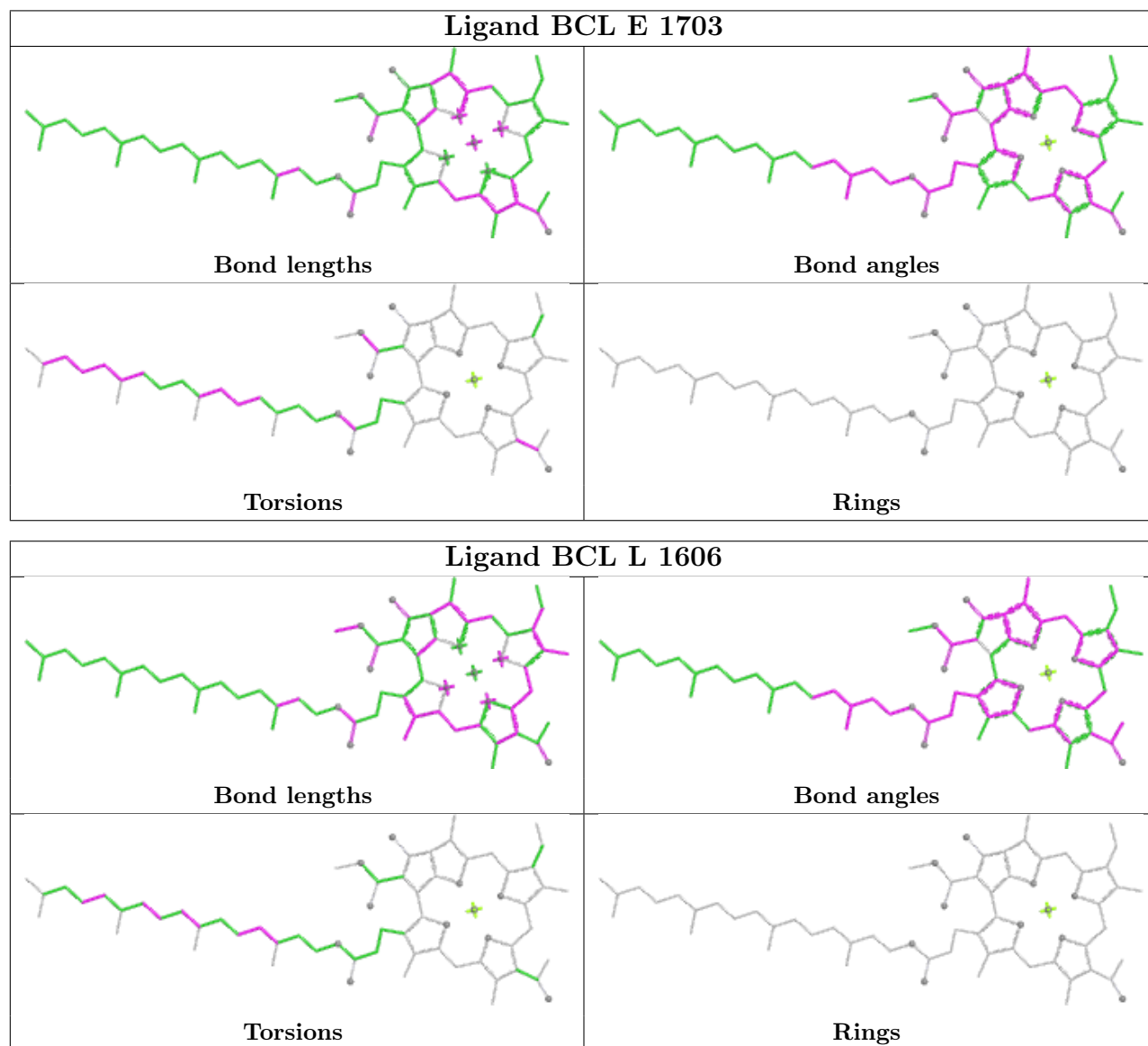
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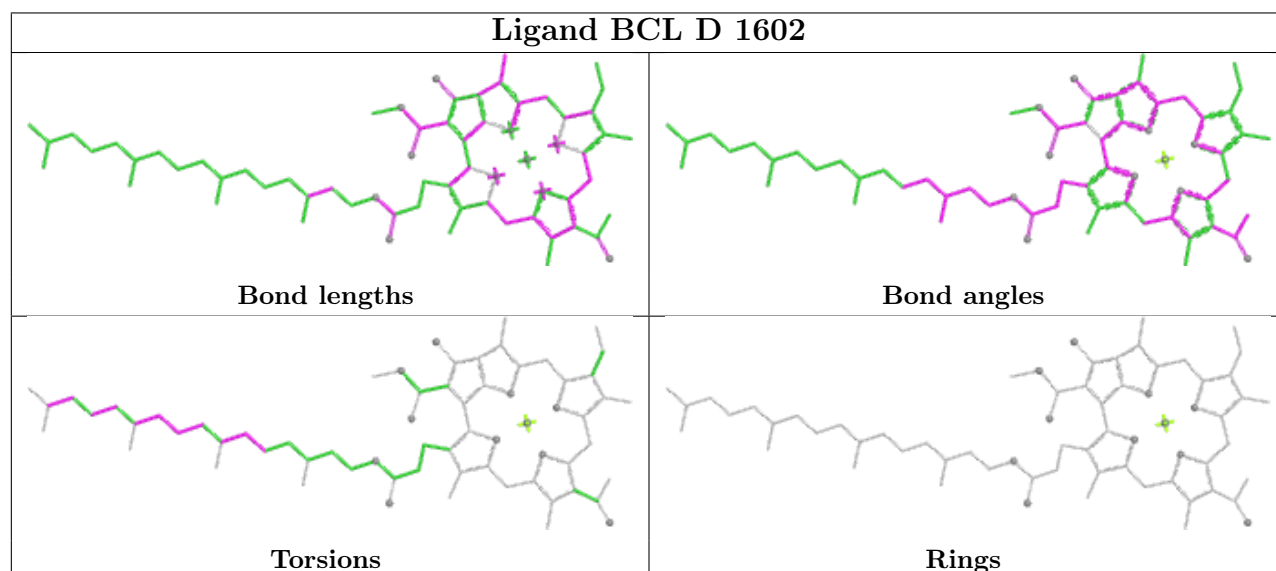
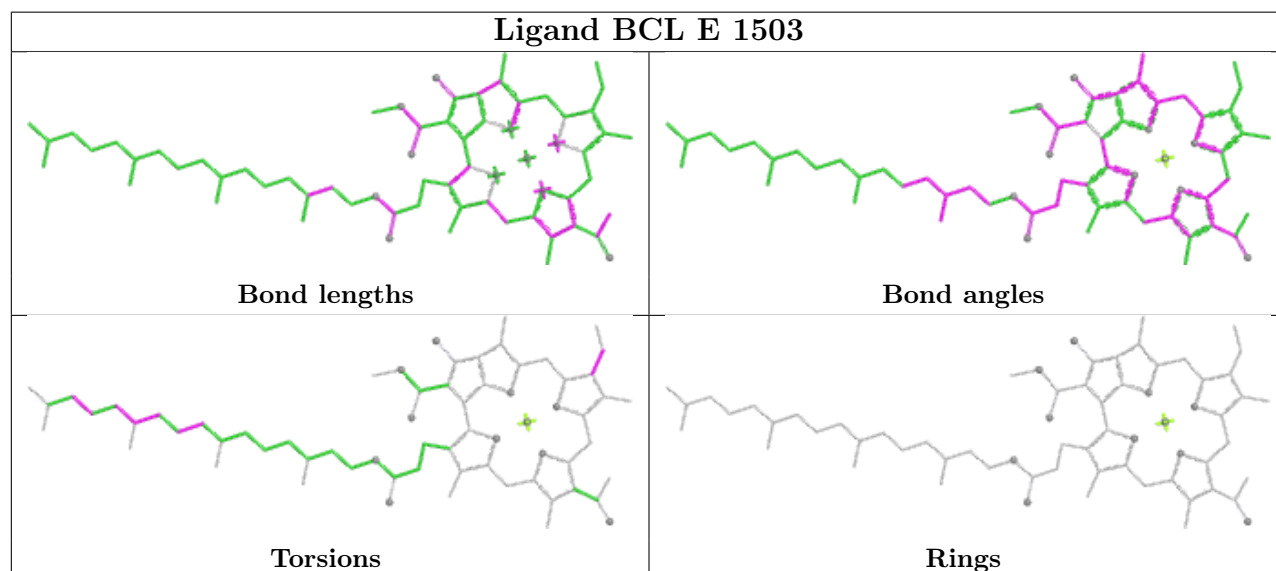
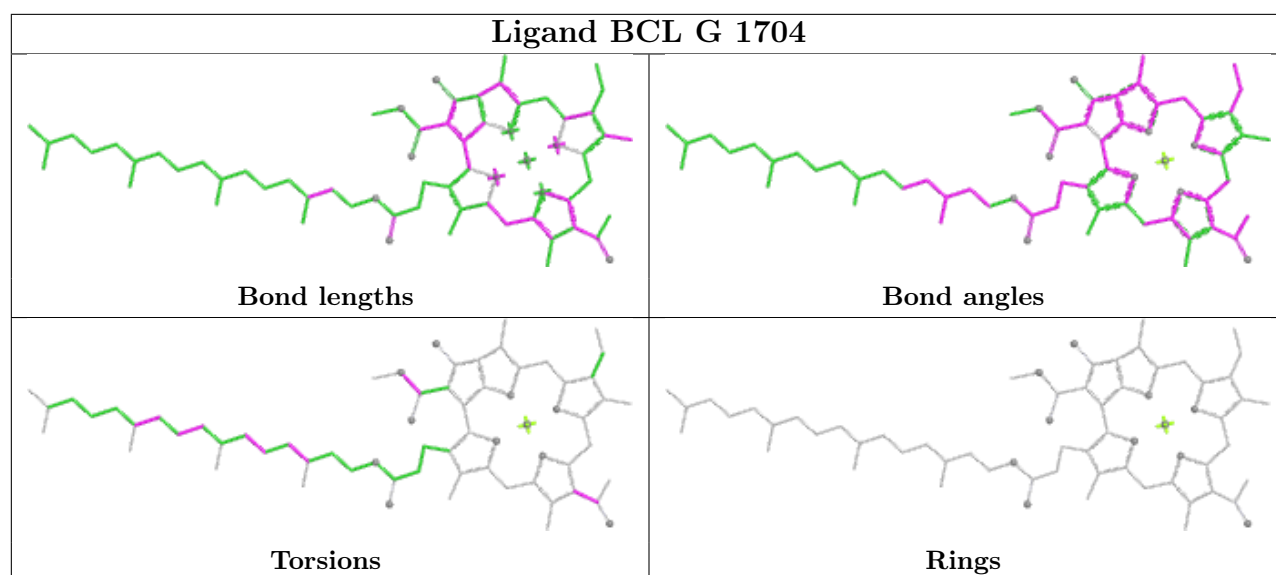
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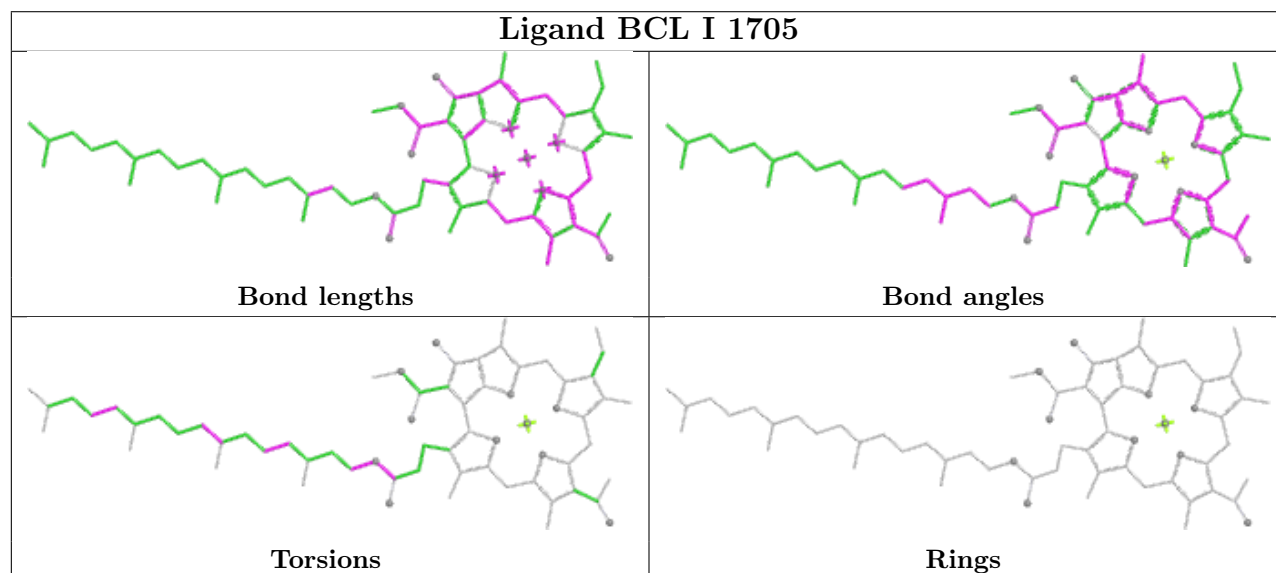
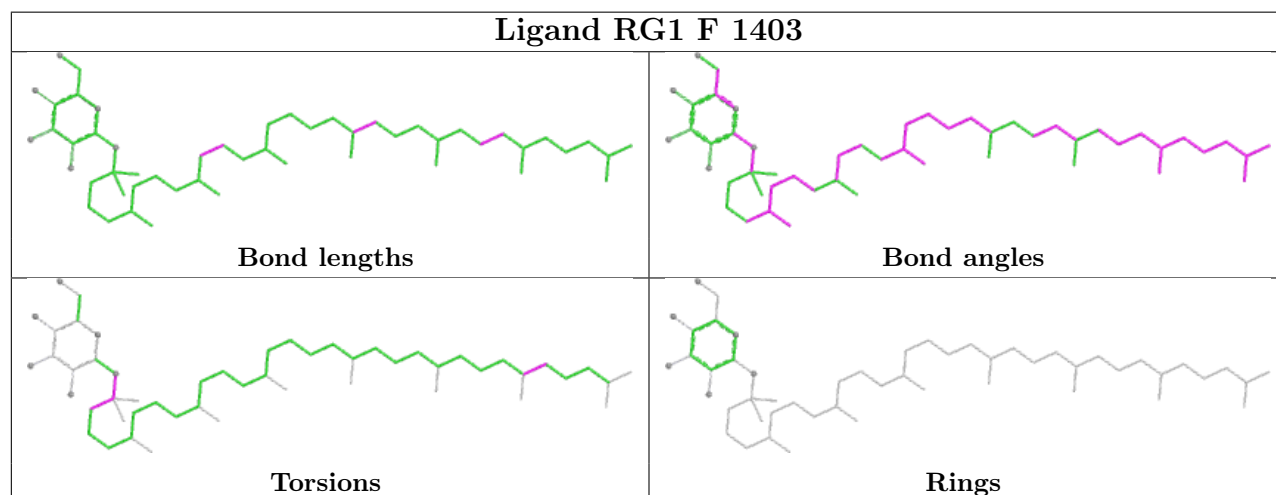
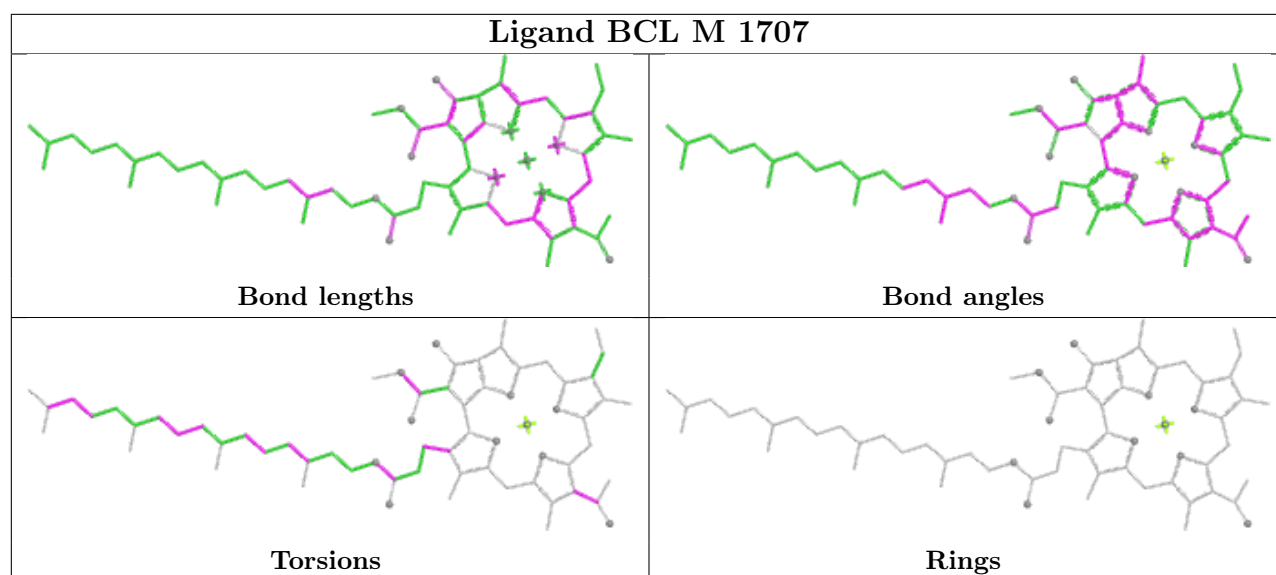
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1501	BCL	16	0
5	D	1402	RG1	5	0
4	N	1807	LDA	2	0
4	C	1815	LDA	6	0
3	K	1706	BCL	5	0
5	S	1409	RG1	5	0
4	I	1812	LDA	7	0
3	I	1505	BCL	9	0
3	P	1608	BCL	11	0
4	A	1816	LDA	8	0
4	B	1801	LDA	2	0
4	G	1824	LDA	14	0
4	R	1818	LDA	12	0
4	O	1820	LDA	7	0
3	A	1701	BCL	6	0
4	G	1814	LDA	3	0
4	K	1810	LDA	8	0
4	K	1826	LDA	4	0
5	P	1408	RG1	4	0
4	J	1805	LDA	1	0
4	A	1817	LDA	3	0
3	G	1504	BCL	3	0
4	I	1825	LDA	6	0
5	J	1405	RG1	1	0
5	N	1407	RG1	4	0
3	R	1509	BCL	6	0
3	F	1603	BCL	9	0
3	O	1508	BCL	11	0
4	E	1823	LDA	6	0
3	H	1604	BCL	8	0
3	K	1506	BCL	9	0
3	O	1708	BCL	9	0
3	C	1702	BCL	8	0
3	M	1507	BCL	2	0

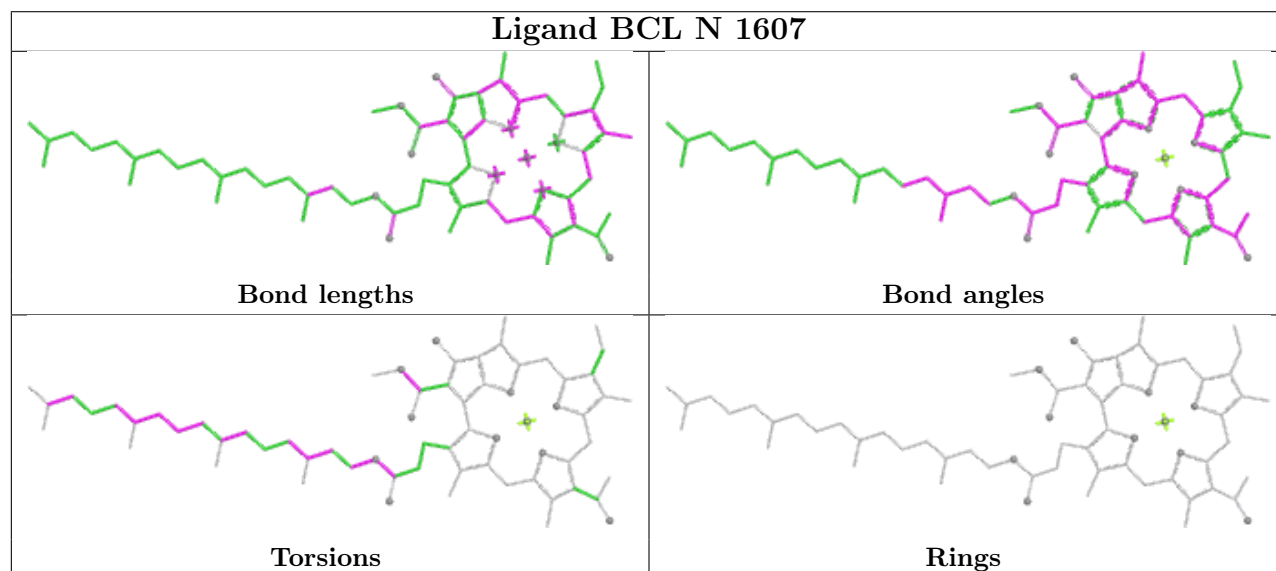
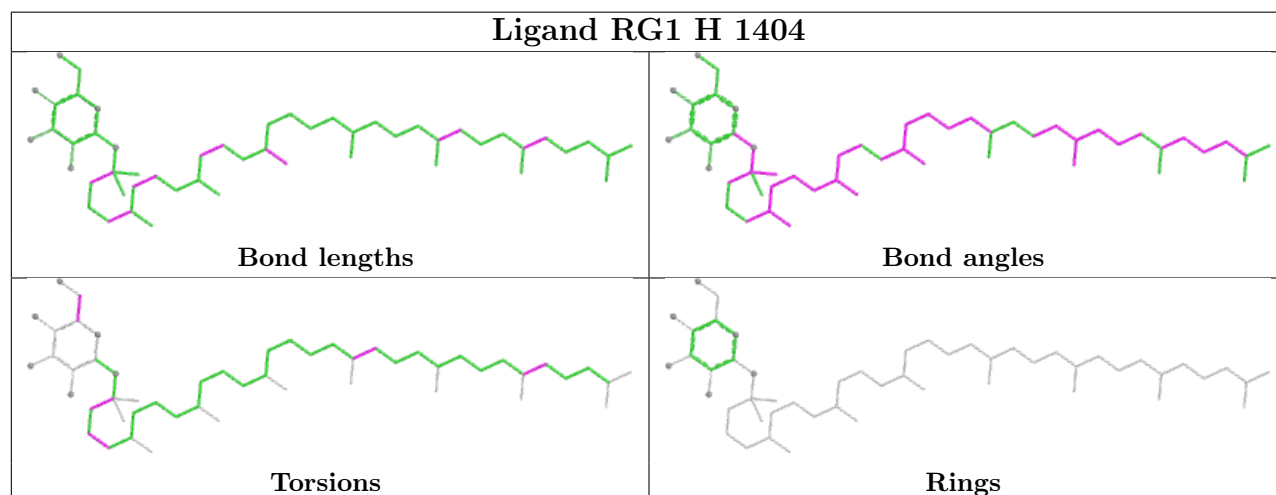
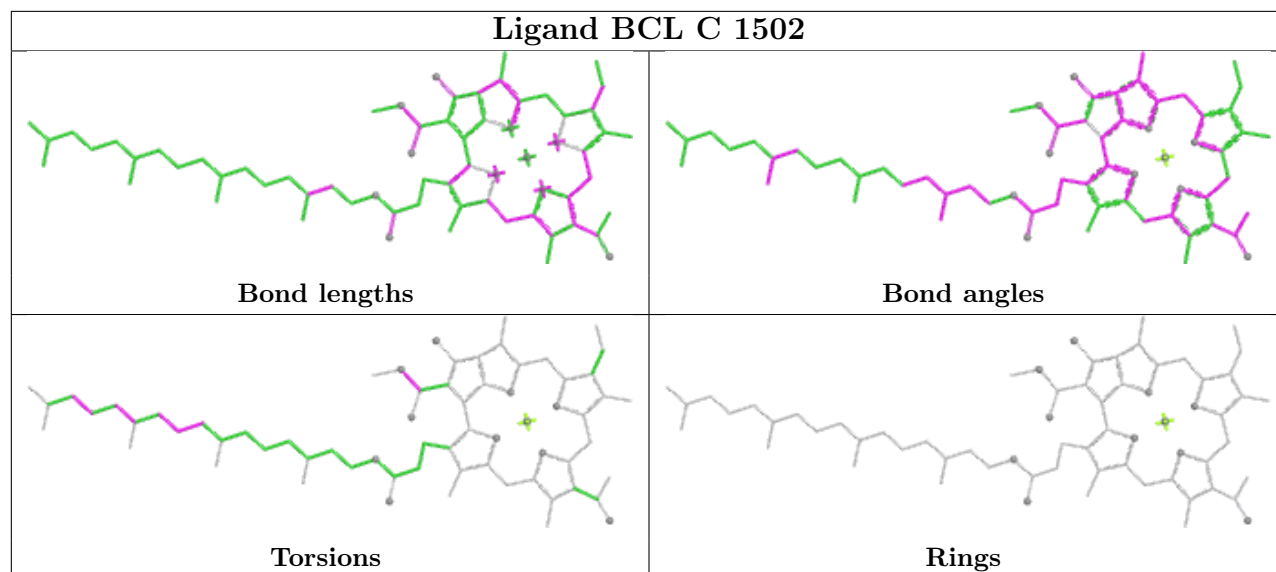
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

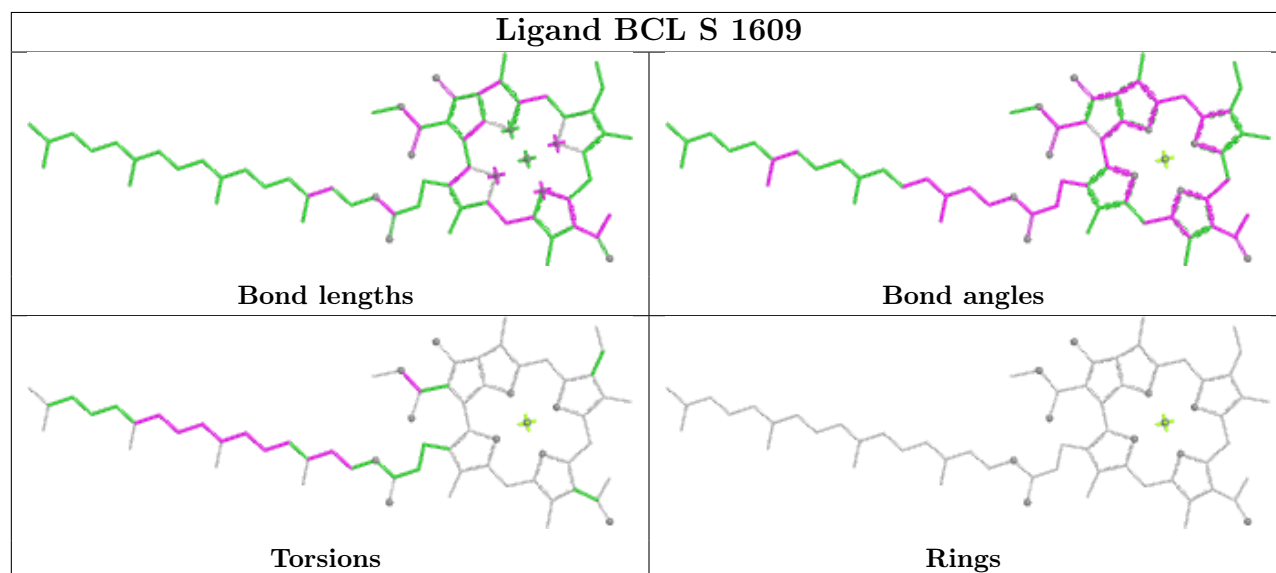
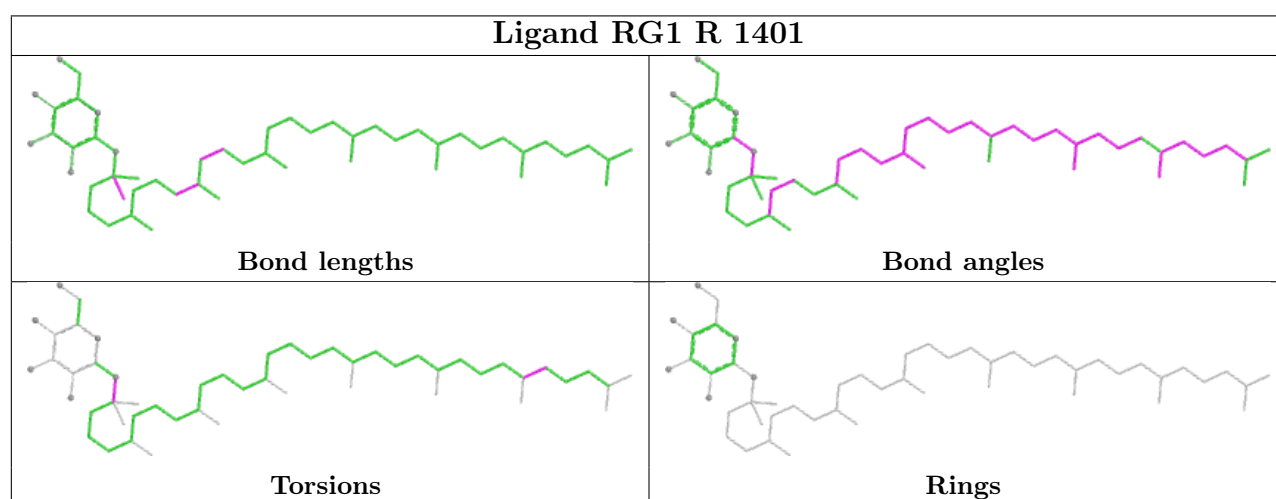
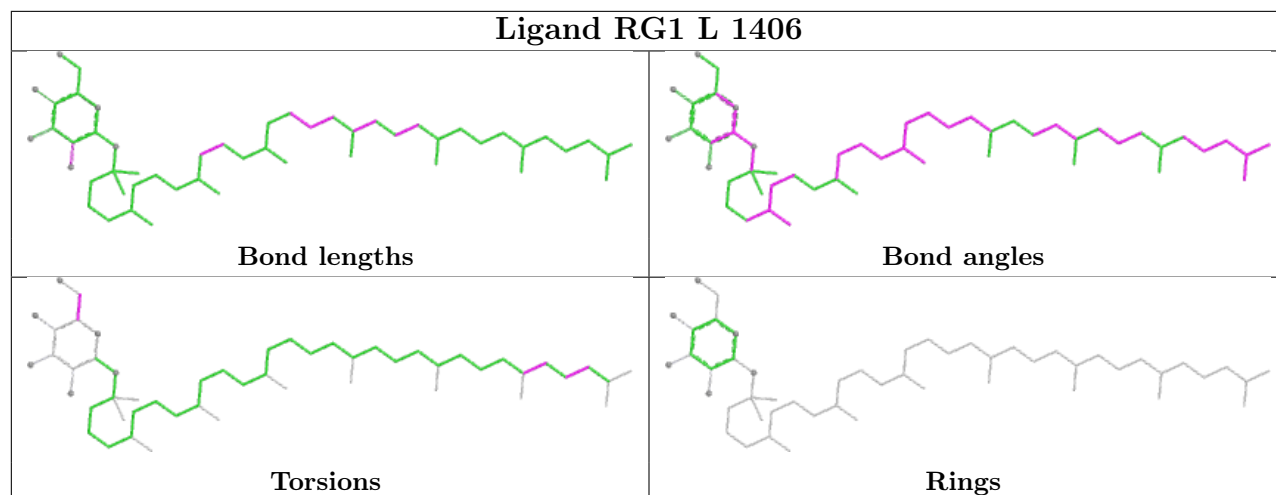
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

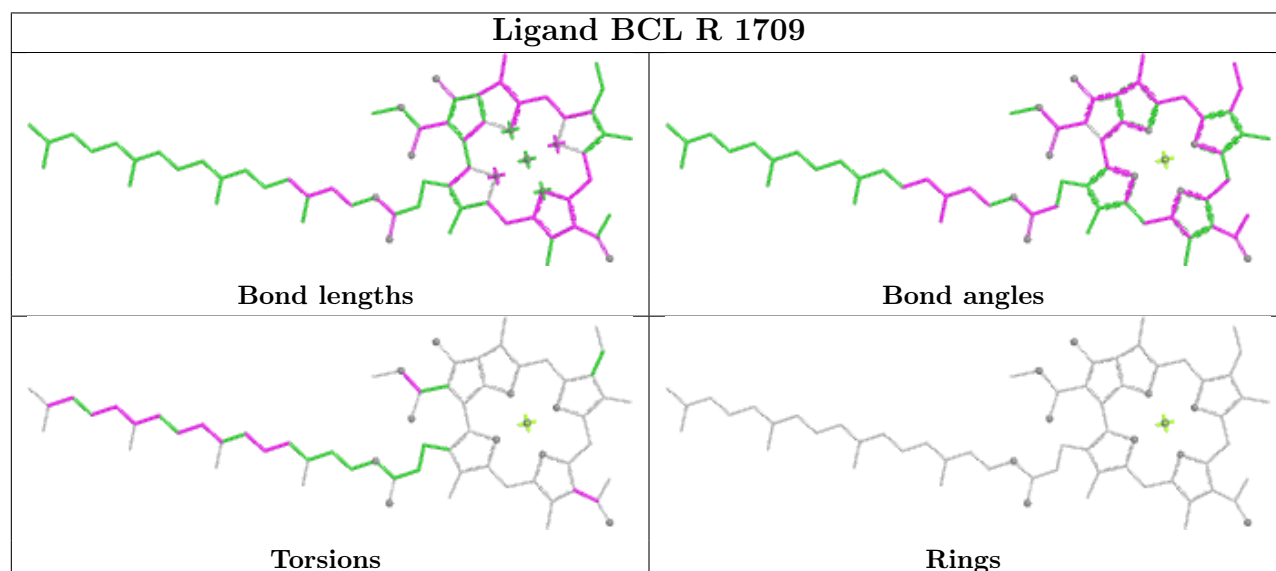
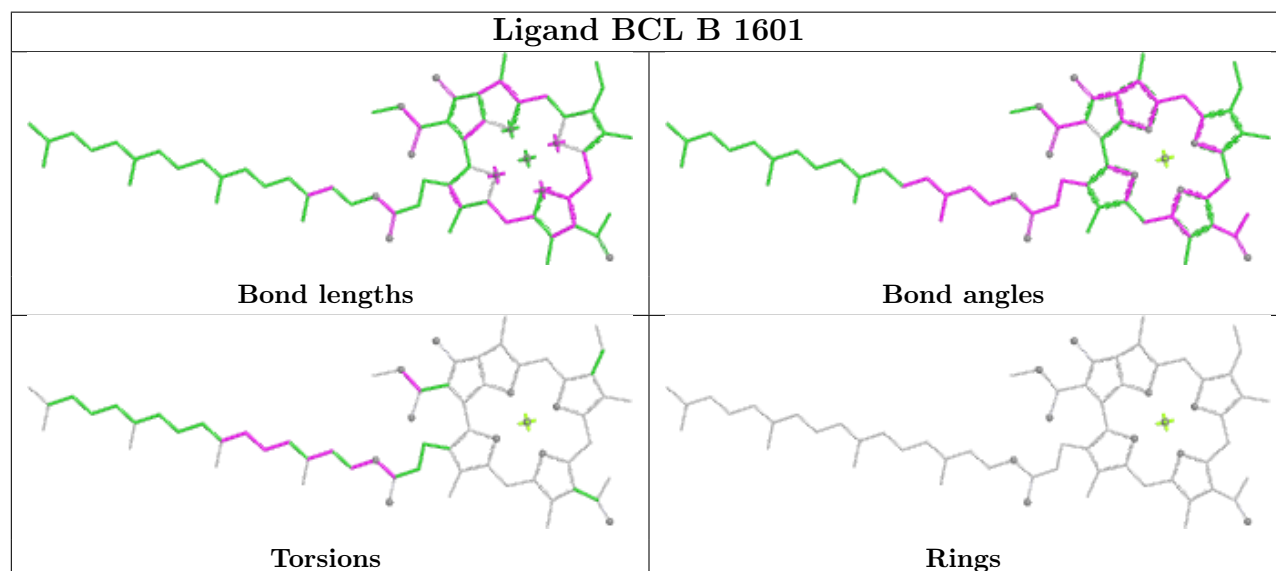
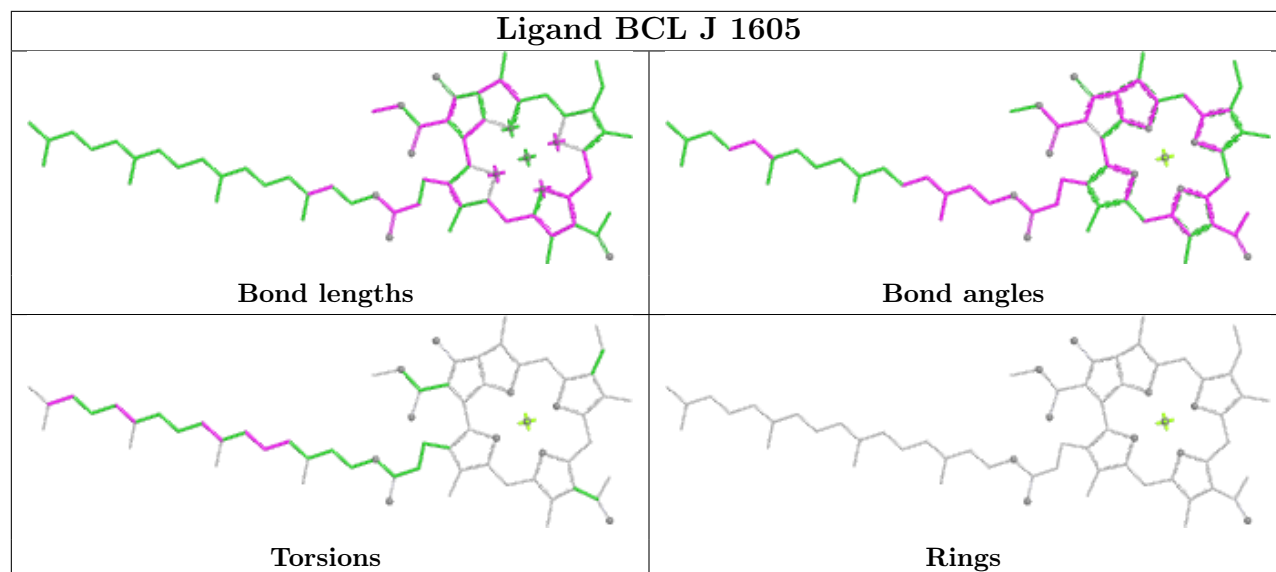


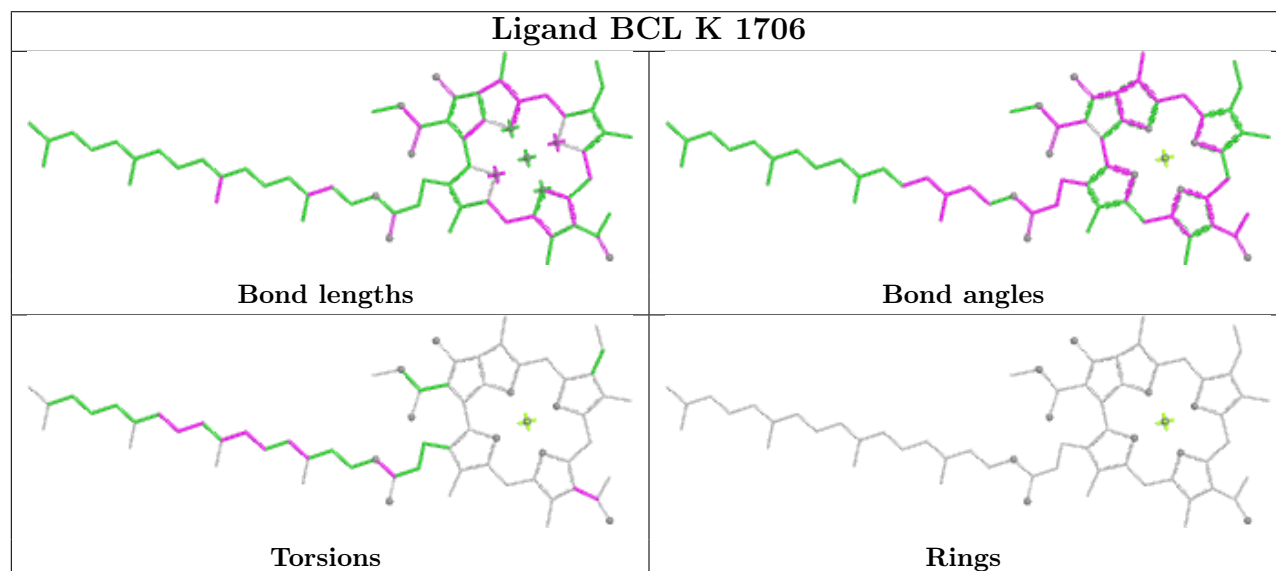
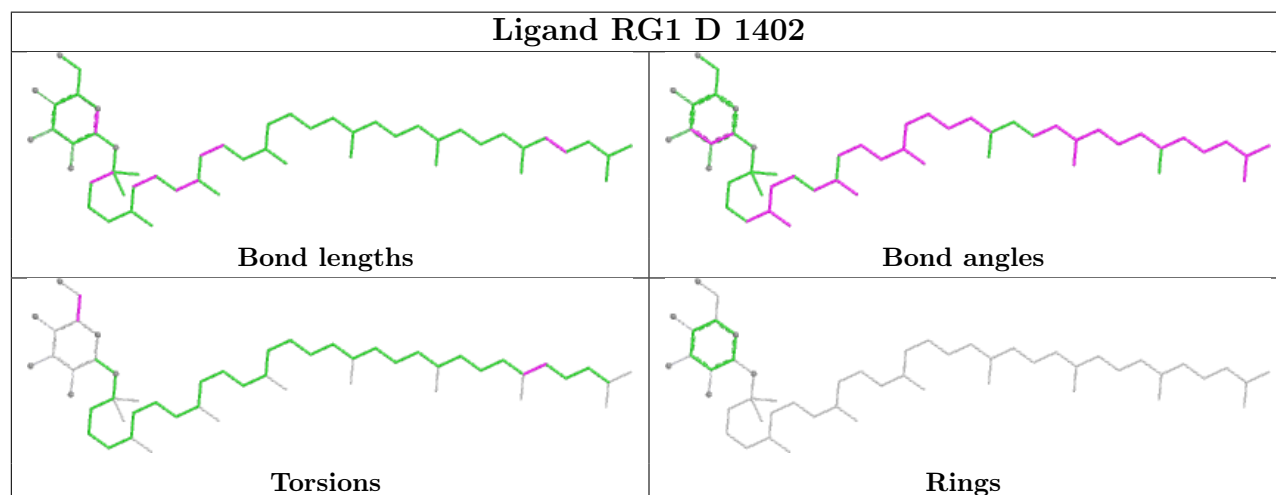
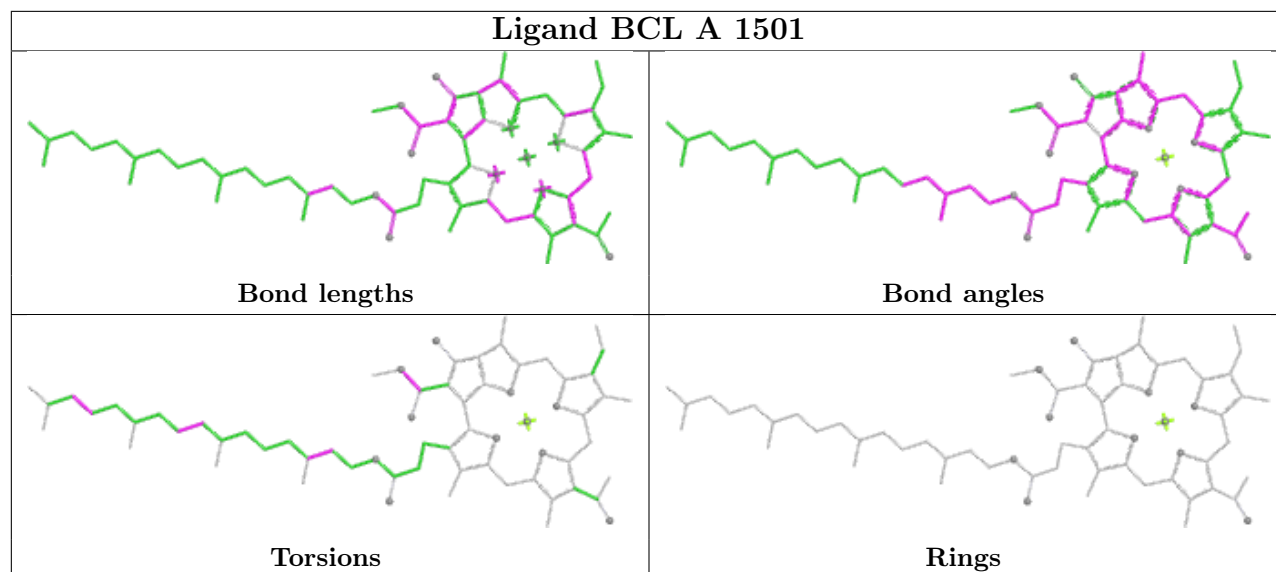


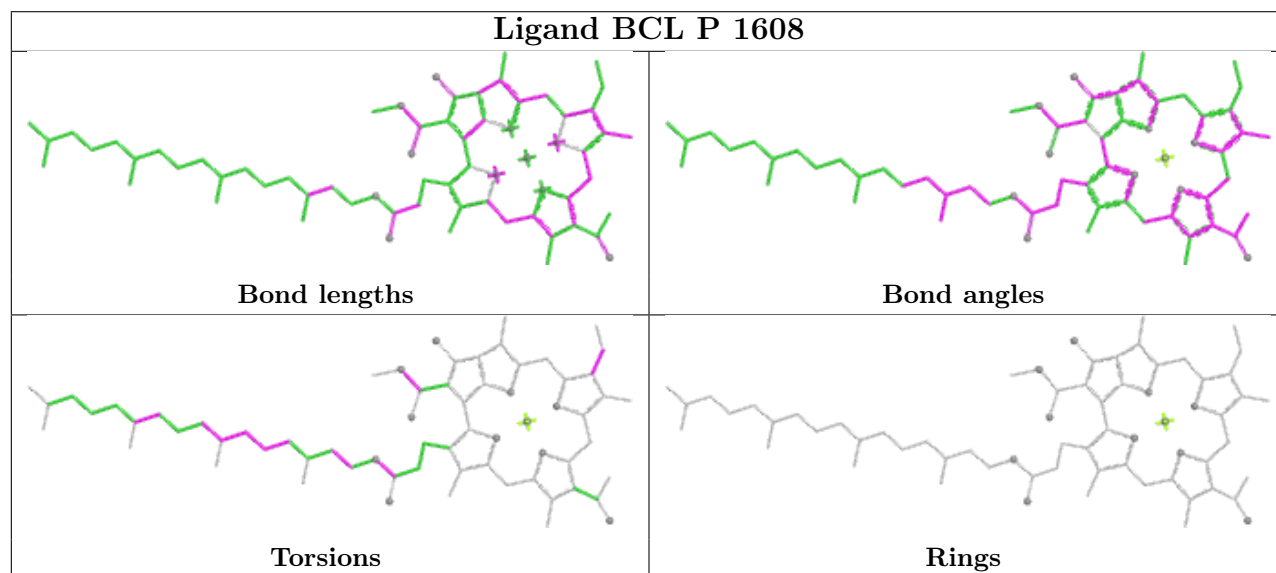
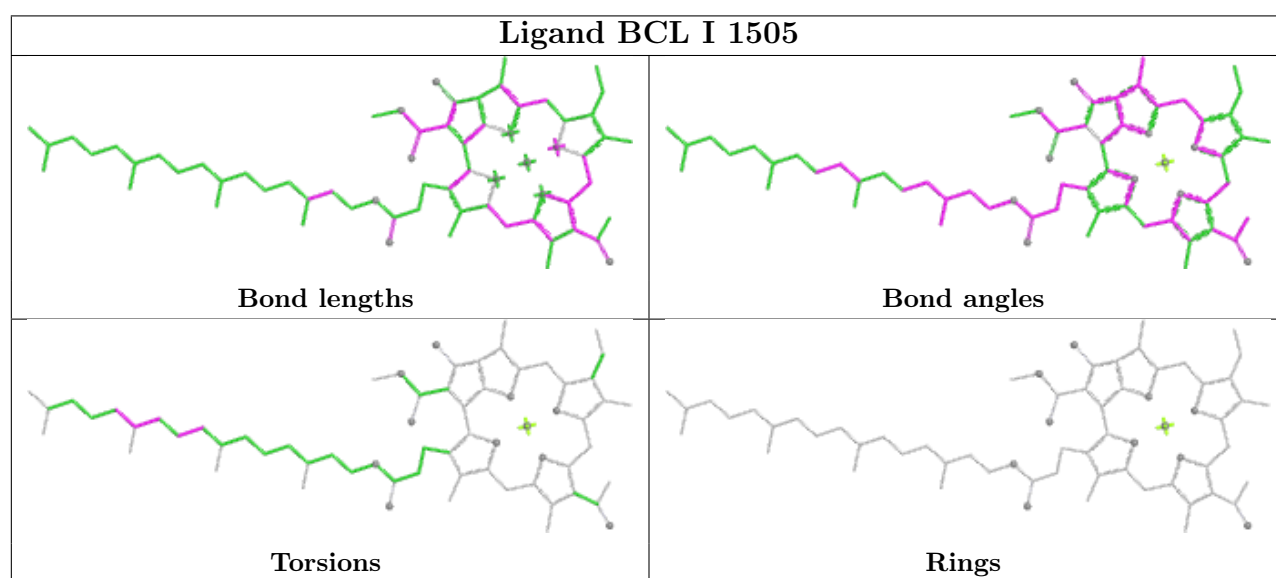
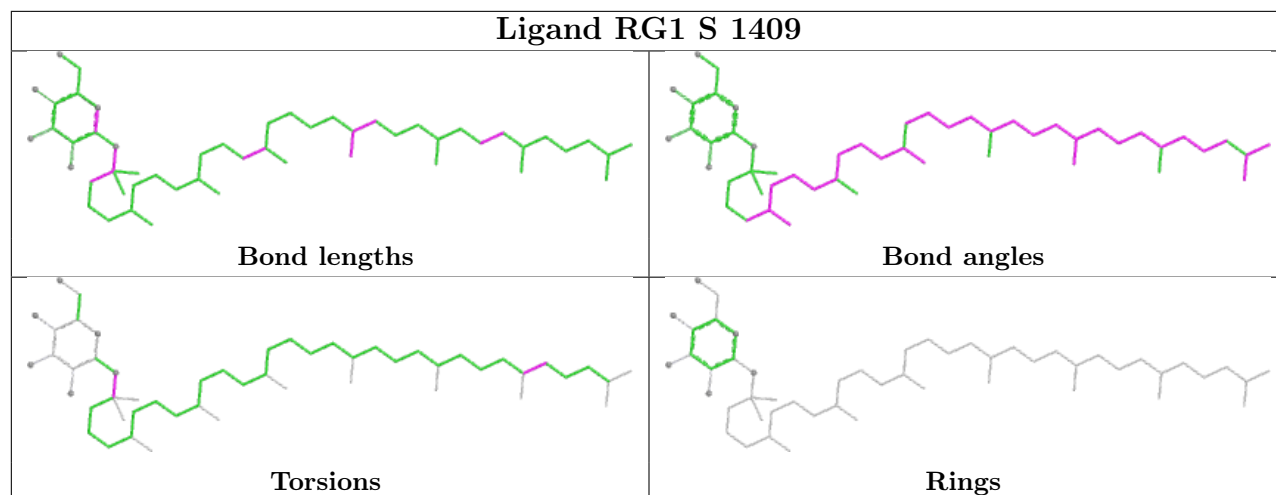


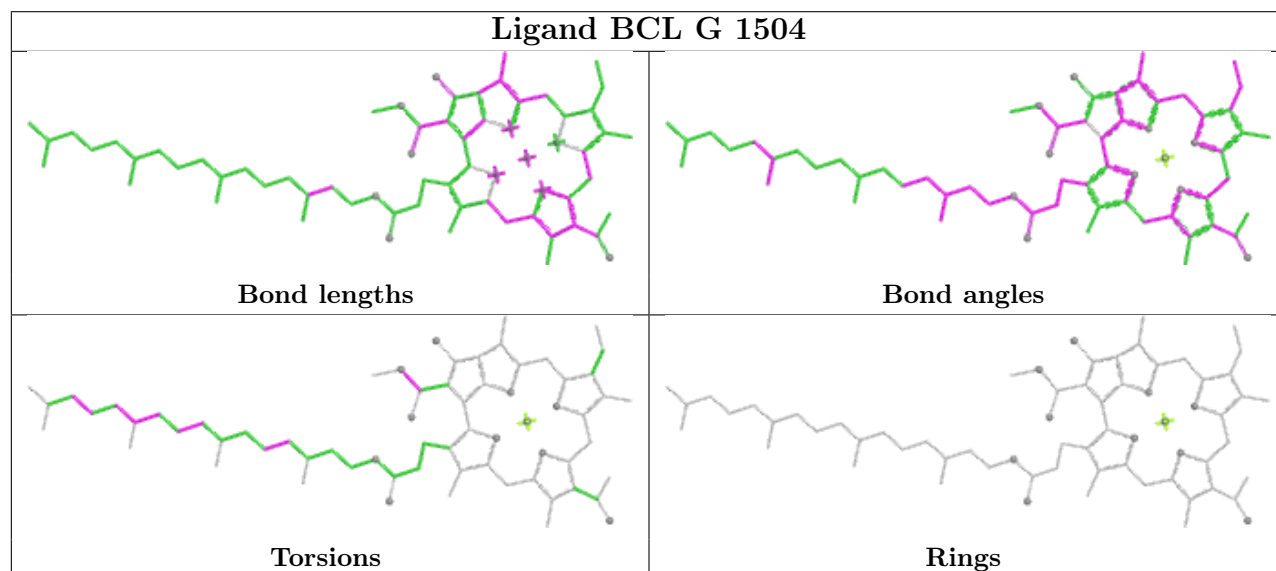
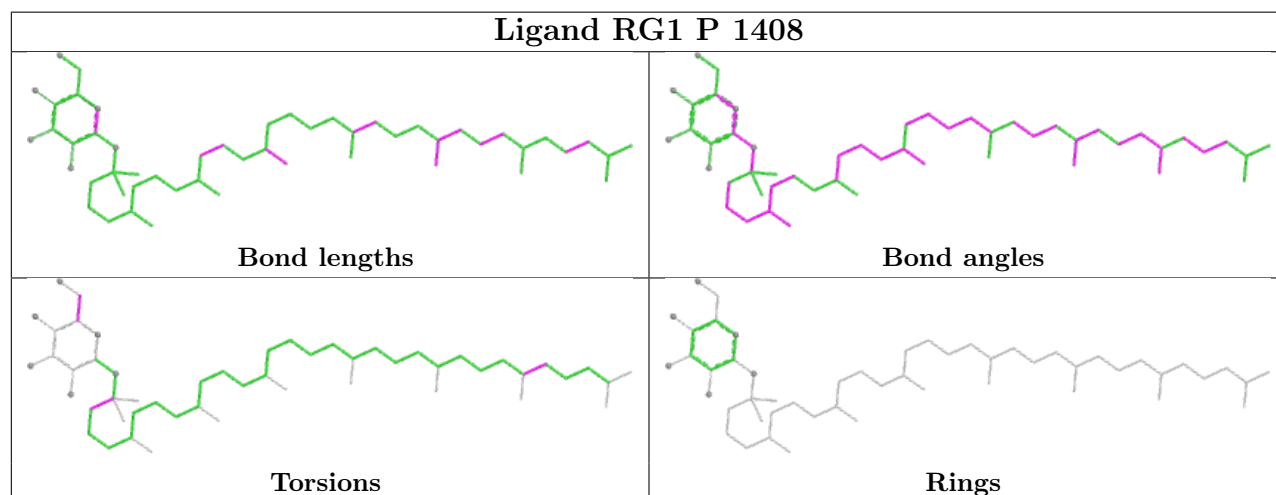
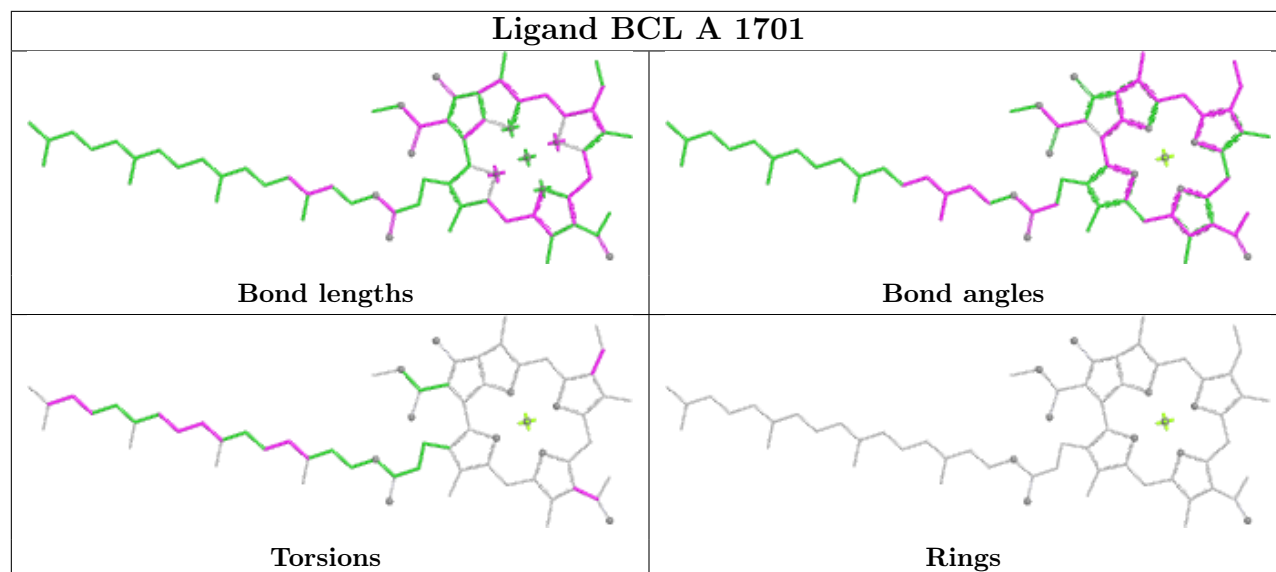


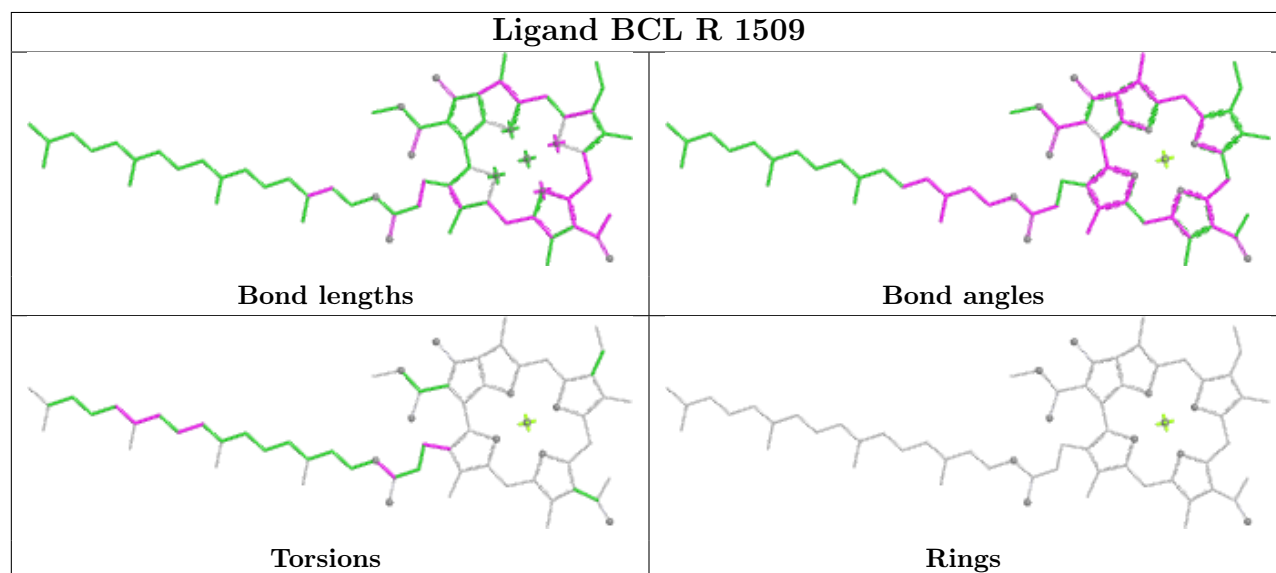
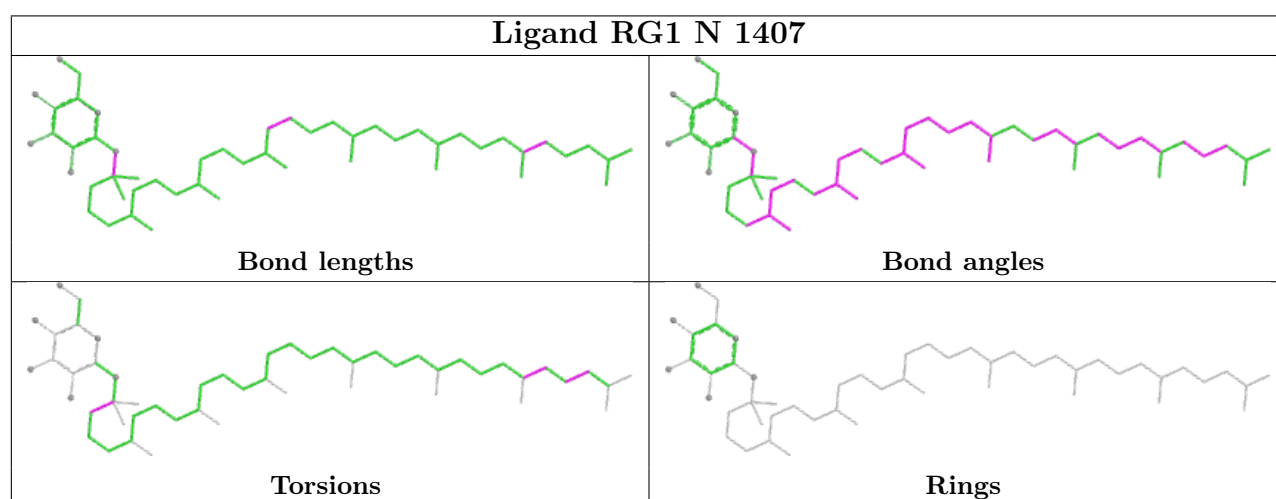
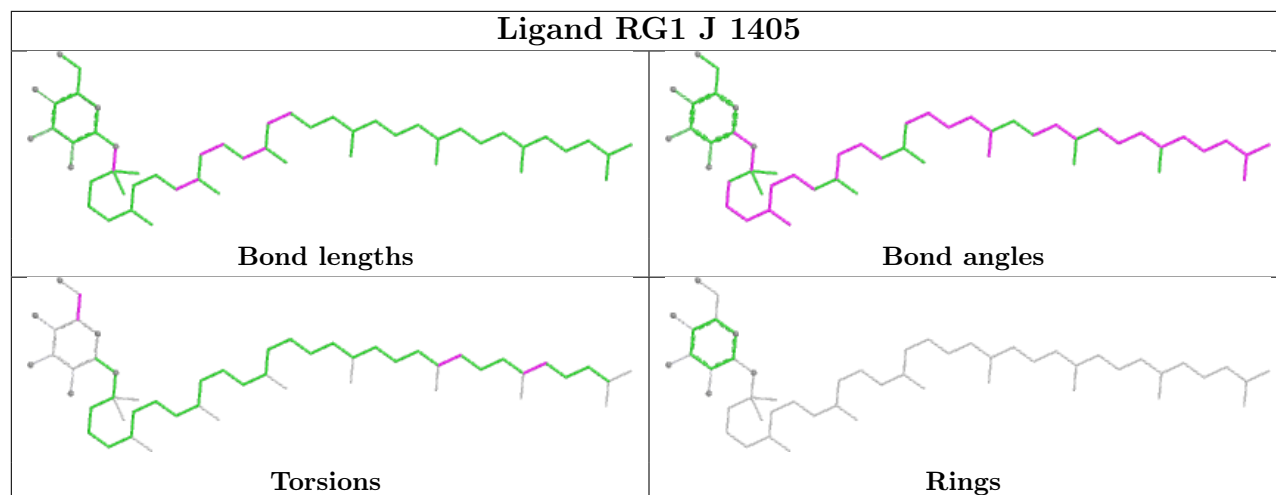


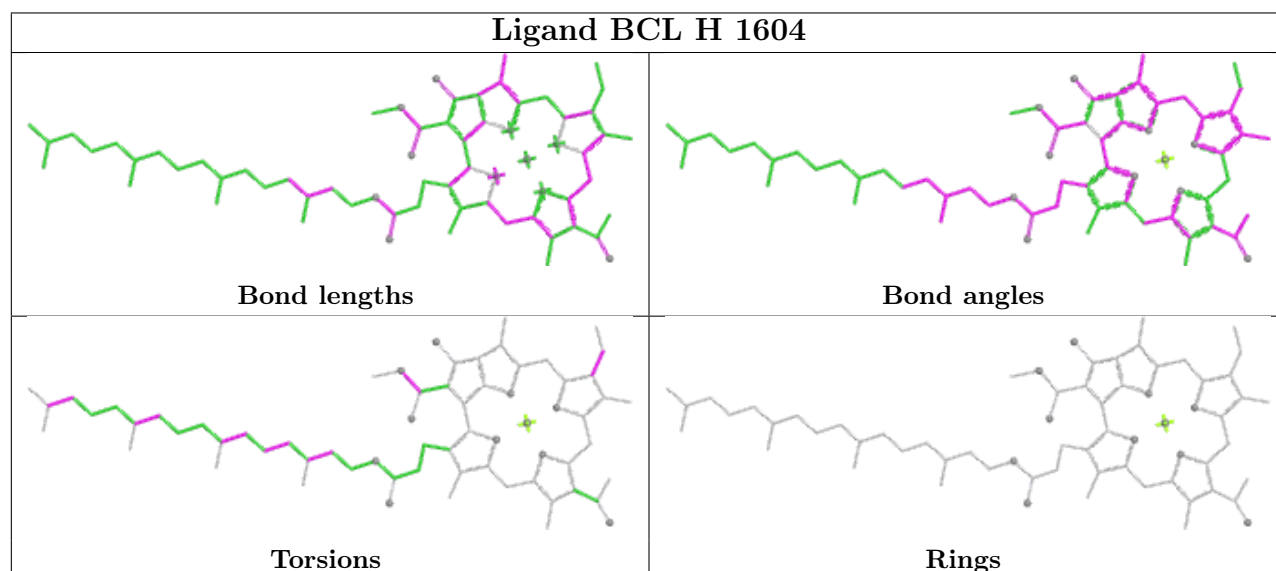
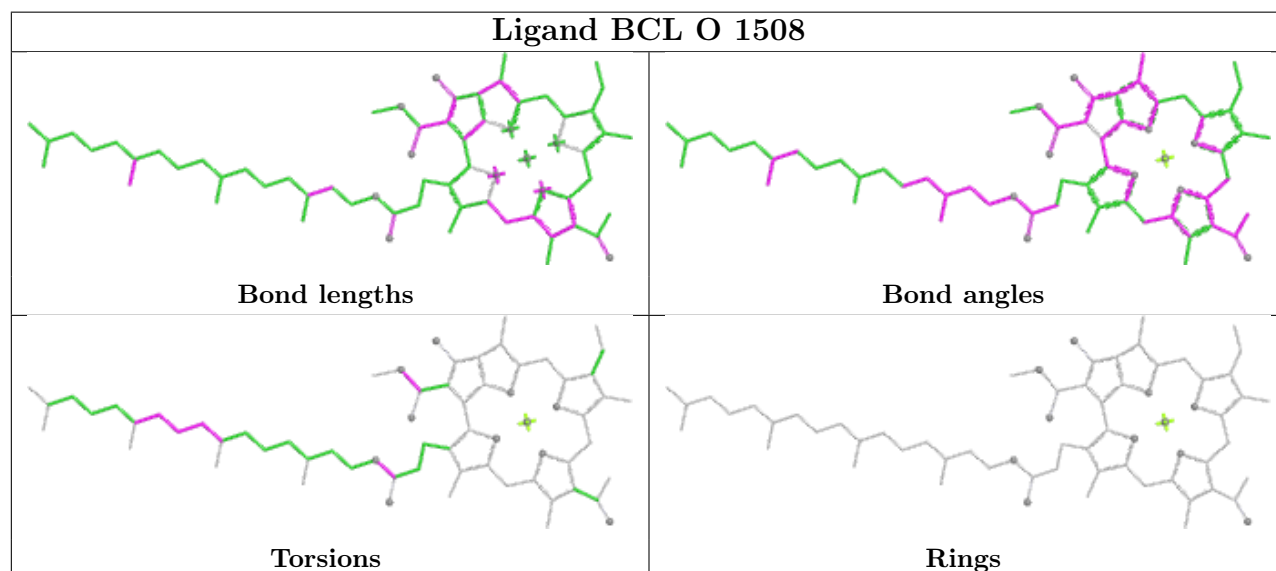
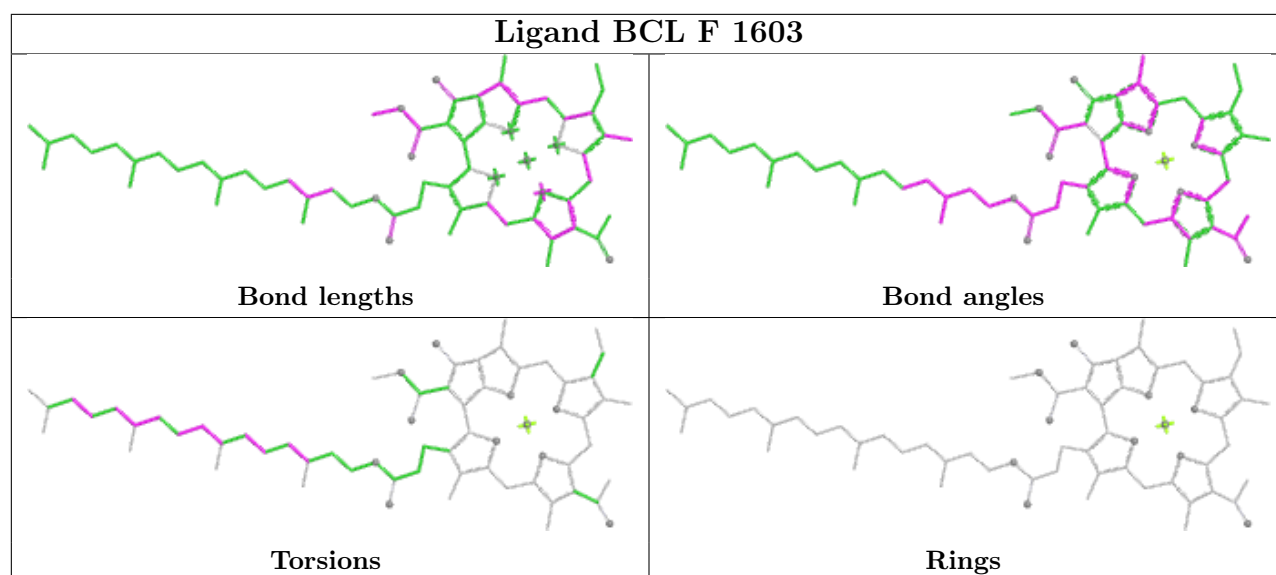


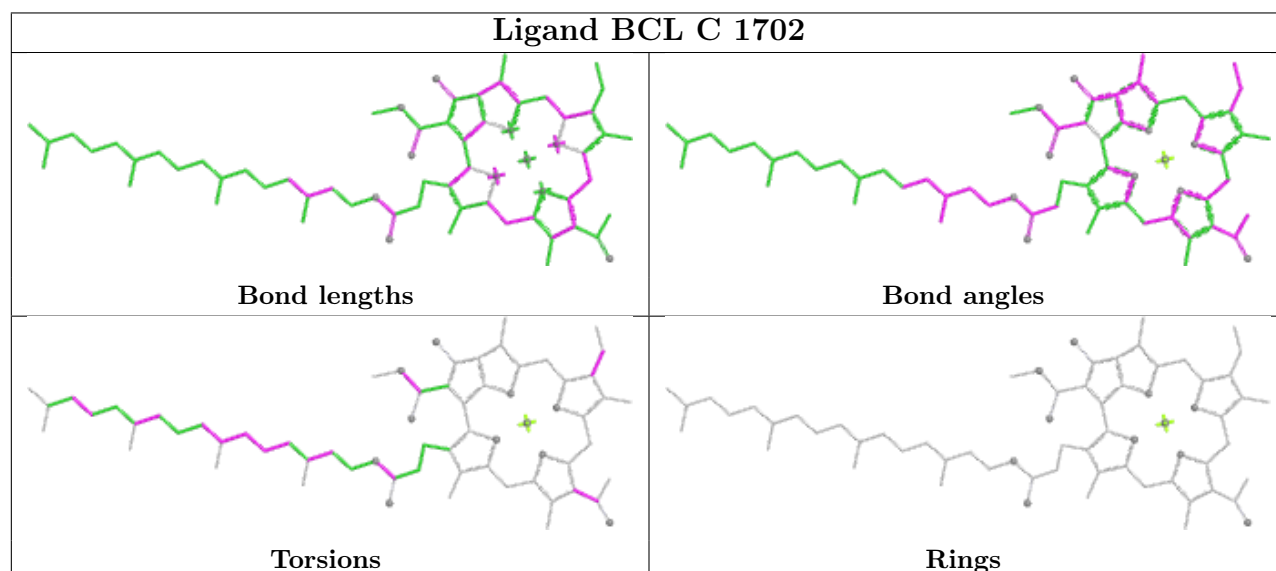
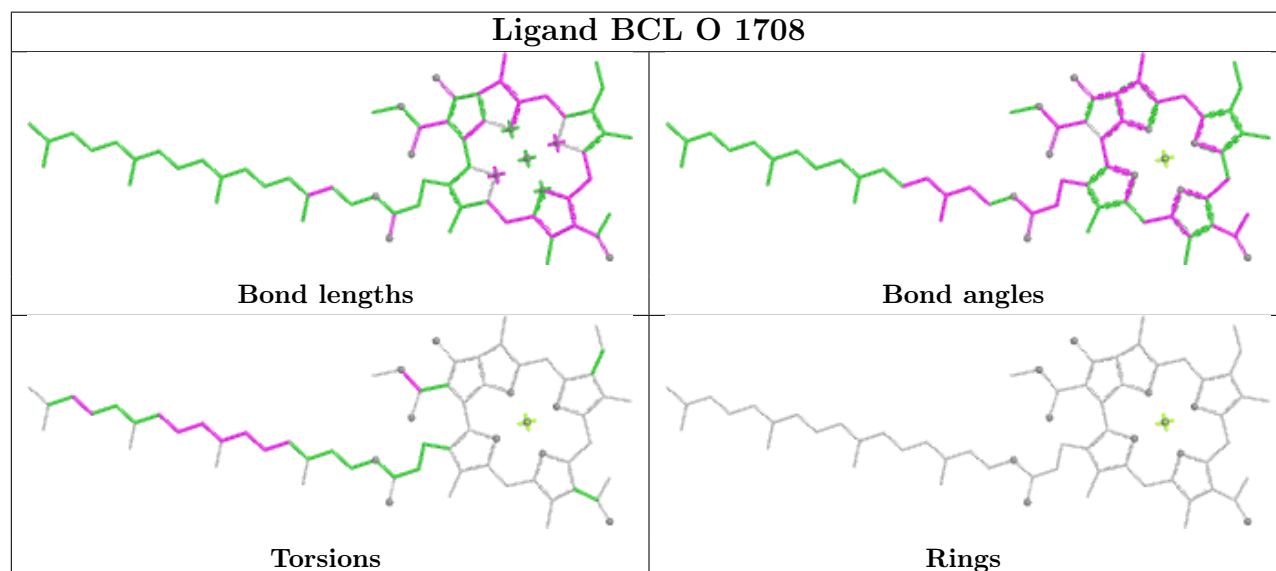
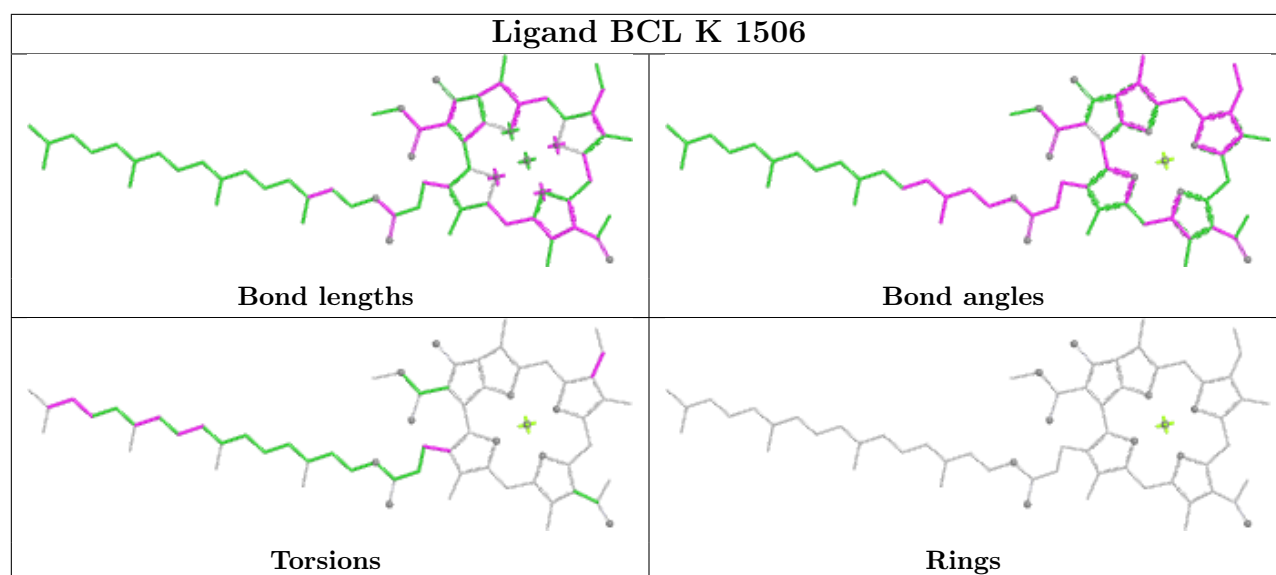


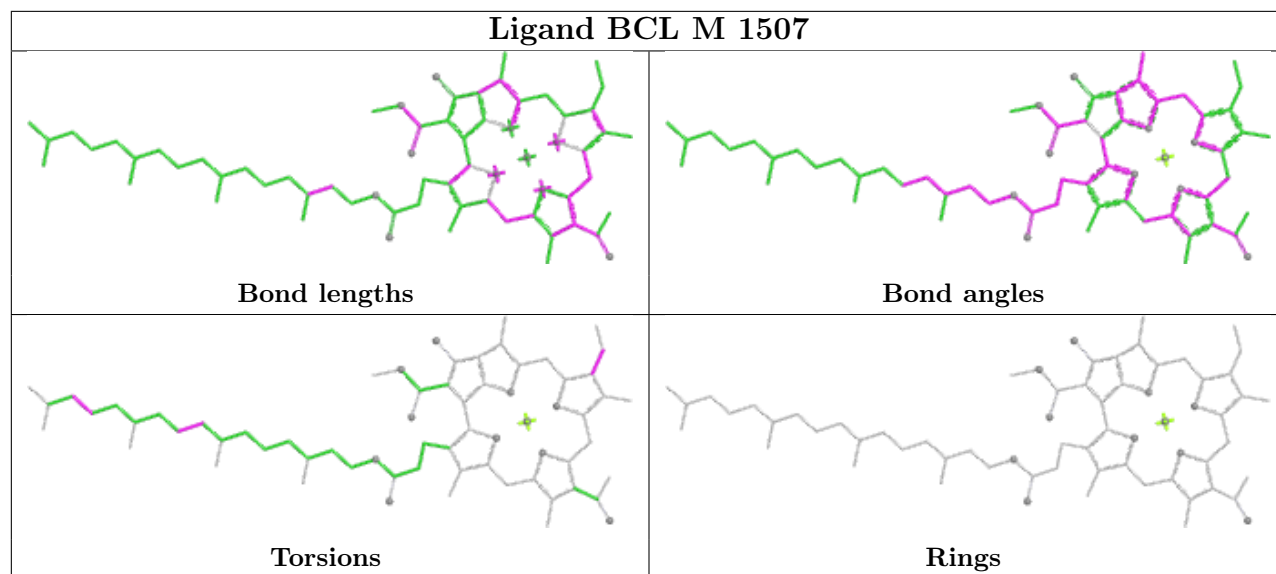












5.7 Other polymers [i](#)

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%)	-0.35	2 (3%) 44 44	35, 41, 88, 98	0
1	C	52/53 (98%)	-0.20	3 (5%) 29 26	34, 41, 88, 102	0
1	E	52/53 (98%)	-0.17	3 (5%) 29 26	35, 40, 88, 101	0
1	G	52/53 (98%)	-0.14	4 (7%) 19 17	33, 40, 87, 99	0
1	I	52/53 (98%)	-0.20	3 (5%) 29 26	34, 39, 88, 100	0
1	K	52/53 (98%)	-0.24	2 (3%) 44 44	33, 40, 88, 100	0
1	M	52/53 (98%)	-0.09	5 (9%) 13 11	35, 40, 88, 101	0
1	O	52/53 (98%)	-0.20	3 (5%) 29 26	34, 41, 87, 100	0
1	R	52/53 (98%)	-0.27	3 (5%) 29 26	35, 41, 87, 97	0
2	B	41/41 (100%)	-0.16	0 100 100	42, 46, 54, 67	0
2	D	41/41 (100%)	-0.32	0 100 100	41, 46, 55, 64	0
2	F	41/41 (100%)	-0.35	0 100 100	38, 45, 52, 65	0
2	H	41/41 (100%)	-0.40	0 100 100	37, 45, 52, 64	0
2	J	41/41 (100%)	-0.35	0 100 100	40, 45, 53, 65	0
2	L	41/41 (100%)	-0.26	0 100 100	39, 43, 52, 65	0
2	N	41/41 (100%)	-0.30	0 100 100	41, 45, 52, 69	0
2	P	41/41 (100%)	-0.26	0 100 100	40, 46, 53, 68	0
2	S	41/41 (100%)	-0.28	0 100 100	41, 46, 54, 67	0
All	All	837/846 (98%)	-0.25	28 (3%) 49 50	33, 43, 79, 102	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	49	VAL	6.5
1	G	49	VAL	5.8
1	E	52	ALA	5.2

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Mol	Chain	Res	Type	RSRZ
1	K	49	VAL	4.8
1	C	49	VAL	4.6
1	O	49	VAL	4.4
1	R	49	VAL	4.4
1	I	49	VAL	4.4
1	A	49	VAL	4.2
1	G	52	ALA	4.1
1	E	49	VAL	4.1
1	C	53	ALA	4.1
1	M	52	ALA	3.8
1	E	53	ALA	3.4
1	C	52	ALA	3.4
1	G	48	GLY	3.3
1	I	50	LYS	3.3
1	O	48	GLY	3.3
1	A	53	ALA	3.1
1	I	52	ALA	3.0
1	O	50	LYS	2.8
1	M	48	GLY	2.7
1	M	50	LYS	2.4
1	R	52	ALA	2.4
1	K	48	GLY	2.4
1	M	51	LYS	2.4
1	G	53	ALA	2.2
1	R	48	GLY	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	C	1	11/12	0.89	0.10	45,47,55,58	0
1	CXM	A	1	11/12	0.92	0.08	45,48,60,62	0
1	CXM	G	1	11/12	0.92	0.07	45,46,52,58	0
1	CXM	R	1	11/12	0.92	0.07	45,48,54,59	0
1	CXM	M	1	11/12	0.93	0.07	40,45,51,52	0
1	CXM	K	1	11/12	0.93	0.07	40,46,54,54	0
1	CXM	O	1	11/12	0.95	0.06	45,47,54,58	0
1	CXM	E	1	11/12	0.95	0.06	41,46,48,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CXM	I	1	11/12	0.97	0.05	38,45,51,52	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($\text{\AA}^2$)	Q<0.9
4	LDA	K	1810	16/16	0.41	0.19	107,110,116,116	0
4	LDA	A	1816	16/16	0.49	0.17	86,87,91,93	0
4	LDA	C	1815	16/16	0.53	0.15	79,96,103,103	0
4	LDA	M	1811	16/16	0.54	0.14	75,77,84,84	0
4	LDA	E	1823	16/16	0.55	0.14	89,99,122,123	0
4	LDA	C	1821	16/16	0.57	0.12	82,90,101,103	0
4	LDA	G	1814	16/16	0.57	0.16	70,74,83,84	0
4	LDA	R	1818	16/16	0.60	0.14	85,90,95,96	0
4	LDA	I	1812	16/16	0.61	0.19	87,106,111,111	0
4	LDA	N	1807	16/16	0.62	0.16	61,66,76,78	0
4	LDA	R	1819	16/16	0.62	0.12	80,83,85,87	0
4	LDA	I	1825	16/16	0.63	0.13	95,101,108,108	0
4	LDA	E	1822	16/16	0.66	0.12	69,91,107,108	0
4	LDA	G	1824	16/16	0.67	0.12	89,105,120,121	0
4	LDA	M	1827	16/16	0.69	0.14	96,101,105,107	0
4	LDA	O	1820	16/16	0.71	0.10	71,80,92,95	0
4	LDA	R	1809	16/16	0.72	0.11	57,63,71,73	0
4	LDA	B	1801	16/16	0.72	0.13	49,62,76,78	0
4	LDA	P	1808	16/16	0.72	0.14	53,61,84,86	0
4	LDA	A	1817	16/16	0.74	0.11	67,69,87,87	0
4	LDA	D	1802	16/16	0.77	0.10	53,57,75,77	0
4	LDA	J	1805	16/16	0.78	0.11	44,54,67,68	0
4	LDA	K	1826	16/16	0.79	0.10	83,88,103,104	0
4	LDA	I	1813	16/16	0.79	0.09	50,54,76,76	0
4	LDA	H	1804	16/16	0.79	0.11	49,57,66,67	0
4	LDA	F	1803	16/16	0.81	0.10	50,56,67,67	0
4	LDA	L	1806	16/16	0.83	0.11	44,52,74,75	0

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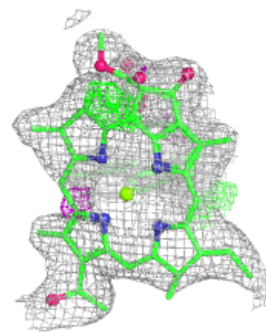
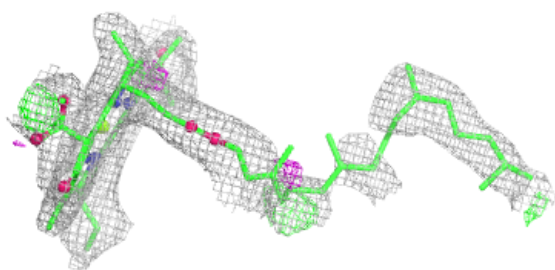
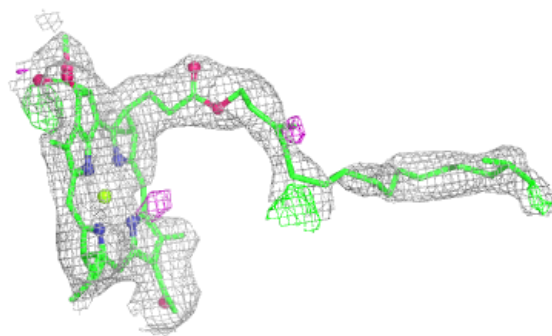
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BCL	R	1709	66/66	0.84	0.09	43,53,78,82	0
3	BCL	G	1704	66/66	0.86	0.09	32,45,73,76	0
3	BCL	C	1702	66/66	0.87	0.08	41,48,78,80	0
3	BCL	M	1707	66/66	0.89	0.08	29,44,74,76	0
3	BCL	A	1701	66/66	0.90	0.07	42,49,80,83	0
3	BCL	O	1708	66/66	0.90	0.08	42,50,79,81	0
3	BCL	N	1607	66/66	0.91	0.08	31,41,63,65	0
3	BCL	I	1705	66/66	0.91	0.07	34,41,73,75	0
3	BCL	E	1703	66/66	0.91	0.07	29,37,69,72	0
5	RG1	P	1408	52/52	0.91	0.07	32,42,75,78	0
5	RG1	R	1401	52/52	0.91	0.07	30,40,74,77	0
3	BCL	K	1706	66/66	0.92	0.07	27,36,78,82	0
5	RG1	N	1407	52/52	0.92	0.06	29,37,69,73	0
3	BCL	F	1603	66/66	0.93	0.07	26,35,62,64	0
3	BCL	J	1605	66/66	0.93	0.07	31,39,64,66	0
3	BCL	K	1506	66/66	0.93	0.06	28,35,47,51	0
5	RG1	D	1402	52/52	0.93	0.06	30,44,77,81	0
5	RG1	F	1403	52/52	0.93	0.07	28,38,77,82	0
5	RG1	J	1405	52/52	0.93	0.07	28,37,76,80	0
5	RG1	L	1406	52/52	0.93	0.06	26,35,74,77	0
3	BCL	P	1608	66/66	0.93	0.07	34,42,66,68	0
3	BCL	R	1509	66/66	0.93	0.06	31,38,49,57	0
3	BCL	A	1501	66/66	0.93	0.06	33,42,51,65	0
5	RG1	S	1409	52/52	0.93	0.06	29,40,77,78	0
3	BCL	D	1602	66/66	0.94	0.07	30,37,64,67	0
3	BCL	E	1503	66/66	0.94	0.05	28,35,46,49	0
5	RG1	H	1404	52/52	0.94	0.07	27,37,78,80	0
3	BCL	H	1604	66/66	0.94	0.07	29,39,63,64	0
3	BCL	L	1606	66/66	0.94	0.06	27,36,66,69	0
3	BCL	S	1609	66/66	0.94	0.07	31,41,69,72	0
3	BCL	I	1505	66/66	0.94	0.06	28,36,42,48	0
3	BCL	B	1601	66/66	0.94	0.07	33,42,67,68	0
3	BCL	O	1508	66/66	0.94	0.05	30,37,46,54	0
3	BCL	M	1507	66/66	0.95	0.05	27,35,41,48	0
3	BCL	C	1502	66/66	0.95	0.05	33,38,50,57	0
3	BCL	G	1504	66/66	0.95	0.05	26,34,44,49	0

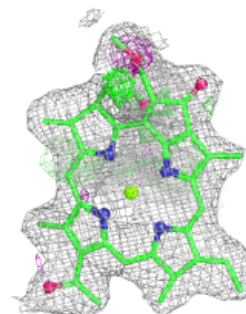
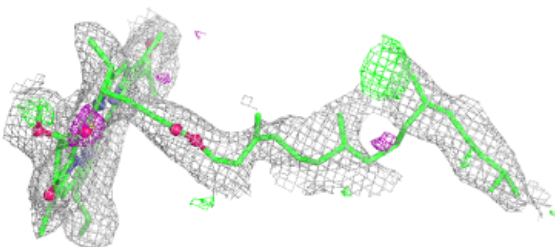
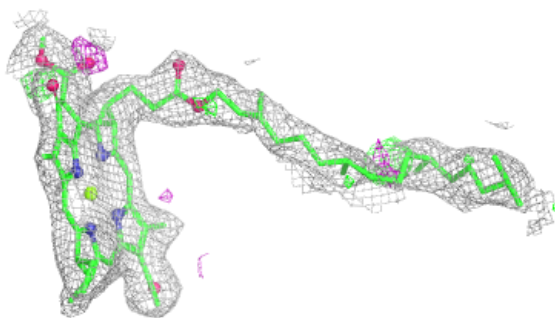
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

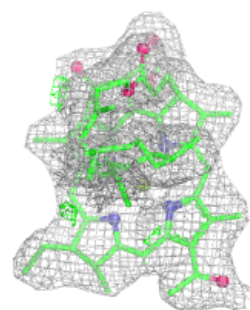
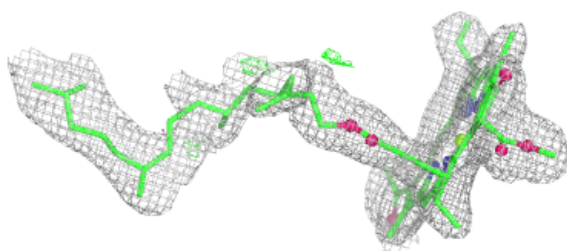
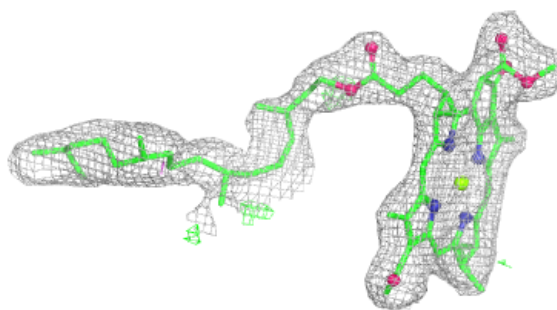
**Electron density around BCL G 1704:**

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

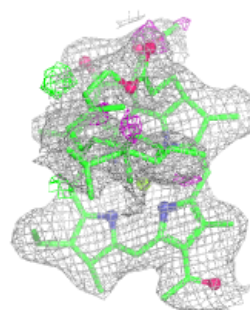
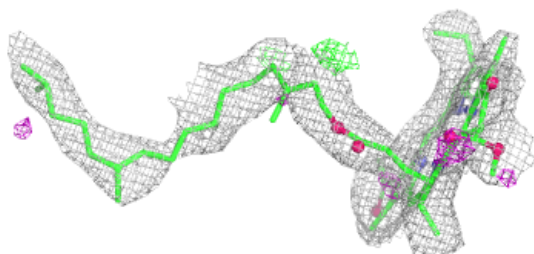
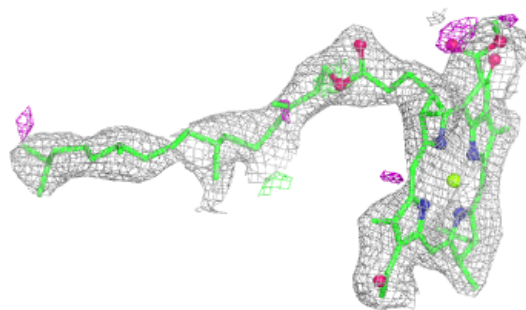


Electron density around BCL C 1702:

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

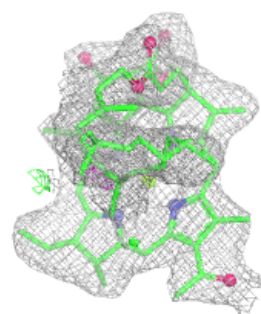
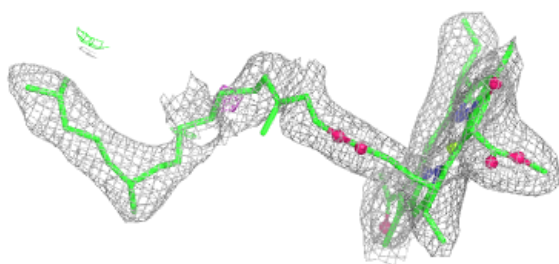
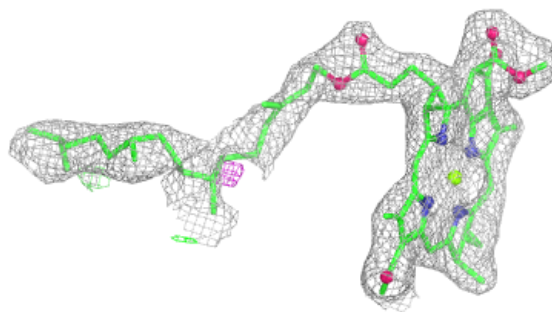
**Electron density around BCL M 1707:**

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

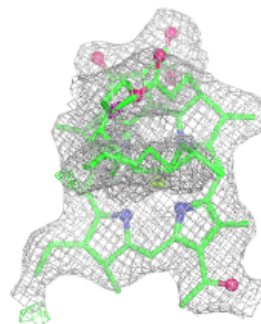
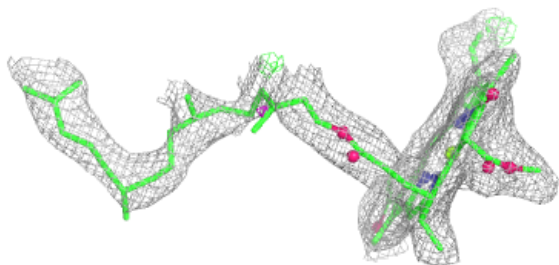
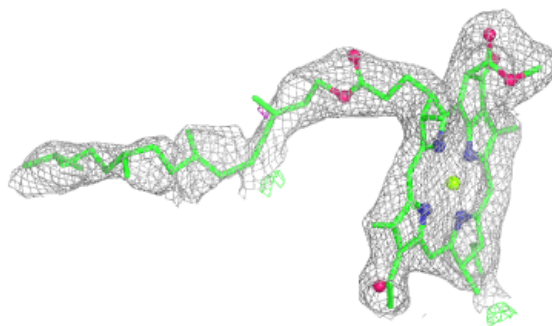


Electron density around BCL A 1701:

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

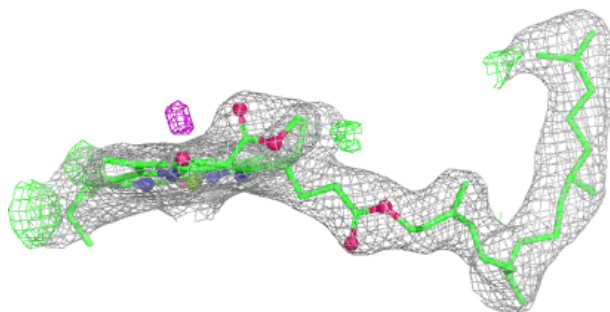
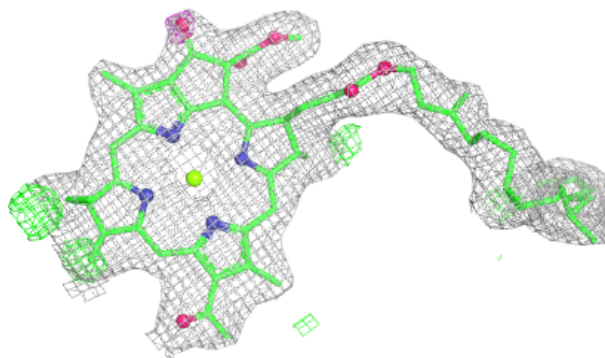
**Electron density around BCL O 1708:**

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

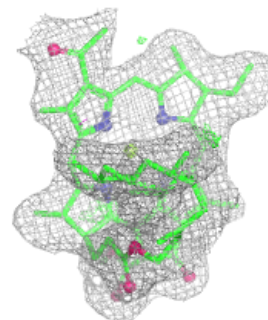
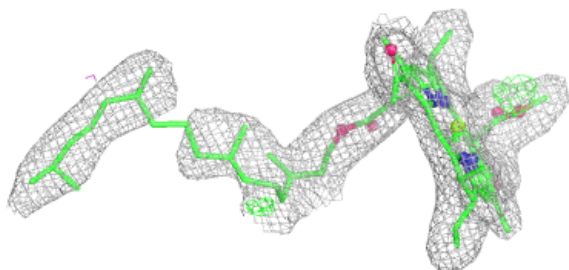
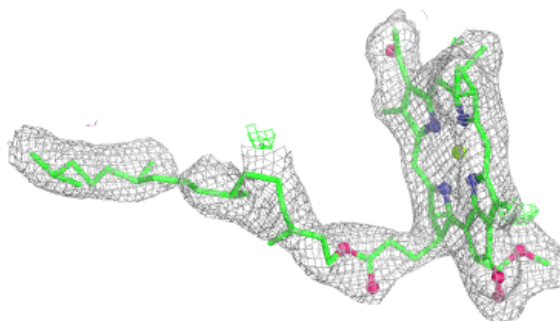


Electron density around BCL N 1607:

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

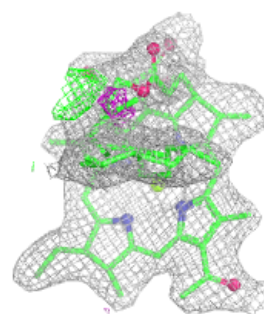
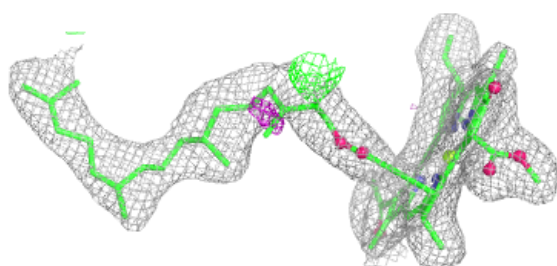
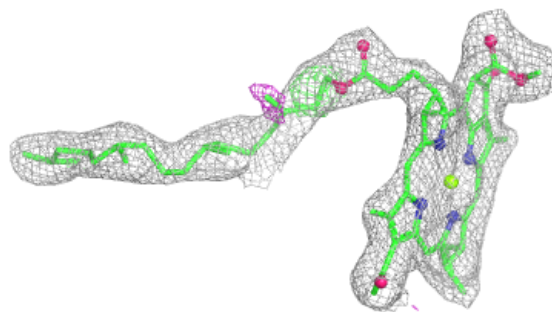
**Electron density around BCL I 1705:**

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

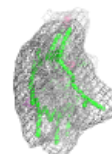
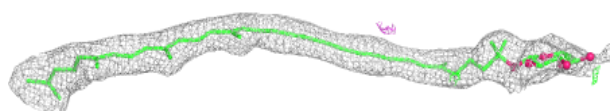
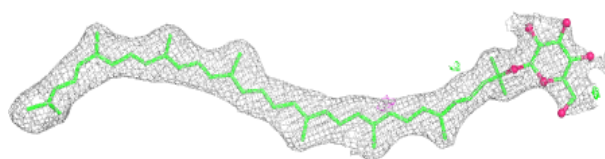


Electron density around BCL E 1703:

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

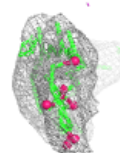
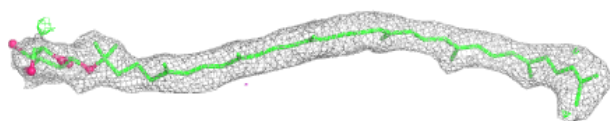
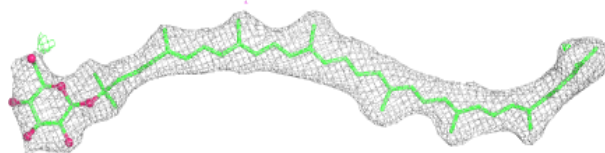
**Electron density around RG1 P 1408:**

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

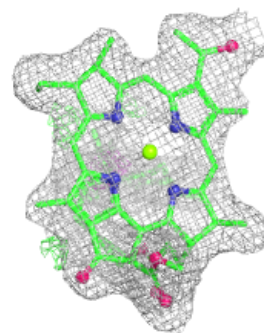
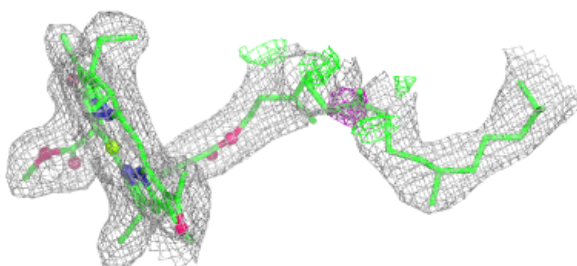
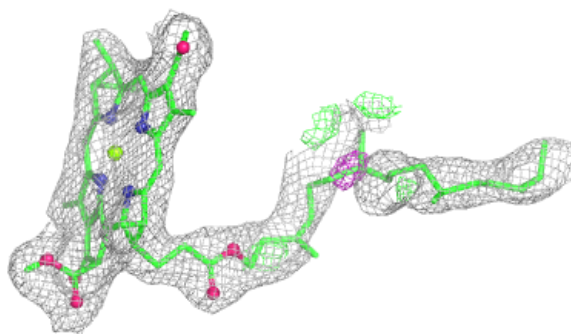


Electron density around RG1 R 1401:

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

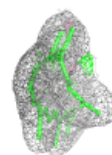
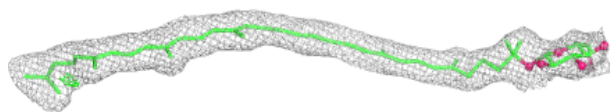
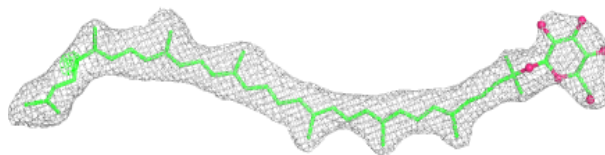
**Electron density around BCL K 1706:**

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

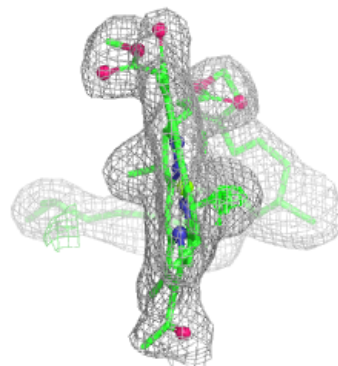
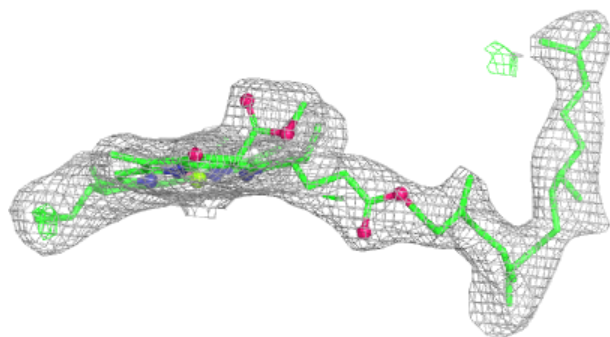
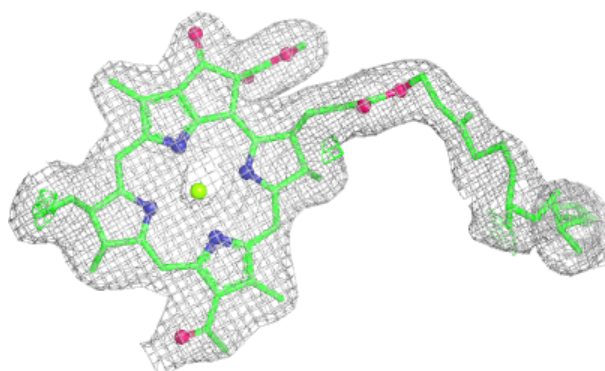


Electron density around RG1 N 1407:

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

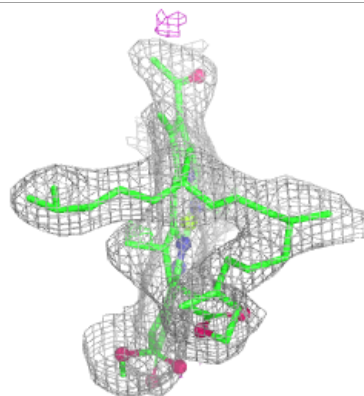
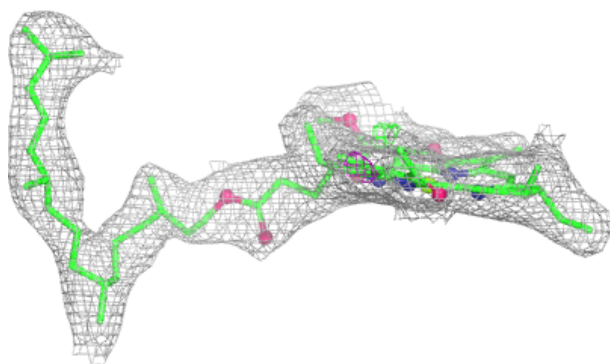
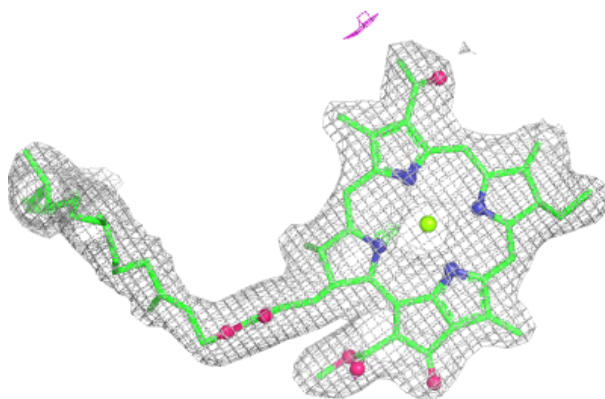
**Electron density around BCL F 1603:**

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

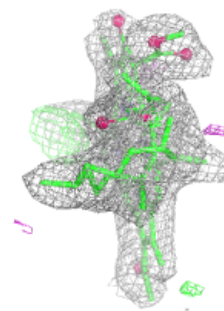
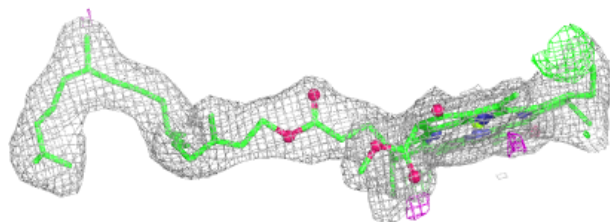
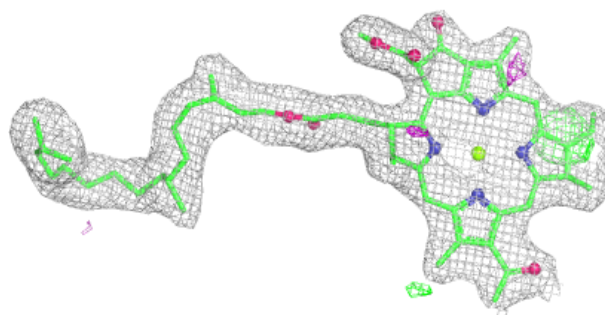


Electron density around BCL J 1605:

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

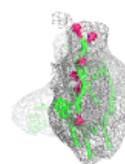
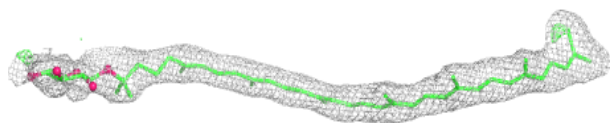
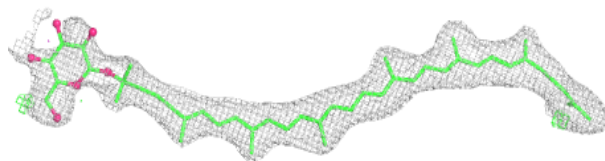
**Electron density around BCL K 1506:**

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

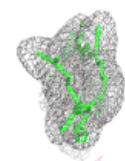
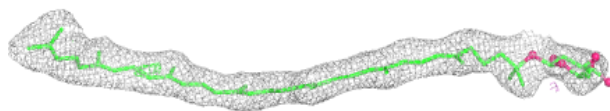
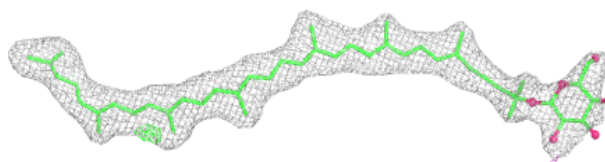


Electron density around RG1 D 1402:

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

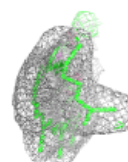
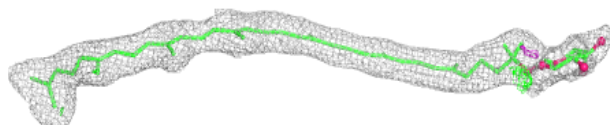
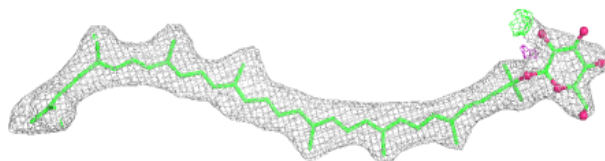
**Electron density around RG1 F 1403:**

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

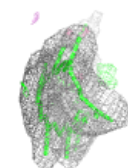
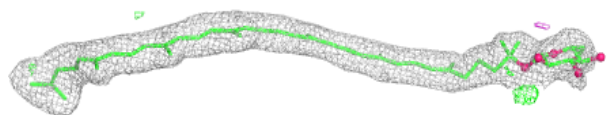
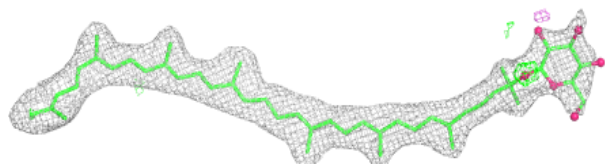


Electron density around RG1 J 1405:

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

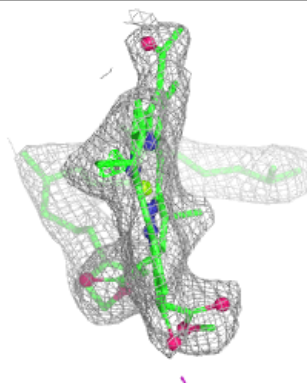
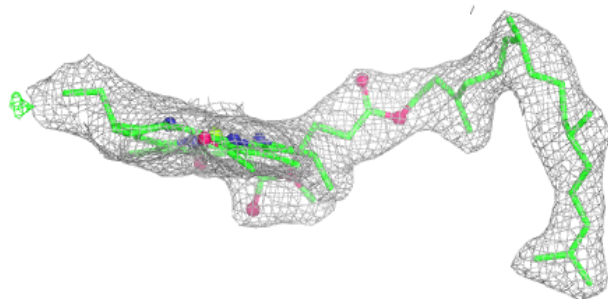
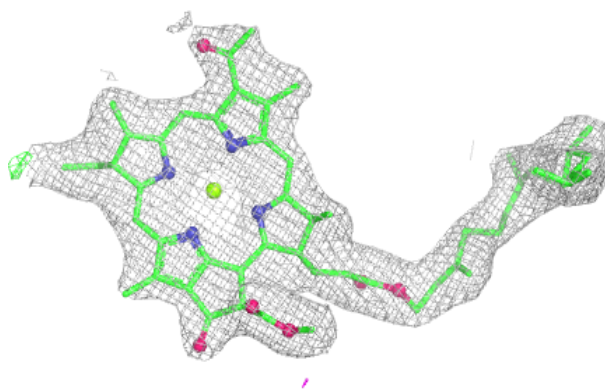
**Electron density around RG1 L 1406:**

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

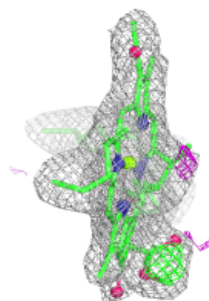
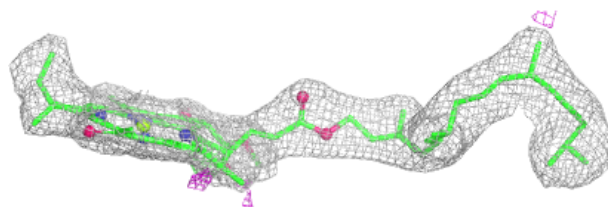


Electron density around BCL P 1608:

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

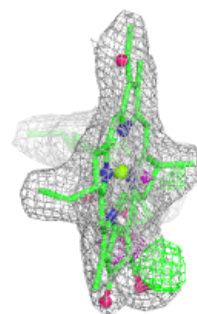
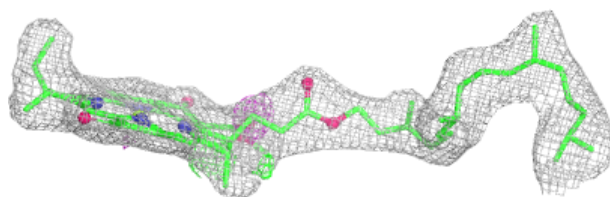
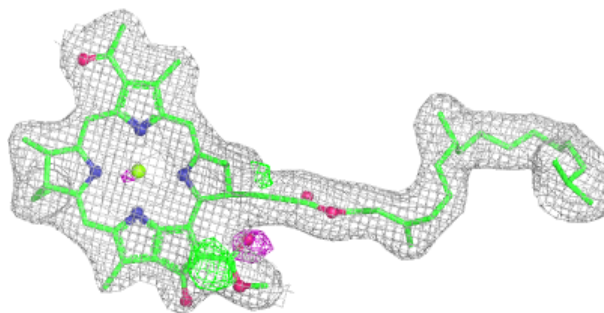
**Electron density around BCL R 1509:**

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

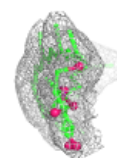
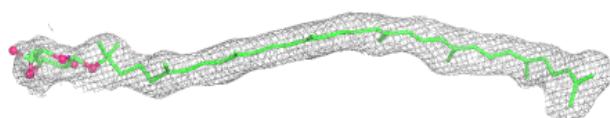
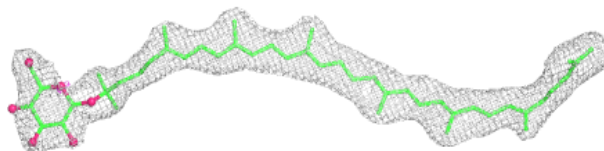


Electron density around BCL A 1501:

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

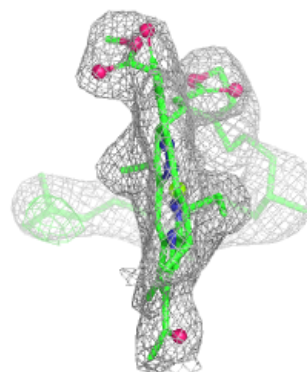
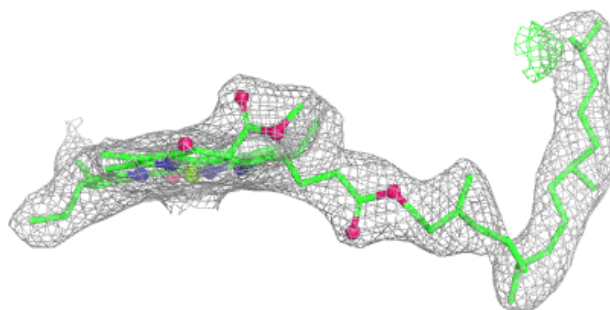
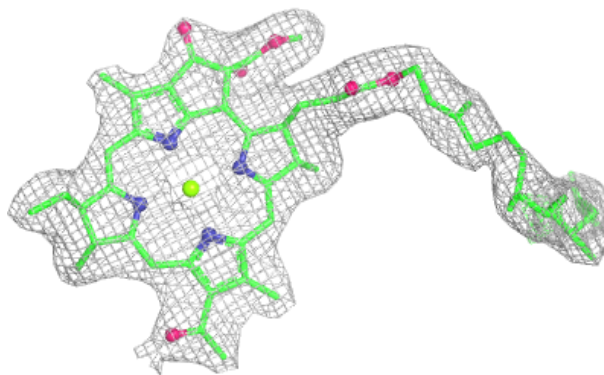
**Electron density around RG1 S 1409:**

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

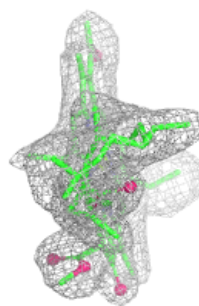
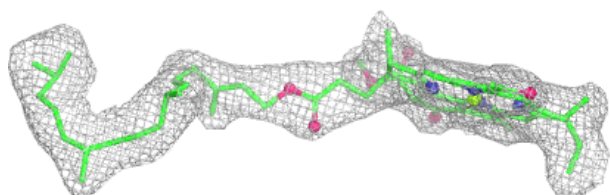
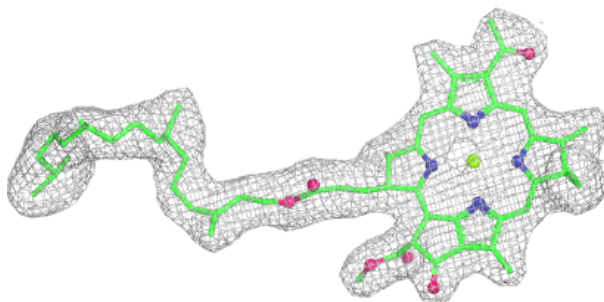


Electron density around BCL D 1602:

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

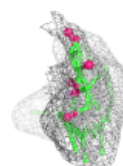
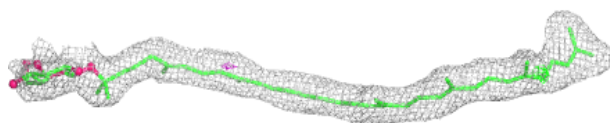
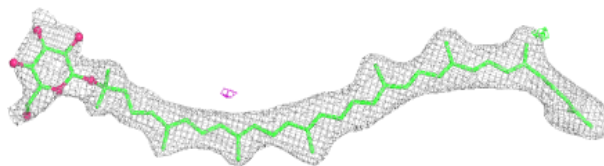
**Electron density around BCL E 1503:**

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

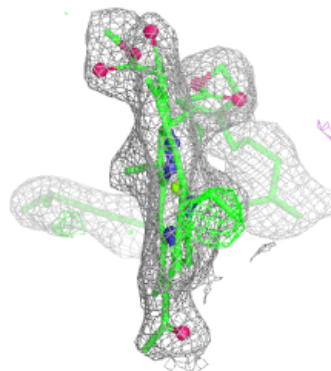
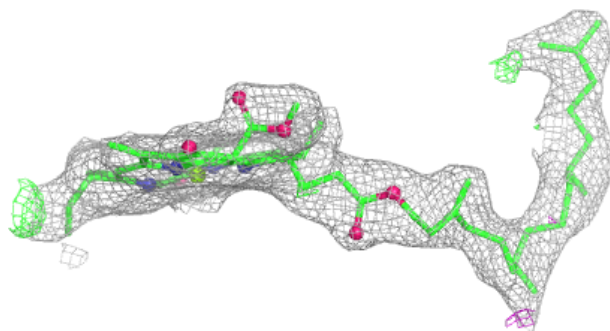
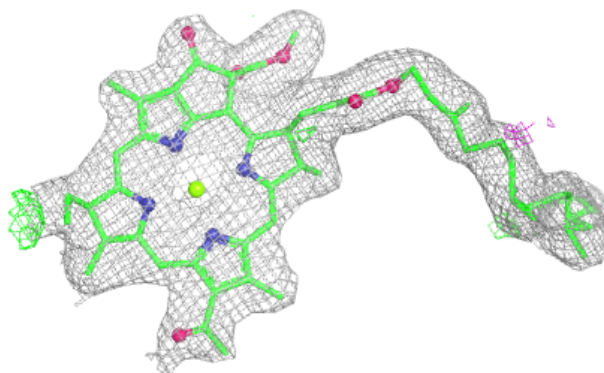


Electron density around RG1 H 1404:

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

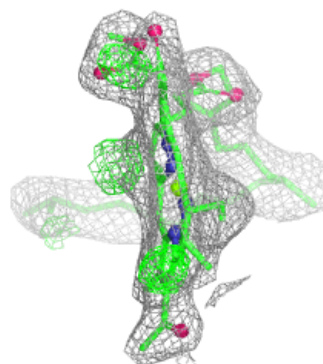
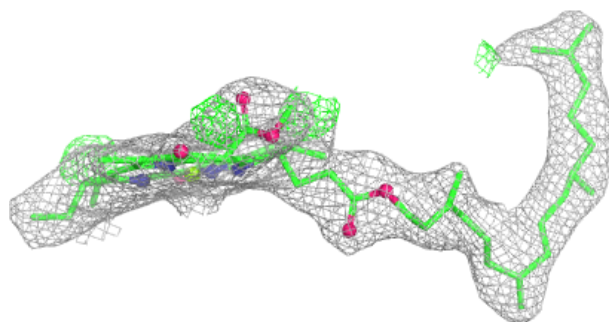
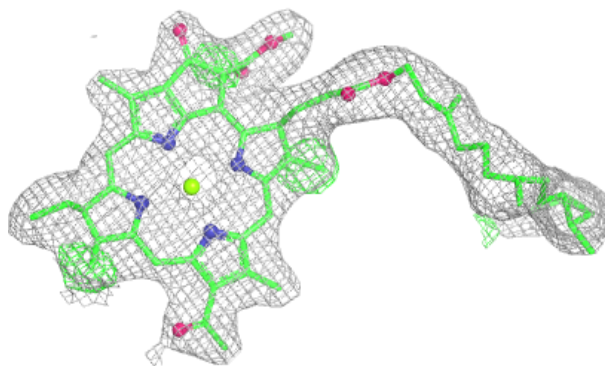
**Electron density around BCL H 1604:**

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

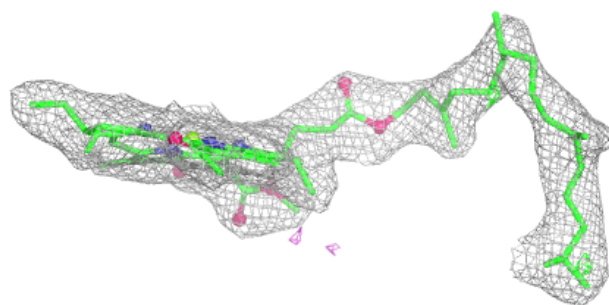
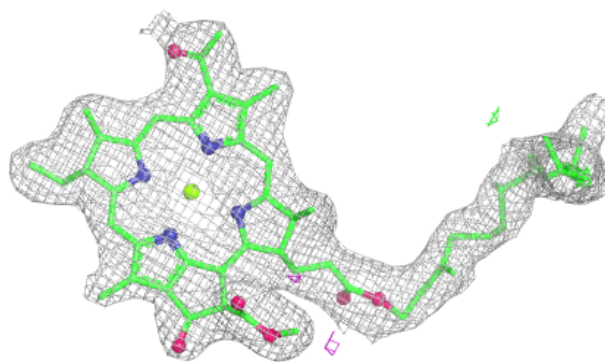


Electron density around BCL L 1606:

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

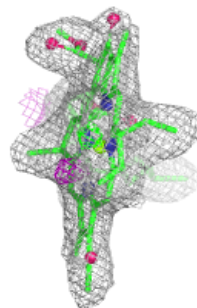
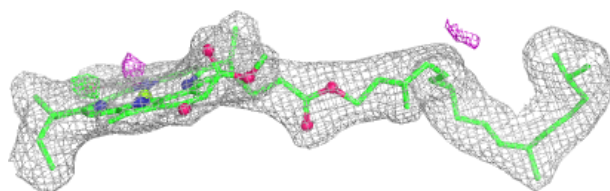
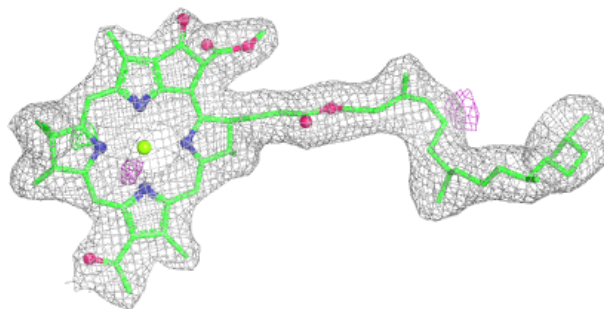
**Electron density around BCL S 1609:**

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

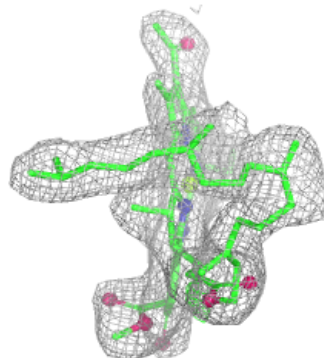
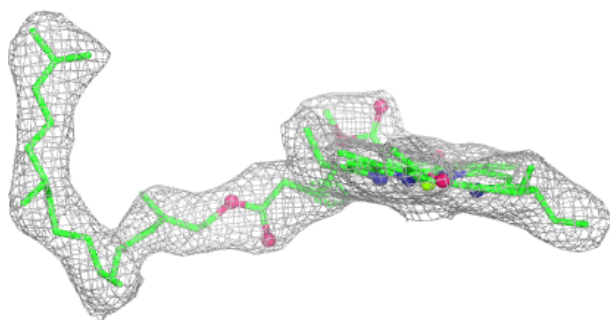
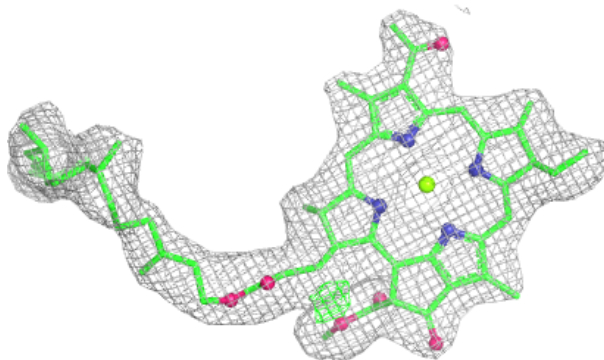


Electron density around BCL I 1505:

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

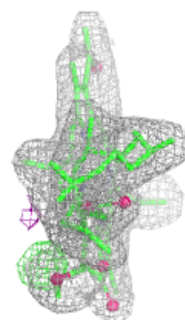
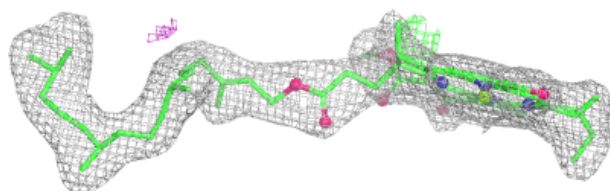
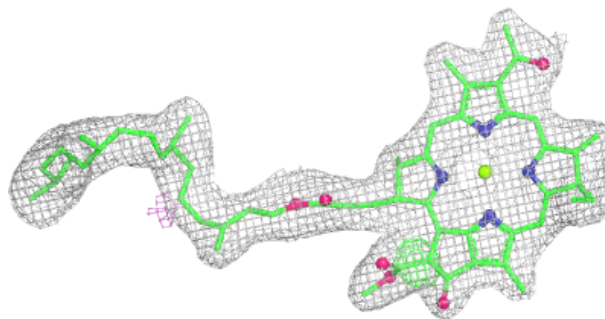
**Electron density around BCL B 1601:**

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

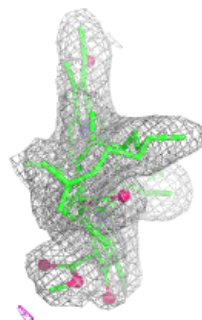
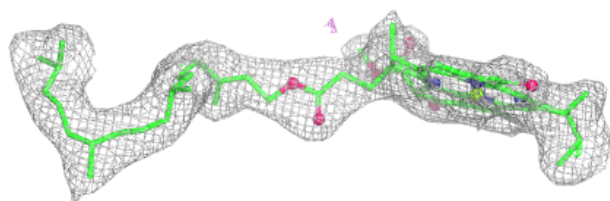
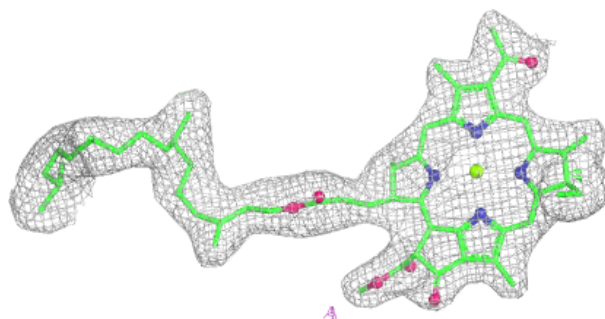


Electron density around BCL O 1508:

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

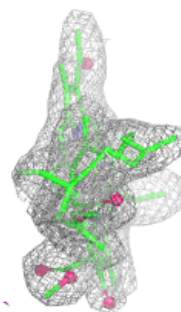
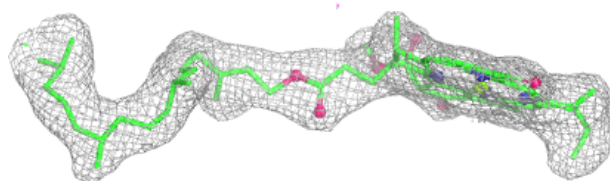
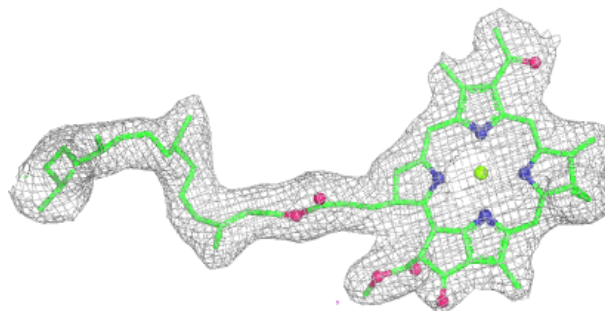
**Electron density around BCL M 1507:**

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

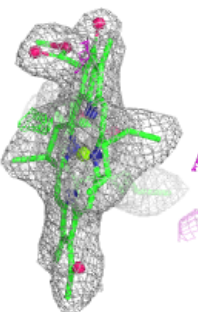
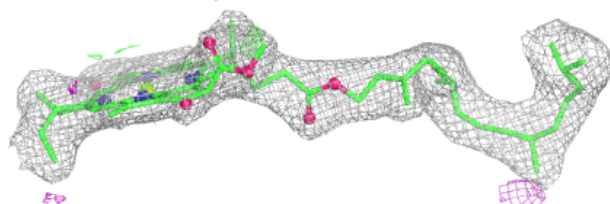
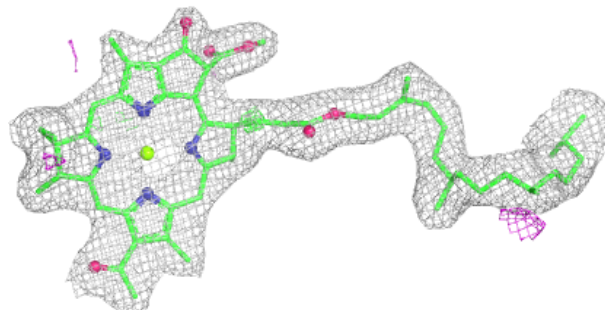


Electron density around BCL C 1502:

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

**Electron density around BCL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.