Full wwPDB EM Validation Report ⓘ

Feb 14, 2023 – 02:18 PM JST

PDB ID	:	7VZG
EMDB ID	:	EMD-32228
Title	:	Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the larger form)
Authors	:	Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.
Deposited on	:	2021-11-16
Resolution	:	2.61 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

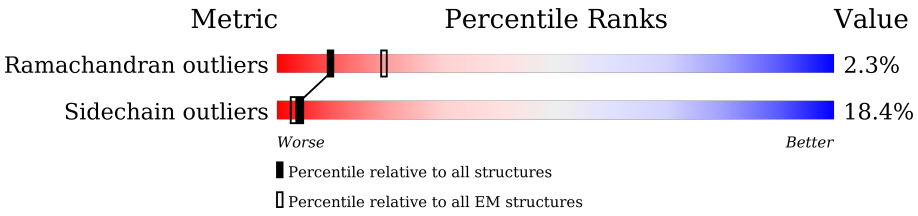
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.61 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	858	63% 31% 5%
1	a	858	67% 26% 7%
2	C	204	49% 36% 9% 5%
3	E	35	66% 29% 6%
3	e	35	71% 26%
4	F	35	43% 57%
4	f	35	71% 23% 6%
5	G	38	74% 16% 11%
5	g	38	74% 24%

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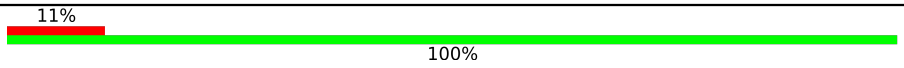
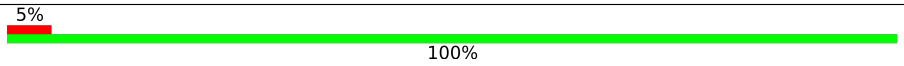
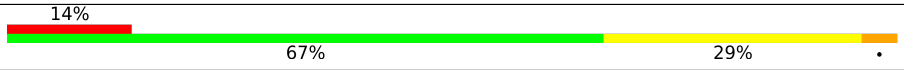
Mol	Chain	Length	Quality of chain
6	H	19	
6	h	19	
7	c	145	
8	B	76	
9	D	70	

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
12	CLA	A	910	X	-	-	-
12	CLA	A	911	X	-	-	-
13	LYC	c	201	-	X	-	-
15	85I	A	916	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 22458 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PscA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	854	Total	C	N	O	S	0	0
			6960	4602	1155	1170	33		
1	a	858	Total	C	N	O	S	0	0
			6984	4616	1160	1175	33		

- Molecule 2 is a protein called Cytochrome c, mono-and diheme variants.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	193	Total	C	N	O	S	0	0
			1474	900	277	288	9		

- Molecule 3 is a protein called PscE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	35	Total	C	N	O	S	0	0
			258	174	40	42	2		
3	e	35	Total	C	N	O	S	0	0
			258	174	40	42	2		

- Molecule 4 is a protein called PscF.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	35	Total	C	N	O	S	0	0
			273	185	43	43	2		
4	f	35	Total	C	N	O	S	0	0
			273	185	43	43	2		

- Molecule 5 is a protein called PscG.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	38	Total	C	N	O	S	0	0
			302	210	45	44	3		

- Molecule 6 is a protein called undefined polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	19	Total	C	N	O	0	0
			95	57	19	19		
6	h	19	Total	C	N	O	0	0
			95	57	19	19		

- Molecule 7 is a protein called Cytochrome c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	145	Total	C	N	O	S	0	0
			1096	679	200	210	7		

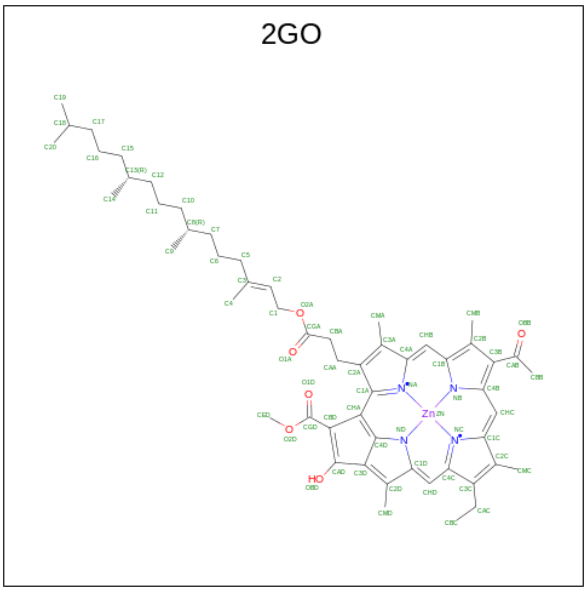
- Molecule 8 is a protein called Photosystem P840 reaction center iron-sulfur protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	76	Total	C	N	O	S	0	0
			568	356	90	114	8		

- Molecule 9 is a protein called PscD'.

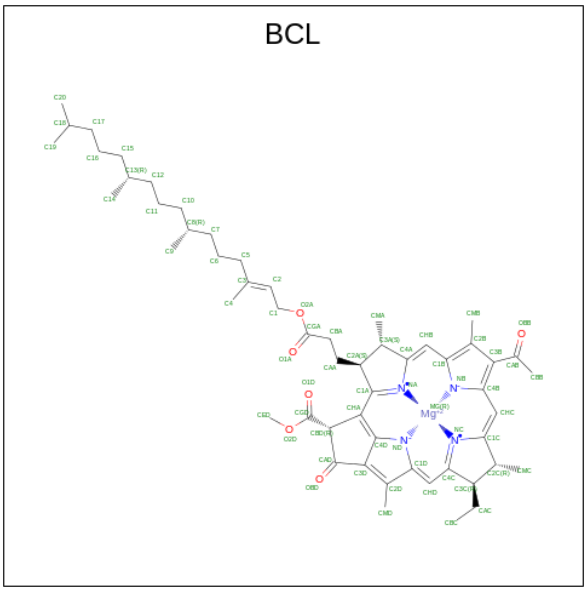
Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	60	Total	C	N	O	S	0	0
			520	330	92	96	2		

- Molecule 10 is [methyl 9-acetyl-14-ethyl-20-hydroxy-4,8,13,18-tetramethyl-3-{3-oxo-3-[(3 ,7,11,15-tetramethylhexadec-2-en-1-yl)oxy]propyl}-3,4,20,21-tetradehydrophorbine-21-ca rboxylatato(2-)-kappa 4 N 23 ,N 24 ,N 25 ,N 26]zinc (three-letter code: 2GO) (formula: $C_{55}H_{70}N_4O_6Zn$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	Zn	0
			66	55	4	6	1	
10	a	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

- Molecule 11 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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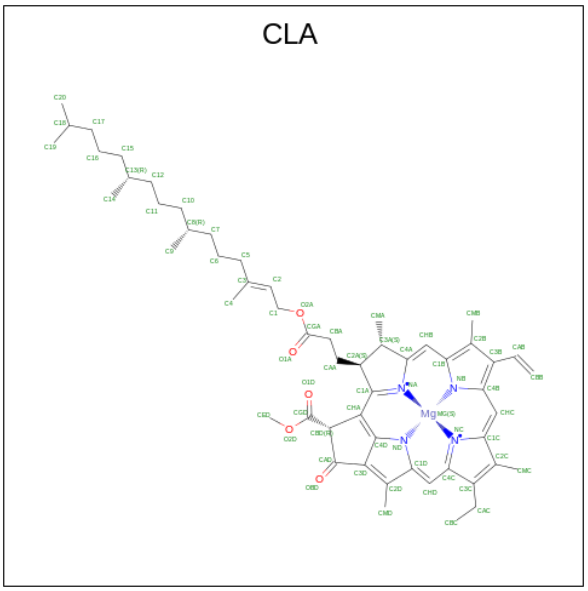
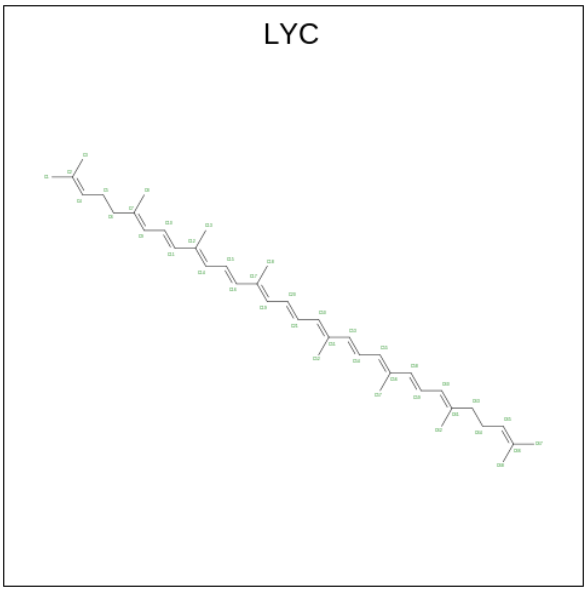
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
11	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	a	1	Total 51	C 41	Mg 1	N 4	O 5	0

- Molecule 13 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$).

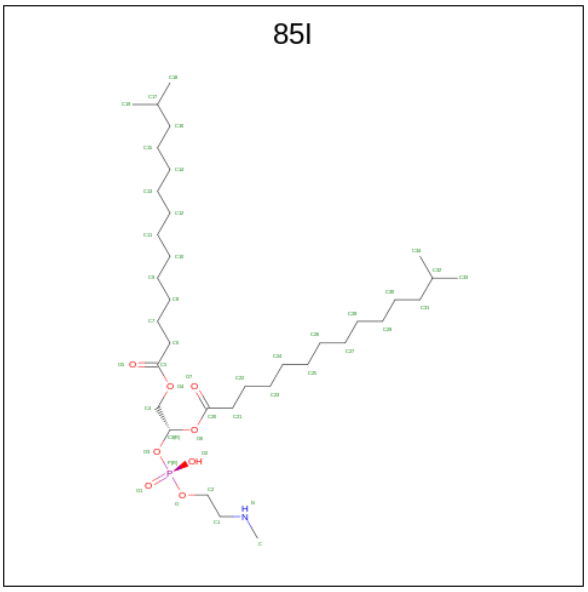


Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 40 40	0
13	c	1	Total C 40 40	0

- Molecule 14 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total Ca 1 1	0
14	a	1	Total Ca 1 1	0

- Molecule 15 is [(2 {R})-2-[2-(methylamino)ethoxy-oxidanyl-phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 85I) (formula: $C_{35}H_{70}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	
15	a	1	Total	C	N	O	P	0
			45	35	1	8	1	

- Molecule 16 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
16	A	13	Total	C	0
			240	240	
16	C	1	Total	C	0
			18	18	
16	E	2	Total	C	0
			26	26	
16	a	13	Total	C	0
			243	243	
16	c	1	Total	C	0
			8	8	

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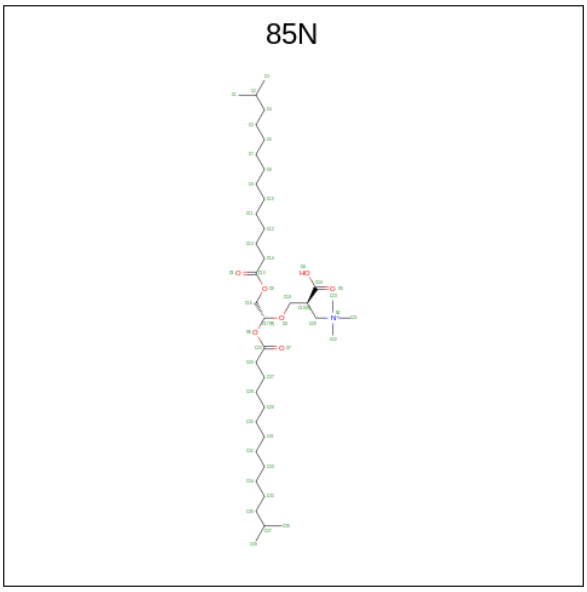
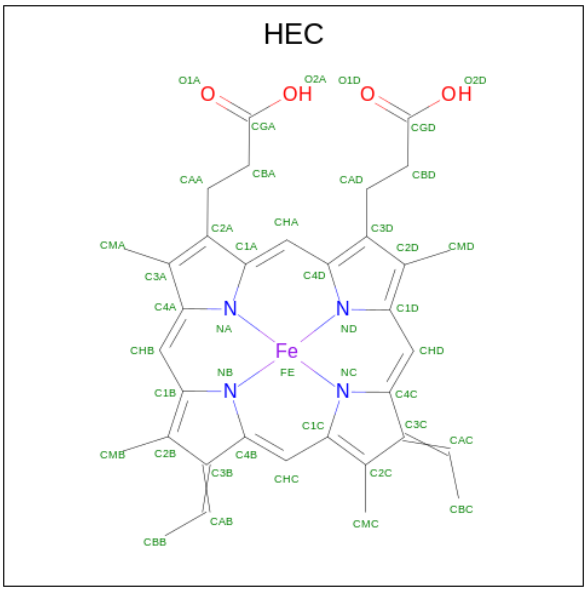
Mol	Chain	Residues	Atoms	AltConf
16	e	2	Total C 26 26	0

- Molecule 17 is [(2 {S})-2-[[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (three-letter code: 85N) (formula: $C_{39}H_{76}NO_7$) (labeled as "Ligand of Interest" by depositor).



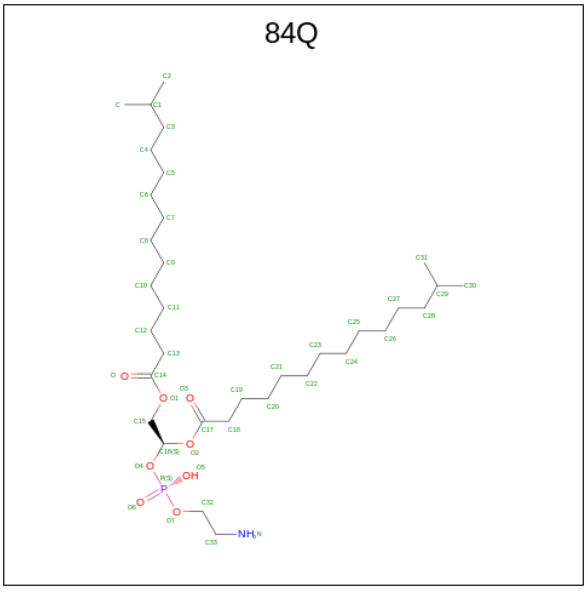
Mol	Chain	Residues	Atoms	AltConf
17	A	1	Total C N O 47 39 1 7	0
17	G	1	Total C N O 38 30 1 7	0
17	a	1	Total C N O 47 39 1 7	0
17	g	1	Total C N O 38 30 1 7	0

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
18	c	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 19 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (three-letter code: 84Q) (formula: $C_{34}H_{68}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	E	1	Total	C	N	O	P	0
			44	34	1	8	1	

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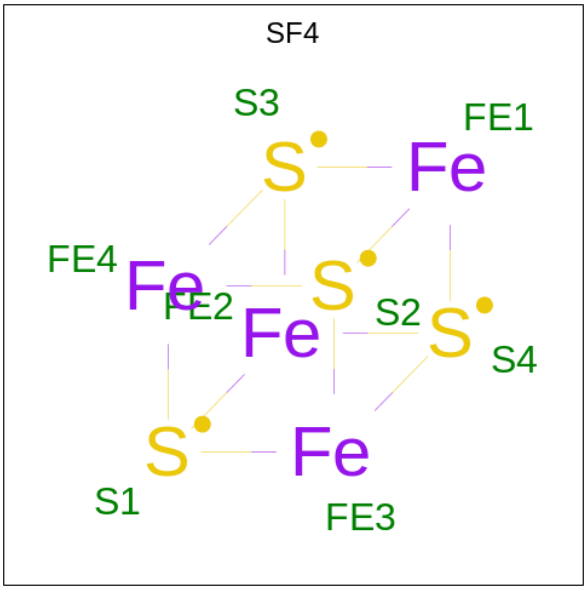
Mol	Chain	Residues	Atoms					AltConf
19	a	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 20 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
20	a	1	Total	Fe	S	0
			8	4	4	
20	B	1	Total	Fe	S	0
			8	4	4	
20	B	1	Total	Fe	S	0
			8	4	4	

- Molecule 21 is water.

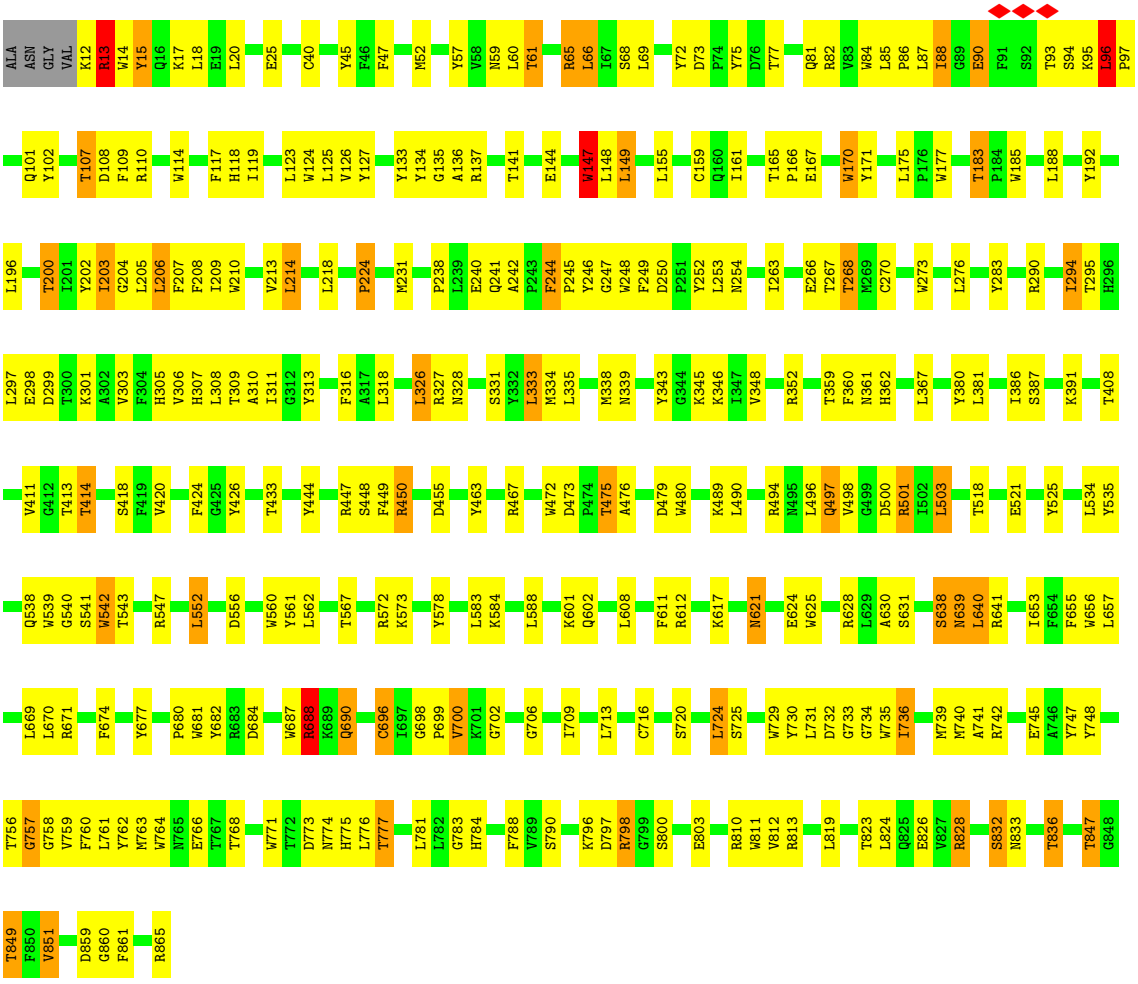
Mol	Chain	Residues	Atoms		AltConf
21	A	3	Total	O	0
			3	3	
21	a	3	Total	O	0
			3	3	

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

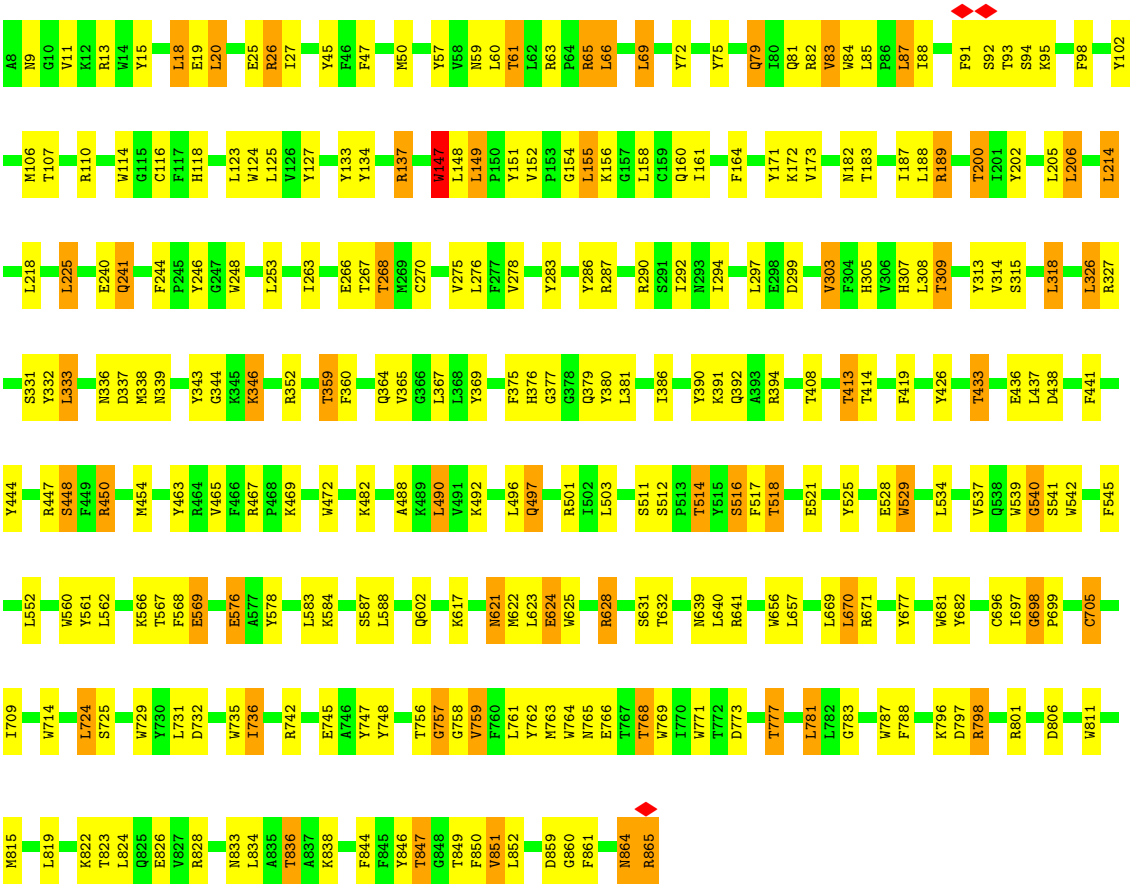
- Molecule 1: PscA

Chain A:



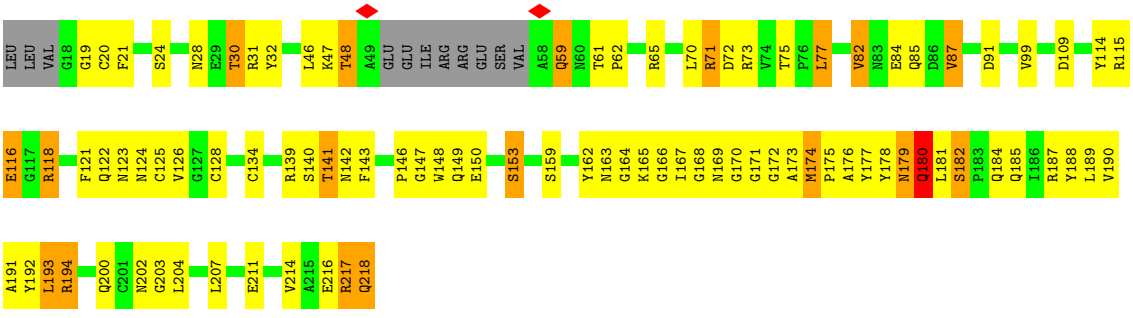
- Molecule 1: PscA

Chain a:



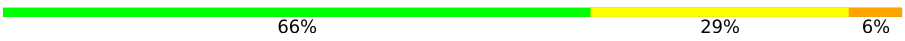
• Molecule 2: Cytochrome c, mono-and diheme variants

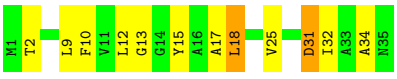
Chain C:



• Molecule 3: PscE

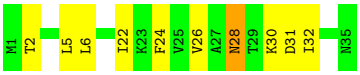
Chain E:





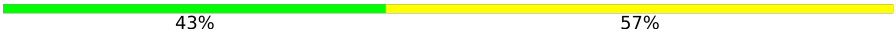
• Molecule 3: PscE

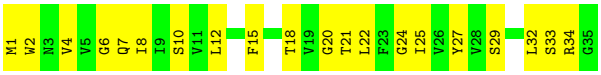
Chain e:



• Molecule 4: PscF

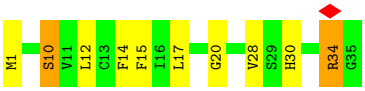
Chain F:





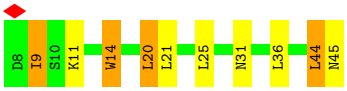
• Molecule 4: PscF

Chain f:



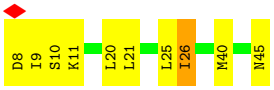
• Molecule 5: PscG

Chain G:



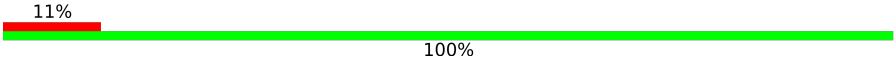
• Molecule 5: PscG

Chain g:



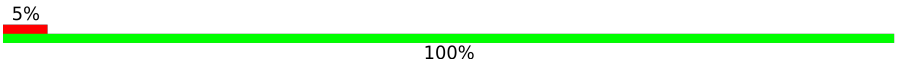
• Molecule 6: undefined polypeptide

Chain H:



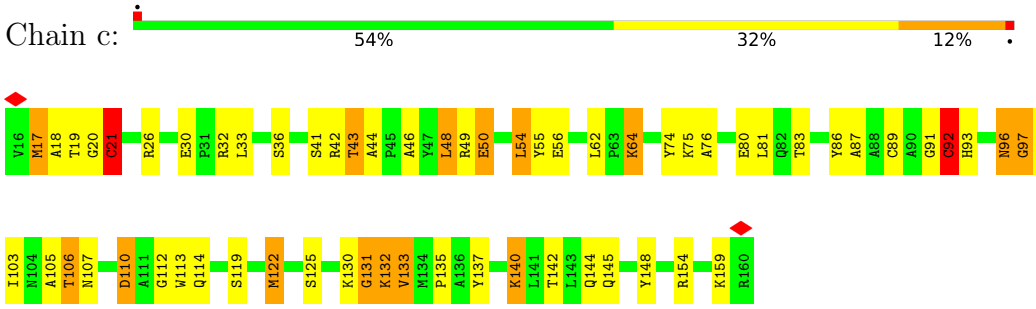
• Molecule 6: undefined polypeptide

Chain h:



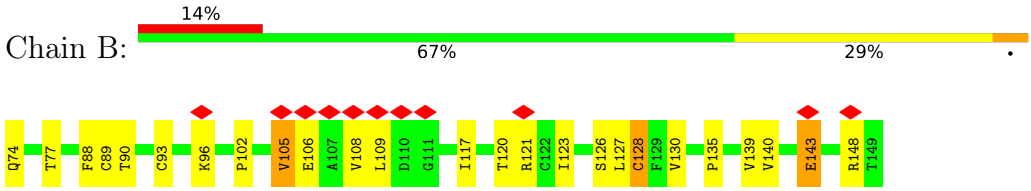
• Molecule 7: Cytochrome c domain-containing protein

Chain c:



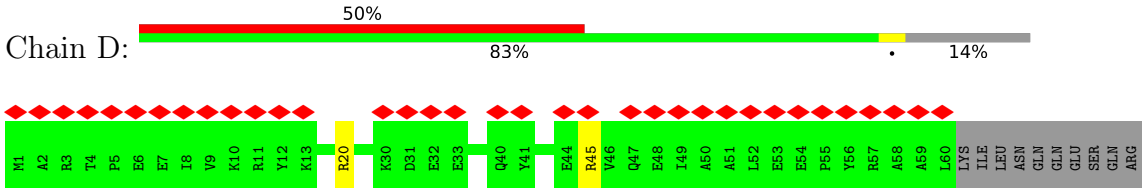
• Molecule 8: Photosystem P840 reaction center iron-sulfur protein

Chain B:



• Molecule 9: PscD'

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.381	Depositor
Minimum map value	-1.010	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.094	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	238.15, 238.15, 238.15	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0825, 1.0825, 1.0825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UNL, BCL, CLA, 84Q, CA, LYC, 85I, HEC, 85N, 2GO, SF4

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	1.97	235/7209 (3.3%)	1.33	86/9827 (0.9%)
1	a	1.85	195/7233 (2.7%)	1.28	90/9860 (0.9%)
2	C	2.35	99/1503 (6.6%)	1.67	34/2037 (1.7%)
3	E	2.16	9/262 (3.4%)	1.43	4/356 (1.1%)
3	e	1.50	2/262 (0.8%)	1.14	1/356 (0.3%)
4	F	2.28	15/279 (5.4%)	1.21	0/379
4	f	1.98	6/279 (2.2%)	1.28	1/379 (0.3%)
5	G	1.49	4/311 (1.3%)	1.60	6/421 (1.4%)
5	g	1.25	0/311	1.16	2/421 (0.5%)
7	c	2.54	75/1115 (6.7%)	1.79	36/1506 (2.4%)
8	B	0.79	0/578	1.11	3/789 (0.4%)
9	D	0.68	0/531	0.92	1/714 (0.1%)
All	All	1.93	640/19873 (3.2%)	1.35	264/27045 (1.0%)

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	1
1	a	0	4
2	C	0	2
7	c	0	1
All	All	0	8

All (640) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	539	TRP	C-O	-15.05	0.94	1.23
7	c	55	TYR	CD1-CE1	-13.98	1.18	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	55	TYR	CD2-CE2	-13.29	1.19	1.39
1	A	309	THR	CB-CG2	-13.11	1.09	1.52
1	A	758	GLY	C-O	-12.39	1.03	1.23
1	a	266	GLU	CD-OE2	-12.23	1.12	1.25
7	c	106	THR	CB-CG2	-12.03	1.12	1.52
1	A	745	GLU	CB-CG	-11.48	1.30	1.52
2	C	141	THR	C-O	-11.40	1.01	1.23
3	E	13	GLY	C-O	-11.31	1.05	1.23
1	a	529	TRP	CB-CG	-11.05	1.30	1.50
1	a	705	CYS	CB-SG	10.70	2.00	1.82
1	a	783	GLY	C-O	-10.62	1.06	1.23
1	A	541	SER	CB-OG	-10.52	1.28	1.42
1	a	860	GLY	C-O	-10.51	1.06	1.23
1	A	266	GLU	CD-OE2	-10.47	1.14	1.25
1	a	758	GLY	C-O	-10.32	1.07	1.23
7	c	20	GLY	C-O	-10.18	1.07	1.23
2	C	179	ASN	C-O	-10.17	1.04	1.23
1	A	766	GLU	CD-OE2	-10.02	1.14	1.25
1	a	852	LEU	C-O	-10.02	1.04	1.23
1	a	757	GLY	C-O	-9.88	1.07	1.23
2	C	140	SER	C-O	-9.86	1.04	1.23
1	a	376	HIS	C-O	-9.82	1.04	1.23
7	c	106	THR	C-O	-9.62	1.05	1.23
1	a	305	HIS	C-O	-9.54	1.05	1.23
7	c	43	THR	CB-CG2	-9.53	1.21	1.52
7	c	112	GLY	C-O	-9.48	1.08	1.23
1	A	638	SER	CB-OG	-9.48	1.29	1.42
1	A	638	SER	C-O	-9.30	1.05	1.23
1	a	541	SER	CB-OG	-9.27	1.30	1.42
2	C	147	GLY	C-O	-9.26	1.08	1.23
7	c	98	GLY	CA-C	-9.23	1.37	1.51
1	a	732	ASP	CB-CG	-9.19	1.32	1.51
4	f	10	SER	CB-OG	-9.14	1.30	1.42
2	C	176	ALA	C-O	-9.13	1.05	1.23
1	a	759	VAL	C-O	-9.10	1.06	1.23
2	C	178	TYR	C-O	-9.07	1.06	1.23
1	A	313	TYR	CD1-CE1	-9.03	1.25	1.39
1	A	306	VAL	C-O	-9.02	1.06	1.23
1	a	748	TYR	CD2-CE2	-9.02	1.25	1.39
1	a	346	LYS	C-O	-9.00	1.06	1.23
1	A	731	LEU	C-O	-8.99	1.06	1.23
1	a	270	CYS	CB-SG	-8.98	1.67	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	182	SER	CB-OG	-8.95	1.30	1.42
1	A	25	GLU	CD-OE1	-8.90	1.15	1.25
2	C	19	GLY	C-O	-8.88	1.09	1.23
7	c	26	ARG	CZ-NH1	-8.81	1.21	1.33
4	F	4	VAL	C-O	-8.77	1.06	1.23
1	A	125	LEU	C-O	-8.75	1.06	1.23
1	a	380	TYR	CD1-CE1	-8.75	1.26	1.39
7	c	96	ASN	C-O	-8.73	1.06	1.23
1	a	369	TYR	CD1-CE1	-8.72	1.26	1.39
7	c	91	GLY	C-O	-8.69	1.09	1.23
1	a	796	LYS	C-O	-8.69	1.06	1.23
1	A	709	ILE	C-O	-8.62	1.06	1.23
1	a	561	TYR	CD2-CE2	-8.61	1.26	1.39
2	C	179	ASN	CG-OD1	-8.57	1.05	1.24
1	A	61	THR	CB-CG2	-8.55	1.24	1.52
1	A	733	GLY	C-O	-8.53	1.09	1.23
1	a	777	THR	CB-CG2	-8.49	1.24	1.52
7	c	56	GLU	CD-OE1	-8.39	1.16	1.25
1	A	266	GLU	CD-OE1	-8.36	1.16	1.25
2	C	30	THR	C-O	-8.33	1.07	1.23
1	A	541	SER	C-O	-8.28	1.07	1.23
1	A	313	TYR	CD2-CE2	-8.25	1.26	1.39
1	A	538	GLN	CD-NE2	-8.24	1.12	1.32
1	a	426	TYR	CD2-CE2	-8.23	1.27	1.39
1	A	860	GLY	C-O	-8.21	1.10	1.23
2	C	142	ASN	CG-ND2	-8.21	1.12	1.32
1	A	542	TRP	C-O	-8.20	1.07	1.23
1	A	631	SER	CB-OG	-8.18	1.31	1.42
4	F	10	SER	CB-OG	-8.17	1.31	1.42
1	a	61	THR	CB-CG2	-8.15	1.25	1.52
2	C	126	VAL	C-O	-8.11	1.07	1.23
1	A	811	TRP	CE3-CZ3	-8.09	1.24	1.38
1	a	133	TYR	CD1-CE1	-8.07	1.27	1.39
1	a	332	TYR	CD2-CE2	-7.99	1.27	1.39
1	a	315	SER	CB-OG	-7.99	1.31	1.42
1	A	748	TYR	CD1-CE1	-7.99	1.27	1.39
2	C	162	TYR	CZ-OH	-7.99	1.24	1.37
2	C	148	TRP	CG-CD1	-7.93	1.25	1.36
1	A	849	THR	CB-CG2	-7.93	1.26	1.52
7	c	86	TYR	CE2-CZ	-7.91	1.28	1.38
1	A	57	TYR	CD1-CE1	-7.91	1.27	1.39
1	a	26	ARG	C-O	-7.90	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	297	LEU	C-O	-7.87	1.08	1.23
1	a	561	TYR	CD1-CE1	-7.86	1.27	1.39
1	A	270	CYS	CB-SG	-7.86	1.68	1.82
1	A	640	LEU	C-O	-7.85	1.08	1.23
2	C	143	PHE	C-O	-7.85	1.08	1.23
1	A	448	SER	CB-OG	-7.84	1.32	1.42
1	A	543	THR	C-O	-7.84	1.08	1.23
7	c	41	SER	CB-OG	-7.84	1.32	1.42
2	C	123	ASN	C-O	-7.82	1.08	1.23
1	A	734	GLY	C-O	-7.79	1.11	1.23
7	c	56	GLU	C-O	-7.77	1.08	1.23
1	A	682	TYR	CE1-CZ	-7.77	1.28	1.38
2	C	153	SER	CB-OG	-7.77	1.32	1.42
2	C	116	GLU	CD-OE2	-7.76	1.17	1.25
4	F	6	GLY	C-O	-7.75	1.11	1.23
1	a	283	TYR	CD2-CE2	-7.74	1.27	1.39
1	a	811	TRP	C-O	-7.73	1.08	1.23
2	C	185	GLN	CD-NE2	-7.73	1.13	1.32
7	c	130	LYS	C-O	-7.71	1.08	1.23
1	A	742	ARG	CZ-NH1	-7.70	1.23	1.33
1	a	364	GLN	CD-NE2	-7.69	1.13	1.32
7	c	55	TYR	CZ-OH	-7.67	1.24	1.37
1	A	362	HIS	C-O	-7.67	1.08	1.23
1	A	747	TYR	CD1-CE1	-7.65	1.27	1.39
2	C	188	TYR	C-O	-7.64	1.08	1.23
2	C	178	TYR	CZ-OH	-7.63	1.24	1.37
2	C	190	VAL	C-O	-7.63	1.08	1.23
1	A	202	TYR	CE2-CZ	-7.63	1.28	1.38
1	a	639	ASN	CB-CG	-7.63	1.33	1.51
1	A	560	TRP	C-O	-7.62	1.08	1.23
1	a	764	TRP	CZ3-CH2	-7.61	1.27	1.40
7	c	26	ARG	C-O	-7.60	1.08	1.23
1	a	542	TRP	CE3-CZ3	-7.59	1.25	1.38
2	C	164	GLY	C-O	-7.58	1.11	1.23
1	A	764	TRP	C-O	-7.58	1.08	1.23
2	C	182	SER	C-O	-7.56	1.08	1.23
1	a	521	GLU	CD-OE1	-7.56	1.17	1.25
2	C	188	TYR	CB-CG	-7.55	1.40	1.51
2	C	166	GLY	C-O	-7.52	1.11	1.23
1	A	655	PHE	C-O	-7.51	1.09	1.23
1	A	294	ILE	C-O	-7.50	1.09	1.23
7	c	42	ARG	C-O	-7.50	1.09	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	639	ASN	CG-OD1	-7.48	1.07	1.24
2	C	121	PHE	C-O	-7.43	1.09	1.23
2	C	173	ALA	C-O	-7.41	1.09	1.23
1	a	433	THR	CB-CG2	-7.40	1.27	1.52
1	a	731	LEU	C-O	-7.39	1.09	1.23
1	A	699	PRO	C-O	-7.37	1.08	1.23
1	A	774	ASN	CG-ND2	-7.36	1.14	1.32
2	C	142	ASN	N-CA	7.35	1.61	1.46
1	a	25	GLU	CD-OE1	-7.34	1.17	1.25
1	A	725	SER	CB-OG	-7.34	1.32	1.42
1	a	134	TYR	CB-CG	-7.34	1.40	1.51
1	A	776	LEU	C-O	-7.33	1.09	1.23
2	C	180	GLN	C-O	-7.32	1.09	1.23
2	C	214	VAL	C-O	-7.32	1.09	1.23
1	a	745	GLU	CB-CG	-7.32	1.38	1.52
7	c	93	HIS	C-O	-7.31	1.09	1.23
1	A	656	TRP	C-O	-7.30	1.09	1.23
2	C	175	PRO	C-O	-7.28	1.08	1.23
1	a	57	TYR	CD2-CE2	-7.27	1.28	1.39
1	A	124	TRP	C-O	-7.27	1.09	1.23
2	C	163	ASN	C-O	-7.27	1.09	1.23
1	a	631	SER	C-O	-7.26	1.09	1.23
2	C	169	ASN	CG-OD1	-7.25	1.08	1.24
1	A	248	TRP	C-O	-7.24	1.09	1.23
2	C	128	CYS	C-O	-7.24	1.09	1.23
7	c	99	GLY	C-O	-7.23	1.12	1.23
1	A	810	ARG	CZ-NH1	-7.23	1.23	1.33
1	a	365	VAL	CB-CG2	-7.22	1.37	1.52
1	A	539	TRP	C-O	-7.21	1.09	1.23
1	A	766	GLU	CD-OE1	-7.20	1.17	1.25
1	A	740	MET	C-O	-7.20	1.09	1.23
1	a	414	THR	CB-CG2	-7.19	1.28	1.52
1	A	245	PRO	C-O	-7.18	1.08	1.23
1	a	364	GLN	CD-OE1	-7.18	1.08	1.24
2	C	181	LEU	C-O	-7.16	1.09	1.23
2	C	72	ASP	C-O	-7.15	1.09	1.23
1	A	756	THR	C-O	-7.14	1.09	1.23
1	A	411	VAL	CB-CG2	-7.14	1.37	1.52
2	C	167	ILE	C-O	-7.13	1.09	1.23
1	a	656	TRP	CB-CG	-7.13	1.37	1.50
1	A	788	PHE	CD2-CE2	-7.10	1.25	1.39
1	a	25	GLU	CD-OE2	-7.10	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	741	ALA	C-O	-7.09	1.09	1.23
2	C	87	VAL	CB-CG2	-7.09	1.38	1.52
4	F	25	ILE	C-O	-7.09	1.09	1.23
1	a	763	MET	C-O	-7.07	1.09	1.23
1	A	796	LYS	C-O	-7.06	1.09	1.23
1	a	748	TYR	CD1-CE1	-7.06	1.28	1.39
1	A	210	TRP	C-O	-7.06	1.09	1.23
1	A	628	ARG	CB-CG	-7.05	1.33	1.52
4	f	20	GLY	C-O	-7.03	1.12	1.23
1	a	765	ASN	CG-OD1	-7.02	1.08	1.24
4	F	10	SER	C-O	-7.02	1.10	1.23
1	a	699	PRO	C-O	-7.02	1.09	1.23
1	A	311	ILE	C-O	-7.01	1.10	1.23
1	a	765	ASN	C-O	-7.01	1.10	1.23
7	c	46	ALA	C-O	-7.00	1.10	1.23
2	C	146	PRO	C-O	-6.99	1.09	1.23
1	a	514	THR	CB-CG2	-6.98	1.29	1.52
1	A	283	TYR	CD2-CE2	-6.97	1.28	1.39
1	a	518	THR	CB-CG2	-6.96	1.29	1.52
1	a	847	THR	CB-CG2	-6.96	1.29	1.52
1	A	540	GLY	C-O	-6.93	1.12	1.23
1	A	762	TYR	CD1-CE1	-6.93	1.28	1.39
1	a	57	TYR	CD1-CE1	-6.93	1.28	1.39
4	f	17	LEU	C-O	-6.92	1.10	1.23
1	A	209	ILE	C-O	-6.91	1.10	1.23
1	a	757	GLY	CA-C	-6.91	1.40	1.51
1	a	202	TYR	CD1-CE1	-6.90	1.28	1.39
1	A	836	THR	CB-CG2	-6.90	1.29	1.52
1	a	528	GLU	CD-OE1	-6.89	1.18	1.25
1	a	173	VAL	CB-CG1	-6.89	1.38	1.52
7	c	43	THR	C-O	-6.87	1.10	1.23
1	A	832	SER	CB-OG	-6.86	1.33	1.42
2	C	148	TRP	C-O	-6.86	1.10	1.23
1	a	742	ARG	CZ-NH1	-6.85	1.24	1.33
1	A	252	TYR	CD2-CE2	-6.84	1.29	1.39
1	a	764	TRP	C-O	-6.83	1.10	1.23
2	C	188	TYR	CE2-CZ	-6.81	1.29	1.38
3	e	28	ASN	C-O	-6.81	1.10	1.23
1	A	203	ILE	C-O	-6.80	1.10	1.23
1	a	413	THR	CB-CG2	-6.80	1.29	1.52
2	C	170	GLY	C-O	-6.80	1.12	1.23
2	C	123	ASN	CG-ND2	-6.79	1.15	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	189	LEU	C-O	-6.79	1.10	1.23
1	A	861	PHE	C-O	-6.78	1.10	1.23
1	a	102	TYR	CD1-CE1	-6.74	1.29	1.39
1	a	624	GLU	CB-CG	-6.73	1.39	1.52
7	c	99	GLY	CA-C	-6.73	1.41	1.51
7	c	26	ARG	CZ-NH2	-6.72	1.24	1.33
1	A	126	VAL	C-O	-6.71	1.10	1.23
1	A	480	TRP	C-O	-6.70	1.10	1.23
1	A	742	ARG	C-O	-6.69	1.10	1.23
1	a	497	GLN	CB-CG	-6.69	1.34	1.52
1	A	497	GLN	CB-CG	-6.68	1.34	1.52
2	C	177	TYR	C-O	-6.67	1.10	1.23
1	a	569	GLU	CB-CG	-6.67	1.39	1.52
2	C	124	ASN	C-O	-6.66	1.10	1.23
1	a	314	VAL	CB-CG2	-6.66	1.38	1.52
1	A	348	VAL	CB-CG2	-6.64	1.38	1.52
1	a	72	TYR	CD2-CE2	-6.62	1.29	1.39
7	c	125	SER	CB-OG	-6.62	1.33	1.42
7	c	55	TYR	CE1-CZ	-6.61	1.29	1.38
2	C	32	TYR	CD1-CE1	-6.60	1.29	1.39
1	a	542	TRP	CD1-NE1	-6.60	1.26	1.38
7	c	113	TRP	CE3-CZ3	-6.59	1.27	1.38
3	E	2	THR	C-O	-6.59	1.10	1.23
1	A	535	TYR	CD1-CE1	-6.59	1.29	1.39
1	A	283	TYR	CD1-CE1	-6.59	1.29	1.39
1	A	307	HIS	C-O	-6.57	1.10	1.23
1	a	313	TYR	CD2-CE2	-6.57	1.29	1.39
1	a	465	VAL	CB-CG2	-6.57	1.39	1.52
1	A	75	TYR	CD1-CE1	-6.57	1.29	1.39
1	a	448	SER	CB-OG	-6.54	1.33	1.42
1	a	756	THR	C-O	-6.54	1.10	1.23
1	A	343	TYR	CD2-CE2	-6.53	1.29	1.39
1	A	202	TYR	CZ-OH	-6.52	1.26	1.37
1	a	72	TYR	CD1-CE1	-6.52	1.29	1.39
1	a	697	ILE	C-O	-6.50	1.11	1.23
2	C	31	ARG	C-O	-6.49	1.11	1.23
1	a	677	TYR	CD2-CE2	-6.49	1.29	1.39
1	A	268	THR	CB-CG2	-6.49	1.30	1.52
1	A	748	TYR	CD2-CE2	-6.47	1.29	1.39
2	C	31	ARG	CZ-NH1	-6.47	1.24	1.33
7	c	105	ALA	C-O	-6.47	1.11	1.23
1	A	102	TYR	CD2-CE2	-6.47	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	PRO	C-O	-6.46	1.10	1.23
7	c	21	CYS	C-O	-6.45	1.11	1.23
7	c	113	TRP	C-O	-6.45	1.11	1.23
7	c	148	TYR	CD1-CE1	-6.45	1.29	1.39
2	C	192	TYR	CD1-CE1	-6.45	1.29	1.39
1	A	118	HIS	C-O	-6.43	1.11	1.23
1	a	438	ASP	CB-CG	-6.43	1.38	1.51
1	A	739	MET	C-O	-6.43	1.11	1.23
1	A	420	VAL	CB-CG1	-6.42	1.39	1.52
1	a	537	VAL	C-O	-6.42	1.11	1.23
2	C	178	TYR	CD1-CE1	-6.42	1.29	1.39
1	a	116	CYS	C-O	-6.42	1.11	1.23
1	a	375	PHE	C-O	-6.42	1.11	1.23
1	A	246	TYR	CE1-CZ	-6.41	1.30	1.38
1	A	192	TYR	CD1-CE1	-6.40	1.29	1.39
1	a	787	TRP	CG-CD1	-6.39	1.27	1.36
1	A	631	SER	C-O	-6.38	1.11	1.23
2	C	20	CYS	C-O	-6.37	1.11	1.23
1	A	677	TYR	CD1-CE1	-6.36	1.29	1.39
1	a	576	GLU	CB-CG	-6.36	1.40	1.52
2	C	21	PHE	C-O	-6.36	1.11	1.23
1	A	119	ILE	C-O	-6.34	1.11	1.23
1	A	630	ALA	C-O	-6.34	1.11	1.23
1	a	541	SER	C-O	-6.34	1.11	1.23
7	c	20	GLY	N-CA	-6.34	1.36	1.46
1	A	213	VAL	CB-CG1	-6.32	1.39	1.52
1	A	207	PHE	C-O	-6.32	1.11	1.23
1	a	512	SER	CB-OG	-6.31	1.34	1.42
1	a	698	GLY	CA-C	-6.29	1.41	1.51
5	G	14	TRP	CB-CG	-6.28	1.39	1.50
1	a	725	SER	CB-OG	-6.28	1.34	1.42
1	A	210	TRP	CG-CD1	-6.28	1.27	1.36
7	c	142	THR	CB-CG2	-6.28	1.31	1.52
2	C	114	TYR	CE1-CZ	-6.28	1.30	1.38
1	a	529	TRP	CG-CD1	-6.27	1.27	1.36
1	A	328	ASN	CG-OD1	-6.27	1.10	1.24
1	a	765	ASN	CG-ND2	-6.26	1.17	1.32
4	F	20	GLY	C-O	-6.26	1.13	1.23
1	A	578	TYR	CD1-CE1	-6.25	1.29	1.39
2	C	71	ARG	CZ-NH1	-6.24	1.25	1.33
1	a	134	TYR	C-O	-6.24	1.11	1.23
1	a	677	TYR	CD1-CE1	-6.24	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	774	ASN	C-O	-6.23	1.11	1.23
1	A	238	PRO	C-O	-6.23	1.10	1.23
1	a	75	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	656	TRP	CG-CD1	-6.20	1.28	1.36
1	a	332	TYR	CD1-CE1	-6.20	1.30	1.39
1	A	625	TRP	CB-CG	-6.19	1.39	1.50
7	c	55	TYR	CB-CG	-6.19	1.42	1.51
1	A	639	ASN	CG-ND2	-6.19	1.17	1.32
1	a	768	THR	CB-CG2	-6.19	1.31	1.52
1	A	308	LEU	C-O	-6.17	1.11	1.23
1	A	732	ASP	CG-OD2	-6.17	1.11	1.25
2	C	165	LYS	C-O	-6.16	1.11	1.23
1	a	444	TYR	CD2-CE2	-6.15	1.30	1.39
2	C	31	ARG	CZ-NH2	-6.15	1.25	1.33
1	A	639	ASN	CB-CG	-6.15	1.36	1.51
1	A	247	GLY	C-O	-6.14	1.13	1.23
2	C	134	CYS	CB-SG	-6.14	1.71	1.82
1	a	309	THR	CB-CG2	-6.13	1.32	1.52
1	A	682	TYR	C-O	-6.12	1.11	1.23
1	a	45	TYR	CD1-CE1	-6.12	1.30	1.39
1	a	102	TYR	CD2-CE2	-6.11	1.30	1.39
1	a	18	LEU	C-O	-6.11	1.11	1.23
7	c	154	ARG	CZ-NH1	-6.10	1.25	1.33
1	A	137	ARG	C-O	-6.09	1.11	1.23
1	A	775	HIS	C-O	-6.09	1.11	1.23
2	C	114	TYR	CZ-OH	-6.09	1.27	1.37
1	A	273	TRP	CB-CG	-6.09	1.39	1.50
1	a	268	THR	CB-CG2	-6.09	1.32	1.52
1	A	561	TYR	CD2-CE2	-6.08	1.30	1.39
7	c	74	TYR	CB-CG	-6.08	1.42	1.51
1	A	246	TYR	CZ-OH	-6.08	1.27	1.37
1	A	762	TYR	CZ-OH	-6.08	1.27	1.37
1	a	134	TYR	CG-CD1	-6.07	1.31	1.39
7	c	140	LYS	C-O	-6.07	1.11	1.23
1	a	202	TYR	CD2-CE2	-6.06	1.30	1.39
7	c	41	SER	C-O	-6.05	1.11	1.23
1	a	134	TYR	CE1-CZ	-6.04	1.30	1.38
1	a	246	TYR	CD1-CE1	-6.04	1.30	1.39
1	A	316	PHE	CD2-CE2	-6.04	1.27	1.39
1	A	25	GLU	CD-OE2	-6.04	1.19	1.25
2	C	142	ASN	CG-OD1	-6.04	1.10	1.24
1	A	127	TYR	CD2-CE2	-6.03	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	ASN	C-O	-6.03	1.11	1.23
1	A	45	TYR	CD1-CE1	-6.02	1.30	1.39
1	a	377	GLY	C-O	-6.02	1.14	1.23
2	C	116	GLU	CG-CD	-6.01	1.43	1.51
1	A	299	ASP	C-O	-5.98	1.11	1.23
1	a	369	TYR	CD2-CE2	-5.97	1.30	1.39
1	A	677	TYR	CD2-CE2	-5.97	1.30	1.39
1	A	133	TYR	CD1-CE1	-5.97	1.30	1.39
7	c	154	ARG	CZ-NH2	-5.97	1.25	1.33
7	c	110	ASP	CG-OD2	-5.96	1.11	1.25
4	F	24	GLY	C-O	-5.96	1.14	1.23
1	a	525	TYR	CD2-CE2	-5.96	1.30	1.39
1	a	426	TYR	CD1-CE1	-5.94	1.30	1.39
2	C	177	TYR	CD1-CE1	-5.94	1.30	1.39
1	A	134	TYR	CD1-CE1	-5.92	1.30	1.39
1	A	208	PHE	C-O	-5.92	1.12	1.23
1	A	295	THR	CB-CG2	-5.92	1.32	1.52
7	c	18	ALA	CA-C	-5.92	1.37	1.52
2	C	174	MET	C-O	-5.92	1.12	1.23
1	A	117	PHE	C-O	-5.92	1.12	1.23
1	A	45	TYR	CD2-CE2	-5.91	1.30	1.39
7	c	107	ASN	CG-ND2	-5.90	1.18	1.32
2	C	163	ASN	CG-OD1	-5.89	1.10	1.24
1	a	696	CYS	C-O	-5.89	1.12	1.23
2	C	188	TYR	CZ-OH	-5.89	1.27	1.37
1	a	307	HIS	C-O	-5.89	1.12	1.23
2	C	124	ASN	CG-OD1	-5.88	1.11	1.24
1	a	769	TRP	CD1-NE1	-5.88	1.27	1.38
1	a	512	SER	C-O	-5.88	1.12	1.23
3	E	25	VAL	C-O	-5.87	1.12	1.23
3	E	15	TYR	C-O	-5.87	1.12	1.23
1	a	771	TRP	CE3-CZ3	-5.87	1.28	1.38
1	A	246	TYR	C-O	-5.86	1.12	1.23
1	a	225	LEU	C-O	-5.86	1.12	1.23
2	C	172	GLY	C-O	-5.86	1.14	1.23
1	A	249	PHE	C-O	-5.86	1.12	1.23
1	A	681	TRP	CE3-CZ3	-5.86	1.28	1.38
1	a	844	PHE	CD1-CE1	-5.85	1.27	1.39
1	A	183	THR	CB-CG2	-5.84	1.33	1.52
4	F	15	PHE	C-O	-5.84	1.12	1.23
1	A	47	PHE	CD1-CE1	-5.84	1.27	1.39
1	a	27	ILE	C-O	-5.83	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	200	THR	CB-CG2	-5.82	1.33	1.52
1	a	850	PHE	CD2-CE2	-5.82	1.27	1.39
1	A	15	TYR	CE1-CZ	-5.82	1.30	1.38
1	A	560	TRP	CB-CG	-5.82	1.39	1.50
1	a	742	ARG	C-O	-5.81	1.12	1.23
7	c	137	TYR	CD2-CE2	-5.81	1.30	1.39
1	A	108	ASP	C-O	-5.80	1.12	1.23
1	a	539	TRP	CB-CG	-5.80	1.39	1.50
1	a	681	TRP	CG-CD1	-5.79	1.28	1.36
7	c	133	VAL	CB-CG1	-5.79	1.40	1.52
2	C	177	TYR	CZ-OH	-5.79	1.28	1.37
1	a	338	MET	C-O	-5.79	1.12	1.23
1	A	305	HIS	C-O	-5.79	1.12	1.23
3	E	10	PHE	C-O	-5.78	1.12	1.23
7	c	107	ASN	CG-OD1	-5.78	1.11	1.24
2	C	184	GLN	CB-CG	-5.77	1.36	1.52
1	a	578	TYR	CD1-CE1	-5.77	1.30	1.39
7	c	55	TYR	CE2-CZ	-5.77	1.31	1.38
1	A	777	THR	CB-CG2	-5.76	1.33	1.52
1	A	501	ARG	C-O	-5.75	1.12	1.23
1	A	639	ASN	C-O	-5.74	1.12	1.23
2	C	165	LYS	CA-C	-5.74	1.38	1.52
1	a	283	TYR	CD1-CE1	-5.74	1.30	1.39
1	a	838	LYS	CB-CG	-5.73	1.37	1.52
1	A	72	TYR	CD1-CE1	-5.72	1.30	1.39
1	A	109	PHE	C-O	-5.72	1.12	1.23
1	a	517	PHE	CD1-CE1	-5.72	1.27	1.39
1	A	561	TYR	C-O	-5.71	1.12	1.23
1	A	783	GLY	C-O	-5.71	1.14	1.23
1	a	352	ARG	CZ-NH2	-5.70	1.25	1.33
1	A	525	TYR	CD1-CE1	-5.70	1.30	1.39
1	a	516	SER	CB-OG	-5.70	1.34	1.42
1	A	414	THR	CB-CG2	-5.69	1.33	1.52
1	a	748	TYR	CZ-OH	-5.69	1.28	1.37
1	A	671	ARG	CZ-NH2	-5.69	1.25	1.33
1	a	621	ASN	CB-CG	-5.68	1.38	1.51
1	a	836	THR	CB-CG2	-5.67	1.33	1.52
1	A	204	GLY	C-O	-5.67	1.14	1.23
1	A	338	MET	C-N	-5.67	1.21	1.34
1	a	628	ARG	CB-CG	-5.66	1.37	1.52
1	A	424	PHE	CD1-CE1	-5.66	1.27	1.39
2	C	185	GLN	C-O	-5.66	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	757	GLY	N-CA	-5.66	1.37	1.46
1	a	379	GLN	CG-CD	-5.65	1.38	1.51
1	A	107	THR	CB-CG2	-5.64	1.33	1.52
1	a	625	TRP	CB-CG	-5.64	1.40	1.50
1	A	252	TYR	CD1-CE1	-5.64	1.30	1.39
1	a	114	TRP	CE3-CZ3	-5.64	1.28	1.38
2	C	114	TYR	C-O	-5.63	1.12	1.23
1	A	102	TYR	CD1-CE1	-5.63	1.30	1.39
1	a	560	TRP	C-O	-5.62	1.12	1.23
1	A	747	TYR	CD2-CE2	-5.62	1.30	1.39
1	a	380	TYR	CD2-CE2	-5.61	1.30	1.39
1	A	735	TRP	CD1-NE1	-5.61	1.28	1.38
1	a	15	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	231	MET	C-O	-5.60	1.12	1.23
1	A	165	THR	C-O	-5.60	1.12	1.23
1	a	20	LEU	C-O	-5.60	1.12	1.23
1	A	310	ALA	C-O	-5.59	1.12	1.23
1	a	540	GLY	N-CA	5.59	1.54	1.46
1	A	847	THR	CB-CG2	-5.59	1.33	1.52
1	a	747	TYR	CD2-CE2	-5.59	1.30	1.39
7	c	154	ARG	C-O	-5.59	1.12	1.23
2	C	211	GLU	CB-CG	-5.58	1.41	1.52
1	a	241	GLN	CB-CG	-5.58	1.37	1.52
4	f	15	PHE	C-O	-5.58	1.12	1.23
1	A	463	TYR	CD1-CE1	-5.57	1.31	1.39
3	e	26	VAL	C-O	-5.56	1.12	1.23
2	C	32	TYR	CD2-CE2	-5.56	1.31	1.39
2	C	114	TYR	CB-CG	-5.55	1.43	1.51
2	C	192	TYR	C-O	-5.55	1.12	1.23
1	a	463	TYR	CD2-CE2	-5.55	1.31	1.39
1	a	846	TYR	CD1-CE1	-5.55	1.31	1.39
2	C	159	SER	CB-OG	-5.55	1.35	1.42
7	c	119	SER	CB-OG	-5.54	1.35	1.42
1	A	688	ARG	C-O	-5.54	1.12	1.23
1	A	57	TYR	CD2-CE2	-5.54	1.31	1.39
1	a	248	TRP	CB-CG	-5.53	1.40	1.50
7	c	97	GLY	N-CA	5.51	1.54	1.46
1	a	339	ASN	C-O	-5.50	1.12	1.23
1	A	764	TRP	CD1-NE1	-5.50	1.28	1.38
1	A	682	TYR	CG-CD1	-5.49	1.32	1.39
1	A	729	TRP	CE3-CZ3	-5.49	1.29	1.38
1	a	171	TYR	CD2-CE2	-5.49	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	539	TRP	CG-CD1	-5.48	1.29	1.36
7	c	21	CYS	CB-SG	-5.47	1.72	1.81
1	A	20	LEU	C-O	-5.46	1.12	1.23
1	A	521	GLU	CB-CG	-5.46	1.41	1.52
1	a	118	HIS	C-O	-5.46	1.12	1.23
7	c	74	TYR	CZ-OH	-5.46	1.28	1.37
1	a	19	GLU	C-O	-5.45	1.12	1.23
7	c	49	ARG	C-O	-5.45	1.12	1.23
1	A	759	VAL	C-O	-5.44	1.13	1.23
3	E	17	ALA	C-O	-5.43	1.13	1.23
1	a	632	THR	C-O	-5.43	1.13	1.23
1	A	542	TRP	CE3-CZ3	-5.43	1.29	1.38
2	C	148	TRP	CD1-NE1	-5.43	1.28	1.38
4	F	18	THR	C-O	-5.43	1.13	1.23
2	C	116	GLU	CB-CG	-5.41	1.41	1.52
1	A	656	TRP	CD1-NE1	-5.41	1.28	1.38
1	a	331	SER	CB-OG	-5.41	1.35	1.42
1	a	419	PHE	CD1-CE1	-5.41	1.28	1.39
1	a	766	GLU	CD-OE1	-5.40	1.19	1.25
1	a	771	TRP	CG-CD1	-5.40	1.29	1.36
1	A	327	ARG	CZ-NH1	-5.40	1.26	1.33
1	A	810	ARG	C-O	-5.39	1.13	1.23
2	C	171	GLY	C-O	-5.38	1.15	1.23
1	a	864	ASN	C-O	-5.38	1.13	1.23
1	A	828	ARG	C-O	-5.38	1.13	1.23
2	C	125	CYS	C-O	-5.38	1.13	1.23
1	A	123	LEU	C-O	-5.38	1.13	1.23
1	a	79	GLN	C-O	-5.38	1.13	1.23
1	A	560	TRP	CD1-NE1	-5.37	1.28	1.38
4	F	22	LEU	C-O	-5.37	1.13	1.23
1	A	472	TRP	CB-CG	-5.36	1.40	1.50
2	C	149	GLN	CD-NE2	-5.36	1.19	1.32
1	a	127	TYR	CD2-CE2	-5.36	1.31	1.39
1	a	164	PHE	CE1-CZ	-5.36	1.27	1.37
7	c	145	GLN	C-O	-5.36	1.13	1.23
1	A	611	PHE	C-O	-5.36	1.13	1.23
1	A	418	SER	CB-OG	-5.35	1.35	1.42
1	a	359	THR	CB-CG2	-5.35	1.34	1.52
7	c	41	SER	CA-CB	-5.35	1.45	1.52
1	A	47	PHE	CE1-CZ	-5.35	1.27	1.37
7	c	131	GLY	C-O	-5.35	1.15	1.23
1	A	177	TRP	CB-CG	-5.33	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	TYR	CD1-CE1	-5.33	1.31	1.39
1	a	47	PHE	CE1-CZ	-5.33	1.27	1.37
5	G	31	ASN	CG-OD1	-5.33	1.12	1.24
4	F	8	ILE	C-O	-5.33	1.13	1.23
2	C	70	LEU	C-O	-5.32	1.13	1.23
1	a	286	TYR	CD2-CE2	-5.31	1.31	1.39
1	a	764	TRP	CE3-CZ3	-5.31	1.29	1.38
1	A	444	TYR	CD1-CE1	-5.31	1.31	1.39
1	a	364	GLN	CB-CG	-5.30	1.38	1.52
1	A	360	PHE	CD1-CE1	-5.29	1.28	1.39
1	A	655	PHE	CB-CG	-5.29	1.42	1.51
1	a	762	TYR	CD2-CE2	-5.29	1.31	1.39
1	A	135	GLY	C-O	-5.29	1.15	1.23
1	A	535	TYR	CD2-CE2	-5.29	1.31	1.39
2	C	168	GLY	C-O	-5.29	1.15	1.23
4	F	7	GLN	CD-OE1	-5.28	1.12	1.24
2	C	148	TRP	CD2-CE2	-5.28	1.35	1.41
1	A	498	VAL	CB-CG2	-5.28	1.41	1.52
1	A	732	ASP	CG-OD1	-5.27	1.13	1.25
4	F	29	SER	C-O	-5.27	1.13	1.23
1	A	241	GLN	C-O	-5.27	1.13	1.23
1	A	309	THR	C-O	-5.27	1.13	1.23
2	C	84	GLU	CD-OE2	-5.26	1.19	1.25
7	c	74	TYR	C-O	-5.25	1.13	1.23
1	A	547	ARG	CZ-NH1	-5.24	1.26	1.33
7	c	36	SER	CB-OG	-5.24	1.35	1.42
3	E	12	LEU	C-O	-5.24	1.13	1.23
1	A	242	ALA	C-O	-5.24	1.13	1.23
5	G	44	LEU	CA-CB	-5.24	1.41	1.53
1	a	568	PHE	CD2-CE2	-5.24	1.28	1.39
1	a	764	TRP	CD2-CE2	-5.23	1.35	1.41
1	a	173	VAL	CB-CG2	-5.23	1.41	1.52
7	c	86	TYR	CZ-OH	-5.23	1.28	1.37
1	a	390	TYR	CD1-CE1	-5.22	1.31	1.39
1	A	812	VAL	C-O	-5.21	1.13	1.23
1	a	766	GLU	CD-OE2	-5.21	1.20	1.25
1	A	674	PHE	CD1-CE1	-5.21	1.28	1.39
1	A	380	TYR	CD2-CE2	-5.21	1.31	1.39
1	A	110	ARG	C-O	-5.20	1.13	1.23
1	A	380	TYR	CE1-CZ	-5.20	1.31	1.38
1	a	133	TYR	CD2-CE2	-5.20	1.31	1.39
1	A	200	THR	CB-CG2	-5.20	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	162	TYR	CE1-CZ	-5.19	1.31	1.38
1	A	774	ASN	CG-OD1	-5.19	1.12	1.24
1	A	472	TRP	CE3-CZ3	-5.19	1.29	1.38
2	C	115	ARG	CD-NE	-5.19	1.37	1.46
2	C	188	TYR	CG-CD1	-5.18	1.32	1.39
1	A	851	VAL	CB-CG2	-5.17	1.42	1.52
1	a	339	ASN	CG-ND2	-5.17	1.20	1.32
1	a	189	ARG	CG-CD	-5.17	1.39	1.51
1	A	681	TRP	C-O	-5.17	1.13	1.23
1	A	730	TYR	CD1-CE1	-5.17	1.31	1.39
7	c	96	ASN	CG-OD1	-5.17	1.12	1.24
2	C	191	ALA	C-O	-5.17	1.13	1.23
4	f	12	LEU	C-O	-5.17	1.13	1.23
2	C	122	GLN	C-O	-5.17	1.13	1.23
1	A	573	LYS	CB-CG	-5.17	1.38	1.52
2	C	192	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	584	LYS	CB-CG	-5.16	1.38	1.52
7	c	148	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	538	GLN	C-O	-5.16	1.13	1.23
1	a	735	TRP	CE3-CZ3	-5.16	1.29	1.38
7	c	50	GLU	CB-CG	-5.16	1.42	1.52
1	a	806	ASP	CB-CG	-5.16	1.41	1.51
1	A	45	TYR	CZ-OH	-5.16	1.29	1.37
1	A	449	PHE	CD1-CE1	-5.16	1.28	1.39
1	a	864	ASN	CA-C	-5.16	1.39	1.52
2	C	162	TYR	CD1-CE1	-5.15	1.31	1.39
4	F	21	THR	C-O	-5.15	1.13	1.23
1	a	732	ASP	CG-OD2	-5.15	1.13	1.25
1	A	690	GLN	C-O	-5.14	1.13	1.23
1	A	702	GLY	C-O	-5.14	1.15	1.23
1	a	682	TYR	CD1-CE1	-5.14	1.31	1.39
2	C	116	GLU	CD-OE1	-5.14	1.20	1.25
1	A	578	TYR	CD2-CE2	-5.13	1.31	1.39
1	A	656	TRP	CE3-CZ3	-5.12	1.29	1.38
1	a	542	TRP	C-O	-5.12	1.13	1.23
1	a	275	VAL	CB-CG1	-5.12	1.42	1.52
1	a	511	SER	C-O	-5.12	1.13	1.23
2	C	114	TYR	CD1-CE1	-5.11	1.31	1.39
1	a	714	TRP	CE3-CZ3	-5.11	1.29	1.38
1	a	436	GLU	CD-OE2	-5.11	1.20	1.25
1	a	278	VAL	CB-CG1	-5.11	1.42	1.52
1	A	171	TYR	CE2-CZ	-5.10	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	681	TRP	CE3-CZ3	-5.10	1.29	1.38
1	A	298	GLU	CD-OE2	-5.10	1.20	1.25
1	A	109	PHE	CB-CG	-5.10	1.42	1.51
7	c	87	ALA	C-O	-5.10	1.13	1.23
1	a	346	LYS	N-CA	5.09	1.56	1.46
1	a	528	GLU	C-O	-5.09	1.13	1.23
2	C	216	GLU	CA-CB	-5.09	1.42	1.53
7	c	113	TRP	CD1-NE1	-5.09	1.29	1.38
4	f	14	PHE	C-O	-5.09	1.13	1.23
7	c	89	CYS	C-O	-5.08	1.13	1.23
1	A	114	TRP	CE3-CZ3	-5.08	1.29	1.38
1	a	545	PHE	CD1-CE1	-5.08	1.29	1.39
3	E	18	LEU	C-O	-5.08	1.13	1.23
7	c	80	GLU	C-O	-5.08	1.13	1.23
7	c	76	ALA	C-O	-5.08	1.13	1.23
1	A	720	SER	CB-OG	-5.07	1.35	1.42
1	A	68	SER	CB-OG	-5.07	1.35	1.42
5	G	20	LEU	C-O	-5.07	1.13	1.23
1	a	25	GLU	C-O	-5.07	1.13	1.23
7	c	83	THR	C-O	-5.07	1.13	1.23
1	A	185	TRP	CB-CG	-5.07	1.41	1.50
1	A	680	PRO	C-O	-5.07	1.13	1.23
1	A	426	TYR	CE1-CZ	-5.06	1.31	1.38
1	A	266	GLU	C-O	-5.06	1.13	1.23
7	c	137	TYR	CD1-CE1	-5.05	1.31	1.39
1	a	343	TYR	CD2-CE2	-5.05	1.31	1.39
7	c	44	ALA	C-O	-5.05	1.13	1.23
1	A	735	TRP	C-O	-5.05	1.13	1.23
1	A	202	TYR	C-O	-5.05	1.13	1.23
1	A	803	GLU	CB-CG	-5.05	1.42	1.52
7	c	135	PRO	C-O	-5.04	1.13	1.23
1	a	488	ALA	C-O	-5.04	1.13	1.23
1	A	732	ASP	CB-CG	-5.03	1.41	1.51
2	C	187	ARG	CZ-NH2	-5.03	1.26	1.33
7	c	75	LYS	C-O	-5.03	1.13	1.23
1	a	732	ASP	C-O	-5.03	1.13	1.23
1	A	621	ASN	CB-CG	-5.03	1.39	1.51
1	A	65	ARG	CZ-NH1	-5.03	1.26	1.33
1	A	75	TYR	CD2-CE2	-5.03	1.31	1.39
7	c	19	THR	CB-CG2	-5.02	1.35	1.52
2	C	82	VAL	CB-CG2	-5.02	1.42	1.52
3	E	9	LEU	C-O	-5.02	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	784	HIS	C-O	-5.02	1.13	1.23
1	a	441	PHE	CD1-CE1	-5.02	1.29	1.39
1	A	733	GLY	N-CA	-5.01	1.38	1.46
7	c	98	GLY	C-O	-5.01	1.15	1.23
1	A	40	CYS	CB-SG	-5.00	1.73	1.81
4	F	27	TYR	CB-CG	-5.00	1.44	1.51
1	a	116	CYS	CB-SG	-5.00	1.73	1.81
7	c	114	GLN	CD-OE1	-5.00	1.12	1.24

All (264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	96	LEU	C-N-CD	-14.30	89.14	120.60
1	A	501	ARG	NE-CZ-NH2	12.92	126.76	120.30
7	c	26	ARG	NE-CZ-NH1	12.53	126.57	120.30
1	a	18	LEU	CA-CB-CG	12.52	144.09	115.30
1	a	18	LEU	CB-CG-CD1	-12.43	89.86	111.00
1	a	801	ARG	NE-CZ-NH1	12.33	126.46	120.30
7	c	26	ARG	NE-CZ-NH2	-12.24	114.18	120.30
1	a	801	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	A	641	ARG	NE-CZ-NH2	-11.94	114.33	120.30
2	C	194	ARG	NE-CZ-NH2	-11.70	114.45	120.30
2	C	194	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	A	798	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	757	GLY	N-CA-C	10.68	139.81	113.10
7	c	110	ASP	CB-CG-OD1	10.31	127.58	118.30
7	c	48	LEU	CB-CG-CD2	-10.12	93.80	111.00
1	A	641	ARG	NE-CZ-NH1	9.91	125.26	120.30
2	C	141	THR	CA-C-N	9.77	138.69	117.20
5	G	44	LEU	CB-CG-CD1	9.74	127.57	111.00
1	A	501	ARG	NE-CZ-NH1	-9.72	115.44	120.30
2	C	179	ASN	O-C-N	-9.63	107.30	122.70
1	a	539	TRP	CA-C-N	9.60	135.40	116.20
7	c	48	LEU	CA-CB-CG	9.60	137.37	115.30
7	c	97	GLY	CA-C-N	-9.53	97.15	116.20
1	a	798	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	a	447	ARG	NE-CZ-NH1	9.27	124.94	120.30
2	C	91	ASP	CB-CG-OD1	9.21	126.59	118.30
1	a	65	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	A	797	ASP	CB-CG-OD1	9.16	126.54	118.30
1	a	346	LYS	N-CA-CB	9.14	127.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	c	48	LEU	CB-CG-CD1	-9.02	95.67	111.00
1	A	500	ASP	CB-CG-OD1	8.99	126.39	118.30
1	a	859	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	450	ARG	NE-CZ-NH1	8.92	124.76	120.30
4	f	12	LEU	CB-CG-CD2	-8.81	96.02	111.00
1	A	639	ASN	CB-CA-C	-8.73	92.94	110.40
7	c	81	LEU	CA-CB-CG	8.63	135.15	115.30
1	a	450	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	65	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	C	71	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	a	757	GLY	N-CA-C	8.39	134.07	113.10
1	a	188	LEU	CA-CB-CG	8.24	134.25	115.30
2	C	118	ARG	NE-CZ-NH2	-8.21	116.19	120.30
3	E	18	LEU	CB-CG-CD2	8.16	124.88	111.00
1	A	739	MET	CA-CB-CG	8.10	127.07	113.30
1	a	539	TRP	O-C-N	-8.10	109.43	123.20
1	A	724	LEU	CA-CB-CG	7.94	133.57	115.30
7	c	106	THR	O-C-N	-7.92	110.03	122.70
2	C	142	ASN	N-CA-CB	7.92	124.85	110.60
1	a	65	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	135	GLY	N-CA-C	-7.79	93.62	113.10
1	a	333	LEU	CB-CG-CD2	7.69	124.07	111.00
1	a	367	LEU	CA-CB-CG	-7.68	97.62	115.30
7	c	21	CYS	N-CA-CB	7.67	124.41	110.60
1	A	108	ASP	CB-CG-OD1	7.64	125.18	118.30
2	C	202	ASN	CB-CA-C	7.64	125.68	110.40
7	c	26	ARG	CG-CD-NE	-7.64	95.76	111.80
1	A	214	LEU	CA-CB-CG	7.58	132.72	115.30
2	C	174	MET	CG-SD-CE	7.56	112.29	100.20
3	E	31	ASP	CB-CG-OD1	7.53	125.08	118.30
1	a	326	LEU	CA-CB-CG	7.53	132.62	115.30
2	C	193	LEU	CA-CB-CG	7.51	132.59	115.30
1	A	450	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	547	ARG	NE-CZ-NH1	7.49	124.05	120.30
2	C	141	THR	CA-C-O	-7.42	104.52	120.10
7	c	131	GLY	N-CA-C	7.41	131.62	113.10
1	A	13	ARG	N-CA-C	7.38	130.93	111.00
1	A	700	VAL	CB-CA-C	-7.34	97.46	111.40
7	c	56	GLU	OE1-CD-OE2	-7.32	114.52	123.30
1	A	501	ARG	CD-NE-CZ	7.31	133.84	123.60
1	A	266	GLU	OE1-CD-OE2	-7.30	114.53	123.30
1	a	364	GLN	N-CA-CB	-7.21	97.62	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	333	LEU	CA-CB-CG	7.19	131.84	115.30
1	a	69	LEU	CA-CB-CG	7.16	131.78	115.30
7	c	91	GLY	C-N-CA	7.16	139.59	121.70
1	a	670	LEU	CA-CB-CG	7.14	131.73	115.30
1	A	638	SER	CB-CA-C	-7.07	96.67	110.10
1	A	724	LEU	CB-CG-CD1	7.07	123.02	111.00
7	c	102	ALA	N-CA-CB	7.05	119.97	110.10
1	A	761	LEU	CB-CG-CD2	7.05	122.98	111.00
1	a	266	GLU	OE1-CD-OE2	-7.03	114.86	123.30
1	a	742	ARG	NE-CZ-NH2	7.00	123.80	120.30
5	G	9	ILE	CG1-CB-CG2	-7.00	96.00	111.40
1	a	450	ARG	NE-CZ-NH2	-6.96	116.82	120.30
2	C	179	ASN	CA-C-N	6.96	132.52	117.20
7	c	106	THR	CA-C-O	6.95	134.70	120.10
1	a	724	LEU	CA-CB-CG	6.95	131.28	115.30
1	a	865	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	a	861	PHE	CB-CA-C	6.89	124.17	110.40
7	c	98	GLY	C-N-CA	6.85	136.68	122.30
1	a	110	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	475	THR	N-CA-CB	6.83	123.27	110.30
1	a	154	GLY	N-CA-C	-6.80	96.09	113.10
1	a	26	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	a	824	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	a	773	ASP	CB-CG-OD1	6.78	124.40	118.30
1	a	851	VAL	CA-CB-CG2	6.77	121.06	110.90
1	A	167	GLU	N-CA-CB	-6.77	98.41	110.60
2	C	207	LEU	CB-CG-CD1	6.76	122.50	111.00
1	A	798	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	88	ILE	N-CA-C	6.67	129.02	111.00
1	a	188	LEU	CB-CG-CD2	-6.66	99.68	111.00
5	G	25	LEU	CB-CG-CD1	-6.66	99.69	111.00
1	A	859	ASP	CB-CG-OD2	6.65	124.28	118.30
3	E	34	ALA	N-CA-CB	6.64	119.39	110.10
1	A	367	LEU	CB-CG-CD1	6.61	122.24	111.00
7	c	26	ARG	CD-NE-CZ	6.61	132.85	123.60
2	C	141	THR	N-CA-C	6.60	128.81	111.00
1	A	196	LEU	CB-CG-CD1	6.57	122.17	111.00
7	c	92	CYS	N-CA-C	-6.54	93.34	111.00
2	C	178	TYR	CB-CG-CD1	-6.52	117.09	121.00
1	a	528	GLU	OE1-CD-OE2	-6.51	115.49	123.30
2	C	71	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	773	ASP	CB-CG-OD1	6.46	124.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	318	LEU	CA-CB-CG	6.41	130.04	115.30
1	A	740	MET	CG-SD-CE	6.40	110.44	100.20
7	c	20	GLY	N-CA-C	-6.40	97.09	113.10
1	a	437	LEU	CA-CB-CG	6.39	129.99	115.30
2	C	178	TYR	CZ-CE2-CD2	-6.36	114.08	119.80
1	a	303	VAL	CG1-CB-CG2	6.35	121.06	110.90
1	a	732	ASP	CB-CG-OD1	6.35	124.01	118.30
1	a	757	GLY	CA-C-N	6.34	128.88	116.20
1	A	333	LEU	CA-CB-CG	6.34	129.87	115.30
7	c	92	CYS	N-CA-CB	6.33	122.00	110.60
7	c	154	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	455	ASP	CB-CG-OD1	6.29	123.97	118.30
7	c	132	LYS	N-CA-CB	6.29	121.92	110.60
1	A	696	CYS	CA-CB-SG	6.23	125.22	114.00
9	D	45	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	851	VAL	CA-CB-CG1	6.17	120.16	110.90
7	c	54	LEU	CA-CB-CG	6.16	129.46	115.30
2	C	218	GLN	N-CA-CB	-6.13	99.57	110.60
8	B	109	LEU	N-CA-C	-6.13	94.45	111.00
7	c	106	THR	N-CA-CB	6.12	121.93	110.30
5	G	36	LEU	CA-CB-CG	6.12	129.38	115.30
1	a	824	LEU	CA-CB-CG	6.12	129.36	115.30
1	A	206	LEU	CB-CG-CD1	6.10	121.38	111.00
1	A	760	PHE	CB-CG-CD1	6.09	125.06	120.80
1	A	96	LEU	C-N-CA	6.08	147.55	122.00
1	a	865	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	C	218	GLN	N-CA-C	6.05	127.33	111.00
1	a	834	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	250	ASP	CB-CG-OD1	6.01	123.71	118.30
1	a	50	MET	CG-SD-CE	-5.95	90.67	100.20
1	a	182	ASN	C-N-CA	-5.93	106.88	121.70
1	A	739	MET	CG-SD-CE	5.92	109.66	100.20
5	g	26	ILE	N-CA-C	-5.91	95.05	111.00
7	c	98	GLY	O-C-N	5.88	133.20	123.20
1	A	763	MET	CB-CG-SD	-5.88	94.77	112.40
1	A	688	ARG	CB-CG-CD	-5.87	96.33	111.60
2	C	109	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	706	GLY	N-CA-C	5.87	127.77	113.10
1	a	339	ASN	CB-CA-C	5.87	122.13	110.40
1	a	798	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	501	ARG	CG-CD-NE	-5.83	99.56	111.80
5	G	25	LEU	CA-CB-CG	5.83	128.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	394	ARG	CB-CA-C	-5.83	98.75	110.40
1	a	299	ASP	CB-CG-OD1	5.79	123.52	118.30
1	A	333	LEU	CB-CG-CD2	5.75	120.78	111.00
1	a	214	LEU	CA-CB-CG	5.75	128.53	115.30
1	a	137	ARG	CB-CG-CD	-5.75	96.66	111.60
1	a	367	LEU	CB-CG-CD2	5.75	120.77	111.00
1	A	367	LEU	CA-CB-CG	-5.74	102.11	115.30
1	a	736	ILE	CG1-CB-CG2	5.73	124.01	111.40
1	A	167	GLU	CB-CA-C	-5.72	98.96	110.40
5	g	21	LEU	CA-CB-CG	-5.72	102.14	115.30
1	A	758	GLY	CA-C-N	5.71	129.76	117.20
1	a	326	LEU	CB-CG-CD1	5.70	120.70	111.00
1	A	813	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	a	852	LEU	CA-CB-CG	5.68	128.37	115.30
7	c	110	ASP	OD1-CG-OD2	-5.67	112.54	123.30
1	a	797	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	196	LEU	C-N-CA	-5.63	107.63	121.70
1	A	447	ARG	NE-CZ-NH1	5.63	123.11	120.30
5	G	44	LEU	N-CA-CB	-5.62	99.15	110.40
1	A	66	LEU	CA-CB-CG	5.62	128.22	115.30
8	B	105	VAL	N-CA-C	5.62	126.16	111.00
1	a	851	VAL	CA-CB-CG1	5.61	119.31	110.90
2	C	180	GLN	N-CA-C	5.60	126.12	111.00
7	c	122	MET	CG-SD-CE	-5.56	91.30	100.20
1	a	364	GLN	CB-CA-C	5.56	121.52	110.40
7	c	32	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	729	TRP	CA-CB-CG	5.55	124.24	113.70
1	A	65	ARG	CG-CD-NE	5.54	123.43	111.80
7	c	96	ASN	CA-C-N	5.53	127.27	116.20
1	a	537	VAL	CB-CA-C	-5.53	100.89	111.40
2	C	207	LEU	CA-CB-CG	5.53	128.02	115.30
1	a	757	GLY	CA-C-O	-5.52	110.67	120.60
1	A	214	LEU	CB-CG-CD1	5.52	120.38	111.00
1	A	736	ILE	CA-CB-CG2	5.52	121.93	110.90
1	a	206	LEU	CA-CB-CG	5.52	127.99	115.30
1	a	337	ASP	CB-CG-OD1	5.51	123.26	118.30
1	a	336	ASN	O-C-N	-5.50	113.90	122.70
2	C	87	VAL	CA-CB-CG1	5.50	119.15	110.90
1	a	327	ARG	C-N-CA	-5.47	108.02	121.70
1	A	761	LEU	CB-CG-CD1	5.46	120.28	111.00
1	a	308	LEU	CB-CG-CD1	5.45	120.27	111.00
1	A	326	LEU	CA-CB-CG	5.43	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	63	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	a	454	MET	CG-SD-CE	5.42	108.87	100.20
1	A	776	LEU	CB-CG-CD2	5.41	120.20	111.00
1	A	742	ARG	NE-CZ-NH2	5.41	123.00	120.30
7	c	133	VAL	CG1-CB-CG2	-5.40	102.27	110.90
1	a	801	ARG	CD-NE-CZ	5.39	131.15	123.60
1	a	65	ARG	CG-CD-NE	5.39	123.12	111.80
1	a	671	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	732	ASP	CB-CG-OD2	5.38	123.14	118.30
1	a	732	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	503	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	309	THR	OG1-CB-CG2	-5.35	97.69	110.00
2	C	216	GLU	CB-CA-C	-5.35	99.70	110.40
1	A	73	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	687	TRP	N-CA-C	5.33	125.39	111.00
1	A	327	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	a	732	ASP	N-CA-CB	-5.32	101.03	110.60
1	A	244	PHE	N-CA-CB	5.31	120.16	110.60
1	A	108	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	a	781	LEU	CA-CB-CG	5.29	127.47	115.30
2	C	128	CYS	CA-CB-SG	5.28	123.51	114.00
1	A	865	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	698	GLY	N-CA-C	5.28	126.30	113.10
1	A	447	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	147	TRP	N-CA-C	5.26	125.21	111.00
1	A	299	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	253	LEU	CA-CB-CG	5.25	127.38	115.30
1	a	266	GLU	CG-CD-OE1	5.25	128.81	118.30
1	a	798	ARG	CG-CD-NE	-5.24	100.80	111.80
3	E	32	ILE	N-CA-C	-5.23	96.88	111.00
1	a	333	LEU	CB-CG-CD1	-5.23	102.11	111.00
7	c	43	THR	OG1-CB-CG2	-5.23	97.97	110.00
3	e	24	PHE	N-CA-C	-5.22	96.92	111.00
2	C	73	ARG	CB-CA-C	-5.21	99.97	110.40
2	C	179	ASN	CB-CA-C	5.21	120.83	110.40
1	a	137	ARG	NE-CZ-NH1	-5.21	117.69	120.30
7	c	19	THR	N-CA-C	-5.21	96.93	111.00
1	a	763	MET	CA-CB-CG	5.21	122.15	113.30
1	a	671	ARG	NE-CZ-NH2	-5.21	117.70	120.30
2	C	141	THR	N-CA-CB	5.20	120.19	110.30
1	A	552	LEU	CA-CB-CG	5.20	127.26	115.30
1	a	63	ARG	NE-CZ-NH2	-5.18	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	20	CYS	N-CA-CB	5.18	119.92	110.60
1	a	447	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	a	698	GLY	C-N-CD	-5.15	109.28	120.60
8	B	140	VAL	N-CA-C	5.14	124.89	111.00
1	a	490	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	713	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	638	SER	C-N-CA	5.12	134.50	121.70
2	C	48	THR	N-CA-C	5.11	124.79	111.00
1	A	166	PRO	C-N-CA	5.10	134.46	121.70
7	c	101	LYS	N-CA-C	-5.10	97.23	111.00
1	a	731	LEU	CB-CG-CD1	5.08	119.64	111.00
1	a	759	VAL	N-CA-C	5.07	124.70	111.00
2	C	179	ASN	N-CA-C	-5.07	97.31	111.00
1	a	344	GLY	C-N-CA	-5.07	109.02	121.70
1	A	170	TRP	N-CA-C	5.07	124.69	111.00
2	C	77	LEU	CA-CB-CG	5.06	126.94	115.30
1	a	66	LEU	CA-CB-CG	5.06	126.93	115.30
7	c	98	GLY	CA-C-N	-5.05	106.10	116.20
1	A	90	GLU	O-C-N	-5.05	114.62	122.70
2	C	59	GLN	CB-CA-C	-5.04	100.33	110.40
1	a	152	VAL	N-CA-C	-5.03	97.41	111.00
7	c	131	GLY	CA-C-O	-5.02	111.56	120.60
1	a	147	TRP	N-CA-C	5.02	124.56	111.00
1	A	327	ARG	CD-NE-CZ	5.01	130.62	123.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ASN	Mainchain
2	C	141	THR	Mainchain
2	C	179	ASN	Mainchain
1	a	360	PHE	Mainchain
1	a	698	GLY	Peptide
1	a	92	SER	Peptide
1	a	93	THR	Peptide
7	c	97	GLY	Mainchain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	852/858 (99%)	792 (93%)	42 (5%)	18 (2%)	7 12
1	a	856/858 (100%)	798 (93%)	46 (5%)	12 (1%)	11 21
2	C	189/204 (93%)	174 (92%)	9 (5%)	6 (3%)	4 5
3	E	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
3	e	33/35 (94%)	32 (97%)	0	1 (3%)	4 6
4	F	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
4	f	33/35 (94%)	30 (91%)	2 (6%)	1 (3%)	4 6
5	G	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5 7
5	g	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
7	c	143/145 (99%)	127 (89%)	8 (6%)	8 (6%)	2 1
8	B	74/76 (97%)	43 (58%)	24 (32%)	7 (10%)	0 0
9	D	58/70 (83%)	58 (100%)	0	0	100 100
All	All	2376/2427 (98%)	2180 (92%)	142 (6%)	54 (2%)	9 10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	97	PRO
1	A	147	TRP
1	A	170	TRP
1	A	346	LYS
2	C	48	THR
2	C	62	PRO
2	C	180	GLN
2	C	203	GLY
1	a	83	VAL
1	a	759	VAL
7	c	99	GLY

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Mol	Chain	Res	Type
7	c	102	ALA
7	c	132	LYS
8	B	102	PRO
8	B	105	VAL
1	A	87	LEU
1	A	136	ALA
1	a	137	ARG
1	a	155	LEU
1	a	346	LYS
7	c	17	MET
7	c	21	CYS
7	c	131	GLY
8	B	128	CYS
1	A	688	ARG
1	a	9	ASN
1	a	87	LEU
7	c	92	CYS
8	B	123	ILE
1	A	94	SER
1	A	155	LEU
1	A	244	PHE
1	A	476	ALA
1	A	542	TRP
5	G	9	ILE
1	a	147	TRP
4	f	34	ARG
8	B	88	PHE
1	A	13	ARG
1	A	96	LEU
1	A	757	GLY
2	C	59	GLN
2	C	217	ARG
7	c	64	LYS
8	B	143	GLU
1	A	149	LEU
1	A	696	CYS
1	a	529	TRP
8	B	135	PRO
1	a	540	GLY
1	a	757	GLY
1	a	149	LEU
3	e	22	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	718/720 (100%)	589 (82%)	129 (18%)	1	2
1	a	720/720 (100%)	585 (81%)	135 (19%)	1	2
2	C	155/166 (93%)	127 (82%)	28 (18%)	1	2
3	E	25/25 (100%)	23 (92%)	2 (8%)	12	23
3	e	25/25 (100%)	18 (72%)	7 (28%)	0	0
4	F	31/31 (100%)	25 (81%)	6 (19%)	1	2
4	f	31/31 (100%)	26 (84%)	5 (16%)	2	3
5	G	31/31 (100%)	25 (81%)	6 (19%)	1	2
5	g	31/31 (100%)	22 (71%)	9 (29%)	0	0
7	c	112/112 (100%)	91 (81%)	21 (19%)	1	2
8	B	65/65 (100%)	47 (72%)	18 (28%)	0	1
9	D	52/62 (84%)	51 (98%)	1 (2%)	57	78
All	All	1996/2019 (99%)	1629 (82%)	367 (18%)	4	2

All (367) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	ARG
1	A	14	TRP
1	A	15	TYR
1	A	17	LYS
1	A	18	LEU
1	A	52	MET
1	A	59	ASN
1	A	60	LEU
1	A	61	THR
1	A	65	ARG
1	A	66	LEU
1	A	69	LEU
1	A	77	THR

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Mol	Chain	Res	Type
1	A	81	GLN
1	A	82	ARG
1	A	84	TRP
1	A	85	LEU
1	A	88	ILE
1	A	90	GLU
1	A	93	THR
1	A	95	LYS
1	A	96	LEU
1	A	101	GLN
1	A	107	THR
1	A	141	THR
1	A	144	GLU
1	A	147	TRP
1	A	148	LEU
1	A	149	LEU
1	A	159	CYS
1	A	161	ILE
1	A	175	LEU
1	A	183	THR
1	A	188	LEU
1	A	200	THR
1	A	203	ILE
1	A	205	LEU
1	A	206	LEU
1	A	214	LEU
1	A	218	LEU
1	A	224	PRO
1	A	240	GLU
1	A	254	ASN
1	A	263	ILE
1	A	267	THR
1	A	268	THR
1	A	276	LEU
1	A	290	ARG
1	A	294	ILE
1	A	301	LYS
1	A	303	VAL
1	A	318	LEU
1	A	326	LEU
1	A	331	SER
1	A	333	LEU

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Mol	Chain	Res	Type
1	A	334	MET
1	A	335	LEU
1	A	339	ASN
1	A	345	LYS
1	A	352	ARG
1	A	359	THR
1	A	381	LEU
1	A	386	ILE
1	A	387	SER
1	A	391	LYS
1	A	408	THR
1	A	413	THR
1	A	414	THR
1	A	433	THR
1	A	450	ARG
1	A	467	ARG
1	A	473	ASP
1	A	475	THR
1	A	479	ASP
1	A	489	LYS
1	A	490	LEU
1	A	494	ARG
1	A	496	LEU
1	A	497	GLN
1	A	501	ARG
1	A	503	LEU
1	A	518	THR
1	A	534	LEU
1	A	552	LEU
1	A	556	ASP
1	A	562	LEU
1	A	567	THR
1	A	572	ARG
1	A	583	LEU
1	A	588	LEU
1	A	601	LYS
1	A	602	GLN
1	A	608	LEU
1	A	612	ARG
1	A	617	LYS
1	A	621	ASN
1	A	624	GLU

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Mol	Chain	Res	Type
1	A	638	SER
1	A	640	LEU
1	A	653	ILE
1	A	657	LEU
1	A	669	LEU
1	A	670	LEU
1	A	684	ASP
1	A	688	ARG
1	A	690	GLN
1	A	700	VAL
1	A	716	CYS
1	A	724	LEU
1	A	736	ILE
1	A	768	THR
1	A	771	TRP
1	A	777	THR
1	A	781	LEU
1	A	790	SER
1	A	798	ARG
1	A	800	SER
1	A	819	LEU
1	A	823	THR
1	A	824	LEU
1	A	826	GLU
1	A	828	ARG
1	A	832	SER
1	A	833	ASN
1	A	836	THR
1	A	847	THR
1	A	849	THR
1	A	851	VAL
2	C	24	SER
2	C	28	ASN
2	C	30	THR
2	C	46	LEU
2	C	47	LYS
2	C	61	THR
2	C	65	ARG
2	C	71	ARG
2	C	75	THR
2	C	77	LEU
2	C	82	VAL

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Mol	Chain	Res	Type
2	C	85	GLN
2	C	87	VAL
2	C	99	VAL
2	C	116	GLU
2	C	118	ARG
2	C	139	ARG
2	C	150	GLU
2	C	153	SER
2	C	174	MET
2	C	180	GLN
2	C	182	SER
2	C	193	LEU
2	C	194	ARG
2	C	200	GLN
2	C	204	LEU
2	C	217	ARG
2	C	218	GLN
3	E	18	LEU
3	E	31	ASP
4	F	1	MET
4	F	2	TRP
4	F	12	LEU
4	F	32	LEU
4	F	33	SER
4	F	34	ARG
5	G	11	LYS
5	G	14	TRP
5	G	20	LEU
5	G	21	LEU
5	G	44	LEU
5	G	45	ASN
1	a	11	VAL
1	a	13	ARG
1	a	18	LEU
1	a	20	LEU
1	a	26	ARG
1	a	59	ASN
1	a	60	LEU
1	a	61	THR
1	a	65	ARG
1	a	66	LEU
1	a	69	LEU

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Mol	Chain	Res	Type
1	a	79	GLN
1	a	81	GLN
1	a	82	ARG
1	a	83	VAL
1	a	84	TRP
1	a	85	LEU
1	a	87	LEU
1	a	88	ILE
1	a	91	PHE
1	a	94	SER
1	a	95	LYS
1	a	98	PHE
1	a	106	MET
1	a	107	THR
1	a	123	LEU
1	a	124	TRP
1	a	125	LEU
1	a	147	TRP
1	a	148	LEU
1	a	149	LEU
1	a	151	TYR
1	a	155	LEU
1	a	156	LYS
1	a	158	LEU
1	a	160	GLN
1	a	161	ILE
1	a	172	LYS
1	a	183	THR
1	a	187	ILE
1	a	189	ARG
1	a	200	THR
1	a	205	LEU
1	a	206	LEU
1	a	214	LEU
1	a	218	LEU
1	a	225	LEU
1	a	240	GLU
1	a	241	GLN
1	a	244	PHE
1	a	253	LEU
1	a	263	ILE
1	a	267	THR

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Mol	Chain	Res	Type
1	a	268	THR
1	a	276	LEU
1	a	287	ARG
1	a	290	ARG
1	a	292	ILE
1	a	294	ILE
1	a	297	LEU
1	a	303	VAL
1	a	309	THR
1	a	318	LEU
1	a	326	LEU
1	a	333	LEU
1	a	359	THR
1	a	381	LEU
1	a	386	ILE
1	a	391	LYS
1	a	392	GLN
1	a	408	THR
1	a	413	THR
1	a	433	THR
1	a	448	SER
1	a	450	ARG
1	a	467	ARG
1	a	469	LYS
1	a	472	TRP
1	a	482	LYS
1	a	490	LEU
1	a	492	LYS
1	a	496	LEU
1	a	497	GLN
1	a	501	ARG
1	a	503	LEU
1	a	514	THR
1	a	516	SER
1	a	518	THR
1	a	534	LEU
1	a	552	LEU
1	a	562	LEU
1	a	566	LYS
1	a	567	THR
1	a	569	GLU
1	a	576	GLU

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Mol	Chain	Res	Type
1	a	583	LEU
1	a	584	LYS
1	a	587	SER
1	a	588	LEU
1	a	602	GLN
1	a	617	LYS
1	a	621	ASN
1	a	622	MET
1	a	623	LEU
1	a	624	GLU
1	a	628	ARG
1	a	640	LEU
1	a	641	ARG
1	a	657	LEU
1	a	669	LEU
1	a	670	LEU
1	a	705	CYS
1	a	709	ILE
1	a	724	LEU
1	a	729	TRP
1	a	736	ILE
1	a	761	LEU
1	a	768	THR
1	a	777	THR
1	a	781	LEU
1	a	788	PHE
1	a	798	ARG
1	a	815	MET
1	a	819	LEU
1	a	822	LYS
1	a	823	THR
1	a	826	GLU
1	a	828	ARG
1	a	833	ASN
1	a	836	THR
1	a	847	THR
1	a	849	THR
1	a	851	VAL
1	a	864	ASN
1	a	865	ARG
7	c	17	MET
7	c	21	CYS

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Mol	Chain	Res	Type
7	c	30	GLU
7	c	33	LEU
7	c	43	THR
7	c	48	LEU
7	c	50	GLU
7	c	54	LEU
7	c	62	LEU
7	c	64	LYS
7	c	92	CYS
7	c	96	ASN
7	c	100	ASN
7	c	103	ILE
7	c	106	THR
7	c	110	ASP
7	c	122	MET
7	c	133	VAL
7	c	140	LYS
7	c	144	GLN
7	c	159	LYS
3	e	2	THR
3	e	5	LEU
3	e	6	LEU
3	e	28	ASN
3	e	30	LYS
3	e	31	ASP
3	e	32	ILE
4	f	1	MET
4	f	10	SER
4	f	28	VAL
4	f	30	HIS
4	f	34	ARG
5	g	8	ASP
5	g	9	ILE
5	g	10	SER
5	g	11	LYS
5	g	20	LEU
5	g	25	LEU
5	g	26	ILE
5	g	40	MET
5	g	45	ASN
8	B	74	GLN
8	B	77	THR

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Mol	Chain	Res	Type
8	B	89	CYS
8	B	90	THR
8	B	93	CYS
8	B	96	LYS
8	B	106	GLU
8	B	108	VAL
8	B	117	ILE
8	B	120	THR
8	B	121	ARG
8	B	126	SER
8	B	127	LEU
8	B	128	CYS
8	B	130	VAL
8	B	139	VAL
8	B	143	GLU
8	B	148	ARG
9	D	20	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	79	GLN
1	A	81	GLN
1	A	101	GLN
1	A	229	GLN
1	A	241	GLN
1	A	255	GLN
1	A	296	HIS
1	A	339	ASN
1	A	364	GLN
1	A	445	GLN
1	A	470	ASN
1	A	483	ASN
1	A	531	GLN
1	A	538	GLN
1	A	550	ASN
1	A	565	GLN
1	A	602	GLN
1	A	619	HIS
1	A	639	ASN
1	A	643	GLN

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Mol	Chain	Res	Type
1	A	755	HIS
1	A	765	ASN
1	A	808	GLN
1	A	825	GLN
1	A	833	ASN
2	C	40	GLN
2	C	59	GLN
2	C	85	GLN
2	C	136	ASN
2	C	149	GLN
2	C	169	ASN
2	C	185	GLN
2	C	200	GLN
3	E	35	ASN
1	a	16	GLN
1	a	59	ASN
1	a	81	GLN
1	a	382	HIS
1	a	445	GLN
1	a	531	GLN
1	a	538	GLN
1	a	550	ASN
1	a	602	GLN
1	a	619	HIS
1	a	621	ASN
1	a	626	ASN
1	a	643	GLN
1	a	712	GLN
1	a	744	ASN
1	a	755	HIS
1	a	765	ASN
1	a	825	GLN
1	a	833	ASN
1	a	864	ASN
7	c	52	GLN
7	c	82	GLN
7	c	96	ASN
7	c	100	ASN
7	c	109	GLN
7	c	144	GLN
7	c	145	GLN
4	f	30	HIS

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Mol	Chain	Res	Type
9	D	21	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 81 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	BCL	A	904	-	38,54,74	2.32	16 (42%)	45,91,115	2.92	22 (48%)
11	BCL	a	907	-	58,74,74	1.94	18 (31%)	69,115,115	3.75	24 (34%)
12	CLA	a	912	21	65,73,73	2.79	17 (26%)	76,113,113	3.23	38 (50%)
12	CLA	a	913	-	65,73,73	2.62	20 (30%)	76,113,113	4.02	34 (44%)
12	CLA	a	914	-	46,54,73	2.87	19 (41%)	53,90,113	3.60	27 (50%)
15	85I	a	920	-	43,44,44	2.22	2 (4%)	47,51,51	2.04	3 (6%)
12	CLA	A	933	-	51,59,73	2.87	18 (35%)	59,96,113	3.90	32 (54%)
11	BCL	A	902	-	58,74,74	2.34	18 (31%)	69,115,115	3.27	29 (42%)
10	2GO	a	903	1	65,74,74	3.45	20 (30%)	76,115,115	3.41	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BCL	A	908	-	58,74,74	2.32	23 (39%)	69,115,115	2.64	24 (34%)
18	HEC	C	301	2	32,50,50	2.95	17 (53%)	24,82,82	3.49	12 (50%)
17	85N	g	101	-	36,37,46	0.79	1 (2%)	40,45,55	0.58	0
18	HEC	c	202	7	32,50,50	2.84	14 (43%)	24,82,82	3.87	11 (45%)
11	BCL	A	907	-	53,69,74	3.09	23 (43%)	63,109,115	4.62	34 (53%)
11	BCL	a	904	-	58,74,74	2.22	15 (25%)	69,115,115	3.26	21 (30%)
12	CLA	A	910	-	65,73,73	2.10	21 (32%)	76,113,113	3.13	31 (40%)
13	LYC	c	201	-	39,39,39	1.65	9 (23%)	44,46,46	5.76	28 (63%)
15	85I	A	916	-	43,44,44	2.15	3 (6%)	47,51,51	2.32	7 (14%)
11	BCL	a	909	-	58,74,74	2.21	18 (31%)	69,115,115	3.75	21 (30%)
17	85N	a	902	-	45,46,46	0.59	0	50,55,55	0.43	0
19	84Q	a	921	-	42,43,43	1.35	2 (4%)	47,50,50	1.04	2 (4%)
12	CLA	A	912	-	46,54,73	2.76	15 (32%)	53,90,113	4.13	29 (54%)
20	SF4	a	917	1	0,12,12	-	-	-		
15	85I	a	919	-	43,44,44	1.41	2 (4%)	47,51,51	1.66	3 (6%)
15	85I	A	917	-	43,44,44	1.57	2 (4%)	47,51,51	2.42	3 (6%)
11	BCL	A	909	-	58,74,74	2.96	22 (37%)	69,115,115	4.47	34 (49%)
11	BCL	A	906	1	44,60,74	2.27	9 (20%)	52,98,115	4.24	19 (36%)
12	CLA	A	911	-	65,73,73	2.71	22 (33%)	76,113,113	3.34	28 (36%)
11	BCL	a	905	-	58,74,74	2.38	14 (24%)	69,115,115	3.54	27 (39%)
15	85I	a	918	-	43,44,44	1.05	2 (4%)	47,51,51	1.69	4 (8%)
20	SF4	B	201	-	0,12,12	-	-	-		
10	2GO	A	901	1	65,74,74	3.57	18 (27%)	76,115,115	3.49	29 (38%)
11	BCL	a	906	-	38,54,74	2.51	15 (39%)	45,91,115	2.77	21 (46%)
11	BCL	a	911	-	58,74,74	2.51	16 (27%)	69,115,115	3.04	30 (43%)
19	84Q	E	101	-	42,43,43	2.09	10 (23%)	47,50,50	1.90	8 (17%)
11	BCL	a	910	-	58,74,74	3.13	15 (25%)	69,115,115	4.29	33 (47%)
15	85I	A	915	-	43,44,44	2.29	10 (23%)	47,51,51	2.44	7 (14%)
17	85N	A	932	-	45,46,46	1.04	1 (2%)	50,55,55	1.82	4 (8%)
13	LYC	A	913	-	39,39,39	2.05	11 (28%)	44,46,46	2.49	18 (40%)
12	CLA	a	915	-	51,59,73	2.93	17 (33%)	59,96,113	3.55	34 (57%)
17	85N	G	101	-	36,37,46	0.72	0	40,45,55	0.77	2 (5%)
11	BCL	a	908	1	58,74,74	2.44	20 (34%)	69,115,115	4.45	30 (43%)
11	BCL	A	905	-	58,74,74	2.40	17 (29%)	69,115,115	3.43	26 (37%)
12	CLA	a	901	21	65,73,73	2.66	21 (32%)	76,113,113	3.57	32 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	BCL	A	903	-	58,74,74	2.60	18 (31%)	69,115,115	3.70	25 (36%)
20	SF4	B	202	8	0,12,12	-	-	-		
12	CLA	A	931	-	65,73,73	3.13	25 (38%)	76,113,113	4.31	38 (50%)

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
11	BCL	A	904	-	-	6/13/113/137	-
11	BCL	a	907	-	-	12/37/137/137	-
12	CLA	a	912	21	-	12/37/115/115	-
12	CLA	a	913	-	-	11/37/115/115	-
12	CLA	a	914	-	-	4/15/93/115	-
15	85I	a	920	-	-	29/47/48/48	-
12	CLA	A	933	-	-	4/21/99/115	-
11	BCL	A	902	-	-	16/37/137/137	-
10	2GO	a	903	1	-	9/37/97/97	-
11	BCL	A	908	-	-	14/37/137/137	-
18	HEC	C	301	2	-	3/10/54/54	-
17	85N	g	101	-	-	19/42/42/51	-
18	HEC	c	202	7	-	3/10/54/54	-
11	BCL	A	907	-	-	16/31/131/137	-
12	CLA	A	910	-	1/1/15/20	13/37/115/115	-
11	BCL	a	904	-	-	12/37/137/137	-
13	LYC	c	201	-	-	16/43/43/43	-
15	85I	A	916	-	1/1/6/7	29/47/48/48	-
11	BCL	a	909	-	-	13/37/137/137	-
17	85N	a	902	-	-	24/51/51/51	-
19	84Q	a	921	-	-	32/46/47/47	-
12	CLA	A	912	-	-	2/15/93/115	-
20	SF4	a	917	1	-	-	0/6/5/5
15	85I	a	919	-	-	36/47/48/48	-
15	85I	A	917	-	-	29/47/48/48	-
12	CLA	A	911	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BCL	A	906	1	-	6/21/121/137	-
11	BCL	A	909	-	-	12/37/137/137	-
11	BCL	a	905	-	-	17/37/137/137	-
15	85I	a	918	-	-	21/47/48/48	-
20	SF4	B	201	-	-	-	0/6/5/5
10	2GO	A	901	1	-	4/37/97/97	-
11	BCL	a	906	-	-	6/13/113/137	-
11	BCL	a	911	-	-	5/37/137/137	-
19	84Q	E	101	-	-	27/46/47/47	-
11	BCL	a	910	-	-	11/37/137/137	-
15	85I	A	915	-	-	19/47/48/48	-
17	85N	A	932	-	-	18/51/51/51	-
13	LYC	A	913	-	-	1/43/43/43	-
12	CLA	a	915	-	-	7/21/99/115	-
17	85N	G	101	-	-	18/42/42/51	-
11	BCL	a	908	1	-	20/37/137/137	-
11	BCL	A	905	-	-	16/37/137/137	-
12	CLA	a	901	21	-	24/37/115/115	-
11	BCL	A	903	-	-	21/37/137/137	-
20	SF4	B	202	8	-	-	0/6/5/5
12	CLA	A	931	-	-	18/37/115/115	-

All (596) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	910	BCL	C4B-NB	-15.65	1.21	1.35
10	A	901	2GO	C4D-ND	-14.73	1.18	1.37
10	A	901	2GO	C2A-C3A	14.60	1.67	1.36
15	a	920	85I	O6-C3	-14.03	1.20	1.44
10	a	903	2GO	C3C-C2C	11.92	1.62	1.36
12	A	931	CLA	C4B-NB	-11.72	1.24	1.35
11	A	909	BCL	C4B-NB	-10.82	1.25	1.35
11	A	903	BCL	C4B-NB	-10.29	1.26	1.35
12	a	912	CLA	C3D-C4D	-10.27	1.21	1.44
15	A	915	85I	C4-C3	-9.77	1.29	1.51
11	A	907	BCL	C1B-NB	-9.44	1.26	1.35
11	a	910	BCL	C1B-NB	-9.40	1.26	1.35
15	A	916	85I	P-O3	9.37	1.85	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	933	CLA	C4B-NB	-9.34	1.26	1.35
12	A	912	CLA	C4B-NB	-9.33	1.26	1.35
10	a	903	2GO	C1D-ND	-9.25	1.25	1.37
12	a	913	CLA	C4B-NB	-9.24	1.27	1.35
10	a	903	2GO	C4D-ND	-9.06	1.25	1.37
12	a	914	CLA	C3D-C4D	-8.99	1.23	1.44
12	A	931	CLA	C3D-C4D	-8.88	1.24	1.44
12	a	915	CLA	C1B-NB	-8.86	1.27	1.35
10	a	903	2GO	C4B-NB	8.81	1.48	1.35
12	A	911	CLA	C1D-ND	8.80	1.48	1.37
19	E	101	84Q	P-O4	8.62	1.83	1.60
11	A	907	BCL	O2A-CGA	8.60	1.58	1.33
11	a	905	BCL	C4B-NB	-8.51	1.27	1.35
10	a	903	2GO	OBD-CAD	-8.49	1.09	1.33
12	A	912	CLA	C3D-C4D	-8.44	1.25	1.44
10	A	901	2GO	C3C-C2C	8.41	1.54	1.36
12	A	933	CLA	C3D-C4D	-8.35	1.25	1.44
11	a	911	BCL	C4B-NB	-8.22	1.27	1.35
12	A	933	CLA	C4D-ND	-8.21	1.26	1.37
12	a	901	CLA	C1C-NC	-8.21	1.25	1.37
12	A	931	CLA	O1D-CGD	-8.17	1.00	1.21
11	a	911	BCL	C1B-NB	-8.04	1.28	1.35
10	a	903	2GO	C2A-C3A	8.01	1.53	1.36
11	A	905	BCL	CAA-C2A	-8.00	1.39	1.54
12	a	913	CLA	C1B-NB	-7.96	1.28	1.35
11	A	909	BCL	C1B-NB	-7.93	1.28	1.35
19	a	921	84Q	O2-C16	-7.90	1.31	1.44
11	A	907	BCL	C4B-NB	-7.90	1.28	1.35
12	a	915	CLA	C3D-C4D	-7.83	1.26	1.44
15	a	919	85I	O6-C3	7.82	1.57	1.44
10	A	901	2GO	OBD-CAD	-7.80	1.11	1.33
11	A	908	BCL	C4B-NB	-7.79	1.28	1.35
12	a	901	CLA	C3D-C4D	-7.69	1.26	1.44
12	a	901	CLA	C1B-NB	-7.69	1.28	1.35
10	A	901	2GO	C1A-NA	-7.63	1.22	1.38
12	a	914	CLA	C1B-NB	-7.55	1.28	1.35
12	A	911	CLA	C1C-NC	-7.52	1.26	1.37
12	a	914	CLA	C4B-NB	-7.48	1.28	1.35
11	a	904	BCL	C3C-C4C	-7.32	1.42	1.51
10	a	903	2GO	C1A-NA	-7.28	1.23	1.38
12	a	901	CLA	C4B-NB	-7.25	1.28	1.35
11	a	908	BCL	CAA-C2A	-7.23	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	916	85I	C4-C3	7.23	1.68	1.51
11	A	902	BCL	C1B-NB	-7.12	1.28	1.35
15	A	917	85I	C4-C3	7.11	1.68	1.51
12	a	915	CLA	CHC-C1C	7.08	1.53	1.35
12	a	912	CLA	C1C-NC	-7.07	1.27	1.37
11	A	902	BCL	C4B-NB	-7.01	1.29	1.35
12	a	912	CLA	C9-C8	-6.99	1.30	1.52
15	A	917	85I	O6-C3	-6.84	1.33	1.44
12	A	911	CLA	C3D-C4D	-6.80	1.28	1.44
18	c	202	HEC	O2A-CGA	-6.79	1.07	1.30
11	a	910	BCL	C3C-C4C	-6.78	1.43	1.51
12	a	913	CLA	C3D-C4D	-6.69	1.29	1.44
13	A	913	LYC	C14-C12	-6.64	1.27	1.35
12	A	910	CLA	C3D-C4D	-6.59	1.29	1.44
11	A	909	BCL	O1A-CGA	-6.58	1.03	1.22
12	A	931	CLA	C1D-ND	6.56	1.45	1.37
11	A	907	BCL	O1D-CGD	-6.49	1.04	1.21
11	a	906	BCL	C4B-NB	-6.36	1.29	1.35
12	a	915	CLA	C4B-NB	-6.31	1.29	1.35
12	a	912	CLA	C4B-NB	-6.30	1.29	1.35
11	a	908	BCL	C2A-C1A	-6.29	1.38	1.52
12	a	913	CLA	C1D-ND	6.26	1.45	1.37
12	A	931	CLA	C4D-ND	-6.14	1.29	1.37
11	A	909	BCL	C3C-C4C	-6.12	1.43	1.51
12	A	933	CLA	O1D-CGD	-6.12	1.05	1.21
11	A	909	BCL	OBB-CAB	-6.12	1.03	1.22
12	a	913	CLA	C1C-NC	-6.09	1.28	1.37
11	A	903	BCL	OBB-CAB	-6.08	1.03	1.22
11	a	904	BCL	C1B-NB	-6.07	1.29	1.35
12	A	911	CLA	C4D-ND	-6.07	1.29	1.37
10	a	903	2GO	OBB-CAB	-6.06	1.04	1.22
11	A	909	BCL	OBD-CAD	-6.05	1.13	1.22
11	A	906	BCL	C4B-NB	-6.03	1.29	1.35
11	A	905	BCL	C2A-C1A	-6.01	1.38	1.52
12	a	912	CLA	OBD-CAD	-5.99	1.12	1.22
11	a	908	BCL	C4B-NB	-5.95	1.29	1.35
11	a	910	BCL	OBB-CAB	-5.91	1.04	1.22
11	A	905	BCL	C4B-NB	-5.87	1.30	1.35
11	A	904	BCL	C4B-NB	-5.83	1.30	1.35
11	a	909	BCL	O1D-CGD	-5.79	1.06	1.21
15	a	918	85I	O6-C3	-5.77	1.34	1.44
12	a	912	CLA	C1B-NB	-5.77	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	906	BCL	O2D-CED	-5.74	1.31	1.45
17	A	932	85N	O3-C17	-5.72	1.21	1.40
11	a	905	BCL	C3C-C4C	-5.69	1.44	1.51
12	A	931	CLA	O2D-CED	-5.64	1.32	1.45
11	a	911	BCL	C3C-C4C	-5.61	1.44	1.51
10	A	901	2GO	C1D-ND	-5.58	1.30	1.37
18	C	301	HEC	O2A-CGA	-5.57	1.12	1.30
12	a	915	CLA	C4D-ND	-5.53	1.30	1.37
11	a	909	BCL	C4B-NB	-5.50	1.30	1.35
15	A	916	85I	O6-C3	5.46	1.53	1.44
12	a	912	CLA	CHC-C1C	5.46	1.49	1.35
11	A	908	BCL	C3C-C4C	-5.39	1.44	1.51
19	E	101	84Q	C15-C16	5.39	1.64	1.51
11	A	903	BCL	C1B-NB	-5.39	1.30	1.35
12	A	911	CLA	C4B-NB	-5.38	1.30	1.35
11	a	909	BCL	C1B-NB	-5.36	1.30	1.35
11	A	906	BCL	C1B-NB	-5.33	1.30	1.35
11	a	911	BCL	OBD-CAD	-5.29	1.14	1.22
11	A	903	BCL	C3C-C4C	-5.29	1.44	1.51
12	a	914	CLA	C1C-NC	-5.28	1.29	1.37
12	A	910	CLA	C1D-ND	5.28	1.44	1.37
12	a	912	CLA	C1D-ND	5.28	1.44	1.37
10	A	901	2GO	C3D-C2D	-5.26	1.30	1.39
11	A	907	BCL	OBD-CAD	-5.18	1.15	1.22
11	A	907	BCL	C5-C3	5.12	1.61	1.51
11	A	903	BCL	O1A-CGA	-5.11	1.07	1.22
11	a	909	BCL	O2D-CED	-5.10	1.33	1.45
11	a	908	BCL	C1B-NB	-5.10	1.30	1.35
12	A	911	CLA	C9-C8	5.07	1.68	1.52
11	a	905	BCL	O1D-CGD	-5.06	1.08	1.21
11	A	902	BCL	C2A-C1A	-5.06	1.40	1.52
11	A	907	BCL	C2-C3	5.03	1.45	1.33
18	c	202	HEC	CAD-C3D	-5.00	1.44	1.52
10	A	901	2GO	C2D-C1D	-4.99	1.31	1.42
12	A	911	CLA	MG-NC	4.98	2.18	2.06
12	A	931	CLA	O2D-CGD	4.98	1.45	1.33
11	a	911	BCL	OBB-CAB	-4.97	1.07	1.22
18	c	202	HEC	C4B-C3B	-4.94	1.34	1.43
12	A	912	CLA	C1B-NB	-4.94	1.30	1.35
18	C	301	HEC	CBB-CAB	-4.89	1.31	1.49
11	a	906	BCL	CAA-C2A	-4.89	1.45	1.54
11	a	904	BCL	C4B-NB	-4.85	1.30	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	906	BCL	C1B-NB	-4.83	1.30	1.35
18	C	301	HEC	O2D-CGD	-4.80	1.14	1.30
12	A	911	CLA	C1B-NB	-4.78	1.30	1.35
10	a	903	2GO	C4C-C3C	4.78	1.53	1.45
11	A	906	BCL	O1D-CGD	-4.76	1.09	1.21
12	a	915	CLA	C1C-NC	-4.75	1.30	1.37
18	C	301	HEC	C1B-NB	-4.74	1.26	1.36
11	A	905	BCL	C3C-C4C	-4.71	1.45	1.51
12	A	910	CLA	C4B-NB	-4.71	1.31	1.35
18	C	301	HEC	CBC-CAC	-4.70	1.31	1.49
11	a	909	BCL	C3C-C4C	-4.70	1.45	1.51
11	a	906	BCL	C3C-C4C	-4.68	1.45	1.51
11	a	904	BCL	O1A-CGA	-4.67	1.08	1.22
11	A	902	BCL	C3C-C4C	-4.67	1.45	1.51
11	a	907	BCL	C2A-C1A	-4.64	1.41	1.52
11	a	905	BCL	O2A-CGA	4.57	1.46	1.33
11	a	905	BCL	OBD-CAD	-4.57	1.15	1.22
11	A	903	BCL	O1D-CGD	-4.56	1.09	1.21
11	A	904	BCL	O2A-CGA	4.56	1.46	1.30
11	A	906	BCL	CBB-CAB	-4.56	1.36	1.49
11	a	910	BCL	O1D-CGD	-4.55	1.09	1.21
12	a	912	CLA	O2D-CED	-4.54	1.34	1.45
11	a	908	BCL	CBB-CAB	-4.54	1.36	1.49
12	A	931	CLA	O2A-CGA	4.53	1.46	1.33
18	C	301	HEC	C3A-C4A	4.53	1.52	1.42
11	A	906	BCL	O1A-CGA	-4.52	1.09	1.22
12	A	912	CLA	C1C-NC	-4.52	1.31	1.37
15	A	915	85I	P-O3	4.49	1.72	1.60
12	A	931	CLA	O1A-CGA	-4.49	1.09	1.22
11	A	908	BCL	C1B-NB	-4.47	1.31	1.35
12	a	915	CLA	C1D-ND	4.47	1.43	1.37
11	a	907	BCL	C4B-NB	-4.47	1.31	1.35
11	A	902	BCL	O2D-CED	-4.43	1.34	1.45
11	A	905	BCL	C1B-NB	-4.42	1.31	1.35
11	a	905	BCL	OBB-CAB	-4.42	1.09	1.22
11	A	909	BCL	MG-NA	4.40	2.16	2.06
18	C	301	HEC	C4B-C3B	-4.39	1.35	1.43
18	c	202	HEC	O2D-CGD	-4.38	1.16	1.30
12	a	914	CLA	O1D-CGD	-4.38	1.10	1.21
12	A	911	CLA	C7-C8	-4.35	1.29	1.52
12	A	912	CLA	MG-NC	4.35	2.16	2.06
12	a	913	CLA	CHC-C1C	4.34	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	912	CLA	O1D-CGD	-4.33	1.10	1.21
11	a	911	BCL	O2D-CED	-4.32	1.35	1.45
12	a	901	CLA	O2A-CGA	4.29	1.45	1.33
11	A	903	BCL	C2A-C1A	-4.27	1.42	1.52
18	c	202	HEC	O1A-CGA	-4.26	1.08	1.22
12	a	901	CLA	CHC-C1C	4.26	1.45	1.35
11	a	904	BCL	O2A-CGA	4.25	1.45	1.33
11	A	907	BCL	O2D-CED	-4.24	1.35	1.45
12	A	933	CLA	C1C-NC	-4.20	1.31	1.37
12	a	912	CLA	O1D-CGD	-4.20	1.10	1.21
18	c	202	HEC	C4D-ND	-4.18	1.27	1.36
10	A	901	2GO	OBB-CAB	-4.15	1.09	1.22
12	A	910	CLA	C1B-NB	-4.15	1.31	1.35
11	A	905	BCL	OBB-CAB	-4.15	1.09	1.22
11	a	910	BCL	O1A-CGA	-4.12	1.10	1.22
11	a	906	BCL	C3B-C2B	4.08	1.46	1.39
11	A	905	BCL	O2D-CED	-4.07	1.35	1.45
11	a	904	BCL	O2D-CED	-4.07	1.35	1.45
12	A	911	CLA	CHC-C1C	4.07	1.45	1.35
11	a	904	BCL	O1D-CGD	-4.04	1.11	1.21
18	C	301	HEC	C3C-C4C	-4.02	1.35	1.43
11	a	911	BCL	C3D-C2D	4.01	1.46	1.39
15	a	919	85I	C4-C3	-4.00	1.42	1.51
11	a	911	BCL	O2A-C1	-4.00	1.34	1.46
10	a	903	2GO	C2D-C1D	-3.99	1.33	1.42
10	A	901	2GO	ZN-NC	3.98	2.25	2.01
11	A	905	BCL	C3A-C2A	-3.98	1.43	1.54
11	a	908	BCL	O1D-CGD	-3.97	1.11	1.21
11	a	908	BCL	O2D-CED	-3.97	1.36	1.45
15	A	915	85I	O4-C5	-3.95	1.21	1.33
11	a	909	BCL	O1A-CGA	-3.94	1.10	1.22
11	A	908	BCL	O1D-CGD	-3.93	1.11	1.21
10	A	901	2GO	ZN-NA	3.92	2.24	2.01
18	c	202	HEC	C1B-NB	-3.92	1.28	1.36
11	A	904	BCL	CAA-C2A	-3.92	1.46	1.54
13	A	913	LYC	C55-C56	-3.91	1.30	1.35
11	a	907	BCL	OBB-CAB	-3.91	1.10	1.22
12	A	933	CLA	O2A-C1	-3.90	1.35	1.46
12	a	915	CLA	C3C-C2C	3.88	1.45	1.36
11	a	911	BCL	O1A-CGA	-3.86	1.11	1.22
12	a	901	CLA	O2D-CED	-3.85	1.36	1.45
11	A	904	BCL	C2A-C1A	-3.85	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	905	BCL	O1D-CGD	-3.83	1.11	1.21
13	c	201	LYC	C14-C12	-3.83	1.30	1.35
11	A	902	BCL	CAA-C2A	-3.82	1.47	1.54
11	A	909	BCL	C4B-CHC	3.81	1.51	1.41
12	a	913	CLA	C3B-C2B	3.81	1.45	1.40
12	a	914	CLA	O2A-CGA	3.80	1.45	1.33
11	A	902	BCL	O2D-CGD	3.79	1.42	1.33
12	A	931	CLA	OBD-CAD	-3.79	1.15	1.22
11	a	910	BCL	O2D-CGD	3.78	1.42	1.33
11	a	905	BCL	O2D-CED	-3.77	1.36	1.45
12	a	915	CLA	MG-NC	3.77	2.15	2.06
12	A	912	CLA	CHC-C1C	3.76	1.44	1.35
11	a	909	BCL	C3B-C2B	3.76	1.46	1.39
12	a	912	CLA	MG-NC	3.75	2.15	2.06
12	a	901	CLA	O1D-CGD	-3.74	1.11	1.21
11	a	910	BCL	O2D-CED	-3.74	1.36	1.45
11	A	907	BCL	C6-C5	3.73	1.65	1.52
12	a	913	CLA	C4D-ND	-3.72	1.32	1.37
10	a	903	2GO	C1C-C2C	3.72	1.51	1.44
13	A	913	LYC	C9-C7	-3.71	1.30	1.34
15	A	915	85I	P-O	-3.70	1.44	1.59
18	C	301	HEC	C1D-ND	-3.69	1.28	1.36
12	a	901	CLA	CHD-C4C	3.68	1.47	1.39
12	a	901	CLA	MG-NC	3.67	2.15	2.06
11	A	908	BCL	C3A-C2A	-3.66	1.44	1.54
11	A	902	BCL	O1A-CGA	-3.65	1.11	1.22
11	A	907	BCL	OBB-CAB	-3.65	1.11	1.22
11	A	909	BCL	C2-C3	3.65	1.41	1.33
11	a	908	BCL	CAA-CBA	-3.65	1.41	1.52
12	A	912	CLA	C4D-ND	-3.65	1.32	1.37
18	C	301	HEC	C3D-C2D	3.64	1.48	1.37
11	a	908	BCL	C3D-C2D	3.63	1.45	1.39
13	c	201	LYC	C19-C17	-3.62	1.31	1.35
11	a	906	BCL	C2A-C1A	-3.62	1.44	1.52
12	a	914	CLA	MG-NC	3.61	2.14	2.06
11	A	909	BCL	C3A-C2A	-3.61	1.44	1.54
11	A	909	BCL	O1D-CGD	-3.60	1.12	1.21
12	a	915	CLA	O1A-CGA	-3.59	1.11	1.22
12	a	913	CLA	CAA-C2A	3.59	1.60	1.54
11	A	903	BCL	C3A-C2A	-3.59	1.44	1.54
12	a	912	CLA	O2A-CGA	3.56	1.43	1.33
10	a	903	2GO	ZN-NC	3.56	2.22	2.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	906	BCL	O2A-CGA	3.55	1.42	1.30
11	a	907	BCL	O2A-CGA	3.55	1.43	1.33
11	A	909	BCL	CAA-CBA	-3.55	1.41	1.52
15	A	915	85I	P-O1	-3.54	1.38	1.50
11	A	904	BCL	C3B-C2B	3.52	1.45	1.39
11	a	908	BCL	C3B-C2B	3.50	1.45	1.39
11	A	904	BCL	C4B-CHC	3.49	1.50	1.41
11	A	908	BCL	C3D-C2D	3.48	1.45	1.39
12	A	933	CLA	CAA-C2A	-3.47	1.47	1.54
12	a	915	CLA	O1D-CGD	-3.46	1.12	1.21
12	A	933	CLA	O1A-CGA	-3.45	1.12	1.22
18	C	301	HEC	CAD-C3D	-3.45	1.47	1.52
12	A	933	CLA	CHC-C1C	3.44	1.43	1.35
11	a	906	BCL	C3D-C2D	3.44	1.45	1.39
12	a	901	CLA	C1D-C2D	3.43	1.52	1.45
11	A	903	BCL	O2A-CGA	3.43	1.43	1.33
11	a	905	BCL	CBB-CAB	-3.43	1.39	1.49
11	a	905	BCL	O1A-CGA	-3.43	1.12	1.22
11	a	907	BCL	O2A-C1	-3.41	1.36	1.46
12	A	910	CLA	O2A-CGA	3.41	1.43	1.33
11	a	907	BCL	CAA-C2A	-3.40	1.47	1.54
11	A	909	BCL	CBD-CGD	-3.40	1.41	1.52
12	A	911	CLA	O1A-CGA	-3.39	1.12	1.22
13	A	913	LYC	C13-C12	-3.39	1.43	1.50
11	a	905	BCL	C3D-C2D	3.38	1.45	1.39
11	a	904	BCL	C3B-C2B	3.38	1.45	1.39
12	A	911	CLA	O2D-CED	-3.37	1.37	1.45
10	a	903	2GO	C1B-NB	3.37	1.40	1.35
11	A	903	BCL	CBB-CAB	-3.37	1.39	1.49
13	c	201	LYC	C13-C12	-3.37	1.43	1.50
18	c	202	HEC	C2B-C3B	3.36	1.44	1.40
12	A	912	CLA	O2A-CGA	3.35	1.43	1.33
12	A	931	CLA	CHC-C1C	3.35	1.43	1.35
11	a	906	BCL	OBB-CAB	-3.35	1.12	1.22
11	A	903	BCL	O2D-CGD	3.34	1.41	1.33
11	A	905	BCL	CBA-CGA	-3.32	1.41	1.50
11	a	908	BCL	CBA-CGA	-3.30	1.41	1.50
12	A	931	CLA	C4D-CHA	3.30	1.50	1.38
12	A	911	CLA	O2A-C1	-3.30	1.36	1.46
18	c	202	HEC	CBA-CGA	-3.29	1.42	1.50
12	a	901	CLA	C7-C8	-3.29	1.35	1.52
11	a	905	BCL	CAC-C3C	-3.28	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	914	CLA	C3C-C2C	3.28	1.43	1.36
11	a	908	BCL	C5-C3	-3.28	1.44	1.51
10	a	903	2GO	O1D-CGD	-3.25	1.14	1.21
18	c	202	HEC	CAA-C2A	-3.23	1.46	1.52
11	A	902	BCL	C3B-C2B	3.23	1.45	1.39
13	A	913	LYC	C19-C17	-3.22	1.31	1.35
11	a	907	BCL	O1D-CGD	-3.20	1.13	1.21
12	a	913	CLA	O1A-CGA	-3.20	1.13	1.22
11	a	907	BCL	MG-NA	-3.19	1.98	2.06
12	a	914	CLA	CHC-C1C	3.19	1.43	1.35
11	A	907	BCL	CMD-C2D	-3.19	1.44	1.51
11	A	908	BCL	CAA-C2A	-3.19	1.48	1.54
11	a	910	BCL	CMB-C2B	-3.18	1.45	1.51
11	A	908	BCL	MG-NC	-3.18	1.98	2.06
13	A	913	LYC	C10-C11	-3.17	1.26	1.34
11	A	908	BCL	CMA-C3A	-3.17	1.46	1.53
11	A	908	BCL	O2A-CGA	3.16	1.42	1.33
11	A	902	BCL	O2A-CGA	3.15	1.42	1.33
11	A	907	BCL	CBB-CAB	-3.13	1.40	1.49
12	A	910	CLA	C7-C8	-3.12	1.36	1.52
11	a	910	BCL	O2A-CGA	3.11	1.42	1.33
11	A	902	BCL	C1B-CHB	3.10	1.49	1.41
18	c	202	HEC	CBC-CAC	-3.10	1.37	1.49
11	A	907	BCL	C2C-C3C	-3.09	1.45	1.54
11	A	908	BCL	C3B-CAB	-3.09	1.41	1.49
12	a	915	CLA	O2D-CED	-3.08	1.38	1.45
12	A	931	CLA	C10-C8	-3.08	1.36	1.52
12	a	901	CLA	O2D-CGD	3.07	1.40	1.33
19	E	101	84Q	C3-C1	-3.07	1.30	1.51
11	a	910	BCL	MG-NA	3.06	2.13	2.06
11	a	909	BCL	C3A-C2A	-3.06	1.45	1.54
12	A	931	CLA	C1D-C2D	-3.04	1.39	1.45
12	A	910	CLA	C3A-C2A	-3.03	1.46	1.54
11	a	907	BCL	C2C-C3C	-3.02	1.46	1.54
10	A	901	2GO	CHA-C1A	3.02	1.51	1.41
18	C	301	HEC	C1C-NC	-3.02	1.29	1.36
12	A	931	CLA	C3D-C2D	3.02	1.47	1.39
12	A	911	CLA	C3B-C2B	3.02	1.44	1.40
10	a	903	2GO	C3D-C2D	-3.01	1.34	1.39
12	a	914	CLA	C2A-C1A	-3.01	1.45	1.52
12	A	910	CLA	C3C-C2C	3.01	1.43	1.36
12	A	910	CLA	C10-C8	-3.01	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	913	CLA	O1D-CGD	-3.00	1.13	1.21
11	a	904	BCL	OBB-CAB	-3.00	1.13	1.22
11	a	908	BCL	OBB-CAB	-2.99	1.13	1.22
11	A	902	BCL	O1D-CGD	-2.98	1.13	1.21
12	A	910	CLA	CHC-C1C	2.97	1.42	1.35
18	c	202	HEC	CMD-C2D	-2.96	1.45	1.51
11	a	911	BCL	C3A-C2A	-2.96	1.46	1.54
11	A	902	BCL	CMB-C2B	-2.96	1.45	1.51
11	A	905	BCL	CAA-CBA	-2.95	1.43	1.52
11	A	909	BCL	CBB-CAB	-2.95	1.40	1.49
12	A	911	CLA	O1D-CGD	-2.95	1.13	1.21
12	A	931	CLA	CHD-C1D	2.95	1.44	1.38
12	a	913	CLA	C10-C8	2.94	1.68	1.52
11	A	903	BCL	O2D-CED	-2.92	1.38	1.45
11	A	902	BCL	C3A-C2A	-2.92	1.46	1.54
12	A	931	CLA	CMA-C3A	-2.92	1.46	1.53
11	A	904	BCL	O2D-CGD	2.91	1.40	1.33
11	A	903	BCL	C3B-CAB	-2.91	1.41	1.49
12	A	931	CLA	C1C-C2C	-2.91	1.38	1.44
11	a	908	BCL	O2D-CGD	2.90	1.40	1.33
12	A	910	CLA	O1D-CGD	-2.89	1.14	1.21
11	a	905	BCL	O2D-CGD	2.89	1.40	1.33
11	A	904	BCL	C3D-C2D	2.89	1.44	1.39
11	A	908	BCL	O2D-CGD	2.88	1.40	1.33
11	A	904	BCL	CMB-C2B	-2.88	1.45	1.51
11	a	905	BCL	C2C-C3C	-2.87	1.46	1.54
13	A	913	LYC	C59-C58	-2.87	1.27	1.34
11	A	908	BCL	C2C-C3C	-2.86	1.46	1.54
12	a	913	CLA	MG-NC	2.86	2.13	2.06
12	A	910	CLA	C1C-NC	-2.86	1.33	1.37
12	A	933	CLA	C3A-C2A	-2.85	1.46	1.54
12	a	914	CLA	C3A-C2A	-2.84	1.46	1.54
11	a	904	BCL	C2C-C3C	-2.84	1.46	1.54
11	A	902	BCL	OBB-CAB	-2.84	1.14	1.22
12	a	901	CLA	CAA-C2A	-2.84	1.48	1.54
11	a	909	BCL	C2C-C3C	-2.83	1.46	1.54
11	a	910	BCL	C4B-CHC	2.82	1.48	1.41
11	a	907	BCL	O1A-CGA	-2.82	1.14	1.22
10	A	901	2GO	CBC-CAC	-2.82	1.38	1.51
12	a	901	CLA	C3C-C2C	2.80	1.42	1.36
19	E	101	84Q	C7-C6	-2.80	1.35	1.51
11	A	903	BCL	CMD-C2D	-2.79	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	908	BCL	O1A-CGA	-2.79	1.14	1.22
11	A	904	BCL	OBB-CAB	-2.78	1.14	1.22
10	A	901	2GO	C4B-NB	2.77	1.39	1.35
12	A	910	CLA	CMB-C2B	-2.76	1.45	1.51
12	A	912	CLA	C3B-C2B	2.76	1.44	1.40
12	A	912	CLA	C1D-C2D	-2.75	1.39	1.45
11	A	908	BCL	MG-NA	-2.74	1.99	2.06
12	A	931	CLA	C1B-NB	2.74	1.37	1.35
15	A	915	85I	O5-C5	-2.74	1.14	1.22
12	A	933	CLA	O2D-CED	-2.74	1.38	1.45
11	a	907	BCL	C3C-C4C	-2.74	1.48	1.51
11	A	906	BCL	OBB-CAB	-2.74	1.14	1.22
11	A	902	BCL	C2C-C3C	-2.73	1.46	1.54
12	a	915	CLA	O2D-CGD	2.72	1.39	1.33
11	A	907	BCL	C1B-CHB	2.71	1.48	1.41
15	A	915	85I	O6-C3	-2.71	1.40	1.44
11	A	907	BCL	O2A-C1	2.71	1.53	1.46
19	E	101	84Q	C9-C8	-2.71	1.36	1.51
12	A	911	CLA	CHD-C1D	2.69	1.43	1.38
12	A	912	CLA	C2A-C1A	-2.69	1.46	1.52
10	a	903	2GO	CHA-C1A	2.69	1.50	1.41
11	a	906	BCL	O1D-CGD	-2.68	1.14	1.21
12	A	912	CLA	C3C-C2C	2.68	1.42	1.36
18	C	301	HEC	CAA-C2A	-2.68	1.47	1.52
12	A	933	CLA	CBA-CGA	-2.68	1.42	1.50
15	A	915	85I	P-O2	-2.68	1.42	1.55
18	C	301	HEC	O1A-CGA	-2.68	1.13	1.22
11	A	908	BCL	O1A-CGA	-2.67	1.14	1.22
11	A	907	BCL	C3A-C2A	-2.67	1.47	1.54
12	A	910	CLA	CAA-C2A	-2.67	1.49	1.54
18	C	301	HEC	CBA-CGA	-2.67	1.44	1.50
11	a	909	BCL	CMD-C2D	-2.66	1.45	1.51
11	a	909	BCL	C5-C3	-2.66	1.45	1.51
12	A	931	CLA	MG-NC	2.66	2.12	2.06
12	A	911	CLA	CMC-C2C	-2.65	1.45	1.50
11	A	907	BCL	C2A-C1A	-2.65	1.46	1.52
15	A	915	85I	C33-C32	-2.63	1.37	1.51
11	a	909	BCL	O2D-CGD	2.63	1.39	1.33
19	E	101	84Q	C9-C10	-2.62	1.36	1.51
12	a	914	CLA	O1A-CGA	-2.61	1.14	1.22
12	a	901	CLA	O1A-CGA	-2.61	1.14	1.22
12	A	910	CLA	CHD-C1D	2.60	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	912	CLA	C1B-CHB	2.59	1.48	1.41
11	A	908	BCL	CBD-CGD	-2.59	1.44	1.52
11	A	905	BCL	O2A-CGA	2.58	1.40	1.33
11	a	909	BCL	CBB-CAB	-2.57	1.42	1.49
11	A	902	BCL	CBB-CAB	-2.56	1.42	1.49
12	a	901	CLA	C5-C3	-2.56	1.46	1.51
12	A	931	CLA	MG-NA	2.55	2.12	2.06
12	A	933	CLA	MG-ND	2.55	2.10	2.05
10	A	901	2GO	C4C-C3C	-2.55	1.40	1.45
11	A	905	BCL	O2A-C1	-2.55	1.39	1.46
13	c	201	LYC	C1-C2	-2.54	1.43	1.50
11	A	907	BCL	C3C-C4C	-2.54	1.48	1.51
11	a	907	BCL	O2D-CED	-2.54	1.39	1.45
13	c	201	LYC	C15-C16	-2.54	1.28	1.34
19	a	921	84Q	P-O4	2.54	1.67	1.60
18	c	202	HEC	C2A-C3A	2.54	1.45	1.37
12	A	931	CLA	C3A-C4A	-2.53	1.43	1.51
12	a	901	CLA	C2-C3	-2.53	1.26	1.33
18	C	301	HEC	CMB-C2B	-2.52	1.45	1.51
12	A	911	CLA	C10-C8	-2.52	1.39	1.52
13	A	913	LYC	C11-C12	-2.52	1.40	1.45
11	a	911	BCL	CBA-CGA	-2.51	1.43	1.50
11	A	906	BCL	C2A-C1A	-2.51	1.46	1.52
10	A	901	2GO	C3B-C2B	-2.50	1.34	1.39
12	A	910	CLA	C3B-C2B	2.50	1.43	1.40
15	a	920	85I	C4-C3	-2.50	1.46	1.51
11	a	910	BCL	C3A-C2A	-2.49	1.47	1.54
12	A	910	CLA	O2D-CGD	2.49	1.39	1.33
12	a	912	CLA	CHD-C4C	2.49	1.44	1.39
11	a	907	BCL	C3B-CAB	-2.49	1.42	1.49
19	E	101	84Q	C6-C5	-2.48	1.37	1.51
11	a	909	BCL	C3A-C4A	-2.48	1.43	1.51
10	a	903	2GO	O1A-CGA	-2.48	1.15	1.22
11	A	905	BCL	C2C-C3C	-2.47	1.47	1.54
11	a	910	BCL	CBB-CAB	-2.47	1.42	1.49
11	a	907	BCL	C1B-CHB	2.47	1.47	1.41
10	A	901	2GO	O1D-CGD	-2.46	1.16	1.21
19	E	101	84Q	C8-C7	-2.45	1.37	1.51
12	a	913	CLA	C5-C3	-2.45	1.46	1.51
11	A	905	BCL	CMB-C2B	-2.45	1.46	1.51
15	a	918	85I	C4-C3	2.45	1.57	1.51
12	A	911	CLA	C3B-CAB	-2.44	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	911	BCL	MG-NA	2.43	2.12	2.06
11	A	902	BCL	OBD-CAD	-2.43	1.18	1.22
11	A	907	BCL	O1A-CGA	-2.43	1.15	1.22
11	A	904	BCL	C3A-C2A	-2.43	1.47	1.54
12	A	910	CLA	CBD-CGD	-2.42	1.44	1.52
10	a	903	2GO	C3B-C2B	-2.42	1.35	1.39
11	a	909	BCL	C2C-C1C	-2.41	1.44	1.51
12	A	933	CLA	C2A-C1A	-2.41	1.46	1.52
19	E	101	84Q	C5-C4	-2.40	1.38	1.51
11	A	903	BCL	C1B-CHB	2.40	1.47	1.41
12	a	913	CLA	C2A-C1A	-2.39	1.46	1.52
12	a	901	CLA	CMC-C2C	-2.39	1.45	1.50
12	a	914	CLA	C4D-CHA	2.39	1.46	1.38
11	a	911	BCL	C2C-C3C	-2.38	1.47	1.54
11	a	906	BCL	CAA-CBA	-2.38	1.45	1.52
17	g	101	85N	O4-C24	-2.37	1.22	1.30
12	A	910	CLA	CMA-C3A	-2.37	1.48	1.53
13	A	913	LYC	C52-C51	-2.36	1.46	1.50
11	a	904	BCL	CAA-CBA	-2.36	1.45	1.52
13	c	201	LYC	C62-C61	-2.36	1.44	1.50
11	a	906	BCL	C3A-C4A	-2.36	1.44	1.51
12	A	910	CLA	C2A-C1A	-2.36	1.46	1.52
11	a	911	BCL	O1D-CGD	-2.35	1.15	1.21
12	A	910	CLA	O2D-CED	-2.35	1.39	1.45
19	E	101	84Q	O-C14	-2.35	1.15	1.22
11	A	904	BCL	CMA-C3A	-2.35	1.48	1.53
11	A	905	BCL	C4B-CHC	2.34	1.47	1.41
11	A	908	BCL	C3A-C4A	-2.34	1.44	1.51
11	a	904	BCL	C2A-C1A	-2.34	1.47	1.52
12	A	931	CLA	C4C-C3C	-2.33	1.41	1.45
18	C	301	HEC	C4D-ND	-2.33	1.31	1.36
10	a	903	2GO	C1A-C2A	2.33	1.50	1.45
12	a	913	CLA	C3A-C2A	-2.32	1.48	1.54
12	A	911	CLA	O2A-CGA	2.32	1.40	1.33
12	A	931	CLA	CBD-CGD	2.31	1.59	1.52
12	a	913	CLA	O2A-CGA	2.31	1.40	1.33
12	a	914	CLA	C4C-C3C	-2.31	1.41	1.45
15	A	915	85I	O7-C20	-2.31	1.15	1.22
11	A	908	BCL	O2D-CED	-2.31	1.39	1.45
12	a	914	CLA	C3D-C2D	2.29	1.45	1.39
11	A	904	BCL	C2D-C1D	2.29	1.47	1.42
11	A	909	BCL	CMD-C2D	-2.29	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	a	904	BCL	CMA-C3A	-2.29	1.48	1.53
11	A	903	BCL	C4B-CHC	2.29	1.47	1.41
11	a	908	BCL	C4-C3	-2.28	1.44	1.50
12	a	915	CLA	O2A-CGA	2.28	1.40	1.33
11	A	908	BCL	CAC-C3C	-2.28	1.49	1.54
12	A	931	CLA	O2A-C1	-2.27	1.39	1.46
11	a	911	BCL	C2A-C1A	-2.26	1.47	1.52
12	a	913	CLA	O2A-C1	-2.26	1.39	1.46
11	A	907	BCL	C3D-CAD	-2.25	1.40	1.46
11	A	908	BCL	OBB-CAB	-2.25	1.15	1.22
11	a	907	BCL	C3A-C4A	-2.24	1.44	1.51
11	a	906	BCL	CBD-CGD	-2.24	1.45	1.52
12	a	914	CLA	C3B-CAB	2.24	1.52	1.47
13	c	201	LYC	C21-C20	-2.23	1.30	1.36
11	A	904	BCL	CAA-CBA	-2.23	1.45	1.52
11	A	904	BCL	C1B-CHB	2.23	1.47	1.41
11	a	907	BCL	CBA-CGA	-2.23	1.44	1.50
11	a	909	BCL	C4-C3	-2.23	1.45	1.50
12	a	913	CLA	C3C-C2C	2.22	1.41	1.36
13	A	913	LYC	C18-C17	-2.21	1.46	1.50
11	a	909	BCL	CMA-C3A	-2.21	1.48	1.53
11	a	908	BCL	O2A-CGA	2.20	1.39	1.33
12	a	915	CLA	C3A-C2A	-2.20	1.48	1.54
11	A	909	BCL	C2A-C1A	-2.20	1.47	1.52
10	a	903	2GO	ZN-NA	2.20	2.14	2.01
10	A	901	2GO	C1C-NC	-2.19	1.34	1.38
11	A	909	BCL	C9-C8	-2.19	1.45	1.52
12	A	933	CLA	C1B-NB	-2.18	1.33	1.35
11	a	905	BCL	C3A-C2A	-2.18	1.48	1.54
11	A	908	BCL	CMB-C2B	-2.18	1.47	1.51
12	a	912	CLA	C2A-C1A	-2.17	1.47	1.52
11	a	906	BCL	C3A-C2A	-2.17	1.48	1.54
11	A	909	BCL	O2D-CED	2.17	1.50	1.45
11	a	910	BCL	OBD-CAD	2.17	1.25	1.22
12	a	901	CLA	C1D-ND	2.17	1.40	1.37
11	A	909	BCL	CBA-CGA	-2.16	1.44	1.50
11	A	908	BCL	CMC-C2C	-2.16	1.48	1.53
13	c	201	LYC	C18-C17	-2.16	1.46	1.50
12	a	913	CLA	C4B-CHC	2.15	1.47	1.41
12	a	915	CLA	C4B-CHC	2.15	1.47	1.41
12	A	933	CLA	MG-NC	2.14	2.11	2.06
12	a	912	CLA	C3D-C2D	2.14	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	914	CLA	CBD-CGD	-2.14	1.45	1.52
11	a	908	BCL	C4B-CHC	2.14	1.46	1.41
11	a	907	BCL	CAA-CBA	-2.14	1.46	1.52
12	A	912	CLA	CHD-C1D	2.14	1.42	1.38
11	a	907	BCL	CMD-C2D	-2.13	1.46	1.51
11	a	906	BCL	C4B-CHC	2.12	1.46	1.41
11	A	906	BCL	O2A-C1	-2.12	1.40	1.46
12	A	933	CLA	C3D-C2D	2.11	1.44	1.39
12	a	912	CLA	C4C-C3C	-2.11	1.41	1.45
13	A	913	LYC	C5-C4	-2.11	1.43	1.50
11	A	905	BCL	C3B-CAB	-2.11	1.43	1.49
11	A	903	BCL	C2C-C3C	-2.10	1.48	1.54
11	A	903	BCL	CAA-CBA	-2.10	1.46	1.52
12	a	914	CLA	CHD-C1D	2.09	1.42	1.38
12	A	933	CLA	C2-C3	-2.09	1.28	1.33
11	A	909	BCL	C2C-C3C	-2.08	1.48	1.54
11	a	908	BCL	C3C-C4C	-2.08	1.49	1.51
12	A	911	CLA	CHD-C4C	2.08	1.44	1.39
11	A	909	BCL	O2A-CGA	2.08	1.39	1.33
12	a	912	CLA	O1A-CGA	-2.07	1.16	1.22
11	A	908	BCL	C5-C3	-2.06	1.47	1.51
11	a	911	BCL	CAC-C3C	-2.06	1.49	1.54
11	a	909	BCL	C2-C3	-2.06	1.28	1.33
12	a	915	CLA	CHD-C1D	2.06	1.42	1.38
18	c	202	HEC	CAA-CBA	-2.06	1.42	1.52
11	A	907	BCL	C1-C2	2.05	1.55	1.49
11	A	904	BCL	CBA-CGA	-2.05	1.45	1.50
11	A	909	BCL	CMB-C2B	-2.05	1.47	1.51
13	c	201	LYC	C63-C64	-2.05	1.46	1.53
12	a	901	CLA	O2A-C1	-2.04	1.40	1.46
12	A	911	CLA	C2A-C1A	-2.03	1.47	1.52
11	A	907	BCL	C6-C7	2.03	1.60	1.52
11	a	904	BCL	C1B-CHB	2.03	1.46	1.41
11	A	907	BCL	C3A-C4A	-2.03	1.45	1.51
12	a	914	CLA	O2D-CED	-2.01	1.40	1.45
11	a	908	BCL	CMC-C2C	-2.01	1.48	1.53
11	a	904	BCL	CAC-C3C	-2.00	1.50	1.54

All (912) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	909	BCL	O2D-CGD-CBD	20.86	148.34	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	908	BCL	C4A-NA-C1A	18.75	115.13	106.71
11	A	906	BCL	O2D-CGD-CBD	18.23	143.66	111.27
12	A	931	CLA	O2D-CGD-CBD	18.08	143.39	111.27
11	a	907	BCL	C4A-NA-C1A	16.51	114.13	106.71
12	a	913	CLA	C1D-ND-C4D	-15.70	95.18	106.33
11	A	906	BCL	O2D-CGD-O1D	-15.50	93.54	123.84
11	a	909	BCL	O2D-CGD-CBD	15.31	138.47	111.27
12	A	912	CLA	C2C-C1C-NC	15.05	124.07	109.97
11	A	905	BCL	O2D-CGD-CBD	14.79	137.54	111.27
13	c	201	LYC	C21-C50-C51	14.72	148.32	127.31
11	A	907	BCL	C4A-NA-C1A	14.54	113.25	106.71
11	A	907	BCL	O2D-CGD-CBD	14.51	137.06	111.27
11	A	903	BCL	O2D-CGD-CBD	14.33	136.73	111.27
12	a	913	CLA	O2D-CGD-CBD	14.11	136.34	111.27
11	a	910	BCL	O2D-CGD-CBD	13.94	136.04	111.27
11	a	904	BCL	O2D-CGD-CBD	13.80	135.79	111.27
11	a	905	BCL	O2D-CGD-CBD	13.73	135.66	111.27
13	c	201	LYC	C53-C51-C50	13.54	139.72	118.94
11	a	910	BCL	C1C-NC-C4C	13.20	112.64	106.71
12	a	913	CLA	O2D-CGD-O1D	-13.12	98.18	123.84
11	a	908	BCL	O2D-CGD-CBD	12.97	134.31	111.27
15	A	917	85I	O4-C4-C3	12.72	142.19	109.54
10	A	901	2GO	CMA-C3A-C4A	-12.61	105.83	125.04
11	A	902	BCL	O2D-CGD-CBD	12.44	133.38	111.27
10	a	903	2GO	CMA-C3A-C4A	-12.44	106.10	125.04
11	A	903	BCL	O2D-CGD-O1D	-12.41	99.57	123.84
12	A	931	CLA	O2D-CGD-O1D	-11.91	100.55	123.84
11	a	907	BCL	O2D-CGD-CBD	11.80	132.25	111.27
13	c	201	LYC	C15-C14-C12	11.80	144.16	127.31
15	A	916	85I	O4-C4-C3	11.67	139.49	109.54
12	A	911	CLA	C1D-ND-C4D	-11.55	98.13	106.33
11	A	909	BCL	O2A-C1-C2	11.44	138.71	108.64
11	a	908	BCL	CBA-CAA-C2A	-11.23	80.73	113.86
10	A	901	2GO	C4A-C3A-C2A	-10.95	95.44	106.96
11	a	907	BCL	C1C-NC-C4C	-10.94	101.79	106.71
11	a	909	BCL	O2D-CGD-O1D	-10.84	102.65	123.84
11	A	909	BCL	O2A-CGA-CBA	10.83	145.89	111.91
10	a	903	2GO	CAD-C3D-C4D	-10.81	102.44	108.47
12	A	933	CLA	O2D-CGD-CBD	10.71	130.29	111.27
12	A	931	CLA	C2D-C1D-ND	-10.66	102.25	110.10
11	a	910	BCL	O2A-CGA-CBA	10.60	145.16	111.91
12	A	933	CLA	O2D-CGD-O1D	-10.55	103.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	905	BCL	O2D-CGD-O1D	-10.51	103.29	123.84
13	c	201	LYC	C21-C20-C19	10.48	144.94	123.47
12	a	901	CLA	O2D-CGD-CBD	10.42	129.78	111.27
13	c	201	LYC	C20-C19-C17	10.31	142.03	127.31
12	a	915	CLA	O2D-CGD-CBD	10.31	129.59	111.27
11	A	907	BCL	O2D-CGD-O1D	-10.21	103.87	123.84
15	a	920	85I	O4-C4-C3	10.19	135.69	109.54
17	A	932	85N	C18-O3-C17	10.16	133.48	113.80
11	A	909	BCL	O1D-CGD-CBD	-10.13	103.75	124.48
15	A	917	85I	P-O3-C3	10.12	161.93	120.90
11	A	908	BCL	O2D-CGD-CBD	10.09	129.19	111.27
12	a	914	CLA	O2D-CGD-CBD	10.06	129.14	111.27
11	a	909	BCL	C4A-NA-C1A	9.86	111.14	106.71
11	a	908	BCL	O2D-CGD-O1D	-9.74	104.80	123.84
11	a	910	BCL	O2A-CGA-O1A	-9.72	99.07	123.59
11	A	906	BCL	C4A-NA-C1A	9.67	111.06	106.71
12	A	931	CLA	CED-O2D-CGD	9.66	137.80	115.94
12	A	912	CLA	C3C-C4C-NC	9.60	121.33	110.57
11	A	907	BCL	C6-C5-C3	9.58	138.58	113.45
15	a	918	85I	O4-C4-C3	9.53	134.01	109.54
18	C	301	HEC	C1D-C2D-C3D	-9.47	100.41	107.00
11	a	904	BCL	C4A-NA-C1A	9.46	110.96	106.71
11	A	905	BCL	O2D-CGD-O1D	-9.34	105.57	123.84
11	A	907	BCL	O2A-CGA-CBA	9.32	141.15	111.91
12	A	931	CLA	C1D-ND-C4D	9.31	112.95	106.33
11	a	904	BCL	O2D-CGD-O1D	-9.27	105.70	123.84
12	A	910	CLA	C2C-C1C-NC	9.21	118.60	109.97
12	a	914	CLA	C3B-C4B-NB	9.19	121.09	109.21
11	a	910	BCL	O2A-C1-C2	9.13	132.62	108.64
10	A	901	2GO	CAC-C3C-C2C	-9.12	111.94	127.53
12	A	911	CLA	C3C-C4C-NC	9.07	120.74	110.57
13	c	201	LYC	C13-C12-C14	-9.06	110.23	122.92
11	a	908	BCL	C1-C2-C3	9.01	141.63	126.04
12	A	933	CLA	C4-C3-C5	8.99	126.27	115.98
12	a	912	CLA	O2D-CGD-O1D	-8.97	106.30	123.84
12	A	910	CLA	O2D-CGD-CBD	8.96	127.19	111.27
12	a	901	CLA	C3C-C4C-NC	8.92	120.57	110.57
11	a	909	BCL	C1-C2-C3	8.88	141.40	126.04
10	A	901	2GO	C1A-NA-C4A	8.85	120.05	106.80
11	A	903	BCL	O2A-CGA-CBA	8.75	139.35	111.91
12	A	911	CLA	C2C-C1C-NC	8.72	118.14	109.97
11	a	910	BCL	C1-O2A-CGA	8.56	138.90	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	902	BCL	C1-O2A-CGA	8.50	138.74	116.44
12	a	901	CLA	C1D-ND-C4D	-8.43	100.34	106.33
15	A	915	85I	O6-C3-C4	-8.41	75.44	107.08
18	c	202	HEC	CMC-C2C-C3C	8.39	135.69	125.82
11	A	907	BCL	C7-C6-C5	8.34	136.00	113.36
11	A	909	BCL	O2D-CGD-O1D	-8.28	107.65	123.84
12	A	933	CLA	CED-O2D-CGD	8.25	134.59	115.94
11	A	904	BCL	C1C-NC-C4C	-8.24	103.00	106.71
11	A	907	BCL	C1C-NC-C4C	-8.24	103.00	106.71
12	a	901	CLA	O2A-CGA-CBA	8.22	137.70	111.91
11	a	905	BCL	O2A-CGA-CBA	8.19	137.61	111.91
15	A	915	85I	P-O3-C3	8.17	154.00	120.90
11	a	910	BCL	O2D-CGD-O1D	-8.17	107.87	123.84
11	A	903	BCL	O2A-C1-C2	8.14	130.02	108.64
15	A	915	85I	O4-C4-C3	8.13	130.42	109.54
11	a	909	BCL	O2A-C1-C2	-8.11	87.33	108.64
10	a	903	2GO	C4C-C3C-C2C	-8.08	95.13	106.90
15	a	919	85I	O3-C3-C4	8.06	137.40	107.08
12	A	910	CLA	CMD-C2D-C1D	8.04	138.88	124.71
12	A	931	CLA	CMC-C2C-C1C	8.03	137.26	125.04
11	a	908	BCL	OBB-CAB-CBB	-7.97	102.22	120.17
12	a	901	CLA	C6-C7-C8	7.96	141.65	115.92
11	a	911	BCL	O2A-C1-C2	7.95	129.53	108.64
11	a	911	BCL	C1-C2-C3	7.93	139.77	126.04
12	a	913	CLA	CMD-C2D-C1D	7.87	138.57	124.71
12	a	915	CLA	O2D-CGD-O1D	-7.83	108.53	123.84
11	a	910	BCL	C4A-NA-C1A	-7.83	103.19	106.71
13	c	201	LYC	C16-C17-C19	7.83	130.96	118.94
12	a	914	CLA	O2D-CGD-O1D	-7.81	108.58	123.84
18	c	202	HEC	C1D-C2D-C3D	-7.80	101.57	107.00
12	A	931	CLA	C4A-NA-C1A	7.79	110.21	106.71
13	c	201	LYC	C52-C51-C50	-7.74	112.08	122.92
11	a	909	BCL	O2A-CGA-O1A	-7.73	104.08	123.59
12	A	933	CLA	C4A-NA-C1A	7.67	110.15	106.71
11	a	911	BCL	C1-O2A-CGA	7.65	136.52	116.44
12	A	911	CLA	C4A-NA-C1A	7.62	110.13	106.71
15	a	920	85I	O6-C3-C4	7.60	135.66	107.08
11	a	908	BCL	C3A-C2A-C1A	7.52	112.60	101.34
11	a	910	BCL	CAD-C3D-C4D	7.50	112.65	108.47
10	A	901	2GO	C2A-C1A-NA	-7.46	105.19	109.01
11	A	905	BCL	C4A-NA-C1A	7.45	110.06	106.71
15	A	916	85I	P-O3-C3	7.44	151.08	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	909	BCL	C4A-NA-C1A	-7.44	103.36	106.71
18	C	301	HEC	C4C-C3C-C2C	7.42	114.36	106.35
11	A	907	BCL	C1-O2A-CGA	7.42	135.90	116.44
12	a	912	CLA	C1D-ND-C4D	-7.36	101.10	106.33
12	a	901	CLA	C2C-C1C-NC	7.36	116.87	109.97
13	c	201	LYC	C15-C16-C17	7.30	146.92	126.42
12	a	901	CLA	C11-C10-C8	-7.27	92.41	115.92
11	A	905	BCL	CBA-CAA-C2A	-7.27	92.40	113.86
12	A	910	CLA	C1D-ND-C4D	-7.23	101.20	106.33
10	a	903	2GO	C4C-CHD-C1D	7.21	132.07	122.56
11	A	907	BCL	CED-O2D-CGD	7.20	132.22	115.94
11	a	910	BCL	C1-C2-C3	-7.17	113.63	126.04
18	c	202	HEC	O2A-CGA-O1A	-7.16	105.45	123.30
12	a	913	CLA	C11-C10-C8	-7.16	92.78	115.92
15	a	919	85I	P-O3-C3	7.14	149.84	120.90
12	A	912	CLA	C1C-C2C-C3C	-7.14	99.45	106.96
11	a	911	BCL	O2A-CGA-CBA	7.14	134.30	111.91
12	a	912	CLA	O2D-CGD-CBD	7.13	123.93	111.27
12	A	912	CLA	C1D-ND-C4D	-7.11	101.28	106.33
12	A	912	CLA	O2D-CGD-O1D	-7.11	109.94	123.84
11	a	907	BCL	C1-C2-C3	-7.10	113.76	126.04
12	a	912	CLA	CMD-C2D-C1D	7.07	137.18	124.71
11	A	907	BCL	C1-C2-C3	7.07	138.27	126.04
12	A	911	CLA	CMD-C2D-C1D	6.99	137.04	124.71
12	A	931	CLA	C1-O2A-CGA	6.97	134.72	116.44
19	E	101	84Q	O1-C15-C16	6.95	127.38	109.54
12	a	914	CLA	C3C-C4C-NC	6.88	118.29	110.57
11	A	903	BCL	C1-O2A-CGA	6.87	134.47	116.44
10	A	901	2GO	C1C-NC-C4C	6.86	115.78	106.49
12	A	911	CLA	CHD-C4C-C3C	-6.86	114.76	124.84
11	A	903	BCL	O1A-CGA-CBA	-6.85	97.03	123.73
12	a	913	CLA	C3D-C2D-C1D	-6.84	96.50	105.83
12	a	901	CLA	CMD-C2D-C1D	6.84	136.76	124.71
11	a	908	BCL	OBB-CAB-C3B	6.78	132.02	119.99
11	A	902	BCL	O2D-CGD-O1D	-6.76	110.61	123.84
11	a	911	BCL	CED-O2D-CGD	6.75	131.20	115.94
11	A	905	BCL	C3A-C2A-C1A	6.75	111.44	101.34
11	a	904	BCL	O2A-CGA-CBA	6.74	133.07	111.91
12	A	931	CLA	CHD-C4C-C3C	-6.73	114.95	124.84
13	c	201	LYC	C18-C17-C16	-6.73	107.48	118.08
12	a	915	CLA	C4-C3-C5	6.72	123.67	115.98
11	A	909	BCL	CAD-C3D-C4D	6.59	112.14	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	902	BCL	C4A-NA-C1A	6.56	109.66	106.71
12	A	911	CLA	C3D-C2D-C1D	-6.54	96.91	105.83
10	a	903	2GO	CHA-CBD-CAD	-6.53	100.71	107.17
12	A	912	CLA	O2D-CGD-CBD	6.53	122.87	111.27
10	a	903	2GO	C1A-NA-C4A	6.52	116.56	106.80
10	a	903	2GO	CAC-C3C-C4C	-6.52	116.36	124.81
12	A	912	CLA	CAC-C3C-C4C	6.48	133.21	124.81
12	a	914	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
11	a	907	BCL	O2D-CGD-O1D	-6.46	111.21	123.84
11	a	907	BCL	CBA-CAA-C2A	-6.45	94.82	113.86
11	a	904	BCL	CED-O2D-CGD	6.44	130.50	115.94
12	a	915	CLA	C4A-NA-C1A	-6.43	103.81	106.71
11	A	909	BCL	C4-C3-C5	-6.42	104.47	115.27
13	A	913	LYC	C18-C17-C19	-6.41	113.94	122.92
13	c	201	LYC	C11-C12-C14	6.40	128.77	118.94
11	a	905	BCL	C4A-NA-C1A	6.40	109.58	106.71
12	a	912	CLA	C2C-C1C-NC	6.40	115.96	109.97
11	a	905	BCL	CHD-C4C-NC	6.39	132.18	125.08
10	a	903	2GO	C1A-C2A-C3A	-6.38	98.20	106.61
11	A	906	BCL	OBB-CAB-C3B	6.35	131.27	119.99
12	A	931	CLA	C2C-C1C-NC	6.33	115.90	109.97
12	A	912	CLA	CMA-C3A-C4A	6.31	128.73	111.77
10	A	901	2GO	CMC-C2C-C1C	-6.29	115.46	125.04
13	c	201	LYC	C20-C21-C50	-6.28	110.61	123.47
11	A	903	BCL	C4A-NA-C1A	6.27	109.53	106.71
12	a	912	CLA	O2A-CGA-CBA	6.27	131.59	111.91
13	c	201	LYC	C52-C51-C53	-6.27	108.20	118.08
11	A	905	BCL	CAA-C2A-C3A	-6.25	95.66	112.78
11	a	905	BCL	C4-C3-C2	-6.25	107.65	123.68
12	A	933	CLA	C3D-C2D-C1D	-6.24	97.31	105.83
12	a	915	CLA	CMD-C2D-C1D	6.23	135.70	124.71
11	A	907	BCL	O1A-CGA-CBA	-6.22	99.48	123.73
12	a	913	CLA	CAC-C3C-C4C	6.20	132.86	124.81
12	A	910	CLA	O2D-CGD-O1D	-6.19	111.73	123.84
11	a	911	BCL	O2D-CGD-CBD	6.18	122.25	111.27
11	a	904	BCL	CHD-C4C-NC	6.17	131.92	125.08
11	a	911	BCL	C1C-NC-C4C	6.16	109.48	106.71
18	c	202	HEC	C4C-C3C-C2C	6.14	112.99	106.35
12	a	915	CLA	C3C-C4C-NC	6.14	117.46	110.57
11	a	907	BCL	C16-C15-C13	-6.13	96.12	115.92
12	a	901	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
12	A	911	CLA	C4C-C3C-C2C	-6.10	98.00	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	903	2GO	CMC-C2C-C1C	-6.05	115.82	125.04
10	a	903	2GO	C16-C15-C13	6.02	135.38	115.92
12	a	901	CLA	O2D-CGD-O1D	-5.96	112.19	123.84
18	c	202	HEC	CMB-C2B-C3B	5.94	132.80	125.82
11	A	909	BCL	C1C-NC-C4C	5.91	109.36	106.71
11	a	909	BCL	C4-C3-C2	-5.90	108.53	123.68
12	A	933	CLA	CMB-C2B-C1B	5.90	137.53	128.46
11	A	907	BCL	C4-C3-C2	-5.90	108.55	123.68
11	a	908	BCL	C2A-C3A-C4A	-5.88	92.37	101.87
12	a	901	CLA	CHD-C1D-ND	-5.87	119.06	124.45
10	A	901	2GO	CAC-C3C-C4C	-5.86	117.20	124.81
11	A	906	BCL	CED-O2D-CGD	5.84	129.14	115.94
11	A	906	BCL	O2A-CGA-O1A	-5.84	108.86	123.59
11	a	909	BCL	C1-O2A-CGA	5.82	131.72	116.44
12	A	933	CLA	O2A-C1-C2	-5.82	93.34	108.64
13	A	913	LYC	C57-C56-C55	5.80	131.04	122.92
11	a	910	BCL	CED-O2D-CGD	5.78	129.01	115.94
11	a	906	BCL	CAC-C3C-C4C	-5.78	99.76	112.58
12	A	931	CLA	O2A-CGA-CBA	5.78	130.04	111.91
12	a	915	CLA	O2A-CGA-O1A	-5.77	109.02	123.59
11	a	904	BCL	C3C-C4C-CHD	-5.77	111.06	123.39
11	a	908	BCL	C5-C3-C2	5.75	132.75	121.12
11	A	909	BCL	O2A-CGA-O1A	-5.73	109.12	123.59
12	a	912	CLA	CED-O2D-CGD	5.72	128.86	115.94
11	a	905	BCL	CED-O2D-CGD	5.70	128.83	115.94
12	a	912	CLA	C3B-C4B-NB	5.69	116.56	109.21
12	a	912	CLA	C3C-C4C-NC	5.65	116.91	110.57
12	a	915	CLA	C3D-C2D-C1D	-5.65	98.12	105.83
12	A	910	CLA	C3C-C4C-NC	5.62	116.88	110.57
11	a	906	BCL	C1C-NC-C4C	-5.62	104.18	106.71
18	C	301	HEC	CMC-C2C-C3C	5.62	132.43	125.82
12	A	933	CLA	C3B-C4B-NB	5.62	116.47	109.21
12	A	933	CLA	C2C-C1C-NC	5.61	115.23	109.97
13	c	201	LYC	C1-C2-C4	-5.59	106.48	122.65
12	a	901	CLA	C4C-C3C-C2C	-5.55	98.81	106.90
11	A	902	BCL	C3C-C4C-CHD	-5.55	111.54	123.39
12	a	914	CLA	C2C-C1C-NC	5.53	115.16	109.97
12	A	912	CLA	C4A-NA-C1A	5.53	109.19	106.71
12	a	915	CLA	CMC-C2C-C1C	5.52	133.45	125.04
11	A	902	BCL	CHD-C4C-NC	5.51	131.20	125.08
12	a	914	CLA	CED-O2D-CGD	5.50	128.38	115.94
11	A	909	BCL	C9-C8-C10	-5.49	91.39	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	904	BCL	C4A-NA-C1A	5.48	109.17	106.71
11	A	905	BCL	C1C-NC-C4C	5.47	109.17	106.71
11	A	905	BCL	CAA-C2A-C1A	-5.46	94.09	111.97
12	a	914	CLA	CHD-C1D-ND	-5.45	119.45	124.45
11	a	905	BCL	C1-C2-C3	5.43	135.43	126.04
15	a	920	85I	P-O3-C3	-5.41	98.96	120.90
11	a	904	BCL	C1-C2-C3	-5.41	116.69	126.04
12	A	910	CLA	C1C-C2C-C3C	-5.39	101.29	106.96
12	A	911	CLA	O2D-CGD-O1D	-5.36	113.35	123.84
12	a	913	CLA	C2D-C1D-ND	5.35	114.05	110.10
19	E	101	84Q	P-O4-C16	5.35	142.59	120.90
11	a	908	BCL	CAA-C2A-C1A	-5.34	94.47	111.97
13	c	201	LYC	C3-C2-C4	5.34	138.07	122.65
12	a	914	CLA	CBA-CAA-C2A	-5.31	98.19	113.86
11	a	909	BCL	CED-O2D-CGD	5.30	127.92	115.94
11	a	906	BCL	C3C-C4C-CHD	-5.28	112.10	123.39
18	c	202	HEC	O2A-CGA-CBA	5.28	131.00	114.03
11	A	907	BCL	CAD-C3D-C4D	-5.27	105.53	108.47
11	a	908	BCL	CED-O2D-CGD	5.26	127.83	115.94
11	A	904	BCL	C3C-C4C-CHD	-5.22	112.25	123.39
13	c	201	LYC	C8-C7-C9	-5.21	109.15	122.59
11	A	906	BCL	C1-O2A-CGA	5.20	130.10	116.44
11	a	910	BCL	C5-C3-C2	5.20	131.64	121.12
11	a	905	BCL	C5-C3-C2	5.20	131.64	121.12
12	A	911	CLA	O2A-CGA-CBA	5.19	128.21	111.91
11	A	903	BCL	CBA-CAA-C2A	5.19	129.18	113.86
12	a	913	CLA	C3C-C4C-NC	5.19	116.39	110.57
12	a	915	CLA	O2A-CGA-CBA	5.16	128.12	111.91
11	a	909	BCL	C5-C3-C2	5.16	131.55	121.12
12	A	910	CLA	CHD-C1D-ND	-5.14	119.73	124.45
11	A	905	BCL	CMA-C3A-C4A	5.13	125.56	111.77
12	a	901	CLA	C3D-C4D-ND	5.12	118.53	110.24
11	A	903	BCL	C3C-C4C-CHD	-5.12	112.46	123.39
12	A	910	CLA	C6-C7-C8	5.11	132.44	115.92
11	a	906	BCL	O2D-CGD-O1D	-5.11	113.85	123.84
11	A	908	BCL	CAA-C2A-C3A	-5.11	98.80	112.78
11	a	909	BCL	O2A-CGA-CBA	5.10	127.93	111.91
11	a	906	BCL	C4A-NA-C1A	5.09	108.99	106.71
10	A	901	2GO	C1-O2A-CGA	5.08	129.78	116.44
11	a	905	BCL	C3C-C4C-CHD	-5.05	112.59	123.39
11	A	902	BCL	O2A-CGA-CBA	5.05	127.75	111.91
12	A	911	CLA	CAC-C3C-C4C	5.03	131.34	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	911	BCL	C4A-NA-C1A	5.02	108.96	106.71
13	A	913	LYC	C13-C12-C11	4.99	125.93	118.08
10	a	903	2GO	CAA-C2A-C3A	-4.98	118.60	127.88
13	c	201	LYC	C14-C15-C16	-4.98	107.67	123.22
12	A	931	CLA	CHD-C4C-NC	4.97	132.03	124.20
11	A	908	BCL	CAD-C3D-C4D	-4.94	105.72	108.47
10	A	901	2GO	CHC-C1C-NC	4.91	130.90	124.68
12	A	910	CLA	C4A-NA-C1A	-4.90	104.50	106.71
11	A	902	BCL	CED-O2D-CGD	4.89	127.00	115.94
12	A	931	CLA	C1C-C2C-C3C	-4.89	101.81	106.96
11	a	905	BCL	CAD-C3D-C4D	-4.87	105.76	108.47
19	a	921	84Q	O1-C15-C16	4.86	122.03	109.54
12	a	913	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
10	A	901	2GO	C4C-CHD-C1D	4.85	128.97	122.56
12	a	915	CLA	CAC-C3C-C4C	4.85	131.10	124.81
13	c	201	LYC	C5-C4-C2	4.85	144.33	127.75
12	a	913	CLA	O2A-CGA-CBA	4.85	127.12	111.91
11	a	908	BCL	CAA-C2A-C3A	-4.85	99.51	112.78
12	A	933	CLA	CAC-C3C-C4C	4.84	131.10	124.81
11	A	903	BCL	OBB-CAB-CBB	-4.83	109.29	120.17
12	A	933	CLA	CMC-C2C-C1C	4.83	132.39	125.04
11	a	904	BCL	C1-O2A-CGA	4.82	129.09	116.44
11	A	909	BCL	O1A-CGA-CBA	-4.82	104.93	123.73
12	a	915	CLA	C3B-C4B-NB	4.81	115.43	109.21
12	a	901	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	A	910	CLA	C11-C10-C8	4.80	131.42	115.92
11	A	904	BCL	CED-O2D-CGD	4.80	126.78	115.94
11	A	904	BCL	O2D-CGD-CBD	4.80	119.79	111.27
12	a	914	CLA	C4C-C3C-C2C	-4.79	99.91	106.90
13	c	201	LYC	C57-C56-C55	-4.78	116.23	122.92
11	a	907	BCL	O2A-CGA-CBA	4.77	126.89	111.91
18	c	202	HEC	O2D-CGD-O1D	-4.76	111.44	123.30
13	c	201	LYC	C10-C11-C12	4.75	139.77	126.42
11	a	905	BCL	OBB-CAB-CBB	-4.75	109.48	120.17
12	a	913	CLA	CHD-C1D-ND	-4.75	120.09	124.45
19	E	101	84Q	O4-C16-C15	4.74	124.93	107.08
17	A	932	85N	O3-C17-O6	4.74	124.04	110.72
12	A	912	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
11	A	905	BCL	C3C-C4C-CHD	-4.73	113.28	123.39
18	C	301	HEC	C3C-C4C-NC	-4.73	102.01	110.94
12	a	913	CLA	C3D-C4D-ND	4.73	117.89	110.24
12	A	910	CLA	C3D-C2D-C1D	-4.73	99.38	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	906	BCL	OBD-CAD-C3D	-4.71	120.16	127.98
11	a	911	BCL	OBB-CAB-C3B	-4.71	111.63	119.99
10	a	903	2GO	C3A-C4A-NA	-4.70	102.95	109.07
12	A	933	CLA	C1-O2A-CGA	4.70	128.77	116.44
11	A	904	BCL	CBC-CAC-C3C	4.69	123.91	113.47
11	A	908	BCL	OBD-CAD-CBD	-4.68	119.20	125.89
12	a	913	CLA	C1-O2A-CGA	4.67	128.70	116.44
11	A	902	BCL	CBC-CAC-C3C	4.67	123.86	113.47
12	A	912	CLA	CMD-C2D-C1D	4.66	132.92	124.71
11	A	908	BCL	C1-C2-C3	-4.64	118.02	126.04
11	a	907	BCL	CED-O2D-CGD	4.63	126.41	115.94
19	a	921	84Q	O4-C16-C15	4.61	124.42	107.08
12	A	912	CLA	CED-O2D-CGD	4.60	126.35	115.94
11	a	908	BCL	CHD-C4C-NC	4.60	130.19	125.08
11	A	907	BCL	C4-C3-C5	4.59	122.98	115.27
18	C	301	HEC	O2A-CGA-O1A	-4.58	111.87	123.30
11	A	909	BCL	C1-O2A-CGA	4.58	128.45	116.44
11	A	908	BCL	O2A-CGA-CBA	4.57	126.25	111.91
13	A	913	LYC	C8-C7-C6	4.57	122.95	115.27
11	A	908	BCL	CMB-C2B-C3B	4.57	133.22	124.68
12	a	912	CLA	O2A-CGA-O1A	-4.56	112.07	123.59
11	a	905	BCL	O1A-CGA-CBA	-4.54	106.03	123.73
12	A	933	CLA	O2A-CGA-O1A	-4.53	112.16	123.59
12	a	912	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
11	A	905	BCL	CED-O2D-CGD	4.52	126.16	115.94
12	A	931	CLA	O1D-CGD-CBD	-4.52	115.24	124.48
12	A	911	CLA	O2A-CGA-O1A	-4.51	112.20	123.59
11	A	909	BCL	OBB-CAB-C3B	-4.51	111.99	119.99
11	A	902	BCL	CAA-CBA-CGA	-4.50	100.09	113.25
11	A	908	BCL	O1D-CGD-CBD	-4.50	115.28	124.48
15	a	918	85I	P-O3-C3	4.48	139.07	120.90
10	a	903	2GO	CHB-C4A-NA	4.47	130.35	124.68
11	A	904	BCL	CAC-C3C-C2C	4.47	125.42	114.26
12	A	931	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
12	A	931	CLA	C3D-C4D-ND	-4.46	103.03	110.24
10	a	903	2GO	C4A-C3A-C2A	-4.46	102.27	106.96
10	A	901	2GO	CHB-C4A-NA	4.45	130.32	124.68
12	a	915	CLA	CED-O2D-CGD	4.44	125.98	115.94
11	a	906	BCL	CAA-C2A-C1A	-4.43	97.46	111.97
11	A	903	BCL	C1-C2-C3	4.43	133.70	126.04
12	A	933	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
13	A	913	LYC	C13-C12-C14	-4.39	116.77	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	913	CLA	C2A-C1A-CHA	-4.39	116.18	123.86
11	a	906	BCL	OBB-CAB-CBB	-4.39	110.30	120.17
12	A	912	CLA	C3D-C4D-ND	4.38	117.33	110.24
11	A	909	BCL	CAA-C2A-C1A	4.37	126.31	111.97
12	a	913	CLA	C4C-C3C-C2C	-4.37	100.53	106.90
12	A	931	CLA	C4D-C3D-CAD	-4.37	102.94	108.10
12	a	914	CLA	O2A-CGA-CBA	4.36	129.48	112.23
11	A	904	BCL	C3D-CAD-CBD	4.36	113.35	107.61
11	a	911	BCL	CAD-C3D-C4D	-4.36	106.04	108.47
10	A	901	2GO	C1A-C2A-C3A	-4.36	100.86	106.61
12	a	912	CLA	C3D-C4D-ND	4.35	117.28	110.24
11	a	911	BCL	CMB-C2B-C3B	4.35	132.81	124.68
10	A	901	2GO	CMC-C2C-C3C	-4.34	114.34	126.12
11	a	908	BCL	CMB-C2B-C3B	4.32	132.77	124.68
12	A	910	CLA	CHD-C4C-C3C	-4.32	118.49	124.84
11	A	903	BCL	CBB-CAB-C3B	4.31	133.15	120.34
11	A	908	BCL	O2D-CGD-O1D	-4.29	115.46	123.84
11	a	910	BCL	OBB-CAB-CBB	-4.28	110.53	120.17
11	a	904	BCL	O1A-CGA-CBA	-4.28	107.02	123.73
12	a	915	CLA	C4C-C3C-C2C	-4.26	100.69	106.90
12	A	912	CLA	C4C-C3C-C2C	-4.26	100.69	106.90
11	A	907	BCL	O2A-C1-C2	4.25	119.80	108.64
12	a	915	CLA	CMB-C2B-C1B	4.25	134.99	128.46
12	A	911	CLA	O2D-CGD-CBD	4.24	118.80	111.27
11	a	910	BCL	C2A-C1A-CHA	-4.24	116.45	123.86
12	A	931	CLA	C4D-CHA-C1A	-4.23	116.11	121.25
12	a	914	CLA	CMC-C2C-C1C	4.20	131.43	125.04
11	A	902	BCL	O1D-CGD-CBD	-4.20	115.90	124.48
11	a	908	BCL	C3D-CAD-CBD	4.19	113.13	107.61
11	a	906	BCL	CAD-C3D-C4D	-4.19	106.13	108.47
11	a	910	BCL	CHD-C4C-NC	4.19	129.73	125.08
11	A	908	BCL	C3D-CAD-CBD	4.17	113.09	107.61
12	A	911	CLA	CHC-C1C-NC	-4.17	117.88	124.20
12	A	933	CLA	CHD-C1D-ND	-4.16	120.63	124.45
11	A	907	BCL	OBB-CAB-C3B	4.16	127.37	119.99
12	A	931	CLA	C4-C3-C5	4.15	122.26	115.27
12	A	911	CLA	C10-C8-C7	4.14	133.92	112.13
11	A	903	BCL	CED-O2D-CGD	4.14	125.30	115.94
12	a	901	CLA	C9-C8-C7	4.13	126.26	111.29
11	A	906	BCL	CMD-C2D-C3D	4.13	132.41	124.68
11	A	908	BCL	C3C-C4C-CHD	-4.13	114.56	123.39
12	a	914	CLA	CMB-C2B-C3B	4.13	132.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	913	CLA	C4-C3-C5	4.12	122.21	115.27
12	a	912	CLA	C6-C7-C8	-4.12	102.59	115.92
13	c	201	LYC	C9-C10-C11	4.11	136.03	123.22
12	a	901	CLA	O2A-CGA-O1A	-4.10	113.23	123.59
11	a	910	BCL	O1D-CGD-CBD	-4.10	116.09	124.48
12	A	912	CLA	CMC-C2C-C1C	4.10	131.28	125.04
12	a	913	CLA	CED-O2D-CGD	4.10	125.21	115.94
10	A	901	2GO	CAA-C2A-C3A	-4.10	120.25	127.88
11	a	905	BCL	CMB-C2B-C1B	4.09	134.75	128.46
12	a	913	CLA	CMC-C2C-C1C	4.08	131.26	125.04
12	a	912	CLA	C4-C3-C2	-4.08	113.21	123.68
12	A	910	CLA	O2A-CGA-CBA	4.08	124.70	111.91
12	a	915	CLA	CHB-C4A-NA	4.07	130.14	124.51
11	A	902	BCL	OBD-CAD-CBD	-4.06	120.09	125.89
11	a	908	BCL	OBD-CAD-C3D	-4.06	121.23	127.98
11	a	904	BCL	CMC-C2C-C1C	4.06	122.68	111.77
11	a	911	BCL	O2D-CGD-O1D	-4.06	115.90	123.84
11	a	907	BCL	CMC-C2C-C1C	4.06	122.68	111.77
11	A	905	BCL	CHD-C4C-NC	4.06	129.58	125.08
12	A	910	CLA	C3B-C4B-NB	4.05	114.44	109.21
11	a	905	BCL	C3D-CAD-CBD	4.04	112.93	107.61
12	A	911	CLA	C6-C7-C8	4.04	128.97	115.92
15	A	915	85I	O3-P-O1	4.04	124.61	109.47
13	c	201	LYC	C57-C56-C58	4.03	124.43	118.08
12	A	912	CLA	CHC-C1C-C2C	-4.03	115.58	126.72
11	A	903	BCL	CHD-C4C-NC	4.03	129.55	125.08
11	a	907	BCL	O1D-CGD-CBD	-4.01	116.28	124.48
11	a	906	BCL	CED-O2D-CGD	4.01	125.01	115.94
11	a	907	BCL	C3C-C4C-CHD	-4.01	114.83	123.39
18	c	202	HEC	CBA-CAA-C2A	-4.00	105.86	112.60
15	A	916	85I	O2-P-O	-4.00	89.16	107.75
12	a	912	CLA	CMB-C2B-C1B	4.00	134.61	128.46
11	A	906	BCL	O2A-CGA-CBA	4.00	124.45	111.91
11	A	905	BCL	C1-O2A-CGA	3.99	126.91	116.44
11	A	905	BCL	O2A-C1-C2	3.98	119.10	108.64
12	a	912	CLA	CAC-C3C-C4C	3.97	129.97	124.81
11	A	902	BCL	O2A-C1-C2	3.97	119.07	108.64
11	a	907	BCL	C4-C3-C5	3.97	121.94	115.27
12	a	914	CLA	CAC-C3C-C4C	3.94	129.93	124.81
11	A	902	BCL	C9-C8-C10	-3.94	97.01	111.29
11	A	904	BCL	CMB-C2B-C1B	3.94	134.52	128.46
12	A	911	CLA	CHD-C1D-ND	-3.93	120.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	a	909	BCL	C6-C5-C3	-3.92	103.17	113.45
11	A	906	BCL	C1-C2-C3	-3.92	119.26	126.04
19	E	101	84Q	O2-C16-C15	-3.91	92.36	107.08
17	A	932	85N	O3-C17-C16	3.91	122.01	107.06
12	A	912	CLA	CAA-CBA-CGA	3.91	124.67	113.25
11	A	905	BCL	O1D-CGD-CBD	-3.89	116.52	124.48
11	a	908	BCL	C3C-C4C-CHD	-3.89	115.08	123.39
11	A	908	BCL	CAA-CBA-CGA	-3.88	101.90	113.25
11	a	909	BCL	CMB-C2B-C3B	3.87	131.93	124.68
11	A	909	BCL	CMB-C2B-C3B	3.87	131.92	124.68
11	A	908	BCL	CHD-C4C-NC	3.86	129.36	125.08
12	a	901	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
12	a	912	CLA	C12-C11-C10	-3.85	95.56	113.24
10	A	901	2GO	C3D-C4D-ND	-3.85	104.57	116.21
12	A	931	CLA	CMB-C2B-C3B	3.83	131.85	124.68
12	a	915	CLA	C2D-C1D-ND	-3.83	107.28	110.10
11	a	907	BCL	C1-O2A-CGA	3.82	126.48	116.44
12	a	912	CLA	C1-C2-C3	-3.82	119.43	126.04
12	a	912	CLA	CHD-C1D-ND	-3.82	120.94	124.45
11	A	907	BCL	C3C-C4C-CHD	-3.82	115.24	123.39
11	a	910	BCL	CAA-C2A-C1A	3.82	124.48	111.97
12	a	913	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
13	c	201	LYC	C6-C7-C9	3.80	133.48	121.98
12	a	901	CLA	O1A-CGA-CBA	-3.80	108.91	123.73
11	A	904	BCL	O1A-CGA-CBA	-3.79	110.89	123.08
11	A	902	BCL	C11-C12-C13	3.78	128.12	115.92
11	a	911	BCL	O1A-CGA-CBA	-3.77	109.01	123.73
18	C	301	HEC	O2A-CGA-CBA	3.77	126.14	114.03
11	A	902	BCL	C14-C13-C12	3.76	124.92	111.29
12	a	912	CLA	C3D-C2D-C1D	-3.76	100.70	105.83
11	A	908	BCL	CAC-C3C-C4C	-3.75	104.26	112.58
11	a	907	BCL	CHB-C4A-NA	3.75	129.70	124.51
12	A	933	CLA	C1D-ND-C4D	-3.74	103.68	106.33
11	a	906	BCL	CAA-CBA-CGA	-3.72	102.63	112.51
12	a	914	CLA	C1D-ND-C4D	-3.71	103.70	106.33
11	A	907	BCL	CAA-CBA-CGA	3.71	124.09	113.25
11	A	904	BCL	O2A-CGA-CBA	3.71	125.95	114.03
11	a	907	BCL	CMB-C2B-C3B	3.70	131.60	124.68
12	a	913	CLA	O2A-CGA-O1A	-3.70	114.27	123.59
12	a	915	CLA	C1-O2A-CGA	3.69	126.12	116.44
11	A	907	BCL	C9-C8-C10	-3.69	97.94	111.29
10	A	901	2GO	C2C-C1C-NC	-3.68	104.28	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	A	910	CLA	C4D-CHA-C1A	-3.68	116.77	121.25
11	a	905	BCL	O2A-C1-C2	3.68	118.30	108.64
12	A	911	CLA	CED-O2D-CGD	3.67	124.24	115.94
11	a	908	BCL	C16-C17-C18	-3.67	98.71	115.98
11	A	902	BCL	C2A-C1A-CHA	-3.66	117.45	123.86
11	a	904	BCL	CMB-C2B-C3B	3.66	131.53	124.68
12	a	901	CLA	CAC-C3C-C2C	3.66	133.79	127.53
15	a	918	85I	O3-C3-C4	3.66	120.84	107.08
12	a	913	CLA	C9-C8-C7	3.65	124.50	111.29
12	A	911	CLA	C1-O2A-CGA	3.64	126.00	116.44
12	A	910	CLA	CGD-CBD-CAD	-3.62	98.99	110.73
11	A	902	BCL	CMA-C3A-C2A	-3.62	99.23	113.83
11	A	907	BCL	C5-C3-C2	3.61	128.43	121.12
12	a	912	CLA	CHD-C4C-C3C	-3.61	119.53	124.84
12	A	911	CLA	C2A-C1A-CHA	-3.61	117.55	123.86
12	a	914	CLA	C3D-C4D-ND	3.61	116.08	110.24
11	A	903	BCL	C6-C7-C8	3.61	127.58	115.92
12	A	933	CLA	CHB-C4A-NA	3.60	129.49	124.51
11	A	903	BCL	C3A-C2A-C1A	3.60	106.73	101.34
10	A	901	2GO	OBB-CAB-CBB	-3.60	112.07	120.17
12	A	933	CLA	C1-C2-C3	-3.60	119.82	126.04
11	a	909	BCL	C3C-C4C-CHD	-3.60	115.70	123.39
12	A	933	CLA	C3C-C4C-NC	3.57	114.58	110.57
11	A	902	BCL	C3A-C2A-C1A	3.57	106.69	101.34
11	a	906	BCL	C3D-CAD-CBD	3.55	112.28	107.61
11	a	905	BCL	CHB-C4A-NA	3.55	129.43	124.51
11	a	905	BCL	CBC-CAC-C3C	-3.54	105.58	113.47
11	A	903	BCL	C6-C5-C3	3.54	122.73	113.45
11	a	909	BCL	OBB-CAB-C3B	3.53	126.26	119.99
11	a	911	BCL	C3D-CAD-CBD	3.53	112.25	107.61
11	A	907	BCL	C9-C8-C7	3.52	124.03	111.29
11	a	911	BCL	C3C-C4C-CHD	-3.51	115.88	123.39
12	a	901	CLA	CED-O2D-CGD	3.51	123.88	115.94
10	a	903	2GO	O2D-CGD-CBD	3.50	118.16	111.80
12	A	910	CLA	C1-O2A-CGA	3.50	125.61	116.44
12	A	933	CLA	C6-C5-C3	-3.49	96.56	113.58
11	a	905	BCL	OBD-CAD-C3D	-3.48	122.20	127.98
12	a	912	CLA	C4-C3-C5	3.48	121.13	115.27
12	A	933	CLA	CBA-CAA-C2A	-3.47	103.62	113.86
12	A	912	CLA	C2A-C1A-CHA	-3.47	117.80	123.86
11	a	910	BCL	C4C-CHD-C1D	-3.47	120.76	125.88
12	a	912	CLA	C9-C8-C10	-3.46	98.76	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	909	BCL	CED-O2D-CGD	3.45	123.74	115.94
12	A	910	CLA	CHC-C1C-C2C	-3.45	117.19	126.72
11	A	905	BCL	CMB-C2B-C3B	3.45	131.13	124.68
12	a	901	CLA	C4-C3-C5	3.42	121.03	115.27
13	A	913	LYC	C64-C65-C66	-3.42	116.07	127.75
11	a	905	BCL	OBB-CAB-C3B	3.42	126.06	119.99
11	A	905	BCL	C2A-C3A-C4A	-3.42	96.35	101.87
12	a	912	CLA	C4A-NA-C1A	-3.41	105.17	106.71
11	a	910	BCL	C16-C15-C13	3.41	126.93	115.92
18	C	301	HEC	CMA-C3A-C2A	3.41	131.37	124.94
11	a	909	BCL	C1C-NC-C4C	-3.40	105.18	106.71
11	A	904	BCL	OBD-CAD-C3D	-3.39	122.35	127.98
11	A	909	BCL	C3D-CAD-CBD	-3.39	103.15	107.61
18	C	301	HEC	CMD-C2D-C3D	3.38	131.31	124.94
12	A	931	CLA	CHA-C4D-ND	3.37	139.56	132.50
11	a	907	BCL	C6-C7-C8	-3.37	105.02	115.92
12	A	931	CLA	O1A-CGA-CBA	-3.37	110.59	123.73
11	A	909	BCL	CMA-C3A-C4A	3.36	120.80	111.77
11	A	902	BCL	CAC-C3C-C4C	-3.36	105.13	112.58
11	A	903	BCL	CAC-C3C-C2C	3.35	122.63	114.26
11	a	910	BCL	C4B-CHC-C1C	3.35	136.74	130.12
11	a	906	BCL	O2D-CGD-CBD	3.35	117.22	111.27
18	c	202	HEC	O2D-CGD-CBD	3.34	124.76	114.03
13	A	913	LYC	C20-C21-C50	3.34	130.31	123.47
12	a	912	CLA	C4D-C3D-CAD	-3.33	104.17	108.10
12	A	931	CLA	C3B-C4B-NB	3.33	113.51	109.21
10	a	903	2GO	C3D-C4D-ND	-3.33	106.13	116.21
12	A	910	CLA	C2A-C1A-CHA	-3.33	118.04	123.86
12	a	914	CLA	CHB-C4A-NA	3.33	129.11	124.51
13	A	913	LYC	C16-C17-C19	3.32	124.03	118.94
11	a	911	BCL	CHD-C4C-NC	3.31	128.76	125.08
11	a	908	BCL	C9-C8-C10	-3.31	99.31	111.29
11	a	907	BCL	C7-C6-C5	-3.30	104.40	113.36
11	A	909	BCL	CHA-C1A-NA	-3.30	118.85	126.40
12	A	912	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
12	a	912	CLA	CHC-C1C-NC	-3.29	119.21	124.20
11	a	904	BCL	O1D-CGD-CBD	-3.28	117.77	124.48
12	a	915	CLA	CMA-C3A-C4A	3.28	120.59	111.77
11	A	902	BCL	C4C-CHD-C1D	-3.28	121.04	125.88
12	A	912	CLA	O2A-CGA-O1A	-3.27	112.88	123.14
12	A	931	CLA	C6-C7-C8	3.27	126.49	115.92
11	A	902	BCL	C4-C3-C2	-3.26	115.32	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	901	CLA	O1D-CGD-CBD	-3.26	117.82	124.48
11	A	905	BCL	C16-C15-C13	-3.25	105.40	115.92
13	A	913	LYC	C58-C56-C55	-3.23	113.98	118.94
12	a	915	CLA	C2A-C1A-CHA	-3.23	118.21	123.86
12	A	912	CLA	C1-O2A-CGA	3.22	126.73	116.11
10	a	903	2GO	OBB-CAB-CBB	-3.22	112.92	120.17
12	A	911	CLA	C2D-C1D-ND	3.22	112.47	110.10
11	A	902	BCL	C1-C2-C3	-3.21	120.49	126.04
18	c	202	HEC	CBD-CAD-C3D	-3.21	107.14	112.62
12	A	931	CLA	C11-C10-C8	3.19	126.23	115.92
12	a	912	CLA	CAA-CBA-CGA	-3.19	103.94	113.25
12	a	912	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
11	A	905	BCL	O2A-CGA-CBA	3.18	121.87	111.91
18	C	301	HEC	O2D-CGD-O1D	-3.17	115.39	123.30
13	A	913	LYC	C1-C2-C4	-3.17	113.49	122.65
12	a	914	CLA	CMD-C2D-C1D	3.17	130.29	124.71
11	a	907	BCL	OBB-CAB-C3B	-3.16	114.39	119.99
12	A	933	CLA	CMD-C2D-C1D	3.15	130.27	124.71
11	A	909	BCL	C3C-C4C-CHD	-3.15	116.67	123.39
11	a	909	BCL	O1D-CGD-CBD	-3.15	118.05	124.48
11	A	909	BCL	C10-C8-C7	3.14	128.67	112.13
11	a	905	BCL	C4-C3-C5	3.14	120.55	115.27
12	a	915	CLA	C4D-CHA-C1A	-3.14	117.43	121.25
11	A	906	BCL	CMC-C2C-C1C	3.13	120.19	111.77
11	A	903	BCL	CMB-C2B-C3B	3.13	130.53	124.68
12	a	901	CLA	CMB-C2B-C1B	3.13	133.27	128.46
11	a	910	BCL	C11-C12-C13	3.12	126.00	115.92
12	A	931	CLA	CHD-C1D-C2D	3.11	132.01	125.48
12	A	931	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
12	A	912	CLA	CMB-C2B-C3B	3.10	130.48	124.68
11	A	902	BCL	C3D-CAD-CBD	3.09	111.68	107.61
11	A	904	BCL	O2D-CGD-O1D	-3.09	117.80	123.84
12	a	913	CLA	C4A-NA-C1A	-3.07	105.32	106.71
12	a	901	CLA	C7-C6-C5	-3.05	105.07	113.36
11	a	907	BCL	CAD-C3D-C4D	-3.05	106.77	108.47
12	a	915	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
11	A	902	BCL	O1A-CGA-CBA	-3.04	111.88	123.73
11	a	905	BCL	C11-C12-C13	3.03	125.70	115.92
15	A	915	85I	O2-P-O	-3.03	93.69	107.75
13	A	913	LYC	C59-C58-C56	-3.02	117.93	126.42
11	A	909	BCL	OBD-CAD-C3D	3.00	132.96	127.98
11	a	909	BCL	CHC-C1C-NC	3.00	128.66	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	912	CLA	C17-C16-C15	-3.00	99.47	113.24
11	a	904	BCL	OBD-CAD-CBD	-2.99	121.62	125.89
10	a	903	2GO	CHA-CBD-CGD	-2.99	115.51	125.12
12	a	914	CLA	C3D-C2D-C1D	-2.98	101.76	105.83
12	a	915	CLA	CHC-C1C-NC	-2.98	119.68	124.20
11	A	909	BCL	C5-C3-C2	2.97	127.14	121.12
11	a	911	BCL	CMD-C2D-C3D	2.97	130.23	124.68
12	A	910	CLA	CMA-C3A-C4A	-2.97	103.80	111.77
11	a	908	BCL	C4C-CHD-C1D	-2.96	121.51	125.88
11	a	904	BCL	CAC-C3C-C2C	-2.95	106.88	114.26
11	a	904	BCL	C4C-CHD-C1D	-2.95	121.52	125.88
12	a	913	CLA	CAA-CBA-CGA	2.94	121.86	113.25
10	A	901	2GO	C4C-C3C-C2C	-2.94	102.61	106.90
13	c	201	LYC	C54-C55-C56	2.94	131.50	127.31
11	A	906	BCL	OBB-CAB-CBB	-2.93	113.57	120.17
12	A	912	CLA	CAA-C2A-C1A	2.92	121.55	111.97
12	a	901	CLA	C14-C13-C15	-2.92	100.71	111.29
11	a	905	BCL	CMA-C3A-C4A	2.91	119.60	111.77
11	A	907	BCL	O1D-CGD-CBD	-2.91	118.53	124.48
10	A	901	2GO	O2A-C1-C2	-2.91	101.00	108.64
11	A	904	BCL	CHD-C4C-NC	2.89	128.29	125.08
10	a	903	2GO	C3C-C4C-NC	2.89	115.94	110.14
11	A	904	BCL	CMA-C3A-C2A	-2.88	102.21	113.83
11	a	907	BCL	O1A-CGA-CBA	-2.87	112.53	123.73
15	a	919	85I	O4-C4-C3	2.87	116.91	109.54
11	a	905	BCL	O2A-CGA-O1A	-2.87	116.35	123.59
12	a	912	CLA	CMC-C2C-C1C	2.87	129.41	125.04
10	A	901	2GO	CHA-C1A-C2A	2.86	132.93	128.18
11	a	911	BCL	C3A-C2A-C1A	2.86	105.62	101.34
12	a	915	CLA	CHD-C4C-C3C	-2.86	120.64	124.84
10	A	901	2GO	CHA-CBD-CAD	-2.85	104.35	107.17
19	E	101	84Q	O7-P-O6	-2.85	97.92	109.07
11	A	908	BCL	OBB-CAB-C3B	-2.85	114.94	119.99
12	a	901	CLA	C6-C5-C3	2.84	120.91	113.45
11	a	907	BCL	CBB-CAB-C3B	2.83	128.75	120.34
11	A	903	BCL	CMC-C2C-C1C	2.83	119.39	111.77
10	A	901	2GO	CBB-CAB-C3B	2.83	128.73	120.34
11	a	904	BCL	CMC-C2C-C3C	-2.82	102.44	113.83
11	A	908	BCL	O2A-C1-C2	2.82	116.04	108.64
11	a	911	BCL	CMA-C3A-C4A	2.81	119.33	111.77
11	a	908	BCL	C4-C3-C5	-2.81	110.55	115.27
11	A	907	BCL	C6-C7-C8	2.81	124.99	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	903	2GO	CMC-C2C-C3C	-2.80	118.53	126.12
11	a	910	BCL	C3A-C2A-C1A	-2.79	97.16	101.34
10	a	903	2GO	O1D-CGD-CBD	-2.78	119.49	124.62
12	a	912	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
11	A	908	BCL	CED-O2D-CGD	2.77	122.20	115.94
12	A	933	CLA	C3D-C4D-ND	2.77	114.72	110.24
11	a	905	BCL	CMC-C2C-C1C	2.76	119.18	111.77
11	a	911	BCL	O2A-CGA-O1A	-2.76	116.64	123.59
11	A	903	BCL	CAA-C2A-C3A	2.75	120.31	112.78
12	a	915	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
12	A	912	CLA	CHC-C1C-NC	-2.74	120.04	124.20
12	a	912	CLA	C9-C8-C7	2.74	121.22	111.29
11	a	911	BCL	CAA-C2A-C1A	2.74	120.96	111.97
19	E	101	84Q	O4-P-O6	2.73	119.70	109.47
12	A	910	CLA	C10-C8-C7	2.73	126.47	112.13
12	a	914	CLA	C1D-CHD-C4C	-2.73	120.18	126.06
12	A	931	CLA	CMD-C2D-C1D	2.73	129.52	124.71
10	A	901	2GO	CAA-C2A-C1A	-2.73	120.55	128.29
12	a	913	CLA	CHA-C4D-ND	-2.72	126.80	132.50
11	a	908	BCL	C4-C3-C2	-2.72	116.69	123.68
11	a	909	BCL	CMA-C3A-C4A	2.72	119.09	111.77
12	a	901	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
11	a	910	BCL	C4-C3-C2	-2.72	116.69	123.68
11	a	907	BCL	C3D-CAD-CBD	2.72	111.18	107.61
12	a	913	CLA	C2C-C1C-NC	2.72	112.52	109.97
11	A	903	BCL	C1C-NC-C4C	-2.71	105.49	106.71
10	A	901	2GO	C1-C2-C3	2.70	130.71	126.04
13	A	913	LYC	C5-C4-C2	2.68	136.92	127.75
10	A	901	2GO	C3A-C4A-NA	-2.68	105.58	109.07
12	a	914	CLA	CHD-C1D-C2D	2.68	131.10	125.48
11	a	911	BCL	OBD-CAD-C3D	-2.68	123.54	127.98
12	A	910	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
11	a	910	BCL	CMB-C2B-C1B	2.67	132.57	128.46
11	a	911	BCL	C6-C5-C3	2.67	120.45	113.45
10	a	903	2GO	CMB-C2B-C1B	-2.66	124.37	128.46
11	A	902	BCL	C4-C3-C5	2.66	119.75	115.27
12	A	931	CLA	CHB-C4A-NA	2.66	128.19	124.51
12	a	914	CLA	CMA-C3A-C2A	-2.65	103.12	113.83
12	A	931	CLA	C16-C15-C13	-2.65	107.37	115.92
12	a	901	CLA	C1-C2-C3	-2.64	121.48	126.04
12	A	931	CLA	C11-C12-C13	-2.64	107.39	115.92
12	a	913	CLA	CMB-C2B-C3B	2.64	129.61	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	905	BCL	C1B-CHB-C4A	-2.63	124.90	130.12
11	A	908	BCL	CHB-C4A-NA	2.63	128.16	124.51
11	A	903	BCL	CBC-CAC-C3C	2.63	119.32	113.47
12	A	933	CLA	CHA-C4D-ND	-2.62	127.03	132.50
11	A	908	BCL	CMA-C3A-C2A	-2.61	103.29	113.83
12	A	933	CLA	C4D-C3D-CAD	-2.61	105.02	108.10
11	a	908	BCL	O2A-CGA-O1A	2.61	130.17	123.59
10	A	901	2GO	CHA-CBD-CGD	-2.60	116.76	125.12
11	a	908	BCL	C4B-C3B-CAB	2.60	132.15	127.13
12	a	915	CLA	C4D-C3D-CAD	-2.60	105.03	108.10
12	a	915	CLA	OBD-CAD-C3D	-2.60	122.27	128.52
11	A	907	BCL	C3D-CAD-CBD	2.60	111.02	107.61
12	A	911	CLA	CMB-C2B-C3B	2.59	129.52	124.68
15	A	915	85I	O-P-O1	-2.58	98.97	109.07
12	A	911	CLA	C3D-C4D-ND	2.58	114.42	110.24
12	A	910	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
11	A	908	BCL	OBB-CAB-CBB	2.58	125.98	120.17
11	A	909	BCL	CAC-C3C-C4C	-2.58	106.86	112.58
12	a	915	CLA	C2C-C1C-NC	2.58	112.39	109.97
11	A	905	BCL	C14-C13-C12	2.58	120.62	111.29
11	A	907	BCL	C15-C13-C14	-2.58	98.63	110.51
11	A	907	BCL	C2C-C3C-C4C	-2.57	97.49	101.34
13	c	201	LYC	C5-C6-C7	2.57	121.43	112.98
11	A	904	BCL	C4C-CHD-C1D	-2.57	122.09	125.88
11	A	906	BCL	CBC-CAC-C3C	2.56	119.17	113.47
11	A	909	BCL	C15-C13-C12	2.56	125.60	112.13
11	A	908	BCL	C7-C6-C5	-2.56	106.40	113.36
12	A	910	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
12	a	912	CLA	CMD-C2D-C3D	-2.56	121.74	127.61
12	A	912	CLA	C3A-C2A-C1A	-2.55	97.52	101.34
11	a	910	BCL	CBA-CAA-C2A	2.54	121.37	113.86
11	A	907	BCL	OBB-CAB-CBB	-2.54	114.45	120.17
12	A	910	CLA	C6-C5-C3	-2.54	106.79	113.45
11	A	902	BCL	C9-C8-C7	-2.54	102.09	111.29
11	A	903	BCL	C2A-C1A-CHA	-2.54	119.42	123.86
11	A	906	BCL	C4-C3-C5	2.54	118.88	115.98
12	a	912	CLA	O1D-CGD-CBD	2.53	129.66	124.48
11	A	908	BCL	C4C-CHD-C1D	-2.53	122.15	125.88
11	a	904	BCL	O2A-C1-C2	2.53	115.28	108.64
11	a	910	BCL	C3C-C4C-CHD	-2.52	118.00	123.39
11	a	909	BCL	C4-C3-C5	2.52	119.51	115.27
11	A	904	BCL	CAA-C2A-C1A	-2.51	103.76	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	913	CLA	C9-C8-C10	-2.51	102.21	111.29
11	A	906	BCL	CBA-CAA-C2A	2.51	121.26	113.86
11	a	908	BCL	CAC-C3C-C2C	-2.50	108.00	114.26
13	A	913	LYC	C18-C17-C16	2.50	122.01	118.08
11	A	906	BCL	CHD-C4C-NC	2.49	127.84	125.08
12	A	911	CLA	C1-C2-C3	-2.49	121.74	126.04
12	A	911	CLA	C6-C5-C3	2.49	119.98	113.45
10	a	903	2GO	C15-C13-C12	-2.48	99.06	112.13
18	c	202	HEC	CMA-C3A-C2A	2.47	129.60	124.94
19	E	101	84Q	C19-C18-C17	2.47	122.61	113.62
12	A	931	CLA	OBD-CAD-C3D	-2.47	122.57	128.52
11	A	907	BCL	C11-C10-C8	2.46	123.86	115.92
12	A	911	CLA	CHB-C4A-NA	2.45	127.90	124.51
12	A	912	CLA	CHD-C4C-NC	-2.45	120.34	124.20
11	a	906	BCL	CBC-CAC-C3C	2.44	118.91	113.47
11	a	911	BCL	C16-C15-C13	2.44	123.82	115.92
10	a	903	2GO	CAC-C3C-C2C	-2.44	123.35	127.53
11	a	911	BCL	C4-C3-C2	2.44	129.94	123.68
11	A	904	BCL	CAD-C3D-C4D	-2.44	107.11	108.47
11	a	908	BCL	C16-C15-C13	-2.44	108.04	115.92
18	C	301	HEC	CBD-CAD-C3D	-2.43	108.47	112.62
12	a	915	CLA	CAA-CBA-CGA	2.43	120.36	113.25
11	a	905	BCL	C4C-CHD-C1D	-2.43	122.30	125.88
12	a	913	CLA	CMA-C3A-C4A	2.43	118.30	111.77
11	A	906	BCL	C3C-C4C-CHD	-2.43	118.21	123.39
13	A	913	LYC	C20-C19-C17	-2.42	123.86	127.31
15	A	917	85I	O3-C3-C4	2.41	116.16	107.08
11	A	908	BCL	O1A-CGA-CBA	-2.41	114.33	123.73
11	A	908	BCL	C1-O2A-CGA	2.40	122.75	116.44
19	E	101	84Q	O5-P-O4	-2.40	97.31	106.78
12	A	931	CLA	C9-C8-C10	2.39	119.96	111.29
13	c	201	LYC	C62-C61-C60	-2.39	116.42	122.59
11	a	904	BCL	C6-C5-C3	2.39	119.73	113.45
12	A	910	CLA	CMC-C2C-C3C	2.39	132.61	126.12
11	a	911	BCL	C4-C3-C5	-2.39	111.25	115.27
11	A	909	BCL	CBA-CAA-C2A	2.38	120.89	113.86
15	A	916	85I	O2-P-O3	2.37	116.14	106.78
12	a	913	CLA	CHC-C1C-NC	-2.37	120.61	124.20
11	A	904	BCL	C2A-C1A-CHA	-2.37	119.72	123.86
11	a	910	BCL	CAC-C3C-C2C	2.36	120.17	114.26
12	A	931	CLA	CHD-C1D-ND	-2.36	122.29	124.45
11	A	909	BCL	CAC-C3C-C2C	2.36	120.15	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	a	901	CLA	CBA-CAA-C2A	2.35	120.80	113.86
12	a	901	CLA	C3B-C4B-NB	2.34	112.24	109.21
11	A	909	BCL	C4B-C3B-CAB	-2.34	122.60	127.13
12	A	933	CLA	C5-C3-C2	-2.34	114.71	120.50
17	A	932	85N	O5-C24-C19	-2.34	117.20	122.93
13	A	913	LYC	C55-C54-C53	-2.33	115.93	123.22
13	c	201	LYC	C59-C58-C56	-2.33	119.86	126.42
15	A	915	85I	O6-C20-C21	2.33	116.53	111.50
11	a	910	BCL	CMC-C2C-C1C	2.33	118.04	111.77
12	A	931	CLA	CAA-C2A-C3A	2.33	119.16	112.78
11	A	909	BCL	C11-C12-C13	2.33	123.45	115.92
12	a	914	CLA	O1A-CGA-CBA	-2.33	114.64	123.73
12	a	915	CLA	CHD-C1D-ND	-2.33	122.31	124.45
12	a	914	CLA	O2A-CGA-O1A	-2.33	115.85	123.14
11	A	905	BCL	CHB-C4A-NA	2.32	127.72	124.51
11	a	910	BCL	CAA-CBA-CGA	2.32	120.02	113.25
10	A	901	2GO	C4B-C3B-CAB	-2.32	122.66	127.13
11	a	908	BCL	C11-C10-C8	-2.31	108.44	115.92
12	a	901	CLA	O2A-C1-C2	-2.31	102.57	108.64
11	a	905	BCL	C6-C5-C3	2.29	119.47	113.45
12	a	912	CLA	C7-C6-C5	2.29	119.58	113.36
12	A	911	CLA	CMA-C3A-C4A	2.29	117.93	111.77
12	a	915	CLA	CBA-CAA-C2A	-2.28	107.12	113.86
15	A	916	85I	C7-C6-C5	-2.28	105.34	113.62
12	A	910	CLA	C1D-CHD-C4C	-2.28	121.15	126.06
11	a	906	BCL	CMC-C2C-C1C	2.27	117.89	111.77
12	a	913	CLA	C4-C3-C2	-2.27	117.85	123.68
17	G	101	85N	O2-C16-C17	-2.27	103.72	109.54
12	a	915	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
11	A	907	BCL	C11-C12-C13	2.26	126.62	115.98
11	A	905	BCL	C9-C8-C10	-2.25	103.14	111.29
11	A	902	BCL	C1B-CHB-C4A	2.25	134.56	130.12
11	A	906	BCL	OBD-CAD-CBD	-2.24	122.69	125.89
11	A	904	BCL	CAC-C3C-C4C	-2.23	107.63	112.58
11	a	911	BCL	CBB-CAB-C3B	2.23	126.95	120.34
11	A	907	BCL	OBD-CAD-CBD	-2.22	122.72	125.89
12	a	912	CLA	C5-C3-C2	2.22	125.62	121.12
12	a	913	CLA	CBC-CAC-C3C	2.22	118.56	112.43
12	a	914	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
11	a	906	BCL	O2A-CGA-CBA	2.21	121.14	114.03
11	a	910	BCL	O1A-CGA-CBA	-2.21	115.11	123.73
11	A	905	BCL	O1A-CGA-CBA	-2.21	115.12	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	918	85I	O6-C3-C4	2.20	115.36	107.08
12	a	915	CLA	C4-C3-C2	-2.20	118.03	123.68
11	a	906	BCL	OBB-CAB-C3B	2.20	123.90	119.99
11	A	907	BCL	CMA-C3A-C4A	2.20	117.68	111.77
12	A	933	CLA	O2A-CGA-CBA	2.19	118.79	111.91
12	a	901	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
11	a	910	BCL	C4-C3-C5	-2.19	111.59	115.27
12	A	931	CLA	C3C-C4C-NC	2.18	113.02	110.57
12	A	912	CLA	CMB-C2B-C1B	2.18	131.82	128.46
11	A	907	BCL	CBA-CAA-C2A	2.17	120.28	113.86
10	a	903	2GO	C1C-C2C-C3C	-2.17	104.68	106.96
11	A	904	BCL	C1B-CHB-C4A	-2.17	125.82	130.12
12	A	933	CLA	CHD-C4C-C3C	-2.17	121.66	124.84
11	a	909	BCL	C9-C8-C7	2.16	119.13	111.29
11	a	904	BCL	C3D-CAD-CBD	2.16	110.45	107.61
12	A	912	CLA	O2A-CGA-CBA	2.16	120.77	112.23
12	a	912	CLA	C6-C5-C3	2.16	119.11	113.45
12	A	933	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
13	c	201	LYC	C63-C61-C60	2.15	128.49	121.98
17	G	101	85N	O3-C17-O6	2.15	116.76	110.72
11	a	908	BCL	CHA-C1A-NA	2.15	131.32	126.40
11	A	909	BCL	CMD-C2D-C3D	2.15	128.70	124.68
11	a	904	BCL	C4-C3-C2	-2.15	118.17	123.68
12	A	931	CLA	C5-C3-C2	-2.14	116.78	121.12
12	a	914	CLA	C4D-CHA-C1A	2.14	123.85	121.25
11	a	907	BCL	O2A-C1-C2	-2.13	103.03	108.64
11	A	906	BCL	CAC-C3C-C4C	2.13	117.31	112.58
15	A	916	85I	O3-C3-C4	2.12	115.07	107.08
11	A	909	BCL	OBD-CAD-CBD	-2.11	122.88	125.89
12	a	912	CLA	C2D-C1D-ND	-2.10	108.56	110.10
11	a	910	BCL	C20-C18-C17	2.10	124.52	111.54
12	a	913	CLA	C2A-C3A-C4A	-2.10	98.48	101.87
13	A	913	LYC	C15-C14-C12	-2.09	124.32	127.31
11	a	906	BCL	CMB-C2B-C3B	2.09	128.59	124.68
10	a	903	2GO	CMD-C2D-C3D	2.09	128.59	124.68
11	a	911	BCL	C15-C13-C12	-2.09	101.15	112.13
11	A	909	BCL	CBB-CAB-C3B	2.09	126.53	120.34
11	a	910	BCL	C14-C13-C15	2.08	118.84	111.29
11	A	907	BCL	C4B-C3B-CAB	2.08	131.14	127.13
12	A	910	CLA	CBA-CAA-C2A	2.08	120.01	113.86
10	a	903	2GO	C6-C7-C8	2.06	122.58	115.92
11	a	906	BCL	CHD-C4C-NC	2.06	127.36	125.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	301	HEC	CAA-C2A-C3A	-2.05	121.35	127.25
11	a	906	BCL	CAC-C3C-C2C	2.05	119.39	114.26
18	C	301	HEC	CAD-C3D-C2D	-2.05	121.36	127.25
11	a	908	BCL	C1-O2A-CGA	-2.04	111.09	116.44
12	A	931	CLA	CMC-C2C-C3C	-2.04	120.58	126.12
12	A	910	CLA	CMB-C2B-C3B	2.04	128.49	124.68
12	a	914	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
12	A	933	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
11	A	909	BCL	C12-C11-C10	2.03	122.56	113.24
10	a	903	2GO	CAA-C2A-C1A	-2.03	122.53	128.29
13	A	913	LYC	C57-C56-C58	-2.03	114.89	118.08
12	A	910	CLA	CAC-C3C-C2C	2.02	130.98	127.53
11	A	904	BCL	C2C-C3C-C4C	-2.02	98.32	101.34
10	A	901	2GO	CAD-C3D-C4D	2.02	109.59	108.47
11	a	906	BCL	O1D-CGD-CBD	2.02	128.61	124.48
11	A	903	BCL	C12-C11-C10	-2.01	103.99	113.24
13	A	913	LYC	C3-C2-C1	2.01	119.05	114.60
12	a	915	CLA	C1-C2-C3	-2.01	122.56	126.04
11	a	911	BCL	CAA-C2A-C3A	2.01	118.28	112.78
11	A	905	BCL	C12-C11-C10	2.01	122.47	113.24
11	A	907	BCL	CAC-C3C-C4C	-2.01	108.13	112.58
12	A	933	CLA	CMD-C2D-C3D	2.01	132.23	127.61
11	a	911	BCL	C4B-C3B-CAB	2.01	131.00	127.13
12	A	911	CLA	C15-C13-C12	2.01	122.69	112.13
11	A	902	BCL	C6-C5-C3	2.00	118.71	113.45
12	a	913	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
12	A	912	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
11	A	905	BCL	CMC-C2C-C3C	-2.00	105.76	113.83
15	A	916	85I	O6-C20-C21	2.00	115.81	111.50

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	910	CLA	C8
12	A	911	CLA	C8
15	A	916	85I	C3

All (646) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	a	903	2GO	C1A-C2A-CAA-CBA
11	A	902	BCL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	A	902	BCL	C11-C12-C13-C14
11	A	903	BCL	C1A-C2A-CAA-CBA
11	A	903	BCL	C2-C3-C5-C6
11	A	903	BCL	C4-C3-C5-C6
11	A	904	BCL	C1A-C2A-CAA-CBA
11	A	904	BCL	CHA-CBD-CGD-O1D
11	A	905	BCL	C1A-C2A-CAA-CBA
11	A	905	BCL	CBA-CGA-O2A-C1
11	A	905	BCL	O1A-CGA-O2A-C1
11	A	905	BCL	CBD-CGD-O2D-CED
11	A	905	BCL	C2-C3-C5-C6
11	A	905	BCL	C4-C3-C5-C6
11	A	906	BCL	CBD-CGD-O2D-CED
11	A	906	BCL	O1D-CGD-O2D-CED
11	A	907	BCL	C2C-C3C-CAC-CBC
11	A	907	BCL	C4C-C3C-CAC-CBC
11	A	907	BCL	CBD-CGD-O2D-CED
11	A	907	BCL	C2-C3-C5-C6
11	A	907	BCL	C4-C3-C5-C6
11	a	904	BCL	C4C-C3C-CAC-CBC
11	a	904	BCL	CBD-CGD-O2D-CED
11	a	905	BCL	C1A-C2A-CAA-CBA
11	a	905	BCL	C3A-C2A-CAA-CBA
11	a	906	BCL	C1A-C2A-CAA-CBA
11	a	907	BCL	C2A-CAA-CBA-CGA
11	a	908	BCL	C1A-C2A-CAA-CBA
11	a	908	BCL	CBD-CGD-O2D-CED
11	a	908	BCL	C2-C3-C5-C6
11	a	908	BCL	C4-C3-C5-C6
11	a	911	BCL	C1A-C2A-CAA-CBA
11	a	911	BCL	C3A-C2A-CAA-CBA
12	A	910	CLA	C2-C3-C5-C6
12	A	910	CLA	C4-C3-C5-C6
12	A	933	CLA	CHA-CBD-CGD-O2D
12	a	912	CLA	CBD-CGD-O2D-CED
12	a	913	CLA	CBD-CGD-O2D-CED
12	a	913	CLA	C6-C7-C8-C9
12	a	915	CLA	C2-C3-C5-C6
12	a	915	CLA	C4-C3-C5-C6
13	c	201	LYC	C4-C5-C6-C7
13	c	201	LYC	C5-C6-C7-C8
13	c	201	LYC	C5-C6-C7-C9

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Mol	Chain	Res	Type	Atoms
13	c	201	LYC	C57-C56-C58-C59
15	A	915	85I	C4-C3-O3-P
15	A	915	85I	O7-C20-O6-C3
15	A	915	85I	C21-C20-O6-C3
15	A	916	85I	N-C1-C2-O
15	A	916	85I	O6-C3-C4-O4
15	A	916	85I	C4-C3-O3-P
15	A	916	85I	C4-C3-O6-C20
15	A	916	85I	O3-C3-O6-C20
15	A	916	85I	O7-C20-O6-C3
15	A	917	85I	C4-C3-O6-C20
15	A	917	85I	C2-O-P-O3
15	A	917	85I	O7-C20-O6-C3
15	a	918	85I	O3-C3-C4-O4
15	a	918	85I	O6-C3-C4-O4
15	a	918	85I	C4-C3-O6-C20
15	a	918	85I	O7-C20-O6-C3
15	a	919	85I	O6-C3-C4-O4
15	a	919	85I	C4-C3-O3-P
15	a	919	85I	O3-C3-O6-C20
15	a	919	85I	C6-C5-O4-C4
15	a	919	85I	C2-O-P-O1
15	a	920	85I	C2-C1-N-C
15	a	920	85I	O3-C3-C4-O4
15	a	920	85I	O6-C3-C4-O4
15	a	920	85I	C4-C3-O6-C20
15	a	920	85I	C2-O-P-O1
15	a	920	85I	C2-O-P-O2
15	a	920	85I	C2-O-P-O3
15	a	920	85I	O7-C20-O6-C3
17	A	932	85N	O3-C17-O6-C25
17	A	932	85N	O2-C16-C17-O6
17	A	932	85N	C16-C17-O3-C18
17	A	932	85N	C20-C19-C24-O4
17	A	932	85N	C20-C19-C24-O5
17	G	101	85N	C19-C20-N1-C21
17	G	101	85N	C19-C20-N1-C22
17	G	101	85N	C19-C20-N1-C23
17	G	101	85N	O3-C18-C19-C20
17	G	101	85N	O3-C18-C19-C24
17	G	101	85N	C20-C19-C24-O4
17	G	101	85N	C20-C19-C24-O5

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Mol	Chain	Res	Type	Atoms
17	a	902	85N	O7-C25-O6-C17
17	a	902	85N	C26-C25-O6-C17
17	a	902	85N	O2-C16-C17-O3
17	g	101	85N	C16-C17-O6-C25
17	g	101	85N	O7-C25-O6-C17
17	g	101	85N	O2-C16-C17-O6
19	E	101	84Q	O3-C17-O2-C16
19	E	101	84Q	O7-C32-C33-N
19	E	101	84Q	O1-C15-C16-O2
19	E	101	84Q	O1-C15-C16-O4
19	a	921	84Q	O4-C16-O2-C17
19	a	921	84Q	O3-C17-O2-C16
19	a	921	84Q	C32-O7-P-O6
19	a	921	84Q	C32-O7-P-O5
19	a	921	84Q	C32-O7-P-O4
19	a	921	84Q	C16-O4-P-O7
19	a	921	84Q	C15-C16-O4-P
19	a	921	84Q	O1-C15-C16-O4
11	a	904	BCL	O1D-CGD-O2D-CED
11	A	902	BCL	O1D-CGD-O2D-CED
11	A	905	BCL	O1D-CGD-O2D-CED
11	a	909	BCL	O1D-CGD-O2D-CED
11	A	902	BCL	CBD-CGD-O2D-CED
11	A	903	BCL	CBD-CGD-O2D-CED
11	a	905	BCL	CBD-CGD-O2D-CED
11	a	909	BCL	CBD-CGD-O2D-CED
12	A	910	CLA	CBD-CGD-O2D-CED
11	A	907	BCL	O1A-CGA-O2A-C1
11	a	907	BCL	O1A-CGA-O2A-C1
11	a	911	BCL	O1A-CGA-O2A-C1
15	a	919	85I	O5-C5-O4-C4
11	A	903	BCL	O1D-CGD-O2D-CED
11	A	907	BCL	O1D-CGD-O2D-CED
12	a	913	CLA	O1D-CGD-O2D-CED
12	A	911	CLA	C3-C5-C6-C7
12	a	913	CLA	C3-C5-C6-C7
11	A	907	BCL	CBA-CGA-O2A-C1
11	a	907	BCL	CBA-CGA-O2A-C1
10	a	903	2GO	C4C-C3C-CAC-CBC
11	a	908	BCL	O1A-CGA-O2A-C1
11	a	908	BCL	O1D-CGD-O2D-CED
12	a	901	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	A	910	CLA	C3-C5-C6-C7
11	a	908	BCL	CBA-CGA-O2A-C1
11	a	911	BCL	CBA-CGA-O2A-C1
12	A	911	CLA	CBD-CGD-O2D-CED
11	A	903	BCL	C2A-CAA-CBA-CGA
11	a	910	BCL	C2A-CAA-CBA-CGA
12	a	912	CLA	C2A-CAA-CBA-CGA
11	a	905	BCL	O1D-CGD-O2D-CED
12	a	912	CLA	O1D-CGD-O2D-CED
11	a	909	BCL	C3-C5-C6-C7
17	g	101	85N	C14-C15-O2-C16
10	A	901	2GO	C1A-C2A-CAA-CBA
10	A	901	2GO	C4C-C3C-CAC-CBC
12	A	910	CLA	O1D-CGD-O2D-CED
15	A	917	85I	O5-C5-O4-C4
17	G	101	85N	O1-C15-O2-C16
17	a	902	85N	C11-C10-C9-C8
11	A	909	BCL	CBD-CGD-O2D-CED
12	a	914	CLA	CBD-CGD-O2D-CED
12	a	915	CLA	CBD-CGD-O2D-CED
17	G	101	85N	C14-C15-O2-C16
15	a	918	85I	C21-C20-O6-C3
12	a	914	CLA	CBA-CGA-O2A-C1
15	A	915	85I	C12-C13-C14-C15
15	A	917	85I	C7-C8-C9-C10
15	A	917	85I	C25-C26-C27-C28
15	A	917	85I	C10-C11-C12-C13
15	A	917	85I	C6-C5-O4-C4
17	g	101	85N	O1-C15-O2-C16
11	A	902	BCL	C4-C3-C5-C6
11	A	902	BCL	C2-C3-C5-C6
12	a	901	CLA	C2A-CAA-CBA-CGA
11	A	902	BCL	CBA-CGA-O2A-C1
19	E	101	84Q	C13-C14-O1-C15
19	a	921	84Q	C13-C14-O1-C15
12	a	914	CLA	O1A-CGA-O2A-C1
15	A	917	85I	C3-O3-P-O
19	E	101	84Q	C16-O4-P-O7
12	A	910	CLA	C13-C15-C16-C17
19	a	921	84Q	C1-C3-C4-C5
19	a	921	84Q	C11-C12-C13-C14
19	E	101	84Q	O-C14-O1-C15

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Mol	Chain	Res	Type	Atoms
19	a	921	84Q	O-C14-O1-C15
11	A	903	BCL	C11-C10-C8-C9
11	A	903	BCL	C14-C13-C15-C16
11	A	907	BCL	C11-C10-C8-C9
11	A	908	BCL	C11-C10-C8-C9
11	a	908	BCL	C14-C13-C15-C16
11	a	910	BCL	C14-C13-C15-C16
12	A	911	CLA	C6-C7-C8-C9
12	A	931	CLA	C6-C7-C8-C9
12	a	901	CLA	C6-C7-C8-C9
13	c	201	LYC	C15-C16-C17-C19
13	c	201	LYC	C55-C56-C58-C59
11	a	908	BCL	C5-C6-C7-C8
12	a	901	CLA	C15-C16-C17-C18
11	a	905	BCL	C15-C16-C17-C18
11	a	909	BCL	C15-C16-C17-C18
15	a	919	85I	C14-C15-C16-C17
17	A	932	85N	C34-C35-C36-C37
17	a	902	85N	C25-C26-C27-C28
15	a	918	85I	C2-C1-N-C
12	A	910	CLA	C8-C10-C11-C12
11	A	909	BCL	C2-C1-O2A-CGA
11	a	907	BCL	C5-C6-C7-C8
11	a	909	BCL	C10-C11-C12-C13
19	E	101	84Q	C18-C17-O2-C16
12	A	911	CLA	C15-C16-C17-C18
11	A	909	BCL	C6-C7-C8-C10
11	a	907	BCL	C11-C12-C13-C15
12	A	910	CLA	C6-C7-C8-C10
12	A	931	CLA	C11-C12-C13-C15
11	A	909	BCL	C3-C5-C6-C7
15	A	915	85I	O5-C5-O4-C4
11	A	905	BCL	C2A-CAA-CBA-CGA
12	A	910	CLA	C5-C6-C7-C8
15	A	917	85I	C29-C30-C31-C32
15	a	920	85I	C29-C30-C31-C32
13	A	913	LYC	C4-C5-C6-C7
11	A	902	BCL	C13-C15-C16-C17
11	a	907	BCL	C10-C11-C12-C13
11	a	909	BCL	C5-C6-C7-C8
12	a	912	CLA	C8-C10-C11-C12
12	A	931	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	a	901	CLA	C5-C6-C7-C8
10	a	903	2GO	C15-C16-C17-C18
12	A	931	CLA	C8-C10-C11-C12
12	A	931	CLA	C13-C15-C16-C17
12	a	901	CLA	C13-C15-C16-C17
15	a	920	85I	C14-C15-C16-C17
15	a	919	85I	C2-O-P-O3
15	A	915	85I	C6-C5-O4-C4
10	a	903	2GO	C13-C15-C16-C17
11	A	905	BCL	C10-C11-C12-C13
12	A	931	CLA	C15-C16-C17-C18
11	A	908	BCL	C2A-CAA-CBA-CGA
12	A	931	CLA	C2A-CAA-CBA-CGA
15	a	919	85I	C15-C16-C17-C19
11	a	905	BCL	C13-C15-C16-C17
15	A	917	85I	C11-C10-C9-C8
17	A	932	85N	C31-C32-C33-C34
19	E	101	84Q	C7-C8-C9-C10
19	a	921	84Q	C9-C10-C11-C12
12	A	931	CLA	C16-C17-C18-C20
17	a	902	85N	C1-C2-C4-C5
15	a	919	85I	C6-C7-C8-C9
15	a	919	85I	C12-C13-C14-C15
15	a	920	85I	C11-C12-C13-C14
17	A	932	85N	C27-C28-C29-C30
19	a	921	84Q	C4-C5-C6-C7
15	a	919	85I	C21-C22-C23-C24
15	A	916	85I	C25-C26-C27-C28
15	a	920	85I	C9-C10-C11-C12
15	A	915	85I	C22-C23-C24-C25
15	A	916	85I	C22-C23-C24-C25
15	a	918	85I	C26-C27-C28-C29
15	a	920	85I	C20-C21-C22-C23
19	E	101	84Q	C17-C18-C19-C20
11	a	909	BCL	C1-C2-C3-C5
15	a	919	85I	C9-C10-C11-C12
11	A	902	BCL	O1A-CGA-O2A-C1
11	A	903	BCL	C16-C17-C18-C20
15	A	917	85I	C30-C31-C32-C34
15	A	915	85I	C10-C11-C12-C13
15	a	919	85I	C11-C10-C9-C8
17	G	101	85N	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
17	a	902	85N	C26-C27-C28-C29
17	g	101	85N	C5-C6-C7-C8
11	A	909	BCL	C11-C10-C8-C9
12	A	911	CLA	O1D-CGD-O2D-CED
15	A	915	85I	C26-C27-C28-C29
15	A	917	85I	C26-C27-C28-C29
17	a	902	85N	C7-C8-C9-C10
19	a	921	84Q	C19-C20-C21-C22
13	c	201	LYC	C15-C16-C17-C18
15	A	916	85I	C27-C28-C29-C30
11	a	908	BCL	C3-C5-C6-C7
15	a	918	85I	C21-C22-C23-C24
15	a	919	85I	C22-C23-C24-C25
17	a	902	85N	C5-C6-C7-C8
15	A	916	85I	C7-C8-C9-C10
15	a	918	85I	C22-C23-C24-C25
15	a	920	85I	C7-C8-C9-C10
17	G	101	85N	C26-C27-C28-C29
19	E	101	84Q	C10-C11-C12-C13
11	a	910	BCL	C16-C17-C18-C19
12	A	931	CLA	C16-C17-C18-C19
19	E	101	84Q	C-C1-C3-C4
12	a	913	CLA	C15-C16-C17-C18
15	A	917	85I	C12-C13-C14-C15
15	a	919	85I	C25-C26-C27-C28
15	a	919	85I	C13-C14-C15-C16
17	a	902	85N	C11-C12-C13-C14
17	g	101	85N	C11-C12-C13-C14
15	A	917	85I	C20-C21-C22-C23
11	a	910	BCL	C10-C11-C12-C13
12	A	931	CLA	C5-C6-C7-C8
15	a	920	85I	C25-C26-C27-C28
17	g	101	85N	C27-C28-C29-C30
19	E	101	84Q	C19-C20-C21-C22
11	a	909	BCL	CBA-CGA-O2A-C1
15	a	919	85I	C10-C11-C12-C13
11	A	904	BCL	C3A-C2A-CAA-CBA
11	A	905	BCL	C3A-C2A-CAA-CBA
11	A	909	BCL	C3A-C2A-CAA-CBA
11	a	906	BCL	C3A-C2A-CAA-CBA
11	a	908	BCL	C3A-C2A-CAA-CBA
12	a	901	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	c	201	LYC	C17-C19-C20-C21
15	a	919	85I	C7-C8-C9-C10
17	a	902	85N	C10-C11-C12-C13
11	a	910	BCL	C16-C17-C18-C20
15	A	916	85I	C30-C31-C32-C33
15	A	917	85I	C15-C16-C17-C19
19	E	101	84Q	C2-C1-C3-C4
15	A	916	85I	C24-C25-C26-C27
15	A	916	85I	C13-C14-C15-C16
15	a	919	85I	C11-C12-C13-C14
19	E	101	84Q	C20-C21-C22-C23
15	A	916	85I	C20-C21-C22-C23
17	a	902	85N	C12-C13-C14-C15
12	A	931	CLA	C4-C3-C5-C6
17	g	101	85N	C26-C27-C28-C29
15	A	916	85I	C11-C10-C9-C8
19	a	921	84Q	C3-C4-C5-C6
12	a	901	CLA	O1D-CGD-O2D-CED
15	a	919	85I	C30-C31-C32-C34
17	a	902	85N	C28-C29-C30-C31
15	A	917	85I	C22-C23-C24-C25
19	a	921	84Q	C6-C7-C8-C9
15	A	916	85I	C12-C13-C14-C15
19	a	921	84Q	C25-C26-C27-C28
15	A	916	85I	C21-C20-O6-C3
15	A	917	85I	C28-C29-C30-C31
12	a	901	CLA	C8-C10-C11-C12
15	A	916	85I	C5-C6-C7-C8
15	a	920	85I	C26-C27-C28-C29
11	A	909	BCL	C11-C10-C8-C7
12	A	911	CLA	C11-C12-C13-C15
12	A	931	CLA	C11-C10-C8-C7
11	a	908	BCL	C13-C15-C16-C17
11	A	903	BCL	C16-C17-C18-C19
15	A	917	85I	C30-C31-C32-C33
15	a	918	85I	C20-C21-C22-C23
11	a	904	BCL	C2A-CAA-CBA-CGA
15	A	917	85I	C21-C22-C23-C24
17	a	902	85N	C17-C16-O2-C15
19	E	101	84Q	C11-C12-C13-C14
19	a	921	84Q	C5-C6-C7-C8
15	a	920	85I	C21-C20-O6-C3

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Mol	Chain	Res	Type	Atoms
17	g	101	85N	C26-C25-O6-C17
11	a	904	BCL	CBA-CGA-O2A-C1
15	A	917	85I	C5-C6-C7-C8
15	a	918	85I	C5-C6-C7-C8
15	A	915	85I	C7-C8-C9-C10
15	a	920	85I	C21-C22-C23-C24
17	a	902	85N	C29-C30-C31-C32
19	E	101	84Q	C3-C4-C5-C6
17	G	101	85N	C1-C2-C4-C5
17	a	902	85N	C3-C2-C4-C5
11	A	903	BCL	C10-C11-C12-C13
11	A	908	BCL	C8-C10-C11-C12
11	a	907	BCL	C11-C12-C13-C14
12	A	912	CLA	CBD-CGD-O2D-CED
19	a	921	84Q	C23-C24-C25-C26
17	A	932	85N	C29-C30-C31-C32
10	a	903	2GO	C2C-C3C-CAC-CBC
11	A	902	BCL	C1A-C2A-CAA-CBA
11	A	908	BCL	C1A-C2A-CAA-CBA
11	A	909	BCL	C1A-C2A-CAA-CBA
11	a	910	BCL	C1A-C2A-CAA-CBA
15	a	919	85I	C30-C31-C32-C33
15	a	920	85I	C30-C31-C32-C33
17	a	902	85N	C30-C31-C32-C33
11	A	905	BCL	C5-C6-C7-C8
12	a	914	CLA	O1D-CGD-O2D-CED
11	A	909	BCL	C15-C16-C17-C18
19	E	101	84Q	C16-C15-O1-C14
15	A	917	85I	C15-C16-C17-C18
11	A	908	BCL	C3-C5-C6-C7
15	A	917	85I	C6-C7-C8-C9
19	a	921	84Q	C10-C11-C12-C13
12	a	901	CLA	CBA-CGA-O2A-C1
11	a	904	BCL	C2C-C3C-CAC-CBC
17	G	101	85N	C7-C8-C9-C10
12	a	912	CLA	C13-C15-C16-C17
15	a	919	85I	C23-C24-C25-C26
11	a	909	BCL	O1A-CGA-O2A-C1
15	a	918	85I	C30-C31-C32-C34
15	A	916	85I	C6-C7-C8-C9
12	A	933	CLA	O1D-CGD-O2D-CED
11	A	909	BCL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
12	a	913	CLA	C16-C17-C18-C19
19	a	921	84Q	C18-C17-O2-C16
15	a	919	85I	C28-C29-C30-C31
17	G	101	85N	C11-C12-C13-C14
19	E	101	84Q	C22-C23-C24-C25
12	A	912	CLA	O1D-CGD-O2D-CED
11	a	908	BCL	C15-C16-C17-C18
15	A	916	85I	C14-C15-C16-C17
11	A	905	BCL	C2-C1-O2A-CGA
15	A	915	85I	C25-C26-C27-C28
17	a	902	85N	C18-C19-C24-O4
11	a	905	BCL	CBA-CGA-O2A-C1
11	A	908	BCL	C12-C13-C15-C16
11	a	908	BCL	C12-C13-C15-C16
11	a	910	BCL	C11-C12-C13-C15
11	a	910	BCL	C12-C13-C15-C16
12	a	901	CLA	C6-C7-C8-C10
12	a	913	CLA	C11-C10-C8-C7
11	A	903	BCL	C6-C7-C8-C9
11	A	905	BCL	C11-C10-C8-C9
11	a	908	BCL	C6-C7-C8-C9
12	A	931	CLA	C11-C12-C13-C14
12	a	912	CLA	C6-C7-C8-C9
12	a	915	CLA	O1D-CGD-O2D-CED
12	a	912	CLA	CBA-CGA-O2A-C1
19	E	101	84Q	C16-O4-P-O5
12	a	913	CLA	C16-C17-C18-C20
17	G	101	85N	C6-C7-C8-C9
11	a	905	BCL	C10-C11-C12-C13
17	a	902	85N	O2-C16-C17-O6
17	g	101	85N	O2-C16-C17-O3
19	a	921	84Q	O1-C15-C16-O2
11	A	903	BCL	C3A-C2A-CAA-CBA
11	A	908	BCL	C3A-C2A-CAA-CBA
15	a	919	85I	C3-O3-P-O
13	c	201	LYC	C58-C59-C60-C61
17	A	932	85N	C28-C29-C30-C31
15	A	916	85I	C30-C31-C32-C34
11	a	904	BCL	C8-C10-C11-C12
17	G	101	85N	C3-C2-C4-C5
19	E	101	84Q	C6-C7-C8-C9
15	A	915	85I	C2-O-P-O3

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Mol	Chain	Res	Type	Atoms
11	a	905	BCL	O1A-CGA-O2A-C1
15	A	915	85I	C30-C31-C32-C33
15	a	919	85I	C15-C16-C17-C18
11	a	908	BCL	C10-C11-C12-C13
17	a	902	85N	C2-C4-C5-C6
10	a	903	2GO	C3A-C2A-CAA-CBA
17	A	932	85N	C25-C26-C27-C28
15	a	920	85I	C30-C31-C32-C34
15	a	918	85I	C11-C12-C13-C14
15	a	918	85I	C12-C13-C14-C15
11	a	911	BCL	C2-C1-O2A-CGA
11	a	905	BCL	C11-C12-C13-C14
19	E	101	84Q	C1-C3-C4-C5
15	A	917	85I	C21-C20-O6-C3
15	a	918	85I	C30-C31-C32-C33
19	a	921	84Q	C2-C1-C3-C4
12	A	911	CLA	C10-C11-C12-C13
15	A	915	85I	C24-C25-C26-C27
11	a	905	BCL	C3-C5-C6-C7
15	a	920	85I	C27-C28-C29-C30
10	A	901	2GO	C10-C11-C12-C13
15	a	919	85I	C29-C30-C31-C32
15	A	915	85I	C21-C22-C23-C24
11	A	902	BCL	C11-C12-C13-C15
11	A	902	BCL	C12-C13-C15-C16
11	A	903	BCL	C6-C7-C8-C10
11	A	903	BCL	C11-C10-C8-C7
11	A	905	BCL	C11-C10-C8-C7
11	a	905	BCL	C11-C12-C13-C15
11	a	908	BCL	C6-C7-C8-C10
12	A	910	CLA	C11-C10-C8-C7
12	A	911	CLA	C11-C10-C8-C7
12	a	901	CLA	C11-C10-C8-C7
11	a	909	BCL	C16-C17-C18-C19
12	A	911	CLA	C16-C17-C18-C19
11	A	902	BCL	C2A-CAA-CBA-CGA
12	a	912	CLA	C3-C5-C6-C7
12	A	910	CLA	C10-C11-C12-C13
12	A	911	CLA	C5-C6-C7-C8
11	a	909	BCL	CAD-CBD-CGD-O2D
12	A	931	CLA	CAD-CBD-CGD-O2D
12	a	912	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
15	A	916	85I	C23-C24-C25-C26
15	a	920	85I	C13-C14-C15-C16
17	a	902	85N	C33-C34-C35-C36
19	E	101	84Q	C24-C25-C26-C27
11	A	906	BCL	CHA-CBD-CGD-O2D
11	a	905	BCL	CHA-CBD-CGD-O2D
12	A	933	CLA	CHA-CBD-CGD-O1D
12	a	915	CLA	CHA-CBD-CGD-O1D
12	a	915	CLA	CHA-CBD-CGD-O2D
11	a	904	BCL	O1A-CGA-O2A-C1
12	a	901	CLA	O1A-CGA-O2A-C1
11	A	903	BCL	C5-C6-C7-C8
15	a	919	85I	O7-C20-O6-C3
11	A	908	BCL	C14-C13-C15-C16
15	A	916	85I	C10-C11-C12-C13
15	A	917	85I	C3-O3-P-O1
19	a	921	84Q	C16-O4-P-O6
17	A	932	85N	C1-C2-C4-C5
15	a	919	85I	N-C1-C2-O
19	E	101	84Q	C32-O7-P-O4
15	a	918	85I	C27-C28-C29-C30
15	A	915	85I	C2-O-P-O1
15	A	917	85I	C2-O-P-O2
15	a	919	85I	C2-O-P-O2
19	E	101	84Q	C27-C28-C29-C31
11	a	905	BCL	C5-C6-C7-C8
11	a	908	BCL	CAD-CBD-CGD-O1D
15	a	920	85I	C1-C2-O-P
19	a	921	84Q	C33-C32-O7-P
15	a	919	85I	C20-C21-C22-C23
15	a	918	85I	C7-C8-C9-C10
19	a	921	84Q	C-C1-C3-C4
11	A	905	BCL	C12-C13-C15-C16
11	A	907	BCL	C6-C7-C8-C10
11	A	907	BCL	C11-C10-C8-C7
11	A	908	BCL	C11-C10-C8-C7
11	a	907	BCL	C11-C10-C8-C7
17	A	932	85N	C19-C18-O3-C17
15	a	918	85I	C23-C24-C25-C26
11	A	907	BCL	C8-C10-C11-C12
11	a	909	BCL	CAA-CBA-CGA-O2A
19	a	921	84Q	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
11	a	904	BCL	C10-C11-C12-C13
10	a	903	2GO	C14-C13-C15-C16
11	A	902	BCL	C14-C13-C15-C16
11	a	907	BCL	C6-C7-C8-C9
11	a	910	BCL	C11-C12-C13-C14
12	A	911	CLA	C11-C12-C13-C14
12	a	913	CLA	C11-C10-C8-C9
17	G	101	85N	C25-C26-C27-C28
12	a	912	CLA	O1A-CGA-O2A-C1
13	c	201	LYC	C9-C10-C11-C12
11	A	908	BCL	C16-C17-C18-C19
17	g	101	85N	C1-C2-C4-C5
15	a	920	85I	C6-C7-C8-C9
11	A	906	BCL	O1A-CGA-O2A-C1
17	A	932	85N	C3-C2-C4-C5
11	a	904	BCL	C2-C1-O2A-CGA
17	a	902	85N	C18-C19-C24-O5
17	g	101	85N	C7-C8-C9-C10
11	A	902	BCL	CAA-CBA-CGA-O2A
15	a	920	85I	C22-C23-C24-C25
15	a	919	85I	C21-C20-O6-C3
15	a	920	85I	C10-C11-C12-C13
10	a	903	2GO	C11-C12-C13-C15
12	a	901	CLA	C11-C12-C13-C14
13	c	201	LYC	C52-C51-C53-C54
10	a	903	2GO	C8-C10-C11-C12
15	A	916	85I	C26-C27-C28-C29
15	a	919	85I	C24-C25-C26-C27
18	c	202	HEC	CAD-CBD-CGD-O2D
15	A	915	85I	C6-C7-C8-C9
12	a	901	CLA	C16-C17-C18-C20
15	a	918	85I	C9-C10-C11-C12
11	a	906	BCL	CAA-CBA-CGA-O1A
15	A	915	85I	O3-C3-C4-O4
15	a	920	85I	C12-C13-C14-C15
12	a	901	CLA	C14-C13-C15-C16
11	a	908	BCL	C2A-CAA-CBA-CGA
19	E	101	84Q	C23-C24-C25-C26
11	A	904	BCL	CAA-CBA-CGA-O2A
11	a	909	BCL	C13-C15-C16-C17
12	a	912	CLA	C4-C3-C5-C6
12	a	901	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	A	903	BCL	C12-C13-C15-C16
12	A	931	CLA	C6-C7-C8-C10
12	a	901	CLA	C12-C13-C15-C16
18	C	301	HEC	CAD-CBD-CGD-O2D
15	A	916	85I	C15-C16-C17-C19
11	A	904	BCL	CAA-CBA-CGA-O1A
12	A	910	CLA	C16-C17-C18-C20
11	a	906	BCL	CAA-CBA-CGA-O2A
13	c	201	LYC	C21-C50-C51-C53
12	a	901	CLA	C2-C1-O2A-CGA
19	a	921	84Q	C27-C28-C29-C30
11	a	904	BCL	CAA-CBA-CGA-O2A
15	a	918	85I	C28-C29-C30-C31
17	g	101	85N	C3-C2-C4-C5
18	C	301	HEC	CAD-CBD-CGD-O1D
15	A	917	85I	C23-C24-C25-C26
12	A	931	CLA	CBD-CGD-O2D-CED
11	A	909	BCL	O1D-CGD-O2D-CED
17	g	101	85N	C11-C10-C9-C8
12	a	901	CLA	CAA-CBA-CGA-O2A
10	A	901	2GO	C16-C17-C18-C20
13	c	201	LYC	C13-C12-C14-C15
13	c	201	LYC	C21-C50-C51-C52
15	A	915	85I	C5-C6-C7-C8
11	A	902	BCL	C8-C10-C11-C12
12	A	931	CLA	C2-C3-C5-C6
12	a	912	CLA	C2-C3-C5-C6
11	A	903	BCL	CAA-CBA-CGA-O2A
11	A	907	BCL	C6-C7-C8-C9
11	A	908	BCL	C6-C7-C8-C9
11	A	909	BCL	C11-C12-C13-C14
11	a	907	BCL	C11-C10-C8-C9
12	a	901	CLA	C11-C10-C8-C9
11	A	903	BCL	CAD-CBD-CGD-O2D
11	A	907	BCL	CAD-CBD-CGD-O2D
12	a	901	CLA	CAD-CBD-CGD-O2D
15	a	918	85I	C24-C25-C26-C27
15	a	920	85I	C11-C10-C9-C8
15	a	919	85I	C26-C27-C28-C29
18	c	202	HEC	CAD-CBD-CGD-O1D
11	A	904	BCL	CHA-CBD-CGD-O2D
11	A	906	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	a	904	BCL	CHA-CBD-CGD-O2D
11	a	905	BCL	CHA-CBD-CGD-O1D
11	a	906	BCL	CHA-CBD-CGD-O1D
11	a	908	BCL	CHA-CBD-CGD-O2D
12	a	913	CLA	CHA-CBD-CGD-O2D
13	c	201	LYC	C11-C12-C14-C15
15	a	919	85I	O4-C5-C6-C7
17	a	902	85N	C13-C14-C15-O2
11	a	910	BCL	CAA-CBA-CGA-O2A
11	a	907	BCL	C6-C7-C8-C10
11	A	907	BCL	C11-C12-C13-C14
12	a	901	CLA	C16-C17-C18-C19
15	A	916	85I	O4-C5-C6-C7
18	C	301	HEC	CAA-CBA-CGA-O2A
12	a	901	CLA	CAA-CBA-CGA-O1A
19	a	921	84Q	C22-C23-C24-C25
15	A	917	85I	N-C1-C2-O
17	g	101	85N	C18-C19-C20-N1
19	a	921	84Q	C27-C28-C29-C31
17	A	932	85N	C4-C5-C6-C7
11	a	907	BCL	C13-C15-C16-C17
12	A	910	CLA	C2A-CAA-CBA-CGA
15	a	919	85I	O5-C5-C6-C7
19	a	921	84Q	C11-C10-C9-C8
18	c	202	HEC	CAA-CBA-CGA-O2A
17	A	932	85N	C2-C4-C5-C6
11	A	903	BCL	CAA-CBA-CGA-O1A
17	g	101	85N	C13-C14-C15-O2
17	a	902	85N	C13-C14-C15-O1
17	g	101	85N	C2-C4-C5-C6
11	a	910	BCL	CAA-CBA-CGA-O1A
11	A	906	BCL	CAD-CBD-CGD-O1D
11	A	908	BCL	CAD-CBD-CGD-O1D
11	a	906	BCL	CAD-CBD-CGD-O1D
12	A	933	CLA	CAD-CBD-CGD-O1D
12	a	915	CLA	CAD-CBD-CGD-O1D
19	E	101	84Q	C33-C32-O7-P
17	g	101	85N	C13-C14-C15-O1
15	a	920	85I	O4-C5-C6-C7
11	A	905	BCL	C14-C13-C15-C16
11	a	905	BCL	C6-C7-C8-C9
11	A	908	BCL	CAA-CBA-CGA-O2A

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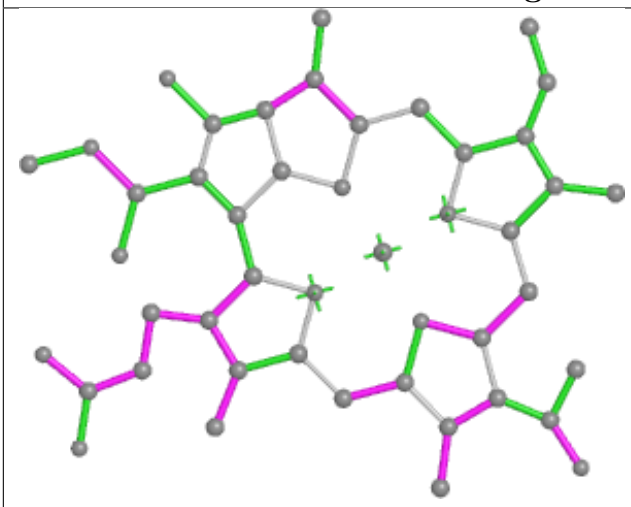
Mol	Chain	Res	Type	Atoms
15	A	916	85I	O6-C20-C21-C22
11	A	908	BCL	C6-C7-C8-C10
11	a	905	BCL	C6-C7-C8-C10
12	a	913	CLA	C6-C7-C8-C10
15	A	916	85I	O5-C5-C6-C7
17	A	932	85N	O7-C25-C26-C27
12	A	931	CLA	C3-C5-C6-C7
13	c	201	LYC	C50-C51-C53-C54
11	A	907	BCL	CAA-CBA-CGA-O2A
17	A	932	85N	O6-C25-C26-C27
17	G	101	85N	C13-C14-C15-O2
15	A	917	85I	C14-C15-C16-C17
11	A	903	BCL	O1A-CGA-O2A-C1
15	A	916	85I	O7-C20-C21-C22

There are no ring outliers.

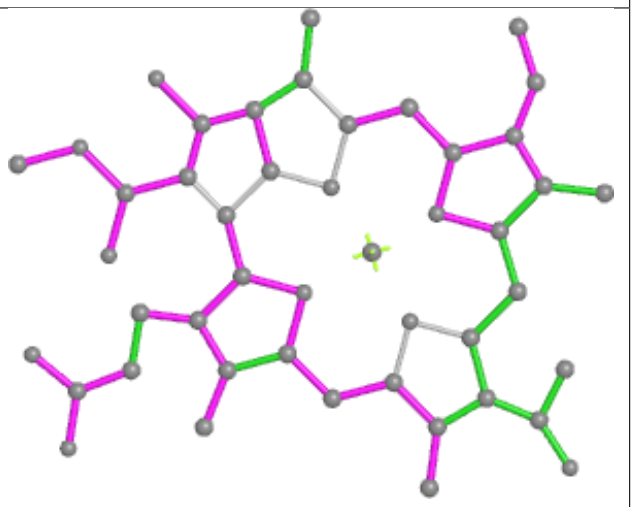
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

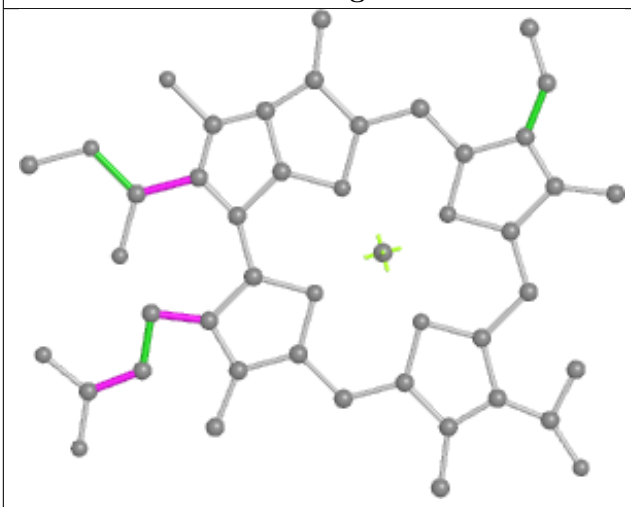
Ligand BCL A 904



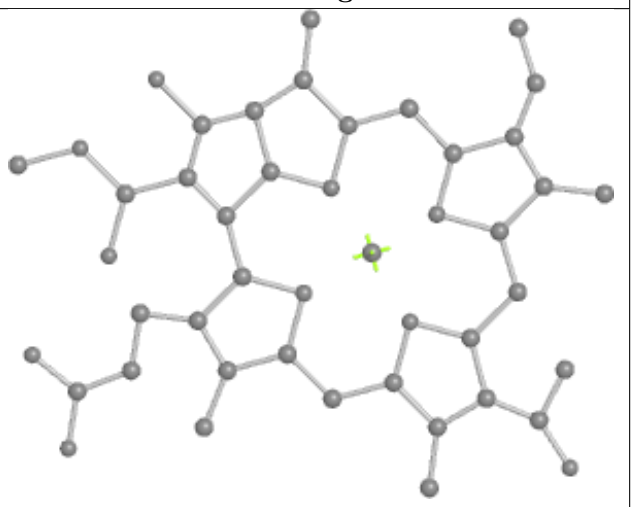
Bond lengths



Bond angles

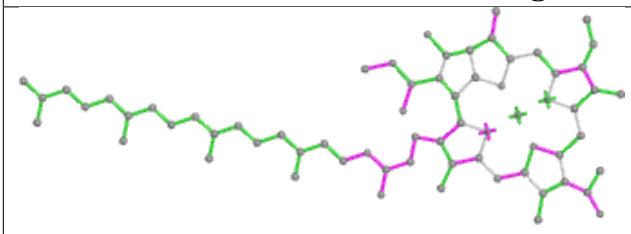


Torsions

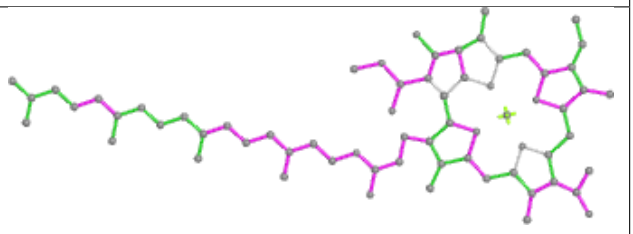


Rings

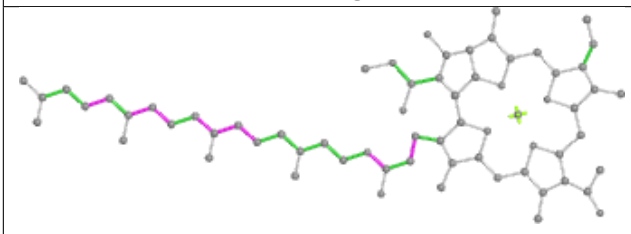
Ligand BCL a 907



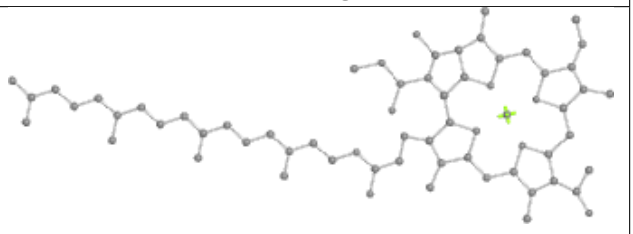
Bond lengths



Bond angles

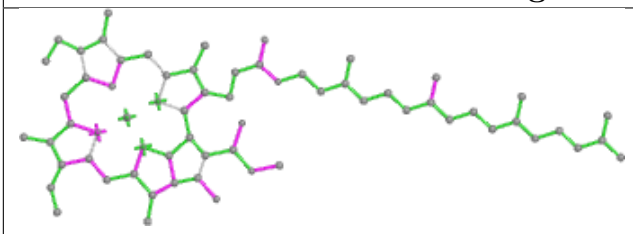


Torsions

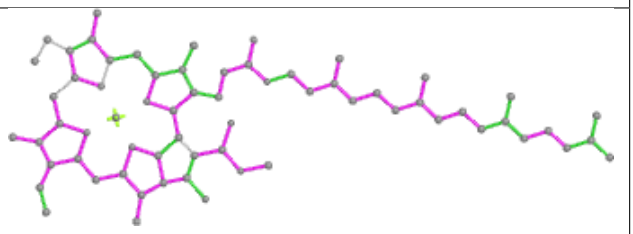


Rings

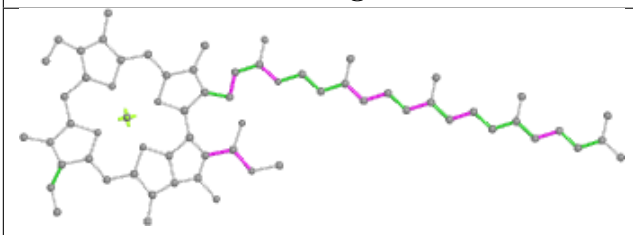
Ligand CLA a 912



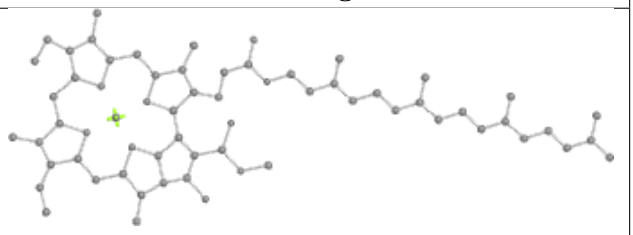
Bond lengths



Bond angles

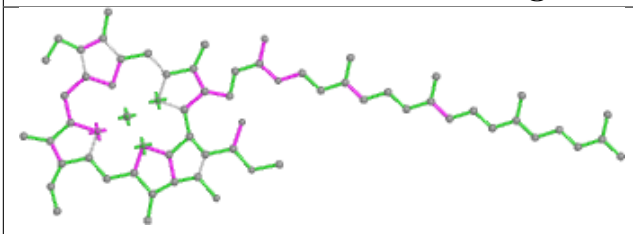


Torsions

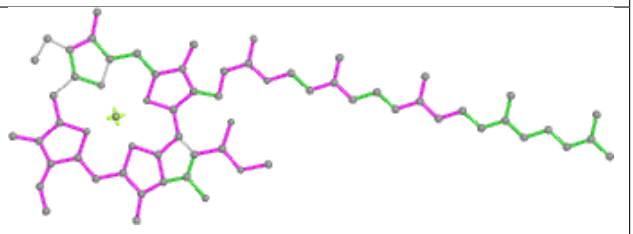


Rings

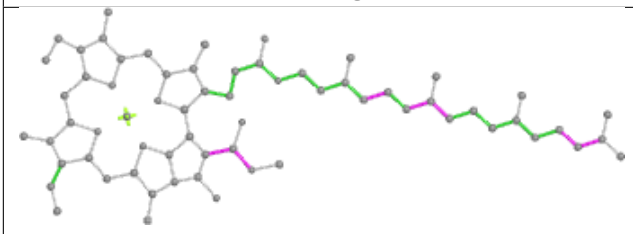
Ligand CLA a 913



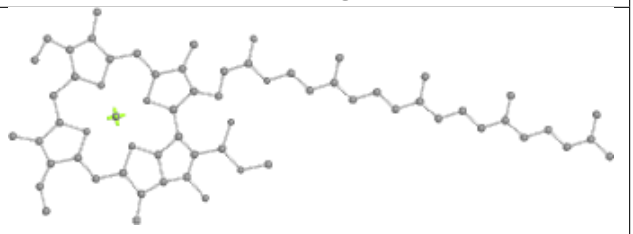
Bond lengths



Bond angles

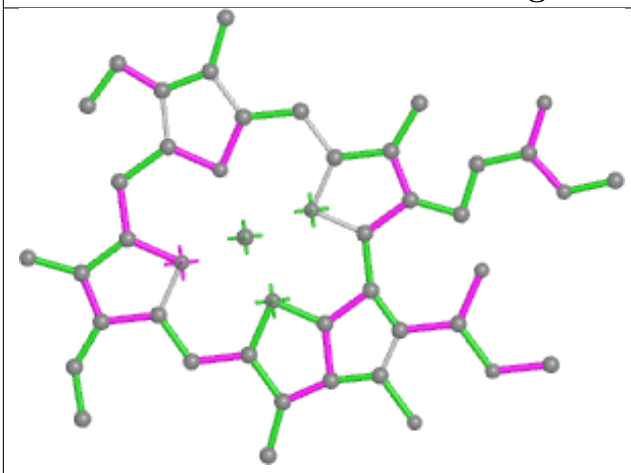


Torsions

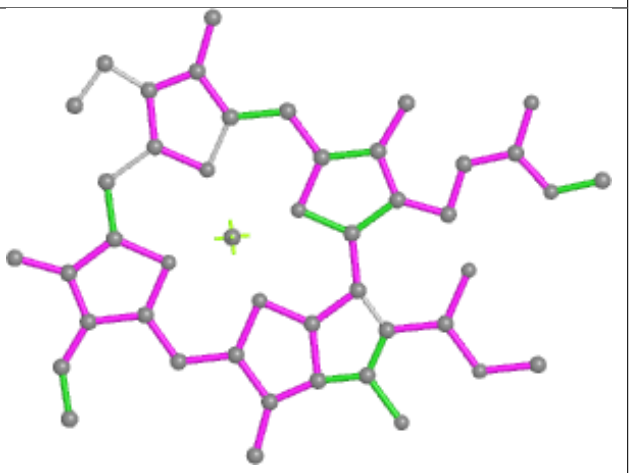


Rings

Ligand CLA a 914



Bond lengths



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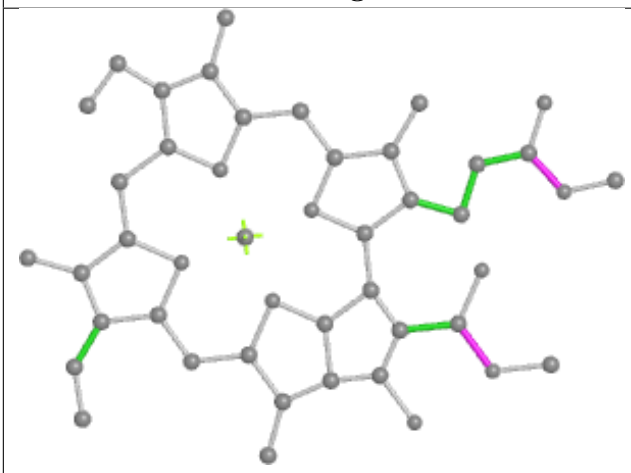
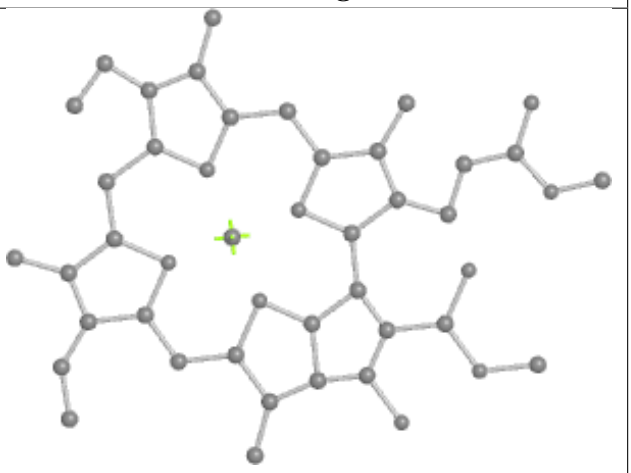
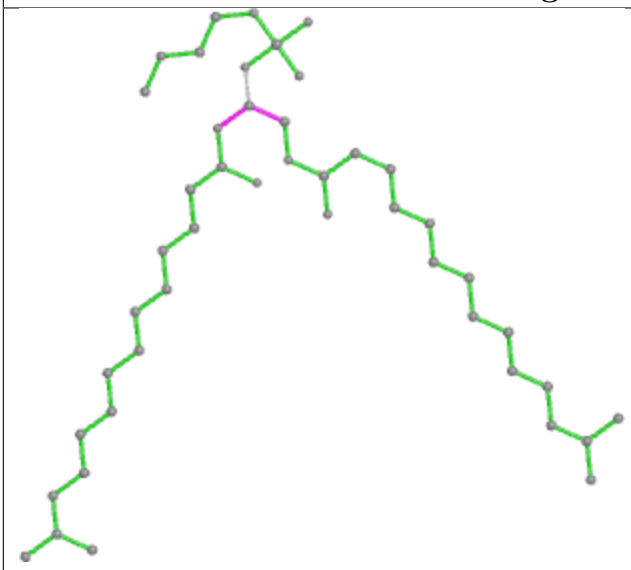


Torsions

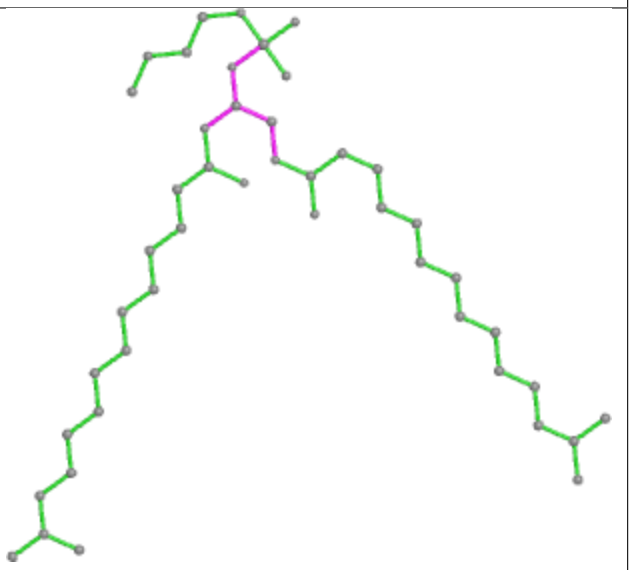


Rings

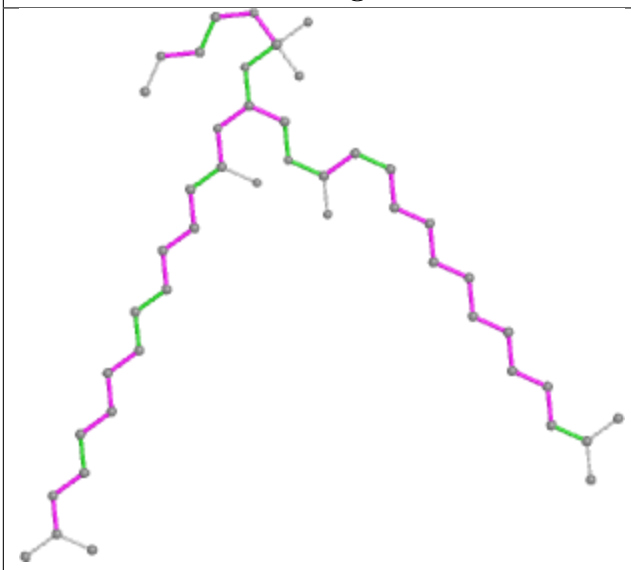
Ligand 85I a 920



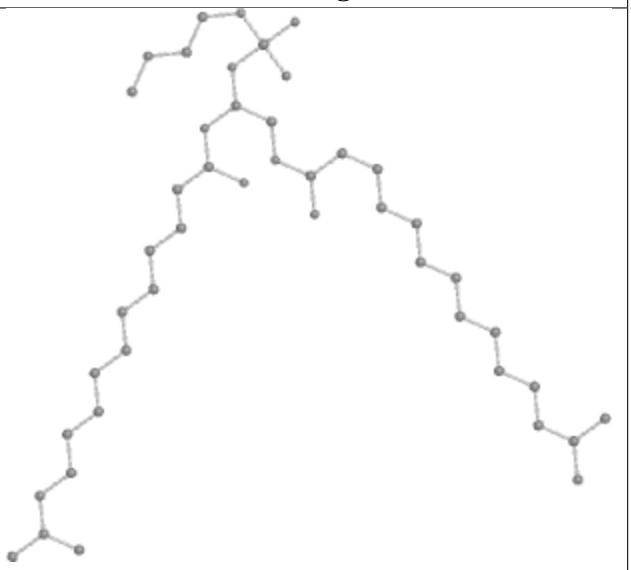
Bond lengths



Bond angles

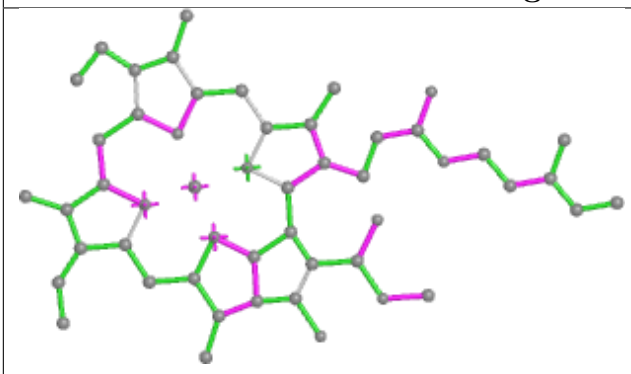


Torsions



Rings

Ligand CLA A 933



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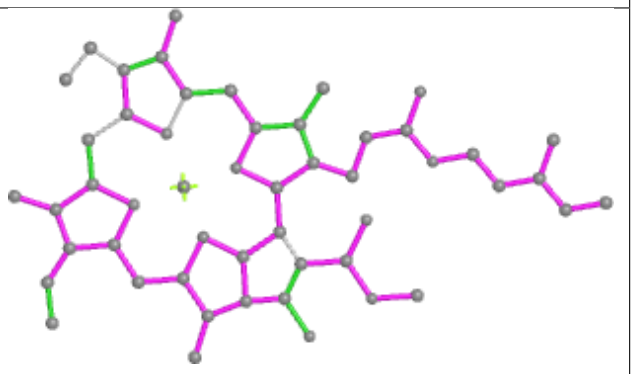
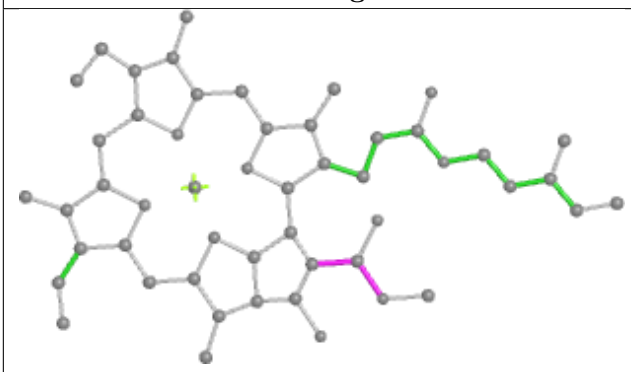
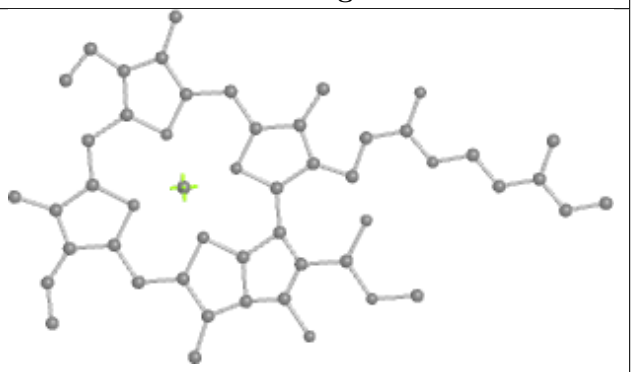


Bond angles

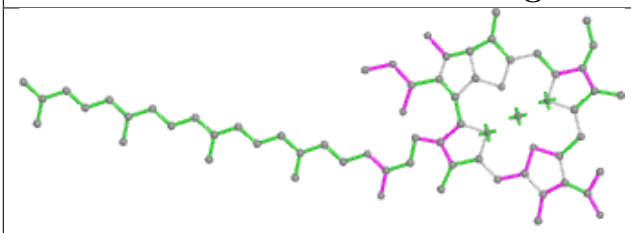


Torsions

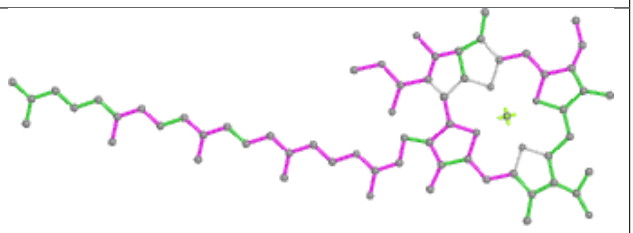


Rings

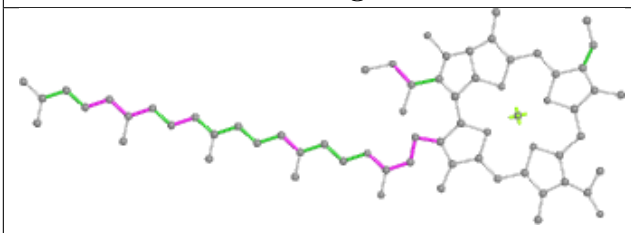
Ligand BCL A 902



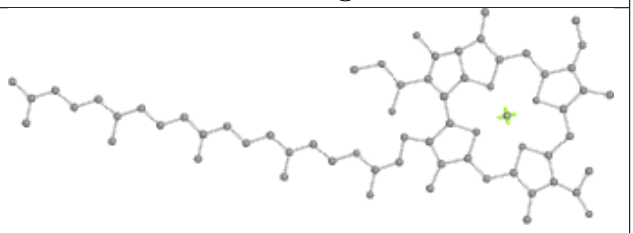
Bond lengths



Bond angles

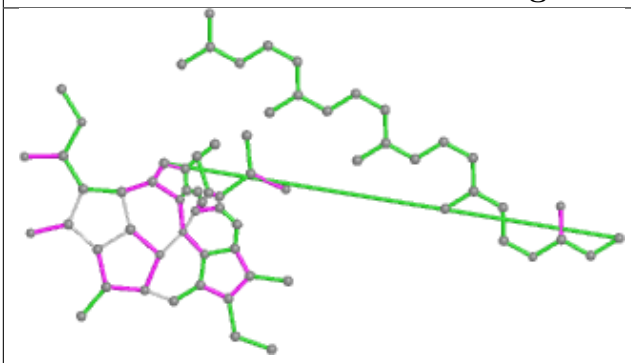


Torsions

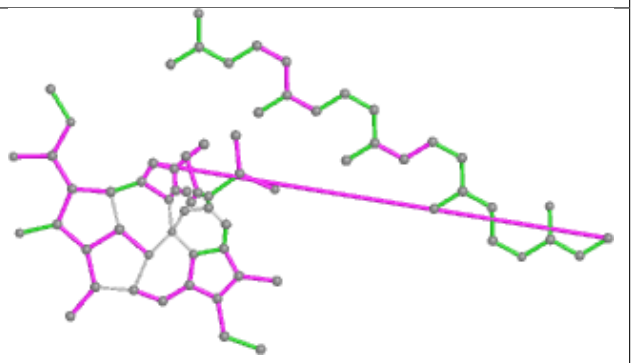


Rings

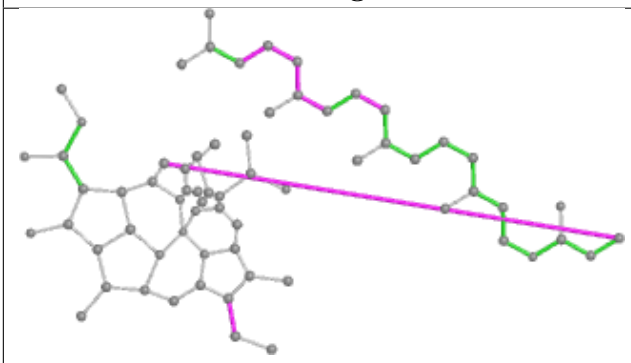
Ligand 2GO a 903



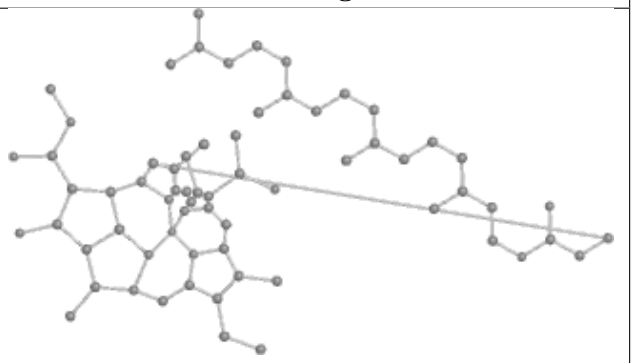
Bond lengths



Bond angles

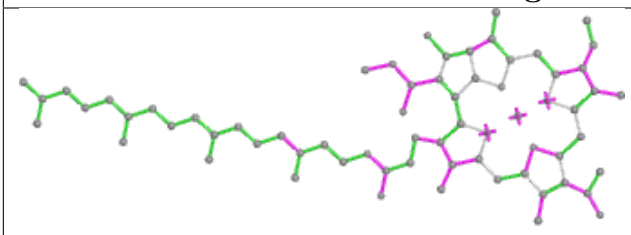


Torsions



Rings

Ligand BCL A 908



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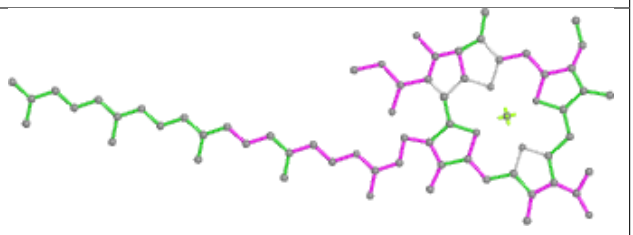
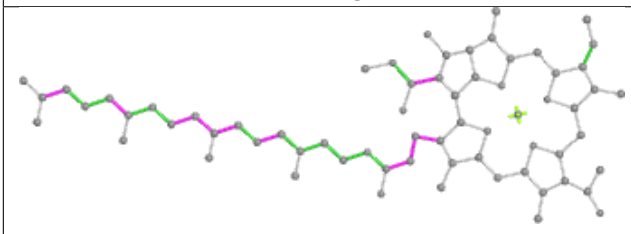
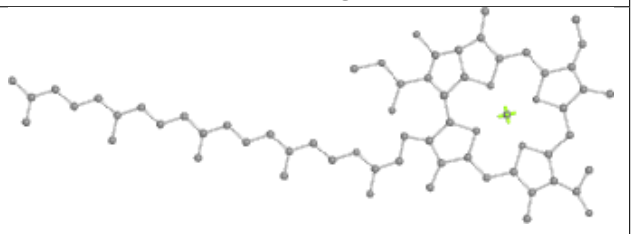


Bond angles

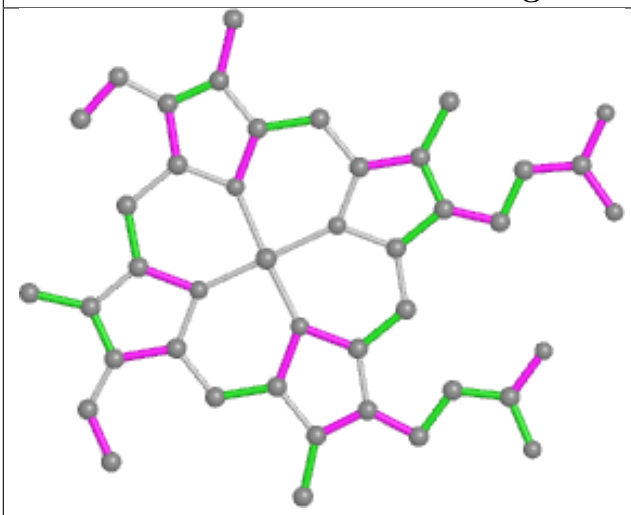


Torsions



Rings

Ligand HEC C 301



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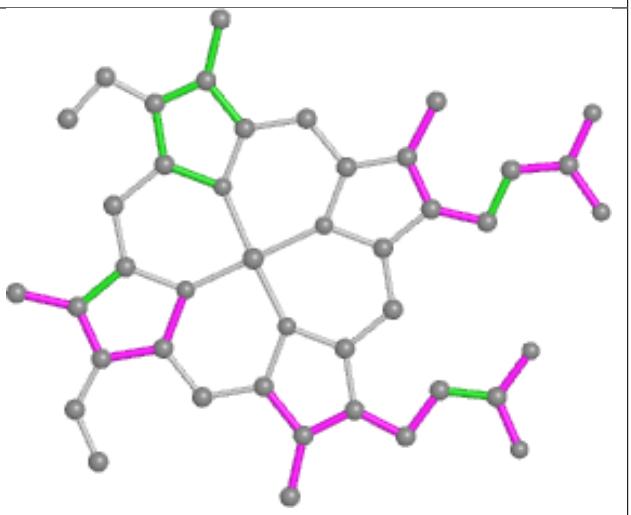
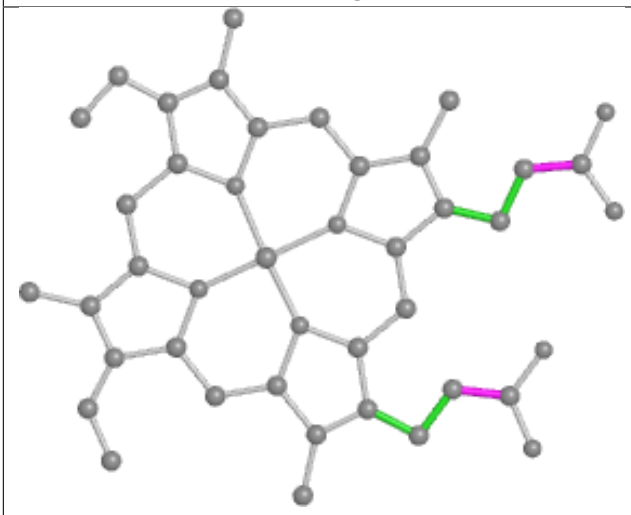
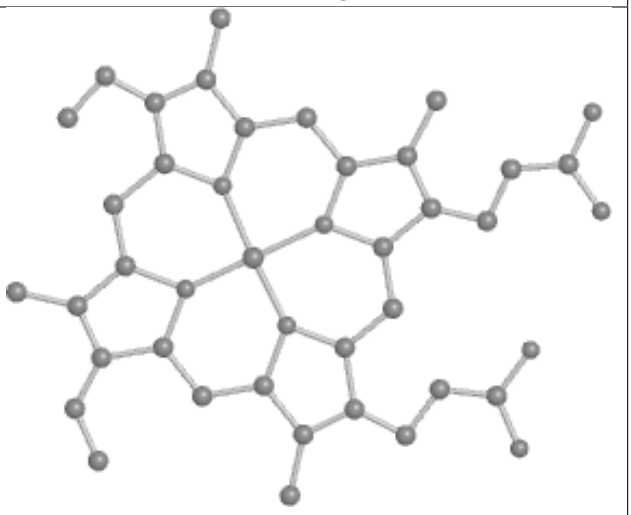


Bond angles

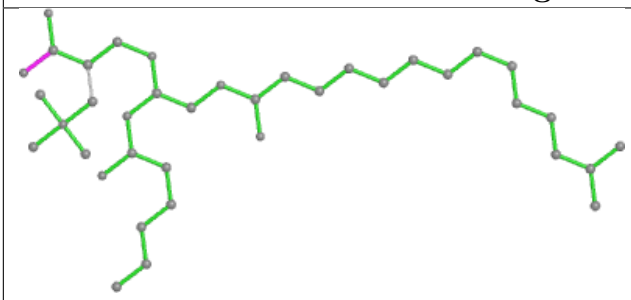


Torsions



Rings

Ligand 85N g 101



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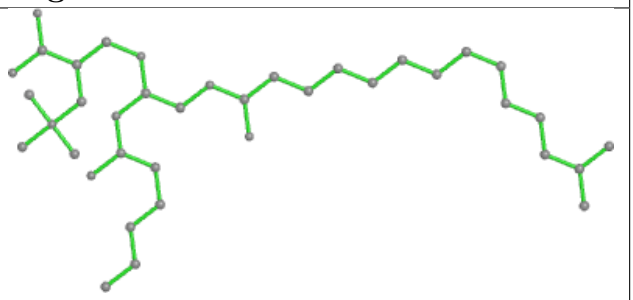
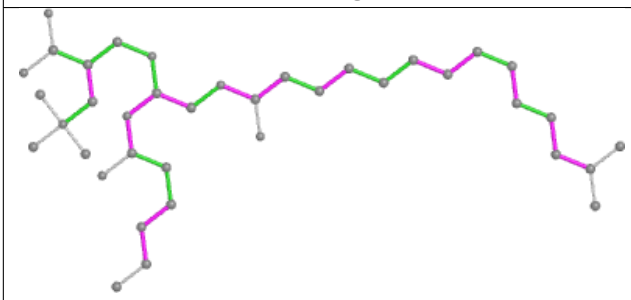
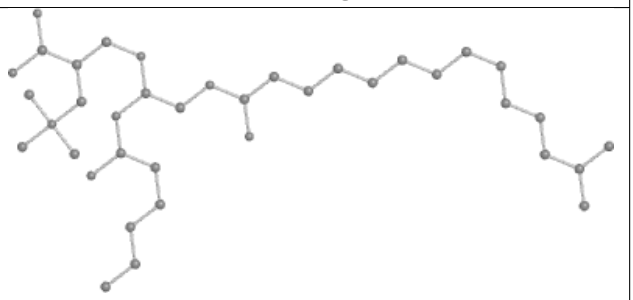


Bond angles

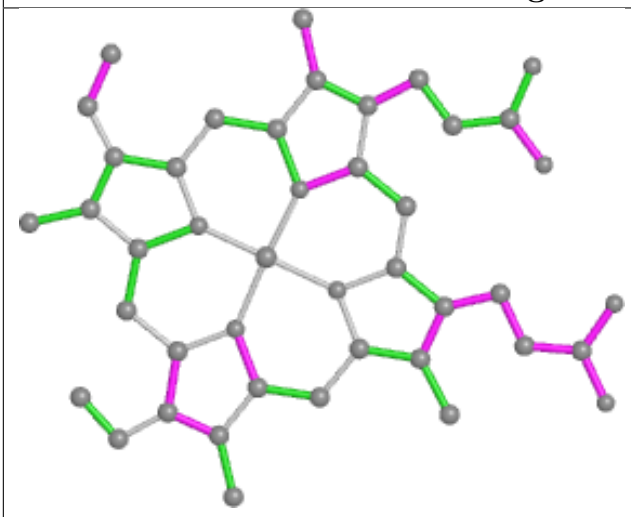


Torsions

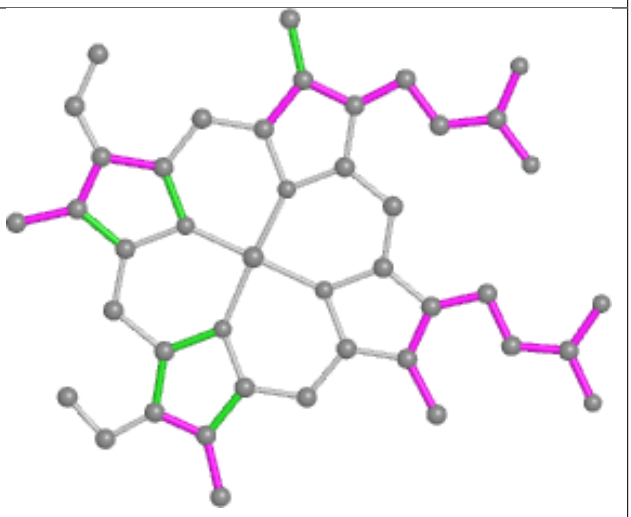


Rings

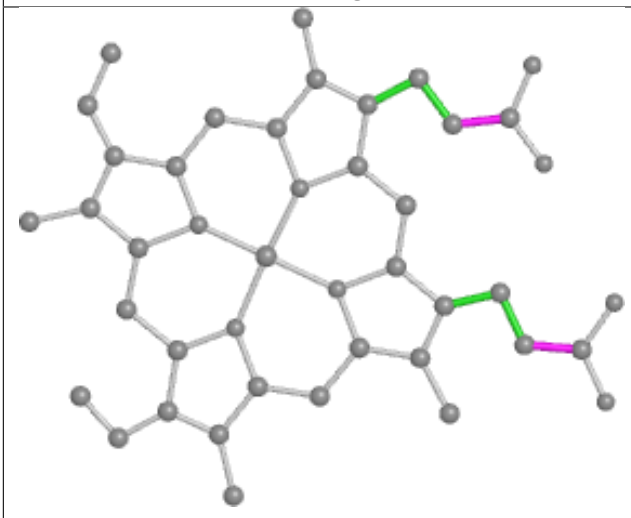
Ligand HEC c 202



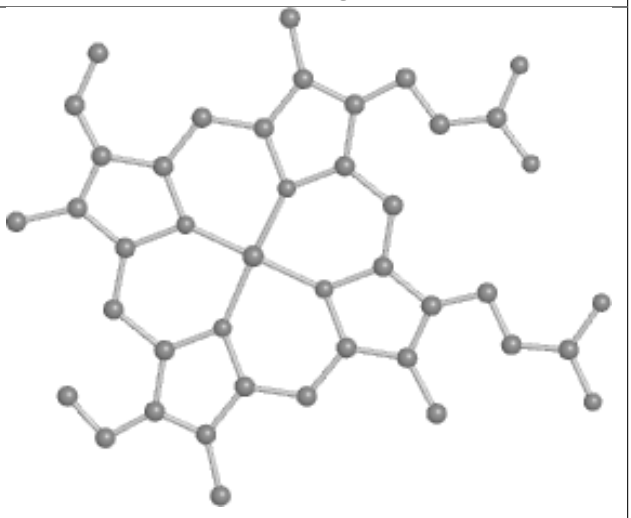
Bond lengths



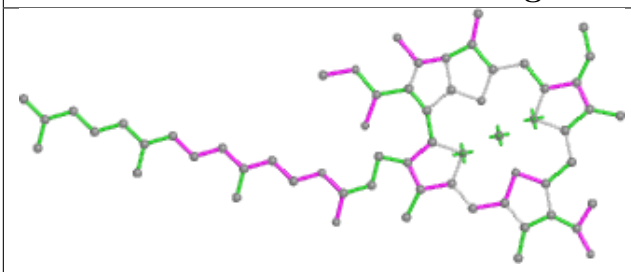
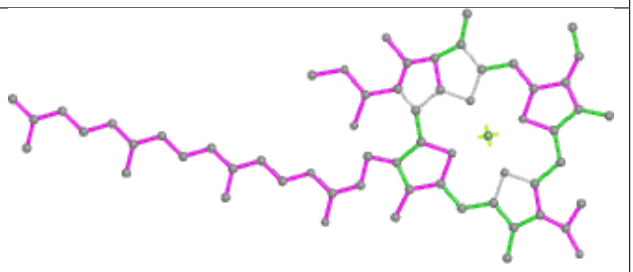
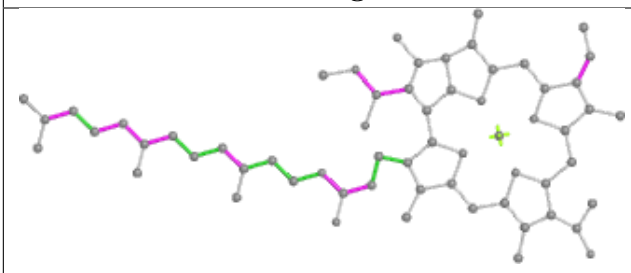
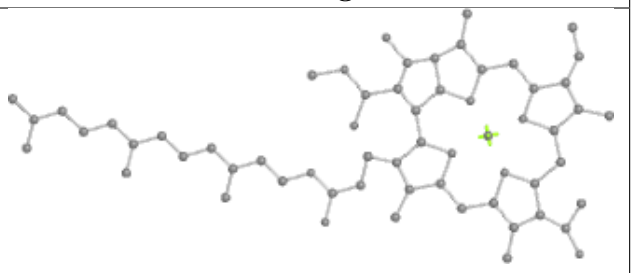
Bond angles

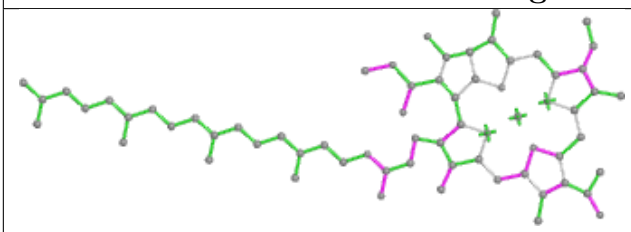
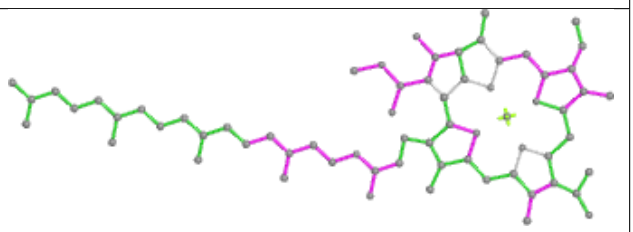
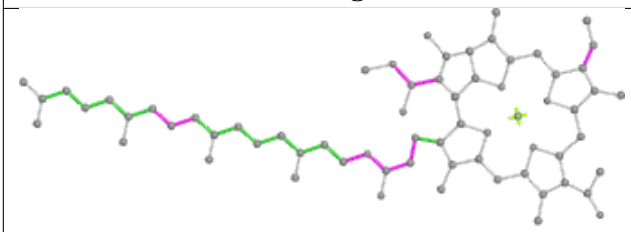
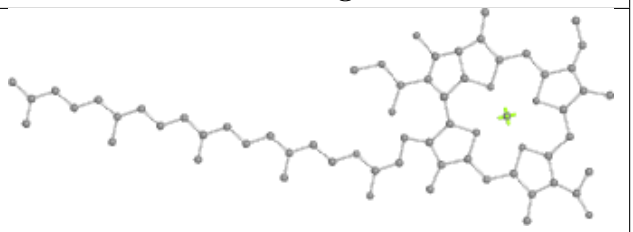


Torsions

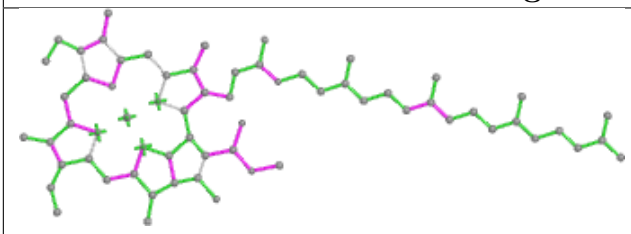


Rings

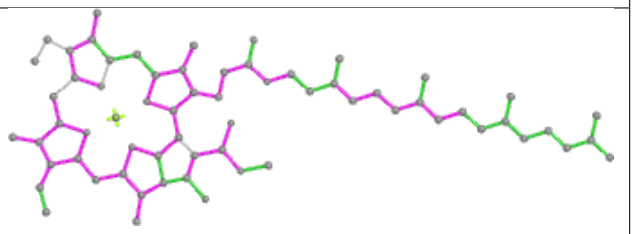
Ligand BCL A 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL a 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

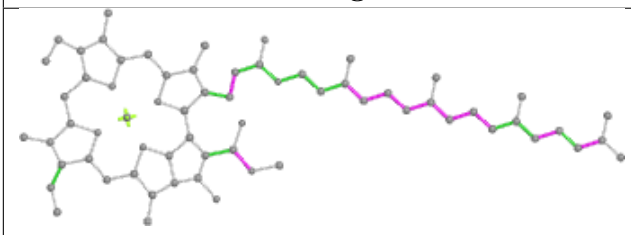
Ligand CLA A 910



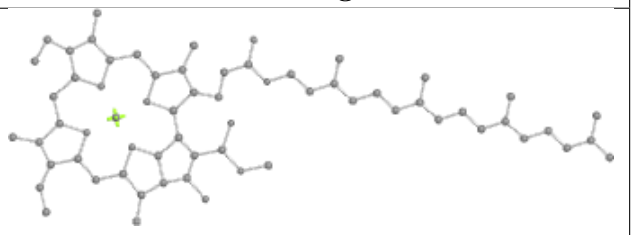
Bond lengths



Bond angles

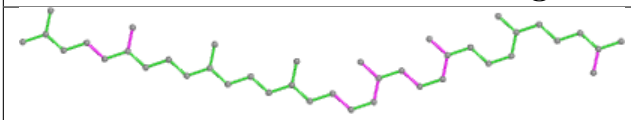


Torsions

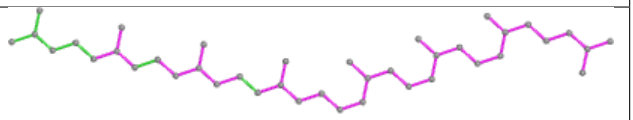


Rings

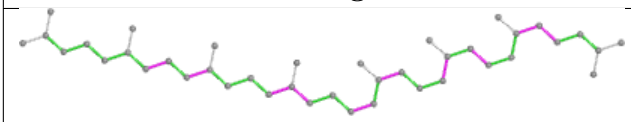
Ligand LYC c 201



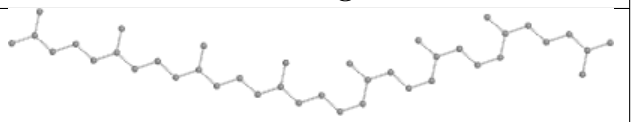
Bond lengths



Bond angles

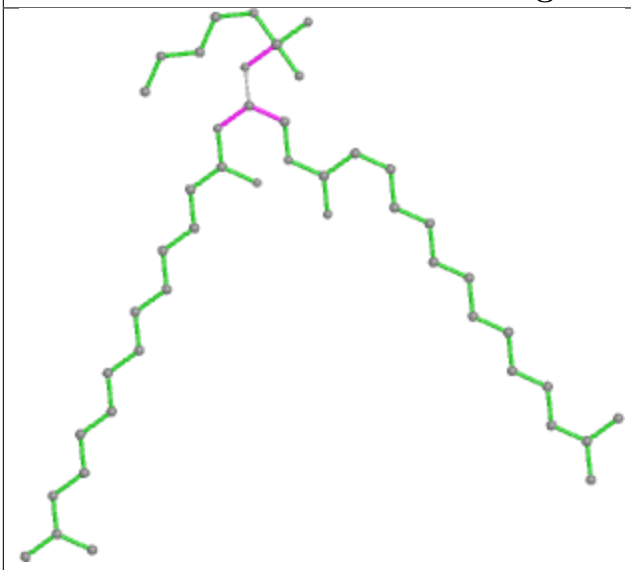


Torsions

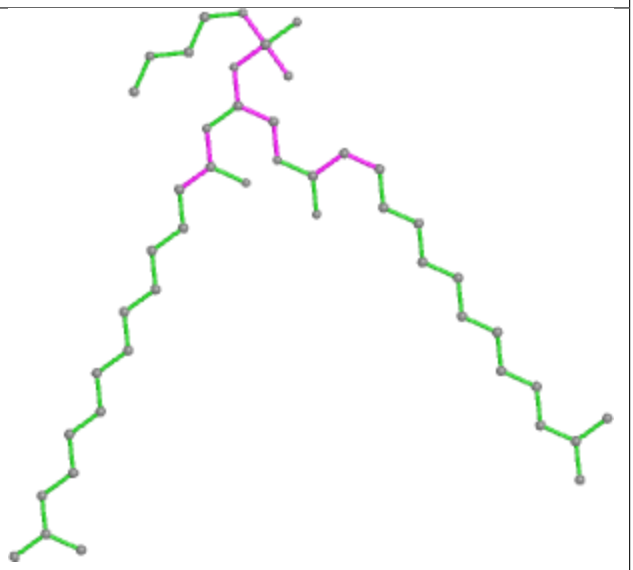


Rings

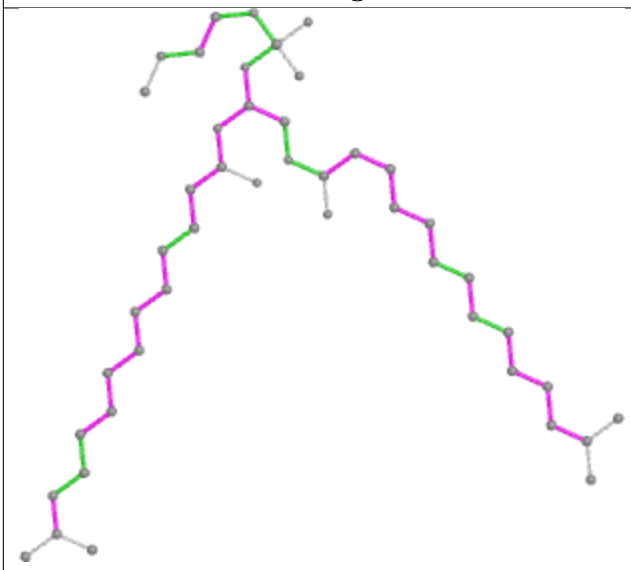
Ligand 85I A 916



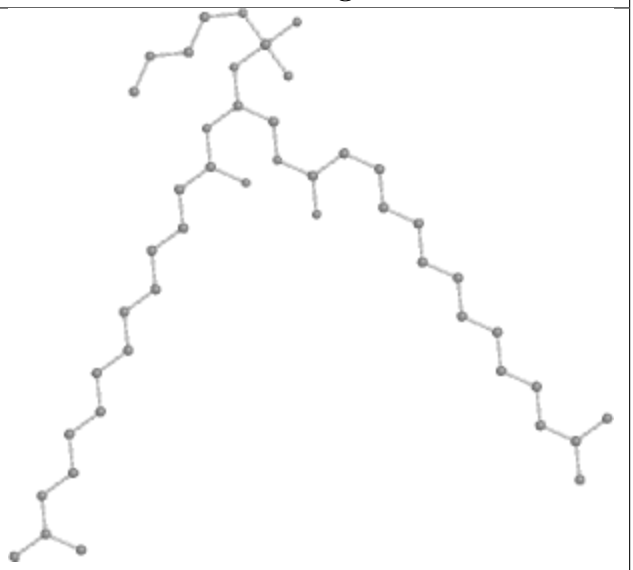
Bond lengths



Bond angles

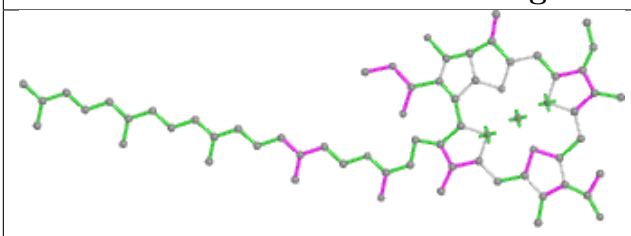


Torsions

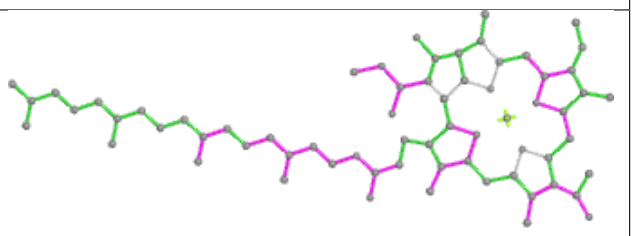


Rings

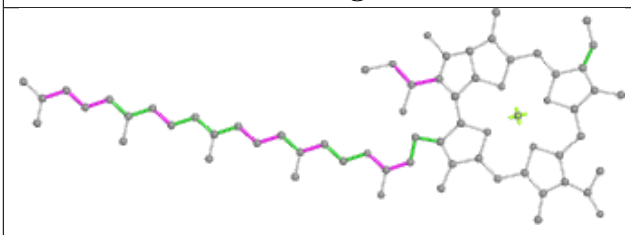
Ligand BCL a 909



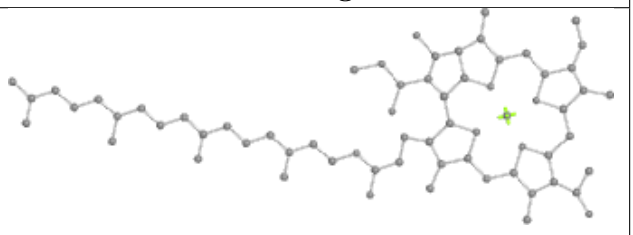
Bond lengths



Bond angles

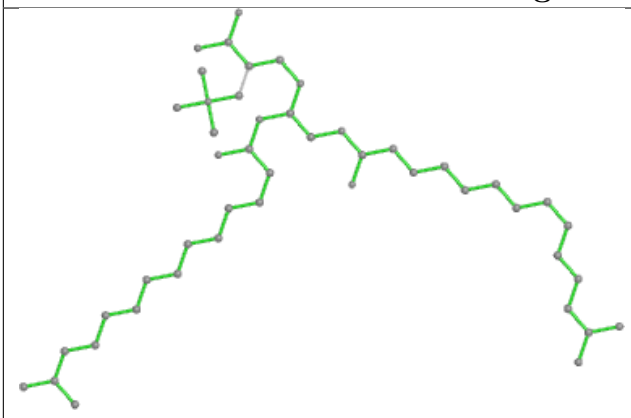


Torsions

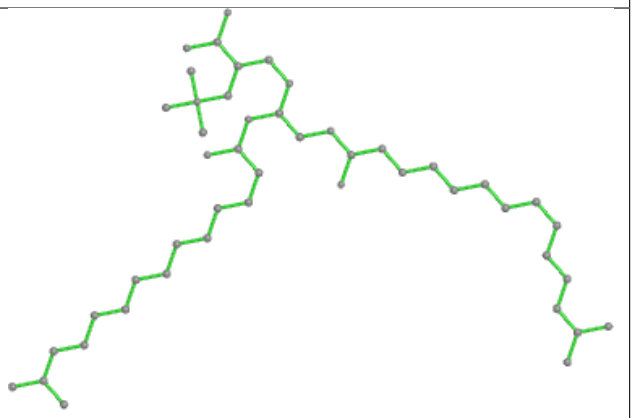


Rings

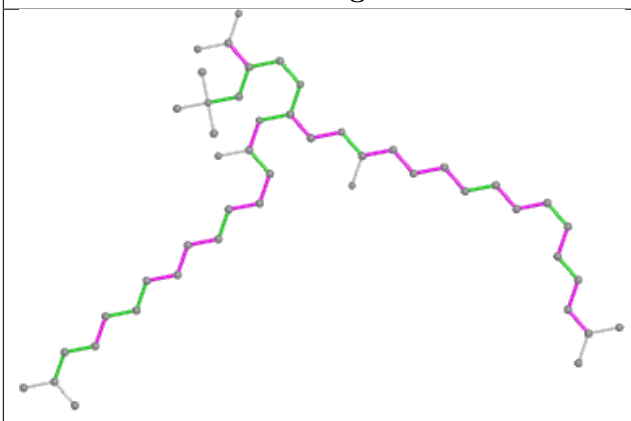
Ligand 85N a 902



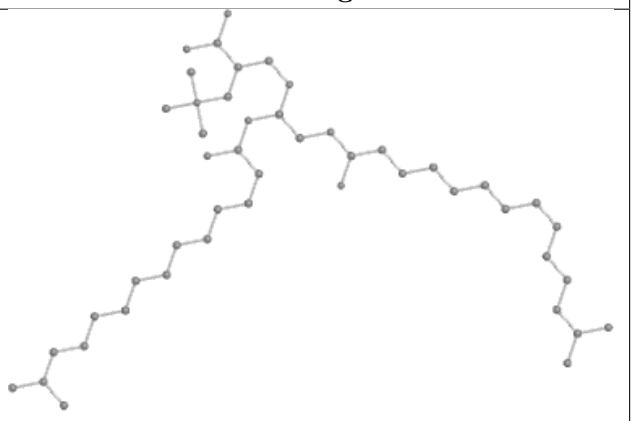
Bond lengths



Bond angles

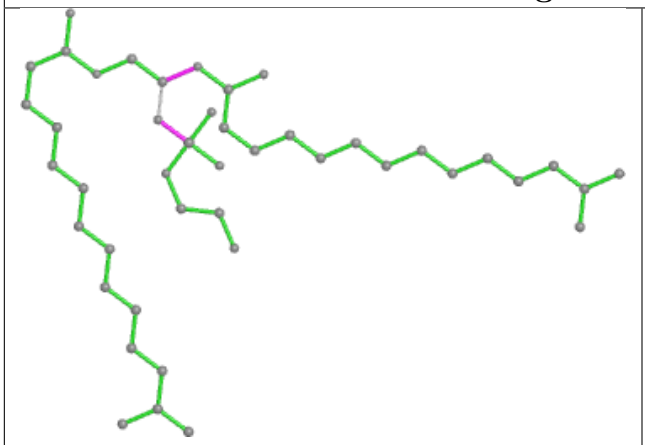


Torsions

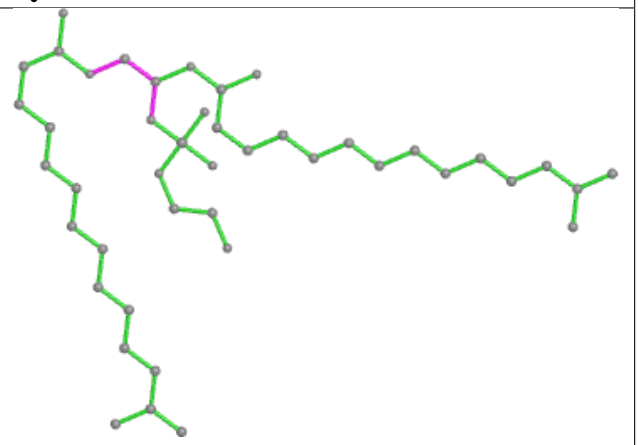


Rings

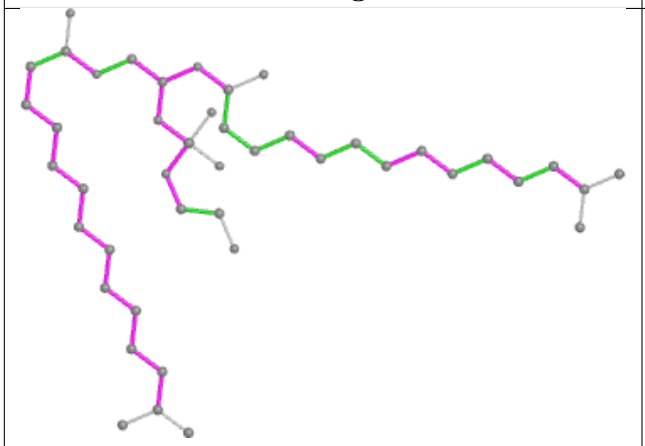
Ligand 84Q a 921



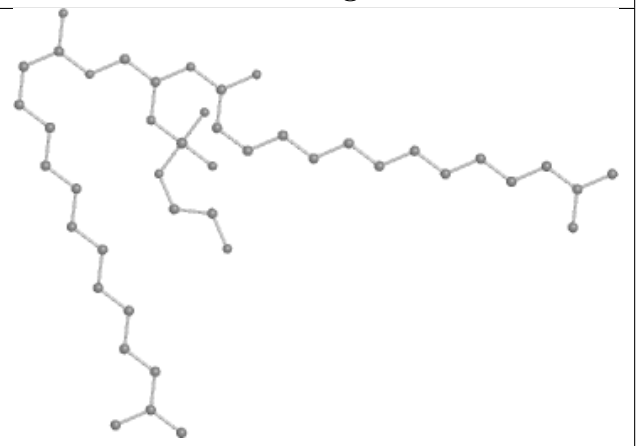
Bond lengths



Bond angles

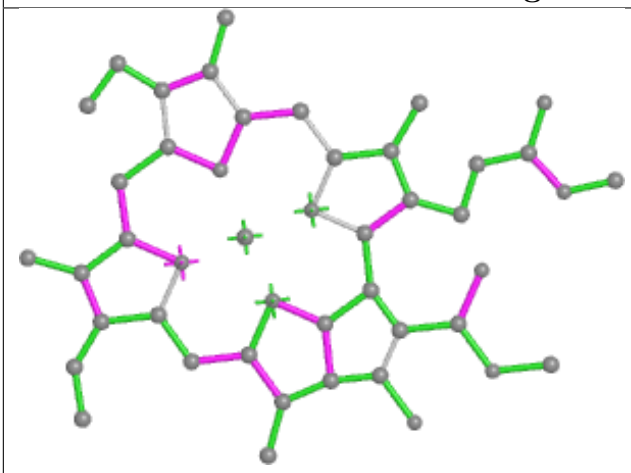


Torsions

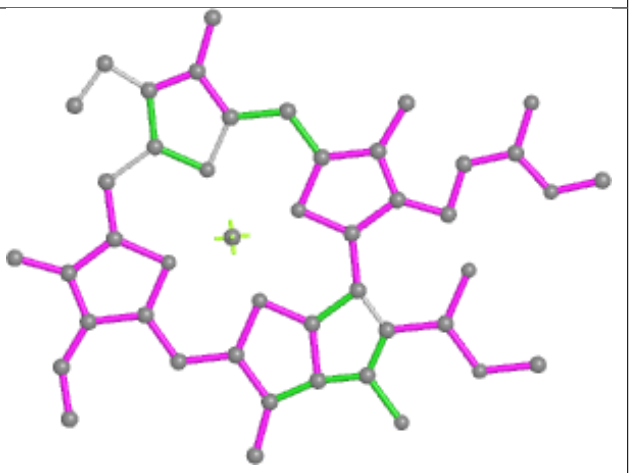


Rings

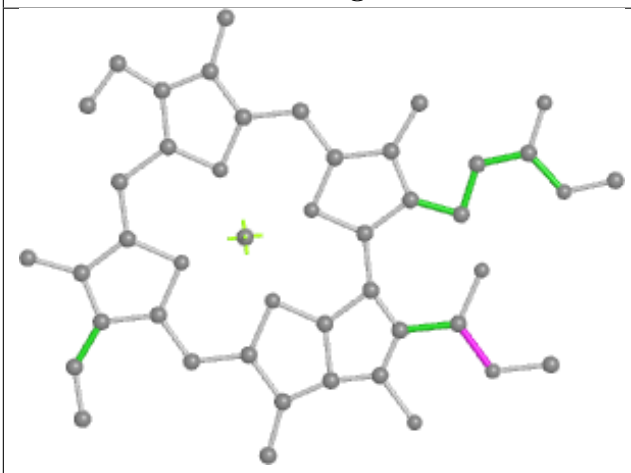
Ligand CLA A 912



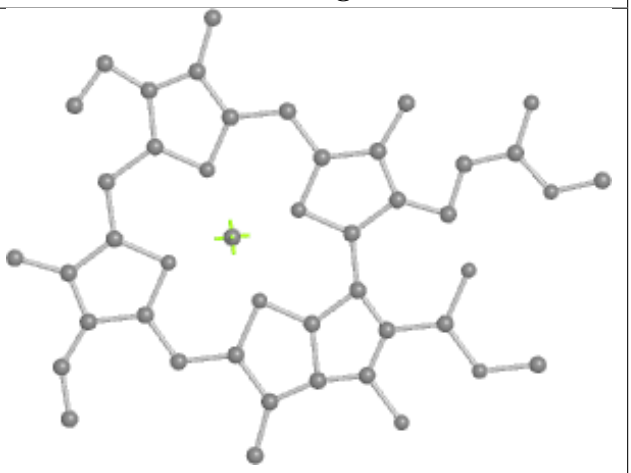
Bond lengths



Bond angles

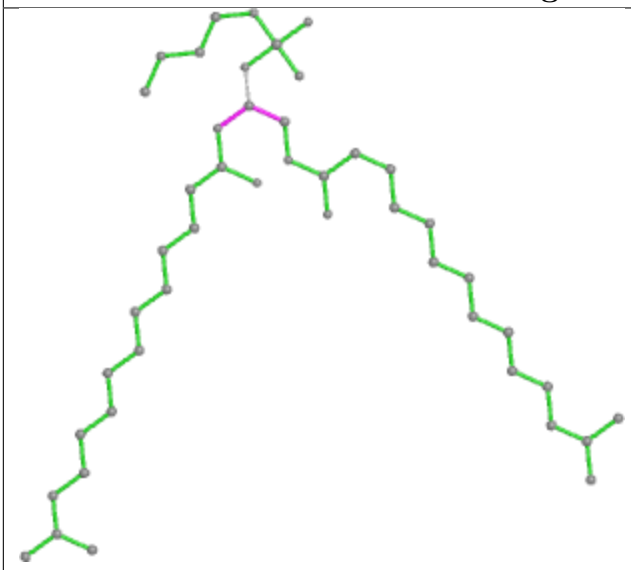


Torsions

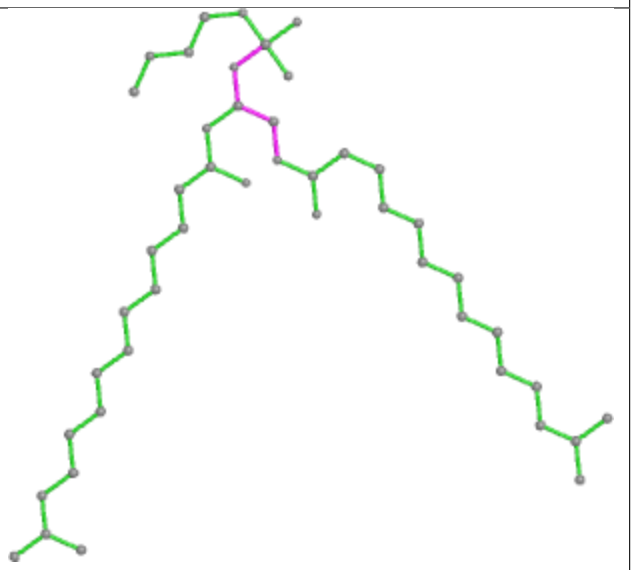


Rings

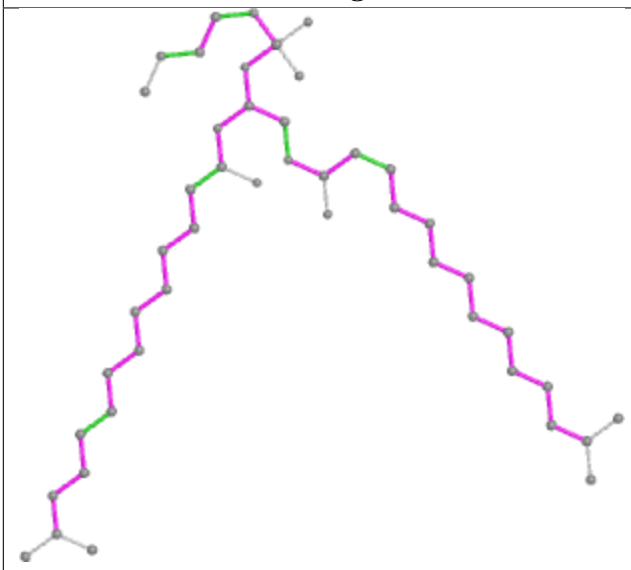
Ligand 85I a 919



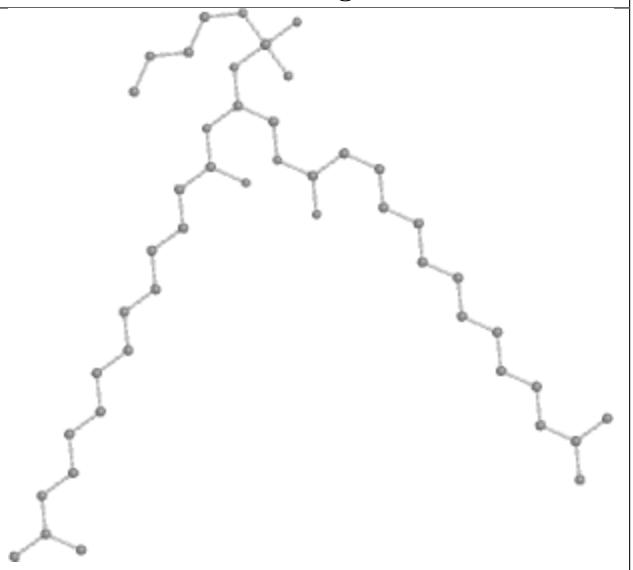
Bond lengths



Bond angles

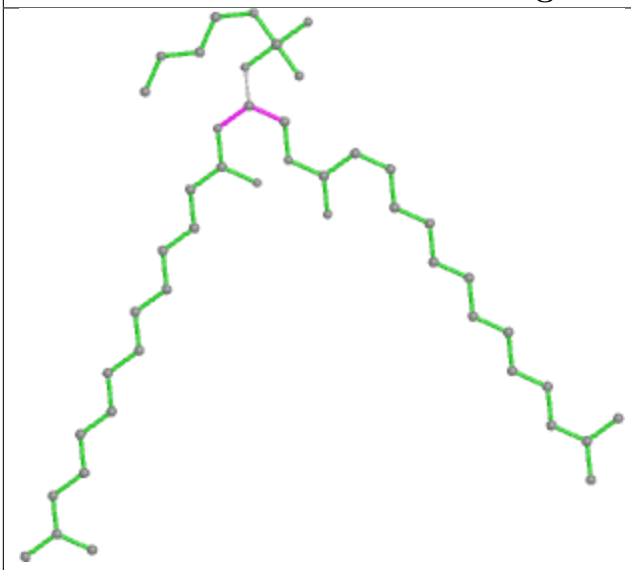


Torsions

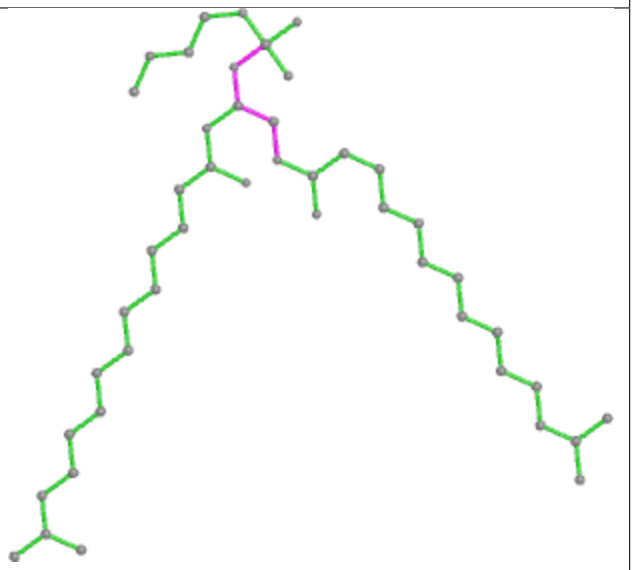


Rings

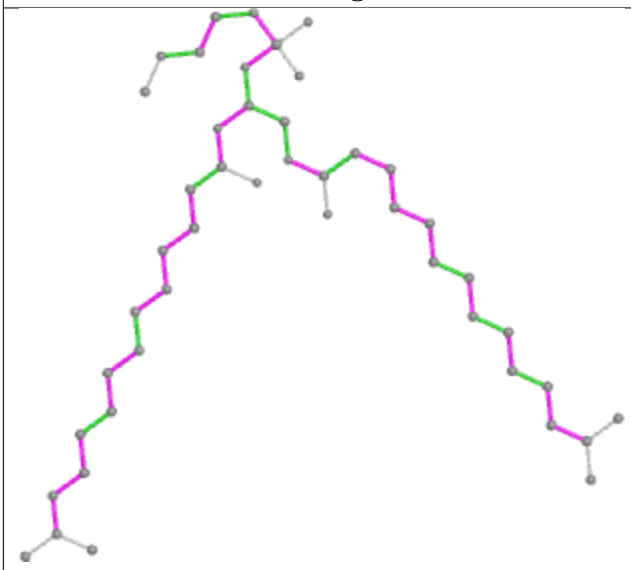
Ligand 85I A 917



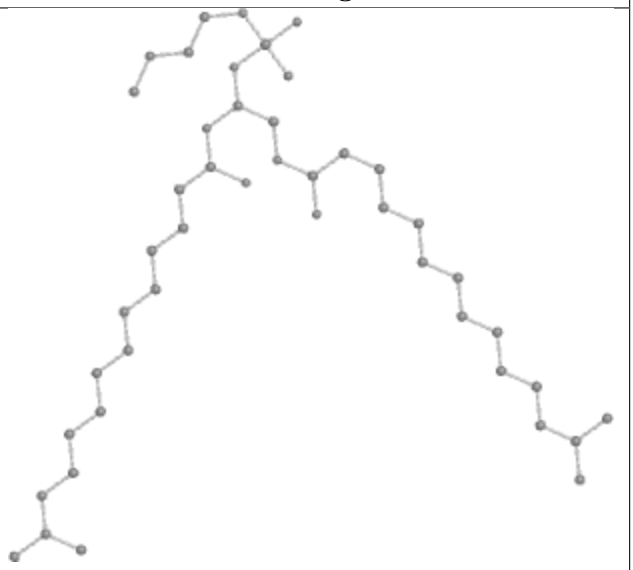
Bond lengths



Bond angles

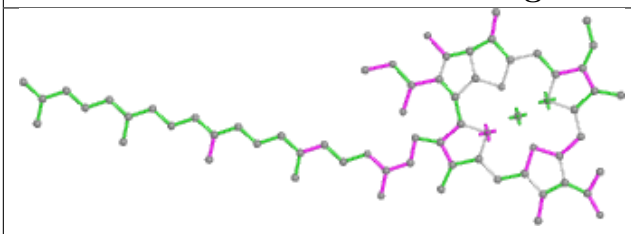


Torsions

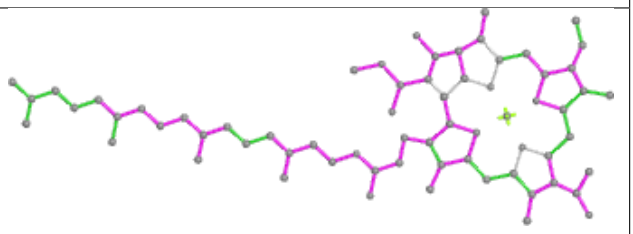


Rings

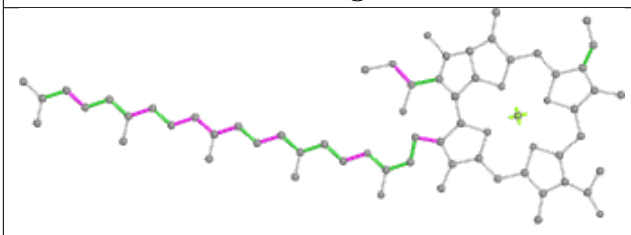
Ligand BCL A 909



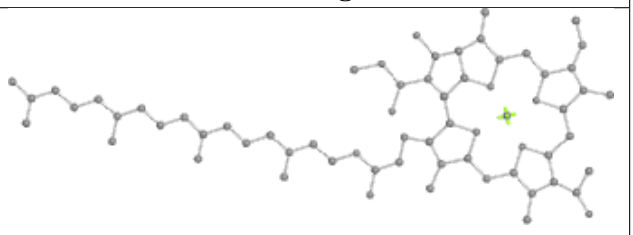
Bond lengths



Bond angles

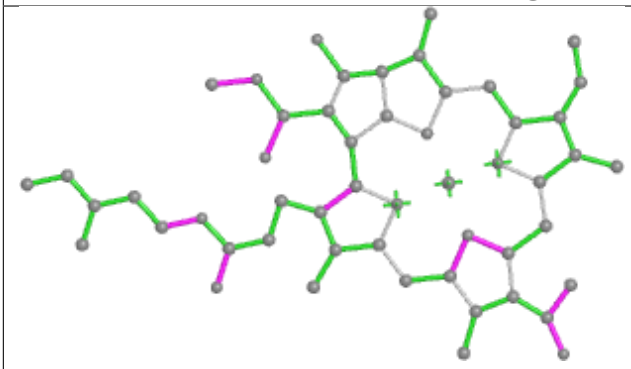


Torsions

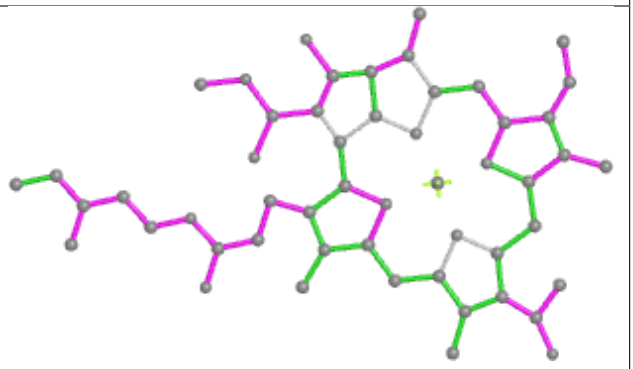


Rings

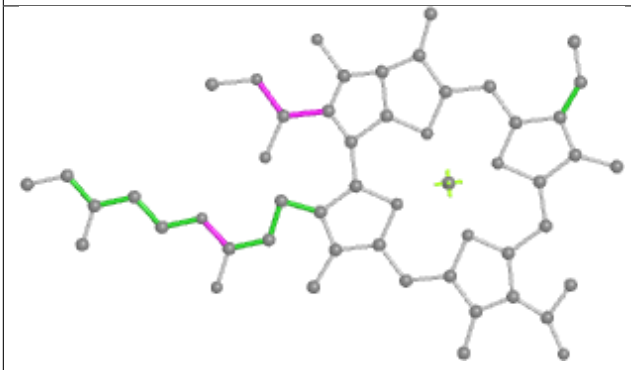
Ligand BCL A 906



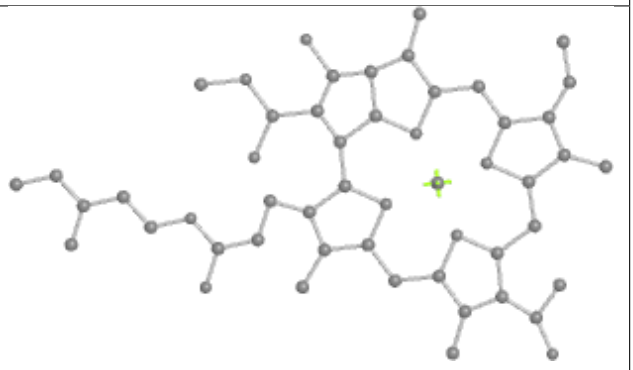
Bond lengths



Bond angles

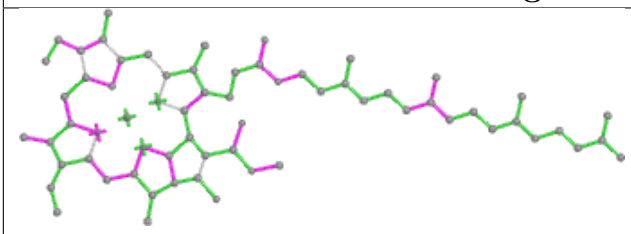


Torsions



Rings

Ligand CLA A 911



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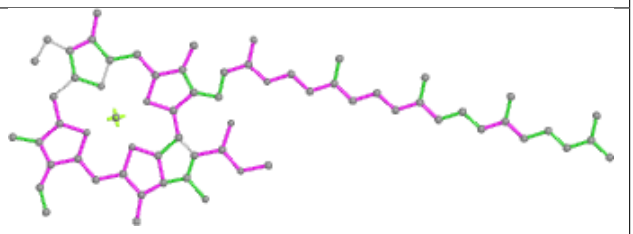
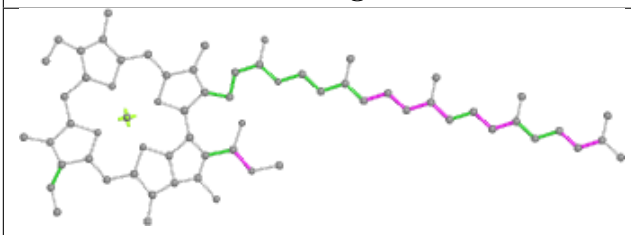
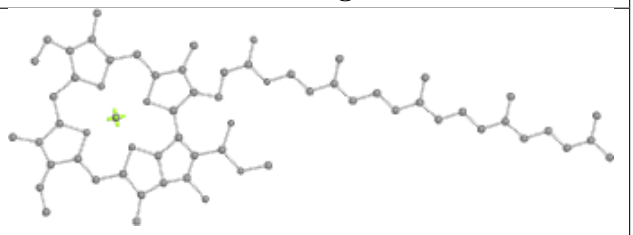


Bond angles

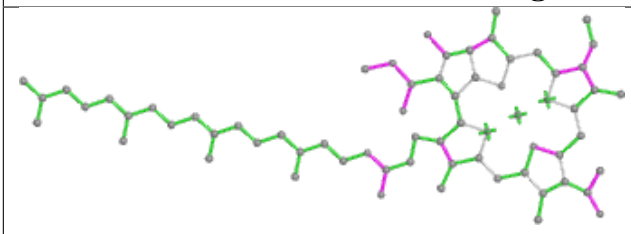


Torsions

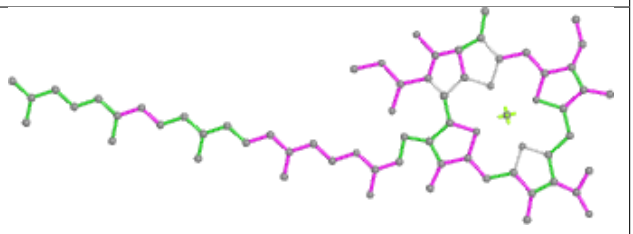


Rings

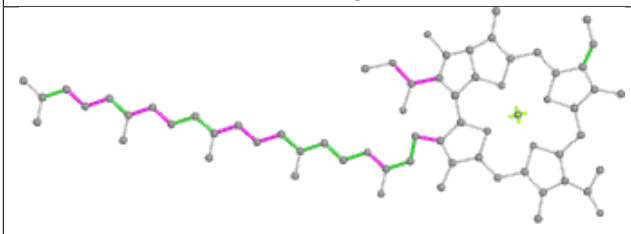
Ligand BCL a 905



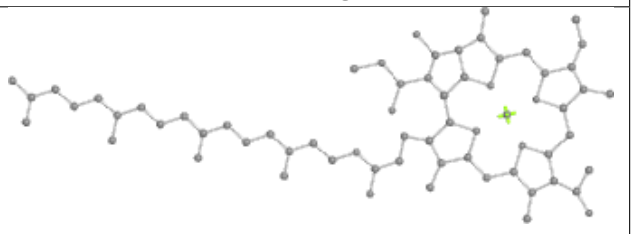
Bond lengths



Bond angles

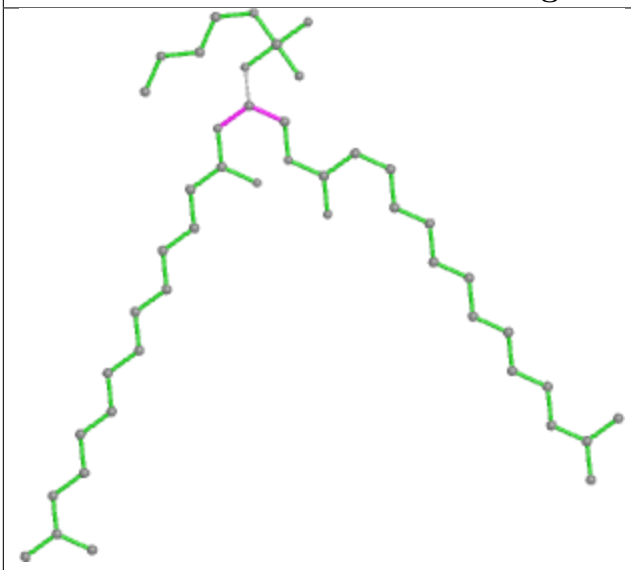


Torsions



Rings

Ligand 85I a 918



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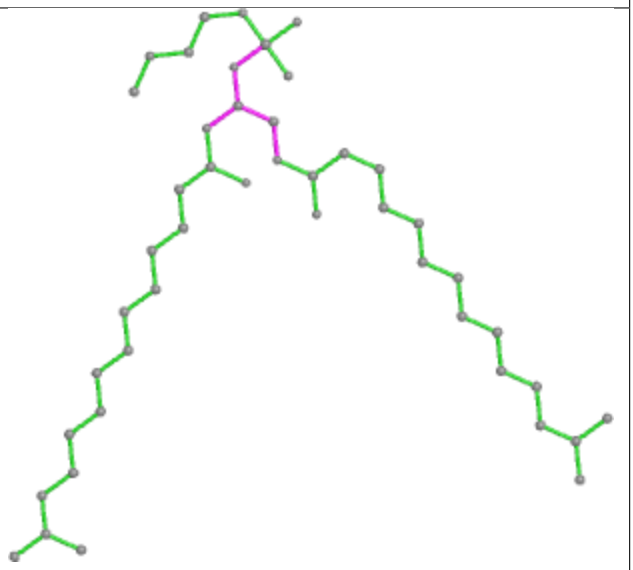
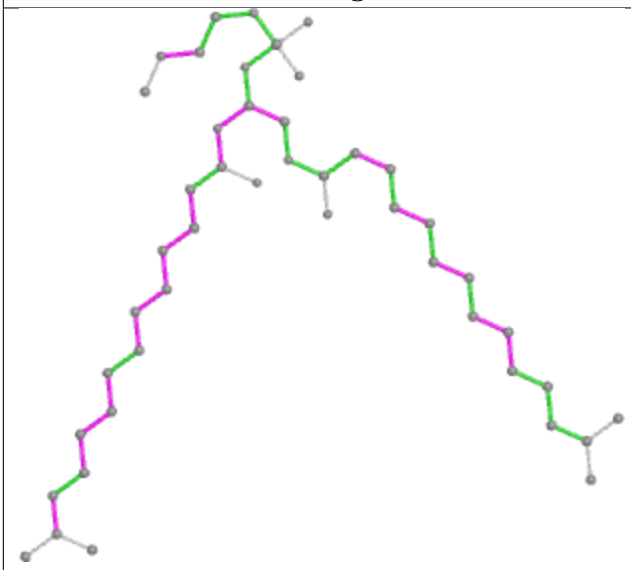
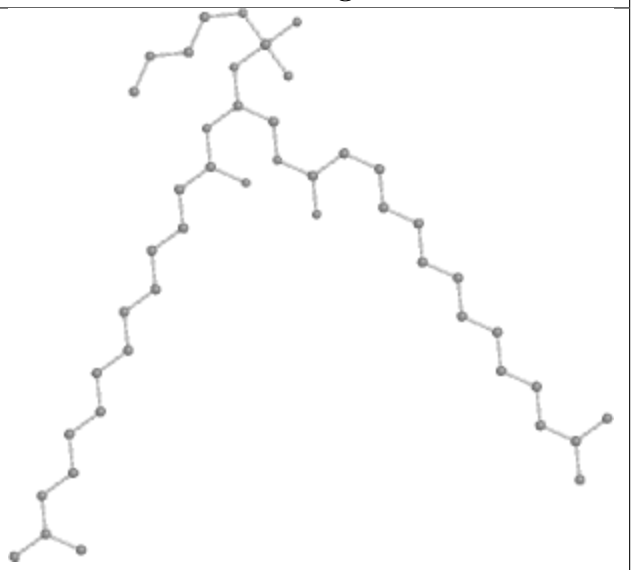


Bond angles

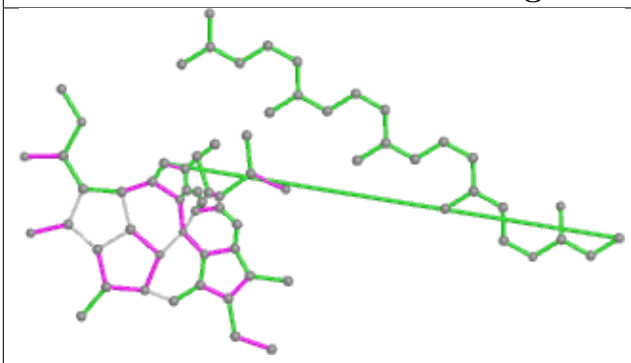


Torsions

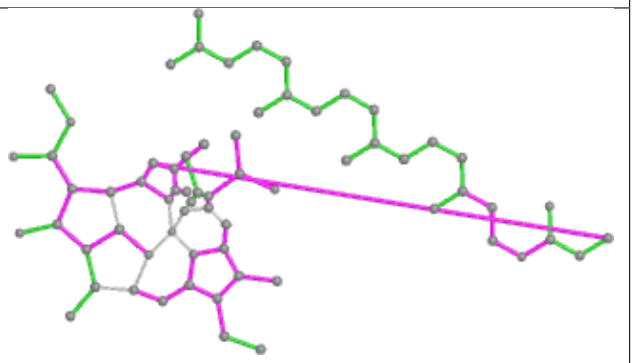


Rings

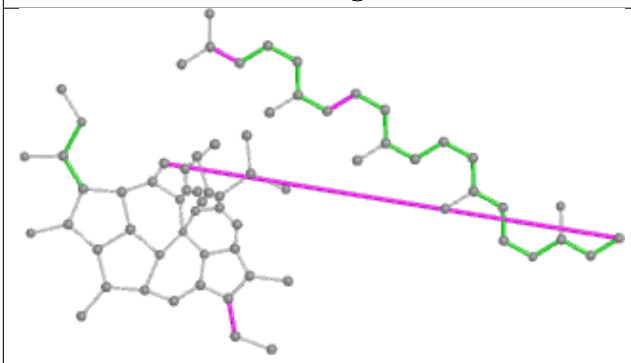
Ligand 2GO A 901



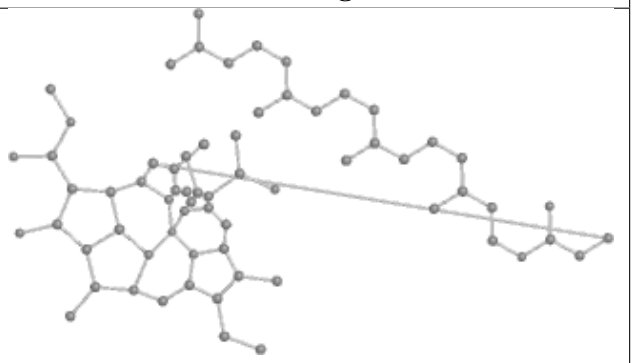
Bond lengths



Bond angles

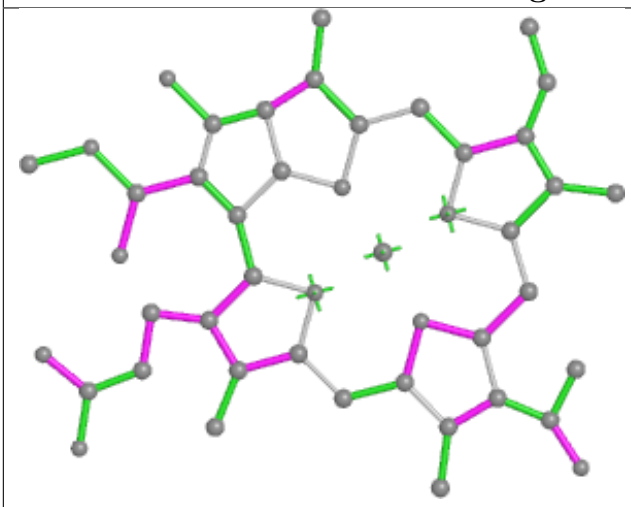


Torsions

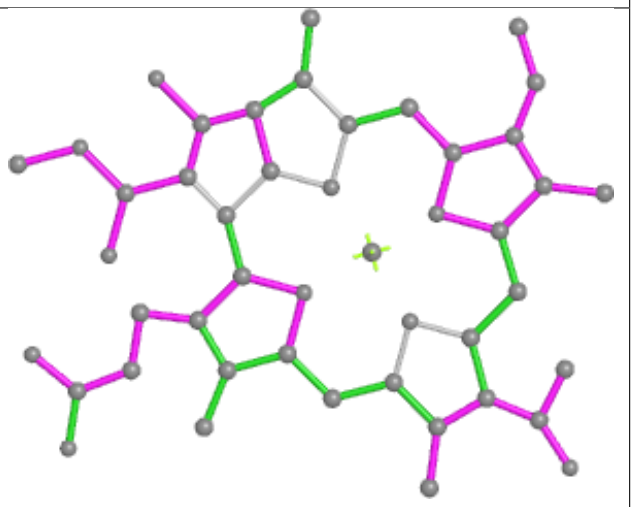


Rings

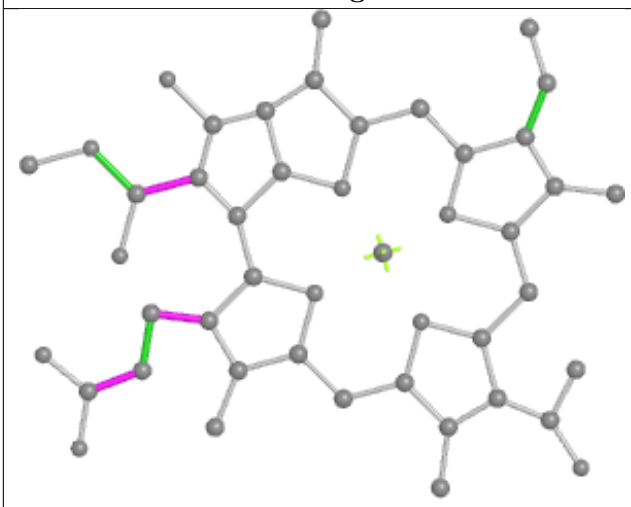
Ligand BCL a 906



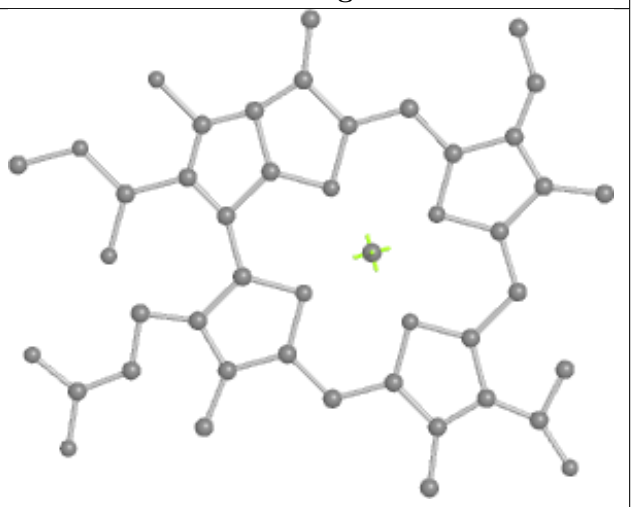
Bond lengths



Bond angles

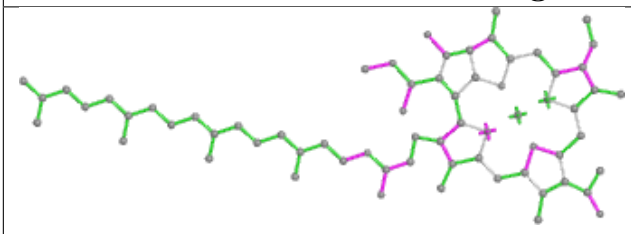


Torsions

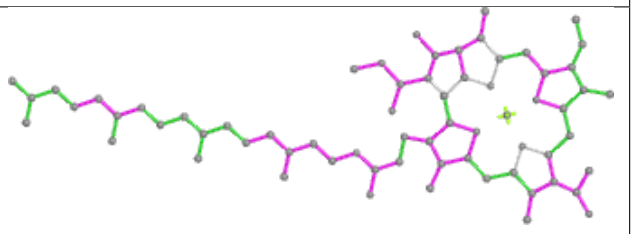


Rings

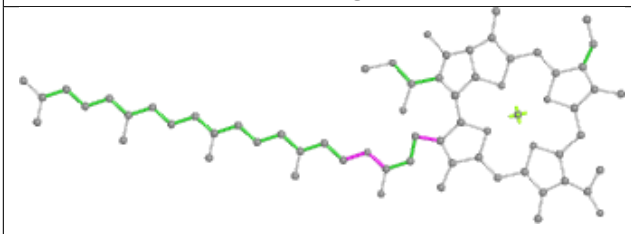
Ligand BCL a 911



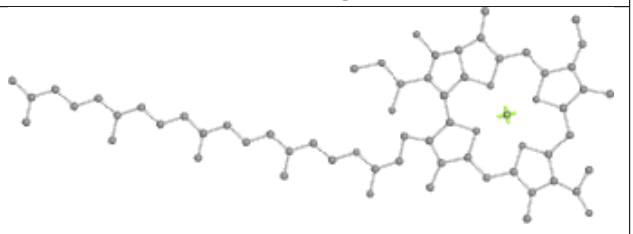
Bond lengths



Bond angles

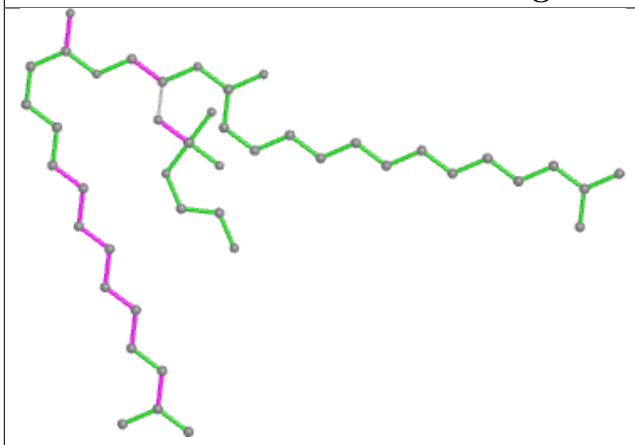


Torsions



Rings

Ligand 84Q E 101



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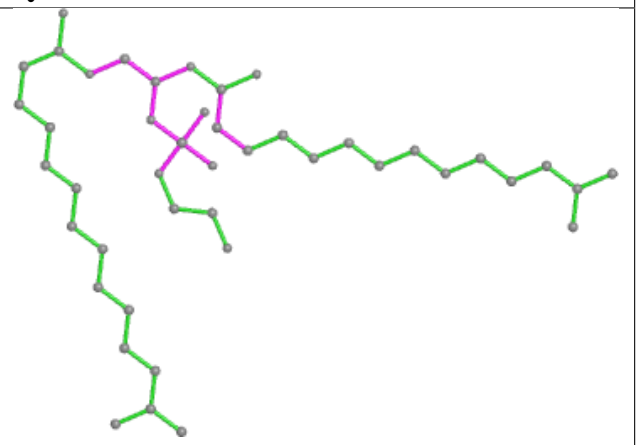
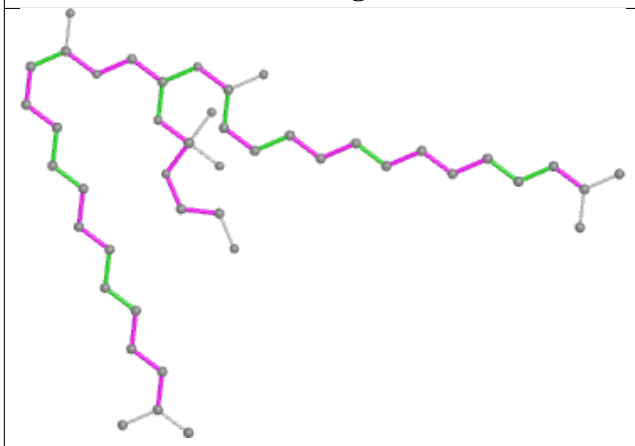


Bond angles



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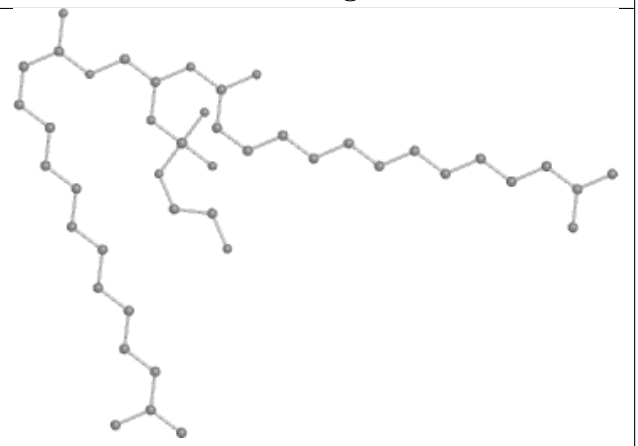
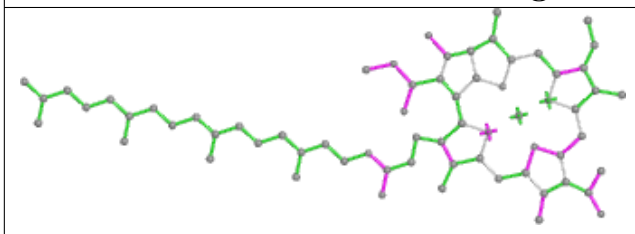
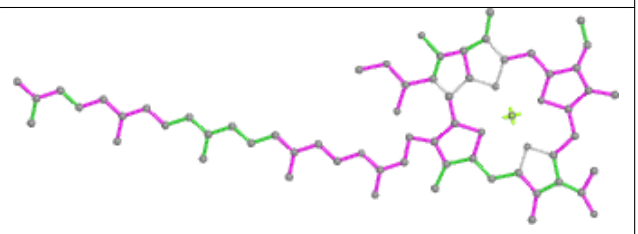


Rings

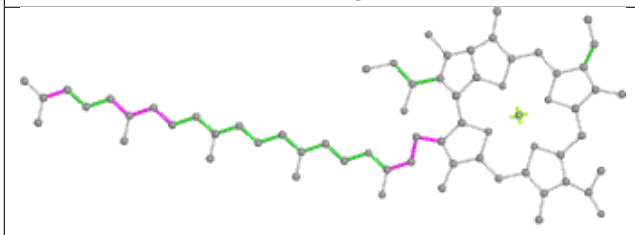
Ligand BCL a 910



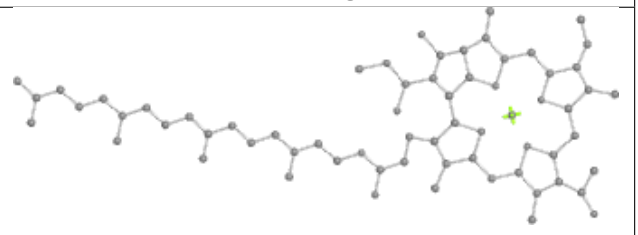
Bond lengths



Bond angles

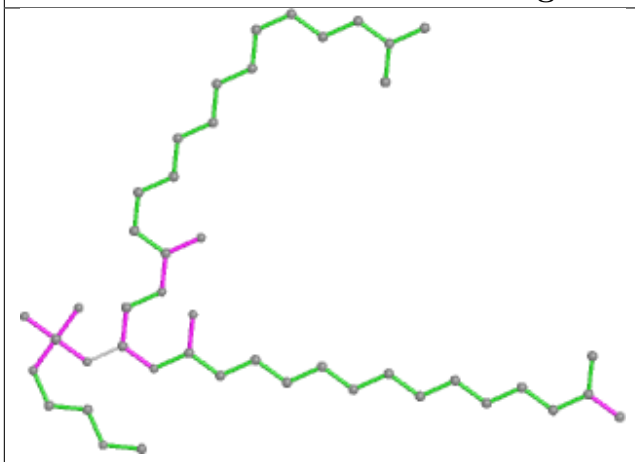


Torsions

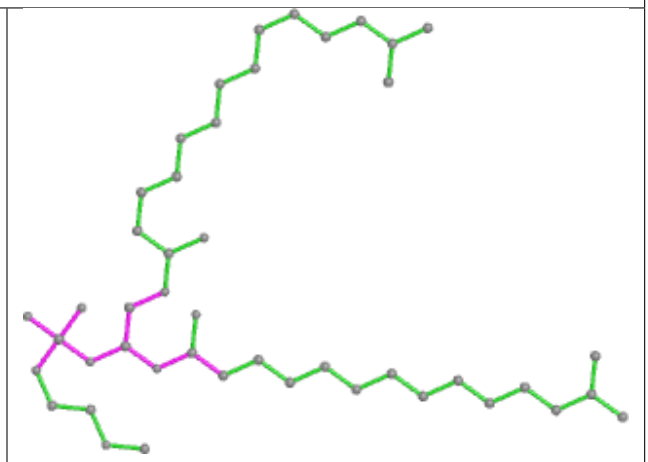


Rings

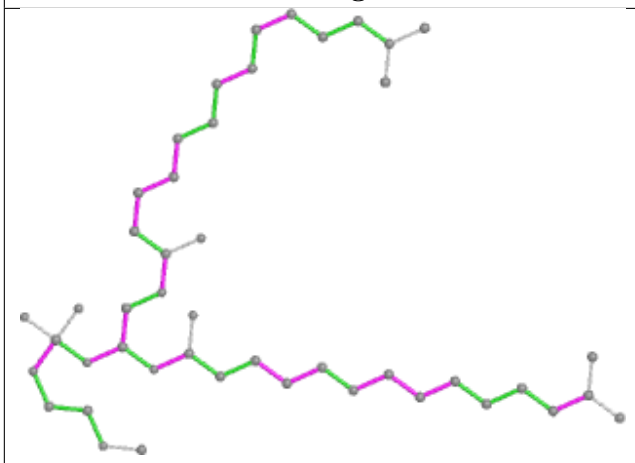
Ligand 85I A 915



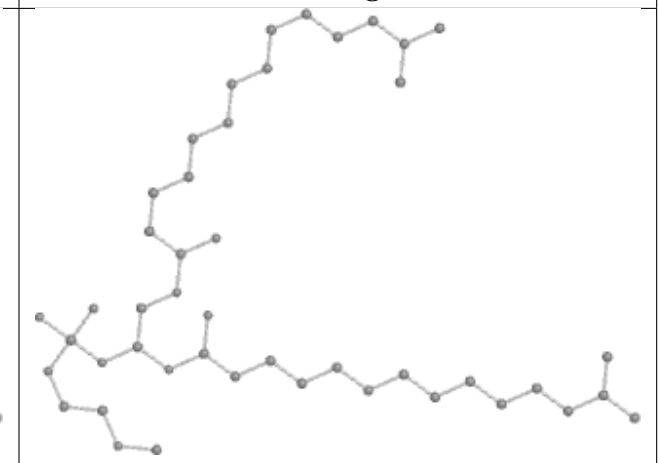
Bond lengths



Bond angles

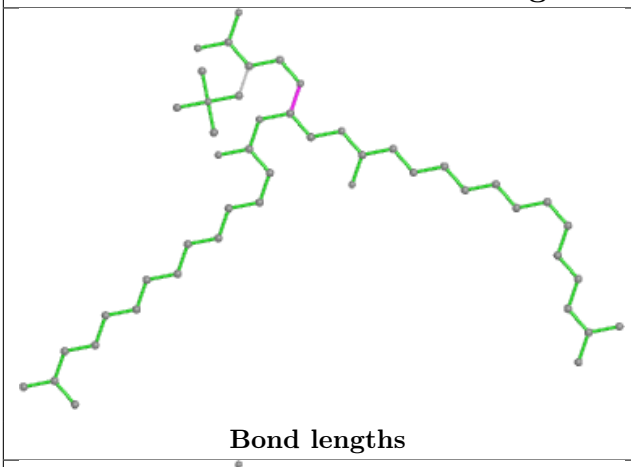


Torsions

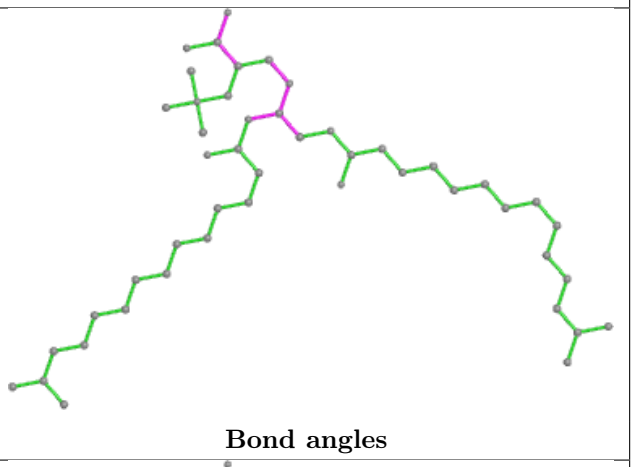


Rings

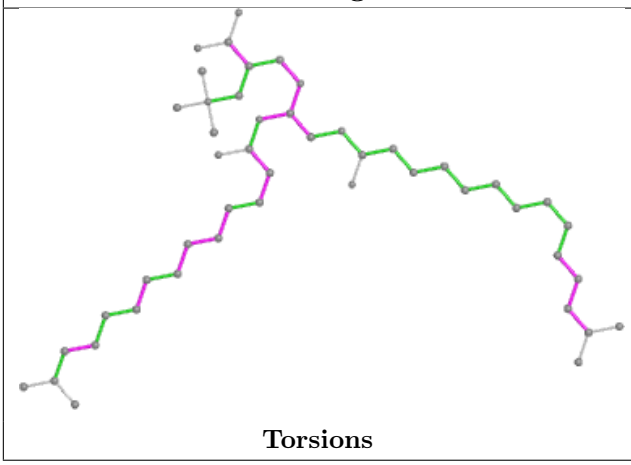
Ligand 85N A 932



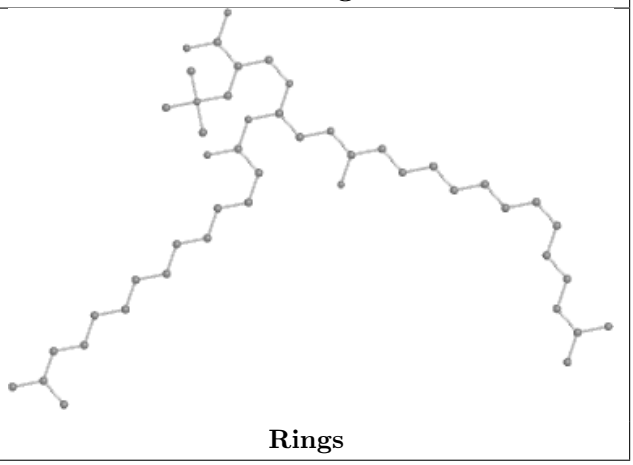
Bond lengths



Bond angles

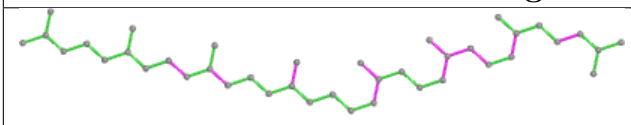


Torsions

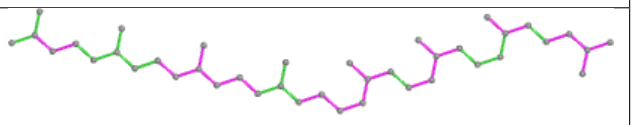


Rings

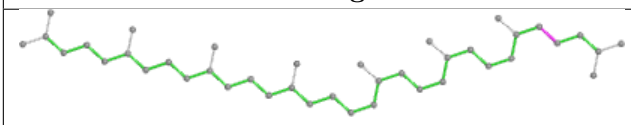
Ligand LYC A 913



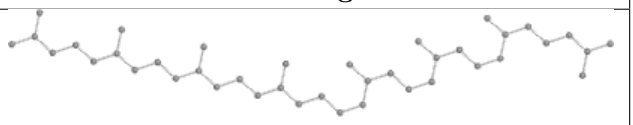
Bond lengths



Bond angles

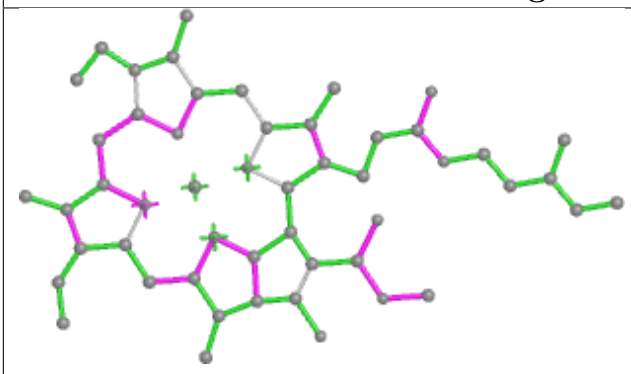


Torsions

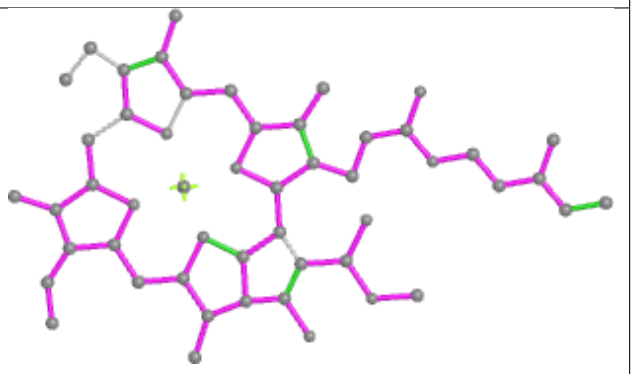


Rings

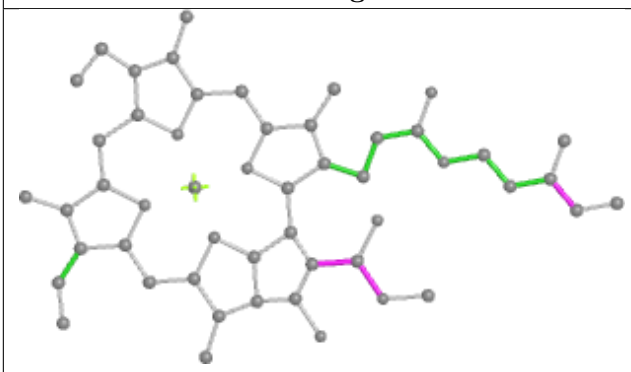
Ligand CLA a 915



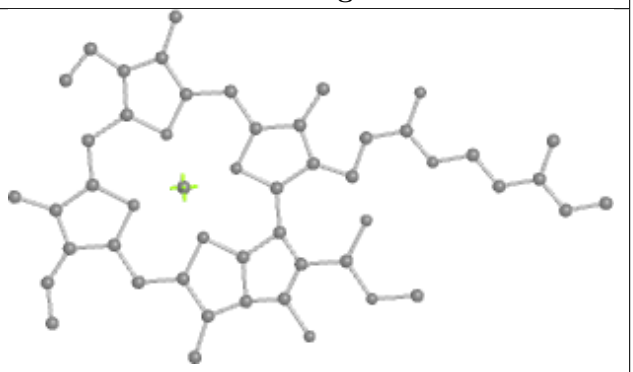
Bond lengths



Bond angles

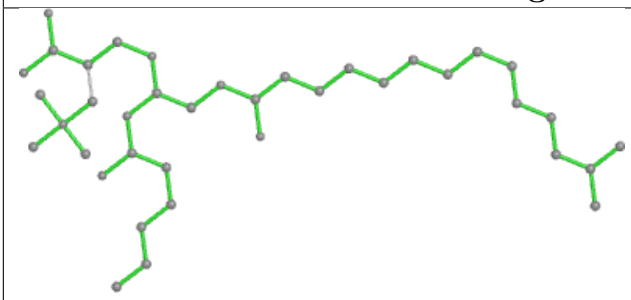


Torsions

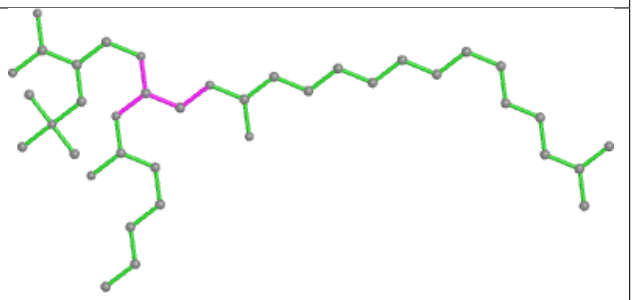


Rings

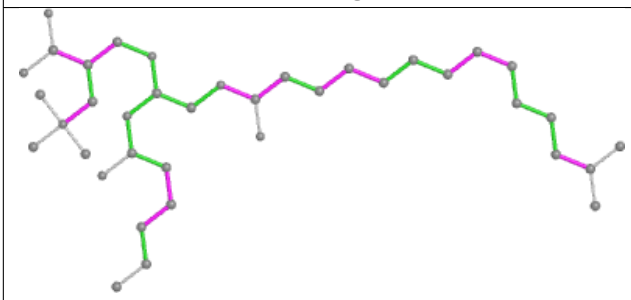
Ligand 85N G 101



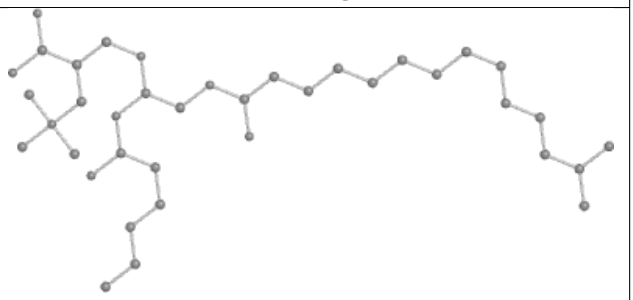
Bond lengths



Bond angles

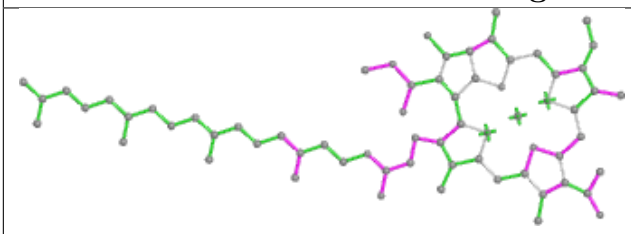


Torsions

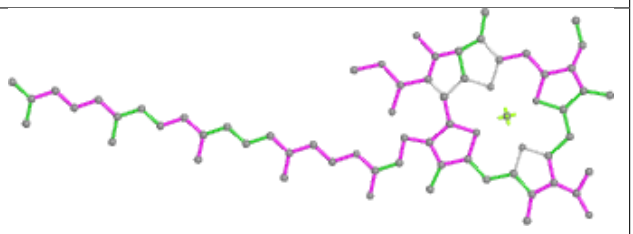


Rings

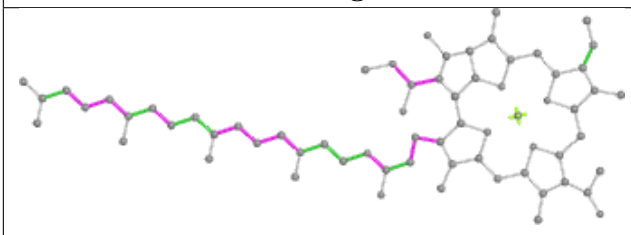
Ligand BCL a 908



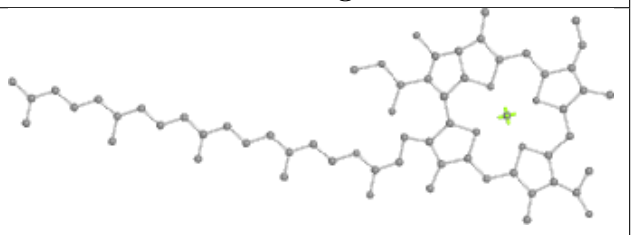
Bond lengths



Bond angles

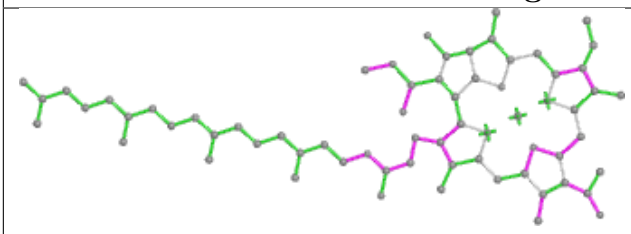


Torsions

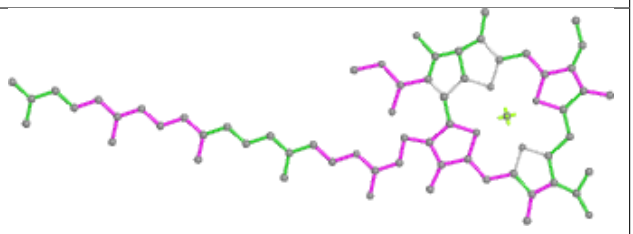


Rings

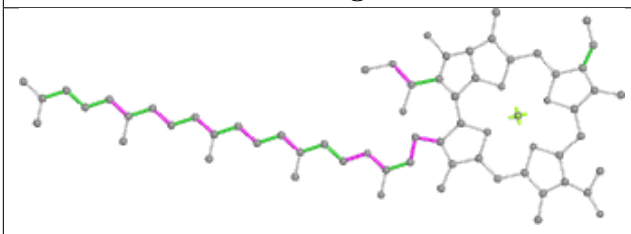
Ligand BCL A 905



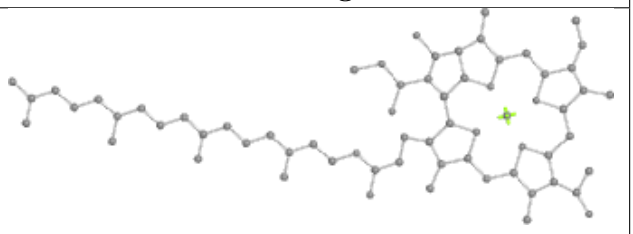
Bond lengths



Bond angles

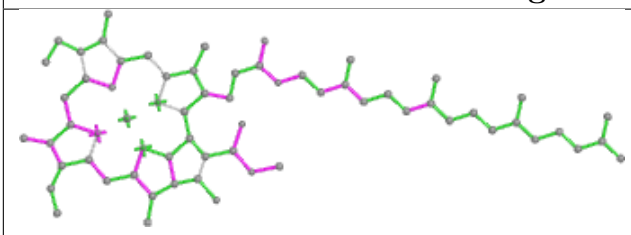


Torsions

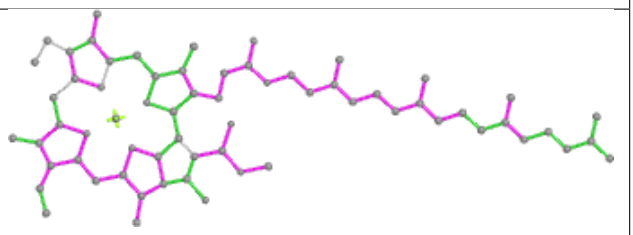


Rings

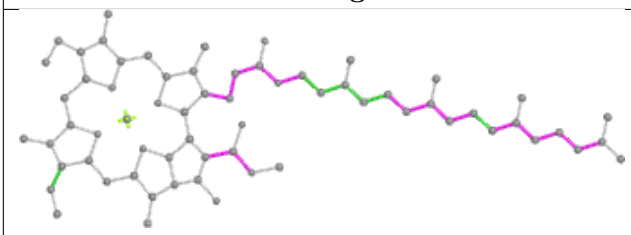
Ligand CLA a 901



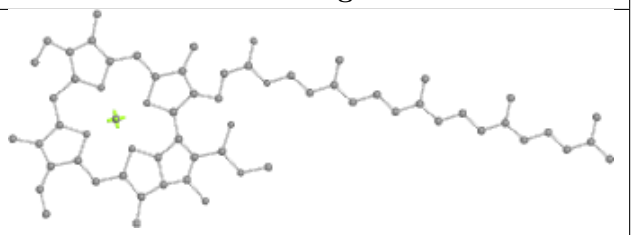
Bond lengths



Bond angles

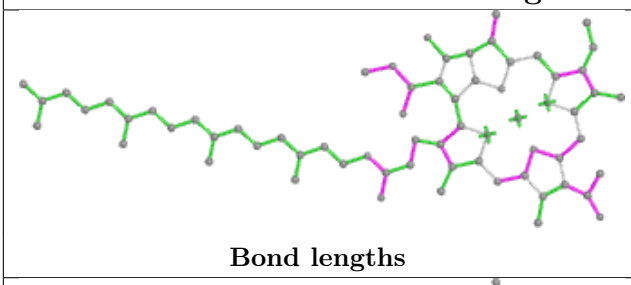


Torsions

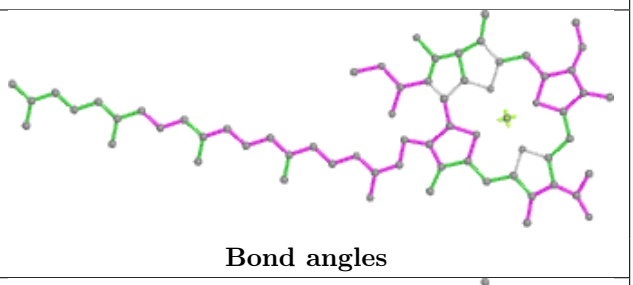


Rings

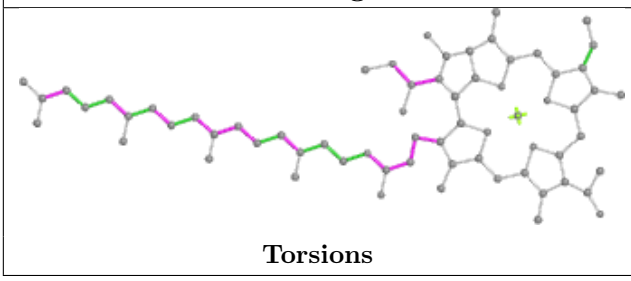
Ligand BCL A 903



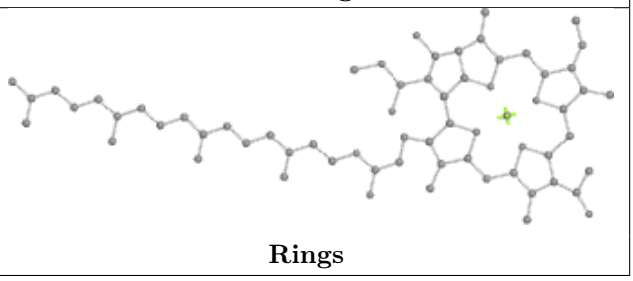
Bond lengths



Bond angles

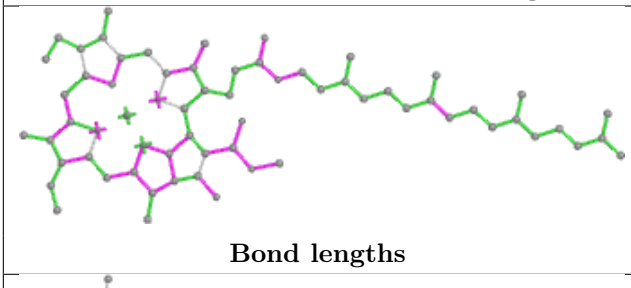


Torsions

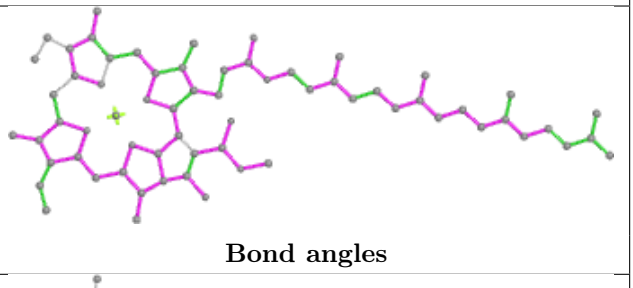


Rings

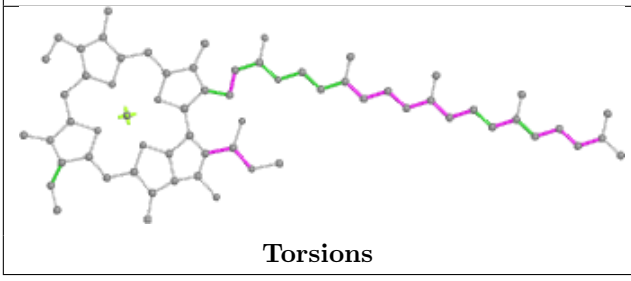
Ligand CLA A 931



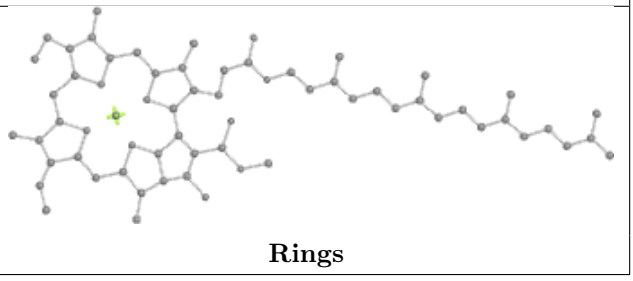
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

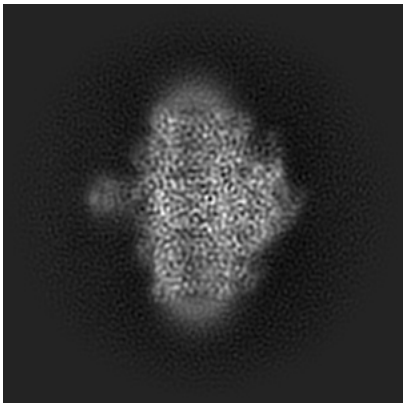
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32228. These allow visual inspection of the internal detail of the map and identification of artifacts.

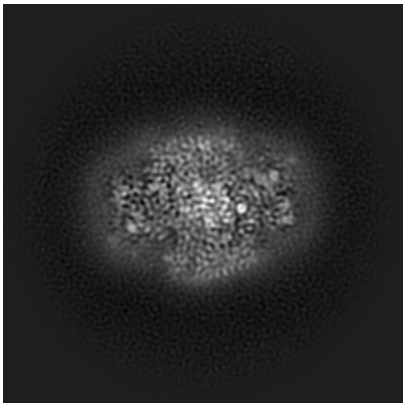
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

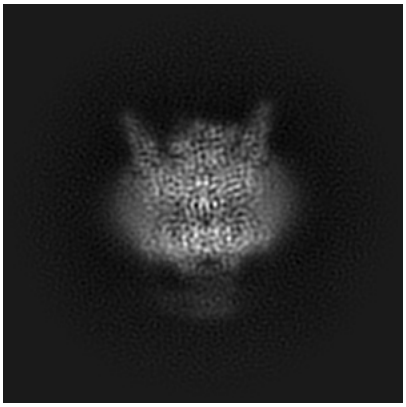
6.1.1 Primary map



X



Y

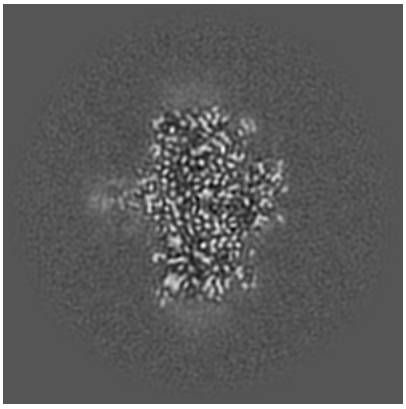


Z

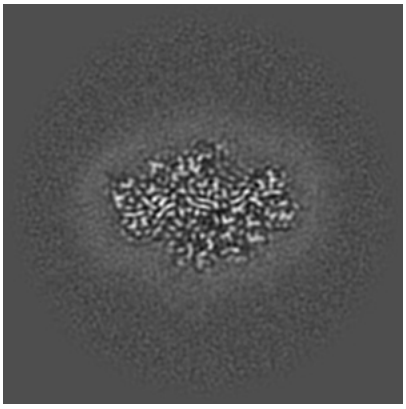
The images above show the map projected in three orthogonal directions.

6.2 Central slices

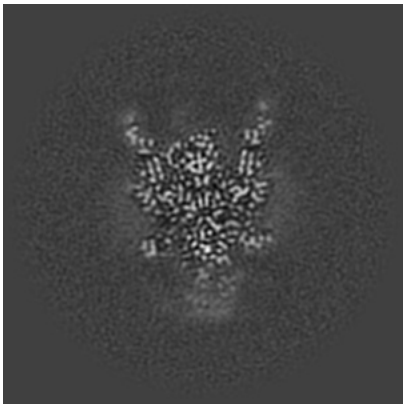
6.2.1 Primary map



X Index: 110



Y Index: 110

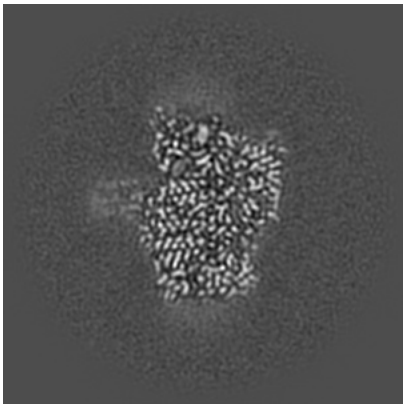


Z Index: 110

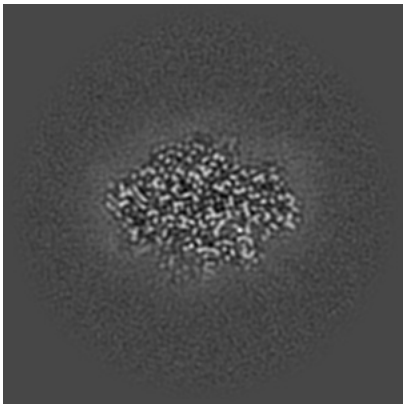
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

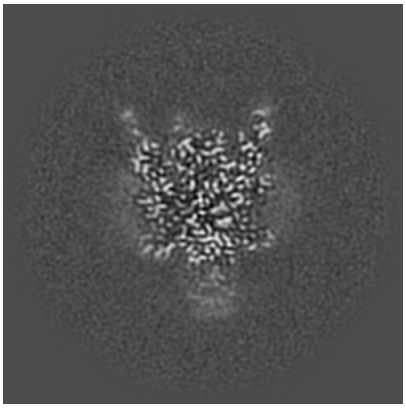
6.3.1 Primary map



X Index: 116



Y Index: 118

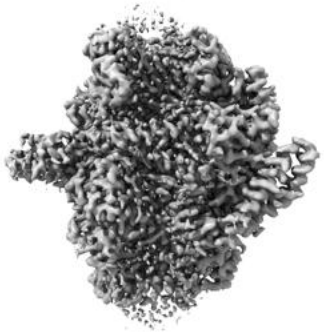


Z Index: 107

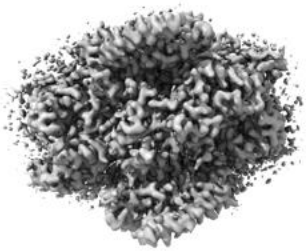
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

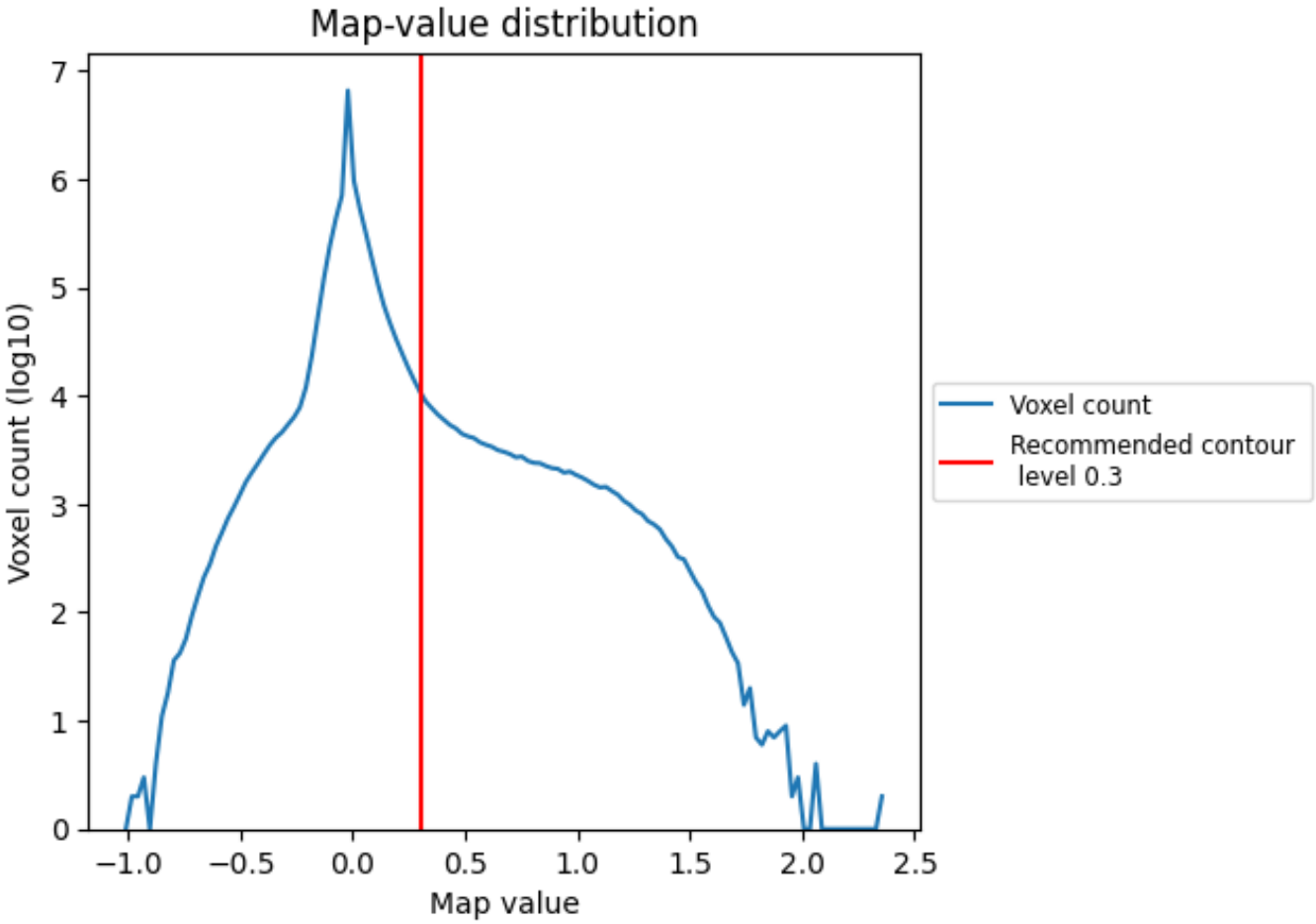
6.5 Mask visualisation (i)

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

7 Map analysis

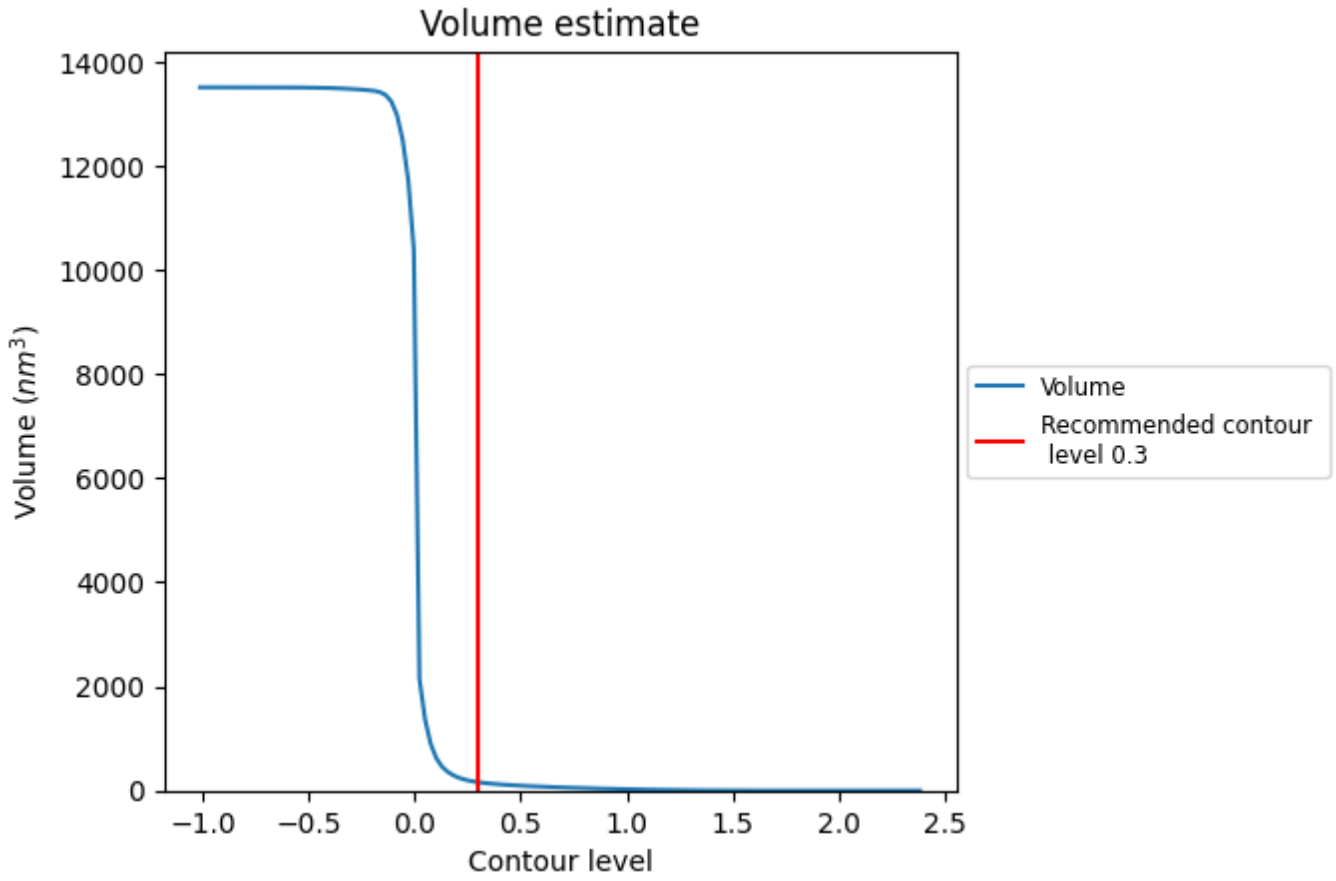
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

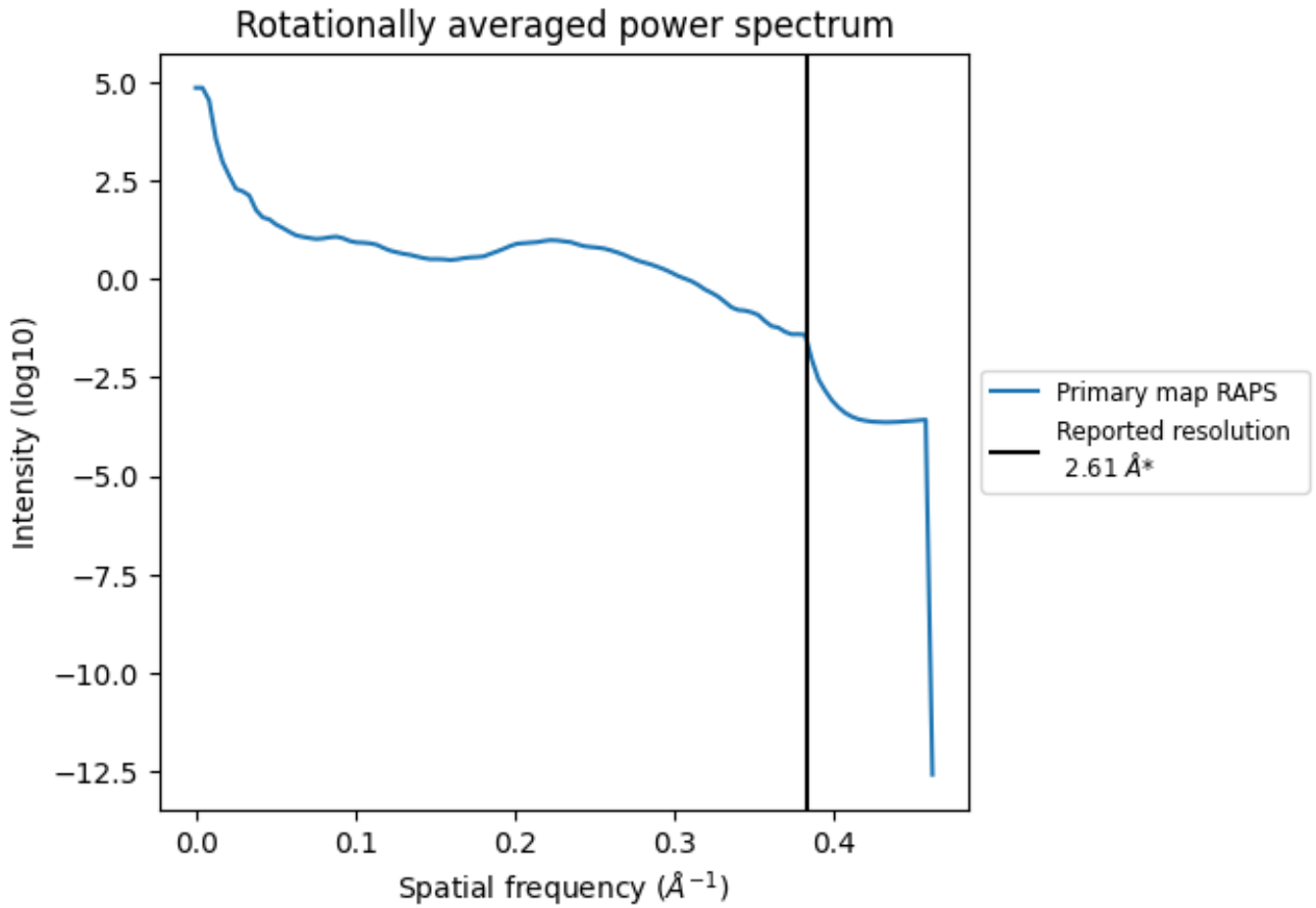
7.2 Volume estimate



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 144 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.383 $Å^{-1}$

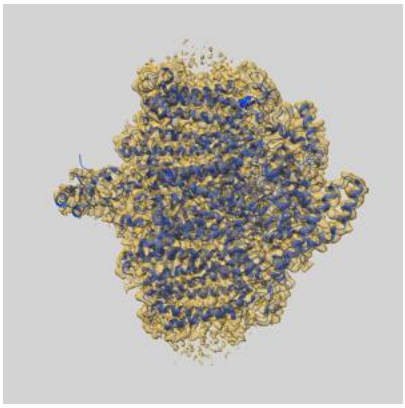
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

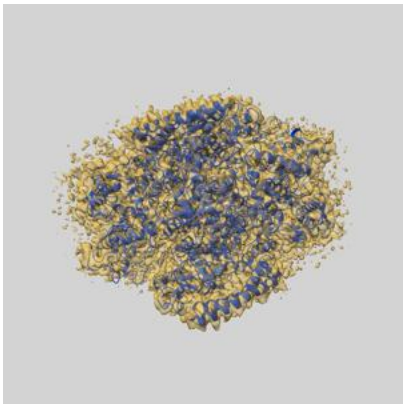
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32228 and PDB model 7VZG. Per-residue inclusion information can be found in section 3 on page 14.

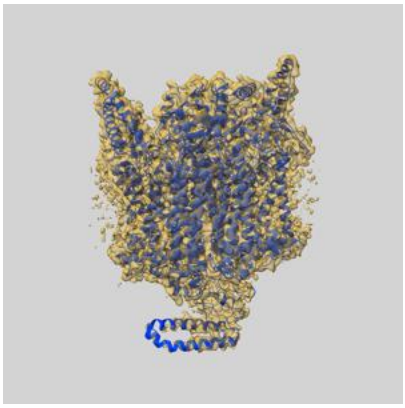
9.1 Map-model overlay



X



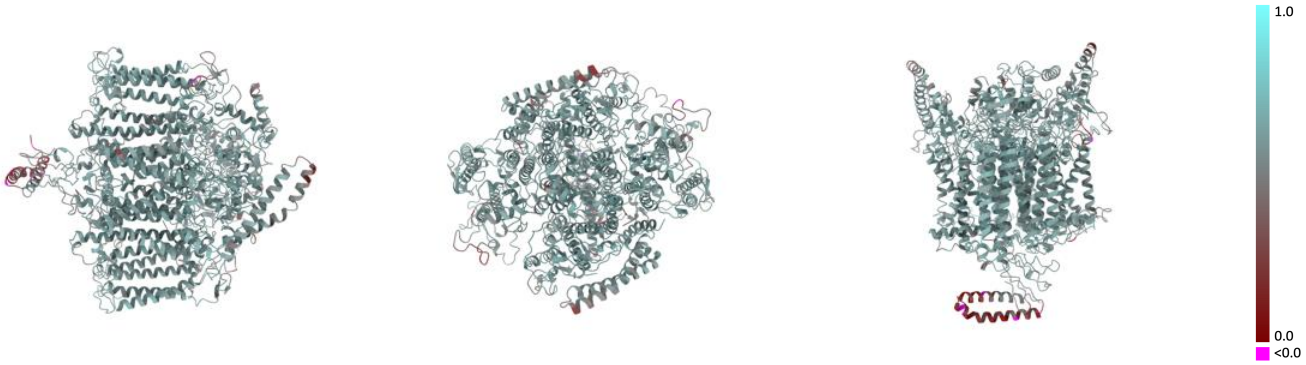
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

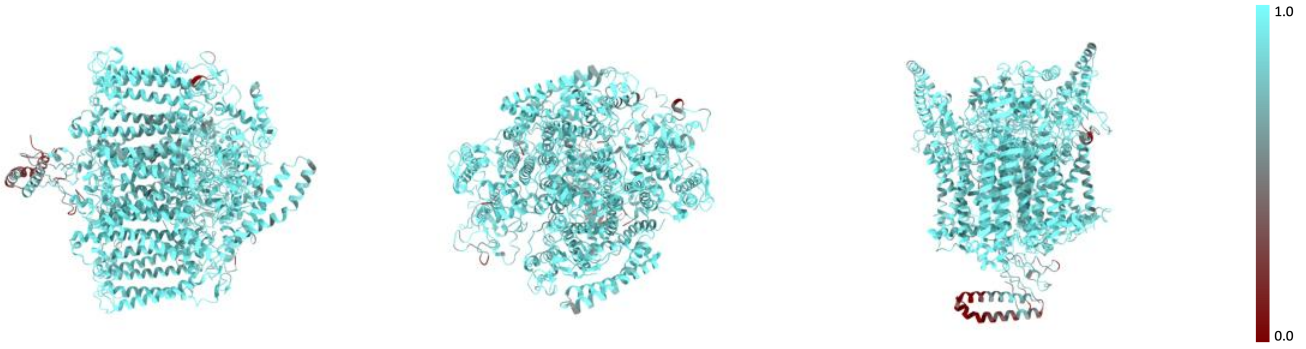
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

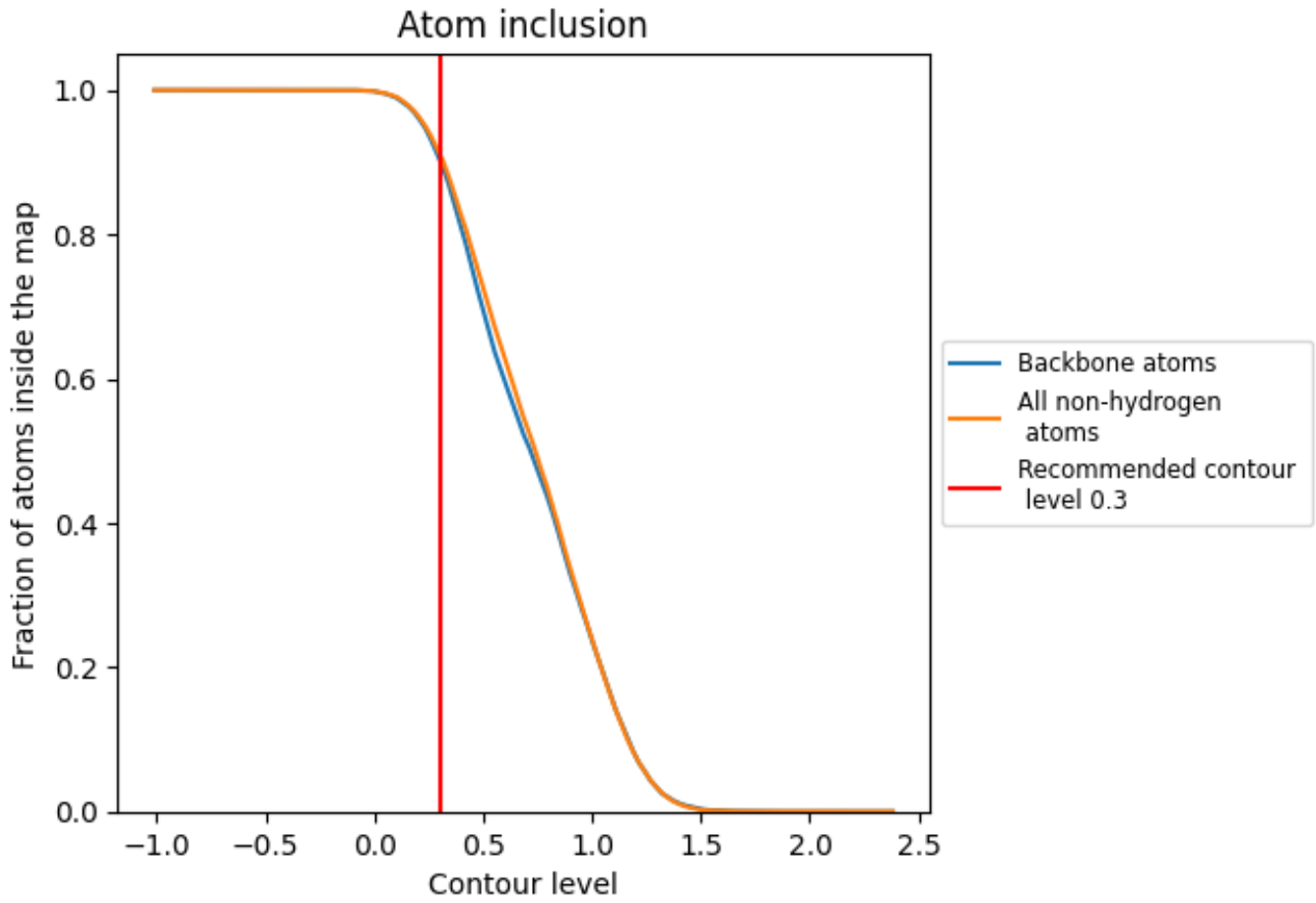
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9117	0.5780
A	0.9439	0.5910
B	0.6696	0.5210
C	0.9323	0.5780
D	0.3566	0.2470
E	0.9080	0.5740
F	0.9331	0.5960
G	0.7092	0.5340
H	0.8421	0.5600
a	0.9437	0.5910
c	0.9258	0.5760
e	0.8901	0.5780
f	0.9442	0.5880
g	0.8309	0.5940
h	0.8526	0.5770