Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:39 AM JST

PDB ID	:	7VZR / pdb_00007vzr
EMDB ID	:	EMD-32229
Title	:	Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the smaller form)
Authors	:	Huang, G.Q.; Dong, S.S.; Qin, X.C.; Sui, S.F.
Deposited on	:	2021-11-16
Resolution	:	2.22 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:

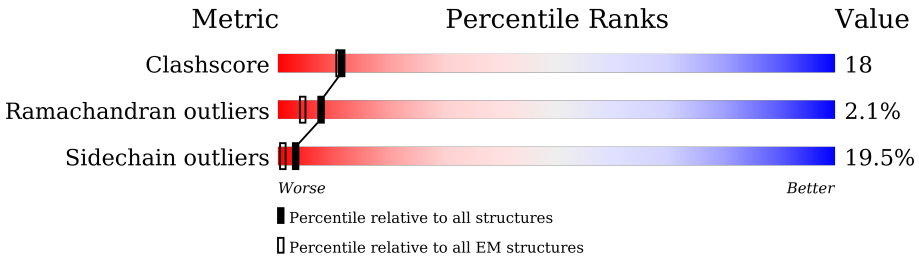
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

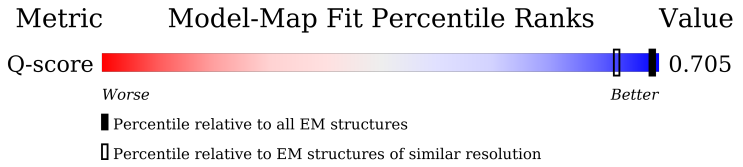
1 Overall quality at a glance

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

The reported resolution of this entry is 2.22 Å.

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





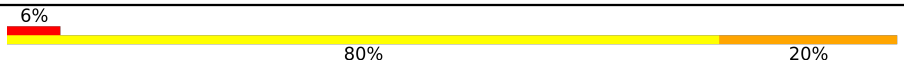
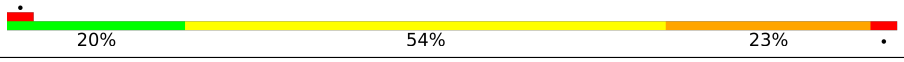
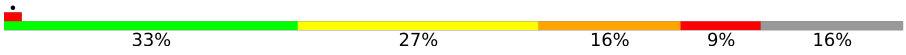
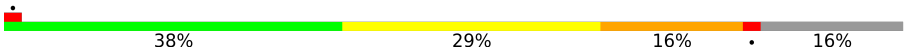
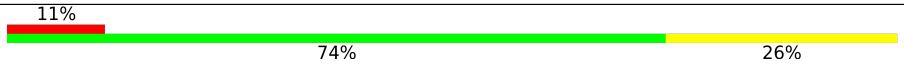
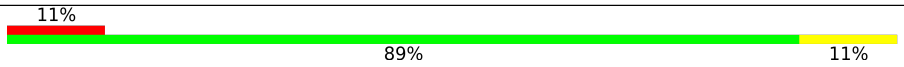
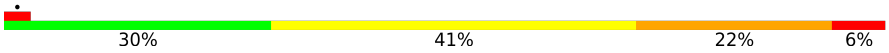
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3277 (1.73 - 2.72)

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	865	52% 32% 11%
1	a	865	58% 29% 9%
2	C	221	37% 33% 11% 7% 13%
3	E	35	23% 60% 17%
3	e	35	46% 43% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	35	
4	f	35	
5	G	45	
5	g	45	
6	H	19	
6	h	19	
7	c	145	

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
10	CLA	A	910	X	-	-	-
10	CLA	A	911	X	-	-	-
11	LYC	c	201	-	X	-	-
14	UNL	A	922	-	-	X	-
14	UNL	A	923	-	-	X	-
14	UNL	A	927	-	-	X	-
14	UNL	C	302	-	-	X	-
14	UNL	a	926	-	-	X	-
14	UNL	a	930	-	-	X	-
14	UNL	a	931	-	-	X	-
16	HEC	C	301	X	X	-	-
16	HEC	c	202	X	-	-	-
18	SF4	a	917	-	-	X	-
8	2GO	A	901	X	-	-	-
8	2GO	a	903	X	-	-	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 21354 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 Photosynthetic reaction center subunit M.

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		

Continued on next page...

Continued from previous page...

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

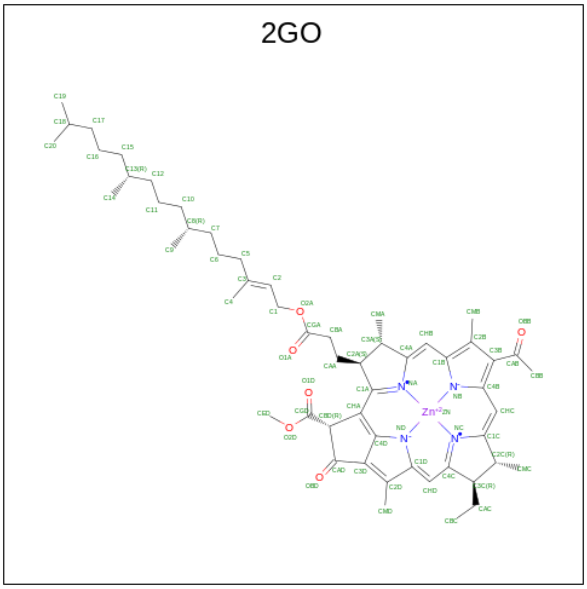
- Molecule 6 is a protein called undefined polypeptide.

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 (T-4-S)-[(3S,4S,13R,14R,21R,23R,25R)-9-acetyl-14-ethyl-21-(methoxycarbonyl)-4,8,13,18-tetramethyl-20-oxo-3-(3-oxo-3-{[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]oxy}propyl)-23,25-didehydro-13,14-dihydrophorbine-23,25-diido-kappa 4 N 23 ,N 24 , N 25 ,N 26]zinc (CCD ID: 2GO) (formula: $C_{55}H_{74}N_4O_6Zn$) (labeled as "Ligand of Interest" by depositor).



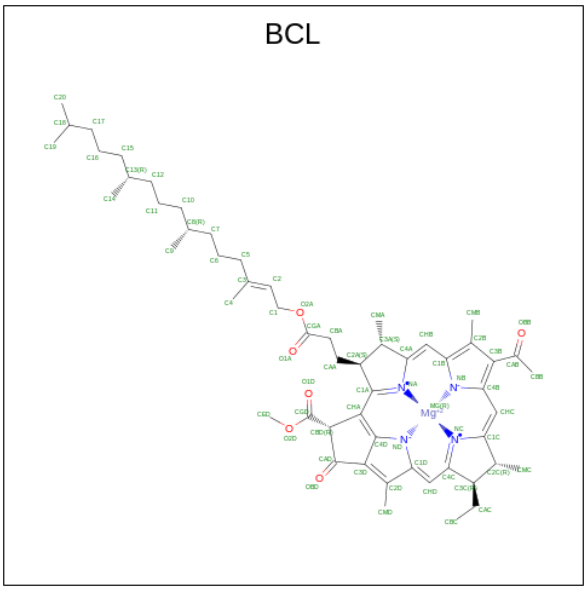
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	Zn	0
			66	55	4	6	1	

Continued on next page...

Continued from previous page...

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

- Molecule 9 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



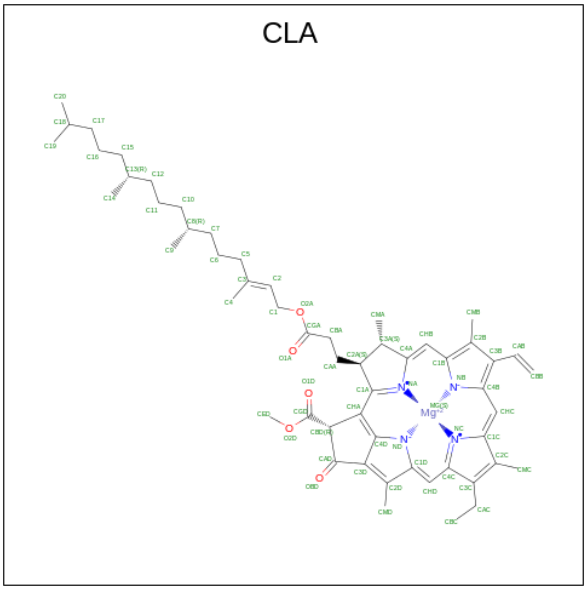
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
9	A	1	Total	C	Mg	N	O	0
			66	55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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
9	a	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



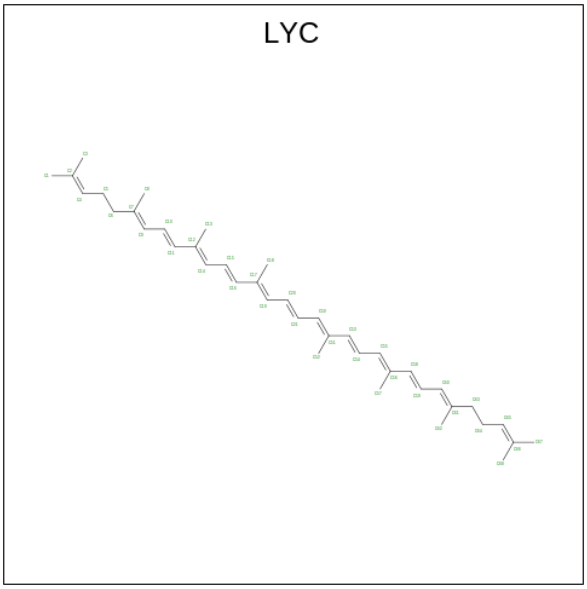
Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

Continued on next page...

Continued from previous page...

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

- Molecule 11 is LYCOPENE (CCD ID: LYC) (formula: $C_{40}H_{56}$).

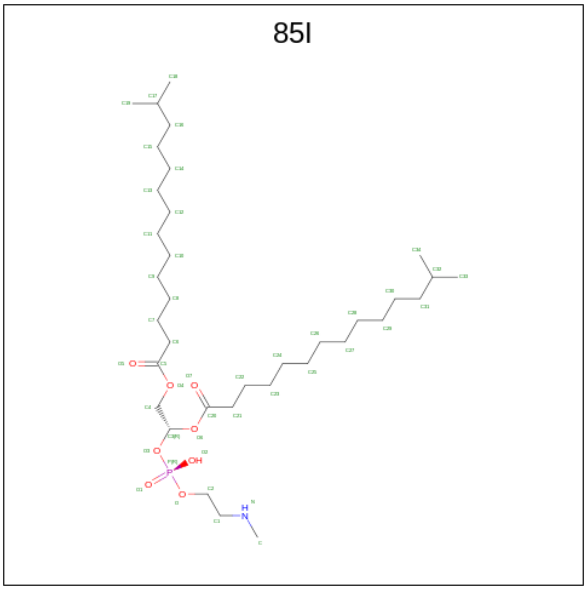


Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total 40	C 40	0
11	c	1	Total 40	C 40	0

- Molecule 12 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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



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

- Molecule 14 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

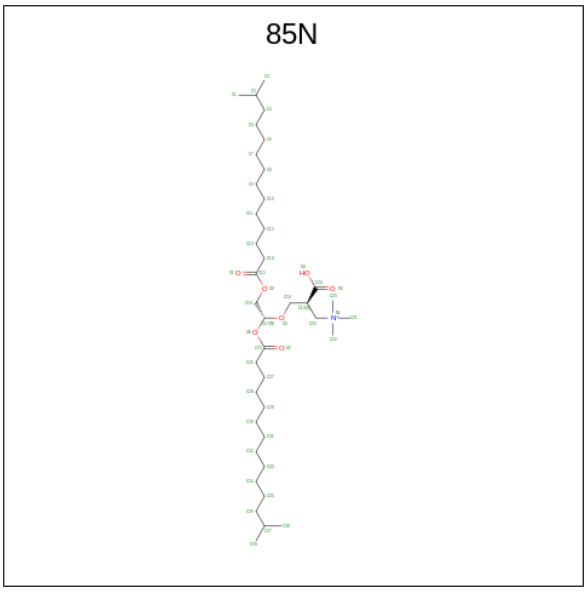
Mol	Chain	Residues	Atoms		AltConf
14	A	13	Total	C	0
			240	240	
14	C	1	Total	C	0
			18	18	
14	E	2	Total	C	0
			26	26	

Continued on next page...

Continued from previous page...

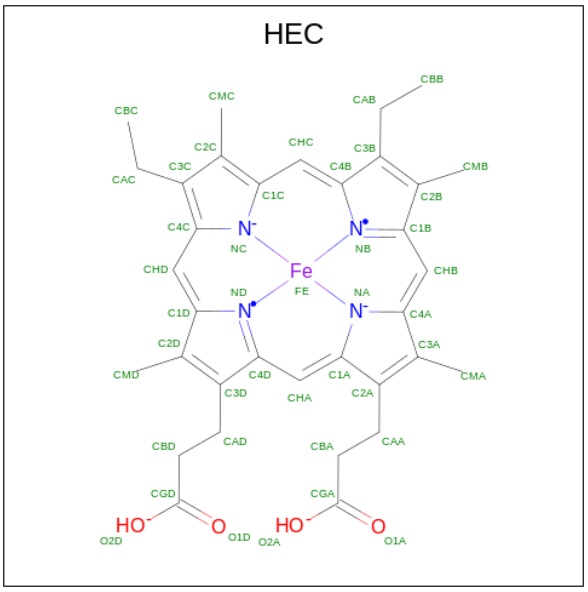
Mol	Chain	Residues	Atoms	AltConf
14	a	13	Total C 243 243	0
14	c	1	Total C 8 8	0
14	e	2	Total C 26 26	0

- Molecule 15 is [(2 {S})-2-[[(1 {R})-1,2-bis(13-methyltetradecanoyloxy)ethoxy]methyl]-3-oxidanyl-3-oxidanylidene-propyl]-trimethyl-azanium (CCD ID: 85N) (formula: $C_{39}H_{76}NO_7$) (labeled as "Ligand of Interest" by depositor).



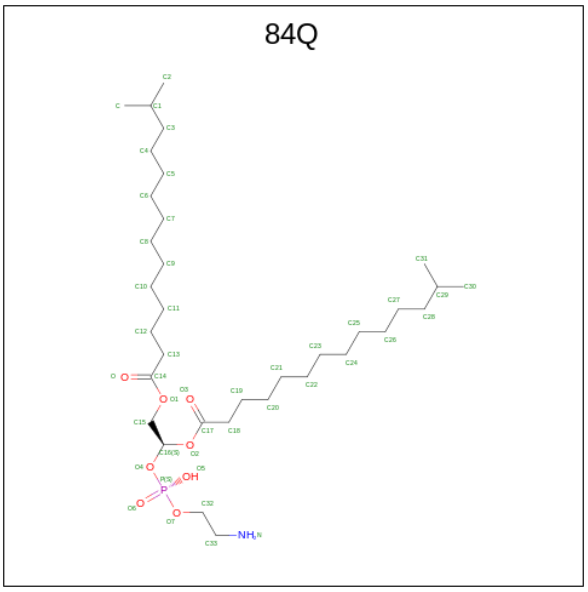
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C N O 47 39 1 7	0
15	G	1	Total C N O 38 30 1 7	0
15	a	1	Total C N O 47 39 1 7	0
15	g	1	Total C N O 38 30 1 7	0

- Molecule 16 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is [(2S)-2-[2-azanylethoxy(oxidanyl)phosphoryl]oxy-2-(13-methyltetradecanoyloxy)ethyl] 13-methyltetradecanoate (CCD ID: 84Q) (formula: $C_{34}H_{68}NO_8P$) (labeled as "Ligand of Interest" by depositor).



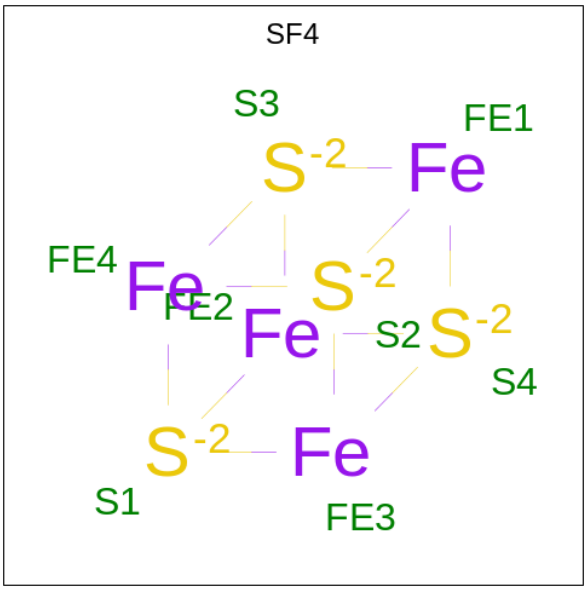
Mol	Chain	Residues	Atoms					AltConf
17	E	1	Total	C	N	O	P	0
			44	34	1	8	1	

Continued on next page...

Continued from previous page...

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

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is water.

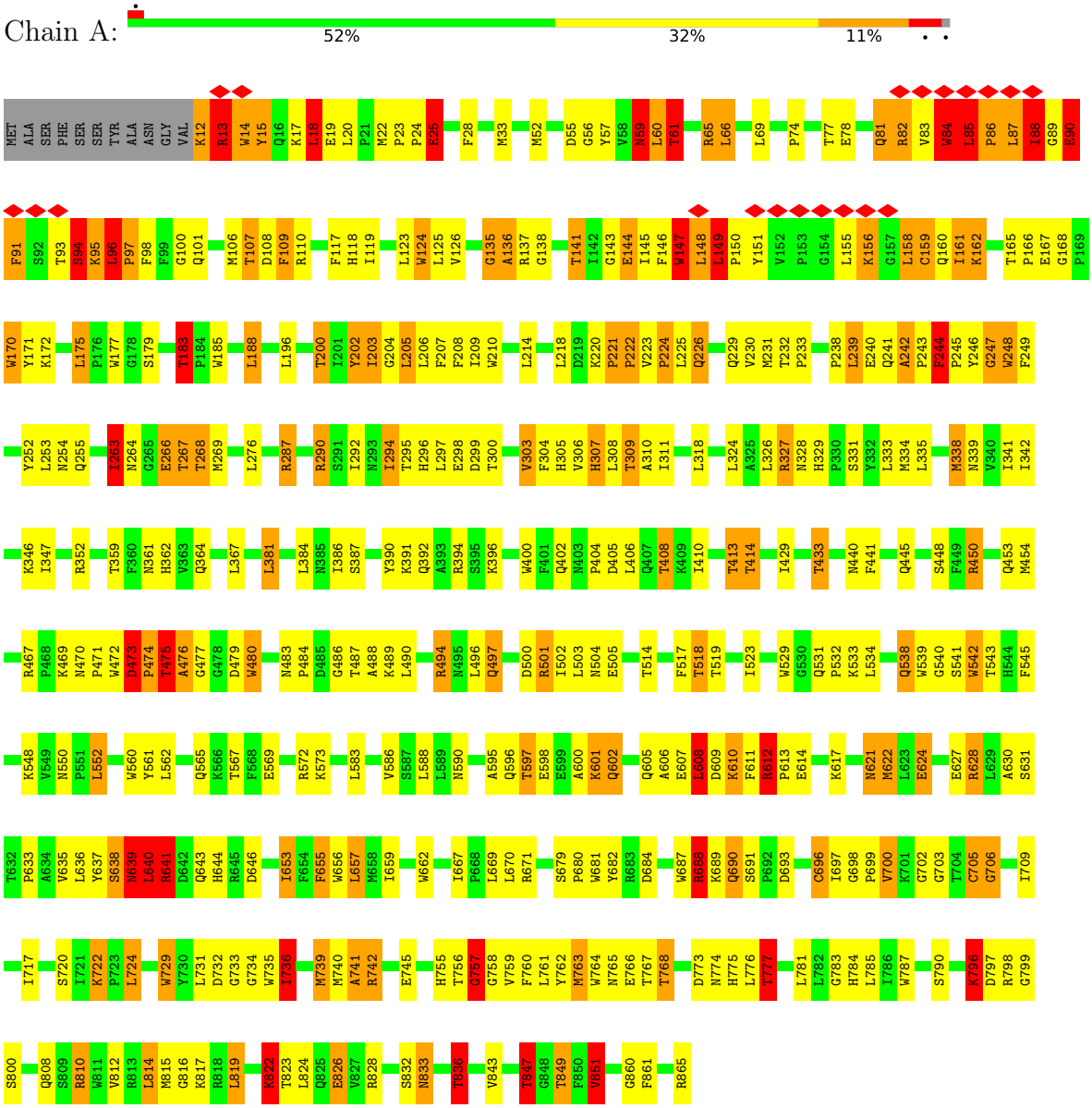
Mol	Chain	Residues	Atoms		AltConf
19	A	3	Total	O	0
			3	3	
19	a	3	Total	O	0
			3	3	

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.

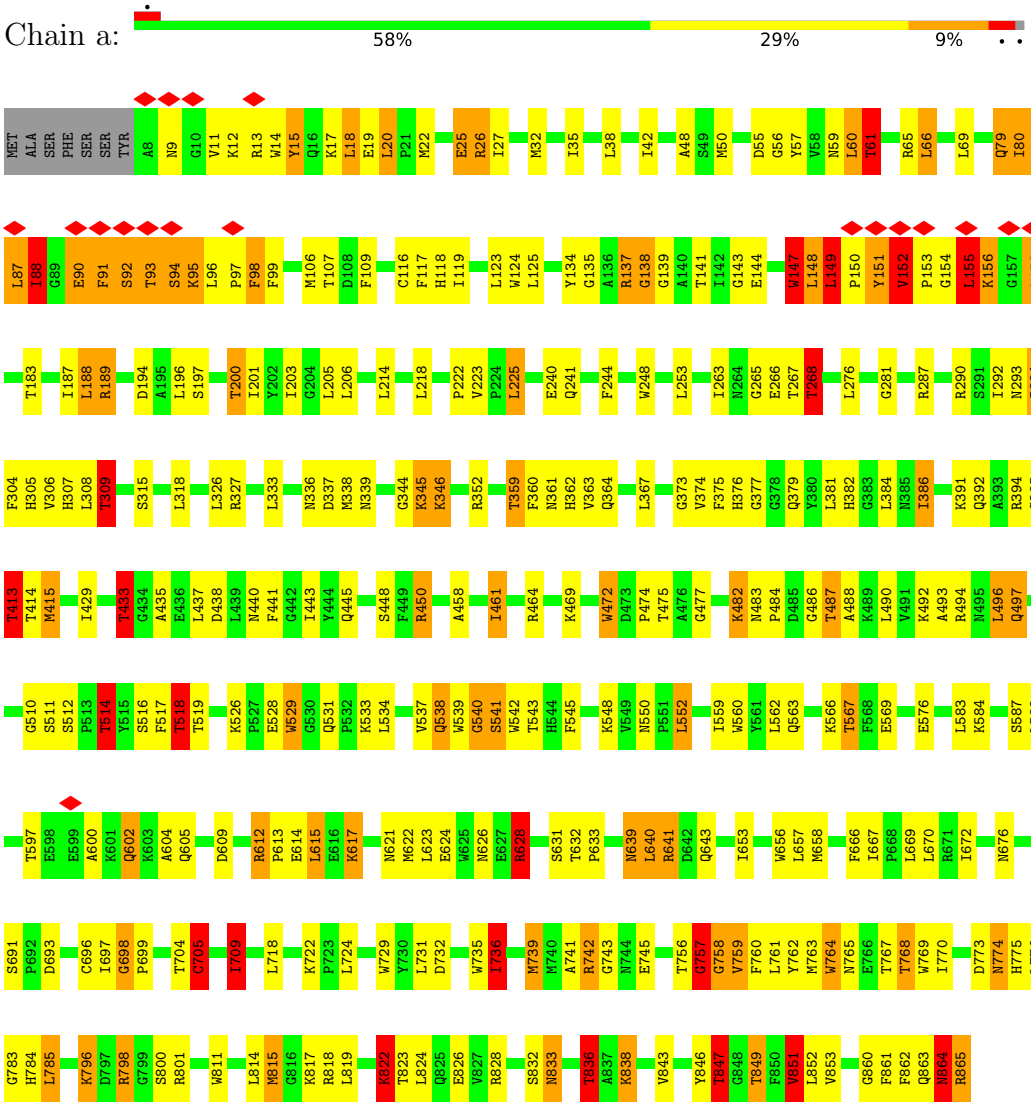
• Molecule 1: Photosynthetic reaction center subunit M

Chain A:



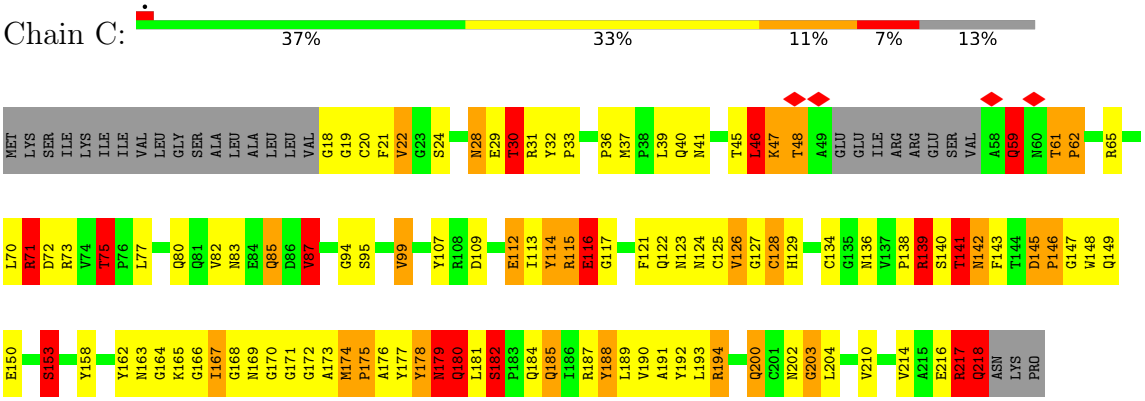
• Molecule 1: Photosynthetic reaction center subunit M

Chain a:



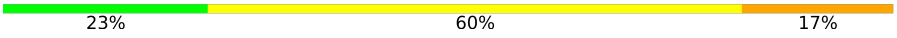
• Molecule 2: Cytochrome c, mono-and diheme variants

Chain C:



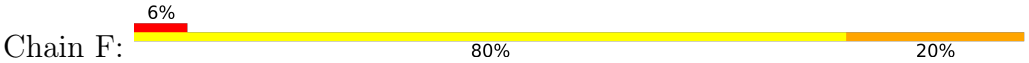
• Molecule 3: PscE

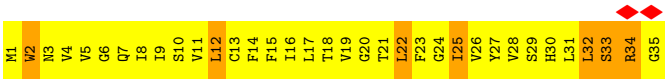
Chain E:



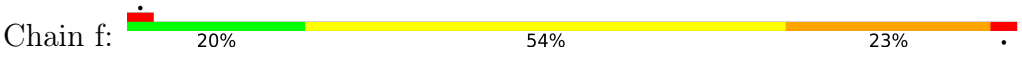
• Molecule 3: PscE

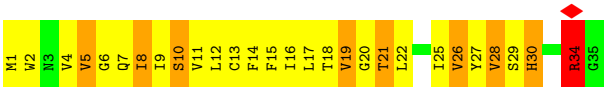
• Molecule 4: PscF



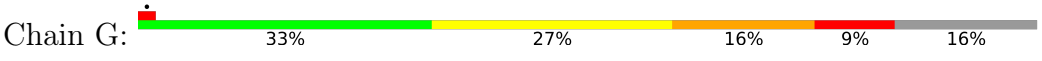


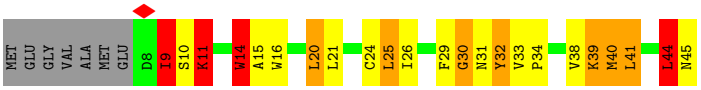
• Molecule 4: PscF



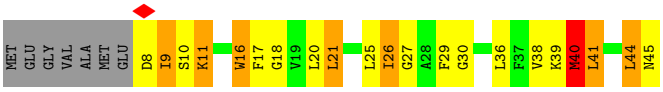


• Molecule 5: PscG



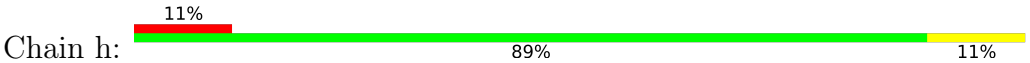


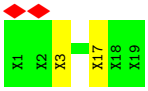
• Molecule 5: PscG



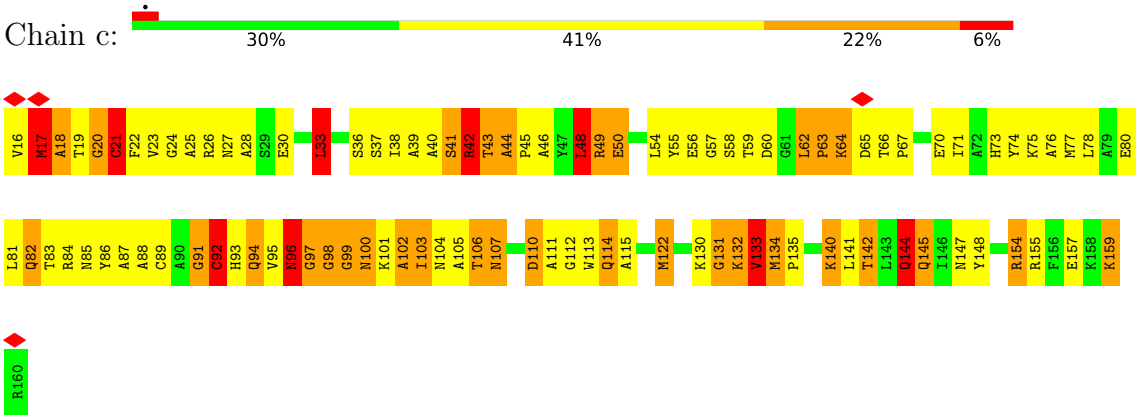
• Molecule 6: undefined polypeptide

• Molecule 6: undefined polypeptide





• Molecule 7: Cytochrome c domain-containing protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	490075	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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	5.661	Depositor
Minimum map value	-2.809	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.48	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: SF4, 85N, 85I, HEC, CA, 84Q, UNL, 2GO, LYC, CLA, BCL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	2.27	241/7209 (3.3%)	1.57	111/9827 (1.1%)
1	a	2.04	178/7233 (2.5%)	1.42	92/9860 (0.9%)
2	C	3.01	114/1503 (7.6%)	2.06	66/2037 (3.2%)
3	E	3.18	26/262 (9.9%)	1.94	7/356 (2.0%)
3	e	2.23	9/262 (3.4%)	1.83	3/356 (0.8%)
4	F	3.38	34/279 (12.2%)	1.79	8/379 (2.1%)
4	f	2.88	22/279 (7.9%)	1.79	9/379 (2.4%)
5	G	2.13	13/311 (4.2%)	1.93	8/421 (1.9%)
5	g	1.68	1/311 (0.3%)	1.56	7/421 (1.7%)
7	c	3.24	127/1115 (11.4%)	2.20	52/1506 (3.5%)
All	All	2.36	765/18764 (4.1%)	1.63	363/25542 (1.4%)

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 (765) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	539	TRP	C-O	-23.08	0.94	1.23
2	C	141	THR	C-O	-19.02	1.01	1.24
1	a	305	HIS	C-O	-15.89	1.05	1.24
2	C	179	ASN	C-O	-15.84	1.04	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	852	LEU	C-O	-15.74	1.04	1.24
4	F	4	VAL	C-O	-15.45	1.06	1.24
1	a	376	HIS	C-O	-15.40	1.04	1.24
7	c	106	THR	C-O	-15.38	1.05	1.23
3	E	13	GLY	C-O	-15.28	1.05	1.24
1	A	731	LEU	C-O	-15.27	1.06	1.24
2	C	140	SER	C-O	-15.19	1.04	1.23
1	a	759	VAL	C-O	-15.15	1.06	1.24
1	A	306	VAL	C-O	-15.08	1.06	1.24
1	A	758	GLY	C-O	-14.81	1.03	1.23
1	A	125	LEU	C-O	-14.64	1.06	1.24
1	A	709	ILE	C-O	-14.48	1.06	1.24
1	A	638	SER	C-O	-14.40	1.05	1.23
1	a	783	GLY	C-O	-14.26	1.06	1.23
1	a	346	LYS	C-O	-14.08	1.06	1.24
2	C	176	ALA	C-O	-14.03	1.06	1.23
2	C	178	TYR	C-O	-14.01	1.06	1.24
2	C	190	VAL	C-O	-13.72	1.08	1.24
1	a	796	LYS	C-O	-13.59	1.06	1.24
2	C	126	VAL	C-O	-13.54	1.08	1.24
7	c	130	LYS	C-O	-13.47	1.08	1.23
1	a	811	TRP	C-O	-13.37	1.08	1.24
2	C	123	ASN	C-O	-13.26	1.08	1.24
2	C	175	PRO	C-O	-13.24	1.08	1.23
1	A	309	THR	CB-CG2	-13.16	1.09	1.52
1	A	245	PRO	C-O	-13.15	1.08	1.24
1	A	764	TRP	C-O	-13.11	1.09	1.24
1	A	655	PHE	C-O	-13.05	1.09	1.24
1	a	537	VAL	C-O	-13.05	1.11	1.24
1	A	796	LYS	C-O	-13.04	1.09	1.23
1	A	238	PRO	C-O	-13.02	1.10	1.23
1	A	560	TRP	C-O	-12.99	1.08	1.24
1	a	26	ARG	C-O	-12.94	1.08	1.24
2	C	121	PHE	C-O	-12.93	1.09	1.24
1	A	542	TRP	C-O	-12.90	1.07	1.24
1	A	362	HIS	C-O	-12.87	1.08	1.24
2	C	30	THR	C-O	-12.86	1.07	1.23
7	c	96	ASN	C-O	-12.85	1.06	1.24
2	C	165	LYS	CA-C	-12.84	1.37	1.52
2	C	188	TYR	C-O	-12.81	1.08	1.24
1	a	860	GLY	C-O	-12.68	1.06	1.23
2	C	147	GLY	C-O	-12.68	1.08	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	112	GLY	C-O	-12.68	1.08	1.23
1	a	731	LEU	C-O	-12.64	1.09	1.24
1	A	294	ILE	C-O	-12.57	1.09	1.24
1	a	758	GLY	C-O	-12.49	1.07	1.23
7	c	26	ARG	C-O	-12.49	1.08	1.23
1	A	311	ILE	C-O	-12.45	1.10	1.24
1	A	209	ILE	C-O	-12.44	1.10	1.24
1	A	543	THR	C-O	-12.35	1.08	1.24
1	a	763	MET	C-O	-12.29	1.09	1.24
4	F	25	ILE	C-O	-12.29	1.09	1.24
7	c	20	GLY	C-O	-12.26	1.07	1.23
1	A	541	SER	C-O	-12.22	1.07	1.24
1	A	860	GLY	C-O	-12.19	1.10	1.23
2	C	143	PHE	C-O	-12.18	1.08	1.24
4	F	10	SER	C-O	-12.13	1.09	1.24
1	A	297	LEU	C-O	-12.11	1.08	1.24
7	c	106	THR	CB-CG2	-12.10	1.12	1.52
7	c	56	GLU	C-O	-12.03	1.08	1.24
4	f	17	LEU	C-O	-11.96	1.10	1.24
1	A	210	TRP	C-O	-11.95	1.10	1.24
1	A	126	VAL	C-O	-11.94	1.10	1.24
1	a	757	GLY	C-O	-11.92	1.07	1.23
1	A	640	LEU	C-O	-11.91	1.08	1.24
7	c	18	ALA	CA-C	-11.88	1.37	1.52
1	A	124	TRP	C-O	-11.88	1.09	1.24
1	A	861	PHE	C-O	-11.87	1.10	1.24
2	C	146	PRO	C-O	-11.87	1.09	1.24
1	a	765	ASN	C-O	-11.86	1.10	1.24
2	C	189	LEU	C-O	-11.83	1.10	1.24
2	C	173	ALA	C-O	-11.75	1.09	1.24
1	A	203	ILE	C-O	-11.70	1.10	1.24
1	A	776	LEU	C-O	-11.67	1.09	1.24
2	C	148	TRP	C-O	-11.59	1.10	1.24
1	A	656	TRP	C-O	-11.54	1.09	1.24
2	C	180	GLN	C-O	-11.52	1.09	1.24
3	E	2	THR	C-O	-11.49	1.10	1.24
1	A	699	PRO	C-O	-11.47	1.08	1.24
1	A	741	ALA	C-O	-11.46	1.09	1.23
7	c	43	THR	C-O	-11.39	1.10	1.23
7	c	46	ALA	C-O	-11.30	1.10	1.23
7	c	113	TRP	C-O	-11.27	1.11	1.24
7	c	42	ARG	C-O	-11.26	1.09	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	742	ARG	C-O	-11.25	1.10	1.23
2	C	163	ASN	C-O	-11.24	1.09	1.24
2	C	72	ASP	C-O	-11.17	1.09	1.24
2	C	167	ILE	C-O	-11.15	1.09	1.24
1	a	116	CYS	C-O	-11.14	1.11	1.24
2	C	128	CYS	C-O	-11.07	1.09	1.24
7	c	93	HIS	C-O	-11.04	1.09	1.24
1	A	539	TRP	C-O	-11.03	1.09	1.24
2	C	142	ASN	N-CA	10.99	1.61	1.46
1	a	375	PHE	C-O	-10.99	1.11	1.24
1	a	697	ILE	C-O	-10.98	1.11	1.24
2	C	181	LEU	C-O	-10.97	1.09	1.23
1	a	631	SER	C-O	-10.90	1.09	1.24
1	A	207	PHE	C-O	-10.89	1.11	1.24
2	C	165	LYS	C-O	-10.86	1.11	1.23
1	A	307	HIS	C-O	-10.84	1.10	1.24
1	A	740	MET	C-O	-10.84	1.09	1.24
2	C	214	VAL	C-O	-10.83	1.09	1.24
2	C	19	GLY	C-O	-10.79	1.09	1.23
7	c	105	ALA	C-O	-10.74	1.11	1.24
1	a	764	TRP	C-O	-10.65	1.10	1.24
1	A	361	ASN	C-O	-10.55	1.11	1.24
7	c	91	GLY	C-O	-10.53	1.09	1.23
1	A	308	LEU	C-O	-10.50	1.11	1.24
7	c	98	GLY	CA-C	-10.48	1.37	1.51
1	A	682	TYR	C-O	-10.47	1.11	1.24
1	A	480	TRP	C-O	-10.46	1.10	1.23
1	A	208	PHE	C-O	-10.40	1.12	1.24
1	A	119	ILE	C-O	-10.39	1.11	1.24
1	A	775	HIS	C-O	-10.36	1.11	1.24
1	A	248	TRP	C-O	-10.33	1.09	1.23
1	A	118	HIS	C-O	-10.32	1.11	1.24
1	A	733	GLY	C-O	-10.32	1.09	1.24
1	A	756	THR	C-O	-10.31	1.09	1.24
1	a	307	HIS	C-O	-10.29	1.12	1.24
3	e	28	ASN	C-O	-10.29	1.10	1.24
1	A	117	PHE	C-O	-10.28	1.12	1.24
3	E	25	VAL	C-O	-10.23	1.12	1.24
7	c	21	CYS	C-O	-10.20	1.11	1.24
2	C	124	ASN	C-O	-10.19	1.10	1.24
2	C	20	CYS	C-O	-10.16	1.11	1.24
1	A	305	HIS	C-O	-10.15	1.12	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	ASP	C-O	-10.12	1.12	1.24
2	C	177	TYR	C-O	-10.12	1.10	1.24
1	A	561	TYR	C-O	-10.10	1.12	1.24
1	A	739	MET	C-O	-10.07	1.11	1.24
4	F	15	PHE	C-O	-10.06	1.12	1.24
1	A	774	ASN	C-O	-10.02	1.11	1.24
1	a	27	ILE	C-O	-10.02	1.12	1.24
1	A	338	MET	C-N	-10.01	1.21	1.33
1	A	538	GLN	CD-NE2	-10.00	1.12	1.33
2	C	182	SER	C-O	-9.98	1.09	1.23
2	C	142	ASN	CG-ND2	-9.96	1.12	1.33
1	a	560	TRP	C-O	-9.94	1.12	1.24
1	A	246	TYR	C-O	-9.93	1.12	1.24
2	C	21	PHE	C-O	-9.90	1.11	1.23
1	A	299	ASP	C-O	-9.87	1.12	1.24
1	A	109	PHE	C-O	-9.80	1.12	1.24
4	F	6	GLY	C-O	-9.79	1.11	1.23
1	a	756	THR	C-O	-9.79	1.10	1.24
1	A	310	ALA	C-O	-9.78	1.12	1.24
1	A	249	PHE	C-O	-9.75	1.12	1.24
2	C	179	ASN	CG-OD1	-9.74	1.05	1.23
7	c	19	THR	CA-C	-9.71	1.43	1.53
1	A	501	ARG	C-O	-9.70	1.12	1.24
3	E	17	ALA	C-O	-9.70	1.12	1.24
2	C	166	GLY	C-O	-9.70	1.11	1.23
4	f	20	GLY	C-O	-9.69	1.12	1.23
1	a	134	TYR	C-O	-9.69	1.11	1.24
2	C	185	GLN	C-O	-9.68	1.12	1.24
1	a	118	HIS	C-O	-9.67	1.12	1.24
2	C	114	TYR	C-O	-9.65	1.12	1.24
7	c	43	THR	CB-CG2	-9.58	1.21	1.52
3	e	26	VAL	C-O	-9.56	1.12	1.24
4	f	15	PHE	C-O	-9.54	1.12	1.24
1	A	810	ARG	C-O	-9.53	1.13	1.24
7	c	56	GLU	CA-C	-9.53	1.40	1.52
2	C	174	MET	C-O	-9.52	1.12	1.24
1	a	742	ARG	C-O	-9.41	1.12	1.23
7	c	49	ARG	C-O	-9.40	1.12	1.24
1	a	696	CYS	C-O	-9.40	1.12	1.24
1	A	231	MET	C-O	-9.39	1.12	1.23
2	C	185	GLN	CD-NE2	-9.39	1.13	1.33
1	a	512	SER	C-O	-9.39	1.12	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	31	ARG	C-O	-9.38	1.10	1.23
4	F	29	SER	C-O	-9.36	1.13	1.24
1	a	364	GLN	CD-NE2	-9.36	1.13	1.33
1	a	864	ASN	CA-C	-9.35	1.39	1.52
4	F	22	LEU	C-O	-9.34	1.13	1.24
1	A	759	VAL	C-O	-9.34	1.12	1.24
7	c	135	PRO	C-O	-9.30	1.13	1.23
1	A	681	TRP	C-O	-9.28	1.13	1.24
1	A	631	SER	C-O	-9.27	1.11	1.24
3	E	10	PHE	C-O	-9.25	1.12	1.24
1	A	812	VAL	C-O	-9.23	1.13	1.24
1	a	541	SER	C-O	-9.22	1.11	1.23
3	E	15	TYR	C-O	-9.22	1.12	1.24
2	C	70	LEU	C-O	-9.20	1.13	1.24
2	C	192	TYR	C-O	-9.19	1.12	1.24
1	A	137	ARG	C-O	-9.19	1.11	1.24
4	F	8	ILE	C-O	-9.17	1.13	1.24
1	A	222	PRO	C-O	-9.15	1.13	1.23
4	F	21	THR	C-O	-9.07	1.13	1.24
1	A	828	ARG	C-O	-9.04	1.13	1.24
4	F	18	THR	C-O	-9.03	1.13	1.24
7	c	154	ARG	C-O	-9.01	1.12	1.24
7	c	41	SER	C-O	-9.00	1.11	1.24
7	c	74	TYR	C-O	-9.00	1.13	1.24
1	A	202	TYR	C-O	-8.98	1.13	1.24
3	E	18	LEU	C-O	-8.98	1.13	1.24
1	A	680	PRO	C-O	-8.98	1.13	1.24
1	A	309	THR	C-O	-8.98	1.13	1.24
1	a	612	ARG	N-CA	-8.96	1.38	1.46
1	A	110	ARG	C-O	-8.95	1.13	1.24
1	A	774	ASN	CG-ND2	-8.96	1.14	1.33
4	f	14	PHE	C-O	-8.94	1.13	1.24
1	a	542	TRP	C-O	-8.93	1.13	1.24
1	A	23	PRO	C-O	-8.91	1.14	1.24
1	a	633	PRO	C-O	-8.86	1.13	1.23
4	f	12	LEU	C-O	-8.86	1.13	1.24
1	A	679	SER	C-O	-8.85	1.16	1.24
7	c	75	LYS	C-O	-8.84	1.13	1.24
1	a	18	LEU	C-O	-8.83	1.11	1.23
1	A	688	ARG	C-O	-8.83	1.12	1.24
1	a	225	LEU	C-O	-8.83	1.12	1.24
7	c	99	GLY	C-O	-8.81	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	339	ASN	C-O	-8.77	1.12	1.24
1	a	79	GLN	C-O	-8.76	1.13	1.23
7	c	87	ALA	C-O	-8.75	1.13	1.24
7	c	74	TYR	CA-C	-8.72	1.41	1.52
7	c	145	GLN	C-O	-8.72	1.13	1.24
7	c	76	ALA	C-O	-8.71	1.13	1.24
1	A	123	LEU	C-O	-8.70	1.13	1.24
2	C	115	ARG	C-O	-8.69	1.14	1.24
1	a	338	MET	C-O	-8.67	1.12	1.24
1	A	20	LEU	C-O	-8.65	1.12	1.23
1	A	630	ALA	C-O	-8.63	1.11	1.24
7	c	97	GLY	N-CA	8.63	1.54	1.45
1	a	19	GLU	C-O	-8.62	1.13	1.23
1	a	632	THR	C-O	-8.61	1.12	1.23
1	A	61	THR	CB-CG2	-8.61	1.24	1.52
1	A	734	GLY	C-O	-8.58	1.11	1.23
1	a	222	PRO	C-O	-8.57	1.14	1.23
3	E	12	LEU	C-O	-8.57	1.13	1.24
1	a	528	GLU	C-O	-8.56	1.13	1.24
1	A	538	GLN	C-O	-8.54	1.13	1.24
1	a	777	THR	CB-CG2	-8.54	1.24	1.52
4	f	13	CYS	C-O	-8.51	1.14	1.24
1	A	205	LEU	C-O	-8.50	1.14	1.24
4	F	20	GLY	C-O	-8.49	1.13	1.23
1	A	242	ALA	C-O	-8.47	1.13	1.24
2	C	122	GLN	C-O	-8.47	1.13	1.24
2	C	191	ALA	C-O	-8.46	1.13	1.24
7	c	89	CYS	C-O	-8.46	1.13	1.24
1	A	501	ARG	CA-C	-8.45	1.42	1.52
1	A	479	ASP	CA-C	-8.43	1.41	1.52
1	A	639	ASN	CG-OD1	-8.43	1.07	1.23
4	F	9	ILE	C-O	-8.43	1.14	1.24
7	c	77	MET	C-O	-8.39	1.14	1.24
1	A	735	TRP	C-O	-8.38	1.13	1.24
1	A	233	PRO	C-O	-8.37	1.13	1.24
7	c	100	ASN	N-CA	-8.36	1.36	1.46
4	F	27	TYR	C-O	-8.34	1.14	1.24
3	E	15	TYR	CA-C	-8.34	1.41	1.52
1	a	377	GLY	C-O	-8.32	1.14	1.23
1	A	639	ASN	C-O	-8.31	1.12	1.23
4	F	26	VAL	C-O	-8.28	1.14	1.24
2	C	125	CYS	C-O	-8.27	1.13	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	C-O	-8.26	1.13	1.24
2	C	123	ASN	CG-ND2	-8.23	1.16	1.33
1	A	165	THR	C-O	-8.21	1.12	1.24
1	a	61	THR	CB-CG2	-8.21	1.25	1.52
2	C	169	ASN	CG-OD1	-8.20	1.07	1.23
1	a	20	LEU	C-O	-8.20	1.12	1.24
7	c	44	ALA	C-O	-8.17	1.13	1.24
1	A	611	PHE	C-O	-8.16	1.13	1.24
2	C	140	SER	CA-C	-8.16	1.42	1.52
3	E	9	LEU	C-O	-8.16	1.13	1.24
4	F	5	VAL	C-O	-8.15	1.14	1.24
4	F	7	GLN	C-O	-8.14	1.14	1.24
7	c	144	GLN	C-O	-8.13	1.14	1.24
2	C	164	GLY	C-O	-8.11	1.11	1.23
1	a	119	ILE	C-O	-8.11	1.14	1.24
1	a	364	GLN	CD-OE1	-8.10	1.08	1.23
1	A	241	GLN	C-O	-8.09	1.13	1.24
1	A	690	GLN	C-O	-8.07	1.13	1.24
2	C	71	ARG	C-O	-8.07	1.14	1.24
7	c	45	PRO	C-O	-8.04	1.13	1.24
1	a	488	ALA	C-O	-8.04	1.13	1.23
7	c	80	GLU	C-O	-8.03	1.13	1.24
1	a	25	GLU	C-O	-8.02	1.13	1.24
7	c	26	ARG	CZ-NH1	-8.01	1.21	1.32
7	c	40	ALA	C-O	-7.99	1.14	1.24
1	A	849	THR	CB-CG2	-7.96	1.26	1.52
1	a	346	LYS	N-CA	7.96	1.56	1.46
1	A	540	GLY	C-O	-7.95	1.12	1.24
1	a	709	ILE	CG1-CD1	-7.95	1.20	1.51
4	F	24	GLY	C-O	-7.92	1.14	1.23
1	a	765	ASN	CG-OD1	-7.91	1.08	1.23
1	a	863	GLN	C-O	-7.91	1.14	1.24
1	A	783	GLY	C-O	-7.88	1.14	1.24
1	a	776	LEU	C-O	-7.88	1.14	1.24
1	a	732	ASP	CB-CG	-7.88	1.32	1.52
1	a	511	SER	C-O	-7.88	1.13	1.24
7	c	105	ALA	CA-C	-7.88	1.42	1.52
1	A	22	MET	C-O	-7.87	1.14	1.24
1	a	864	ASN	C-O	-7.85	1.13	1.23
7	c	39	ALA	C-O	-7.85	1.15	1.24
5	G	20	LEU	C-O	-7.85	1.13	1.24
1	A	204	GLY	C-O	-7.84	1.14	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	757	GLY	CA-C	-7.84	1.40	1.51
1	a	656	TRP	C-O	-7.83	1.14	1.24
2	C	162	TYR	C-O	-7.83	1.15	1.24
1	A	298	GLU	C-O	-7.82	1.14	1.24
7	c	38	ILE	C-O	-7.81	1.14	1.24
1	a	784	HIS	C-O	-7.80	1.14	1.24
4	f	10	SER	C-O	-7.80	1.15	1.24
1	a	613	PRO	C-O	-7.79	1.13	1.24
7	c	140	LYS	C-O	-7.77	1.11	1.23
7	c	111	ALA	C-O	-7.76	1.14	1.24
4	F	17	LEU	C-O	-7.75	1.14	1.24
1	A	784	HIS	C-O	-7.74	1.13	1.24
1	A	244	PHE	CA-C	-7.73	1.43	1.52
1	A	657	LEU	C-O	-7.73	1.14	1.24
2	C	182	SER	CA-C	7.73	1.61	1.52
1	A	221	PRO	C-O	-7.73	1.15	1.24
1	A	488	ALA	C-O	-7.72	1.15	1.24
1	A	697	ILE	C-O	-7.70	1.15	1.24
1	A	243	PRO	C-O	-7.69	1.14	1.23
4	f	21	THR	C-O	-7.69	1.15	1.24
1	a	117	PHE	C-O	-7.68	1.15	1.24
1	a	769	TRP	C-O	-7.67	1.14	1.24
7	c	25	ALA	C-O	-7.67	1.14	1.23
1	a	765	ASN	CG-ND2	-7.65	1.17	1.33
3	E	8	CYS	C-O	-7.65	1.15	1.24
7	c	99	GLY	CA-C	-7.63	1.41	1.51
5	G	44	LEU	CA-CB	-7.63	1.41	1.53
7	c	83	THR	C-O	-7.63	1.13	1.24
2	C	114	TYR	N-CA	-7.62	1.36	1.46
2	C	170	GLY	C-O	-7.62	1.12	1.24
2	C	192	TYR	CA-C	-7.62	1.42	1.52
7	c	130	LYS	CA-C	-7.61	1.43	1.52
1	a	732	ASP	C-O	-7.59	1.13	1.24
1	A	364	GLN	N-CA	-7.59	1.37	1.46
3	E	22	ILE	C-O	-7.59	1.15	1.24
2	C	149	GLN	C-O	-7.58	1.15	1.24
1	A	639	ASN	CG-ND2	-7.55	1.17	1.33
4	f	22	LEU	C-O	-7.55	1.15	1.24
1	A	327	ARG	C-O	-7.54	1.15	1.24
7	c	142	THR	C-O	-7.54	1.13	1.23
1	a	739	MET	C-O	-7.54	1.14	1.24
7	c	114	GLN	C-O	-7.53	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	7	GLN	C-O	-7.53	1.15	1.24
1	a	363	VAL	C-O	-7.53	1.15	1.24
4	F	16	ILE	C-O	-7.51	1.14	1.24
1	a	548	LYS	C-O	-7.49	1.14	1.24
1	a	433	THR	CB-CG2	-7.48	1.27	1.52
1	A	732	ASP	CG-OD2	-7.46	1.11	1.25
7	c	23	VAL	C-O	-7.45	1.15	1.24
1	a	22	MET	C-O	-7.45	1.16	1.24
3	E	29	THR	C-O	-7.44	1.14	1.24
3	E	16	ALA	C-O	-7.43	1.14	1.24
1	a	639	ASN	CB-CG	-7.42	1.33	1.52
7	c	134	MET	C-O	-7.41	1.14	1.24
1	A	239	LEU	C-O	-7.36	1.15	1.24
1	A	745	GLU	CB-CG	-7.36	1.30	1.52
1	A	653	ILE	CG1-CD1	-7.35	1.23	1.51
1	a	362	HIS	C-O	-7.35	1.14	1.24
3	E	34	ALA	N-CA	7.35	1.55	1.46
1	a	698	GLY	CA-C	-7.33	1.41	1.51
1	a	615	LEU	C-O	-7.33	1.14	1.24
1	A	814	LEU	C-O	-7.32	1.15	1.24
1	a	139	GLY	C-O	-7.29	1.16	1.23
1	A	20	LEU	CA-C	-7.28	1.44	1.53
7	c	141	LEU	C-O	-7.28	1.14	1.23
7	c	28	ALA	C-O	-7.26	1.14	1.24
1	A	329	HIS	C-O	-7.25	1.14	1.24
1	a	414	THR	CB-CG2	-7.25	1.28	1.52
1	A	166	PRO	C-O	-7.24	1.15	1.24
1	a	487	THR	C-O	-7.23	1.15	1.23
7	c	107	ASN	CG-ND2	-7.22	1.18	1.33
2	C	179	ASN	C-N	-7.22	1.23	1.33
7	c	110	ASP	CG-OD2	-7.22	1.11	1.25
1	a	852	LEU	N-CA	-7.21	1.37	1.46
2	C	172	GLY	C-O	-7.20	1.14	1.23
1	A	785	LEU	C-O	-7.19	1.15	1.24
2	C	217	ARG	CA-C	-7.17	1.43	1.52
7	c	133	VAL	C-O	-7.17	1.15	1.23
7	c	37	SER	C-O	-7.17	1.14	1.24
4	F	30	HIS	C-O	-7.16	1.15	1.24
4	F	17	LEU	N-CA	-7.13	1.37	1.46
2	C	124	ASN	CA-C	-7.12	1.42	1.52
7	c	26	ARG	CZ-NH2	-7.11	1.24	1.33
1	A	640	LEU	CA-C	-7.10	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	216	GLU	CA-CB	-7.07	1.42	1.53
1	A	700	VAL	CA-C	-7.07	1.44	1.52
1	a	364	GLN	N-CA	-7.06	1.37	1.46
1	a	514	THR	CB-CG2	-7.06	1.29	1.52
1	A	304	PHE	C-O	-7.04	1.15	1.24
1	A	328	ASN	CG-OD1	-7.04	1.10	1.23
1	a	847	THR	CB-CG2	-7.04	1.29	1.52
7	c	103	ILE	C-O	-7.02	1.14	1.24
1	a	518	THR	CB-CG2	-7.01	1.29	1.52
1	a	699	PRO	C-O	-7.01	1.09	1.23
2	C	112	GLU	N-CA	-7.01	1.37	1.46
3	E	23	LYS	C-O	-6.99	1.15	1.24
4	f	11	VAL	C-O	-6.99	1.16	1.24
4	F	14	PHE	C-O	-6.99	1.16	1.24
1	a	394	ARG	CA-C	-6.98	1.43	1.52
3	e	11	VAL	C-O	6.98	1.32	1.24
1	A	836	THR	CB-CG2	-6.97	1.29	1.52
1	a	764	TRP	N-CA	-6.96	1.37	1.46
4	f	5	VAL	C-O	-6.94	1.15	1.24
7	c	36	SER	C-O	-6.93	1.15	1.24
1	A	742	ARG	CZ-NH1	-6.93	1.23	1.32
1	a	266	GLU	CD-OE2	-6.93	1.12	1.25
1	A	136	ALA	C-O	-6.93	1.15	1.24
3	E	21	ILE	C-O	-6.90	1.16	1.24
1	a	413	THR	CB-CG2	-6.86	1.29	1.52
7	c	18	ALA	C-O	-6.86	1.16	1.24
7	c	82	GLN	C-O	-6.83	1.15	1.24
2	C	187	ARG	C-O	-6.82	1.15	1.24
2	C	171	GLY	C-O	-6.82	1.15	1.23
1	A	541	SER	CB-OG	-6.80	1.28	1.42
2	C	129	HIS	C-O	-6.79	1.14	1.24
1	a	666	PHE	C-O	-6.78	1.15	1.24
7	c	73	HIS	C-O	-6.77	1.15	1.24
3	e	22	ILE	C-O	-6.77	1.16	1.24
1	a	732	ASP	C-N	-6.76	1.24	1.33
7	c	55	TYR	CD1-CE1	-6.76	1.18	1.38
1	a	689	LYS	C-O	-6.74	1.16	1.24
2	C	29	GLU	C-O	-6.74	1.14	1.23
2	C	142	ASN	CG-OD1	-6.74	1.10	1.23
7	c	88	ALA	C-O	-6.73	1.14	1.23
3	E	28	ASN	C-O	-6.72	1.15	1.24
5	G	14	TRP	CA-C	-6.69	1.44	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	c	48	LEU	C-O	-6.68	1.15	1.24
1	A	232	THR	C-O	-6.68	1.15	1.24
1	A	328	ASN	C-O	-6.68	1.14	1.23
1	a	775	HIS	C-O	-6.68	1.15	1.24
1	a	308	LEU	N-CA	-6.66	1.38	1.46
4	F	3	ASN	CA-C	-6.65	1.44	1.52
2	C	124	ASN	CG-OD1	-6.62	1.10	1.23
7	c	122	MET	SD-CE	-6.62	1.63	1.79
2	C	163	ASN	CG-OD1	-6.61	1.10	1.23
1	a	364	GLN	C-O	-6.60	1.15	1.24
1	a	134	TYR	CA-C	-6.60	1.43	1.52
2	C	149	GLN	CD-NE2	-6.58	1.19	1.33
5	G	25	LEU	C-O	-6.58	1.16	1.24
1	a	732	ASP	N-CA	-6.57	1.37	1.46
7	c	81	LEU	C-O	-6.57	1.15	1.24
1	a	541	SER	N-CA	-6.56	1.37	1.46
4	F	19	VAL	C-O	-6.55	1.16	1.24
1	A	487	THR	C-O	-6.55	1.15	1.23
2	C	162	TYR	CZ-OH	-6.55	1.24	1.38
1	a	759	VAL	CA-CB	6.54	1.63	1.54
1	A	268	THR	CB-CG2	-6.53	1.31	1.52
7	c	107	ASN	CG-OD1	-6.52	1.11	1.23
7	c	131	GLY	C-O	-6.51	1.15	1.23
1	A	691	SER	C-N	-6.50	1.28	1.33
1	a	394	ARG	CA-CB	-6.50	1.44	1.54
3	E	24	PHE	C-O	-6.49	1.16	1.24
1	A	810	ARG	CZ-NH1	-6.48	1.23	1.32
1	a	785	LEU	C-O	-6.48	1.15	1.24
7	c	141	LEU	CA-C	-6.47	1.45	1.52
4	f	26	VAL	C-O	-6.46	1.16	1.24
1	A	224	PRO	C-O	-6.46	1.10	1.23
1	A	223	VAL	C-O	-6.45	1.16	1.24
2	C	31	ARG	CZ-NH2	-6.45	1.25	1.33
1	a	225	LEU	N-CA	-6.45	1.39	1.46
1	a	811	TRP	N-CA	-6.45	1.38	1.46
1	A	702	GLY	C-O	-6.44	1.15	1.24
1	A	25	GLU	C-O	-6.43	1.15	1.24
1	a	308	LEU	C-O	-6.43	1.16	1.24
1	A	135	GLY	C-O	-6.42	1.15	1.23
1	a	612	ARG	CA-CB	-6.42	1.46	1.53
1	a	529	TRP	CB-CG	-6.42	1.30	1.50
7	c	55	TYR	CD2-CE2	-6.40	1.19	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	28	ASN	C-O	-6.40	1.15	1.24
1	A	299	ASP	N-CA	-6.39	1.38	1.46
1	a	50	MET	SD-CE	-6.38	1.63	1.79
1	A	732	ASP	CG-OD1	-6.38	1.13	1.25
1	a	137	ARG	C-O	-6.38	1.16	1.24
1	A	732	ASP	N-CA	-6.37	1.37	1.46
1	a	339	ASN	CG-ND2	-6.37	1.19	1.33
7	c	97	GLY	C-O	-6.36	1.15	1.23
1	A	226	GLN	C-O	-6.36	1.15	1.23
1	a	248	TRP	C-O	-6.35	1.15	1.24
1	A	763	MET	SD-CE	-6.34	1.63	1.79
7	c	142	THR	CB-CG2	-6.33	1.31	1.52
1	A	689	LYS	C-O	-6.33	1.16	1.24
1	A	628	ARG	CB-CG	-6.32	1.33	1.52
1	a	540	GLY	N-CA	6.32	1.54	1.45
7	c	55	TYR	CZ-OH	-6.31	1.24	1.38
1	A	91	PHE	N-CA	6.29	1.54	1.46
7	c	154	ARG	CZ-NH2	-6.27	1.25	1.33
1	A	364	GLN	C-O	-6.27	1.16	1.24
1	a	756	THR	CA-C	-6.27	1.44	1.52
1	A	700	VAL	C-O	-6.27	1.16	1.24
7	c	71	ILE	C-O	-6.26	1.16	1.24
5	G	26	ILE	C-O	-6.26	1.17	1.24
2	C	178	TYR	CZ-OH	-6.25	1.25	1.38
1	A	172	LYS	C-O	-6.25	1.17	1.24
1	a	732	ASP	CG-OD2	-6.25	1.13	1.25
1	a	768	THR	CB-CG2	-6.24	1.31	1.52
2	C	46	LEU	C-O	-6.24	1.16	1.24
7	c	103	ILE	N-CA	-6.23	1.37	1.46
2	C	123	ASN	N-CA	-6.22	1.39	1.46
3	e	26	VAL	N-CA	-6.22	1.38	1.46
1	a	815	MET	C-O	-6.21	1.16	1.24
1	a	309	THR	CB-CG2	-6.21	1.32	1.52
4	f	8	ILE	C-O	-6.21	1.17	1.24
2	C	116	GLU	C-O	-6.21	1.16	1.24
1	a	742	ARG	CZ-NH1	-6.20	1.24	1.32
5	G	31	ASN	C-O	-6.19	1.17	1.24
1	A	225	LEU	C-O	-6.18	1.15	1.23
7	c	59	THR	C-O	-6.17	1.15	1.23
1	A	144	GLU	C-O	-6.17	1.16	1.23
1	A	633	PRO	C-O	-6.17	1.16	1.23
1	A	659	ILE	CG1-CD1	-6.17	1.27	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	706	GLY	C-O	-6.16	1.16	1.24
4	F	7	GLN	N-CA	-6.16	1.38	1.46
7	c	98	GLY	C-O	-6.15	1.15	1.23
1	a	268	THR	CB-CG2	-6.15	1.32	1.52
7	c	93	HIS	CA-C	-6.15	1.44	1.52
1	a	742	ARG	CA-C	-6.15	1.44	1.52
7	c	39	ALA	CA-C	-6.13	1.45	1.52
7	c	58	SER	CA-C	-6.13	1.45	1.52
1	A	705	CYS	C-O	-6.13	1.16	1.23
2	C	115	ARG	CD-NE	-6.13	1.37	1.46
1	a	861	PHE	C-O	-6.12	1.16	1.24
7	c	27	ASN	C-O	-6.11	1.16	1.23
3	e	27	ALA	C-O	-6.10	1.16	1.24
1	A	638	SER	CB-OG	-6.10	1.29	1.42
1	A	657	LEU	N-CA	-6.09	1.38	1.46
1	A	18	LEU	C-O	-6.09	1.16	1.23
1	A	246	TYR	CA-C	-6.09	1.45	1.52
1	a	529	TRP	C-O	-6.09	1.16	1.24
7	c	20	GLY	N-CA	-6.09	1.36	1.45
5	G	15	ALA	C-O	-6.08	1.16	1.24
1	A	170	TRP	C-O	-6.08	1.16	1.24
1	A	816	GLY	C-O	-6.08	1.16	1.23
1	A	470	ASN	CA-C	-6.07	1.45	1.52
1	a	697	ILE	N-CA	-6.07	1.38	1.46
1	a	352	ARG	CZ-NH2	-6.07	1.25	1.33
1	A	172	LYS	N-CA	-6.07	1.40	1.46
1	a	376	HIS	CA-C	-6.06	1.44	1.52
4	f	6	GLY	C-O	-6.06	1.16	1.23
1	A	637	TYR	C-O	-6.05	1.16	1.24
7	c	94	GLN	C-O	-6.05	1.16	1.24
1	A	471	PRO	C-O	-6.04	1.16	1.24
1	A	639	ASN	CB-CG	-6.04	1.36	1.52
3	E	11	VAL	C-O	-6.03	1.16	1.24
1	A	671	ARG	CZ-NH2	-6.02	1.25	1.33
2	C	127	GLY	C-O	-6.02	1.15	1.23
1	a	538	GLN	CD-NE2	-6.02	1.20	1.33
1	A	606	ALA	C-O	-6.00	1.16	1.24
2	C	181	LEU	CA-C	-6.00	1.45	1.52
1	A	479	ASP	C-O	-6.00	1.16	1.23
1	A	295	THR	CB-CG2	-5.99	1.32	1.52
1	A	817	LYS	C-O	-5.99	1.17	1.24
1	a	223	VAL	C-O	-5.99	1.17	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	306	VAL	C-O	-5.98	1.17	1.24
1	a	732	ASP	CA-CB	-5.98	1.43	1.53
4	F	13	CYS	C-O	-5.98	1.17	1.24
1	a	541	SER	CB-OG	-5.98	1.30	1.42
5	G	33	VAL	C-O	-5.97	1.16	1.24
1	a	497	GLN	CB-CG	-5.96	1.34	1.52
1	A	295	THR	C-O	-5.96	1.16	1.24
1	A	497	GLN	CB-CG	-5.96	1.34	1.52
1	A	610	LYS	C-O	-5.96	1.16	1.24
5	G	31	ASN	CG-OD1	-5.95	1.12	1.23
2	C	115	ARG	N-CA	-5.94	1.39	1.46
1	A	502	ILE	C-O	-5.93	1.17	1.24
5	G	24	CYS	C-O	-5.93	1.17	1.24
1	A	732	ASP	C-O	-5.92	1.16	1.24
1	A	470	ASN	C-O	-5.91	1.16	1.24
1	A	266	GLU	CD-OE2	-5.90	1.14	1.25
1	A	183	THR	CB-CG2	-5.90	1.33	1.52
4	F	7	GLN	CD-OE1	-5.90	1.12	1.23
5	g	41	LEU	C-O	-5.89	1.16	1.24
1	a	361	ASN	C-O	-5.89	1.16	1.24
7	c	49	ARG	N-CA	-5.89	1.39	1.46
7	c	95	VAL	C-O	-5.89	1.16	1.24
1	a	200	THR	CB-CG2	-5.88	1.33	1.52
7	c	78	LEU	C-O	-5.88	1.17	1.24
4	f	10	SER	CB-OG	-5.86	1.30	1.42
1	a	538	GLN	C-O	-5.84	1.17	1.24
2	C	71	ARG	CA-C	-5.84	1.44	1.52
1	A	777	THR	CB-CG2	-5.83	1.33	1.52
2	C	168	GLY	C-O	-5.83	1.15	1.23
1	A	860	GLY	C-N	-5.82	1.25	1.33
1	A	249	PHE	N-CA	-5.82	1.39	1.46
2	C	116	GLU	CA-CB	-5.81	1.44	1.53
7	c	96	ASN	CG-OD1	-5.81	1.12	1.23
1	A	202	TYR	N-CA	-5.81	1.39	1.46
2	C	31	ARG	CZ-NH1	-5.81	1.24	1.32
1	a	705	CYS	CB-SG	5.80	2.00	1.81
5	G	41	LEU	C-O	-5.79	1.15	1.24
1	A	774	ASN	CG-OD1	-5.79	1.12	1.23
2	C	182	SER	CB-OG	-5.79	1.30	1.42
4	F	8	ILE	N-CA	-5.77	1.39	1.46
4	f	19	VAL	C-O	-5.77	1.16	1.24
1	A	763	MET	C-N	-5.76	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	836	THR	CB-CG2	-5.76	1.33	1.52
4	f	16	ILE	C-O	-5.76	1.17	1.24
1	A	414	THR	CB-CG2	-5.75	1.33	1.52
1	A	822	LYS	C-O	-5.73	1.17	1.24
1	a	415	MET	SD-CE	-5.72	1.65	1.79
1	A	759	VAL	C-N	-5.72	1.26	1.33
1	A	107	THR	CB-CG2	-5.71	1.33	1.52
2	C	164	GLY	C-N	-5.71	1.26	1.33
3	E	17	ALA	CA-C	-5.70	1.45	1.52
1	A	560	TRP	N-CA	-5.70	1.39	1.46
3	e	26	VAL	CA-C	-5.70	1.45	1.52
1	a	732	ASP	CG-OD1	-5.70	1.14	1.25
4	f	28	VAL	C-O	-5.70	1.17	1.24
1	A	548	LYS	C-O	-5.69	1.16	1.24
7	c	97	GLY	C-N	-5.67	1.25	1.33
1	a	759	VAL	C-N	-5.67	1.26	1.33
1	A	476	ALA	C-O	-5.66	1.16	1.24
1	A	766	GLU	CD-OE2	-5.65	1.14	1.25
1	A	145	ILE	N-CA	-5.65	1.39	1.46
7	c	114	GLN	CD-NE2	-5.65	1.21	1.33
5	G	30	GLY	C-O	-5.65	1.17	1.23
7	c	85	ASN	C-O	-5.65	1.16	1.23
2	C	112	GLU	CA-CB	-5.64	1.44	1.53
1	a	621	ASN	CB-CG	-5.63	1.38	1.52
1	A	847	THR	CB-CG2	-5.63	1.33	1.52
3	E	21	ILE	N-CA	-5.63	1.40	1.46
7	c	38	ILE	CA-C	-5.63	1.45	1.52
1	a	379	GLN	CG-CD	-5.61	1.38	1.52
1	a	15	TYR	C-O	-5.59	1.16	1.24
7	c	75	LYS	N-CA	-5.59	1.39	1.46
1	A	810	ARG	CA-CB	-5.58	1.44	1.53
1	A	606	ALA	CA-C	-5.58	1.45	1.52
1	A	361	ASN	CG-ND2	-5.57	1.21	1.33
2	C	73	ARG	C-O	-5.57	1.16	1.24
7	c	107	ASN	C-O	-5.57	1.16	1.23
1	a	537	VAL	CA-C	-5.56	1.45	1.52
7	c	100	ASN	C-O	-5.56	1.17	1.24
1	a	363	VAL	N-CA	-5.56	1.39	1.46
1	a	486	GLY	C-O	-5.56	1.16	1.24
1	A	230	VAL	CA-C	-5.55	1.45	1.52
4	F	11	VAL	C-O	-5.55	1.17	1.24
4	F	23	PHE	C-O	-5.55	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	71	ARG	CZ-NH1	-5.54	1.25	1.32
2	C	139	ARG	C-O	-5.54	1.14	1.24
1	a	757	GLY	C-N	-5.54	1.25	1.33
7	c	104	ASN	C-O	-5.54	1.15	1.23
7	c	114	GLN	CD-OE1	-5.53	1.13	1.23
3	e	9	LEU	C-O	-5.53	1.17	1.24
1	A	631	SER	CA-C	-5.52	1.45	1.52
1	a	438	ASP	CB-CG	-5.52	1.38	1.52
1	A	328	ASN	N-CA	-5.51	1.39	1.46
1	A	138	GLY	C-O	-5.51	1.17	1.24
1	a	394	ARG	C-O	-5.51	1.17	1.23
1	A	657	LEU	CA-C	-5.50	1.45	1.52
2	C	147	GLY	N-CA	-5.50	1.39	1.45
7	c	154	ARG	CZ-NH1	-5.50	1.25	1.32
1	a	18	LEU	CA-C	-5.50	1.44	1.53
1	a	337	ASP	C-O	-5.50	1.16	1.24
1	A	22	MET	C-N	-5.49	1.26	1.33
1	A	703	GLY	C-O	-5.49	1.16	1.23
1	A	143	GLY	C-O	-5.48	1.18	1.24
3	E	32	ILE	C-O	-5.47	1.18	1.24
7	c	107	ASN	N-CA	5.47	1.53	1.46
7	c	22	PHE	C-O	-5.47	1.16	1.23
7	c	57	GLY	C-O	-5.47	1.16	1.23
7	c	58	SER	C-O	-5.46	1.17	1.23
7	c	110	ASP	C-O	-5.46	1.17	1.24
1	A	740	MET	CA-C	-5.45	1.45	1.52
2	C	142	ASN	C-O	-5.45	1.15	1.23
4	f	29	SER	C-O	-5.45	1.16	1.24
1	A	294	ILE	CB-CG1	-5.45	1.42	1.53
1	A	538	GLN	CD-OE1	-5.44	1.13	1.23
1	A	609	ASP	C-O	-5.44	1.17	1.24
1	A	757	GLY	CA-C	-5.43	1.44	1.51
1	a	757	GLY	N-CA	-5.42	1.37	1.45
7	c	132	LYS	C-O	-5.42	1.17	1.24
7	c	145	GLN	CA-C	5.42	1.60	1.52
1	A	311	ILE	N-CA	-5.41	1.40	1.46
1	a	359	THR	CB-CG2	-5.41	1.34	1.52
1	A	622	MET	CB-CG	-5.41	1.36	1.52
7	c	63	PRO	C-O	-5.40	1.17	1.24
1	A	24	PRO	C-O	-5.40	1.17	1.24
1	A	202	TYR	CZ-OH	-5.40	1.26	1.38
1	a	364	GLN	C-N	-5.39	1.27	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	189	LEU	N-CA	-5.38	1.40	1.46
1	A	341	ILE	CG1-CD1	-5.36	1.30	1.51
1	a	482	LYS	C-O	-5.36	1.16	1.23
1	A	230	VAL	C-O	-5.36	1.18	1.23
7	c	100	ASN	CG-ND2	-5.35	1.22	1.33
2	C	109	ASP	C-N	-5.34	1.27	1.34
1	a	774	ASN	C-O	-5.34	1.17	1.24
5	G	29	PHE	C-O	-5.33	1.18	1.24
2	C	187	ARG	CZ-NH2	-5.33	1.26	1.33
1	a	691	SER	C-O	-5.33	1.17	1.24
2	C	169	ASN	C-O	-5.33	1.17	1.24
7	c	80	GLU	CA-C	-5.33	1.45	1.52
1	A	742	ARG	CZ-NH2	-5.33	1.26	1.33
1	A	177	TRP	C-O	-5.31	1.16	1.23
1	A	108	ASP	N-CA	-5.31	1.40	1.46
1	a	612	ARG	C-O	-5.31	1.19	1.24
2	C	180	GLN	CD-NE2	-5.31	1.22	1.33
1	a	482	LYS	CA-CB	-5.31	1.46	1.53
3	E	24	PHE	N-CA	-5.30	1.39	1.46
4	F	28	VAL	C-O	-5.30	1.17	1.24
1	a	305	HIS	CD2-NE2	-5.30	1.32	1.37
3	E	20	GLY	C-N	-5.29	1.27	1.33
1	a	542	TRP	CD1-NE1	-5.29	1.26	1.37
7	c	42	ARG	CZ-NH2	-5.29	1.26	1.33
7	c	86	TYR	C-O	-5.28	1.17	1.23
4	F	12	LEU	C-O	-5.28	1.18	1.24
4	f	9	ILE	C-O	-5.28	1.18	1.24
2	C	124	ASN	CA-CB	-5.27	1.45	1.53
1	A	606	ALA	N-CA	-5.27	1.39	1.46
4	F	10	SER	CB-OG	-5.26	1.31	1.42
2	C	48	THR	C-O	-5.25	1.17	1.24
7	c	48	LEU	CB-CG	-5.25	1.43	1.53
1	A	200	THR	CB-CG2	-5.24	1.35	1.52
1	a	116	CYS	CA-C	-5.24	1.46	1.52
7	c	97	GLY	CA-C	5.24	1.59	1.52
1	A	631	SER	CB-OG	-5.24	1.31	1.42
1	A	757	GLY	C-O	-5.23	1.16	1.23
7	c	24	GLY	C-O	-5.23	1.15	1.23
1	a	614	GLU	C-O	-5.22	1.17	1.24
2	C	113	ILE	C-O	-5.22	1.18	1.24
1	A	679	SER	CA-CB	-5.22	1.46	1.53
1	a	135	GLY	C-O	-5.21	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	TRP	C-N	-5.21	1.26	1.33
1	a	510	GLY	C-O	-5.21	1.16	1.23
1	A	612	ARG	C-O	-5.20	1.19	1.24
1	a	307	HIS	CA-C	-5.18	1.46	1.52
1	A	764	TRP	N-CA	-5.18	1.40	1.46
2	C	184	GLN	CB-CG	-5.18	1.36	1.52
1	A	177	TRP	CA-C	-5.17	1.45	1.52
1	A	735	TRP	C-N	-5.16	1.27	1.33
2	C	149	GLN	CD-OE1	-5.16	1.13	1.23
7	c	21	CYS	CA-C	-5.15	1.45	1.52
1	A	247	GLY	C-O	-5.14	1.13	1.23
1	A	19	GLU	C-O	-5.13	1.17	1.23
1	a	838	LYS	CB-CG	-5.12	1.37	1.52
2	C	31	ARG	NE-CZ	-5.12	1.27	1.33
2	C	188	TYR	CB-CG	-5.12	1.40	1.51
1	a	315	SER	CB-OG	-5.12	1.31	1.42
1	a	346	LYS	CA-C	-5.11	1.46	1.52
1	a	138	GLY	C-O	-5.10	1.16	1.24
7	c	19	THR	CB-CG2	-5.09	1.35	1.52
1	a	628	ARG	CB-CG	-5.09	1.37	1.52
7	c	84	ARG	CA-CB	-5.09	1.46	1.53
4	F	31	LEU	C-O	-5.08	1.18	1.24
4	f	18	THR	CA-C	-5.08	1.46	1.52
1	A	655	PHE	N-CA	-5.08	1.40	1.46
1	A	448	SER	CB-OG	-5.07	1.32	1.42
7	c	155	ARG	C-O	-5.07	1.17	1.24
1	a	774	ASN	CA-C	-5.06	1.45	1.52
3	e	29	THR	N-CA	-5.05	1.39	1.46
7	c	102	ALA	C-O	-5.05	1.17	1.24
7	c	41	SER	CB-OG	-5.04	1.32	1.42
1	A	328	ASN	CA-CB	5.04	1.60	1.53
1	a	567	THR	CB-CG2	-5.04	1.35	1.52
2	C	165	LYS	CA-CB	-5.03	1.45	1.53
2	C	122	GLN	C-N	-5.03	1.27	1.33
1	a	134	TYR	CB-CG	-5.03	1.40	1.51
7	c	94	GLN	N-CA	5.03	1.52	1.46
1	A	621	ASN	CB-CG	-5.03	1.39	1.52
2	C	153	SER	CB-OG	-5.02	1.32	1.42
1	a	764	TRP	CZ3-CH2	-5.02	1.27	1.40
2	C	162	TYR	N-CA	-5.01	1.40	1.46
2	C	214	VAL	N-CA	-5.01	1.39	1.46
1	A	762	TYR	CZ-OH	-5.01	1.27	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	147	GLY	CA-C	-5.01	1.46	1.52
3	E	7	ALA	C-O	5.01	1.29	1.24
1	a	196	LEU	C-N	-5.01	1.26	1.34
7	c	41	SER	CA-CB	-5.00	1.45	1.53
1	a	828	ARG	CA-C	-5.00	1.47	1.52

All (363) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	96	LEU	CA-C-N	22.20	147.59	119.84
1	A	96	LEU	C-N-CA	22.20	147.59	119.84
1	A	473	ASP	CA-C-N	17.04	136.90	120.03
1	A	473	ASP	C-N-CA	17.04	136.90	120.03
2	C	141	THR	CA-C-O	-14.88	104.56	120.63
2	C	141	THR	N-CA-C	14.46	128.82	111.33
3	e	24	PHE	N-CA-C	-13.76	96.95	113.88
7	c	133	VAL	N-CA-C	13.00	122.74	111.56
1	A	13	ARG	N-CA-C	12.73	130.94	113.37
7	c	106	THR	CA-C-O	12.63	134.72	120.96
2	C	179	ASN	O-C-N	-11.51	107.29	122.59
1	A	757	GLY	N-CA-C	11.23	139.80	113.18
1	A	244	PHE	CA-C-N	-11.14	107.38	119.19
1	A	244	PHE	C-N-CA	-11.14	107.38	119.19
7	c	106	THR	O-C-N	-10.86	110.02	123.06
2	C	142	ASN	N-CA-C	10.62	123.33	110.91
1	a	85	LEU	CA-C-N	10.59	133.08	119.84
1	a	85	LEU	C-N-CA	10.59	133.08	119.84
1	a	539	TRP	O-C-N	-10.42	109.44	122.68
7	c	60	ASP	N-CA-C	10.35	123.61	111.71
1	A	700	VAL	CB-CA-C	-10.02	97.45	111.28
1	A	221	PRO	CA-C-N	9.91	129.67	119.76
1	A	221	PRO	C-N-CA	9.91	129.67	119.76
1	a	346	LYS	N-CA-CB	9.80	127.05	110.49
1	A	687	TRP	N-CA-C	9.58	125.42	112.68
1	A	88	ILE	N-CA-C	9.47	129.04	109.34
7	c	91	GLY	CA-C-N	9.45	139.58	121.54
7	c	91	GLY	C-N-CA	9.45	139.58	121.54
3	E	33	ALA	N-CA-C	9.32	123.97	112.23
1	a	537	VAL	N-CA-C	9.29	122.31	108.46
2	C	22	VAL	CA-C-N	-9.28	113.09	122.27
2	C	22	VAL	C-N-CA	-9.28	113.09	122.27
1	a	327	ARG	CA-C-N	-9.04	108.06	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	327	ARG	C-N-CA	-9.04	108.06	122.79
7	c	19	THR	N-CA-C	-9.03	96.98	109.71
1	A	706	GLY	N-CA-C	8.98	127.79	115.30
2	C	116	GLU	N-CA-C	8.84	122.18	111.40
1	a	757	GLY	N-CA-C	8.82	134.08	113.18
7	c	159	LYS	CA-C-O	-8.79	111.83	121.94
1	A	96	LEU	C-N-CD	-8.75	89.13	125.00
7	c	96	ASN	N-CA-C	8.74	123.67	112.92
1	A	85	LEU	CA-C-N	8.64	130.64	119.84
1	A	85	LEU	C-N-CA	8.64	130.64	119.84
1	A	475	THR	N-CA-C	-8.61	99.46	111.52
1	A	338	MET	CA-C-N	-8.58	109.30	123.37
1	A	338	MET	C-N-CA	-8.58	109.30	123.37
2	C	124	ASN	N-CA-C	8.55	124.10	112.90
1	a	344	GLY	CA-C-N	-8.54	109.03	122.17
1	a	344	GLY	C-N-CA	-8.54	109.03	122.17
5	g	16	TRP	N-CA-C	-8.45	101.44	112.68
1	a	705	CYS	N-CA-C	8.40	121.24	109.15
1	A	501	ARG	NE-CZ-NH2	8.38	126.74	119.20
4	f	2	TRP	N-CA-C	-8.30	103.17	113.38
2	C	202	ASN	CB-CA-C	8.29	125.66	109.33
1	A	167	GLU	N-CA-CB	-8.28	98.38	110.47
1	A	135	GLY	N-CA-C	-8.26	93.61	113.18
1	a	364	GLN	N-CA-CB	-8.26	97.58	110.30
7	c	21	CYS	N-CA-CB	8.25	124.44	110.49
1	A	639	ASN	CB-CA-C	-8.24	92.92	111.30
1	a	861	PHE	CB-CA-C	8.22	124.19	110.79
7	c	92	CYS	N-CA-C	-8.21	93.31	110.80
7	c	98	GLY	O-C-N	8.14	133.28	122.70
7	c	106	THR	N-CA-CB	8.02	121.91	109.48
2	C	142	ASN	N-CA-CB	8.01	124.83	111.53
1	A	156	LYS	N-CA-C	-7.97	102.08	112.68
1	a	18	LEU	CA-CB-CG	7.93	144.06	116.30
1	a	528	GLU	N-CA-C	-7.87	98.23	109.96
1	a	482	LYS	N-CA-C	7.86	120.34	109.18
7	c	101	LYS	N-CA-C	-7.84	97.25	109.25
2	C	178	TYR	N-CA-C	7.82	122.51	112.34
1	A	167	GLU	N-CA-C	7.79	122.91	113.41
7	c	98	GLY	CA-C-N	7.79	136.67	121.41
7	c	98	GLY	C-N-CA	7.79	136.67	121.41
7	c	111	ALA	CA-C-N	7.78	128.42	119.94
7	c	111	ALA	C-N-CA	7.78	128.42	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	295	THR	N-CA-C	7.77	122.45	112.34
7	c	131	GLY	N-CA-C	7.77	131.60	113.18
4	f	18	THR	N-CA-C	7.75	119.81	111.36
1	a	345	LYS	N-CA-C	7.67	122.40	112.12
1	a	22	MET	CA-C-N	7.59	125.20	119.66
1	a	22	MET	C-N-CA	7.59	125.20	119.66
1	A	638	SER	CA-C-N	7.57	134.46	121.29
1	A	638	SER	C-N-CA	7.57	134.46	121.29
1	A	361	ASN	CA-C-N	7.56	131.02	120.29
1	A	361	ASN	C-N-CA	7.56	131.02	120.29
7	c	134	MET	CA-C-N	7.51	127.43	119.85
7	c	134	MET	C-N-CA	7.51	127.43	119.85
7	c	133	VAL	CA-C-O	-7.51	113.52	120.73
1	A	475	THR	N-CA-CB	7.47	123.27	111.91
7	c	62	LEU	CA-C-N	7.43	129.12	119.84
7	c	62	LEU	C-N-CA	7.43	129.12	119.84
7	c	96	ASN	CA-C-O	-7.42	110.87	119.56
1	a	759	VAL	N-CA-C	7.38	124.69	109.34
5	g	44	LEU	N-CA-C	7.37	120.92	110.23
7	c	26	ARG	CG-CD-NE	-7.37	95.80	112.00
5	G	11	LYS	N-CA-C	-7.34	103.21	111.14
2	C	165	LYS	CB-CA-C	7.29	121.37	110.14
3	E	32	ILE	N-CA-C	-7.29	96.92	107.78
1	A	245	PRO	CA-C-O	-7.27	108.66	119.34
5	G	44	LEU	N-CA-CB	-7.23	99.14	110.06
1	a	154	GLY	N-CA-C	-7.22	96.06	113.18
2	C	180	GLN	N-CA-C	7.19	126.11	110.80
1	a	690	GLN	N-CA-C	7.18	121.87	113.18
1	A	641	ARG	CA-C-N	-7.18	110.92	122.62
1	A	641	ARG	C-N-CA	-7.18	110.92	122.62
2	C	202	ASN	N-CA-C	-7.11	98.34	109.72
1	a	732	ASP	CA-C-N	7.09	131.32	121.26
1	a	732	ASP	C-N-CA	7.09	131.32	121.26
1	A	145	ILE	N-CA-C	-7.08	103.76	110.42
1	a	782	LEU	CA-C-N	7.06	127.63	119.94
1	a	782	LEU	C-N-CA	7.06	127.63	119.94
1	a	612	ARG	N-CA-C	7.05	122.42	113.25
1	A	91	PHE	CA-CB-CG	7.04	120.84	113.80
2	C	141	THR	O-C-N	-6.96	114.74	122.12
1	a	88	ILE	N-CA-C	6.96	123.82	109.34
1	a	18	LEU	CB-CG-CD1	-6.96	89.83	110.70
4	F	10	SER	CA-C-N	6.95	130.28	120.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	10	SER	C-N-CA	6.95	130.28	120.42
1	A	732	ASP	N-CA-C	6.89	121.54	113.20
1	A	166	PRO	CA-C-N	6.89	134.43	122.09
1	A	166	PRO	C-N-CA	6.89	134.43	122.09
5	g	26	ILE	N-CA-C	-6.88	95.03	109.34
1	A	682	TYR	N-CA-C	6.84	119.61	111.33
1	A	698	GLY	N-CA-C	6.83	126.27	112.34
7	c	106	THR	N-CA-C	6.81	120.25	110.24
7	c	92	CYS	N-CA-CB	6.79	121.97	110.49
7	c	20	GLY	N-CA-C	-6.79	97.10	113.18
7	c	132	LYS	N-CA-CB	6.78	121.94	110.49
2	C	141	THR	N-CA-CB	6.77	120.22	110.06
1	A	147	TRP	N-CA-C	6.76	125.19	110.80
1	A	501	ARG	CD-NE-CZ	6.75	133.85	124.40
1	A	736	ILE	CA-CB-CG2	6.73	121.94	110.50
3	e	28	ASN	N-CA-C	6.69	120.75	112.59
5	G	40	MET	N-CA-C	-6.64	102.32	111.28
1	A	90	GLU	O-C-N	-6.61	114.63	122.96
1	A	709	ILE	CA-C-O	-6.61	113.84	120.85
1	A	327	ARG	N-CA-C	6.61	119.33	111.33
1	a	83	VAL	N-CA-C	6.61	123.08	109.34
1	a	759	VAL	CA-C-N	6.59	129.40	120.44
1	a	759	VAL	C-N-CA	6.59	129.40	120.44
2	C	48	THR	N-CA-C	6.57	124.79	110.80
2	C	190	VAL	CA-C-O	-6.52	114.31	121.29
1	a	732	ASP	N-CA-CB	-6.52	101.05	110.56
1	A	170	TRP	N-CA-C	6.51	124.67	110.80
1	A	688	ARG	CB-CG-CD	-6.50	96.35	111.30
1	A	739	MET	CA-CB-CG	6.49	127.08	114.10
2	C	202	ASN	CA-C-O	-6.49	113.78	121.11
1	A	608	LEU	N-CA-C	-6.47	104.07	112.23
1	a	147	TRP	N-CA-C	6.47	124.58	110.80
1	a	14	TRP	N-CA-C	-6.46	105.41	113.55
1	a	197	SER	N-CA-C	6.44	120.98	112.35
2	C	216	GLU	CB-CA-C	-6.44	99.67	110.81
1	A	690	GLN	N-CA-C	6.41	120.36	112.54
2	C	218	GLN	N-CA-CB	-6.41	99.60	110.50
1	a	336	ASN	O-C-N	-6.41	113.90	122.43
1	A	638	SER	CB-CA-C	-6.40	96.66	109.79
1	a	686	GLU	CA-C-N	-6.40	111.90	122.79
1	a	686	GLU	C-N-CA	-6.40	111.90	122.79
1	a	137	ARG	CB-CG-CD	-6.38	96.64	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	741	ALA	N-CA-C	6.38	119.61	110.24
1	a	852	LEU	CA-C-O	-6.33	112.95	120.10
2	C	117	GLY	CA-C-O	-6.32	113.96	120.66
2	C	179	ASN	N-CA-C	-6.32	97.34	110.80
1	A	244	PHE	N-CA-C	6.32	123.77	109.81
2	C	71	ARG	CG-CD-NE	-6.29	98.17	112.00
1	a	851	VAL	CA-CB-CG2	6.27	121.05	110.40
2	C	121	PHE	CA-C-N	6.26	129.29	120.28
2	C	121	PHE	C-N-CA	6.26	129.29	120.28
1	A	734	GLY	N-CA-C	6.26	120.55	112.54
2	C	125	CYS	CA-C-N	6.26	129.30	120.42
2	C	125	CYS	C-N-CA	6.26	129.30	120.42
1	a	537	VAL	CB-CA-C	-6.24	100.89	110.50
1	A	94	SER	N-CA-C	6.22	124.04	110.80
1	a	822	LYS	N-CA-C	6.22	119.97	112.38
5	g	36	LEU	N-CA-C	6.21	119.33	111.69
1	a	698	GLY	CA-C-O	-6.19	116.45	122.46
4	f	5	VAL	CA-C-N	6.17	126.67	119.94
4	f	5	VAL	C-N-CA	6.17	126.67	119.94
1	a	762	TYR	CA-C-N	6.16	128.44	120.44
1	a	762	TYR	C-N-CA	6.16	128.44	120.44
1	a	394	ARG	CB-CA-C	-6.15	98.74	109.07
2	C	129	HIS	CA-C-N	6.14	131.95	121.87
2	C	129	HIS	C-N-CA	6.14	131.95	121.87
1	a	731	LEU	N-CA-C	6.14	117.97	111.28
1	A	310	ALA	CA-C-N	6.13	128.28	120.56
1	A	310	ALA	C-N-CA	6.13	128.28	120.56
2	C	191	ALA	N-CA-C	6.11	118.73	111.71
1	A	65	ARG	NE-CZ-NH1	6.09	127.59	121.50
1	A	59	ASN	CA-CB-CG	6.08	118.68	112.60
7	c	26	ARG	CD-NE-CZ	6.07	132.90	124.40
1	A	501	ARG	NE-CZ-NH1	-6.07	115.43	121.50
1	a	633	PRO	N-CA-C	6.06	120.60	111.14
1	a	539	TRP	CA-C-O	-6.06	114.61	120.92
1	A	136	ALA	N-CA-C	-6.06	97.89	110.80
2	C	216	GLU	N-CA-CB	-6.05	102.20	110.56
7	c	48	LEU	CA-CB-CG	6.03	137.41	116.30
1	A	548	LYS	CA-C-O	6.02	126.60	119.56
1	A	640	LEU	CA-C-N	6.00	133.00	121.54
1	A	640	LEU	C-N-CA	6.00	133.00	121.54
1	a	160	GLN	N-CA-C	-5.99	105.54	114.64
2	C	146	PRO	CA-C-N	5.99	126.59	120.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	146	PRO	C-N-CA	5.99	126.59	120.00
1	A	239	LEU	N-CA-C	5.98	121.24	111.37
1	A	763	MET	CB-CG-SD	-5.98	94.75	112.70
2	C	47	LYS	CA-C-N	5.97	132.94	121.54
2	C	47	LYS	C-N-CA	5.97	132.94	121.54
1	a	196	LEU	CA-C-N	-5.97	112.38	119.78
1	a	196	LEU	C-N-CA	-5.97	112.38	119.78
1	A	633	PRO	N-CA-C	5.94	120.40	111.14
1	a	736	ILE	CA-CB-CG2	5.91	120.55	110.50
2	C	75	THR	N-CA-CB	5.90	118.63	110.01
1	a	339	ASN	CB-CA-C	5.89	122.14	110.42
1	a	377	GLY	CA-C-N	5.88	127.49	120.14
1	a	377	GLY	C-N-CA	5.88	127.49	120.14
1	A	167	GLU	CB-CA-C	-5.87	98.97	109.24
2	C	22	VAL	O-C-N	-5.86	115.25	122.57
7	c	100	ASN	N-CA-CB	-5.86	101.77	110.90
2	C	218	GLN	N-CA-C	5.83	127.33	111.00
1	A	413	THR	CA-C-N	-5.83	110.78	120.68
1	A	413	THR	C-N-CA	-5.83	110.78	120.68
1	A	196	LEU	CA-C-N	-5.82	107.60	121.80
1	A	196	LEU	C-N-CA	-5.82	107.60	121.80
2	C	141	THR	CA-C-N	-5.82	114.14	122.93
2	C	141	THR	C-N-CA	-5.82	114.14	122.93
5	G	16	TRP	N-CA-C	-5.81	105.03	111.36
1	A	294	ILE	CA-CB-CG2	5.80	120.37	110.50
1	A	309	THR	OG1-CB-CG2	-5.80	97.69	109.30
2	C	163	ASN	N-CA-C	5.80	119.54	112.23
1	a	852	LEU	CA-C-N	5.79	129.79	120.30
1	a	852	LEU	C-N-CA	5.79	129.79	120.30
1	A	851	VAL	CA-CB-CG1	5.77	120.20	110.40
1	a	374	VAL	CA-C-N	5.73	128.23	120.38
1	a	374	VAL	C-N-CA	5.73	128.23	120.38
5	G	32	TYR	N-CA-C	5.73	120.39	113.17
7	c	106	THR	CA-CB-OG1	5.71	118.16	109.60
1	a	437	LEU	CA-C-N	5.71	130.23	122.07
1	a	437	LEU	C-N-CA	5.71	130.23	122.07
1	a	757	GLY	CA-C-O	-5.71	110.64	120.57
2	C	112	GLU	N-CA-C	5.71	117.58	111.36
1	A	486	GLY	N-CA-C	5.70	124.13	115.63
5	g	40	MET	CA-C-N	5.70	128.70	120.38
5	g	40	MET	C-N-CA	5.70	128.70	120.38
1	a	472	TRP	CA-C-N	-5.69	114.23	121.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	472	TRP	C-N-CA	-5.69	114.23	121.74
1	a	362	HIS	CA-C-N	5.67	128.48	120.42
1	a	362	HIS	C-N-CA	5.67	128.48	120.42
7	c	115	ALA	CA-C-N	-5.67	113.59	122.73
7	c	115	ALA	C-N-CA	-5.67	113.59	122.73
2	C	145	ASP	CA-C-N	5.67	125.34	119.05
2	C	145	ASP	C-N-CA	5.67	125.34	119.05
1	A	501	ARG	CG-CD-NE	-5.67	99.53	112.00
1	A	611	PHE	N-CA-C	-5.66	106.36	113.72
2	C	45	THR	N-CA-C	-5.66	105.72	113.30
1	a	698	GLY	CA-C-N	5.66	140.58	127.00
1	a	698	GLY	C-N-CA	5.66	140.58	127.00
7	c	43	THR	OG1-CB-CG2	-5.65	97.99	109.30
7	c	48	LEU	CB-CG-CD2	-5.64	93.78	110.70
2	C	71	ARG	N-CA-CB	5.64	119.02	110.28
1	a	709	ILE	CA-CB-CG2	5.64	120.08	110.50
7	c	130	LYS	CA-C-N	5.63	132.45	121.41
7	c	130	LYS	C-N-CA	5.63	132.45	121.41
5	G	44	LEU	CB-CG-CD1	5.63	127.58	110.70
1	A	722	LYS	N-CA-C	5.62	120.40	112.75
5	g	11	LYS	N-CA-C	-5.62	105.06	111.07
7	c	26	ARG	N-CA-C	5.60	118.36	109.96
1	A	729	TRP	CA-CB-CG	5.60	124.24	113.60
2	C	20	CYS	N-CA-CB	5.59	119.94	110.49
7	c	26	ARG	NE-CZ-NH2	-5.58	114.18	119.20
7	c	102	ALA	N-CA-CB	5.58	119.92	110.49
1	A	539	TRP	CA-C-N	5.57	129.66	120.25
1	A	539	TRP	C-N-CA	5.57	129.66	120.25
2	C	129	HIS	N-CA-C	5.56	119.76	112.92
3	E	11	VAL	N-CA-C	-5.56	104.94	111.00
1	a	801	ARG	NE-CZ-NH2	-5.56	114.20	119.20
2	C	30	THR	N-CA-CB	5.53	118.13	110.17
4	F	29	SER	N-CA-C	-5.53	105.16	111.07
1	A	238	PRO	CA-C-O	-5.52	115.19	121.98
1	a	308	LEU	CA-C-O	-5.52	115.01	120.70
5	G	9	ILE	N-CA-C	5.52	120.81	109.34
1	A	244	PHE	N-CA-CB	5.51	120.18	110.37
1	A	263	ILE	CB-CA-C	-5.51	103.33	112.26
1	a	364	GLN	CB-CA-C	5.46	121.52	110.38
2	C	164	GLY	O-C-N	-5.45	116.85	122.68
1	a	764	TRP	CA-C-N	5.44	128.02	120.29
1	a	764	TRP	C-N-CA	5.44	128.02	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	641	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	A	759	VAL	N-CA-C	5.43	120.64	109.34
7	c	81	LEU	CA-CB-CG	5.38	135.14	116.30
4	f	14	PHE	CA-C-N	5.37	127.92	120.29
4	f	14	PHE	C-N-CA	5.37	127.92	120.29
3	e	29	THR	N-CA-C	-5.37	104.01	110.88
1	A	287	ARG	CA-C-N	5.36	125.90	120.38
1	A	287	ARG	C-N-CA	5.36	125.90	120.38
1	A	822	LYS	N-CA-C	5.36	118.61	111.75
1	A	785	LEU	CA-C-N	5.35	127.30	120.56
1	A	785	LEU	C-N-CA	5.35	127.30	120.56
3	E	33	ALA	CA-C-O	-5.35	113.48	119.79
7	c	112	GLY	CA-C-O	-5.35	114.91	120.90
1	A	474	PRO	N-CA-C	-5.33	103.41	111.41
1	a	367	LEU	CA-CB-CG	-5.33	97.63	116.30
4	f	15	PHE	CA-C-N	5.33	127.99	120.42
4	f	15	PHE	C-N-CA	5.33	127.99	120.42
2	C	174	MET	N-CA-C	-5.33	98.04	109.81
7	c	33	LEU	N-CA-C	5.32	118.03	110.10
4	F	5	VAL	CA-C-N	5.32	126.78	120.14
4	F	5	VAL	C-N-CA	5.32	126.78	120.14
1	a	19	GLU	N-CA-C	5.31	118.66	110.42
1	A	91	PHE	CA-C-N	5.30	128.38	120.90
1	A	91	PHE	C-N-CA	5.30	128.38	120.90
7	c	26	ARG	CB-CG-CD	5.30	123.50	111.30
2	C	73	ARG	CB-CA-C	-5.30	99.97	109.24
1	a	152	VAL	N-CA-C	-5.29	97.44	108.88
2	C	216	GLU	CA-C-N	5.29	131.65	121.54
2	C	216	GLU	C-N-CA	5.29	131.65	121.54
1	a	305	HIS	CA-C-O	-5.29	114.82	120.42
2	C	30	THR	CB-CA-C	-5.28	99.82	109.54
3	E	34	ALA	N-CA-CB	5.26	119.39	110.49
1	A	709	ILE	N-CA-CB	5.26	118.47	110.58
2	C	194	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	a	851	VAL	CA-CB-CG1	5.25	119.32	110.40
2	C	71	ARG	N-CA-C	5.23	117.89	111.82
2	C	179	ASN	CB-CA-C	5.23	120.83	110.42
2	C	48	THR	N-CA-CB	5.22	119.31	110.49
1	A	65	ARG	CG-CD-NE	5.20	123.45	112.00
3	E	27	ALA	N-CA-C	5.20	116.95	111.28
1	A	242	ALA	CA-C-N	5.20	125.13	119.78
1	A	242	ALA	C-N-CA	5.20	125.13	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	19	GLY	CA-C-N	5.20	131.47	121.54
2	C	19	GLY	C-N-CA	5.20	131.47	121.54
1	A	500	ASP	N-CA-C	5.19	117.82	110.50
1	a	768	THR	CA-CB-OG1	5.19	117.38	109.60
7	c	131	GLY	CA-C-O	-5.18	111.55	120.57
2	C	174	MET	CG-SD-CE	5.17	112.27	100.90
1	A	84	TRP	N-CA-C	-5.17	107.04	113.55
1	a	698	GLY	C-N-CD	-5.16	109.26	120.60
7	c	103	ILE	N-CA-CB	-5.15	103.42	112.08
2	C	87	VAL	CA-CB-CG1	5.14	119.14	110.40
1	a	188	LEU	CA-CB-CG	5.14	134.29	116.30
1	a	528	GLU	CA-C-O	-5.14	114.79	120.70
2	C	203	GLY	N-CA-C	5.14	125.36	113.18
7	c	41	SER	N-CA-C	5.13	119.40	113.20
4	F	25	ILE	CA-C-N	5.12	127.01	120.56
4	F	25	ILE	C-N-CA	5.12	127.01	120.56
1	a	775	HIS	N-CA-C	-5.10	105.36	112.45
1	A	472	TRP	N-CA-C	5.09	118.59	112.38
1	a	798	ARG	CG-CD-NE	-5.09	100.81	112.00
4	f	13	CYS	N-CA-C	-5.08	105.82	111.36
1	A	860	GLY	O-C-N	-5.08	117.17	123.21
1	a	742	ARG	NE-CZ-NH2	5.07	123.77	119.20
2	C	59	GLN	CB-CA-C	-5.07	100.33	110.42
4	F	3	ASN	N-CA-C	-5.07	105.45	111.69
1	A	168	GLY	N-CA-C	5.06	122.66	112.34
7	c	135	PRO	N-CA-C	5.05	119.42	111.38
1	A	529	TRP	N-CA-C	5.05	121.56	110.80
1	a	65	ARG	CG-CD-NE	5.04	123.10	112.00
3	E	31	ASP	N-CA-C	5.03	119.37	113.23
1	a	697	ILE	CA-C-N	5.03	129.34	121.64
1	a	697	ILE	C-N-CA	5.03	129.34	121.64
5	G	41	LEU	N-CA-C	5.02	119.17	113.19
7	c	26	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	A	706	GLY	CA-C-N	5.01	128.87	120.64
1	A	706	GLY	C-N-CA	5.01	128.87	120.64
1	A	736	ILE	CB-CG1-CD1	-5.01	103.28	113.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	639	ASN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6960	0	6807	263	0
1	a	6984	0	6830	222	0
2	C	1474	0	1403	57	0
3	E	258	0	279	6	0
3	e	258	0	279	15	0
4	F	273	0	290	9	0
4	f	273	0	290	12	0
5	G	302	0	318	23	0
5	g	302	0	318	27	0
6	H	95	0	23	8	0
6	h	95	0	20	5	0
7	c	1096	0	1079	50	0
8	A	66	0	68	2	0
8	a	66	0	69	1	0
9	A	489	0	507	46	0
9	a	508	0	553	44	0
10	A	292	0	287	20	0
10	a	292	0	284	17	0
11	A	40	0	56	6	0
11	c	40	0	55	5	0
12	A	1	0	0	0	0
12	a	1	0	0	0	0
13	A	135	0	0	5	0
13	a	135	0	0	5	0
14	A	240	0	0	15	0
14	C	18	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	E	26	0	0	0	0
14	a	243	0	0	9	0
14	c	8	0	0	1	0
14	e	26	0	0	1	0
15	A	47	0	0	8	0
15	G	38	0	0	7	0
15	a	47	0	0	3	0
15	g	38	0	0	1	0
16	C	43	0	31	9	0
16	c	43	0	31	5	0
17	E	44	0	0	0	0
17	a	44	0	0	0	0
18	a	8	0	0	4	0
19	A	3	0	0	0	0
19	a	3	0	0	0	0
All	All	21354	0	19877	738	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (738) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD12	1:A:86:PRO:CD	1.38	1.47
5:G:40:MET:HE1	15:G:101:85N:C22	1.47	1.43
1:a:150:PRO:HA	1:a:156:LYS:NZ	1.27	1.42
1:a:150:PRO:CA	1:a:156:LYS:HZ1	1.32	1.41
5:G:40:MET:CE	15:G:101:85N:C22	1.95	1.41
2:C:128:CYS:SG	16:C:301:HEC:CAC	2.09	1.40
1:a:150:PRO:CA	1:a:156:LYS:NZ	1.84	1.40
1:A:826:GLU:OE1	15:A:932:85N:C22	1.78	1.32
1:a:150:PRO:C	1:a:156:LYS:HZ1	1.40	1.28
1:A:85:LEU:CD1	1:A:86:PRO:HD2	1.67	1.25
7:c:98:GLY:HA2	7:c:107:ASN:CA	1.66	1.25
1:a:12:LYS:NZ	1:a:693:ASP:OD2	1.69	1.25
1:a:149:LEU:O	1:a:156:LYS:NZ	1.75	1.20
2:C:128:CYS:SG	16:C:301:HEC:HAC	1.76	1.19
1:A:94:SER:HB2	1:A:97:PRO:HA	1.19	1.17
9:A:908:BCL:HBA1	9:A:908:BCL:HBD	1.21	1.16
9:a:904:BCL:H203	7:c:16:VAL:CG2	1.77	1.15
1:A:88:ILE:HA	1:A:95:LYS:NZ	1.62	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:CD1	1:A:86:PRO:CD	2.25	1.12
1:A:88:ILE:HA	1:A:95:LYS:HZ3	1.12	1.11
7:c:49:ARG:HH11	7:c:63:PRO:HG2	1.06	1.10
5:G:34:PRO:HB3	5:G:44:LEU:HD22	1.22	1.09
7:c:98:GLY:CA	7:c:107:ASN:HA	1.83	1.09
1:A:66:LEU:HD13	10:A:911:CLA:CED	1.85	1.05
7:c:98:GLY:HA3	7:c:107:ASN:OD1	1.57	1.04
1:A:83:VAL:HG21	1:A:106:MET:HE1	1.37	1.04
1:a:152:VAL:HB	1:a:155:LEU:HD21	1.39	1.03
1:a:640:LEU:H	1:a:865:ARG:HG3	1.25	1.01
4:f:4:VAL:O	4:f:8:ILE:HD12	1.62	1.00
9:A:903:BCL:HAA1	9:A:903:BCL:HBD	1.42	1.00
1:A:865:ARG:NH1	2:C:83:ASN:OD1	1.95	0.99
9:a:904:BCL:H203	7:c:16:VAL:HG21	1.42	0.99
9:A:902:BCL:HBB3	11:A:913:LYC:H62	1.43	0.98
1:A:91:PHE:HB3	1:A:95:LYS:HB3	1.46	0.98
7:c:18:ALA:HB2	11:c:201:LYC:H622	1.42	0.97
1:A:639:ASN:HD22	1:A:643:GLN:HB2	1.29	0.97
1:a:475:THR:HA	5:g:39:LYS:HG2	1.46	0.96
1:A:28:PHE:CE2	9:A:905:BCL:HED2	2.01	0.95
5:G:40:MET:HE2	15:G:101:85N:C22	1.94	0.95
1:a:445:GLN:HE22	1:a:514:THR:HG22	1.28	0.93
9:A:906:BCL:HMB1	9:A:906:BCL:HBB3	1.49	0.93
1:A:85:LEU:HD12	1:A:86:PRO:HD3	1.50	0.92
1:A:149:LEU:H	1:A:150:PRO:CD	1.82	0.92
9:A:908:BCL:HBA1	9:A:908:BCL:CBD	1.99	0.92
5:G:34:PRO:HB3	5:G:44:LEU:CD2	2.00	0.91
5:G:41:LEU:HG	5:G:44:LEU:HD23	1.52	0.91
7:c:98:GLY:HA2	7:c:107:ASN:HA	0.93	0.90
1:A:66:LEU:CD1	10:A:911:CLA:CED	2.50	0.90
5:g:30:GLY:HA3	15:g:101:85N:O4	1.70	0.90
5:G:34:PRO:CB	5:G:44:LEU:HD22	2.01	0.90
1:A:483:ASN:HB3	1:A:484:PRO:HD2	1.51	0.90
1:A:88:ILE:CA	1:A:95:LYS:NZ	2.36	0.89
9:a:908:BCL:H193	3:e:5:LEU:HD21	1.55	0.88
7:c:98:GLY:HA2	7:c:107:ASN:CB	2.04	0.88
5:G:32:TYR:OH	6:H:6:UNK:O	1.91	0.87
7:c:49:ARG:NH1	7:c:63:PRO:HG2	1.89	0.87
1:A:13:ARG:HH11	1:A:13:ARG:HB2	1.38	0.87
1:A:477:GLY:H	5:G:41:LEU:HD13	1.38	0.87
1:A:94:SER:HB2	1:A:97:PRO:CA	2.03	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:908:BCL:C19	3:e:5:LEU:HD21	2.04	0.86
7:c:33:LEU:O	7:c:33:LEU:HD23	1.76	0.85
1:A:109:PHE:CD1	14:A:922:UNL:C16	2.59	0.85
1:A:94:SER:CB	1:A:97:PRO:HA	2.06	0.85
1:A:88:ILE:CA	1:A:95:LYS:HZ3	1.87	0.85
1:a:149:LEU:C	1:a:156:LYS:HZ3	1.84	0.85
9:a:904:BCL:H203	7:c:16:VAL:HG23	1.59	0.84
7:c:98:GLY:CA	7:c:107:ASN:OD1	2.24	0.84
1:A:433:THR:HG21	1:A:739:MET:HG2	1.59	0.84
1:A:85:LEU:CD1	1:A:86:PRO:HD3	2.04	0.84
1:a:150:PRO:HA	1:a:156:LYS:HZ2	1.02	0.84
4:F:34:ARG:HA	4:F:34:ARG:NE	1.93	0.83
1:a:501:ARG:HD2	5:g:44:LEU:HD23	1.59	0.83
1:A:613:PRO:O	1:A:614:GLU:HB3	1.79	0.83
1:a:149:LEU:C	1:a:156:LYS:NZ	2.36	0.83
1:a:445:GLN:HE22	1:a:514:THR:CG2	1.91	0.83
1:A:156:LYS:HD2	1:A:156:LYS:O	1.79	0.83
1:A:158:LEU:HD22	1:A:158:LEU:O	1.78	0.83
1:A:765:ASN:O	1:A:768:THR:HG23	1.79	0.82
1:A:88:ILE:C	1:A:95:LYS:NZ	2.38	0.82
9:A:907:BCL:HBB3	9:A:907:BCL:HMB1	1.61	0.81
1:A:83:VAL:HG12	1:A:88:ILE:HD12	1.63	0.81
1:A:149:LEU:N	1:A:150:PRO:CD	2.41	0.80
1:a:149:LEU:N	1:a:150:PRO:CD	2.44	0.80
1:a:149:LEU:H	1:a:150:PRO:CD	1.93	0.80
1:A:66:LEU:HD13	10:A:911:CLA:HED1	1.62	0.80
1:a:641:ARG:CG	1:a:865:ARG:HH11	1.94	0.80
1:a:641:ARG:HD3	1:a:865:ARG:HH11	1.46	0.80
7:c:18:ALA:CB	11:c:201:LYC:H622	2.11	0.80
1:a:641:ARG:HD3	1:a:865:ARG:NH1	1.96	0.80
1:A:307:HIS:ND1	9:A:902:BCL:HBB1	1.96	0.79
9:A:903:BCL:HAA1	9:A:903:BCL:CBD	2.04	0.79
1:a:641:ARG:CD	1:a:865:ARG:HH11	1.94	0.79
1:A:696:CYS:HG	18:a:917:SF4:FE4	0.97	0.79
1:A:78:GLU:CD	2:C:62:PRO:HG2	2.09	0.78
1:a:150:PRO:CA	1:a:156:LYS:HZ2	1.75	0.78
5:G:34:PRO:CB	5:G:44:LEU:CD2	2.61	0.78
1:A:141:THR:HG22	1:A:162:LYS:HG2	1.64	0.78
1:a:641:ARG:CD	1:a:865:ARG:NH1	2.46	0.78
1:A:82:ARG:HA	1:A:88:ILE:HG13	1.66	0.78
1:a:12:LYS:HZ1	1:a:693:ASP:CG	1.89	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:150:PRO:C	1:a:156:LYS:NZ	2.26	0.77
1:A:641:ARG:HG2	2:C:39:LEU:CD1	2.14	0.77
14:A:926:UNL:C2	14:A:927:UNL:C	2.63	0.77
1:a:440:ASN:HB2	1:a:514:THR:HG21	1.67	0.77
1:A:760:PHE:CE2	10:A:931:CLA:HED3	2.20	0.76
1:a:501:ARG:CD	5:g:44:LEU:HD23	2.15	0.76
1:A:13:ARG:HB2	1:A:13:ARG:NH1	2.00	0.76
10:A:910:CLA:HED3	1:a:760:PHE:CE2	2.21	0.75
1:A:88:ILE:C	1:A:95:LYS:HZ3	1.93	0.74
1:a:639:ASN:HB3	1:a:641:ARG:H	1.51	0.74
2:C:128:CYS:SG	16:C:301:HEC:CBC	2.75	0.73
1:A:429:ILE:O	1:A:433:THR:HG23	1.89	0.73
1:A:833:ASN:C	1:A:833:ASN:HD22	1.97	0.73
1:a:493:ALA:HA	1:a:496:LEU:HD22	1.71	0.73
1:a:705:CYS:HB3	18:a:917:SF4:S4	2.29	0.73
2:C:87:VAL:HG22	2:C:179:ASN:O	1.89	0.72
7:c:33:LEU:HD23	7:c:33:LEU:C	2.12	0.72
1:a:158:LEU:HD13	1:a:158:LEU:C	2.14	0.72
5:g:40:MET:HG3	5:g:40:MET:O	1.88	0.72
1:a:475:THR:HA	5:g:39:LYS:CG	2.19	0.72
1:A:149:LEU:H	1:A:150:PRO:HD3	1.51	0.72
9:a:909:BCL:HBB3	9:a:909:BCL:HMB1	1.72	0.72
1:A:627:GLU:HB3	2:C:46:LEU:HD22	1.71	0.71
1:A:826:GLU:OE1	15:A:932:85N:C19	2.39	0.71
4:F:2:TRP:HA	4:F:2:TRP:CE3	2.24	0.71
2:C:87:VAL:CG2	2:C:179:ASN:O	2.39	0.71
1:a:13:ARG:O	1:a:17:LYS:HE2	1.91	0.71
1:a:55:ASP:OD1	7:c:42:ARG:NH2	2.23	0.71
1:A:148:LEU:H	1:A:148:LEU:HD23	1.55	0.70
1:a:149:LEU:H	1:a:150:PRO:HD3	1.55	0.70
2:C:107:TYR:CG	2:C:218:GLN:HB2	2.27	0.70
9:a:905:BCL:H92	14:a:931:UNL:C	2.22	0.70
14:a:932:UNL:C16	14:a:933:UNL:C17	2.69	0.70
7:c:133:VAL:HG22	16:c:202:HEC:HMD2	1.72	0.70
9:A:904:BCL:HMB1	9:A:904:BCL:HBB3	1.72	0.69
1:A:627:GLU:HB3	2:C:46:LEU:CD2	2.22	0.69
1:a:12:LYS:NZ	1:a:693:ASP:CG	2.49	0.69
1:a:641:ARG:HG3	1:a:865:ARG:NH1	2.07	0.69
1:A:741:ALA:O	1:A:757:GLY:O	2.10	0.69
1:A:87:LEU:O	1:A:87:LEU:HD12	1.93	0.69
1:a:155:LEU:HD23	1:a:155:LEU:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:HD12	1:A:86:PRO:HD2	0.73	0.69
7:c:98:GLY:HA3	7:c:107:ASN:CG	2.16	0.69
1:A:57:TYR:O	1:A:61:THR:HG22	1.92	0.69
1:a:152:VAL:CG1	1:a:155:LEU:HD11	2.23	0.69
1:A:109:PHE:HD1	14:A:922:UNL:C16	2.05	0.68
1:A:287:ARG:NH1	1:A:287:ARG:HG3	2.06	0.68
9:a:904:BCL:C20	7:c:16:VAL:HG23	2.22	0.68
2:C:59:GLN:CD	2:C:59:GLN:H	2.01	0.68
1:a:294:ILE:HG13	1:a:297:LEU:HD23	1.74	0.68
9:A:905:BCL:HBB2	9:A:905:BCL:HMB3	1.74	0.68
1:A:494:ARG:HD2	1:A:586:VAL:HG13	1.75	0.68
1:A:641:ARG:HG2	2:C:39:LEU:HD12	1.75	0.68
1:a:640:LEU:HD22	1:a:865:ARG:HB2	1.76	0.68
1:A:141:THR:HB	1:A:161:ILE:O	1.94	0.67
1:a:88:ILE:O	1:a:95:LYS:HD2	1.94	0.67
9:A:902:BCL:CBB	11:A:913:LYC:H62	2.19	0.67
1:A:810:ARG:HG2	3:e:35:ASN:HA	1.75	0.67
9:A:906:BCL:HBB3	9:A:906:BCL:CMB	2.23	0.67
1:A:66:LEU:CD1	10:A:911:CLA:HED3	2.23	0.67
1:A:135:GLY:O	1:A:175:LEU:HD22	1.94	0.67
4:f:34:ARG:HG3	4:f:34:ARG:O	1.94	0.67
1:A:597:THR:HG22	1:A:600:ALA:H	1.60	0.67
1:a:150:PRO:N	1:a:156:LYS:NZ	2.43	0.67
7:c:98:GLY:CA	7:c:107:ASN:CG	2.69	0.66
1:A:763:MET:HE1	10:A:931:CLA:HED2	1.77	0.66
1:a:705:CYS:CB	18:a:917:SF4:S4	2.83	0.66
1:A:84:TRP:HE3	1:A:84:TRP:O	1.79	0.66
4:F:2:TRP:HA	4:F:2:TRP:HE3	1.56	0.66
1:a:658:MET:HE2	1:a:658:MET:HA	1.77	0.66
2:C:107:TYR:CD1	2:C:218:GLN:HB2	2.31	0.66
1:A:826:GLU:CD	15:A:932:85N:C22	2.69	0.66
1:a:152:VAL:HB	1:a:155:LEU:CD2	2.23	0.66
1:A:149:LEU:N	1:A:150:PRO:HD2	2.09	0.65
9:a:905:BCL:CHB	9:a:905:BCL:H11	2.26	0.65
6:H:2:UNK:CB	14:c:203:UNL:C4	2.73	0.65
1:A:441:PHE:CE2	6:H:3:UNK:CB	2.80	0.65
16:c:202:HEC:HMB3	16:c:202:HEC:HBB3	1.77	0.65
1:A:135:GLY:O	1:A:175:LEU:CD2	2.45	0.65
1:a:487:THR:HB	6:h:17:UNK:O	1.97	0.64
1:A:342:ILE:HD12	1:A:347:ILE:HG13	1.79	0.64
1:A:531:GLN:HE21	1:A:533:LYS:HE3	1.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:155:LEU:HD22	1:a:155:LEU:N	2.11	0.64
1:a:864:ASN:C	1:a:864:ASN:HD22	2.06	0.64
7:c:96:ASN:C	7:c:96:ASN:HD22	2.06	0.64
7:c:144:GLN:NE2	7:c:147:ASN:HD22	1.95	0.64
2:C:71:ARG:HB2	2:C:75:THR:HG23	1.79	0.64
2:C:134:CYS:HA	2:C:142:ASN:OD1	1.97	0.64
1:A:158:LEU:HD22	1:A:158:LEU:C	2.20	0.63
1:A:28:PHE:CD2	9:A:905:BCL:HED2	2.32	0.63
1:A:13:ARG:HH11	1:A:13:ARG:CB	2.09	0.63
3:e:18:LEU:HD23	14:e:101:UNL:C4	2.29	0.63
9:A:902:BCL:HHC	9:A:902:BCL:HBB2	1.79	0.63
1:a:150:PRO:O	1:a:156:LYS:NZ	2.30	0.63
1:a:641:ARG:CG	1:a:865:ARG:NH1	2.58	0.63
2:C:128:CYS:SG	16:C:301:HEC:C3C	2.86	0.63
1:A:392:GLN:O	1:A:394:ARG:NH1	2.31	0.63
9:a:905:BCL:CBB	9:a:905:BCL:HMB3	2.30	0.62
1:A:109:PHE:CD1	14:A:922:UNL:C15	2.81	0.62
1:A:843:VAL:O	1:A:847:THR:HG23	1.99	0.62
1:a:109:PHE:HD1	14:a:926:UNL:C7	2.12	0.62
1:a:158:LEU:HD22	1:a:158:LEU:O	2.00	0.62
5:G:34:PRO:HB2	5:G:44:LEU:CG	2.30	0.62
1:a:309:THR:HG22	1:a:373:GLY:HA3	1.80	0.62
1:A:220:LYS:O	1:A:267:THR:HG21	2.00	0.62
1:a:441:PHE:CE2	6:h:3:UNK:CB	2.83	0.62
1:A:83:VAL:CG2	1:A:106:MET:HE1	2.23	0.61
1:a:85:LEU:H	1:a:85:LEU:CD2	2.13	0.61
1:a:773:ASP:O	1:a:777:THR:HG22	2.01	0.61
13:A:917:85I:C33	10:a:901:CLA:H141	2.30	0.61
5:G:30:GLY:CA	15:G:101:85N:O5	2.48	0.61
1:A:160:GLN:O	1:A:160:GLN:HG3	2.00	0.61
1:a:415:MET:HG2	1:a:667:ILE:HD13	1.83	0.61
1:a:615:LEU:HG	1:a:615:LEU:O	1.99	0.61
1:A:78:GLU:OE2	2:C:62:PRO:HG2	2.01	0.61
1:A:156:LYS:HD2	1:A:156:LYS:C	2.21	0.61
1:A:66:LEU:HD13	10:A:911:CLA:HED2	1.77	0.61
1:a:158:LEU:HD13	1:a:158:LEU:O	2.00	0.61
1:a:501:ARG:NH1	5:g:44:LEU:O	2.34	0.60
4:f:4:VAL:O	4:f:4:VAL:HG12	2.01	0.60
9:a:904:BCL:C20	7:c:16:VAL:CG2	2.66	0.60
1:A:729:TRP:HB3	1:A:736:ILE:HD11	1.83	0.60
1:A:87:LEU:HD12	1:A:95:LYS:HG3	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LEU:H	1:A:148:LEU:CD2	2.14	0.60
5:G:40:MET:HE3	15:G:101:85N:C22	2.24	0.60
1:A:33:MET:HB3	9:A:902:BCL:C9	2.32	0.60
1:a:155:LEU:HD22	1:a:155:LEU:H	1.65	0.60
1:a:474:PRO:O	1:a:475:THR:OG1	2.15	0.60
1:A:88:ILE:C	1:A:95:LYS:HZ1	2.08	0.60
1:A:550:ASN:HD21	1:A:552:LEU:HB2	1.67	0.60
1:A:156:LYS:NZ	1:A:160:GLN:HB3	2.17	0.59
1:A:242:ALA:HB3	1:A:247:GLY:HA3	1.82	0.59
1:A:252:TYR:CE1	2:C:36:PRO:HB3	2.37	0.59
1:A:532:PRO:HB2	1:A:622:MET:HE1	1.83	0.59
1:A:94:SER:CB	1:A:97:PRO:CA	2.73	0.59
14:A:923:UNL:C10	2:C:22:VAL:O	2.50	0.59
1:a:93:THR:O	1:a:97:PRO:HA	2.01	0.59
5:g:38:VAL:HG12	5:g:38:VAL:O	2.01	0.59
1:a:487:THR:CB	6:h:17:UNK:O	2.50	0.59
1:A:639:ASN:ND2	1:A:643:GLN:HB2	2.11	0.58
1:a:458:ALA:HA	1:a:461:ILE:HD12	1.85	0.58
1:A:826:GLU:O	15:A:932:85N:C18	2.52	0.58
1:a:94:SER:C	1:a:96:LEU:H	2.12	0.58
1:a:61:THR:HG21	9:a:910:BCL:HAA2	1.86	0.58
1:a:445:GLN:NE2	1:a:514:THR:HG22	2.08	0.58
7:c:133:VAL:HG22	16:c:202:HEC:CMD	2.34	0.58
1:A:88:ILE:O	1:A:88:ILE:HG22	2.03	0.58
1:A:610:LYS:O	1:A:610:LYS:HG2	2.04	0.58
1:a:149:LEU:HA	1:a:152:VAL:HG23	1.85	0.58
1:A:82:ARG:O	1:A:82:ARG:HG3	1.99	0.58
9:A:907:BCL:HBB3	9:A:907:BCL:CMB	2.33	0.58
2:C:116:GLU:HG2	2:C:188:TYR:CD2	2.38	0.58
9:a:905:BCL:HHD	9:a:909:BCL:HBB2	1.85	0.58
9:A:908:BCL:HBA1	9:A:908:BCL:CHA	2.31	0.57
7:c:44:ALA:O	7:c:48:LEU:HD22	2.04	0.57
1:A:696:CYS:SG	18:a:917:SF4:S1	3.01	0.57
1:a:843:VAL:O	1:a:847:THR:HG23	2.04	0.57
1:A:85:LEU:HD13	1:A:86:PRO:HD3	1.86	0.57
10:a:913:CLA:HBD	10:a:913:CLA:HAA1	1.85	0.57
14:a:930:UNL:C	14:a:931:UNL:C8	2.83	0.57
5:G:9:ILE:HD12	5:G:9:ILE:H	1.70	0.56
5:G:34:PRO:HB2	5:G:44:LEU:CD1	2.35	0.56
9:A:908:BCL:HMB1	9:A:908:BCL:HBB3	1.87	0.56
1:a:531:GLN:HE21	1:a:533:LYS:HE2	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:904:BCL:HED3	10:a:914:CLA:HMB1	1.87	0.56
1:A:147:TRP:CD1	1:A:147:TRP:C	2.83	0.56
9:A:907:BCL:CMB	9:A:907:BCL:CBB	2.83	0.56
5:g:9:ILE:CD1	5:g:9:ILE:H	2.18	0.56
1:a:443:ILE:O	5:g:27:GLY:C	2.49	0.56
1:a:143:GLY:O	1:a:147:TRP:HA	2.05	0.56
1:a:203:ILE:HD12	9:a:909:BCL:HED2	1.86	0.56
1:a:818:ARG:HG3	1:a:818:ARG:HH11	1.71	0.56
1:A:826:GLU:OE1	15:A:932:85N:C21	2.53	0.56
14:a:929:UNL:C9	14:a:929:UNL:C13	2.83	0.56
1:A:595:ALA:HB3	1:A:601:LYS:HG2	1.88	0.56
1:A:149:LEU:H	1:A:150:PRO:HD2	1.64	0.56
14:C:302:UNL:C19	14:C:302:UNL:C14	2.84	0.56
2:C:107:TYR:CG	2:C:218:GLN:CB	2.89	0.55
4:f:30:HIS:C	4:f:30:HIS:CD2	2.84	0.55
1:A:88:ILE:CG2	1:A:109:PHE:HZ	2.18	0.55
1:A:441:PHE:CD2	6:H:3:UNK:CB	2.90	0.55
1:a:640:LEU:H	1:a:865:ARG:CG	2.11	0.55
1:A:185:TRP:HB2	1:A:188:LEU:HD22	1.89	0.55
15:A:932:85N:C8	15:A:932:85N:C4	2.85	0.55
14:a:931:UNL:C	14:a:931:UNL:C5	2.85	0.55
9:A:906:BCL:CMB	9:A:906:BCL:CBB	2.85	0.55
1:A:450:ARG:HH21	1:A:518:THR:HG22	1.72	0.55
1:a:672:ILE:HG12	1:a:709:ILE:HG13	1.89	0.55
1:a:433:THR:HG21	1:a:739:MET:HG2	1.89	0.55
1:a:641:ARG:HG3	1:a:865:ARG:HH11	1.66	0.55
1:a:735:TRP:O	1:a:758:GLY:HA2	2.07	0.55
1:A:89:GLY:O	1:A:95:LYS:HE2	2.07	0.55
1:A:636:LEU:HD21	13:A:915:85I:O7	2.07	0.55
1:a:409:LYS:O	1:a:413:THR:HG23	2.07	0.55
2:C:59:GLN:H	2:C:59:GLN:NE2	2.05	0.54
1:a:85:LEU:N	1:a:85:LEU:HD23	2.22	0.54
1:a:494:ARG:NH1	1:a:590:ASN:OD1	2.39	0.54
1:A:14:TRP:CD1	1:A:14:TRP:C	2.85	0.54
1:A:156:LYS:HZ2	1:A:160:GLN:HB3	1.71	0.54
1:A:501:ARG:HB3	1:A:517:PHE:HB3	1.89	0.54
1:A:847:THR:O	1:A:851:VAL:HG13	2.06	0.54
15:A:932:85N:C18	15:A:932:85N:C21	2.85	0.54
1:a:559:ILE:O	1:a:563:GLN:HG3	2.07	0.54
2:C:37:MET:HE1	2:C:80:GLN:HB3	1.89	0.54
1:a:147:TRP:CD1	1:a:147:TRP:C	2.85	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:151:TYR:N	1:a:151:TYR:CD1	2.72	0.54
1:A:519:THR:H	1:A:538:GLN:HE21	1.55	0.54
4:f:25:ILE:HG22	4:f:25:ILE:O	2.07	0.54
1:A:755:HIS:HD2	1:A:757:GLY:H	1.55	0.54
2:C:182:SER:H	2:C:185:GLN:HE21	1.56	0.54
10:A:910:CLA:NC	1:a:722:LYS:HD3	2.23	0.54
1:A:309:THR:HG23	9:A:903:BCL:HMC1	1.88	0.54
14:A:919:UNL:C10	14:A:919:UNL:C6	2.85	0.54
1:A:639:ASN:ND2	1:A:643:GLN:HE21	2.04	0.54
1:A:158:LEU:C	1:A:158:LEU:HD13	2.33	0.54
14:A:918:UNL:C8	14:A:918:UNL:C12	2.86	0.54
15:G:101:85N:C22	15:G:101:85N:C24	2.85	0.54
1:a:382:HIS:CE1	1:a:386:ILE:HD13	2.43	0.54
15:a:902:85N:C27	15:a:902:85N:C16	2.85	0.54
1:A:88:ILE:HA	1:A:95:LYS:HZ2	1.66	0.53
2:C:116:GLU:HG2	2:C:188:TYR:CE2	2.43	0.53
1:a:48:ALA:HB2	7:c:20:GLY:CA	2.38	0.53
1:a:849:THR:O	1:a:853:VAL:HG23	2.08	0.53
1:A:624:GLU:OE2	1:A:628:ARG:NH1	2.38	0.53
5:G:30:GLY:HA3	15:G:101:85N:O5	2.07	0.53
7:c:98:GLY:CA	7:c:107:ASN:CB	2.81	0.53
1:A:13:ARG:HG3	1:A:13:ARG:O	2.09	0.53
4:f:26:VAL:HG12	4:f:26:VAL:O	2.08	0.53
10:A:911:CLA:HAA1	10:A:911:CLA:HBD	1.90	0.53
9:a:905:BCL:HMB3	9:a:905:BCL:HBB2	1.90	0.53
1:A:814:LEU:HD13	3:e:34:ALA:HA	1.89	0.53
1:a:832:SER:HA	13:a:920:85I:O2	2.09	0.53
1:A:445:GLN:NE2	1:A:514:THR:OG1	2.34	0.53
1:A:720:SER:O	1:A:724:LEU:HD22	2.09	0.53
3:e:21:ILE:C	3:e:23:LYS:H	2.16	0.53
1:A:94:SER:CB	1:A:98:PHE:N	2.72	0.53
1:a:676:ASN:HA	1:a:709:ILE:CD1	2.38	0.53
5:g:9:ILE:CD1	5:g:9:ILE:N	2.72	0.53
5:G:14:TRP:HA	5:G:14:TRP:CE3	2.43	0.53
4:F:33:SER:HB2	13:a:920:85I:O3	2.09	0.53
8:a:903:2GO:H21	8:a:903:2GO:H25	1.91	0.53
7:c:100:ASN:C	7:c:100:ASN:HD22	2.16	0.53
7:c:114:GLN:HG3	7:c:157:GLU:HG3	1.91	0.53
10:A:910:CLA:HMB1	10:A:910:CLA:HBB1	1.91	0.53
2:C:59:GLN:HB2	2:C:61:THR:HG22	1.90	0.53
1:A:269:MET:HB2	9:A:906:BCL:HED2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:908:BCL:H191	3:e:5:LEU:HD21	1.91	0.52
1:A:33:MET:HB3	9:A:902:BCL:H92	1.92	0.52
1:A:151:TYR:N	1:A:151:TYR:CD1	2.74	0.52
9:A:908:BCL:HHC	9:A:908:BCL:OBB	2.10	0.52
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.73	0.52
1:A:688:ARG:CG	1:A:688:ARG:HH11	2.21	0.52
1:a:609:ASP:HA	1:a:612:ARG:NH1	2.24	0.52
5:g:16:TRP:C	5:g:18:GLY:H	2.17	0.52
1:A:171:TYR:CD1	1:A:171:TYR:C	2.86	0.52
1:A:612:ARG:HB3	1:A:613:PRO:HD3	1.91	0.52
1:a:85:LEU:CD2	1:a:85:LEU:N	2.73	0.52
1:a:155:LEU:CD2	1:a:155:LEU:N	2.72	0.52
1:a:526:LYS:NZ	1:a:626:ASN:HD21	2.07	0.52
1:A:148:LEU:CD2	1:A:148:LEU:N	2.73	0.52
1:A:826:GLU:OE1	15:A:932:85N:N1	2.39	0.52
14:A:927:UNL:C9	14:A:927:UNL:C5	2.85	0.52
2:C:167:ILE:HB	1:a:345:LYS:HE3	1.92	0.51
1:A:287:ARG:HH11	1:A:287:ARG:CG	2.23	0.51
7:c:49:ARG:HD3	7:c:70:GLU:OE2	2.10	0.51
1:A:639:ASN:HB3	1:A:641:ARG:H	1.74	0.51
1:a:149:LEU:N	1:a:150:PRO:HD2	2.21	0.51
1:A:612:ARG:HB3	1:A:613:PRO:CD	2.39	0.51
1:a:141:THR:OG1	1:a:144:GLU:HG3	2.10	0.51
1:A:440:ASN:O	6:H:5:UNK:CB	2.58	0.51
1:A:612:ARG:HH11	1:A:612:ARG:CG	2.24	0.51
2:C:136:ASN:HD22	1:a:743:GLY:H	1.59	0.51
1:A:25:GLU:CD	1:A:25:GLU:H	2.19	0.51
1:a:687:TRP:O	1:a:688:ARG:HB2	2.10	0.51
1:A:483:ASN:HB3	1:A:484:PRO:CD	2.33	0.51
1:A:742:ARG:HG3	1:A:761:LEU:CD2	2.40	0.51
1:a:293:ASN:HA	1:a:395:SER:HB2	1.91	0.51
1:a:729:TRP:HB2	1:a:736:ILE:HD11	1.92	0.51
1:A:151:TYR:N	1:A:151:TYR:HD1	2.06	0.51
1:A:640:LEU:HB2	1:A:865:ARG:HA	1.91	0.51
13:A:915:85I:C4	13:A:915:85I:C21	2.85	0.51
1:a:57:TYR:O	1:a:61:THR:CG2	2.59	0.51
1:a:676:ASN:HA	1:a:709:ILE:HD13	1.93	0.51
1:A:440:ASN:ND2	6:H:5:UNK:CB	2.74	0.50
1:a:93:THR:HB	1:a:98:PHE:N	2.26	0.50
3:e:23:LYS:O	3:e:23:LYS:HG2	2.10	0.50
7:c:48:LEU:HD22	7:c:48:LEU:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:916:85I:C11	13:A:917:85I:C14	2.88	0.50
2:C:87:VAL:HG21	2:C:179:ASN:O	2.11	0.50
1:A:89:GLY:C	1:A:95:LYS:HE2	2.36	0.50
1:A:244:PHE:CD1	1:A:244:PHE:O	2.63	0.50
10:a:901:CLA:H191	4:f:21:THR:HG22	1.93	0.50
1:a:617:LYS:HA	1:a:617:LYS:HZ2	1.77	0.50
1:A:179:SER:O	1:A:183:THR:HG22	2.12	0.50
7:c:63:PRO:C	7:c:65:ASP:H	2.18	0.50
1:a:38:LEU:HD23	10:a:913:CLA:HBC1	1.93	0.50
1:A:693:ASP:OD1	1:A:693:ASP:N	2.44	0.50
5:g:29:PHE:CD1	5:g:29:PHE:C	2.90	0.49
1:a:152:VAL:HB	1:a:155:LEU:HD11	1.94	0.49
1:a:592:ILE:HD11	1:a:605:GLN:HA	1.94	0.49
7:c:41:SER:HB2	7:c:148:TYR:OH	2.12	0.49
1:A:381:LEU:HD21	9:A:903:BCL:HAA2	1.94	0.49
1:A:81:GLN:HG3	1:A:89:GLY:HA2	1.93	0.49
14:C:302:UNL:C14	14:C:302:UNL:C18	2.85	0.49
1:a:833:ASN:C	1:a:833:ASN:HD22	2.19	0.49
7:c:142:THR:H	7:c:145:GLN:HE21	1.61	0.49
1:A:226:GLN:O	1:A:226:GLN:HG2	2.12	0.49
13:A:917:85I:C25	4:f:26:VAL:HG22	2.42	0.49
1:A:605:GLN:O	1:A:605:GLN:HG3	2.13	0.49
2:C:178:TYR:CD1	2:C:178:TYR:C	2.91	0.49
1:a:150:PRO:HA	1:a:156:LYS:CE	2.33	0.49
1:A:441:PHE:HE2	6:H:3:UNK:CB	2.26	0.49
10:A:931:CLA:H142	10:A:931:CLA:H12	1.93	0.49
1:A:221:PRO:CB	1:A:222:PRO:HD2	2.42	0.49
1:A:597:THR:O	1:A:600:ALA:N	2.46	0.49
1:a:592:ILE:HG13	1:a:604:ALA:HB1	1.95	0.49
1:A:56:GLY:H	1:A:59:ASN:ND2	2.11	0.48
1:A:324:LEU:O	1:A:327:ARG:HG2	2.13	0.48
1:a:440:ASN:HB2	1:a:514:THR:CG2	2.40	0.48
9:a:911:BCL:H3A	9:a:911:BCL:H12	1.94	0.48
1:a:25:GLU:CD	1:a:25:GLU:H	2.21	0.48
1:a:94:SER:O	1:a:96:LEU:N	2.40	0.48
1:A:148:LEU:HG	1:A:148:LEU:O	2.12	0.48
1:A:688:ARG:CG	1:A:688:ARG:NH1	2.72	0.48
2:C:46:LEU:HD13	2:C:46:LEU:HA	1.64	0.48
1:a:94:SER:C	1:a:96:LEU:N	2.71	0.48
1:A:156:LYS:NZ	1:A:160:GLN:OE1	2.44	0.48
1:A:221:PRO:CB	1:A:222:PRO:CD	2.90	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLY:O	1:a:800:SER:HB2	2.14	0.48
2:C:128:CYS:HG	1:a:764:TRP:HH2	1.61	0.48
1:a:158:LEU:C	1:a:158:LEU:CD1	2.85	0.48
1:A:635:VAL:O	3:E:3:ALA:HB2	2.13	0.48
2:C:217:ARG:HA	2:C:217:ARG:NE	2.29	0.48
1:a:81:GLN:HE21	1:a:81:GLN:HB2	1.46	0.48
1:a:450:ARG:NH2	1:a:504:ASN:OD1	2.47	0.48
1:A:74:PRO:HB3	1:A:338:MET:HE3	1.96	0.48
3:E:32:ILE:CD1	1:a:818:ARG:HD3	2.44	0.48
1:a:152:VAL:HG11	1:a:155:LEU:HD11	1.96	0.48
3:e:21:ILE:C	3:e:23:LYS:N	2.70	0.48
1:A:15:TYR:CD1	1:A:15:TYR:N	2.80	0.48
1:A:94:SER:CB	1:A:98:PHE:H	2.27	0.48
2:C:30:THR:HB	2:C:32:TYR:H	1.79	0.47
9:a:909:BCL:HAA1	9:a:909:BCL:HBD	1.95	0.47
2:C:175:PRO:HD3	16:C:301:HEC:HBC2	1.96	0.47
1:A:612:ARG:NH1	1:A:612:ARG:HG3	2.30	0.47
1:A:300:THR:HA	1:A:303:VAL:HG23	1.97	0.47
1:A:573:LYS:HB2	1:A:573:LYS:HE3	1.42	0.47
9:A:907:BCL:HMB1	9:A:907:BCL:CBB	2.37	0.47
1:a:475:THR:CA	5:g:39:LYS:HG2	2.33	0.47
1:a:501:ARG:HD3	5:g:44:LEU:HD23	1.93	0.47
7:c:98:GLY:HA2	7:c:107:ASN:CG	2.34	0.47
4:F:32:LEU:HD12	4:F:32:LEU:HA	1.69	0.47
1:a:42:ILE:HG13	10:a:913:CLA:HMD3	1.95	0.47
1:a:304:PHE:HA	9:a:904:BCL:HBB3	1.97	0.47
9:a:911:BCL:O1A	10:a:913:CLA:HMD1	2.14	0.47
5:g:16:TRP:C	5:g:18:GLY:N	2.70	0.47
1:A:202:TYR:HE2	9:A:905:BCL:H192	1.79	0.47
1:A:253:LEU:HD23	1:A:255:GLN:HE22	1.79	0.47
1:A:729:TRP:CB	1:A:736:ILE:HD11	2.44	0.47
1:a:152:VAL:CB	1:a:155:LEU:HD21	2.21	0.47
9:a:905:BCL:H12	14:a:931:UNL:C1	2.45	0.47
1:A:454:MET:HE1	1:A:523:ILE:HB	1.96	0.47
9:A:905:BCL:H61	9:A:905:BCL:H41	1.57	0.47
10:A:910:CLA:C1C	1:a:722:LYS:HD3	2.45	0.47
1:a:109:PHE:CD1	14:a:926:UNL:C7	2.94	0.47
1:a:818:ARG:HG3	1:a:818:ARG:NH1	2.27	0.47
9:a:908:BCL:H41	9:a:908:BCL:H62	1.29	0.47
5:g:9:ILE:N	5:g:9:ILE:HD12	2.29	0.47
1:A:644:HIS:HE1	1:A:646:ASP:OD1	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:5:VAL:O	4:f:5:VAL:HG12	2.15	0.47
9:A:902:BCL:HBA1	9:A:902:BCL:H3A	1.60	0.47
1:a:35:ILE:HD11	11:c:201:LYC:H131	1.97	0.47
1:A:148:LEU:HD23	1:A:148:LEU:N	2.24	0.47
1:A:610:LYS:HB3	1:A:610:LYS:HE3	1.44	0.47
1:A:799:GLY:HA3	1:a:704:THR:C	2.39	0.47
15:a:902:85N:C3	13:a:920:85I:C33	2.93	0.46
1:A:405:ASP:OD1	3:E:33:ALA:O	2.33	0.46
1:A:655:PHE:C	1:A:655:PHE:CD2	2.93	0.46
2:C:85:GLN:H	2:C:85:GLN:HG2	1.51	0.46
1:a:543:THR:HB	1:a:545:PHE:CE2	2.50	0.46
1:A:264:ASN:HA	1:A:267:THR:HG23	1.98	0.46
11:A:913:LYC:H10	11:A:913:LYC:H81	1.54	0.46
14:A:918:UNL:C17	14:A:918:UNL:C6	2.94	0.46
1:a:503:LEU:HD13	1:a:517:PHE:CE1	2.50	0.46
1:a:847:THR:O	1:a:851:VAL:HG13	2.15	0.46
9:a:907:BCL:H172	9:a:907:BCL:H13	1.73	0.46
9:a:910:BCL:H43	9:a:910:BCL:H12	1.72	0.46
1:A:66:LEU:CD1	10:A:911:CLA:HED2	2.40	0.46
1:a:156:LYS:HA	1:a:156:LYS:HD3	1.46	0.46
1:a:640:LEU:HB2	1:a:865:ARG:CB	2.46	0.46
1:A:480:TRP:CE2	6:H:15:UNK:HA	2.51	0.46
1:A:773:ASP:O	1:A:777:THR:HG23	2.15	0.46
1:A:815:MET:O	1:A:819:LEU:HB2	2.14	0.46
1:a:477:GLY:HA2	5:g:41:LEU:HD11	1.98	0.46
7:c:144:GLN:HA	7:c:144:GLN:HE21	1.79	0.46
2:C:94:GLY:HA2	2:C:99:VAL:HG13	1.97	0.46
1:a:90:GLU:HB2	1:a:94:SER:HB2	1.97	0.46
1:A:220:LYS:HD2	1:A:263:ILE:HD13	1.97	0.46
1:A:406:LEU:O	1:A:410:ILE:HG13	2.15	0.46
1:A:696:CYS:HB3	1:A:705:CYS:HA	1.98	0.46
1:a:441:PHE:HE2	6:h:3:UNK:CB	2.27	0.46
1:a:550:ASN:HD21	1:a:552:LEU:HB2	1.80	0.46
1:A:595:ALA:CB	1:A:601:LYS:HG2	2.46	0.46
9:A:904:BCL:HMB1	9:A:904:BCL:CBB	2.43	0.46
1:a:639:ASN:HB2	1:a:643:GLN:H	1.79	0.46
1:A:55:ASP:HA	1:A:59:ASN:HD21	1.80	0.46
1:a:147:TRP:CD1	1:a:147:TRP:O	2.69	0.46
1:a:429:ILE:O	1:a:433:THR:HG22	2.15	0.46
1:A:109:PHE:CE1	14:A:922:UNL:C16	2.97	0.46
1:A:760:PHE:CD2	10:A:931:CLA:HED3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:923:UNL:C7	14:A:923:UNL:C11	2.94	0.46
2:C:41:ASN:ND2	2:C:85:GLN:HG3	2.31	0.46
1:a:189:ARG:CG	1:a:194:ASP:HB3	2.46	0.45
1:a:822:LYS:HE3	1:a:822:LYS:HB3	1.87	0.45
1:A:475:THR:HA	5:G:39:LYS:HG2	1.98	0.45
1:a:832:SER:HA	13:a:920:85I:C4	2.46	0.45
1:A:14:TRP:CD1	1:A:14:TRP:O	2.69	0.45
1:A:57:TYR:O	1:A:61:THR:CG2	2.64	0.45
1:A:98:PHE:CG	1:A:98:PHE:O	2.70	0.45
1:a:150:PRO:O	1:a:156:LYS:CE	2.65	0.45
4:f:27:TYR:O	4:f:27:TYR:CG	2.68	0.45
5:G:10:SER:OG	15:a:902:85N:C18	2.65	0.45
1:a:639:ASN:ND2	1:a:643:GLN:HE21	2.14	0.45
1:A:722:LYS:HE2	10:A:931:CLA:NB	2.31	0.45
1:A:796:LYS:HE2	1:a:838:LYS:HE2	1.99	0.45
2:C:114:TYR:HB2	2:C:210:VAL:HG21	1.98	0.45
1:a:822:LYS:H	1:a:822:LYS:HG2	1.33	0.45
10:a:915:CLA:C6	7:c:17:MET:HG2	2.47	0.45
7:c:144:GLN:HE21	7:c:147:ASN:HD22	1.62	0.45
1:A:90:GLU:HB2	1:A:100:GLY:O	2.16	0.45
1:A:171:TYR:CD1	1:A:171:TYR:O	2.70	0.45
1:a:189:ARG:HG2	1:a:194:ASP:HB3	1.98	0.45
1:a:519:THR:H	1:a:538:GLN:HE21	1.65	0.45
1:A:504:ASN:OD1	1:A:518:THR:HG22	2.17	0.45
1:a:15:TYR:O	1:a:15:TYR:CD2	2.69	0.45
1:a:201:ILE:HG13	1:a:281:GLY:HA3	1.98	0.45
9:a:908:BCL:H171	3:e:1:MET:HE2	1.99	0.45
4:f:19:VAL:O	4:f:19:VAL:HG12	2.16	0.45
1:A:729:TRP:HB3	1:A:736:ILE:CD1	2.47	0.45
1:a:98:PHE:CD1	1:a:98:PHE:C	2.92	0.45
5:g:17:PHE:O	5:g:17:PHE:CD2	2.70	0.45
5:g:29:PHE:CD1	5:g:29:PHE:O	2.69	0.45
1:A:742:ARG:HG3	1:A:761:LEU:HD21	1.98	0.45
4:F:34:ARG:NE	4:F:34:ARG:CA	2.71	0.45
5:G:34:PRO:HB2	5:G:44:LEU:CD2	2.41	0.45
1:a:38:LEU:HD23	10:a:913:CLA:CBC	2.47	0.45
1:A:612:ARG:CG	1:A:612:ARG:NH1	2.77	0.44
1:A:85:LEU:HD13	1:A:85:LEU:HA	1.54	0.44
1:A:85:LEU:HA	1:A:86:PRO:HD3	1.76	0.44
1:A:85:LEU:CG	1:A:86:PRO:HD2	2.42	0.44
1:a:602:GLN:HE21	1:a:602:GLN:N	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:907:BCL:HBB2	9:a:907:BCL:HMB3	1.99	0.44
10:a:912:CLA:H92	10:a:912:CLA:H52	1.98	0.44
7:c:134:MET:HB2	16:c:202:HEC:C4D	2.47	0.44
5:g:17:PHE:O	5:g:17:PHE:CG	2.69	0.44
1:A:94:SER:C	1:A:96:LEU:H	2.25	0.44
1:A:396:LYS:HE3	1:A:400:TRP:CZ2	2.53	0.44
9:a:911:BCL:CBB	9:a:911:BCL:HMB1	2.47	0.44
7:c:63:PRO:C	7:c:65:ASP:N	2.74	0.44
11:A:913:LYC:H20	11:A:913:LYC:H181	1.57	0.44
1:a:152:VAL:CB	1:a:155:LEU:HD11	2.46	0.44
1:A:98:PHE:O	1:A:98:PHE:CD1	2.70	0.44
1:A:644:HIS:CE1	1:A:646:ASP:OD1	2.70	0.44
1:A:688:ARG:HH11	1:A:688:ARG:HG2	1.82	0.44
10:A:933:CLA:ND	2:C:18:GLY:HA3	2.33	0.44
1:a:628:ARG:HH11	1:a:628:ARG:HB2	1.83	0.44
1:A:220:LYS:HD2	1:A:263:ILE:CD1	2.47	0.44
1:a:609:ASP:HA	1:a:612:ARG:HH12	1.81	0.44
1:A:88:ILE:HG21	1:A:109:PHE:CZ	2.53	0.44
1:A:96:LEU:HA	1:A:97:PRO:HD2	1.52	0.44
1:A:833:ASN:ND2	1:A:836:THR:CG2	2.81	0.44
9:a:905:BCL:CBB	9:a:905:BCL:CMB	2.94	0.44
9:a:908:BCL:H71	14:a:930:UNL:C21	2.48	0.44
10:a:914:CLA:HAA1	10:a:914:CLA:HBD	2.00	0.44
1:A:12:LYS:HE2	1:A:12:LYS:HB3	1.69	0.44
1:A:367:LEU:HD13	1:A:662:TRP:HZ3	1.82	0.43
1:A:473:ASP:HA	1:A:474:PRO:HD2	1.40	0.43
2:C:138:PRO:HB3	1:a:862:PHE:HB3	2.00	0.43
3:E:32:ILE:CG2	1:a:817:LYS:HE3	2.48	0.43
4:F:22:LEU:HD13	10:a:912:CLA:H172	2.00	0.43
5:G:34:PRO:HB2	5:G:44:LEU:HD13	1.99	0.43
1:a:93:THR:HB	1:a:98:PHE:H	1.83	0.43
1:a:818:ARG:HA	1:a:818:ARG:HD2	1.63	0.43
10:a:915:CLA:C5	7:c:17:MET:HG2	2.48	0.43
1:A:494:ARG:NH1	1:A:590:ASN:OD1	2.51	0.43
1:a:155:LEU:HD23	1:a:155:LEU:C	2.43	0.43
1:a:640:LEU:HB2	1:a:865:ARG:CG	2.48	0.43
1:A:239:LEU:HD21	1:A:248:TRP:CE2	2.53	0.43
2:C:95:SER:O	2:C:99:VAL:HG22	2.18	0.43
1:a:138:GLY:O	1:a:166:PRO:HD3	2.18	0.43
1:a:475:THR:HG22	5:g:39:LYS:HD3	2.01	0.43
1:a:833:ASN:ND2	1:a:836:THR:HG23	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:82:GLN:O	7:c:82:GLN:HG3	2.17	0.43
1:A:28:PHE:CZ	9:A:905:BCL:HED2	2.49	0.43
1:A:87:LEU:O	1:A:95:LYS:HG3	2.18	0.43
1:A:266:GLU:HB2	9:A:906:BCL:C1D	2.49	0.43
1:A:822:LYS:HB3	1:A:822:LYS:HE2	1.62	0.43
1:a:48:ALA:HB2	7:c:20:GLY:HA3	2.00	0.43
9:a:908:BCL:H161	9:a:908:BCL:H141	1.49	0.43
1:A:787:TRP:CG	8:A:901:2GO:H27	2.53	0.43
1:A:607:GLU:O	1:A:607:GLU:HG2	2.17	0.43
1:A:808:GLN:HG3	1:a:415:MET:HE1	2.01	0.43
3:E:32:ILE:HG22	1:a:814:LEU:HD12	2.00	0.43
5:G:11:LYS:HA	5:G:11:LYS:HD2	1.63	0.43
1:a:48:ALA:HB2	7:c:20:GLY:HA2	2.01	0.43
1:a:143:GLY:HA3	1:a:159:CYS:SG	2.59	0.43
1:a:244:PHE:CD1	1:a:244:PHE:C	2.90	0.43
1:a:409:LYS:O	1:a:413:THR:CG2	2.67	0.43
5:g:9:ILE:H	5:g:9:ILE:HD13	1.84	0.43
9:A:908:BCL:HHD	9:A:908:BCL:HAC1	1.68	0.43
2:C:153:SER:HB2	16:c:202:HEC:O2D	2.18	0.43
4:F:34:ARG:HB3	4:F:35:GLY:H	1.52	0.43
1:A:59:ASN:HD22	1:A:60:LEU:N	2.16	0.43
2:C:139:ARG:HA	2:C:139:ARG:HD2	1.84	0.43
2:C:141:THR:O	2:C:141:THR:CG2	2.66	0.43
1:a:150:PRO:HB2	1:a:151:TYR:CE1	2.53	0.43
9:a:905:BCL:H192	9:a:905:BCL:H161	1.72	0.43
3:e:22:ILE:HG21	3:e:22:ILE:HD13	1.61	0.43
1:A:797:ASP:HA	1:a:705:CYS:O	2.19	0.43
9:A:909:BCL:H162	9:A:909:BCL:H141	1.62	0.43
1:a:152:VAL:N	1:a:153:PRO:HD3	2.34	0.43
1:a:435:ALA:HB2	1:a:541:SER:HB2	2.01	0.43
1:a:475:THR:HA	5:g:39:LYS:CD	2.48	0.43
1:A:78:GLU:HG3	2:C:62:PRO:HB2	2.02	0.42
1:A:159:CYS:SG	1:A:159:CYS:O	2.77	0.42
1:A:202:TYR:CE2	9:A:905:BCL:H192	2.54	0.42
1:A:390:TYR:CZ	1:A:402:GLN:HG2	2.54	0.42
11:A:913:LYC:H131	11:A:913:LYC:H15	1.60	0.42
2:C:32:TYR:HA	2:C:33:PRO:HD3	1.86	0.42
2:C:115:ARG:HH11	2:C:115:ARG:HD3	1.64	0.42
1:A:608:LEU:HD11	1:A:612:ARG:HH21	1.83	0.42
9:A:905:BCL:H12	9:A:905:BCL:HBA2	1.89	0.42
10:A:931:CLA:HAB	10:A:931:CLA:HHC	1.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:C:301:HEC:CMB	16:C:301:HEC:HBB3	2.48	0.42
9:a:904:BCL:H112	9:a:904:BCL:H91	1.77	0.42
1:A:292:ILE:HD12	1:A:292:ILE:H	1.84	0.42
1:a:477:GLY:C	5:g:41:LEU:HD12	2.44	0.42
1:a:526:LYS:HZ1	1:a:626:ASN:HD21	1.67	0.42
9:a:908:BCL:H12	9:a:908:BCL:HBA1	1.85	0.42
1:A:124:TRP:NE1	14:A:924:UNL:C10	2.82	0.42
1:A:290:ARG:H	14:A:920:UNL:C21	2.32	0.42
2:C:99:VAL:HG11	2:C:158:TYR:CZ	2.54	0.42
1:a:742:ARG:HB2	1:a:745:GLU:HG3	2.01	0.42
10:a:901:CLA:C19	4:f:21:THR:HG22	2.49	0.42
1:A:88:ILE:HG21	1:A:109:PHE:HZ	1.85	0.42
1:A:595:ALA:O	1:A:596:GLN:HB2	2.20	0.42
7:c:33:LEU:C	7:c:33:LEU:CD2	2.85	0.42
2:C:71:ARG:HB2	2:C:75:THR:CG2	2.48	0.42
1:a:96:LEU:HB2	1:a:99:PHE:HB2	2.00	0.42
9:a:907:BCL:H141	9:a:907:BCL:H161	1.50	0.42
9:a:909:BCL:HBB3	9:a:909:BCL:CMB	2.43	0.42
2:C:145:ASP:HA	2:C:146:PRO:HD3	1.78	0.42
1:a:57:TYR:O	1:a:61:THR:HG23	2.20	0.42
1:a:847:THR:HB	9:a:910:BCL:H91	2.01	0.42
1:A:171:TYR:O	1:A:171:TYR:HD1	2.03	0.42
1:A:266:GLU:HG3	9:A:906:BCL:HED3	2.02	0.42
1:a:718:LEU:H	1:a:718:LEU:HG	1.79	0.42
9:a:908:BCL:H12	9:a:908:BCL:O1D	2.20	0.42
1:A:91:PHE:HB3	1:A:95:LYS:CB	2.33	0.42
8:A:901:2GO:H21	8:A:901:2GO:H25	2.02	0.42
1:a:32:MET:HB2	9:a:907:BCL:HED1	2.02	0.42
9:a:904:BCL:HBC3	9:a:911:BCL:H91	2.02	0.42
1:A:602:GLN:HE21	1:A:602:GLN:HB3	1.40	0.41
1:A:610:LYS:O	1:A:610:LYS:CG	2.68	0.41
9:A:907:BCL:HAA1	9:A:907:BCL:HBD	2.02	0.41
10:A:931:CLA:H52	1:a:781:LEU:HD23	2.02	0.41
1:a:265:GLY:O	1:a:268:THR:HG23	2.19	0.41
7:c:66:THR:HA	7:c:67:PRO:HD3	1.83	0.41
3:e:6:LEU:HD12	3:e:6:LEU:HA	1.89	0.41
1:A:469:LYS:HE2	1:A:477:GLY:C	2.45	0.41
1:a:56:GLY:O	1:a:60:LEU:HB2	2.20	0.41
1:a:147:TRP:NE1	1:a:148:LEU:HD22	2.34	0.41
1:a:440:ASN:CB	1:a:514:THR:HG21	2.42	0.41
7:c:18:ALA:HB2	11:c:201:LYC:C62	2.30	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:909:BCL:C2B	9:A:909:BCL:H52	2.51	0.41
1:a:66:LEU:HD13	10:a:913:CLA:HED1	2.03	0.41
1:a:150:PRO:HB2	1:a:151:TYR:CD1	2.55	0.41
1:a:741:ALA:O	1:a:757:GLY:O	2.39	0.41
1:A:146:PHE:O	1:A:148:LEU:HD22	2.19	0.41
1:A:296:HIS:H	1:A:296:HIS:CD2	2.39	0.41
4:F:25:ILE:HD13	13:a:919:85I:C29	2.50	0.41
1:a:487:THR:HG22	6:h:17:UNK:O	2.21	0.41
1:a:774:ASN:HA	1:a:777:THR:HG23	2.03	0.41
1:A:640:LEU:HA	1:A:640:LEU:HD12	1.57	0.41
1:A:640:LEU:HB3	1:A:865:ARG:HG3	2.02	0.41
9:A:902:BCL:H43	9:A:902:BCL:H12	1.89	0.41
9:A:902:BCL:HAA1	9:A:902:BCL:HBD	2.03	0.41
1:a:729:TRP:CB	1:a:736:ILE:HD11	2.51	0.41
3:e:22:ILE:O	3:e:22:ILE:CG2	2.67	0.41
5:g:21:LEU:HD12	5:g:21:LEU:HA	1.65	0.41
1:a:85:LEU:H	1:a:85:LEU:HD22	1.85	0.41
1:a:91:PHE:H	1:a:94:SER:CB	2.33	0.41
1:a:504:ASN:OD1	1:a:518:THR:HG22	2.21	0.41
7:c:91:GLY:H	7:c:94:GLN:H	1.69	0.41
1:A:796:LYS:HG3	1:a:796:LYS:CG	2.50	0.41
2:C:37:MET:HE1	2:C:80:GLN:CB	2.50	0.41
1:a:91:PHE:HB2	1:a:95:LYS:H	1.85	0.41
1:a:475:THR:HA	5:g:39:LYS:HD3	2.01	0.41
11:c:201:LYC:H54	11:c:201:LYC:H521	1.64	0.41
1:A:545:PHE:HB2	14:A:928:UNL:C17	2.51	0.41
1:A:643:GLN:HB2	1:A:643:GLN:HE21	1.55	0.41
2:C:128:CYS:CB	16:C:301:HEC:CAC	2.94	0.41
2:C:174:MET:HB2	16:C:301:HEC:C4D	2.50	0.41
1:a:92:SER:O	1:a:93:THR:C	2.63	0.41
1:a:149:LEU:H	1:a:150:PRO:HD2	1.80	0.41
1:a:159:CYS:SG	1:a:159:CYS:O	2.78	0.41
1:a:483:ASN:HB3	1:a:484:PRO:CD	2.51	0.41
9:a:904:BCL:H43	9:a:904:BCL:H12	1.87	0.41
10:a:912:CLA:H42	10:a:912:CLA:H11	1.81	0.41
1:A:404:PRO:O	1:A:408:THR:HG22	2.20	0.41
1:A:429:ILE:O	1:A:433:THR:CG2	2.65	0.41
7:c:48:LEU:HD22	7:c:48:LEU:N	2.33	0.41
9:A:907:BCL:H91	9:A:907:BCL:H112	1.67	0.40
9:A:908:BCL:HBD	9:A:908:BCL:CBA	2.15	0.40
9:a:908:BCL:H111	9:a:908:BCL:H142	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:911:BCL:H2C	9:a:911:BCL:HBC2	1.82	0.40
7:c:50:GLU:O	7:c:50:GLU:HG3	2.11	0.40
3:e:5:LEU:HD12	3:e:5:LEU:HA	1.84	0.40
11:A:913:LYC:H521	11:A:913:LYC:H54	1.83	0.40
3:E:32:ILE:CG2	1:a:814:LEU:HD12	2.52	0.40
1:a:80:ILE:HG21	1:a:83:VAL:HG13	2.03	0.40
3:e:23:LYS:O	3:e:23:LYS:CG	2.69	0.40
2:C:128:CYS:CB	16:C:301:HEC:HAC	2.48	0.40
1:a:767:THR:HA	1:a:770:ILE:HB	2.04	0.40
9:A:905:BCL:CBB	9:A:905:BCL:CMB	2.98	0.40
2:C:200:GLN:HE21	2:C:200:GLN:HB2	1.39	0.40
1:a:472:TRP:O	1:a:474:PRO:HD3	2.21	0.40
1:a:597:THR:O	1:a:600:ALA:N	2.54	0.40
1:A:18:LEU:O	10:A:912:CLA:HAA2	2.21	0.40
1:A:90:GLU:HG2	1:A:91:PHE:N	2.36	0.40
1:A:146:PHE:O	1:A:148:LEU:CD2	2.69	0.40
1:A:453:GLN:NE2	1:A:533:LYS:HD3	2.36	0.40
1:A:477:GLY:H	5:G:41:LEU:CD1	2.20	0.40
1:A:767:THR:O	1:A:768:THR:C	2.63	0.40
9:A:903:BCL:H2	14:A:927:UNL:C9	2.52	0.40
1:a:91:PHE:O	1:a:94:SER:HB3	2.22	0.40
1:a:846:TYR:CD1	9:a:910:BCL:H162	2.55	0.40
10:a:912:CLA:H162	10:a:912:CLA:H202	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	852/865 (98%)	793 (93%)	41 (5%)	18 (2%)	5 3
1	a	856/865 (99%)	798 (93%)	46 (5%)	12 (1%)	9 7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	189/221 (86%)	174 (92%)	9 (5%)	6 (3%)	3 1
3	E	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
3	e	33/35 (94%)	32 (97%)	0	1 (3%)	3 1
4	F	33/35 (94%)	31 (94%)	2 (6%)	0	100 100
4	f	33/35 (94%)	30 (91%)	2 (6%)	1 (3%)	3 1
5	G	36/45 (80%)	32 (89%)	3 (8%)	1 (3%)	4 2
5	g	36/45 (80%)	32 (89%)	4 (11%)	0	100 100
7	c	143/145 (99%)	127 (89%)	8 (6%)	8 (6%)	1 0
All	All	2244/2326 (96%)	2080 (93%)	117 (5%)	47 (2%)	8 3

All (47) 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
7	c	102	ALA
7	c	132	LYS
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
1	A	688	ARG
1	a	9	ASN
1	a	87	LEU
7	c	92	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
1	A	13	ARG
1	A	96	LEU
1	A	757	GLY
2	C	59	GLN
2	C	217	ARG
7	c	64	LYS
1	A	149	LEU
1	A	696	CYS
1	a	529	TRP
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	718/726 (99%)	582 (81%)	136 (19%)	1	1
1	a	720/726 (99%)	583 (81%)	137 (19%)	1	1
2	C	155/180 (86%)	126 (81%)	29 (19%)	1	1
3	E	25/25 (100%)	20 (80%)	5 (20%)	1	1
3	e	25/25 (100%)	18 (72%)	7 (28%)	0	0
4	F	31/31 (100%)	25 (81%)	6 (19%)	1	1
4	f	31/31 (100%)	26 (84%)	5 (16%)	2	2
5	G	31/36 (86%)	22 (71%)	9 (29%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	g	31/36 (86%)	21 (68%)	10 (32%)	0 0
7	c	112/112 (100%)	90 (80%)	22 (20%)	1 1
All	All	1879/1928 (98%)	1513 (80%)	366 (20%)	3 1

All (366) 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	25	GLU
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
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	158	LEU
1	A	159	CYS
1	A	161	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	LYS
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	229	GLN
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	303	VAL
1	A	318	LEU
1	A	326	LEU
1	A	331	SER
1	A	333	LEU
1	A	334	MET
1	A	335	LEU
1	A	339	ASN
1	A	352	ARG
1	A	359	THR
1	A	381	LEU
1	A	384	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	475	THR
1	A	489	LYS
1	A	490	LEU
1	A	494	ARG
1	A	496	LEU
1	A	497	GLN
1	A	503	LEU
1	A	505	GLU
1	A	518	THR
1	A	534	LEU
1	A	552	LEU
1	A	562	LEU
1	A	565	GLN
1	A	567	THR
1	A	569	GLU
1	A	572	ARG
1	A	583	LEU
1	A	588	LEU
1	A	597	THR
1	A	598	GLU
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
1	A	638	SER
1	A	640	LEU
1	A	641	ARG
1	A	653	ILE
1	A	657	LEU
1	A	667	ILE
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	717	ILE
1	A	724	LEU
1	A	736	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	768	THR
1	A	777	THR
1	A	781	LEU
1	A	790	SER
1	A	796	LYS
1	A	798	ARG
1	A	800	SER
1	A	819	LEU
1	A	822	LYS
1	A	823	THR
1	A	824	LEU
1	A	826	GLU
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	40	GLN
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
2	C	85	GLN
2	C	87	VAL
2	C	99	VAL
2	C	112	GLU
2	C	116	GLU
2	C	126	VAL
2	C	139	ARG
2	C	150	GLU
2	C	153	SER
2	C	180	GLN
2	C	182	SER
2	C	193	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	194	ARG
2	C	200	GLN
2	C	204	LEU
2	C	217	ARG
2	C	218	GLN
3	E	9	LEU
3	E	18	LEU
3	E	23	LYS
3	E	30	LYS
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	25	LEU
5	G	38	VAL
5	G	39	LYS
5	G	44	LEU
5	G	45	ASN
1	a	11	VAL
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	66	LEU
1	a	69	LEU
1	a	79	GLN
1	a	80	ILE
1	a	81	GLN
1	a	82	ARG
1	a	83	VAL
1	a	84	TRP
1	a	85	LEU
1	a	87	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	88	ILE
1	a	90	GLU
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	152	VAL
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	173	VAL
1	a	183	THR
1	a	187	ILE
1	a	188	LEU
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	253	LEU
1	a	263	ILE
1	a	267	THR
1	a	268	THR
1	a	276	LEU
1	a	287	ARG
1	a	290	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	384	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	461	ILE
1	a	464	ARG
1	a	469	LYS
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
1	a	583	LEU
1	a	584	LYS
1	a	587	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	588	LEU
1	a	602	GLN
1	a	617	LYS
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	653	ILE
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	736	ILE
1	a	761	LEU
1	a	768	THR
1	a	777	THR
1	a	781	LEU
1	a	785	LEU
1	a	798	ARG
1	a	815	MET
1	a	819	LEU
1	a	822	LYS
1	a	823	THR
1	a	824	LEU
1	a	826	GLU
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
7	c	30	GLU
7	c	33	LEU
7	c	42	ARG
7	c	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	154	ARG
7	c	159	LYS
3	e	2	THR
3	e	5	LEU
3	e	6	LEU
3	e	22	ILE
3	e	28	ASN
3	e	30	LYS
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	21	LEU
5	g	25	LEU
5	g	26	ILE
5	g	40	MET
5	g	45	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) 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	241	GLN
1	A	255	GLN
1	A	261	ASN
1	A	296	HIS
1	A	362	HIS
1	A	364	GLN
1	A	379	GLN
1	A	392	GLN
1	A	445	GLN
1	A	470	ASN
1	A	531	GLN
1	A	538	GLN
1	A	550	ASN
1	A	565	GLN
1	A	602	GLN
1	A	639	ASN
1	A	643	GLN
1	A	644	HIS
1	A	675	HIS
1	A	755	HIS
1	A	808	GLN
1	A	825	GLN
1	A	833	ASN
2	C	40	GLN
2	C	59	GLN
2	C	78	ASN
2	C	81	GLN
2	C	85	GLN
2	C	122	GLN
2	C	123	ASN
2	C	136	ASN
2	C	149	GLN
2	C	169	ASN
2	C	180	GLN
2	C	185	GLN
2	C	200	GLN
2	C	202	ASN
3	E	35	ASN
5	G	45	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	16	GLN
1	a	59	ASN
1	a	81	GLN
1	a	160	GLN
1	a	254	ASN
1	a	296	HIS
1	a	329	HIS
1	a	362	HIS
1	a	364	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	644	HIS
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	94	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
5	g	45	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 2 are monoatomic and 32 are unknown - leaving 45 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	$\#\|Z\| > 2$
9	BCL	A	909	1	69,74,74	3.31	29 (42%)	83,115,115	4.39	38 (45%)
11	LYC	A	913	-	39,39,39	2.05	11 (28%)	44,46,46	2.49	18 (40%)
8	2GO	A	901	1	71,74,74	2.80	22 (30%)	83,115,115	2.56	26 (31%)
10	CLA	a	913	1	69,73,73	2.51	21 (30%)	83,113,113	3.96	36 (43%)
15	85N	g	101	-	36,37,46	0.79	1 (2%)	40,45,55	0.58	0
15	85N	G	101	-	36,37,46	0.72	0	40,45,55	0.77	2 (5%)
9	BCL	a	904	1	69,74,74	2.67	20 (28%)	83,115,115	3.47	30 (36%)
17	84Q	E	101	-	42,43,43	2.09	10 (23%)	47,50,50	1.90	8 (17%)
10	CLA	a	901	19	69,73,73	2.63	23 (33%)	83,113,113	3.71	36 (43%)
13	85I	A	915	-	43,44,44	2.29	10 (23%)	47,51,51	2.44	7 (14%)
9	BCL	a	909	1	69,74,74	2.52	26 (37%)	83,115,115	3.88	33 (39%)
10	CLA	A	910	1	69,73,73	2.50	21 (30%)	83,113,113	3.61	40 (48%)
13	85I	a	918	-	43,44,44	1.06	2 (4%)	47,51,51	1.69	4 (8%)
9	BCL	A	908	1	69,74,74	2.52	30 (43%)	83,115,115	2.99	33 (39%)
9	BCL	A	907	1	64,69,74	3.34	29 (45%)	77,109,115	4.61	43 (55%)
18	SF4	a	917	1	0,12,12	-	-	-		
9	BCL	A	904	1	49,54,74	2.57	22 (44%)	59,91,115	3.09	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	A	911	1	69,73,73	2.61	22 (31%)	83,113,113	3.34	34 (40%)
15	85N	a	902	-	45,46,46	0.59	0	50,55,55	0.42	0
13	85I	a	920	-	43,44,44	2.21	2 (4%)	47,51,51	2.04	3 (6%)
10	CLA	a	914	1	50,54,73	2.92	21 (42%)	60,90,113	3.84	30 (50%)
10	CLA	A	933	1	55,59,73	2.81	21 (38%)	66,96,113	4.25	36 (54%)
11	LYC	c	201	-	39,39,39	1.65	9 (23%)	44,46,46	5.75	28 (63%)
9	BCL	A	902	1	69,74,74	2.81	24 (34%)	83,115,115	3.37	36 (43%)
9	BCL	a	905	1	69,74,74	2.82	21 (30%)	83,115,115	3.88	36 (43%)
10	CLA	a	915	1	55,59,73	2.94	21 (38%)	66,96,113	3.54	37 (56%)
16	HEC	c	202	7	50,50,50	3.71	27 (54%)	68,82,82	3.32	33 (48%)
16	HEC	C	301	2	50,50,50	3.85	32 (64%)	68,82,82	3.46	39 (57%)
9	BCL	a	911	1	69,74,74	2.85	28 (40%)	83,115,115	3.50	35 (42%)
10	CLA	A	912	1	50,54,73	2.69	16 (32%)	60,90,113	4.18	31 (51%)
8	2GO	a	903	1	71,74,74	2.46	18 (25%)	83,115,115	2.26	29 (34%)
9	BCL	A	905	1	69,74,74	2.71	21 (30%)	83,115,115	3.98	36 (43%)
9	BCL	A	903	1	69,74,74	2.89	22 (31%)	83,115,115	3.82	36 (43%)
13	85I	A	916	-	43,44,44	2.22	3 (6%)	47,51,51	1.93	6 (12%)
9	BCL	a	908	1	69,74,74	2.96	26 (37%)	83,115,115	4.42	38 (45%)
9	BCL	a	907	1	69,74,74	2.64	27 (39%)	83,115,115	3.82	31 (37%)
10	CLA	A	931	1	69,73,73	3.00	26 (37%)	83,113,113	4.40	44 (53%)
9	BCL	A	906	1	55,60,74	3.00	20 (36%)	66,98,115	4.75	29 (43%)
17	84Q	a	921	-	42,43,43	1.35	2 (4%)	47,50,50	1.04	2 (4%)
10	CLA	a	912	19	69,73,73	2.76	19 (27%)	83,113,113	3.58	42 (50%)
9	BCL	a	910	1	69,74,74	3.21	22 (31%)	83,115,115	4.00	40 (48%)
9	BCL	a	906	1	49,54,74	2.89	22 (44%)	59,91,115	3.46	28 (47%)
15	85N	A	932	-	45,46,46	1.04	1 (2%)	50,55,55	1.82	4 (8%)
13	85I	A	917	-	43,44,44	1.57	2 (4%)	47,51,51	2.42	3 (6%)
13	85I	a	919	-	43,44,44	1.41	2 (4%)	47,51,51	1.66	3 (6%)

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
9	BCL	A	909	1	-	12/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LYC	A	913	-	-	1/43/43/43	-
8	2GO	A	901	1	2/2/21/25	5/41/137/137	-
10	CLA	a	913	1	-	11/39/115/115	-
15	85N	g	101	-	-	19/42/42/51	-
15	85N	G	101	-	-	18/42/42/51	-
9	BCL	a	904	1	-	12/41/137/137	-
17	84Q	E	101	-	-	27/46/47/47	-
10	CLA	a	901	19	-	25/39/115/115	-
13	85I	A	915	-	-	19/47/48/48	-
10	CLA	A	910	1	1/1/15/20	9/39/115/115	-
9	BCL	a	909	1	-	13/41/137/137	-
13	85I	a	918	-	-	21/47/48/48	-
9	BCL	A	908	1	-	14/41/137/137	-
9	BCL	A	907	1	-	16/35/131/137	-
18	SF4	a	917	1	-	-	0/6/5/5
10	CLA	A	911	1	1/1/15/20	11/39/115/115	-
9	BCL	A	904	1	-	6/17/113/137	-
15	85N	a	902	-	-	25/51/51/51	-
13	85I	a	920	-	-	30/47/48/48	-
10	CLA	a	914	1	-	4/17/93/115	-
10	CLA	A	933	1	-	6/23/99/115	-
11	LYC	c	201	-	-	16/43/43/43	-
9	BCL	A	902	1	-	18/41/137/137	-
9	BCL	a	905	1	-	17/41/137/137	-
10	CLA	a	915	1	-	9/23/99/115	-
16	HEC	c	202	7	1/1/3/7	7/14/54/54	-
16	HEC	C	301	2	1/1/3/7	7/14/54/54	-
9	BCL	a	911	1	-	5/41/137/137	-
10	CLA	A	912	1	-	2/17/93/115	-
8	2GO	a	903	1	2/2/21/25	5/41/137/137	-
9	BCL	A	905	1	-	16/41/137/137	-
9	BCL	A	903	1	-	21/41/137/137	-
13	85I	A	916	-	-	27/47/48/48	-
9	BCL	a	908	1	-	20/41/137/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	a	907	1	-	12/41/137/137	-
10	CLA	A	931	1	-	18/39/115/115	-
9	BCL	A	906	1	-	6/25/121/137	-
17	84Q	a	921	-	-	32/46/47/47	-
10	CLA	a	912	19	-	12/39/115/115	-
9	BCL	a	910	1	-	11/41/137/137	-
9	BCL	a	906	1	-	6/17/113/137	-
15	85N	A	932	-	-	18/51/51/51	-
13	85I	A	917	-	-	29/47/48/48	-
13	85I	a	919	-	-	36/47/48/48	-

All (754) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	920	85I	O6-C3	-14.01	1.20	1.44
9	a	910	BCL	C4B-NB	-13.44	1.21	1.37
10	A	931	CLA	C4B-NB	-10.59	1.24	1.37
10	a	912	CLA	C3D-C4D	-10.25	1.21	1.44
9	A	909	BCL	C4B-NB	-9.97	1.25	1.37
13	A	915	85I	C4-C3	-9.76	1.29	1.51
9	a	904	BCL	C3D-C4D	-9.67	1.22	1.44
9	a	910	BCL	C3D-C4D	-9.66	1.22	1.44
9	A	903	BCL	C4B-NB	-9.61	1.26	1.37
13	A	916	85I	P-O3	9.38	1.85	1.60
16	C	301	HEC	FE-ND	9.28	2.23	1.94
9	a	907	BCL	C1D-ND	-9.03	1.26	1.37
10	a	914	CLA	C3D-C4D	-8.99	1.23	1.44
9	A	907	BCL	C1B-NB	-8.96	1.26	1.37
10	A	912	CLA	C4B-NB	-8.90	1.26	1.37
10	A	931	CLA	C3D-C4D	-8.88	1.24	1.44
10	A	933	CLA	C4B-NB	-8.88	1.26	1.37
9	a	910	BCL	C1B-NB	-8.85	1.26	1.37
9	a	905	BCL	C3D-C4D	-8.78	1.24	1.44
10	A	911	CLA	C1D-ND	8.78	1.48	1.37
10	a	913	CLA	C4B-NB	-8.76	1.27	1.37
9	A	909	BCL	OBB-CAB	-8.76	1.03	1.23
9	A	903	BCL	OBB-CAB	-8.73	1.03	1.23
8	A	901	2GO	C3C-C4C	-8.69	1.40	1.51
8	a	903	2GO	OBB-CAB	-8.66	1.04	1.23
8	A	901	2GO	C4D-ND	-8.64	1.18	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	907	BCL	O2A-CGA	8.61	1.58	1.33
10	A	910	CLA	C3D-C4D	-8.60	1.24	1.44
17	E	101	84Q	P-O4	8.60	1.83	1.60
10	a	915	CLA	C1B-NB	-8.52	1.27	1.37
9	a	910	BCL	OBB-CAB	-8.50	1.04	1.23
13	A	916	85I	C4-C3	8.49	1.71	1.51
9	a	908	BCL	C3D-C4D	-8.45	1.25	1.44
9	A	903	BCL	C3D-C4D	-8.44	1.25	1.44
10	A	912	CLA	C3D-C4D	-8.42	1.25	1.44
10	A	933	CLA	C3D-C4D	-8.34	1.25	1.44
10	A	910	CLA	C1B-NB	-8.33	1.27	1.37
9	a	907	BCL	C3D-C4D	-8.32	1.25	1.44
9	A	902	BCL	C3D-C4D	-8.27	1.25	1.44
9	A	909	BCL	C3D-C4D	-8.24	1.25	1.44
16	c	202	HEC	C4B-NB	-8.23	1.26	1.40
10	A	933	CLA	C4D-ND	-8.22	1.26	1.37
10	a	901	CLA	C1C-NC	-8.21	1.25	1.37
9	a	905	BCL	C4B-NB	-8.20	1.27	1.37
10	A	931	CLA	O1D-CGD	-8.18	1.00	1.21
9	a	911	BCL	C4B-NB	-8.05	1.27	1.37
9	A	905	BCL	CAA-C2A	-8.02	1.39	1.54
17	a	921	84Q	O2-C16	-7.91	1.31	1.44
9	a	911	BCL	C1B-NB	-7.89	1.28	1.37
10	A	910	CLA	C4B-NB	-7.88	1.28	1.37
9	A	906	BCL	C3D-C4D	-7.87	1.26	1.44
13	a	919	85I	O6-C3	7.86	1.58	1.44
9	A	907	BCL	C4B-NB	-7.85	1.28	1.37
10	a	913	CLA	C1B-NB	-7.84	1.28	1.37
9	A	909	BCL	C1B-NB	-7.83	1.28	1.37
10	a	915	CLA	C3D-C4D	-7.83	1.26	1.44
9	A	908	BCL	C4B-NB	-7.78	1.28	1.37
10	a	901	CLA	C1B-NB	-7.72	1.28	1.37
9	a	909	BCL	C3D-C4D	-7.70	1.26	1.44
16	C	301	HEC	C4C-NC	-7.70	1.24	1.39
10	a	901	CLA	C3D-C4D	-7.69	1.26	1.44
9	a	906	BCL	C3D-C4D	-7.65	1.26	1.44
9	A	906	BCL	C1D-ND	-7.63	1.28	1.37
9	A	902	BCL	C1D-ND	-7.60	1.28	1.37
10	a	914	CLA	C1B-NB	-7.59	1.28	1.37
10	a	914	CLA	C4B-NB	-7.55	1.28	1.37
10	A	911	CLA	C1C-NC	-7.54	1.26	1.37
9	A	905	BCL	C3D-C4D	-7.48	1.27	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	904	BCL	C3D-C4D	-7.41	1.27	1.44
10	a	901	CLA	C4B-NB	-7.40	1.28	1.37
16	c	202	HEC	C4A-NA	-7.37	1.25	1.39
9	a	904	BCL	C3C-C4C	-7.35	1.42	1.51
9	A	909	BCL	C4D-ND	-7.29	1.27	1.37
8	a	903	2GO	OBD-CAD	-7.29	1.09	1.22
9	A	902	BCL	C1B-NB	-7.28	1.28	1.37
9	a	911	BCL	C3D-C4D	-7.28	1.27	1.44
9	a	908	BCL	CAA-C2A	-7.26	1.40	1.54
16	c	202	HEC	FE-ND	7.23	2.17	1.94
10	a	915	CLA	CHC-C1C	7.21	1.53	1.38
9	a	908	BCL	C4D-ND	-7.21	1.27	1.37
9	A	902	BCL	C4B-NB	-7.17	1.29	1.37
9	a	908	BCL	C1D-ND	-7.16	1.29	1.37
9	a	911	BCL	OBB-CAB	-7.15	1.07	1.23
8	A	901	2GO	C1D-C2D	-7.13	1.31	1.45
13	A	917	85I	C4-C3	7.10	1.68	1.51
9	a	908	BCL	CBB-CAB	-7.10	1.36	1.50
9	A	906	BCL	CBB-CAB	-7.10	1.36	1.50
10	a	912	CLA	C1C-NC	-7.05	1.27	1.37
16	c	202	HEC	FE-NB	7.03	2.16	1.94
10	a	912	CLA	C9-C8	-6.98	1.30	1.52
9	A	907	BCL	C4D-ND	-6.96	1.28	1.37
9	A	907	BCL	C3D-C4D	-6.88	1.28	1.44
13	A	917	85I	O6-C3	-6.87	1.32	1.44
9	A	908	BCL	C3D-C4D	-6.83	1.28	1.44
10	A	911	CLA	C3D-C4D	-6.81	1.28	1.44
9	a	911	BCL	C1D-ND	-6.80	1.29	1.37
9	a	905	BCL	C1D-ND	-6.80	1.29	1.37
16	C	301	HEC	C1D-ND	-6.79	1.28	1.40
16	C	301	HEC	FE-NB	6.79	2.15	1.94
16	c	202	HEC	O2A-CGA	-6.79	1.07	1.30
9	a	910	BCL	C3C-C4C	-6.75	1.43	1.51
8	A	901	2GO	ZN-NC	6.74	2.25	2.03
10	a	915	CLA	C4B-NB	-6.69	1.29	1.37
11	A	913	LYC	C14-C12	-6.69	1.26	1.35
10	a	913	CLA	C3D-C4D	-6.68	1.29	1.44
10	a	912	CLA	C4B-NB	-6.68	1.29	1.37
9	a	906	BCL	C4B-NB	-6.67	1.29	1.37
8	A	901	2GO	ZN-NA	6.62	2.24	2.03
10	A	931	CLA	C1D-ND	6.61	1.45	1.37
9	A	909	BCL	O1A-CGA	-6.61	1.02	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	904	BCL	C1B-NB	-6.52	1.29	1.37
9	A	907	BCL	O1D-CGD	-6.50	1.04	1.21
8	A	901	2GO	C3D-C4D	-6.49	1.29	1.44
9	A	907	BCL	C1D-ND	-6.49	1.29	1.37
9	A	906	BCL	C4B-NB	-6.44	1.29	1.37
9	a	905	BCL	OBB-CAB	-6.42	1.09	1.23
9	a	908	BCL	C4B-NB	-6.41	1.29	1.37
9	A	905	BCL	C4B-NB	-6.38	1.29	1.37
9	a	904	BCL	C1D-ND	-6.38	1.29	1.37
16	c	202	HEC	C4B-C3B	-6.35	1.34	1.45
9	A	904	BCL	C4B-NB	-6.32	1.30	1.37
16	C	301	HEC	FE-NA	6.31	2.16	1.95
10	a	912	CLA	C1B-NB	-6.29	1.30	1.37
9	a	908	BCL	C2A-C1A	-6.27	1.38	1.52
10	a	913	CLA	C1D-ND	6.23	1.45	1.37
9	a	905	BCL	C4D-ND	-6.19	1.29	1.37
10	A	931	CLA	C4D-ND	-6.17	1.29	1.37
8	A	901	2GO	OBD-CAD	-6.16	1.11	1.22
10	A	933	CLA	O1D-CGD	-6.15	1.05	1.21
8	a	903	2GO	C3D-C4D	-6.13	1.30	1.44
9	a	909	BCL	C4B-NB	-6.13	1.30	1.37
10	a	913	CLA	C1C-NC	-6.11	1.28	1.37
9	A	909	BCL	C3C-C4C	-6.10	1.43	1.51
16	c	202	HEC	CHA-C1A	6.04	1.50	1.38
10	a	914	CLA	MG-NB	6.04	2.17	2.05
8	A	901	2GO	OBB-CAB	-6.02	1.09	1.23
9	A	905	BCL	C2A-C1A	-6.01	1.38	1.52
16	C	301	HEC	C1B-NB	-6.01	1.26	1.38
9	A	906	BCL	C1B-NB	-6.01	1.30	1.37
10	A	911	CLA	C4B-NB	-6.00	1.30	1.37
10	A	911	CLA	C4D-ND	-6.00	1.29	1.37
10	a	912	CLA	OBD-CAD	-5.99	1.12	1.22
9	A	905	BCL	OBB-CAB	-5.99	1.10	1.23
16	C	301	HEC	C4B-NB	-5.99	1.30	1.40
8	a	903	2GO	C1D-C2D	-5.98	1.33	1.45
8	a	903	2GO	ZN-NC	5.96	2.22	2.03
9	A	903	BCL	C1B-NB	-5.95	1.30	1.37
9	a	909	BCL	C1B-NB	-5.93	1.30	1.37
9	A	905	BCL	C1D-ND	-5.91	1.30	1.37
13	a	918	85I	O6-C3	-5.82	1.34	1.44
16	c	202	HEC	C1A-NA	-5.80	1.28	1.39
9	a	909	BCL	O1D-CGD	-5.78	1.06	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	908	BCL	C1B-NB	-5.78	1.30	1.37
9	A	906	BCL	O2D-CED	-5.76	1.31	1.45
16	C	301	HEC	C4B-C3B	-5.76	1.35	1.45
15	A	932	85N	O3-C17	-5.73	1.21	1.40
9	a	905	BCL	C3C-C4C	-5.70	1.44	1.51
8	a	903	2GO	C1D-ND	-5.67	1.25	1.38
9	a	907	BCL	OBB-CAB	-5.67	1.10	1.23
10	A	912	CLA	C1B-NB	-5.64	1.30	1.37
10	A	931	CLA	O2D-CED	-5.64	1.32	1.45
9	a	911	BCL	C3C-C4C	-5.61	1.44	1.51
10	A	911	CLA	C1B-NB	-5.58	1.30	1.37
9	a	906	BCL	C1B-NB	-5.57	1.30	1.37
9	a	904	BCL	C4B-NB	-5.57	1.30	1.37
16	C	301	HEC	O2A-CGA	-5.56	1.12	1.30
8	a	903	2GO	C4D-ND	-5.56	1.25	1.38
16	C	301	HEC	C3D-C2D	5.55	1.48	1.36
10	a	915	CLA	C4D-ND	-5.53	1.30	1.37
9	a	909	BCL	C1D-ND	-5.53	1.31	1.37
9	A	909	BCL	C1D-ND	-5.51	1.31	1.37
9	a	910	BCL	C1D-ND	-5.47	1.31	1.37
9	a	907	BCL	C4D-ND	-5.46	1.30	1.37
9	A	909	BCL	CHC-C4B	5.45	1.51	1.39
16	c	202	HEC	C4D-ND	-5.44	1.27	1.38
9	a	905	BCL	CBB-CAB	-5.42	1.39	1.50
9	A	908	BCL	C3C-C4C	-5.42	1.44	1.51
17	E	101	84Q	C15-C16	5.38	1.64	1.51
9	A	908	BCL	C1B-NB	-5.38	1.31	1.37
9	a	906	BCL	C4D-ND	-5.38	1.30	1.37
9	A	903	BCL	CBB-CAB	-5.37	1.39	1.50
9	A	907	BCL	OBB-CAB	-5.34	1.11	1.23
9	a	907	BCL	C4B-NB	-5.34	1.31	1.37
9	A	903	BCL	C3C-C4C	-5.31	1.44	1.51
10	a	912	CLA	C1D-ND	5.29	1.44	1.37
9	A	905	BCL	C1B-NB	-5.27	1.31	1.37
10	a	914	CLA	C1C-NC	-5.26	1.30	1.37
9	A	903	BCL	C1D-ND	-5.23	1.31	1.37
16	c	202	HEC	C1B-NB	-5.21	1.28	1.38
9	A	908	BCL	C1D-ND	-5.18	1.31	1.37
9	A	909	BCL	CHB-C4A	-5.18	1.25	1.37
9	a	906	BCL	C1D-ND	-5.16	1.31	1.37
10	a	912	CLA	CHC-C1C	5.16	1.49	1.38
9	A	905	BCL	C4D-ND	-5.14	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	903	BCL	O1A-CGA	-5.13	1.07	1.22
9	a	911	BCL	C4D-ND	-5.11	1.30	1.37
9	A	907	BCL	C5-C3	5.10	1.61	1.51
9	a	909	BCL	O2D-CED	-5.09	1.33	1.45
9	A	902	BCL	C2A-C1A	-5.08	1.40	1.52
9	a	905	BCL	O1D-CGD	-5.05	1.08	1.21
9	A	906	BCL	C4D-ND	-5.05	1.30	1.37
16	C	301	HEC	C1C-NC	-5.03	1.30	1.39
9	A	907	BCL	C2-C3	5.02	1.45	1.33
9	A	904	BCL	CHC-C4B	5.01	1.50	1.39
9	A	902	BCL	C4D-ND	-5.00	1.30	1.37
10	A	911	CLA	MG-NC	5.00	2.18	2.06
9	A	909	BCL	OBD-CAD	-4.99	1.13	1.22
9	A	907	BCL	CHC-C1C	-4.99	1.26	1.37
10	A	931	CLA	O2D-CGD	4.98	1.45	1.33
9	A	907	BCL	CBB-CAB	-4.96	1.40	1.50
9	a	906	BCL	CAA-C2A	-4.92	1.45	1.54
8	a	903	2GO	C4B-NB	4.88	1.48	1.38
9	a	906	BCL	OBB-CAB	-4.88	1.12	1.23
13	A	916	85I	O6-C3	4.86	1.52	1.44
10	A	910	CLA	C4D-ND	-4.84	1.31	1.37
8	A	901	2GO	C3A-C2A	4.81	1.67	1.54
16	C	301	HEC	FE-NC	4.79	2.11	1.95
16	C	301	HEC	O2D-CGD	-4.79	1.14	1.30
16	C	301	HEC	CHD-C4C	4.77	1.50	1.39
9	A	909	BCL	CBB-CAB	-4.75	1.40	1.50
9	A	906	BCL	O1D-CGD	-4.74	1.09	1.21
9	A	905	BCL	C3C-C4C	-4.74	1.45	1.51
10	a	915	CLA	C1C-NC	-4.71	1.30	1.37
9	a	904	BCL	C4D-ND	-4.69	1.31	1.37
9	a	904	BCL	O1A-CGA	-4.68	1.08	1.22
9	a	909	BCL	C3C-C4C	-4.67	1.45	1.51
9	a	906	BCL	C3C-C4C	-4.65	1.45	1.51
9	A	902	BCL	C3C-C4C	-4.65	1.45	1.51
9	a	907	BCL	C2A-C1A	-4.64	1.41	1.52
16	C	301	HEC	CBB-CAB	-4.60	1.31	1.51
9	A	903	BCL	O1D-CGD	-4.59	1.09	1.21
9	a	905	BCL	O2A-CGA	4.57	1.46	1.33
10	a	912	CLA	O2D-CED	-4.57	1.34	1.45
9	A	904	BCL	O2A-CGA	4.57	1.46	1.30
9	A	902	BCL	CHB-C1B	4.55	1.49	1.39
10	A	931	CLA	O2A-CGA	4.55	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	910	BCL	O1D-CGD	-4.53	1.09	1.21
9	A	906	BCL	O1A-CGA	-4.53	1.09	1.22
10	A	912	CLA	C1C-NC	-4.52	1.31	1.37
13	A	915	85I	P-O3	4.50	1.72	1.60
10	A	931	CLA	O1A-CGA	-4.49	1.09	1.22
16	c	202	HEC	C1D-ND	-4.48	1.32	1.40
10	a	915	CLA	C1D-ND	4.45	1.43	1.37
9	a	904	BCL	OBB-CAB	-4.41	1.13	1.23
16	C	301	HEC	CBC-CAC	-4.41	1.31	1.51
16	C	301	HEC	C4C-C3C	-4.41	1.35	1.44
9	a	911	BCL	OBD-CAD	-4.40	1.14	1.22
10	A	910	CLA	O2D-CED	-4.40	1.35	1.45
9	A	902	BCL	O2D-CED	-4.40	1.35	1.45
9	A	909	BCL	MG-NA	4.39	2.16	2.06
9	a	908	BCL	OBB-CAB	-4.38	1.13	1.23
16	c	202	HEC	O2D-CGD	-4.38	1.16	1.30
10	a	914	CLA	O1D-CGD	-4.37	1.10	1.21
10	A	912	CLA	MG-NC	4.34	2.16	2.06
9	a	911	BCL	O2D-CED	-4.33	1.35	1.45
10	A	912	CLA	O1D-CGD	-4.33	1.10	1.21
9	A	907	BCL	OBD-CAD	-4.32	1.15	1.22
10	a	901	CLA	O2A-CGA	4.30	1.45	1.33
16	c	202	HEC	O1A-CGA	-4.30	1.07	1.22
9	a	904	BCL	O2A-CGA	4.27	1.45	1.33
9	A	903	BCL	C2A-C1A	-4.26	1.42	1.52
9	A	907	BCL	O2D-CED	-4.25	1.35	1.45
10	A	910	CLA	C1C-NC	-4.24	1.31	1.37
10	a	912	CLA	O1D-CGD	-4.21	1.10	1.21
9	A	902	BCL	OBB-CAB	-4.18	1.14	1.23
9	a	910	BCL	CHC-C4B	4.17	1.48	1.39
10	A	910	CLA	O1D-CGD	-4.16	1.10	1.21
16	c	202	HEC	CAC-C3C	-4.15	1.40	1.51
10	A	933	CLA	C1C-NC	-4.15	1.31	1.37
9	a	909	BCL	CBB-CAB	-4.12	1.42	1.50
9	A	904	BCL	OBB-CAB	-4.12	1.14	1.23
9	A	902	BCL	CBB-CAB	-4.12	1.42	1.50
9	a	910	BCL	O1A-CGA	-4.10	1.10	1.22
9	A	905	BCL	O2D-CED	-4.10	1.35	1.45
10	A	910	CLA	CHB-C1B	4.10	1.48	1.39
9	A	902	BCL	MG-NB	4.10	2.13	2.05
9	a	904	BCL	O2D-CED	-4.06	1.35	1.45
9	a	904	BCL	O1D-CGD	-4.03	1.11	1.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	907	BCL	CHB-C1B	4.03	1.48	1.39
9	A	906	BCL	OBB-CAB	-4.02	1.14	1.23
9	A	905	BCL	C3A-C2A	-4.01	1.43	1.54
16	c	202	HEC	FE-NA	4.00	2.08	1.95
13	a	919	85I	C4-C3	-4.00	1.42	1.51
9	a	908	BCL	O2D-CED	-3.99	1.35	1.45
9	a	911	BCL	O2A-C1	-3.98	1.34	1.46
13	A	915	85I	O4-C5	-3.97	1.21	1.33
9	a	908	BCL	O1D-CGD	-3.97	1.11	1.21
16	c	202	HEC	C2A-C3A	3.96	1.45	1.36
9	a	910	BCL	CBB-CAB	-3.96	1.42	1.50
9	a	909	BCL	O1A-CGA	-3.94	1.10	1.22
9	A	908	BCL	O1D-CGD	-3.94	1.11	1.21
9	A	904	BCL	CAA-C2A	-3.92	1.46	1.54
16	c	202	HEC	FE-NC	3.91	2.08	1.95
11	A	913	LYC	C55-C56	-3.90	1.30	1.35
10	a	915	CLA	C3C-C2C	3.89	1.45	1.36
10	A	933	CLA	O2A-C1	-3.89	1.35	1.46
10	A	912	CLA	CHB-C1B	3.89	1.48	1.39
9	A	906	BCL	C1B-C2B	-3.87	1.34	1.43
10	a	915	CLA	CHB-C4A	-3.87	1.28	1.37
10	a	901	CLA	O2D-CED	-3.87	1.36	1.45
9	a	911	BCL	O1A-CGA	-3.86	1.11	1.22
9	A	904	BCL	C2A-C1A	-3.86	1.43	1.52
10	A	911	CLA	CHB-C4A	-3.85	1.28	1.37
9	A	902	BCL	CAA-C2A	-3.84	1.47	1.54
9	A	905	BCL	O1D-CGD	-3.83	1.11	1.21
9	a	911	BCL	CHD-C1D	3.83	1.45	1.38
11	c	201	LYC	C14-C12	-3.82	1.30	1.35
10	A	931	CLA	OBD-CAD	-3.82	1.15	1.22
9	A	904	BCL	C4D-ND	-3.81	1.32	1.37
9	a	910	BCL	O2D-CGD	3.80	1.42	1.33
9	a	905	BCL	OBD-CAD	-3.79	1.15	1.22
16	C	301	HEC	C4A-C3A	3.79	1.52	1.45
10	a	914	CLA	O2A-CGA	3.79	1.45	1.33
9	a	907	BCL	CHB-C1B	3.78	1.47	1.39
9	A	902	BCL	O2D-CGD	3.77	1.42	1.33
9	a	905	BCL	O2D-CED	-3.76	1.36	1.45
9	a	910	BCL	O2D-CED	-3.75	1.36	1.45
10	a	912	CLA	MG-NC	3.75	2.15	2.06
9	a	910	BCL	C4D-ND	-3.75	1.32	1.37
10	a	915	CLA	MG-NC	3.74	2.15	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	907	BCL	C6-C5	3.73	1.65	1.52
10	a	913	CLA	CHC-C1C	3.73	1.46	1.38
9	A	906	BCL	CHC-C1C	-3.72	1.28	1.37
10	a	901	CLA	O1D-CGD	-3.72	1.11	1.21
11	A	913	LYC	C9-C7	-3.72	1.30	1.34
10	a	913	CLA	C4D-ND	-3.70	1.32	1.37
13	A	915	85I	P-O	-3.70	1.44	1.59
9	A	908	BCL	C3A-C2A	-3.68	1.44	1.54
9	A	903	BCL	CHB-C1B	3.68	1.47	1.39
10	a	901	CLA	MG-NC	3.68	2.15	2.06
10	A	912	CLA	C4D-ND	-3.68	1.32	1.37
10	a	901	CLA	CHD-C4C	3.67	1.47	1.39
9	a	908	BCL	CAA-CBA	-3.66	1.41	1.52
9	a	906	BCL	C2A-C1A	-3.66	1.44	1.52
10	a	901	CLA	CHC-C1C	3.65	1.45	1.38
10	A	933	CLA	C1B-NB	-3.65	1.33	1.37
9	A	909	BCL	MG-ND	-3.65	1.98	2.05
9	a	909	BCL	C4D-ND	-3.64	1.32	1.37
9	A	909	BCL	C2-C3	3.64	1.41	1.33
9	A	902	BCL	O1A-CGA	-3.63	1.11	1.22
9	A	909	BCL	C3A-C2A	-3.62	1.44	1.54
8	A	901	2GO	C1D-ND	-3.62	1.30	1.38
9	A	905	BCL	CHC-C4B	3.62	1.47	1.39
10	a	913	CLA	CAA-C2A	3.61	1.60	1.54
10	a	914	CLA	MG-NC	3.61	2.14	2.06
9	A	909	BCL	O1D-CGD	-3.61	1.12	1.21
10	a	915	CLA	O1A-CGA	-3.59	1.11	1.22
16	C	301	HEC	C4D-ND	-3.59	1.31	1.38
11	c	201	LYC	C19-C17	-3.59	1.31	1.35
9	a	907	BCL	O2A-CGA	3.58	1.43	1.33
9	A	903	BCL	C3A-C2A	-3.58	1.44	1.54
10	a	912	CLA	O2A-CGA	3.57	1.43	1.33
9	a	906	BCL	O2A-CGA	3.56	1.42	1.30
10	A	911	CLA	C10-C8	-3.56	1.33	1.52
16	c	202	HEC	C3B-C2B	3.55	1.44	1.36
13	A	915	85I	P-O1	-3.54	1.38	1.50
9	A	909	BCL	CAA-CBA	-3.54	1.41	1.52
9	A	903	BCL	CHC-C4B	3.54	1.47	1.39
9	A	904	BCL	CHB-C1B	3.50	1.47	1.39
8	a	903	2GO	ZN-NA	3.50	2.14	2.03
9	A	904	BCL	C1B-NB	-3.49	1.33	1.37
16	C	301	HEC	C4A-NA	-3.49	1.33	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	933	CLA	CAA-C2A	-3.48	1.47	1.54
10	a	915	CLA	O1D-CGD	-3.47	1.12	1.21
9	a	911	BCL	CHC-C1C	-3.47	1.29	1.37
9	A	903	BCL	C4D-ND	-3.45	1.33	1.37
9	a	905	BCL	O1A-CGA	-3.44	1.12	1.22
9	a	906	BCL	MG-NB	3.43	2.12	2.05
10	A	933	CLA	O1A-CGA	-3.42	1.12	1.22
9	A	903	BCL	O2A-CGA	3.42	1.43	1.33
9	A	909	BCL	CBD-CGD	-3.41	1.41	1.52
9	a	907	BCL	O2A-C1	-3.41	1.36	1.46
10	A	911	CLA	O1A-CGA	-3.40	1.12	1.22
10	a	901	CLA	C1D-C2D	3.40	1.52	1.45
11	A	913	LYC	C13-C12	-3.39	1.43	1.50
10	A	911	CLA	O2D-CED	-3.39	1.37	1.45
11	c	201	LYC	C13-C12	-3.39	1.43	1.50
10	a	913	CLA	CHC-C4B	3.38	1.47	1.39
10	a	915	CLA	CHC-C4B	3.38	1.47	1.39
9	a	908	BCL	CHC-C4B	3.38	1.47	1.39
9	A	908	BCL	CHB-C4A	-3.37	1.29	1.37
9	a	907	BCL	CHD-C1D	3.37	1.44	1.38
9	a	907	BCL	CAA-C2A	-3.36	1.47	1.54
10	A	911	CLA	CHC-C1C	3.36	1.45	1.38
9	A	903	BCL	O2D-CGD	3.35	1.41	1.33
9	a	910	BCL	CHB-C4A	-3.35	1.29	1.37
9	A	905	BCL	CBA-CGA	-3.34	1.40	1.50
9	A	908	BCL	C4D-ND	-3.34	1.33	1.37
9	A	908	BCL	OBB-CAB	-3.33	1.15	1.23
10	A	912	CLA	O2A-CGA	3.33	1.43	1.33
8	A	901	2GO	C3D-C2D	-3.33	1.30	1.39
9	a	906	BCL	CHC-C4B	3.32	1.46	1.39
10	A	931	CLA	C4D-CHA	3.31	1.50	1.38
10	A	911	CLA	O2A-C1	-3.30	1.36	1.46
10	a	901	CLA	C7-C8	-3.30	1.35	1.52
16	c	202	HEC	CBA-CGA	-3.30	1.42	1.50
9	a	905	BCL	CHB-C4A	-3.30	1.29	1.37
9	a	908	BCL	CHC-C1C	-3.30	1.29	1.37
9	a	907	BCL	C1B-NB	-3.29	1.33	1.37
10	a	914	CLA	C3C-C2C	3.29	1.43	1.36
9	a	908	BCL	CBA-CGA	-3.29	1.41	1.50
9	a	905	BCL	CAC-C3C	-3.29	1.47	1.54
9	a	906	BCL	C3B-C4B	3.27	1.47	1.41
9	A	906	BCL	CHB-C4A	-3.27	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	904	BCL	CHB-C1B	3.25	1.46	1.39
9	a	908	BCL	C5-C3	-3.23	1.44	1.51
9	A	908	BCL	CAA-C2A	-3.21	1.48	1.54
9	a	909	BCL	CHC-C1C	-3.21	1.30	1.37
9	a	907	BCL	O1D-CGD	-3.21	1.13	1.21
9	A	907	BCL	CMD-C2D	-3.20	1.44	1.50
9	a	905	BCL	C1B-NB	-3.20	1.33	1.37
9	a	907	BCL	MG-NA	-3.19	1.98	2.06
16	c	202	HEC	CHB-C4A	3.18	1.44	1.38
10	A	910	CLA	CHD-C1D	3.18	1.44	1.38
10	a	913	CLA	O1A-CGA	-3.18	1.13	1.22
9	A	908	BCL	CMA-C3A	-3.18	1.46	1.53
9	A	908	BCL	MG-NC	-3.18	1.98	2.06
9	a	907	BCL	MG-NB	3.18	2.12	2.05
9	a	909	BCL	CHB-C1B	3.17	1.46	1.39
11	A	913	LYC	C19-C17	-3.16	1.31	1.35
8	a	903	2GO	C4C-NC	3.16	1.35	1.28
9	A	908	BCL	O2A-CGA	3.16	1.42	1.33
11	A	913	LYC	C10-C11	-3.15	1.26	1.34
9	A	906	BCL	CHB-C1B	3.15	1.46	1.39
9	a	907	BCL	CHC-C4B	3.15	1.46	1.39
9	A	902	BCL	O2A-CGA	3.15	1.42	1.33
10	A	910	CLA	CHC-C4B	3.12	1.46	1.39
10	a	901	CLA	CHB-C1B	3.12	1.46	1.39
9	a	910	BCL	O2A-CGA	3.11	1.42	1.33
16	c	202	HEC	C1B-C2B	-3.11	1.38	1.44
9	A	907	BCL	C2C-C3C	-3.09	1.45	1.54
9	A	902	BCL	CHC-C1C	-3.09	1.30	1.37
10	A	910	CLA	MG-NB	3.08	2.11	2.05
10	A	910	CLA	CHD-C4C	3.08	1.46	1.39
9	a	911	BCL	C1D-C2D	-3.07	1.39	1.45
10	a	915	CLA	O2D-CED	-3.07	1.38	1.45
10	A	931	CLA	C10-C8	-3.07	1.36	1.52
17	E	101	84Q	C3-C1	-3.07	1.30	1.51
9	a	909	BCL	C3A-C2A	-3.06	1.45	1.54
9	a	910	BCL	MG-NA	3.06	2.13	2.06
10	A	910	CLA	MG-NC	3.06	2.13	2.06
16	c	202	HEC	CBC-CAC	-3.05	1.37	1.51
10	a	901	CLA	O2D-CGD	3.05	1.40	1.33
10	A	931	CLA	CHB-C1B	3.04	1.46	1.39
9	A	909	BCL	CHD-C1D	3.03	1.44	1.38
9	a	907	BCL	C2C-C3C	-3.03	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	931	CLA	C1D-C2D	-3.03	1.39	1.45
10	A	931	CLA	C3D-C2D	3.02	1.47	1.39
16	c	202	HEC	CBA-CAA	-3.01	1.42	1.52
9	A	902	BCL	CHD-C1D	3.01	1.44	1.38
16	c	202	HEC	C4C-NC	-3.01	1.33	1.39
10	a	914	CLA	C2A-C1A	-3.00	1.45	1.52
10	A	912	CLA	CHC-C1C	3.00	1.44	1.38
10	a	913	CLA	O1D-CGD	-2.99	1.13	1.21
9	a	904	BCL	CHC-C4B	2.99	1.46	1.39
9	a	911	BCL	C3A-C2A	-2.99	1.46	1.54
16	C	301	HEC	CHD-C1D	2.98	1.44	1.38
9	A	902	BCL	O1D-CGD	-2.97	1.13	1.21
10	A	911	CLA	O1D-CGD	-2.96	1.13	1.21
10	A	912	CLA	CHB-C4A	-2.96	1.30	1.37
9	A	903	BCL	O2D-CED	-2.95	1.38	1.45
9	A	906	BCL	CHD-C1D	2.94	1.44	1.38
9	a	908	BCL	CHB-C1B	2.94	1.46	1.39
9	A	905	BCL	CAA-CBA	-2.94	1.43	1.52
9	A	905	BCL	CHB-C4A	-2.93	1.30	1.37
9	a	908	BCL	O2D-CGD	2.93	1.40	1.33
10	a	913	CLA	C10-C8	2.93	1.68	1.52
10	a	915	CLA	CHB-C1B	2.93	1.46	1.39
10	A	931	CLA	CHD-C1D	2.93	1.44	1.38
10	a	915	CLA	C3B-C4B	-2.93	1.36	1.42
8	A	901	2GO	ZN-NB	2.92	2.13	2.03
10	A	931	CLA	CMA-C3A	-2.91	1.46	1.53
9	A	902	BCL	C3A-C2A	-2.90	1.46	1.54
9	A	904	BCL	O2D-CGD	2.90	1.40	1.33
10	A	931	CLA	MG-NB	2.90	2.11	2.05
9	a	905	BCL	O2D-CGD	2.90	1.40	1.33
10	A	931	CLA	C1C-C2C	-2.88	1.39	1.44
10	a	913	CLA	MG-NC	2.87	2.13	2.06
9	A	908	BCL	O2D-CGD	2.87	1.40	1.33
9	A	903	BCL	CHC-C1C	-2.87	1.30	1.37
9	A	908	BCL	C2C-C3C	-2.87	1.46	1.54
8	A	901	2GO	CHD-C1D	2.87	1.44	1.38
9	a	909	BCL	C2C-C3C	-2.87	1.46	1.54
9	a	905	BCL	C2C-C3C	-2.86	1.46	1.54
10	a	914	CLA	C3A-C2A	-2.86	1.46	1.54
10	A	933	CLA	C3A-C2A	-2.85	1.46	1.54
11	A	913	LYC	C59-C58	-2.85	1.27	1.34
8	a	903	2GO	CHB-C1B	2.85	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	904	BCL	C2C-C3C	-2.85	1.46	1.54
10	a	901	CLA	CAA-C2A	-2.83	1.48	1.54
9	a	907	BCL	O1A-CGA	-2.83	1.14	1.22
17	E	101	84Q	C7-C6	-2.80	1.35	1.51
10	a	914	CLA	CHB-C4A	-2.80	1.31	1.37
9	a	908	BCL	O1A-CGA	-2.79	1.14	1.22
10	A	910	CLA	CHC-C1C	2.79	1.44	1.38
10	a	901	CLA	C3C-C2C	2.79	1.42	1.36
9	A	903	BCL	CMD-C2D	-2.78	1.44	1.50
10	A	912	CLA	C1D-C2D	-2.77	1.39	1.45
10	a	914	CLA	CHB-C1B	2.77	1.45	1.39
9	a	907	BCL	C3C-C4C	-2.75	1.48	1.51
9	a	911	BCL	C3D-C2D	2.74	1.46	1.39
8	a	903	2GO	C2C-C3C	2.74	1.62	1.54
10	A	933	CLA	O2D-CED	-2.73	1.38	1.45
9	A	908	BCL	MG-NA	-2.73	1.99	2.06
9	a	907	BCL	C1D-C2D	-2.73	1.39	1.45
10	a	915	CLA	O2D-CGD	2.73	1.39	1.33
9	a	910	BCL	CMB-C2B	-2.73	1.45	1.50
16	C	301	HEC	C1C-C2C	-2.73	1.36	1.43
10	A	933	CLA	CHB-C4A	-2.72	1.31	1.37
13	A	915	85I	O5-C5	-2.72	1.14	1.22
9	A	908	BCL	CHC-C1C	-2.71	1.31	1.37
13	A	915	85I	O6-C3	-2.71	1.40	1.44
9	A	902	BCL	CHB-C4A	-2.71	1.31	1.37
9	A	902	BCL	C2C-C3C	-2.70	1.46	1.54
10	A	911	CLA	CHD-C1D	2.70	1.43	1.38
10	A	912	CLA	C3C-C2C	2.70	1.42	1.36
9	a	904	BCL	CHC-C1C	-2.70	1.31	1.37
10	a	912	CLA	MG-NB	2.69	2.11	2.05
17	E	101	84Q	C9-C8	-2.69	1.36	1.51
10	A	912	CLA	C2A-C1A	-2.69	1.46	1.52
9	A	907	BCL	C3A-C2A	-2.68	1.47	1.54
10	A	910	CLA	O2A-CGA	2.68	1.41	1.33
16	C	301	HEC	O1A-CGA	-2.68	1.13	1.22
9	A	907	BCL	CHC-C4B	2.68	1.45	1.39
10	A	933	CLA	CBA-CGA	-2.68	1.42	1.50
9	a	906	BCL	O1D-CGD	-2.68	1.14	1.21
9	A	907	BCL	O2A-C1	2.68	1.53	1.46
13	A	915	85I	P-O2	-2.67	1.42	1.55
9	A	908	BCL	O1A-CGA	-2.67	1.14	1.22
8	A	901	2GO	ZN-ND	2.66	2.12	2.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	906	BCL	CHD-C1D	2.65	1.43	1.38
10	A	911	CLA	CMC-C2C	-2.65	1.45	1.50
9	a	909	BCL	C5-C3	-2.65	1.45	1.51
16	C	301	HEC	C3B-C2B	2.64	1.42	1.36
16	C	301	HEC	CBA-CGA	-2.64	1.44	1.50
10	A	931	CLA	MG-NC	2.64	2.12	2.06
9	a	905	BCL	CHC-C4B	2.63	1.45	1.39
10	a	901	CLA	O1A-CGA	-2.63	1.14	1.22
9	a	909	BCL	CMD-C2D	-2.63	1.45	1.50
13	A	915	85I	C33-C32	-2.63	1.37	1.51
9	A	907	BCL	C2A-C1A	-2.63	1.46	1.52
17	E	101	84Q	C9-C10	-2.62	1.36	1.51
9	a	909	BCL	O2D-CGD	2.62	1.39	1.33
9	a	911	BCL	CHB-C4A	-2.62	1.31	1.37
10	a	914	CLA	O1A-CGA	-2.61	1.14	1.22
9	A	908	BCL	CBD-CGD	-2.60	1.44	1.52
9	A	907	BCL	C3C-C4C	-2.60	1.48	1.51
10	A	933	CLA	CHC-C1C	2.60	1.43	1.38
10	A	931	CLA	MG-NA	2.59	2.12	2.06
9	A	905	BCL	O2A-CGA	2.59	1.40	1.33
9	a	911	BCL	CBB-CAB	-2.58	1.45	1.50
8	a	903	2GO	O1D-CGD	-2.58	1.14	1.21
10	a	901	CLA	C5-C3	-2.58	1.45	1.51
16	C	301	HEC	CHB-C1B	2.57	1.45	1.39
9	a	907	BCL	CHB-C4A	-2.57	1.31	1.37
16	C	301	HEC	CHC-C1C	2.56	1.45	1.39
8	A	901	2GO	C4C-NC	2.56	1.34	1.28
10	A	910	CLA	C1D-C2D	-2.56	1.40	1.45
16	C	301	HEC	C1A-NA	-2.56	1.34	1.39
10	A	933	CLA	MG-ND	2.56	2.10	2.05
17	a	921	84Q	P-O4	2.56	1.67	1.60
9	a	907	BCL	O2D-CED	-2.55	1.39	1.45
8	A	901	2GO	C3B-C4B	-2.54	1.36	1.41
9	A	905	BCL	O2A-C1	-2.54	1.39	1.46
10	A	931	CLA	C3A-C4A	-2.54	1.43	1.51
10	a	901	CLA	C2-C3	-2.54	1.26	1.33
16	c	202	HEC	CAD-C3D	-2.54	1.44	1.51
11	c	201	LYC	C1-C2	-2.53	1.43	1.50
11	A	913	LYC	C11-C12	-2.53	1.40	1.45
9	A	902	BCL	CMB-C2B	-2.52	1.45	1.50
10	a	913	CLA	CHB-C1B	2.52	1.45	1.39
10	A	910	CLA	C1D-ND	2.52	1.40	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	c	201	LYC	C15-C16	-2.52	1.28	1.34
9	A	906	BCL	C2A-C1A	-2.51	1.46	1.52
16	c	202	HEC	CMD-C2D	-2.51	1.45	1.50
9	a	910	BCL	C3A-C2A	-2.51	1.47	1.54
9	a	911	BCL	C1B-C2B	-2.51	1.37	1.43
10	a	912	CLA	CHD-C4C	2.51	1.45	1.39
8	a	903	2GO	O1A-CGA	-2.50	1.15	1.22
13	a	920	85I	C4-C3	-2.50	1.46	1.51
9	a	910	BCL	CHB-C1B	2.50	1.45	1.39
9	a	908	BCL	C3D-C2D	2.49	1.45	1.39
9	a	911	BCL	CBA-CGA	-2.49	1.43	1.50
9	A	905	BCL	C2C-C3C	-2.48	1.47	1.54
10	a	901	CLA	MG-NB	2.48	2.10	2.05
17	E	101	84Q	C6-C5	-2.48	1.37	1.51
9	a	904	BCL	CBB-CAB	-2.48	1.45	1.50
9	a	909	BCL	C3A-C4A	-2.47	1.43	1.51
16	C	301	HEC	CMB-C2B	-2.47	1.45	1.50
9	a	908	BCL	MG-ND	2.46	2.10	2.05
13	a	918	85I	C4-C3	2.46	1.57	1.51
10	A	911	CLA	CHB-C1B	2.46	1.44	1.39
9	A	909	BCL	C3B-C4B	2.46	1.45	1.41
17	E	101	84Q	C8-C7	-2.46	1.37	1.51
10	a	913	CLA	C5-C3	-2.45	1.46	1.51
9	a	911	BCL	CHB-C1B	2.45	1.44	1.39
10	a	913	CLA	CHB-C4A	-2.44	1.31	1.37
10	A	931	CLA	CHC-C1C	2.43	1.43	1.38
9	A	904	BCL	CMB-C2B	-2.42	1.45	1.50
9	A	906	BCL	MG-ND	2.42	2.10	2.05
9	A	907	BCL	O1A-CGA	-2.42	1.15	1.22
9	A	907	BCL	CHB-C4A	-2.42	1.31	1.37
10	A	910	CLA	CBB-CAB	-2.41	1.18	1.30
10	a	914	CLA	C4D-CHA	2.41	1.47	1.38
9	A	904	BCL	C3A-C2A	-2.41	1.47	1.54
9	a	910	BCL	MG-NB	2.40	2.10	2.05
9	A	909	BCL	CHB-C1B	2.40	1.44	1.39
9	a	909	BCL	C2C-C1C	-2.40	1.44	1.51
9	A	908	BCL	C3D-C2D	2.40	1.45	1.39
9	a	911	BCL	MG-NA	2.39	2.12	2.06
17	E	101	84Q	C5-C4	-2.39	1.38	1.51
9	a	906	BCL	CHB-C1B	2.39	1.44	1.39
15	g	101	85N	O4-C24	-2.39	1.22	1.30
9	a	906	BCL	CAA-CBA	-2.39	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	901	2GO	C1B-C2B	-2.38	1.37	1.43
9	a	906	BCL	C3D-C2D	2.38	1.45	1.39
10	a	901	CLA	CMC-C2C	-2.38	1.45	1.50
10	A	933	CLA	C2A-C1A	-2.38	1.46	1.52
10	a	913	CLA	C2A-C1A	-2.37	1.46	1.52
11	c	201	LYC	C62-C61	-2.37	1.44	1.50
9	a	911	BCL	C2C-C3C	-2.37	1.47	1.54
9	A	904	BCL	CMA-C3A	-2.36	1.48	1.53
9	A	905	BCL	CBB-CAB	-2.36	1.45	1.50
9	a	906	BCL	C3A-C4A	-2.35	1.44	1.51
9	a	911	BCL	O1D-CGD	-2.35	1.15	1.21
10	A	931	CLA	C4C-C3C	-2.35	1.41	1.45
17	E	101	84Q	O-C14	-2.35	1.15	1.22
9	a	905	BCL	C3D-C2D	2.35	1.45	1.39
9	a	904	BCL	CAA-CBA	-2.35	1.45	1.52
8	A	901	2GO	C3B-C2B	-2.34	1.35	1.42
11	A	913	LYC	C52-C51	-2.34	1.46	1.50
9	A	908	BCL	C3A-C4A	-2.34	1.44	1.51
10	a	913	CLA	C3A-C2A	-2.34	1.47	1.54
10	a	913	CLA	O2A-CGA	2.33	1.40	1.33
9	A	907	BCL	CHD-C1D	2.32	1.42	1.38
9	A	908	BCL	CAC-C3C	-2.32	1.49	1.54
8	a	903	2GO	C3B-C2B	-2.32	1.35	1.42
9	a	904	BCL	C2A-C1A	-2.31	1.47	1.52
10	a	914	CLA	C4C-C3C	-2.31	1.41	1.45
8	A	901	2GO	C1A-NA	-2.31	1.22	1.29
9	a	911	BCL	C3B-C4B	2.31	1.45	1.41
10	A	911	CLA	O2A-CGA	2.30	1.40	1.33
10	a	914	CLA	C3D-C2D	2.30	1.45	1.39
9	A	908	BCL	O2D-CED	-2.30	1.39	1.45
13	A	915	85I	O7-C20	-2.30	1.15	1.22
10	A	931	CLA	CBD-CGD	2.30	1.59	1.52
10	a	914	CLA	CHC-C1C	2.29	1.43	1.38
10	A	931	CLA	O2A-C1	-2.28	1.39	1.46
9	a	908	BCL	C4-C3	-2.28	1.44	1.50
10	a	915	CLA	O2A-CGA	2.28	1.40	1.33
10	a	912	CLA	CHC-C4B	2.27	1.44	1.39
10	a	913	CLA	O2A-C1	-2.27	1.39	1.46
9	a	911	BCL	C2A-C1A	-2.27	1.47	1.52
10	A	911	CLA	CHC-C4B	2.27	1.44	1.39
9	a	909	BCL	C4-C3	-2.26	1.44	1.50
9	a	904	BCL	CMA-C3A	-2.25	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	906	BCL	CBD-CGD	-2.25	1.45	1.52
9	a	909	BCL	CHC-C4B	2.24	1.44	1.39
9	A	904	BCL	C1D-ND	-2.24	1.35	1.37
9	a	907	BCL	C3A-C4A	-2.24	1.44	1.51
9	A	903	BCL	CHB-C4A	-2.24	1.32	1.37
16	c	202	HEC	C4C-C3C	-2.24	1.40	1.44
8	A	901	2GO	C4D-CHA	-2.24	1.30	1.38
9	a	907	BCL	CBA-CGA	-2.24	1.44	1.50
16	C	301	HEC	CHC-C4B	2.24	1.43	1.38
9	A	904	BCL	CAA-CBA	-2.23	1.45	1.52
9	A	909	BCL	C2A-C1A	-2.23	1.47	1.52
11	A	913	LYC	C18-C17	-2.23	1.46	1.50
9	A	909	BCL	CMD-C2D	-2.22	1.46	1.50
9	A	909	BCL	C9-C8	-2.22	1.45	1.52
10	a	913	CLA	C3C-C2C	2.21	1.41	1.36
9	a	909	BCL	CHB-C4A	-2.21	1.32	1.37
11	c	201	LYC	C21-C20	-2.21	1.30	1.36
9	A	905	BCL	C3B-C4B	2.20	1.45	1.41
9	a	908	BCL	O2A-CGA	2.20	1.39	1.33
8	a	903	2GO	CHC-C1C	-2.20	1.32	1.37
9	a	909	BCL	CMA-C3A	-2.19	1.48	1.53
10	A	910	CLA	C1C-C2C	-2.19	1.40	1.44
9	a	904	BCL	MG-NB	2.19	2.10	2.05
9	A	908	BCL	CHD-C1D	2.19	1.42	1.38
10	a	915	CLA	MG-NB	2.18	2.10	2.05
9	A	908	BCL	CHD-C4C	2.18	1.45	1.39
11	c	201	LYC	C18-C17	-2.18	1.46	1.50
9	A	904	BCL	CHB-C4A	-2.17	1.32	1.37
9	A	908	BCL	CMC-C2C	-2.17	1.48	1.53
10	a	912	CLA	C2A-C1A	-2.17	1.47	1.52
9	a	905	BCL	C3A-C2A	-2.17	1.48	1.54
10	a	915	CLA	C3A-C2A	-2.17	1.48	1.54
10	a	901	CLA	C1D-ND	2.17	1.40	1.37
10	A	910	CLA	C3D-C2D	2.17	1.45	1.39
10	a	914	CLA	CBD-CGD	-2.16	1.45	1.52
9	a	909	BCL	CHD-C1D	2.16	1.42	1.38
9	a	906	BCL	C3A-C2A	-2.16	1.48	1.54
9	A	909	BCL	O2D-CED	2.16	1.50	1.45
10	a	912	CLA	C3D-C2D	2.16	1.45	1.39
9	A	904	BCL	CHC-C1C	-2.15	1.32	1.37
9	A	904	BCL	CHD-C1D	2.15	1.42	1.38
9	a	905	BCL	CHC-C1C	-2.15	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	909	BCL	CBA-CGA	-2.14	1.44	1.50
9	A	904	BCL	C4D-CHA	2.14	1.46	1.38
10	A	933	CLA	MG-NB	2.14	2.10	2.05
10	a	912	CLA	C4C-C3C	-2.13	1.41	1.45
9	a	907	BCL	CAA-CBA	-2.13	1.46	1.52
10	A	933	CLA	MG-NC	2.13	2.11	2.06
9	a	908	BCL	C3B-C4B	2.13	1.45	1.41
9	A	903	BCL	C2C-C3C	-2.13	1.48	1.54
10	A	912	CLA	CHD-C1D	2.13	1.42	1.38
16	C	301	HEC	C4D-C3D	2.12	1.48	1.45
9	A	906	BCL	O2A-C1	-2.11	1.40	1.46
9	A	906	BCL	MG-NB	-2.11	2.01	2.05
10	A	933	CLA	C3D-C2D	2.11	1.44	1.39
10	A	910	CLA	O2D-CGD	2.10	1.38	1.33
11	A	913	LYC	C5-C4	-2.10	1.43	1.50
16	C	301	HEC	C2A-C3A	2.10	1.41	1.36
10	A	911	CLA	C9-C8	2.10	1.59	1.52
9	A	902	BCL	OBD-CAD	-2.10	1.18	1.22
9	a	909	BCL	C2-C3	-2.09	1.28	1.33
9	A	908	BCL	CHC-C4B	2.09	1.44	1.39
10	a	912	CLA	O1A-CGA	-2.09	1.16	1.22
9	A	909	BCL	O2A-CGA	2.09	1.39	1.33
9	A	903	BCL	CAA-CBA	-2.09	1.46	1.52
9	A	908	BCL	C5-C3	-2.08	1.47	1.51
10	a	914	CLA	CHD-C1D	2.08	1.42	1.38
10	A	911	CLA	CHD-C4C	2.07	1.44	1.39
10	A	933	CLA	C2-C3	-2.07	1.28	1.33
9	A	906	BCL	CHC-C4B	2.07	1.44	1.39
10	a	915	CLA	CHD-C1D	2.07	1.42	1.38
8	A	901	2GO	C1A-CHA	2.07	1.51	1.43
9	A	907	BCL	C1-C2	2.06	1.55	1.49
9	A	909	BCL	C2C-C3C	-2.06	1.48	1.54
9	a	906	BCL	CHB-C4A	-2.06	1.32	1.37
10	A	912	CLA	C3B-C4B	-2.05	1.38	1.42
9	a	910	BCL	CHD-C4C	2.05	1.45	1.39
8	a	903	2GO	C1A-NA	-2.05	1.23	1.29
9	A	904	BCL	CBA-CGA	-2.05	1.45	1.50
9	a	911	BCL	CAC-C3C	-2.05	1.49	1.54
11	c	201	LYC	C63-C64	-2.05	1.46	1.53
10	A	911	CLA	C2A-C1A	-2.04	1.47	1.52
9	a	911	BCL	CHD-C4C	2.04	1.45	1.39
8	a	903	2GO	ZN-ND	2.04	2.10	2.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	a	907	BCL	CBB-CAB	-2.04	1.46	1.50
9	a	908	BCL	C3C-C4C	-2.04	1.49	1.51
9	A	904	BCL	C3D-C2D	2.04	1.44	1.39
10	a	914	CLA	O2D-CED	-2.04	1.40	1.45
10	A	933	CLA	CHC-C4B	2.03	1.44	1.39
10	a	901	CLA	O2A-C1	-2.03	1.40	1.46
9	a	909	BCL	C2A-C1A	-2.03	1.47	1.52
9	A	907	BCL	C6-C7	2.02	1.60	1.52
9	A	907	BCL	C3A-C4A	-2.02	1.45	1.51
8	A	901	2GO	CBC-CAC	-2.01	1.38	1.51
9	A	908	BCL	CBB-CAB	-2.01	1.46	1.50
9	a	910	BCL	C4D-CHA	2.01	1.45	1.38
9	a	908	BCL	CMC-C2C	-2.01	1.48	1.53
9	a	907	BCL	CMD-C2D	-2.01	1.46	1.50

All (1130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	909	BCL	O2D-CGD-CBD	20.86	148.33	111.27
9	a	908	BCL	C4A-NA-C1A	18.67	115.10	106.71
9	A	906	BCL	O2D-CGD-CBD	18.23	143.67	111.27
10	A	931	CLA	O2D-CGD-CBD	18.08	143.39	111.27
9	a	907	BCL	C4A-NA-C1A	16.53	114.14	106.71
10	a	913	CLA	C1D-ND-C4D	-15.69	95.19	106.33
9	A	906	BCL	O2D-CGD-O1D	-15.51	93.51	123.84
9	a	909	BCL	O2D-CGD-CBD	15.31	138.47	111.27
10	A	912	CLA	C2C-C1C-NC	15.09	124.11	109.97
9	A	905	BCL	O2D-CGD-CBD	14.78	137.52	111.27
11	c	201	LYC	C21-C50-C51	14.71	148.31	127.31
9	A	907	BCL	C4A-NA-C1A	14.57	113.26	106.71
9	A	907	BCL	O2D-CGD-CBD	14.50	137.03	111.27
9	A	903	BCL	O2D-CGD-CBD	14.33	136.73	111.27
10	a	913	CLA	O2D-CGD-CBD	14.11	136.34	111.27
9	a	910	BCL	O2D-CGD-CBD	13.95	136.06	111.27
9	a	904	BCL	O2D-CGD-CBD	13.80	135.79	111.27
9	a	905	BCL	O2D-CGD-CBD	13.71	135.63	111.27
11	c	201	LYC	C53-C51-C50	13.56	139.75	118.94
9	A	906	BCL	CHD-C1D-ND	-13.50	112.05	124.45
9	a	910	BCL	C1C-NC-C4C	13.25	112.67	106.71
9	A	906	BCL	C2D-C1D-ND	13.25	119.87	110.10
10	a	913	CLA	O2D-CGD-O1D	-13.14	98.15	123.84
9	a	908	BCL	O2D-CGD-CBD	12.95	134.28	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	908	BCL	C2B-C1B-NB	12.82	118.83	110.23
10	A	910	CLA	O2D-CGD-O1D	-12.76	98.89	123.84
13	A	917	85I	O4-C4-C3	12.74	142.25	109.54
9	A	902	BCL	O2D-CGD-CBD	12.47	133.43	111.27
9	A	903	BCL	O2D-CGD-O1D	-12.40	99.59	123.84
10	A	910	CLA	O2D-CGD-CBD	11.97	132.54	111.27
10	A	931	CLA	O2D-CGD-O1D	-11.90	100.56	123.84
9	a	911	BCL	C2D-C1D-ND	11.85	118.84	110.10
11	c	201	LYC	C15-C14-C12	11.82	144.19	127.31
9	a	907	BCL	O2D-CGD-CBD	11.81	132.26	111.27
10	a	912	CLA	C2B-C1B-NB	11.68	118.06	110.23
10	A	911	CLA	C1D-ND-C4D	-11.56	98.12	106.33
9	A	909	BCL	O2A-C1-C2	11.47	138.78	108.64
10	a	914	CLA	C3B-C4B-NB	11.42	121.11	110.52
10	A	933	CLA	C2B-C1B-NB	11.37	117.85	110.23
9	a	908	BCL	CBA-CAA-C2A	-11.23	80.73	113.86
9	a	905	BCL	C2B-C1B-NB	10.90	117.54	110.23
9	a	906	BCL	C2B-C1B-NB	10.89	117.53	110.23
9	a	907	BCL	C1C-NC-C4C	-10.88	101.81	106.71
9	a	909	BCL	O2D-CGD-O1D	-10.83	102.67	123.84
9	A	909	BCL	O2A-CGA-CBA	10.82	145.86	111.91
10	A	933	CLA	O2D-CGD-CBD	10.70	130.28	111.27
10	A	931	CLA	C2D-C1D-ND	-10.69	102.22	110.10
9	A	905	BCL	C2B-C1B-NB	10.63	117.36	110.23
9	a	910	BCL	O2A-CGA-CBA	10.58	145.11	111.91
10	A	933	CLA	O2D-CGD-O1D	-10.54	103.23	123.84
9	a	905	BCL	O2D-CGD-O1D	-10.51	103.29	123.84
10	a	914	CLA	C2B-C1B-NB	10.48	117.26	110.23
11	c	201	LYC	C21-C20-C19	10.48	144.93	123.47
10	a	901	CLA	O2D-CGD-CBD	10.45	129.83	111.27
10	a	915	CLA	O2D-CGD-CBD	10.31	129.58	111.27
11	c	201	LYC	C20-C19-C17	10.30	142.00	127.31
9	A	907	BCL	O2D-CGD-O1D	-10.19	103.91	123.84
13	a	920	85I	O4-C4-C3	10.17	135.66	109.54
15	A	932	85N	C18-O3-C17	10.17	133.50	113.80
9	A	909	BCL	C2B-C1B-NB	10.15	117.04	110.23
9	A	909	BCL	O1D-CGD-CBD	-10.14	103.74	124.48
13	A	917	85I	P-O3-C3	10.14	161.99	120.90
10	A	910	CLA	CED-O2D-CGD	10.13	138.85	115.94
9	A	908	BCL	O2D-CGD-CBD	10.08	129.19	111.27
16	C	301	HEC	C4C-NC-C1C	10.07	115.21	105.35
10	a	914	CLA	O2D-CGD-CBD	10.06	129.14	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	909	BCL	C4A-NA-C1A	9.83	111.12	106.71
10	a	901	CLA	C2B-C1B-NB	9.75	116.77	110.23
9	a	908	BCL	O2D-CGD-O1D	-9.73	104.82	123.84
9	a	910	BCL	O2A-CGA-O1A	-9.72	99.07	123.59
10	A	931	CLA	CED-O2D-CGD	9.66	137.79	115.94
9	A	906	BCL	C4A-NA-C1A	9.66	111.05	106.71
10	A	912	CLA	C3C-C4C-NC	9.59	121.32	110.57
9	A	907	BCL	C6-C5-C3	9.59	138.59	113.45
13	A	916	85I	O4-C4-C3	9.56	134.07	109.54
13	a	918	85I	O4-C4-C3	9.53	134.00	109.54
9	A	902	BCL	C2B-C1B-NB	9.51	116.61	110.23
9	a	904	BCL	C4A-NA-C1A	9.50	110.98	106.71
9	a	906	BCL	CMD-C2D-C1D	9.36	141.21	124.71
9	A	905	BCL	O2D-CGD-O1D	-9.34	105.57	123.84
10	A	931	CLA	C3B-C2B-C1B	-9.34	95.89	107.16
10	A	931	CLA	C1D-ND-C4D	9.32	112.95	106.33
9	A	907	BCL	O2A-CGA-CBA	9.32	141.15	111.91
9	a	905	BCL	CHD-C1D-ND	-9.28	115.93	124.45
9	a	904	BCL	O2D-CGD-O1D	-9.27	105.71	123.84
9	a	909	BCL	CHD-C1D-ND	-9.14	116.05	124.45
9	a	910	BCL	O2A-C1-C2	9.13	132.64	108.64
9	A	905	BCL	CHD-C1D-ND	-9.08	116.11	124.45
10	A	911	CLA	C3C-C4C-NC	9.06	120.74	110.57
9	A	906	BCL	C3D-C2D-C1D	-9.03	93.51	105.83
11	c	201	LYC	C13-C12-C14	-9.03	110.27	122.92
9	a	908	BCL	C1-C2-C3	9.02	141.64	126.04
10	A	933	CLA	C4-C3-C5	9.02	126.29	115.98
10	a	912	CLA	O2D-CGD-O1D	-9.00	106.25	123.84
9	a	911	BCL	C3D-C2D-C1D	-8.94	93.63	105.83
9	a	909	BCL	C1-C2-C3	8.90	141.43	126.04
10	a	901	CLA	C3C-C4C-NC	8.89	120.54	110.57
9	A	907	BCL	C3D-C2D-C1D	-8.78	93.85	105.83
9	a	904	BCL	CHD-C1D-ND	-8.75	116.41	124.45
9	A	903	BCL	O2A-CGA-CBA	8.74	139.34	111.91
10	A	911	CLA	C2C-C1C-NC	8.69	118.11	109.97
9	A	906	BCL	C1D-ND-C4D	-8.63	100.20	106.33
9	A	905	BCL	C2D-C1D-ND	8.61	116.45	110.10
9	A	903	BCL	CMD-C2D-C1D	8.56	139.79	124.71
16	c	202	HEC	CAC-C3C-C4C	-8.54	113.06	124.92
16	C	301	HEC	C1C-C2C-C3C	-8.53	96.85	106.83
9	a	910	BCL	C1-O2A-CGA	8.53	138.83	116.44
9	A	902	BCL	C1-O2A-CGA	8.50	138.74	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	931	CLA	C2B-C1B-NB	8.48	115.92	110.23
10	a	901	CLA	C1D-ND-C4D	-8.45	100.33	106.33
13	A	915	85I	O6-C3-C4	-8.41	75.45	107.08
10	A	933	CLA	C3B-C2B-C1B	-8.39	97.03	107.16
9	a	907	BCL	C2B-C1B-NB	8.37	115.84	110.23
9	A	907	BCL	C1C-NC-C4C	-8.34	102.96	106.71
9	A	907	BCL	C7-C6-C5	8.33	135.99	113.36
9	A	907	BCL	C2D-C1D-ND	8.30	116.22	110.10
9	A	904	BCL	C1C-NC-C4C	-8.28	102.98	106.71
9	A	909	BCL	O2D-CGD-O1D	-8.27	107.67	123.84
8	A	901	2GO	C1A-NA-C4A	8.25	120.03	106.96
9	A	905	BCL	CMD-C2D-C1D	8.24	139.23	124.71
9	a	911	BCL	C2B-C1B-NB	8.23	115.75	110.23
10	A	933	CLA	CED-O2D-CGD	8.23	134.56	115.94
16	c	202	HEC	C1C-C2C-C3C	-8.23	97.21	106.83
10	a	901	CLA	O2A-CGA-CBA	8.20	137.65	111.91
9	a	905	BCL	O2A-CGA-CBA	8.19	137.62	111.91
9	a	910	BCL	O2D-CGD-O1D	-8.19	107.83	123.84
13	A	915	85I	P-O3-C3	8.16	153.97	120.90
9	A	905	BCL	C3D-C2D-C1D	-8.15	94.71	105.83
9	A	903	BCL	O2A-C1-C2	8.13	130.00	108.64
9	a	908	BCL	C2B-C1B-NB	8.12	115.68	110.23
13	A	915	85I	O4-C4-C3	8.12	130.39	109.54
9	a	909	BCL	O2A-C1-C2	-8.11	87.32	108.64
10	A	912	CLA	C2B-C1B-NB	8.10	115.66	110.23
13	a	919	85I	O3-C3-C4	8.08	137.46	107.08
10	A	931	CLA	CMC-C2C-C1C	8.00	137.22	125.04
10	A	933	CLA	CMB-C2B-C1B	7.99	137.53	125.37
9	A	907	BCL	CMD-C2D-C1D	7.97	138.76	124.71
16	c	202	HEC	C1D-ND-C4D	7.96	113.30	105.07
9	a	911	BCL	O2A-C1-C2	7.96	129.56	108.64
10	a	901	CLA	C6-C7-C8	7.96	141.65	115.92
9	a	909	BCL	CMD-C2D-C1D	7.96	138.74	124.71
10	A	912	CLA	C3B-C2B-C1B	-7.95	97.56	107.16
9	a	911	BCL	C1-C2-C3	7.94	139.77	126.04
9	A	903	BCL	CHD-C1D-ND	-7.91	117.19	124.45
9	a	908	BCL	OBB-CAB-CBB	-7.89	102.23	119.73
10	a	913	CLA	CMD-C2D-C1D	7.87	138.59	124.71
10	a	915	CLA	O2D-CGD-O1D	-7.83	108.53	123.84
10	A	931	CLA	C4A-NA-C1A	7.83	110.22	106.71
11	c	201	LYC	C16-C17-C19	7.82	130.94	118.94
9	A	904	BCL	CMD-C2D-C1D	7.82	138.49	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	914	CLA	O2D-CGD-O1D	-7.81	108.56	123.84
9	a	909	BCL	O2A-CGA-O1A	-7.74	104.05	123.59
11	c	201	LYC	C52-C51-C50	-7.74	112.08	122.92
9	a	910	BCL	C4A-NA-C1A	-7.72	103.24	106.71
9	a	908	BCL	CHD-C1D-ND	-7.70	117.38	124.45
10	A	910	CLA	C2C-C1C-NC	7.67	117.16	109.97
9	a	911	BCL	C1-O2A-CGA	7.67	136.56	116.44
9	a	905	BCL	CMD-C2D-C1D	7.64	138.18	124.71
13	a	920	85I	O6-C3-C4	7.61	135.72	107.08
10	A	911	CLA	C4A-NA-C1A	7.59	110.12	106.71
10	A	933	CLA	C4A-NA-C1A	7.59	110.12	106.71
9	a	906	BCL	CHD-C1D-ND	-7.56	117.50	124.45
9	A	909	BCL	C4A-NA-C1A	-7.51	103.33	106.71
9	a	908	BCL	C3A-C2A-C1A	7.50	112.57	101.34
9	A	907	BCL	C1-O2A-CGA	7.42	135.92	116.44
10	a	912	CLA	C1D-ND-C4D	-7.38	101.09	106.33
10	a	901	CLA	C2C-C1C-NC	7.36	116.87	109.97
9	A	905	BCL	C4A-NA-C1A	7.36	110.02	106.71
9	a	905	BCL	C3D-C2D-C1D	-7.36	95.79	105.83
8	A	901	2GO	C4C-NC-C1C	7.32	115.77	107.00
16	C	301	HEC	C3C-C4C-NC	-7.30	101.98	110.15
11	c	201	LYC	C15-C16-C17	7.29	146.91	126.42
10	a	901	CLA	C11-C10-C8	-7.27	92.43	115.92
9	A	905	BCL	CBA-CAA-C2A	-7.26	92.43	113.86
9	a	909	BCL	C2B-C1B-NB	7.22	115.07	110.23
9	A	907	BCL	CED-O2D-CGD	7.21	132.24	115.94
10	A	912	CLA	C1C-C2C-C3C	-7.17	99.42	106.96
9	a	910	BCL	C1-C2-C3	-7.17	113.65	126.04
10	a	913	CLA	C11-C10-C8	-7.16	92.78	115.92
10	a	912	CLA	O2D-CGD-CBD	7.15	123.97	111.27
16	c	202	HEC	O2A-CGA-O1A	-7.15	105.48	123.30
9	a	911	BCL	O2A-CGA-CBA	7.15	134.34	111.91
9	a	908	BCL	C3D-C2D-C1D	-7.14	96.09	105.83
13	a	919	85I	P-O3-C3	7.13	149.82	120.90
10	A	912	CLA	O2D-CGD-O1D	-7.12	109.92	123.84
9	a	907	BCL	C1-C2-C3	-7.12	113.74	126.04
10	a	912	CLA	CHB-C1B-NB	-7.08	116.76	124.26
9	A	907	BCL	C1-C2-C3	7.08	138.29	126.04
10	a	912	CLA	CMD-C2D-C1D	7.07	137.18	124.71
10	A	912	CLA	C1D-ND-C4D	-7.04	101.33	106.33
9	a	906	BCL	C3D-C2D-C1D	-7.01	96.27	105.83
9	A	909	BCL	C3D-C2D-C1D	-7.00	96.28	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	911	CLA	CMD-C2D-C1D	6.99	137.03	124.71
9	A	908	BCL	CHD-C1D-ND	-6.99	118.03	124.45
10	A	931	CLA	C1-O2A-CGA	6.97	134.72	116.44
17	E	101	84Q	O1-C15-C16	6.93	127.33	109.54
10	a	914	CLA	C3C-C4C-NC	6.89	118.30	110.57
9	A	903	BCL	C1-O2A-CGA	6.87	134.47	116.44
10	a	913	CLA	C3D-C2D-C1D	-6.86	96.47	105.83
16	c	202	HEC	C1B-C2B-C3B	-6.85	99.76	106.96
10	A	911	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
10	a	901	CLA	CMD-C2D-C1D	6.84	136.77	124.71
9	A	903	BCL	O1A-CGA-CBA	-6.84	97.06	123.73
9	A	905	BCL	C3A-C2A-C1A	6.77	111.48	101.34
9	A	902	BCL	O2D-CGD-O1D	-6.77	110.61	123.84
10	A	931	CLA	CHD-C4C-C3C	-6.76	114.90	124.84
11	c	201	LYC	C18-C17-C16	-6.75	107.44	118.08
9	a	911	BCL	CED-O2D-CGD	6.74	131.18	115.94
9	a	904	BCL	O2A-CGA-CBA	6.73	133.03	111.91
9	a	911	BCL	CHD-C1D-ND	-6.73	118.27	124.45
10	A	933	CLA	CHB-C1B-NB	-6.71	117.15	124.26
10	a	915	CLA	C4-C3-C5	6.68	123.62	115.98
9	a	908	BCL	CMD-C2D-C1D	6.64	136.41	124.71
9	A	904	BCL	C3D-C2D-C1D	-6.64	96.77	105.83
10	a	912	CLA	C3B-C4B-NB	6.56	116.60	110.52
10	a	913	CLA	C3B-C2B-C1B	-6.55	99.26	107.16
10	A	912	CLA	O2D-CGD-CBD	6.54	122.90	111.27
10	A	911	CLA	C3D-C2D-C1D	-6.54	96.90	105.83
10	A	910	CLA	C3B-C2B-C1B	-6.52	99.29	107.16
10	A	933	CLA	C3B-C4B-NB	6.49	116.53	110.52
10	A	912	CLA	CAC-C3C-C4C	6.47	133.21	124.81
9	a	907	BCL	O2D-CGD-O1D	-6.47	111.19	123.84
10	a	914	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
9	a	911	BCL	CMD-C2D-C1D	6.46	136.09	124.71
9	a	907	BCL	CBA-CAA-C2A	-6.45	94.82	113.86
9	A	907	BCL	CHD-C1D-ND	-6.44	118.54	124.45
9	a	904	BCL	CED-O2D-CGD	6.43	130.48	115.94
9	A	905	BCL	C1D-ND-C4D	-6.43	101.77	106.33
9	A	909	BCL	C4-C3-C5	-6.42	104.46	115.27
10	A	910	CLA	CMD-C2D-C1D	6.42	136.03	124.71
10	a	912	CLA	C2C-C1C-NC	6.42	115.98	109.97
9	A	902	BCL	C4A-NA-C1A	6.41	109.59	106.71
11	A	913	LYC	C18-C17-C19	-6.41	113.95	122.92
9	A	903	BCL	C4A-NA-C1A	6.40	109.58	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	905	BCL	C4A-NA-C1A	6.39	109.58	106.71
10	a	912	CLA	C3B-C2B-C1B	-6.38	99.46	107.16
11	c	201	LYC	C11-C12-C14	6.36	128.71	118.94
9	a	905	BCL	CHD-C4C-NC	6.33	132.11	125.08
16	c	202	HEC	C4A-NA-C1A	6.33	111.55	105.35
10	a	915	CLA	C4A-NA-C1A	-6.32	103.87	106.71
10	A	912	CLA	CMA-C3A-C4A	6.31	128.73	111.77
11	c	201	LYC	C52-C51-C53	-6.29	108.16	118.08
11	c	201	LYC	C20-C21-C50	-6.29	110.60	123.47
10	A	931	CLA	C2C-C1C-NC	6.29	115.86	109.97
10	a	915	CLA	CMB-C2B-C1B	6.27	134.91	125.37
10	a	912	CLA	O2A-CGA-CBA	6.26	131.54	111.91
16	C	301	HEC	C1D-C2D-C3D	-6.26	100.38	106.96
9	a	908	BCL	OBB-CAB-C3B	6.25	131.98	120.41
9	A	902	BCL	CHD-C1D-ND	-6.25	118.71	124.45
10	A	910	CLA	C1D-ND-C4D	-6.25	101.90	106.33
9	a	905	BCL	C4-C3-C2	-6.25	107.66	123.68
10	A	933	CLA	C3D-C2D-C1D	-6.24	97.32	105.83
9	A	903	BCL	C2B-C1B-NB	6.24	114.41	110.23
10	a	915	CLA	CMD-C2D-C1D	6.23	135.70	124.71
9	A	905	BCL	CAA-C2A-C3A	-6.23	95.72	112.78
9	A	907	BCL	O1A-CGA-CBA	-6.22	99.46	123.73
10	a	913	CLA	CAC-C3C-C4C	6.22	132.88	124.81
9	a	911	BCL	O2D-CGD-CBD	6.17	122.24	111.27
9	a	911	BCL	C1C-NC-C4C	6.17	109.48	106.71
9	a	905	BCL	CMB-C2B-C1B	6.16	134.76	125.37
10	a	915	CLA	C3C-C4C-NC	6.15	117.47	110.57
9	a	904	BCL	CHD-C4C-NC	6.15	131.90	125.08
9	a	907	BCL	C16-C15-C13	-6.13	96.12	115.92
10	a	901	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
10	A	911	CLA	C4C-C3C-C2C	-6.10	98.01	106.90
9	a	910	BCL	CMD-C2D-C1D	6.09	135.45	124.71
8	a	903	2GO	CGD-CBD-CAD	6.08	130.43	110.73
10	a	912	CLA	CMB-C2B-C1B	6.06	134.60	125.37
10	A	910	CLA	C3C-C4C-NC	6.05	117.35	110.57
8	a	903	2GO	C1A-NA-C4A	6.03	116.52	106.96
9	a	904	BCL	CMD-C2D-C1D	6.03	135.34	124.71
9	A	909	BCL	CHC-C4B-NB	-6.03	117.87	124.26
8	a	903	2GO	C16-C15-C13	6.03	135.41	115.92
9	A	904	BCL	CMB-C2B-C1B	6.00	134.50	125.37
9	A	902	BCL	CMD-C2D-C1D	5.97	135.23	124.71
9	a	907	BCL	CMD-C2D-C1D	5.96	135.22	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	901	CLA	O2D-CGD-O1D	-5.96	112.19	123.84
9	A	903	BCL	CBB-CAB-C3B	5.94	133.12	120.43
9	a	909	BCL	C4-C3-C2	-5.89	108.56	123.68
9	A	907	BCL	C4-C3-C2	-5.89	108.57	123.68
10	a	901	CLA	CHD-C1D-ND	-5.89	119.04	124.45
9	A	906	BCL	OBB-CAB-C3B	5.88	131.29	120.41
9	a	908	BCL	C2A-C3A-C4A	-5.88	92.37	101.87
16	C	301	HEC	C2D-C1D-ND	5.88	116.80	109.84
9	A	909	BCL	C1C-NC-C4C	5.86	109.34	106.71
10	A	911	CLA	C3B-C2B-C1B	-5.85	100.10	107.16
9	A	909	BCL	CMD-C2D-C1D	5.85	135.02	124.71
9	A	906	BCL	CED-O2D-CGD	5.85	129.16	115.94
8	A	901	2GO	C2B-C1B-NB	-5.85	101.59	109.02
9	A	906	BCL	O2A-CGA-O1A	-5.84	108.85	123.59
10	A	933	CLA	O2A-C1-C2	-5.82	93.34	108.64
9	a	909	BCL	C1-O2A-CGA	5.81	131.68	116.44
11	A	913	LYC	C57-C56-C55	5.79	131.03	122.92
10	a	915	CLA	O2A-CGA-O1A	-5.78	109.00	123.59
9	a	910	BCL	CED-O2D-CGD	5.78	129.01	115.94
9	a	906	BCL	CAC-C3C-C4C	-5.78	99.76	112.58
10	A	931	CLA	O2A-CGA-CBA	5.78	130.03	111.91
9	a	904	BCL	C3C-C4C-CHD	-5.77	111.06	123.39
9	a	908	BCL	C5-C3-C2	5.76	132.77	121.12
9	a	904	BCL	C2B-C1B-NB	5.75	114.09	110.23
8	A	901	2GO	C4D-ND-C1D	5.73	116.82	106.69
9	A	909	BCL	O2A-CGA-O1A	-5.72	109.16	123.59
10	a	912	CLA	CED-O2D-CGD	5.72	128.87	115.94
10	A	910	CLA	C2B-C1B-NB	5.70	114.05	110.23
9	a	905	BCL	CED-O2D-CGD	5.70	128.82	115.94
9	A	904	BCL	CHD-C1D-ND	-5.68	119.23	124.45
10	a	912	CLA	C3C-C4C-NC	5.67	116.93	110.57
10	a	915	CLA	C3D-C2D-C1D	-5.66	98.10	105.83
10	A	933	CLA	C2C-C1C-NC	5.65	115.27	109.97
16	C	301	HEC	C4B-NB-C1B	5.65	110.91	105.07
9	a	909	BCL	C3D-C2D-C1D	-5.59	98.20	105.83
9	a	908	BCL	C2D-C1D-ND	5.58	114.21	110.10
11	c	201	LYC	C1-C2-C4	-5.58	106.53	122.65
9	a	907	BCL	CHC-C4B-NB	-5.58	118.36	124.26
9	A	902	BCL	C3C-C4C-CHD	-5.56	111.51	123.39
10	a	901	CLA	C4C-C3C-C2C	-5.55	98.81	106.90
10	a	914	CLA	C2C-C1C-NC	5.55	115.17	109.97
16	C	301	HEC	CAD-C3D-C4D	5.54	134.35	124.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	902	BCL	CHD-C4C-NC	5.53	131.22	125.08
10	A	912	CLA	C4A-NA-C1A	5.53	109.19	106.71
9	A	904	BCL	C4A-NA-C1A	5.52	109.19	106.71
10	a	914	CLA	CED-O2D-CGD	5.52	128.42	115.94
9	a	906	BCL	C1C-NC-C4C	-5.51	104.23	106.71
10	a	915	CLA	CMC-C2C-C1C	5.51	133.43	125.04
10	a	914	CLA	CHD-C1D-ND	-5.50	119.40	124.45
9	A	909	BCL	C9-C8-C10	-5.49	91.41	111.29
8	A	901	2GO	C3B-C4B-NB	-5.49	102.53	109.62
9	A	905	BCL	CAA-C2A-C1A	-5.46	94.08	111.97
9	A	907	BCL	C2B-C1B-NB	5.45	113.89	110.23
9	A	905	BCL	C1C-NC-C4C	5.45	109.15	106.71
9	a	905	BCL	C1-C2-C3	5.44	135.46	126.04
9	a	907	BCL	CHB-C1B-NB	-5.43	118.51	124.26
10	A	910	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
9	a	904	BCL	C1-C2-C3	-5.41	116.68	126.04
13	a	920	85I	P-O3-C3	-5.41	98.98	120.90
10	a	913	CLA	C2D-C1D-ND	5.39	114.08	110.10
16	C	301	HEC	C4A-C3A-C2A	-5.39	99.07	106.94
16	C	301	HEC	CHD-C1D-ND	-5.38	117.74	124.37
10	a	901	CLA	C3B-C2B-C1B	-5.38	100.67	107.16
10	A	911	CLA	O2D-CGD-O1D	-5.37	113.34	123.84
17	E	101	84Q	P-O4-C16	5.35	142.59	120.90
9	a	908	BCL	CAA-C2A-C1A	-5.33	94.50	111.97
9	a	904	BCL	CHC-C4B-NB	-5.32	118.62	124.26
11	c	201	LYC	C3-C2-C4	5.32	138.03	122.65
10	a	915	CLA	C3B-C4B-NB	5.32	115.45	110.52
10	a	914	CLA	CBA-CAA-C2A	-5.31	98.19	113.86
9	a	909	BCL	CED-O2D-CGD	5.30	127.92	115.94
8	A	901	2GO	C2D-C1D-ND	-5.28	101.77	110.37
9	a	906	BCL	C3C-C4C-CHD	-5.28	112.12	123.39
16	c	202	HEC	O2A-CGA-CBA	5.26	130.95	114.03
9	a	908	BCL	CED-O2D-CGD	5.25	127.82	115.94
13	A	916	85I	P-O3-C3	5.24	142.14	120.90
9	a	904	BCL	C3D-C2D-C1D	-5.23	98.69	105.83
9	A	904	BCL	C3C-C4C-CHD	-5.23	112.23	123.39
9	a	910	BCL	C5-C3-C2	5.22	131.68	121.12
10	a	913	CLA	C3C-C4C-NC	5.21	116.42	110.57
9	A	906	BCL	C1-O2A-CGA	5.21	130.12	116.44
8	A	901	2GO	C1B-NB-C4B	5.21	114.61	106.52
9	a	905	BCL	CHB-C1B-NB	-5.20	118.76	124.26
11	c	201	LYC	C8-C7-C9	-5.19	109.19	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	903	BCL	CBA-CAA-C2A	5.19	129.19	113.86
10	A	911	CLA	O2A-CGA-CBA	5.19	128.19	111.91
9	a	905	BCL	C5-C3-C2	5.19	131.61	121.12
8	A	901	2GO	C2A-C1A-CHA	5.18	132.92	123.86
10	a	901	CLA	CMB-C2B-C1B	5.17	133.25	125.37
9	a	906	BCL	CHC-C4B-NB	-5.17	118.78	124.26
10	a	915	CLA	O2A-CGA-CBA	5.17	128.14	111.91
9	A	908	BCL	C3D-C2D-C1D	-5.17	98.77	105.83
9	a	909	BCL	C5-C3-C2	5.14	131.52	121.12
9	A	905	BCL	CMA-C3A-C4A	5.14	125.59	111.77
10	a	901	CLA	C3D-C4D-ND	5.13	118.53	110.24
16	c	202	HEC	C1D-C2D-C3D	-5.13	101.57	106.96
9	A	903	BCL	C3C-C4C-CHD	-5.12	112.45	123.39
9	a	907	BCL	CHD-C1D-ND	-5.11	119.76	124.45
9	a	909	BCL	O2A-CGA-CBA	5.11	127.93	111.91
9	a	906	BCL	O2D-CGD-O1D	-5.11	113.86	123.84
8	A	901	2GO	C1-O2A-CGA	5.09	129.81	116.44
9	A	908	BCL	CAA-C2A-C3A	-5.08	98.86	112.78
9	A	906	BCL	CMD-C2D-C1D	5.07	133.65	124.71
9	A	902	BCL	O2A-CGA-CBA	5.05	127.75	111.91
9	a	905	BCL	C3C-C4C-CHD	-5.05	112.61	123.39
9	a	906	BCL	C4A-NA-C1A	5.04	108.97	106.71
9	a	907	BCL	C1D-ND-C4D	5.02	109.90	106.33
10	A	911	CLA	CAC-C3C-C4C	5.00	131.30	124.81
11	A	913	LYC	C13-C12-C11	4.99	125.94	118.08
11	c	201	LYC	C14-C15-C16	-4.99	107.65	123.22
8	A	901	2GO	C2A-C1A-NA	-4.97	105.20	110.99
10	A	931	CLA	CHD-C4C-NC	4.97	132.04	124.20
9	A	903	BCL	C3D-C2D-C1D	-4.96	99.06	105.83
10	A	910	CLA	CHD-C1D-ND	-4.96	119.90	124.45
9	a	911	BCL	C4A-NA-C1A	4.91	108.91	106.71
8	a	903	2GO	C3B-C4B-NB	-4.90	103.28	109.62
9	A	902	BCL	CED-O2D-CGD	4.89	127.00	115.94
10	A	931	CLA	C1C-C2C-C3C	-4.89	101.82	106.96
17	a	921	84Q	O1-C15-C16	4.87	122.05	109.54
10	a	913	CLA	CHD-C4C-C3C	-4.86	117.70	124.84
11	c	201	LYC	C5-C4-C2	4.85	144.34	127.75
10	a	913	CLA	O2A-CGA-CBA	4.85	127.14	111.91
9	A	905	BCL	CHC-C4B-NB	-4.85	119.12	124.26
10	a	915	CLA	CAC-C3C-C4C	4.85	131.10	124.81
10	A	911	CLA	CHC-C4B-NB	4.85	129.39	124.26
10	a	901	CLA	CHC-C4B-NB	-4.84	119.13	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	908	BCL	CAA-C2A-C3A	-4.83	99.54	112.78
10	A	933	CLA	CAC-C3C-C4C	4.83	131.08	124.81
9	A	904	BCL	O2D-CGD-CBD	4.83	119.85	111.27
9	A	909	BCL	O1A-CGA-CBA	-4.82	104.94	123.73
9	A	904	BCL	CED-O2D-CGD	4.81	126.81	115.94
9	a	904	BCL	C1-O2A-CGA	4.81	129.06	116.44
10	A	933	CLA	CMC-C2C-C1C	4.80	132.36	125.04
10	a	914	CLA	C4C-C3C-C2C	-4.80	99.90	106.90
10	a	901	CLA	C3D-C2D-C1D	-4.79	99.30	105.83
8	a	903	2GO	C4D-C3D-CAD	-4.77	102.47	108.10
11	c	201	LYC	C57-C56-C55	-4.77	116.25	122.92
16	c	202	HEC	O2D-CGD-O1D	-4.75	111.45	123.30
9	a	911	BCL	OBB-CAB-C3B	-4.75	111.61	120.41
9	a	907	BCL	O2A-CGA-CBA	4.75	126.82	111.91
10	A	912	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
16	C	301	HEC	C4C-C3C-C2C	4.75	114.36	106.89
15	A	932	85N	O3-C17-O6	4.75	124.05	110.72
17	E	101	84Q	O4-C16-C15	4.75	124.94	107.08
16	c	202	HEC	C1A-CHA-C4D	4.75	136.29	126.06
11	c	201	LYC	C10-C11-C12	4.74	139.73	126.42
9	A	908	BCL	C2D-C1D-ND	4.73	113.59	110.10
10	a	913	CLA	C3D-C4D-ND	4.73	117.89	110.24
9	A	905	BCL	C3C-C4C-CHD	-4.73	113.29	123.39
10	a	913	CLA	CHD-C1D-ND	-4.72	120.11	124.45
8	a	903	2GO	C2B-C1B-NB	-4.72	103.02	109.02
10	A	910	CLA	C9-C8-C7	4.72	128.37	111.29
9	a	910	BCL	CMB-C2B-C1B	4.70	132.53	125.37
9	A	908	BCL	CMD-C2D-C1D	4.70	133.00	124.71
9	A	909	BCL	CHD-C1D-ND	-4.70	120.13	124.45
10	A	910	CLA	C1-O2A-CGA	4.69	128.75	116.44
10	A	933	CLA	C1-O2A-CGA	4.69	128.75	116.44
16	C	301	HEC	C2A-C1A-NA	4.69	114.89	110.32
9	A	904	BCL	CBC-CAC-C3C	4.69	123.90	113.47
9	A	903	BCL	OBB-CAB-CBB	-4.68	109.36	119.73
10	a	913	CLA	C1-O2A-CGA	4.67	128.71	116.44
16	C	301	HEC	CHA-C1A-NA	-4.67	119.39	124.44
16	c	202	HEC	CMC-C2C-C3C	4.66	135.69	125.61
9	A	902	BCL	CBC-CAC-C3C	4.66	123.84	113.47
16	c	202	HEC	CHA-C1A-NA	-4.66	119.40	124.44
10	a	915	CLA	C2B-C1B-NB	4.65	113.35	110.23
10	A	912	CLA	CMD-C2D-C1D	4.64	132.89	124.71
9	a	904	BCL	C1D-ND-C4D	-4.64	103.04	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	907	BCL	CED-O2D-CGD	4.63	126.41	115.94
9	a	908	BCL	CHD-C4C-NC	4.63	130.22	125.08
9	A	908	BCL	C1-C2-C3	-4.62	118.06	126.04
17	a	921	84Q	O4-C16-C15	4.61	124.44	107.08
9	a	905	BCL	OBB-CAB-CBB	-4.61	109.52	119.73
16	C	301	HEC	O2A-CGA-O1A	-4.60	111.84	123.30
10	A	912	CLA	CED-O2D-CGD	4.60	126.33	115.94
9	A	907	BCL	C4-C3-C5	4.58	122.97	115.27
9	A	908	BCL	O2A-CGA-CBA	4.58	126.27	111.91
9	A	909	BCL	OBB-CAB-C3B	-4.57	111.95	120.41
10	a	912	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
9	A	909	BCL	C1-O2A-CGA	4.55	128.39	116.44
10	a	912	CLA	O2A-CGA-O1A	-4.55	112.11	123.59
11	A	913	LYC	C8-C7-C6	4.55	122.92	115.27
10	a	915	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
9	A	905	BCL	CED-O2D-CGD	4.53	126.19	115.94
10	A	931	CLA	O1D-CGD-CBD	-4.53	115.21	124.48
9	a	905	BCL	O1A-CGA-CBA	-4.53	106.06	123.73
10	A	933	CLA	O2A-CGA-O1A	-4.52	112.19	123.59
9	A	902	BCL	CAA-CBA-CGA	-4.51	100.07	113.25
9	A	908	BCL	O1D-CGD-CBD	-4.50	115.28	124.48
10	A	911	CLA	O2A-CGA-O1A	-4.49	112.25	123.59
13	a	918	85I	P-O3-C3	4.49	139.10	120.90
16	c	202	HEC	CHA-C4D-C3D	4.48	131.43	124.84
9	a	908	BCL	CHC-C4B-NB	-4.48	119.52	124.26
9	A	904	BCL	CAC-C3C-C2C	4.46	125.40	114.26
10	A	931	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
10	A	931	CLA	C3D-C4D-ND	-4.44	103.06	110.24
10	a	915	CLA	CED-O2D-CGD	4.43	125.97	115.94
9	A	903	BCL	C1-C2-C3	4.43	133.70	126.04
16	C	301	HEC	C1B-C2B-C3B	-4.42	102.31	106.96
9	A	905	BCL	CAB-C3B-C2B	-4.42	121.71	128.34
9	a	906	BCL	CAA-C2A-C1A	-4.41	97.51	111.97
10	A	910	CLA	CMC-C2C-C1C	4.41	131.76	125.04
9	a	909	BCL	C2D-C1D-ND	4.41	113.36	110.10
10	A	933	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
11	A	913	LYC	C13-C12-C14	-4.40	116.76	122.92
10	a	913	CLA	C2A-C1A-CHA	-4.39	116.19	123.86
8	A	901	2GO	CGD-CBD-CAD	4.38	124.91	110.73
10	A	912	CLA	C3D-C4D-ND	4.37	117.31	110.24
10	a	913	CLA	C4C-C3C-C2C	-4.36	100.54	106.90
10	a	912	CLA	C3D-C4D-ND	4.36	117.30	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	909	BCL	CAA-C2A-C1A	4.36	126.27	111.97
10	a	914	CLA	O2A-CGA-CBA	4.36	129.47	112.23
10	A	931	CLA	C4D-C3D-CAD	-4.35	102.97	108.10
9	a	904	BCL	CHB-C1B-NB	-4.31	119.70	124.26
16	C	301	HEC	C4C-CHD-C1D	4.30	136.53	126.34
9	A	908	BCL	O2D-CGD-O1D	-4.29	115.46	123.84
10	A	910	CLA	O2A-CGA-O1A	-4.28	112.80	123.59
9	a	904	BCL	O1A-CGA-CBA	-4.28	107.05	123.73
9	A	907	BCL	O2A-C1-C2	4.27	119.85	108.64
10	a	915	CLA	C4C-C3C-C2C	-4.26	100.68	106.90
10	a	914	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
9	a	906	BCL	OBB-CAB-CBB	-4.26	110.30	119.73
10	A	931	CLA	C4D-CHA-C1A	-4.25	116.08	121.25
10	a	914	CLA	CHC-C4B-NB	-4.25	119.76	124.26
10	A	912	CLA	C4C-C3C-C2C	-4.25	100.70	106.90
10	A	911	CLA	O2D-CGD-CBD	4.24	118.80	111.27
10	a	914	CLA	CHB-C1B-NB	-4.23	119.78	124.26
16	c	202	HEC	CAC-C3C-C2C	4.23	133.63	126.86
9	A	902	BCL	O1D-CGD-CBD	-4.22	115.85	124.48
9	a	910	BCL	C2A-C1A-CHA	-4.22	116.49	123.86
10	a	914	CLA	CMC-C2C-C1C	4.21	131.45	125.04
10	A	912	CLA	CMB-C2B-C1B	4.21	131.78	125.37
10	A	910	CLA	CBA-CAA-C2A	4.21	126.29	113.86
9	a	910	BCL	CHD-C4C-NC	4.20	129.74	125.08
10	a	913	CLA	C2B-C1B-NB	4.20	113.05	110.23
10	A	933	CLA	CHD-C1D-ND	-4.19	120.61	124.45
9	a	910	BCL	OBB-CAB-CBB	-4.17	110.49	119.73
10	A	911	CLA	CHC-C1C-NC	-4.16	117.89	124.20
8	a	903	2GO	C3C-C4C-NC	4.15	115.93	111.10
8	a	903	2GO	C2C-C3C-C4C	-4.15	95.13	101.34
9	A	903	BCL	CED-O2D-CGD	4.14	125.31	115.94
10	A	910	CLA	C4A-NA-C1A	4.14	108.57	106.71
16	c	202	HEC	C3D-C4D-ND	-4.14	106.35	110.36
10	a	901	CLA	C9-C8-C7	4.13	126.26	111.29
10	a	913	CLA	C4-C3-C5	4.13	122.22	115.27
10	A	931	CLA	C4-C3-C5	4.13	122.22	115.27
9	A	908	BCL	C3C-C4C-CHD	-4.13	114.57	123.39
10	a	912	CLA	C6-C7-C8	-4.13	102.58	115.92
10	A	912	CLA	CMC-C2C-C1C	4.12	131.31	125.04
10	A	910	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
11	c	201	LYC	C9-C10-C11	4.11	136.06	123.22
8	a	903	2GO	C4D-ND-C1D	4.10	113.95	106.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	915	CLA	CHB-C4A-NA	4.10	130.18	124.51
10	a	901	CLA	O2A-CGA-O1A	-4.10	113.25	123.59
9	a	910	BCL	O1D-CGD-CBD	-4.09	116.11	124.48
10	a	913	CLA	CMC-C2C-C1C	4.09	131.26	125.04
10	a	913	CLA	CED-O2D-CGD	4.08	125.17	115.94
10	a	912	CLA	C4-C3-C2	-4.08	113.22	123.68
16	c	202	HEC	CAA-C2A-C1A	4.07	132.56	124.89
9	A	903	BCL	CHD-C4C-NC	4.06	129.59	125.08
9	a	907	BCL	CMC-C2C-C1C	4.06	122.67	111.77
9	a	904	BCL	CMC-C2C-C1C	4.05	122.66	111.77
9	a	911	BCL	O2D-CGD-O1D	-4.04	115.94	123.84
13	A	915	85I	O3-P-O1	4.04	124.61	109.47
9	a	907	BCL	C3C-C4C-CHD	-4.03	114.79	123.39
11	c	201	LYC	C57-C56-C58	4.03	124.42	118.08
9	A	905	BCL	CHD-C4C-NC	4.02	129.54	125.08
10	A	912	CLA	CHC-C1C-C2C	-4.01	115.58	126.73
9	A	906	BCL	O2A-CGA-CBA	4.01	124.48	111.91
9	A	907	BCL	CHB-C1B-NB	-4.01	120.02	124.26
9	a	907	BCL	O1D-CGD-CBD	-4.01	116.29	124.48
9	a	906	BCL	CED-O2D-CGD	4.00	124.99	115.94
13	A	916	85I	O2-P-O	-4.00	89.18	107.75
9	a	908	BCL	CAB-C3B-C2B	-3.99	122.37	128.34
10	A	931	CLA	CHC-C4B-NB	3.98	128.47	124.26
9	A	905	BCL	C1-O2A-CGA	3.98	126.89	116.44
9	A	905	BCL	O2A-C1-C2	3.98	119.09	108.64
9	a	907	BCL	C4-C3-C5	3.98	121.97	115.27
8	A	901	2GO	C2A-C3A-C4A	-3.97	95.45	101.87
9	a	911	BCL	CAB-C3B-C2B	-3.96	122.41	128.34
10	A	931	CLA	CMB-C2B-C1B	3.96	131.40	125.37
10	a	912	CLA	CAC-C3C-C4C	3.96	129.95	124.81
9	A	902	BCL	C9-C8-C10	-3.96	96.96	111.29
9	A	902	BCL	O2A-C1-C2	3.96	119.03	108.64
10	a	914	CLA	CAC-C3C-C4C	3.95	129.94	124.81
9	A	902	BCL	CMB-C2B-C1B	3.95	131.39	125.37
9	a	911	BCL	C1D-ND-C4D	-3.95	103.53	106.33
10	A	911	CLA	CHD-C1D-ND	-3.95	120.83	124.45
9	A	906	BCL	C1-C2-C3	-3.94	119.23	126.04
9	a	906	BCL	CMB-C2B-C1B	3.93	131.36	125.37
9	a	909	BCL	C6-C5-C3	-3.93	103.16	113.45
17	E	101	84Q	O2-C16-C15	-3.92	92.35	107.08
9	a	907	BCL	CBB-CAB-C3B	3.92	128.79	120.43
9	a	908	BCL	C3C-C4C-CHD	-3.91	115.03	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	909	BCL	CHC-C4B-NB	-3.91	120.12	124.26
15	A	932	85N	O3-C17-C16	3.91	122.01	107.06
16	C	301	HEC	CHD-C4C-C3C	3.91	133.89	125.36
10	A	912	CLA	CAA-CBA-CGA	3.90	124.65	113.25
8	A	901	2GO	CBB-CAB-C3B	3.88	128.72	120.43
9	A	905	BCL	O1D-CGD-CBD	-3.88	116.54	124.48
8	a	903	2GO	O2D-CGD-CBD	3.87	118.15	111.27
16	c	202	HEC	C4C-C3C-C2C	3.87	112.98	106.89
9	A	908	BCL	CAA-CBA-CGA	-3.87	101.95	113.25
10	a	912	CLA	C12-C11-C10	-3.85	95.53	113.24
10	A	910	CLA	CBC-CAC-C3C	-3.85	101.81	112.43
9	a	910	BCL	C4D-C3D-CAD	3.85	112.63	108.10
9	A	908	BCL	CHD-C4C-NC	3.84	129.34	125.08
10	a	912	CLA	C1-C2-C3	-3.83	119.41	126.04
10	a	901	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
9	a	906	BCL	CHB-C1B-NB	-3.83	120.20	124.26
9	A	907	BCL	C3C-C4C-CHD	-3.83	115.22	123.39
9	a	907	BCL	C1-O2A-CGA	3.82	126.47	116.44
10	a	915	CLA	C2D-C1D-ND	-3.82	107.29	110.10
10	a	912	CLA	CHD-C1D-ND	-3.82	120.95	124.45
9	a	910	BCL	CAA-C2A-C1A	3.81	124.46	111.97
10	a	913	CLA	C4D-CHA-C1A	-3.81	116.61	121.25
11	c	201	LYC	C6-C7-C9	3.79	133.46	121.98
10	a	901	CLA	O1A-CGA-CBA	-3.79	108.94	123.73
10	a	913	CLA	CMB-C2B-C1B	3.78	131.13	125.37
9	a	911	BCL	O1A-CGA-CBA	-3.78	109.00	123.73
9	A	904	BCL	O1A-CGA-CBA	-3.78	110.95	123.08
16	C	301	HEC	O2A-CGA-CBA	3.78	126.16	114.03
10	a	914	CLA	C1D-ND-C4D	-3.77	103.65	106.33
9	A	902	BCL	C11-C12-C13	3.77	128.10	115.92
10	A	933	CLA	C1D-ND-C4D	-3.76	103.66	106.33
9	A	907	BCL	OBB-CAB-C3B	3.76	127.37	120.41
9	a	907	BCL	CHB-C4A-NA	3.76	129.71	124.51
9	A	908	BCL	CHB-C1B-NB	-3.76	120.28	124.26
9	A	902	BCL	C14-C13-C12	3.75	124.89	111.29
10	a	912	CLA	C3D-C2D-C1D	-3.75	100.72	105.83
9	A	908	BCL	CAC-C3C-C4C	-3.74	104.28	112.58
10	A	911	CLA	C2B-C1B-NB	3.72	112.73	110.23
9	a	904	BCL	C3D-C4D-ND	3.71	116.25	110.24
9	a	906	BCL	CAA-CBA-CGA	-3.71	102.67	112.51
10	a	913	CLA	O2A-CGA-O1A	-3.71	114.24	123.59
10	a	915	CLA	C1-O2A-CGA	3.70	126.16	116.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	902	BCL	C3D-C2D-C1D	-3.70	100.78	105.83
9	a	904	BCL	C2D-C1D-ND	3.70	112.83	110.10
9	A	904	BCL	O2A-CGA-CBA	3.70	125.92	114.03
9	A	907	BCL	CAA-CBA-CGA	3.70	124.07	113.25
16	c	202	HEC	C2C-C1C-NC	3.70	115.71	110.08
9	A	907	BCL	C9-C8-C10	-3.69	97.93	111.29
10	A	911	CLA	CED-O2D-CGD	3.69	124.27	115.94
9	A	902	BCL	CHB-C1B-NB	-3.69	120.36	124.26
9	a	905	BCL	O2A-C1-C2	3.68	118.31	108.64
16	C	301	HEC	C3A-C4A-NA	3.68	116.48	109.69
10	a	901	CLA	CAC-C3C-C2C	3.67	133.81	127.53
9	A	902	BCL	C2A-C1A-CHA	-3.67	117.44	123.86
9	a	907	BCL	C3D-C2D-C1D	-3.67	100.83	105.83
13	a	918	85I	O3-C3-C4	3.66	120.84	107.08
9	a	908	BCL	C16-C17-C18	-3.66	98.75	115.98
10	A	911	CLA	C6-C7-C8	3.66	127.74	115.92
8	a	903	2GO	CAC-C3C-C2C	3.64	123.36	114.26
10	a	914	CLA	C3D-C4D-ND	3.64	116.13	110.24
10	a	913	CLA	C9-C8-C7	3.64	124.47	111.29
10	A	911	CLA	C1-O2A-CGA	3.63	125.98	116.44
9	A	903	BCL	C3A-C2A-C1A	3.62	106.77	101.34
10	A	910	CLA	C11-C10-C8	3.61	127.59	115.92
9	A	902	BCL	CMA-C3A-C2A	-3.61	99.27	113.83
9	A	903	BCL	C6-C7-C8	3.61	127.58	115.92
10	A	911	CLA	C2A-C1A-CHA	-3.61	117.55	123.86
9	A	907	BCL	C5-C3-C2	3.61	128.41	121.12
10	a	912	CLA	CHD-C4C-C3C	-3.61	119.54	124.84
10	A	933	CLA	C1-C2-C3	-3.60	119.81	126.04
9	a	909	BCL	C3C-C4C-CHD	-3.60	115.70	123.39
10	A	933	CLA	C3C-C4C-NC	3.60	114.61	110.57
10	A	933	CLA	CHB-C4A-NA	3.58	129.47	124.51
9	a	906	BCL	C2D-C1D-ND	3.58	112.75	110.10
9	A	902	BCL	C3A-C2A-C1A	3.57	106.68	101.34
10	A	910	CLA	CMB-C2B-C1B	3.56	130.80	125.37
9	a	905	BCL	CHB-C4A-NA	3.56	129.43	124.51
10	A	910	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
9	a	905	BCL	CBC-CAC-C3C	-3.55	105.57	113.47
9	A	903	BCL	C6-C5-C3	3.54	122.75	113.45
9	a	911	BCL	C3C-C4C-CHD	-3.53	115.84	123.39
10	a	901	CLA	CED-O2D-CGD	3.52	123.91	115.94
9	A	907	BCL	C9-C8-C7	3.51	124.02	111.29
16	C	301	HEC	CAA-C2A-C3A	-3.51	121.34	127.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	301	HEC	CAD-C3D-C2D	-3.50	121.35	127.88
10	A	933	CLA	C6-C5-C3	-3.49	96.56	113.58
16	C	301	HEC	CAA-C2A-C1A	3.48	131.45	124.89
10	A	912	CLA	C2A-C1A-CHA	-3.48	117.78	123.86
10	A	933	CLA	CBA-CAA-C2A	-3.47	103.61	113.86
10	a	912	CLA	C4-C3-C5	3.47	121.11	115.27
9	A	903	BCL	C1D-ND-C4D	-3.47	103.87	106.33
8	A	901	2GO	OBB-CAB-CBB	-3.46	112.05	119.73
9	a	906	BCL	OBD-CAD-C3D	-3.46	120.19	128.52
9	A	909	BCL	C4D-C3D-CAD	3.46	112.17	108.10
16	C	301	HEC	CMC-C2C-C1C	3.46	130.63	125.37
10	A	910	CLA	O2A-CGA-CBA	3.46	122.75	111.91
10	a	912	CLA	C9-C8-C10	-3.46	98.78	111.29
9	A	909	BCL	CED-O2D-CGD	3.44	123.71	115.94
10	a	901	CLA	C4-C3-C5	3.43	121.05	115.27
10	A	931	CLA	CHB-C1B-NB	-3.43	120.63	124.26
9	A	903	BCL	C2D-C1D-ND	3.42	112.62	110.10
11	A	913	LYC	C64-C65-C66	-3.41	116.08	127.75
9	A	905	BCL	C2A-C3A-C4A	-3.41	96.36	101.87
10	a	912	CLA	C4A-NA-C1A	-3.41	105.17	106.71
9	a	910	BCL	C16-C15-C13	3.39	126.88	115.92
10	A	910	CLA	CAC-C3C-C4C	3.38	129.20	124.81
10	A	931	CLA	CHA-C4D-ND	3.38	139.56	132.50
9	a	909	BCL	C1C-NC-C4C	-3.37	105.19	106.71
9	A	904	BCL	C2B-C1B-NB	3.37	112.49	110.23
9	a	907	BCL	C6-C7-C8	-3.36	105.05	115.92
9	A	909	BCL	CHB-C1B-C2B	-3.36	117.74	127.24
11	A	913	LYC	C20-C21-C50	3.36	130.36	123.47
9	A	905	BCL	C3D-C4D-ND	3.36	115.67	110.24
9	a	905	BCL	CHC-C4B-NB	-3.36	120.70	124.26
9	A	909	BCL	CMA-C3A-C4A	3.36	120.80	111.77
10	A	931	CLA	O1A-CGA-CBA	-3.35	110.64	123.73
10	a	914	CLA	CHB-C4A-NA	3.35	129.15	124.51
9	A	903	BCL	CAC-C3C-C2C	3.35	122.62	114.26
9	A	902	BCL	CAC-C3C-C4C	-3.35	105.16	112.58
9	a	911	BCL	CHD-C4C-NC	3.34	128.78	125.08
16	C	301	HEC	CMB-C2B-C1B	3.34	130.12	125.04
9	a	906	BCL	O2D-CGD-CBD	3.33	117.19	111.27
16	c	202	HEC	O2D-CGD-CBD	3.33	124.73	114.03
9	A	902	BCL	CHC-C4B-NB	-3.33	120.73	124.26
9	a	908	BCL	C9-C8-C10	-3.32	99.28	111.29
16	c	202	HEC	C1A-C2A-C3A	-3.32	102.81	107.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	909	BCL	CHA-C1A-NA	-3.31	118.81	126.40
10	a	912	CLA	C4D-C3D-CAD	-3.31	104.19	108.10
10	A	910	CLA	CHC-C1C-NC	-3.30	119.19	124.20
10	a	912	CLA	CHC-C1C-NC	-3.30	119.19	124.20
10	A	910	CLA	CHC-C4B-NB	3.30	127.75	124.26
9	a	907	BCL	C7-C6-C5	-3.30	104.41	113.36
11	A	913	LYC	C16-C17-C19	3.30	124.00	118.94
10	A	912	CLA	C1D-CHD-C4C	-3.29	118.96	126.06
9	a	904	BCL	O1D-CGD-CBD	-3.29	117.76	124.48
10	a	901	CLA	O1D-CGD-CBD	-3.28	117.78	124.48
10	A	931	CLA	C6-C7-C8	3.28	126.51	115.92
10	A	912	CLA	O2A-CGA-O1A	-3.28	112.87	123.14
10	a	915	CLA	CMA-C3A-C4A	3.28	120.58	111.77
9	A	902	BCL	C4-C3-C2	-3.27	115.29	123.68
8	a	903	2GO	CHD-C1D-C2D	3.27	132.33	125.48
9	a	907	BCL	CAB-C3B-C2B	-3.27	123.44	128.34
10	A	911	CLA	CMB-C2B-C1B	3.25	130.32	125.37
9	A	905	BCL	C16-C15-C13	-3.25	105.42	115.92
10	A	910	CLA	C4D-CHA-C1A	-3.25	117.30	121.25
11	A	913	LYC	C58-C56-C55	-3.24	113.96	118.94
16	C	301	HEC	C1A-CHA-C4D	3.24	133.05	126.06
10	a	915	CLA	C2A-C1A-CHA	-3.24	118.19	123.86
16	C	301	HEC	C4A-NA-C1A	-3.24	102.17	105.35
9	a	907	BCL	OBB-CAB-C3B	-3.23	114.42	120.41
10	A	911	CLA	C2D-C1D-ND	3.23	112.48	110.10
10	A	912	CLA	C1-O2A-CGA	3.23	126.75	116.11
16	C	301	HEC	C4A-CHB-C1B	3.22	133.01	126.06
8	a	903	2GO	CAA-C2A-C1A	3.22	122.53	111.97
9	A	905	BCL	CMB-C2B-C1B	3.21	130.26	125.37
9	A	902	BCL	C1-C2-C3	-3.21	120.49	126.04
10	A	910	CLA	CHB-C4A-NA	3.21	128.95	124.51
10	A	910	CLA	CHB-C1B-NB	-3.21	120.86	124.26
16	C	301	HEC	C1C-CHC-C4B	3.21	133.94	126.34
9	a	905	BCL	C4D-CHA-C1A	3.21	125.15	121.25
10	A	931	CLA	C3B-C4B-NB	3.20	113.49	110.52
9	a	910	BCL	C3D-C2D-C1D	-3.20	101.47	105.83
16	C	301	HEC	O2D-CGD-O1D	-3.19	115.35	123.30
10	A	931	CLA	C11-C10-C8	3.18	126.21	115.92
10	a	912	CLA	CAA-CBA-CGA	-3.18	103.95	113.25
9	a	909	BCL	OBB-CAB-C3B	3.17	126.28	120.41
9	A	905	BCL	O2A-CGA-CBA	3.17	121.87	111.91
8	A	901	2GO	C3D-C4D-ND	-3.17	104.60	110.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	909	BCL	C3C-C4C-CHD	-3.17	116.62	123.39
10	a	912	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
9	a	909	BCL	O1D-CGD-CBD	-3.16	118.02	124.48
11	A	913	LYC	C1-C2-C4	-3.16	113.53	122.65
10	A	933	CLA	CMD-C2D-C1D	3.15	130.27	124.71
9	a	905	BCL	C4-C3-C5	3.15	120.57	115.27
10	a	914	CLA	CMD-C2D-C1D	3.15	130.26	124.71
16	C	301	HEC	CMC-C2C-C3C	3.15	132.41	125.61
9	A	906	BCL	CMC-C2C-C1C	3.14	120.22	111.77
9	A	909	BCL	C10-C8-C7	3.14	128.65	112.13
10	a	915	CLA	C4D-CHA-C1A	-3.13	117.44	121.25
16	c	202	HEC	CMD-C2D-C1D	3.13	129.81	125.04
10	A	931	CLA	C1D-CHD-C4C	-3.12	119.32	126.06
9	a	910	BCL	C11-C12-C13	3.12	126.01	115.92
10	A	931	CLA	CHD-C1D-C2D	3.12	132.02	125.48
9	A	908	BCL	CMB-C2B-C1B	3.11	130.11	125.37
9	A	904	BCL	O2D-CGD-O1D	-3.10	117.77	123.84
16	C	301	HEC	C1D-ND-C4D	3.10	108.27	105.07
8	A	901	2GO	CHD-C1D-C2D	3.09	131.97	125.48
9	a	905	BCL	C2D-C1D-ND	3.08	112.37	110.10
16	c	202	HEC	C2B-C1B-NB	3.08	113.57	109.88
8	a	903	2GO	OBB-CAB-CBB	-3.07	112.93	119.73
9	a	905	BCL	CAB-C3B-C2B	-3.07	123.74	128.34
9	a	910	BCL	C4D-CHA-C1A	-3.07	117.52	121.25
9	a	911	BCL	CBB-CAB-C3B	3.07	126.98	120.43
10	a	915	CLA	CHB-C1B-NB	-3.05	121.02	124.26
10	A	933	CLA	CHC-C4B-NB	-3.05	121.03	124.26
9	A	902	BCL	O1A-CGA-CBA	-3.04	111.86	123.73
16	c	202	HEC	C4B-NB-C1B	3.04	108.21	105.07
10	a	901	CLA	C7-C6-C5	-3.03	105.12	113.36
9	a	905	BCL	OBB-CAB-C3B	3.03	126.02	120.41
9	a	908	BCL	OBD-CAD-C3D	-3.03	121.23	128.52
10	a	915	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
11	A	913	LYC	C59-C58-C56	-3.03	117.90	126.42
9	a	909	BCL	CHC-C1C-NC	3.02	128.69	124.51
13	A	915	85I	O2-P-O	-3.02	93.70	107.75
9	a	905	BCL	C11-C12-C13	3.02	125.67	115.92
9	A	908	BCL	C3B-C2B-C1B	-3.02	96.67	106.39
10	a	915	CLA	CHC-C1C-NC	-3.00	119.64	124.20
10	a	912	CLA	C17-C16-C15	-3.00	99.44	113.24
10	a	913	CLA	C4A-NA-C1A	-3.00	105.36	106.71
9	A	909	BCL	C5-C3-C2	2.98	127.15	121.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	911	CLA	C3B-C4B-NB	-2.98	107.75	110.52
16	C	301	HEC	CAB-C3B-C4B	-2.97	120.95	124.81
11	c	201	LYC	C54-C55-C56	2.95	131.53	127.31
9	a	904	BCL	CAC-C3C-C2C	-2.95	106.88	114.26
9	A	908	BCL	OBB-CAB-C3B	-2.95	114.94	120.41
10	a	914	CLA	C3D-C2D-C1D	-2.95	101.80	105.83
10	a	913	CLA	CAA-CBA-CGA	2.94	121.83	113.25
9	a	905	BCL	CHD-C1D-C2D	2.94	131.64	125.48
16	c	202	HEC	CHA-C1A-C2A	2.93	129.68	124.94
10	A	911	CLA	C10-C8-C7	2.92	127.48	112.13
9	A	907	BCL	O1D-CGD-CBD	-2.92	118.52	124.48
10	A	912	CLA	CAA-C2A-C1A	2.92	121.53	111.97
9	a	905	BCL	C3B-C2B-C1B	-2.91	97.00	106.39
10	a	901	CLA	C14-C13-C15	-2.91	100.74	111.29
9	A	903	BCL	CMB-C2B-C1B	2.91	129.80	125.37
9	A	904	BCL	CHD-C4C-NC	2.91	128.31	125.08
9	a	905	BCL	CMA-C3A-C4A	2.91	119.59	111.77
8	A	901	2GO	O2A-C1-C2	-2.90	101.02	108.64
9	a	906	BCL	C4B-C3B-C2B	-2.90	103.70	108.36
13	a	919	85I	O4-C4-C3	2.89	116.96	109.54
9	a	911	BCL	C3A-C2A-C1A	2.89	105.67	101.34
9	A	906	BCL	C3D-C4D-ND	2.89	114.91	110.24
9	A	904	BCL	CMA-C3A-C2A	-2.89	102.19	113.83
9	a	905	BCL	O2A-CGA-O1A	-2.88	116.32	123.59
9	A	903	BCL	C3D-C4D-ND	2.88	114.90	110.24
9	A	903	BCL	CMD-C2D-C3D	-2.87	121.00	127.61
8	a	903	2GO	C2D-C1D-ND	-2.87	105.69	110.37
9	a	910	BCL	C3D-C4D-ND	2.87	114.88	110.24
16	c	202	HEC	C4C-CHD-C1D	2.87	133.14	126.34
10	a	912	CLA	CMC-C2C-C1C	2.87	129.40	125.04
17	E	101	84Q	O7-P-O6	-2.86	97.89	109.07
9	a	910	BCL	C2B-C1B-NB	2.86	112.15	110.23
9	A	909	BCL	CBB-CAB-C3B	2.86	126.53	120.43
10	a	901	CLA	C6-C5-C3	2.85	120.94	113.45
9	a	907	BCL	O1A-CGA-CBA	-2.85	112.60	123.73
10	a	915	CLA	CHD-C4C-C3C	-2.85	120.65	124.84
10	A	910	CLA	CHD-C4C-C3C	-2.83	120.67	124.84
10	A	910	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
9	a	904	BCL	CMC-C2C-C3C	-2.83	102.42	113.83
9	A	908	BCL	O2A-C1-C2	2.82	116.06	108.64
9	A	903	BCL	CMC-C2C-C1C	2.82	119.36	111.77
9	a	908	BCL	C4-C3-C5	-2.82	110.53	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	907	BCL	C6-C7-C8	2.81	125.01	115.92
9	A	908	BCL	OBB-CAB-CBB	2.81	125.97	119.73
8	A	901	2GO	C3C-C2C-C1C	2.80	106.39	101.87
9	a	911	BCL	CMA-C3A-C4A	2.80	119.29	111.77
9	a	910	BCL	C3A-C2A-C1A	-2.79	97.16	101.34
9	A	906	BCL	OBB-CAB-CBB	-2.79	113.55	119.73
10	A	933	CLA	C3D-C4D-ND	2.78	114.73	110.24
10	A	912	CLA	CHC-C1C-NC	-2.78	119.99	124.20
10	a	912	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
9	A	909	BCL	CMB-C2B-C1B	2.78	129.60	125.37
9	A	906	BCL	CAB-C3B-C2B	-2.77	124.19	128.34
9	a	904	BCL	C4B-C3B-C2B	-2.77	103.90	108.36
9	A	908	BCL	CED-O2D-CGD	2.77	122.19	115.94
9	a	911	BCL	O2A-CGA-O1A	-2.76	116.62	123.59
10	a	915	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
9	a	905	BCL	CMC-C2C-C1C	2.75	119.17	111.77
9	a	908	BCL	C3D-C4D-ND	2.75	114.69	110.24
9	A	903	BCL	CAA-C2A-C3A	2.75	120.30	112.78
16	C	301	HEC	CMA-C3A-C4A	2.75	129.55	124.71
9	A	909	BCL	C2D-C1D-ND	2.75	112.13	110.10
9	a	910	BCL	C4-C3-C2	-2.74	116.65	123.68
17	E	101	84Q	O4-P-O6	2.74	119.73	109.47
10	a	912	CLA	C9-C8-C7	2.74	121.20	111.29
10	a	901	CLA	CAA-C2A-C3A	-2.73	105.30	112.78
10	a	913	CLA	C2C-C1C-NC	2.73	112.53	109.97
8	A	901	2GO	CAA-C2A-C3A	2.73	120.25	112.78
9	a	911	BCL	CAA-C2A-C1A	2.73	120.91	111.97
8	a	903	2GO	CBB-CAB-C3B	2.73	126.25	120.43
10	a	913	CLA	CHA-C4D-ND	-2.72	126.80	132.50
9	a	909	BCL	CMA-C3A-C4A	2.72	119.09	111.77
9	a	908	BCL	C4-C3-C2	-2.72	116.70	123.68
9	A	907	BCL	CHC-C4B-NB	-2.72	121.38	124.26
9	A	903	BCL	C1C-NC-C4C	-2.71	105.49	106.71
10	a	914	CLA	C1D-CHD-C4C	-2.71	120.21	126.06
10	A	931	CLA	CMD-C2D-C1D	2.71	129.48	124.71
10	A	910	CLA	C6-C7-C8	2.70	124.65	115.92
10	a	914	CLA	CHD-C1D-C2D	2.69	131.13	125.48
11	A	913	LYC	C5-C4-C2	2.69	136.94	127.75
8	A	901	2GO	CHB-C1B-NB	2.69	128.71	124.17
9	A	908	BCL	CMB-C2B-C3B	2.69	133.19	125.93
9	A	904	BCL	CHB-C1B-NB	-2.68	121.42	124.26
8	A	901	2GO	C1-C2-C3	2.68	130.67	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	902	BCL	C4-C3-C5	2.68	119.77	115.27
9	a	911	BCL	C4D-CHA-C1A	-2.68	117.99	121.25
16	C	301	HEC	CAB-C3B-C2B	2.67	132.10	127.53
9	a	911	BCL	C6-C5-C3	2.66	120.44	113.45
9	A	908	BCL	CHB-C4A-NA	2.66	128.19	124.51
9	A	904	BCL	C4D-CHA-C1A	-2.66	118.02	121.25
9	A	902	BCL	CHD-C1D-C2D	2.65	131.04	125.48
10	a	914	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
16	C	301	HEC	CHB-C4A-C3A	-2.65	119.92	125.48
10	A	931	CLA	C16-C15-C13	-2.65	107.36	115.92
10	A	931	CLA	CHB-C4A-NA	2.64	128.16	124.51
10	A	931	CLA	C11-C12-C13	-2.64	107.39	115.92
10	a	901	CLA	C1-C2-C3	-2.63	121.49	126.04
9	a	905	BCL	OBD-CAD-C3D	-2.63	122.19	128.52
16	C	301	HEC	CAC-C3C-C4C	-2.63	121.27	124.92
16	c	202	HEC	C4A-C3A-C2A	-2.63	103.10	106.94
10	A	933	CLA	C4D-C3D-CAD	-2.62	105.01	108.10
9	A	903	BCL	CBC-CAC-C3C	2.62	119.30	113.47
9	A	905	BCL	CHB-C1B-C2B	-2.61	119.85	127.24
10	A	933	CLA	CHA-C4D-ND	-2.61	127.03	132.50
8	A	901	2GO	CAA-C2A-C1A	2.61	120.54	111.97
10	A	910	CLA	CAA-C2A-C3A	2.61	119.93	112.78
9	A	908	BCL	CMA-C3A-C2A	-2.61	103.30	113.83
16	C	301	HEC	CBC-CAC-C3C	2.60	119.60	112.43
9	A	907	BCL	C2C-C3C-C4C	-2.60	97.45	101.34
9	a	908	BCL	O2A-CGA-O1A	2.60	130.15	123.59
9	A	906	BCL	CBC-CAC-C3C	2.59	119.24	113.47
8	a	903	2GO	C2A-C1A-CHA	2.59	128.39	123.86
9	A	904	BCL	C2D-C1D-ND	2.59	112.01	110.10
13	A	915	85I	O-P-O1	-2.59	98.96	109.07
16	c	202	HEC	CHC-C4B-C3B	-2.59	120.47	125.33
10	a	915	CLA	C2C-C1C-NC	2.59	112.39	109.97
9	A	904	BCL	OBD-CAD-C3D	-2.59	122.30	128.52
9	A	905	BCL	C14-C13-C12	2.58	120.64	111.29
10	a	915	CLA	C4D-C3D-CAD	-2.58	105.05	108.10
9	A	909	BCL	CAC-C3C-C4C	-2.58	106.86	112.58
9	A	904	BCL	CHC-C4B-NB	-2.58	121.53	124.26
9	A	908	BCL	C7-C6-C5	-2.57	106.37	113.36
11	c	201	LYC	C5-C6-C7	2.57	121.44	112.98
10	a	915	CLA	OBD-CAD-C3D	-2.57	122.33	128.52
9	A	907	BCL	C15-C13-C14	-2.57	98.66	110.51
10	A	911	CLA	C3D-C4D-ND	2.57	114.39	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	C	301	HEC	CBB-CAB-C3B	-2.56	105.36	112.43
9	a	909	BCL	CBB-CAB-C3B	-2.56	114.95	120.43
9	A	909	BCL	C15-C13-C12	2.56	125.60	112.13
9	a	910	BCL	C4B-C3B-C2B	-2.56	104.24	108.36
9	a	911	BCL	CMB-C2B-C3B	2.56	132.84	125.93
10	a	912	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
9	A	903	BCL	C2A-C1A-CHA	-2.56	119.39	123.86
9	A	908	BCL	C3D-C4D-ND	2.56	114.37	110.24
8	A	901	2GO	CMA-C3A-C2A	2.55	124.12	113.83
10	A	912	CLA	C3A-C2A-C1A	-2.54	97.53	101.34
9	a	910	BCL	CBA-CAA-C2A	2.54	121.37	113.86
9	a	908	BCL	CMB-C2B-C3B	2.54	132.79	125.93
9	A	907	BCL	CAB-C3B-C2B	-2.54	124.53	128.34
9	A	907	BCL	C4B-C3B-C2B	-2.54	104.28	108.36
10	a	912	CLA	O1D-CGD-CBD	2.54	129.68	124.48
9	A	902	BCL	C9-C8-C7	-2.53	102.12	111.29
9	a	905	BCL	C1D-ND-C4D	2.53	108.13	106.33
10	A	910	CLA	C3A-C2A-C1A	-2.53	97.55	101.34
9	a	904	BCL	O2A-C1-C2	2.52	115.26	108.64
9	A	906	BCL	C4-C3-C5	2.52	118.86	115.98
9	a	909	BCL	C4-C3-C5	2.52	119.51	115.27
9	a	904	BCL	CHD-C1D-C2D	2.51	130.75	125.48
9	a	908	BCL	CAC-C3C-C2C	-2.51	107.98	114.26
11	A	913	LYC	C18-C17-C16	2.51	122.04	118.08
9	A	906	BCL	CBA-CAA-C2A	2.51	121.28	113.86
10	A	910	CLA	C3D-C4D-ND	2.51	114.30	110.24
9	A	904	BCL	CAA-C2A-C1A	-2.51	103.76	111.97
9	a	910	BCL	C3C-C4C-CHD	-2.51	118.04	123.39
9	A	909	BCL	C3B-C2B-C1B	-2.50	98.32	106.39
16	c	202	HEC	CHC-C4B-NB	2.50	127.46	124.37
10	A	910	CLA	C6-C5-C3	2.50	120.02	113.45
9	a	908	BCL	CBB-CAB-C3B	2.50	125.78	120.43
10	A	911	CLA	C1-C2-C3	-2.50	121.72	126.04
10	a	913	CLA	C9-C8-C10	-2.50	102.25	111.29
8	a	903	2GO	C15-C13-C12	-2.49	99.04	112.13
9	A	906	BCL	CHD-C4C-NC	2.49	127.84	125.08
10	A	911	CLA	C6-C5-C3	2.48	119.97	113.45
9	A	907	BCL	C1D-ND-C4D	-2.48	104.57	106.33
9	A	906	BCL	CBB-CAB-C3B	-2.48	115.13	120.43
17	E	101	84Q	C19-C18-C17	2.48	122.63	113.62
9	A	907	BCL	C11-C10-C8	2.47	123.91	115.92
10	A	911	CLA	CHB-C4A-NA	2.47	127.93	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	911	BCL	CHB-C1B-NB	-2.46	121.65	124.26
10	A	931	CLA	OBD-CAD-C3D	-2.46	122.59	128.52
9	A	906	BCL	C4D-CHA-C1A	2.46	124.25	121.25
9	a	906	BCL	CBC-CAC-C3C	2.46	118.94	113.47
9	a	906	BCL	CBB-CAB-C3B	2.46	125.68	120.43
16	c	202	HEC	CMB-C2B-C3B	2.46	132.78	126.12
10	a	901	CLA	CHB-C1B-NB	-2.45	121.66	124.26
9	a	911	BCL	C4-C3-C2	2.44	129.95	123.68
8	a	903	2GO	O1D-CGD-CBD	-2.44	119.49	124.48
9	a	909	BCL	CHD-C1D-C2D	2.44	130.59	125.48
16	c	202	HEC	CBA-CAA-C2A	-2.44	105.86	112.63
10	A	912	CLA	CHD-C4C-NC	-2.43	120.37	124.20
9	a	908	BCL	C16-C15-C13	-2.43	108.06	115.92
10	A	910	CLA	C2D-C1D-ND	2.43	111.89	110.10
9	a	910	BCL	CBB-CAB-C3B	2.43	125.62	120.43
9	a	910	BCL	C1D-CHD-C4C	-2.43	120.77	126.62
11	A	913	LYC	C20-C19-C17	-2.43	123.85	127.31
9	a	911	BCL	C16-C15-C13	2.42	123.75	115.92
9	a	906	BCL	CMD-C2D-C3D	-2.42	122.04	127.61
9	A	906	BCL	C3C-C4C-CHD	-2.42	118.22	123.39
9	a	909	BCL	CAB-C3B-C2B	-2.42	124.71	128.34
10	a	915	CLA	CAA-CBA-CGA	2.42	120.33	113.25
9	a	909	BCL	C1D-ND-C4D	-2.42	104.62	106.33
10	a	913	CLA	CMA-C3A-C4A	2.42	118.27	111.77
9	A	905	BCL	C3B-C2B-C1B	-2.41	98.61	106.39
9	A	908	BCL	C1-O2A-CGA	2.41	122.77	116.44
9	A	908	BCL	O1A-CGA-CBA	-2.41	114.35	123.73
13	A	917	85I	O3-C3-C4	2.40	116.12	107.08
9	A	909	BCL	CBA-CAA-C2A	2.40	120.96	113.86
10	A	931	CLA	C9-C8-C10	2.40	119.97	111.29
9	a	904	BCL	C6-C5-C3	2.39	119.73	113.45
16	c	202	HEC	CHA-C4D-ND	-2.39	121.82	124.42
9	a	911	BCL	C4-C3-C5	-2.39	111.25	115.27
17	E	101	84Q	O5-P-O4	-2.39	97.34	106.78
11	c	201	LYC	C62-C61-C60	-2.39	116.44	122.59
8	a	903	2GO	C1B-NB-C4B	2.38	110.23	106.52
9	A	907	BCL	OBB-CAB-CBB	-2.38	114.45	119.73
10	a	914	CLA	CMB-C2B-C3B	2.38	132.36	126.59
9	a	910	BCL	CAC-C3C-C2C	2.38	120.20	114.26
10	a	913	CLA	CHC-C1C-NC	-2.37	120.61	124.20
13	A	916	85I	O2-P-O3	2.36	116.09	106.78
9	a	907	BCL	CHD-C1D-C2D	2.35	130.42	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	904	BCL	C2A-C1A-CHA	-2.35	119.74	123.86
10	a	901	CLA	CBA-CAA-C2A	2.35	120.80	113.86
13	A	915	85I	O6-C20-C21	2.35	116.56	111.50
9	A	909	BCL	CAC-C3C-C2C	2.35	120.12	114.26
11	c	201	LYC	C59-C58-C56	-2.34	119.83	126.42
15	A	932	85N	O5-C24-C19	-2.34	117.19	122.93
10	A	933	CLA	C5-C3-C2	-2.34	114.71	120.50
8	a	903	2GO	C3D-C4D-ND	-2.34	106.15	110.51
9	A	908	BCL	CHC-C4B-NB	-2.34	121.78	124.26
9	A	903	BCL	CHB-C1B-C2B	-2.34	120.63	127.24
10	A	931	CLA	CHD-C1D-ND	-2.34	122.30	124.45
10	a	914	CLA	O1A-CGA-CBA	-2.33	114.63	123.73
11	A	913	LYC	C55-C54-C53	-2.33	115.95	123.22
9	a	910	BCL	CAA-CBA-CGA	2.33	120.06	113.25
9	a	908	BCL	CHB-C1B-C2B	-2.33	120.67	127.24
9	a	910	BCL	CMC-C2C-C1C	2.33	118.02	111.77
9	A	909	BCL	C11-C12-C13	2.32	123.43	115.92
10	A	931	CLA	CAA-C2A-C3A	2.32	119.13	112.78
10	a	914	CLA	O2A-CGA-O1A	-2.32	115.88	123.14
9	A	902	BCL	C1D-CHD-C4C	-2.32	121.03	126.62
9	a	908	BCL	C11-C10-C8	-2.31	108.44	115.92
10	a	901	CLA	O2A-C1-C2	-2.31	102.56	108.64
10	A	911	CLA	CMA-C3A-C4A	2.31	117.97	111.77
9	A	904	BCL	C4B-C3B-C2B	-2.31	104.65	108.36
10	a	915	CLA	CHD-C1D-ND	-2.30	122.34	124.45
10	A	910	CLA	CAA-CBA-CGA	2.30	119.98	113.25
16	C	301	HEC	CHB-C1B-NB	-2.30	121.92	124.42
10	a	915	CLA	CBA-CAA-C2A	-2.29	107.09	113.86
15	G	101	85N	O2-C16-C17	-2.29	103.66	109.54
10	a	913	CLA	C4-C3-C2	-2.29	117.81	123.68
9	a	905	BCL	C6-C5-C3	2.29	119.45	113.45
10	a	912	CLA	C7-C6-C5	2.28	119.56	113.36
9	A	902	BCL	C4B-C3B-C2B	-2.28	104.69	108.36
9	a	906	BCL	CMC-C2C-C1C	2.28	117.90	111.77
9	A	905	BCL	CHB-C4A-NA	2.28	127.66	124.51
8	a	903	2GO	C1D-CHD-C4C	2.27	132.09	126.62
13	A	916	85I	C7-C6-C5	-2.27	105.37	113.62
9	A	907	BCL	C11-C12-C13	2.26	126.64	115.98
9	A	905	BCL	C9-C8-C10	-2.26	103.12	111.29
9	A	906	BCL	CMB-C2B-C1B	2.25	128.79	125.37
9	A	908	BCL	CHB-C1B-C2B	-2.24	120.90	127.24
9	A	903	BCL	CHD-C1D-C2D	2.24	130.18	125.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	202	HEC	CHD-C1D-ND	-2.24	121.61	124.37
9	A	902	BCL	CAB-C3B-C2B	-2.24	124.99	128.34
9	A	909	BCL	CMB-C2B-C3B	2.24	131.97	125.93
9	a	909	BCL	CMB-C2B-C3B	2.23	131.96	125.93
9	A	904	BCL	CAC-C3C-C4C	-2.23	107.63	112.58
10	a	912	CLA	C5-C3-C2	2.23	125.63	121.12
9	A	908	BCL	C1D-ND-C4D	-2.22	104.76	106.33
10	a	913	CLA	CBC-CAC-C3C	2.22	118.54	112.43
10	A	931	CLA	C3C-C4C-NC	2.21	113.05	110.57
8	A	901	2GO	CMA-C3A-C4A	-2.21	105.83	111.77
10	a	901	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
13	a	918	85I	O6-C3-C4	2.21	115.38	107.08
9	a	906	BCL	O2A-CGA-CBA	2.21	121.11	114.03
9	a	910	BCL	O1A-CGA-CBA	-2.20	115.14	123.73
10	a	915	CLA	C4-C3-C2	-2.20	118.03	123.68
10	a	914	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
9	A	905	BCL	O1A-CGA-CBA	-2.20	115.15	123.73
10	A	933	CLA	O2A-CGA-CBA	2.19	118.79	111.91
9	A	907	BCL	C4D-C3D-CAD	-2.19	105.51	108.10
9	A	907	BCL	CMA-C3A-C4A	2.19	117.66	111.77
8	a	903	2GO	C3B-C2B-C1B	2.18	113.43	106.39
10	A	933	CLA	CHD-C4C-C3C	-2.18	121.63	124.84
10	A	931	CLA	CHC-C4B-C3B	-2.18	118.01	127.71
10	A	931	CLA	CMB-C2B-C3B	2.18	131.87	126.59
9	a	910	BCL	C4-C3-C5	-2.18	111.60	115.27
9	A	907	BCL	C4D-CHA-C1A	2.18	123.90	121.25
10	A	912	CLA	CHB-C1B-C2B	-2.18	121.09	127.24
9	A	907	BCL	CBA-CAA-C2A	2.17	120.27	113.86
9	a	909	BCL	C9-C8-C7	2.17	119.14	111.29
10	A	912	CLA	O2A-CGA-CBA	2.16	120.77	112.23
9	a	909	BCL	C4B-C3B-C2B	-2.16	104.89	108.36
15	G	101	85N	O3-C17-O6	2.16	116.77	110.72
11	c	201	LYC	C63-C61-C60	2.15	128.49	121.98
10	A	933	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
9	A	906	BCL	CHC-C4B-NB	2.15	126.53	124.26
10	A	931	CLA	C5-C3-C2	-2.15	116.76	121.12
9	a	908	BCL	CHA-C1A-NA	2.15	131.32	126.40
9	a	904	BCL	C4-C3-C2	-2.15	118.16	123.68
10	a	912	CLA	C6-C5-C3	2.15	119.09	113.45
9	a	907	BCL	O2A-C1-C2	-2.14	103.00	108.64
8	a	903	2GO	CAA-C2A-C3A	2.13	118.62	112.78
16	C	301	HEC	CMD-C2D-C1D	2.13	128.28	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	a	908	BCL	C1D-CHD-C4C	-2.13	121.49	126.62
9	A	906	BCL	CAC-C3C-C4C	2.12	117.29	112.58
10	a	914	CLA	C4D-CHA-C1A	2.12	123.83	121.25
9	A	907	BCL	CMB-C2B-C1B	2.12	128.59	125.37
8	a	903	2GO	CHD-C1D-ND	-2.12	121.30	124.86
8	a	903	2GO	CMA-C3A-C4A	-2.12	106.09	111.77
9	a	904	BCL	C1D-CHD-C4C	-2.11	121.53	126.62
10	A	911	CLA	CHB-C1B-NB	-2.11	122.02	124.26
8	a	903	2GO	C3A-C2A-C1A	-2.11	98.18	101.34
16	c	202	HEC	C4A-CHB-C1B	2.11	130.60	126.06
9	a	910	BCL	C14-C13-C15	2.10	118.91	111.29
10	A	910	CLA	CHD-C4C-NC	-2.10	120.90	124.20
9	A	903	BCL	C3B-C2B-C1B	-2.10	99.63	106.39
8	A	901	2GO	CHA-C1A-NA	-2.10	121.59	126.40
9	a	911	BCL	C15-C13-C12	-2.10	101.10	112.13
9	a	907	BCL	CMB-C2B-C3B	2.10	131.59	125.93
9	a	910	BCL	C20-C18-C17	2.09	124.47	111.54
9	a	910	BCL	CMD-C2D-C3D	-2.09	122.80	127.61
10	A	910	CLA	C4-C3-C5	2.09	118.78	115.27
10	a	913	CLA	C2A-C3A-C4A	-2.08	98.50	101.87
10	a	912	CLA	C2D-C1D-ND	-2.08	108.57	110.10
11	A	913	LYC	C15-C14-C12	-2.08	124.34	127.31
9	A	906	BCL	CMD-C2D-C3D	2.08	132.39	127.61
9	a	911	BCL	OBD-CAD-C3D	-2.08	123.52	128.52
9	a	906	BCL	CHD-C4C-NC	2.07	127.38	125.08
8	a	903	2GO	C6-C7-C8	2.07	122.60	115.92
9	a	904	BCL	CMB-C2B-C3B	2.07	131.51	125.93
8	A	901	2GO	CAC-C3C-C4C	2.07	117.17	112.58
9	a	906	BCL	CAC-C3C-C2C	2.06	119.41	114.26
10	A	911	CLA	C9-C8-C10	2.06	118.74	111.29
10	a	912	CLA	C4B-CHC-C1C	2.06	131.22	126.34
8	a	903	2GO	CHA-C1A-NA	-2.06	121.69	126.40
10	a	915	CLA	C4B-CHC-C1C	2.05	131.21	126.34
10	A	933	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
9	a	909	BCL	CMD-C2D-C3D	-2.05	122.91	127.61
9	a	908	BCL	C1-O2A-CGA	-2.04	111.08	116.44
9	A	909	BCL	C12-C11-C10	2.03	122.55	113.24
9	a	906	BCL	O1D-CGD-CBD	2.03	128.63	124.48
9	A	908	BCL	C4D-C3D-CAD	-2.02	105.71	108.10
10	a	913	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
10	a	915	CLA	C1-C2-C3	-2.02	122.54	126.04
10	A	931	CLA	CMC-C2C-C3C	-2.02	120.62	126.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	902	BCL	C6-C5-C3	2.02	118.74	113.45
9	A	903	BCL	C12-C11-C10	-2.01	103.99	113.24
10	A	911	CLA	C15-C13-C12	2.01	122.71	112.13
10	A	912	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
9	A	907	BCL	CAC-C3C-C4C	-2.01	108.12	112.58
13	A	916	85I	O6-C20-C21	2.01	115.83	111.50
9	A	905	BCL	C12-C11-C10	2.01	122.47	113.24
9	a	911	BCL	CAA-C2A-C3A	2.01	118.28	112.78
10	a	901	CLA	CHB-C1B-C2B	-2.01	121.56	127.24
11	A	913	LYC	C3-C2-C1	2.01	119.04	114.60
10	A	933	CLA	CMD-C2D-C3D	2.01	132.23	127.61
11	A	913	LYC	C57-C56-C58	-2.01	114.92	118.08
9	A	904	BCL	C2C-C3C-C4C	-2.00	98.34	101.34
9	A	905	BCL	CMC-C2C-C3C	-2.00	105.76	113.83

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	901	2GO	CBD
8	A	901	2GO	ND
8	a	903	2GO	CBD
8	a	903	2GO	ND
10	A	910	CLA	C8
10	A	911	CLA	C8
16	C	301	HEC	NA
16	c	202	HEC	NA

All (654) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	902	BCL	C1A-C2A-CAA-CBA
9	A	902	BCL	C3A-C2A-CAA-CBA
9	A	902	BCL	CBD-CGD-O2D-CED
9	A	902	BCL	C11-C12-C13-C14
9	A	903	BCL	C1A-C2A-CAA-CBA
9	A	903	BCL	C2-C3-C5-C6
9	A	903	BCL	C4-C3-C5-C6
9	A	904	BCL	C1A-C2A-CAA-CBA
9	A	904	BCL	CHA-CBD-CGD-O1D
9	A	905	BCL	C1A-C2A-CAA-CBA
9	A	905	BCL	CBA-CGA-O2A-C1
9	A	905	BCL	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	905	BCL	CBD-CGD-O2D-CED
9	A	905	BCL	C2-C3-C5-C6
9	A	905	BCL	C4-C3-C5-C6
9	A	906	BCL	CBD-CGD-O2D-CED
9	A	906	BCL	O1D-CGD-O2D-CED
9	A	907	BCL	C2C-C3C-CAC-CBC
9	A	907	BCL	C4C-C3C-CAC-CBC
9	A	907	BCL	CBD-CGD-O2D-CED
9	A	907	BCL	C2-C3-C5-C6
9	A	907	BCL	C4-C3-C5-C6
9	a	904	BCL	C4C-C3C-CAC-CBC
9	a	904	BCL	CBD-CGD-O2D-CED
9	a	905	BCL	C1A-C2A-CAA-CBA
9	a	905	BCL	C3A-C2A-CAA-CBA
9	a	906	BCL	C1A-C2A-CAA-CBA
9	a	907	BCL	C2A-CAA-CBA-CGA
9	a	908	BCL	C1A-C2A-CAA-CBA
9	a	908	BCL	CBD-CGD-O2D-CED
9	a	908	BCL	C2-C3-C5-C6
9	a	908	BCL	C4-C3-C5-C6
9	a	911	BCL	C1A-C2A-CAA-CBA
9	a	911	BCL	C3A-C2A-CAA-CBA
10	A	933	CLA	CHA-CBD-CGD-O2D
10	a	912	CLA	CBD-CGD-O2D-CED
10	a	913	CLA	CBD-CGD-O2D-CED
10	a	913	CLA	C6-C7-C8-C9
10	a	915	CLA	C2B-C3B-CAB-CBB
10	a	915	CLA	C2-C3-C5-C6
10	a	915	CLA	C4-C3-C5-C6
11	c	201	LYC	C4-C5-C6-C7
11	c	201	LYC	C5-C6-C7-C8
11	c	201	LYC	C5-C6-C7-C9
11	c	201	LYC	C57-C56-C58-C59
13	A	915	85I	C4-C3-O3-P
13	A	915	85I	O7-C20-O6-C3
13	A	915	85I	C21-C20-O6-C3
13	A	916	85I	N-C1-C2-O
13	A	916	85I	O3-C3-O6-C20
13	A	916	85I	C3-O3-P-O
13	A	916	85I	O7-C20-O6-C3
13	A	917	85I	C4-C3-O6-C20
13	A	917	85I	C2-O-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	917	85I	O7-C20-O6-C3
13	a	918	85I	O3-C3-C4-O4
13	a	918	85I	O6-C3-C4-O4
13	a	918	85I	C4-C3-O6-C20
13	a	918	85I	O7-C20-O6-C3
13	a	919	85I	O6-C3-C4-O4
13	a	919	85I	C4-C3-O3-P
13	a	919	85I	O3-C3-O6-C20
13	a	919	85I	C6-C5-O4-C4
13	a	919	85I	C2-O-P-O1
13	a	920	85I	C2-C1-N-C
13	a	920	85I	O3-C3-C4-O4
13	a	920	85I	O6-C3-C4-O4
13	a	920	85I	C4-C3-O6-C20
13	a	920	85I	C2-O-P-O1
13	a	920	85I	C2-O-P-O2
13	a	920	85I	C2-O-P-O3
13	a	920	85I	O7-C20-O6-C3
15	A	932	85N	O3-C17-O6-C25
15	A	932	85N	O2-C16-C17-O6
15	A	932	85N	C16-C17-O3-C18
15	A	932	85N	C20-C19-C24-O4
15	A	932	85N	C20-C19-C24-O5
15	G	101	85N	C19-C20-N1-C21
15	G	101	85N	C19-C20-N1-C22
15	G	101	85N	C19-C20-N1-C23
15	G	101	85N	O3-C18-C19-C20
15	G	101	85N	O3-C18-C19-C24
15	G	101	85N	C20-C19-C24-O4
15	G	101	85N	C20-C19-C24-O5
15	a	902	85N	O7-C25-O6-C17
15	a	902	85N	C26-C25-O6-C17
15	a	902	85N	O2-C16-C17-O3
15	g	101	85N	C16-C17-O6-C25
15	g	101	85N	O7-C25-O6-C17
15	g	101	85N	O2-C16-C17-O6
17	E	101	84Q	O3-C17-O2-C16
17	E	101	84Q	O7-C32-C33-N
17	E	101	84Q	O1-C15-C16-O2
17	E	101	84Q	O1-C15-C16-O4
17	a	921	84Q	O4-C16-O2-C17
17	a	921	84Q	O3-C17-O2-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	a	921	84Q	C32-O7-P-O6
17	a	921	84Q	C32-O7-P-O5
17	a	921	84Q	C32-O7-P-O4
17	a	921	84Q	C16-O4-P-O7
17	a	921	84Q	C15-C16-O4-P
17	a	921	84Q	O1-C15-C16-O4
9	a	904	BCL	O1D-CGD-O2D-CED
16	c	202	HEC	C4B-C3B-CAB-CBB
9	A	902	BCL	O1D-CGD-O2D-CED
9	A	905	BCL	O1D-CGD-O2D-CED
9	a	909	BCL	O1D-CGD-O2D-CED
9	A	903	BCL	CBD-CGD-O2D-CED
9	a	905	BCL	CBD-CGD-O2D-CED
9	a	909	BCL	CBD-CGD-O2D-CED
9	A	907	BCL	O1A-CGA-O2A-C1
9	a	907	BCL	O1A-CGA-O2A-C1
9	a	911	BCL	O1A-CGA-O2A-C1
13	a	919	85I	O5-C5-O4-C4
9	A	903	BCL	O1D-CGD-O2D-CED
9	A	907	BCL	O1D-CGD-O2D-CED
10	a	913	CLA	O1D-CGD-O2D-CED
16	c	202	HEC	C2C-C3C-CAC-CBC
16	c	202	HEC	C4C-C3C-CAC-CBC
10	A	911	CLA	C3-C5-C6-C7
10	a	913	CLA	C3-C5-C6-C7
9	A	907	BCL	CBA-CGA-O2A-C1
9	a	907	BCL	CBA-CGA-O2A-C1
9	a	908	BCL	O1A-CGA-O2A-C1
9	a	908	BCL	O1D-CGD-O2D-CED
16	c	202	HEC	C2B-C3B-CAB-CBB
10	a	901	CLA	CBD-CGD-O2D-CED
9	a	908	BCL	CBA-CGA-O2A-C1
9	a	911	BCL	CBA-CGA-O2A-C1
10	A	911	CLA	CBD-CGD-O2D-CED
9	A	903	BCL	C2A-CAA-CBA-CGA
9	a	910	BCL	C2A-CAA-CBA-CGA
10	a	912	CLA	C2A-CAA-CBA-CGA
9	a	905	BCL	O1D-CGD-O2D-CED
10	a	912	CLA	O1D-CGD-O2D-CED
9	a	909	BCL	C3-C5-C6-C7
15	g	101	85N	C14-C15-O2-C16
13	A	917	85I	O5-C5-O4-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	G	101	85N	O1-C15-O2-C16
15	a	902	85N	C11-C10-C9-C8
9	A	909	BCL	CBD-CGD-O2D-CED
10	a	914	CLA	CBD-CGD-O2D-CED
10	a	915	CLA	CBD-CGD-O2D-CED
15	G	101	85N	C14-C15-O2-C16
13	a	918	85I	C21-C20-O6-C3
16	C	301	HEC	C2B-C3B-CAB-CBB
10	a	914	CLA	CBA-CGA-O2A-C1
13	A	915	85I	C12-C13-C14-C15
13	A	917	85I	C7-C8-C9-C10
13	A	917	85I	C25-C26-C27-C28
13	A	917	85I	C10-C11-C12-C13
13	A	917	85I	C6-C5-O4-C4
15	g	101	85N	O1-C15-O2-C16
9	A	902	BCL	C4-C3-C5-C6
9	A	902	BCL	C2-C3-C5-C6
10	a	901	CLA	C2A-CAA-CBA-CGA
9	A	902	BCL	CBA-CGA-O2A-C1
13	A	916	85I	C21-C20-O6-C3
17	E	101	84Q	C13-C14-O1-C15
17	a	921	84Q	C13-C14-O1-C15
10	a	914	CLA	O1A-CGA-O2A-C1
13	A	917	85I	C3-O3-P-O
17	E	101	84Q	C16-O4-P-O7
10	A	910	CLA	C13-C15-C16-C17
17	a	921	84Q	C1-C3-C4-C5
17	a	921	84Q	C11-C12-C13-C14
17	E	101	84Q	O-C14-O1-C15
17	a	921	84Q	O-C14-O1-C15
9	A	903	BCL	C11-C10-C8-C9
9	A	903	BCL	C14-C13-C15-C16
9	A	907	BCL	C11-C10-C8-C9
9	A	908	BCL	C11-C10-C8-C9
9	a	908	BCL	C14-C13-C15-C16
9	a	910	BCL	C14-C13-C15-C16
10	A	910	CLA	C6-C7-C8-C9
10	A	911	CLA	C6-C7-C8-C9
10	A	931	CLA	C6-C7-C8-C9
10	a	901	CLA	C6-C7-C8-C9
11	c	201	LYC	C15-C16-C17-C19
11	c	201	LYC	C55-C56-C58-C59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
16	C	301	HEC	C2C-C3C-CAC-CBC
9	a	908	BCL	C5-C6-C7-C8
10	A	910	CLA	C5-C6-C7-C8
9	a	905	BCL	C15-C16-C17-C18
9	a	909	BCL	C15-C16-C17-C18
10	a	901	CLA	C15-C16-C17-C18
13	a	919	85I	C14-C15-C16-C17
15	A	932	85N	C34-C35-C36-C37
15	a	902	85N	C25-C26-C27-C28
13	a	918	85I	C2-C1-N-C
9	A	909	BCL	C2-C1-O2A-CGA
9	a	907	BCL	C5-C6-C7-C8
9	a	909	BCL	C10-C11-C12-C13
17	E	101	84Q	C18-C17-O2-C16
10	A	911	CLA	C15-C16-C17-C18
9	A	909	BCL	C6-C7-C8-C10
9	a	907	BCL	C11-C12-C13-C15
10	A	910	CLA	C11-C10-C8-C7
10	A	931	CLA	C11-C12-C13-C15
9	A	909	BCL	C3-C5-C6-C7
13	A	915	85I	O5-C5-O4-C4
9	A	905	BCL	C2A-CAA-CBA-CGA
13	A	917	85I	C29-C30-C31-C32
13	a	920	85I	C29-C30-C31-C32
11	A	913	LYC	C4-C5-C6-C7
10	A	931	CLA	O1D-CGD-O2D-CED
9	A	902	BCL	C13-C15-C16-C17
9	a	907	BCL	C10-C11-C12-C13
9	a	909	BCL	C5-C6-C7-C8
10	a	912	CLA	C8-C10-C11-C12
10	a	901	CLA	C5-C6-C7-C8
8	a	903	2GO	C15-C16-C17-C18
10	A	931	CLA	C8-C10-C11-C12
10	A	931	CLA	C13-C15-C16-C17
10	a	901	CLA	C13-C15-C16-C17
13	a	920	85I	C14-C15-C16-C17
13	a	919	85I	C2-O-P-O3
13	A	915	85I	C6-C5-O4-C4
10	A	910	CLA	O1D-CGD-O2D-CED
8	a	903	2GO	C13-C15-C16-C17
9	A	905	BCL	C10-C11-C12-C13
10	A	931	CLA	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	A	908	BCL	C2A-CAA-CBA-CGA
10	A	931	CLA	C2A-CAA-CBA-CGA
13	a	919	85I	C15-C16-C17-C19
9	a	905	BCL	C13-C15-C16-C17
13	A	917	85I	C11-C10-C9-C8
15	A	932	85N	C31-C32-C33-C34
17	E	101	84Q	C7-C8-C9-C10
17	a	921	84Q	C9-C10-C11-C12
10	A	931	CLA	C16-C17-C18-C20
15	a	902	85N	C1-C2-C4-C5
13	a	919	85I	C6-C7-C8-C9
13	a	919	85I	C12-C13-C14-C15
13	a	920	85I	C11-C12-C13-C14
15	A	932	85N	C27-C28-C29-C30
17	a	921	84Q	C4-C5-C6-C7
13	a	919	85I	C21-C22-C23-C24
13	A	916	85I	C25-C26-C27-C28
13	a	920	85I	C9-C10-C11-C12
13	A	915	85I	C22-C23-C24-C25
13	A	916	85I	C22-C23-C24-C25
13	a	920	85I	C20-C21-C22-C23
17	E	101	84Q	C17-C18-C19-C20
9	a	909	BCL	C1-C2-C3-C5
13	a	918	85I	C26-C27-C28-C29
13	a	919	85I	C9-C10-C11-C12
9	A	902	BCL	O1A-CGA-O2A-C1
9	A	903	BCL	C16-C17-C18-C20
10	A	910	CLA	C16-C17-C18-C19
13	A	917	85I	C30-C31-C32-C34
13	A	915	85I	C10-C11-C12-C13
13	a	919	85I	C11-C10-C9-C8
15	G	101	85N	C10-C11-C12-C13
15	a	902	85N	C26-C27-C28-C29
9	A	909	BCL	C11-C10-C8-C9
10	A	911	CLA	O1D-CGD-O2D-CED
13	A	915	85I	C26-C27-C28-C29
13	A	917	85I	C26-C27-C28-C29
15	a	902	85N	C7-C8-C9-C10
15	g	101	85N	C5-C6-C7-C8
17	a	921	84Q	C19-C20-C21-C22
11	c	201	LYC	C15-C16-C17-C18
9	a	908	BCL	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	916	85I	C27-C28-C29-C30
13	a	918	85I	C21-C22-C23-C24
13	a	919	85I	C22-C23-C24-C25
15	a	902	85N	C5-C6-C7-C8
13	A	916	85I	C7-C8-C9-C10
13	a	918	85I	C22-C23-C24-C25
13	a	920	85I	C7-C8-C9-C10
15	G	101	85N	C26-C27-C28-C29
15	a	902	85N	C11-C12-C13-C14
17	E	101	84Q	C10-C11-C12-C13
9	a	910	BCL	C16-C17-C18-C19
10	A	931	CLA	C16-C17-C18-C19
17	E	101	84Q	C-C1-C3-C4
10	a	913	CLA	C15-C16-C17-C18
13	A	917	85I	C12-C13-C14-C15
13	a	919	85I	C25-C26-C27-C28
13	a	919	85I	C13-C14-C15-C16
15	g	101	85N	C11-C12-C13-C14
13	A	917	85I	C20-C21-C22-C23
10	A	931	CLA	C5-C6-C7-C8
13	a	920	85I	C25-C26-C27-C28
15	g	101	85N	C27-C28-C29-C30
17	E	101	84Q	C19-C20-C21-C22
9	a	909	BCL	CBA-CGA-O2A-C1
13	a	919	85I	C10-C11-C12-C13
9	A	904	BCL	C3A-C2A-CAA-CBA
9	A	905	BCL	C3A-C2A-CAA-CBA
9	A	909	BCL	C3A-C2A-CAA-CBA
9	a	906	BCL	C3A-C2A-CAA-CBA
9	a	908	BCL	C3A-C2A-CAA-CBA
10	a	901	CLA	C3A-C2A-CAA-CBA
9	a	910	BCL	C10-C11-C12-C13
11	c	201	LYC	C17-C19-C20-C21
13	a	919	85I	C7-C8-C9-C10
15	a	902	85N	C10-C11-C12-C13
9	a	910	BCL	C16-C17-C18-C20
13	A	916	85I	C30-C31-C32-C33
13	A	917	85I	C15-C16-C17-C19
17	E	101	84Q	C2-C1-C3-C4
13	A	916	85I	C24-C25-C26-C27
13	A	916	85I	C13-C14-C15-C16
13	a	919	85I	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	E	101	84Q	C20-C21-C22-C23
13	A	916	85I	C20-C21-C22-C23
15	a	902	85N	C12-C13-C14-C15
10	A	931	CLA	C4-C3-C5-C6
15	g	101	85N	C26-C27-C28-C29
10	a	901	CLA	O1D-CGD-O2D-CED
17	a	921	84Q	C3-C4-C5-C6
13	a	919	85I	C30-C31-C32-C34
13	A	916	85I	C11-C10-C9-C8
10	A	933	CLA	C2B-C3B-CAB-CBB
15	a	902	85N	C28-C29-C30-C31
13	A	917	85I	C22-C23-C24-C25
17	a	921	84Q	C6-C7-C8-C9
17	a	921	84Q	C25-C26-C27-C28
13	A	916	85I	C12-C13-C14-C15
13	A	917	85I	C28-C29-C30-C31
10	a	901	CLA	C8-C10-C11-C12
13	A	916	85I	C5-C6-C7-C8
9	A	909	BCL	C11-C10-C8-C7
10	A	911	CLA	C11-C12-C13-C15
10	A	931	CLA	C11-C10-C8-C7
13	a	920	85I	C26-C27-C28-C29
9	A	903	BCL	C16-C17-C18-C19
13	A	917	85I	C30-C31-C32-C33
13	a	918	85I	C20-C21-C22-C23
9	a	904	BCL	C2A-CAA-CBA-CGA
16	C	301	HEC	C4C-C3C-CAC-CBC
9	a	908	BCL	C13-C15-C16-C17
13	A	917	85I	C21-C22-C23-C24
15	a	902	85N	C17-C16-O2-C15
17	E	101	84Q	C11-C12-C13-C14
17	a	921	84Q	C5-C6-C7-C8
13	a	920	85I	C21-C20-O6-C3
15	g	101	85N	C26-C25-O6-C17
9	a	904	BCL	CBA-CGA-O2A-C1
13	A	917	85I	C5-C6-C7-C8
13	a	918	85I	C5-C6-C7-C8
13	A	915	85I	C7-C8-C9-C10
13	a	920	85I	C21-C22-C23-C24
15	a	902	85N	C29-C30-C31-C32
17	E	101	84Q	C3-C4-C5-C6
15	G	101	85N	C1-C2-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a	902	85N	C3-C2-C4-C5
9	A	903	BCL	C10-C11-C12-C13
9	A	908	BCL	C8-C10-C11-C12
9	a	907	BCL	C11-C12-C13-C14
10	A	912	CLA	CBD-CGD-O2D-CED
17	a	921	84Q	C23-C24-C25-C26
15	A	932	85N	C29-C30-C31-C32
8	A	901	2GO	C1A-C2A-CAA-CBA
9	A	908	BCL	C1A-C2A-CAA-CBA
9	A	909	BCL	C1A-C2A-CAA-CBA
9	a	910	BCL	C1A-C2A-CAA-CBA
10	A	910	CLA	C16-C17-C18-C20
13	a	919	85I	C30-C31-C32-C33
13	a	920	85I	C30-C31-C32-C33
15	a	902	85N	C30-C31-C32-C33
10	a	914	CLA	O1D-CGD-O2D-CED
9	A	905	BCL	C5-C6-C7-C8
9	A	909	BCL	C15-C16-C17-C18
17	E	101	84Q	C16-C15-O1-C14
13	A	917	85I	C15-C16-C17-C18
9	A	908	BCL	C3-C5-C6-C7
13	A	917	85I	C6-C7-C8-C9
10	a	901	CLA	CBA-CGA-O2A-C1
9	a	904	BCL	C2C-C3C-CAC-CBC
15	G	101	85N	C7-C8-C9-C10
17	a	921	84Q	C10-C11-C12-C13
10	a	912	CLA	C13-C15-C16-C17
13	a	919	85I	C23-C24-C25-C26
10	a	913	CLA	C16-C17-C18-C19
13	a	918	85I	C30-C31-C32-C34
13	A	916	85I	C6-C7-C8-C9
10	A	933	CLA	O1D-CGD-O2D-CED
9	A	909	BCL	C8-C10-C11-C12
9	a	909	BCL	O1A-CGA-O2A-C1
17	a	921	84Q	C18-C17-O2-C16
13	a	919	85I	C28-C29-C30-C31
15	G	101	85N	C11-C12-C13-C14
17	E	101	84Q	C22-C23-C24-C25
10	A	912	CLA	O1D-CGD-O2D-CED
9	a	908	BCL	C15-C16-C17-C18
13	A	916	85I	C14-C15-C16-C17
13	A	915	85I	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	a	902	85N	C18-C19-C24-O4
9	a	905	BCL	CBA-CGA-O2A-C1
9	A	908	BCL	C12-C13-C15-C16
9	a	908	BCL	C12-C13-C15-C16
9	a	910	BCL	C11-C12-C13-C15
9	a	910	BCL	C12-C13-C15-C16
10	a	901	CLA	C6-C7-C8-C10
10	a	913	CLA	C11-C10-C8-C7
9	A	903	BCL	C6-C7-C8-C9
9	A	905	BCL	C11-C10-C8-C9
9	a	908	BCL	C6-C7-C8-C9
10	A	931	CLA	C11-C12-C13-C14
10	a	912	CLA	C6-C7-C8-C9
10	a	915	CLA	O1D-CGD-O2D-CED
10	a	912	CLA	CBA-CGA-O2A-C1
10	A	933	CLA	C4B-C3B-CAB-CBB
10	a	915	CLA	C4B-C3B-CAB-CBB
17	E	101	84Q	C16-O4-P-O5
9	a	905	BCL	C10-C11-C12-C13
10	a	913	CLA	C16-C17-C18-C20
15	a	902	85N	O2-C16-C17-O6
15	g	101	85N	O2-C16-C17-O3
17	a	921	84Q	O1-C15-C16-O2
15	G	101	85N	C6-C7-C8-C9
9	A	903	BCL	C3A-C2A-CAA-CBA
9	A	908	BCL	C3A-C2A-CAA-CBA
13	a	919	85I	C3-O3-P-O
11	c	201	LYC	C58-C59-C60-C61
9	A	902	BCL	C2B-C3B-CAB-CBB
15	A	932	85N	C28-C29-C30-C31
13	A	916	85I	C30-C31-C32-C34
9	a	904	BCL	C8-C10-C11-C12
15	G	101	85N	C3-C2-C4-C5
17	E	101	84Q	C6-C7-C8-C9
13	A	915	85I	C2-O-P-O3
9	a	905	BCL	O1A-CGA-O2A-C1
13	A	915	85I	C30-C31-C32-C33
13	a	919	85I	C15-C16-C17-C18
10	a	901	CLA	C2B-C3B-CAB-CBB
9	a	908	BCL	C10-C11-C12-C13
15	a	902	85N	C2-C4-C5-C6
13	a	920	85I	C30-C31-C32-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	a	918	85I	C11-C12-C13-C14
13	a	918	85I	C12-C13-C14-C15
9	A	905	BCL	C2-C1-O2A-CGA
9	a	911	BCL	C2-C1-O2A-CGA
15	A	932	85N	C25-C26-C27-C28
9	a	905	BCL	C11-C12-C13-C14
13	A	917	85I	C21-C20-O6-C3
16	C	301	HEC	C4B-C3B-CAB-CBB
13	a	918	85I	C30-C31-C32-C33
17	a	921	84Q	C2-C1-C3-C4
17	E	101	84Q	C1-C3-C4-C5
8	A	901	2GO	C4C-C3C-CAC-CBC
10	A	911	CLA	C10-C11-C12-C13
13	A	915	85I	C24-C25-C26-C27
9	a	905	BCL	C3-C5-C6-C7
8	A	901	2GO	C10-C11-C12-C13
13	a	919	85I	C29-C30-C31-C32
13	A	915	85I	C21-C22-C23-C24
13	a	920	85I	C27-C28-C29-C30
9	A	902	BCL	C11-C12-C13-C15
9	A	902	BCL	C12-C13-C15-C16
9	A	903	BCL	C6-C7-C8-C10
9	A	903	BCL	C11-C10-C8-C7
9	A	905	BCL	C11-C10-C8-C7
9	a	905	BCL	C11-C12-C13-C15
9	a	908	BCL	C6-C7-C8-C10
10	a	901	CLA	C11-C10-C8-C7
9	a	909	BCL	C16-C17-C18-C19
10	A	911	CLA	C16-C17-C18-C19
9	A	902	BCL	C2A-CAA-CBA-CGA
10	a	912	CLA	C3-C5-C6-C7
9	a	909	BCL	CAD-CBD-CGD-O2D
10	A	931	CLA	CAD-CBD-CGD-O2D
10	a	912	CLA	CAD-CBD-CGD-O2D
13	A	916	85I	C23-C24-C25-C26
13	a	920	85I	C13-C14-C15-C16
15	a	902	85N	C33-C34-C35-C36
9	A	903	BCL	C5-C6-C7-C8
17	E	101	84Q	C24-C25-C26-C27
9	A	906	BCL	CHA-CBD-CGD-O2D
9	a	905	BCL	CHA-CBD-CGD-O2D
10	A	933	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	915	CLA	CHA-CBD-CGD-O1D
10	a	915	CLA	CHA-CBD-CGD-O2D
9	a	904	BCL	O1A-CGA-O2A-C1
10	a	901	CLA	O1A-CGA-O2A-C1
13	a	919	85I	O7-C20-O6-C3
9	A	908	BCL	C14-C13-C15-C16
13	A	916	85I	C10-C11-C12-C13
13	A	917	85I	C3-O3-P-O1
17	a	921	84Q	C16-O4-P-O6
15	A	932	85N	C1-C2-C4-C5
13	a	919	85I	N-C1-C2-O
17	E	101	84Q	C32-O7-P-O4
13	a	918	85I	C27-C28-C29-C30
13	A	915	85I	C2-O-P-O1
13	A	917	85I	C2-O-P-O2
13	a	919	85I	C2-O-P-O2
17	E	101	84Q	C27-C28-C29-C31
9	a	905	BCL	C5-C6-C7-C8
9	a	908	BCL	CAD-CBD-CGD-O1D
13	a	920	85I	C1-C2-O-P
17	a	921	84Q	C33-C32-O7-P
13	a	919	85I	C20-C21-C22-C23
13	a	918	85I	C7-C8-C9-C10
9	A	907	BCL	C8-C10-C11-C12
17	a	921	84Q	C-C1-C3-C4
9	A	905	BCL	C12-C13-C15-C16
9	A	907	BCL	C6-C7-C8-C10
9	A	907	BCL	C11-C10-C8-C7
9	A	908	BCL	C11-C10-C8-C7
9	a	907	BCL	C11-C10-C8-C7
10	A	911	CLA	C11-C10-C8-C7
15	A	932	85N	C19-C18-O3-C17
13	a	918	85I	C23-C24-C25-C26
9	a	909	BCL	CAA-CBA-CGA-O2A
17	a	921	84Q	C7-C8-C9-C10
9	a	904	BCL	C10-C11-C12-C13
8	a	903	2GO	C14-C13-C15-C16
9	A	902	BCL	C14-C13-C15-C16
9	a	907	BCL	C6-C7-C8-C9
9	a	910	BCL	C11-C12-C13-C14
10	A	911	CLA	C11-C12-C13-C14
10	a	913	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	G	101	85N	C25-C26-C27-C28
11	c	201	LYC	C9-C10-C11-C12
13	a	920	85I	C6-C7-C8-C9
10	a	912	CLA	O1A-CGA-O2A-C1
9	A	908	BCL	C16-C17-C18-C19
15	g	101	85N	C1-C2-C4-C5
9	A	906	BCL	O1A-CGA-O2A-C1
15	A	932	85N	C3-C2-C4-C5
9	a	904	BCL	C2-C1-O2A-CGA
15	a	902	85N	C18-C19-C24-O5
15	g	101	85N	C7-C8-C9-C10
9	A	902	BCL	CAA-CBA-CGA-O2A
13	a	919	85I	C21-C20-O6-C3
13	a	920	85I	C22-C23-C24-C25
13	a	920	85I	C10-C11-C12-C13
8	a	903	2GO	C11-C12-C13-C15
10	a	901	CLA	C11-C12-C13-C14
11	c	201	LYC	C52-C51-C53-C54
8	a	903	2GO	C8-C10-C11-C12
13	A	916	85I	C26-C27-C28-C29
13	a	919	85I	C24-C25-C26-C27
13	A	915	85I	C6-C7-C8-C9
16	c	202	HEC	CAD-CBD-CGD-O2D
10	a	901	CLA	C16-C17-C18-C20
9	a	906	BCL	CAA-CBA-CGA-O1A
13	A	915	85I	O3-C3-C4-O4
13	a	918	85I	C9-C10-C11-C12
13	a	920	85I	C12-C13-C14-C15
10	a	901	CLA	C14-C13-C15-C16
9	a	908	BCL	C2A-CAA-CBA-CGA
17	E	101	84Q	C23-C24-C25-C26
9	A	904	BCL	CAA-CBA-CGA-O2A
10	a	912	CLA	C4-C3-C5-C6
10	a	901	CLA	C1A-C2A-CAA-CBA
9	A	903	BCL	C12-C13-C15-C16
10	A	931	CLA	C6-C7-C8-C10
10	a	901	CLA	C12-C13-C15-C16
9	a	909	BCL	C13-C15-C16-C17
16	C	301	HEC	CAD-CBD-CGD-O2D
13	A	916	85I	C15-C16-C17-C19
9	A	904	BCL	CAA-CBA-CGA-O1A
10	A	910	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	A	911	CLA	C5-C6-C7-C8
9	a	906	BCL	CAA-CBA-CGA-O2A
11	c	201	LYC	C21-C50-C51-C53
9	A	902	BCL	C4B-C3B-CAB-CBB
10	a	901	CLA	C2-C1-O2A-CGA
13	a	918	85I	C28-C29-C30-C31
9	A	909	BCL	O1D-CGD-O2D-CED
9	a	904	BCL	CAA-CBA-CGA-O2A
16	C	301	HEC	CAD-CBD-CGD-O1D
15	g	101	85N	C3-C2-C4-C5
17	a	921	84Q	C27-C28-C29-C30
13	A	917	85I	C23-C24-C25-C26
10	A	931	CLA	CBD-CGD-O2D-CED
15	g	101	85N	C11-C10-C9-C8
10	a	901	CLA	CAA-CBA-CGA-O2A
8	A	901	2GO	C16-C17-C18-C20
11	c	201	LYC	C13-C12-C14-C15
11	c	201	LYC	C21-C50-C51-C52
13	A	915	85I	C5-C6-C7-C8
9	A	902	BCL	C8-C10-C11-C12
10	A	931	CLA	C2-C3-C5-C6
10	a	912	CLA	C2-C3-C5-C6
9	A	907	BCL	C6-C7-C8-C9
9	A	908	BCL	C6-C7-C8-C9
9	A	909	BCL	C11-C12-C13-C14
9	a	907	BCL	C11-C10-C8-C9
10	A	910	CLA	C11-C10-C8-C9
10	a	901	CLA	C11-C10-C8-C9
9	A	903	BCL	CAA-CBA-CGA-O2A
9	A	903	BCL	CAD-CBD-CGD-O2D
9	A	907	BCL	CAD-CBD-CGD-O2D
10	a	901	CLA	CAD-CBD-CGD-O2D
13	a	918	85I	C24-C25-C26-C27
13	a	920	85I	C11-C10-C9-C8
13	a	919	85I	C26-C27-C28-C29
16	c	202	HEC	CAD-CBD-CGD-O1D
8	A	901	2GO	CHA-CBD-CGD-O1D
9	A	904	BCL	CHA-CBD-CGD-O2D
9	A	906	BCL	CHA-CBD-CGD-O1D
9	a	904	BCL	CHA-CBD-CGD-O2D
9	a	905	BCL	CHA-CBD-CGD-O1D
9	a	906	BCL	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	a	908	BCL	CHA-CBD-CGD-O2D
10	a	913	CLA	CHA-CBD-CGD-O2D
11	c	201	LYC	C11-C12-C14-C15
13	a	919	85I	O4-C5-C6-C7
15	a	902	85N	C13-C14-C15-O2
9	a	910	BCL	CAA-CBA-CGA-O2A
9	a	907	BCL	C6-C7-C8-C10
9	A	907	BCL	C11-C12-C13-C14
10	a	901	CLA	C16-C17-C18-C19
13	A	916	85I	O4-C5-C6-C7
16	C	301	HEC	CAA-CBA-CGA-O2A
10	a	901	CLA	CAA-CBA-CGA-O1A
17	a	921	84Q	C22-C23-C24-C25
17	a	921	84Q	C27-C28-C29-C31
13	A	917	85I	N-C1-C2-O
15	g	101	85N	C18-C19-C20-N1
15	A	932	85N	C4-C5-C6-C7
9	a	907	BCL	C13-C15-C16-C17
13	a	919	85I	O5-C5-C6-C7
17	a	921	84Q	C11-C10-C9-C8
15	A	932	85N	C2-C4-C5-C6
9	A	903	BCL	CAA-CBA-CGA-O1A
15	g	101	85N	C13-C14-C15-O2
16	c	202	HEC	CAA-CBA-CGA-O2A
9	a	910	BCL	CAA-CBA-CGA-O1A
15	a	902	85N	C13-C14-C15-O1
9	A	906	BCL	CAD-CBD-CGD-O1D
9	A	908	BCL	CAD-CBD-CGD-O1D
9	a	906	BCL	CAD-CBD-CGD-O1D
10	A	933	CLA	CAD-CBD-CGD-O1D
10	a	915	CLA	CAD-CBD-CGD-O1D
17	E	101	84Q	C33-C32-O7-P
15	g	101	85N	C13-C14-C15-O1
13	a	920	85I	O4-C5-C6-C7
15	g	101	85N	C2-C4-C5-C6
9	A	905	BCL	C14-C13-C15-C16
9	a	905	BCL	C6-C7-C8-C9
9	A	908	BCL	CAA-CBA-CGA-O2A
13	A	916	85I	O6-C20-C21-C22
13	A	916	85I	O5-C5-C6-C7
9	A	908	BCL	C6-C7-C8-C10
9	a	905	BCL	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
10	a	913	CLA	C6-C7-C8-C10
15	A	932	85N	O7-C25-C26-C27
10	A	931	CLA	C3-C5-C6-C7
11	c	201	LYC	C50-C51-C53-C54
9	A	907	BCL	CAA-CBA-CGA-O2A
15	A	932	85N	O6-C25-C26-C27
15	G	101	85N	C13-C14-C15-O2
13	A	917	85I	C14-C15-C16-C17
9	A	903	BCL	O1A-CGA-O2A-C1
13	A	916	85I	O7-C20-C21-C22
13	a	920	85I	O5-C5-C6-C7
15	a	902	85N	C14-C15-O2-C16

There are no ring outliers.

41 monomers are involved in 182 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	909	BCL	2	0
11	A	913	LYC	6	0
8	A	901	2GO	2	0
10	a	913	CLA	6	0
15	g	101	85N	1	0
15	G	101	85N	7	0
9	a	904	BCL	10	0
10	a	901	CLA	3	0
13	A	915	85I	2	0
9	a	909	BCL	5	0
10	A	910	CLA	4	0
9	A	908	BCL	7	0
9	A	907	BCL	6	0
18	a	917	SF4	4	0
9	A	904	BCL	2	0
10	A	911	CLA	7	0
15	a	902	85N	3	0
13	a	920	85I	4	0
10	a	914	CLA	2	0
10	A	933	CLA	1	0
11	c	201	LYC	5	0
9	A	902	BCL	9	0
9	a	905	BCL	8	0
10	a	915	CLA	2	0
16	c	202	HEC	5	0

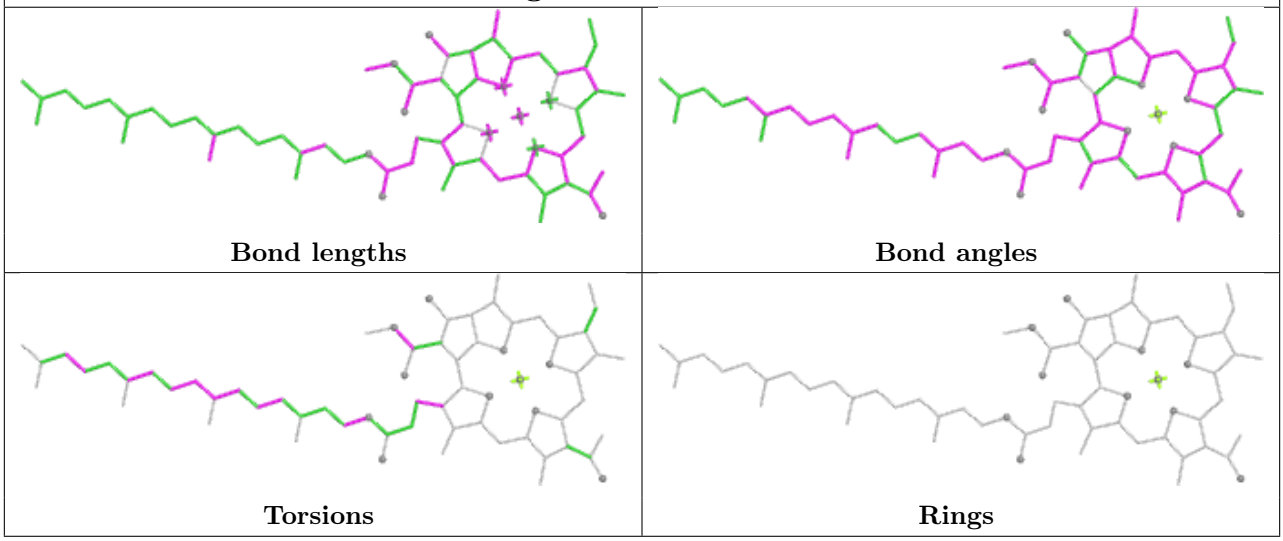
Continued on next page...

Continued from previous page...

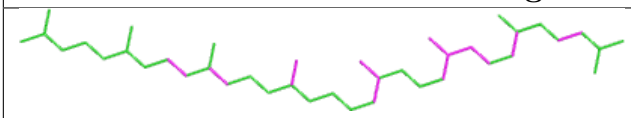
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	C	301	HEC	9	0
9	a	911	BCL	5	0
10	A	912	CLA	1	0
8	a	903	2GO	1	0
9	A	905	BCL	9	0
9	A	903	BCL	5	0
13	A	916	85I	1	0
9	a	908	BCL	10	0
9	a	907	BCL	4	0
10	A	931	CLA	7	0
9	A	906	BCL	6	0
10	a	912	CLA	4	0
9	a	910	BCL	4	0
15	A	932	85N	8	0
13	A	917	85I	3	0
13	a	919	85I	1	0

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

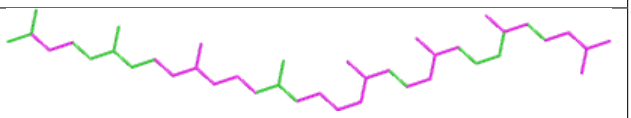
Ligand BCL A 909



Ligand LYC A 913

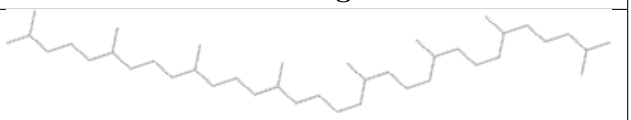


Bond lengths



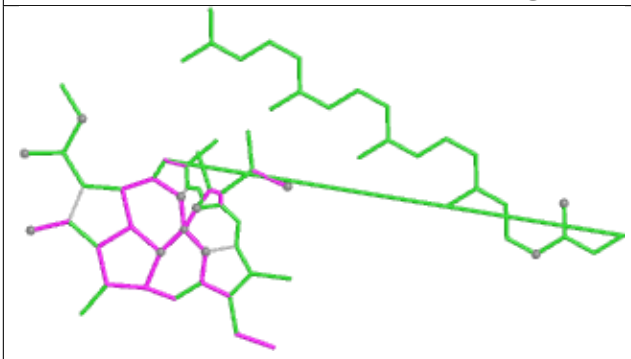
Bond angles

Torsions

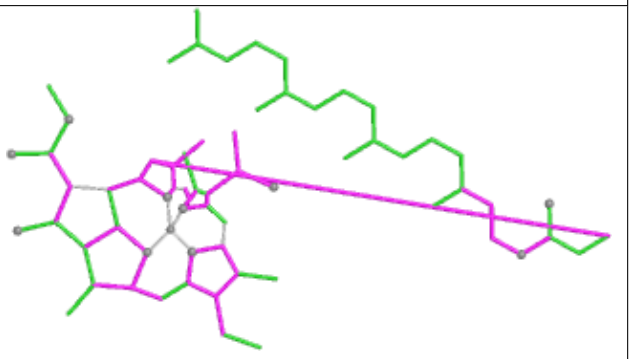


Rings

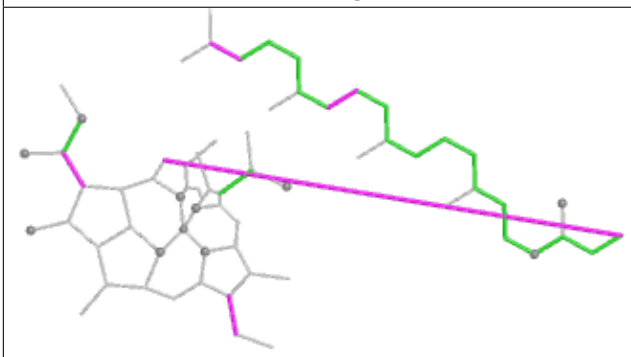
Ligand 2GO A 901



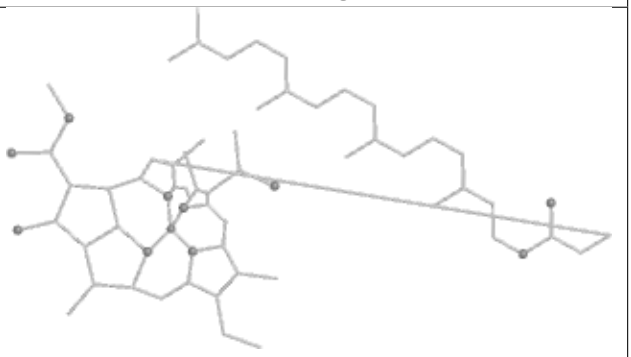
Bond lengths



Bond angles

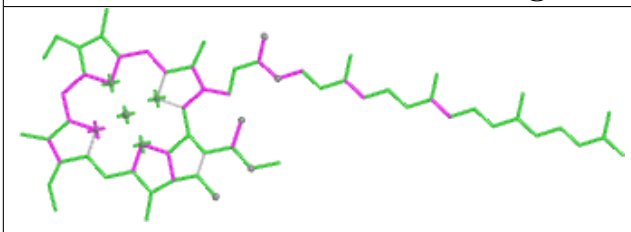


Torsions

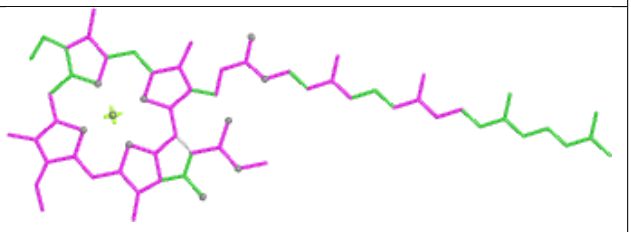


Rings

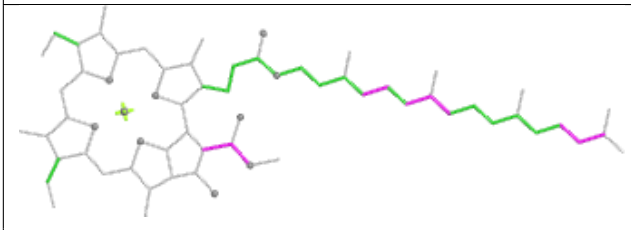
Ligand CLA a 913



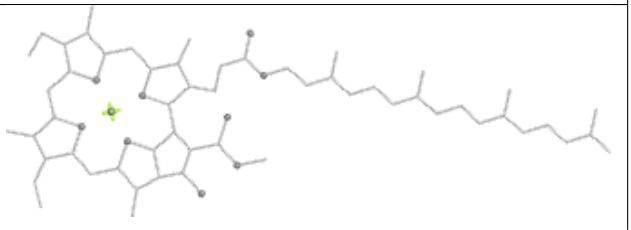
Bond lengths



Bond angles

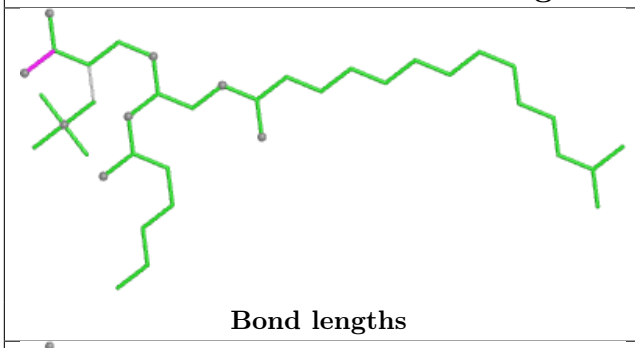


Torsions

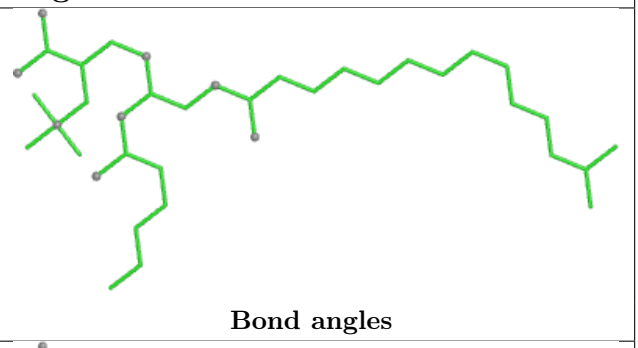


Rings

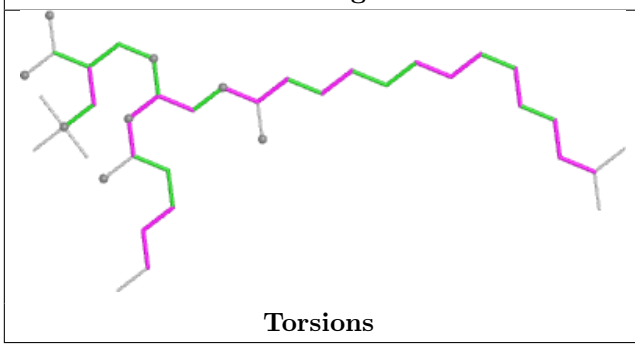
Ligand 85N g 101



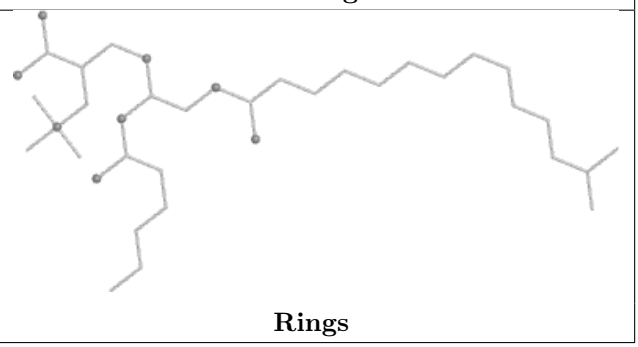
Bond lengths



Bond angles

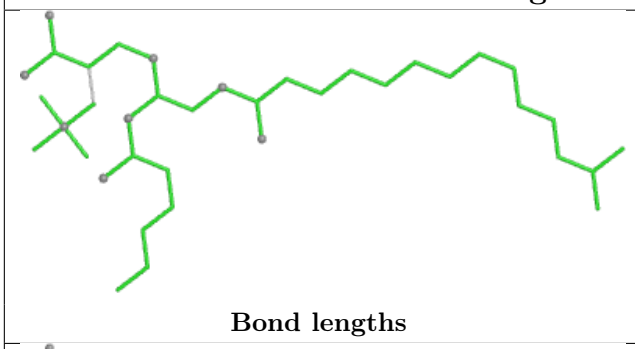


Torsions

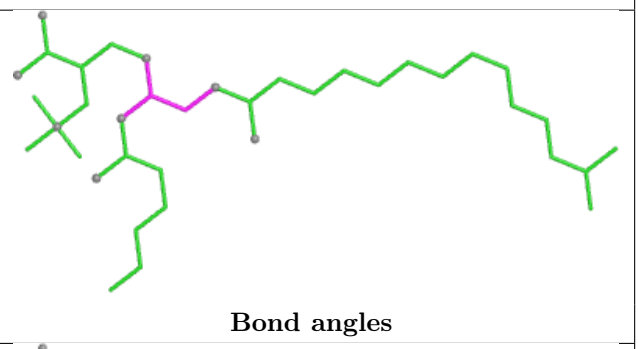


Rings

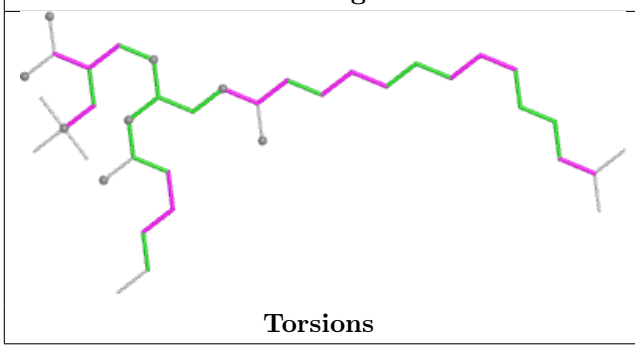
Ligand 85N G 101



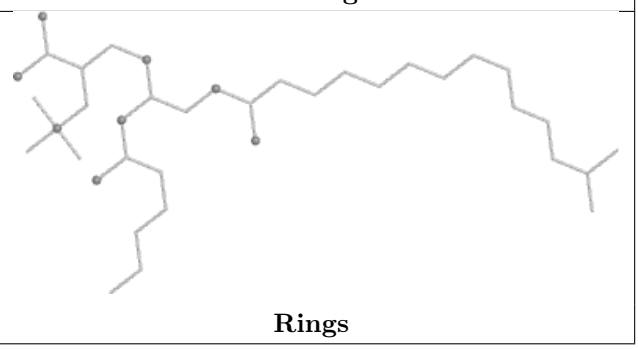
Bond lengths



Bond angles

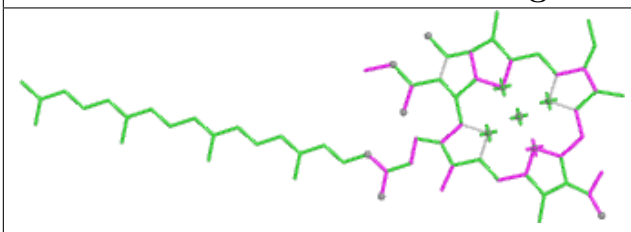


Torsions

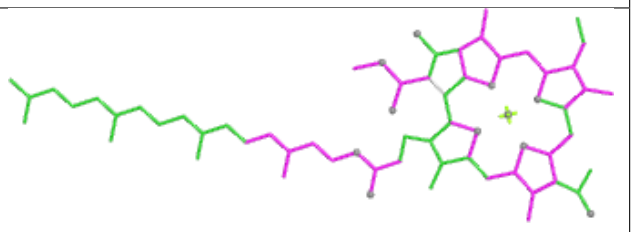


Rings

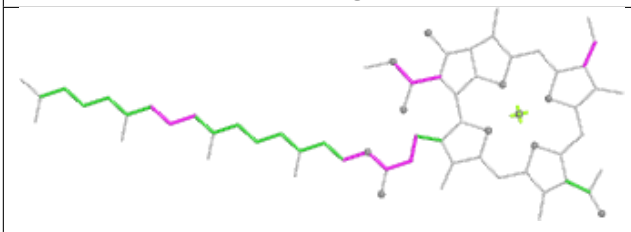
Ligand BCL a 904



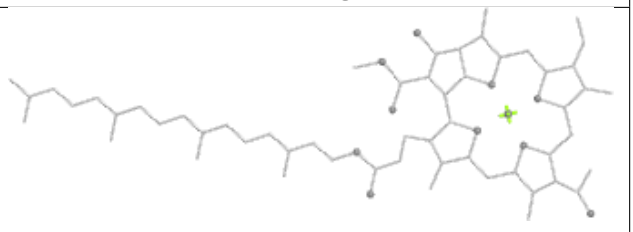
Bond lengths



Bond angles

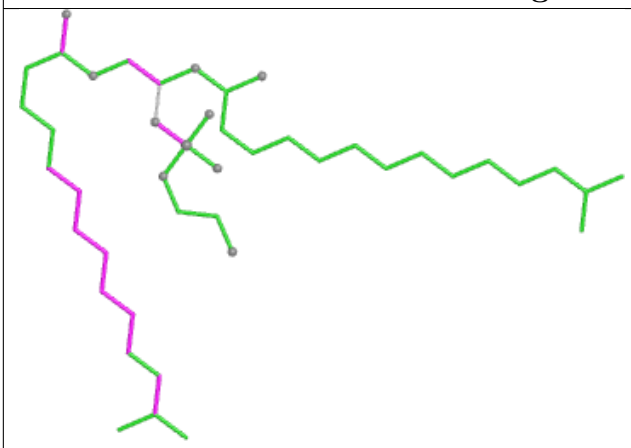


Torsions

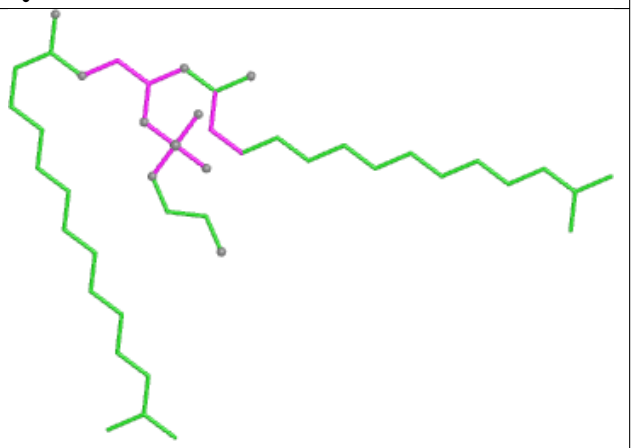


Rings

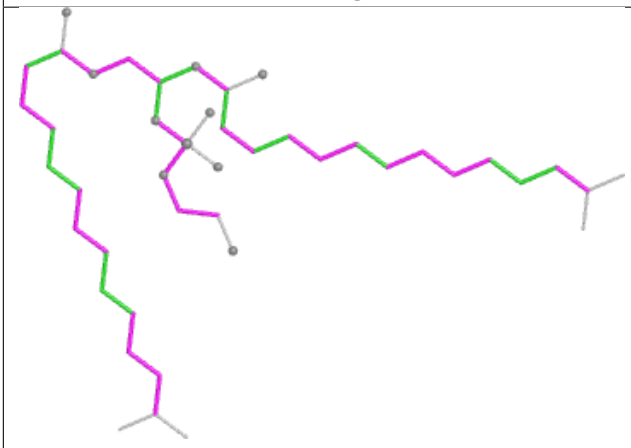
Ligand 84Q E 101



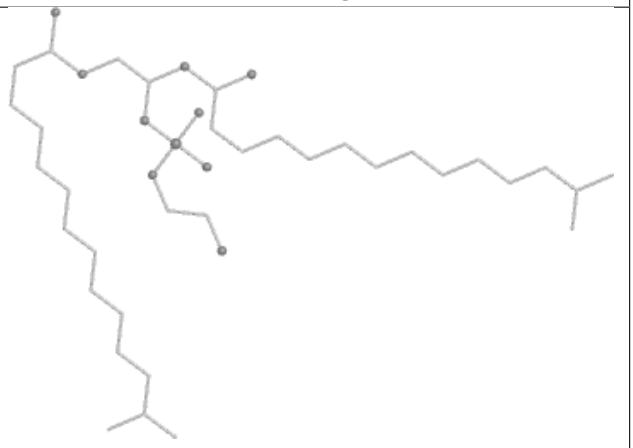
Bond lengths



Bond angles

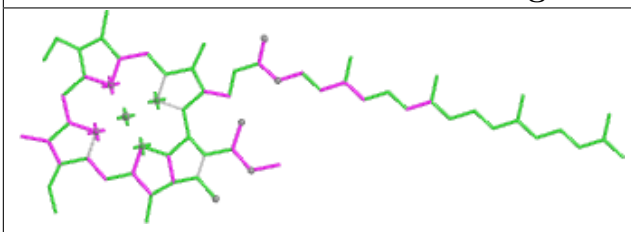


Torsions

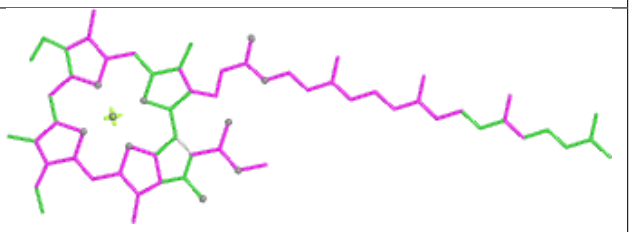


Rings

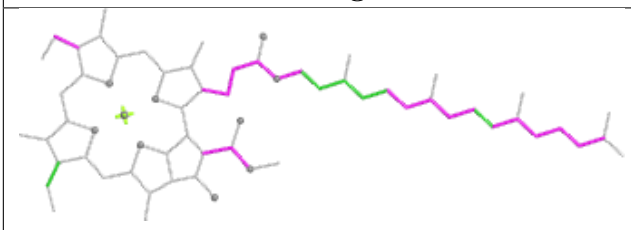
Ligand CLA a 901



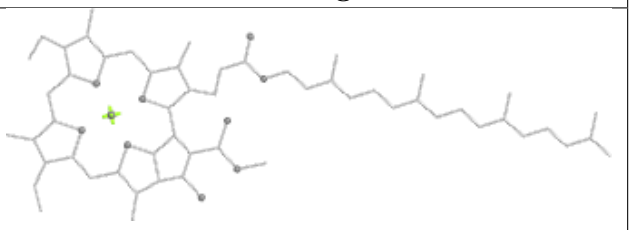
Bond lengths



Bond angles



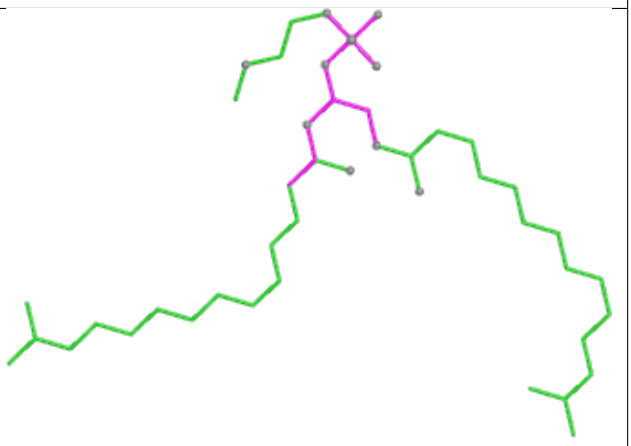
Torsions



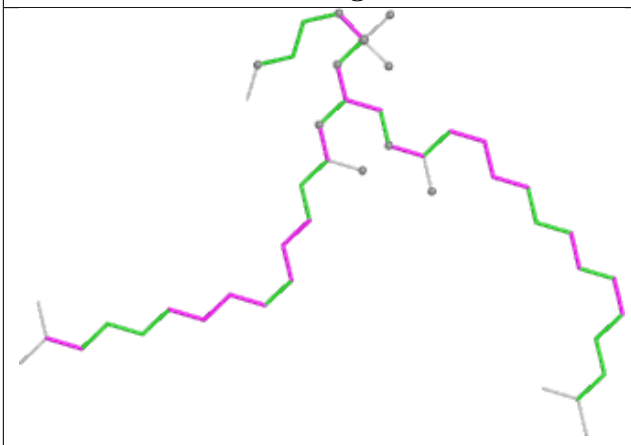
Rings

Ligand 85I A 915

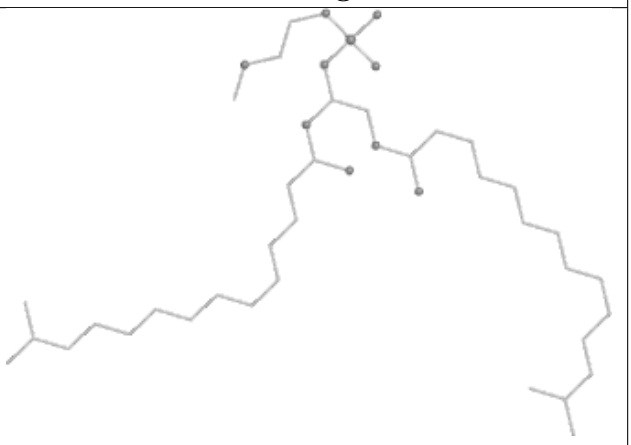
Bond lengths



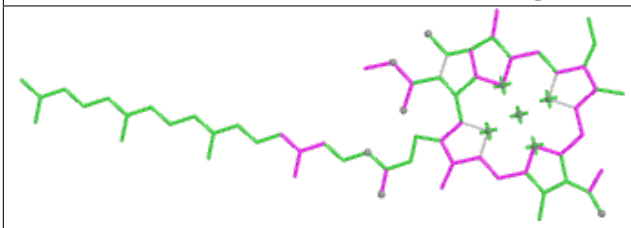
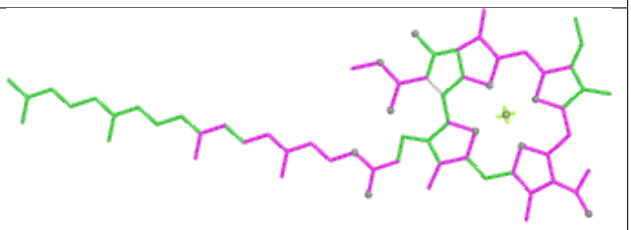
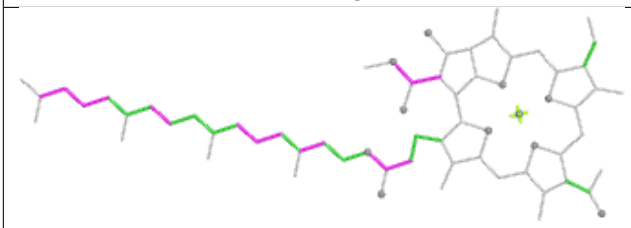
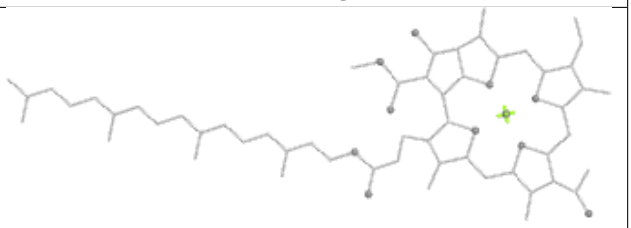
Bond angles

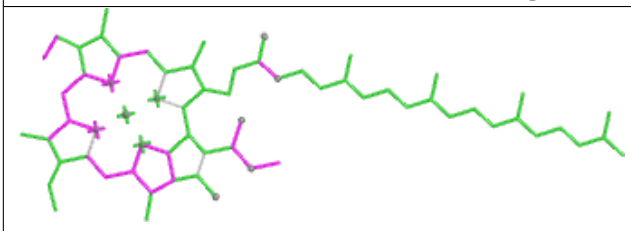
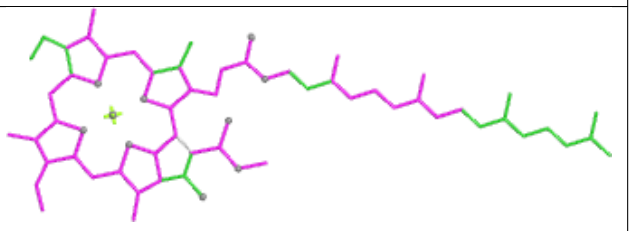
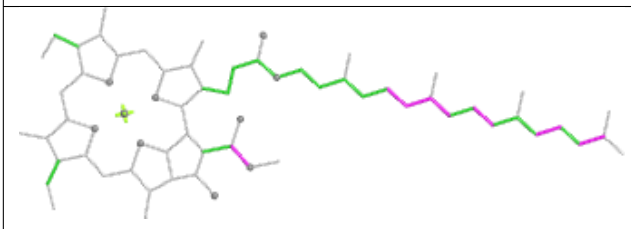
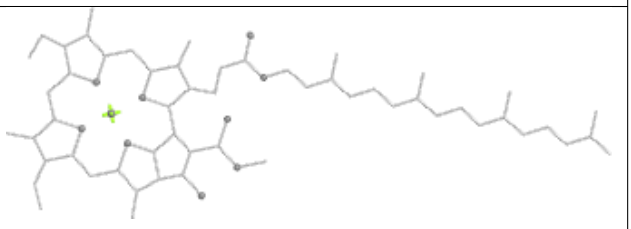


Torsions

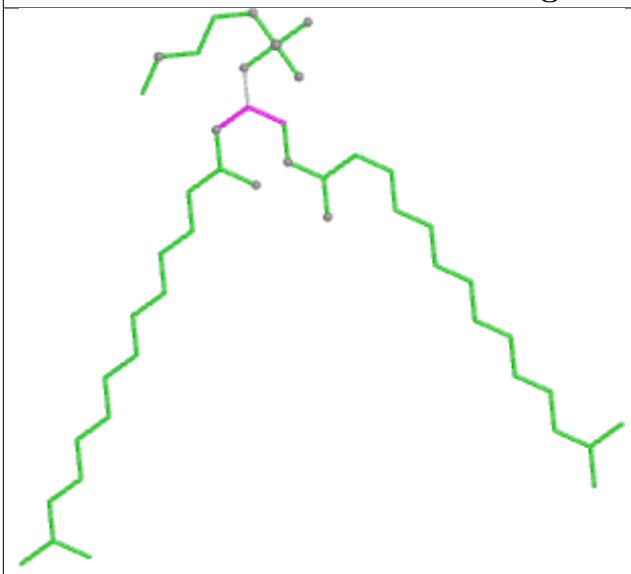


Rings

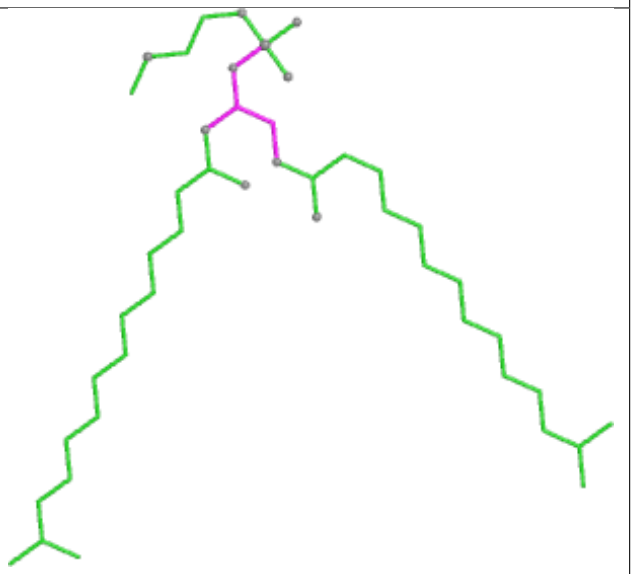
Ligand BCL a 909	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 910	
	
Bond lengths	Bond angles
	
Torsions	Rings

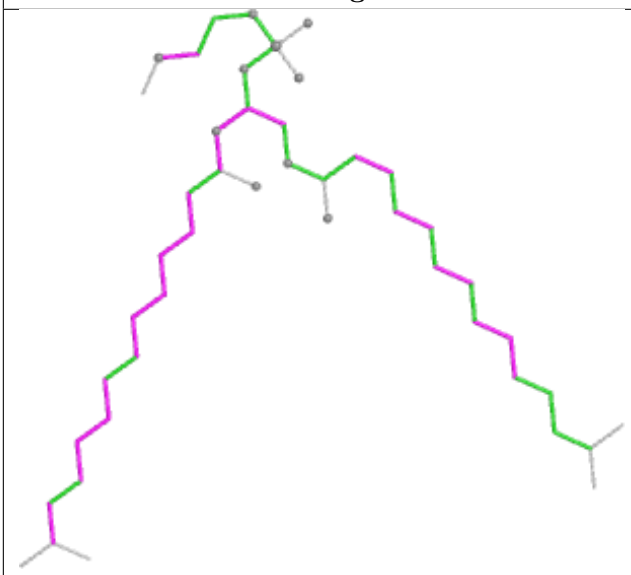
Ligand 85I a 918



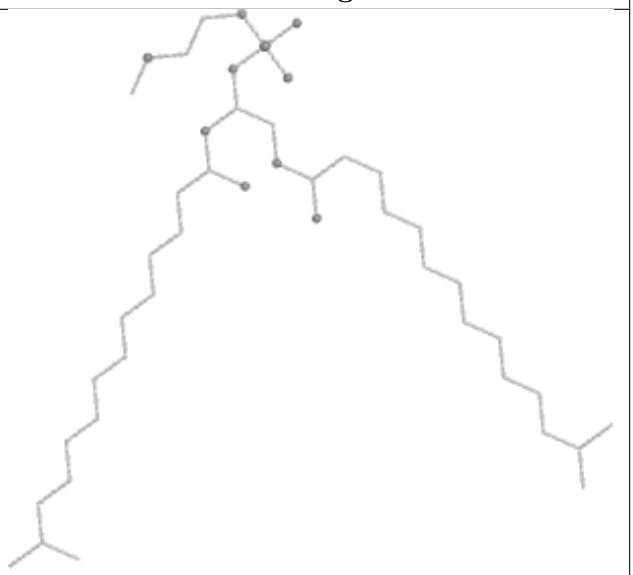
Bond lengths



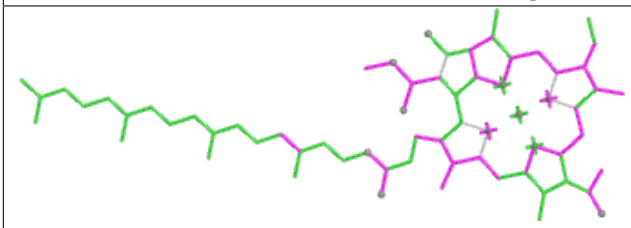
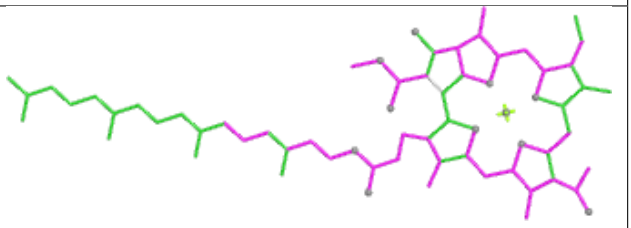
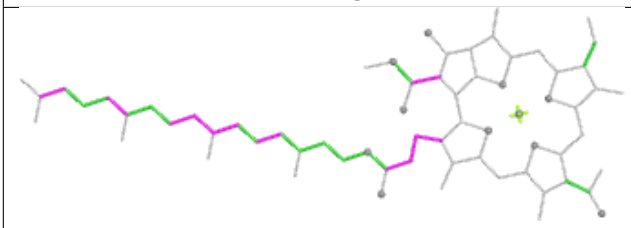
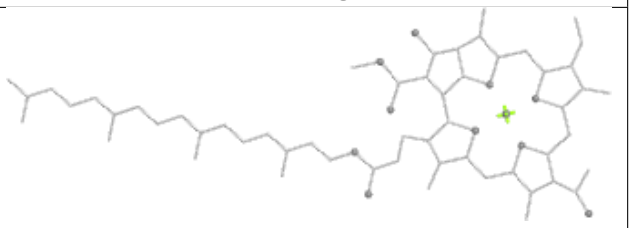
Bond angles

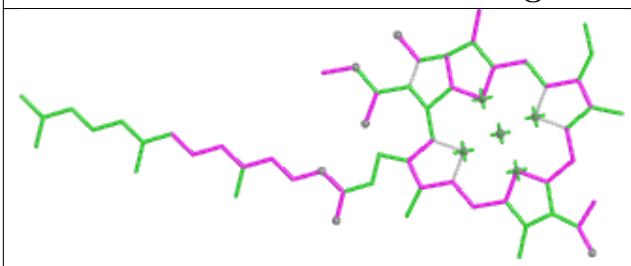
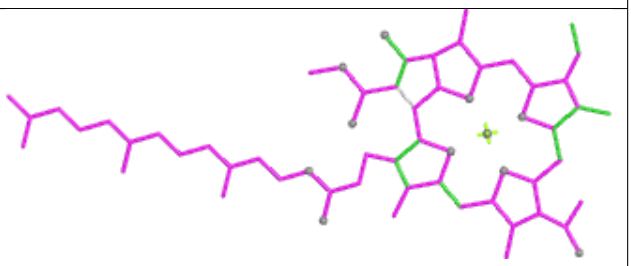
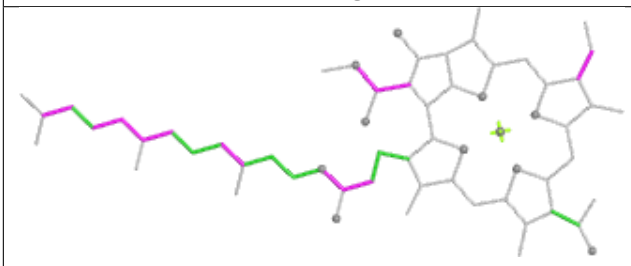
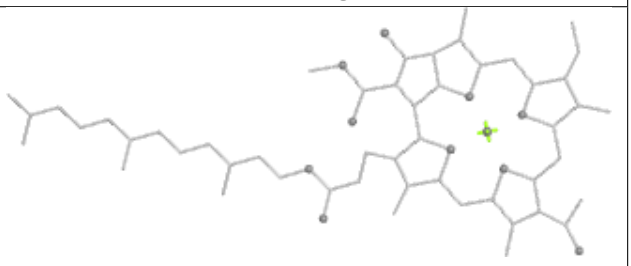


Torsions

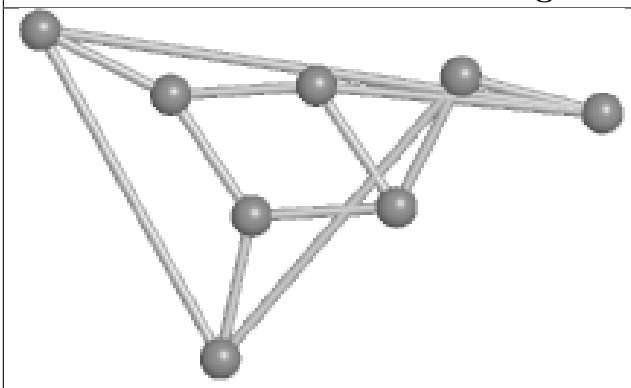


Rings

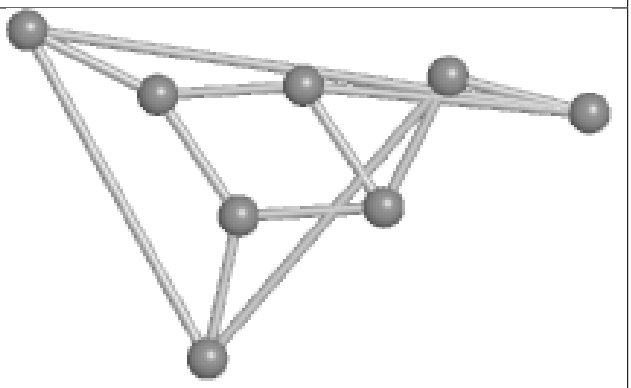
Ligand BCL A 908	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL A 907	
 Bond lengths	 Bond angles
 Torsions	 Rings

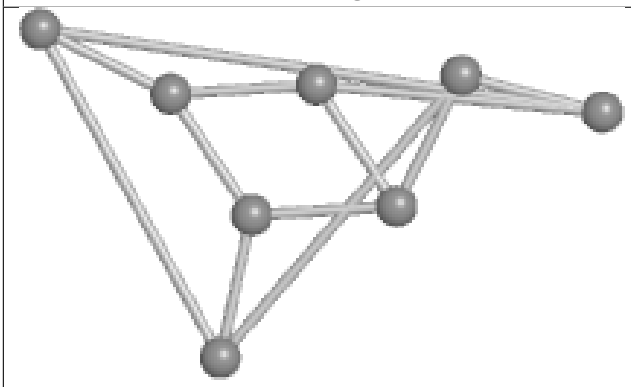
Ligand SF4 a 917



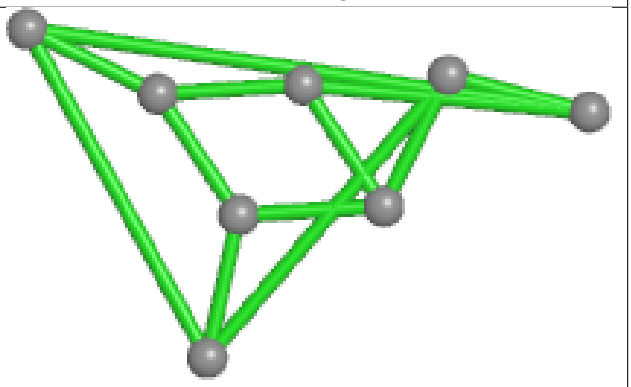
Bond lengths



Bond angles

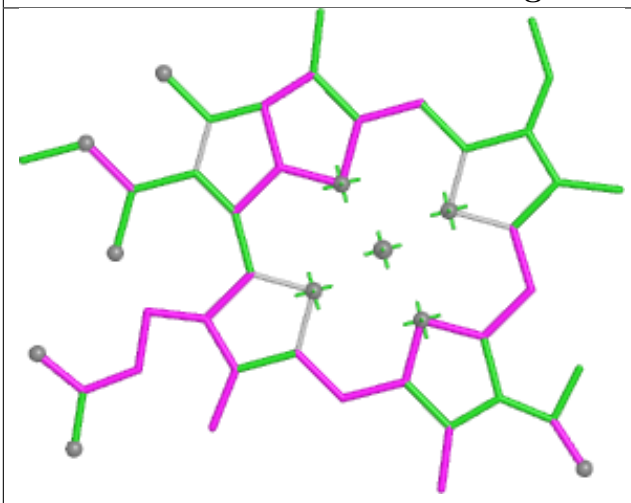


Torsions

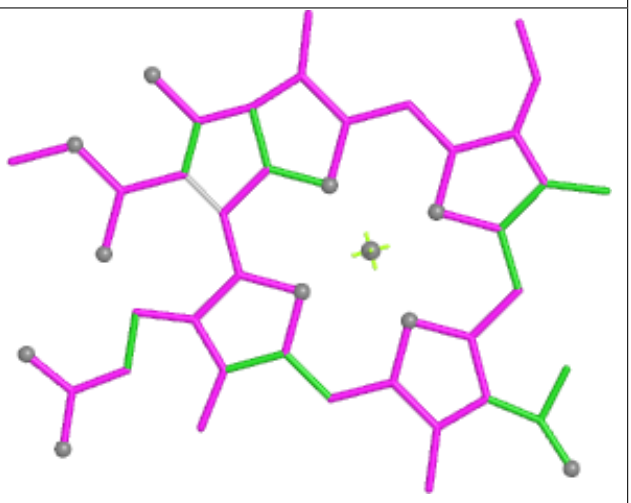


Rings

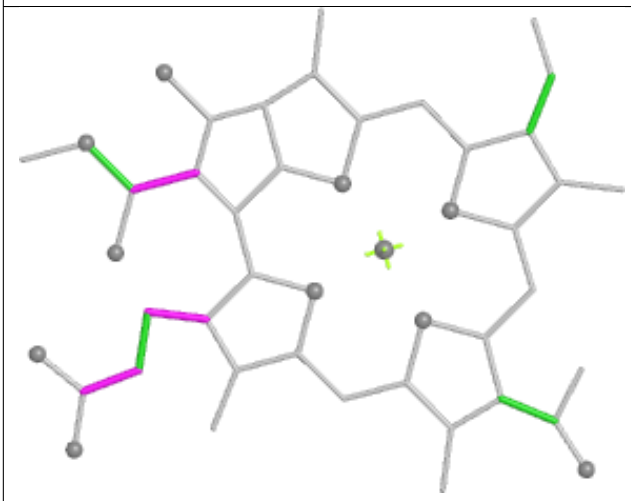
Ligand BCL A 904



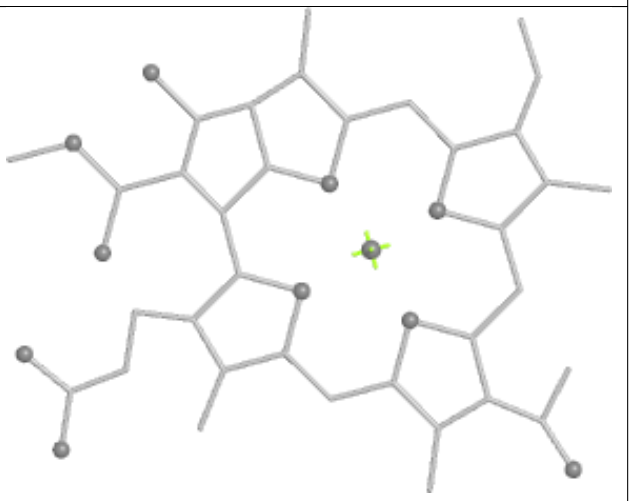
Bond lengths



Bond angles

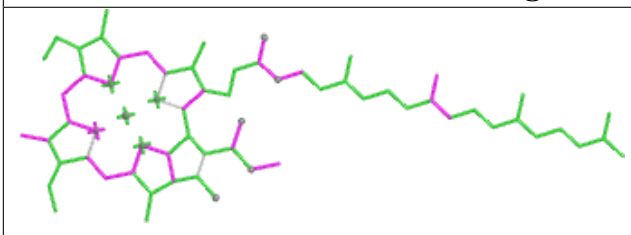


Torsions

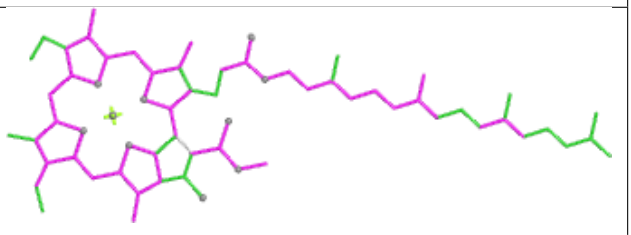


Rings

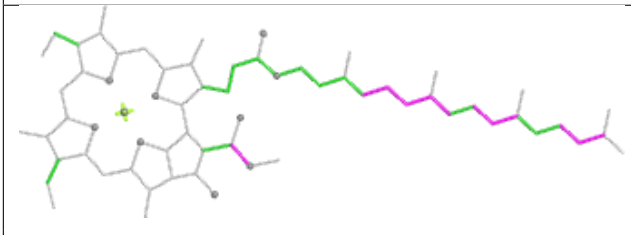
Ligand CLA A 911



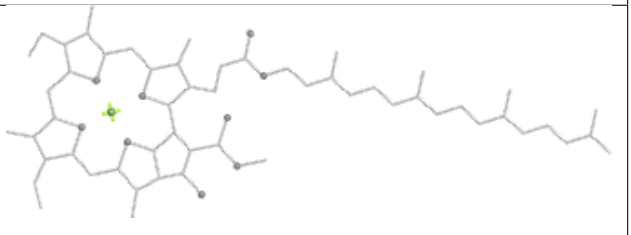
Bond lengths



Bond angles

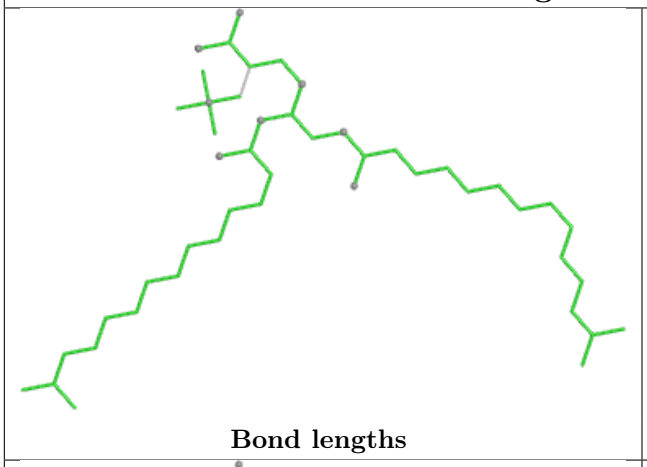


Torsions

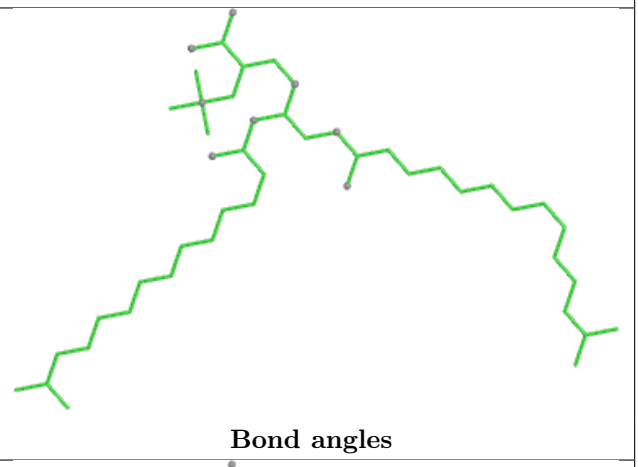


Rings

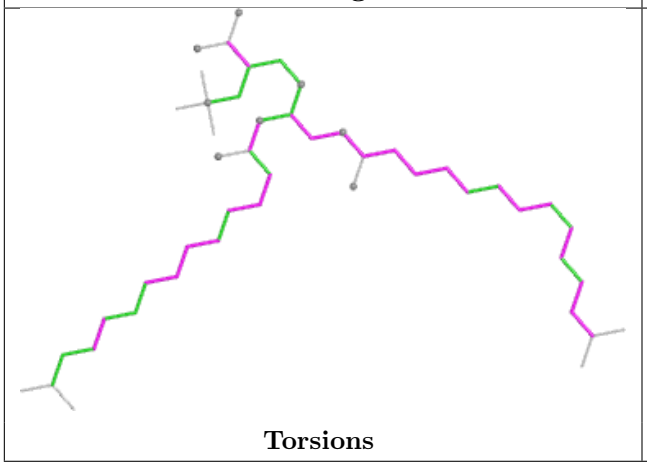
Ligand 85N a 902



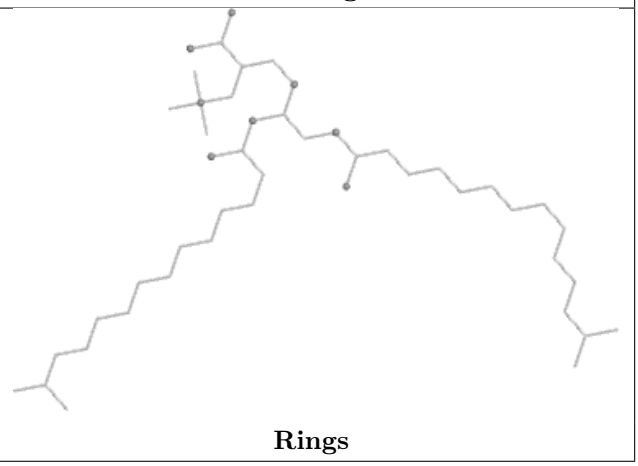
Bond lengths



Bond angles

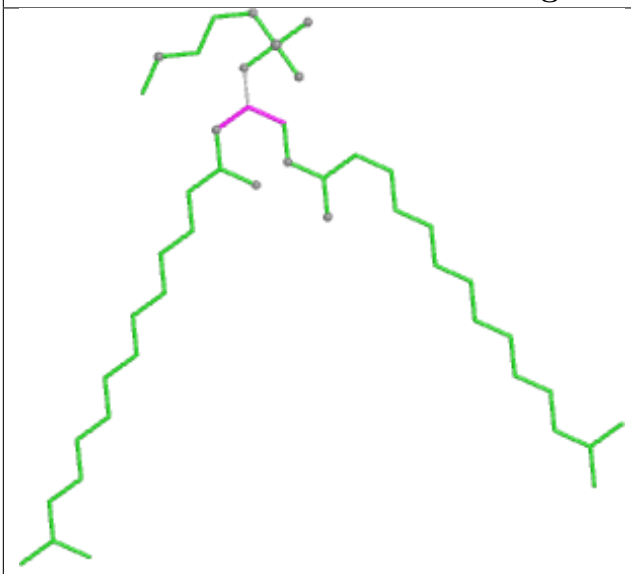


Torsions

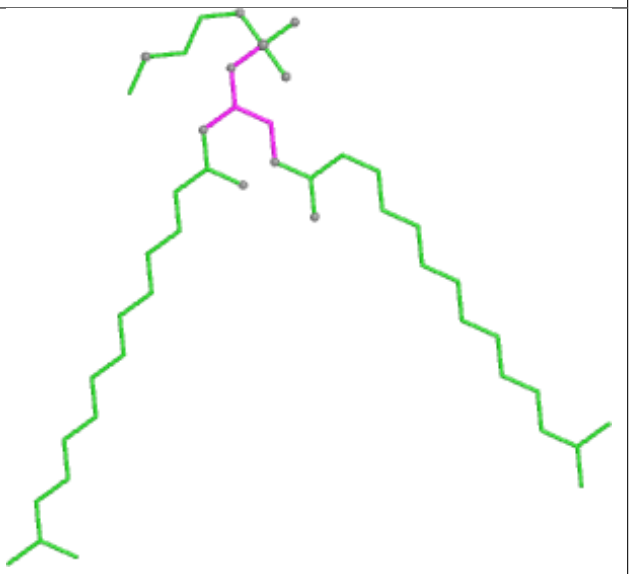


Rings

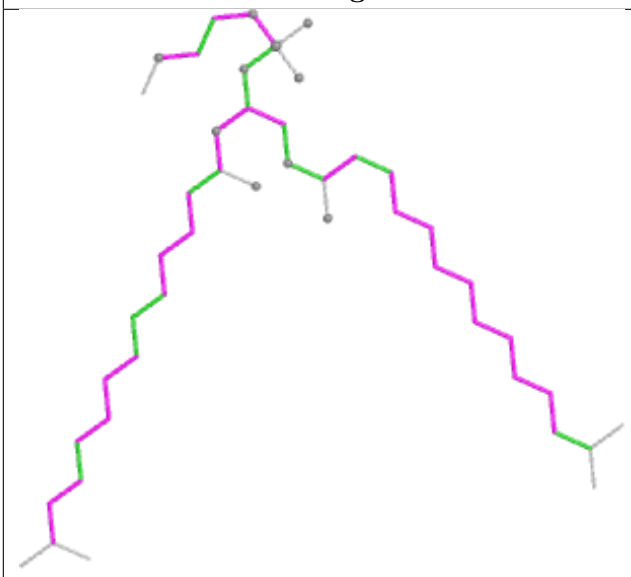
Ligand 85I a 920



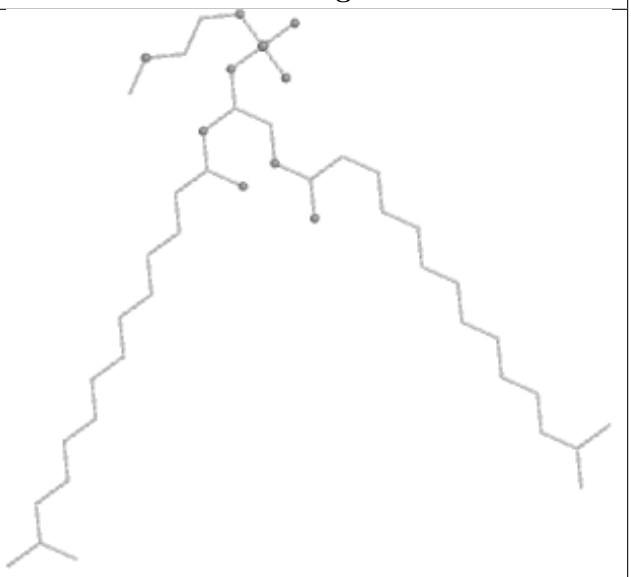
Bond lengths



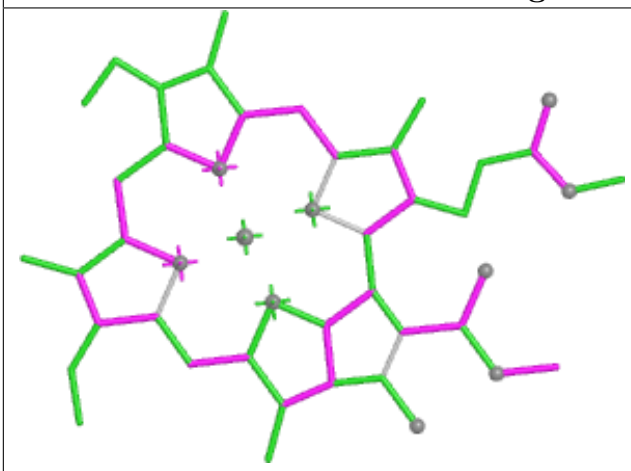
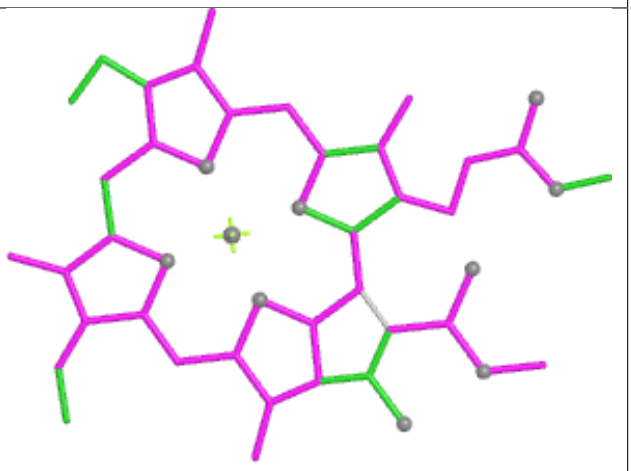
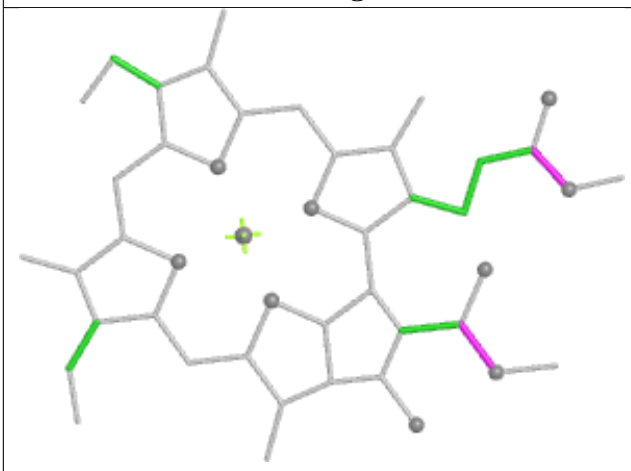
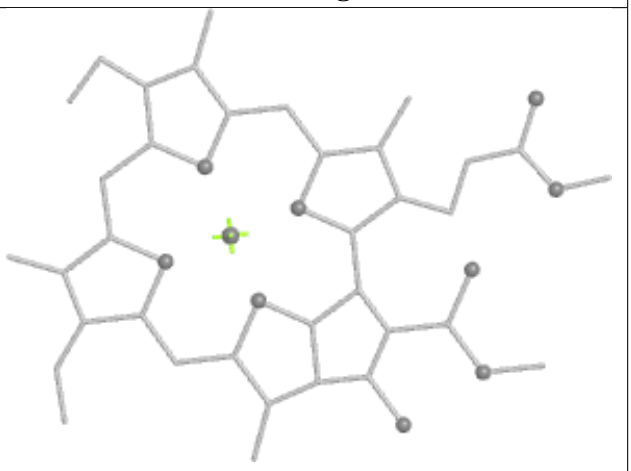
Bond angles



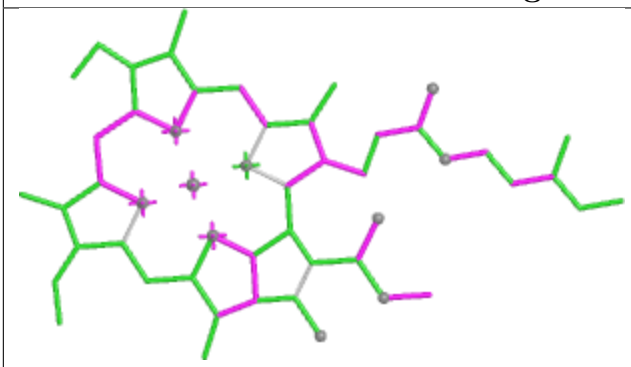
Torsions



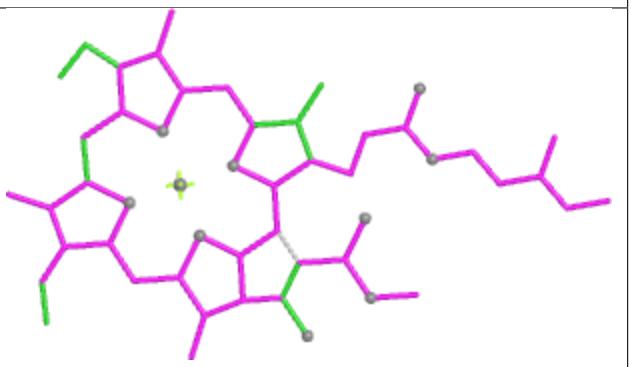
Rings

Ligand CLA a 914	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

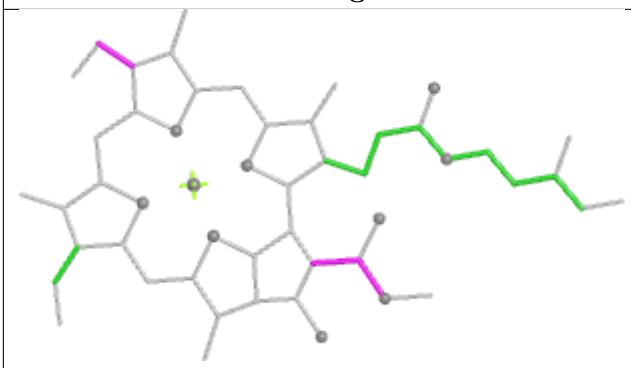
Ligand CLA A 933



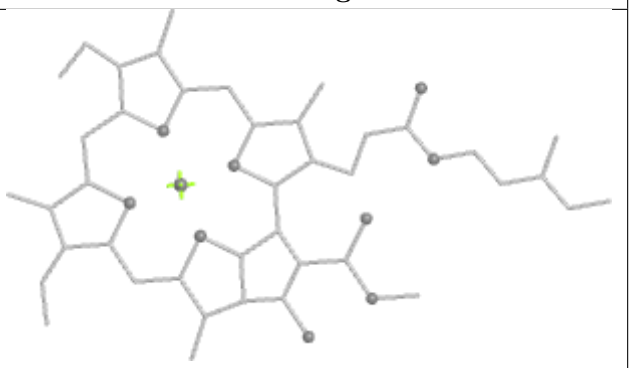
Bond lengths



Bond angles

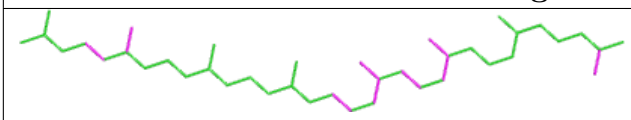


Torsions

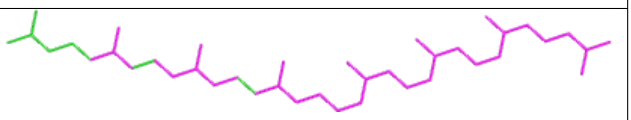


Rings

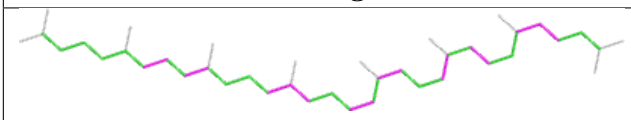
Ligand LYC c 201



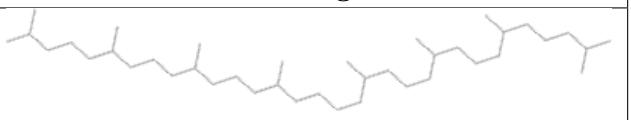
Bond lengths



Bond angles

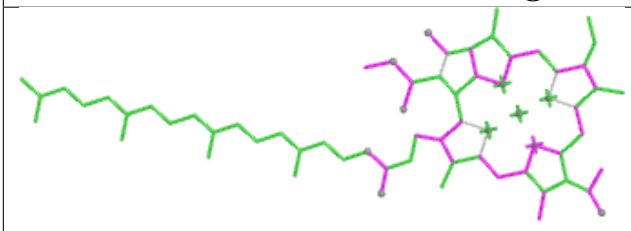


Torsions

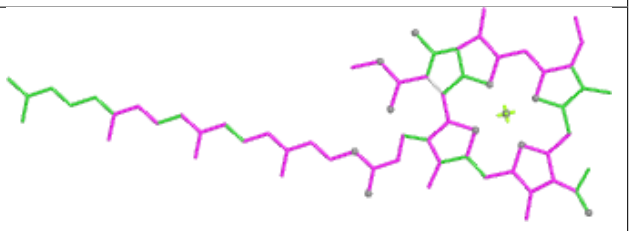


Rings

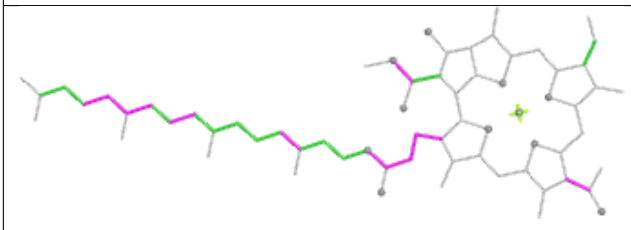
Ligand BCL A 902



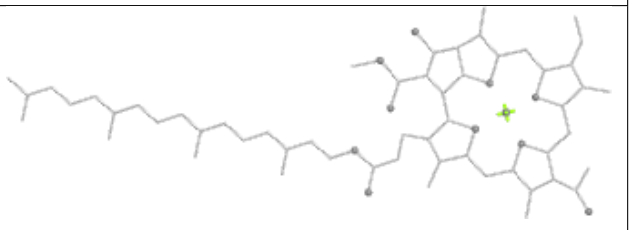
Bond lengths



Bond angles

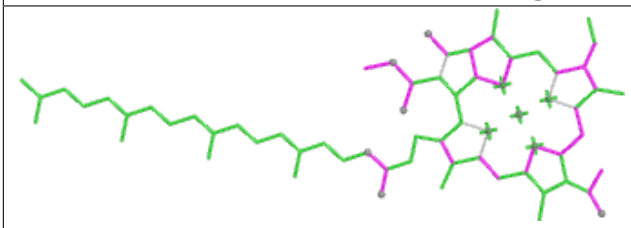


Torsions

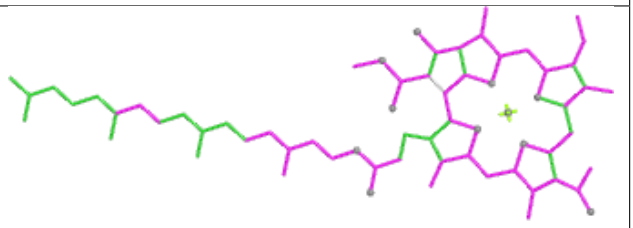


Rings

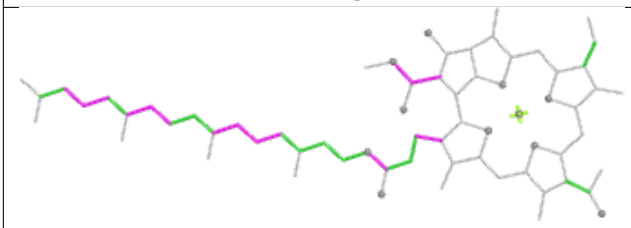
Ligand BCL a 905



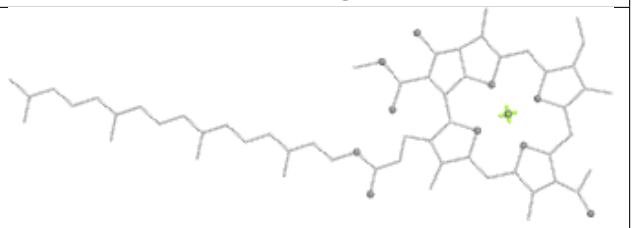
Bond lengths



Bond angles

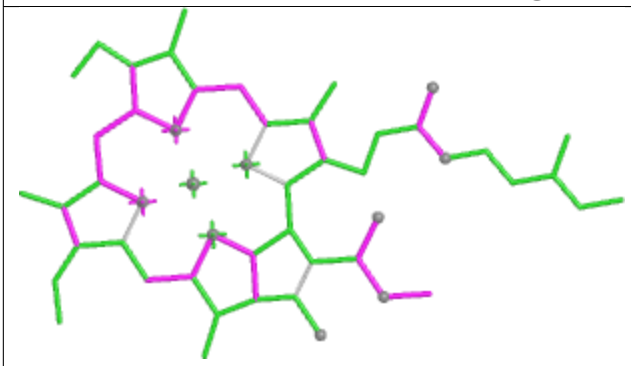


Torsions

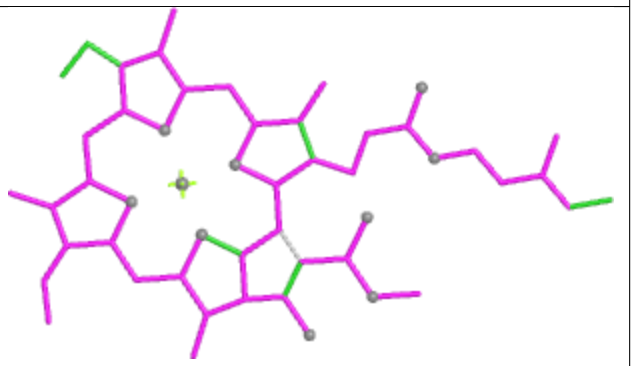


Rings

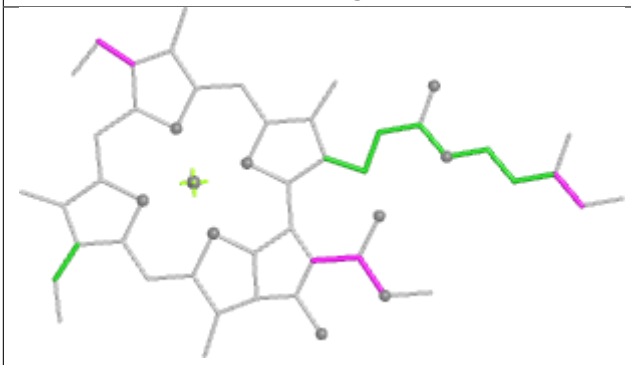
Ligand CLA a 915



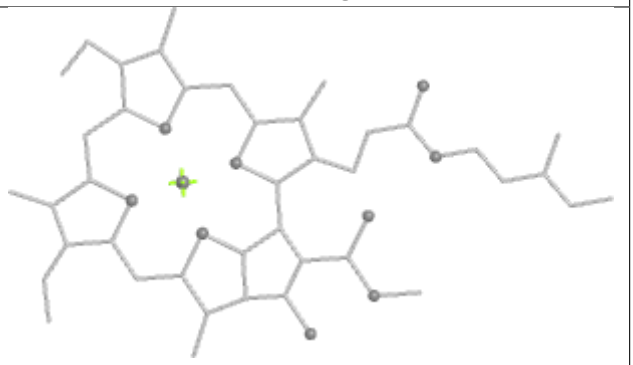
Bond lengths



Bond angles

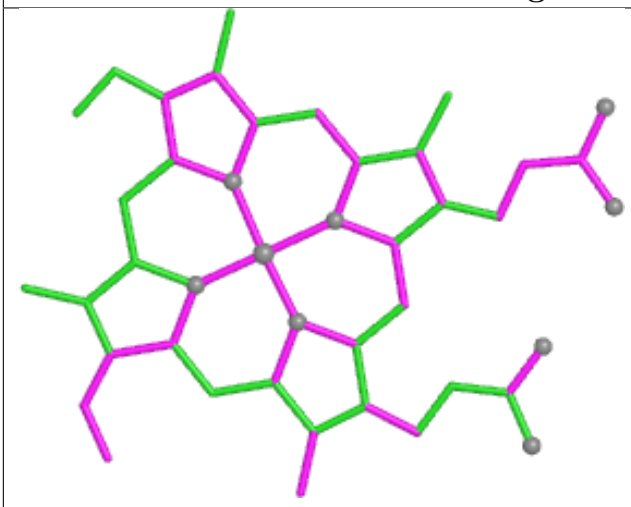


Torsions

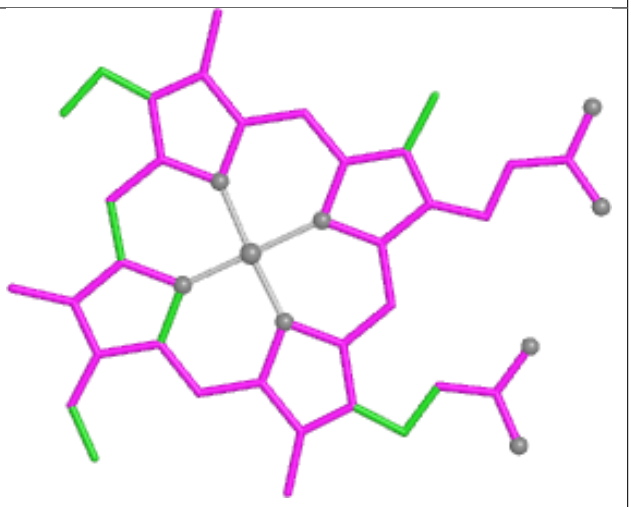


Rings

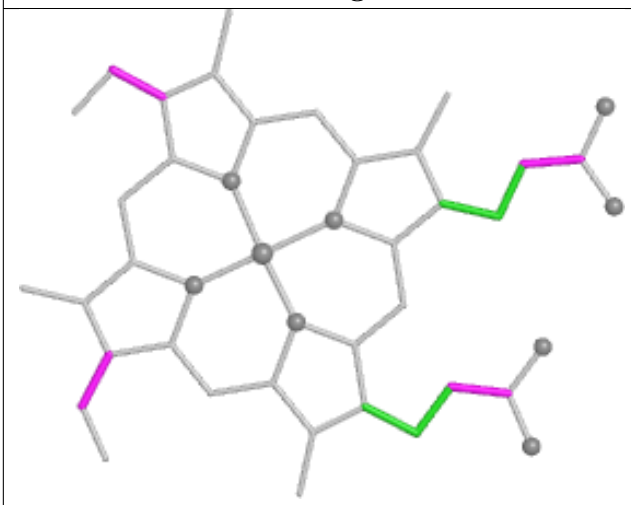
Ligand HEC c 202



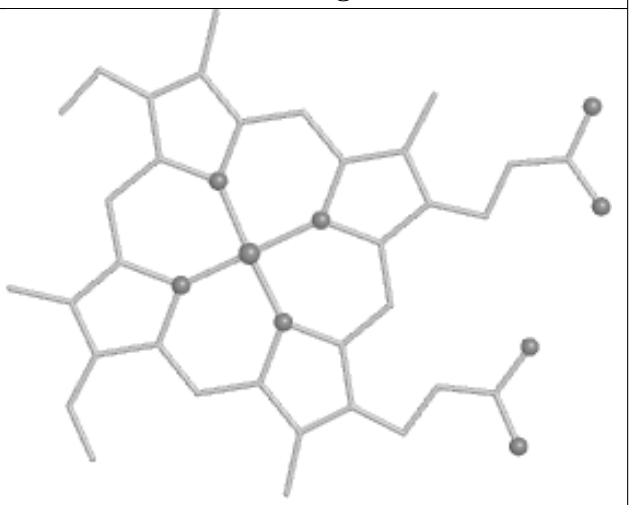
Bond lengths



Bond angles

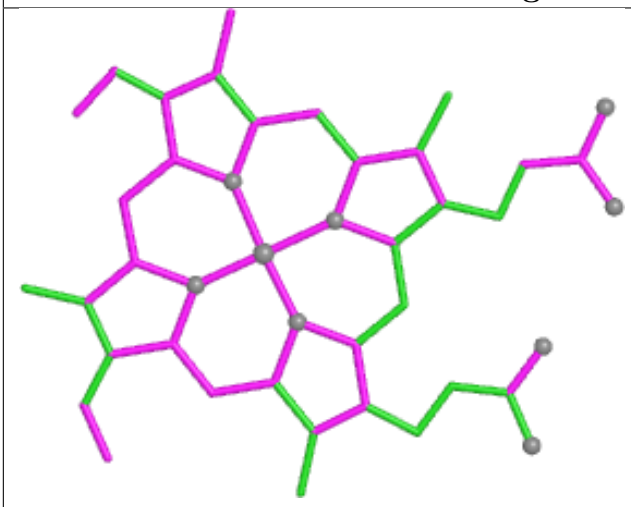


Torsions

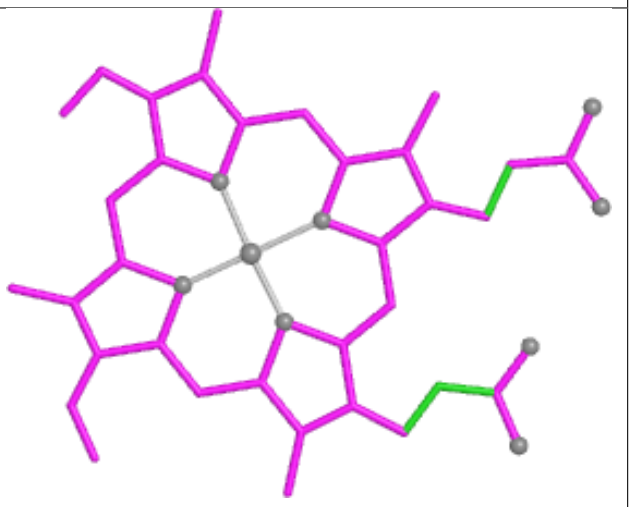


Rings

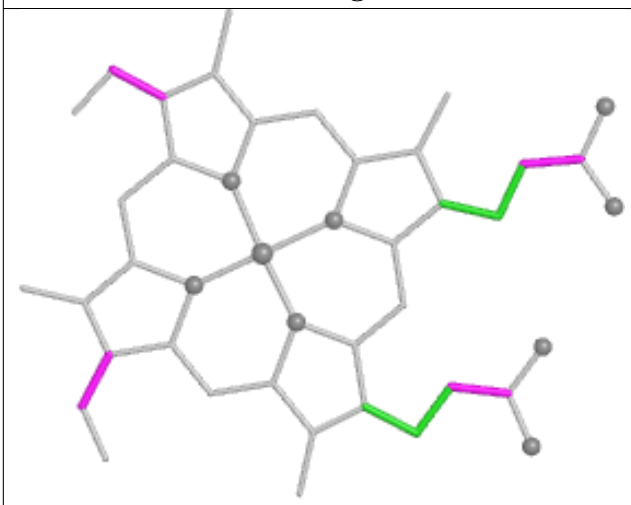
Ligand HEC C 301



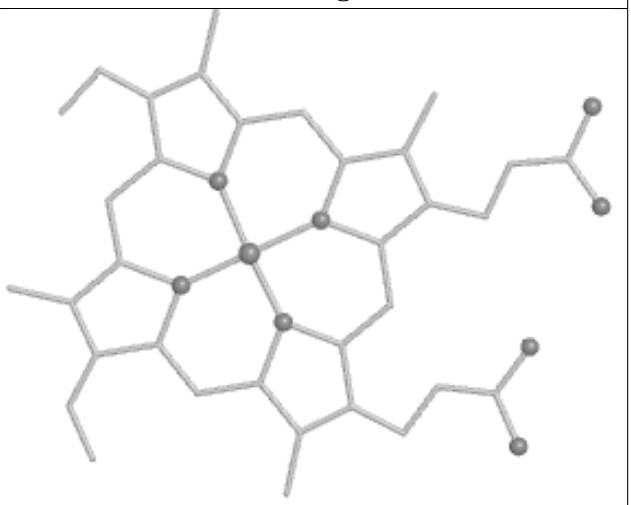
Bond lengths



Bond angles

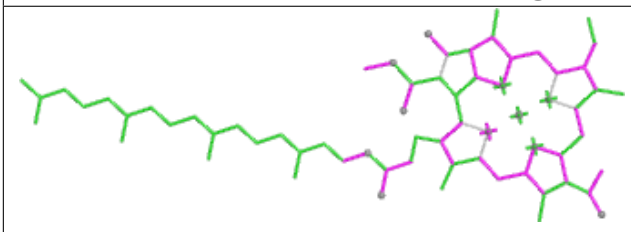


Torsions

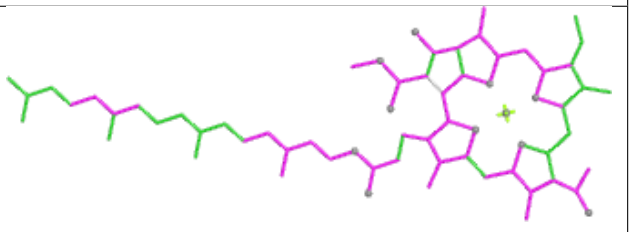


Rings

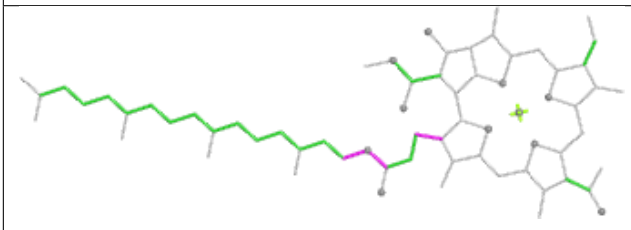
Ligand BCL a 911



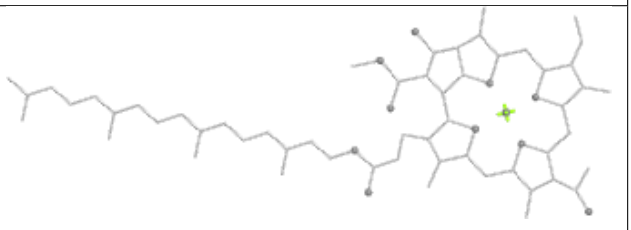
Bond lengths



Bond angles

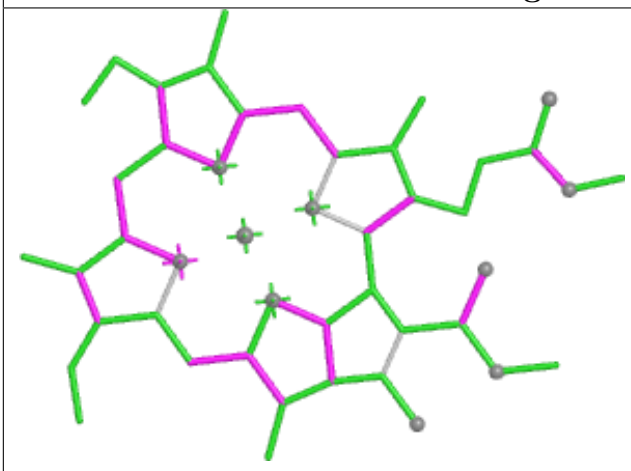


Torsions

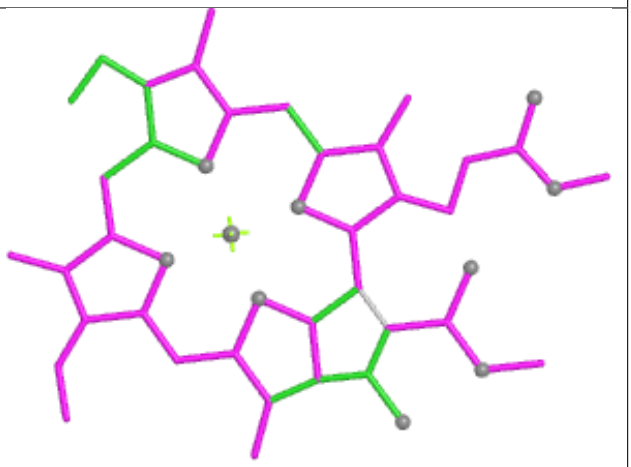


Rings

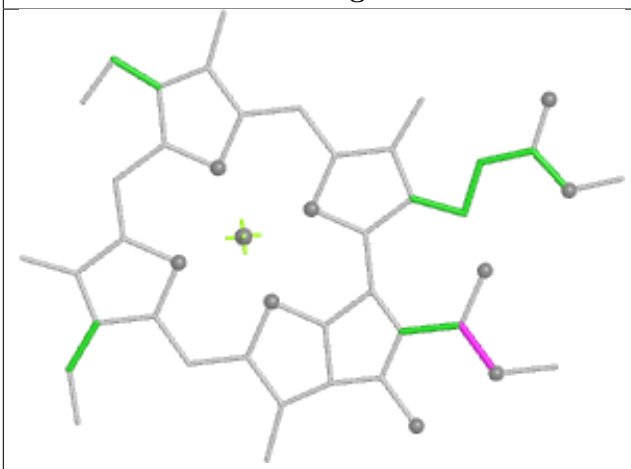
Ligand CLA A 912



Bond lengths



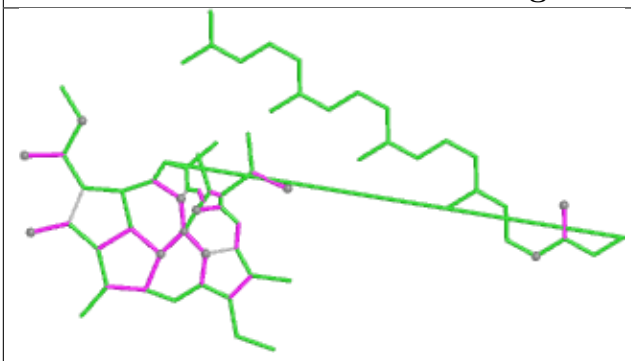
Bond angles



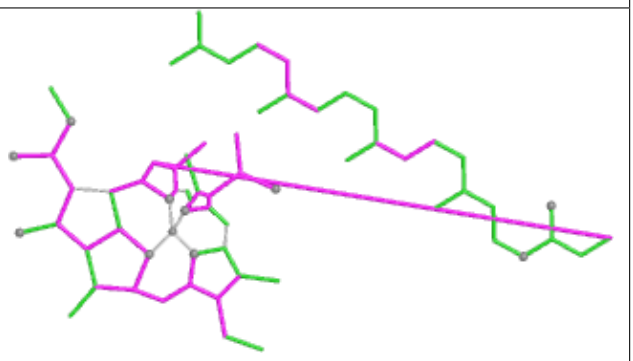
Torsions

Rings

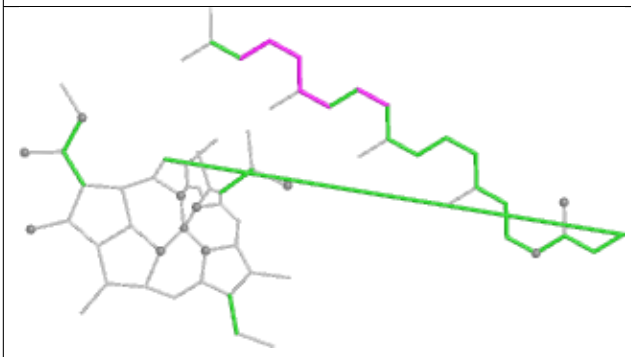
Ligand 2GO a 903



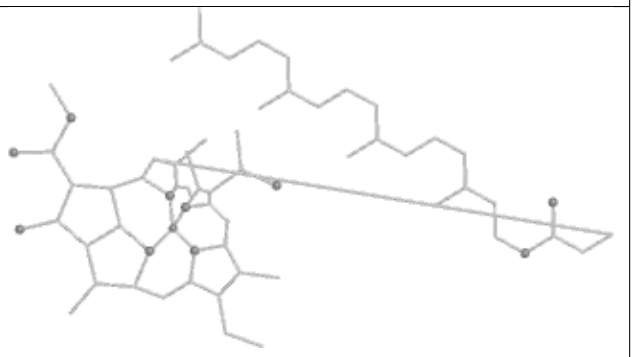
Bond lengths



Bond angles

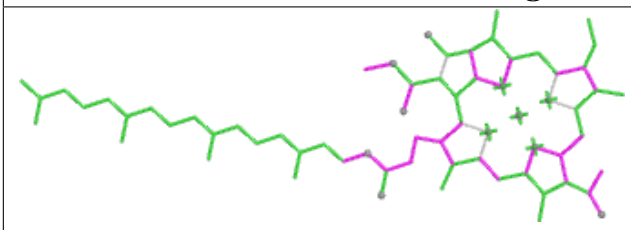


Torsions

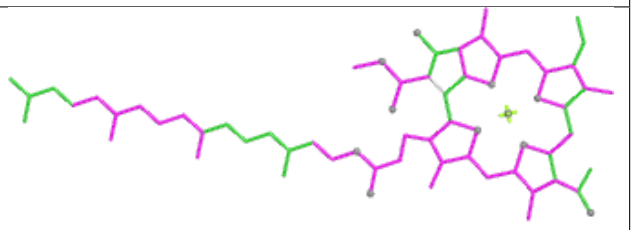


Rings

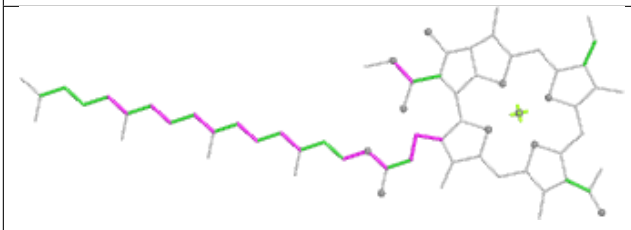
Ligand BCL A 905



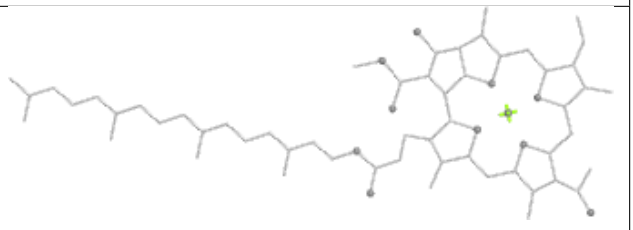
Bond lengths



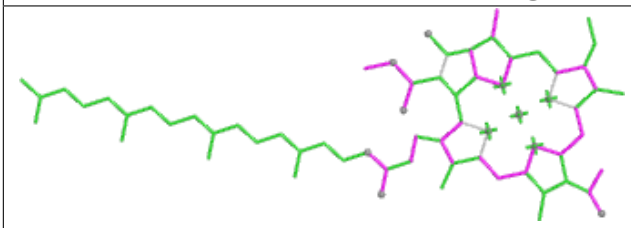
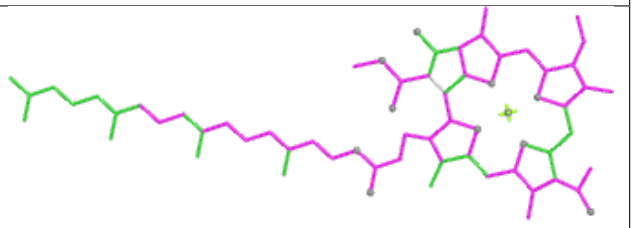
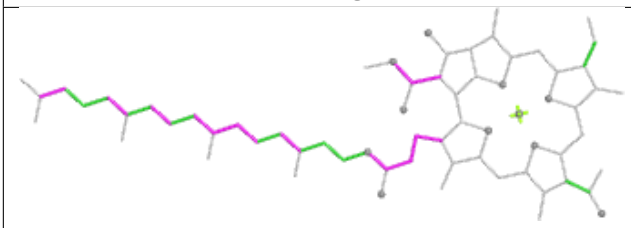
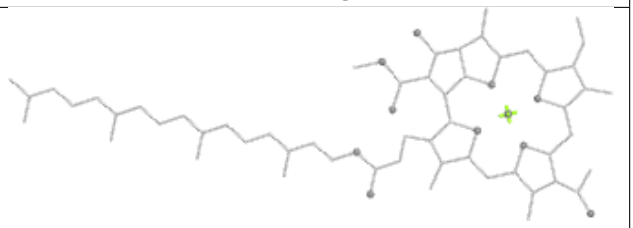
Bond angles



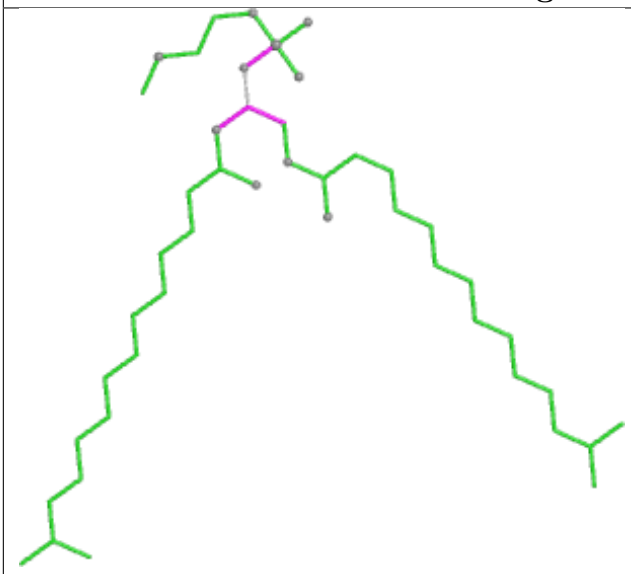
Torsions



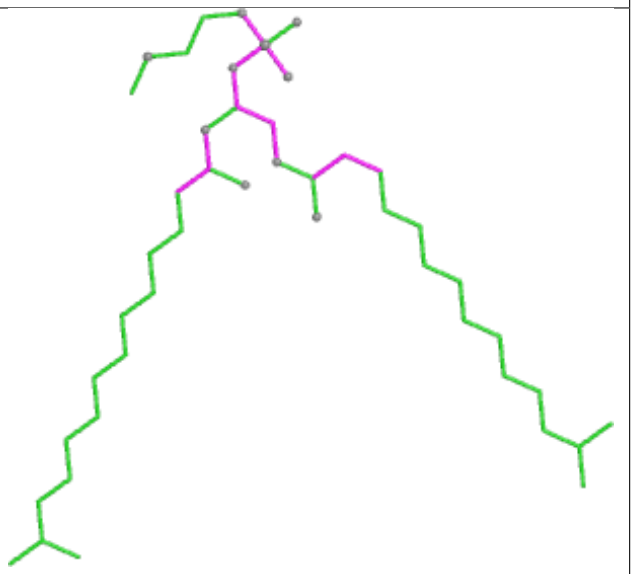
Rings

Ligand BCL A 903	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

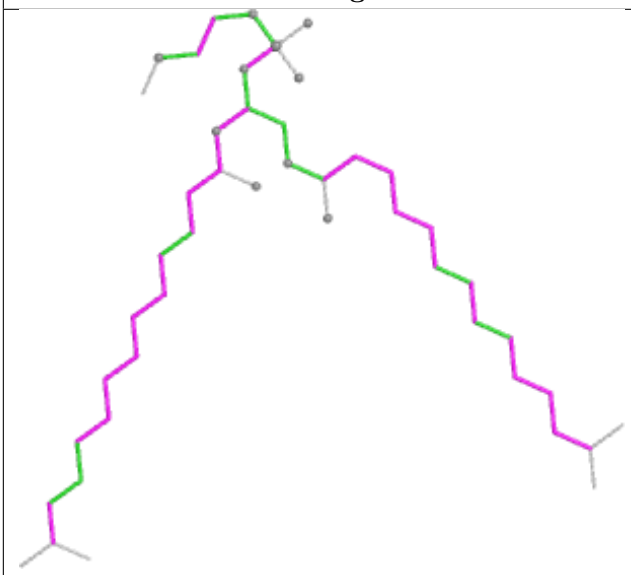
Ligand 85I A 916



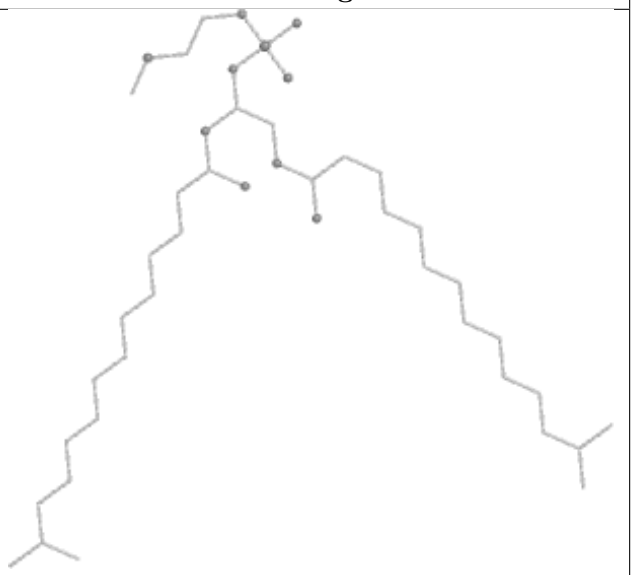
Bond lengths



Bond angles

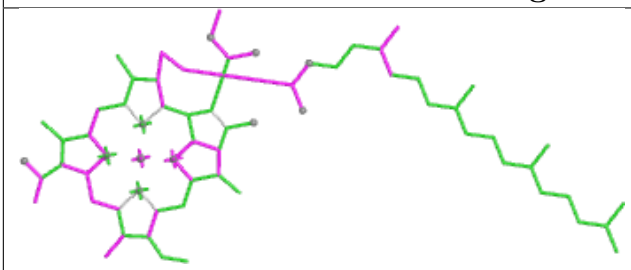


Torsions

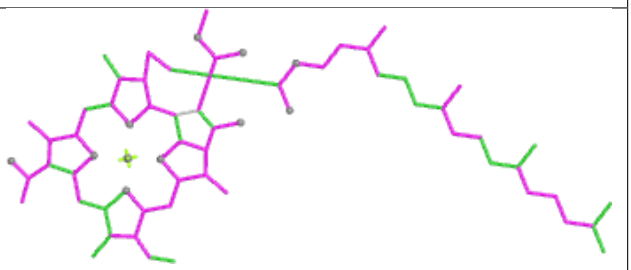


Rings

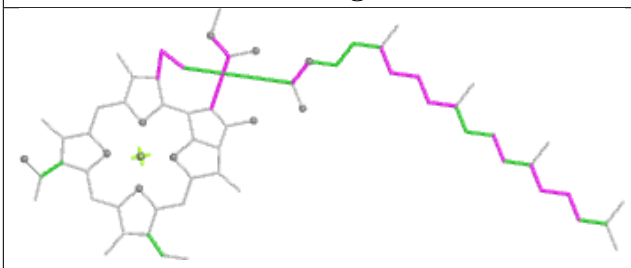
Ligand BCL a 908



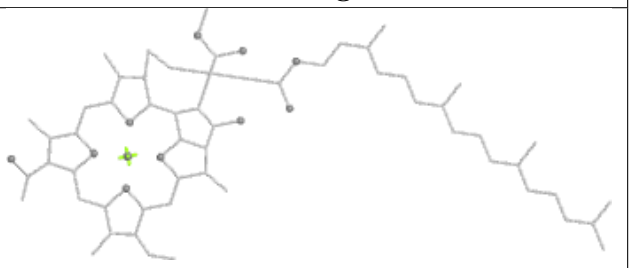
Bond lengths



Bond angles

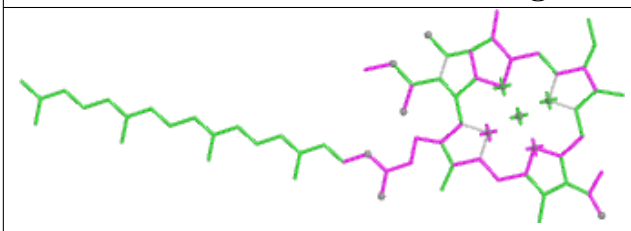


Torsions

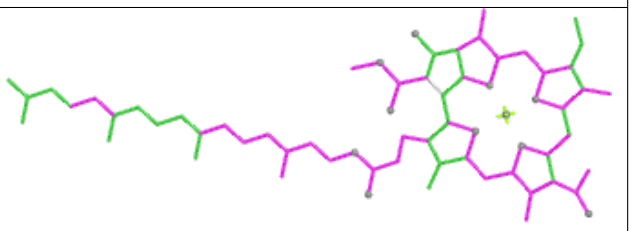


Rings

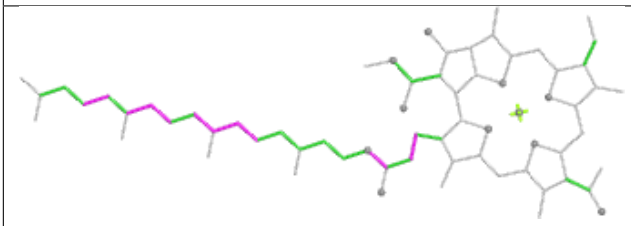
Ligand BCL a 907



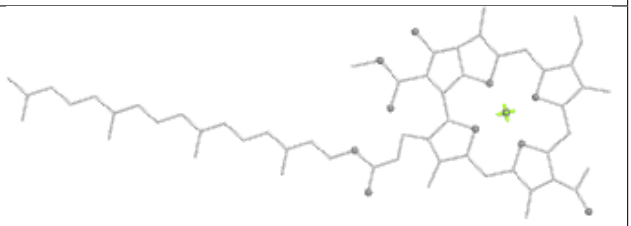
Bond lengths



Bond angles

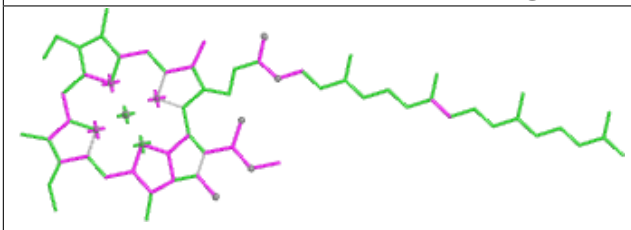


Torsions

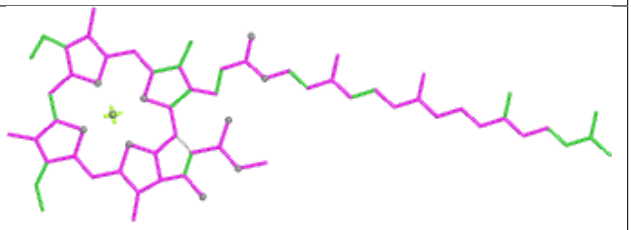


Rings

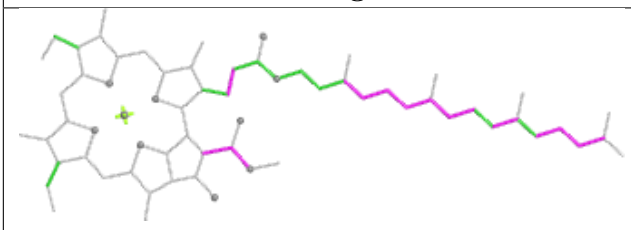
Ligand CLA A 931



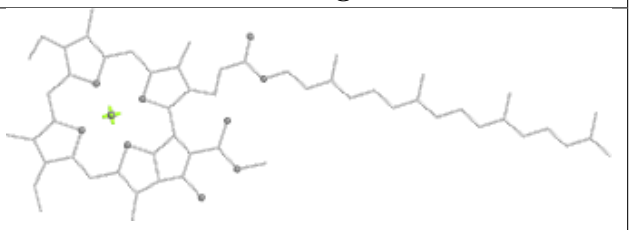
Bond lengths



Bond angles

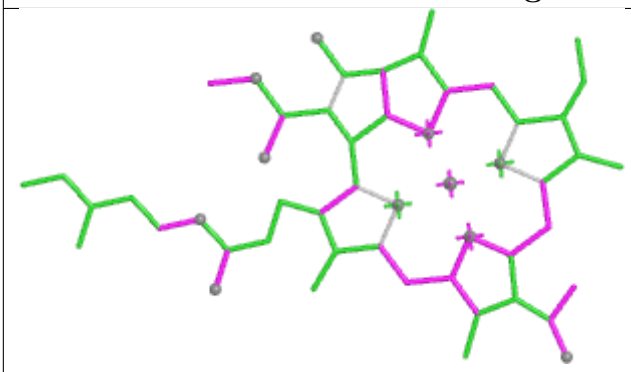


Torsions

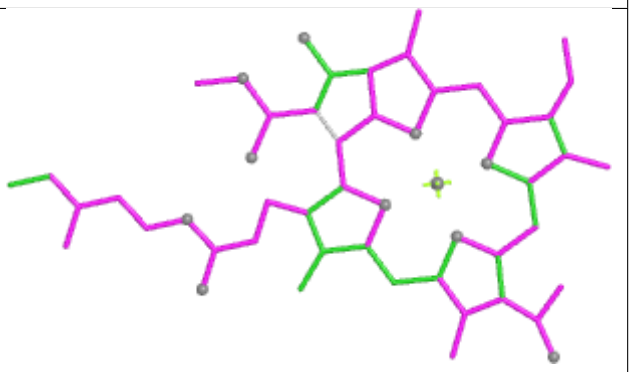


Rings

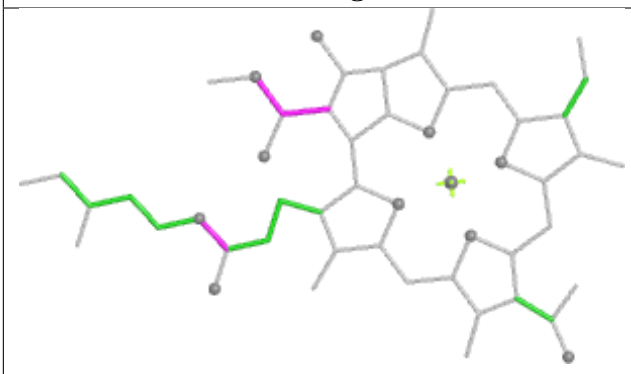
Ligand BCL A 906



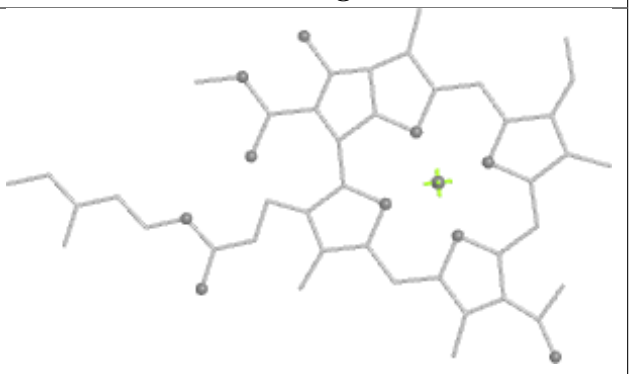
Bond lengths



Bond angles

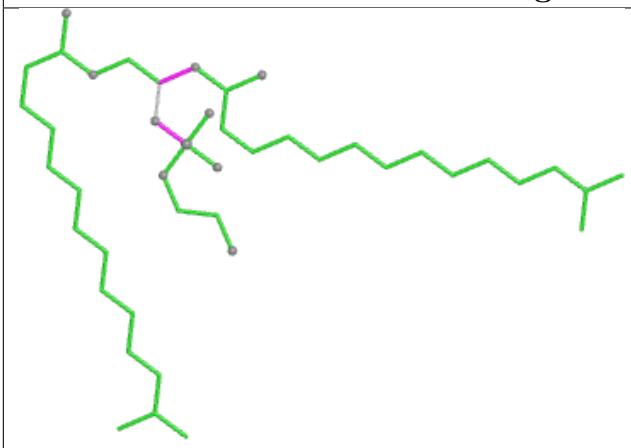


Torsions

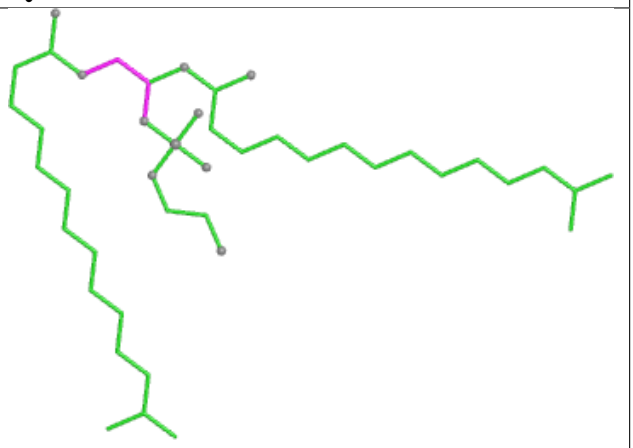


Rings

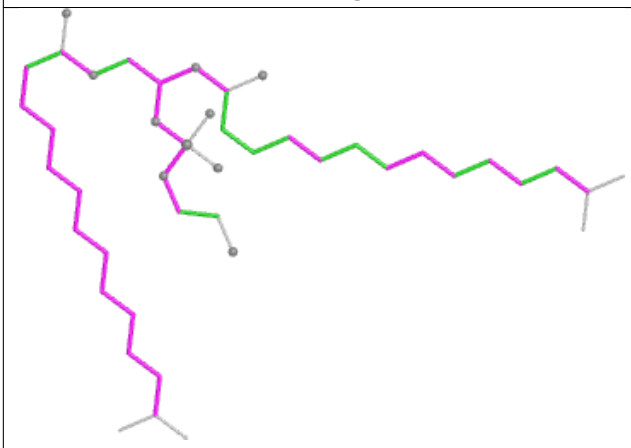
Ligand 84Q a 921



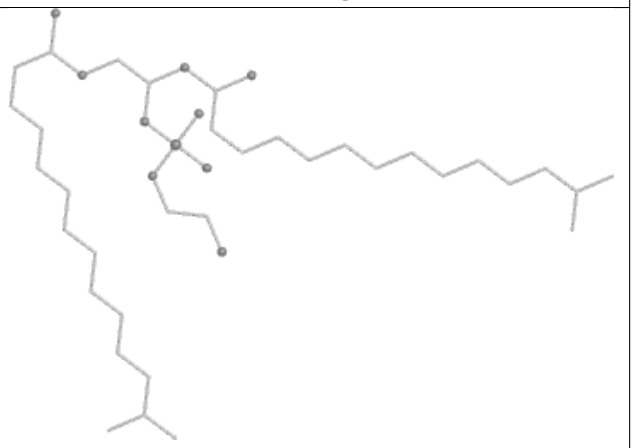
Bond lengths



Bond angles

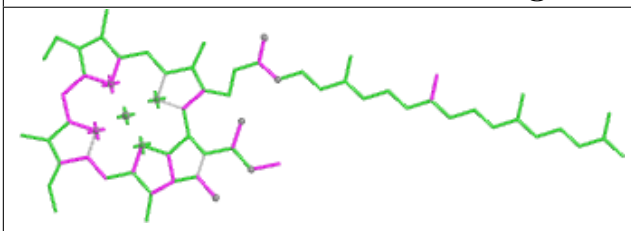


Torsions

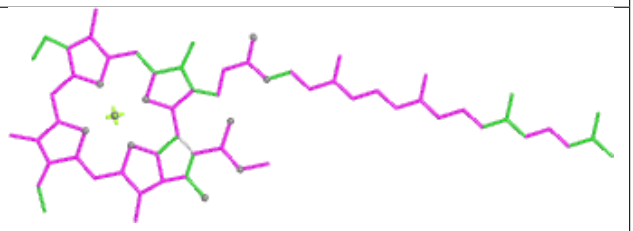


Rings

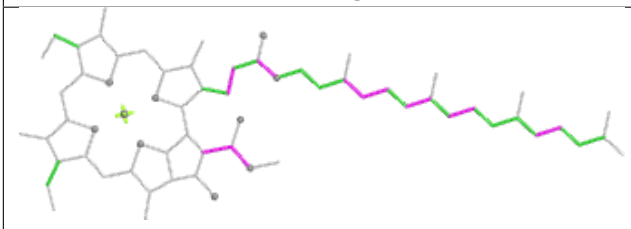
Ligand CLA a 912



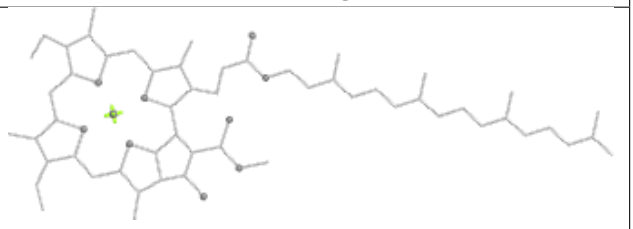
Bond lengths



Bond angles

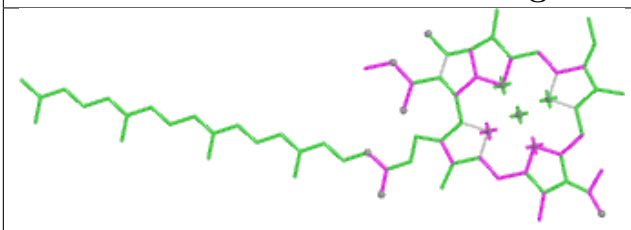


Torsions

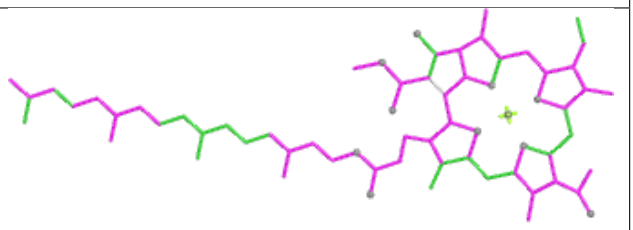


Rings

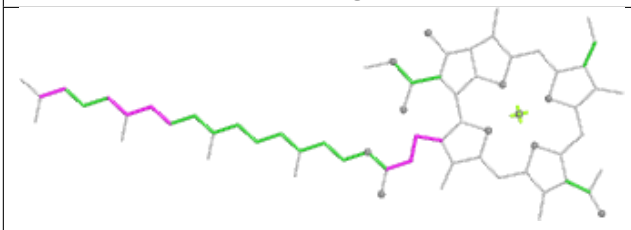
Ligand BCL a 910



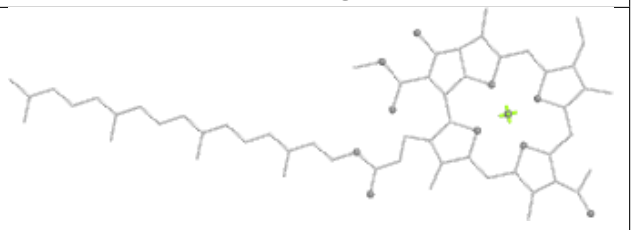
Bond lengths



Bond angles

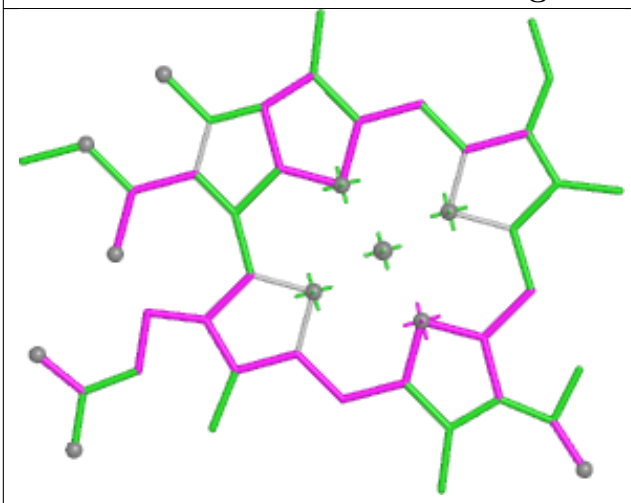


Torsions

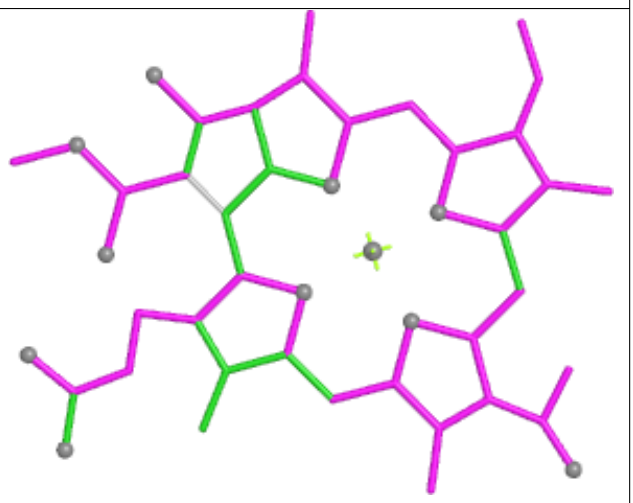


Rings

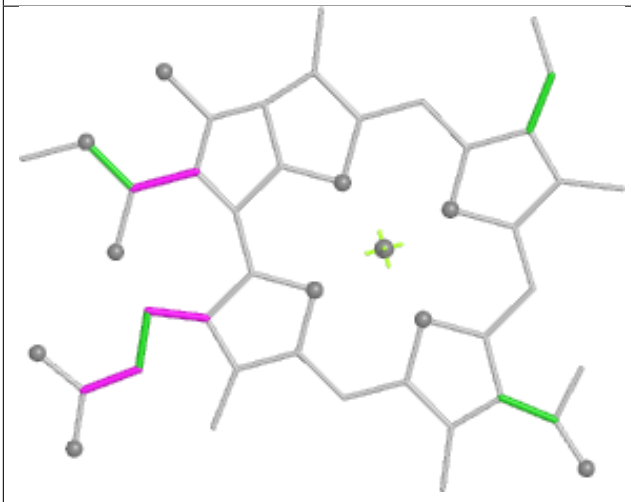
Ligand BCL a 906



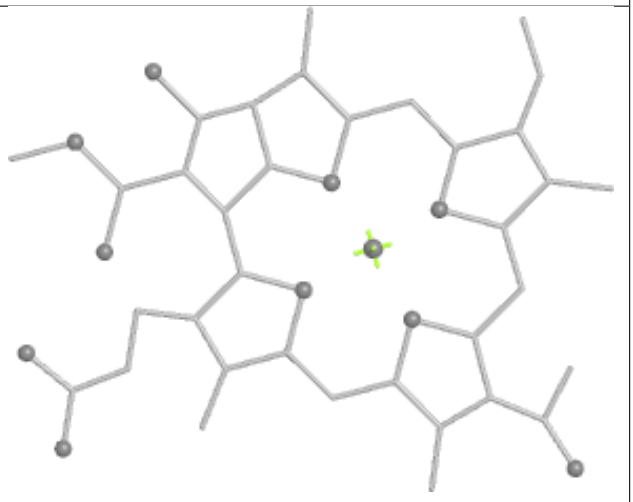
Bond lengths



Bond angles

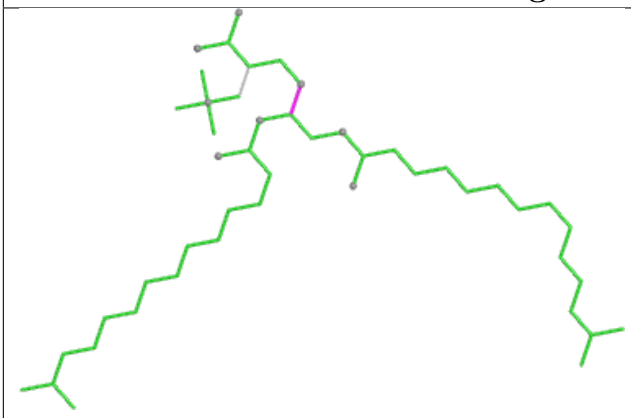


Torsions

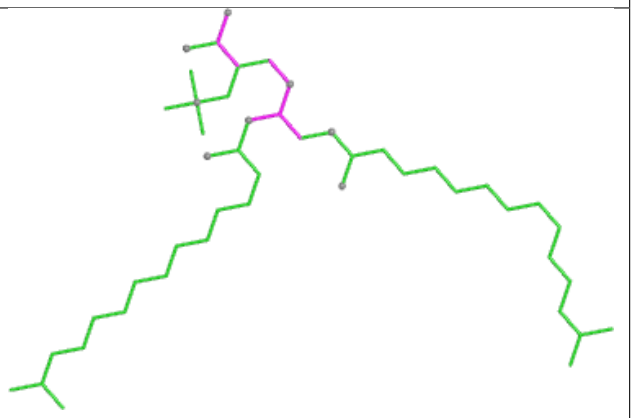


Rings

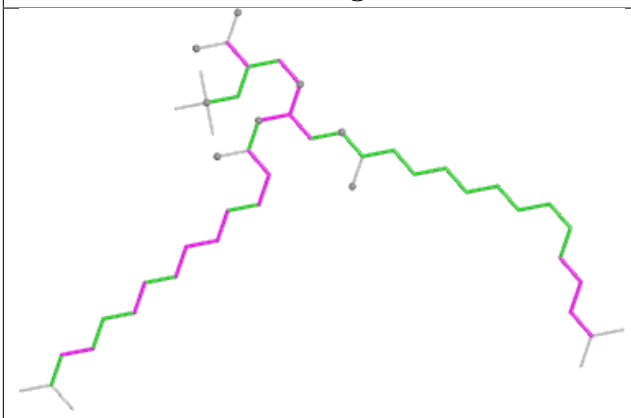
Ligand 85N A 932



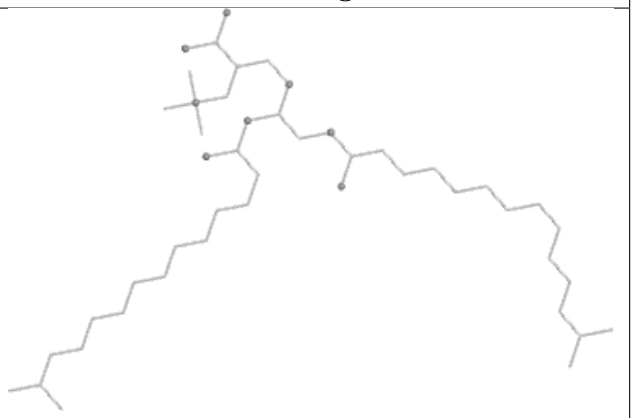
Bond lengths



Bond angles

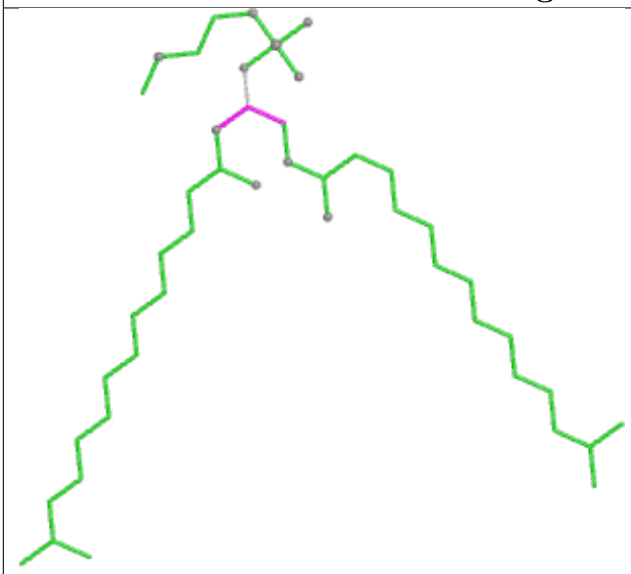


Torsions

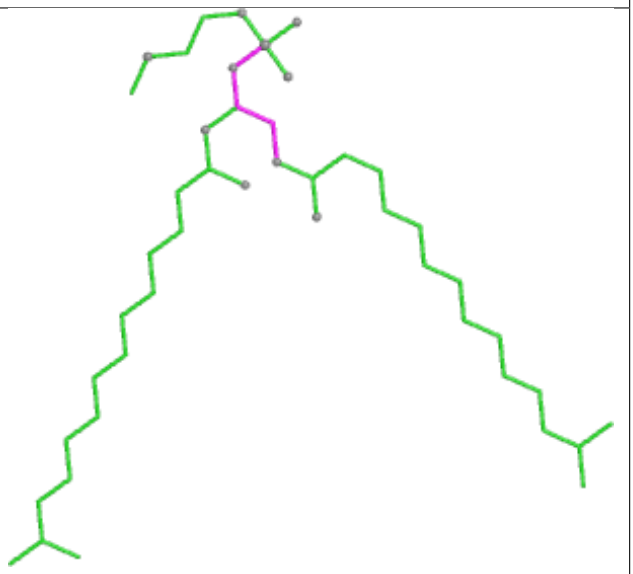


Rings

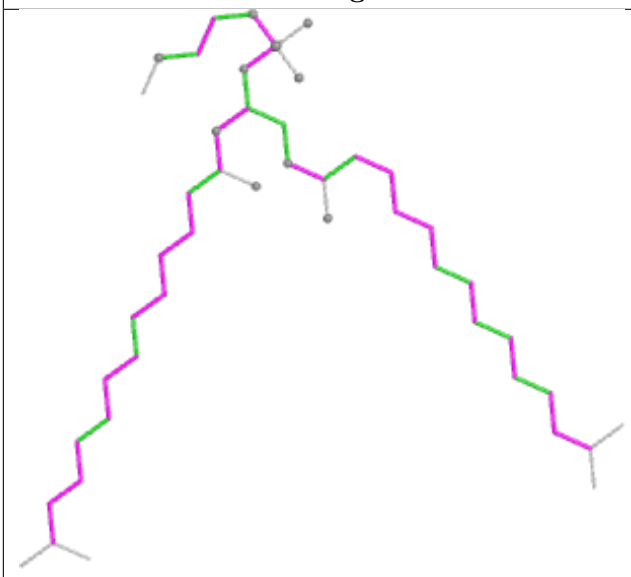
Ligand 85I A 917



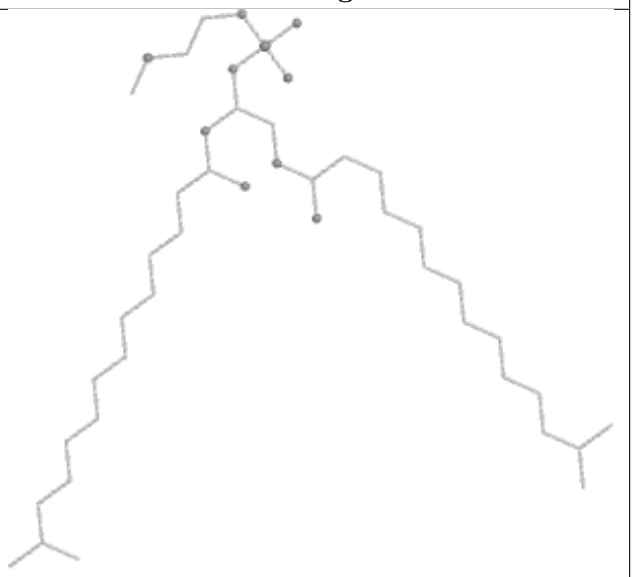
Bond lengths



Bond angles

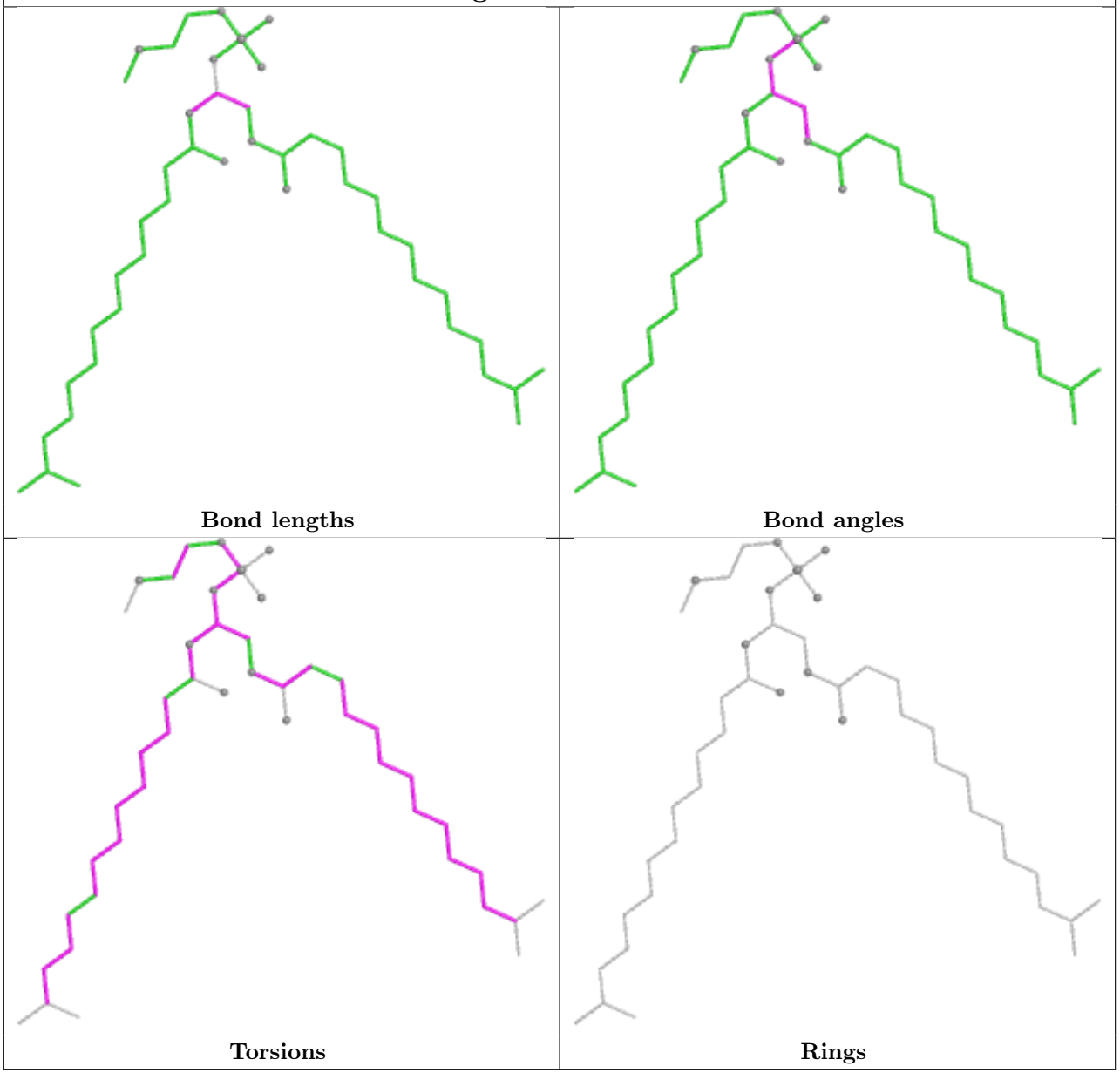


Torsions



Rings

Ligand 85I a 919



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.

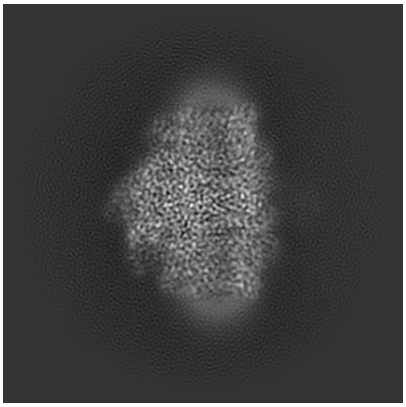
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32229. These allow visual inspection of the internal detail of the map and identification of artifacts.

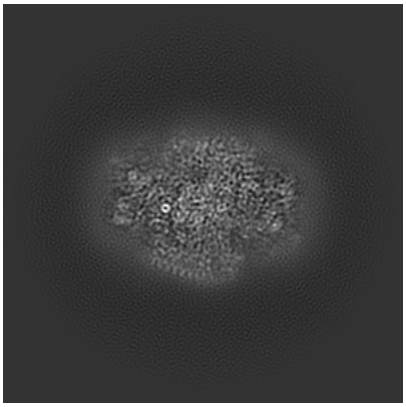
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

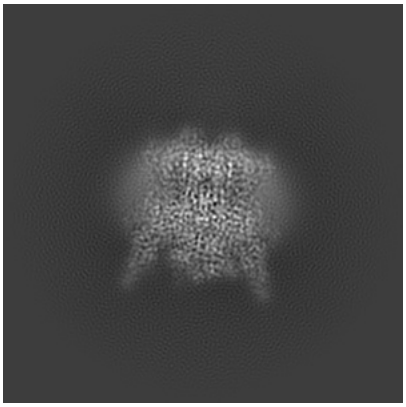
6.1.1 Primary map



X



Y

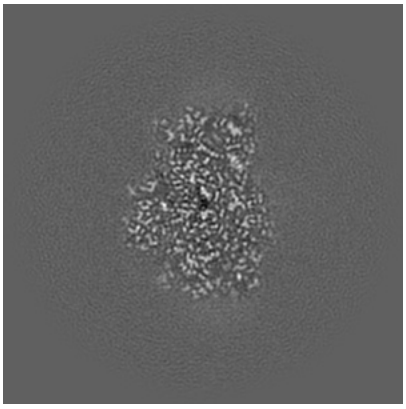


Z

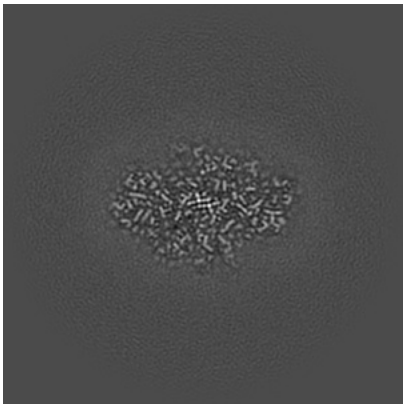
The images above show the map projected in three orthogonal directions.

6.2 Central slices

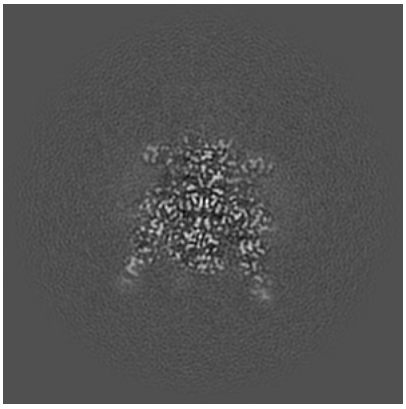
6.2.1 Primary map



X Index: 110



Y Index: 110

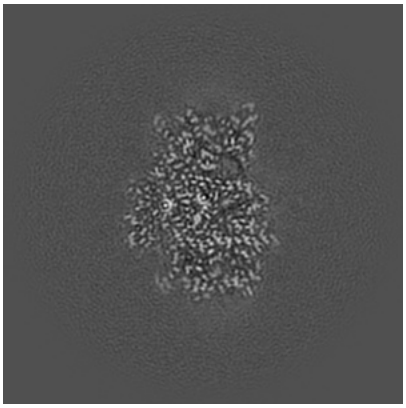


Z Index: 110

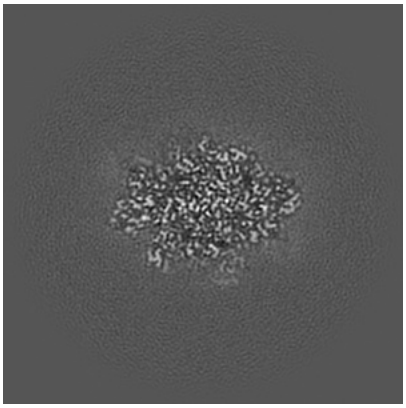
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

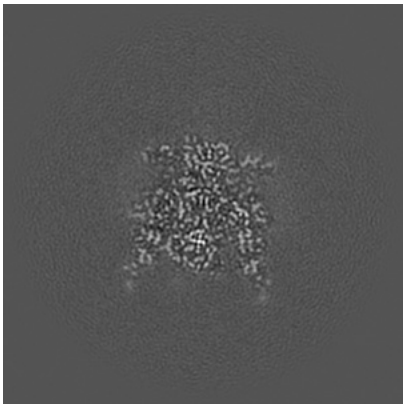
6.3.1 Primary map



X Index: 108



Y Index: 101

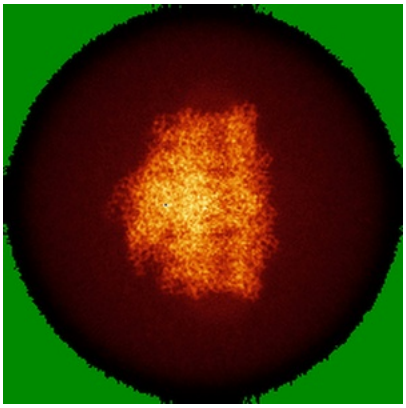


Z Index: 109

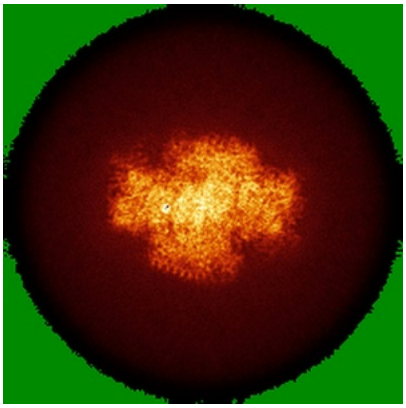
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

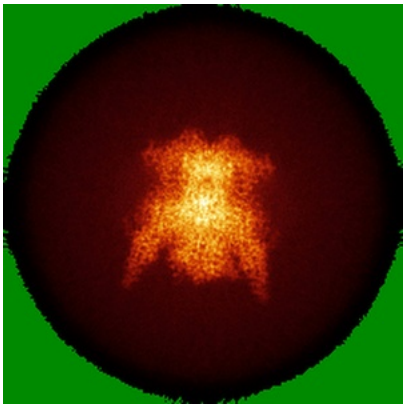
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.48. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

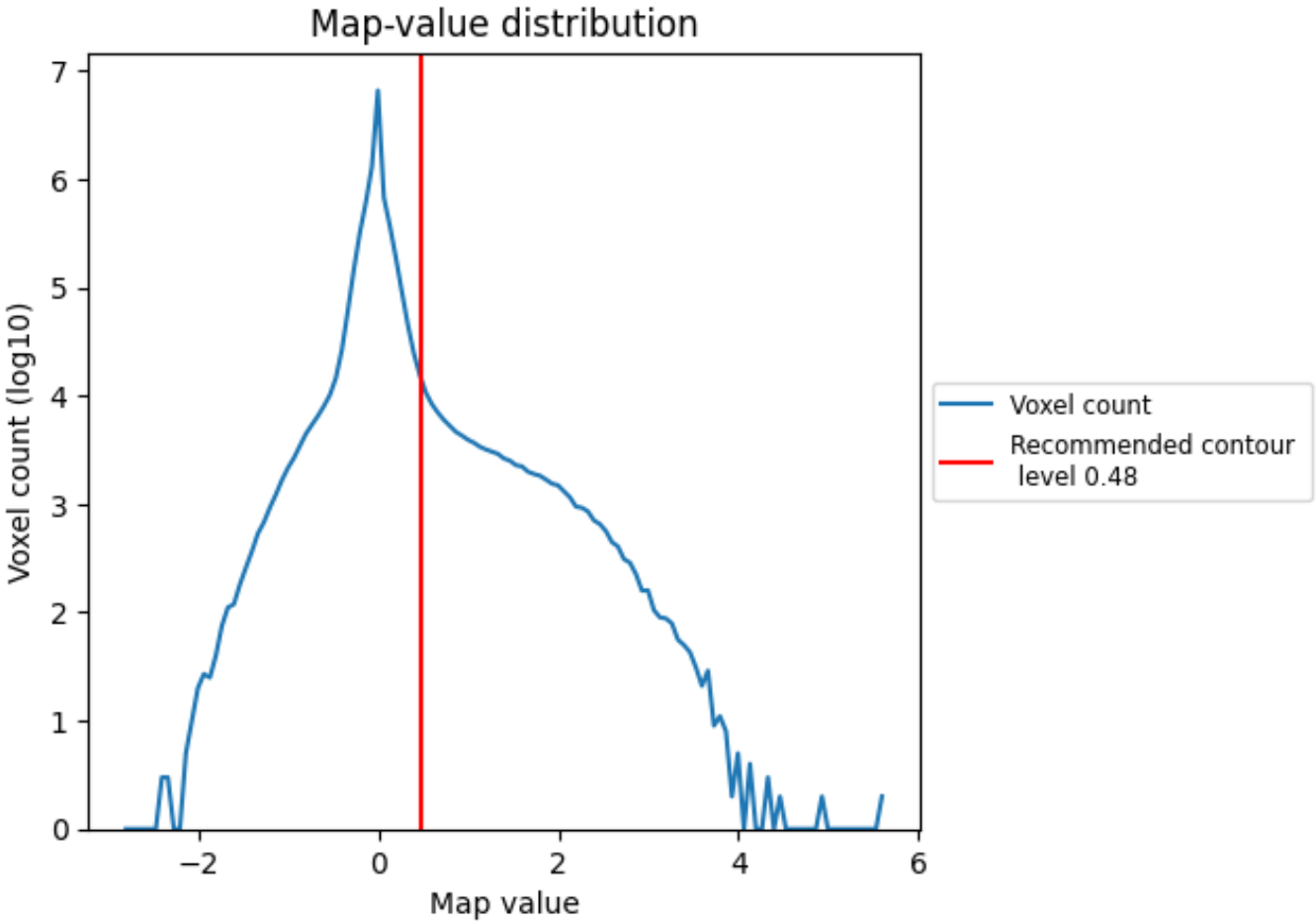
6.6 Mask visualisation (i)

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

7 Map analysis

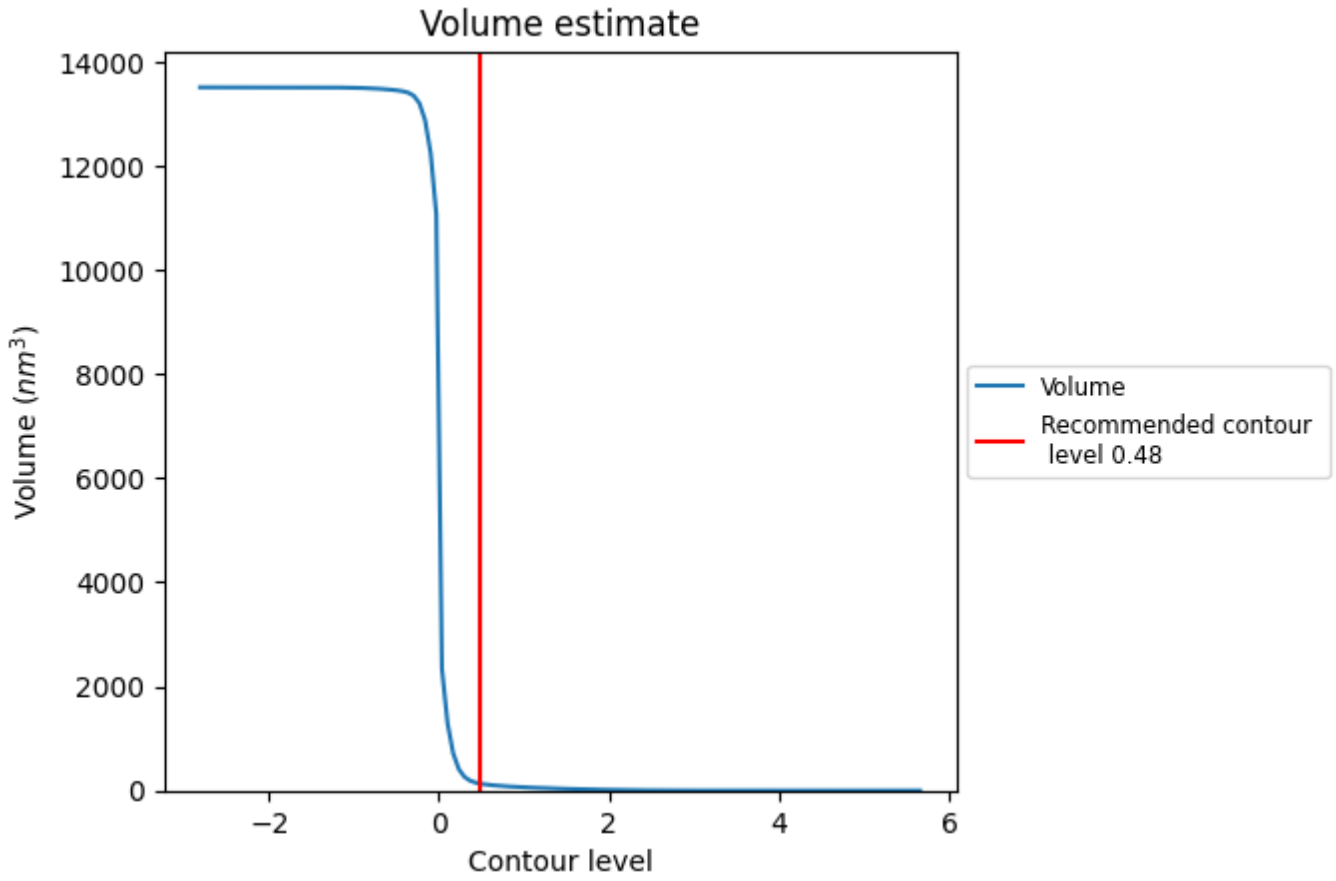
This section contains the results of statistical analysis of the map.

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.

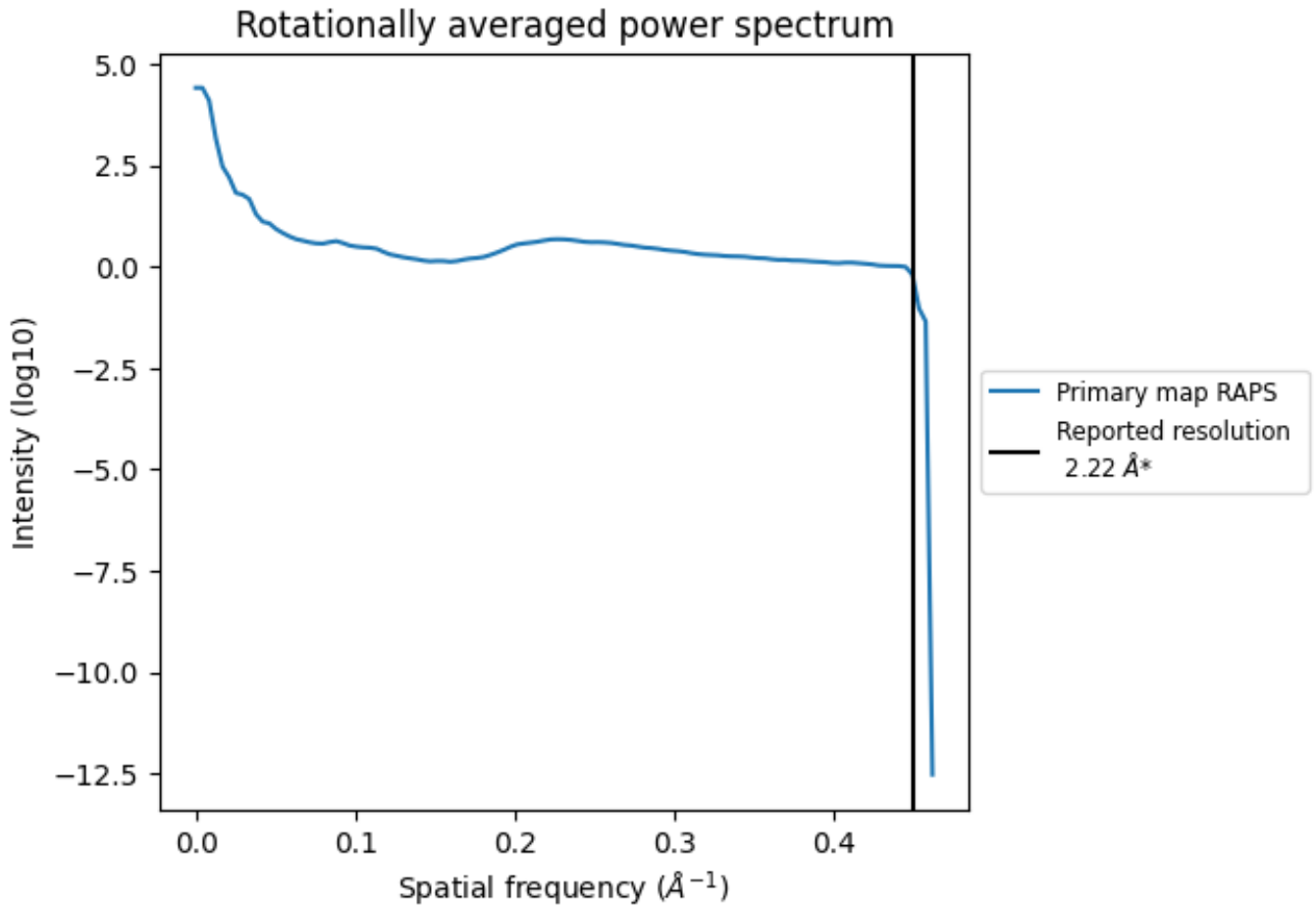
7.2 Volume estimate



The volume at the recommended contour level is 136 nm^3; this corresponds to an approximate mass of 123 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 0.450 $Å^{-1}$

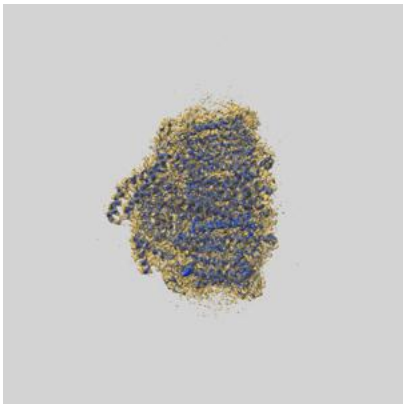
8 Fourier-Shell correlation

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

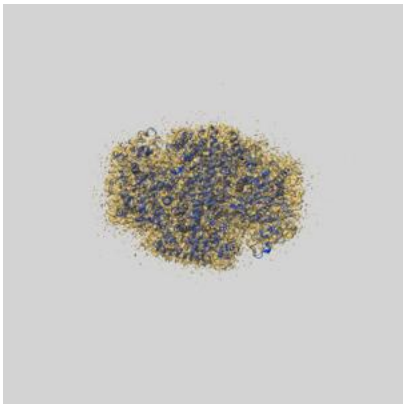
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32229 and PDB model 7VZR. Per-residue inclusion information can be found in section 3 on page 13.

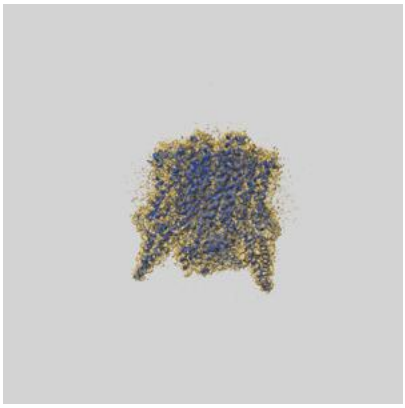
9.1 Map-model overlay



X



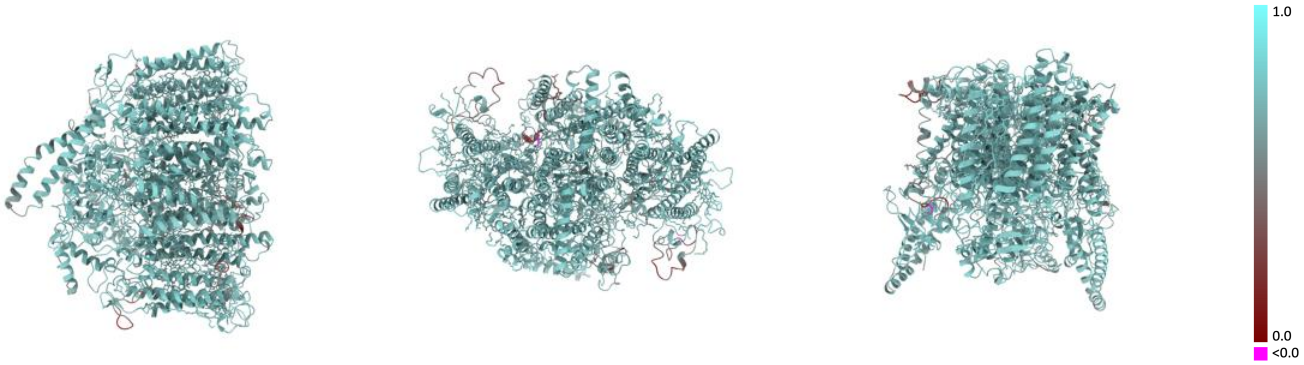
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.48 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.

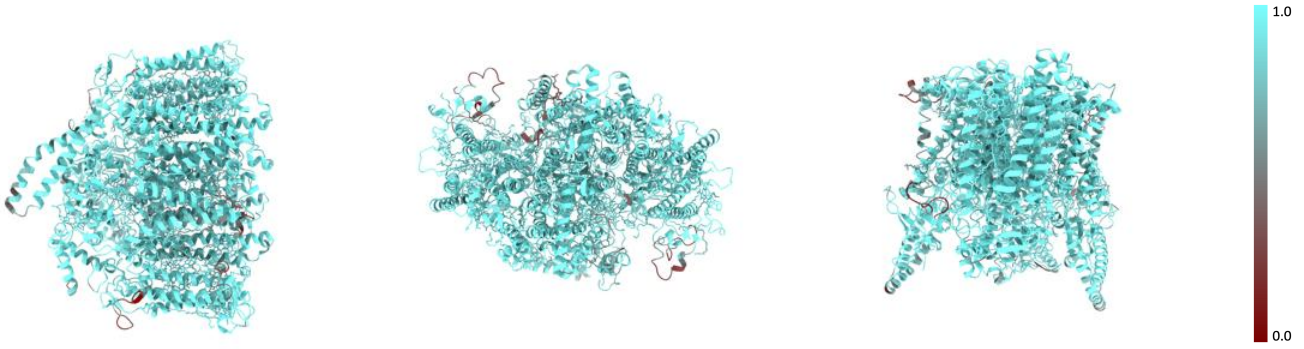
9.2 Q-score mapped to coordinate model (i)



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.

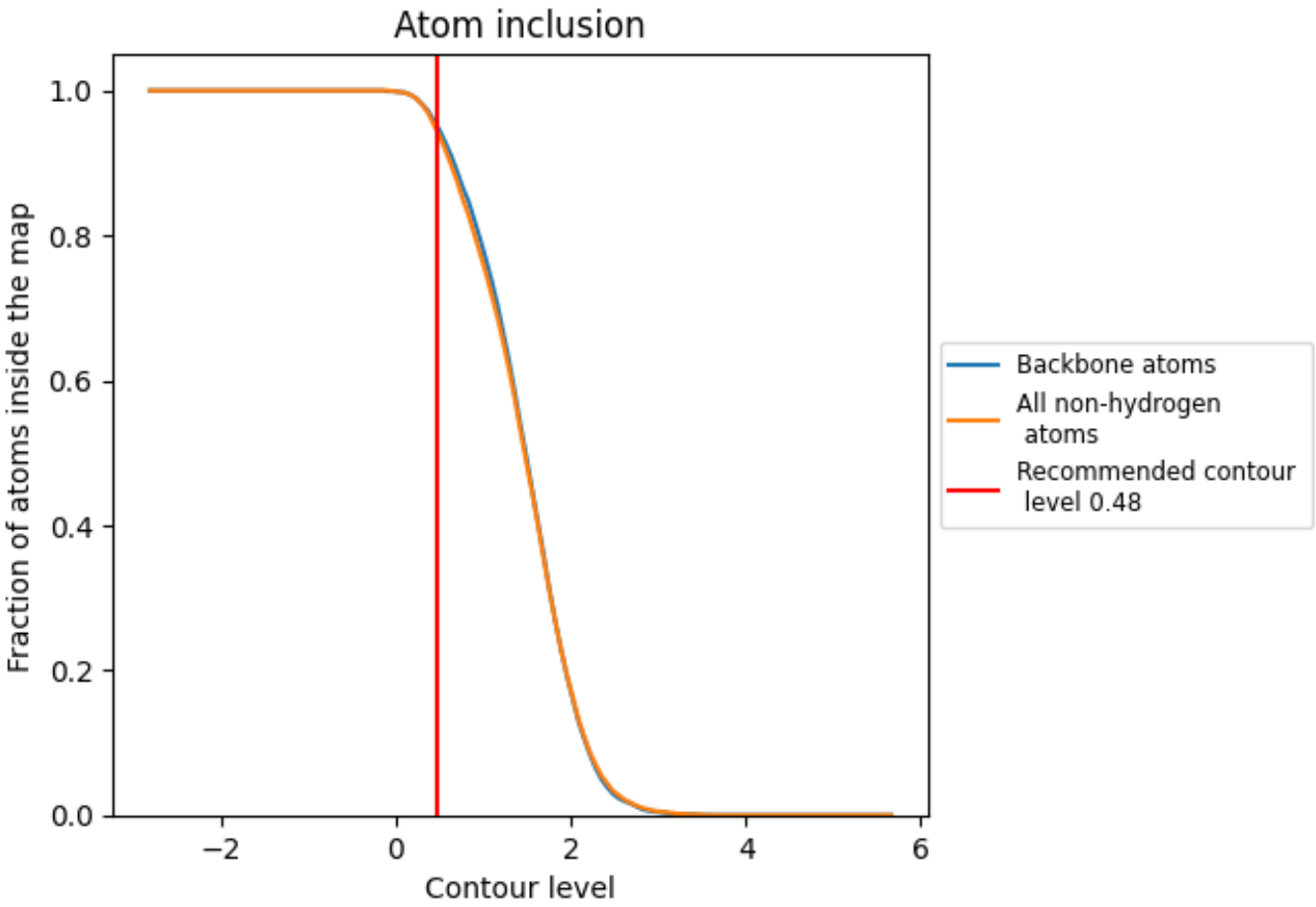
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.48).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9420	0.7050
A	0.9520	0.7100
C	0.9580	0.7210
E	0.9630	0.7140
F	0.9260	0.6700
G	0.7980	0.6490
H	0.8740	0.6670
a	0.9500	0.7060
c	0.9400	0.7060
e	0.9680	0.6970
f	0.9180	0.6770
g	0.7540	0.5870
h	0.8530	0.6610