Full wwPDB EM Validation Report ⓘ

Sep 27, 2023 – 12:21 PM JST

PDB ID	:	8HJU
EMDB ID	:	EMD-34838
Title	:	Cryo-EM structure of native RC-LH complex from Roseiflexus castenholzii at 10,000 lux
Authors	:	Xu, X.; Xin, J.
Deposited on	:	2022-11-23
Resolution	:	2.80 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:

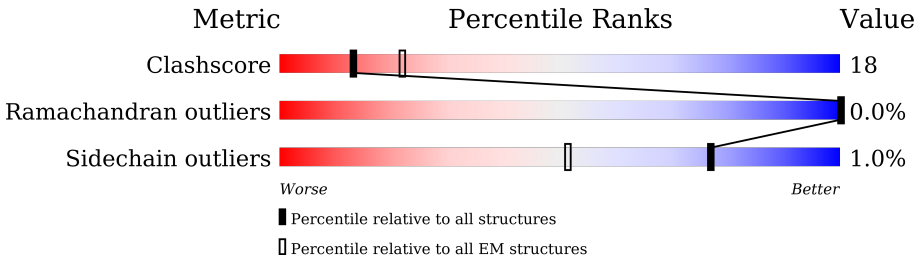
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	0	55	67% 22% 11%
1	2	55	71% 18% 11%
1	4	55	64% 25% 11%
1	6	55	69% 20% 11%
1	8	55	64% 25% 11%
1	B	55	67% 22% 11%
1	E	55	65% 24% 11%
1	G	55	69% 20% 11%

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Mol	Chain	Length	Quality of chain
1	I	55	64% 25% 11%
1	K	55	71% 18% 11%
1	O	55	69% 20% 11%
1	Q	55	71% 18% 11%
1	S	55	73% 16% 11%
1	U	55	58% 31% 11%
1	W	55	62% 27% 11%
2	1	42	50% 33% 17%
2	3	42	71% 19% 10%
2	5	42	64% 26% 10%
2	7	42	64% 24% 10%
2	9	42	67% 21% 10%
2	A	42	62% 26% 10%
2	D	42	60% 29% 10%
2	F	42	67% 21% 10%
2	H	42	60% 31% 10%
2	J	42	50% 38% 10%
2	N	42	52% 36% 10%
2	P	42	60% 29% 10%
2	R	42	60% 31% 10%
2	T	42	60% 29% 10%
2	V	42	7% 62% 29% 10%
3	L	315	72% 24%
4	M	307	76% 24%
5	C	320	63% 34%

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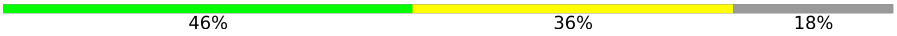
Mol	Chain	Length	Quality of chain
6	X	32	
7	Y	39	
8	Z	63	

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
11	BPH	M	704	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 23917 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 Beta subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	2	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	4	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	6	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	8	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	B	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	E	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	G	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	I	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	K	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	O	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	Q	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	S	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	U	49	Total	C	N	O	S	0	0
			407	275	68	63	1		
1	W	49	Total	C	N	O	S	0	0
			407	275	68	63	1		

- Molecule 2 is a protein called Alpha subunit of light-harvesting 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	35	Total	C	N	O	S	0	0
			271	181	45	44	1		
2	3	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	5	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	7	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	9	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	A	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	D	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	F	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	H	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	J	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	N	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	P	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	R	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	T	38	Total	C	N	O	S	0	0
			300	201	51	47	1		
2	V	38	Total	C	N	O	S	0	0
			300	201	51	47	1		

- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	302	Total	C	N	O	S	0	0
			2389	1597	386	398	8		

- Molecule 4 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	306	Total	C	N	O	S	0	0
			2488	1673	399	409	7		

- Molecule 5 is a protein called MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	315	Total	C	N	O	S	0	0
			2404	1532	407	443	22		

- Molecule 6 is a protein called SUBUNIT X.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	26	Total	C	N	O	S	0	0
			206	145	26	31	4		

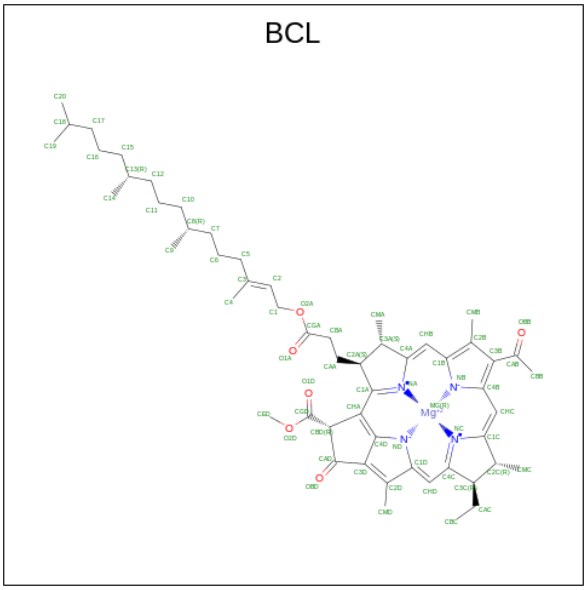
- Molecule 7 is a protein called SUBUNIT Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	32	Total	C	N	O	S	0	0
			259	181	36	39	3		

- Molecule 8 is a protein called SUBUNIT Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	47	Total	C	N	O	S	0	0
			362	242	59	60	1		

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



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

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Mol	Chain	Residues	Atoms					AltConf
9	0	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	5	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	9	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	B	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	D	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	E	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
9	F	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	H	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	I	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	J	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	K	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	R	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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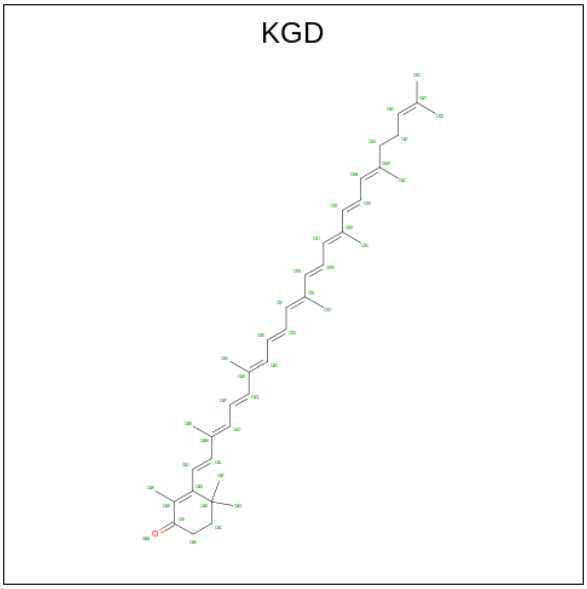
Mol	Chain	Residues	Atoms					AltConf
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	U	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	X	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is beta,psi-caroten-4-one (three-letter code: KGD) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
10	0	1	Total	C	O	0
			41	40	1	
10	0	1	Total	C	O	0
			41	40	1	
10	2	1	Total	C	O	0
			41	40	1	
10	2	1	Total	C	O	0
			41	40	1	
10	3	1	Total	C	O	0
			41	40	1	
10	4	1	Total	C	O	0
			41	40	1	

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Mol	Chain	Residues	Atoms			AltConf
10	5	1	Total	C	O	0
			41	40	1	
10	6	1	Total	C	O	0
			41	40	1	
10	8	1	Total	C	O	0
			41	40	1	
10	9	1	Total	C	O	0
			41	40	1	
10	A	1	Total	C	O	0
			41	40	1	
10	A	1	Total	C	O	0
			41	40	1	
10	B	1	Total	C	O	0
			41	40	1	
10	E	1	Total	C	O	0
			41	40	1	
10	F	1	Total	C	O	0
			41	40	1	
10	G	1	Total	C	O	0
			41	40	1	
10	H	1	Total	C	O	0
			41	40	1	
10	I	1	Total	C	O	0
			41	40	1	
10	J	1	Total	C	O	0
			41	40	1	
10	K	1	Total	C	O	0
			41	40	1	
10	N	1	Total	C	O	0
			41	40	1	
10	O	1	Total	C	O	0
			41	40	1	
10	P	1	Total	C	O	0
			41	40	1	
10	Q	1	Total	C	O	0
			41	40	1	
10	S	1	Total	C	O	0
			41	40	1	
10	S	1	Total	C	O	0
			41	40	1	
10	T	1	Total	C	O	0
			41	40	1	

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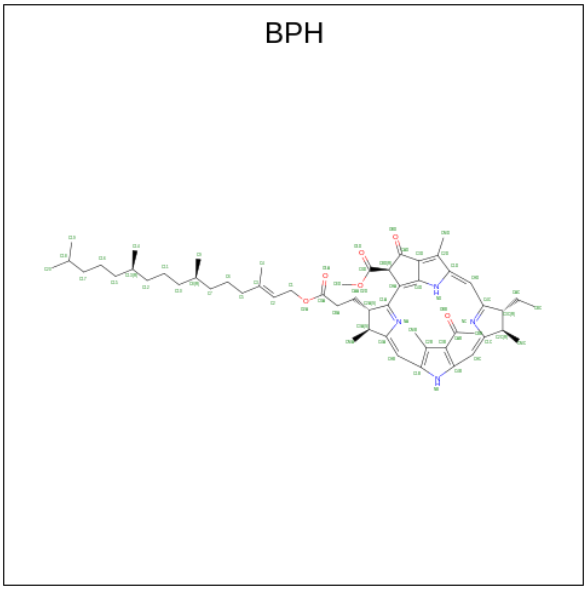
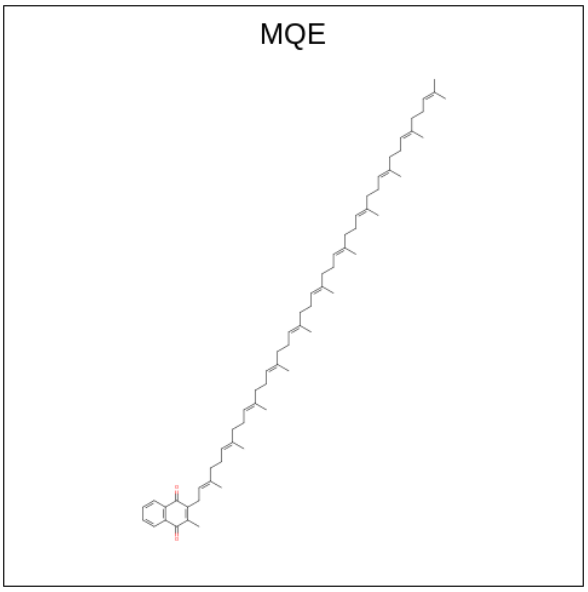
Mol	Chain	Residues	Atoms	AltConf
10	U	1	Total C O 41 40 1	0
10	W	1	Total C O 41 40 1	0
10	C	1	Total C O 41 40 1	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



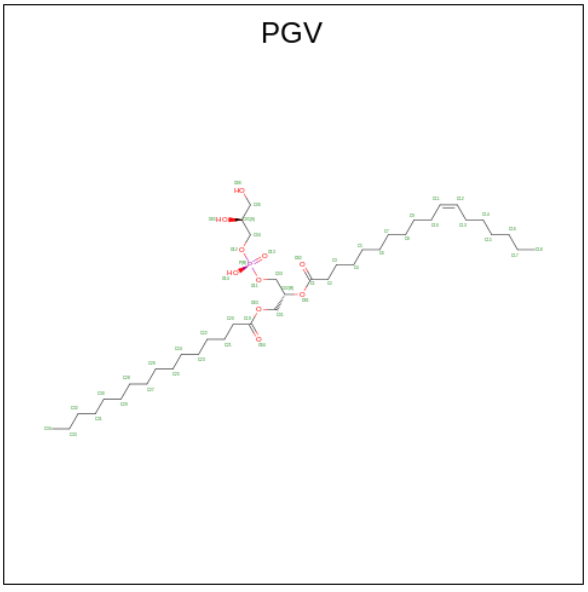
Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total C N O 65 55 4 6	0
11	L	1	Total C N O 65 55 4 6	0
11	M	1	Total C N O 65 55 4 6	0

- Molecule 12 is 2-methyl-3-[(2E,6E,10E,14E,18E,22E,26E,30E,34E,38E)-3,7,11,15,19,23,27,31,35,39,43-undecamethyltetratetraconta-2,6,10,14,18,22,26,30,34,38,42-undecaen-1-yl]naphthalene-1,4-dione (three-letter code: MQE) (formula: $C_{66}H_{96}O_2$).



Mol	Chain	Residues	Atoms			AltConf
12	L	1	Total	C	O	0
			68	66	2	
12	M	1	Total	C	O	0
			68	66	2	
12	M	1	Total	C	O	0
			24	22	2	

- Molecule 13 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).

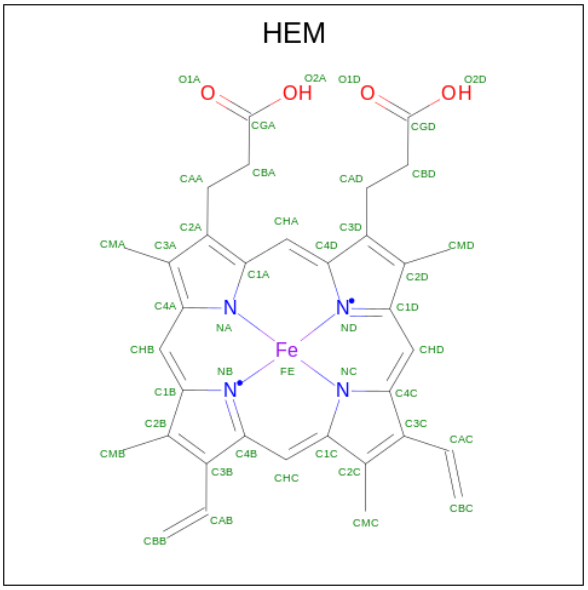


Mol	Chain	Residues	Atoms				AltConf
13	L	1	Total	C	O	P	0
			32	21	10	1	
13	L	1	Total	C	O	P	0
			42	31	10	1	
13	M	1	Total	C	O	P	0
			34	23	10	1	
13	P	1	Total	C	O	P	0
			37	26	10	1	
13	P	1	Total	C	O	P	0
			41	30	10	1	
13	C	1	Total	C	O	P	0
			45	34	10	1	
13	Z	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
14	M	1	Total	Fe	0
			1	1	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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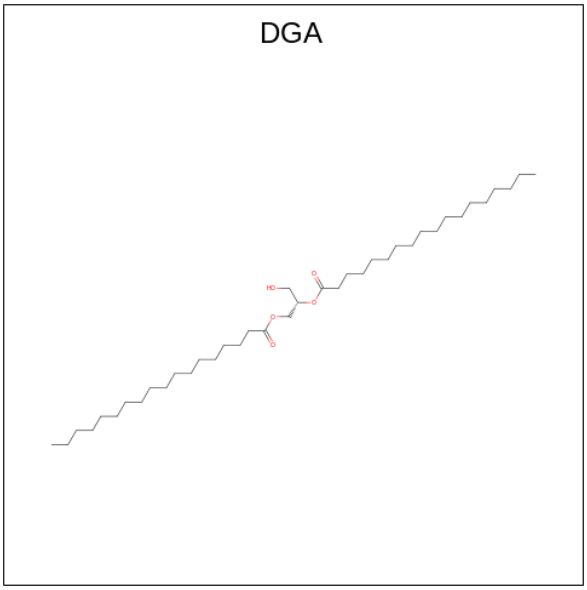
Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
15	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



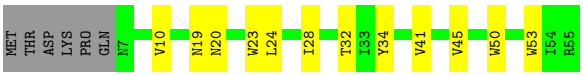
Mol	Chain	Residues	Atoms			AltConf
16	Y	1	Total	C	O	0
			37	32	5	

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.

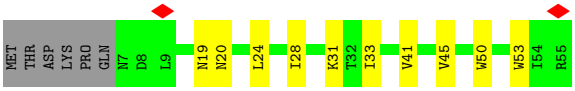
• Molecule 1: Beta subunit of light-harvesting 1

Chain 0:



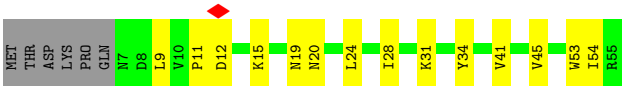
• Molecule 1: Beta subunit of light-harvesting 1

Chain 2:



• Molecule 1: Beta subunit of light-harvesting 1

Chain 4:

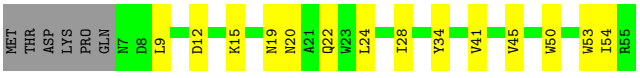


• Molecule 1: Beta subunit of light-harvesting 1

Chain 6:

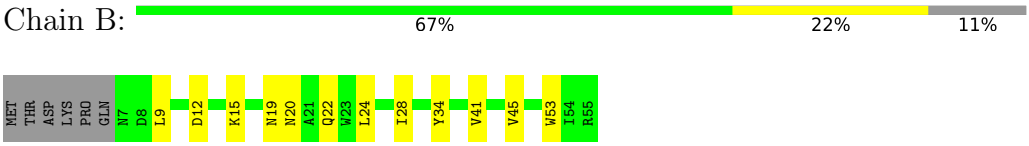
• Molecule 1: Beta subunit of light-harvesting 1

Chain 8:



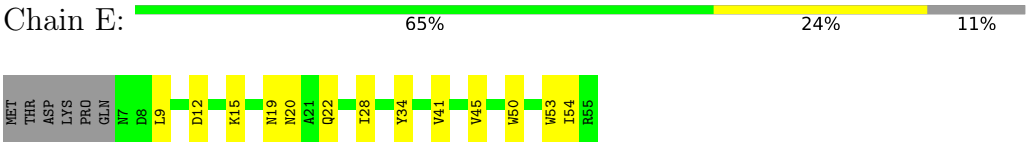
• Molecule 1: Beta subunit of light-harvesting 1

Chain B:



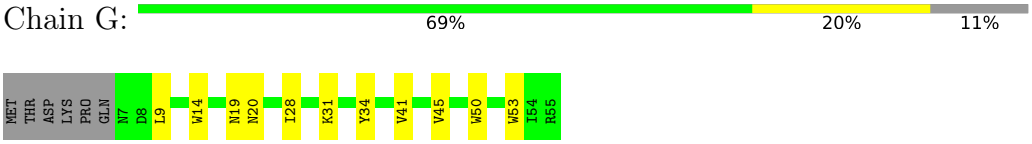
• Molecule 1: Beta subunit of light-harvesting 1

Chain E:



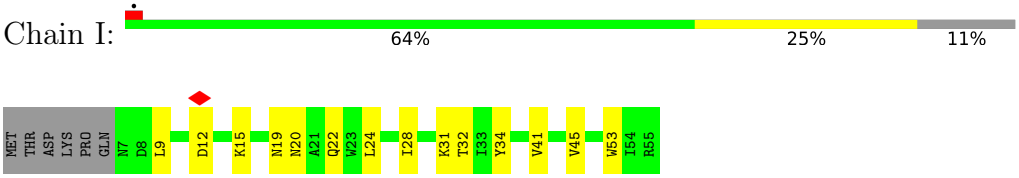
• Molecule 1: Beta subunit of light-harvesting 1

Chain G:



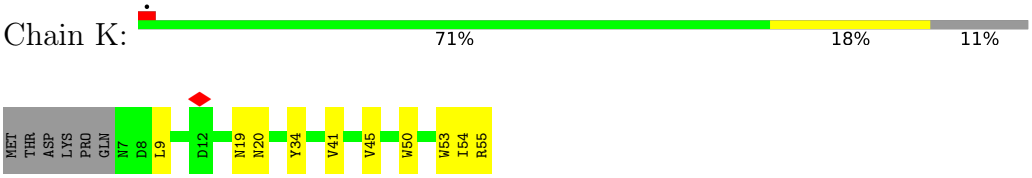
• Molecule 1: Beta subunit of light-harvesting 1

Chain I:



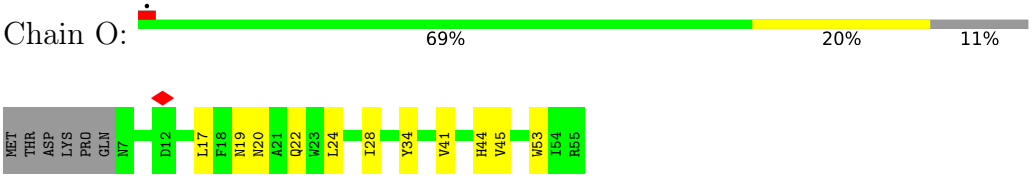
• Molecule 1: Beta subunit of light-harvesting 1

Chain K:



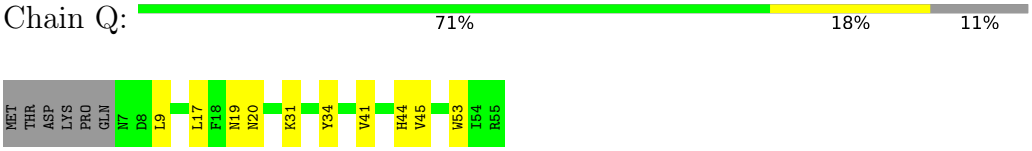
• Molecule 1: Beta subunit of light-harvesting 1

Chain O:



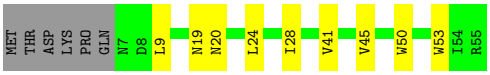
• Molecule 1: Beta subunit of light-harvesting 1

Chain Q:



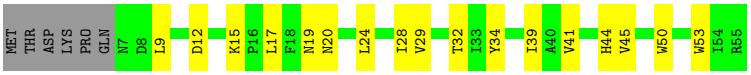
• Molecule 1: Beta subunit of light-harvesting 1

Chain S:



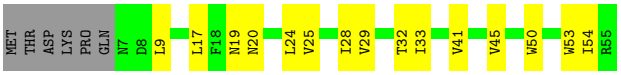
• Molecule 1: Beta subunit of light-harvesting 1

Chain U:



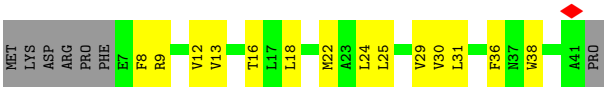
• Molecule 1: Beta subunit of light-harvesting 1

Chain W:



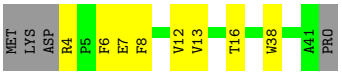
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 1:



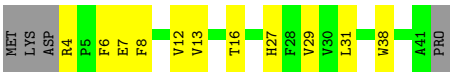
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 3:



• Molecule 2: Alpha subunit of light-harvesting 1

Chain 5:

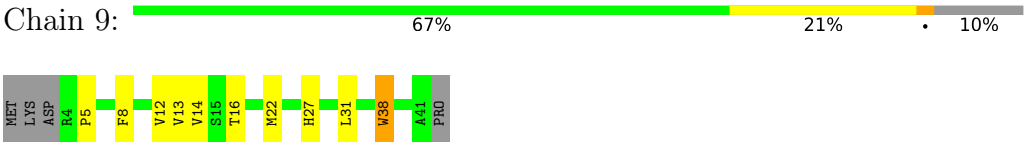


• Molecule 2: Alpha subunit of light-harvesting 1

Chain 7:

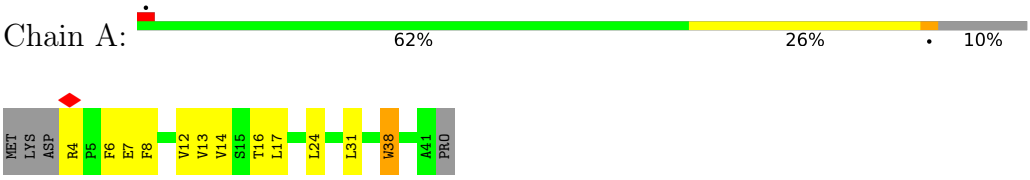
• Molecule 2: Alpha subunit of light-harvesting 1

Chain 9:



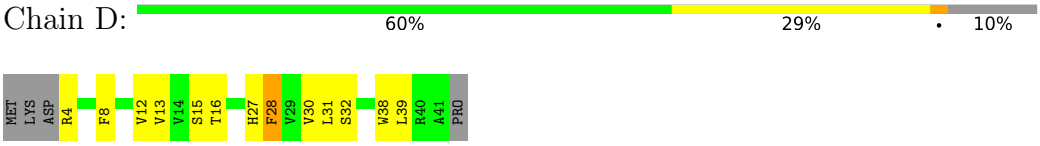
• Molecule 2: Alpha subunit of light-harvesting 1

Chain A:



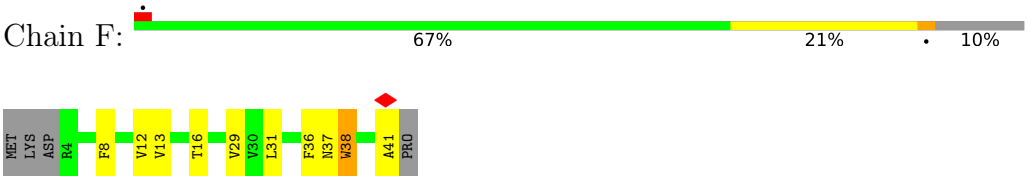
• Molecule 2: Alpha subunit of light-harvesting 1

Chain D:



• Molecule 2: Alpha subunit of light-harvesting 1

Chain F:

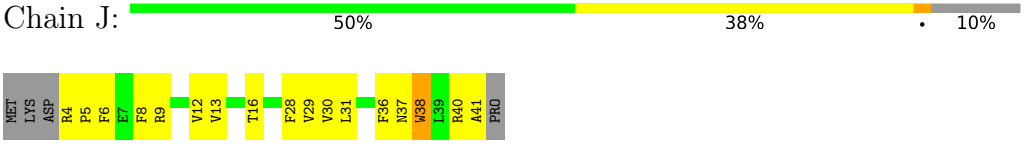


• Molecule 2: Alpha subunit of light-harvesting 1

Chain H:

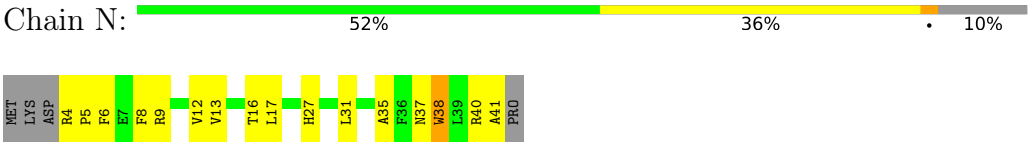
• Molecule 2: Alpha subunit of light-harvesting 1

Chain J:



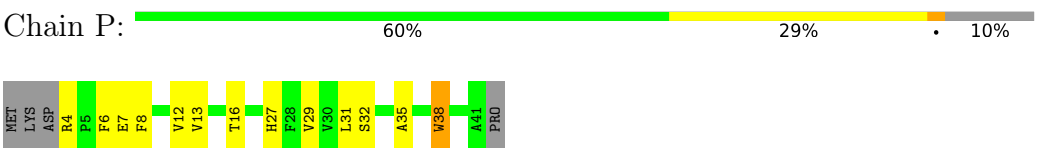
• Molecule 2: Alpha subunit of light-harvesting 1

Chain N:



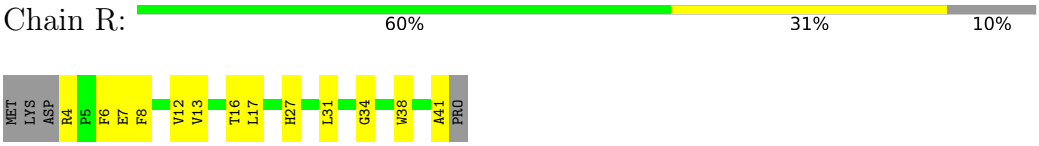
• Molecule 2: Alpha subunit of light-harvesting 1

Chain P:



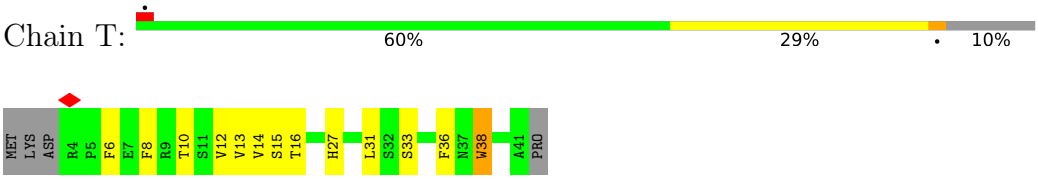
• Molecule 2: Alpha subunit of light-harvesting 1

Chain R:



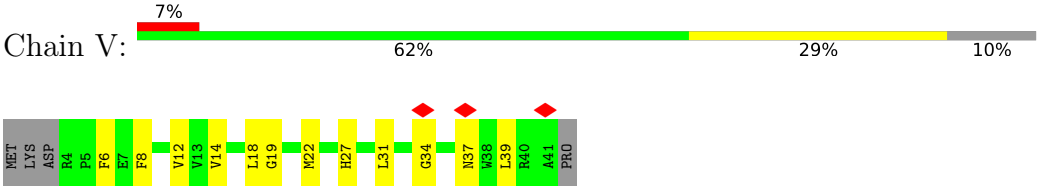
• Molecule 2: Alpha subunit of light-harvesting 1

Chain T:



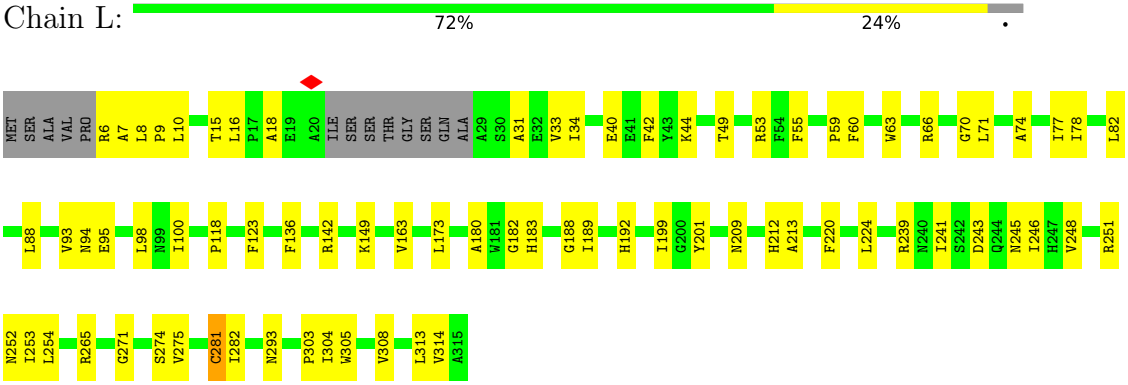
• Molecule 2: Alpha subunit of light-harvesting 1

Chain V:



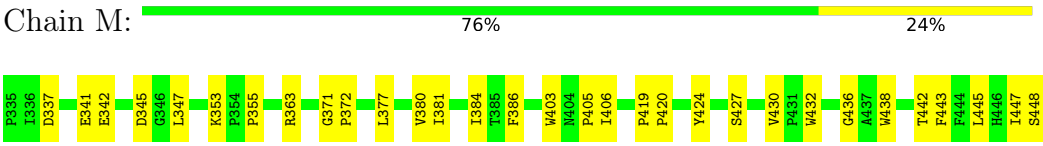
• Molecule 3: Reaction center protein L chain

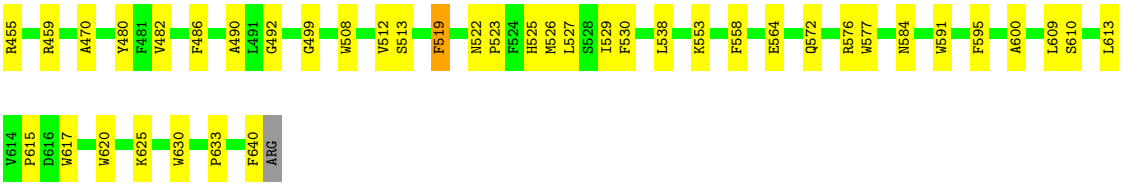
Chain L:



• Molecule 4: Reaction center protein M chain

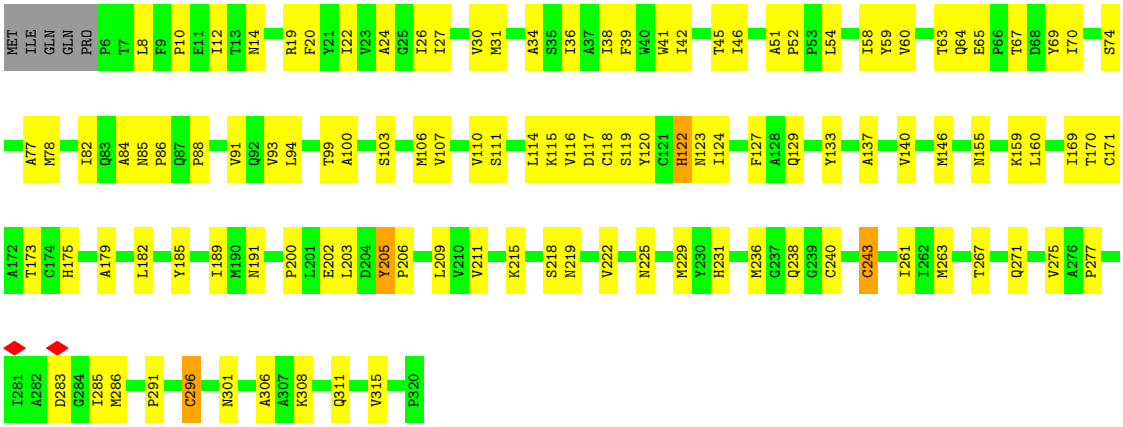
Chain M:





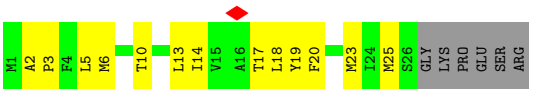
• Molecule 5: MULTIHEME_CYTC DOMAIN-CONTAINING PROTEIN

Chain C:



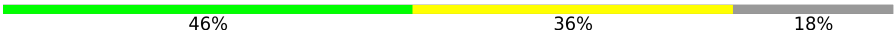
• Molecule 6: SUBUNIT X

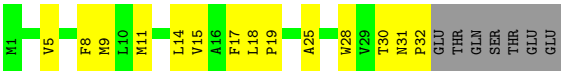
Chain X:



• Molecule 7: SUBUNIT Y

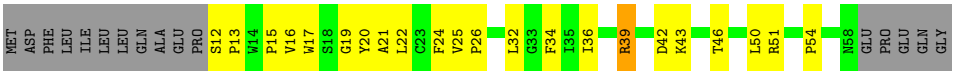
Chain Y:





• Molecule 8: SUBUNIT Z

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372029	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.00, 50.00, 50.00, 50.00, 50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.122	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, DGA, KGD, BPH, BCL, PGV, HEM, MQE

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	0	0.40	0/423	0.42	0/585
1	2	0.37	0/423	0.39	0/585
1	4	0.38	0/423	0.39	0/585
1	6	0.36	0/423	0.38	0/585
1	8	0.34	0/423	0.39	0/585
1	B	0.36	0/423	0.39	0/585
1	E	0.35	0/423	0.39	0/585
1	G	0.37	0/423	0.40	0/585
1	I	0.38	0/423	0.39	0/585
1	K	0.35	0/423	0.40	0/585
1	O	0.39	0/423	0.40	0/585
1	Q	0.36	0/423	0.39	0/585
1	S	0.37	0/423	0.39	0/585
1	U	0.36	0/423	0.39	0/585
1	W	0.40	0/423	0.39	0/585
2	1	0.46	0/276	0.54	0/375
2	3	0.34	0/307	0.44	0/417
2	5	0.44	0/307	0.55	0/417
2	7	0.35	0/307	0.48	0/417
2	9	0.39	0/307	0.53	0/417
2	A	0.38	0/307	0.49	0/417
2	D	0.36	0/307	0.58	0/417
2	F	0.37	0/307	0.51	0/417
2	H	0.35	0/307	0.46	0/417
2	J	0.43	0/307	0.50	0/417
2	N	0.37	0/307	0.45	0/417
2	P	0.36	0/307	0.45	0/417
2	R	0.38	0/307	0.50	0/417
2	T	0.35	0/307	0.46	0/417
2	V	0.34	0/307	0.55	0/417
3	L	0.48	0/2473	0.55	1/3375 (0.0%)
4	M	0.43	0/2597	0.48	0/3566

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
5	C	0.44	0/2469	0.53	0/3371
6	X	0.35	0/211	0.48	0/285
7	Y	0.50	0/268	0.64	0/370
8	Z	0.50	0/374	0.54	0/513
All	All	0.41	0/19311	0.48	1/26468 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	281	CYS	CA-CB-SG	5.04	123.08	114.00

There are no chirality outliers.

There are no planarity outliers.

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	0	407	0	407	8	0
1	2	407	0	407	10	0
1	4	407	0	407	14	0
1	6	407	0	407	7	0
1	8	407	0	407	10	0
1	B	407	0	407	10	0
1	E	407	0	407	11	0
1	G	407	0	407	9	0
1	I	407	0	407	11	0
1	K	407	0	407	9	0
1	O	407	0	407	10	0
1	Q	407	0	407	8	0
1	S	407	0	407	7	0
1	U	407	0	407	18	0
1	W	407	0	407	21	0
2	1	271	0	287	15	0
2	3	300	0	316	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	5	300	0	316	10	0
2	7	300	0	316	9	0
2	9	300	0	316	9	0
2	A	300	0	316	13	0
2	D	300	0	316	15	0
2	F	300	0	316	9	0
2	H	300	0	316	12	0
2	J	300	0	316	20	0
2	N	300	0	316	22	0
2	P	300	0	316	15	0
2	R	300	0	316	18	0
2	T	300	0	316	13	0
2	V	300	0	316	23	0
3	L	2389	0	2348	87	0
4	M	2488	0	2373	74	0
5	C	2404	0	2360	117	0
6	X	206	0	224	25	0
7	Y	259	0	272	16	0
8	Z	362	0	366	56	0
9	0	132	0	148	7	0
9	1	66	0	74	8	0
9	2	132	0	148	11	0
9	3	66	0	74	5	0
9	4	132	0	148	7	0
9	5	66	0	74	6	0
9	6	132	0	148	8	0
9	7	66	0	74	7	0
9	8	132	0	148	9	0
9	9	66	0	74	5	0
9	A	132	0	148	8	0
9	B	66	0	74	5	0
9	D	132	0	148	8	0
9	E	66	0	74	5	0
9	F	132	0	148	6	0
9	G	66	0	74	5	0
9	H	132	0	148	10	0
9	I	66	0	74	6	0
9	J	132	0	148	10	0
9	K	66	0	74	7	0
9	L	132	0	148	13	0
9	M	66	0	74	10	0
9	N	132	0	148	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	O	66	0	74	3	0
9	P	66	0	74	8	0
9	Q	132	0	148	10	0
9	R	66	0	74	9	0
9	S	132	0	148	10	0
9	T	66	0	74	11	0
9	U	132	0	148	14	0
9	W	132	0	148	15	0
9	X	66	0	74	11	0
10	0	82	0	0	10	0
10	2	82	0	0	6	0
10	3	41	0	0	8	0
10	4	41	0	0	2	0
10	5	41	0	0	5	0
10	6	41	0	0	1	0
10	8	41	0	0	4	0
10	9	41	0	0	4	0
10	A	82	0	0	8	0
10	B	41	0	0	3	0
10	C	41	0	0	20	0
10	E	41	0	0	3	0
10	F	41	0	0	6	0
10	G	41	0	0	0	0
10	H	41	0	0	5	0
10	I	41	0	0	4	0
10	J	41	0	0	7	0
10	K	41	0	0	0	0
10	N	41	0	0	4	0
10	O	41	0	0	3	0
10	P	41	0	0	6	0
10	Q	41	0	0	1	0
10	S	82	0	0	7	0
10	T	41	0	0	6	0
10	U	41	0	0	3	0
10	W	41	0	0	5	0
11	L	130	0	152	13	0
11	M	65	0	76	37	0
12	L	68	0	0	2	0
12	M	92	0	0	17	0
13	C	45	0	60	5	0
13	L	74	0	89	1	0
13	M	34	0	37	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	78	0	93	31	0
13	Z	39	0	48	8	0
14	M	1	0	0	0	0
15	C	172	0	120	19	0
16	Y	37	0	59	1	0
All	All	23917	0	23045	858	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 (858) 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)
10:P:102:KGD:CAE	9:S:103:BCL:HBB2	1.46	1.46
5:C:243:CYS:SG	15:C:404:HEM:CAC	2.05	1.44
9:P:101:BCL:HBB2	10:S:101:KGD:CBC	1.56	1.36
10:5:102:KGD:CAE	9:8:102:BCL:HBB2	1.56	1.34
5:C:36:ILE:HG12	10:C:401:KGD:CAF	1.56	1.33
10:F:103:KGD:CAE	9:I:101:BCL:HBB2	1.60	1.32
10:N:103:KGD:CAE	9:Q:102:BCL:HBB2	1.58	1.31
10:3:102:KGD:CAE	9:6:102:BCL:HBB2	1.63	1.27
10:C:401:KGD:CAG	7:Y:11:MET:SD	2.22	1.27
2:V:39:LEU:CD2	6:X:6:MET:HG2	1.65	1.26
9:3:101:BCL:HBB2	10:5:102:KGD:CBC	1.66	1.23
5:C:243:CYS:SG	15:C:404:HEM:HAC	1.69	1.22
10:H:103:KGD:CAE	9:K:101:BCL:HBB2	1.68	1.21
5:C:31:MET:HE1	10:C:401:KGD:CBI	1.75	1.15
10:2:101:KGD:CAE	9:4:102:BCL:HBB2	1.76	1.14
13:P:103:PGV:C30	13:Z:101:PGV:C8	2.24	1.14
8:Z:39:ARG:HH11	8:Z:43:LYS:CG	1.61	1.13
10:T:102:KGD:CAE	9:W:103:BCL:HBB2	1.79	1.11
12:M:701:MQE:CBZ	13:P:104:PGV:H92	1.81	1.10
9:W:102:BCL:H171	6:X:17:THR:HG22	1.20	1.09
10:A:104:KGD:CAE	9:G:101:BCL:HBB2	1.81	1.09
5:C:36:ILE:CG1	10:C:401:KGD:CAF	2.30	1.08
11:M:704:BPH:HHC	11:M:704:BPH:HBB3	1.34	1.08
5:C:31:MET:HE1	10:C:401:KGD:CBO	1.82	1.08
2:V:39:LEU:HD23	6:X:6:MET:CG	1.82	1.07
10:S:101:KGD:CAE	9:U:102:BCL:HBB2	1.83	1.07
12:M:701:MQE:CBT	13:P:104:PGV:H261	1.83	1.07
5:C:31:MET:HE1	10:C:401:KGD:CBL	1.83	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:103:KGD:CAE	9:E:101:BCL:HBB2	1.85	1.05
4:M:490:ALA:HA	13:M:706:PGV:H032	1.36	1.05
2:V:39:LEU:HD23	6:X:6:MET:HG2	1.33	1.05
9:H:101:BCL:HBB2	10:J:103:KGD:CBC	1.86	1.04
10:0:104:KGD:CAE	9:B:101:BCL:HBB2	1.85	1.04
10:P:102:KGD:CAE	9:S:103:BCL:CBB	2.34	1.03
2:V:39:LEU:HD23	6:X:6:MET:SD	1.99	1.03
10:5:102:KGD:CAE	9:8:102:BCL:CBB	2.37	1.01
2:V:39:LEU:HD21	6:X:6:MET:HG2	1.38	1.00
8:Z:39:ARG:HH11	8:Z:43:LYS:HG3	1.26	0.99
9:5:101:BCL:HBB2	10:9:101:KGD:CBC	1.97	0.94
4:M:424:TYR:CD1	4:M:430:VAL:HG12	2.03	0.94
3:L:10:LEU:HD23	8:Z:50:LEU:HD12	1.49	0.93
5:C:36:ILE:CD1	10:C:401:KGD:CAF	2.47	0.92
5:C:31:MET:CE	10:C:401:KGD:CBO	2.48	0.91
3:L:6:ARG:HH12	3:L:33:VAL:HG21	1.36	0.90
4:M:490:ALA:HB2	13:M:706:PGV:H042	1.54	0.89
8:Z:22:LEU:O	8:Z:26:PRO:HG2	1.71	0.89
5:C:31:MET:CE	10:C:401:KGD:CBI	2.50	0.88
2:P:7:GLU:HB2	13:P:103:PGV:O14	1.73	0.88
8:Z:39:ARG:HH11	8:Z:43:LYS:HG2	1.37	0.88
12:M:701:MQE:CBT	13:P:104:PGV:C26	2.51	0.87
3:L:220:PHE:HB3	11:M:704:BPH:HBB2	1.56	0.87
2:V:39:LEU:CD2	6:X:6:MET:CG	2.47	0.87
8:Z:39:ARG:NH1	8:Z:43:LYS:CG	2.40	0.85
4:M:620:TRP:CZ2	8:Z:19:GLY:HA2	2.12	0.85
12:M:701:MQE:CCF	13:P:104:PGV:C12	2.55	0.84
5:C:236:MET:HG2	5:C:301:ASN:HA	1.59	0.84
2:F:29:VAL:HA	13:M:706:PGV:O13	1.78	0.84
12:M:701:MQE:CAG	8:Z:34:PHE:CZ	2.61	0.84
5:C:31:MET:CE	10:C:401:KGD:CBL	2.56	0.84
12:M:701:MQE:CBA	13:P:104:PGV:C12	2.56	0.83
10:N:103:KGD:CAE	9:Q:102:BCL:CBB	2.52	0.83
9:W:102:BCL:C17	6:X:17:THR:HG22	2.07	0.83
1:2:33:ILE:HG12	10:2:101:KGD:CAU	2.09	0.82
8:Z:25:VAL:HG23	8:Z:26:PRO:HD3	1.61	0.82
3:L:254:LEU:HD11	11:M:704:BPH:HED3	1.61	0.82
12:M:701:MQE:CAG	8:Z:34:PHE:HZ	1.93	0.81
3:L:7:ALA:HB1	3:L:15:THR:HG21	1.60	0.81
10:F:103:KGD:CAE	9:I:101:BCL:CBB	2.54	0.80
11:L:1005:BPH:HED1	13:C:406:PGV:C12	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:39:ARG:NH1	8:Z:43:LYS:HG3	1.97	0.80
4:M:538:LEU:HD13	12:M:701:MQE:CBY	2.12	0.80
9:0:102:BCL:HBB2	10:9:101:KGD:CAE	2.11	0.79
9:P:101:BCL:CBB	10:S:101:KGD:CBC	2.52	0.79
10:3:102:KGD:CAE	9:6:102:BCL:CBB	2.55	0.79
12:M:701:MQE:CBG	8:Z:34:PHE:HZ	1.95	0.78
10:3:102:KGD:OAA	2:5:6:PHE:CD2	2.36	0.78
3:L:7:ALA:HB1	3:L:15:THR:CG2	2.15	0.77
2:D:32:SER:HB3	4:M:427:SER:HA	1.64	0.77
6:X:10:THR:O	6:X:14:ILE:HG12	1.84	0.77
2:J:37:ASN:HA	2:J:41:ALA:HA	1.65	0.77
9:T:101:BCL:H203	2:V:14:VAL:HG11	1.68	0.76
1:W:50:TRP:CE3	6:X:5:LEU:HD12	2.20	0.76
5:C:243:CYS:SG	15:C:404:HEM:CBC	2.74	0.76
9:D:101:BCL:HBB2	10:F:103:KGD:CBC	2.15	0.75
3:L:10:LEU:HD11	3:L:16:LEU:HD22	1.69	0.75
4:M:424:TYR:CE1	4:M:430:VAL:HG12	2.22	0.75
7:Y:11:MET:O	7:Y:15:VAL:HG23	1.85	0.75
1:2:33:ILE:CG1	10:2:101:KGD:CAU	2.65	0.75
2:R:4:ARG:NH1	2:R:7:GLU:HA	2.02	0.75
11:M:704:BPH:H4C2	11:M:704:BPH:C14	2.16	0.74
8:Z:21:ALA:O	8:Z:26:PRO:HD2	1.87	0.74
2:1:36:PHE:HB3	1:2:50:TRP:CH2	2.21	0.74
13:P:103:PGV:H062	13:P:104:PGV:O14	1.87	0.74
10:W:101:KGD:CAJ	9:X:101:BCL:H141	2.17	0.74
2:J:36:PHE:O	1:K:50:TRP:CZ2	2.41	0.74
3:L:201:TYR:O	5:C:240:CYS:HB3	1.87	0.73
3:L:254:LEU:HD11	11:M:704:BPH:CED	2.17	0.73
10:J:103:KGD:CAE	9:O:101:BCL:HBB2	2.18	0.73
3:L:98:LEU:HD11	2:P:29:VAL:HG22	1.70	0.72
4:M:490:ALA:CA	13:M:706:PGV:H032	2.16	0.72
11:M:704:BPH:HHC	11:M:704:BPH:CBB	2.14	0.72
2:N:37:ASN:HA	2:N:41:ALA:HA	1.70	0.72
5:C:243:CYS:SG	15:C:404:HEM:C3C	2.82	0.72
9:W:102:BCL:H171	6:X:17:THR:CG2	2.13	0.72
2:R:4:ARG:HH11	2:R:7:GLU:HA	1.55	0.71
5:C:173:THR:O	5:C:296:CYS:HB3	1.89	0.71
5:C:211:VAL:HG21	5:C:222:VAL:HG22	1.72	0.71
1:4:12:ASP:HA	1:4:15:LYS:HG3	1.73	0.71
2:N:4:ARG:HH22	1:O:22:GLN:HE22	1.39	0.71
1:4:12:ASP:HA	1:4:15:LYS:CD	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:101:BCL:CBB	10:J:103:KGD:CBC	2.68	0.70
9:2:103:BCL:HBA1	10:C:401:KGD:CAZ	2.20	0.70
5:C:19:ARG:HD3	6:X:25:MET:SD	2.32	0.70
12:M:701:MQE:CBX	13:P:104:PGV:H91	2.23	0.69
3:L:6:ARG:NH1	3:L:33:VAL:HG21	2.05	0.69
4:M:345:ASP:OD1	4:M:353:LYS:HE3	1.93	0.69
6:X:2:ALA:O	6:X:6:MET:HG3	1.93	0.69
5:C:229:MET:SD	15:C:404:HEM:NC	2.66	0.68
8:Z:16:VAL:HG23	8:Z:19:GLY:H	1.57	0.68
2:T:27:HIS:CE1	9:U:101:BCL:HMD1	2.28	0.68
5:C:34:ALA:O	5:C:38:ILE:HG22	1.94	0.68
9:7:101:BCL:H192	2:9:14:VAL:HG11	1.76	0.68
4:M:492:GLY:HA3	13:M:706:PGV:H32	1.76	0.68
9:L:1002:BCL:C20	13:P:104:PGV:H291	2.23	0.68
2:V:8:PHE:CE2	1:W:25:VAL:HB	2.29	0.68
5:C:114:LEU:HD22	5:C:179:ALA:HA	1.77	0.67
9:W:102:BCL:H51	9:X:101:BCL:H12	1.76	0.67
8:Z:42:ASP:OD1	8:Z:46:THR:HG23	1.94	0.67
4:M:353:LYS:HA	4:M:372:PRO:HB3	1.75	0.67
9:3:101:BCL:CBB	10:5:102:KGD:CBC	2.60	0.67
13:P:104:PGV:H202	13:Z:101:PGV:H41	1.76	0.67
4:M:355:PRO:HB3	4:M:371:GLY:HA2	1.76	0.67
3:L:59:PRO:HG2	3:L:71:LEU:HD13	1.76	0.67
4:M:610:SER:HB3	4:M:617:TRP:HE1	1.60	0.67
8:Z:25:VAL:CG2	8:Z:26:PRO:HD3	2.24	0.66
7:Y:18:LEU:HB3	7:Y:19:PRO:HD3	1.78	0.66
8:Z:20:TYR:HD1	8:Z:24:PHE:CD2	2.13	0.66
1:I:31:LYS:HB2	9:K:101:BCL:H42	1.76	0.66
11:M:704:BPH:C4	11:M:704:BPH:H142	2.25	0.66
9:T:101:BCL:C1D	9:U:101:BCL:HMD2	2.26	0.66
1:U:50:TRP:CH2	1:W:54:ILE:HG23	2.30	0.66
10:P:102:KGD:CAI	9:S:103:BCL:HBB2	2.25	0.65
10:0:104:KGD:CAE	9:B:101:BCL:CBB	2.69	0.65
2:3:13:VAL:HG22	9:3:101:BCL:H18	1.79	0.65
1:I:12:ASP:HA	1:I:15:LYS:HE2	1.78	0.65
13:P:103:PGV:O12	13:P:103:PGV:O06	2.11	0.65
12:L:1004:MQE:CAO	7:Y:14:LEU:HB3	2.27	0.65
4:M:523:PRO:HA	4:M:526:MET:HE2	1.77	0.65
12:M:701:MQE:CCF	13:P:104:PGV:C11	2.74	0.65
9:M:703:BCL:H201	11:M:704:BPH:H202	1.77	0.65
2:F:13:VAL:HG22	9:F:101:BCL:H18	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:490:ALA:HB2	13:M:706:PGV:C04	2.26	0.65
2:N:13:VAL:HG22	9:N:101:BCL:H18	1.79	0.65
1:4:12:ASP:HA	1:4:15:LYS:CG	2.27	0.65
8:Z:39:ARG:HH22	13:Z:101:PGV:H05	1.62	0.65
2:D:38:TRP:CH2	2:D:39:LEU:HD12	2.32	0.65
12:M:701:MQE:CBG	8:Z:34:PHE:CZ	2.79	0.65
2:9:13:VAL:HG22	9:9:102:BCL:H18	1.79	0.64
9:J:101:BCL:HBB2	10:N:103:KGD:CBD	2.27	0.64
5:C:106:MET:HG2	15:C:402:HEM:C4B	2.33	0.64
8:Z:39:ARG:NH1	8:Z:43:LYS:HG2	2.11	0.64
2:R:13:VAL:HG22	9:R:101:BCL:H18	1.79	0.64
4:M:490:ALA:HA	13:M:706:PGV:C03	2.21	0.64
1:W:50:TRP:CZ3	6:X:5:LEU:HD12	2.33	0.64
2:5:4:ARG:NH1	2:5:7:GLU:HA	2.13	0.64
2:7:13:VAL:HG22	9:7:101:BCL:H18	1.79	0.64
3:L:188:GLY:O	3:L:192:HIS:ND1	2.29	0.64
5:C:59:TYR:O	5:C:308:LYS:HE3	1.96	0.64
2:F:16:THR:HG23	9:F:101:BCL:H52	1.80	0.64
2:J:13:VAL:HG22	9:J:101:BCL:H18	1.79	0.64
2:5:13:VAL:HG22	9:5:101:BCL:H18	1.79	0.64
2:H:13:VAL:HG22	9:H:101:BCL:H18	1.79	0.64
4:M:625:LYS:HG3	8:Z:15:PRO:HD3	1.80	0.64
2:D:13:VAL:HG22	9:D:101:BCL:H18	1.79	0.64
2:1:16:THR:HG23	9:1:101:BCL:H52	1.80	0.64
2:D:31:LEU:HD22	2:D:38:TRP:CE3	2.33	0.64
3:L:314:VAL:HG13	3:L:314:VAL:O	1.98	0.64
9:2:103:BCL:HAC2	10:C:401:KGD:CBO	2.28	0.64
2:3:12:VAL:HG11	10:3:102:KGD:CAK	2.28	0.64
2:3:16:THR:HG23	9:3:101:BCL:H52	1.80	0.63
2:J:16:THR:HG23	9:J:101:BCL:H52	1.80	0.63
3:L:253:ILE:HG22	3:L:254:LEU:CD1	2.28	0.63
2:P:13:VAL:HG22	9:P:101:BCL:H18	1.79	0.63
2:T:13:VAL:HG22	9:T:101:BCL:H18	1.79	0.63
2:9:16:THR:HG23	9:9:102:BCL:H52	1.80	0.63
11:M:704:BPH:H4C2	11:M:704:BPH:H141	1.81	0.63
2:1:13:VAL:HG22	9:1:101:BCL:H18	1.79	0.63
3:L:8:LEU:HD12	3:L:18:ALA:HA	1.80	0.63
2:1:29:VAL:HG12	5:C:46:ILE:HD11	1.81	0.63
2:A:13:VAL:HG22	9:A:101:BCL:H18	1.79	0.63
2:A:16:THR:HG23	9:A:101:BCL:H52	1.80	0.63
10:A:104:KGD:CAE	9:G:101:BCL:CBB	2.69	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:40:ARG:HB2	2:N:35:ALA:HB2	1.80	0.63
1:U:12:ASP:HA	1:U:15:LYS:HE3	1.79	0.63
2:7:16:THR:HG23	9:7:101:BCL:H52	1.80	0.63
2:D:16:THR:HG23	9:D:101:BCL:H52	1.80	0.63
1:B:19:ASN:H	1:B:22:GLN:HE21	1.45	0.63
5:C:182:LEU:HB2	15:C:403:HEM:HBD1	1.80	0.63
5:C:106:MET:HG2	15:C:402:HEM:NB	2.13	0.63
9:L:1002:BCL:H201	13:P:104:PGV:H291	1.81	0.63
2:N:4:ARG:NH1	1:O:17:LEU:O	2.31	0.63
3:L:220:PHE:HB3	11:M:704:BPH:CBB	2.28	0.63
1:W:53:TRP:CD1	1:W:54:ILE:HG13	2.34	0.63
5:C:263:MET:O	5:C:267:THR:HG23	1.99	0.62
6:X:14:ILE:O	6:X:18:LEU:HG	1.99	0.62
3:L:254:LEU:CD1	11:M:704:BPH:HED3	2.30	0.62
2:P:16:THR:HG23	9:P:101:BCL:H52	1.80	0.62
5:C:185:TYR:HA	5:C:189:ILE:HD11	1.81	0.62
2:T:16:THR:HG23	9:T:101:BCL:H52	1.80	0.62
2:F:12:VAL:HG11	10:F:103:KGD:CAK	2.29	0.62
2:N:16:THR:HG23	9:N:101:BCL:H52	1.80	0.62
10:F:103:KGD:OAA	2:H:6:PHE:CD1	2.53	0.62
2:5:16:THR:HG23	9:5:101:BCL:H52	1.80	0.62
3:L:239:ARG:HB2	3:L:241:ILE:HG12	1.82	0.62
3:L:254:LEU:CD1	11:M:704:BPH:CED	2.78	0.62
4:M:424:TYR:HD1	4:M:430:VAL:HG12	1.57	0.62
3:L:180:ALA:HB3	3:L:183:HIS:CD2	2.35	0.62
2:5:4:ARG:HH11	2:5:7:GLU:HA	1.65	0.61
1:W:53:TRP:CE2	9:W:102:BCL:H2C	2.35	0.61
2:H:16:THR:HG23	9:H:101:BCL:H52	1.80	0.61
2:H:31:LEU:HD22	2:H:38:TRP:CE3	2.36	0.61
1:U:39:ILE:HD11	9:W:103:BCL:H122	1.83	0.61
5:C:60:VAL:HG23	5:C:306:ALA:O	2.00	0.61
8:Z:15:PRO:HB2	8:Z:20:TYR:CE1	2.36	0.61
8:Z:39:ARG:NH1	13:Z:101:PGV:O05	2.34	0.61
3:L:10:LEU:CD2	8:Z:50:LEU:HD12	2.27	0.61
9:9:102:BCL:H192	2:A:14:VAL:HG11	1.82	0.61
9:H:101:BCL:HBB2	10:J:103:KGD:CAY	2.30	0.61
11:M:704:BPH:H4C2	11:M:704:BPH:H142	1.82	0.61
4:M:445:LEU:HD11	9:M:703:BCL:H141	1.82	0.60
5:C:64:GLN:NE2	5:C:65:GLU:OE1	2.33	0.60
2:J:36:PHE:HB3	1:K:50:TRP:CH2	2.37	0.60
10:S:101:KGD:OAA	2:T:6:PHE:CD1	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:36:ILE:HD11	10:C:401:KGD:CAF	2.31	0.60
5:C:69:TYR:CE1	5:C:115:LYS:HD3	2.37	0.60
10:0:104:KGD:OAA	2:A:6:PHE:CE2	2.54	0.60
2:5:31:LEU:HB2	2:5:38:TRP:CZ3	2.37	0.60
3:L:220:PHE:CD2	11:M:704:BPH:HBB1	2.37	0.60
2:A:17:LEU:HD11	4:M:381:ILE:HG23	1.83	0.59
3:L:253:ILE:HG22	3:L:254:LEU:HD13	1.84	0.59
3:L:254:LEU:HG	11:M:704:BPH:H151	1.83	0.59
2:P:27:HIS:CE1	9:Q:101:BCL:HMD1	2.37	0.59
2:V:39:LEU:HD21	9:X:101:BCL:HMC2	1.84	0.59
1:K:34:TYR:OH	9:K:101:BCL:OBD	2.15	0.59
4:M:625:LYS:HB2	8:Z:15:PRO:HG3	1.84	0.59
8:Z:21:ALA:O	8:Z:25:VAL:HG22	2.02	0.59
2:H:4:ARG:HH22	1:I:22:GLN:HE22	1.50	0.59
3:L:66:ARG:NH1	8:Z:42:ASP:OD2	2.35	0.59
7:Y:8:PHE:HA	7:Y:11:MET:HG2	1.85	0.59
11:M:704:BPH:H7C2	11:M:704:BPH:C12	2.31	0.59
9:A:101:BCL:H201	4:M:377:LEU:HD21	1.85	0.59
4:M:615:PRO:HB3	5:C:215:LYS:HE2	1.85	0.58
12:M:701:MQE:CCF	13:P:104:PGV:H11	2.31	0.58
7:Y:8:PHE:O	7:Y:11:MET:HG2	2.02	0.58
4:M:600:ALA:HB2	11:M:704:BPH:HBC1	1.85	0.58
1:U:50:TRP:CE3	10:U:103:KGD:CAZ	2.86	0.58
2:1:22:MET:SD	9:2:102:BCL:HED1	2.43	0.58
2:A:4:ARG:NH1	1:B:22:GLN:OE1	2.37	0.58
13:P:103:PGV:H231	13:Z:101:PGV:H32	1.86	0.58
2:R:4:ARG:NH1	2:R:8:PHE:H	2.01	0.58
1:E:34:TYR:OH	9:E:101:BCL:OBD	2.15	0.58
2:V:6:PHE:HB3	9:W:103:BCL:HBB1	1.84	0.58
1:4:12:ASP:HA	1:4:15:LYS:HD2	1.86	0.58
11:L:1005:BPH:HBC3	9:M:703:BCL:H43	1.86	0.58
5:C:94:LEU:HA	5:C:315:VAL:HG21	1.85	0.58
1:6:12:ASP:HA	1:6:15:LYS:HE3	1.85	0.58
11:M:704:BPH:H142	11:M:704:BPH:H7C2	1.84	0.57
1:4:31:LYS:HB2	9:6:102:BCL:H42	1.85	0.57
9:1:101:BCL:H92	9:2:102:BCL:H101	1.86	0.57
4:M:420:PRO:HG3	4:M:430:VAL:HG21	1.85	0.57
1:E:28:ILE:HD11	1:G:14:TRP:CH2	2.38	0.57
2:3:4:ARG:HE	2:3:7:GLU:HA	1.70	0.57
2:R:16:THR:HG21	9:R:101:BCL:H171	1.86	0.57
1:I:34:TYR:OH	9:I:101:BCL:OBD	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:34:TYR:OH	9:O:101:BCL:OBD	2.15	0.57
9:2:103:BCL:HBB3	5:C:20:PHE:CZ	2.40	0.57
4:M:424:TYR:CE1	4:M:430:VAL:CG1	2.88	0.57
13:P:103:PGV:H062	13:P:104:PGV:P	2.45	0.57
2:A:4:ARG:HE	2:A:7:GLU:HA	1.69	0.57
2:H:9:ARG:HD3	2:J:5:PRO:O	2.05	0.57
1:W:53:TRP:CD2	9:W:102:BCL:H2C	2.40	0.57
10:S:101:KGD:CAK	10:S:101:KGD:CAL	2.83	0.56
9:T:101:BCL:HMD1	1:U:44:HIS:CE1	2.40	0.56
2:V:8:PHE:CE2	5:C:8:LEU:HD11	2.39	0.56
5:C:211:VAL:CG2	5:C:222:VAL:HG22	2.36	0.56
5:C:229:MET:SD	15:C:404:HEM:NB	2.78	0.56
1:8:22:GLN:HG2	2:9:5:PRO:HB3	1.88	0.56
2:F:29:VAL:HG22	13:M:706:PGV:O13	2.06	0.56
9:M:703:BCL:H202	11:M:704:BPH:H162	1.88	0.56
10:T:102:KGD:CAE	9:W:103:BCL:CBB	2.70	0.56
1:W:32:THR:HG1	6:X:20:PHE:HE1	1.48	0.56
7:Y:5:VAL:O	7:Y:9:MET:HG2	2.05	0.56
10:0:104:KGD:CAK	2:9:12:VAL:HG11	2.36	0.56
5:C:120:TYR:OH	15:C:403:HEM:O2A	2.24	0.56
9:0:101:BCL:HMD1	2:9:27:HIS:CE1	2.41	0.56
1:6:22:GLN:HG2	2:7:5:PRO:HB3	1.88	0.56
1:0:32:THR:HG21	10:0:104:KGD:CAN	2.36	0.55
10:T:102:KGD:CAN	1:U:32:THR:HG21	2.35	0.55
5:C:88:PRO:HB2	5:C:91:VAL:HG13	1.87	0.55
10:2:101:KGD:CAC	9:4:102:BCL:HBB2	2.34	0.55
9:R:101:BCL:CHC	9:U:101:BCL:HBB3	2.36	0.55
5:C:82:ILE:HD13	5:C:100:ALA:HA	1.88	0.55
10:2:101:KGD:CBF	10:2:101:KGD:CAZ	2.85	0.55
10:5:102:KGD:CAI	9:8:102:BCL:HBB2	2.33	0.55
9:M:703:BCL:HBD	9:M:703:BCL:HAA2	1.87	0.55
2:P:4:ARG:HG3	1:Q:17:LEU:HD23	1.89	0.55
11:M:704:BPH:H172	11:M:704:BPH:H122	1.88	0.55
2:V:8:PHE:HE2	1:W:25:VAL:HB	1.69	0.55
2:A:12:VAL:HG11	10:A:103:KGD:CAK	2.37	0.55
1:B:19:ASN:H	1:B:22:GLN:NE2	2.04	0.55
2:T:27:HIS:NE2	9:U:101:BCL:HMD1	2.21	0.55
9:T:101:BCL:OBD	9:U:101:BCL:HBD	2.07	0.55
5:C:41:TRP:O	5:C:45:THR:HG22	2.06	0.55
4:M:620:TRP:HZ2	8:Z:19:GLY:HA2	1.65	0.54
5:C:206:PRO:HA	5:C:261:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:TYR:OH	9:G:101:BCL:OBD	2.15	0.54
9:T:101:BCL:HBB2	10:W:101:KGD:CBD	2.37	0.54
5:C:67:THR:HA	5:C:69:TYR:CE1	2.42	0.54
3:L:241:ILE:HG23	3:L:245:ASN:HB2	1.89	0.54
2:N:40:ARG:HB2	2:P:35:ALA:HB2	1.89	0.53
2:5:29:VAL:HG22	3:L:303:PRO:O	2.08	0.53
3:L:293:ASN:O	5:C:191:ASN:ND2	2.42	0.53
9:L:1001:BCL:HAC2	9:L:1002:BCL:H2	1.91	0.53
10:F:103:KGD:CAK	10:F:103:KGD:CAL	2.87	0.53
2:J:31:LEU:HB2	2:J:38:TRP:CZ3	2.44	0.53
1:4:12:ASP:OD1	1:4:15:LYS:HD2	2.08	0.53
2:9:31:LEU:HB2	2:9:38:TRP:CZ3	2.44	0.53
11:M:704:BPH:HBB3	11:M:704:BPH:CHC	2.22	0.53
5:C:54:LEU:HD21	5:C:63:THR:HB	1.90	0.53
5:C:86:PRO:O	5:C:99:THR:HG22	2.09	0.53
1:0:10:VAL:HG22	1:0:23:TRP:HB2	1.89	0.53
10:B:102:KGD:CAK	10:B:102:KGD:CAL	2.87	0.53
10:B:102:KGD:CAX	1:E:54:ILE:HG21	2.39	0.53
5:C:229:MET:HB3	15:C:404:HEM:C4B	2.44	0.53
5:C:20:PHE:HE1	10:C:401:KGD:CBF	2.21	0.52
3:L:163:VAL:HB	11:L:1003:BPH:HAC1	1.90	0.52
9:T:101:BCL:CHD	9:U:101:BCL:HMD2	2.39	0.52
1:B:12:ASP:HA	1:B:15:LYS:HE3	1.91	0.52
10:W:101:KGD:CAG	9:X:101:BCL:H141	2.39	0.52
1:2:33:ILE:HG13	10:2:101:KGD:CAU	2.40	0.52
9:L:1002:BCL:H203	13:P:104:PGV:H291	1.90	0.52
10:T:102:KGD:CAF	10:U:103:KGD:OAA	2.57	0.52
1:0:34:TYR:OH	9:0:102:BCL:OBD	2.15	0.52
9:H:102:BCL:H192	10:J:103:KGD:CBG	2.40	0.52
3:L:74:ALA:O	3:L:78:ILE:HG13	2.09	0.52
4:M:452:TRP:CH2	11:M:704:BPH:H112	2.44	0.52
3:L:93:VAL:HG12	3:L:94:ASN:N	2.25	0.52
2:V:39:LEU:HD23	6:X:6:MET:CE	2.38	0.52
1:8:12:ASP:HA	1:8:15:LYS:HE2	1.92	0.52
3:L:93:VAL:HG22	2:P:32:SER:HB3	1.92	0.52
3:L:265:ARG:HH22	7:Y:31:ASN:HD21	1.57	0.52
8:Z:12:SER:N	8:Z:13:PRO:CD	2.73	0.52
5:C:123:ASN:HB3	5:C:129:GLN:HE21	1.75	0.51
2:H:9:ARG:HG3	2:J:6:PHE:CZ	2.45	0.51
11:M:704:BPH:H122	11:M:704:BPH:C17	2.41	0.51
1:U:50:TRP:CZ2	1:W:54:ILE:HG23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:78:MET:O	5:C:82:ILE:HG13	2.10	0.51
10:0:104:KGD:OAA	2:A:6:PHE:CD2	2.64	0.51
10:E:102:KGD:CAL	10:E:102:KGD:CAK	2.87	0.51
5:C:31:MET:HE2	10:C:401:KGD:CBO	2.37	0.51
5:C:58:ILE:HA	5:C:311:GLN:HG3	1.92	0.51
1:W:50:TRP:CE3	6:X:5:LEU:CD1	2.91	0.51
3:L:77:ILE:HG23	2:R:17:LEU:HD21	1.92	0.51
5:C:200:PRO:O	5:C:205:TYR:OH	2.28	0.51
3:L:271:GLY:O	3:L:274:SER:OG	2.29	0.51
4:M:538:LEU:HD21	4:M:591:TRP:HB3	1.93	0.51
2:F:31:LEU:HB2	2:F:38:TRP:CZ3	2.46	0.51
4:M:453:TRP:NE1	4:M:470:ALA:O	2.44	0.51
1:B:34:TYR:OH	9:B:101:BCL:OBD	2.15	0.50
2:F:37:ASN:HA	2:F:41:ALA:HA	1.92	0.50
11:M:704:BPH:C14	11:M:704:BPH:C4	2.86	0.50
8:Z:20:TYR:O	8:Z:21:ALA:C	2.50	0.50
4:M:345:ASP:OD1	4:M:353:LYS:CE	2.59	0.50
5:C:285:ILE:HG13	5:C:286:MET:HG3	1.92	0.50
8:Z:25:VAL:CG2	8:Z:26:PRO:CD	2.89	0.50
8:Z:32:LEU:O	8:Z:36:ILE:HG13	2.11	0.50
9:W:102:BCL:H202	6:X:17:THR:HA	1.94	0.50
8:Z:20:TYR:HD1	8:Z:24:PHE:HD2	1.55	0.50
2:D:31:LEU:HD22	2:D:38:TRP:CZ3	2.46	0.50
8:Z:22:LEU:O	8:Z:26:PRO:CG	2.54	0.50
9:5:101:BCL:H192	2:7:14:VAL:HG11	1.93	0.50
2:J:9:ARG:HD3	2:N:5:PRO:O	2.12	0.50
7:Y:25:ALA:HB3	16:Y:101:DGA:HA82	1.94	0.50
12:M:701:MQE:CBA	13:P:104:PGV:C11	2.89	0.50
3:L:88:LEU:HD13	12:M:701:MQE:CCN	2.41	0.50
4:M:564:GLU:OE2	4:M:584:ASN:HB2	2.12	0.50
10:A:103:KGD:CAK	10:A:103:KGD:CAL	2.87	0.50
11:M:704:BPH:H7C2	11:M:704:BPH:C13	2.42	0.50
10:O:102:KGD:CAG	9:Q:102:BCL:CAD	2.89	0.50
10:S:101:KGD:OAA	2:T:6:PHE:CE1	2.65	0.50
5:C:20:PHE:CE1	10:C:401:KGD:CBA	2.95	0.50
2:A:31:LEU:HB2	2:A:38:TRP:CZ3	2.47	0.49
2:N:4:ARG:HH22	1:O:22:GLN:NE2	2.08	0.49
1:U:19:ASN:OD1	1:U:20:ASN:N	2.44	0.49
10:P:102:KGD:OAA	2:R:6:PHE:CD2	2.65	0.49
10:Q:103:KGD:CAK	10:Q:103:KGD:CAL	2.87	0.49
5:C:229:MET:SD	15:C:404:HEM:ND	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:TRP:CE3	10:E:102:KGD:CAZ	2.95	0.49
1:I:31:LYS:CB	9:K:101:BCL:H42	2.41	0.49
2:V:27:HIS:CE1	9:W:102:BCL:HMD1	2.47	0.49
5:C:78:MET:HA	5:C:127:PHE:HE2	1.76	0.49
7:Y:14:LEU:O	7:Y:17:PHE:HB2	2.12	0.49
10:H:103:KGD:CAG	10:I:102:KGD:OAA	2.61	0.49
3:L:42:PHE:CD2	8:Z:54:PRO:HB2	2.47	0.49
2:T:36:PHE:CZ	1:U:53:TRP:HB3	2.47	0.49
3:L:254:LEU:CD1	11:M:704:BPH:HED1	2.42	0.49
12:M:701:MQE:CAG	8:Z:34:PHE:CE2	2.96	0.49
5:C:218:SER:OG	5:C:219:ASN:N	2.45	0.49
5:C:275:VAL:HG21	5:C:291:PRO:HD3	1.94	0.49
8:Z:20:TYR:HA	8:Z:24:PHE:CD2	2.47	0.49
2:J:28:PHE:CE2	13:L:1006:PGV:H232	2.48	0.49
2:N:17:LEU:HD22	13:P:103:PGV:C27	2.43	0.49
1:W:29:VAL:HG22	10:W:101:KGD:CAL	2.42	0.49
10:A:104:KGD:CAG	10:E:102:KGD:OAA	2.61	0.49
2:A:17:LEU:CD2	4:M:384:ILE:HB	2.42	0.49
9:D:101:BCL:H203	9:D:101:BCL:H162	1.71	0.49
2:J:9:ARG:HG3	2:N:6:PHE:CZ	2.48	0.49
3:L:248:VAL:HG13	4:M:342:GLU:HG2	1.95	0.49
1:2:31:LYS:HB2	9:4:102:BCL:H42	1.95	0.48
2:9:8:PHE:O	2:9:12:VAL:HG23	2.13	0.48
2:A:8:PHE:O	2:A:12:VAL:HG23	2.13	0.48
3:L:241:ILE:CG2	3:L:245:ASN:HB2	2.43	0.48
2:R:8:PHE:O	2:R:12:VAL:HG23	2.13	0.48
1:U:24:LEU:HB2	1:W:17:LEU:HD11	1.95	0.48
2:7:8:PHE:O	2:7:12:VAL:HG23	2.13	0.48
2:N:8:PHE:O	2:N:12:VAL:HG23	2.14	0.48
2:1:8:PHE:CE1	9:2:103:BCL:HMC2	2.48	0.48
9:1:101:BCL:HBB2	10:3:102:KGD:CBC	2.44	0.48
2:3:8:PHE:O	2:3:12:VAL:HG23	2.13	0.48
8:Z:15:PRO:HG2	8:Z:20:TYR:CE1	2.48	0.48
2:1:8:PHE:O	2:1:12:VAL:HG23	2.13	0.48
2:1:31:LEU:HB2	2:1:38:TRP:CZ3	2.48	0.48
2:D:8:PHE:O	2:D:12:VAL:HG23	2.13	0.48
2:F:8:PHE:O	2:F:12:VAL:HG23	2.14	0.48
9:N:102:BCL:H71	9:N:102:BCL:H112	1.60	0.48
1:U:34:TYR:OH	9:U:102:BCL:OBD	2.14	0.48
5:C:129:GLN:HG3	5:C:133:TYR:HE1	1.78	0.48
9:M:703:BCL:C20	11:M:704:BPH:H162	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:8:PHE:O	2:T:12:VAL:HG23	2.13	0.48
8:Z:20:TYR:HD1	8:Z:24:PHE:CE2	2.31	0.48
2:5:8:PHE:O	2:5:12:VAL:HG23	2.14	0.48
2:F:36:PHE:O	1:G:50:TRP:CZ2	2.66	0.48
3:L:59:PRO:HD2	3:L:71:LEU:HB2	1.95	0.48
4:M:452:TRP:HH2	11:M:704:BPH:H112	1.78	0.48
1:Q:19:ASN:OD1	1:Q:20:ASN:N	2.44	0.48
2:1:9:ARG:HG3	2:3:6:PHE:CE1	2.49	0.48
9:8:101:BCL:H202	10:8:103:KGD:CAL	2.43	0.48
2:J:8:PHE:O	2:J:12:VAL:HG23	2.13	0.48
2:5:4:ARG:HG3	2:5:4:ARG:O	2.14	0.48
2:J:40:ARG:HB2	2:N:35:ALA:CB	2.43	0.48
3:L:118:PRO:HD2	2:T:33:SER:HA	1.96	0.48
3:L:209:ASN:HB3	3:L:212:HIS:HB3	1.95	0.48
1:E:28:ILE:HD13	9:G:101:BCL:HBA1	1.95	0.48
2:H:8:PHE:O	2:H:12:VAL:HG23	2.13	0.48
4:M:610:SER:CB	4:M:617:TRP:HE1	2.25	0.48
11:L:1005:BPH:HED1	13:C:406:PGV:C13	2.43	0.48
11:M:704:BPH:H193	11:M:704:BPH:H161	1.71	0.48
2:P:8:PHE:O	2:P:12:VAL:HG23	2.13	0.47
2:R:13:VAL:O	2:R:16:THR:HG22	2.14	0.47
2:V:12:VAL:HG11	10:W:101:KGD:CAK	2.44	0.47
1:4:19:ASN:OD1	1:4:20:ASN:N	2.44	0.47
10:9:101:KGD:CBA	10:9:101:KGD:CBK	2.92	0.47
5:C:170:THR:OG1	5:C:171:CYS:N	2.47	0.47
1:S:24:LEU:HB2	1:U:17:LEU:HD11	1.95	0.47
5:C:117:ASP:OD1	5:C:118:CYS:N	2.47	0.47
5:C:155:ASN:O	5:C:159:LYS:HE2	2.15	0.47
10:0:104:KGD:CAC	9:B:101:BCL:HBB2	2.43	0.47
1:8:50:TRP:CE3	10:8:103:KGD:CAZ	2.98	0.47
3:L:78:ILE:CG1	2:R:17:LEU:HD11	2.45	0.47
9:N:101:BCL:H162	9:N:101:BCL:H203	1.71	0.47
9:R:101:BCL:H203	9:R:101:BCL:H162	1.71	0.47
8:Z:25:VAL:HG23	8:Z:26:PRO:CD	2.41	0.47
2:5:27:HIS:CE1	9:6:101:BCL:HMD1	2.49	0.47
2:D:27:HIS:O	2:D:31:LEU:HG	2.14	0.47
12:L:1004:MQE:CAO	7:Y:14:LEU:CB	2.92	0.47
4:M:609:LEU:HD22	4:M:613:LEU:HD12	1.97	0.47
4:M:630:TRP:CE2	4:M:633:PRO:HB3	2.50	0.47
2:N:9:ARG:HG3	2:P:6:PHE:CZ	2.50	0.47
2:V:8:PHE:O	2:V:12:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:18:LEU:O	2:V:22:MET:HG2	2.13	0.47
5:C:20:PHE:HE1	10:C:401:KGD:CBA	2.28	0.47
5:C:146:MET:HG2	15:C:403:HEM:CBB	2.44	0.47
8:Z:15:PRO:HG2	8:Z:20:TYR:HE1	1.78	0.47
1:0:19:ASN:OD1	1:0:20:ASN:N	2.44	0.47
1:0:50:TRP:CE3	10:0:103:KGD:CAZ	2.98	0.47
2:1:25:LEU:HD21	5:C:39:PHE:CZ	2.50	0.47
5:C:82:ILE:HD11	5:C:103:SER:CB	2.44	0.47
5:C:111:SER:O	5:C:115:LYS:N	2.48	0.47
5:C:189:ILE:HD12	5:C:231:HIS:CE1	2.50	0.47
5:C:211:VAL:HG12	15:C:404:HEM:HAA1	1.97	0.47
8:Z:39:ARG:HH12	13:Z:101:PGV:C05	2.27	0.47
1:G:31:LYS:HB2	9:I:101:BCL:H42	1.97	0.47
2:J:4:ARG:HH21	2:J:8:PHE:H	1.63	0.47
11:L:1005:BPH:HED3	13:C:406:PGV:H151	1.97	0.47
5:C:78:MET:HA	5:C:127:PHE:CE2	2.50	0.47
9:A:101:BCL:HBB2	10:A:104:KGD:CBD	2.44	0.47
9:B:101:BCL:H62	9:B:101:BCL:H41	1.62	0.47
1:K:19:ASN:OD1	1:K:20:ASN:N	2.44	0.47
3:L:55:PHE:HD1	9:T:101:BCL:H201	1.79	0.47
5:C:146:MET:HG2	15:C:403:HEM:HBB2	1.96	0.47
5:C:271:GLN:HA	5:C:275:VAL:HB	1.97	0.47
9:9:102:BCL:H203	9:9:102:BCL:H162	1.71	0.47
3:L:59:PRO:HA	2:T:10:THR:HG23	1.97	0.47
9:Q:102:BCL:H62	9:Q:102:BCL:H41	1.62	0.47
5:C:119:SER:N	5:C:124:ILE:HD11	2.30	0.47
9:0:101:BCL:HBB3	9:7:101:BCL:CHC	2.46	0.46
1:2:19:ASN:OD1	1:2:20:ASN:N	2.44	0.46
1:G:19:ASN:OD1	1:G:20:ASN:N	2.44	0.46
13:P:103:PGV:H201	13:P:103:PGV:H22	1.97	0.46
1:S:19:ASN:OD1	1:S:20:ASN:N	2.44	0.46
3:L:34:ILE:HB	8:Z:51:ARG:HD2	1.97	0.46
10:3:102:KGD:CAK	10:3:102:KGD:CAL	2.91	0.46
1:6:34:TYR:OH	9:6:102:BCL:OBD	2.15	0.46
9:L:1001:BCL:H141	9:L:1001:BCL:H161	1.53	0.46
10:B:102:KGD:CAF	9:E:101:BCL:C3	2.94	0.46
10:H:103:KGD:OAA	2:J:6:PHE:CD1	2.68	0.46
2:J:29:VAL:HG22	8:Z:17:TRP:HB2	1.97	0.46
11:L:1005:BPH:H162	11:L:1005:BPH:H193	1.66	0.46
5:C:26:ILE:O	5:C:30:VAL:HG12	2.16	0.46
5:C:93:VAL:O	5:C:94:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:8:19:ASN:OD1	1:8:20:ASN:N	2.44	0.46
2:H:39:LEU:HD23	2:H:39:LEU:HA	1.75	0.46
9:L:1002:BCL:H143	9:L:1002:BCL:H161	1.60	0.46
11:M:704:BPH:C12	11:M:704:BPH:C17	2.93	0.46
5:C:77:ALA:HB3	5:C:124:ILE:HG22	1.96	0.46
5:C:169:ILE:HG12	15:C:405:HEM:HBC2	1.98	0.46
4:M:386:PHE:HB2	4:M:448:SER:OG	2.15	0.46
2:P:31:LEU:HB2	2:P:38:TRP:CZ3	2.51	0.46
5:C:70:ILE:HD13	5:C:107:VAL:HG23	1.96	0.46
5:C:111:SER:HB2	5:C:116:VAL:O	2.16	0.46
10:I:102:KGD:CAS	10:I:102:KGD:CBC	2.94	0.46
10:I:102:KGD:CAS	1:K:54:ILE:HG21	2.46	0.46
4:M:432:TRP:HA	4:M:436:GLY:HA3	1.97	0.46
4:M:482:VAL:HA	4:M:486:PHE:HB2	1.97	0.46
2:T:31:LEU:HB2	2:T:38:TRP:CZ3	2.51	0.46
9:X:101:BCL:H111	9:X:101:BCL:H142	1.51	0.46
1:8:34:TYR:OH	9:8:102:BCL:OBD	2.15	0.46
9:E:101:BCL:H62	9:E:101:BCL:H41	1.62	0.46
2:J:4:ARG:NH2	2:J:8:PHE:H	2.14	0.46
3:L:142:ARG:NH2	4:M:577:TRP:O	2.49	0.46
2:7:31:LEU:HB2	2:7:38:TRP:CZ3	2.51	0.46
2:N:17:LEU:HD11	13:P:103:PGV:H292	1.98	0.46
9:U:101:BCL:H191	1:W:33:ILE:HD13	1.97	0.46
2:1:30:VAL:HA	5:C:46:ILE:CD1	2.46	0.45
2:R:34:GLY:HA2	2:R:41:ALA:HB1	1.97	0.45
3:L:63:TRP:CH2	3:L:149:LYS:HE2	2.51	0.45
2:P:7:GLU:CB	13:P:103:PGV:O14	2.56	0.45
5:C:67:THR:HB	5:C:70:ILE:HD12	1.97	0.45
7:Y:30:THR:C	7:Y:32:PRO:HD3	2.36	0.45
1:4:11:PRO:O	1:4:15:LYS:HG3	2.16	0.45
10:6:103:KGD:CAK	10:6:103:KGD:CAL	2.93	0.45
4:M:347:LEU:HD11	4:M:380:VAL:HG21	1.97	0.45
5:C:10:PRO:O	5:C:14:ASN:HB2	2.16	0.45
2:J:12:VAL:HG11	10:J:103:KGD:CAK	2.46	0.45
3:L:7:ALA:O	3:L:15:THR:HG22	2.15	0.45
2:N:31:LEU:HB2	2:N:38:TRP:CZ3	2.51	0.45
9:S:102:BCL:H71	9:S:102:BCL:H112	1.60	0.45
5:C:191:ASN:O	13:C:406:PGV:O14	2.34	0.45
9:X:101:BCL:H143	9:X:101:BCL:H161	1.59	0.45
4:M:527:LEU:HD11	8:Z:26:PRO:HB3	1.98	0.45
10:T:102:KGD:CAK	1:U:29:VAL:CG2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:20:PHE:CZ	5:C:24:ALA:HB2	2.51	0.45
8:Z:15:PRO:HD2	8:Z:20:TYR:OH	2.16	0.45
9:0:102:BCL:H62	9:0:102:BCL:H41	1.62	0.45
9:1:101:BCL:HMB2	10:3:102:KGD:CAS	2.47	0.45
11:M:704:BPH:CBB	11:M:704:BPH:CHC	2.86	0.45
9:N:101:BCL:H191	13:P:103:PGV:H41	1.98	0.45
1:W:19:ASN:OD1	1:W:20:ASN:N	2.44	0.45
10:J:103:KGD:OAA	2:N:6:PHE:CD2	2.70	0.45
3:L:136:PHE:CE1	9:L:1002:BCL:H121	2.51	0.45
9:R:101:BCL:HMB1	9:R:101:BCL:HBB3	1.99	0.45
9:3:101:BCL:HMB1	9:3:101:BCL:HBB3	1.99	0.45
10:4:103:KGD:CAU	9:6:102:BCL:H162	2.46	0.45
3:L:93:VAL:C	3:L:95:GLU:H	2.19	0.45
11:M:704:BPH:H4C2	11:M:704:BPH:O2A	2.17	0.45
2:R:31:LEU:HB2	2:R:38:TRP:CZ3	2.52	0.45
9:X:101:BCL:HMB1	9:X:101:BCL:HBB3	1.99	0.45
2:1:30:VAL:HG22	5:C:46:ILE:HD13	1.99	0.45
9:G:101:BCL:H62	9:G:101:BCL:H41	1.62	0.45
9:H:101:BCL:HBB3	9:H:101:BCL:HMB1	1.99	0.45
3:L:173:LEU:HD23	7:Y:9:MET:HE3	1.99	0.45
9:L:1001:BCL:HBA2	4:M:530:PHE:HD1	1.82	0.45
9:L:1002:BCL:H151	11:L:1003:BPH:HHB	1.99	0.45
5:C:88:PRO:HB2	5:C:91:VAL:CG1	2.46	0.45
9:4:101:BCL:H112	9:4:101:BCL:H71	1.60	0.45
3:L:224:LEU:HD13	11:M:704:BPH:ND	2.32	0.45
11:M:704:BPH:H6C1	11:M:704:BPH:H4C1	1.69	0.45
1:2:31:LYS:CB	9:4:102:BCL:H42	2.47	0.44
9:2:102:BCL:H112	9:2:102:BCL:H71	1.60	0.44
9:A:101:BCL:HMB1	9:A:101:BCL:HBB3	1.99	0.44
9:F:102:BCL:H112	9:F:102:BCL:H71	1.60	0.44
9:H:102:BCL:H112	9:H:102:BCL:H71	1.60	0.44
3:L:49:THR:O	3:L:53:ARG:HG2	2.18	0.44
9:F:101:BCL:HMB1	9:F:101:BCL:HBB3	1.99	0.44
5:C:106:MET:HA	5:C:110:VAL:HB	1.99	0.44
6:X:20:PHE:CD2	9:X:101:BCL:H91	2.52	0.44
11:M:704:BPH:ND	11:M:704:BPH:NC	2.60	0.44
10:0:104:KGD:CAK	10:0:104:KGD:CAL	2.93	0.44
9:5:101:BCL:HMB1	9:5:101:BCL:HBB3	1.99	0.44
3:L:40:GLU:CD	4:M:576:ARG:HH12	2.20	0.44
3:L:239:ARG:HB2	3:L:241:ILE:CG1	2.47	0.44
4:M:525:HIS:CE1	4:M:529:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:101:BCL:HMB1	9:N:101:BCL:HBB3	1.99	0.44
5:C:12:ILE:HG22	5:C:22:ILE:HD11	1.98	0.44
5:C:84:ALA:O	5:C:86:PRO:HD3	2.17	0.44
9:D:101:BCL:HMB1	9:D:101:BCL:HBB3	1.99	0.44
3:L:34:ILE:HD12	8:Z:51:ARG:HB2	1.99	0.44
4:M:522:ASN:HB3	4:M:525:HIS:HB3	1.99	0.44
9:T:101:BCL:HBB3	9:T:101:BCL:HMB1	1.99	0.44
5:C:277:PRO:HG2	5:C:283:ASP:O	2.17	0.44
6:X:2:ALA:N	6:X:3:PRO:HD2	2.32	0.44
2:R:16:THR:HG21	9:R:101:BCL:H193	1.99	0.44
5:C:118:CYS:HB3	5:C:122:HIS:HE1	1.83	0.44
8:Z:43:LYS:HE3	8:Z:43:LYS:HB3	1.71	0.44
10:A:104:KGD:CAK	2:D:12:VAL:HG11	2.47	0.44
1:B:19:ASN:OD1	1:B:20:ASN:N	2.44	0.44
1:E:12:ASP:HA	1:E:15:LYS:HE3	2.00	0.44
3:L:275:VAL:HG11	11:L:1003:BPH:H2C	2.00	0.44
9:L:1001:BCL:H142	9:L:1001:BCL:H112	1.67	0.44
1:2:53:TRP:CD2	9:2:102:BCL:H2C	2.53	0.44
9:2:102:BCL:HMC3	5:C:42:ILE:HG23	2.00	0.44
1:S:53:TRP:CD2	9:S:102:BCL:H2C	2.53	0.44
2:7:28:PHE:HB3	4:M:405:PRO:HD3	2.00	0.43
4:M:420:PRO:HB3	4:M:430:VAL:HG11	1.99	0.43
9:N:101:BCL:HMD1	1:O:44:HIS:CE1	2.52	0.43
1:Q:53:TRP:CD2	9:Q:101:BCL:H2C	2.53	0.43
5:C:122:HIS:CE1	15:C:402:HEM:NB	2.84	0.43
1:8:53:TRP:CD2	9:8:101:BCL:H2C	2.53	0.43
9:J:101:BCL:HBB3	9:J:101:BCL:HMB1	1.99	0.43
3:L:180:ALA:C	3:L:182:GLY:H	2.22	0.43
4:M:337:ASP:O	4:M:341:GLU:HG2	2.18	0.43
4:M:363:ARG:HG3	7:Y:31:ASN:O	2.18	0.43
1:S:50:TRP:CE3	10:S:104:KGD:CAZ	3.02	0.43
1:U:15:LYS:HE3	1:U:15:LYS:HB2	1.87	0.43
9:2:103:BCL:CAC	10:C:401:KGD:CBO	2.94	0.43
9:7:101:BCL:HBB3	9:7:101:BCL:HMB1	1.99	0.43
9:D:102:BCL:H2C	1:E:53:TRP:CD2	2.53	0.43
3:L:6:ARG:HH12	3:L:9:PRO:HD2	1.82	0.43
3:L:251:ARG:HD2	4:M:371:GLY:HA3	2.01	0.43
1:Q:31:LYS:HB2	9:S:103:BCL:H42	1.99	0.43
6:X:13:LEU:C	6:X:13:LEU:HD23	2.39	0.43
1:6:19:ASN:OD1	1:6:20:ASN:N	2.44	0.43
9:9:102:BCL:HMB1	9:9:102:BCL:HBB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:102:KGD:CBN	9:J:102:BCL:HMB1	2.48	0.43
4:M:553:LYS:HD3	4:M:553:LYS:HA	1.61	0.43
2:V:19:GLY:HA3	9:X:101:BCL:H42	2.00	0.43
8:Z:39:ARG:HH12	13:Z:101:PGV:C04	2.31	0.43
10:0:103:KGD:CAK	10:0:103:KGD:CAL	2.93	0.43
9:1:101:BCL:HMB1	9:1:101:BCL:HBB3	1.99	0.43
1:2:41:VAL:O	1:2:45:VAL:HG23	2.19	0.43
1:6:41:VAL:O	1:6:45:VAL:HG23	2.19	0.43
9:F:102:BCL:H2C	1:G:53:TRP:CD2	2.53	0.43
9:J:101:BCL:H203	9:J:101:BCL:H162	1.71	0.43
9:N:101:BCL:H202	2:P:6:PHE:CE2	2.53	0.43
1:W:41:VAL:O	1:W:45:VAL:HG23	2.19	0.43
5:C:218:SER:O	5:C:222:VAL:HG23	2.18	0.43
2:1:18:LEU:HD22	10:C:401:KGD:CAQ	2.47	0.43
1:6:53:TRP:CD2	9:6:101:BCL:H2C	2.53	0.43
9:8:101:BCL:H161	10:8:103:KGD:CAO	2.48	0.43
3:L:308:VAL:HG23	3:L:308:VAL:O	2.18	0.43
2:N:4:ARG:NH2	1:O:22:GLN:HE22	2.13	0.43
9:S:102:BCL:H192	10:T:102:KGD:CBG	2.48	0.43
5:C:137:ALA:O	5:C:140:VAL:HG22	2.19	0.43
1:I:19:ASN:OD1	1:I:20:ASN:N	2.44	0.43
9:J:102:BCL:H2C	1:K:53:TRP:CD2	2.53	0.43
3:L:60:PHE:CE2	9:R:101:BCL:H201	2.53	0.43
9:S:103:BCL:H62	9:S:103:BCL:H41	1.62	0.43
1:4:53:TRP:CD2	9:4:101:BCL:H2C	2.53	0.43
2:D:38:TRP:CZ2	2:D:39:LEU:HD12	2.52	0.43
9:H:102:BCL:H2C	1:I:53:TRP:CD2	2.53	0.43
1:I:41:VAL:O	1:I:45:VAL:HG23	2.19	0.43
2:R:4:ARG:HG3	2:R:4:ARG:O	2.19	0.43
5:C:77:ALA:CB	5:C:124:ILE:HG22	2.49	0.43
2:3:4:ARG:NH1	2:3:7:GLU:HG2	2.34	0.43
9:A:102:BCL:H71	9:A:102:BCL:H112	1.60	0.43
3:L:31:ALA:HB1	8:Z:50:LEU:HB3	2.00	0.43
3:L:60:PHE:O	3:L:70:GLY:HA2	2.18	0.43
1:U:53:TRP:CD2	9:U:101:BCL:H2C	2.53	0.43
9:6:101:BCL:H112	9:6:101:BCL:H71	1.60	0.43
2:D:15:SER:HB2	9:E:101:BCL:HBC2	2.01	0.43
9:J:102:BCL:H71	9:J:102:BCL:H112	1.60	0.43
3:L:118:PRO:HA	3:L:123:PHE:CG	2.54	0.43
3:L:308:VAL:HG21	4:M:406:ILE:HG21	2.00	0.43
9:W:103:BCL:H62	9:W:103:BCL:H41	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:20:PHE:CE2	9:X:101:BCL:C9	3.02	0.43
9:2:103:BCL:H41	9:2:103:BCL:H62	1.62	0.42
1:4:53:TRP:CD1	1:4:54:ILE:HG13	2.53	0.42
1:E:19:ASN:OD1	1:E:20:ASN:N	2.44	0.42
1:E:41:VAL:O	1:E:45:VAL:HG23	2.19	0.42
1:K:41:VAL:O	1:K:45:VAL:HG23	2.19	0.42
3:L:241:ILE:HB	4:M:558:PHE:CE1	2.54	0.42
9:P:101:BCL:H203	9:P:101:BCL:H162	1.71	0.42
8:Z:15:PRO:CD	8:Z:20:TYR:OH	2.67	0.42
9:A:102:BCL:H2C	1:B:53:TRP:CD2	2.53	0.42
9:D:102:BCL:H112	9:D:102:BCL:H71	1.60	0.42
2:N:17:LEU:HD22	13:P:103:PGV:H272	2.00	0.42
5:C:69:TYR:CE1	5:C:115:LYS:CD	3.02	0.42
5:C:236:MET:O	5:C:238:GLN:N	2.52	0.42
9:1:101:BCL:H203	9:1:101:BCL:H162	1.71	0.42
1:G:41:VAL:O	1:G:45:VAL:HG23	2.19	0.42
9:L:1001:BCL:HBB3	11:L:1003:BPH:H141	2.01	0.42
11:L:1003:BPH:OBB	11:L:1003:BPH:HHC	2.20	0.42
4:M:438:TRP:O	4:M:442:THR:OG1	2.24	0.42
4:M:508:TRP:CE2	4:M:512:VAL:HG21	2.54	0.42
11:M:704:BPH:C14	11:M:704:BPH:H7C2	2.48	0.42
10:P:102:KGD:OAA	2:R:6:PHE:HB2	2.20	0.42
9:R:101:BCL:OBD	9:S:102:BCL:HBD	2.19	0.42
1:S:41:VAL:O	1:S:45:VAL:HG23	2.19	0.42
5:C:36:ILE:HD13	10:C:401:KGD:CAF	2.44	0.42
1:0:53:TRP:CD2	9:0:101:BCL:H2C	2.53	0.42
9:1:101:BCL:HBC3	9:1:101:BCL:H2C	1.88	0.42
1:4:41:VAL:O	1:4:45:VAL:HG23	2.19	0.42
9:8:102:BCL:H41	9:8:102:BCL:H62	1.62	0.42
2:D:28:PHE:HD1	2:D:28:PHE:O	2.03	0.42
9:J:101:BCL:HMB3	9:N:102:BCL:CHB	2.49	0.42
3:L:78:ILE:HG12	2:R:17:LEU:HD11	2.01	0.42
4:M:519:PHE:O	4:M:525:HIS:ND1	2.52	0.42
2:H:4:ARG:NH1	2:H:7:GLU:HG2	2.34	0.42
4:M:363:ARG:NH2	7:Y:28:TRP:CD1	2.88	0.42
4:M:480:TYR:HB2	9:M:703:BCL:H62	2.01	0.42
10:O:102:KGD:CAG	9:Q:102:BCL:C3D	2.97	0.42
9:P:101:BCL:HMB1	9:P:101:BCL:HBB3	1.99	0.42
13:P:103:PGV:H22	13:P:103:PGV:C20	2.50	0.42
9:U:101:BCL:H91	9:W:103:BCL:H91	2.01	0.42
1:0:41:VAL:O	1:0:45:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:ARG:HG3	1:K:55:ARG:HH22	1.83	0.42
9:N:102:BCL:H2C	1:O:53:TRP:CD2	2.53	0.42
10:U:103:KGD:CAG	9:W:103:BCL:H62	2.50	0.42
5:C:85:ASN:O	5:C:99:THR:HG21	2.19	0.42
5:C:209:LEU:HB3	5:C:225:ASN:HD22	1.84	0.42
1:B:41:VAL:O	1:B:45:VAL:HG23	2.19	0.42
3:L:100:ILE:HD12	3:L:189:ILE:HD12	2.02	0.42
1:Q:41:VAL:O	1:Q:45:VAL:HG23	2.19	0.42
1:U:41:VAL:O	1:U:45:VAL:HG23	2.19	0.42
5:C:175:HIS:HA	5:C:182:LEU:HD11	2.02	0.42
6:X:19:TYR:CE2	6:X:23:MET:HE1	2.54	0.42
2:7:24:LEU:HD21	2:9:22:MET:HE1	2.00	0.42
2:H:27:HIS:O	2:H:31:LEU:HG	2.20	0.42
10:H:103:KGD:CAN	1:I:32:THR:HG21	2.50	0.42
3:L:93:VAL:CG2	2:P:32:SER:HB3	2.49	0.42
9:L:1001:BCL:H112	9:L:1001:BCL:H3A	2.01	0.42
2:N:9:ARG:HD2	13:P:103:PGV:H032	2.01	0.42
1:O:41:VAL:O	1:O:45:VAL:HG23	2.19	0.42
5:C:27:ILE:O	5:C:31:MET:HB2	2.20	0.42
5:C:51:ALA:HA	5:C:52:PRO:HD3	1.96	0.42
5:C:160:LEU:HD12	15:C:405:HEM:HBD1	2.01	0.42
1:8:41:VAL:O	1:8:45:VAL:HG23	2.19	0.42
9:A:101:BCL:HBC3	9:A:101:BCL:H2C	1.88	0.42
3:L:253:ILE:HD11	4:M:459:ARG:HB2	2.01	0.42
11:L:1003:BPH:HBC3	11:L:1003:BPH:HHD	2.02	0.42
4:M:513:SER:CB	9:M:703:BCL:H3C	2.50	0.42
9:O:101:BCL:H62	9:O:101:BCL:H41	1.62	0.42
2:V:8:PHE:HE2	1:W:25:VAL:CG1	2.33	0.42
2:V:27:HIS:O	2:V:31:LEU:HG	2.20	0.42
5:C:74:SER:HA	5:C:124:ILE:HG21	2.02	0.42
5:C:118:CYS:HB2	5:C:124:ILE:HD12	2.02	0.42
5:C:202:GLU:HG3	5:C:203:LEU:HG	2.01	0.42
9:0:101:BCL:CHB	9:7:101:BCL:HMB3	2.50	0.42
10:8:103:KGD:OAA	10:9:101:KGD:CAG	2.67	0.42
2:N:40:ARG:HB2	2:P:35:ALA:CB	2.50	0.42
10:4:103:KGD:CAL	10:4:103:KGD:CAK	2.96	0.41
3:L:246:ILE:HD12	3:L:246:ILE:HA	1.87	0.41
4:M:443:PHE:CE2	4:M:447:ILE:HD11	2.55	0.41
2:1:30:VAL:HA	5:C:46:ILE:HD13	2.01	0.41
1:4:34:TYR:OH	9:4:102:BCL:OBD	2.15	0.41
2:J:30:VAL:HG21	9:J:102:BCL:HHD	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:212:HIS:CD2	9:L:1002:BCL:HMA3	2.55	0.41
9:F:101:BCL:H203	9:F:101:BCL:H162	1.71	0.41
9:K:101:BCL:H62	9:K:101:BCL:H41	1.62	0.41
4:M:419:PRO:HD3	4:M:499:GLY:HA2	2.01	0.41
9:M:703:BCL:HMB1	9:M:703:BCL:HBB3	2.02	0.41
2:V:8:PHE:CD2	5:C:8:LEU:HD11	2.56	0.41
3:L:199:ILE:HG21	3:L:282:ILE:HD11	2.03	0.41
11:L:1005:BPH:H9C2	11:L:1005:BPH:H6C2	1.82	0.41
9:M:703:BCL:H41	9:M:703:BCL:H61	1.71	0.41
9:U:101:BCL:H201	1:W:33:ILE:CG2	2.51	0.41
8:Z:39:ARG:HE	8:Z:43:LYS:HG3	1.85	0.41
2:7:32:SER:HB3	4:M:403:TRP:O	2.19	0.41
9:7:101:BCL:H203	9:7:101:BCL:H162	1.71	0.41
3:L:44:LYS:HD3	3:L:44:LYS:HA	1.82	0.41
1:O:19:ASN:OD1	1:O:20:ASN:N	2.44	0.41
13:P:103:PGV:H231	13:Z:101:PGV:C3	2.51	0.41
9:R:101:BCL:H203	2:T:14:VAL:HG11	2.02	0.41
2:V:34:GLY:HA2	2:V:37:ASN:HA	2.03	0.41
5:C:122:HIS:HA	5:C:133:TYR:CE2	2.55	0.41
1:4:24:LEU:O	1:4:28:ILE:HG13	2.21	0.41
1:8:9:LEU:HB2	1:8:20:ASN:OD1	2.21	0.41
5:C:69:TYR:CD2	5:C:70:ILE:HG13	2.55	0.41
1:B:9:LEU:HB2	1:B:20:ASN:OD1	2.21	0.41
2:D:4:ARG:HH12	1:E:22:GLN:HE22	1.68	0.41
3:L:8:LEU:HD13	8:Z:50:LEU:HD11	2.03	0.41
12:M:701:MQE:CAM	8:Z:34:PHE:HZ	2.28	0.41
2:1:24:LEU:HD23	10:3:102:KGD:CAZ	2.51	0.41
1:6:24:LEU:O	1:6:28:ILE:HG13	2.21	0.41
2:D:31:LEU:HD22	2:D:38:TRP:CD2	2.55	0.41
3:L:82:LEU:HD23	3:L:82:LEU:HA	1.84	0.41
11:M:704:BPH:H3A	11:M:704:BPH:HBA2	1.81	0.41
13:P:104:PGV:C1	13:P:104:PGV:O11	2.69	0.41
1:2:24:LEU:O	1:2:28:ILE:HG13	2.21	0.41
9:5:101:BCL:H162	9:5:101:BCL:H203	1.71	0.41
1:8:53:TRP:CD1	1:8:54:ILE:HG13	2.56	0.41
1:B:24:LEU:O	1:B:28:ILE:HG13	2.21	0.41
1:E:9:LEU:HB2	1:E:20:ASN:OD1	2.21	0.41
1:I:9:LEU:HB2	1:I:20:ASN:OD1	2.21	0.41
1:I:24:LEU:O	1:I:28:ILE:HG13	2.21	0.41
1:K:9:LEU:HB2	1:K:20:ASN:OD1	2.21	0.41
3:L:241:ILE:HG22	3:L:243:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:252:ASN:O	4:M:455:ARG:NH2	2.53	0.41
4:M:363:ARG:NH2	7:Y:28:TRP:CE2	2.89	0.41
4:M:377:LEU:HD22	4:M:377:LEU:O	2.20	0.41
2:N:27:HIS:CE1	9:N:102:BCL:HMD1	2.55	0.41
1:O:24:LEU:O	1:O:28:ILE:HG13	2.21	0.41
10:P:102:KGD:OAA	2:R:6:PHE:CG	2.74	0.41
2:R:27:HIS:CE1	9:S:102:BCL:HMD1	2.55	0.41
1:S:24:LEU:O	1:S:28:ILE:HG13	2.21	0.41
1:U:24:LEU:O	1:U:28:ILE:HG13	2.21	0.41
9:H:101:BCL:H162	9:H:101:BCL:H203	1.71	0.41
9:K:101:BCL:H93	9:K:101:BCL:H111	1.83	0.41
3:L:201:TYR:O	5:C:240:CYS:CB	2.65	0.41
4:M:564:GLU:OE1	4:M:572:GLN:NE2	2.51	0.41
9:P:101:BCL:HMD1	1:Q:44:HIS:CE1	2.55	0.41
5:C:263:MET:HB3	15:C:405:HEM:C4B	2.55	0.41
1:4:9:LEU:HB2	1:4:20:ASN:OD1	2.21	0.40
2:D:30:VAL:HG21	9:D:102:BCL:HHD	2.02	0.40
3:L:8:LEU:HA	3:L:8:LEU:HD23	1.65	0.40
4:M:424:TYR:HE1	4:M:430:VAL:HB	1.85	0.40
9:N:101:BCL:H191	13:P:103:PGV:H62	2.02	0.40
1:S:9:LEU:HB2	1:S:20:ASN:OD1	2.21	0.40
1:U:9:LEU:HB2	1:U:20:ASN:OD1	2.21	0.40
1:G:28:ILE:HD13	9:I:101:BCL:HBA1	2.03	0.40
10:H:103:KGD:CAE	9:K:101:BCL:CBB	2.64	0.40
9:I:101:BCL:H62	9:I:101:BCL:H41	1.62	0.40
3:L:313:LEU:HD13	3:L:313:LEU:HA	1.89	0.40
10:O:102:KGD:CAF	9:Q:102:BCL:H71	2.52	0.40
1:Q:34:TYR:OH	9:Q:102:BCL:OBD	2.15	0.40
1:W:24:LEU:O	1:W:28:ILE:HG13	2.21	0.40
1:8:24:LEU:O	1:8:28:ILE:HG13	2.21	0.40
3:L:213:ALA:HB3	13:C:406:PGV:H11	2.03	0.40
4:M:625:LYS:HA	4:M:625:LYS:HD3	1.99	0.40
4:M:640:PHE:HD2	5:C:238:GLN:HA	1.86	0.40
13:P:103:PGV:H221	8:Z:39:ARG:HG3	2.04	0.40
9:T:101:BCL:H203	9:T:101:BCL:H162	1.71	0.40
2:V:8:PHE:HE2	1:W:25:VAL:CB	2.34	0.40
8:Z:39:ARG:CZ	8:Z:43:LYS:HG3	2.50	0.40
1:0:24:LEU:O	1:0:28:ILE:HG13	2.21	0.40
2:A:24:LEU:HD13	4:M:443:PHE:HE2	1.85	0.40
1:G:9:LEU:HB2	1:G:20:ASN:OD1	2.21	0.40
11:L:1005:BPH:NC	11:L:1005:BPH:ND	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:103:KGD:CAK	10:N:103:KGD:CAL	2.97	0.40
9:P:101:BCL:OBD	9:Q:101:BCL:HBD	2.22	0.40
2:T:15:SER:HB2	9:U:102:BCL:HBC2	2.04	0.40
9:X:101:BCL:HBC3	9:X:101:BCL:H2C	1.88	0.40
9:8:101:BCL:H112	9:8:101:BCL:H71	1.60	0.40
3:L:6:ARG:HH11	3:L:8:LEU:HD23	1.86	0.40
1:Q:9:LEU:HB2	1:Q:20:ASN:OD1	2.21	0.40
9:U:101:BCL:H112	9:U:101:BCL:H71	1.60	0.40
1:W:9:LEU:HB2	1:W:20:ASN:OD1	2.21	0.40
6:X:13:LEU:O	6:X:17:THR:HG23	2.22	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	0	47/55 (86%)	47 (100%)	0	0	100	100
1	2	47/55 (86%)	47 (100%)	0	0	100	100
1	4	47/55 (86%)	47 (100%)	0	0	100	100
1	6	47/55 (86%)	47 (100%)	0	0	100	100
1	8	47/55 (86%)	47 (100%)	0	0	100	100
1	B	47/55 (86%)	47 (100%)	0	0	100	100
1	E	47/55 (86%)	47 (100%)	0	0	100	100
1	G	47/55 (86%)	47 (100%)	0	0	100	100
1	I	47/55 (86%)	47 (100%)	0	0	100	100
1	K	47/55 (86%)	47 (100%)	0	0	100	100
1	O	47/55 (86%)	47 (100%)	0	0	100	100
1	Q	47/55 (86%)	47 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	47/55 (86%)	47 (100%)	0	0	100	100
1	U	47/55 (86%)	47 (100%)	0	0	100	100
1	W	47/55 (86%)	47 (100%)	0	0	100	100
2	1	33/42 (79%)	32 (97%)	1 (3%)	0	100	100
2	3	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	5	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	7	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	9	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	A	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	D	36/42 (86%)	36 (100%)	0	0	100	100
2	F	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	H	36/42 (86%)	36 (100%)	0	0	100	100
2	J	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	N	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	P	36/42 (86%)	35 (97%)	1 (3%)	0	100	100
2	R	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
2	T	36/42 (86%)	33 (92%)	3 (8%)	0	100	100
2	V	36/42 (86%)	34 (94%)	2 (6%)	0	100	100
3	L	298/315 (95%)	279 (94%)	18 (6%)	1 (0%)	41	72
4	M	304/307 (99%)	293 (96%)	11 (4%)	0	100	100
5	C	313/320 (98%)	290 (93%)	23 (7%)	0	100	100
6	X	24/32 (75%)	24 (100%)	0	0	100	100
7	Y	30/39 (77%)	30 (100%)	0	0	100	100
8	Z	45/63 (71%)	40 (89%)	5 (11%)	0	100	100
All	All	2256/2531 (89%)	2173 (96%)	82 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	304	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	0	43/49 (88%)	43 (100%)	0	100	100
1	2	43/49 (88%)	43 (100%)	0	100	100
1	4	43/49 (88%)	43 (100%)	0	100	100
1	6	43/49 (88%)	43 (100%)	0	100	100
1	8	43/49 (88%)	43 (100%)	0	100	100
1	B	43/49 (88%)	43 (100%)	0	100	100
1	E	43/49 (88%)	43 (100%)	0	100	100
1	G	43/49 (88%)	43 (100%)	0	100	100
1	I	43/49 (88%)	43 (100%)	0	100	100
1	K	43/49 (88%)	43 (100%)	0	100	100
1	O	43/49 (88%)	43 (100%)	0	100	100
1	Q	43/49 (88%)	43 (100%)	0	100	100
1	S	43/49 (88%)	43 (100%)	0	100	100
1	U	43/49 (88%)	43 (100%)	0	100	100
1	W	43/49 (88%)	43 (100%)	0	100	100
2	1	30/37 (81%)	30 (100%)	0	100	100
2	3	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	5	33/37 (89%)	33 (100%)	0	100	100
2	7	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	9	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	A	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	D	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	F	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	H	33/37 (89%)	33 (100%)	0	100	100
2	J	33/37 (89%)	32 (97%)	1 (3%)	41	75
2	N	33/37 (89%)	32 (97%)	1 (3%)	41	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	P	33/37 (89%)	32 (97%)	1 (3%)	41 75
2	R	33/37 (89%)	33 (100%)	0	100 100
2	T	33/37 (89%)	32 (97%)	1 (3%)	41 75
2	V	33/37 (89%)	33 (100%)	0	100 100
3	L	243/253 (96%)	241 (99%)	2 (1%)	81 94
4	M	244/245 (100%)	242 (99%)	2 (1%)	81 94
5	C	257/262 (98%)	253 (98%)	4 (2%)	62 88
6	X	23/28 (82%)	23 (100%)	0	100 100
7	Y	29/36 (81%)	29 (100%)	0	100 100
8	Z	36/50 (72%)	35 (97%)	1 (3%)	43 77
All	All	1969/2164 (91%)	1950 (99%)	19 (1%)	77 93

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	38	TRP
2	7	38	TRP
2	9	38	TRP
2	A	38	TRP
2	D	28	PHE
2	F	38	TRP
2	J	38	TRP
3	L	281	CYS
3	L	305	TRP
4	M	519	PHE
4	M	595	PHE
2	N	38	TRP
2	P	38	TRP
2	T	38	TRP
5	C	122	HIS
5	C	205	TYR
5	C	243	CYS
5	C	296	CYS
8	Z	39	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	89	GLN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 97 ligands modelled in this entry, 1 is monoatomic - leaving 96 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	$\#\|Z\| > 2$
12	MQE	M	705	-	25,25,69	1.62	5 (20%)	31,34,87	1.18	3 (9%)
10	KGD	9	101	-	41,41,41	1.55	3 (7%)	49,53,53	2.10	17 (34%)
9	BCL	U	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
9	BCL	9	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	28 (35%)
9	BCL	4	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
10	KGD	4	103	-	41,41,41	1.21	2 (4%)	49,53,53	1.98	11 (22%)
10	KGD	C	401	-	41,41,41	1.57	2 (4%)	49,53,53	2.30	14 (28%)
15	HEM	C	405	5	41,50,50	1.32	3 (7%)	45,82,82	1.98	10 (22%)
10	KGD	T	102	-	41,41,41	1.73	10 (24%)	49,53,53	2.18	14 (28%)
13	PGV	Z	101	-	38,38,50	0.89	2 (5%)	41,44,56	0.95	4 (9%)
15	HEM	C	402	5	41,50,50	1.31	3 (7%)	45,82,82	1.95	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	KGD	S	101	-	41,41,41	1.33	2 (4%)	49,53,53	1.78	14 (28%)
9	BCL	Q	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	26 (33%)
10	KGD	3	102	-	41,41,41	1.15	2 (4%)	49,53,53	1.96	15 (30%)
9	BCL	A	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	29 (37%)
9	BCL	N	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	28 (35%)
13	PGV	M	706	-	33,33,50	1.02	3 (9%)	36,39,56	1.02	3 (8%)
12	MQE	M	701	-	69,69,69	0.94	2 (2%)	84,87,87	1.57	14 (16%)
9	BCL	R	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.30	28 (35%)
9	BCL	G	101	-	64,74,74	1.74	11 (17%)	78,115,115	2.15	27 (34%)
9	BCL	E	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.15	26 (33%)
10	KGD	G	102	-	41,41,41	1.42	3 (7%)	49,53,53	1.95	14 (28%)
9	BCL	M	703	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	W	103	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	26 (33%)
9	BCL	W	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.31	29 (37%)
9	BCL	H	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.30	28 (35%)
13	PGV	L	1006	-	31,31,50	1.04	2 (6%)	34,37,56	1.09	3 (8%)
10	KGD	U	103	-	41,41,41	1.20	1 (2%)	49,53,53	1.77	11 (22%)
9	BCL	K	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
10	KGD	A	104	-	41,41,41	1.51	5 (12%)	49,53,53	1.95	12 (24%)
9	BCL	8	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	29 (37%)
10	KGD	2	101	-	41,41,41	1.64	10 (24%)	49,53,53	2.04	10 (20%)
10	KGD	A	103	-	41,41,41	1.44	5 (12%)	49,53,53	1.85	16 (32%)
9	BCL	4	101	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	28 (35%)
13	PGV	L	1007	-	41,41,50	1.06	2 (4%)	44,47,56	0.94	3 (6%)
9	BCL	0	101	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	28 (35%)
9	BCL	U	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	28 (35%)
9	BCL	T	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
11	BPH	L	1003	-	51,70,70	1.12	6 (11%)	52,101,101	1.61	12 (23%)
10	KGD	E	102	-	41,41,41	1.22	2 (4%)	49,53,53	1.69	9 (18%)
9	BCL	5	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	8	102	-	64,74,74	1.74	13 (20%)	78,115,115	2.14	26 (33%)
9	BCL	3	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	28 (35%)
9	BCL	2	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	28 (35%)
10	KGD	5	102	-	41,41,41	1.23	1 (2%)	49,53,53	1.79	12 (24%)
9	BCL	Q	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	29 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	HEM	C	403	5	41,50,50	1.30	3 (7%)	45,82,82	1.91	9 (20%)
9	BCL	7	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	B	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	26 (33%)
10	KGD	K	102	-	41,41,41	1.22	2 (4%)	49,53,53	1.88	11 (22%)
9	BCL	F	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.31	28 (35%)
9	BCL	L	1002	-	64,74,74	1.72	10 (15%)	78,115,115	2.52	28 (35%)
11	BPH	M	704	-	51,70,70	0.95	4 (7%)	52,101,101	1.37	8 (15%)
10	KGD	2	104	-	41,41,41	1.22	4 (9%)	49,53,53	1.79	15 (30%)
10	KGD	H	103	-	41,41,41	1.61	7 (17%)	49,53,53	2.04	15 (30%)
10	KGD	P	102	-	41,41,41	1.42	3 (7%)	49,53,53	2.07	15 (30%)
9	BCL	F	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	2	103	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
9	BCL	P	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
10	KGD	Q	103	-	41,41,41	1.49	6 (14%)	49,53,53	2.04	14 (28%)
16	DGA	Y	101	-	36,36,43	0.72	1 (2%)	38,38,45	0.77	0
15	HEM	C	404	5	41,50,50	1.38	3 (7%)	45,82,82	2.24	12 (26%)
9	BCL	H	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.31	29 (37%)
10	KGD	J	103	-	41,41,41	1.26	1 (2%)	49,53,53	1.75	12 (24%)
9	BCL	6	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
9	BCL	D	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.30	28 (35%)
10	KGD	F	103	-	41,41,41	1.43	3 (7%)	49,53,53	1.90	10 (20%)
9	BCL	0	102	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	26 (33%)
10	KGD	O	102	-	41,41,41	1.38	3 (7%)	49,53,53	1.60	12 (24%)
13	PGV	P	104	-	40,40,50	1.44	6 (15%)	43,46,56	1.24	5 (11%)
9	BCL	J	102	-	64,74,74	1.75	13 (20%)	78,115,115	2.29	29 (37%)
9	BCL	O	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	27 (34%)
10	KGD	8	103	-	41,41,41	1.19	4 (9%)	49,53,53	1.97	13 (26%)
13	PGV	C	406	-	44,44,50	0.91	2 (4%)	47,50,56	0.99	4 (8%)
9	BCL	S	103	-	64,74,74	1.74	12 (18%)	78,115,115	2.15	27 (34%)
9	BCL	6	101	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	29 (37%)
9	BCL	D	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.30	28 (35%)
9	BCL	S	102	-	64,74,74	1.75	12 (18%)	78,115,115	2.30	28 (35%)
13	PGV	P	103	-	36,36,50	1.49	6 (16%)	39,42,56	1.07	3 (7%)
9	BCL	N	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.31	28 (35%)
10	KGD	0	103	-	41,41,41	1.56	6 (14%)	49,53,53	2.17	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	KGD	I	102	-	41,41,41	1.36	2 (4%)	49,53,53	1.80	14 (28%)
11	BPH	L	1005	-	51,70,70	1.07	5 (9%)	52,101,101	1.38	7 (13%)
9	BCL	J	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	A	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.31	28 (35%)
9	BCL	L	1001	-	64,74,74	1.79	11 (17%)	78,115,115	2.44	28 (35%)
9	BCL	I	101	-	64,74,74	1.74	12 (18%)	78,115,115	2.14	26 (33%)
9	BCL	1	101	-	64,74,74	1.74	13 (20%)	78,115,115	2.31	28 (35%)
10	KGD	0	104	-	41,41,41	1.37	3 (7%)	49,53,53	1.83	13 (26%)
12	MQE	L	1004	-	69,69,69	0.64	0	84,87,87	1.34	12 (14%)
10	KGD	S	104	-	41,41,41	1.35	2 (4%)	49,53,53	1.88	15 (30%)
10	KGD	6	103	-	41,41,41	1.56	8 (19%)	49,53,53	2.14	13 (26%)
9	BCL	X	101	-	64,74,74	1.75	13 (20%)	78,115,115	2.29	28 (35%)
10	KGD	N	103	-	41,41,41	1.50	3 (7%)	49,53,53	1.98	15 (30%)
10	KGD	B	102	-	41,41,41	1.67	9 (21%)	49,53,53	2.18	17 (34%)
10	KGD	W	101	-	41,41,41	1.37	3 (7%)	49,53,53	2.06	13 (26%)

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
12	MQE	M	705	-	-	1/13/33/85	0/2/2/2
10	KGD	9	101	-	-	6/36/56/56	0/1/1/1
9	BCL	U	102	-	-	18/37/137/137	-
9	BCL	9	102	-	-	19/37/137/137	-
9	BCL	4	102	-	-	18/37/137/137	-
10	KGD	4	103	-	-	6/36/56/56	0/1/1/1
10	KGD	C	401	-	-	13/36/56/56	0/1/1/1
15	HEM	C	405	5	-	4/12/54/54	-
10	KGD	T	102	-	-	6/36/56/56	0/1/1/1
13	PGV	Z	101	-	-	13/43/43/55	-
15	HEM	C	402	5	-	4/12/54/54	-
10	KGD	S	101	-	-	5/36/56/56	0/1/1/1
9	BCL	Q	102	-	-	18/37/137/137	-
10	KGD	3	102	-	-	5/36/56/56	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	A	102	-	-	9/37/137/137	-
9	BCL	N	102	-	-	9/37/137/137	-
13	PGV	M	706	-	-	10/38/38/55	-
12	MQE	M	701	-	-	14/65/85/85	0/2/2/2
9	BCL	R	101	-	-	19/37/137/137	-
9	BCL	G	101	-	-	18/37/137/137	-
9	BCL	E	101	-	-	18/37/137/137	-
10	KGD	G	102	-	-	11/36/56/56	0/1/1/1
9	BCL	M	703	-	-	16/37/137/137	-
9	BCL	W	103	-	-	18/37/137/137	-
9	BCL	W	102	-	-	11/37/137/137	-
9	BCL	H	101	-	-	19/37/137/137	-
13	PGV	L	1006	-	-	16/36/36/55	-
10	KGD	U	103	-	-	7/36/56/56	0/1/1/1
9	BCL	K	101	-	-	18/37/137/137	-
10	KGD	A	104	-	-	4/36/56/56	0/1/1/1
9	BCL	8	101	-	-	9/37/137/137	-
10	KGD	2	101	-	-	7/36/56/56	0/1/1/1
10	KGD	A	103	-	-	3/36/56/56	0/1/1/1
9	BCL	4	101	-	-	9/37/137/137	-
13	PGV	L	1007	-	-	16/46/46/55	-
9	BCL	0	101	-	-	9/37/137/137	-
9	BCL	U	101	-	-	9/37/137/137	-
9	BCL	T	101	-	-	19/37/137/137	-
11	BPH	L	1003	-	-	10/37/105/105	0/5/6/6
10	KGD	E	102	-	-	4/36/56/56	0/1/1/1
9	BCL	5	101	-	-	19/37/137/137	-
9	BCL	8	102	-	-	18/37/137/137	-
9	BCL	3	101	-	-	19/37/137/137	-
9	BCL	2	102	-	-	9/37/137/137	-
10	KGD	5	102	-	-	8/36/56/56	0/1/1/1
9	BCL	Q	101	-	-	9/37/137/137	-
15	HEM	C	403	5	-	4/12/54/54	-
9	BCL	7	101	-	-	19/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	B	101	-	-	18/37/137/137	-
10	KGD	K	102	-	-	10/36/56/56	0/1/1/1
9	BCL	F	102	-	-	9/37/137/137	-
9	BCL	L	1002	-	-	22/37/137/137	-
11	BPH	M	704	-	-	16/37/105/105	0/5/6/6
10	KGD	2	104	-	-	3/36/56/56	0/1/1/1
10	KGD	H	103	-	-	3/36/56/56	0/1/1/1
10	KGD	P	102	-	-	6/36/56/56	0/1/1/1
9	BCL	F	101	-	-	19/37/137/137	-
9	BCL	2	103	-	-	18/37/137/137	-
9	BCL	P	101	-	-	19/37/137/137	-
10	KGD	Q	103	-	-	9/36/56/56	0/1/1/1
16	DGA	Y	101	-	-	13/38/38/45	-
15	HEM	C	404	5	-	4/12/54/54	-
9	BCL	H	102	-	-	9/37/137/137	-
10	KGD	J	103	-	-	5/36/56/56	0/1/1/1
9	BCL	6	102	-	-	18/37/137/137	-
9	BCL	D	102	-	-	9/37/137/137	-
10	KGD	F	103	-	-	3/36/56/56	0/1/1/1
9	BCL	0	102	-	-	18/37/137/137	-
10	KGD	O	102	-	-	11/36/56/56	0/1/1/1
13	PGV	P	104	-	-	22/45/45/55	-
9	BCL	J	102	-	-	9/37/137/137	-
9	BCL	O	101	-	-	18/37/137/137	-
10	KGD	8	103	-	-	13/36/56/56	0/1/1/1
13	PGV	C	406	-	-	16/49/49/55	-
9	BCL	S	103	-	-	18/37/137/137	-
9	BCL	6	101	-	-	9/37/137/137	-
9	BCL	D	101	-	-	19/37/137/137	-
9	BCL	S	102	-	-	9/37/137/137	-
13	PGV	P	103	-	-	15/41/41/55	-
9	BCL	N	101	-	-	19/37/137/137	-
10	KGD	0	103	-	-	4/36/56/56	0/1/1/1
10	KGD	I	102	-	-	4/36/56/56	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BPH	L	1005	-	-	15/37/105/105	0/5/6/6
9	BCL	J	101	-	-	19/37/137/137	-
9	BCL	A	101	-	-	19/37/137/137	-
9	BCL	L	1001	-	-	14/37/137/137	-
9	BCL	I	101	-	-	18/37/137/137	-
9	BCL	1	101	-	-	19/37/137/137	-
10	KGD	0	104	-	-	5/36/56/56	0/1/1/1
12	MQE	L	1004	-	-	15/65/85/85	0/2/2/2
10	KGD	S	104	-	-	7/36/56/56	0/1/1/1
10	KGD	6	103	-	-	8/36/56/56	0/1/1/1
9	BCL	X	101	-	-	22/37/137/137	-
10	KGD	N	103	-	-	6/36/56/56	0/1/1/1
10	KGD	B	102	-	-	7/36/56/56	0/1/1/1
10	KGD	W	101	-	-	6/36/56/56	0/1/1/1

All (769) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	1001	BCL	MG-ND	-6.52	1.92	2.05
10	T	102	KGD	CAB-CAD	-6.26	1.45	1.53
9	6	101	BCL	MG-ND	-6.18	1.93	2.05
9	0	101	BCL	MG-ND	-6.17	1.93	2.05
9	Q	101	BCL	MG-ND	-6.16	1.93	2.05
9	4	101	BCL	MG-ND	-6.15	1.93	2.05
9	2	102	BCL	MG-ND	-6.15	1.93	2.05
9	8	101	BCL	MG-ND	-6.15	1.93	2.05
9	A	102	BCL	MG-ND	-6.14	1.93	2.05
9	S	102	BCL	MG-ND	-6.14	1.93	2.05
9	F	102	BCL	MG-ND	-6.13	1.93	2.05
9	U	101	BCL	MG-ND	-6.13	1.93	2.05
9	H	102	BCL	MG-ND	-6.12	1.93	2.05
9	D	102	BCL	MG-ND	-6.12	1.93	2.05
9	N	102	BCL	MG-ND	-6.12	1.93	2.05
9	W	102	BCL	MG-ND	-6.11	1.93	2.05
9	J	102	BCL	MG-ND	-6.10	1.93	2.05
10	C	401	KGD	CAE-CAI	-6.06	1.42	1.50
9	M	703	BCL	MG-ND	-6.05	1.93	2.05
10	9	101	KGD	CAB-CAD	-6.05	1.45	1.53
9	B	101	BCL	MG-ND	-5.99	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	102	BCL	MG-ND	-5.99	1.93	2.05
9	E	101	BCL	MG-ND	-5.98	1.93	2.05
9	K	101	BCL	MG-ND	-5.97	1.94	2.05
9	O	101	BCL	MG-ND	-5.96	1.94	2.05
9	4	102	BCL	MG-ND	-5.96	1.94	2.05
9	U	102	BCL	MG-ND	-5.95	1.94	2.05
9	L	1002	BCL	MG-ND	-5.95	1.94	2.05
9	Q	102	BCL	MG-ND	-5.95	1.94	2.05
9	I	101	BCL	MG-ND	-5.95	1.94	2.05
9	W	103	BCL	MG-ND	-5.94	1.94	2.05
9	S	103	BCL	MG-ND	-5.94	1.94	2.05
9	6	102	BCL	MG-ND	-5.94	1.94	2.05
9	G	101	BCL	MG-ND	-5.94	1.94	2.05
9	0	102	BCL	MG-ND	-5.92	1.94	2.05
9	2	103	BCL	MG-ND	-5.92	1.94	2.05
10	C	401	KGD	CAF-CAB	-5.92	1.42	1.53
9	A	101	BCL	MG-ND	-5.92	1.94	2.05
9	X	101	BCL	MG-ND	-5.88	1.94	2.05
9	5	101	BCL	MG-ND	-5.88	1.94	2.05
9	J	101	BCL	MG-ND	-5.88	1.94	2.05
9	N	101	BCL	MG-ND	-5.88	1.94	2.05
9	D	101	BCL	MG-ND	-5.87	1.94	2.05
9	T	101	BCL	MG-ND	-5.87	1.94	2.05
9	7	101	BCL	MG-ND	-5.86	1.94	2.05
9	F	101	BCL	MG-ND	-5.86	1.94	2.05
9	9	102	BCL	MG-ND	-5.86	1.94	2.05
9	3	101	BCL	MG-ND	-5.86	1.94	2.05
9	P	101	BCL	MG-ND	-5.85	1.94	2.05
9	H	101	BCL	MG-ND	-5.85	1.94	2.05
9	1	101	BCL	MG-ND	-5.84	1.94	2.05
9	R	101	BCL	MG-ND	-5.84	1.94	2.05
10	H	103	KGD	CAB-CAD	-5.33	1.46	1.53
10	P	102	KGD	CAB-CAD	-5.15	1.46	1.53
10	J	103	KGD	CAB-CAD	-5.04	1.46	1.53
10	A	103	KGD	CAB-CAD	-4.89	1.47	1.53
9	L	1002	BCL	OBD-CAD	4.76	1.30	1.22
13	P	103	PGV	C2-C1	-4.70	1.37	1.50
10	N	103	KGD	CAB-CAD	-4.68	1.47	1.53
10	S	104	KGD	CAB-CAD	-4.65	1.47	1.53
10	G	102	KGD	CAB-CAD	-4.64	1.47	1.53
15	C	404	HEM	C4D-ND	-4.63	1.32	1.40
9	L	1001	BCL	OBD-CAD	4.57	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	102	BCL	C4D-ND	-4.57	1.31	1.37
9	W	103	BCL	C4D-ND	-4.55	1.31	1.37
9	2	103	BCL	C4D-ND	-4.54	1.31	1.37
9	O	101	BCL	C4D-ND	-4.53	1.31	1.37
9	U	102	BCL	C4D-ND	-4.53	1.31	1.37
9	X	101	BCL	C4D-ND	-4.53	1.31	1.37
9	W	102	BCL	C4D-ND	-4.53	1.31	1.37
9	4	102	BCL	C4D-ND	-4.52	1.31	1.37
9	D	101	BCL	C4D-ND	-4.52	1.31	1.37
9	L	1001	BCL	C4D-ND	-4.52	1.31	1.37
9	M	703	BCL	C4D-ND	-4.52	1.31	1.37
9	6	102	BCL	C4D-ND	-4.51	1.31	1.37
9	N	101	BCL	C4D-ND	-4.51	1.31	1.37
9	J	101	BCL	C4D-ND	-4.50	1.31	1.37
9	H	101	BCL	C4D-ND	-4.50	1.31	1.37
9	9	102	BCL	C4D-ND	-4.49	1.31	1.37
9	N	102	BCL	C4D-ND	-4.49	1.31	1.37
9	8	101	BCL	C4D-ND	-4.49	1.31	1.37
9	U	102	BCL	OBD-CAD	4.49	1.30	1.22
9	R	101	BCL	C4D-ND	-4.49	1.31	1.37
9	0	102	BCL	C4D-ND	-4.49	1.31	1.37
9	P	101	BCL	C4D-ND	-4.48	1.31	1.37
9	8	102	BCL	C4D-ND	-4.48	1.31	1.37
9	J	102	BCL	C4D-ND	-4.48	1.31	1.37
9	B	101	BCL	C4D-ND	-4.48	1.31	1.37
9	I	101	BCL	C4D-ND	-4.48	1.31	1.37
9	F	101	BCL	C4D-ND	-4.47	1.31	1.37
9	T	101	BCL	C4D-ND	-4.47	1.31	1.37
9	U	101	BCL	C4D-ND	-4.47	1.31	1.37
9	M	703	BCL	O1D-CGD	-4.46	1.10	1.21
9	Q	101	BCL	C4D-ND	-4.46	1.31	1.37
9	G	101	BCL	C4D-ND	-4.46	1.31	1.37
9	H	102	BCL	OBD-CAD	4.46	1.30	1.22
9	5	101	BCL	C4D-ND	-4.46	1.31	1.37
9	K	101	BCL	C4D-ND	-4.46	1.31	1.37
9	A	102	BCL	C4D-ND	-4.45	1.31	1.37
9	J	102	BCL	OBD-CAD	4.45	1.30	1.22
9	U	101	BCL	OBD-CAD	4.45	1.30	1.22
9	A	101	BCL	C4D-ND	-4.45	1.31	1.37
9	E	101	BCL	C4D-ND	-4.45	1.31	1.37
9	H	102	BCL	C4D-ND	-4.45	1.31	1.37
9	S	103	BCL	C4D-ND	-4.45	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	0	101	BCL	C4D-ND	-4.45	1.31	1.37
9	3	101	BCL	C4D-ND	-4.45	1.31	1.37
9	1	101	BCL	C4D-ND	-4.45	1.31	1.37
9	I	101	BCL	OBD-CAD	4.45	1.30	1.22
9	4	101	BCL	C4D-ND	-4.45	1.31	1.37
9	7	101	BCL	C4D-ND	-4.44	1.31	1.37
9	2	103	BCL	OBD-CAD	4.44	1.30	1.22
9	D	102	BCL	C4D-ND	-4.44	1.31	1.37
9	2	102	BCL	C4D-ND	-4.44	1.31	1.37
9	6	101	BCL	OBD-CAD	4.44	1.30	1.22
9	6	102	BCL	OBD-CAD	4.44	1.30	1.22
9	8	101	BCL	OBD-CAD	4.43	1.30	1.22
9	4	102	BCL	OBD-CAD	4.43	1.30	1.22
9	D	102	BCL	OBD-CAD	4.43	1.30	1.22
9	0	102	BCL	OBD-CAD	4.43	1.30	1.22
9	4	101	BCL	OBD-CAD	4.43	1.30	1.22
9	O	101	BCL	OBD-CAD	4.43	1.30	1.22
9	9	102	BCL	OBD-CAD	4.43	1.30	1.22
9	G	101	BCL	OBD-CAD	4.42	1.30	1.22
9	A	101	BCL	OBD-CAD	4.42	1.30	1.22
9	F	102	BCL	C4D-ND	-4.42	1.31	1.37
9	F	102	BCL	OBD-CAD	4.42	1.30	1.22
9	A	102	BCL	OBD-CAD	4.42	1.30	1.22
9	S	102	BCL	OBD-CAD	4.42	1.30	1.22
9	H	101	BCL	OBD-CAD	4.42	1.30	1.22
9	B	101	BCL	OBD-CAD	4.42	1.30	1.22
9	E	101	BCL	OBD-CAD	4.42	1.30	1.22
9	W	102	BCL	OBD-CAD	4.42	1.30	1.22
9	S	102	BCL	C4D-ND	-4.41	1.31	1.37
9	0	101	BCL	OBD-CAD	4.41	1.30	1.22
9	3	101	BCL	OBD-CAD	4.41	1.30	1.22
9	5	101	BCL	OBD-CAD	4.41	1.30	1.22
9	7	101	BCL	OBD-CAD	4.41	1.30	1.22
9	Q	101	BCL	OBD-CAD	4.41	1.30	1.22
9	6	101	BCL	C4D-ND	-4.40	1.31	1.37
9	N	102	BCL	OBD-CAD	4.40	1.30	1.22
9	1	101	BCL	OBD-CAD	4.40	1.30	1.22
9	Q	102	BCL	OBD-CAD	4.40	1.30	1.22
9	X	101	BCL	OBD-CAD	4.40	1.30	1.22
9	2	102	BCL	OBD-CAD	4.40	1.30	1.22
9	S	103	BCL	OBD-CAD	4.40	1.30	1.22
9	R	101	BCL	OBD-CAD	4.40	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	103	BCL	OBD-CAD	4.39	1.30	1.22
9	P	101	BCL	OBD-CAD	4.39	1.30	1.22
9	8	102	BCL	OBD-CAD	4.39	1.30	1.22
9	K	101	BCL	OBD-CAD	4.38	1.30	1.22
9	D	101	BCL	OBD-CAD	4.38	1.30	1.22
9	N	101	BCL	OBD-CAD	4.37	1.30	1.22
9	F	101	BCL	OBD-CAD	4.37	1.30	1.22
9	T	101	BCL	OBD-CAD	4.37	1.30	1.22
9	J	101	BCL	OBD-CAD	4.37	1.30	1.22
9	M	703	BCL	OBD-CAD	4.37	1.30	1.22
10	U	103	KGD	CAB-CAD	-4.31	1.47	1.53
10	5	102	KGD	CAB-CAD	-4.31	1.47	1.53
10	O	102	KGD	CAB-CAD	-4.28	1.47	1.53
9	3	101	BCL	O1D-CGD	-4.27	1.10	1.21
9	R	101	BCL	O1D-CGD	-4.26	1.10	1.21
13	P	103	PGV	O03-C01	-4.25	1.35	1.45
9	L	1002	BCL	C4D-ND	-4.25	1.31	1.37
9	9	102	BCL	O1D-CGD	-4.24	1.10	1.21
9	1	101	BCL	O1D-CGD	-4.24	1.10	1.21
9	X	101	BCL	O1D-CGD	-4.23	1.10	1.21
9	F	101	BCL	O1D-CGD	-4.23	1.10	1.21
9	H	101	BCL	O1D-CGD	-4.23	1.10	1.21
9	D	101	BCL	O1D-CGD	-4.23	1.10	1.21
9	N	101	BCL	O1D-CGD	-4.22	1.10	1.21
9	7	101	BCL	O1D-CGD	-4.22	1.10	1.21
9	J	101	BCL	O1D-CGD	-4.21	1.10	1.21
9	5	101	BCL	O1D-CGD	-4.21	1.10	1.21
9	A	101	BCL	O1D-CGD	-4.21	1.10	1.21
9	P	101	BCL	O1D-CGD	-4.21	1.10	1.21
9	T	101	BCL	O1D-CGD	-4.20	1.10	1.21
15	C	403	HEM	C4D-ND	-4.20	1.33	1.40
15	C	402	HEM	C4D-ND	-4.19	1.33	1.40
15	C	405	HEM	C4D-ND	-4.19	1.33	1.40
10	I	102	KGD	CAB-CAD	-4.15	1.48	1.53
9	D	102	BCL	O1D-CGD	-4.15	1.10	1.21
9	W	102	BCL	O1D-CGD	-4.15	1.10	1.21
9	6	101	BCL	O1D-CGD	-4.15	1.10	1.21
9	4	101	BCL	O1D-CGD	-4.14	1.10	1.21
9	S	102	BCL	O1D-CGD	-4.14	1.10	1.21
9	0	101	BCL	O1D-CGD	-4.13	1.10	1.21
9	4	102	BCL	O1D-CGD	-4.13	1.10	1.21
9	A	102	BCL	O1D-CGD	-4.13	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	6	102	BCL	O1D-CGD	-4.13	1.10	1.21
9	J	102	BCL	O1D-CGD	-4.12	1.10	1.21
9	W	103	BCL	O1D-CGD	-4.12	1.10	1.21
9	L	1002	BCL	O1D-CGD	-4.12	1.10	1.21
9	O	101	BCL	O1D-CGD	-4.12	1.10	1.21
9	8	101	BCL	O1D-CGD	-4.11	1.10	1.21
9	N	102	BCL	O1D-CGD	-4.11	1.10	1.21
9	2	102	BCL	O1D-CGD	-4.11	1.10	1.21
9	Q	101	BCL	O1D-CGD	-4.11	1.10	1.21
9	I	101	BCL	O1D-CGD	-4.11	1.10	1.21
9	B	101	BCL	O1D-CGD	-4.11	1.10	1.21
9	S	103	BCL	O1D-CGD	-4.11	1.10	1.21
9	U	101	BCL	O1D-CGD	-4.11	1.10	1.21
9	H	102	BCL	O1D-CGD	-4.10	1.10	1.21
9	K	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	0	102	BCL	O1D-CGD	-4.10	1.10	1.21
9	Q	102	BCL	O1D-CGD	-4.10	1.10	1.21
9	G	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	2	103	BCL	O1D-CGD	-4.10	1.10	1.21
9	E	101	BCL	O1D-CGD	-4.10	1.10	1.21
9	F	102	BCL	O1D-CGD	-4.09	1.11	1.21
9	U	102	BCL	O1D-CGD	-4.09	1.11	1.21
9	8	102	BCL	O1D-CGD	-4.08	1.11	1.21
9	L	1001	BCL	O1D-CGD	-4.04	1.11	1.21
10	S	101	KGD	CAB-CAD	-4.01	1.48	1.53
10	E	102	KGD	CAB-CAD	-3.87	1.48	1.53
13	L	1007	PGV	O01-C02	-3.79	1.37	1.46
10	0	103	KGD	CAB-CAD	-3.79	1.48	1.53
10	W	101	KGD	CAB-CAD	-3.77	1.48	1.53
10	O	102	KGD	CAG-CAB	-3.77	1.46	1.53
13	P	104	PGV	P-O11	3.72	1.74	1.59
13	P	104	PGV	C01-C02	3.62	1.61	1.50
10	Q	103	KGD	CAB-CAD	-3.52	1.48	1.53
10	A	104	KGD	CAB-CAD	-3.49	1.49	1.53
10	B	102	KGD	CAB-CAD	-3.43	1.49	1.53
10	0	104	KGD	CAB-CAD	-3.43	1.49	1.53
10	F	103	KGD	CAE-CAI	-3.42	1.46	1.50
9	W	102	BCL	O2D-CED	3.41	1.53	1.45
10	2	101	KGD	CAU-CAR	-3.41	1.43	1.50
10	2	101	KGD	CBA-CAW	3.40	1.37	1.34
9	2	102	BCL	O2D-CED	3.39	1.53	1.45
9	B	101	BCL	O2D-CED	3.38	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	8	102	BCL	O2D-CED	3.38	1.53	1.45
9	F	102	BCL	O2D-CED	3.37	1.53	1.45
9	2	103	BCL	O2D-CED	3.37	1.53	1.45
9	G	101	BCL	O2D-CED	3.37	1.53	1.45
9	E	101	BCL	O2D-CED	3.37	1.53	1.45
9	U	101	BCL	O2D-CED	3.37	1.53	1.45
9	I	101	BCL	O2D-CED	3.37	1.53	1.45
9	O	101	BCL	O2D-CED	3.37	1.53	1.45
9	J	102	BCL	O2D-CED	3.37	1.53	1.45
9	S	103	BCL	O2D-CED	3.37	1.53	1.45
9	W	103	BCL	O2D-CED	3.36	1.53	1.45
9	A	102	BCL	O2D-CED	3.36	1.53	1.45
9	Q	102	BCL	O2D-CED	3.36	1.53	1.45
9	4	102	BCL	O2D-CED	3.36	1.53	1.45
9	U	102	BCL	O2D-CED	3.36	1.53	1.45
9	Q	101	BCL	O2D-CED	3.35	1.53	1.45
9	6	102	BCL	O2D-CED	3.35	1.53	1.45
9	D	102	BCL	O2D-CED	3.34	1.53	1.45
9	N	102	BCL	O2D-CED	3.34	1.53	1.45
9	S	102	BCL	O2D-CED	3.34	1.53	1.45
9	0	102	BCL	O2D-CED	3.34	1.53	1.45
9	K	101	BCL	O2D-CED	3.34	1.53	1.45
9	0	101	BCL	O2D-CED	3.34	1.53	1.45
9	6	101	BCL	O2D-CED	3.33	1.53	1.45
13	P	104	PGV	O01-C02	-3.33	1.38	1.46
10	2	101	KGD	CBK-CBH	-3.32	1.44	1.50
9	4	101	BCL	O2D-CED	3.32	1.53	1.45
9	H	102	BCL	O2D-CED	3.31	1.53	1.45
9	8	101	BCL	O2D-CED	3.31	1.53	1.45
10	F	103	KGD	CAB-CAD	-3.31	1.49	1.53
9	5	101	BCL	O2D-CED	3.30	1.53	1.45
9	3	101	BCL	O2D-CED	3.28	1.53	1.45
9	P	101	BCL	O2D-CED	3.28	1.53	1.45
9	X	101	BCL	O2D-CED	3.28	1.53	1.45
9	X	101	BCL	O2A-CGA	-3.28	1.23	1.33
9	T	101	BCL	O2D-CED	3.27	1.53	1.45
15	C	404	HEM	C1D-ND	-3.27	1.32	1.38
9	L	1001	BCL	O2D-CED	3.27	1.53	1.45
9	A	101	BCL	O2D-CED	3.27	1.53	1.45
9	J	101	BCL	O2D-CED	3.27	1.53	1.45
9	F	101	BCL	O2D-CED	3.26	1.53	1.45
9	Q	101	BCL	O2A-CGA	-3.26	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	101	BCL	O2D-CED	3.26	1.53	1.45
9	L	1001	BCL	O2D-CGD	-3.26	1.25	1.33
9	7	101	BCL	O2D-CED	3.25	1.53	1.45
9	N	101	BCL	O2D-CED	3.25	1.53	1.45
9	D	101	BCL	O2D-CED	3.25	1.53	1.45
9	M	703	BCL	O2D-CGD	-3.25	1.25	1.33
9	9	102	BCL	O2D-CED	3.25	1.53	1.45
9	1	101	BCL	O2D-CED	3.25	1.53	1.45
9	H	101	BCL	O2D-CED	3.25	1.53	1.45
9	J	102	BCL	O2D-CGD	-3.24	1.25	1.33
9	0	101	BCL	O2A-CGA	-3.24	1.23	1.33
9	W	102	BCL	O2D-CGD	-3.23	1.25	1.33
9	U	101	BCL	O2D-CGD	-3.23	1.25	1.33
9	A	102	BCL	O2A-CGA	-3.23	1.23	1.33
9	N	102	BCL	O2A-CGA	-3.23	1.23	1.33
9	J	102	BCL	O2A-CGA	-3.23	1.23	1.33
9	M	703	BCL	O2D-CED	3.23	1.52	1.45
9	H	102	BCL	O2A-CGA	-3.23	1.23	1.33
9	4	101	BCL	O2A-CGA	-3.22	1.23	1.33
9	W	102	BCL	O2A-CGA	-3.22	1.23	1.33
9	L	1002	BCL	O2D-CGD	-3.22	1.25	1.33
10	2	101	KGD	CBF-CBH	-3.22	1.39	1.45
9	2	102	BCL	O2D-CGD	-3.22	1.25	1.33
9	D	102	BCL	O2A-CGA	-3.22	1.23	1.33
9	A	102	BCL	O2D-CGD	-3.22	1.25	1.33
9	U	101	BCL	O2A-CGA	-3.22	1.23	1.33
10	0	103	KGD	CBJ-CBH	-3.22	1.31	1.35
9	2	102	BCL	O2A-CGA	-3.22	1.23	1.33
9	S	102	BCL	O2A-CGA	-3.21	1.23	1.33
9	4	101	BCL	O2D-CGD	-3.21	1.25	1.33
9	P	101	BCL	O2A-CGA	-3.21	1.23	1.33
9	8	101	BCL	O2A-CGA	-3.20	1.23	1.33
9	Q	101	BCL	O2D-CGD	-3.20	1.25	1.33
9	N	102	BCL	O2D-CGD	-3.20	1.25	1.33
9	D	102	BCL	O2D-CGD	-3.20	1.25	1.33
9	H	102	BCL	O2D-CGD	-3.20	1.25	1.33
9	3	101	BCL	O2A-CGA	-3.20	1.24	1.33
9	F	102	BCL	O2A-CGA	-3.20	1.24	1.33
9	6	101	BCL	O2A-CGA	-3.19	1.24	1.33
9	D	101	BCL	O2A-CGA	-3.19	1.24	1.33
9	8	101	BCL	O2D-CGD	-3.19	1.25	1.33
9	D	101	BCL	O2D-CGD	-3.19	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	102	BCL	O2D-CGD	-3.19	1.25	1.33
9	7	101	BCL	O2A-CGA	-3.19	1.24	1.33
9	T	101	BCL	O2D-CGD	-3.19	1.25	1.33
9	J	101	BCL	O2D-CGD	-3.19	1.25	1.33
9	A	101	BCL	O2A-CGA	-3.19	1.24	1.33
9	9	102	BCL	O2A-CGA	-3.19	1.24	1.33
9	X	101	BCL	O2D-CGD	-3.18	1.25	1.33
9	N	101	BCL	O2A-CGA	-3.18	1.24	1.33
9	S	102	BCL	O2D-CGD	-3.18	1.25	1.33
9	T	101	BCL	O2A-CGA	-3.18	1.24	1.33
9	H	101	BCL	O2D-CGD	-3.18	1.25	1.33
9	8	102	BCL	O2D-CGD	-3.18	1.25	1.33
9	J	101	BCL	O2A-CGA	-3.18	1.24	1.33
9	F	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	R	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	1	101	BCL	O2A-CGA	-3.17	1.24	1.33
9	9	102	BCL	O2D-CGD	-3.17	1.25	1.33
9	0	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	7	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	A	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	6	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	3	101	BCL	O2D-CGD	-3.17	1.25	1.33
9	E	101	BCL	O2D-CGD	-3.16	1.25	1.33
9	R	101	BCL	O2A-CGA	-3.16	1.24	1.33
9	F	101	BCL	O2A-CGA	-3.16	1.24	1.33
9	Q	102	BCL	O2D-CGD	-3.16	1.25	1.33
9	U	102	BCL	O2D-CGD	-3.16	1.25	1.33
9	H	101	BCL	O2A-CGA	-3.16	1.24	1.33
9	B	101	BCL	O2D-CGD	-3.16	1.25	1.33
9	5	101	BCL	O2D-CGD	-3.16	1.25	1.33
9	5	101	BCL	O2A-CGA	-3.16	1.24	1.33
9	S	103	BCL	O2D-CGD	-3.16	1.25	1.33
9	N	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	P	101	BCL	O2D-CGD	-3.15	1.25	1.33
11	L	1005	BPH	C3D-C2D	-3.15	1.33	1.39
9	I	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	G	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	K	101	BCL	O2D-CGD	-3.15	1.25	1.33
9	O	101	BCL	O2D-CGD	-3.14	1.25	1.33
11	L	1003	BPH	C3D-C2D	-3.14	1.33	1.39
9	1	101	BCL	O2D-CGD	-3.14	1.25	1.33
9	2	103	BCL	O2D-CGD	-3.13	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	102	BCL	O2D-CGD	-3.13	1.25	1.33
9	L	1001	BCL	O2A-CGA	-3.13	1.24	1.33
9	0	102	BCL	O2D-CGD	-3.13	1.25	1.33
9	W	103	BCL	O2D-CGD	-3.12	1.25	1.33
9	6	102	BCL	O2D-CGD	-3.11	1.25	1.33
10	6	103	KGD	CAS-CAW	-3.10	1.44	1.51
10	3	102	KGD	CAB-CAD	-3.09	1.49	1.53
9	L	1001	BCL	O1A-CGA	-3.09	1.13	1.22
9	X	101	BCL	O1A-CGA	-3.07	1.13	1.22
15	C	405	HEM	C1D-ND	-3.06	1.32	1.38
10	Q	103	KGD	CAE-CAI	-3.06	1.46	1.50
9	L	1002	BCL	O2D-CED	3.05	1.52	1.45
10	6	103	KGD	CBA-CAW	-3.05	1.31	1.34
9	9	102	BCL	O1A-CGA	-3.05	1.13	1.22
9	1	101	BCL	O1A-CGA	-3.05	1.13	1.22
9	F	101	BCL	O1A-CGA	-3.05	1.13	1.22
9	3	101	BCL	O1A-CGA	-3.05	1.13	1.22
9	7	101	BCL	O1A-CGA	-3.04	1.13	1.22
10	6	103	KGD	CBJ-CBH	-3.04	1.31	1.35
9	P	101	BCL	O1A-CGA	-3.04	1.13	1.22
9	A	101	BCL	O1A-CGA	-3.04	1.13	1.22
9	N	101	BCL	O1A-CGA	-3.04	1.13	1.22
9	J	101	BCL	O1A-CGA	-3.03	1.13	1.22
9	5	101	BCL	O1A-CGA	-3.03	1.13	1.22
15	C	403	HEM	C1D-ND	-3.03	1.32	1.38
9	R	101	BCL	O1A-CGA	-3.03	1.13	1.22
9	D	101	BCL	O1A-CGA	-3.03	1.13	1.22
11	M	704	BPH	C3D-C2D	-3.03	1.34	1.39
9	H	101	BCL	O1A-CGA	-3.02	1.13	1.22
13	C	406	PGV	O03-C01	-3.02	1.38	1.45
9	T	101	BCL	O1A-CGA	-3.02	1.13	1.22
15	C	402	HEM	C1D-ND	-3.01	1.32	1.38
9	L	1002	BCL	O2A-CGA	-2.99	1.24	1.33
9	8	102	BCL	O2A-CGA	-2.99	1.24	1.33
9	B	101	BCL	O2A-CGA	-2.98	1.24	1.33
9	E	101	BCL	O2A-CGA	-2.97	1.24	1.33
10	B	102	KGD	CAF-CAB	-2.97	1.47	1.53
9	K	101	BCL	O2A-CGA	-2.97	1.24	1.33
9	O	101	BCL	O2A-CGA	-2.97	1.24	1.33
9	0	102	BCL	O2A-CGA	-2.97	1.24	1.33
9	U	102	BCL	O2A-CGA	-2.97	1.24	1.33
9	G	101	BCL	O2A-CGA	-2.96	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	405	HEM	C1B-NB	-2.96	1.35	1.40
9	4	102	BCL	O2A-CGA	-2.96	1.24	1.33
10	6	103	KGD	CAB-CAD	-2.96	1.49	1.53
9	Q	102	BCL	O2A-CGA	-2.96	1.24	1.33
9	2	103	BCL	O2A-CGA	-2.96	1.24	1.33
9	S	103	BCL	O2A-CGA	-2.95	1.24	1.33
9	I	101	BCL	O2A-CGA	-2.95	1.24	1.33
15	C	404	HEM	C1B-NB	-2.95	1.35	1.40
9	W	103	BCL	O2A-CGA	-2.95	1.24	1.33
9	6	102	BCL	O2A-CGA	-2.95	1.24	1.33
12	M	705	MQE	CAY-CAX	-2.93	1.46	1.51
13	P	104	PGV	O05-C05	-2.92	1.34	1.43
11	L	1003	BPH	CMD-C2D	-2.92	1.44	1.51
9	M	703	BCL	O1A-CGA	-2.92	1.13	1.22
10	2	104	KGD	CAB-CAD	-2.91	1.49	1.53
9	M	703	BCL	O2A-CGA	-2.90	1.24	1.33
9	6	101	BCL	O1A-CGA	-2.89	1.14	1.22
9	F	102	BCL	O1A-CGA	-2.89	1.14	1.22
9	Q	101	BCL	O1A-CGA	-2.89	1.14	1.22
9	8	101	BCL	O1A-CGA	-2.89	1.14	1.22
15	C	402	HEM	C1B-NB	-2.89	1.35	1.40
9	S	102	BCL	O1A-CGA	-2.88	1.14	1.22
9	J	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	H	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	2	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	D	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	N	102	BCL	O1A-CGA	-2.87	1.14	1.22
9	4	101	BCL	O1A-CGA	-2.86	1.14	1.22
9	0	101	BCL	O1A-CGA	-2.86	1.14	1.22
9	A	102	BCL	O1A-CGA	-2.85	1.14	1.22
9	U	101	BCL	O1A-CGA	-2.85	1.14	1.22
9	W	102	BCL	O1A-CGA	-2.83	1.14	1.22
9	Q	102	BCL	O1A-CGA	-2.82	1.14	1.22
10	A	104	KGD	CAE-CAI	-2.80	1.47	1.50
9	2	102	BCL	C1D-C2D	-2.80	1.39	1.45
9	0	102	BCL	O1A-CGA	-2.80	1.14	1.22
9	6	102	BCL	O1A-CGA	-2.79	1.14	1.22
9	8	102	BCL	O1A-CGA	-2.79	1.14	1.22
9	E	101	BCL	O1A-CGA	-2.79	1.14	1.22
9	4	102	BCL	O1A-CGA	-2.79	1.14	1.22
9	K	101	BCL	O1A-CGA	-2.79	1.14	1.22
9	S	103	BCL	O1A-CGA	-2.79	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	103	BCL	O1A-CGA	-2.79	1.14	1.22
9	2	103	BCL	O1A-CGA	-2.79	1.14	1.22
10	4	103	KGD	CAB-CAD	-2.79	1.49	1.53
9	4	101	BCL	C1D-C2D	-2.78	1.39	1.45
9	I	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	U	102	BCL	O1A-CGA	-2.78	1.14	1.22
10	K	102	KGD	CAB-CAD	-2.78	1.49	1.53
9	B	101	BCL	O1A-CGA	-2.78	1.14	1.22
9	6	101	BCL	C1D-C2D	-2.77	1.39	1.45
9	G	101	BCL	O1A-CGA	-2.77	1.14	1.22
9	L	1002	BCL	O1A-CGA	-2.77	1.14	1.22
9	H	102	BCL	C1D-C2D	-2.77	1.39	1.45
13	P	104	PGV	O02-C1	-2.76	1.14	1.22
9	O	101	BCL	O1A-CGA	-2.76	1.14	1.22
9	S	102	BCL	C1D-C2D	-2.76	1.39	1.45
10	Q	103	KGD	CAG-CAB	-2.76	1.48	1.53
9	D	102	BCL	C1D-C2D	-2.75	1.39	1.45
10	B	102	KGD	CBN-CBL	-2.75	1.40	1.45
9	0	101	BCL	C1D-C2D	-2.74	1.39	1.45
9	Q	101	BCL	C1D-C2D	-2.74	1.39	1.45
9	0	102	BCL	C3B-C2B	-2.74	1.34	1.39
9	G	101	BCL	C3B-C2B	-2.74	1.34	1.39
9	F	102	BCL	C1D-C2D	-2.74	1.39	1.45
9	8	101	BCL	C1D-C2D	-2.73	1.39	1.45
11	L	1005	BPH	CMD-C2D	-2.73	1.45	1.51
9	U	101	BCL	C1D-C2D	-2.73	1.39	1.45
9	W	102	BCL	C1D-C2D	-2.72	1.39	1.45
9	4	102	BCL	C3B-C2B	-2.72	1.34	1.39
9	J	102	BCL	C1D-C2D	-2.72	1.40	1.45
9	I	101	BCL	C3B-C2B	-2.72	1.34	1.39
9	6	102	BCL	C3B-C2B	-2.72	1.34	1.39
9	B	101	BCL	C3B-C2B	-2.72	1.34	1.39
9	Q	102	BCL	C3B-C2B	-2.72	1.34	1.39
9	N	102	BCL	C1D-C2D	-2.72	1.40	1.45
9	E	101	BCL	C3B-C2B	-2.72	1.34	1.39
9	L	1001	BCL	C1D-C2D	-2.71	1.40	1.45
10	A	104	KGD	CAS-CAW	-2.71	1.45	1.51
10	P	102	KGD	CAE-CAI	-2.71	1.47	1.50
10	2	101	KGD	CAS-CAW	-2.71	1.45	1.51
9	A	102	BCL	C1D-C2D	-2.71	1.40	1.45
10	B	102	KGD	CBF-CBH	-2.70	1.40	1.45
10	B	102	KGD	CBJ-CBH	-2.70	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	102	BCL	C3B-C2B	-2.70	1.34	1.39
9	8	102	BCL	C3B-C2B	-2.70	1.34	1.39
9	K	101	BCL	C3B-C2B	-2.70	1.34	1.39
9	W	103	BCL	C3B-C2B	-2.70	1.34	1.39
10	2	104	KGD	CBO-CBL	-2.70	1.45	1.50
10	G	102	KGD	CBJ-CBH	-2.69	1.32	1.35
11	L	1003	BPH	C3A-C2A	-2.69	1.52	1.54
9	O	101	BCL	C3B-C2B	-2.68	1.34	1.39
13	P	103	PGV	O05-C05	-2.68	1.35	1.43
9	2	103	BCL	C3B-C2B	-2.68	1.34	1.39
15	C	403	HEM	C1B-NB	-2.67	1.35	1.40
9	S	103	BCL	C3B-C2B	-2.67	1.34	1.39
10	8	103	KGD	CAB-CAD	-2.66	1.50	1.53
12	M	705	MQE	CCH-CBR	-2.66	1.35	1.39
10	0	104	KGD	CAE-CAI	-2.65	1.47	1.50
10	0	103	KGD	CBN-CBL	-2.65	1.40	1.45
10	3	102	KGD	CAE-CAI	-2.64	1.47	1.50
9	J	101	BCL	C1D-C2D	-2.64	1.40	1.45
10	6	103	KGD	CBN-CBL	-2.64	1.40	1.45
9	M	703	BCL	C1D-C2D	-2.62	1.40	1.45
9	L	1002	BCL	C1D-C2D	-2.62	1.40	1.45
10	W	101	KGD	CAE-CAI	-2.62	1.47	1.50
12	M	701	MQE	CAY-CAX	-2.61	1.47	1.51
9	H	101	BCL	C1D-C2D	-2.60	1.40	1.45
11	M	704	BPH	CMD-C2D	-2.60	1.45	1.51
13	P	104	PGV	O12-C04	-2.60	1.34	1.44
9	R	101	BCL	C1D-C2D	-2.60	1.40	1.45
9	N	101	BCL	C1D-C2D	-2.60	1.40	1.45
9	F	101	BCL	C1D-C2D	-2.59	1.40	1.45
9	T	101	BCL	C1D-C2D	-2.58	1.40	1.45
9	3	101	BCL	C1D-C2D	-2.58	1.40	1.45
9	1	101	BCL	C1D-C2D	-2.58	1.40	1.45
9	A	101	BCL	C1D-C2D	-2.57	1.40	1.45
9	X	101	BCL	C1D-C2D	-2.57	1.40	1.45
9	P	101	BCL	C1D-C2D	-2.57	1.40	1.45
10	6	103	KGD	CBF-CBH	-2.57	1.40	1.45
9	7	101	BCL	C1D-C2D	-2.57	1.40	1.45
9	D	101	BCL	C1D-C2D	-2.56	1.40	1.45
10	T	102	KGD	CAO-CAM	-2.55	1.32	1.35
12	M	705	MQE	CAY-CBL	-2.55	1.47	1.50
9	5	101	BCL	C1D-C2D	-2.55	1.40	1.45
9	9	102	BCL	C1D-C2D	-2.54	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	4	102	BCL	C1D-C2D	-2.52	1.40	1.45
10	2	101	KGD	CBO-CBL	-2.51	1.45	1.50
9	W	103	BCL	C1D-C2D	-2.51	1.40	1.45
9	8	102	BCL	C1D-C2D	-2.51	1.40	1.45
9	G	101	BCL	C1D-C2D	-2.51	1.40	1.45
9	E	101	BCL	C1D-C2D	-2.51	1.40	1.45
9	K	101	BCL	C1D-C2D	-2.49	1.40	1.45
16	Y	101	DGA	OG2-CG2	-2.49	1.40	1.46
9	0	102	BCL	C1D-C2D	-2.49	1.40	1.45
9	2	103	BCL	C1D-C2D	-2.48	1.40	1.45
10	9	101	KGD	CAD-CAH	-2.48	1.32	1.35
9	S	103	BCL	C1D-C2D	-2.48	1.40	1.45
9	6	102	BCL	C1D-C2D	-2.48	1.40	1.45
9	O	101	BCL	C1D-C2D	-2.48	1.40	1.45
10	B	102	KGD	CAE-CAI	-2.48	1.47	1.50
9	Q	102	BCL	C1D-C2D	-2.48	1.40	1.45
10	N	103	KGD	CAS-CAW	-2.47	1.46	1.51
9	B	101	BCL	C1D-C2D	-2.47	1.40	1.45
9	U	102	BCL	C1D-C2D	-2.47	1.40	1.45
9	I	101	BCL	C1D-C2D	-2.47	1.40	1.45
13	L	1007	PGV	P-O12	2.43	1.69	1.59
12	M	705	MQE	CCG-CBP	-2.43	1.36	1.39
9	L	1001	BCL	C3D-C4D	-2.43	1.38	1.44
9	H	102	BCL	C3B-C2B	-2.43	1.35	1.39
9	W	102	BCL	C3B-C2B	-2.42	1.35	1.39
12	M	705	MQE	CBR-CBP	-2.41	1.36	1.40
10	T	102	KGD	CAI-CAH	-2.41	1.42	1.47
10	0	103	KGD	CBI-CBL	-2.41	1.32	1.35
9	8	101	BCL	C3B-C2B	-2.40	1.35	1.39
9	0	101	BCL	C3B-C2B	-2.40	1.35	1.39
9	A	102	BCL	C3B-C2B	-2.40	1.35	1.39
9	L	1002	BCL	C3B-CAB	2.39	1.55	1.49
9	2	102	BCL	C3B-C2B	-2.39	1.35	1.39
9	S	102	BCL	C3B-C2B	-2.39	1.35	1.39
9	A	101	BCL	C3B-C2B	-2.39	1.35	1.39
10	H	103	KGD	CAS-CAW	-2.39	1.46	1.51
10	T	102	KGD	CAS-CAW	-2.38	1.46	1.51
10	K	102	KGD	CAE-CAI	-2.38	1.47	1.50
10	B	102	KGD	CAS-CAW	-2.38	1.46	1.51
9	Q	101	BCL	C3B-C2B	-2.38	1.35	1.39
10	2	101	KGD	CAI-CAH	-2.38	1.43	1.47
9	4	101	BCL	C3B-C2B	-2.38	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	706	PGV	O05-C05	-2.38	1.36	1.43
9	J	102	BCL	C3B-C2B	-2.38	1.35	1.39
9	U	101	BCL	C3B-C2B	-2.38	1.35	1.39
9	7	101	BCL	C3B-C2B	-2.37	1.35	1.39
9	N	102	BCL	C3B-C2B	-2.36	1.35	1.39
9	H	102	BCL	C3D-C4D	-2.36	1.38	1.44
10	0	103	KGD	CAV-CAR	-2.36	1.32	1.35
9	A	102	BCL	C3D-C4D	-2.36	1.38	1.44
10	H	103	KGD	CAG-CAB	-2.36	1.49	1.53
13	P	103	PGV	O01-C02	-2.36	1.40	1.46
9	5	101	BCL	C3B-C2B	-2.36	1.35	1.39
9	D	102	BCL	C3B-C2B	-2.35	1.35	1.39
9	T	101	BCL	C3B-C2B	-2.35	1.35	1.39
9	6	101	BCL	C3B-C2B	-2.35	1.35	1.39
13	L	1006	PGV	P-O11	2.35	1.68	1.59
10	P	102	KGD	CAC-CAB	-2.35	1.48	1.54
9	F	102	BCL	C3B-C2B	-2.35	1.35	1.39
9	5	101	BCL	C3D-C4D	-2.35	1.38	1.44
9	D	101	BCL	C3D-C4D	-2.35	1.38	1.44
9	P	101	BCL	C3B-C2B	-2.34	1.35	1.39
13	C	406	PGV	O05-C05	-2.34	1.36	1.43
9	1	101	BCL	C3B-C2B	-2.34	1.35	1.39
9	F	102	BCL	C3D-C4D	-2.34	1.38	1.44
9	E	101	BCL	C3D-C4D	-2.33	1.38	1.44
9	U	101	BCL	C3D-C4D	-2.33	1.38	1.44
9	S	102	BCL	C3D-C4D	-2.33	1.38	1.44
9	1	101	BCL	C3D-C4D	-2.33	1.38	1.44
10	T	102	KGD	CAD-CAH	-2.33	1.32	1.35
9	X	101	BCL	C3B-C2B	-2.33	1.35	1.39
9	P	101	BCL	C3D-C4D	-2.33	1.38	1.44
9	R	101	BCL	C3D-C4D	-2.33	1.38	1.44
9	A	101	BCL	C3D-C4D	-2.33	1.38	1.44
9	3	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	G	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	N	102	BCL	C3D-C4D	-2.32	1.38	1.44
9	4	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	3	101	BCL	C3B-C2B	-2.32	1.35	1.39
9	6	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	N	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	8	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	H	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	B	101	BCL	C3D-C4D	-2.32	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	9	102	BCL	C3B-C2B	-2.32	1.35	1.39
9	2	102	BCL	C3D-C4D	-2.32	1.38	1.44
9	0	101	BCL	C3D-C4D	-2.32	1.38	1.44
9	Q	101	BCL	C3D-C4D	-2.31	1.39	1.44
9	N	101	BCL	C3B-C2B	-2.31	1.35	1.39
9	S	103	BCL	C3D-C4D	-2.31	1.39	1.44
9	J	101	BCL	C3D-C4D	-2.31	1.39	1.44
9	2	103	BCL	C3D-C4D	-2.31	1.39	1.44
9	4	102	BCL	C3D-C4D	-2.31	1.39	1.44
10	I	102	KGD	CAE-CAI	-2.31	1.47	1.50
9	0	102	BCL	C3D-C4D	-2.31	1.39	1.44
9	R	101	BCL	C3B-C2B	-2.31	1.35	1.39
9	D	101	BCL	C3B-C2B	-2.31	1.35	1.39
9	F	101	BCL	C3B-C2B	-2.31	1.35	1.39
9	U	102	BCL	C3D-C4D	-2.31	1.39	1.44
9	8	102	BCL	C3D-C4D	-2.31	1.39	1.44
9	K	101	BCL	C3D-C4D	-2.30	1.39	1.44
9	W	103	BCL	C3D-C4D	-2.30	1.39	1.44
9	X	101	BCL	C3D-C4D	-2.30	1.39	1.44
9	9	102	BCL	C3D-C4D	-2.30	1.39	1.44
9	H	101	BCL	C3B-C2B	-2.30	1.35	1.39
9	6	102	BCL	C3D-C4D	-2.30	1.39	1.44
10	6	103	KGD	CAE-CAI	-2.30	1.47	1.50
9	F	101	BCL	C3D-C4D	-2.30	1.39	1.44
9	J	102	BCL	C3D-C4D	-2.29	1.39	1.44
9	O	101	BCL	C3D-C4D	-2.29	1.39	1.44
9	T	101	BCL	C3D-C4D	-2.29	1.39	1.44
9	D	102	BCL	C3D-C4D	-2.29	1.39	1.44
9	M	703	BCL	C3D-C4D	-2.29	1.39	1.44
9	Q	102	BCL	C3D-C4D	-2.29	1.39	1.44
13	Z	101	PGV	P-O11	2.29	1.68	1.59
9	7	101	BCL	C3D-C4D	-2.29	1.39	1.44
10	A	103	KGD	CBC-CAY	-2.28	1.44	1.50
9	I	101	BCL	C3D-C4D	-2.28	1.39	1.44
9	J	101	BCL	C3B-C2B	-2.28	1.35	1.39
9	W	102	BCL	C3D-C4D	-2.28	1.39	1.44
10	B	102	KGD	CBA-CAW	-2.27	1.31	1.34
10	A	104	KGD	CBA-CAW	-2.27	1.31	1.34
10	Q	103	KGD	CBA-CAW	-2.26	1.31	1.34
11	L	1005	BPH	CMB-C2B	-2.26	1.46	1.51
10	Q	103	KGD	CBF-CBH	-2.25	1.41	1.45
11	L	1005	BPH	O2D-CED	-2.23	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	706	PGV	P-O12	2.22	1.68	1.59
10	F	103	KGD	CAI-CAH	-2.22	1.43	1.47
10	8	103	KGD	CBJ-CBH	-2.22	1.32	1.35
10	2	101	KGD	CBC-CAY	-2.21	1.44	1.50
11	L	1003	BPH	CBD-CGD	-2.20	1.49	1.52
10	4	103	KGD	CAE-CAI	-2.19	1.48	1.50
10	N	103	KGD	CBJ-CBH	-2.19	1.32	1.35
10	2	101	KGD	CAD-CAH	-2.19	1.32	1.35
9	M	703	BCL	C3D-C2D	-2.19	1.33	1.39
10	T	102	KGD	CBI-CBL	-2.17	1.32	1.35
10	0	104	KGD	CAO-CAM	-2.17	1.32	1.35
10	H	103	KGD	CBJ-CBH	-2.17	1.32	1.35
10	Q	103	KGD	CBJ-CBH	-2.16	1.32	1.35
10	8	103	KGD	CAE-CAI	-2.16	1.48	1.50
10	0	103	KGD	CBA-CAW	-2.16	1.31	1.34
10	2	104	KGD	CBJ-CBH	-2.16	1.32	1.35
13	M	706	PGV	O03-C01	-2.16	1.40	1.45
9	F	101	BCL	C2C-C3C	-2.15	1.48	1.54
10	T	102	KGD	CBJ-CBH	-2.14	1.32	1.35
9	R	101	BCL	C2C-C3C	-2.13	1.48	1.54
9	7	101	BCL	C2C-C3C	-2.13	1.48	1.54
9	P	101	BCL	C2C-C3C	-2.13	1.48	1.54
9	H	101	BCL	C2C-C3C	-2.13	1.48	1.54
9	1	101	BCL	C2C-C3C	-2.13	1.48	1.54
11	L	1003	BPH	O2D-CED	-2.13	1.40	1.45
10	9	101	KGD	CAO-CAM	-2.13	1.33	1.35
9	T	101	BCL	C2C-C3C	-2.12	1.48	1.54
9	X	101	BCL	C2C-C3C	-2.12	1.48	1.54
9	5	101	BCL	C2C-C3C	-2.12	1.48	1.54
9	N	101	BCL	C2C-C3C	-2.12	1.48	1.54
9	9	102	BCL	C2C-C3C	-2.11	1.48	1.54
9	3	101	BCL	C2C-C3C	-2.11	1.48	1.54
9	A	101	BCL	C2C-C3C	-2.11	1.48	1.54
10	S	101	KGD	CBC-CAY	-2.11	1.44	1.50
9	M	703	BCL	C3B-C2B	-2.10	1.35	1.39
13	Z	101	PGV	P-O12	2.10	1.67	1.59
10	E	102	KGD	CAF-CAB	-2.10	1.49	1.53
9	D	101	BCL	C2C-C3C	-2.10	1.48	1.54
9	6	101	BCL	C2C-C3C	-2.09	1.48	1.54
9	S	102	BCL	C2C-C3C	-2.09	1.48	1.54
10	A	104	KGD	CBJ-CBH	-2.09	1.33	1.35
9	J	101	BCL	C2C-C3C	-2.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	101	BCL	C2C-C3C	-2.09	1.48	1.54
9	9	102	BCL	C3D-C2D	-2.09	1.33	1.39
9	J	102	BCL	C2C-C3C	-2.09	1.48	1.54
9	N	102	BCL	C2C-C3C	-2.09	1.48	1.54
9	F	102	BCL	C2C-C3C	-2.08	1.48	1.54
10	6	103	KGD	CBI-CBL	-2.08	1.33	1.35
10	T	102	KGD	CAV-CAR	-2.08	1.33	1.35
9	4	101	BCL	C2C-C3C	-2.08	1.48	1.54
9	3	101	BCL	C3D-C2D	-2.08	1.33	1.39
9	H	102	BCL	C2C-C3C	-2.08	1.48	1.54
9	A	102	BCL	C2C-C3C	-2.08	1.48	1.54
10	S	104	KGD	CAF-CAB	-2.08	1.49	1.53
9	D	101	BCL	C3D-C2D	-2.08	1.33	1.39
9	0	101	BCL	C2C-C3C	-2.08	1.48	1.54
10	B	102	KGD	CAV-CAR	-2.08	1.33	1.35
9	7	101	BCL	C3D-C2D	-2.08	1.33	1.39
13	P	103	PGV	P-O13	-2.08	1.43	1.50
9	8	101	BCL	C2C-C3C	-2.07	1.48	1.54
9	A	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	1	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	R	101	BCL	C3D-C2D	-2.07	1.33	1.39
9	P	101	BCL	C3D-C2D	-2.07	1.33	1.39
13	P	103	PGV	O12-C04	-2.07	1.36	1.44
9	H	101	BCL	C3D-C2D	-2.07	1.33	1.39
11	L	1005	BPH	CHA-CBD	-2.07	1.49	1.52
9	2	102	BCL	C2C-C3C	-2.07	1.48	1.54
10	A	103	KGD	CAO-CAM	-2.07	1.33	1.35
9	F	101	BCL	C3D-C2D	-2.07	1.33	1.39
12	M	701	MQE	CBY-CAW	-2.07	1.45	1.50
10	G	102	KGD	CBN-CBL	-2.07	1.41	1.45
9	X	101	BCL	C3D-C2D	-2.06	1.33	1.39
9	D	102	BCL	C2C-C3C	-2.06	1.48	1.54
10	A	103	KGD	CAE-CAI	-2.06	1.48	1.50
9	U	101	BCL	C2C-C3C	-2.06	1.48	1.54
9	T	101	BCL	C3D-C2D	-2.06	1.33	1.39
13	L	1006	PGV	P-O12	2.06	1.67	1.59
11	L	1003	BPH	CMB-C2B	-2.06	1.46	1.51
9	J	101	BCL	C3D-C2D	-2.06	1.33	1.39
10	2	104	KGD	CBK-CBH	-2.05	1.46	1.50
9	W	102	BCL	C2C-C3C	-2.05	1.48	1.54
10	T	102	KGD	CAQ-CAR	-2.05	1.41	1.45
10	H	103	KGD	CBI-CBL	-2.05	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	5	101	BCL	C3D-C2D	-2.05	1.33	1.39
10	8	103	KGD	CBA-CAW	-2.05	1.32	1.34
9	6	102	BCL	C3D-C2D	-2.04	1.33	1.39
9	Q	102	BCL	C3D-C2D	-2.04	1.33	1.39
9	S	103	BCL	C3D-C2D	-2.04	1.33	1.39
9	I	101	BCL	C3D-C2D	-2.04	1.33	1.39
9	N	101	BCL	C3D-C2D	-2.04	1.33	1.39
9	W	103	BCL	C3D-C2D	-2.04	1.33	1.39
10	W	101	KGD	CAN-CAM	-2.04	1.46	1.50
10	H	103	KGD	CAV-CAR	-2.03	1.33	1.35
9	8	102	BCL	C3D-C2D	-2.03	1.33	1.39
9	K	101	BCL	C3D-C2D	-2.03	1.33	1.39
9	E	101	BCL	C3D-C2D	-2.03	1.33	1.39
9	4	102	BCL	C3D-C2D	-2.02	1.33	1.39
10	O	102	KGD	CBJ-CBH	-2.02	1.33	1.35
10	T	102	KGD	CAK-CAH	-2.02	1.46	1.50
9	U	101	BCL	C3D-C2D	-2.02	1.33	1.39
9	D	102	BCL	C3D-C2D	-2.02	1.33	1.39
10	A	103	KGD	CAL-CAM	-2.02	1.41	1.45
11	M	704	BPH	CMB-C2B	-2.02	1.46	1.51
9	J	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	O	101	BCL	C3D-C2D	-2.01	1.33	1.39
9	U	102	BCL	C3D-C2D	-2.01	1.33	1.39
9	B	101	BCL	C3D-C2D	-2.01	1.33	1.39
10	2	101	KGD	CBN-CBL	-2.01	1.41	1.45
9	Q	101	BCL	C3D-C2D	-2.01	1.33	1.39
9	2	103	BCL	C3D-C2D	-2.01	1.33	1.39
9	0	102	BCL	C3D-C2D	-2.01	1.33	1.39
11	M	704	BPH	CHA-CBD	-2.01	1.50	1.52
9	M	703	BCL	C2C-C3C	-2.00	1.48	1.54
9	8	101	BCL	C3D-C2D	-2.00	1.33	1.39
9	L	1001	BCL	C3D-C2D	-2.00	1.33	1.39
10	H	103	KGD	CBF-CBH	-2.00	1.41	1.45
9	8	102	BCL	C2C-C3C	-2.00	1.48	1.54

All (1855) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	401	KGD	CBB-CAV-CAR	-8.48	115.21	127.31
9	L	1001	BCL	CMB-C2B-C1B	-8.24	115.81	128.46
9	L	1002	BCL	CMB-C2B-C1B	-7.79	116.49	128.46
10	C	401	KGD	CBM-CBJ-CBH	-7.37	116.79	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	404	HEM	CHC-C4B-NB	6.79	131.81	124.43
9	L	1001	BCL	O2D-CGD-O1D	-6.27	111.58	123.84
9	M	703	BCL	CMB-C2B-C1B	-6.02	119.21	128.46
10	P	102	KGD	CAJ-CAL-CAM	-5.99	117.19	126.23
10	2	101	KGD	CBB-CAV-CAR	-5.88	118.92	127.31
9	Q	101	BCL	O2D-CGD-CBD	5.77	121.53	111.27
9	8	101	BCL	O2D-CGD-CBD	5.76	121.50	111.27
9	H	102	BCL	O2D-CGD-CBD	5.76	121.50	111.27
9	0	101	BCL	O2D-CGD-CBD	5.75	121.49	111.27
9	4	101	BCL	O2D-CGD-CBD	5.75	121.49	111.27
9	2	102	BCL	O2D-CGD-CBD	5.75	121.49	111.27
9	W	102	BCL	O2D-CGD-CBD	5.75	121.49	111.27
9	A	102	BCL	O2D-CGD-CBD	5.75	121.48	111.27
9	N	102	BCL	O2D-CGD-CBD	5.75	121.48	111.27
9	F	102	BCL	O2D-CGD-CBD	5.75	121.48	111.27
9	J	102	BCL	O2D-CGD-CBD	5.74	121.47	111.27
9	6	101	BCL	O2D-CGD-CBD	5.74	121.47	111.27
9	L	1002	BCL	C2D-C1D-ND	5.73	114.33	110.10
9	D	102	BCL	O2D-CGD-CBD	5.73	121.45	111.27
9	S	102	BCL	O2D-CGD-CBD	5.72	121.44	111.27
9	U	101	BCL	O2D-CGD-CBD	5.72	121.43	111.27
9	5	101	BCL	C1D-ND-C4D	-5.72	102.27	106.33
9	A	101	BCL	C1D-ND-C4D	-5.71	102.28	106.33
9	F	101	BCL	C1D-ND-C4D	-5.71	102.28	106.33
9	1	101	BCL	C1D-ND-C4D	-5.71	102.28	106.33
9	N	101	BCL	C1D-ND-C4D	-5.71	102.28	106.33
9	L	1001	BCL	CAC-C3C-C2C	-5.70	100.01	114.26
9	J	101	BCL	C1D-ND-C4D	-5.70	102.28	106.33
9	P	101	BCL	CMB-C2B-C1B	-5.70	119.70	128.46
9	5	101	BCL	CMB-C2B-C1B	-5.68	119.73	128.46
9	A	101	BCL	CMB-C2B-C1B	-5.67	119.74	128.46
9	7	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	3	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	T	101	BCL	C1D-ND-C4D	-5.67	102.31	106.33
9	9	102	BCL	CMB-C2B-C1B	-5.66	119.76	128.46
9	F	101	BCL	CMB-C2B-C1B	-5.66	119.76	128.46
10	H	103	KGD	CBG-CBI-CBL	-5.66	119.23	127.31
9	1	101	BCL	CMB-C2B-C1B	-5.66	119.77	128.46
9	N	101	BCL	CMB-C2B-C1B	-5.66	119.77	128.46
9	R	101	BCL	CMB-C2B-C1B	-5.66	119.77	128.46
9	T	101	BCL	CMB-C2B-C1B	-5.66	119.77	128.46
9	D	101	BCL	C1D-ND-C4D	-5.65	102.32	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	101	BCL	C1D-ND-C4D	-5.65	102.32	106.33
9	7	101	BCL	CMB-C2B-C1B	-5.65	119.78	128.46
9	H	101	BCL	CMB-C2B-C1B	-5.65	119.78	128.46
9	3	101	BCL	CMB-C2B-C1B	-5.64	119.79	128.46
9	P	101	BCL	C1D-ND-C4D	-5.64	102.33	106.33
9	L	1002	BCL	C1D-ND-C4D	-5.63	102.33	106.33
9	J	101	BCL	CMB-C2B-C1B	-5.63	119.81	128.46
9	D	101	BCL	CMB-C2B-C1B	-5.63	119.81	128.46
9	9	102	BCL	C1D-ND-C4D	-5.63	102.34	106.33
9	X	101	BCL	C1D-ND-C4D	-5.63	102.34	106.33
9	R	101	BCL	C1D-ND-C4D	-5.62	102.34	106.33
9	X	101	BCL	CMB-C2B-C1B	-5.62	119.83	128.46
9	E	101	BCL	C1D-ND-C4D	-5.58	102.37	106.33
9	B	101	BCL	C1D-ND-C4D	-5.56	102.39	106.33
9	K	101	BCL	C1D-ND-C4D	-5.56	102.39	106.33
9	G	101	BCL	C1D-ND-C4D	-5.55	102.39	106.33
10	F	103	KGD	CAP-CAO-CAM	-5.53	119.41	127.31
9	8	102	BCL	C1D-ND-C4D	-5.53	102.41	106.33
9	4	102	BCL	C1D-ND-C4D	-5.53	102.41	106.33
9	W	102	BCL	CMB-C2B-C1B	-5.53	119.97	128.46
9	S	103	BCL	C1D-ND-C4D	-5.52	102.41	106.33
10	P	102	KGD	CAP-CAO-CAM	-5.52	119.43	127.31
10	8	103	KGD	CAP-CAO-CAM	-5.52	119.43	127.31
9	0	101	BCL	CMB-C2B-C1B	-5.52	119.98	128.46
9	N	102	BCL	CMB-C2B-C1B	-5.52	119.98	128.46
9	4	101	BCL	CMB-C2B-C1B	-5.52	119.99	128.46
9	A	102	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
9	6	101	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
12	M	701	MQE	CAY-CBL-CBB	-5.51	117.63	126.79
9	H	102	BCL	CMB-C2B-C1B	-5.50	120.00	128.46
9	2	102	BCL	CMB-C2B-C1B	-5.50	120.00	128.46
9	U	102	BCL	C1D-ND-C4D	-5.50	102.43	106.33
9	U	101	BCL	CMB-C2B-C1B	-5.49	120.02	128.46
9	8	101	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
9	F	102	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
9	D	102	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
9	Q	101	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
9	S	102	BCL	CMB-C2B-C1B	-5.49	120.03	128.46
9	W	103	BCL	C1D-ND-C4D	-5.48	102.44	106.33
9	J	102	BCL	CMB-C2B-C1B	-5.47	120.05	128.46
9	6	102	BCL	C1D-ND-C4D	-5.47	102.45	106.33
9	0	102	BCL	C1D-ND-C4D	-5.47	102.45	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	405	HEM	C4D-ND-C1D	5.47	110.72	105.07
9	2	103	BCL	C1D-ND-C4D	-5.47	102.45	106.33
9	I	101	BCL	C1D-ND-C4D	-5.46	102.46	106.33
9	O	101	BCL	C1D-ND-C4D	-5.45	102.46	106.33
9	Q	102	BCL	C1D-ND-C4D	-5.44	102.47	106.33
10	W	101	KGD	CAJ-CAL-CAM	-5.42	118.05	126.23
15	C	404	HEM	C4D-ND-C1D	5.40	110.65	105.07
10	N	103	KGD	CBG-CBI-CBL	-5.37	119.64	127.31
9	M	703	BCL	C1D-ND-C4D	-5.36	102.53	106.33
10	2	101	KGD	CAJ-CAL-CAM	-5.35	118.15	126.23
10	6	103	KGD	CBB-CAV-CAR	-5.33	119.70	127.31
9	4	101	BCL	C1D-ND-C4D	-5.33	102.55	106.33
9	L	1001	BCL	CMB-C2B-C3B	5.32	134.63	124.68
9	H	102	BCL	C1D-ND-C4D	-5.32	102.56	106.33
10	3	102	KGD	CBF-CBH-CBJ	-5.32	110.78	118.94
9	F	102	BCL	C1D-ND-C4D	-5.31	102.56	106.33
9	S	102	BCL	C1D-ND-C4D	-5.31	102.56	106.33
9	6	101	BCL	C1D-ND-C4D	-5.31	102.56	106.33
10	T	102	KGD	CAJ-CAL-CAM	-5.29	118.24	126.23
9	N	101	BCL	C2D-C1D-ND	5.29	114.00	110.10
9	0	101	BCL	C1D-ND-C4D	-5.29	102.58	106.33
9	L	1002	BCL	CMB-C2B-C3B	5.28	134.56	124.68
9	D	102	BCL	C1D-ND-C4D	-5.28	102.58	106.33
9	2	102	BCL	C1D-ND-C4D	-5.27	102.59	106.33
9	F	101	BCL	C2D-C1D-ND	5.26	113.98	110.10
9	U	101	BCL	C1D-ND-C4D	-5.26	102.60	106.33
9	1	101	BCL	C2D-C1D-ND	5.25	113.97	110.10
9	Q	101	BCL	C1D-ND-C4D	-5.25	102.61	106.33
9	T	101	BCL	C2D-C1D-ND	5.25	113.97	110.10
9	A	102	BCL	C1D-ND-C4D	-5.24	102.61	106.33
9	N	102	BCL	C1D-ND-C4D	-5.24	102.61	106.33
15	C	403	HEM	CHB-C1B-NB	5.23	130.84	124.38
9	7	101	BCL	C2D-C1D-ND	5.23	113.96	110.10
9	P	101	BCL	C2D-C1D-ND	5.23	113.95	110.10
9	8	101	BCL	C1D-ND-C4D	-5.22	102.62	106.33
9	J	101	BCL	C2D-C1D-ND	5.22	113.95	110.10
9	H	101	BCL	C2D-C1D-ND	5.22	113.95	110.10
9	J	102	BCL	C1D-ND-C4D	-5.22	102.63	106.33
10	Q	103	KGD	CAJ-CAL-CAM	-5.21	118.36	126.23
15	C	402	HEM	CHB-C1B-NB	5.21	130.82	124.38
9	M	703	BCL	O2D-CGD-O1D	-5.20	113.67	123.84
9	3	101	BCL	C2D-C1D-ND	5.20	113.93	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	101	BCL	C2D-C1D-ND	5.20	113.93	110.10
9	6	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
10	W	101	KGD	CBG-CBI-CBL	-5.19	119.90	127.31
9	X	101	BCL	C2D-C1D-ND	5.19	113.93	110.10
9	9	102	BCL	C2D-C1D-ND	5.18	113.92	110.10
9	5	101	BCL	C2D-C1D-ND	5.18	113.92	110.10
9	F	102	BCL	C2D-C1D-ND	5.18	113.92	110.10
9	M	703	BCL	C2D-C1D-ND	5.18	113.92	110.10
9	W	102	BCL	C1D-ND-C4D	-5.18	102.66	106.33
9	D	101	BCL	C2D-C1D-ND	5.18	113.92	110.10
10	2	101	KGD	CAP-CAO-CAM	-5.17	119.93	127.31
15	C	404	HEM	CHB-C1B-NB	5.17	130.77	124.38
9	6	102	BCL	CAC-C3C-C2C	-5.16	101.36	114.26
9	I	101	BCL	CAC-C3C-C2C	-5.16	101.37	114.26
9	G	101	BCL	CAC-C3C-C2C	-5.16	101.38	114.26
9	R	101	BCL	C2D-C1D-ND	5.16	113.90	110.10
9	S	103	BCL	CAC-C3C-C2C	-5.16	101.38	114.26
9	K	101	BCL	CAC-C3C-C2C	-5.15	101.39	114.26
9	0	102	BCL	CAC-C3C-C2C	-5.15	101.39	114.26
9	H	102	BCL	C2D-C1D-ND	5.15	113.90	110.10
9	M	703	BCL	O2D-CGD-CBD	5.15	120.42	111.27
9	W	103	BCL	CAC-C3C-C2C	-5.15	101.40	114.26
9	U	102	BCL	CAC-C3C-C2C	-5.15	101.40	114.26
9	2	103	BCL	CAC-C3C-C2C	-5.14	101.41	114.26
9	E	101	BCL	CAC-C3C-C2C	-5.14	101.41	114.26
9	O	101	BCL	CAC-C3C-C2C	-5.14	101.42	114.26
9	Q	102	BCL	CAC-C3C-C2C	-5.14	101.42	114.26
9	B	101	BCL	CAC-C3C-C2C	-5.14	101.42	114.26
9	S	102	BCL	C2D-C1D-ND	5.13	113.89	110.10
9	8	102	BCL	CAC-C3C-C2C	-5.13	101.43	114.26
9	T	101	BCL	O2D-CGD-O1D	-5.13	113.80	123.84
9	4	102	BCL	CAC-C3C-C2C	-5.13	101.43	114.26
10	B	102	KGD	CBF-CBH-CBJ	-5.13	111.07	118.94
9	P	101	BCL	O2D-CGD-O1D	-5.13	113.81	123.84
9	N	101	BCL	O2D-CGD-O1D	-5.13	113.81	123.84
9	F	101	BCL	O2D-CGD-O1D	-5.12	113.82	123.84
9	2	102	BCL	C2D-C1D-ND	5.11	113.87	110.10
9	3	101	BCL	O2D-CGD-O1D	-5.11	113.84	123.84
9	D	102	BCL	C2D-C1D-ND	5.11	113.87	110.10
9	5	101	BCL	O2D-CGD-O1D	-5.11	113.85	123.84
9	R	101	BCL	O2D-CGD-O1D	-5.11	113.85	123.84
9	1	101	BCL	O2D-CGD-O1D	-5.11	113.85	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	D	101	BCL	O2D-CGD-O1D	-5.11	113.85	123.84
9	J	101	BCL	O2D-CGD-O1D	-5.11	113.86	123.84
10	5	102	KGD	CAJ-CAL-CAM	-5.11	118.52	126.23
9	4	101	BCL	C2D-C1D-ND	5.10	113.86	110.10
9	A	102	BCL	C2D-C1D-ND	5.10	113.86	110.10
10	G	102	KGD	CAP-CAO-CAM	-5.10	120.03	127.31
9	7	101	BCL	O2D-CGD-O1D	-5.10	113.86	123.84
9	X	101	BCL	O2D-CGD-O1D	-5.10	113.86	123.84
9	E	101	BCL	O2D-CGD-O1D	-5.10	113.87	123.84
9	H	101	BCL	O2D-CGD-O1D	-5.09	113.88	123.84
9	S	103	BCL	O2D-CGD-O1D	-5.09	113.88	123.84
9	9	102	BCL	O2D-CGD-O1D	-5.09	113.88	123.84
9	A	101	BCL	O2D-CGD-O1D	-5.09	113.88	123.84
9	0	102	BCL	O2D-CGD-O1D	-5.09	113.88	123.84
9	0	101	BCL	C2D-C1D-ND	5.09	113.85	110.10
9	B	101	BCL	O2D-CGD-O1D	-5.09	113.89	123.84
9	4	102	BCL	O2D-CGD-O1D	-5.09	113.89	123.84
9	6	102	BCL	O2D-CGD-O1D	-5.09	113.89	123.84
9	W	103	BCL	O2D-CGD-O1D	-5.09	113.89	123.84
9	2	103	BCL	O2D-CGD-O1D	-5.08	113.90	123.84
9	Q	102	BCL	O2D-CGD-O1D	-5.08	113.90	123.84
9	N	102	BCL	C2D-C1D-ND	5.08	113.85	110.10
9	G	101	BCL	O2D-CGD-O1D	-5.08	113.90	123.84
9	U	102	BCL	O2D-CGD-O1D	-5.08	113.91	123.84
9	O	101	BCL	O2D-CGD-O1D	-5.07	113.92	123.84
9	8	102	BCL	O2D-CGD-O1D	-5.07	113.92	123.84
9	K	101	BCL	O2D-CGD-O1D	-5.07	113.93	123.84
9	I	101	BCL	O2D-CGD-O1D	-5.06	113.94	123.84
9	U	101	BCL	C2D-C1D-ND	5.05	113.83	110.10
9	8	101	BCL	C2D-C1D-ND	5.05	113.83	110.10
15	C	405	HEM	CHC-C4B-NB	5.05	129.92	124.43
9	J	102	BCL	C2D-C1D-ND	5.04	113.82	110.10
9	Q	101	BCL	C2D-C1D-ND	5.03	113.81	110.10
9	W	102	BCL	C2D-C1D-ND	5.03	113.81	110.10
9	G	101	BCL	C2D-C1D-ND	5.02	113.80	110.10
9	S	103	BCL	C2D-C1D-ND	5.01	113.80	110.10
9	4	102	BCL	C2D-C1D-ND	5.00	113.79	110.10
9	E	101	BCL	C2D-C1D-ND	5.00	113.79	110.10
9	B	101	BCL	C2D-C1D-ND	5.00	113.79	110.10
9	T	101	BCL	O2D-CGD-CBD	4.99	120.14	111.27
10	J	103	KGD	CBG-CBI-CBL	-4.99	120.19	127.31
9	J	101	BCL	O2D-CGD-CBD	4.99	120.13	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	7	101	BCL	O2D-CGD-CBD	4.99	120.13	111.27
9	P	101	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	5	101	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	9	102	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	D	101	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	N	101	BCL	O2D-CGD-CBD	4.98	120.12	111.27
9	A	101	BCL	O2D-CGD-CBD	4.98	120.11	111.27
9	I	101	BCL	C2D-C1D-ND	4.98	113.77	110.10
9	K	101	BCL	C2D-C1D-ND	4.98	113.77	110.10
9	F	101	BCL	O2D-CGD-CBD	4.98	120.11	111.27
9	U	102	BCL	C2D-C1D-ND	4.97	113.77	110.10
9	R	101	BCL	O2D-CGD-CBD	4.97	120.10	111.27
9	H	101	BCL	O2D-CGD-CBD	4.97	120.10	111.27
9	3	101	BCL	O2D-CGD-CBD	4.96	120.08	111.27
9	0	102	BCL	C2D-C1D-ND	4.96	113.76	110.10
9	8	102	BCL	C2D-C1D-ND	4.96	113.76	110.10
9	1	101	BCL	O2D-CGD-CBD	4.96	120.08	111.27
9	2	103	BCL	C2D-C1D-ND	4.95	113.75	110.10
9	X	101	BCL	O2D-CGD-CBD	4.94	120.05	111.27
15	C	403	HEM	C4D-ND-C1D	4.94	110.17	105.07
9	9	102	BCL	CAC-C3C-C2C	-4.94	101.92	114.26
9	3	101	BCL	CAC-C3C-C2C	-4.94	101.92	114.26
9	A	101	BCL	CAC-C3C-C2C	-4.94	101.92	114.26
9	H	101	BCL	CAC-C3C-C2C	-4.94	101.93	114.26
9	P	101	BCL	CAC-C3C-C2C	-4.93	101.93	114.26
9	J	101	BCL	CAC-C3C-C2C	-4.93	101.93	114.26
9	F	101	BCL	CAC-C3C-C2C	-4.93	101.94	114.26
9	R	101	BCL	CAC-C3C-C2C	-4.93	101.95	114.26
9	O	101	BCL	C2D-C1D-ND	4.93	113.73	110.10
9	T	101	BCL	CAC-C3C-C2C	-4.92	101.95	114.26
9	N	101	BCL	CAC-C3C-C2C	-4.92	101.96	114.26
9	W	103	BCL	C2D-C1D-ND	4.92	113.73	110.10
9	5	101	BCL	CAC-C3C-C2C	-4.92	101.97	114.26
9	X	101	BCL	CAC-C3C-C2C	-4.92	101.97	114.26
9	1	101	BCL	CAC-C3C-C2C	-4.92	101.97	114.26
9	7	101	BCL	CAC-C3C-C2C	-4.91	101.98	114.26
10	S	104	KGD	CAP-CAO-CAM	-4.91	120.30	127.31
9	6	101	BCL	O2D-CGD-O1D	-4.91	114.24	123.84
15	C	403	HEM	CHC-C4B-NB	4.91	129.76	124.43
9	D	101	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
9	0	101	BCL	O2D-CGD-O1D	-4.91	114.25	123.84
9	6	102	BCL	C2D-C1D-ND	4.91	113.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	102	BCL	O2D-CGD-O1D	-4.90	114.25	123.84
9	Q	101	BCL	O2D-CGD-O1D	-4.90	114.26	123.84
9	8	101	BCL	O2D-CGD-O1D	-4.89	114.27	123.84
10	G	102	KGD	CBG-CBI-CBL	-4.89	120.33	127.31
10	6	103	KGD	CBG-CBI-CBL	-4.89	120.33	127.31
9	Q	102	BCL	C2D-C1D-ND	4.89	113.71	110.10
9	A	102	BCL	O2D-CGD-O1D	-4.89	114.28	123.84
9	F	102	BCL	O2D-CGD-O1D	-4.89	114.28	123.84
9	4	101	BCL	O2D-CGD-O1D	-4.89	114.29	123.84
9	S	102	BCL	O2D-CGD-O1D	-4.88	114.29	123.84
9	D	102	BCL	O2D-CGD-O1D	-4.88	114.30	123.84
9	2	102	BCL	O2D-CGD-O1D	-4.87	114.31	123.84
9	N	102	BCL	O2D-CGD-O1D	-4.87	114.31	123.84
9	W	102	BCL	O2D-CGD-O1D	-4.87	114.32	123.84
9	J	102	BCL	O2D-CGD-O1D	-4.85	114.35	123.84
9	U	101	BCL	O2D-CGD-O1D	-4.85	114.36	123.84
10	0	104	KGD	CBG-CBI-CBL	-4.84	120.41	127.31
10	4	103	KGD	CAJ-CAL-CAM	-4.82	118.95	126.23
10	U	103	KGD	CAJ-CAL-CAM	-4.80	118.99	126.23
9	L	1002	BCL	O2D-CGD-O1D	-4.79	114.47	123.84
9	E	101	BCL	O2D-CGD-CBD	4.79	119.78	111.27
9	0	102	BCL	O2D-CGD-CBD	4.79	119.78	111.27
9	Q	102	BCL	O2D-CGD-CBD	4.78	119.76	111.27
9	8	102	BCL	O2D-CGD-CBD	4.78	119.76	111.27
9	B	101	BCL	O2D-CGD-CBD	4.78	119.76	111.27
9	S	103	BCL	O2D-CGD-CBD	4.78	119.76	111.27
9	K	101	BCL	O2D-CGD-CBD	4.78	119.76	111.27
9	G	101	BCL	O2D-CGD-CBD	4.76	119.73	111.27
9	U	102	BCL	O2D-CGD-CBD	4.76	119.73	111.27
9	4	102	BCL	O2D-CGD-CBD	4.76	119.73	111.27
9	2	103	BCL	O2D-CGD-CBD	4.76	119.72	111.27
9	W	103	BCL	O2D-CGD-CBD	4.76	119.72	111.27
10	0	103	KGD	CBF-CBH-CBJ	-4.76	111.64	118.94
9	O	101	BCL	O2D-CGD-CBD	4.75	119.72	111.27
9	L	1002	BCL	OBB-CAB-CBB	-4.75	109.47	120.17
9	6	102	BCL	O2D-CGD-CBD	4.75	119.71	111.27
9	I	101	BCL	O2D-CGD-CBD	4.75	119.70	111.27
9	2	102	BCL	C1C-NC-C4C	-4.74	104.57	106.71
9	W	102	BCL	C1C-NC-C4C	-4.74	104.58	106.71
10	E	102	KGD	CAJ-CAL-CAM	-4.73	119.09	126.23
10	H	103	KGD	CAJ-CAL-CAM	-4.72	119.10	126.23
10	0	103	KGD	CBB-CAV-CAR	-4.72	120.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	102	BCL	C1C-NC-C4C	-4.72	104.58	106.71
9	D	102	BCL	C1C-NC-C4C	-4.72	104.59	106.71
15	C	405	HEM	CHB-C1B-NB	4.70	130.19	124.38
9	0	101	BCL	C1C-NC-C4C	-4.70	104.59	106.71
10	S	101	KGD	CBG-CBI-CBL	-4.70	120.61	127.31
9	H	102	BCL	C1C-NC-C4C	-4.68	104.60	106.71
10	4	103	KGD	CBB-CAV-CAR	-4.66	120.66	127.31
15	C	402	HEM	CHC-C4B-NB	4.65	129.49	124.43
9	M	703	BCL	C1C-NC-C4C	-4.65	104.62	106.71
9	U	101	BCL	C1C-NC-C4C	-4.65	104.62	106.71
9	L	1001	BCL	OBB-CAB-CBB	-4.65	109.71	120.17
9	N	102	BCL	C1C-NC-C4C	-4.64	104.62	106.71
10	9	101	KGD	CBG-CBI-CBL	-4.64	120.68	127.31
10	Q	103	KGD	CBG-CBI-CBL	-4.64	120.69	127.31
10	B	102	KGD	CBG-CBI-CBL	-4.64	120.69	127.31
10	0	103	KGD	CBG-CBB-CAV	-4.63	113.99	123.47
9	J	102	BCL	C1C-NC-C4C	-4.63	104.63	106.71
10	W	101	KGD	CAP-CAO-CAM	-4.63	120.71	127.31
10	4	103	KGD	CAP-CAO-CAM	-4.62	120.71	127.31
9	6	101	BCL	C1C-NC-C4C	-4.62	104.63	106.71
9	A	102	BCL	C1C-NC-C4C	-4.61	104.63	106.71
9	Q	101	BCL	C1C-NC-C4C	-4.61	104.63	106.71
9	L	1002	BCL	O2D-CGD-CBD	4.61	119.46	111.27
9	4	101	BCL	C1C-NC-C4C	-4.61	104.63	106.71
10	T	102	KGD	CAE-CAI-CAH	-4.60	114.41	118.65
9	4	101	BCL	CAC-C3C-C2C	-4.59	102.78	114.26
9	U	101	BCL	CAC-C3C-C2C	-4.59	102.78	114.26
9	N	102	BCL	CAC-C3C-C2C	-4.59	102.79	114.26
10	A	103	KGD	CBG-CBI-CBL	-4.59	120.76	127.31
9	8	101	BCL	C1C-NC-C4C	-4.59	104.64	106.71
9	D	102	BCL	CAC-C3C-C2C	-4.59	102.80	114.26
9	2	102	BCL	CAC-C3C-C2C	-4.59	102.80	114.26
9	H	102	BCL	CAC-C3C-C2C	-4.59	102.80	114.26
15	C	402	HEM	C4D-ND-C1D	4.59	109.81	105.07
9	Q	101	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
9	A	102	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
9	0	101	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
9	W	102	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
9	J	102	BCL	CAC-C3C-C2C	-4.58	102.82	114.26
9	S	102	BCL	CAC-C3C-C2C	-4.58	102.82	114.26
10	8	103	KGD	CBB-CAV-CAR	-4.57	120.78	127.31
9	6	101	BCL	CAC-C3C-C2C	-4.57	102.84	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	T	102	KGD	CBB-CAV-CAR	-4.57	120.79	127.31
9	8	101	BCL	CAC-C3C-C2C	-4.57	102.84	114.26
9	F	102	BCL	CAC-C3C-C2C	-4.56	102.86	114.26
10	Q	103	KGD	CBF-CBH-CBJ	-4.56	111.95	118.94
9	S	102	BCL	C1C-NC-C4C	-4.56	104.66	106.71
10	2	101	KGD	CAE-CAI-CAH	-4.54	114.46	118.65
9	L	1002	BCL	CAC-C3C-C2C	-4.54	102.91	114.26
10	9	101	KGD	CAJ-CAL-CAM	-4.53	119.39	126.23
10	O	102	KGD	CBG-CBI-CBL	-4.53	120.85	127.31
10	6	103	KGD	CAJ-CAL-CAM	-4.52	119.40	126.23
10	0	103	KGD	CBG-CBI-CBL	-4.49	120.91	127.31
10	3	102	KGD	CBG-CBI-CBL	-4.47	120.94	127.31
9	L	1001	BCL	C1D-ND-C4D	-4.46	103.17	106.33
11	L	1003	BPH	O2D-CGD-CBD	4.44	116.62	111.00
9	L	1002	BCL	C4A-NA-C1A	-4.40	104.73	106.71
15	C	404	HEM	CBA-CAA-C2A	-4.40	105.11	112.62
9	A	101	BCL	C1C-NC-C4C	-4.38	104.74	106.71
10	2	101	KGD	CBG-CBI-CBL	-4.37	121.07	127.31
15	C	402	HEM	CBA-CAA-C2A	-4.37	105.17	112.62
9	1	101	BCL	C1C-NC-C4C	-4.36	104.75	106.71
9	J	101	BCL	C1C-NC-C4C	-4.36	104.75	106.71
9	0	102	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
9	8	102	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
9	W	103	BCL	CMB-C2B-C1B	-4.35	121.77	128.46
10	S	104	KGD	CAJ-CAL-CAM	-4.35	119.66	126.23
9	Q	102	BCL	CMB-C2B-C1B	-4.35	121.78	128.46
9	T	101	BCL	C1C-NC-C4C	-4.34	104.75	106.71
9	B	101	BCL	CMB-C2B-C1B	-4.34	121.79	128.46
9	6	102	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
10	A	104	KGD	CBB-CAV-CAR	-4.34	121.12	127.31
9	K	101	BCL	CMB-C2B-C1B	-4.34	121.80	128.46
10	J	103	KGD	CBB-CAV-CAR	-4.33	121.13	127.31
9	G	101	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
9	D	101	BCL	C1C-NC-C4C	-4.33	104.76	106.71
10	T	102	KGD	CBG-CBI-CBL	-4.33	121.13	127.31
9	E	101	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
9	U	102	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
9	4	102	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
9	S	103	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
9	I	101	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
9	O	101	BCL	CMB-C2B-C1B	-4.31	121.83	128.46
9	2	103	BCL	CMB-C2B-C1B	-4.31	121.84	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	3	101	BCL	C1C-NC-C4C	-4.31	104.77	106.71
9	7	101	BCL	C1C-NC-C4C	-4.31	104.77	106.71
9	R	101	BCL	C1C-NC-C4C	-4.30	104.77	106.71
9	M	703	BCL	CAC-C3C-C2C	-4.30	103.51	114.26
9	F	101	BCL	C1C-NC-C4C	-4.30	104.77	106.71
9	L	1002	BCL	C2A-C3A-C4A	-4.29	94.94	101.87
10	H	103	KGD	CAP-CAO-CAM	-4.27	121.22	127.31
9	5	101	BCL	C1C-NC-C4C	-4.25	104.80	106.71
9	N	101	BCL	C1C-NC-C4C	-4.23	104.80	106.71
10	4	103	KGD	CBG-CBI-CBL	-4.18	121.35	127.31
10	E	102	KGD	CBG-CBI-CBL	-4.17	121.35	127.31
10	A	104	KGD	CBG-CBB-CAV	-4.17	114.93	123.47
9	H	101	BCL	C1C-NC-C4C	-4.16	104.83	106.71
9	P	101	BCL	C1C-NC-C4C	-4.16	104.83	106.71
9	9	102	BCL	C1C-NC-C4C	-4.16	104.84	106.71
10	4	103	KGD	CAE-CAI-CAH	-4.16	114.82	118.65
9	X	101	BCL	C1C-NC-C4C	-4.16	104.84	106.71
10	8	103	KGD	CBG-CBI-CBL	-4.15	121.38	127.31
10	B	102	KGD	CAP-CAO-CAM	-4.15	121.39	127.31
10	9	101	KGD	CBF-CBH-CBJ	-4.14	112.59	118.94
10	K	102	KGD	CBG-CBI-CBL	-4.13	121.42	127.31
10	9	101	KGD	CBB-CAV-CAR	-4.13	121.42	127.31
10	A	104	KGD	CBG-CBI-CBL	-4.12	121.42	127.31
9	4	101	BCL	CHD-C1D-ND	-4.11	120.68	124.45
9	2	102	BCL	CHD-C1D-ND	-4.11	120.68	124.45
10	I	102	KGD	CAJ-CAL-CAM	-4.10	120.05	126.23
9	D	102	BCL	CHD-C1D-ND	-4.10	120.69	124.45
9	6	101	BCL	CHD-C1D-ND	-4.09	120.70	124.45
9	K	101	BCL	CHD-C1D-ND	-4.08	120.70	124.45
9	S	102	BCL	CHD-C1D-ND	-4.08	120.70	124.45
9	L	1002	BCL	CHD-C1D-ND	-4.08	120.71	124.45
9	Q	101	BCL	CHD-C1D-ND	-4.07	120.71	124.45
9	F	102	BCL	CHD-C1D-ND	-4.07	120.72	124.45
9	L	1001	BCL	CHA-C1A-NA	-4.06	117.09	126.40
9	H	102	BCL	CHD-C1D-ND	-4.06	120.72	124.45
9	M	703	BCL	CMB-C2B-C3B	4.06	132.28	124.68
9	0	101	BCL	CHD-C1D-ND	-4.06	120.72	124.45
9	L	1001	BCL	O2D-CGD-CBD	4.06	118.48	111.27
9	G	101	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	E	101	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	S	103	BCL	CHD-C1D-ND	-4.05	120.73	124.45
9	8	102	BCL	CHD-C1D-ND	-4.05	120.73	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	102	BCL	CHD-C1D-ND	-4.04	120.74	124.45
9	J	102	BCL	CHD-C1D-ND	-4.04	120.74	124.45
9	4	102	BCL	CHD-C1D-ND	-4.04	120.74	124.45
9	U	101	BCL	CHD-C1D-ND	-4.04	120.74	124.45
9	W	103	BCL	CHD-C1D-ND	-4.03	120.75	124.45
9	B	101	BCL	CHD-C1D-ND	-4.03	120.75	124.45
9	8	101	BCL	CHD-C1D-ND	-4.02	120.76	124.45
9	O	101	BCL	CHD-C1D-ND	-4.01	120.77	124.45
9	W	102	BCL	CHD-C1D-ND	-4.01	120.77	124.45
9	Q	102	BCL	CHD-C1D-ND	-4.01	120.77	124.45
9	U	102	BCL	CHD-C1D-ND	-4.01	120.77	124.45
10	K	102	KGD	CAP-CAO-CAM	-4.00	121.60	127.31
9	2	103	BCL	CHD-C1D-ND	-4.00	120.78	124.45
9	N	102	BCL	CHD-C1D-ND	-4.00	120.78	124.45
9	I	101	BCL	CHD-C1D-ND	-4.00	120.78	124.45
9	M	703	BCL	OBB-CAB-CBB	-3.99	111.19	120.17
10	5	102	KGD	CAP-CAO-CAM	-3.99	121.62	127.31
10	C	401	KGD	CBM-CBN-CBL	-3.98	115.22	126.42
9	6	102	BCL	CHD-C1D-ND	-3.98	120.80	124.45
9	0	102	BCL	CHD-C1D-ND	-3.98	120.80	124.45
10	5	102	KGD	CBG-CBI-CBL	-3.97	121.64	127.31
10	N	103	KGD	CAJ-CAL-CAM	-3.97	120.23	126.23
9	M	703	BCL	CHD-C1D-ND	-3.95	120.83	124.45
10	K	102	KGD	CBF-CBH-CBJ	-3.92	112.92	118.94
10	T	102	KGD	CAP-CAO-CAM	-3.92	121.72	127.31
10	W	101	KGD	CBB-CAV-CAR	-3.92	121.72	127.31
9	F	101	BCL	CHD-C1D-ND	-3.90	120.87	124.45
9	J	101	BCL	CHD-C1D-ND	-3.90	120.87	124.45
10	6	103	KGD	CAE-CAI-CAH	-3.90	115.06	118.65
9	U	101	BCL	OBB-CAB-CBB	-3.90	111.40	120.17
10	0	103	KGD	CAP-CAO-CAM	-3.89	121.75	127.31
9	F	102	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	7	101	BCL	CHD-C1D-ND	-3.89	120.88	124.45
9	E	101	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	H	102	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	I	101	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	8	101	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
9	N	102	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	W	103	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	6	101	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	U	102	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
9	2	102	BCL	OBB-CAB-CBB	-3.88	111.44	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	4	101	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
9	Q	102	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
9	S	103	BCL	OBB-CAB-CBB	-3.88	111.44	120.17
9	T	101	BCL	CHD-C1D-ND	-3.88	120.89	124.45
9	Q	101	BCL	OBB-CAB-CBB	-3.88	111.45	120.17
9	A	102	BCL	OBB-CAB-CBB	-3.87	111.45	120.17
9	D	102	BCL	OBB-CAB-CBB	-3.87	111.45	120.17
9	J	102	BCL	OBB-CAB-CBB	-3.87	111.45	120.17
9	6	102	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	0	102	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	2	103	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	G	101	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	W	102	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
9	4	102	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
9	S	102	BCL	OBB-CAB-CBB	-3.87	111.47	120.17
9	B	101	BCL	OBB-CAB-CBB	-3.86	111.47	120.17
9	O	101	BCL	OBB-CAB-CBB	-3.86	111.48	120.17
9	N	101	BCL	CHD-C1D-ND	-3.86	120.91	124.45
9	8	102	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
9	H	101	BCL	CHD-C1D-ND	-3.85	120.91	124.45
9	0	101	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
9	5	101	BCL	CHD-C1D-ND	-3.85	120.92	124.45
10	P	102	KGD	CBG-CBI-CBL	-3.85	121.82	127.31
9	5	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
9	K	101	BCL	OBB-CAB-CBB	-3.85	111.51	120.17
9	R	101	BCL	OBB-CAB-CBB	-3.84	111.52	120.17
9	A	101	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
9	X	101	BCL	OBB-CAB-CBB	-3.84	111.53	120.17
9	A	101	BCL	CHD-C1D-ND	-3.84	120.93	124.45
9	1	101	BCL	CHD-C1D-ND	-3.83	120.93	124.45
9	9	102	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
10	N	103	KGD	CBB-CAV-CAR	-3.83	121.84	127.31
9	F	101	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
9	H	101	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
9	J	101	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
9	D	101	BCL	OBB-CAB-CBB	-3.83	111.55	120.17
9	7	101	BCL	OBB-CAB-CBB	-3.83	111.56	120.17
9	3	101	BCL	CHD-C1D-ND	-3.83	120.94	124.45
10	Q	103	KGD	CAE-CAI-CAH	-3.83	115.12	118.65
9	R	101	BCL	CHD-C1D-ND	-3.82	120.94	124.45
9	3	101	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
9	1	101	BCL	OBB-CAB-CBB	-3.82	111.57	120.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	101	BCL	OBB-CAB-CBB	-3.82	111.57	120.17
9	P	101	BCL	CHD-C1D-ND	-3.82	120.94	124.45
10	2	104	KGD	CBB-CAV-CAR	-3.82	121.86	127.31
9	N	101	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
9	T	101	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
9	X	101	BCL	CHD-C1D-ND	-3.81	120.95	124.45
9	D	101	BCL	CHD-C1D-ND	-3.80	120.96	124.45
9	9	102	BCL	CHD-C1D-ND	-3.79	120.97	124.45
10	F	103	KGD	CBM-CBJ-CBH	-3.79	121.90	127.31
10	K	102	KGD	CAL-CAJ-CAD	-3.79	116.57	127.20
10	T	102	KGD	CBG-CBB-CAV	-3.78	115.73	123.47
10	U	103	KGD	CAP-CAO-CAM	-3.77	121.92	127.31
10	0	103	KGD	CAL-CAJ-CAD	-3.77	116.62	127.20
10	F	103	KGD	CBG-CBI-CBL	-3.76	121.94	127.31
10	6	103	KGD	CBF-CBH-CBJ	-3.75	113.18	118.94
10	2	104	KGD	CBF-CBH-CBJ	-3.75	113.19	118.94
10	B	102	KGD	CBB-CAV-CAR	-3.75	121.96	127.31
10	3	102	KGD	CAP-CAO-CAM	-3.75	121.97	127.31
10	W	101	KGD	CAE-CAI-CAH	-3.73	115.21	118.65
11	L	1005	BPH	CMD-C2D-C3D	3.73	131.65	124.68
10	6	103	KGD	CAP-CAO-CAM	-3.71	122.02	127.31
9	L	1001	BCL	C16-C15-C13	-3.70	103.97	115.92
10	H	103	KGD	CBB-CAV-CAR	-3.69	122.04	127.31
10	P	102	KGD	CBF-CBH-CBJ	-3.69	113.28	118.94
10	O	102	KGD	CAJ-CAL-CAM	-3.68	120.67	126.23
10	3	102	KGD	CAJ-CAL-CAM	-3.68	120.67	126.23
11	M	704	BPH	CMD-C2D-C3D	3.68	131.57	124.68
10	A	104	KGD	CAJ-CAL-CAM	-3.67	120.69	126.23
10	F	103	KGD	CBG-CBB-CAV	-3.67	115.96	123.47
10	8	103	KGD	CBB-CBG-CBI	-3.66	115.98	123.47
10	T	102	KGD	CBF-CBH-CBJ	-3.65	113.34	118.94
10	A	104	KGD	CAP-CAO-CAM	-3.65	122.10	127.31
10	5	102	KGD	CBB-CAV-CAR	-3.64	122.11	127.31
10	B	102	KGD	CBG-CBB-CAV	-3.64	116.01	123.47
9	M	703	BCL	C4D-CHA-C1A	3.64	125.67	121.25
10	K	102	KGD	CAE-CAI-CAH	-3.63	115.30	118.65
10	S	101	KGD	CAJ-CAL-CAM	-3.62	120.76	126.23
11	L	1003	BPH	CMB-C2B-C3B	3.62	131.46	124.68
10	A	104	KGD	CAE-CAI-CAH	-3.62	115.31	118.65
9	L	1001	BCL	C2D-C1D-ND	3.61	112.77	110.10
10	J	103	KGD	CAJ-CAL-CAM	-3.60	120.79	126.23
10	S	104	KGD	CBG-CBI-CBL	-3.60	122.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	704	BPH	O2D-CGD-CBD	3.60	115.56	111.00
9	5	101	BCL	CMB-C2B-C3B	3.60	131.41	124.68
9	R	101	BCL	CMB-C2B-C3B	3.60	131.41	124.68
9	P	101	BCL	CMB-C2B-C3B	3.59	131.40	124.68
9	1	101	BCL	CMB-C2B-C3B	3.59	131.40	124.68
10	9	101	KGD	CAL-CAJ-CAD	-3.59	117.12	127.20
9	L	1002	BCL	CHA-C1A-NA	-3.59	118.18	126.40
9	F	101	BCL	CMB-C2B-C3B	3.58	131.38	124.68
9	L	1002	BCL	C16-C15-C13	-3.58	104.34	115.92
9	3	101	BCL	CMB-C2B-C3B	3.58	131.38	124.68
9	D	101	BCL	CMB-C2B-C3B	3.58	131.38	124.68
9	X	101	BCL	CMB-C2B-C3B	3.58	131.38	124.68
9	N	101	BCL	CMB-C2B-C3B	3.58	131.37	124.68
9	A	101	BCL	CMB-C2B-C3B	3.58	131.37	124.68
9	J	101	BCL	CMB-C2B-C3B	3.58	131.37	124.68
9	T	101	BCL	CMB-C2B-C3B	3.57	131.36	124.68
9	7	101	BCL	CMB-C2B-C3B	3.57	131.35	124.68
9	L	1001	BCL	O2A-CGA-O1A	-3.57	114.59	123.59
9	9	102	BCL	CMB-C2B-C3B	3.56	131.34	124.68
9	U	101	BCL	C16-C15-C13	-3.56	104.41	115.92
9	H	102	BCL	C16-C15-C13	-3.56	104.42	115.92
9	N	102	BCL	C16-C15-C13	-3.56	104.42	115.92
9	H	101	BCL	CMB-C2B-C3B	3.56	131.33	124.68
9	0	101	BCL	C16-C15-C13	-3.55	104.45	115.92
9	Q	101	BCL	C16-C15-C13	-3.55	104.45	115.92
9	2	102	BCL	C16-C15-C13	-3.55	104.45	115.92
9	6	101	BCL	C16-C15-C13	-3.55	104.45	115.92
9	D	102	BCL	C16-C15-C13	-3.55	104.46	115.92
9	J	102	BCL	C16-C15-C13	-3.54	104.46	115.92
9	8	101	BCL	C16-C15-C13	-3.54	104.47	115.92
9	A	102	BCL	C16-C15-C13	-3.54	104.47	115.92
9	4	101	BCL	C16-C15-C13	-3.54	104.47	115.92
10	S	101	KGD	CAP-CAO-CAM	-3.54	122.26	127.31
9	S	102	BCL	C16-C15-C13	-3.53	104.50	115.92
9	F	102	BCL	C16-C15-C13	-3.53	104.50	115.92
10	I	102	KGD	CBB-CAV-CAR	-3.53	122.27	127.31
10	2	101	KGD	CBM-CBJ-CBH	-3.52	122.28	127.31
15	C	404	HEM	C4B-CHC-C1C	-3.52	117.91	122.56
10	0	104	KGD	CAJ-CAL-CAM	-3.52	120.92	126.23
9	L	1002	BCL	C2A-C1A-CHA	3.50	129.98	123.86
10	B	102	KGD	CAJ-CAL-CAM	-3.50	120.95	126.23
10	G	102	KGD	CAL-CAJ-CAD	-3.50	117.38	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	103	KGD	CAP-CAO-CAM	-3.49	122.33	127.31
9	L	1002	BCL	C7-C6-C5	-3.47	103.92	113.36
10	C	401	KGD	CAJ-CAL-CAM	-3.47	120.99	126.23
10	H	103	KGD	CBF-CBH-CBJ	-3.47	113.62	118.94
11	L	1003	BPH	CMD-C2D-C3D	3.47	131.16	124.68
9	X	101	BCL	O2A-CGA-O1A	-3.46	114.85	123.59
9	4	101	BCL	CMB-C2B-C3B	3.46	131.15	124.68
12	M	705	MQE	CAY-CAX-CBQ	-3.46	114.80	118.50
9	0	101	BCL	CMB-C2B-C3B	3.45	131.14	124.68
10	0	104	KGD	CAL-CAJ-CAD	-3.45	117.50	127.20
9	F	102	BCL	CMB-C2B-C3B	3.45	131.13	124.68
9	6	101	BCL	CMB-C2B-C3B	3.45	131.13	124.68
9	A	102	BCL	CMB-C2B-C3B	3.45	131.13	124.68
9	W	102	BCL	C16-C15-C13	-3.45	104.78	115.92
10	E	102	KGD	CBB-CAV-CAR	-3.45	122.39	127.31
10	0	104	KGD	CAP-CAO-CAM	-3.44	122.39	127.31
9	H	102	BCL	CMB-C2B-C3B	3.44	131.12	124.68
9	W	102	BCL	CMB-C2B-C3B	3.44	131.12	124.68
10	N	103	KGD	CBF-CBH-CBJ	-3.44	113.66	118.94
9	N	102	BCL	CMB-C2B-C3B	3.44	131.11	124.68
10	Q	103	KGD	CAZ-CAW-CAS	3.44	121.05	115.27
9	U	101	BCL	CMB-C2B-C3B	3.44	131.11	124.68
9	2	102	BCL	CMB-C2B-C3B	3.44	131.11	124.68
10	2	104	KGD	CAJ-CAL-CAM	-3.44	121.04	126.23
9	J	102	BCL	CMB-C2B-C3B	3.43	131.10	124.68
9	8	101	BCL	CMB-C2B-C3B	3.42	131.08	124.68
9	K	101	BCL	C4D-CHA-C1A	3.42	125.41	121.25
9	D	102	BCL	CMB-C2B-C3B	3.42	131.07	124.68
9	Q	101	BCL	CMB-C2B-C3B	3.42	131.07	124.68
15	C	403	HEM	CHB-C1B-C2B	-3.41	117.28	126.72
9	U	102	BCL	C4D-CHA-C1A	3.41	125.39	121.25
9	W	103	BCL	C4D-CHA-C1A	3.40	125.39	121.25
9	8	102	BCL	C4D-CHA-C1A	3.40	125.39	121.25
10	A	103	KGD	CAJ-CAL-CAM	-3.40	121.10	126.23
9	G	101	BCL	C4D-CHA-C1A	3.40	125.39	121.25
9	Q	102	BCL	C4D-CHA-C1A	3.40	125.38	121.25
9	S	102	BCL	CMB-C2B-C3B	3.40	131.03	124.68
15	C	402	HEM	CHB-C1B-C2B	-3.39	117.34	126.72
9	I	101	BCL	C4D-CHA-C1A	3.39	125.37	121.25
9	4	102	BCL	C4D-CHA-C1A	3.38	125.37	121.25
9	W	102	BCL	C7-C6-C5	-3.38	104.18	113.36
9	L	1001	BCL	C2A-C3A-C4A	-3.38	96.41	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	103	BCL	C4D-CHA-C1A	3.38	125.36	121.25
9	0	102	BCL	C4D-CHA-C1A	3.38	125.36	121.25
9	F	102	BCL	C7-C6-C5	-3.37	104.19	113.36
9	J	101	BCL	O2A-CGA-O1A	-3.37	115.08	123.59
9	H	101	BCL	O2A-CGA-O1A	-3.37	115.08	123.59
9	2	103	BCL	C4D-CHA-C1A	3.37	125.35	121.25
9	E	101	BCL	C4D-CHA-C1A	3.37	125.35	121.25
9	6	102	BCL	C4D-CHA-C1A	3.37	125.35	121.25
9	R	101	BCL	O2A-CGA-O1A	-3.37	115.10	123.59
9	B	101	BCL	C4D-CHA-C1A	3.36	125.34	121.25
9	J	102	BCL	C7-C6-C5	-3.36	104.23	113.36
9	4	101	BCL	C7-C6-C5	-3.36	104.23	113.36
9	N	101	BCL	O2A-CGA-O1A	-3.36	115.11	123.59
10	0	103	KGD	CAJ-CAL-CAM	-3.36	121.16	126.23
9	T	101	BCL	O2A-CGA-O1A	-3.36	115.12	123.59
9	O	101	BCL	C4D-CHA-C1A	3.36	125.34	121.25
9	U	101	BCL	C7-C6-C5	-3.36	104.24	113.36
9	5	101	BCL	O2A-CGA-O1A	-3.36	115.12	123.59
9	P	101	BCL	O2A-CGA-O1A	-3.36	115.12	123.59
9	D	102	BCL	C7-C6-C5	-3.36	104.25	113.36
9	N	102	BCL	C7-C6-C5	-3.35	104.25	113.36
9	F	101	BCL	O2A-CGA-O1A	-3.35	115.13	123.59
9	1	101	BCL	O2A-CGA-O1A	-3.35	115.13	123.59
9	D	101	BCL	O2A-CGA-O1A	-3.35	115.13	123.59
9	9	102	BCL	O2A-CGA-O1A	-3.35	115.13	123.59
9	S	102	BCL	C7-C6-C5	-3.35	104.26	113.36
10	U	103	KGD	CBG-CBI-CBL	-3.35	122.53	127.31
10	P	102	KGD	CAE-CAC-CAB	-3.35	107.80	113.18
9	A	102	BCL	C7-C6-C5	-3.35	104.26	113.36
9	0	101	BCL	C7-C6-C5	-3.35	104.26	113.36
9	2	102	BCL	C7-C6-C5	-3.35	104.27	113.36
9	A	101	BCL	O2A-CGA-O1A	-3.34	115.15	123.59
9	8	101	BCL	C7-C6-C5	-3.34	104.28	113.36
9	H	102	BCL	C7-C6-C5	-3.34	104.28	113.36
10	B	102	KGD	CAZ-CAW-CAS	3.34	120.89	115.27
9	3	101	BCL	O2A-CGA-O1A	-3.34	115.16	123.59
9	6	101	BCL	C7-C6-C5	-3.34	104.28	113.36
9	7	101	BCL	O2A-CGA-O1A	-3.34	115.16	123.59
9	Q	101	BCL	C7-C6-C5	-3.34	104.29	113.36
10	3	102	KGD	CAE-CAI-CAH	-3.34	115.58	118.65
9	P	101	BCL	C4D-CHA-C1A	3.34	125.31	121.25
10	8	103	KGD	CBM-CBJ-CBH	-3.33	122.56	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	101	BCL	C4D-CHA-C1A	3.32	125.29	121.25
10	F	103	KGD	CAL-CAJ-CAD	-3.32	117.88	127.20
10	K	102	KGD	CAZ-CAW-CAS	3.32	120.86	115.27
10	W	101	KGD	CAL-CAJ-CAD	-3.32	117.89	127.20
10	9	101	KGD	CBK-CBH-CBF	3.32	123.30	118.08
10	5	102	KGD	CBG-CBB-CAV	-3.31	116.69	123.47
10	S	104	KGD	CAL-CAJ-CAD	-3.31	117.91	127.20
9	2	103	BCL	C4B-CHC-C1C	-3.31	123.56	130.12
10	P	102	KGD	CAE-CAI-CAH	-3.31	115.60	118.65
9	9	102	BCL	C4D-CHA-C1A	3.31	125.27	121.25
9	H	101	BCL	C4D-CHA-C1A	3.31	125.27	121.25
10	I	102	KGD	CAL-CAJ-CAD	-3.30	117.92	127.20
9	4	102	BCL	C4B-CHC-C1C	-3.30	123.58	130.12
9	3	101	BCL	C4D-CHA-C1A	3.30	125.26	121.25
9	O	101	BCL	C4B-CHC-C1C	-3.29	123.59	130.12
9	S	103	BCL	C4B-CHC-C1C	-3.29	123.60	130.12
9	Q	102	BCL	C16-C15-C13	-3.29	105.28	115.92
9	U	102	BCL	C4B-CHC-C1C	-3.29	123.60	130.12
10	6	103	KGD	CBB-CBG-CBI	-3.29	116.73	123.47
9	L	1001	BCL	CHB-C4A-NA	-3.29	119.96	124.51
9	I	101	BCL	C4B-CHC-C1C	-3.29	123.60	130.12
9	K	101	BCL	C4B-CHC-C1C	-3.29	123.61	130.12
9	W	103	BCL	C4B-CHC-C1C	-3.29	123.61	130.12
9	X	101	BCL	C4D-CHA-C1A	3.29	125.25	121.25
9	4	102	BCL	C16-C15-C13	-3.29	105.30	115.92
9	O	101	BCL	C16-C15-C13	-3.28	105.30	115.92
9	A	101	BCL	C4D-CHA-C1A	3.28	125.25	121.25
9	B	101	BCL	C16-C15-C13	-3.28	105.31	115.92
9	8	102	BCL	C16-C15-C13	-3.28	105.31	115.92
9	T	101	BCL	C4D-CHA-C1A	3.28	125.24	121.25
9	G	101	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
9	G	101	BCL	C16-C15-C13	-3.28	105.31	115.92
10	S	101	KGD	CBB-CAV-CAR	-3.28	122.63	127.31
9	W	103	BCL	C16-C15-C13	-3.28	105.32	115.92
9	6	102	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
9	1	101	BCL	C11-C10-C8	-3.28	105.32	115.92
9	U	102	BCL	C16-C15-C13	-3.28	105.32	115.92
9	K	101	BCL	C16-C15-C13	-3.28	105.32	115.92
9	0	102	BCL	C16-C15-C13	-3.28	105.33	115.92
9	0	102	BCL	C4B-CHC-C1C	-3.28	123.63	130.12
9	S	103	BCL	C16-C15-C13	-3.28	105.33	115.92
9	E	101	BCL	C16-C15-C13	-3.28	105.33	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	701	MQE	CBA-CBN-CBM	-3.27	119.78	127.66
9	5	101	BCL	C4D-CHA-C1A	3.27	125.23	121.25
9	F	101	BCL	C4D-CHA-C1A	3.27	125.23	121.25
9	6	102	BCL	C16-C15-C13	-3.27	105.35	115.92
9	D	101	BCL	C4D-CHA-C1A	3.27	125.23	121.25
9	E	101	BCL	C4B-CHC-C1C	-3.27	123.64	130.12
9	8	102	BCL	C4B-CHC-C1C	-3.27	123.64	130.12
9	Q	102	BCL	C4B-CHC-C1C	-3.27	123.65	130.12
9	N	101	BCL	C11-C10-C8	-3.27	105.36	115.92
9	I	101	BCL	C16-C15-C13	-3.27	105.36	115.92
9	1	101	BCL	C4D-CHA-C1A	3.26	125.22	121.25
9	H	101	BCL	C11-C10-C8	-3.26	105.37	115.92
9	2	103	BCL	C16-C15-C13	-3.26	105.37	115.92
9	J	101	BCL	C4D-CHA-C1A	3.26	125.22	121.25
9	R	101	BCL	C11-C10-C8	-3.26	105.38	115.92
9	J	101	BCL	C11-C10-C8	-3.26	105.38	115.92
9	9	102	BCL	C11-C10-C8	-3.26	105.38	115.92
9	W	102	BCL	C11-C10-C8	-3.26	105.38	115.92
9	T	101	BCL	C11-C10-C8	-3.26	105.39	115.92
9	F	101	BCL	C11-C10-C8	-3.26	105.39	115.92
10	S	101	KGD	CAE-CAC-CAB	-3.26	107.95	113.18
10	F	103	KGD	CAE-CAI-CAH	-3.26	115.65	118.65
9	D	101	BCL	C11-C10-C8	-3.26	105.40	115.92
9	7	101	BCL	C11-C10-C8	-3.25	105.40	115.92
9	3	101	BCL	C11-C10-C8	-3.25	105.41	115.92
9	P	101	BCL	C11-C10-C8	-3.25	105.41	115.92
9	5	101	BCL	C11-C10-C8	-3.25	105.41	115.92
9	A	101	BCL	C11-C10-C8	-3.25	105.41	115.92
9	B	101	BCL	C4B-CHC-C1C	-3.25	123.68	130.12
10	0	104	KGD	CAE-CAI-CAH	-3.25	115.66	118.65
9	N	101	BCL	C4D-CHA-C1A	3.25	125.20	121.25
9	7	101	BCL	C4D-CHA-C1A	3.25	125.20	121.25
9	L	1002	BCL	CMC-C2C-C3C	-3.24	100.75	113.83
12	M	701	MQE	CAO-CBI-CAZ	-3.24	119.86	127.66
9	H	102	BCL	C4B-CHC-C1C	-3.23	123.72	130.12
9	A	102	BCL	C4B-CHC-C1C	-3.23	123.73	130.12
9	N	102	BCL	C4B-CHC-C1C	-3.22	123.74	130.12
10	9	101	KGD	CBG-CBB-CAV	-3.22	116.89	123.47
9	A	102	BCL	C4D-CHA-C1A	3.21	125.16	121.25
10	S	104	KGD	CBF-CBH-CBJ	-3.21	114.01	118.94
9	8	101	BCL	C4B-CHC-C1C	-3.21	123.76	130.12
9	Q	101	BCL	C4B-CHC-C1C	-3.21	123.76	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	404	HEM	CHC-C4B-C3B	-3.21	119.66	124.57
9	7	101	BCL	C7-C6-C5	-3.21	104.65	113.36
9	S	102	BCL	C4B-CHC-C1C	-3.20	123.77	130.12
10	J	103	KGD	CAC-CAB-CAD	-3.20	105.55	110.48
9	X	101	BCL	C16-C15-C13	-3.20	105.57	115.92
9	U	101	BCL	C4B-CHC-C1C	-3.20	123.78	130.12
11	L	1005	BPH	O2D-CGD-CBD	3.20	115.05	111.00
9	W	102	BCL	C4B-CHC-C1C	-3.20	123.78	130.12
9	8	101	BCL	C4D-CHA-C1A	3.20	125.14	121.25
9	3	101	BCL	C7-C6-C5	-3.20	104.68	113.36
9	J	101	BCL	C7-C6-C5	-3.19	104.68	113.36
9	N	101	BCL	C7-C6-C5	-3.19	104.68	113.36
9	0	101	BCL	C4B-CHC-C1C	-3.19	123.79	130.12
9	W	102	BCL	C4D-CHA-C1A	3.19	125.14	121.25
9	F	101	BCL	C7-C6-C5	-3.19	104.69	113.36
10	E	102	KGD	CBF-CBH-CBJ	-3.19	114.04	118.94
9	F	102	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
9	4	101	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
9	4	101	BCL	C4D-CHA-C1A	3.19	125.13	121.25
9	6	101	BCL	C4D-CHA-C1A	3.19	125.13	121.25
10	N	103	KGD	CAL-CAJ-CAD	-3.19	118.24	127.20
10	I	102	KGD	CBG-CBI-CBL	-3.19	122.76	127.31
9	F	102	BCL	C4D-CHA-C1A	3.19	125.13	121.25
10	A	103	KGD	CAL-CAJ-CAD	-3.19	118.25	127.20
9	D	101	BCL	C7-C6-C5	-3.19	104.70	113.36
10	2	104	KGD	CBG-CBB-CAV	-3.19	116.94	123.47
9	2	102	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
9	5	101	BCL	C7-C6-C5	-3.19	104.70	113.36
9	9	102	BCL	C7-C6-C5	-3.19	104.70	113.36
9	A	101	BCL	C7-C6-C5	-3.19	104.71	113.36
9	P	101	BCL	C7-C6-C5	-3.18	104.71	113.36
12	M	701	MQE	CAJ-CBC-CAP	-3.18	119.99	127.66
10	B	102	KGD	CAE-CAI-CAH	-3.18	115.72	118.65
9	J	102	BCL	C4B-CHC-C1C	-3.18	123.81	130.12
9	H	102	BCL	C4D-CHA-C1A	3.18	125.12	121.25
9	S	102	BCL	C4D-CHA-C1A	3.18	125.12	121.25
9	X	101	BCL	C7-C6-C5	-3.18	104.72	113.36
9	6	101	BCL	C4B-CHC-C1C	-3.18	123.82	130.12
9	Q	101	BCL	C4D-CHA-C1A	3.18	125.12	121.25
9	T	101	BCL	C7-C6-C5	-3.18	104.72	113.36
9	R	101	BCL	C7-C6-C5	-3.18	104.72	113.36
10	9	101	KGD	CAP-CAO-CAM	-3.18	122.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	9	101	KGD	CAE-CAI-CAH	-3.18	115.72	118.65
9	1	101	BCL	C7-C6-C5	-3.18	104.73	113.36
9	D	102	BCL	C4B-CHC-C1C	-3.17	123.83	130.12
9	N	102	BCL	C4D-CHA-C1A	3.17	125.11	121.25
9	2	102	BCL	C4D-CHA-C1A	3.17	125.11	121.25
9	L	1001	BCL	C7-C6-C5	-3.17	104.75	113.36
9	H	101	BCL	C7-C6-C5	-3.17	104.75	113.36
11	L	1003	BPH	O2D-CGD-O1D	-3.17	117.64	123.84
9	D	102	BCL	C4D-CHA-C1A	3.17	125.10	121.25
12	M	701	MQE	CAL-CBF-CAV	-3.16	120.05	127.66
9	0	101	BCL	C4D-CHA-C1A	3.16	125.09	121.25
10	2	104	KGD	CBJ-CBM-CBN	-3.15	113.38	123.22
9	J	102	BCL	C4D-CHA-C1A	3.15	125.08	121.25
9	U	101	BCL	C4D-CHA-C1A	3.15	125.08	121.25
9	X	101	BCL	C11-C10-C8	-3.14	105.77	115.92
15	C	402	HEM	CAD-CBD-CGD	-3.13	106.86	113.60
10	8	103	KGD	CAJ-CAL-CAM	-3.13	121.50	126.23
9	W	103	BCL	CHA-C1A-NA	-3.13	119.23	126.40
10	B	102	KGD	CAL-CAJ-CAD	-3.13	118.42	127.20
9	K	101	BCL	CHA-C1A-NA	-3.13	119.24	126.40
11	L	1003	BPH	CAA-CBA-CGA	-3.12	104.13	113.25
9	Q	102	BCL	CHA-C1A-NA	-3.12	119.26	126.40
9	G	101	BCL	CHA-C1A-NA	-3.12	119.26	126.40
9	I	101	BCL	CHA-C1A-NA	-3.11	119.27	126.40
9	U	102	BCL	CHA-C1A-NA	-3.11	119.27	126.40
9	8	102	BCL	CHA-C1A-NA	-3.11	119.27	126.40
9	4	102	BCL	CHA-C1A-NA	-3.11	119.28	126.40
9	2	103	BCL	CHA-C1A-NA	-3.11	119.28	126.40
9	6	102	BCL	CHA-C1A-NA	-3.11	119.28	126.40
10	C	401	KGD	CBG-CBI-CBL	-3.10	122.88	127.31
9	S	103	BCL	CHA-C1A-NA	-3.10	119.29	126.40
9	O	101	BCL	CHA-C1A-NA	-3.10	119.29	126.40
9	B	101	BCL	CHA-C1A-NA	-3.10	119.30	126.40
10	3	102	KGD	CBK-CBH-CBF	3.09	122.95	118.08
9	0	102	BCL	CHA-C1A-NA	-3.09	119.32	126.40
12	L	1004	MQE	CAY-CBL-CBB	-3.08	121.66	126.79
9	E	101	BCL	CHA-C1A-NA	-3.08	119.33	126.40
9	L	1001	BCL	C11-C10-C8	-3.08	105.96	115.92
10	B	102	KGD	CBA-CBE-CBF	-3.07	113.62	123.22
10	U	103	KGD	CAE-CAI-CAH	-3.07	115.82	118.65
10	P	102	KGD	CBG-CBB-CAV	-3.07	117.19	123.47
10	A	103	KGD	CAE-CAC-CAB	-3.07	108.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	103	KGD	CBG-CBB-CAV	-3.06	117.20	123.47
9	L	1001	BCL	CHD-C1D-ND	-3.06	121.64	124.45
10	A	104	KGD	CAL-CAJ-CAD	-3.06	118.60	127.20
15	C	404	HEM	CHB-C1B-C2B	-3.05	118.28	126.72
10	I	102	KGD	CAP-CAO-CAM	-3.05	122.96	127.31
10	I	102	KGD	CBF-CBH-CBJ	-3.03	114.29	118.94
10	A	103	KGD	CBB-CAV-CAR	-3.03	122.98	127.31
10	F	103	KGD	CBB-CAV-CAR	-3.03	122.99	127.31
15	C	405	HEM	CHB-C1B-C2B	-3.02	118.38	126.72
9	M	703	BCL	CHA-C1A-NA	-3.01	119.50	126.40
10	I	102	KGD	CAE-CAI-CAH	-3.01	115.88	118.65
10	G	102	KGD	CAJ-CAL-CAM	-3.00	121.70	126.23
9	2	102	BCL	O2A-CGA-O1A	-3.00	116.02	123.59
9	S	102	BCL	O2A-CGA-O1A	-3.00	116.03	123.59
9	F	102	BCL	O2A-CGA-O1A	-3.00	116.03	123.59
12	M	701	MQE	CAS-CBH-CAW	-2.99	120.45	127.66
9	N	102	BCL	O2A-CGA-O1A	-2.99	116.04	123.59
12	L	1004	MQE	CBO-CCB-CCC	-2.99	120.46	127.66
12	L	1004	MQE	CAK-CBE-CAQ	-2.99	120.47	127.66
9	8	101	BCL	O2A-CGA-O1A	-2.98	116.07	123.59
9	J	102	BCL	O2A-CGA-O1A	-2.98	116.07	123.59
9	0	101	BCL	O2A-CGA-O1A	-2.98	116.07	123.59
10	0	103	KGD	CBK-CBH-CBF	2.98	122.77	118.08
9	L	1002	BCL	C3D-C2D-C1D	-2.98	101.77	105.83
10	H	103	KGD	CAE-CAC-CAB	-2.97	108.41	113.18
10	G	102	KGD	CBB-CAV-CAR	-2.97	123.06	127.31
9	W	102	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
9	H	102	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
15	C	404	HEM	CBD-CAD-C3D	-2.97	104.37	112.63
9	Q	101	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
9	D	102	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
9	M	703	BCL	CMA-C3A-C4A	-2.97	103.79	111.77
10	2	104	KGD	CAE-CAI-CAH	-2.97	115.91	118.65
9	L	1001	BCL	CED-O2D-CGD	-2.97	109.22	115.94
9	4	101	BCL	O2A-CGA-O1A	-2.97	116.09	123.59
9	6	101	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
9	A	102	BCL	O2A-CGA-O1A	-2.97	116.10	123.59
9	U	101	BCL	O2A-CGA-O1A	-2.97	116.11	123.59
9	9	102	BCL	C16-C15-C13	-2.96	106.34	115.92
10	9	101	KGD	CAC-CAB-CAD	-2.96	105.92	110.48
11	L	1003	BPH	C1-C2-C3	-2.96	120.92	126.04
10	4	103	KGD	CAL-CAJ-CAD	-2.96	118.88	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	6	103	KGD	CAZ-CAW-CAS	2.96	120.25	115.27
9	F	101	BCL	C16-C15-C13	-2.96	106.35	115.92
9	R	101	BCL	C16-C15-C13	-2.96	106.35	115.92
9	N	101	BCL	C16-C15-C13	-2.96	106.36	115.92
9	P	101	BCL	C16-C15-C13	-2.96	106.36	115.92
9	T	101	BCL	C16-C15-C13	-2.96	106.36	115.92
10	2	104	KGD	CAZ-CAW-CAS	2.96	120.25	115.27
9	7	101	BCL	C16-C15-C13	-2.96	106.37	115.92
10	U	103	KGD	CBF-CBH-CBJ	-2.95	114.41	118.94
9	H	101	BCL	C16-C15-C13	-2.95	106.37	115.92
9	5	101	BCL	C16-C15-C13	-2.95	106.37	115.92
9	P	101	BCL	CHA-C1A-NA	-2.95	119.64	126.40
9	1	101	BCL	C16-C15-C13	-2.95	106.37	115.92
10	G	102	KGD	CBF-CBH-CBJ	-2.95	114.41	118.94
9	D	101	BCL	C16-C15-C13	-2.95	106.38	115.92
9	M	703	BCL	CMC-C2C-C3C	-2.95	101.93	113.83
9	9	102	BCL	CHA-C1A-NA	-2.95	119.64	126.40
9	L	1002	BCL	C4D-CHA-C1A	2.95	124.83	121.25
9	A	101	BCL	C16-C15-C13	-2.95	106.40	115.92
10	N	103	KGD	CAP-CAO-CAM	-2.94	123.11	127.31
9	J	101	BCL	C16-C15-C13	-2.94	106.41	115.92
9	H	101	BCL	CHA-C1A-NA	-2.94	119.66	126.40
9	F	101	BCL	CHA-C1A-NA	-2.94	119.66	126.40
10	3	102	KGD	CAL-CAJ-CAD	-2.94	118.94	127.20
10	2	104	KGD	CAL-CAJ-CAD	-2.94	118.94	127.20
9	X	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
9	3	101	BCL	C16-C15-C13	-2.94	106.42	115.92
9	D	101	BCL	CHA-C1A-NA	-2.94	119.67	126.40
10	8	103	KGD	CAL-CAJ-CAD	-2.94	118.95	127.20
13	P	104	PGV	O01-C1-C2	2.94	117.83	111.50
10	4	103	KGD	CBM-CBJ-CBH	-2.93	123.12	127.31
9	R	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
10	H	103	KGD	CBG-CBB-CAV	-2.93	117.47	123.47
10	Q	103	KGD	CBB-CAV-CAR	-2.93	123.13	127.31
9	A	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
9	N	101	BCL	CHA-C1A-NA	-2.93	119.69	126.40
9	3	101	BCL	CHA-C1A-NA	-2.92	119.70	126.40
9	T	101	BCL	CHA-C1A-NA	-2.92	119.70	126.40
10	C	401	KGD	OAA-CAI-CAH	2.92	123.55	120.96
9	1	101	BCL	CHA-C1A-NA	-2.92	119.71	126.40
12	M	701	MQE	CAM-CBG-CAT	-2.92	120.63	127.66
10	6	103	KGD	CBM-CBJ-CBH	-2.92	123.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	101	BCL	CHA-C1A-NA	-2.92	119.72	126.40
9	7	101	BCL	CHA-C1A-NA	-2.91	119.72	126.40
9	5	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
15	C	402	HEM	CHA-C4D-ND	2.91	127.98	124.38
9	3	101	BCL	CMC-C2C-C3C	-2.90	102.11	113.83
10	4	103	KGD	CBB-CBG-CBI	-2.90	117.53	123.47
9	X	101	BCL	CMC-C2C-C3C	-2.90	102.12	113.83
9	A	101	BCL	CMC-C2C-C3C	-2.90	102.13	113.83
9	F	101	BCL	CMC-C2C-C3C	-2.90	102.13	113.83
9	7	101	BCL	CMC-C2C-C3C	-2.90	102.14	113.83
9	N	101	BCL	CMC-C2C-C3C	-2.89	102.15	113.83
10	A	103	KGD	CAN-CAM-CAO	2.89	126.98	122.92
10	O	102	KGD	CAL-CAJ-CAD	-2.89	119.08	127.20
9	R	101	BCL	CMC-C2C-C3C	-2.89	102.16	113.83
9	M	703	BCL	C7-C6-C5	-2.89	105.50	113.36
9	1	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
9	P	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
9	J	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
10	A	104	KGD	CAZ-CAW-CAS	2.89	120.13	115.27
9	T	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
10	Q	103	KGD	CAP-CAO-CAM	-2.89	123.19	127.31
9	D	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
9	H	101	BCL	CMC-C2C-C3C	-2.89	102.18	113.83
9	9	102	BCL	CMC-C2C-C3C	-2.89	102.19	113.83
10	C	401	KGD	CAL-CAJ-CAD	-2.89	119.10	127.20
9	5	101	BCL	CMC-C2C-C3C	-2.88	102.20	113.83
10	3	102	KGD	CBG-CBB-CAV	-2.88	117.57	123.47
9	M	703	BCL	C3D-C2D-C1D	-2.88	101.90	105.83
10	W	101	KGD	CBM-CBJ-CBH	-2.87	123.21	127.31
11	L	1005	BPH	O2D-CGD-O1D	-2.87	118.23	123.84
9	L	1002	BCL	C11-C10-C8	-2.87	106.66	115.92
11	M	704	BPH	C1-C2-C3	-2.86	121.09	126.04
10	K	102	KGD	CBG-CBB-CAV	-2.86	117.62	123.47
9	D	102	BCL	CMC-C2C-C3C	-2.85	102.33	113.83
10	J	103	KGD	CAL-CAJ-CAD	-2.85	119.20	127.20
9	U	101	BCL	CMC-C2C-C3C	-2.85	102.34	113.83
15	C	405	HEM	CHC-C4B-C3B	-2.85	120.21	124.57
9	4	101	BCL	CMC-C2C-C3C	-2.85	102.35	113.83
9	2	102	BCL	CMC-C2C-C3C	-2.84	102.35	113.83
9	N	102	BCL	CMC-C2C-C3C	-2.84	102.35	113.83
9	H	102	BCL	CMC-C2C-C3C	-2.84	102.36	113.83
9	S	102	BCL	CMC-C2C-C3C	-2.84	102.36	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	102	BCL	CMC-C2C-C3C	-2.84	102.36	113.83
9	Q	101	BCL	CMC-C2C-C3C	-2.84	102.36	113.83
9	W	102	BCL	CMC-C2C-C3C	-2.84	102.37	113.83
9	6	101	BCL	CMC-C2C-C3C	-2.84	102.37	113.83
10	I	102	KGD	CBG-CBB-CAV	-2.84	117.66	123.47
9	T	101	BCL	C11-C12-C13	-2.84	106.74	115.92
9	R	101	BCL	C11-C12-C13	-2.84	106.74	115.92
9	N	101	BCL	C3D-C2D-C1D	-2.84	101.96	105.83
9	0	101	BCL	CMC-C2C-C3C	-2.84	102.39	113.83
9	J	102	BCL	CMC-C2C-C3C	-2.84	102.39	113.83
9	8	101	BCL	CMC-C2C-C3C	-2.83	102.39	113.83
9	F	102	BCL	CMC-C2C-C3C	-2.83	102.39	113.83
10	S	104	KGD	CAE-CAI-CAH	-2.83	116.04	118.65
9	D	101	BCL	C11-C12-C13	-2.83	106.76	115.92
10	N	103	KGD	CAE-CAC-CAB	-2.83	108.63	113.18
9	N	101	BCL	C11-C12-C13	-2.83	106.76	115.92
9	3	101	BCL	C11-C12-C13	-2.83	106.77	115.92
9	7	101	BCL	C11-C12-C13	-2.83	106.77	115.92
9	H	101	BCL	C11-C12-C13	-2.83	106.77	115.92
10	T	102	KGD	CAL-CAJ-CAD	-2.83	119.25	127.20
10	G	102	KGD	CBJ-CBM-CBN	-2.83	114.39	123.22
9	5	101	BCL	C11-C12-C13	-2.83	106.78	115.92
9	9	102	BCL	C11-C12-C13	-2.83	106.78	115.92
9	P	101	BCL	C3D-C2D-C1D	-2.83	101.97	105.83
9	1	101	BCL	C11-C12-C13	-2.82	106.79	115.92
9	A	101	BCL	C11-C12-C13	-2.82	106.79	115.92
11	L	1005	BPH	C1-C2-C3	-2.82	121.16	126.04
9	L	1001	BCL	C1B-CHB-C4A	-2.82	124.53	130.12
10	0	104	KGD	CBB-CAV-CAR	-2.82	123.29	127.31
9	P	101	BCL	C11-C12-C13	-2.82	106.81	115.92
12	L	1004	MQE	CAL-CBF-CAV	-2.82	120.88	127.66
9	F	101	BCL	C11-C12-C13	-2.82	106.82	115.92
9	X	101	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
9	J	101	BCL	C11-C12-C13	-2.81	106.82	115.92
10	F	103	KGD	CAJ-CAL-CAM	-2.81	121.98	126.23
9	5	101	BCL	C4B-CHC-C1C	-2.81	124.55	130.12
9	D	101	BCL	C3D-C2D-C1D	-2.81	101.99	105.83
10	C	401	KGD	CBN-CBL-CBI	2.81	123.25	118.94
10	S	104	KGD	CBG-CBB-CAV	-2.81	117.72	123.47
9	H	101	BCL	C4B-CHC-C1C	-2.80	124.56	130.12
9	F	101	BCL	C3D-C2D-C1D	-2.80	102.00	105.83
9	P	101	BCL	C4B-CHC-C1C	-2.80	124.57	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	103	KGD	CAL-CAJ-CAD	-2.80	119.33	127.20
9	T	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
9	1	101	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
15	C	405	HEM	CHA-C4D-ND	2.80	127.84	124.38
9	9	102	BCL	C3D-C2D-C1D	-2.80	102.01	105.83
9	U	102	BCL	C7-C6-C5	-2.80	105.77	113.36
9	F	101	BCL	C4B-CHC-C1C	-2.79	124.58	130.12
9	O	101	BCL	C7-C6-C5	-2.79	105.77	113.36
9	Q	102	BCL	C7-C6-C5	-2.79	105.77	113.36
10	8	103	KGD	CAE-CAI-CAH	-2.79	116.08	118.65
9	8	102	BCL	C7-C6-C5	-2.79	105.78	113.36
9	B	101	BCL	C7-C6-C5	-2.79	105.78	113.36
9	5	101	BCL	C3D-C2D-C1D	-2.79	102.02	105.83
9	E	101	BCL	C7-C6-C5	-2.79	105.78	113.36
9	H	101	BCL	C3D-C2D-C1D	-2.79	102.02	105.83
9	G	101	BCL	C7-C6-C5	-2.79	105.78	113.36
9	3	101	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
9	J	101	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
9	T	101	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
9	6	102	BCL	C7-C6-C5	-2.79	105.79	113.36
9	2	103	BCL	C7-C6-C5	-2.79	105.79	113.36
9	W	103	BCL	C7-C6-C5	-2.79	105.79	113.36
9	I	101	BCL	C7-C6-C5	-2.79	105.79	113.36
9	A	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
9	K	101	BCL	CMC-C2C-C3C	-2.78	102.60	113.83
9	X	101	BCL	C4B-CHC-C1C	-2.78	124.60	130.12
9	0	102	BCL	C7-C6-C5	-2.78	105.80	113.36
9	7	101	BCL	C3D-C2D-C1D	-2.78	102.03	105.83
10	A	104	KGD	CBF-CBH-CBJ	-2.78	114.67	118.94
10	0	103	KGD	CBJ-CBM-CBN	-2.78	114.53	123.22
9	D	101	BCL	C4B-CHC-C1C	-2.78	124.61	130.12
9	0	102	BCL	CMC-C2C-C3C	-2.78	102.60	113.83
9	6	102	BCL	CMC-C2C-C3C	-2.78	102.61	113.83
12	M	701	MQE	CAI-CBD-CAR	-2.78	120.96	127.66
9	Q	102	BCL	CMC-C2C-C3C	-2.78	102.61	113.83
9	K	101	BCL	C7-C6-C5	-2.78	105.81	113.36
9	S	103	BCL	CMC-C2C-C3C	-2.78	102.62	113.83
9	2	103	BCL	CMC-C2C-C3C	-2.78	102.62	113.83
9	4	102	BCL	C7-C6-C5	-2.78	105.81	113.36
9	N	101	BCL	C4B-CHC-C1C	-2.78	124.61	130.12
9	3	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
9	7	101	BCL	C4B-CHC-C1C	-2.78	124.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	703	BCL	C4B-CHC-C1C	-2.78	124.62	130.12
9	G	101	BCL	CMC-C2C-C3C	-2.78	102.63	113.83
9	S	103	BCL	C7-C6-C5	-2.78	105.82	113.36
9	W	103	BCL	CMC-C2C-C3C	-2.78	102.63	113.83
9	J	101	BCL	C3D-C2D-C1D	-2.78	102.04	105.83
9	U	102	BCL	CMC-C2C-C3C	-2.78	102.63	113.83
9	I	101	BCL	CMC-C2C-C3C	-2.77	102.64	113.83
9	O	101	BCL	CMC-C2C-C3C	-2.77	102.64	113.83
9	R	101	BCL	C3D-C2D-C1D	-2.77	102.05	105.83
9	1	101	BCL	C4B-CHC-C1C	-2.77	124.63	130.12
9	A	101	BCL	C4B-CHC-C1C	-2.77	124.63	130.12
9	B	101	BCL	CMC-C2C-C3C	-2.77	102.65	113.83
9	M	703	BCL	C11-C10-C8	-2.77	106.97	115.92
9	L	1002	BCL	C1B-CHB-C4A	-2.77	124.63	130.12
10	S	101	KGD	CBG-CBB-CAV	-2.77	117.80	123.47
9	8	102	BCL	CMC-C2C-C3C	-2.77	102.67	113.83
9	9	102	BCL	C4B-CHC-C1C	-2.77	124.64	130.12
10	G	102	KGD	CAE-CAC-CAB	-2.77	108.74	113.18
9	4	102	BCL	CMC-C2C-C3C	-2.77	102.67	113.83
9	W	102	BCL	C11-C12-C13	-2.76	106.98	115.92
9	R	101	BCL	C4B-CHC-C1C	-2.76	124.65	130.12
9	E	101	BCL	CMC-C2C-C3C	-2.76	102.70	113.83
9	L	1002	BCL	C3C-C2C-C1C	2.76	106.32	101.87
9	8	101	BCL	CHA-C1A-NA	-2.76	120.09	126.40
9	A	102	BCL	CHA-C1A-NA	-2.76	120.09	126.40
10	Q	103	KGD	CBK-CBH-CBJ	2.76	126.78	122.92
9	F	102	BCL	CHA-C1A-NA	-2.75	120.10	126.40
10	9	101	KGD	CBJ-CBM-CBN	-2.75	114.64	123.22
9	4	101	BCL	CHA-C1A-NA	-2.75	120.10	126.40
9	W	102	BCL	CHA-C1A-NA	-2.75	120.10	126.40
9	2	102	BCL	CHA-C1A-NA	-2.75	120.10	126.40
9	Q	101	BCL	CHA-C1A-NA	-2.75	120.10	126.40
9	H	102	BCL	CHA-C1A-NA	-2.75	120.11	126.40
10	0	103	KGD	CBN-CBL-CBI	-2.74	114.73	118.94
9	D	102	BCL	CHA-C1A-NA	-2.74	120.12	126.40
9	L	1002	BCL	O2A-CGA-O1A	-2.74	116.68	123.59
9	6	101	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	S	102	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	N	102	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	J	102	BCL	CHA-C1A-NA	-2.74	120.13	126.40
9	S	103	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
9	U	101	BCL	CHA-C1A-NA	-2.73	120.14	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	0	101	BCL	CHA-C1A-NA	-2.73	120.14	126.40
9	B	101	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
9	U	102	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
9	G	101	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
12	M	701	MQE	CBO-CCB-CCC	-2.72	121.10	127.66
9	I	101	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
10	J	103	KGD	CAP-CAO-CAM	-2.72	123.43	127.31
10	8	103	KGD	CAN-CAM-CAL	-2.72	113.79	118.08
9	2	103	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
9	4	102	BCL	C3D-C2D-C1D	-2.72	102.12	105.83
10	C	401	KGD	CAE-CAC-CAB	-2.71	108.82	113.18
9	O	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
10	S	104	KGD	CAZ-CAW-CAS	2.71	119.83	115.27
10	0	103	KGD	CAC-CAB-CAD	-2.71	106.31	110.48
9	E	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
9	K	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
9	F	102	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
9	L	1001	BCL	C4B-CHC-C1C	-2.71	124.75	130.12
10	B	102	KGD	CBK-CBH-CBF	2.70	122.34	118.08
10	H	103	KGD	CAL-CAJ-CAD	-2.70	119.61	127.20
9	Q	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
9	0	102	BCL	C3D-C2D-C1D	-2.70	102.14	105.83
12	L	1004	MQE	CAJ-CBC-CAP	-2.70	121.16	127.66
9	A	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
9	6	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
10	U	103	KGD	CBB-CAV-CAR	-2.70	123.46	127.31
9	H	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
9	W	103	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
10	O	102	KGD	CBM-CBJ-CBH	-2.69	123.47	127.31
9	W	102	BCL	CED-O2D-CGD	-2.68	109.87	115.94
9	6	101	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
10	W	101	KGD	CBF-CBH-CBJ	-2.68	114.83	118.94
9	8	102	BCL	C3D-C2D-C1D	-2.68	102.18	105.83
9	M	703	BCL	C16-C15-C13	-2.68	107.27	115.92
10	T	102	KGD	CBN-CBL-CBI	-2.68	114.84	118.94
9	N	102	BCL	C3D-C2D-C1D	-2.67	102.18	105.83
9	L	1002	BCL	CED-O2D-CGD	-2.67	109.89	115.94
15	C	403	HEM	CHA-C4D-ND	2.67	127.68	124.38
10	8	103	KGD	CAL-CAM-CAO	2.66	123.02	118.94
10	G	102	KGD	CAC-CAB-CAD	-2.66	106.39	110.48
9	U	101	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
9	M	703	BCL	C11-C12-C13	-2.66	107.33	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	102	KGD	CAE-CAC-CAB	-2.65	108.92	113.18
9	S	102	BCL	C3D-C2D-C1D	-2.65	102.21	105.83
10	C	401	KGD	CAP-CAO-CAM	-2.65	123.53	127.31
9	0	101	BCL	C3D-C2D-C1D	-2.65	102.21	105.83
9	X	101	BCL	C11-C12-C13	-2.65	107.36	115.92
10	N	103	KGD	CAZ-CAW-CAS	2.65	119.72	115.27
9	8	101	BCL	C3D-C2D-C1D	-2.65	102.22	105.83
9	L	1002	BCL	CBB-CAB-C3B	2.65	128.20	120.34
10	3	102	KGD	CAE-CAC-CAB	-2.65	108.93	113.18
9	J	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
9	2	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
9	D	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
9	W	102	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
10	6	103	KGD	CBJ-CBM-CBN	-2.63	115.00	123.22
9	A	102	BCL	CMA-C3A-C4A	-2.63	104.70	111.77
9	4	101	BCL	C3D-C2D-C1D	-2.63	102.24	105.83
9	0	101	BCL	C11-C10-C8	-2.63	107.42	115.92
9	N	102	BCL	C11-C10-C8	-2.63	107.43	115.92
9	J	102	BCL	C11-C10-C8	-2.63	107.43	115.92
9	0	101	BCL	CMA-C3A-C4A	-2.62	104.72	111.77
9	F	102	BCL	C11-C10-C8	-2.62	107.44	115.92
9	Q	101	BCL	C3D-C2D-C1D	-2.62	102.25	105.83
9	F	102	BCL	CMA-C3A-C4A	-2.62	104.72	111.77
9	U	101	BCL	C11-C10-C8	-2.62	107.44	115.92
10	K	102	KGD	CAJ-CAL-CAM	-2.62	122.27	126.23
9	4	101	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
9	N	102	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
9	Q	101	BCL	C11-C10-C8	-2.62	107.45	115.92
9	4	101	BCL	C11-C10-C8	-2.62	107.45	115.92
9	8	101	BCL	C11-C10-C8	-2.62	107.45	115.92
9	L	1002	BCL	CGD-CBD-CAD	-2.62	102.25	110.73
9	2	102	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
9	S	102	BCL	C11-C10-C8	-2.62	107.46	115.92
9	H	102	BCL	C11-C10-C8	-2.62	107.46	115.92
10	B	102	KGD	CBK-CBH-CBJ	2.62	126.59	122.92
9	S	102	BCL	CMA-C3A-C4A	-2.62	104.74	111.77
9	2	102	BCL	C11-C10-C8	-2.62	107.46	115.92
10	3	102	KGD	CAZ-CAW-CAS	2.62	119.67	115.27
9	W	102	BCL	CMA-C3A-C4A	-2.61	104.75	111.77
10	W	101	KGD	CAP-CAQ-CAR	-2.61	119.08	126.42
9	A	102	BCL	C11-C10-C8	-2.61	107.48	115.92
9	6	101	BCL	CMA-C3A-C4A	-2.61	104.76	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	102	BCL	CMA-C3A-C4A	-2.61	104.76	111.77
10	2	104	KGD	CBK-CBH-CBJ	2.61	126.58	122.92
10	T	102	KGD	CAO-CAP-CAQ	-2.61	115.08	123.22
12	L	1004	MQE	CAO-CBI-CAZ	-2.61	121.38	127.66
9	D	102	BCL	C11-C10-C8	-2.61	107.49	115.92
9	8	101	BCL	CMA-C3A-C4A	-2.61	104.77	111.77
15	C	405	HEM	CBA-CAA-C2A	-2.60	108.17	112.62
9	U	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
10	P	102	KGD	OAA-CAI-CAH	2.60	123.27	120.96
9	D	102	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	6	101	BCL	C11-C10-C8	-2.60	107.50	115.92
13	L	1006	PGV	O01-C1-C2	2.60	117.11	111.50
9	Q	101	BCL	CMA-C3A-C4A	-2.60	104.78	111.77
9	F	102	BCL	C11-C12-C13	-2.60	107.52	115.92
10	N	103	KGD	CAP-CAQ-CAR	-2.60	119.12	126.42
9	J	102	BCL	CMA-C3A-C4A	-2.60	104.79	111.77
10	G	102	KGD	CBM-CBJ-CBH	-2.60	123.60	127.31
9	8	101	BCL	C11-C12-C13	-2.60	107.53	115.92
10	Q	103	KGD	CBA-CBE-CBF	-2.60	115.11	123.22
10	S	101	KGD	CAL-CAJ-CAD	-2.60	119.91	127.20
9	J	102	BCL	C11-C12-C13	-2.60	107.53	115.92
9	N	102	BCL	C11-C12-C13	-2.60	107.53	115.92
9	A	102	BCL	C11-C12-C13	-2.60	107.53	115.92
9	Q	101	BCL	C11-C12-C13	-2.59	107.53	115.92
9	U	101	BCL	C11-C12-C13	-2.59	107.54	115.92
11	L	1005	BPH	CMC-C2C-C1C	-2.59	108.70	114.38
9	0	101	BCL	C11-C12-C13	-2.59	107.55	115.92
9	2	102	BCL	C11-C12-C13	-2.59	107.55	115.92
9	H	102	BCL	C11-C12-C13	-2.59	107.55	115.92
10	5	102	KGD	CAC-CAB-CAD	-2.59	106.50	110.48
9	S	102	BCL	C11-C12-C13	-2.59	107.56	115.92
9	6	101	BCL	C11-C12-C13	-2.59	107.56	115.92
15	C	405	HEM	C4B-CHC-C1C	-2.58	119.15	122.56
9	4	101	BCL	C11-C12-C13	-2.58	107.57	115.92
11	M	704	BPH	O2D-CGD-O1D	-2.58	118.79	123.84
10	I	102	KGD	CAZ-CAW-CAS	2.58	119.61	115.27
10	C	401	KGD	CAE-CAI-CAH	-2.58	116.27	118.65
9	D	102	BCL	C11-C12-C13	-2.58	107.59	115.92
10	K	102	KGD	CBJ-CBM-CBN	-2.57	115.18	123.22
13	L	1007	PGV	P-O12-C04	-2.57	106.61	121.68
10	G	102	KGD	CAZ-CAW-CAS	2.56	119.58	115.27
13	L	1006	PGV	O14-P-O13	2.56	124.89	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	9	101	KGD	CBN-CBL-CBI	-2.56	115.02	118.94
15	C	405	HEM	CBD-CAD-C3D	-2.56	105.53	112.63
9	M	703	BCL	C2A-C1A-CHA	2.55	128.32	123.86
10	T	102	KGD	CAC-CAB-CAD	-2.55	106.56	110.48
13	M	706	PGV	O14-P-O13	2.55	124.85	112.24
9	O	101	BCL	O2A-CGA-O1A	-2.55	117.16	123.59
10	9	101	KGD	CAN-CAM-CAO	2.55	126.49	122.92
10	N	103	KGD	CAC-CAB-CAD	-2.55	106.56	110.48
9	2	103	BCL	O2A-CGA-O1A	-2.54	117.17	123.59
10	S	101	KGD	CAK-CAH-CAI	-2.54	111.70	115.48
9	L	1001	BCL	C1C-NC-C4C	-2.54	105.56	106.71
10	W	101	KGD	CBG-CBB-CAV	-2.54	118.27	123.47
9	6	102	BCL	O2A-CGA-O1A	-2.54	117.18	123.59
10	6	103	KGD	CAL-CAJ-CAD	-2.54	120.07	127.20
10	S	101	KGD	CBF-CBH-CBJ	-2.54	115.05	118.94
10	H	103	KGD	CAZ-CAW-CAS	2.53	119.53	115.27
9	W	103	BCL	O2A-CGA-O1A	-2.53	117.20	123.59
10	P	102	KGD	CAN-CAM-CAL	-2.53	114.08	118.08
9	E	101	BCL	O2A-CGA-O1A	-2.53	117.20	123.59
9	I	101	BCL	O2A-CGA-O1A	-2.53	117.20	123.59
10	0	103	KGD	CAN-CAM-CAO	2.53	126.47	122.92
9	Q	102	BCL	O2A-CGA-O1A	-2.53	117.21	123.59
9	G	101	BCL	O2A-CGA-O1A	-2.53	117.21	123.59
9	0	102	BCL	O2A-CGA-O1A	-2.53	117.21	123.59
10	2	104	KGD	CBG-CBI-CBL	-2.52	123.71	127.31
10	N	103	KGD	CBG-CBB-CAV	-2.52	118.31	123.47
9	U	102	BCL	O2A-CGA-O1A	-2.52	117.23	123.59
10	8	103	KGD	CAE-CAC-CAB	-2.52	109.14	113.18
9	L	1001	BCL	C2A-C1A-CHA	2.52	128.26	123.86
13	Z	101	PGV	O14-P-O13	2.52	124.69	112.24
10	N	103	KGD	CBM-CBJ-CBH	-2.52	123.72	127.31
10	S	101	KGD	CAC-CAB-CAD	-2.52	106.61	110.48
10	O	102	KGD	CAP-CAQ-CAR	-2.51	119.35	126.42
9	S	103	BCL	O2A-CGA-O1A	-2.51	117.25	123.59
9	8	102	BCL	O2A-CGA-O1A	-2.51	117.25	123.59
12	L	1004	MQE	CAI-CBD-CAR	-2.51	121.61	127.66
9	4	102	BCL	O2A-CGA-O1A	-2.51	117.26	123.59
9	K	101	BCL	O2A-CGA-O1A	-2.51	117.26	123.59
9	B	101	BCL	O2A-CGA-O1A	-2.51	117.26	123.59
10	A	103	KGD	CBB-CBG-CBI	-2.51	118.34	123.47
9	A	102	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
9	J	102	BCL	C2A-C3A-C4A	-2.50	97.83	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	101	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
9	L	1002	BCL	CMA-C3A-C4A	-2.50	105.06	111.77
9	W	102	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
9	D	102	BCL	C2A-C3A-C4A	-2.50	97.84	101.87
9	6	102	BCL	C3C-C2C-C1C	2.50	105.90	101.87
9	Q	102	BCL	C3C-C2C-C1C	2.49	105.89	101.87
10	G	102	KGD	CAO-CAP-CAQ	-2.49	115.44	123.22
9	F	102	BCL	C2A-C3A-C4A	-2.49	97.85	101.87
9	2	102	BCL	C2A-C3A-C4A	-2.49	97.85	101.87
10	A	103	KGD	CBM-CBJ-CBH	-2.49	123.76	127.31
9	0	101	BCL	C2A-C3A-C4A	-2.49	97.85	101.87
9	2	103	BCL	C3C-C2C-C1C	2.49	105.89	101.87
10	F	103	KGD	CBF-CBH-CBJ	-2.49	115.12	118.94
9	8	101	BCL	C2A-C3A-C4A	-2.49	97.85	101.87
9	I	101	BCL	C3C-C2C-C1C	2.49	105.88	101.87
9	B	101	BCL	C3C-C2C-C1C	2.48	105.88	101.87
10	A	103	KGD	CBF-CBH-CBJ	-2.48	115.13	118.94
9	8	102	BCL	C1C-NC-C4C	-2.48	105.59	106.71
9	N	102	BCL	C2A-C3A-C4A	-2.48	97.86	101.87
9	U	101	BCL	C2A-C3A-C4A	-2.48	97.86	101.87
9	W	103	BCL	C3C-C2C-C1C	2.48	105.88	101.87
9	S	102	BCL	C2A-C3A-C4A	-2.48	97.87	101.87
9	H	102	BCL	C2A-C3A-C4A	-2.48	97.87	101.87
9	S	103	BCL	C3C-C2C-C1C	2.48	105.87	101.87
9	4	102	BCL	C3C-C2C-C1C	2.47	105.86	101.87
9	K	101	BCL	C3C-C2C-C1C	2.47	105.86	101.87
9	O	101	BCL	C3C-C2C-C1C	2.47	105.86	101.87
9	8	102	BCL	C3C-C2C-C1C	2.47	105.86	101.87
9	U	102	BCL	C3C-C2C-C1C	2.47	105.86	101.87
10	0	103	KGD	CAE-CAI-CAH	-2.47	116.38	118.65
9	Q	102	BCL	C1C-NC-C4C	-2.47	105.60	106.71
15	C	405	HEM	C4B-C3B-C2B	-2.47	105.16	107.11
10	N	103	KGD	CBM-CBN-CBL	-2.47	119.48	126.42
9	0	102	BCL	C3C-C2C-C1C	2.47	105.85	101.87
9	E	101	BCL	C1C-NC-C4C	-2.47	105.60	106.71
9	W	103	BCL	CMB-C2B-C3B	2.47	129.29	124.68
9	4	101	BCL	C2A-C3A-C4A	-2.47	97.89	101.87
9	6	101	BCL	C2A-C3A-C4A	-2.46	97.89	101.87
9	I	101	BCL	C1C-NC-C4C	-2.46	105.60	106.71
9	O	101	BCL	C1C-NC-C4C	-2.46	105.60	106.71
9	6	102	BCL	CMB-C2B-C3B	2.46	129.28	124.68
9	L	1001	BCL	C1-C2-C3	-2.46	121.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	0	104	KGD	CBG-CBB-CAV	-2.45	118.45	123.47
9	G	101	BCL	C3C-C2C-C1C	2.45	105.83	101.87
9	K	101	BCL	CMB-C2B-C3B	2.45	129.27	124.68
9	B	101	BCL	CMB-C2B-C3B	2.45	129.27	124.68
9	4	102	BCL	CMB-C2B-C3B	2.45	129.26	124.68
9	Q	102	BCL	CMB-C2B-C3B	2.45	129.26	124.68
9	E	101	BCL	C3C-C2C-C1C	2.45	105.83	101.87
10	U	103	KGD	CBJ-CBM-CBN	-2.45	115.57	123.22
9	M	703	BCL	CGD-CBD-CAD	-2.45	102.80	110.73
15	C	402	HEM	C4B-C3B-C2B	-2.45	105.17	107.11
9	W	103	BCL	C1C-NC-C4C	-2.45	105.61	106.71
11	L	1003	BPH	C11-C12-C13	-2.45	108.00	115.92
15	C	403	HEM	CHC-C4B-C3B	-2.45	120.82	124.57
12	L	1004	MQE	CBA-CBN-CBM	-2.45	121.77	127.66
9	O	101	BCL	CMB-C2B-C3B	2.45	129.26	124.68
9	U	102	BCL	CMB-C2B-C3B	2.45	129.25	124.68
10	O	102	KGD	CAN-CAM-CAO	2.44	126.35	122.92
9	S	103	BCL	CMB-C2B-C3B	2.44	129.25	124.68
9	2	103	BCL	CMB-C2B-C3B	2.44	129.25	124.68
9	8	102	BCL	CMB-C2B-C3B	2.44	129.24	124.68
9	E	101	BCL	CMB-C2B-C3B	2.44	129.24	124.68
9	I	101	BCL	CMB-C2B-C3B	2.44	129.24	124.68
10	8	103	KGD	CAZ-CAW-CAS	2.44	119.37	115.27
9	G	101	BCL	CMB-C2B-C3B	2.44	129.24	124.68
9	2	103	BCL	C1C-NC-C4C	-2.44	105.61	106.71
9	G	101	BCL	C11-C10-C8	-2.43	108.05	115.92
9	0	102	BCL	CMB-C2B-C3B	2.43	129.23	124.68
9	0	102	BCL	C11-C10-C8	-2.43	108.05	115.92
9	W	103	BCL	C11-C10-C8	-2.43	108.06	115.92
9	4	102	BCL	C11-C10-C8	-2.43	108.06	115.92
9	8	102	BCL	C11-C10-C8	-2.43	108.08	115.92
10	3	102	KGD	CBB-CAV-CAR	-2.43	123.85	127.31
9	B	101	BCL	C11-C10-C8	-2.43	108.08	115.92
10	E	102	KGD	CAP-CAO-CAM	-2.43	123.85	127.31
9	S	103	BCL	C11-C10-C8	-2.43	108.08	115.92
9	I	101	BCL	C11-C10-C8	-2.42	108.08	115.92
9	2	103	BCL	C11-C10-C8	-2.42	108.09	115.92
9	U	102	BCL	C11-C10-C8	-2.42	108.09	115.92
9	K	101	BCL	C1C-NC-C4C	-2.42	105.62	106.71
9	6	102	BCL	C11-C10-C8	-2.42	108.09	115.92
9	O	101	BCL	C11-C10-C8	-2.42	108.09	115.92
9	E	101	BCL	C11-C10-C8	-2.42	108.11	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	102	BCL	C11-C10-C8	-2.42	108.11	115.92
9	K	101	BCL	C11-C10-C8	-2.42	108.11	115.92
9	S	103	BCL	C1C-NC-C4C	-2.42	105.62	106.71
13	P	104	PGV	O14-P-O13	2.41	124.16	112.24
9	4	102	BCL	C1C-NC-C4C	-2.41	105.62	106.71
9	G	101	BCL	CMD-C2D-C1D	2.41	128.96	124.71
9	2	103	BCL	CMD-C2D-C1D	2.41	128.96	124.71
9	B	101	BCL	C1C-NC-C4C	-2.40	105.62	106.71
9	M	703	BCL	CMD-C2D-C1D	2.40	128.95	124.71
9	K	101	BCL	C11-C12-C13	-2.40	108.15	115.92
9	1	101	BCL	CMA-C3A-C4A	-2.40	105.32	111.77
9	T	101	BCL	CMA-C3A-C4A	-2.40	105.32	111.77
9	G	101	BCL	C1C-NC-C4C	-2.40	105.63	106.71
9	I	101	BCL	C11-C12-C13	-2.40	108.16	115.92
9	E	101	BCL	C11-C12-C13	-2.40	108.16	115.92
9	2	103	BCL	C11-C12-C13	-2.40	108.17	115.92
9	O	101	BCL	C11-C12-C13	-2.40	108.17	115.92
13	L	1007	PGV	P-O11-C03	-2.40	107.62	121.68
9	0	102	BCL	C11-C12-C13	-2.40	108.17	115.92
9	B	101	BCL	C11-C12-C13	-2.40	108.17	115.92
10	A	103	KGD	CAC-CAB-CAD	-2.40	106.79	110.48
9	Q	102	BCL	C11-C12-C13	-2.40	108.17	115.92
11	M	704	BPH	CBC-CAC-C3C	-2.40	108.94	113.77
10	H	103	KGD	CAC-CAB-CAD	-2.40	106.79	110.48
9	8	102	BCL	C11-C12-C13	-2.40	108.17	115.92
9	M	703	BCL	O2A-CGA-O1A	-2.39	117.55	123.59
9	U	102	BCL	CMD-C2D-C1D	2.39	128.93	124.71
9	U	102	BCL	C1C-NC-C4C	-2.39	105.63	106.71
9	U	102	BCL	C11-C12-C13	-2.39	108.18	115.92
9	W	103	BCL	C11-C12-C13	-2.39	108.19	115.92
12	M	701	MQE	CAK-CBE-CAQ	-2.39	121.90	127.66
9	4	102	BCL	C11-C12-C13	-2.39	108.19	115.92
9	0	102	BCL	C1C-NC-C4C	-2.39	105.63	106.71
9	0	102	BCL	CMD-C2D-C1D	2.39	128.93	124.71
9	9	102	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
9	3	101	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
9	4	102	BCL	CMD-C2D-C1D	2.39	128.93	124.71
9	6	102	BCL	C11-C12-C13	-2.39	108.20	115.92
9	J	101	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
9	S	103	BCL	C11-C12-C13	-2.39	108.20	115.92
9	E	101	BCL	CMD-C2D-C1D	2.39	128.92	124.71
10	O	102	KGD	CBB-CAV-CAR	-2.39	123.90	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	101	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
9	G	101	BCL	C11-C12-C13	-2.39	108.20	115.92
9	F	101	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
9	I	101	BCL	CMD-C2D-C1D	2.39	128.92	124.71
9	D	101	BCL	CMA-C3A-C4A	-2.39	105.36	111.77
9	M	703	BCL	C12-C11-C10	-2.39	102.28	113.24
13	L	1006	PGV	P-O12-C04	-2.38	107.71	121.68
9	H	101	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
9	N	101	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
9	P	101	BCL	CMA-C3A-C4A	-2.38	105.37	111.77
9	8	102	BCL	CMD-C2D-C1D	2.38	128.91	124.71
9	A	101	BCL	CMA-C3A-C4A	-2.38	105.38	111.77
9	O	101	BCL	CMA-C3A-C4A	-2.38	105.38	111.77
9	6	102	BCL	CMD-C2D-C1D	2.38	128.90	124.71
9	B	101	BCL	CMD-C2D-C1D	2.38	128.90	124.71
9	K	101	BCL	CMD-C2D-C1D	2.38	128.90	124.71
13	L	1007	PGV	O14-P-O13	2.37	123.98	112.24
9	W	103	BCL	CMD-C2D-C1D	2.37	128.90	124.71
9	8	102	BCL	CMA-C3A-C4A	-2.37	105.39	111.77
9	5	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
9	K	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
9	7	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
9	L	1001	BCL	C11-C12-C13	-2.37	108.25	115.92
9	6	102	BCL	C1C-NC-C4C	-2.37	105.64	106.71
10	A	104	KGD	CAE-CAC-CAB	-2.37	109.38	113.18
9	S	103	BCL	CMD-C2D-C1D	2.37	128.89	124.71
9	O	101	BCL	CMD-C2D-C1D	2.37	128.89	124.71
13	Z	101	PGV	P-O12-C04	-2.37	107.79	121.68
9	0	102	BCL	CMA-C3A-C4A	-2.37	105.41	111.77
9	U	102	BCL	CMA-C3A-C4A	-2.37	105.41	111.77
9	6	102	BCL	CMA-C3A-C4A	-2.37	105.41	111.77
10	P	102	KGD	CAL-CAJ-CAD	-2.36	120.56	127.20
9	G	101	BCL	CMA-C3A-C4A	-2.36	105.42	111.77
10	0	104	KGD	CAE-CAC-CAB	-2.36	109.39	113.18
9	Q	102	BCL	CMD-C2D-C1D	2.36	128.87	124.71
10	U	103	KGD	CAE-CAC-CAB	-2.36	109.39	113.18
9	Q	102	BCL	CMA-C3A-C4A	-2.36	105.43	111.77
10	5	102	KGD	CBE-CBF-CBH	-2.36	119.79	126.42
10	3	102	KGD	CBK-CBH-CBJ	2.36	126.22	122.92
9	I	101	BCL	CMA-C3A-C4A	-2.35	105.44	111.77
9	W	103	BCL	CMA-C3A-C4A	-2.35	105.44	111.77
9	B	101	BCL	CMA-C3A-C4A	-2.35	105.45	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	0	104	KGD	CBB-CBG-CBI	-2.35	118.65	123.47
10	5	102	KGD	CBM-CBJ-CBH	-2.35	123.95	127.31
13	M	706	PGV	P-O11-C03	-2.35	107.89	121.68
13	C	406	PGV	O01-C1-C2	2.35	116.57	111.50
9	E	101	BCL	CMA-C3A-C4A	-2.35	105.45	111.77
9	2	103	BCL	CMA-C3A-C4A	-2.35	105.46	111.77
10	2	104	KGD	CAE-CAC-CAB	-2.35	109.41	113.18
10	P	102	KGD	CAT-CAX-CAY	-2.35	119.73	127.75
9	A	102	BCL	CHC-C1C-NC	2.35	127.75	124.51
9	S	103	BCL	CMA-C3A-C4A	-2.35	105.47	111.77
10	B	102	KGD	CBM-CBN-CBL	-2.34	119.83	126.42
9	4	102	BCL	CMA-C3A-C4A	-2.34	105.47	111.77
10	W	101	KGD	CAZ-CAW-CAS	2.34	119.21	115.27
10	A	104	KGD	CBN-CBL-CBI	-2.34	115.35	118.94
15	C	403	HEM	C4B-CHC-C1C	-2.34	119.47	122.56
9	S	102	BCL	CHC-C1C-NC	2.34	127.74	124.51
10	P	102	KGD	CBM-CBN-CBL	-2.34	119.85	126.42
9	8	101	BCL	CHC-C1C-NC	2.34	127.74	124.51
9	X	101	BCL	C1B-CHB-C4A	-2.34	125.49	130.12
11	L	1003	BPH	CMC-C2C-C1C	-2.33	109.28	114.38
9	Q	101	BCL	CHC-C1C-NC	2.33	127.73	124.51
11	L	1005	BPH	CMB-C2B-C3B	2.33	129.03	124.68
9	N	102	BCL	CHC-C1C-NC	2.32	127.72	124.51
10	T	102	KGD	CAZ-CAW-CAS	2.32	119.18	115.27
10	E	102	KGD	CAZ-CAW-CAS	2.32	119.17	115.27
12	M	701	MQE	CAS-CAN-CBB	-2.32	105.34	112.98
15	C	404	HEM	CMA-C3A-C4A	-2.32	124.90	128.46
10	0	104	KGD	CAN-CAM-CAO	2.32	126.17	122.92
10	G	102	KGD	CBB-CBG-CBI	-2.32	118.72	123.47
12	M	705	MQE	CAY-CBL-CBB	-2.32	122.93	126.79
10	S	101	KGD	CAN-CAM-CAO	2.31	126.16	122.92
10	Q	103	KGD	CBJ-CBM-CBN	-2.31	116.01	123.22
9	H	102	BCL	CHC-C1C-NC	2.31	127.70	124.51
12	L	1004	MQE	CAM-CBG-CAT	-2.31	122.11	127.66
9	M	703	BCL	CHC-C1C-NC	2.30	127.70	124.51
9	L	1001	BCL	C2C-C3C-C4C	-2.30	97.89	101.34
13	C	406	PGV	O14-P-O13	2.30	123.60	112.24
10	C	401	KGD	CAQ-CAR-CAV	2.30	122.47	118.94
10	2	104	KGD	CAC-CAB-CAD	-2.30	106.94	110.48
10	I	102	KGD	CAE-CAC-CAB	-2.29	109.50	113.18
10	2	104	KGD	CAN-CAM-CAO	2.29	126.13	122.92
10	S	104	KGD	CBB-CAV-CAR	-2.29	124.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	103	KGD	CAZ-CAW-CAS	2.29	119.12	115.27
10	J	103	KGD	CAZ-CAW-CAS	2.29	119.12	115.27
9	U	101	BCL	CHC-C1C-NC	2.29	127.68	124.51
9	W	102	BCL	CHC-C1C-NC	2.29	127.67	124.51
9	4	101	BCL	CHC-C1C-NC	2.29	127.67	124.51
9	6	101	BCL	CHC-C1C-NC	2.28	127.67	124.51
10	N	103	KGD	CAN-CAM-CAO	2.28	126.12	122.92
9	J	102	BCL	CHC-C1C-NC	2.28	127.66	124.51
10	0	103	KGD	CBA-CBE-CBF	-2.28	116.11	123.22
9	0	101	BCL	CHC-C1C-NC	2.28	127.66	124.51
15	C	404	HEM	CHA-C4D-ND	2.28	127.19	124.38
10	J	103	KGD	CBM-CBJ-CBH	-2.28	124.06	127.31
9	F	102	BCL	CHC-C1C-NC	2.28	127.66	124.51
10	B	102	KGD	CBJ-CBM-CBN	-2.28	116.11	123.22
10	4	103	KGD	CAZ-CAW-CAS	2.27	119.09	115.27
9	2	102	BCL	CHC-C1C-NC	2.27	127.65	124.51
13	M	706	PGV	P-O12-C04	-2.27	108.36	121.68
9	L	1001	BCL	CMC-C2C-C3C	-2.27	104.67	113.83
13	Z	101	PGV	P-O11-C03	-2.27	108.38	121.68
13	C	406	PGV	P-O11-C03	-2.27	108.38	121.68
10	W	101	KGD	CAE-CAC-CAB	-2.27	109.54	113.18
11	M	704	BPH	CMA-C3A-C4A	-2.27	109.42	114.38
13	C	406	PGV	P-O12-C04	-2.26	108.41	121.68
9	D	102	BCL	CHC-C1C-NC	2.26	127.64	124.51
9	L	1001	BCL	C12-C11-C10	-2.26	102.85	113.24
10	H	103	KGD	CAE-CAI-CAH	-2.26	116.57	118.65
10	2	101	KGD	CAL-CAJ-CAD	-2.26	120.87	127.20
10	Q	103	KGD	CBG-CBB-CAV	-2.25	118.86	123.47
10	O	102	KGD	CAZ-CAW-CAS	2.25	119.06	115.27
9	N	101	BCL	CMD-C2D-C1D	2.25	128.67	124.71
15	C	403	HEM	C4B-C3B-C2B	-2.25	105.33	107.11
9	9	102	BCL	C3C-C4C-CHD	-2.25	118.59	123.39
9	L	1001	BCL	CMA-C3A-C4A	-2.25	105.73	111.77
10	3	102	KGD	CBA-CBE-CBF	2.24	130.22	123.22
10	S	101	KGD	CBM-CBJ-CBH	-2.24	124.11	127.31
10	4	103	KGD	CBF-CBH-CBJ	-2.24	115.50	118.94
13	P	104	PGV	P-O12-C04	-2.24	108.55	121.68
12	L	1004	MQE	CAS-CBH-CAW	-2.24	122.27	127.66
10	6	103	KGD	CBA-CBE-CBF	-2.24	116.23	123.22
9	D	101	BCL	C3C-C4C-CHD	-2.24	118.61	123.39
9	T	101	BCL	CMD-C2D-C1D	2.24	128.65	124.71
9	6	101	BCL	C3C-C2C-C1C	2.23	105.48	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	101	BCL	C3C-C4C-CHD	-2.23	118.62	123.39
9	5	101	BCL	C3C-C4C-CHD	-2.23	118.62	123.39
9	4	101	BCL	C3C-C2C-C1C	2.23	105.47	101.87
9	D	102	BCL	C3C-C2C-C1C	2.23	105.47	101.87
15	C	402	HEM	CHC-C4B-C3B	-2.23	121.16	124.57
13	P	103	PGV	P-O12-C04	-2.23	108.60	121.68
10	H	103	KGD	CBM-CBJ-CBH	-2.23	124.13	127.31
9	J	101	BCL	CMD-C2D-C1D	2.23	128.64	124.71
9	1	101	BCL	CMD-C2D-C1D	2.23	128.64	124.71
9	A	101	BCL	C3C-C4C-CHD	-2.23	118.63	123.39
10	5	102	KGD	CAL-CAJ-CAD	-2.23	120.95	127.20
10	0	103	KGD	CAZ-CAW-CAS	2.23	119.02	115.27
9	R	101	BCL	C3C-C4C-CHD	-2.23	118.64	123.39
9	X	101	BCL	C3C-C4C-CHD	-2.22	118.64	123.39
9	1	101	BCL	C3C-C4C-CHD	-2.22	118.64	123.39
11	L	1003	BPH	C16-C15-C13	-2.22	108.73	115.92
9	0	101	BCL	C3C-C2C-C1C	2.22	105.46	101.87
9	H	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
9	7	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
9	D	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
9	T	101	BCL	C3C-C4C-CHD	-2.22	118.64	123.39
10	G	102	KGD	CBA-CBE-CBF	-2.22	116.28	123.22
10	0	103	KGD	CAE-CAC-CAB	-2.22	109.61	113.18
9	N	101	BCL	C3C-C4C-CHD	-2.22	118.65	123.39
9	F	101	BCL	CMD-C2D-C1D	2.22	128.63	124.71
10	J	103	KGD	CAE-CAI-CAH	-2.22	116.61	118.65
9	3	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
9	H	101	BCL	C3C-C4C-CHD	-2.22	118.65	123.39
10	N	103	KGD	CAE-CAI-CAH	-2.22	116.61	118.65
9	X	101	BCL	CGD-CBD-CAD	-2.22	103.55	110.73
13	P	103	PGV	O14-P-O13	2.22	123.20	112.24
9	7	101	BCL	C3C-C4C-CHD	-2.22	118.66	123.39
10	5	102	KGD	CBF-CBH-CBJ	-2.22	115.54	118.94
9	P	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
9	A	101	BCL	CMD-C2D-C1D	2.22	128.62	124.71
9	N	102	BCL	C3C-C2C-C1C	2.22	105.45	101.87
9	3	101	BCL	C3C-C4C-CHD	-2.22	118.66	123.39
9	9	102	BCL	CMD-C2D-C1D	2.21	128.62	124.71
9	P	101	BCL	C3C-C4C-CHD	-2.21	118.66	123.39
11	L	1003	BPH	CMA-C3A-C4A	-2.21	109.53	114.38
9	H	102	BCL	C3C-C2C-C1C	2.21	105.44	101.87
10	0	103	KGD	CAO-CAP-CAQ	-2.21	116.31	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	X	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
10	2	101	KGD	CBE-CBF-CBH	-2.21	120.20	126.42
10	S	104	KGD	CBA-CBE-CBF	-2.21	116.32	123.22
9	R	101	BCL	CMD-C2D-C1D	2.21	128.61	124.71
9	Q	101	BCL	C3C-C2C-C1C	2.21	105.44	101.87
9	S	102	BCL	C3C-C2C-C1C	2.21	105.44	101.87
10	3	102	KGD	CBJ-CBM-CBN	-2.21	116.33	123.22
9	L	1002	BCL	C4B-CHC-C1C	-2.21	125.75	130.12
10	5	102	KGD	CAZ-CAW-CAS	2.21	118.98	115.27
10	Q	103	KGD	CAN-CAM-CAO	2.21	126.01	122.92
10	O	102	KGD	CBJ-CBM-CBN	-2.21	116.33	123.22
9	F	101	BCL	C3C-C4C-CHD	-2.20	118.68	123.39
9	H	101	BCL	C12-C11-C10	-2.20	103.12	113.24
9	D	101	BCL	C12-C11-C10	-2.20	103.12	113.24
9	T	101	BCL	C12-C11-C10	-2.20	103.12	113.24
9	F	102	BCL	C3C-C2C-C1C	2.20	105.42	101.87
9	1	101	BCL	C12-C11-C10	-2.20	103.13	113.24
9	N	101	BCL	C12-C11-C10	-2.20	103.14	113.24
9	R	101	BCL	C12-C11-C10	-2.20	103.14	113.24
10	0	104	KGD	CAQ-CAR-CAV	-2.20	115.57	118.94
9	A	101	BCL	C12-C11-C10	-2.20	103.15	113.24
10	6	103	KGD	CBK-CBH-CBJ	2.20	126.00	122.92
9	8	101	BCL	C3C-C2C-C1C	2.20	105.42	101.87
9	7	101	BCL	C12-C11-C10	-2.20	103.15	113.24
9	9	102	BCL	C12-C11-C10	-2.20	103.15	113.24
9	5	101	BCL	CMD-C2D-C1D	2.19	128.58	124.71
9	J	101	BCL	C12-C11-C10	-2.19	103.16	113.24
12	L	1004	MQE	CAY-CAX-CBQ	-2.19	116.15	118.50
9	3	101	BCL	C12-C11-C10	-2.19	103.16	113.24
9	F	101	BCL	C12-C11-C10	-2.19	103.17	113.24
10	A	103	KGD	CAL-CAM-CAO	-2.19	115.58	118.94
10	H	103	KGD	CBM-CBN-CBL	-2.19	120.26	126.42
11	L	1005	BPH	CMA-C3A-C4A	-2.19	109.58	114.38
9	U	101	BCL	C3C-C2C-C1C	2.19	105.40	101.87
9	J	102	BCL	C3C-C2C-C1C	2.19	105.40	101.87
9	2	102	BCL	C3C-C2C-C1C	2.19	105.40	101.87
9	A	102	BCL	C3C-C2C-C1C	2.19	105.40	101.87
9	5	101	BCL	C12-C11-C10	-2.19	103.20	113.24
10	A	104	KGD	CBM-CBJ-CBH	-2.18	124.19	127.31
9	P	101	BCL	C12-C11-C10	-2.18	103.20	113.24
12	M	701	MQE	CAJ-CAD-CAQ	-2.18	105.80	112.98
10	T	102	KGD	CBK-CBH-CBF	2.18	121.51	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	102	KGD	CAN-CAM-CAO	2.18	125.97	122.92
9	0	102	BCL	C12-C11-C10	-2.18	103.23	113.24
9	M	703	BCL	C1-O2A-CGA	2.18	122.16	116.44
10	0	104	KGD	CBF-CBH-CBJ	-2.18	115.60	118.94
9	2	103	BCL	C12-C11-C10	-2.18	103.24	113.24
10	2	104	KGD	OAA-CAI-CAH	2.17	122.89	120.96
9	E	101	BCL	C12-C11-C10	-2.17	103.25	113.24
9	W	103	BCL	C12-C11-C10	-2.17	103.25	113.24
10	K	102	KGD	CBB-CAV-CAR	-2.17	124.21	127.31
9	6	102	BCL	C12-C11-C10	-2.17	103.26	113.24
9	O	101	BCL	C12-C11-C10	-2.17	103.26	113.24
9	G	101	BCL	C12-C11-C10	-2.17	103.26	113.24
9	8	102	BCL	C12-C11-C10	-2.17	103.26	113.24
9	J	101	BCL	CGD-CBD-CAD	-2.17	103.70	110.73
9	R	101	BCL	CGD-CBD-CAD	-2.17	103.70	110.73
9	U	102	BCL	C12-C11-C10	-2.17	103.27	113.24
9	1	101	BCL	CGD-CBD-CAD	-2.17	103.71	110.73
9	D	101	BCL	CGD-CBD-CAD	-2.17	103.71	110.73
9	W	102	BCL	C2A-C1A-CHA	2.17	127.65	123.86
9	K	101	BCL	C12-C11-C10	-2.17	103.28	113.24
9	H	101	BCL	CGD-CBD-CAD	-2.17	103.71	110.73
9	N	101	BCL	CGD-CBD-CAD	-2.17	103.71	110.73
10	0	104	KGD	CBE-CBF-CBH	-2.17	120.33	126.42
9	4	102	BCL	C12-C11-C10	-2.17	103.28	113.24
9	B	101	BCL	C12-C11-C10	-2.17	103.28	113.24
9	Q	102	BCL	C12-C11-C10	-2.17	103.28	113.24
9	I	101	BCL	C12-C11-C10	-2.17	103.29	113.24
9	S	103	BCL	C12-C11-C10	-2.17	103.29	113.24
9	S	102	BCL	C2A-C1A-CHA	2.17	127.64	123.86
10	S	101	KGD	CAP-CAQ-CAR	-2.16	120.33	126.42
9	F	101	BCL	CGD-CBD-CAD	-2.16	103.72	110.73
9	T	101	BCL	CGD-CBD-CAD	-2.16	103.72	110.73
9	8	101	BCL	C2A-C1A-CHA	2.16	127.64	123.86
9	5	101	BCL	CGD-CBD-CAD	-2.16	103.73	110.73
10	U	103	KGD	CAZ-CAW-CAS	2.16	118.91	115.27
9	9	102	BCL	CGD-CBD-CAD	-2.16	103.73	110.73
10	E	102	KGD	CBA-CBE-CBF	-2.16	116.48	123.22
9	7	101	BCL	CGD-CBD-CAD	-2.16	103.74	110.73
9	3	101	BCL	CGD-CBD-CAD	-2.16	103.74	110.73
10	I	102	KGD	CAO-CAP-CAQ	-2.16	116.48	123.22
9	P	101	BCL	CGD-CBD-CAD	-2.16	103.74	110.73
10	W	101	KGD	CAN-CAM-CAO	2.15	125.94	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	103	KGD	CAE-CAC-CAB	-2.15	109.72	113.18
9	A	101	BCL	CGD-CBD-CAD	-2.15	103.77	110.73
11	M	704	BPH	CMC-C2C-C1C	-2.15	109.67	114.38
9	W	102	BCL	C3C-C2C-C1C	2.15	105.34	101.87
10	9	101	KGD	CAZ-CAW-CAS	2.15	118.88	115.27
9	2	102	BCL	C2A-C1A-CHA	2.15	127.61	123.86
9	4	101	BCL	C2A-C1A-CHA	2.15	127.61	123.86
9	0	101	BCL	C12-C11-C10	-2.14	103.39	113.24
9	F	101	BCL	CBB-CAB-C3B	2.14	126.70	120.34
9	W	102	BCL	C12-C11-C10	-2.14	103.40	113.24
10	A	103	KGD	CAQ-CAR-CAV	-2.14	115.66	118.94
9	F	102	BCL	C2A-C1A-CHA	2.14	127.60	123.86
9	S	102	BCL	CED-O2D-CGD	-2.14	111.10	115.94
9	5	101	BCL	CBB-CAB-C3B	2.14	126.69	120.34
10	K	102	KGD	CBK-CBH-CBJ	2.14	125.92	122.92
9	0	101	BCL	C2A-C1A-CHA	2.14	127.60	123.86
9	A	102	BCL	C2A-C1A-CHA	2.14	127.60	123.86
9	6	101	BCL	C2A-C1A-CHA	2.14	127.59	123.86
9	Q	101	BCL	C2A-C1A-CHA	2.14	127.59	123.86
9	D	101	BCL	CBB-CAB-C3B	2.14	126.68	120.34
9	F	102	BCL	C12-C11-C10	-2.13	103.43	113.24
10	B	102	KGD	CBN-CBL-CBI	-2.13	115.67	118.94
9	R	101	BCL	CBB-CAB-C3B	2.13	126.68	120.34
9	2	102	BCL	C12-C11-C10	-2.13	103.43	113.24
9	4	101	BCL	C12-C11-C10	-2.13	103.44	113.24
9	9	102	BCL	CBB-CAB-C3B	2.13	126.67	120.34
9	8	101	BCL	C12-C11-C10	-2.13	103.44	113.24
9	J	101	BCL	CBB-CAB-C3B	2.13	126.67	120.34
9	2	102	BCL	CED-O2D-CGD	-2.13	111.12	115.94
9	D	102	BCL	C12-C11-C10	-2.13	103.45	113.24
9	D	102	BCL	CED-O2D-CGD	-2.13	111.12	115.94
9	1	101	BCL	CBB-CAB-C3B	2.13	126.67	120.34
9	P	101	BCL	CBB-CAB-C3B	2.13	126.67	120.34
9	F	102	BCL	CED-O2D-CGD	-2.13	111.12	115.94
9	H	102	BCL	C12-C11-C10	-2.13	103.45	113.24
9	U	101	BCL	C12-C11-C10	-2.13	103.45	113.24
9	N	102	BCL	C12-C11-C10	-2.13	103.45	113.24
9	H	102	BCL	C2A-C1A-CHA	2.13	127.58	123.86
9	X	101	BCL	CBB-CAB-C3B	2.13	126.66	120.34
9	0	101	BCL	CED-O2D-CGD	-2.13	111.12	115.94
9	3	101	BCL	CBB-CAB-C3B	2.13	126.66	120.34
9	J	102	BCL	C12-C11-C10	-2.13	103.46	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	102	BCL	CED-O2D-CGD	-2.13	111.12	115.94
9	6	101	BCL	C12-C11-C10	-2.13	103.47	113.24
9	D	102	BCL	C2A-C1A-CHA	2.13	127.58	123.86
10	P	102	KGD	CAQ-CAR-CAV	-2.13	115.68	118.94
13	P	104	PGV	C01-O03-C19	2.13	124.99	117.12
10	S	101	KGD	CAZ-CAW-CAS	2.13	118.85	115.27
10	9	101	KGD	CAQ-CAR-CAV	-2.12	115.68	118.94
9	U	101	BCL	CED-O2D-CGD	-2.12	111.13	115.94
9	H	101	BCL	CBB-CAB-C3B	2.12	126.65	120.34
9	N	102	BCL	C2A-C1A-CHA	2.12	127.57	123.86
9	S	102	BCL	C12-C11-C10	-2.12	103.48	113.24
9	J	102	BCL	CED-O2D-CGD	-2.12	111.14	115.94
9	Q	101	BCL	C12-C11-C10	-2.12	103.49	113.24
12	M	705	MQE	CAS-CBH-CAW	-2.12	122.55	127.66
10	5	102	KGD	CAE-CAI-CAH	-2.12	116.70	118.65
9	7	101	BCL	CBB-CAB-C3B	2.12	126.63	120.34
10	S	104	KGD	CAE-CAC-CAB	-2.12	109.78	113.18
9	J	102	BCL	C2A-C1A-CHA	2.12	127.56	123.86
9	N	101	BCL	CBB-CAB-C3B	2.12	126.63	120.34
9	8	101	BCL	CED-O2D-CGD	-2.12	111.15	115.94
9	A	102	BCL	C12-C11-C10	-2.12	103.51	113.24
10	3	102	KGD	CAN-CAM-CAO	2.12	125.89	122.92
9	A	101	BCL	CBB-CAB-C3B	2.12	126.62	120.34
9	6	101	BCL	CED-O2D-CGD	-2.12	111.15	115.94
9	U	101	BCL	C2A-C1A-CHA	2.12	127.56	123.86
9	L	1002	BCL	CMD-C2D-C1D	2.11	128.44	124.71
9	A	102	BCL	CED-O2D-CGD	-2.11	111.16	115.94
9	L	1001	BCL	C4A-NA-C1A	-2.11	105.76	106.71
15	C	403	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
9	X	101	BCL	C2A-C3A-C4A	-2.11	98.46	101.87
10	P	102	KGD	CBK-CBH-CBF	2.11	121.40	118.08
10	C	401	KGD	CBG-CBB-CAV	2.11	127.79	123.47
9	T	101	BCL	CBB-CAB-C3B	2.11	126.60	120.34
9	4	101	BCL	CED-O2D-CGD	-2.11	111.17	115.94
9	H	102	BCL	CED-O2D-CGD	-2.11	111.17	115.94
9	Q	101	BCL	CED-O2D-CGD	-2.10	111.18	115.94
10	8	103	KGD	CBJ-CBM-CBN	-2.10	116.67	123.22
10	Q	103	KGD	OAA-CAI-CAH	2.10	122.82	120.96
9	4	101	BCL	CAA-CBA-CGA	-2.10	107.13	113.25
10	B	102	KGD	CBD-CAY-CBC	2.10	119.23	114.60
9	2	103	BCL	CED-O2D-CGD	-2.09	111.20	115.94
9	6	102	BCL	CED-O2D-CGD	-2.09	111.20	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	401	KGD	CAZ-CAW-CAS	2.09	118.79	115.27
9	I	101	BCL	CED-O2D-CGD	-2.09	111.21	115.94
10	J	103	KGD	CAP-CAQ-CAR	-2.09	120.56	126.42
10	A	103	KGD	CBM-CBN-CBL	-2.08	120.56	126.42
9	H	102	BCL	CAA-CBA-CGA	-2.08	107.16	113.25
9	O	101	BCL	CED-O2D-CGD	-2.08	111.22	115.94
9	0	101	BCL	CAA-CBA-CGA	-2.08	107.17	113.25
9	S	102	BCL	CAA-CBA-CGA	-2.08	107.17	113.25
9	8	101	BCL	CAA-CBA-CGA	-2.08	107.17	113.25
9	A	102	BCL	CAA-CBA-CGA	-2.08	107.17	113.25
9	5	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
9	N	101	BCL	CED-O2D-CGD	-2.08	111.24	115.94
9	N	102	BCL	CAA-CBA-CGA	-2.08	107.18	113.25
9	A	101	BCL	CED-O2D-CGD	-2.08	111.24	115.94
9	P	101	BCL	CHC-C1C-NC	2.08	127.39	124.51
9	1	101	BCL	CED-O2D-CGD	-2.08	111.24	115.94
10	A	103	KGD	CAO-CAP-CAQ	-2.08	116.74	123.22
9	H	101	BCL	CED-O2D-CGD	-2.07	111.25	115.94
9	9	102	BCL	CED-O2D-CGD	-2.07	111.25	115.94
9	K	101	BCL	CED-O2D-CGD	-2.07	111.25	115.94
9	Q	102	BCL	CED-O2D-CGD	-2.07	111.25	115.94
9	2	102	BCL	CAA-CBA-CGA	-2.07	107.19	113.25
9	D	102	BCL	CAA-CBA-CGA	-2.07	107.20	113.25
9	J	102	BCL	CAA-CBA-CGA	-2.07	107.20	113.25
9	7	101	BCL	CED-O2D-CGD	-2.07	111.25	115.94
11	L	1003	BPH	O2A-CGA-CBA	2.07	118.41	111.91
9	F	102	BCL	CAA-CBA-CGA	-2.07	107.20	113.25
9	5	101	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	J	101	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	8	102	BCL	CED-O2D-CGD	-2.07	111.26	115.94
13	Z	101	PGV	O01-C1-C2	2.07	115.96	111.50
9	Q	101	BCL	CAA-CBA-CGA	-2.07	107.21	113.25
9	X	101	BCL	CHC-C1C-NC	2.07	127.37	124.51
10	E	102	KGD	CBK-CBH-CBF	2.07	121.33	118.08
12	L	1004	MQE	CCA-CBB-CAN	2.07	118.75	115.27
9	W	103	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	S	103	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	G	101	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	H	101	BCL	CHC-C1C-NC	2.06	127.37	124.51
9	6	101	BCL	CAA-CBA-CGA	-2.06	107.22	113.25
9	W	102	BCL	CAA-CBA-CGA	-2.06	107.22	113.25
9	U	101	BCL	CAA-CBA-CGA	-2.06	107.22	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	404	HEM	C3D-C4D-ND	-2.06	107.87	110.17
10	0	103	KGD	CAL-CAM-CAO	-2.06	115.77	118.94
9	0	102	BCL	CED-O2D-CGD	-2.06	111.27	115.94
9	3	101	BCL	CED-O2D-CGD	-2.06	111.27	115.94
13	P	104	PGV	C22-C21-C20	-2.06	105.78	113.19
9	F	101	BCL	CED-O2D-CGD	-2.06	111.28	115.94
9	4	102	BCL	CED-O2D-CGD	-2.06	111.28	115.94
9	B	101	BCL	CED-O2D-CGD	-2.06	111.28	115.94
9	E	101	BCL	CED-O2D-CGD	-2.06	111.28	115.94
9	U	102	BCL	CED-O2D-CGD	-2.06	111.28	115.94
10	T	102	KGD	CAF-CAB-CAD	-2.06	106.96	110.30
10	I	102	KGD	CBJ-CBM-CBN	-2.06	116.80	123.22
9	X	101	BCL	CED-O2D-CGD	-2.06	111.28	115.94
9	9	102	BCL	CHC-C1C-NC	2.06	127.36	124.51
10	2	101	KGD	CAO-CAP-CAQ	-2.06	116.80	123.22
9	P	101	BCL	CED-O2D-CGD	-2.06	111.29	115.94
9	T	101	BCL	CHC-C1C-NC	2.06	127.35	124.51
11	M	704	BPH	C11-C12-C13	-2.06	109.28	115.92
10	S	104	KGD	CAO-CAP-CAQ	-2.05	116.81	123.22
10	A	103	KGD	CAZ-CAW-CAS	2.05	118.72	115.27
9	F	101	BCL	CHC-C1C-NC	2.05	127.35	124.51
9	R	101	BCL	CED-O2D-CGD	-2.05	111.30	115.94
9	D	101	BCL	CED-O2D-CGD	-2.05	111.30	115.94
11	L	1003	BPH	O2A-CGA-O1A	-2.05	118.42	123.59
10	9	101	KGD	CAO-CAP-CAQ	-2.05	116.82	123.22
9	N	101	BCL	CHC-C1C-NC	2.05	127.34	124.51
9	6	102	BCL	CGD-CBD-CAD	-2.04	104.11	110.73
9	7	101	BCL	CHC-C1C-NC	2.04	127.34	124.51
9	8	102	BCL	CGD-CBD-CAD	-2.04	104.11	110.73
10	J	103	KGD	CAN-CAM-CAO	2.04	125.78	122.92
9	E	101	BCL	CGD-CBD-CAD	-2.04	104.12	110.73
9	T	101	BCL	CED-O2D-CGD	-2.04	111.32	115.94
9	S	103	BCL	CGD-CBD-CAD	-2.04	104.12	110.73
10	P	102	KGD	CAC-CAB-CAD	-2.04	107.34	110.48
10	2	101	KGD	CBJ-CBM-CBN	-2.04	116.85	123.22
9	B	101	BCL	CGD-CBD-CAD	-2.04	104.13	110.73
10	4	103	KGD	CBJ-CBM-CBN	-2.04	116.86	123.22
9	4	102	BCL	CGD-CBD-CAD	-2.04	104.14	110.73
9	O	101	BCL	CGD-CBD-CAD	-2.04	104.14	110.73
9	2	103	BCL	CGD-CBD-CAD	-2.04	104.14	110.73
9	U	102	BCL	CGD-CBD-CAD	-2.04	104.14	110.73
9	Q	102	BCL	CGD-CBD-CAD	-2.04	104.14	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	W	103	BCL	CGD-CBD-CAD	-2.03	104.14	110.73
9	K	101	BCL	CGD-CBD-CAD	-2.03	104.15	110.73
9	W	102	BCL	C5-C3-C2	2.03	125.23	121.12
9	3	101	BCL	CHC-C1C-NC	2.03	127.32	124.51
10	H	103	KGD	CBK-CBH-CBJ	2.03	125.77	122.92
10	O	102	KGD	CBB-CBG-CBI	-2.03	119.31	123.47
9	I	101	BCL	CGD-CBD-CAD	-2.03	104.16	110.73
10	I	102	KGD	CBM-CBJ-CBH	-2.03	124.42	127.31
10	0	103	KGD	CBO-CBL-CBI	2.03	125.76	122.92
9	G	101	BCL	CGD-CBD-CAD	-2.03	104.17	110.73
10	2	104	KGD	CBN-CBL-CBI	-2.03	115.83	118.94
10	Q	103	KGD	CBK-CBH-CBF	2.03	121.27	118.08
9	J	101	BCL	CHC-C1C-NC	2.02	127.31	124.51
13	P	103	PGV	P-O11-C03	-2.02	109.81	121.68
9	2	103	BCL	CHC-C1C-NC	2.02	127.31	124.51
9	6	102	BCL	CHC-C1C-NC	2.02	127.31	124.51
10	H	103	KGD	CAP-CAQ-CAR	-2.02	120.74	126.42
9	R	101	BCL	CHC-C1C-NC	2.02	127.31	124.51
9	S	103	BCL	CHC-C1C-NC	2.02	127.31	124.51
9	D	101	BCL	CHC-C1C-NC	2.02	127.30	124.51
10	O	102	KGD	CAQ-CAR-CAV	-2.02	115.84	118.94
10	I	102	KGD	CBN-CBL-CBI	-2.02	115.85	118.94
9	0	102	BCL	CGD-CBD-CAD	-2.02	104.20	110.73
10	S	104	KGD	CAQ-CAR-CAV	-2.02	115.85	118.94
9	1	101	BCL	CHC-C1C-NC	2.01	127.30	124.51
12	M	701	MQE	CBA-CAU-CAZ	-2.01	106.36	112.98
10	S	104	KGD	CAC-CAB-CAD	-2.01	107.38	110.48
9	4	102	BCL	CHC-C1C-NC	2.01	127.30	124.51
15	C	404	HEM	CAD-CBD-CGD	-2.01	109.27	113.60
10	O	102	KGD	CBF-CBH-CBJ	-2.01	115.86	118.94
10	9	101	KGD	CAK-CAH-CAD	-2.01	120.88	124.11
9	U	102	BCL	CHC-C1C-NC	2.01	127.29	124.51
9	Q	101	BCL	C1-C2-C3	-2.01	122.57	126.04
9	8	101	BCL	C1-C2-C3	-2.01	122.57	126.04
9	K	101	BCL	CHC-C1C-NC	2.01	127.29	124.51
9	J	102	BCL	C1-C2-C3	-2.01	122.57	126.04
9	M	703	BCL	CBB-CAB-C3B	2.01	126.30	120.34
12	M	701	MQE	CCD-CCI-CCM	-2.01	105.29	111.88
9	G	101	BCL	CHC-C1C-NC	2.00	127.28	124.51
9	H	102	BCL	C1-C2-C3	-2.00	122.58	126.04
10	S	104	KGD	CBJ-CBM-CBN	-2.00	116.97	123.22
9	A	101	BCL	CHC-C1C-NC	2.00	127.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	O	101	BCL	CHC-C1C-NC	2.00	127.28	124.51
9	6	101	BCL	C1-C2-C3	-2.00	122.58	126.04
9	A	102	BCL	C1-C2-C3	-2.00	122.58	126.04

There are no chirality outliers.

All (1150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	0	101	BCL	C4C-C3C-CAC-CBC
9	0	102	BCL	C4C-C3C-CAC-CBC
9	0	102	BCL	C4-C3-C5-C6
9	1	101	BCL	CHA-CBD-CGD-O1D
9	2	102	BCL	C4C-C3C-CAC-CBC
9	2	103	BCL	C4C-C3C-CAC-CBC
9	2	103	BCL	C4-C3-C5-C6
9	3	101	BCL	CHA-CBD-CGD-O1D
9	4	101	BCL	C4C-C3C-CAC-CBC
9	4	102	BCL	C4C-C3C-CAC-CBC
9	4	102	BCL	C4-C3-C5-C6
9	5	101	BCL	CHA-CBD-CGD-O1D
9	6	101	BCL	C4C-C3C-CAC-CBC
9	6	102	BCL	C4C-C3C-CAC-CBC
9	6	102	BCL	C4-C3-C5-C6
9	7	101	BCL	CHA-CBD-CGD-O1D
9	8	101	BCL	C4C-C3C-CAC-CBC
9	8	102	BCL	C4C-C3C-CAC-CBC
9	8	102	BCL	C4-C3-C5-C6
9	9	102	BCL	CHA-CBD-CGD-O1D
9	A	101	BCL	CHA-CBD-CGD-O1D
9	A	102	BCL	C4C-C3C-CAC-CBC
9	B	101	BCL	C4C-C3C-CAC-CBC
9	B	101	BCL	C4-C3-C5-C6
9	D	101	BCL	CHA-CBD-CGD-O1D
9	D	102	BCL	C4C-C3C-CAC-CBC
9	E	101	BCL	C4C-C3C-CAC-CBC
9	E	101	BCL	C4-C3-C5-C6
9	F	101	BCL	CHA-CBD-CGD-O1D
9	F	102	BCL	C4C-C3C-CAC-CBC
9	G	101	BCL	C4C-C3C-CAC-CBC
9	G	101	BCL	C4-C3-C5-C6
9	H	101	BCL	CHA-CBD-CGD-O1D
9	H	102	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
9	I	101	BCL	C4C-C3C-CAC-CBC
9	I	101	BCL	C4-C3-C5-C6
9	J	101	BCL	CHA-CBD-CGD-O1D
9	J	102	BCL	C4C-C3C-CAC-CBC
9	K	101	BCL	C4C-C3C-CAC-CBC
9	K	101	BCL	C4-C3-C5-C6
9	L	1001	BCL	C4C-C3C-CAC-CBC
9	L	1001	BCL	C1-C2-C3-C4
9	L	1002	BCL	C2C-C3C-CAC-CBC
9	L	1002	BCL	CHA-CBD-CGD-O1D
9	L	1002	BCL	CBD-CGD-O2D-CED
9	L	1002	BCL	C1-C2-C3-C4
9	L	1002	BCL	C1-C2-C3-C5
9	L	1002	BCL	C2-C3-C5-C6
9	N	101	BCL	CHA-CBD-CGD-O1D
9	N	102	BCL	C4C-C3C-CAC-CBC
9	O	101	BCL	C4C-C3C-CAC-CBC
9	O	101	BCL	C4-C3-C5-C6
9	P	101	BCL	CHA-CBD-CGD-O1D
9	Q	101	BCL	C4C-C3C-CAC-CBC
9	Q	102	BCL	C4C-C3C-CAC-CBC
9	Q	102	BCL	C4-C3-C5-C6
9	R	101	BCL	CHA-CBD-CGD-O1D
9	S	102	BCL	C4C-C3C-CAC-CBC
9	S	103	BCL	C4C-C3C-CAC-CBC
9	S	103	BCL	C4-C3-C5-C6
9	T	101	BCL	CHA-CBD-CGD-O1D
9	U	101	BCL	C4C-C3C-CAC-CBC
9	U	102	BCL	C4C-C3C-CAC-CBC
9	U	102	BCL	C4-C3-C5-C6
9	W	102	BCL	C4C-C3C-CAC-CBC
9	W	102	BCL	C6-C7-C8-C9
9	W	103	BCL	C4C-C3C-CAC-CBC
9	W	103	BCL	C4-C3-C5-C6
9	X	101	BCL	CHA-CBD-CGD-O1D
9	X	101	BCL	C1-C2-C3-C5
10	2	101	KGD	CAP-CAQ-CAR-CAU
10	2	101	KGD	CAP-CAQ-CAR-CAV
10	2	101	KGD	CBH-CBJ-CBM-CBN
10	3	102	KGD	CAJ-CAL-CAM-CAN
10	4	103	KGD	CAJ-CAL-CAM-CAN
10	4	103	KGD	CAJ-CAL-CAM-CAO

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Mol	Chain	Res	Type	Atoms
10	4	103	KGD	CAP-CAQ-CAR-CAU
10	4	103	KGD	CAW-CAS-CAT-CAX
10	5	102	KGD	CBE-CBF-CBH-CBJ
10	5	102	KGD	CBE-CBF-CBH-CBK
10	8	103	KGD	CAH-CAD-CAJ-CAL
10	8	103	KGD	CAJ-CAL-CAM-CAN
10	8	103	KGD	CAJ-CAL-CAM-CAO
10	8	103	KGD	CAP-CAQ-CAR-CAU
10	8	103	KGD	CAP-CAQ-CAR-CAV
10	8	103	KGD	CAR-CAV-CBB-CBG
10	8	103	KGD	CBE-CBF-CBH-CBJ
10	8	103	KGD	CBE-CBF-CBH-CBK
10	9	101	KGD	CAT-CAS-CAW-CAZ
10	9	101	KGD	CAT-CAS-CAW-CBA
10	A	104	KGD	CAW-CAS-CAT-CAX
10	B	102	KGD	CAW-CAS-CAT-CAX
10	B	102	KGD	CAT-CAS-CAW-CAZ
10	B	102	KGD	CAT-CAS-CAW-CBA
10	E	102	KGD	CAW-CAS-CAT-CAX
10	F	103	KGD	CAJ-CAL-CAM-CAN
10	F	103	KGD	CAJ-CAL-CAM-CAO
10	G	102	KGD	CAJ-CAL-CAM-CAN
10	G	102	KGD	CAJ-CAL-CAM-CAO
10	G	102	KGD	CBE-CBF-CBH-CBJ
10	G	102	KGD	CBE-CBF-CBH-CBK
10	G	102	KGD	CBO-CBL-CBN-CBM
10	I	102	KGD	CAB-CAD-CAJ-CAL
10	I	102	KGD	CAS-CAT-CAX-CAY
10	J	103	KGD	CAJ-CAL-CAM-CAN
10	K	102	KGD	CAH-CAD-CAJ-CAL
10	K	102	KGD	CAJ-CAL-CAM-CAN
10	K	102	KGD	CAJ-CAL-CAM-CAO
10	K	102	KGD	CAW-CAS-CAT-CAX
10	K	102	KGD	CAT-CAS-CAW-CAZ
10	K	102	KGD	CAT-CAS-CAW-CBA
10	K	102	KGD	CBE-CBF-CBH-CBJ
10	K	102	KGD	CBE-CBF-CBH-CBK
10	N	103	KGD	CBE-CBF-CBH-CBJ
10	N	103	KGD	CBE-CBF-CBH-CBK
10	O	102	KGD	CAP-CAQ-CAR-CAU
10	O	102	KGD	CAP-CAQ-CAR-CAV
10	O	102	KGD	CAW-CBA-CBE-CBF

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Mol	Chain	Res	Type	Atoms
10	O	102	KGD	CBE-CBF-CBH-CBJ
10	O	102	KGD	CBE-CBF-CBH-CBK
10	P	102	KGD	CAJ-CAL-CAM-CAN
10	P	102	KGD	CAJ-CAL-CAM-CAO
10	Q	103	KGD	CAH-CAD-CAJ-CAL
10	Q	103	KGD	CAJ-CAL-CAM-CAN
10	Q	103	KGD	CAJ-CAL-CAM-CAO
10	Q	103	KGD	CAP-CAQ-CAR-CAU
10	Q	103	KGD	CAT-CAS-CAW-CAZ
10	Q	103	KGD	CAT-CAS-CAW-CBA
10	S	101	KGD	CAB-CAD-CAJ-CAL
10	S	101	KGD	CAH-CAD-CAJ-CAL
10	S	101	KGD	CAW-CAS-CAT-CAX
10	T	102	KGD	CBE-CBF-CBH-CBJ
10	T	102	KGD	CBE-CBF-CBH-CBK
10	T	102	KGD	CBI-CBL-CBN-CBM
10	T	102	KGD	CBO-CBL-CBN-CBM
10	U	103	KGD	CBE-CBF-CBH-CBJ
10	U	103	KGD	CBE-CBF-CBH-CBK
10	W	101	KGD	CAP-CAQ-CAR-CAU
10	W	101	KGD	CAP-CAQ-CAR-CAV
10	C	401	KGD	CAJ-CAL-CAM-CAN
10	C	401	KGD	CAW-CBA-CBE-CBF
10	C	401	KGD	CBE-CBF-CBH-CBJ
10	C	401	KGD	CBE-CBF-CBH-CBK
11	L	1003	BPH	C4C-C3C-CAC-CBC
11	L	1003	BPH	C2C-C3C-CAC-CBC
11	M	704	BPH	O2A-C1-C2-C3
12	M	701	MQE	CAR-CAE-CAL-CBF
12	M	701	MQE	CAT-CAF-CAK-CBE
12	M	701	MQE	CAW-CAG-CAM-CBG
13	L	1006	PGV	O03-C01-C02-O01
13	L	1006	PGV	O12-C04-C05-C06
13	L	1007	PGV	C03-O11-P-O14
13	M	706	PGV	O12-C04-C05-C06
13	P	104	PGV	C03-O11-P-O12
13	P	104	PGV	C03-O11-P-O13
13	P	104	PGV	C03-O11-P-O14
13	P	104	PGV	O12-C04-C05-O05
13	P	104	PGV	C04-C05-C06-O06
13	C	406	PGV	C04-C05-C06-O06
13	C	406	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
13	C	406	PGV	C2-C1-O01-C02
13	Z	101	PGV	O12-C04-C05-O05
13	Z	101	PGV	C2-C1-O01-C02
15	C	402	HEM	C2B-C3B-CAB-CBB
15	C	403	HEM	C2B-C3B-CAB-CBB
15	C	404	HEM	C2B-C3B-CAB-CBB
15	C	404	HEM	C4B-C3B-CAB-CBB
15	C	405	HEM	C2B-C3B-CAB-CBB
15	C	405	HEM	C4B-C3B-CAB-CBB
16	Y	101	DGA	CB2-CB1-OG2-CG2
11	L	1005	BPH	CBD-CGD-O2D-CED
9	1	101	BCL	O1A-CGA-O2A-C1
9	3	101	BCL	O1A-CGA-O2A-C1
9	5	101	BCL	O1A-CGA-O2A-C1
9	7	101	BCL	O1A-CGA-O2A-C1
9	9	102	BCL	O1A-CGA-O2A-C1
9	A	101	BCL	O1A-CGA-O2A-C1
9	D	101	BCL	O1A-CGA-O2A-C1
9	F	101	BCL	O1A-CGA-O2A-C1
9	H	101	BCL	O1A-CGA-O2A-C1
9	J	101	BCL	O1A-CGA-O2A-C1
9	N	101	BCL	O1A-CGA-O2A-C1
9	P	101	BCL	O1A-CGA-O2A-C1
9	R	101	BCL	O1A-CGA-O2A-C1
9	T	101	BCL	O1A-CGA-O2A-C1
9	X	101	BCL	O1A-CGA-O2A-C1
13	P	103	PGV	O04-C19-O03-C01
9	L	1001	BCL	CBD-CGD-O2D-CED
9	0	101	BCL	O1A-CGA-O2A-C1
9	2	102	BCL	O1A-CGA-O2A-C1
9	4	101	BCL	O1A-CGA-O2A-C1
9	6	101	BCL	O1A-CGA-O2A-C1
9	8	101	BCL	O1A-CGA-O2A-C1
9	A	102	BCL	O1A-CGA-O2A-C1
9	D	102	BCL	O1A-CGA-O2A-C1
9	F	102	BCL	O1A-CGA-O2A-C1
9	H	102	BCL	O1A-CGA-O2A-C1
9	J	102	BCL	O1A-CGA-O2A-C1
9	N	102	BCL	O1A-CGA-O2A-C1
9	Q	101	BCL	O1A-CGA-O2A-C1
9	S	102	BCL	O1A-CGA-O2A-C1
9	U	101	BCL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
9	W	102	BCL	O1A-CGA-O2A-C1
16	Y	101	DGA	OA1-CA1-OG1-CG1
11	M	704	BPH	CBD-CGD-O2D-CED
13	Z	101	PGV	O02-C1-O01-C02
16	Y	101	DGA	OB1-CB1-OG2-CG2
13	P	103	PGV	C20-C19-O03-C01
11	L	1005	BPH	O1D-CGD-O2D-CED
9	W	102	BCL	CBD-CGD-O2D-CED
12	L	1004	MQE	CAM-CAG-CAW-CBY
12	L	1004	MQE	CAM-CAG-CAW-CBH
9	1	101	BCL	CBD-CGD-O2D-CED
9	3	101	BCL	CBD-CGD-O2D-CED
9	5	101	BCL	CBD-CGD-O2D-CED
9	7	101	BCL	CBD-CGD-O2D-CED
9	9	102	BCL	CBD-CGD-O2D-CED
9	A	101	BCL	CBD-CGD-O2D-CED
9	D	101	BCL	CBD-CGD-O2D-CED
9	F	101	BCL	CBD-CGD-O2D-CED
9	H	101	BCL	CBD-CGD-O2D-CED
9	J	101	BCL	CBD-CGD-O2D-CED
9	N	101	BCL	CBD-CGD-O2D-CED
9	P	101	BCL	CBD-CGD-O2D-CED
9	R	101	BCL	CBD-CGD-O2D-CED
9	T	101	BCL	CBD-CGD-O2D-CED
9	X	101	BCL	CBD-CGD-O2D-CED
9	L	1001	BCL	C2A-CAA-CBA-CGA
11	L	1005	BPH	C2A-CAA-CBA-CGA
9	1	101	BCL	O1D-CGD-O2D-CED
9	3	101	BCL	O1D-CGD-O2D-CED
9	5	101	BCL	O1D-CGD-O2D-CED
9	7	101	BCL	O1D-CGD-O2D-CED
9	9	102	BCL	O1D-CGD-O2D-CED
9	A	101	BCL	O1D-CGD-O2D-CED
9	D	101	BCL	O1D-CGD-O2D-CED
9	F	101	BCL	O1D-CGD-O2D-CED
9	H	101	BCL	O1D-CGD-O2D-CED
9	J	101	BCL	O1D-CGD-O2D-CED
9	M	703	BCL	O1D-CGD-O2D-CED
9	N	101	BCL	O1D-CGD-O2D-CED
9	P	101	BCL	O1D-CGD-O2D-CED
9	R	101	BCL	O1D-CGD-O2D-CED
9	T	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	L	1001	BCL	C3-C5-C6-C7
9	0	101	BCL	CBA-CGA-O2A-C1
9	1	101	BCL	CBA-CGA-O2A-C1
9	2	102	BCL	CBA-CGA-O2A-C1
9	3	101	BCL	CBA-CGA-O2A-C1
9	4	101	BCL	CBA-CGA-O2A-C1
9	5	101	BCL	CBA-CGA-O2A-C1
9	6	101	BCL	CBA-CGA-O2A-C1
9	7	101	BCL	CBA-CGA-O2A-C1
9	8	101	BCL	CBA-CGA-O2A-C1
9	9	102	BCL	CBA-CGA-O2A-C1
9	A	101	BCL	CBA-CGA-O2A-C1
9	A	102	BCL	CBA-CGA-O2A-C1
9	D	101	BCL	CBA-CGA-O2A-C1
9	D	102	BCL	CBA-CGA-O2A-C1
9	F	101	BCL	CBA-CGA-O2A-C1
9	F	102	BCL	CBA-CGA-O2A-C1
9	H	101	BCL	CBA-CGA-O2A-C1
9	H	102	BCL	CBA-CGA-O2A-C1
9	J	101	BCL	CBA-CGA-O2A-C1
9	J	102	BCL	CBA-CGA-O2A-C1
9	N	101	BCL	CBA-CGA-O2A-C1
9	N	102	BCL	CBA-CGA-O2A-C1
9	P	101	BCL	CBA-CGA-O2A-C1
9	Q	101	BCL	CBA-CGA-O2A-C1
9	R	101	BCL	CBA-CGA-O2A-C1
9	S	102	BCL	CBA-CGA-O2A-C1
9	T	101	BCL	CBA-CGA-O2A-C1
9	U	101	BCL	CBA-CGA-O2A-C1
9	W	102	BCL	CBA-CGA-O2A-C1
9	X	101	BCL	CBA-CGA-O2A-C1
13	P	104	PGV	C20-C19-O03-C01
16	Y	101	DGA	CA2-CA1-OG1-CG1
9	X	101	BCL	O1D-CGD-O2D-CED
9	L	1001	BCL	C1-C2-C3-C5
9	L	1002	BCL	O1D-CGD-O2D-CED
13	L	1007	PGV	O04-C19-O03-C01
13	P	104	PGV	O04-C19-O03-C01
10	0	103	KGD	CBB-CBG-CBI-CBL
10	2	101	KGD	CAW-CBA-CBE-CBF
10	8	103	KGD	CAW-CBA-CBE-CBF
10	U	103	KGD	CAW-CBA-CBE-CBF

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Mol	Chain	Res	Type	Atoms
9	M	703	BCL	CBD-CGD-O2D-CED
9	0	102	BCL	O1D-CGD-O2D-CED
9	2	103	BCL	O1D-CGD-O2D-CED
9	4	102	BCL	O1D-CGD-O2D-CED
9	6	102	BCL	O1D-CGD-O2D-CED
9	8	102	BCL	O1D-CGD-O2D-CED
9	B	101	BCL	O1D-CGD-O2D-CED
9	E	101	BCL	O1D-CGD-O2D-CED
9	G	101	BCL	O1D-CGD-O2D-CED
9	I	101	BCL	O1D-CGD-O2D-CED
9	K	101	BCL	O1D-CGD-O2D-CED
9	O	101	BCL	O1D-CGD-O2D-CED
9	Q	102	BCL	O1D-CGD-O2D-CED
9	S	103	BCL	O1D-CGD-O2D-CED
9	U	102	BCL	O1D-CGD-O2D-CED
9	W	103	BCL	O1D-CGD-O2D-CED
13	L	1006	PGV	O12-C04-C05-O05
13	M	706	PGV	O12-C04-C05-O05
11	L	1005	BPH	CBA-CGA-O2A-C1
9	0	102	BCL	CBD-CGD-O2D-CED
9	2	103	BCL	CBD-CGD-O2D-CED
9	4	102	BCL	CBD-CGD-O2D-CED
9	6	102	BCL	CBD-CGD-O2D-CED
9	8	102	BCL	CBD-CGD-O2D-CED
9	B	101	BCL	CBD-CGD-O2D-CED
9	E	101	BCL	CBD-CGD-O2D-CED
9	G	101	BCL	CBD-CGD-O2D-CED
9	I	101	BCL	CBD-CGD-O2D-CED
9	K	101	BCL	CBD-CGD-O2D-CED
9	O	101	BCL	CBD-CGD-O2D-CED
9	Q	102	BCL	CBD-CGD-O2D-CED
9	S	103	BCL	CBD-CGD-O2D-CED
9	U	102	BCL	CBD-CGD-O2D-CED
9	W	103	BCL	CBD-CGD-O2D-CED
9	X	101	BCL	C3-C5-C6-C7
13	L	1007	PGV	C20-C19-O03-C01
10	2	104	KGD	CAT-CAS-CAW-CAZ
10	3	102	KGD	CAT-CAS-CAW-CAZ
10	6	103	KGD	CAT-CAS-CAW-CAZ
12	L	1004	MQE	CCL-CCC-CCD-CCI
9	0	102	BCL	C2-C3-C5-C6
9	2	103	BCL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
9	4	102	BCL	C2-C3-C5-C6
9	6	102	BCL	C2-C3-C5-C6
9	8	102	BCL	C2-C3-C5-C6
9	B	101	BCL	C2-C3-C5-C6
9	E	101	BCL	C2-C3-C5-C6
9	G	101	BCL	C2-C3-C5-C6
9	I	101	BCL	C2-C3-C5-C6
9	K	101	BCL	C2-C3-C5-C6
9	O	101	BCL	C2-C3-C5-C6
9	Q	102	BCL	C2-C3-C5-C6
9	S	103	BCL	C2-C3-C5-C6
9	U	102	BCL	C2-C3-C5-C6
9	W	103	BCL	C2-C3-C5-C6
10	2	104	KGD	CAT-CAS-CAW-CBA
10	3	102	KGD	CAT-CAS-CAW-CBA
10	6	103	KGD	CAT-CAS-CAW-CBA
12	L	1004	MQE	CCB-CCC-CCD-CCI
11	L	1005	BPH	O1A-CGA-O2A-C1
10	5	102	KGD	CAW-CAS-CAT-CAX
10	G	102	KGD	CAW-CAS-CAT-CAX
10	I	102	KGD	CAW-CAS-CAT-CAX
10	S	104	KGD	CAW-CAS-CAT-CAX
10	C	401	KGD	CAW-CAS-CAT-CAX
12	L	1004	MQE	CAP-CAC-CAI-CBD
12	L	1004	MQE	CAV-CAH-CAO-CBI
12	L	1004	MQE	CCC-CCD-CCI-CCM
12	M	701	MQE	CAV-CAH-CAO-CBI
12	M	701	MQE	CBB-CAN-CAS-CBH
12	M	705	MQE	CBB-CAN-CAS-CBH
13	P	104	PGV	O12-C04-C05-C06
13	Z	101	PGV	O12-C04-C05-C06
9	M	703	BCL	C3-C5-C6-C7
9	L	1001	BCL	CBA-CGA-O2A-C1
13	Z	101	PGV	C1-C2-C3-C4
9	1	101	BCL	C15-C16-C17-C18
9	3	101	BCL	C15-C16-C17-C18
9	5	101	BCL	C15-C16-C17-C18
9	7	101	BCL	C15-C16-C17-C18
9	9	102	BCL	C15-C16-C17-C18
9	A	101	BCL	C15-C16-C17-C18
9	D	101	BCL	C15-C16-C17-C18
9	F	101	BCL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
9	H	101	BCL	C15-C16-C17-C18
9	J	101	BCL	C15-C16-C17-C18
9	N	101	BCL	C15-C16-C17-C18
9	P	101	BCL	C15-C16-C17-C18
9	R	101	BCL	C15-C16-C17-C18
9	T	101	BCL	C15-C16-C17-C18
10	S	104	KGD	CAT-CAS-CAW-CAZ
9	L	1001	BCL	C6-C7-C8-C9
9	L	1002	BCL	C11-C10-C8-C9
10	0	104	KGD	CAJ-CAL-CAM-CAN
10	6	103	KGD	CAJ-CAL-CAM-CAN
10	B	102	KGD	CBO-CBL-CBN-CBM
10	J	103	KGD	CBE-CBF-CBH-CBK
10	N	103	KGD	CAP-CAQ-CAR-CAU
10	O	102	KGD	CBO-CBL-CBN-CBM
10	S	104	KGD	CAJ-CAL-CAM-CAN
10	6	103	KGD	CAJ-CAL-CAM-CAO
10	W	101	KGD	CAJ-CAL-CAM-CAO
9	X	101	BCL	C5-C6-C7-C8
9	W	102	BCL	O1D-CGD-O2D-CED
9	L	1001	BCL	C13-C15-C16-C17
13	P	104	PGV	O05-C05-C06-O06
13	P	103	PGV	C19-C20-C21-C22
9	0	101	BCL	CBD-CGD-O2D-CED
9	2	102	BCL	CBD-CGD-O2D-CED
9	4	101	BCL	CBD-CGD-O2D-CED
9	6	101	BCL	CBD-CGD-O2D-CED
9	8	101	BCL	CBD-CGD-O2D-CED
9	A	102	BCL	CBD-CGD-O2D-CED
9	D	102	BCL	CBD-CGD-O2D-CED
9	F	102	BCL	CBD-CGD-O2D-CED
9	H	102	BCL	CBD-CGD-O2D-CED
9	J	102	BCL	CBD-CGD-O2D-CED
9	N	102	BCL	CBD-CGD-O2D-CED
9	Q	101	BCL	CBD-CGD-O2D-CED
9	S	102	BCL	CBD-CGD-O2D-CED
9	U	101	BCL	CBD-CGD-O2D-CED
11	L	1005	BPH	C13-C15-C16-C17
11	M	704	BPH	C11-C10-C8-C7
11	M	704	BPH	O1D-CGD-O2D-CED
9	X	101	BCL	C10-C11-C12-C13
10	8	103	KGD	CAW-CAS-CAT-CAX

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Mol	Chain	Res	Type	Atoms
10	Q	103	KGD	CAW-CAS-CAT-CAX
10	U	103	KGD	CAW-CAS-CAT-CAX
12	L	1004	MQE	CAZ-CAU-CBA-CBN
12	M	701	MQE	CAQ-CAD-CAJ-CBC
12	M	701	MQE	CCC-CCD-CCI-CCM
9	L	1001	BCL	C8-C10-C11-C12
9	M	703	BCL	C5-C6-C7-C8
11	M	704	BPH	C5-C6-C7-C8
9	M	703	BCL	C15-C16-C17-C18
13	L	1006	PGV	C03-O11-P-O12
13	L	1007	PGV	C03-O11-P-O12
13	M	706	PGV	C03-O11-P-O12
13	P	103	PGV	C04-O12-P-O11
12	M	701	MQE	CAL-CAE-CAR-CBV
12	M	701	MQE	CAO-CAH-CAV-CBX
9	1	101	BCL	C2A-CAA-CBA-CGA
9	3	101	BCL	C2A-CAA-CBA-CGA
9	5	101	BCL	C2A-CAA-CBA-CGA
9	7	101	BCL	C2A-CAA-CBA-CGA
9	9	102	BCL	C2A-CAA-CBA-CGA
9	A	101	BCL	C2A-CAA-CBA-CGA
9	D	101	BCL	C2A-CAA-CBA-CGA
9	F	101	BCL	C2A-CAA-CBA-CGA
9	H	101	BCL	C2A-CAA-CBA-CGA
9	J	101	BCL	C2A-CAA-CBA-CGA
9	N	101	BCL	C2A-CAA-CBA-CGA
9	P	101	BCL	C2A-CAA-CBA-CGA
9	R	101	BCL	C2A-CAA-CBA-CGA
9	T	101	BCL	C2A-CAA-CBA-CGA
9	X	101	BCL	C2A-CAA-CBA-CGA
16	Y	101	DGA	CA5-CA6-CA7-CA8
13	C	406	PGV	C01-C02-O01-C1
13	P	103	PGV	C25-C26-C27-C28
12	M	701	MQE	CAL-CAE-CAR-CBD
9	1	101	BCL	C11-C12-C13-C14
9	3	101	BCL	C11-C12-C13-C14
9	5	101	BCL	C11-C12-C13-C14
9	7	101	BCL	C11-C12-C13-C14
9	9	102	BCL	C11-C12-C13-C14
9	A	101	BCL	C11-C12-C13-C14
9	D	101	BCL	C11-C12-C13-C14
9	F	101	BCL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
9	H	101	BCL	C11-C12-C13-C14
9	J	101	BCL	C11-C12-C13-C14
9	L	1002	BCL	C11-C12-C13-C14
9	N	101	BCL	C11-C12-C13-C14
9	P	101	BCL	C11-C12-C13-C14
9	R	101	BCL	C11-C12-C13-C14
9	T	101	BCL	C11-C12-C13-C14
9	X	101	BCL	C6-C7-C8-C9
10	W	101	KGD	CAJ-CAL-CAM-CAN
10	4	103	KGD	CAP-CAQ-CAR-CAV
10	B	102	KGD	CBI-CBL-CBN-CBM
10	J	103	KGD	CAJ-CAL-CAM-CAO
10	Q	103	KGD	CAP-CAQ-CAR-CAV
13	P	103	PGV	C2-C1-O01-C02
13	P	103	PGV	C26-C27-C28-C29
16	Y	101	DGA	CB9-CAB-CBB-CCB
9	X	101	BCL	C16-C17-C18-C19
12	L	1004	MQE	CBM-CBJ-CBO-CCB
9	J	102	BCL	O1D-CGD-O2D-CED
9	S	102	BCL	O1D-CGD-O2D-CED
9	0	101	BCL	O1D-CGD-O2D-CED
9	0	102	BCL	C3-C5-C6-C7
9	2	103	BCL	C3-C5-C6-C7
9	4	102	BCL	C3-C5-C6-C7
9	6	102	BCL	C3-C5-C6-C7
9	8	102	BCL	C3-C5-C6-C7
9	B	101	BCL	C3-C5-C6-C7
9	E	101	BCL	C3-C5-C6-C7
9	G	101	BCL	C3-C5-C6-C7
9	I	101	BCL	C3-C5-C6-C7
9	K	101	BCL	C3-C5-C6-C7
9	O	101	BCL	C3-C5-C6-C7
9	Q	102	BCL	C3-C5-C6-C7
9	S	103	BCL	C3-C5-C6-C7
9	U	102	BCL	C3-C5-C6-C7
9	W	103	BCL	C3-C5-C6-C7
9	4	101	BCL	O1D-CGD-O2D-CED
9	6	101	BCL	O1D-CGD-O2D-CED
9	8	101	BCL	O1D-CGD-O2D-CED
9	A	102	BCL	O1D-CGD-O2D-CED
9	F	102	BCL	O1D-CGD-O2D-CED
9	H	102	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
9	N	102	BCL	O1D-CGD-O2D-CED
9	Q	101	BCL	O1D-CGD-O2D-CED
9	U	101	BCL	O1D-CGD-O2D-CED
9	1	101	BCL	C3A-C2A-CAA-CBA
9	3	101	BCL	C3A-C2A-CAA-CBA
9	5	101	BCL	C3A-C2A-CAA-CBA
9	7	101	BCL	C3A-C2A-CAA-CBA
9	9	102	BCL	C3A-C2A-CAA-CBA
9	A	101	BCL	C3A-C2A-CAA-CBA
9	D	101	BCL	C3A-C2A-CAA-CBA
9	F	101	BCL	C3A-C2A-CAA-CBA
9	H	101	BCL	C3A-C2A-CAA-CBA
9	J	101	BCL	C3A-C2A-CAA-CBA
9	L	1002	BCL	C3A-C2A-CAA-CBA
9	N	101	BCL	C3A-C2A-CAA-CBA
9	P	101	BCL	C3A-C2A-CAA-CBA
9	R	101	BCL	C3A-C2A-CAA-CBA
9	T	101	BCL	C3A-C2A-CAA-CBA
9	X	101	BCL	C3A-C2A-CAA-CBA
9	2	102	BCL	O1D-CGD-O2D-CED
9	D	102	BCL	O1D-CGD-O2D-CED
13	L	1007	PGV	C7-C8-C9-C10
10	0	104	KGD	CAT-CAS-CAW-CBA
11	L	1003	BPH	C2-C3-C5-C6
13	C	406	PGV	C22-C23-C24-C25
9	0	102	BCL	C16-C17-C18-C19
9	2	103	BCL	C16-C17-C18-C19
9	4	102	BCL	C16-C17-C18-C19
9	6	102	BCL	C16-C17-C18-C19
9	8	102	BCL	C16-C17-C18-C19
9	B	101	BCL	C16-C17-C18-C19
9	E	101	BCL	C16-C17-C18-C19
9	G	101	BCL	C16-C17-C18-C19
9	I	101	BCL	C16-C17-C18-C19
9	K	101	BCL	C16-C17-C18-C19
9	O	101	BCL	C16-C17-C18-C19
9	Q	102	BCL	C16-C17-C18-C19
9	S	103	BCL	C16-C17-C18-C19
9	U	102	BCL	C16-C17-C18-C19
9	W	103	BCL	C16-C17-C18-C19
13	Z	101	PGV	C2-C3-C4-C5
13	P	103	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
13	L	1007	PGV	C5-C6-C7-C8
13	C	406	PGV	C14-C15-C16-C17
11	L	1005	BPH	C15-C16-C17-C18
10	4	103	KGD	CAB-CAD-CAJ-CAL
10	6	103	KGD	CAB-CAD-CAJ-CAL
10	9	101	KGD	CAB-CAD-CAJ-CAL
10	9	101	KGD	CAH-CAD-CAJ-CAL
10	A	103	KGD	CAH-CAD-CAJ-CAL
10	E	102	KGD	CAH-CAD-CAJ-CAL
10	G	102	KGD	CAB-CAD-CAJ-CAL
10	G	102	KGD	CAH-CAD-CAJ-CAL
10	H	103	KGD	CAH-CAD-CAJ-CAL
10	I	102	KGD	CAH-CAD-CAJ-CAL
10	J	103	KGD	CAH-CAD-CAJ-CAL
10	K	102	KGD	CAB-CAD-CAJ-CAL
10	Q	103	KGD	CAB-CAD-CAJ-CAL
10	S	104	KGD	CAH-CAD-CAJ-CAL
11	M	704	BPH	C8-C10-C11-C12
16	Y	101	DGA	CB4-CB5-CB6-CB7
11	M	704	BPH	C10-C11-C12-C13
13	L	1006	PGV	C21-C22-C23-C24
10	0	104	KGD	CAT-CAS-CAW-CAZ
9	1	101	BCL	C11-C12-C13-C15
9	3	101	BCL	C11-C12-C13-C15
9	5	101	BCL	C11-C12-C13-C15
9	7	101	BCL	C11-C12-C13-C15
9	9	102	BCL	C11-C12-C13-C15
9	A	101	BCL	C11-C12-C13-C15
9	D	101	BCL	C11-C12-C13-C15
9	F	101	BCL	C11-C12-C13-C15
9	H	101	BCL	C11-C12-C13-C15
9	J	101	BCL	C11-C12-C13-C15
9	L	1002	BCL	C11-C12-C13-C15
9	N	101	BCL	C11-C12-C13-C15
9	P	101	BCL	C11-C12-C13-C15
9	R	101	BCL	C11-C12-C13-C15
9	T	101	BCL	C11-C12-C13-C15
9	X	101	BCL	C6-C7-C8-C10
11	L	1003	BPH	C11-C10-C8-C7
9	W	102	BCL	C15-C16-C17-C18
10	W	101	KGD	CAM-CAO-CAP-CAQ
9	L	1002	BCL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
9	0	102	BCL	C16-C17-C18-C20
9	2	103	BCL	C16-C17-C18-C20
9	4	102	BCL	C16-C17-C18-C20
9	6	102	BCL	C16-C17-C18-C20
9	8	102	BCL	C16-C17-C18-C20
9	B	101	BCL	C16-C17-C18-C20
9	E	101	BCL	C16-C17-C18-C20
9	G	101	BCL	C16-C17-C18-C20
9	I	101	BCL	C16-C17-C18-C20
9	K	101	BCL	C16-C17-C18-C20
9	O	101	BCL	C16-C17-C18-C20
9	Q	102	BCL	C16-C17-C18-C20
9	S	103	BCL	C16-C17-C18-C20
9	U	102	BCL	C16-C17-C18-C20
9	W	103	BCL	C16-C17-C18-C20
13	C	406	PGV	C5-C6-C7-C8
15	C	402	HEM	C4B-C3B-CAB-CBB
15	C	403	HEM	C4B-C3B-CAB-CBB
9	X	101	BCL	C16-C17-C18-C20
13	C	406	PGV	C12-C13-C14-C15
11	L	1003	BPH	C4-C3-C5-C6
11	M	704	BPH	C4-C3-C5-C6
12	L	1004	MQE	CAS-CAN-CBB-CCA
10	S	104	KGD	CAT-CAS-CAW-CBA
12	M	701	MQE	CAO-CAH-CAV-CBF
9	1	101	BCL	C11-C10-C8-C9
9	3	101	BCL	C11-C10-C8-C9
9	5	101	BCL	C11-C10-C8-C9
9	7	101	BCL	C11-C10-C8-C9
9	9	102	BCL	C11-C10-C8-C9
9	A	101	BCL	C11-C10-C8-C9
9	D	101	BCL	C11-C10-C8-C9
9	F	101	BCL	C11-C10-C8-C9
9	H	101	BCL	C11-C10-C8-C9
9	J	101	BCL	C11-C10-C8-C9
9	N	101	BCL	C11-C10-C8-C9
9	P	101	BCL	C11-C10-C8-C9
9	R	101	BCL	C11-C10-C8-C9
9	T	101	BCL	C11-C10-C8-C9
11	L	1003	BPH	C11-C10-C8-C9
9	0	101	BCL	C2A-CAA-CBA-CGA
9	2	102	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
9	4	101	BCL	C2A-CAA-CBA-CGA
9	6	101	BCL	C2A-CAA-CBA-CGA
9	8	101	BCL	C2A-CAA-CBA-CGA
9	A	102	BCL	C2A-CAA-CBA-CGA
9	D	102	BCL	C2A-CAA-CBA-CGA
9	F	102	BCL	C2A-CAA-CBA-CGA
9	H	102	BCL	C2A-CAA-CBA-CGA
9	J	102	BCL	C2A-CAA-CBA-CGA
9	N	102	BCL	C2A-CAA-CBA-CGA
9	Q	101	BCL	C2A-CAA-CBA-CGA
9	S	102	BCL	C2A-CAA-CBA-CGA
9	U	101	BCL	C2A-CAA-CBA-CGA
9	W	102	BCL	C2A-CAA-CBA-CGA
10	6	103	KGD	CBO-CBL-CBN-CBM
10	3	102	KGD	CAJ-CAL-CAM-CAO
10	N	103	KGD	CAP-CAQ-CAR-CAV
9	0	102	BCL	C1A-C2A-CAA-CBA
9	1	101	BCL	C1A-C2A-CAA-CBA
9	2	103	BCL	C1A-C2A-CAA-CBA
9	3	101	BCL	C1A-C2A-CAA-CBA
9	4	102	BCL	C1A-C2A-CAA-CBA
9	5	101	BCL	C1A-C2A-CAA-CBA
9	6	102	BCL	C1A-C2A-CAA-CBA
9	7	101	BCL	C1A-C2A-CAA-CBA
9	8	102	BCL	C1A-C2A-CAA-CBA
9	9	102	BCL	C1A-C2A-CAA-CBA
9	A	101	BCL	C1A-C2A-CAA-CBA
9	B	101	BCL	C1A-C2A-CAA-CBA
9	D	101	BCL	C1A-C2A-CAA-CBA
9	E	101	BCL	C1A-C2A-CAA-CBA
9	F	101	BCL	C1A-C2A-CAA-CBA
9	G	101	BCL	C1A-C2A-CAA-CBA
9	H	101	BCL	C1A-C2A-CAA-CBA
9	I	101	BCL	C1A-C2A-CAA-CBA
9	J	101	BCL	C1A-C2A-CAA-CBA
9	K	101	BCL	C1A-C2A-CAA-CBA
9	L	1002	BCL	C1A-C2A-CAA-CBA
9	N	101	BCL	C1A-C2A-CAA-CBA
9	O	101	BCL	C1A-C2A-CAA-CBA
9	P	101	BCL	C1A-C2A-CAA-CBA
9	Q	102	BCL	C1A-C2A-CAA-CBA
9	R	101	BCL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
9	S	103	BCL	C1A-C2A-CAA-CBA
9	T	101	BCL	C1A-C2A-CAA-CBA
9	U	102	BCL	C1A-C2A-CAA-CBA
9	W	103	BCL	C1A-C2A-CAA-CBA
9	X	101	BCL	C1A-C2A-CAA-CBA
11	L	1005	BPH	C16-C17-C18-C20
10	N	103	KGD	CAM-CAO-CAP-CAQ
9	0	102	BCL	C2C-C3C-CAC-CBC
9	2	103	BCL	C2C-C3C-CAC-CBC
9	4	102	BCL	C2C-C3C-CAC-CBC
9	6	102	BCL	C2C-C3C-CAC-CBC
9	8	102	BCL	C2C-C3C-CAC-CBC
9	B	101	BCL	C2C-C3C-CAC-CBC
9	E	101	BCL	C2C-C3C-CAC-CBC
9	G	101	BCL	C2C-C3C-CAC-CBC
9	I	101	BCL	C2C-C3C-CAC-CBC
9	K	101	BCL	C2C-C3C-CAC-CBC
9	O	101	BCL	C2C-C3C-CAC-CBC
9	Q	102	BCL	C2C-C3C-CAC-CBC
9	S	103	BCL	C2C-C3C-CAC-CBC
9	U	102	BCL	C2C-C3C-CAC-CBC
9	W	103	BCL	C2C-C3C-CAC-CBC
15	C	405	HEM	C2A-CAA-CBA-CGA
13	L	1007	PGV	C14-C15-C16-C17
13	C	406	PGV	C3-C4-C5-C6
13	Z	101	PGV	O03-C01-C02-C03
16	Y	101	DGA	OG1-CG1-CG2-CG3
13	C	406	PGV	O05-C05-C06-O06
13	P	104	PGV	C11-C10-C9-C8
13	C	406	PGV	C11-C10-C9-C8
13	L	1006	PGV	C20-C19-O03-C01
16	Y	101	DGA	OG1-CG1-CG2-OG2
11	M	704	BPH	CHA-CBD-CGD-O1D
11	M	704	BPH	CHA-CBD-CGD-O2D
9	1	101	BCL	C11-C10-C8-C7
9	3	101	BCL	C11-C10-C8-C7
9	5	101	BCL	C11-C10-C8-C7
9	7	101	BCL	C11-C10-C8-C7
9	9	102	BCL	C11-C10-C8-C7
9	A	101	BCL	C11-C10-C8-C7
9	D	101	BCL	C11-C10-C8-C7
9	F	101	BCL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
9	H	101	BCL	C11-C10-C8-C7
9	J	101	BCL	C11-C10-C8-C7
9	L	1002	BCL	C6-C7-C8-C10
9	L	1002	BCL	C11-C10-C8-C7
9	M	703	BCL	C12-C13-C15-C16
9	N	101	BCL	C11-C10-C8-C7
9	P	101	BCL	C11-C10-C8-C7
9	R	101	BCL	C11-C10-C8-C7
9	T	101	BCL	C11-C10-C8-C7
9	0	101	BCL	C11-C12-C13-C14
9	2	102	BCL	C11-C12-C13-C14
9	2	103	BCL	C14-C13-C15-C16
9	4	101	BCL	C11-C12-C13-C14
9	6	101	BCL	C11-C12-C13-C14
9	8	101	BCL	C11-C12-C13-C14
9	A	102	BCL	C11-C12-C13-C14
9	D	102	BCL	C11-C12-C13-C14
9	F	102	BCL	C11-C12-C13-C14
9	H	102	BCL	C11-C12-C13-C14
9	J	102	BCL	C11-C12-C13-C14
9	M	703	BCL	C11-C10-C8-C9
9	N	102	BCL	C11-C12-C13-C14
9	Q	101	BCL	C11-C12-C13-C14
9	S	102	BCL	C11-C12-C13-C14
9	U	101	BCL	C11-C12-C13-C14
11	M	704	BPH	C11-C12-C13-C14
10	B	102	KGD	CBH-CBJ-CBM-CBN
13	P	104	PGV	C1-C2-C3-C4
13	L	1006	PGV	C3-C4-C5-C6
10	5	102	KGD	CAJ-CAL-CAM-CAN
10	0	104	KGD	CAJ-CAL-CAM-CAO
10	2	101	KGD	CBE-CBF-CBH-CBJ
10	J	103	KGD	CBE-CBF-CBH-CBJ
9	M	703	BCL	C10-C11-C12-C13
13	L	1006	PGV	C2-C1-O01-C02
13	P	104	PGV	C2-C1-O01-C02
13	P	104	PGV	C7-C8-C9-C10
9	X	101	BCL	C8-C10-C11-C12
13	C	406	PGV	C2-C3-C4-C5
9	M	703	BCL	C4-C3-C5-C6
13	P	104	PGV	C24-C25-C26-C27
10	2	104	KGD	CBB-CBG-CBI-CBL

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Mol	Chain	Res	Type	Atoms
10	K	102	KGD	CAW-CBA-CBE-CBF
11	L	1005	BPH	C10-C11-C12-C13
13	L	1006	PGV	O03-C01-C02-C03
13	M	706	PGV	C25-C26-C27-C28
13	P	103	PGV	C23-C24-C25-C26
9	X	101	BCL	C4-C3-C5-C6
11	M	704	BPH	C2-C3-C5-C6
12	L	1004	MQE	CAS-CAN-CBB-CBL
13	L	1006	PGV	O04-C19-O03-C01
13	L	1007	PGV	O03-C01-C02-O01
9	1	101	BCL	C16-C17-C18-C20
9	3	101	BCL	C16-C17-C18-C20
9	5	101	BCL	C16-C17-C18-C20
9	7	101	BCL	C16-C17-C18-C20
9	D	101	BCL	C16-C17-C18-C20
9	F	101	BCL	C16-C17-C18-C20
9	H	101	BCL	C16-C17-C18-C20
9	P	101	BCL	C16-C17-C18-C20
9	T	101	BCL	C16-C17-C18-C20
10	0	103	KGD	CAW-CAS-CAT-CAX
10	N	103	KGD	CAW-CAS-CAT-CAX
9	0	102	BCL	C14-C13-C15-C16
9	4	102	BCL	C14-C13-C15-C16
9	6	102	BCL	C14-C13-C15-C16
9	8	102	BCL	C14-C13-C15-C16
9	B	101	BCL	C14-C13-C15-C16
9	E	101	BCL	C14-C13-C15-C16
9	G	101	BCL	C14-C13-C15-C16
9	I	101	BCL	C14-C13-C15-C16
9	K	101	BCL	C14-C13-C15-C16
9	O	101	BCL	C14-C13-C15-C16
9	Q	102	BCL	C14-C13-C15-C16
9	S	103	BCL	C14-C13-C15-C16
9	U	102	BCL	C14-C13-C15-C16
9	W	103	BCL	C14-C13-C15-C16
11	M	704	BPH	C6-C7-C8-C9
13	L	1006	PGV	C02-C03-O11-P
13	P	103	PGV	C05-C04-O12-P
13	P	104	PGV	C05-C04-O12-P
11	L	1005	BPH	C16-C17-C18-C19
10	6	103	KGD	CAH-CAD-CAJ-CAL
10	8	103	KGD	CAB-CAD-CAJ-CAL

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Mol	Chain	Res	Type	Atoms
10	H	103	KGD	CAB-CAD-CAJ-CAL
10	S	104	KGD	CAB-CAD-CAJ-CAL
10	U	103	KGD	CAB-CAD-CAJ-CAL
10	C	401	KGD	CAB-CAD-CAJ-CAL
10	C	401	KGD	CAH-CAD-CAJ-CAL
10	2	101	KGD	CBE-CBF-CBH-CBK
9	1	101	BCL	C4C-C3C-CAC-CBC
9	3	101	BCL	C4C-C3C-CAC-CBC
9	5	101	BCL	C4C-C3C-CAC-CBC
9	7	101	BCL	C4C-C3C-CAC-CBC
9	9	102	BCL	C4C-C3C-CAC-CBC
9	A	101	BCL	C4C-C3C-CAC-CBC
9	D	101	BCL	C4C-C3C-CAC-CBC
9	F	101	BCL	C4C-C3C-CAC-CBC
9	H	101	BCL	C4C-C3C-CAC-CBC
9	J	101	BCL	C4C-C3C-CAC-CBC
9	N	101	BCL	C4C-C3C-CAC-CBC
9	P	101	BCL	C4C-C3C-CAC-CBC
9	R	101	BCL	C4C-C3C-CAC-CBC
9	T	101	BCL	C4C-C3C-CAC-CBC
9	X	101	BCL	C4C-C3C-CAC-CBC
13	L	1006	PGV	C22-C23-C24-C25
9	9	102	BCL	C16-C17-C18-C20
9	A	101	BCL	C16-C17-C18-C20
9	J	101	BCL	C16-C17-C18-C20
9	N	101	BCL	C16-C17-C18-C20
9	R	101	BCL	C16-C17-C18-C20
9	0	102	BCL	C6-C7-C8-C10
9	2	102	BCL	C11-C12-C13-C15
9	2	103	BCL	C6-C7-C8-C10
9	4	101	BCL	C11-C12-C13-C15
9	4	102	BCL	C6-C7-C8-C10
9	6	101	BCL	C11-C12-C13-C15
9	6	102	BCL	C6-C7-C8-C10
9	8	102	BCL	C6-C7-C8-C10
9	A	102	BCL	C11-C12-C13-C15
9	B	101	BCL	C6-C7-C8-C10
9	D	102	BCL	C11-C12-C13-C15
9	E	101	BCL	C6-C7-C8-C10
9	G	101	BCL	C6-C7-C8-C10
9	I	101	BCL	C6-C7-C8-C10
9	J	102	BCL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
9	K	101	BCL	C6-C7-C8-C10
9	M	703	BCL	C11-C10-C8-C7
9	N	102	BCL	C11-C12-C13-C15
9	O	101	BCL	C6-C7-C8-C10
9	Q	101	BCL	C11-C12-C13-C15
9	Q	102	BCL	C6-C7-C8-C10
9	S	102	BCL	C11-C12-C13-C15
9	S	103	BCL	C6-C7-C8-C10
9	U	102	BCL	C6-C7-C8-C10
9	W	103	BCL	C6-C7-C8-C10
11	L	1005	BPH	C12-C13-C15-C16
11	M	704	BPH	C6-C7-C8-C10
11	M	704	BPH	C11-C12-C13-C15
10	B	102	KGD	CBB-CBG-CBI-CBL
9	L	1002	BCL	C16-C17-C18-C20
13	C	406	PGV	C02-C03-O11-P
13	P	103	PGV	C3-C4-C5-C6
13	Z	101	PGV	C22-C23-C24-C25
13	L	1006	PGV	O02-C1-O01-C02
9	M	703	BCL	CHA-CBD-CGD-O2D
13	Z	101	PGV	O03-C01-C02-O01
13	P	103	PGV	C4-C5-C6-C7
13	P	104	PGV	C23-C24-C25-C26
11	L	1003	BPH	C10-C11-C12-C13
9	0	102	BCL	C6-C7-C8-C9
9	2	103	BCL	C6-C7-C8-C9
9	4	102	BCL	C6-C7-C8-C9
9	6	102	BCL	C6-C7-C8-C9
9	8	102	BCL	C6-C7-C8-C9
9	B	101	BCL	C6-C7-C8-C9
9	E	101	BCL	C6-C7-C8-C9
9	G	101	BCL	C6-C7-C8-C9
9	I	101	BCL	C6-C7-C8-C9
9	K	101	BCL	C6-C7-C8-C9
9	O	101	BCL	C6-C7-C8-C9
9	Q	102	BCL	C6-C7-C8-C9
9	S	103	BCL	C6-C7-C8-C9
9	U	102	BCL	C6-C7-C8-C9
9	W	103	BCL	C6-C7-C8-C9
11	L	1005	BPH	C14-C13-C15-C16
13	L	1007	PGV	C2-C3-C4-C5
11	L	1005	BPH	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
10	E	102	KGD	CAJ-CAL-CAM-CAN
10	S	104	KGD	CAJ-CAL-CAM-CAO
13	M	706	PGV	C21-C22-C23-C24
10	A	104	KGD	CBB-CBG-CBI-CBL
10	G	102	KGD	CAM-CAO-CAP-CAQ
13	C	406	PGV	C03-O11-P-O12
13	Z	101	PGV	C04-O12-P-O11
13	L	1006	PGV	C03-O11-P-O13
13	M	706	PGV	C03-O11-P-O13
13	P	103	PGV	C04-O12-P-O13
16	Y	101	DGA	CA8-CA9-CAA-CBA
13	P	104	PGV	O02-C1-O01-C02
9	0	101	BCL	C11-C12-C13-C15
9	0	102	BCL	C12-C13-C15-C16
9	2	103	BCL	C12-C13-C15-C16
9	4	102	BCL	C12-C13-C15-C16
9	6	102	BCL	C12-C13-C15-C16
9	8	101	BCL	C11-C12-C13-C15
9	8	102	BCL	C12-C13-C15-C16
9	B	101	BCL	C12-C13-C15-C16
9	E	101	BCL	C12-C13-C15-C16
9	F	102	BCL	C11-C12-C13-C15
9	G	101	BCL	C12-C13-C15-C16
9	H	102	BCL	C11-C12-C13-C15
9	I	101	BCL	C12-C13-C15-C16
9	K	101	BCL	C12-C13-C15-C16
9	L	1001	BCL	C6-C7-C8-C10
9	O	101	BCL	C12-C13-C15-C16
9	Q	102	BCL	C12-C13-C15-C16
9	S	103	BCL	C12-C13-C15-C16
9	U	101	BCL	C11-C12-C13-C15
9	U	102	BCL	C12-C13-C15-C16
9	W	102	BCL	C6-C7-C8-C10
9	W	103	BCL	C12-C13-C15-C16
11	L	1003	BPH	C12-C13-C15-C16
13	P	103	PGV	C20-C21-C22-C23
13	Z	101	PGV	C5-C6-C7-C8
13	M	706	PGV	C20-C19-O03-C01
9	L	1002	BCL	C6-C7-C8-C9
13	C	406	PGV	C25-C26-C27-C28
13	M	706	PGV	O04-C19-O03-C01
10	3	102	KGD	CBA-CBE-CBF-CBH

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Mol	Chain	Res	Type	Atoms
10	9	101	KGD	CBA-CBE-CBF-CBH
10	G	102	KGD	CBI-CBL-CBN-CBM
9	M	703	BCL	CAA-CBA-CGA-O2A
9	0	102	BCL	C2-C1-O2A-CGA
9	2	103	BCL	C2-C1-O2A-CGA
9	4	102	BCL	C2-C1-O2A-CGA
9	6	102	BCL	C2-C1-O2A-CGA
9	8	102	BCL	C2-C1-O2A-CGA
9	B	101	BCL	C2-C1-O2A-CGA
9	E	101	BCL	C2-C1-O2A-CGA
9	G	101	BCL	C2-C1-O2A-CGA
9	I	101	BCL	C2-C1-O2A-CGA
9	K	101	BCL	C2-C1-O2A-CGA
9	O	101	BCL	C2-C1-O2A-CGA
9	Q	102	BCL	C2-C1-O2A-CGA
9	S	103	BCL	C2-C1-O2A-CGA
9	U	102	BCL	C2-C1-O2A-CGA
9	W	103	BCL	C2-C1-O2A-CGA
9	6	102	BCL	C15-C16-C17-C18
9	E	101	BCL	C15-C16-C17-C18
9	I	101	BCL	C15-C16-C17-C18
9	S	103	BCL	C15-C16-C17-C18
9	U	102	BCL	C15-C16-C17-C18
9	W	103	BCL	C15-C16-C17-C18
9	L	1001	BCL	O1A-CGA-O2A-C1
9	0	102	BCL	C15-C16-C17-C18
9	K	101	BCL	C15-C16-C17-C18
9	Q	102	BCL	C15-C16-C17-C18
9	2	103	BCL	C15-C16-C17-C18
9	B	101	BCL	C15-C16-C17-C18
9	4	102	BCL	C15-C16-C17-C18
9	8	102	BCL	C15-C16-C17-C18
9	G	101	BCL	C15-C16-C17-C18
9	O	101	BCL	C15-C16-C17-C18
10	W	101	KGD	CAW-CAS-CAT-CAX
12	L	1004	MQE	CBB-CAN-CAS-CBH
13	L	1007	PGV	C04-O12-P-O11
13	L	1007	PGV	O03-C01-C02-C03
11	L	1003	BPH	C14-C13-C15-C16
10	0	103	KGD	CAR-CAV-CBB-CBG
10	5	102	KGD	CAW-CBA-CBE-CBF
10	T	102	KGD	CBH-CBJ-CBM-CBN

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Mol	Chain	Res	Type	Atoms
9	1	101	BCL	C16-C17-C18-C19
9	3	101	BCL	C16-C17-C18-C19
9	5	101	BCL	C16-C17-C18-C19
9	7	101	BCL	C16-C17-C18-C19
9	9	102	BCL	C16-C17-C18-C19
9	A	101	BCL	C16-C17-C18-C19
9	D	101	BCL	C16-C17-C18-C19
9	F	101	BCL	C16-C17-C18-C19
9	H	101	BCL	C16-C17-C18-C19
9	J	101	BCL	C16-C17-C18-C19
9	N	101	BCL	C16-C17-C18-C19
9	P	101	BCL	C16-C17-C18-C19
9	R	101	BCL	C16-C17-C18-C19
9	T	101	BCL	C16-C17-C18-C19
13	Z	101	PGV	C05-C04-O12-P
10	E	102	KGD	CAJ-CAL-CAM-CAO
10	P	102	KGD	CBI-CBL-CBN-CBM
10	C	401	KGD	CAJ-CAL-CAM-CAO
15	C	403	HEM	CAD-CBD-CGD-O2D
10	2	101	KGD	CAR-CAV-CBB-CBG
10	G	102	KGD	CAW-CBA-CBE-CBF
12	L	1004	MQE	CAQ-CAD-CAJ-CBC
9	L	1002	BCL	C16-C17-C18-C19
12	M	701	MQE	CCL-CCC-CCD-CCI
15	C	402	HEM	CAA-CBA-CGA-O1A
13	P	104	PGV	C21-C22-C23-C24
15	C	403	HEM	CAD-CBD-CGD-O1D
9	L	1001	BCL	C3A-C2A-CAA-CBA
9	X	101	BCL	C11-C12-C13-C14
15	C	402	HEM	CAA-CBA-CGA-O2A
10	C	401	KGD	CBG-CBI-CBL-CBO
15	C	404	HEM	CAA-CBA-CGA-O1A
13	L	1007	PGV	C9-C10-C11-C12
10	P	102	KGD	CBE-CBF-CBH-CBK
13	L	1006	PGV	C20-C21-C22-C23
10	P	102	KGD	CBH-CBJ-CBM-CBN
13	P	104	PGV	C26-C27-C28-C29
13	P	103	PGV	C01-C02-C03-O11
10	5	102	KGD	CAT-CAS-CAW-CAZ
10	C	401	KGD	CBG-CBI-CBL-CBN
10	A	104	KGD	CAR-CAV-CBB-CBG
10	F	103	KGD	CBB-CBG-CBI-CBL

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Mol	Chain	Res	Type	Atoms
10	O	102	KGD	CAM-CAO-CAP-CAQ
10	T	102	KGD	CBB-CBG-CBI-CBL
9	0	102	BCL	O1A-CGA-O2A-C1
9	6	102	BCL	O1A-CGA-O2A-C1
9	8	102	BCL	O1A-CGA-O2A-C1
9	I	101	BCL	O1A-CGA-O2A-C1
9	K	101	BCL	O1A-CGA-O2A-C1
10	A	103	KGD	CAW-CAS-CAT-CAX
10	S	101	KGD	CAT-CAS-CAW-CAZ
10	C	401	KGD	CAT-CAS-CAW-CAZ
9	L	1002	BCL	C2-C1-O2A-CGA
9	2	103	BCL	O1A-CGA-O2A-C1
9	4	102	BCL	O1A-CGA-O2A-C1
9	B	101	BCL	O1A-CGA-O2A-C1
9	E	101	BCL	O1A-CGA-O2A-C1
9	G	101	BCL	O1A-CGA-O2A-C1
9	O	101	BCL	O1A-CGA-O2A-C1
9	Q	102	BCL	O1A-CGA-O2A-C1
9	S	103	BCL	O1A-CGA-O2A-C1
9	U	102	BCL	O1A-CGA-O2A-C1
9	W	103	BCL	O1A-CGA-O2A-C1
9	J	101	BCL	C8-C10-C11-C12
9	3	101	BCL	C8-C10-C11-C12
9	5	101	BCL	C8-C10-C11-C12
9	7	101	BCL	C8-C10-C11-C12
9	9	102	BCL	C8-C10-C11-C12
9	A	101	BCL	C8-C10-C11-C12
9	D	101	BCL	C8-C10-C11-C12
9	1	101	BCL	C8-C10-C11-C12
9	F	101	BCL	C8-C10-C11-C12
9	N	101	BCL	C8-C10-C11-C12
11	L	1003	BPH	C2A-CAA-CBA-CGA
9	R	101	BCL	C8-C10-C11-C12
9	H	101	BCL	C8-C10-C11-C12
9	P	101	BCL	C8-C10-C11-C12
9	T	101	BCL	C8-C10-C11-C12
10	9	101	KGD	CAM-CAO-CAP-CAQ
10	U	103	KGD	CBB-CBG-CBI-CBL
10	8	103	KGD	CAT-CAS-CAW-CAZ
12	L	1004	MQE	CAL-CAE-CAR-CBV
10	5	102	KGD	CAJ-CAL-CAM-CAO
15	C	404	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
16	Y	101	DGA	CB2-CB3-CB4-CB5
9	1	101	BCL	C2-C3-C5-C6
9	3	101	BCL	C2-C3-C5-C6
9	5	101	BCL	C2-C3-C5-C6
9	7	101	BCL	C2-C3-C5-C6
9	9	102	BCL	C2-C3-C5-C6
9	A	101	BCL	C2-C3-C5-C6
9	D	101	BCL	C2-C3-C5-C6
9	F	101	BCL	C2-C3-C5-C6
9	H	101	BCL	C2-C3-C5-C6
9	J	101	BCL	C2-C3-C5-C6
9	N	101	BCL	C2-C3-C5-C6
9	P	101	BCL	C2-C3-C5-C6
9	R	101	BCL	C2-C3-C5-C6
9	T	101	BCL	C2-C3-C5-C6
10	C	401	KGD	CAT-CAS-CAW-CBA
9	X	101	BCL	C1-C2-C3-C4
13	L	1007	PGV	C21-C22-C23-C24
10	O	102	KGD	CAT-CAS-CAW-CAZ
10	5	102	KGD	CAT-CAS-CAW-CBA
11	M	704	BPH	C11-C10-C8-C9
13	C	406	PGV	C11-C12-C13-C14
9	M	703	BCL	CAD-CBD-CGD-O2D
9	G	101	BCL	CBA-CGA-O2A-C1
9	0	102	BCL	CBA-CGA-O2A-C1
9	2	103	BCL	CBA-CGA-O2A-C1
9	8	102	BCL	CBA-CGA-O2A-C1
9	E	101	BCL	CBA-CGA-O2A-C1
9	I	101	BCL	CBA-CGA-O2A-C1
9	K	101	BCL	CBA-CGA-O2A-C1
9	O	101	BCL	CBA-CGA-O2A-C1
9	Q	102	BCL	CBA-CGA-O2A-C1
9	S	103	BCL	CBA-CGA-O2A-C1
9	U	102	BCL	CBA-CGA-O2A-C1
9	W	103	BCL	CBA-CGA-O2A-C1
10	8	103	KGD	CAT-CAS-CAW-CBA
10	6	103	KGD	CBI-CBL-CBN-CBM
10	A	104	KGD	CBE-CBF-CBH-CBJ
10	P	102	KGD	CBE-CBF-CBH-CBJ
10	0	104	KGD	CAW-CAS-CAT-CAX
15	C	405	HEM	CAA-CBA-CGA-O1A
9	6	102	BCL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	L	1007	PGV	O01-C02-C03-O11
11	L	1005	BPH	O2A-C1-C2-C3
9	4	102	BCL	CBA-CGA-O2A-C1
9	B	101	BCL	CBA-CGA-O2A-C1
13	M	706	PGV	C19-C20-C21-C22
9	0	101	BCL	CHA-CBD-CGD-O1D
9	2	102	BCL	CHA-CBD-CGD-O1D
9	4	101	BCL	CHA-CBD-CGD-O1D
9	6	101	BCL	CHA-CBD-CGD-O1D
9	8	101	BCL	CHA-CBD-CGD-O1D
9	A	102	BCL	CHA-CBD-CGD-O1D
9	D	102	BCL	CHA-CBD-CGD-O1D
9	F	102	BCL	CHA-CBD-CGD-O1D
9	H	102	BCL	CHA-CBD-CGD-O1D
9	J	102	BCL	CHA-CBD-CGD-O1D
9	L	1001	BCL	CHA-CBD-CGD-O2D
9	N	102	BCL	CHA-CBD-CGD-O1D
9	Q	101	BCL	CHA-CBD-CGD-O1D
9	S	102	BCL	CHA-CBD-CGD-O1D
9	U	101	BCL	CHA-CBD-CGD-O1D
9	W	102	BCL	CHA-CBD-CGD-O1D
10	C	401	KGD	CBB-CBG-CBI-CBL
10	O	102	KGD	CAT-CAS-CAW-CBA
12	L	1004	MQE	CAL-CAE-CAR-CBD
13	M	706	PGV	C1-C2-C3-C4
12	M	701	MQE	CCB-CCC-CCD-CCI
16	Y	101	DGA	CA3-CA4-CA5-CA6
10	O	102	KGD	CAW-CAS-CAT-CAX
12	M	701	MQE	CAP-CAC-CAI-CBD
13	P	104	PGV	C25-C26-C27-C28
9	W	102	BCL	C16-C17-C18-C19
10	0	103	KGD	CBI-CBL-CBN-CBM
10	H	103	KGD	CBE-CBF-CBH-CBJ
10	O	102	KGD	CBI-CBL-CBN-CBM
13	L	1006	PGV	C04-O12-P-O13
13	L	1007	PGV	C04-O12-P-O13
9	L	1002	BCL	CAA-CBA-CGA-O1A
9	M	703	BCL	CAD-CBD-CGD-O1D
13	L	1007	PGV	C01-C02-O01-C1
13	P	104	PGV	O01-C1-C2-C3
9	M	703	BCL	C6-C7-C8-C9
9	M	703	BCL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
11	L	1005	BPH	C11-C12-C13-C14
9	L	1002	BCL	CAA-CBA-CGA-O2A
13	P	104	PGV	O02-C1-C2-C3
9	1	101	BCL	CAA-CBA-CGA-O2A
9	3	101	BCL	CAA-CBA-CGA-O2A
9	5	101	BCL	CAA-CBA-CGA-O2A
9	7	101	BCL	CAA-CBA-CGA-O2A
9	9	102	BCL	CAA-CBA-CGA-O2A
9	D	101	BCL	CAA-CBA-CGA-O2A
9	F	101	BCL	CAA-CBA-CGA-O2A
9	H	101	BCL	CAA-CBA-CGA-O2A
9	J	101	BCL	CAA-CBA-CGA-O2A
9	N	101	BCL	CAA-CBA-CGA-O2A
16	Y	101	DGA	CA7-CA8-CA9-CAA
10	U	103	KGD	CAT-CAS-CAW-CAZ
9	A	101	BCL	CAA-CBA-CGA-O2A
9	P	101	BCL	CAA-CBA-CGA-O2A
9	R	101	BCL	CAA-CBA-CGA-O2A
9	T	101	BCL	CAA-CBA-CGA-O2A
10	A	103	KGD	CAJ-CAL-CAM-CAO
10	S	101	KGD	CBE-CBF-CBH-CBJ
13	Z	101	PGV	C23-C24-C25-C26
9	X	101	BCL	CAA-CBA-CGA-O2A
9	L	1002	BCL	C2A-CAA-CBA-CGA

There are no ring outliers.

91 monomers are involved in 442 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	9	101	KGD	4	0
9	U	102	BCL	3	0
9	9	102	BCL	5	0
9	4	102	BCL	5	0
10	4	103	KGD	2	0
10	C	401	KGD	20	0
15	C	405	HEM	3	0
10	T	102	KGD	6	0
13	Z	101	PGV	8	0
15	C	402	HEM	3	0
10	S	101	KGD	6	0
9	Q	102	BCL	7	0
10	3	102	KGD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	102	BCL	2	0
9	N	102	BCL	4	0
13	M	706	PGV	8	0
12	M	701	MQE	17	0
9	R	101	BCL	9	0
9	G	101	BCL	5	0
9	E	101	BCL	5	0
9	M	703	BCL	10	0
9	W	103	BCL	7	0
9	W	102	BCL	8	0
9	H	101	BCL	7	0
13	L	1006	PGV	1	0
10	U	103	KGD	3	0
9	K	101	BCL	7	0
10	A	104	KGD	5	0
9	8	101	BCL	4	0
10	2	101	KGD	6	0
10	A	103	KGD	3	0
9	4	101	BCL	2	0
9	0	101	BCL	4	0
9	U	101	BCL	11	0
9	T	101	BCL	11	0
11	L	1003	BPH	6	0
10	E	102	KGD	3	0
9	5	101	BCL	6	0
9	8	102	BCL	5	0
9	3	101	BCL	5	0
9	2	102	BCL	5	0
10	5	102	KGD	5	0
9	Q	101	BCL	3	0
15	C	403	HEM	4	0
9	7	101	BCL	7	0
9	B	101	BCL	5	0
9	F	102	BCL	2	0
9	L	1002	BCL	8	0
11	M	704	BPH	37	0
10	H	103	KGD	5	0
10	P	102	KGD	6	0
9	F	101	BCL	4	0
9	2	103	BCL	6	0
9	P	101	BCL	8	0
10	Q	103	KGD	1	0

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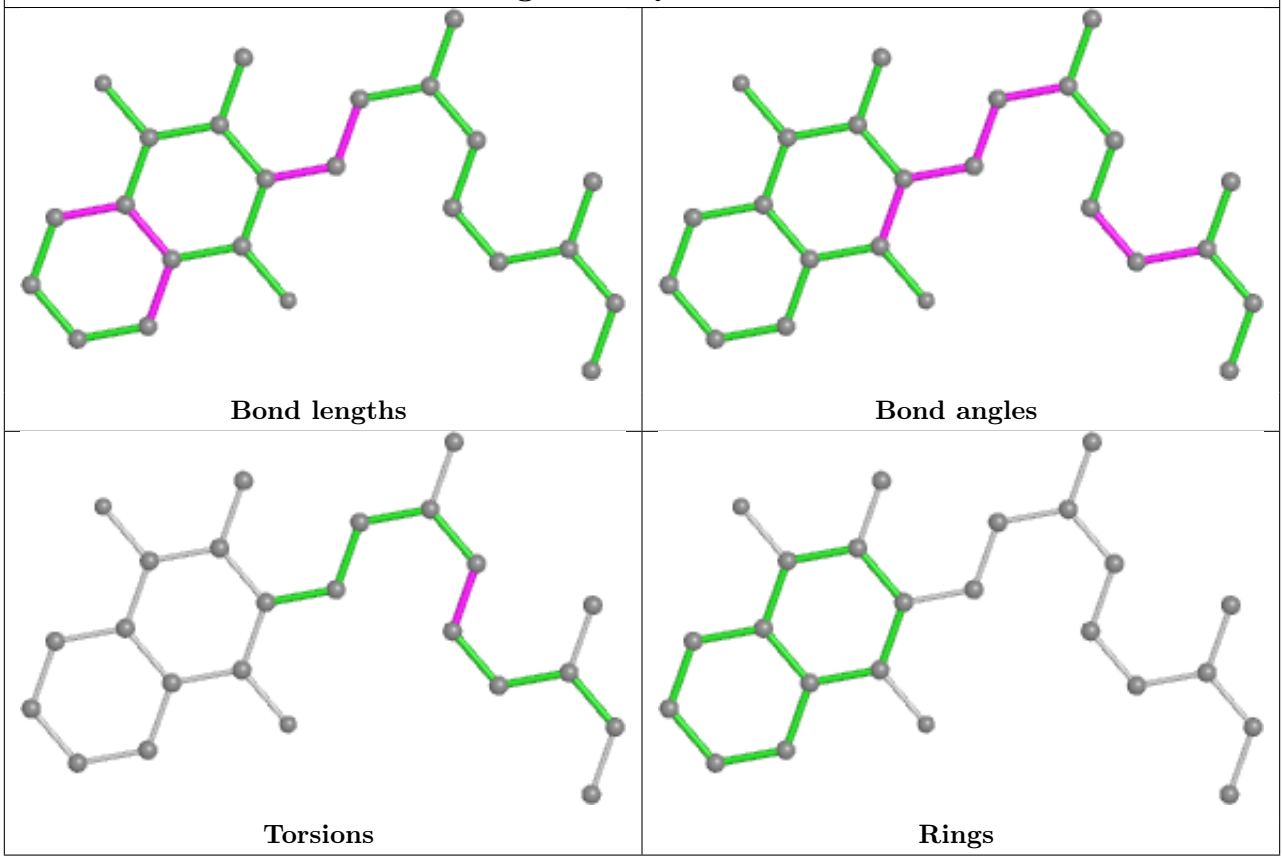
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Y	101	DGA	1	0
15	C	404	HEM	9	0
9	H	102	BCL	3	0
10	J	103	KGD	7	0
9	6	102	BCL	5	0
9	D	102	BCL	3	0
10	F	103	KGD	6	0
9	0	102	BCL	3	0
10	O	102	KGD	3	0
13	P	104	PGV	16	0
9	J	102	BCL	4	0
9	O	101	BCL	3	0
10	8	103	KGD	4	0
13	C	406	PGV	5	0
9	S	103	BCL	5	0
9	6	101	BCL	3	0
9	D	101	BCL	5	0
9	S	102	BCL	5	0
13	P	103	PGV	17	0
9	N	101	BCL	8	0
10	0	103	KGD	2	0
10	I	102	KGD	4	0
11	L	1005	BPH	7	0
9	J	101	BCL	6	0
9	A	101	BCL	6	0
9	L	1001	BCL	6	0
9	I	101	BCL	6	0
9	1	101	BCL	8	0
10	0	104	KGD	8	0
12	L	1004	MQE	2	0
10	S	104	KGD	1	0
10	6	103	KGD	1	0
9	X	101	BCL	11	0
10	N	103	KGD	4	0
10	B	102	KGD	3	0
10	W	101	KGD	5	0

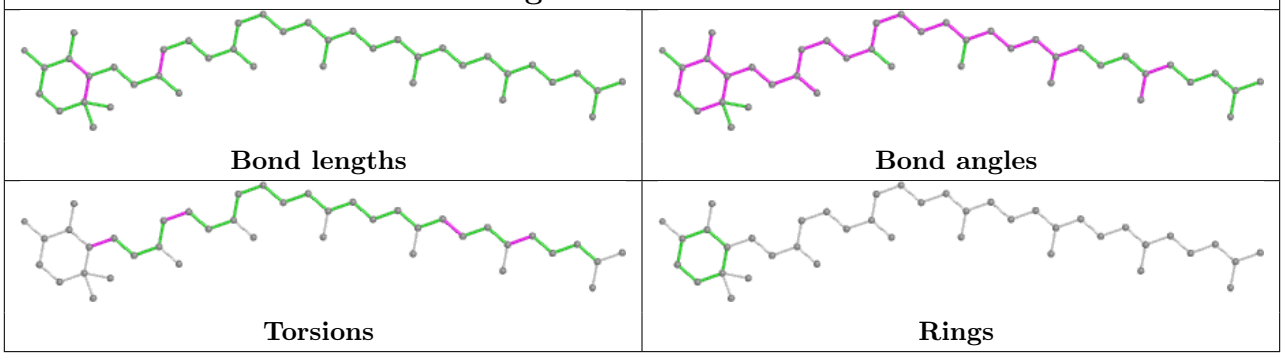
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

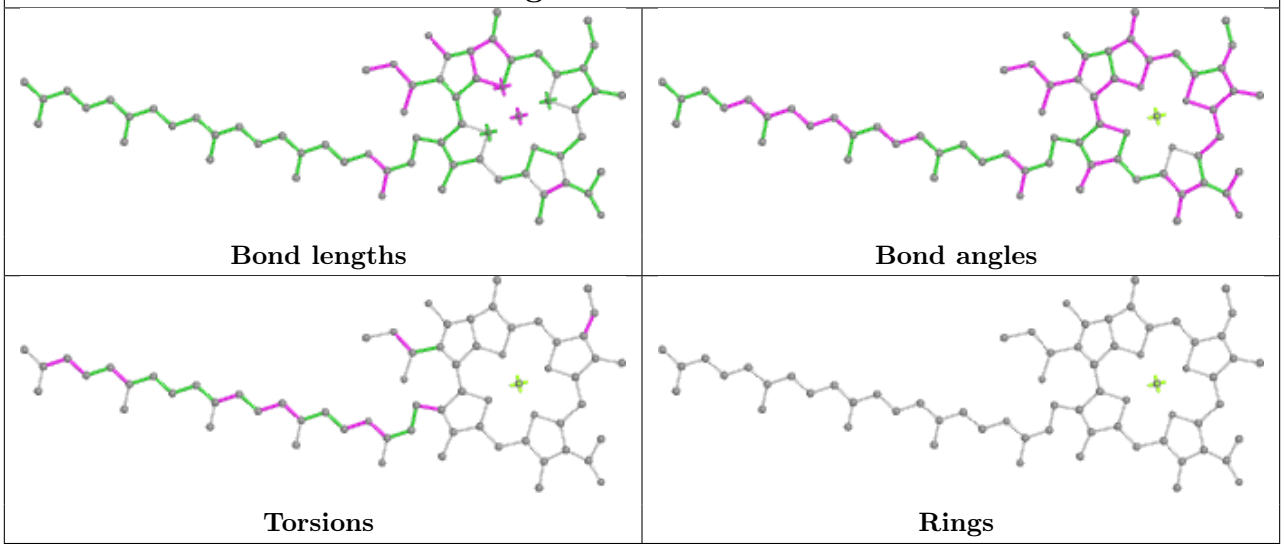
Ligand MQE M 705



Ligand KGD 9 101



Ligand BCL U 102



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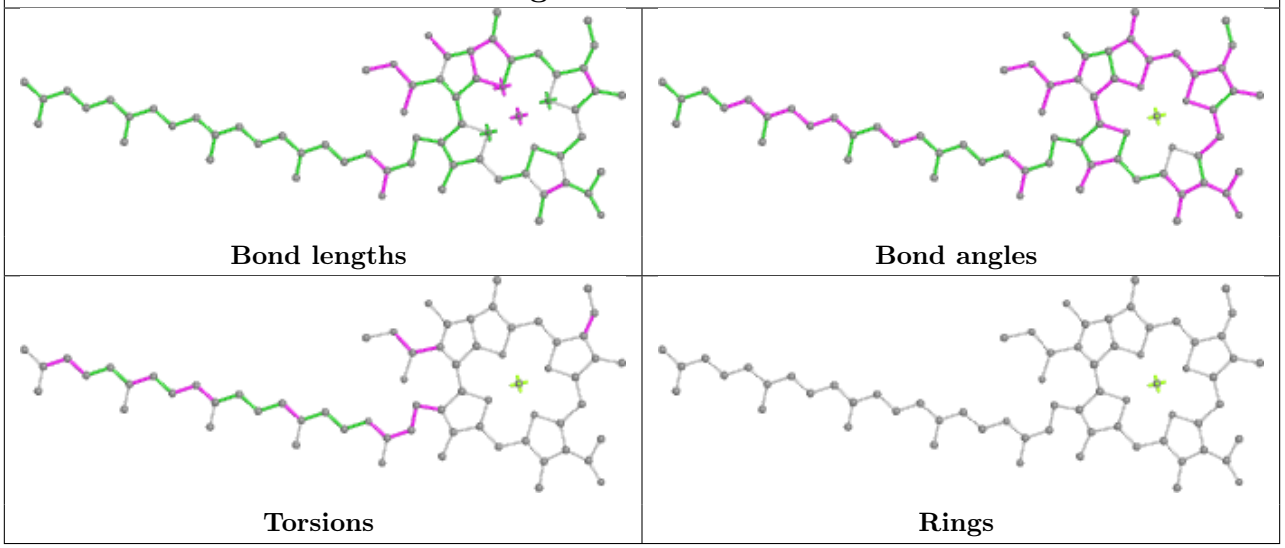

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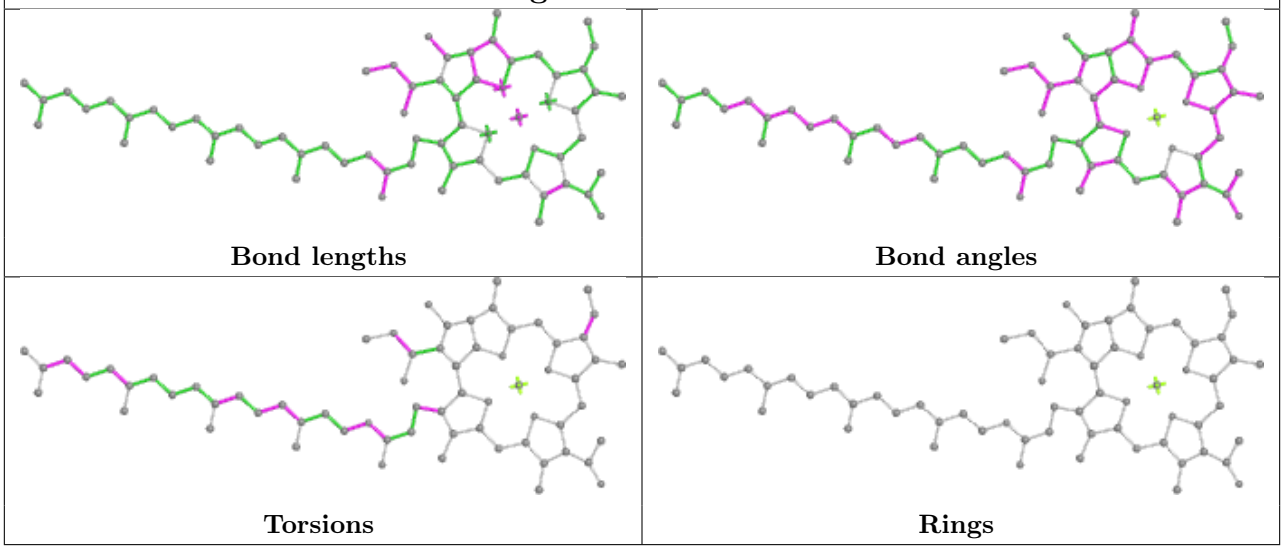

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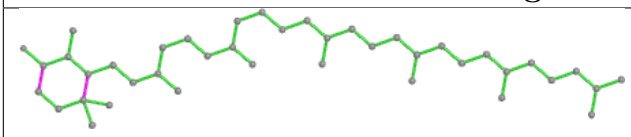
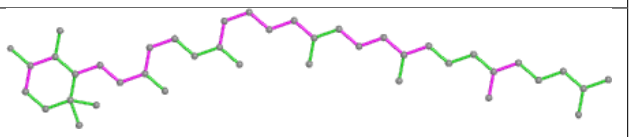
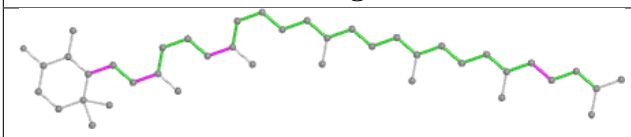
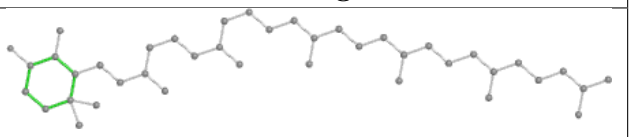
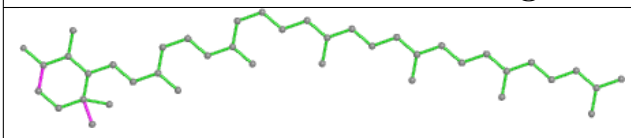
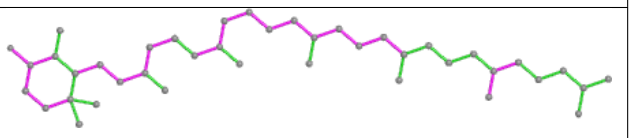
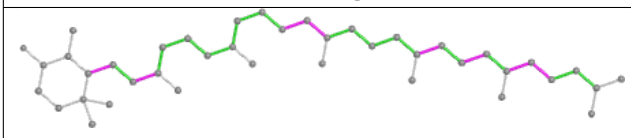
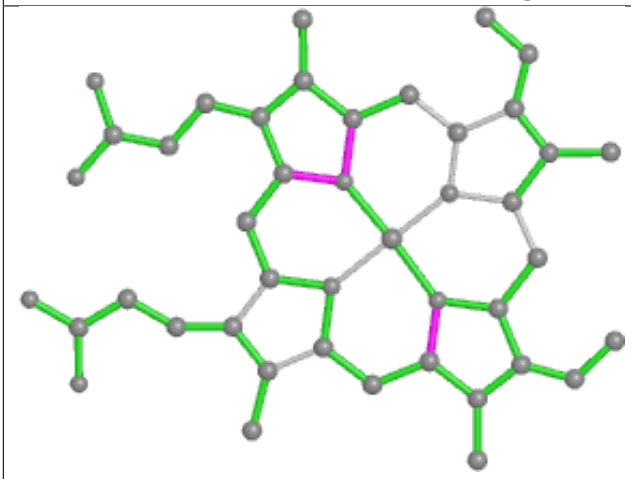
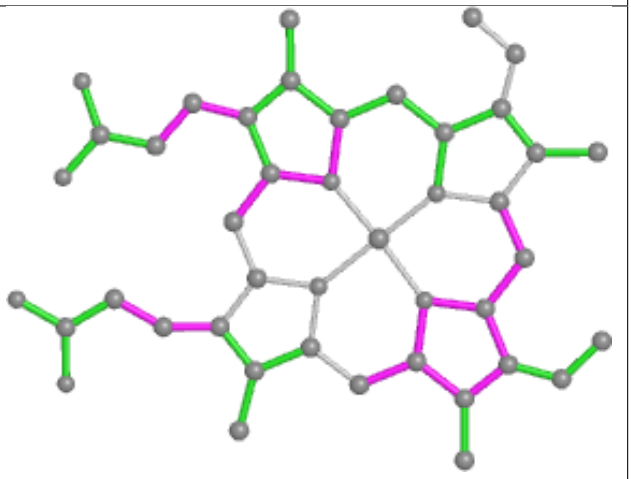
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KGD C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

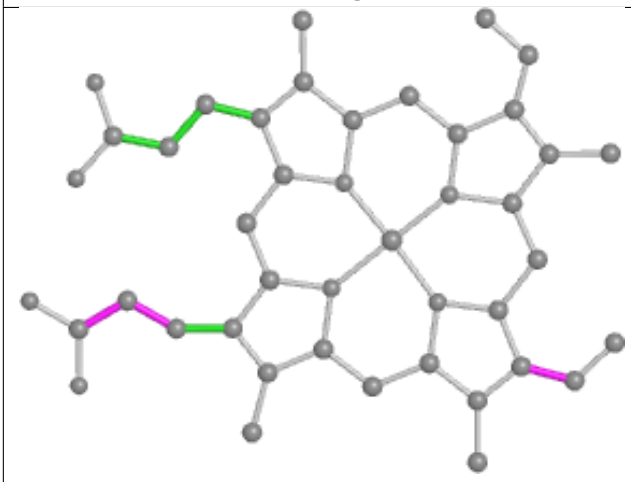
Ligand HEM C 405



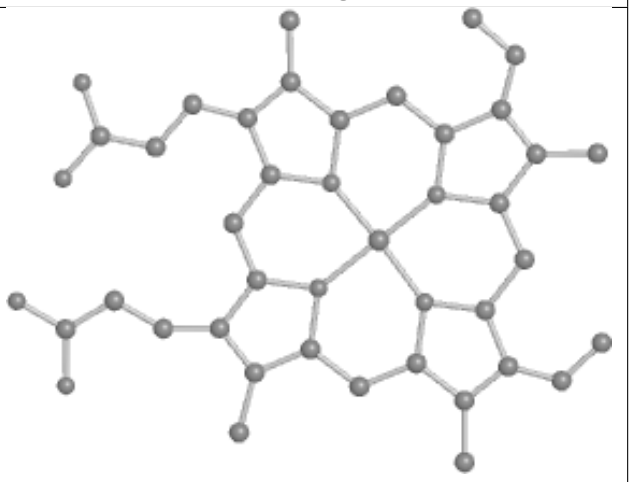
Bond lengths



Bond angles

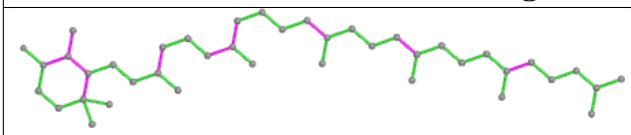


Torsions

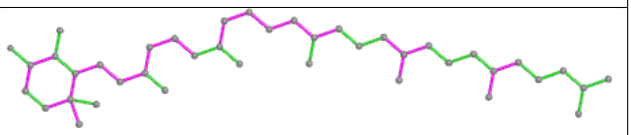


Rings

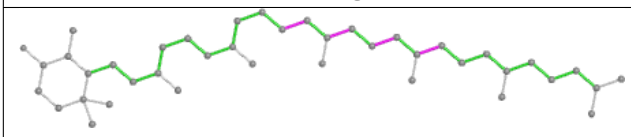
Ligand KGD T 102



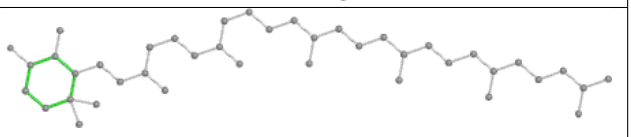
Bond lengths



Bond angles

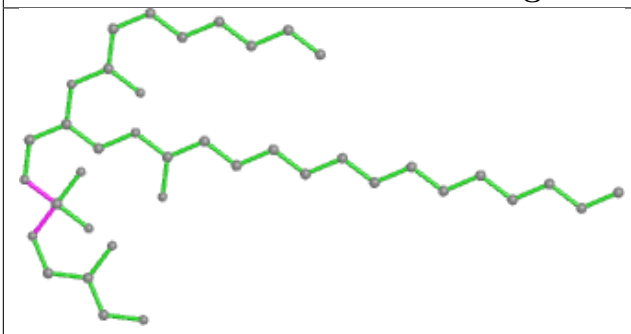


Torsions

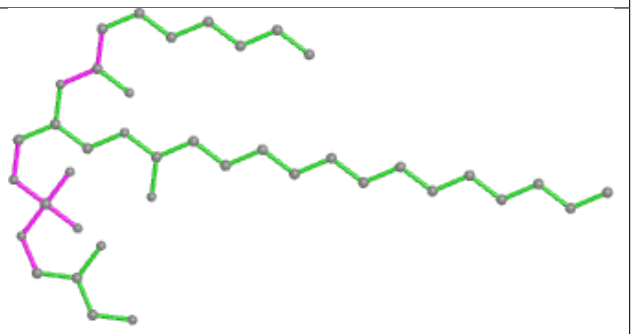


Rings

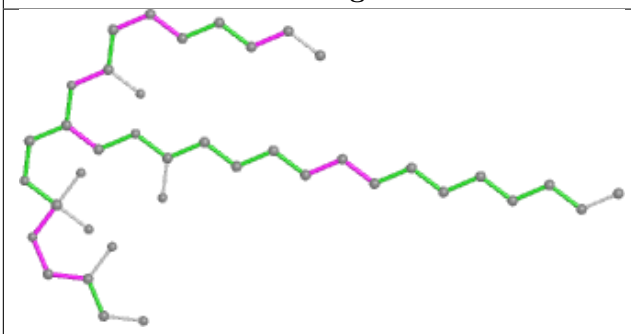
Ligand PGV Z 101



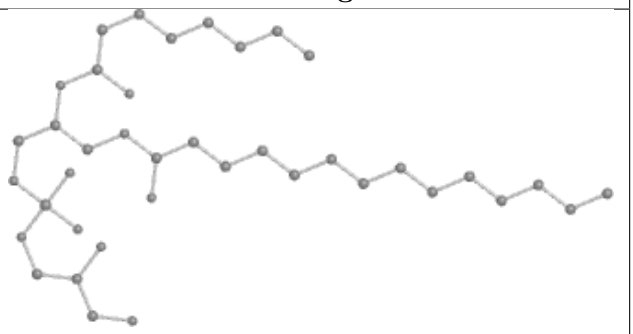
Bond lengths



Bond angles

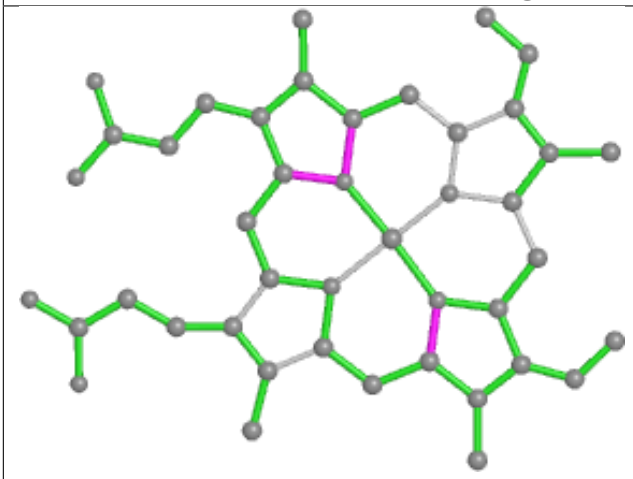


Torsions



Rings

Ligand HEM C 402



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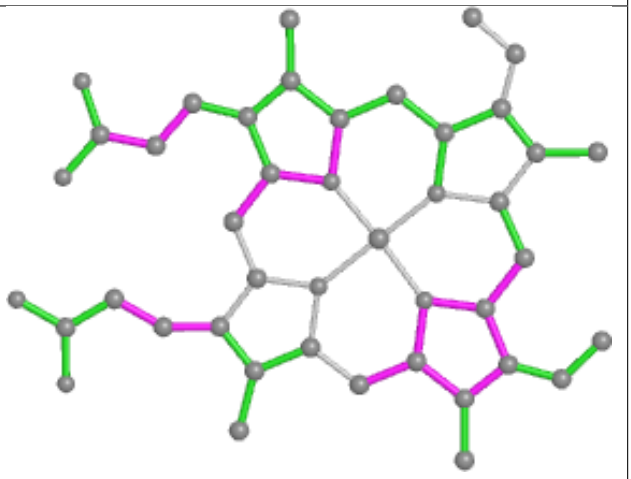
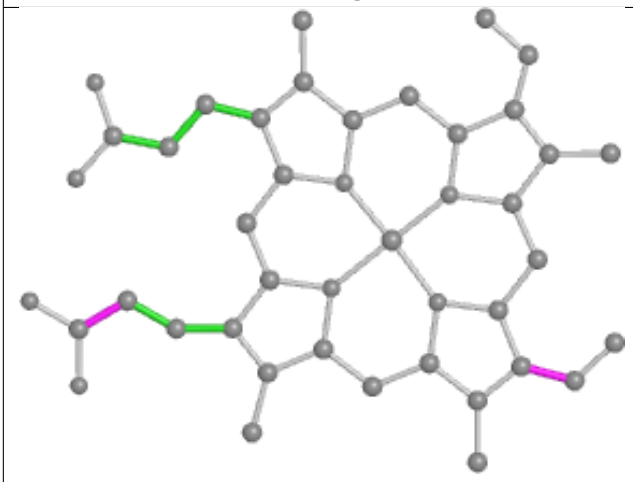
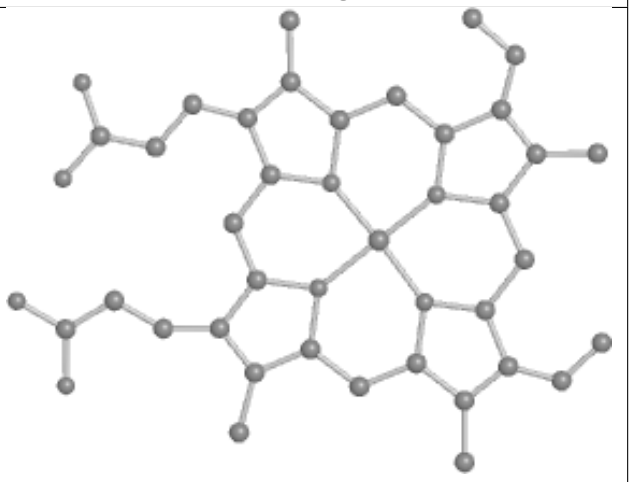


Bond angles

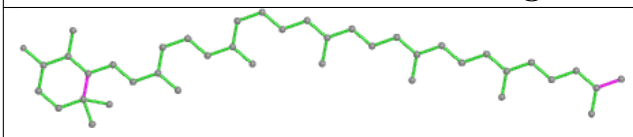


Torsions

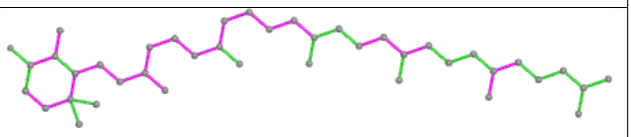


Rings

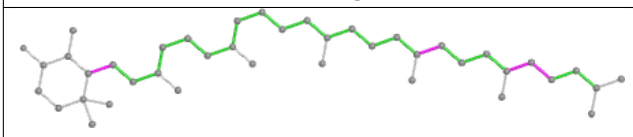
Ligand KGD S 101



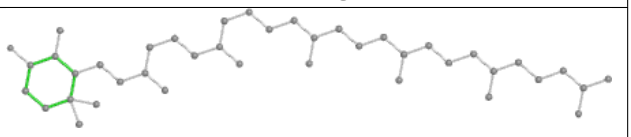
Bond lengths



Bond angles

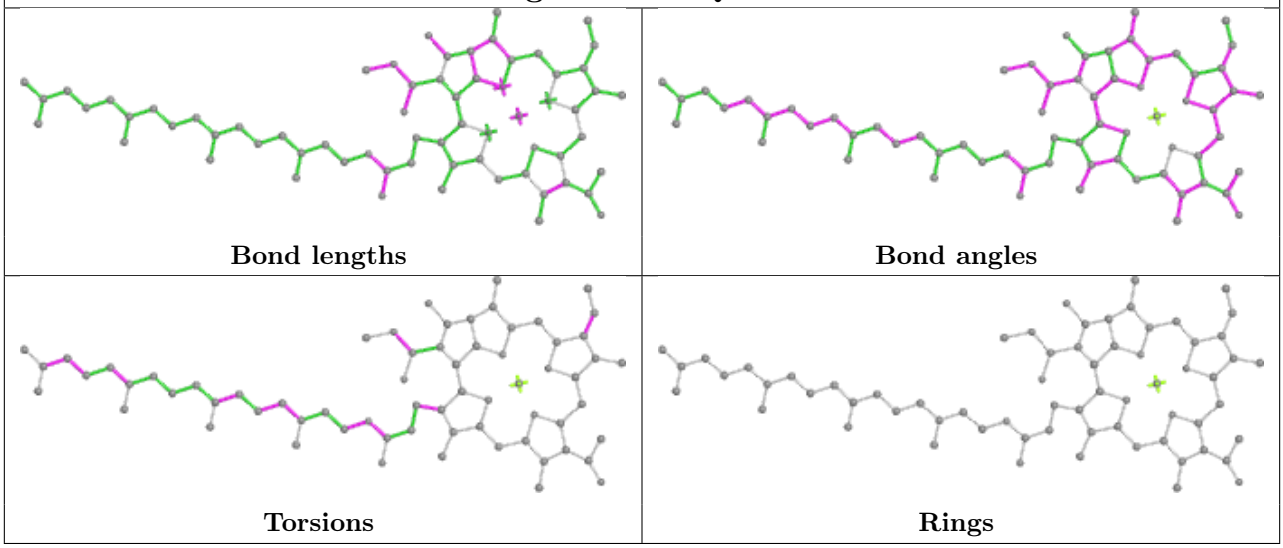


Torsions

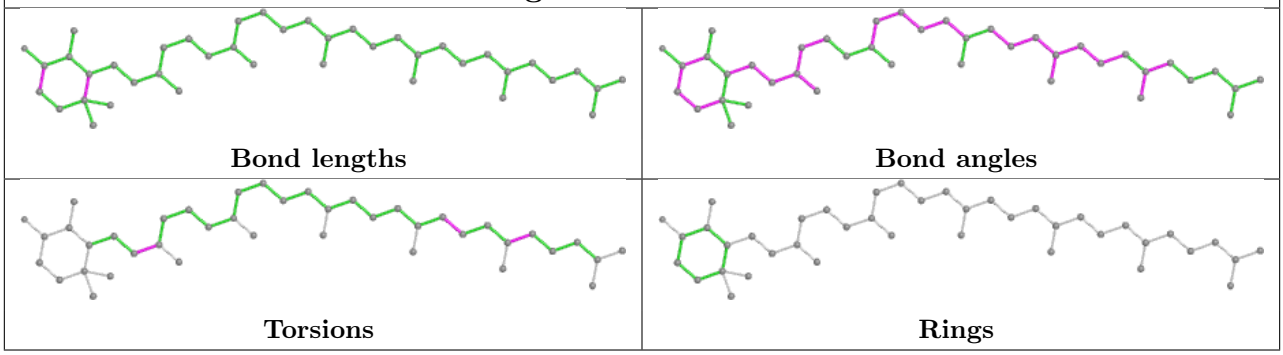


Rings

Ligand BCL Q 102



Ligand KGD 3 102



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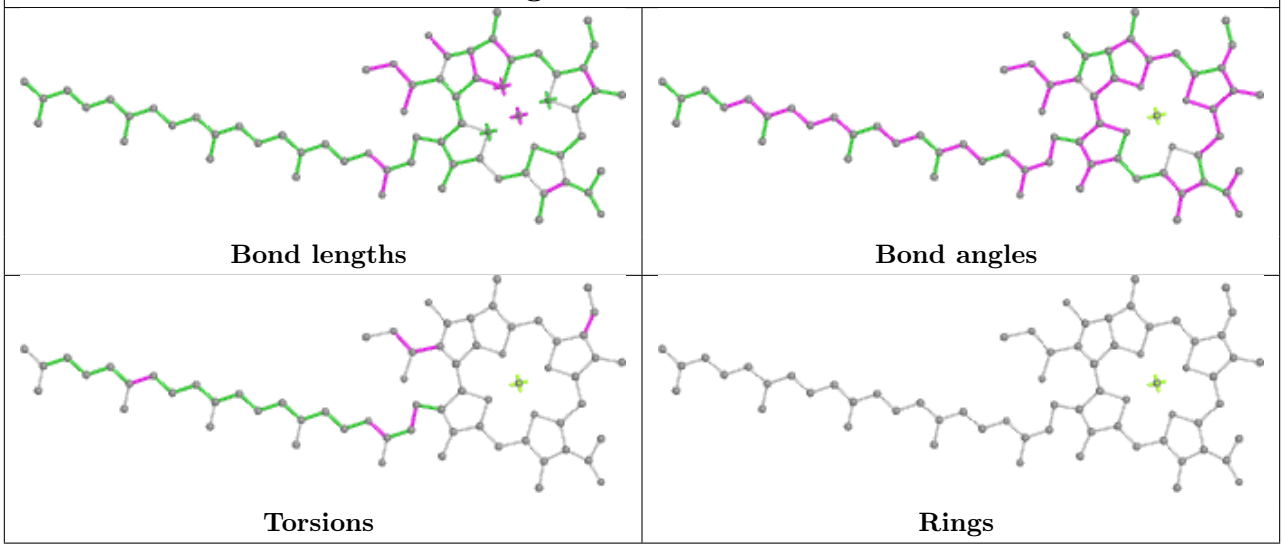

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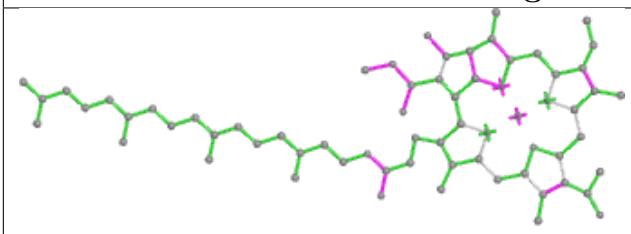

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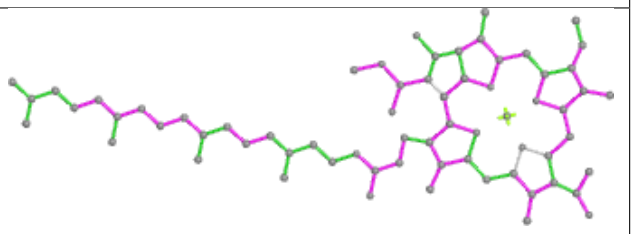
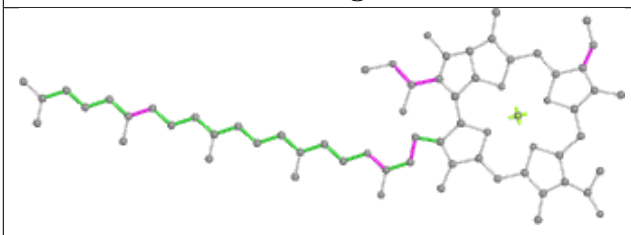
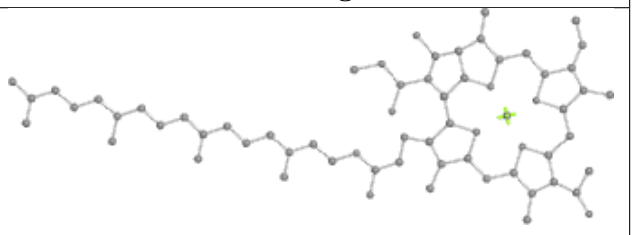


Bond angles

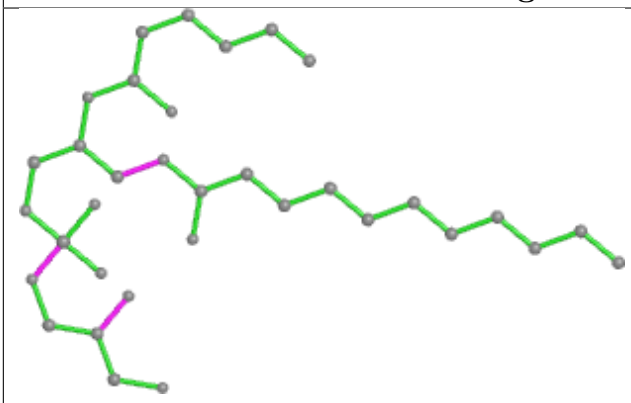


Torsions

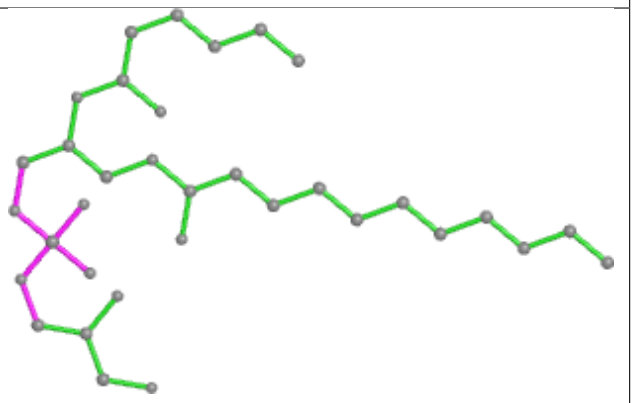


Rings

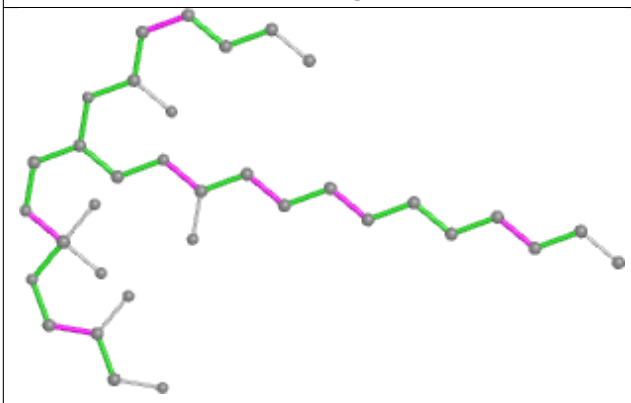
Ligand PGV M 706



Bond lengths



Bond angles



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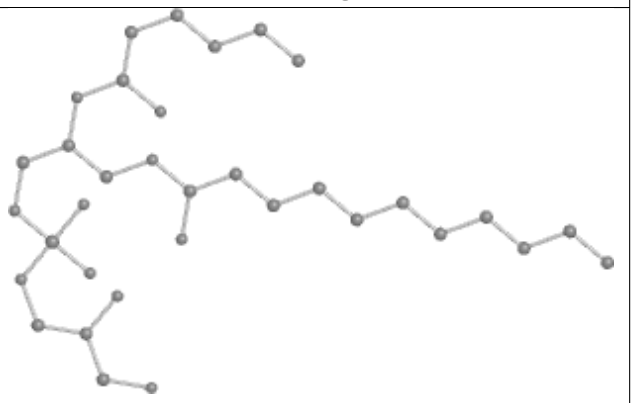
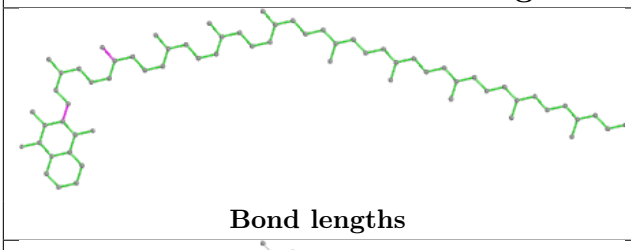
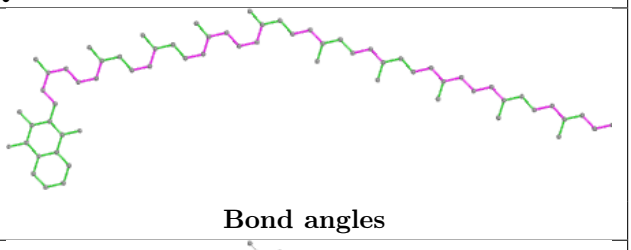
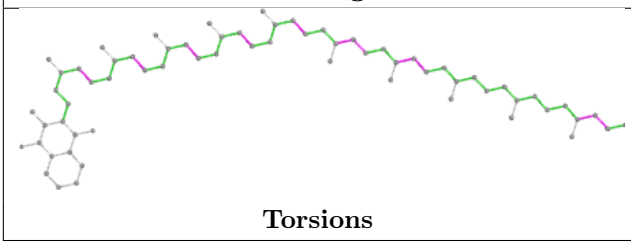


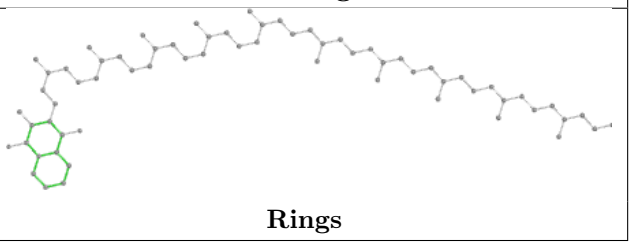
Rings

Ligand MQE M 701

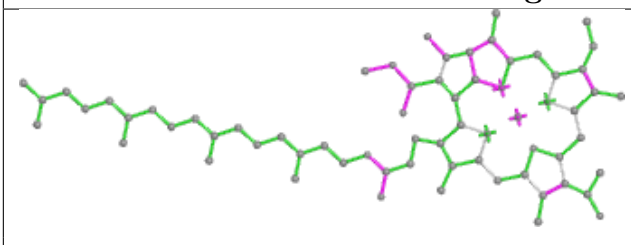

Bond lengths

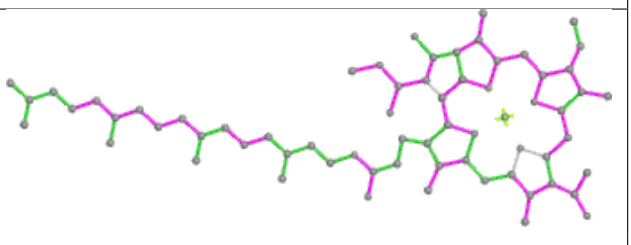

Bond angles

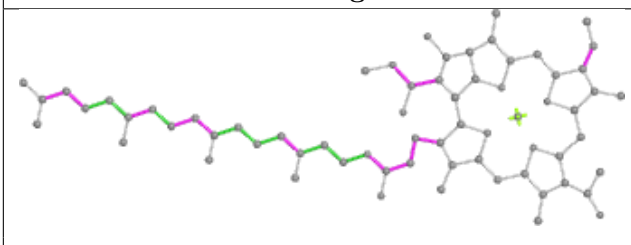

Torsions

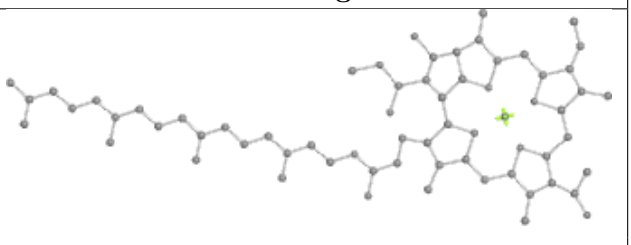

Rings

Ligand BCL R 101

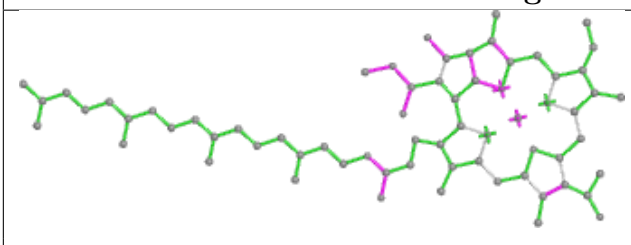

Bond lengths

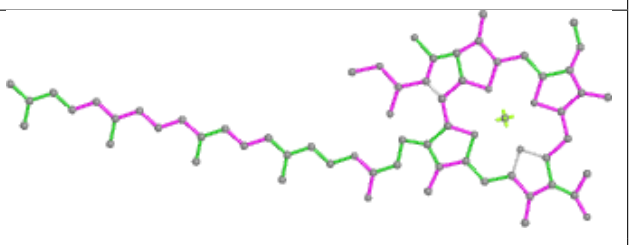

Bond angles

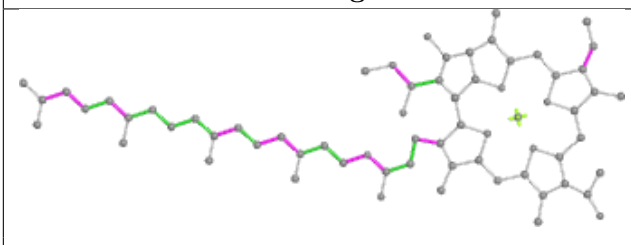

Torsions

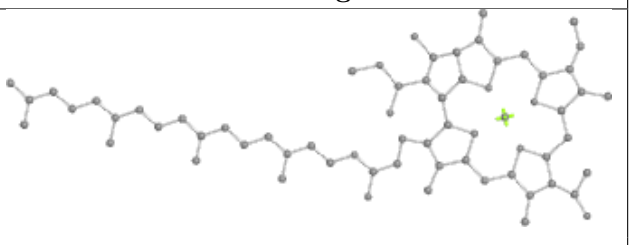

Rings

Ligand BCL G 101

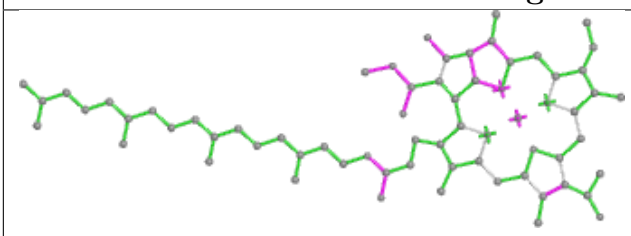

Bond lengths


Bond angles

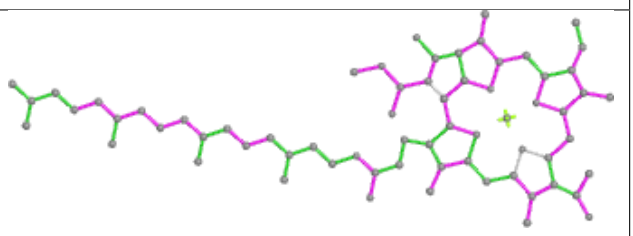

Torsions


Rings

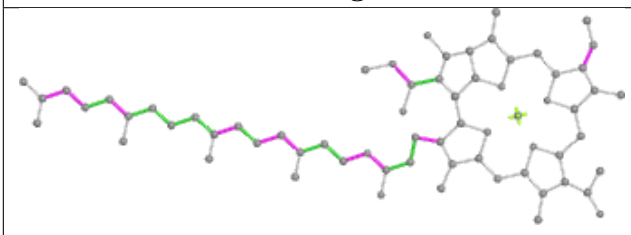
Ligand BCL E 101



Bond lengths



Bond angles



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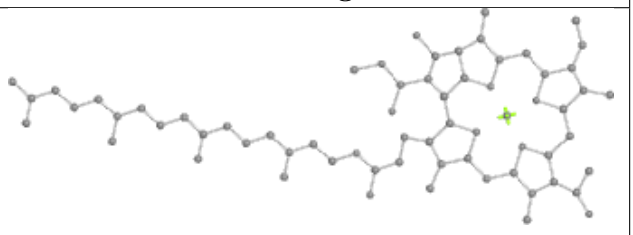
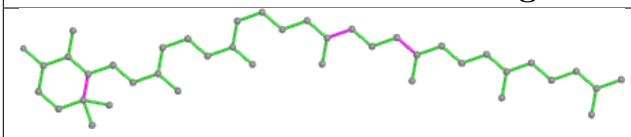


Rings

Ligand KGD G 102



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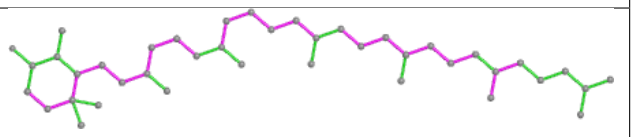
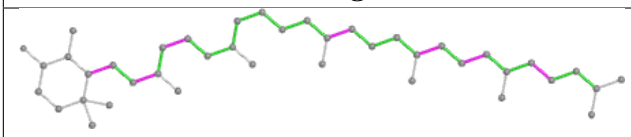
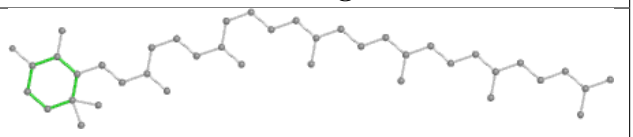


Bond angles

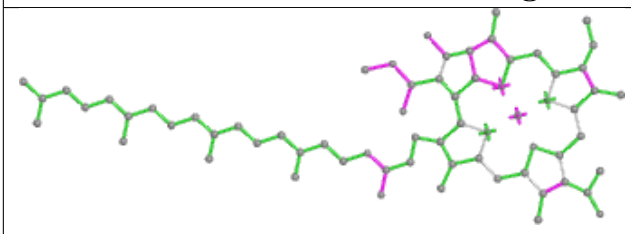


Torsions

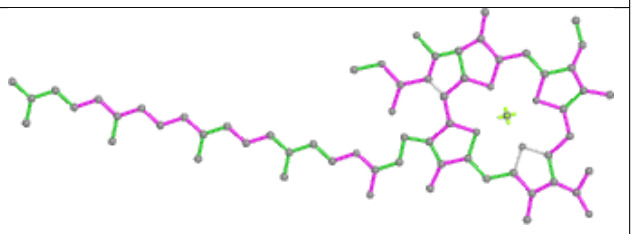


Rings

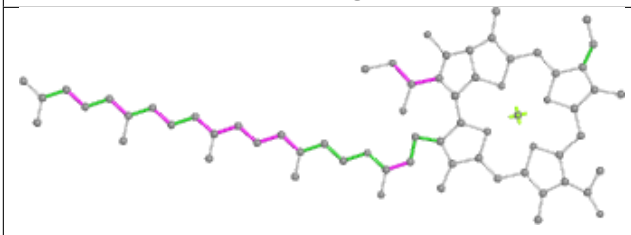
Ligand BCL M 703



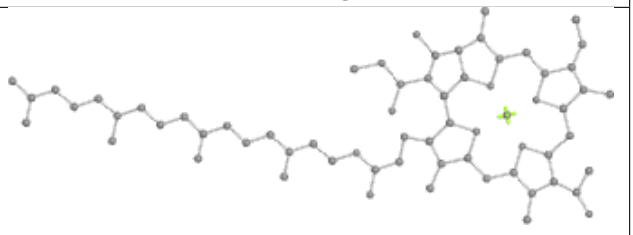
Bond lengths



Bond angles

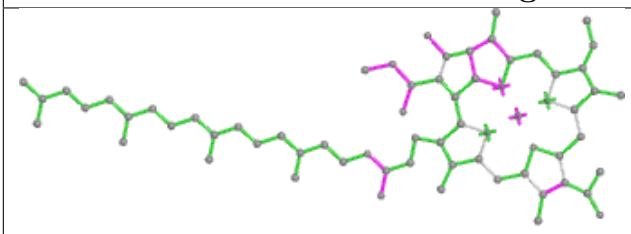


Torsions

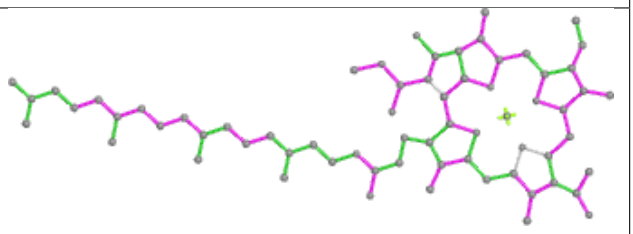


Rings

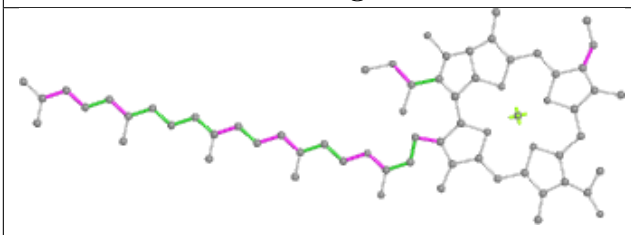
Ligand BCL W 103



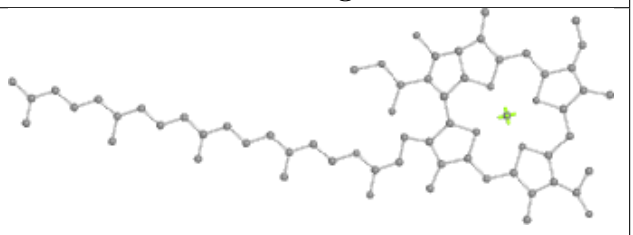
Bond lengths



Bond angles

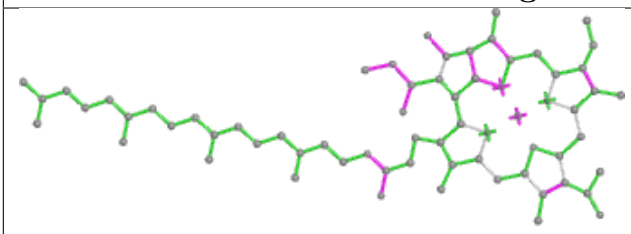


Torsions

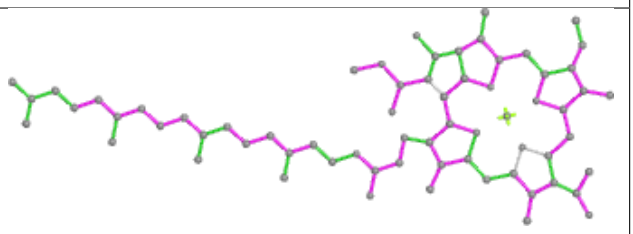


Rings

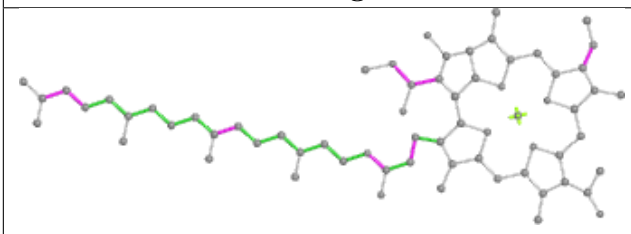
Ligand BCL W 102



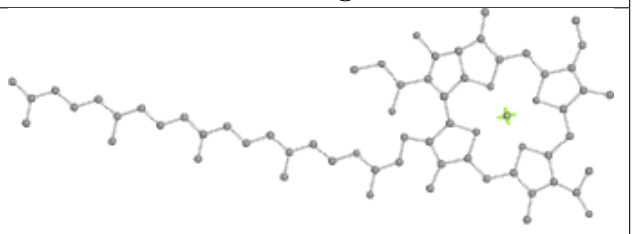
Bond lengths



Bond angles

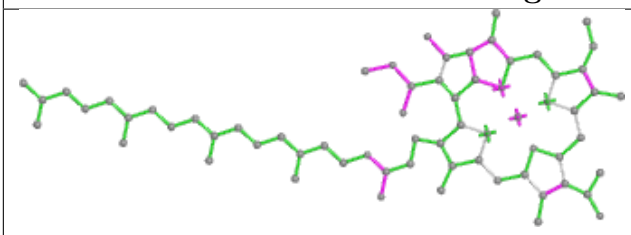


Torsions



Rings

Ligand BCL H 101



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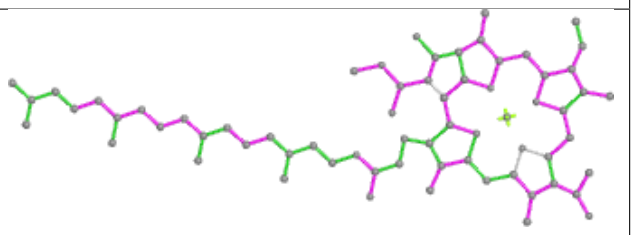

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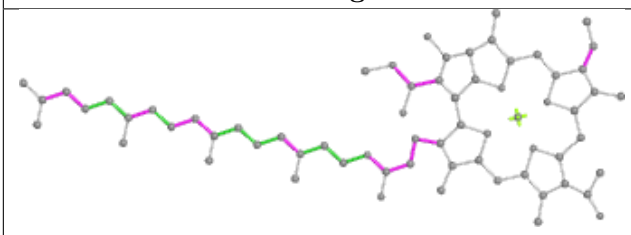

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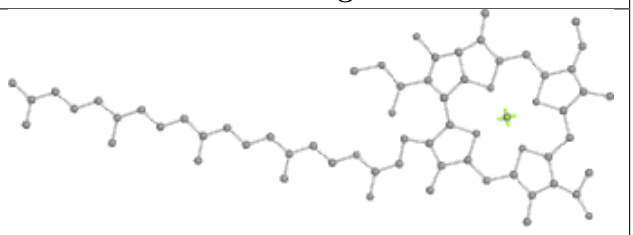
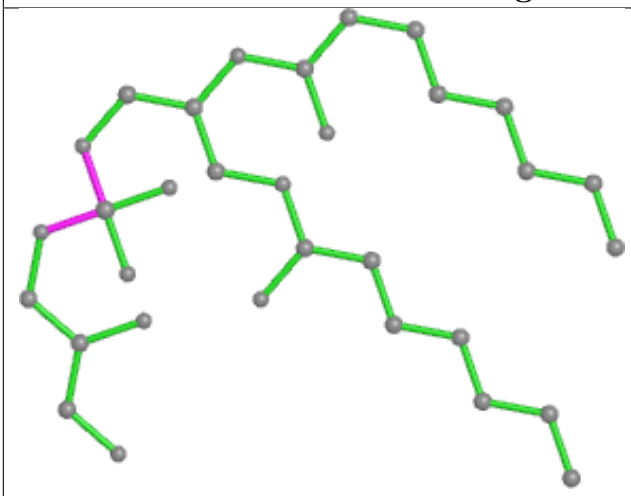


Rings

Ligand PGV L 1006



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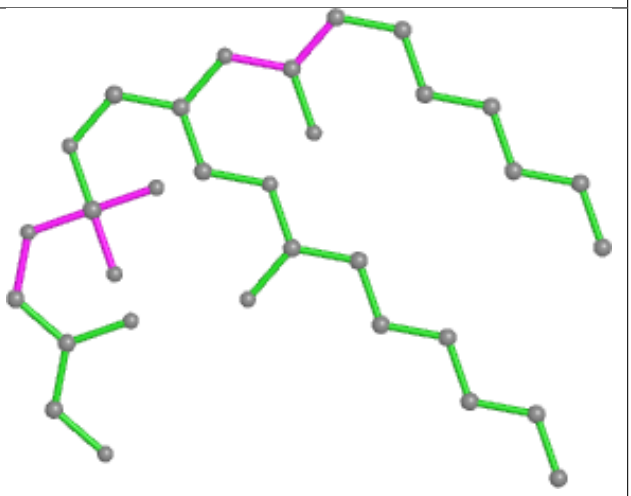

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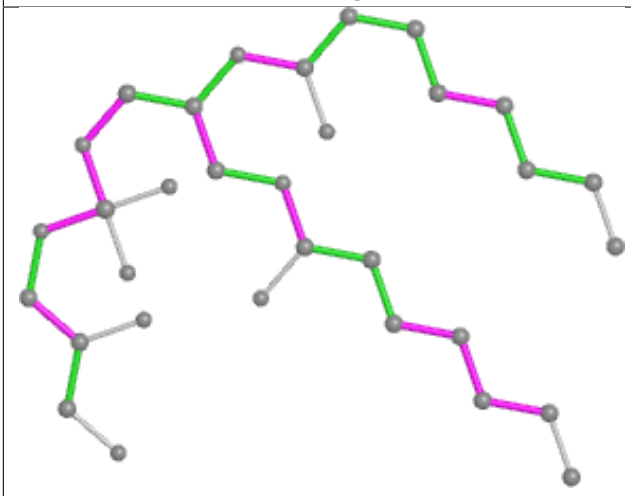

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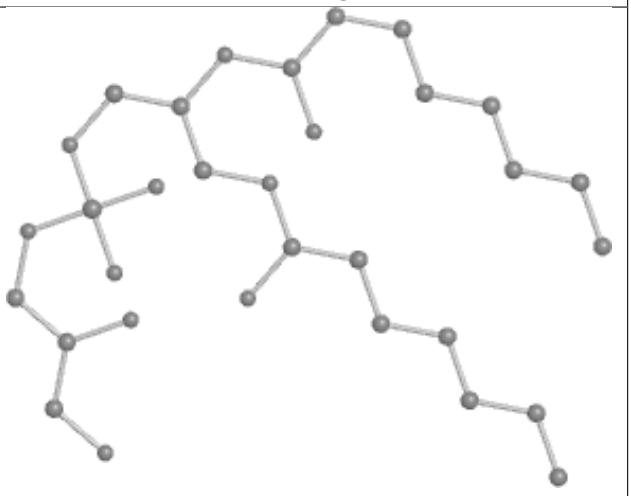
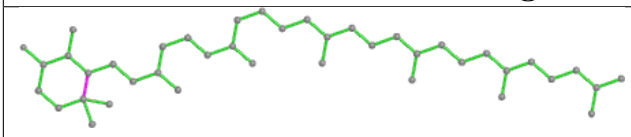


Rings

Ligand KGD U 103



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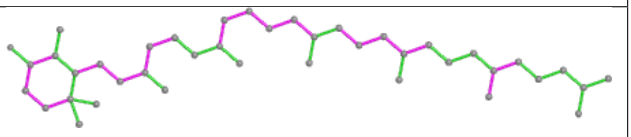
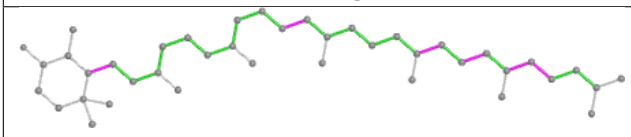


Bond angles



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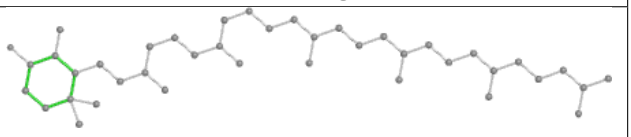
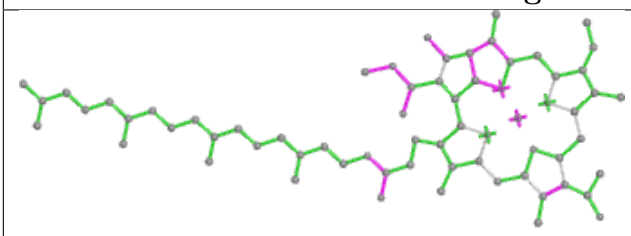


Rings

Ligand BCL K 101



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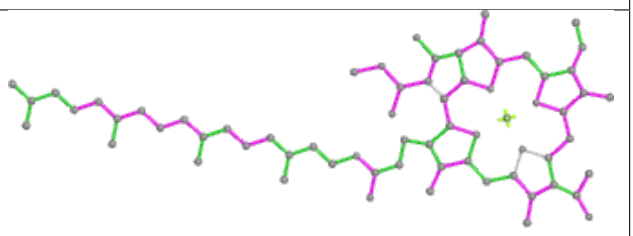

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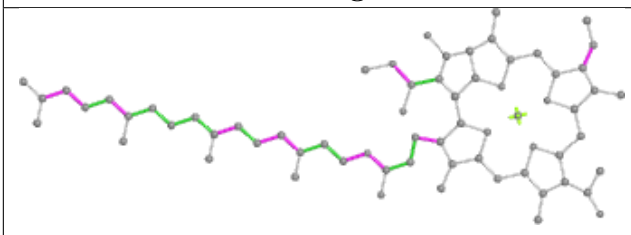

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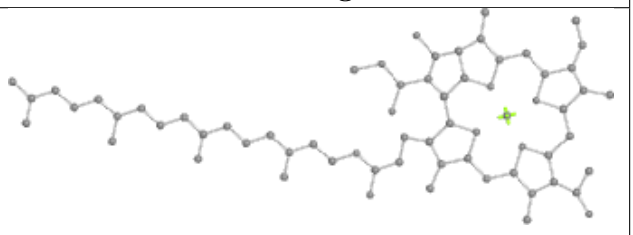
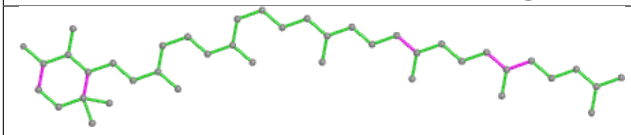


Rings

Ligand KGD A 104



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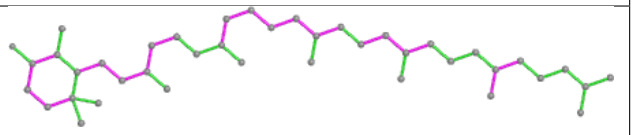
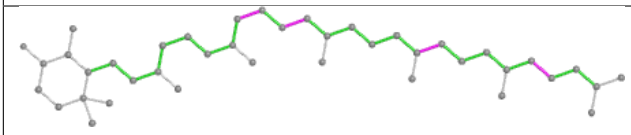


Bond angles



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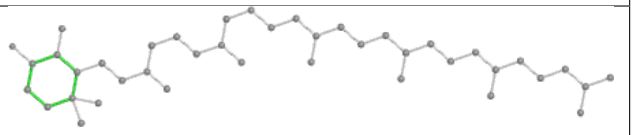
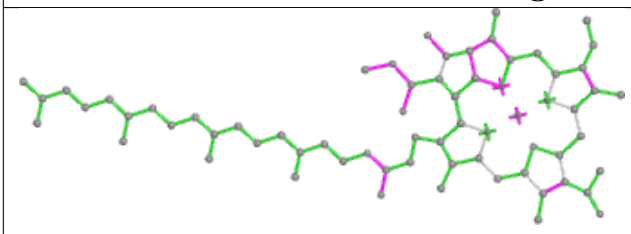


Rings

Ligand BCL 8 101



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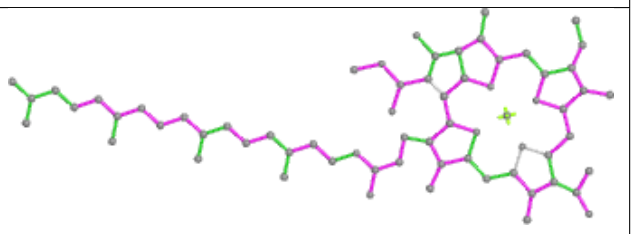

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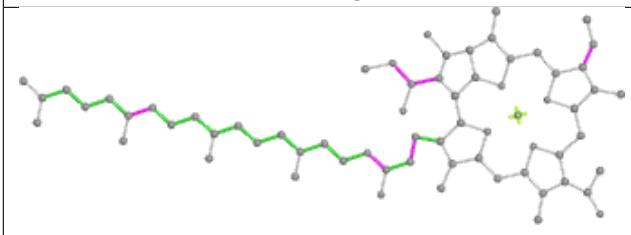

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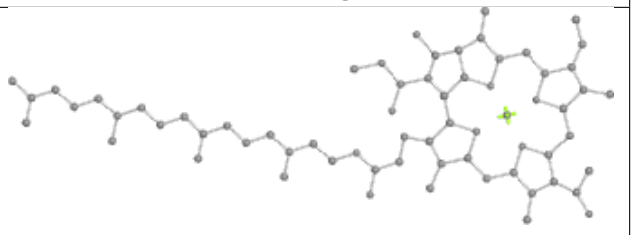
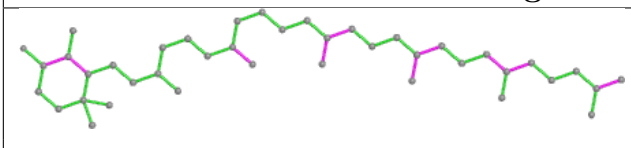


Rings

Ligand KGD 2 101



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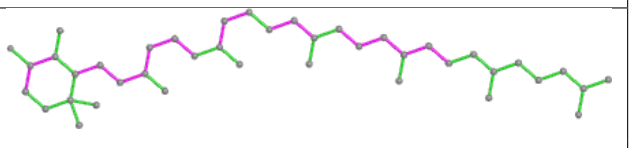
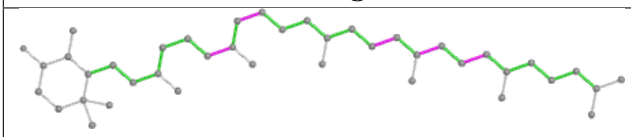


Bond angles



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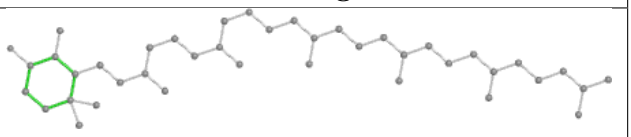
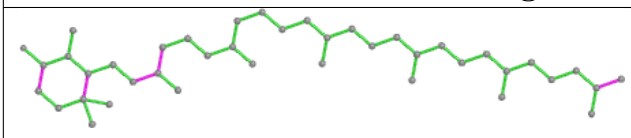


Rings

Ligand KGD A 103



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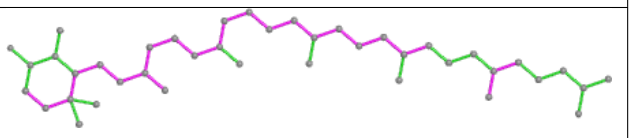
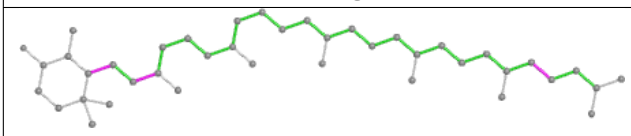
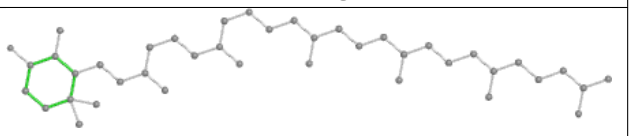


Bond angles

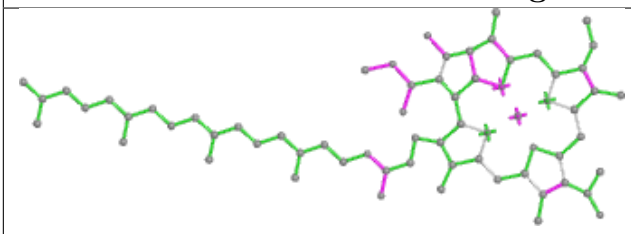


Torsions



Rings

Ligand BCL 4 101



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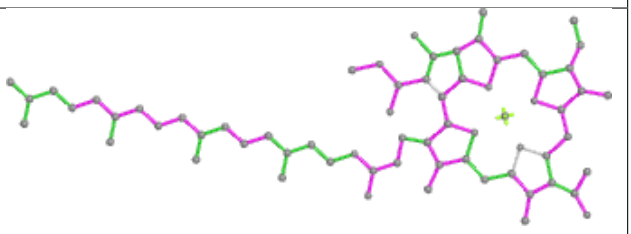
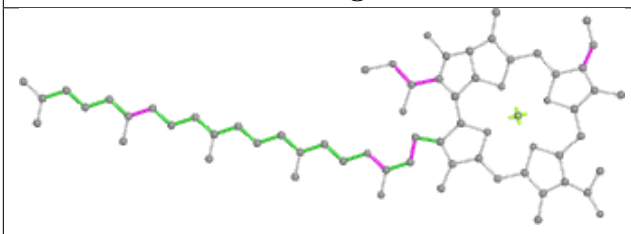
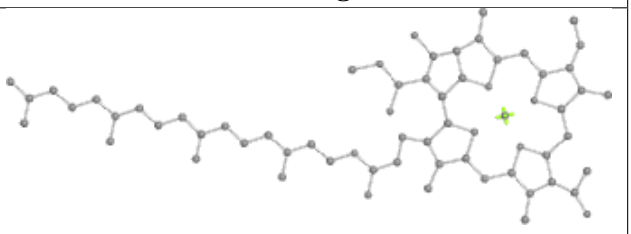


Bond angles

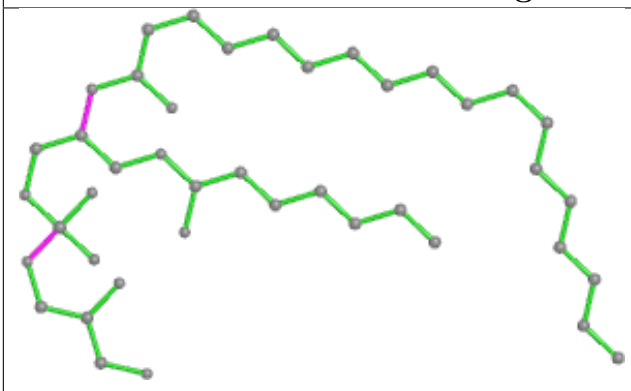


Torsions



Rings

Ligand PGV L 1007



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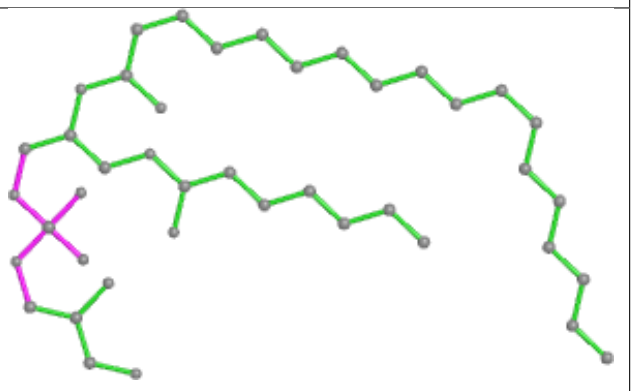
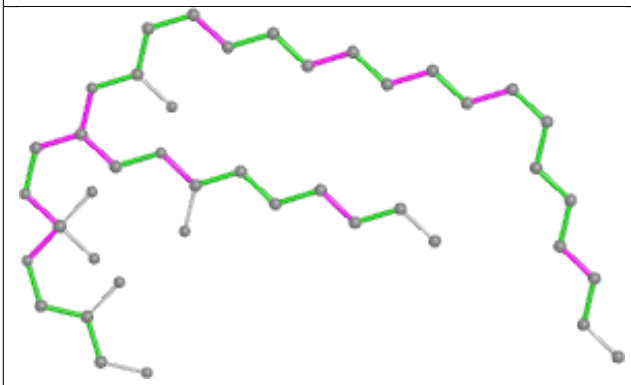


Bond angles



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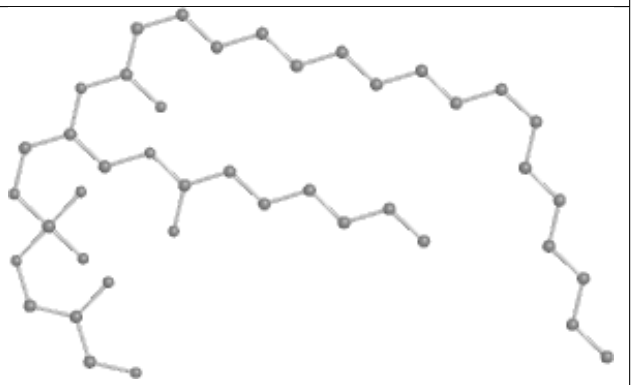
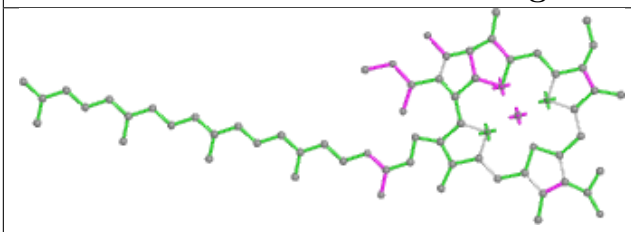


Rings

Ligand BCL 0 101



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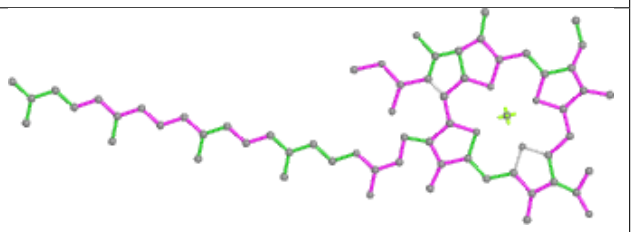
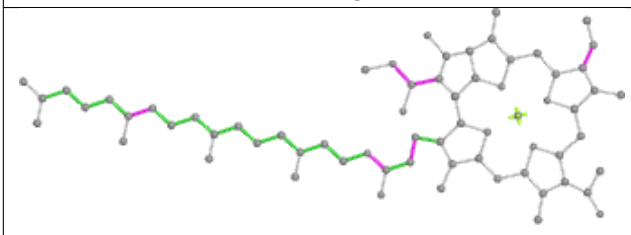
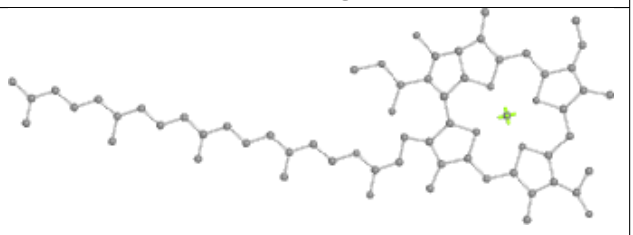


Bond angles

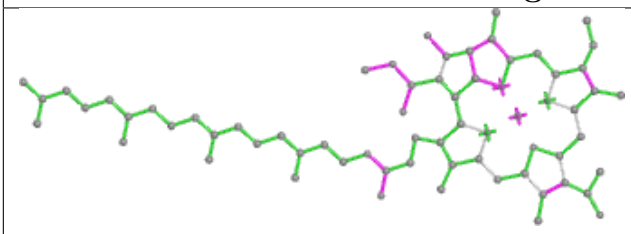


Torsions



Rings

Ligand BCL U 101



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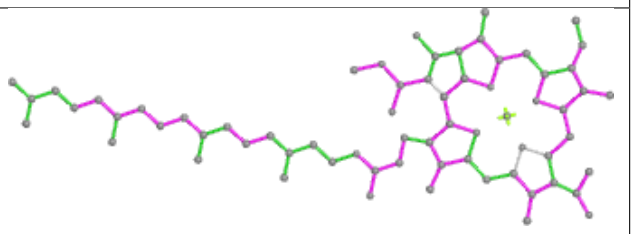
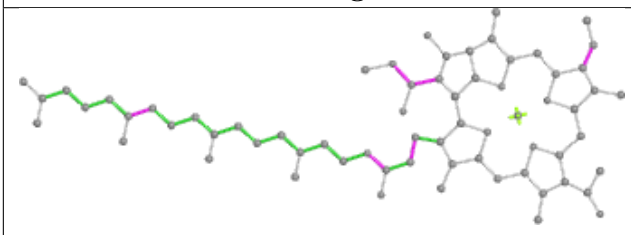


Bond angles



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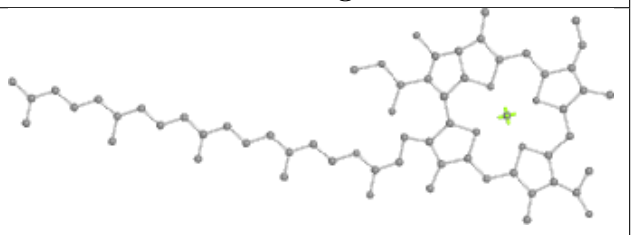
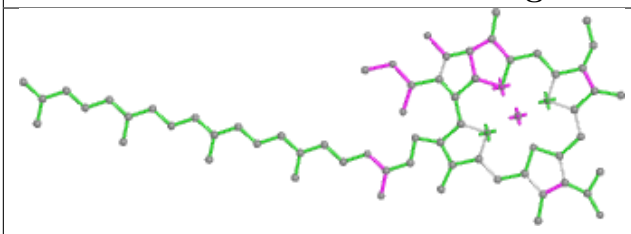
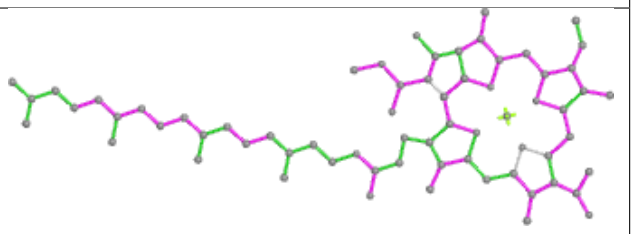


Rings

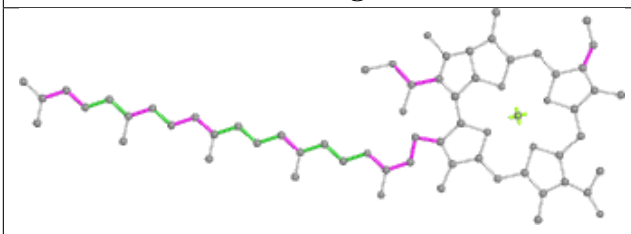
Ligand BCL T 101



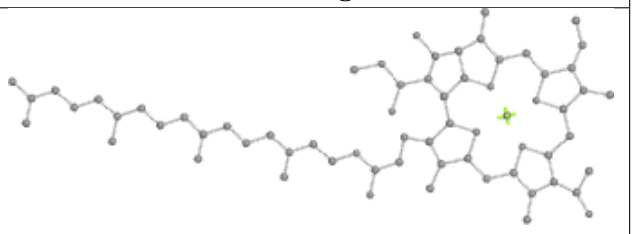
Bond lengths



Bond angles

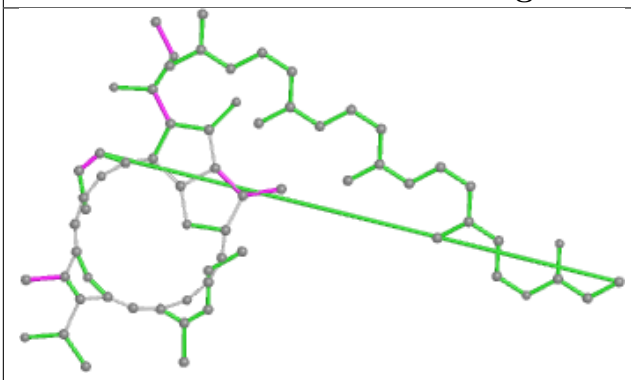


Torsions

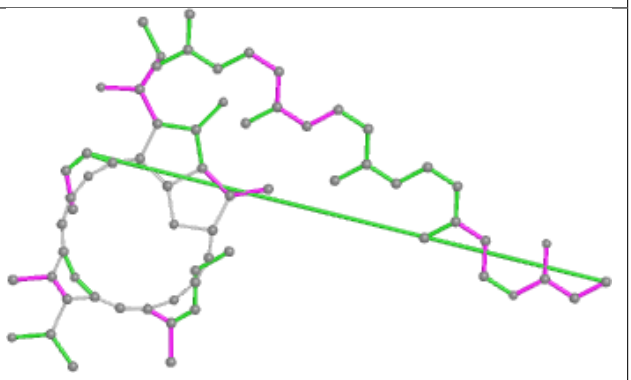


Rings

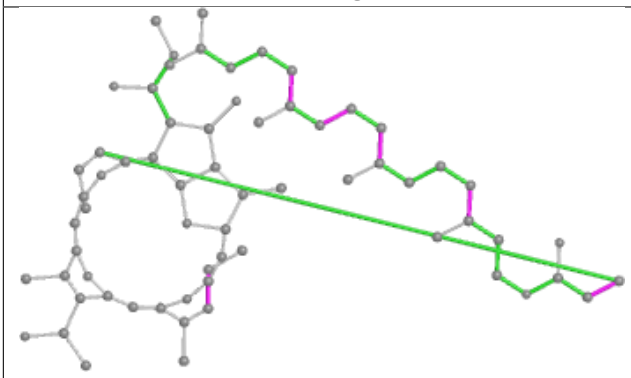
Ligand BPH L 1003



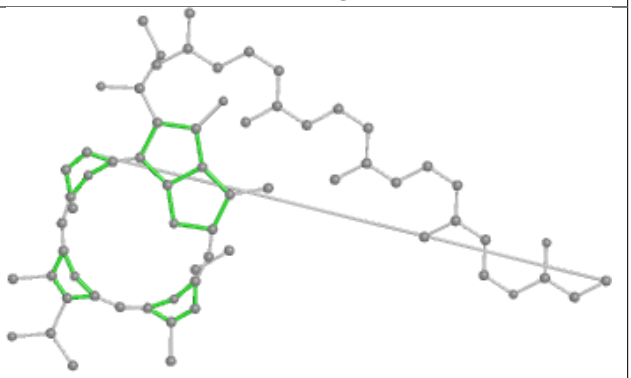
Bond lengths



Bond angles

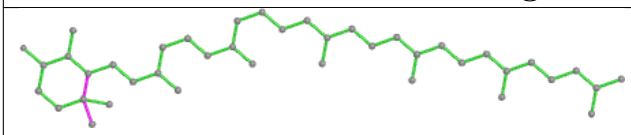


Torsions

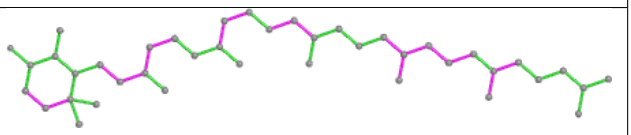


Rings

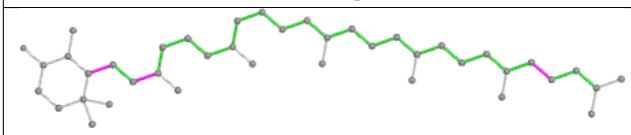
Ligand KGD E 102



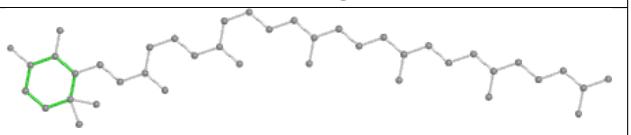
Bond lengths



Bond angles

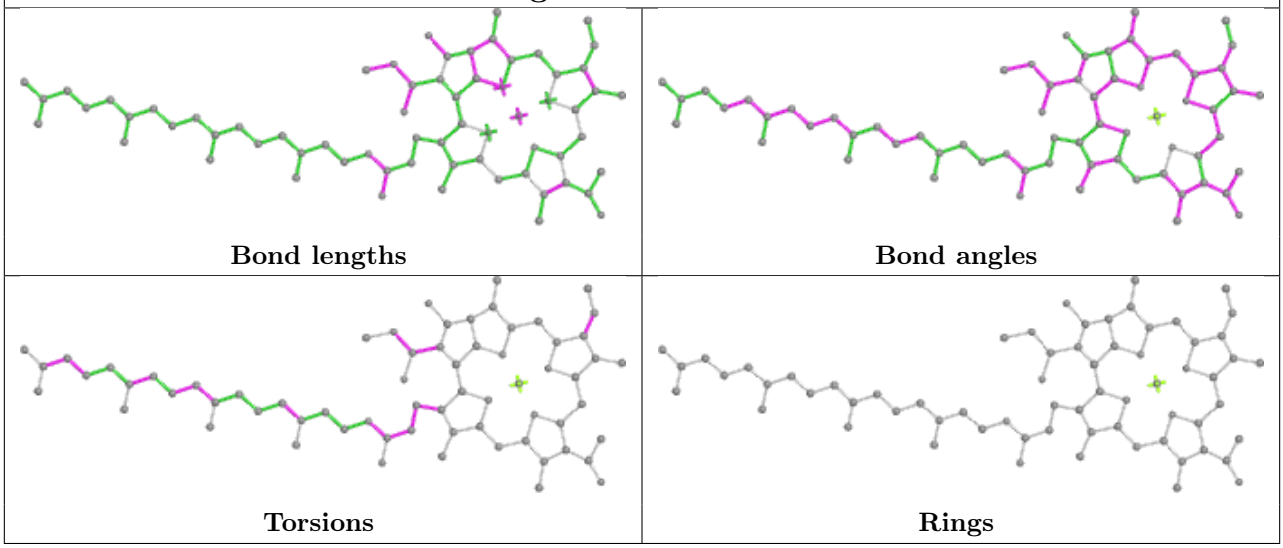


Torsions

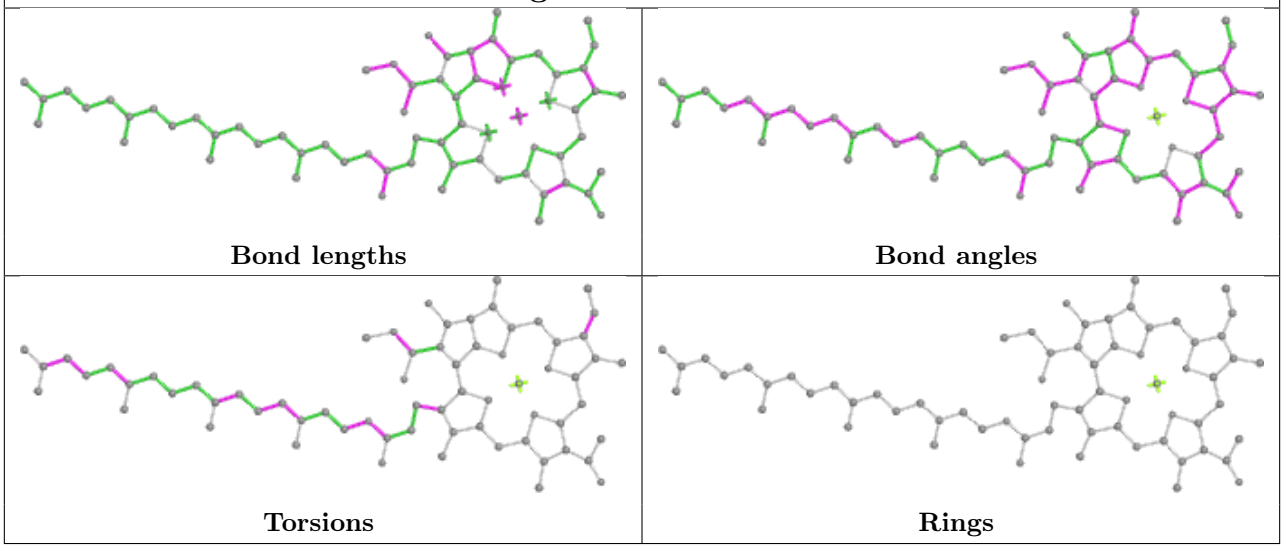


Rings

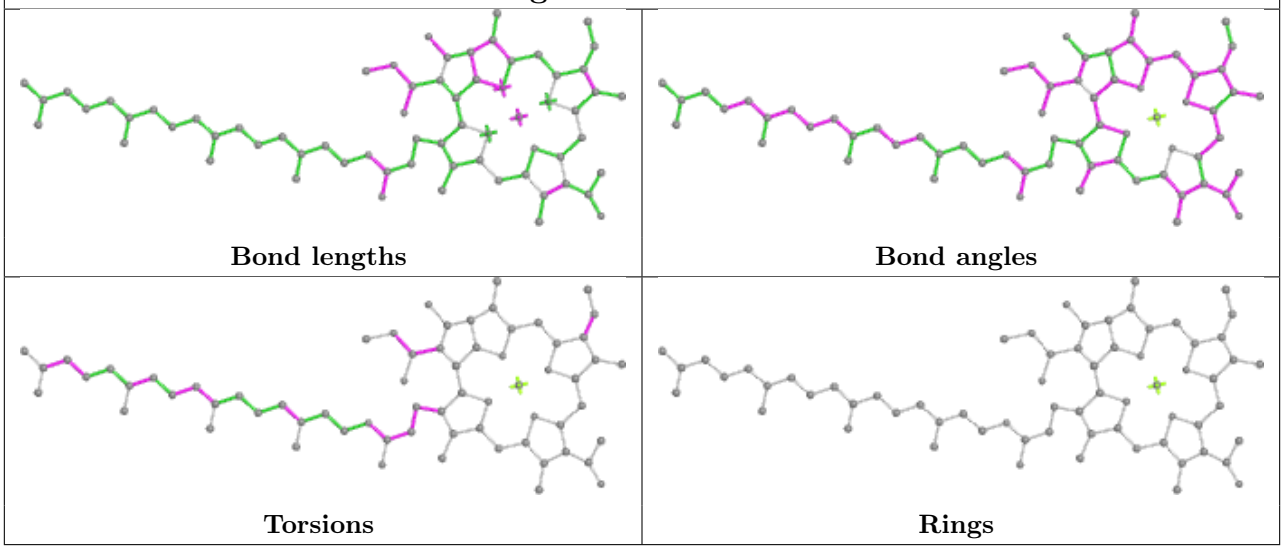
Ligand BCL 5 101



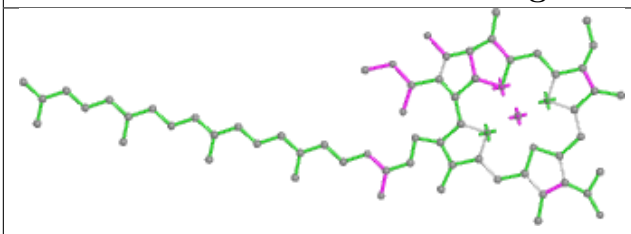
Ligand BCL 8 102



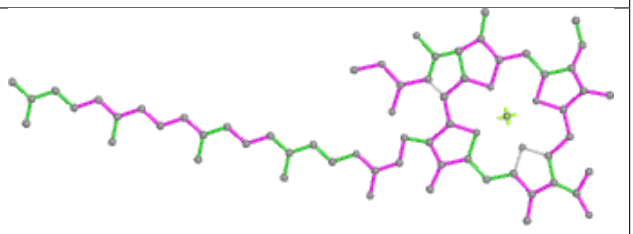
Ligand BCL 3 101



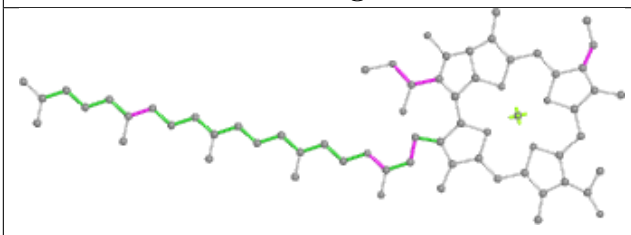
Ligand BCL 2 102



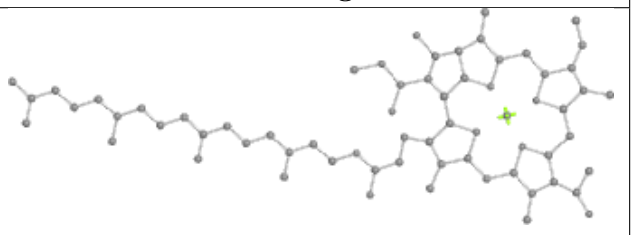
Bond lengths



Bond angles

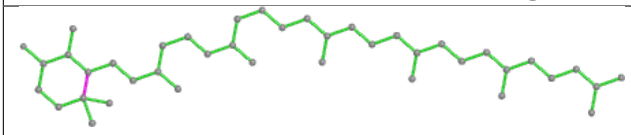


Torsions

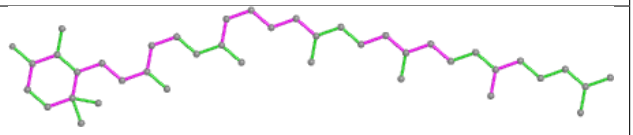


Rings

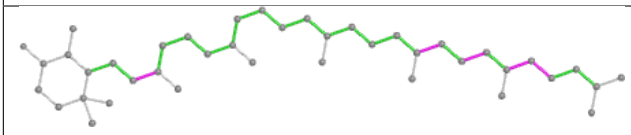
Ligand KGD 5 102



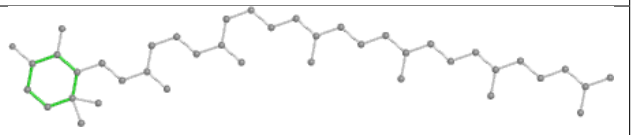
Bond lengths



Bond angles

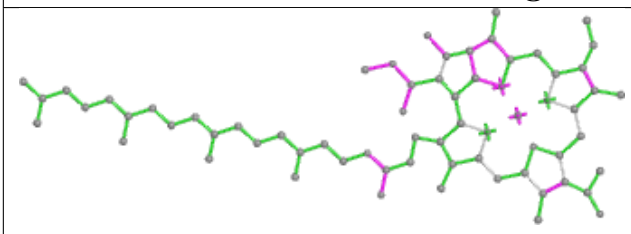


Torsions

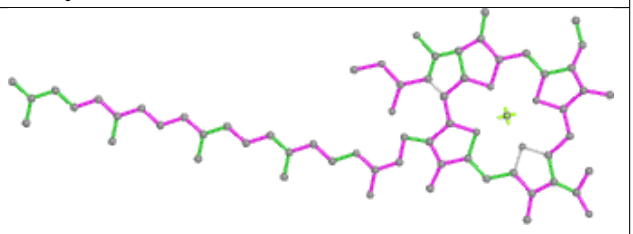


Rings

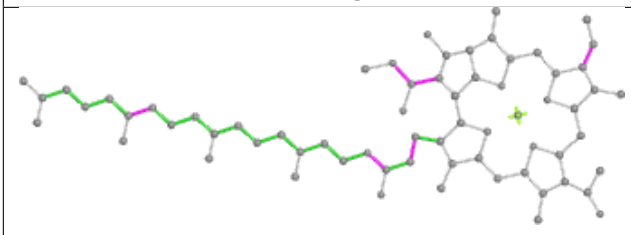
Ligand BCL Q 101



Bond lengths



Bond angles



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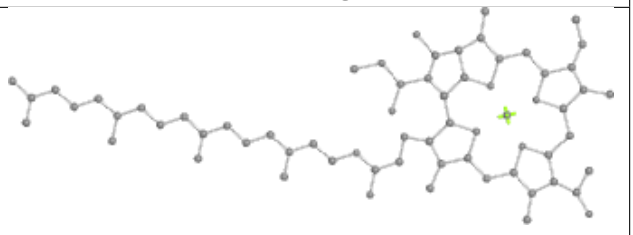
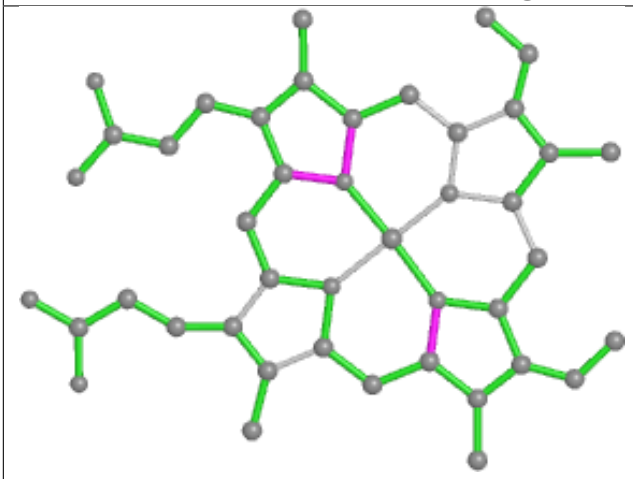
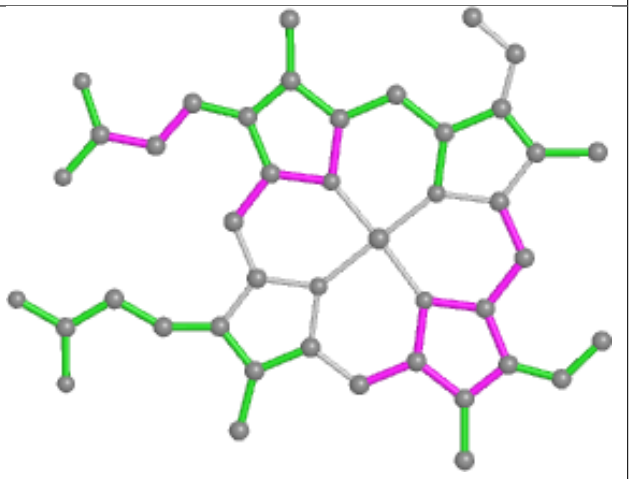


Rings

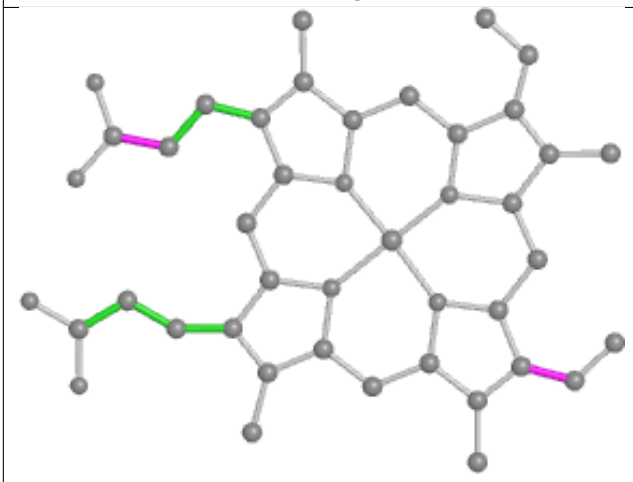
Ligand HEM C 403



Bond lengths



Bond angles



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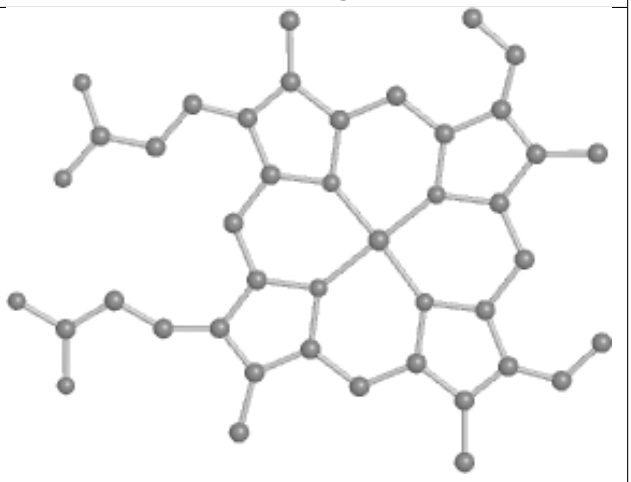
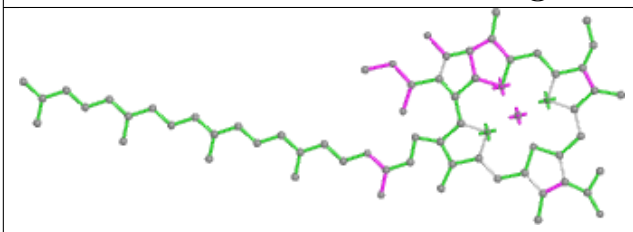
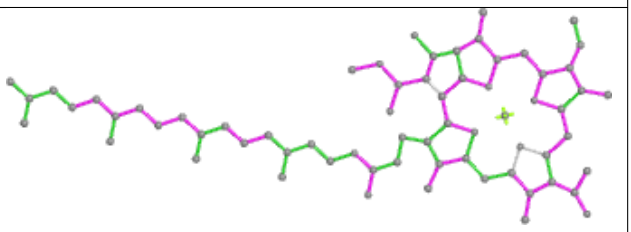


Rings

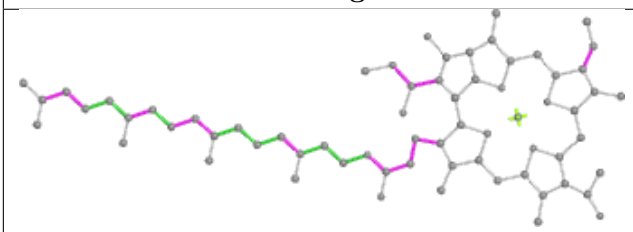
Ligand BCL 7 101



Bond lengths



Bond angles



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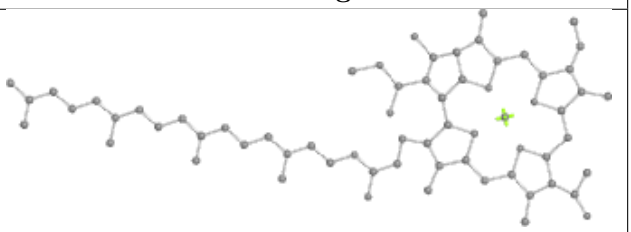
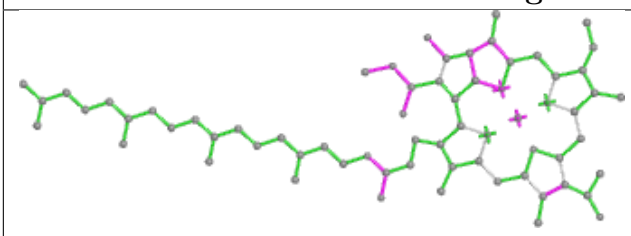
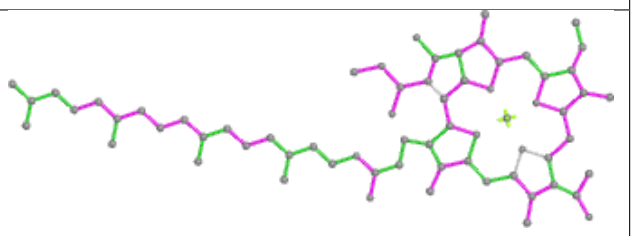


Rings

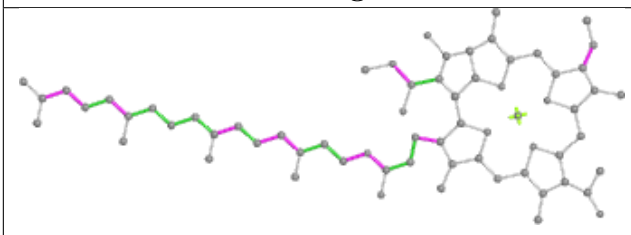
Ligand BCL B 101



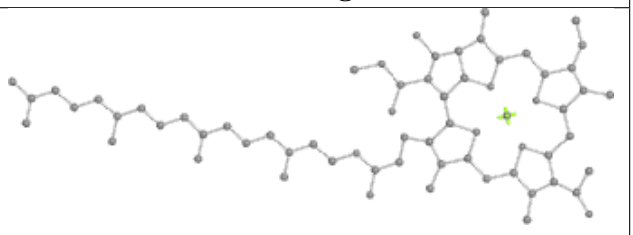
Bond lengths



Bond angles

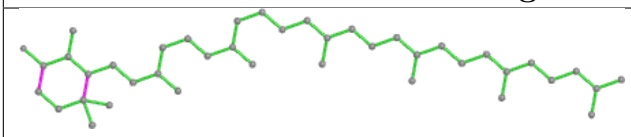


Torsions

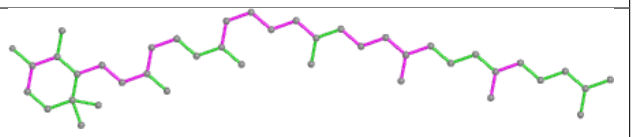


Rings

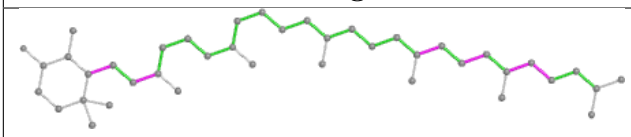
Ligand KGD K 102



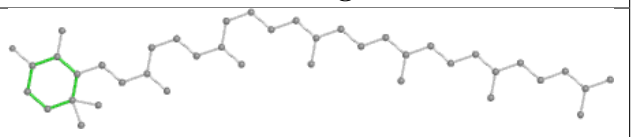
Bond lengths



Bond angles

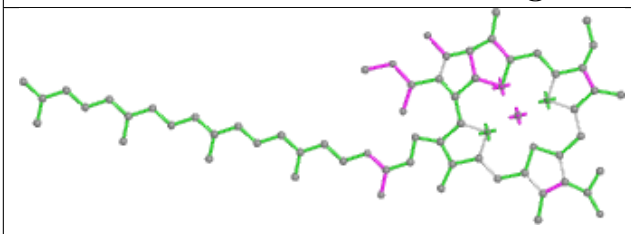


Torsions

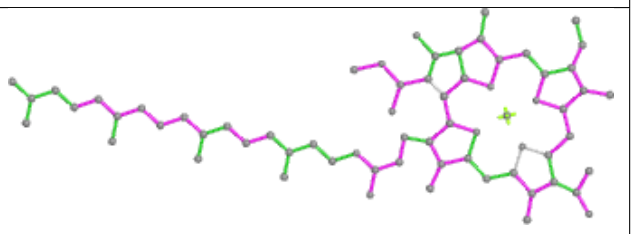


Rings

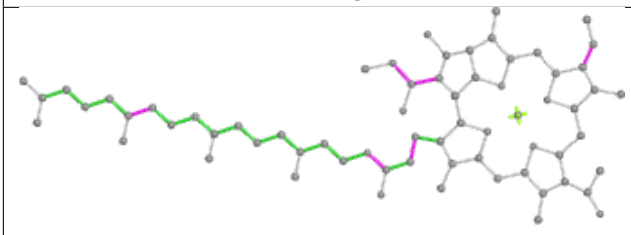
Ligand BCL F 102



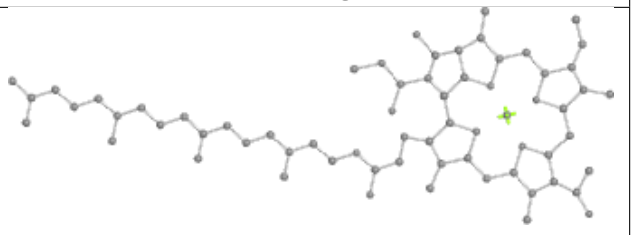
Bond lengths



Bond angles

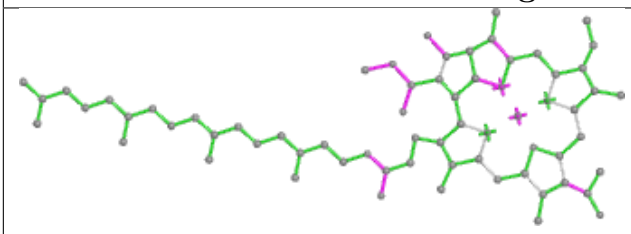


Torsions



Rings

Ligand BCL L 1002



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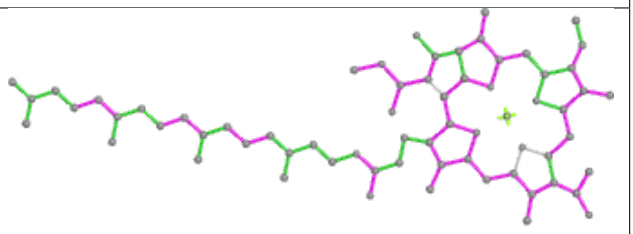
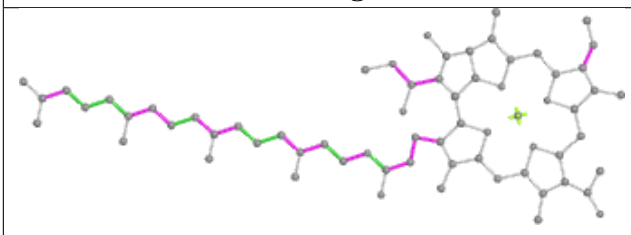


Bond angles



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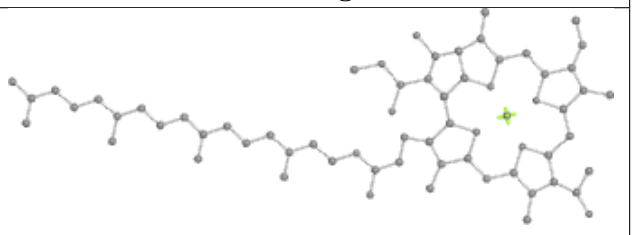
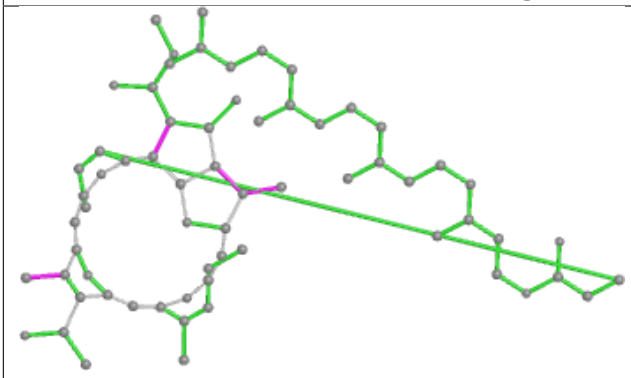


Rings

Ligand BPH M 704



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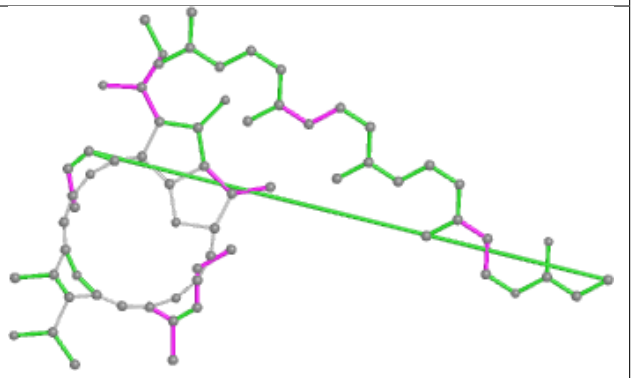
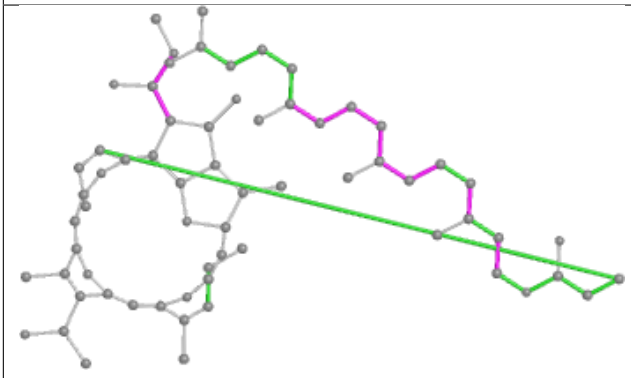
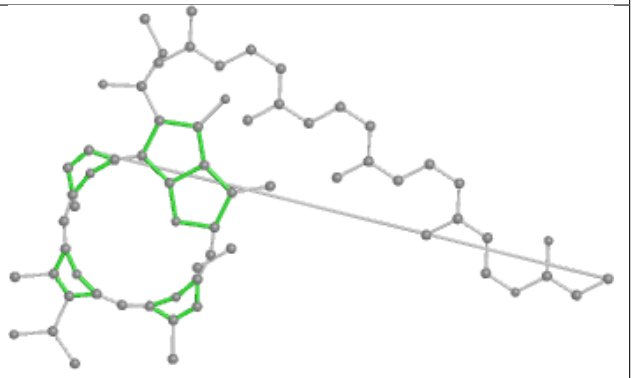


Bond angles

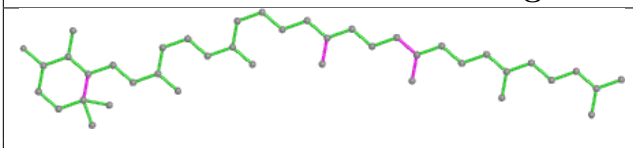


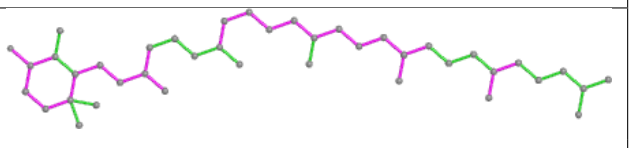
Torsions

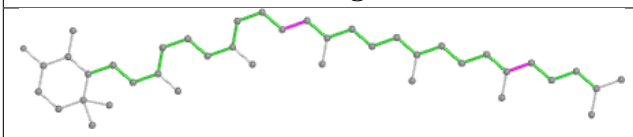


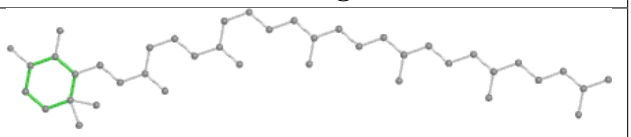
Rings

Ligand KGD 2 104

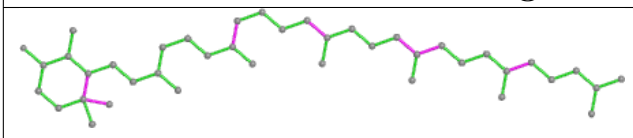

Bond lengths


Bond angles


Torsions


Rings

Ligand KGD H 103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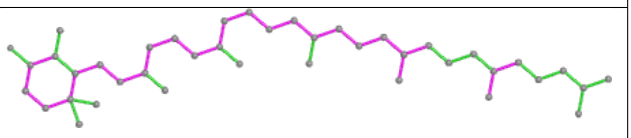
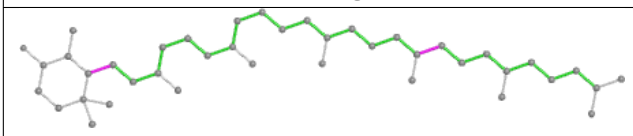
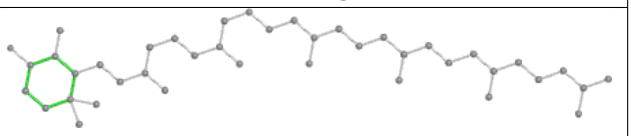
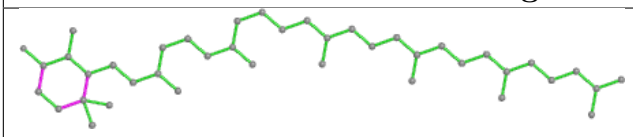
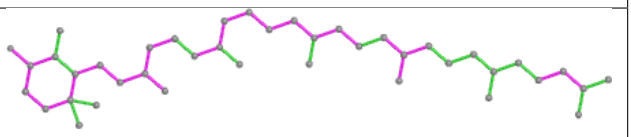

Bond angles

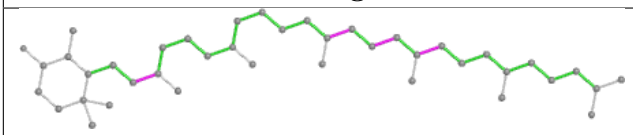

Torsions

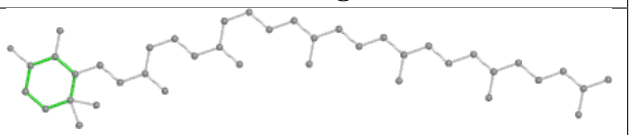

Rings

Ligand KGD P 102

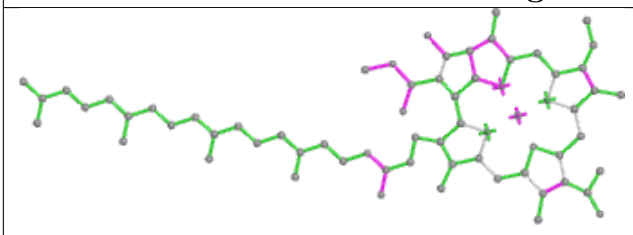

Bond lengths


Bond angles


Torsions


Rings

Ligand BCL F 101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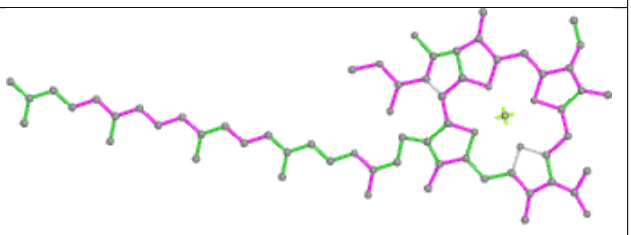
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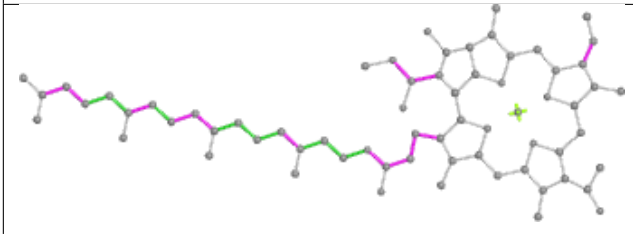
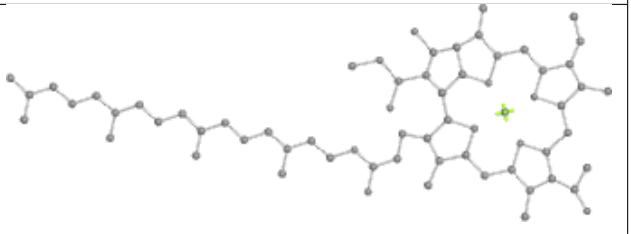
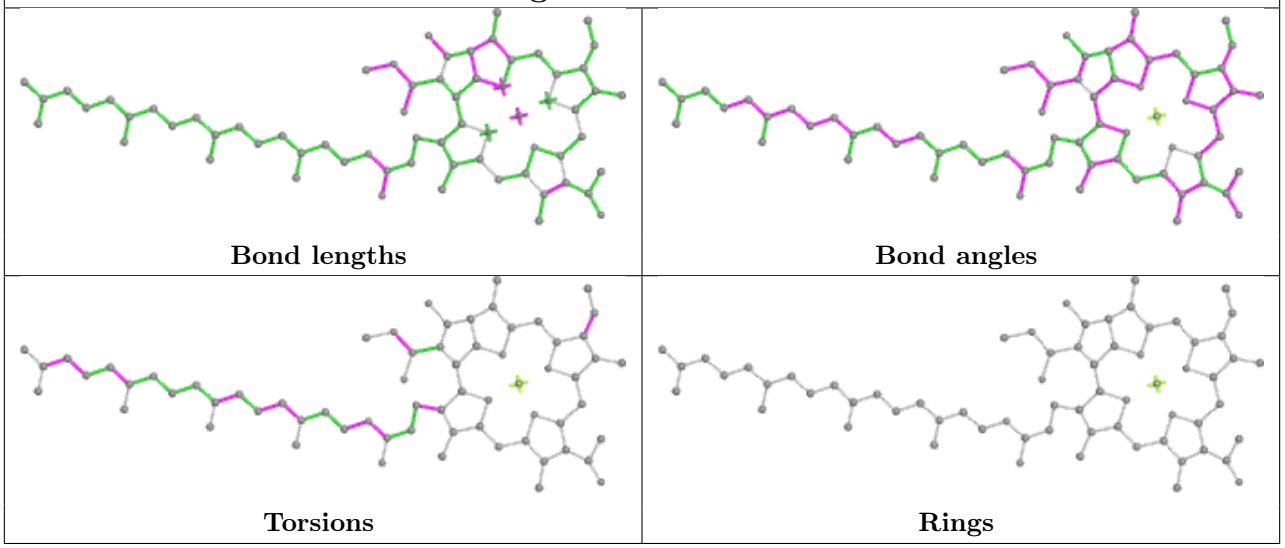
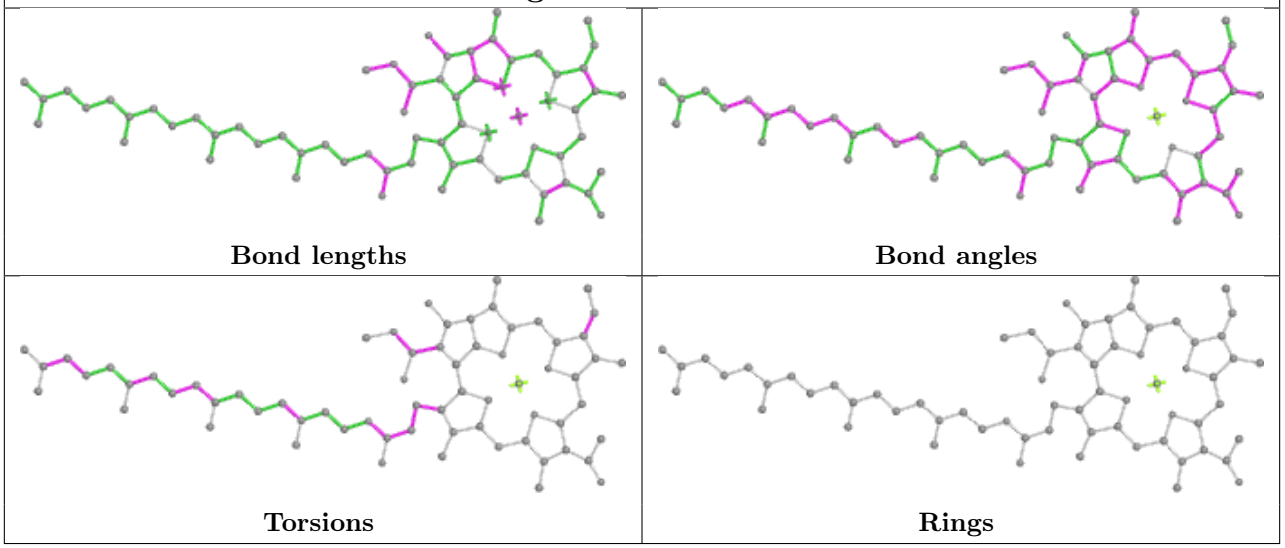

Torsions


Rings

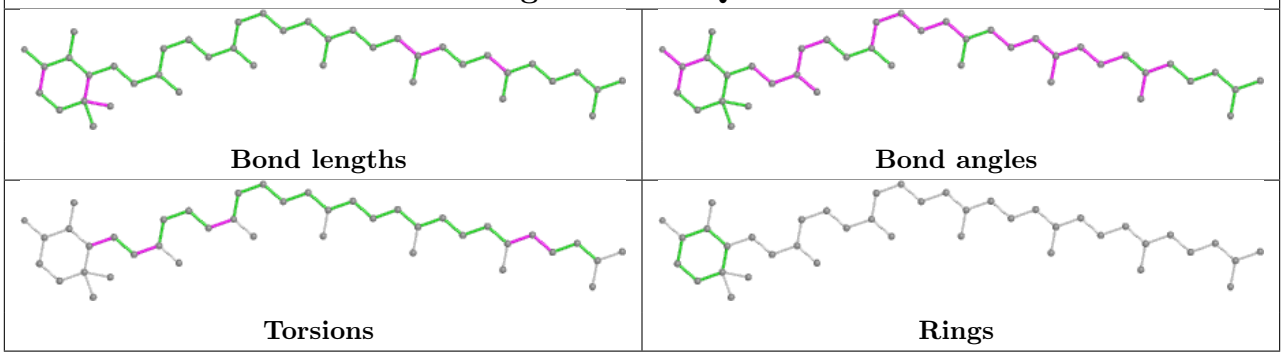
Ligand BCL 2 103

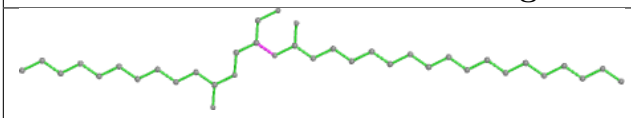
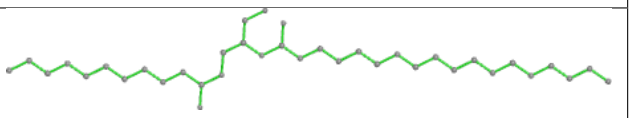
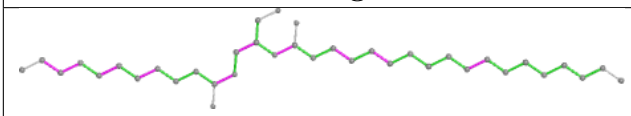
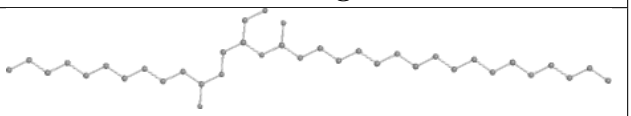


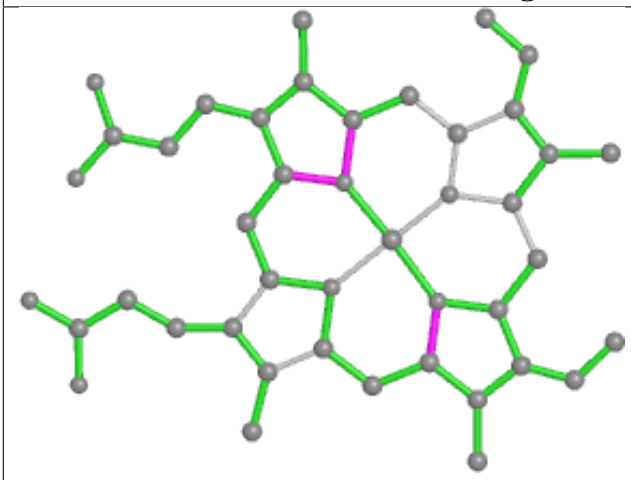
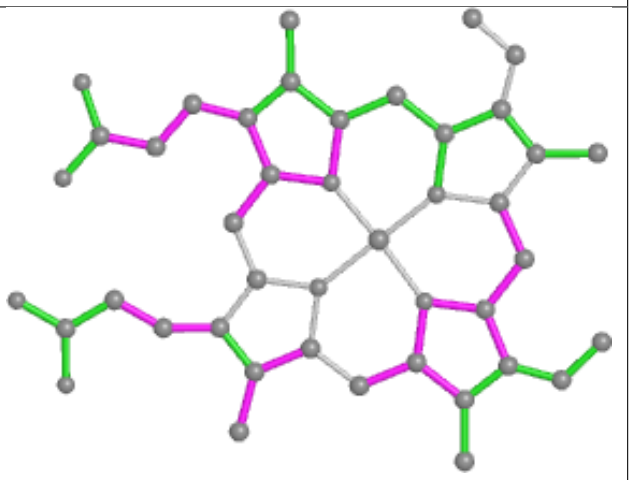
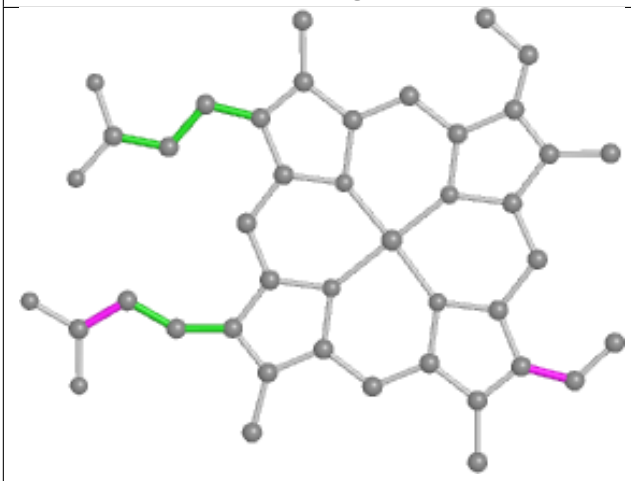
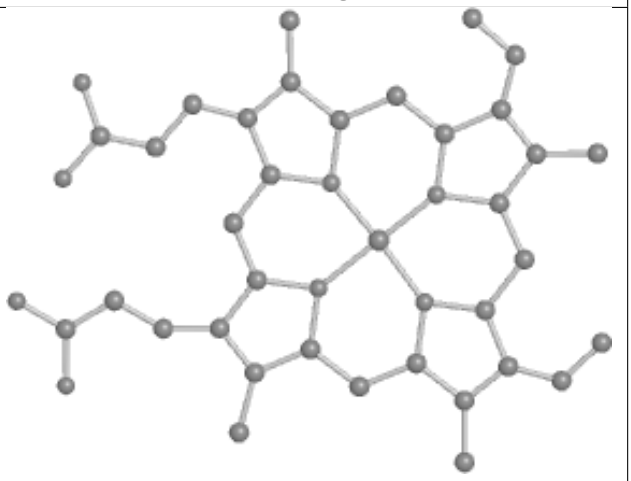
Ligand BCL P 101



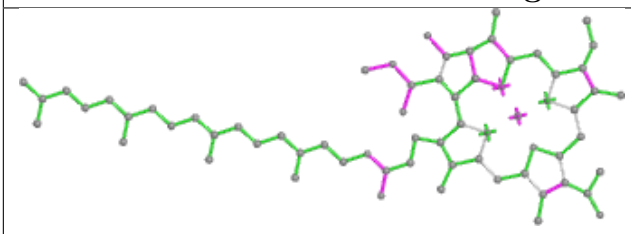
Ligand KGD Q 103



Ligand DGA Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM C 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCL H 102



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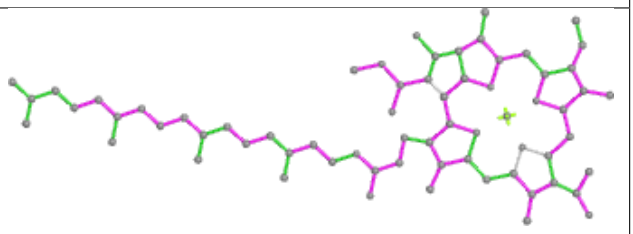
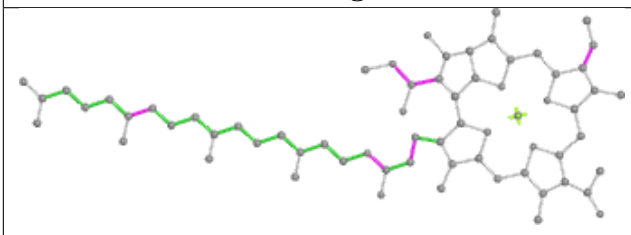


Bond angles



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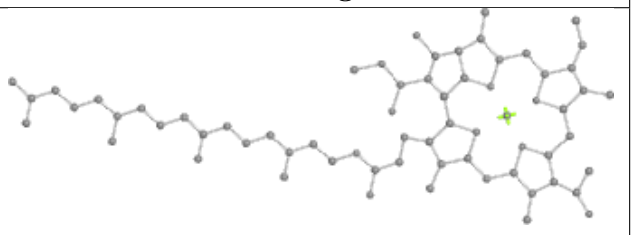
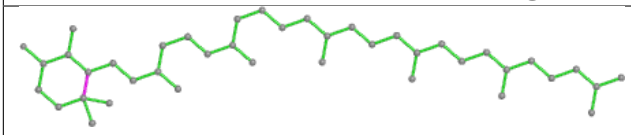


Rings

Ligand KGD J 103



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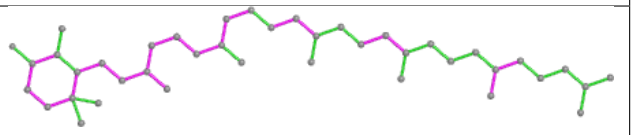
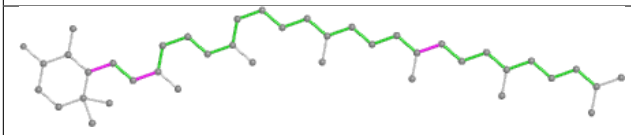


Bond angles



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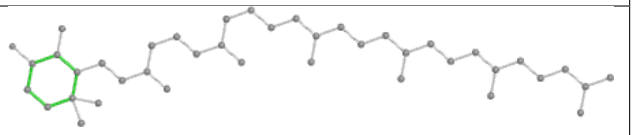
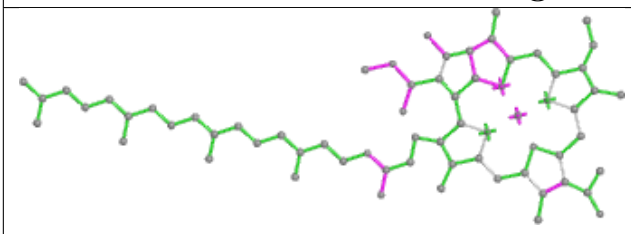


Rings

Ligand BCL 6 102



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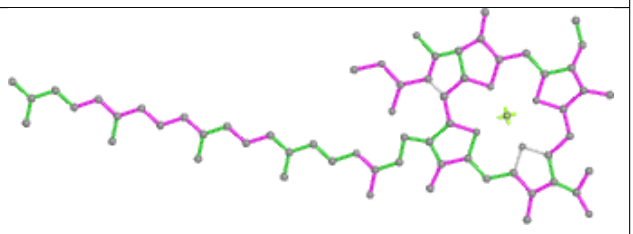
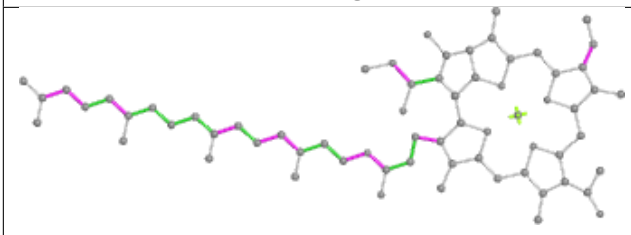


Bond angles



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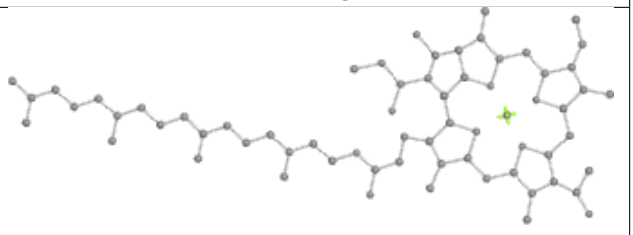
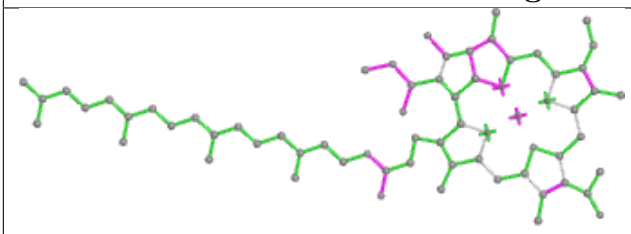


Rings

Ligand BCL D 102



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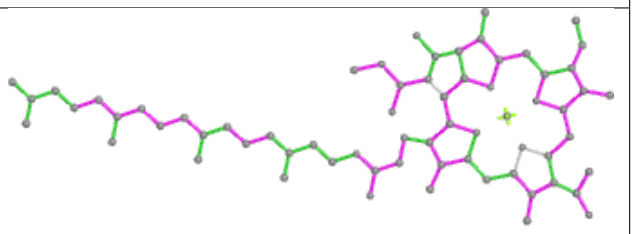
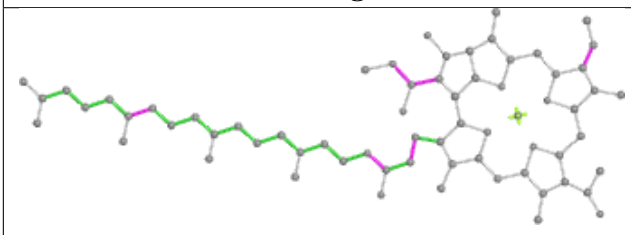


Bond angles



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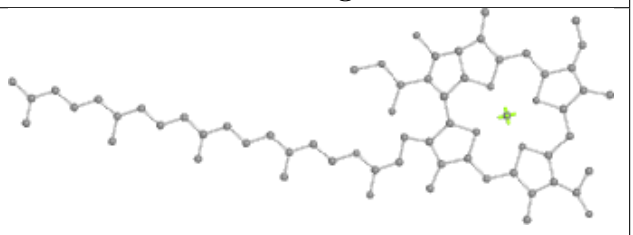
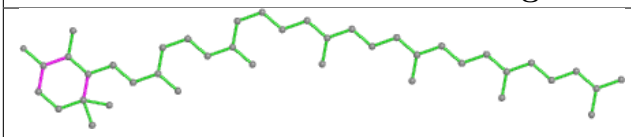


Rings

Ligand KGD F 103



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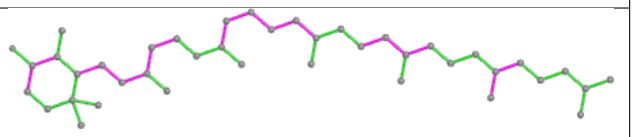
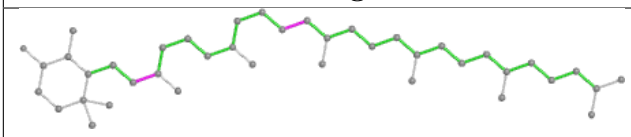


Bond angles



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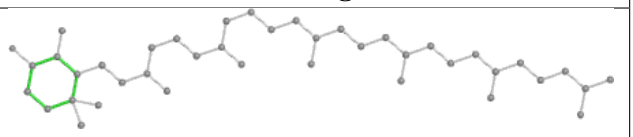
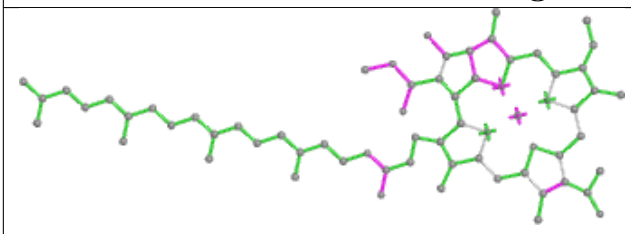


Rings

Ligand BCL 0 102



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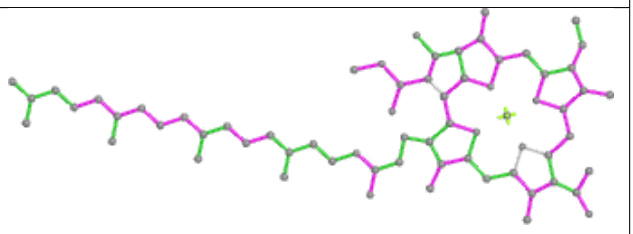
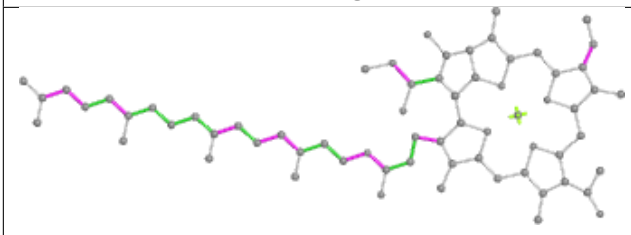


Bond angles



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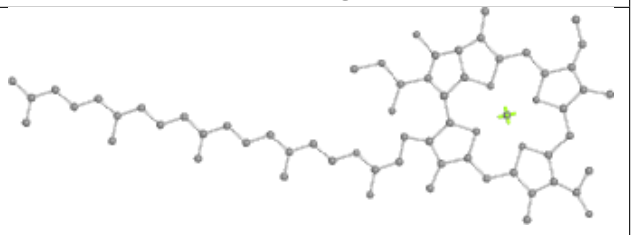
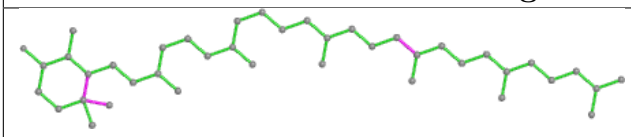


Rings

Ligand KGD O 102



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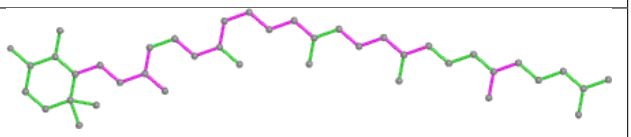
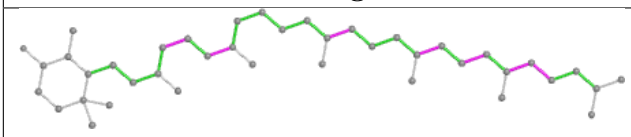


Bond angles



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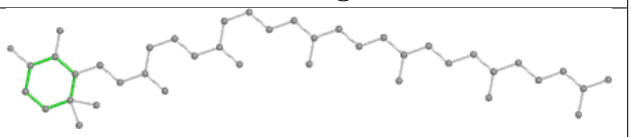
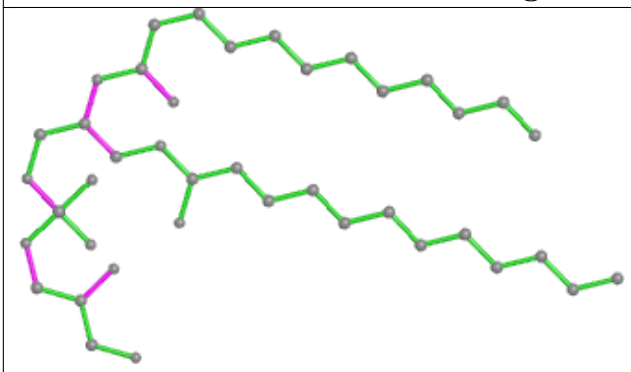


Rings

Ligand PGV P 104



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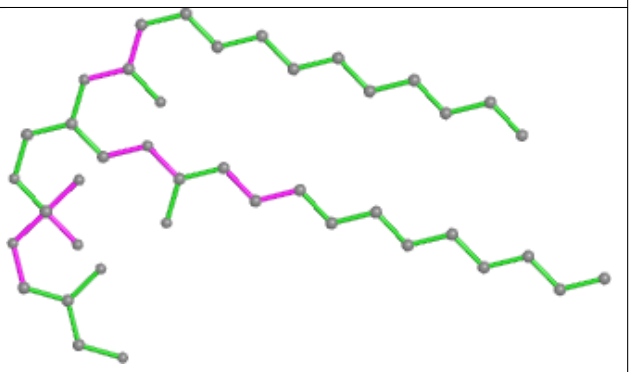

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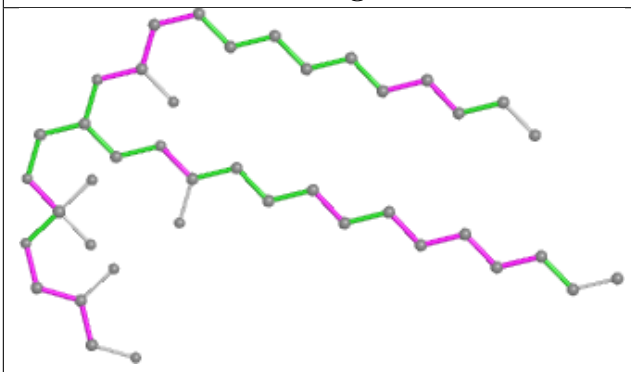

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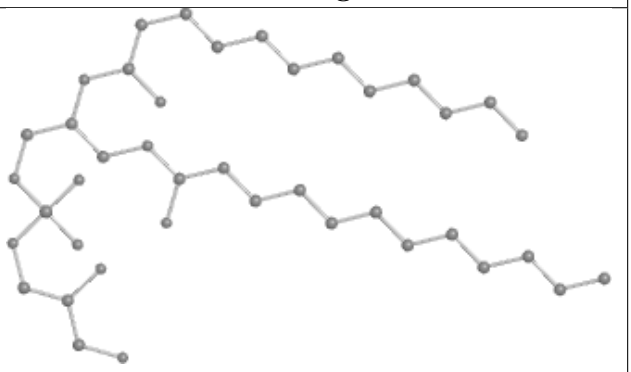
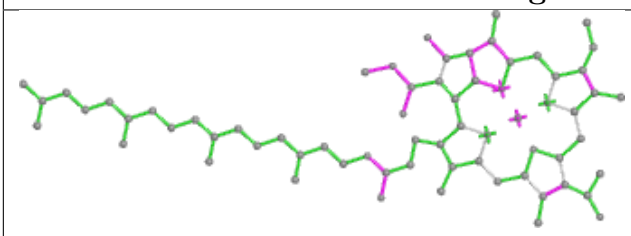


Rings

Ligand BCL J 102



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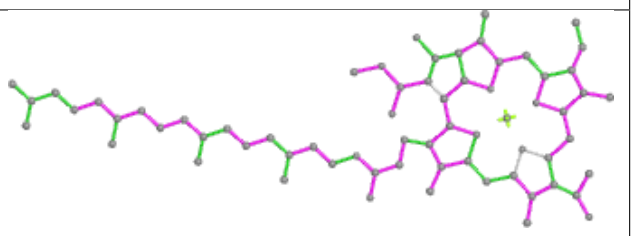
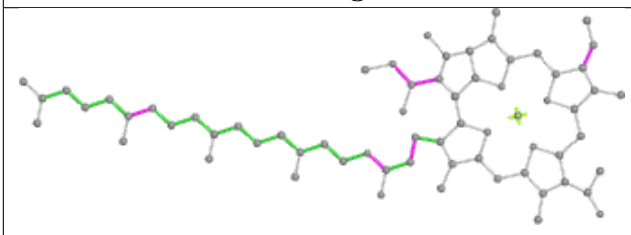
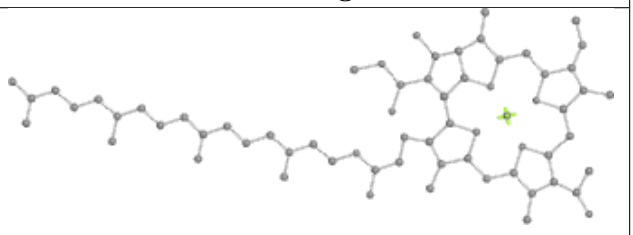


Bond angles

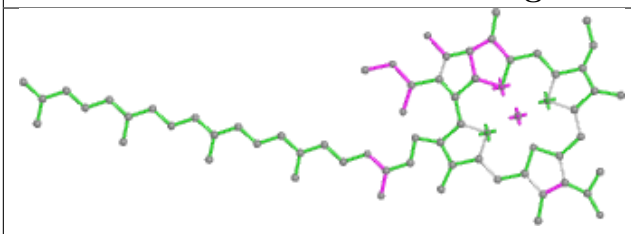


Torsions

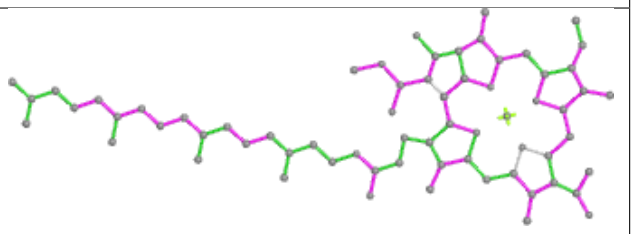


Rings

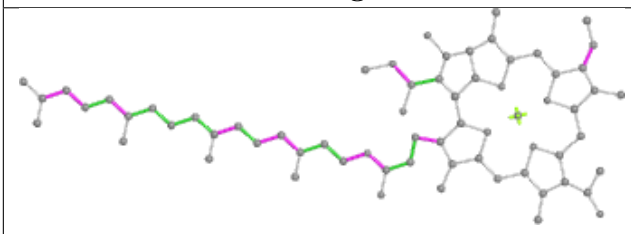
Ligand BCL O 101



Bond lengths



Bond angles



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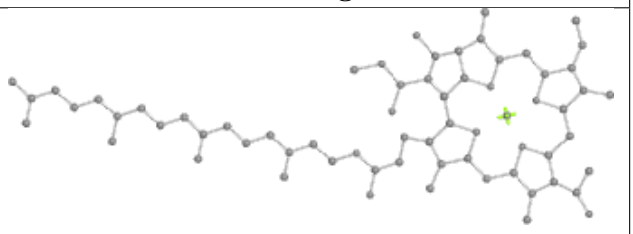
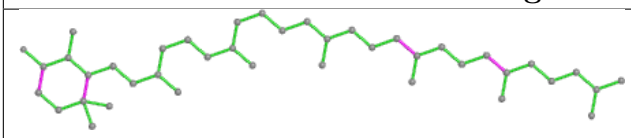
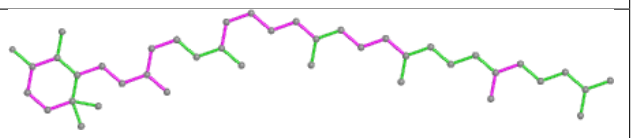


Rings

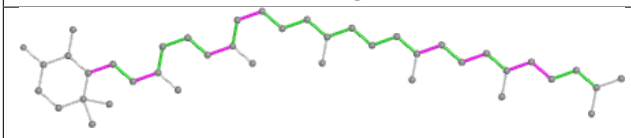
Ligand KGD 8 103



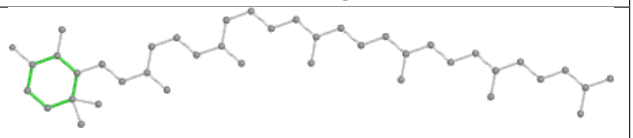
Bond lengths



Bond angles

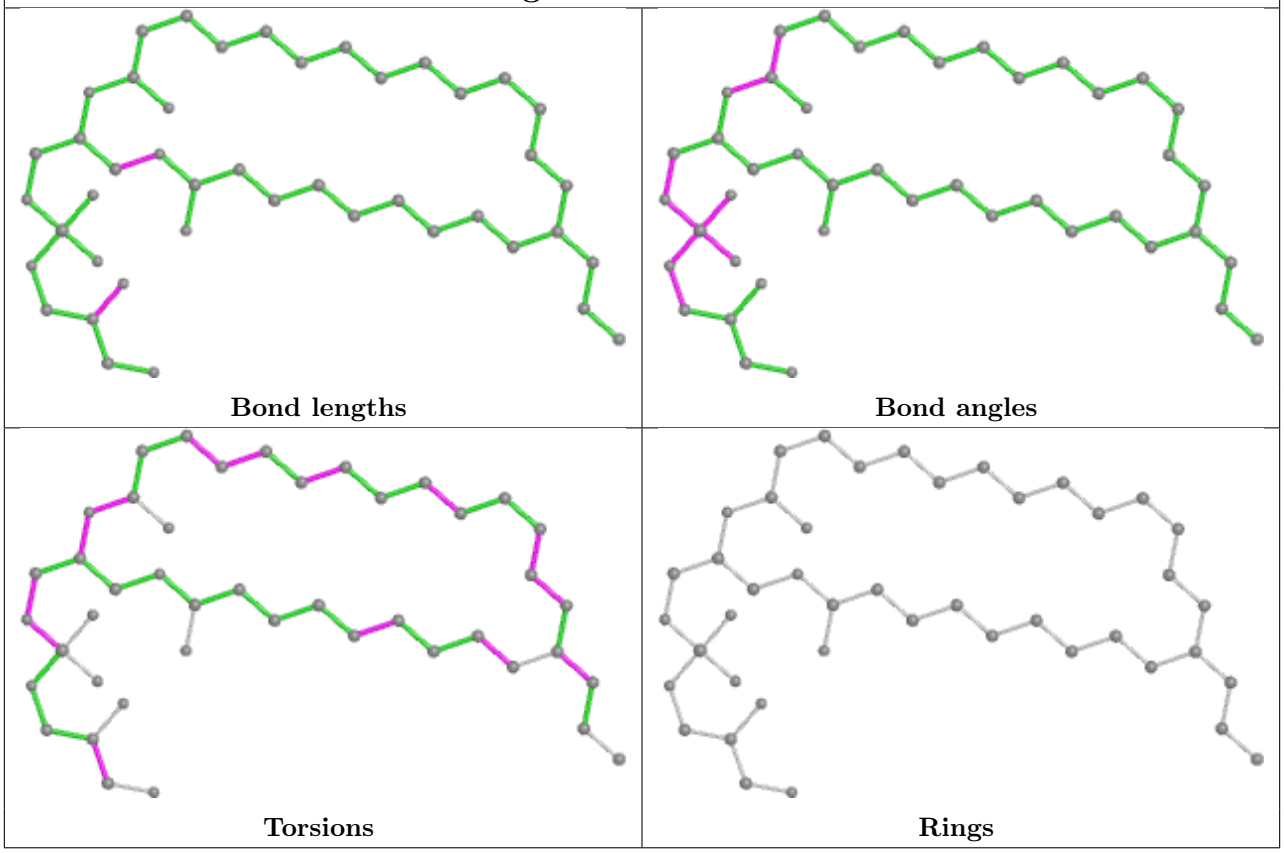


Torsions

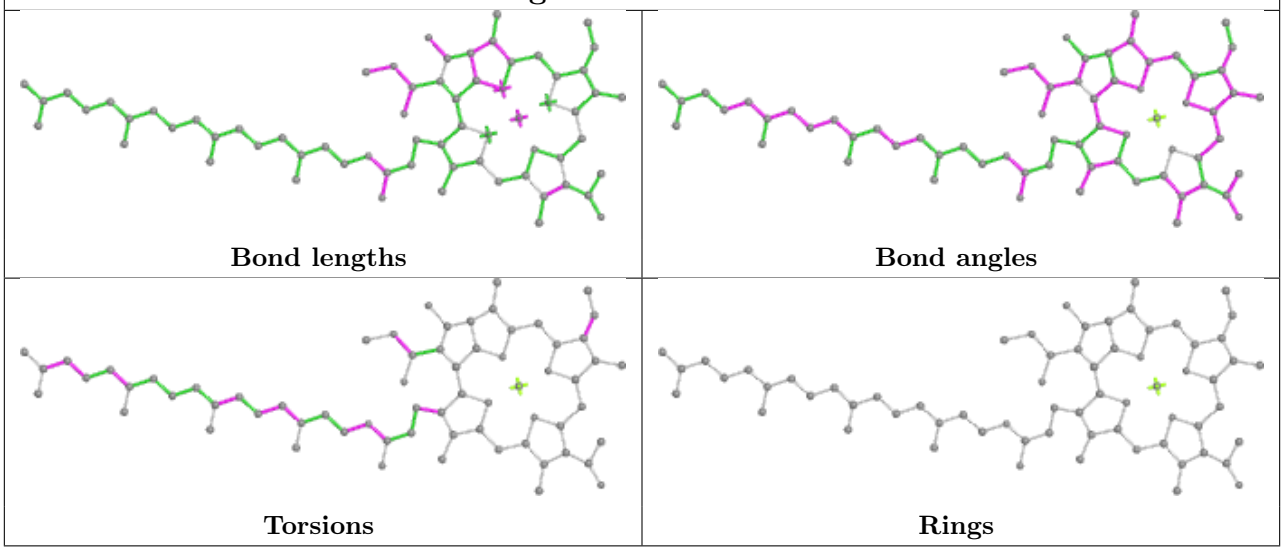


Rings

Ligand PGV C 406



Ligand BCL S 103



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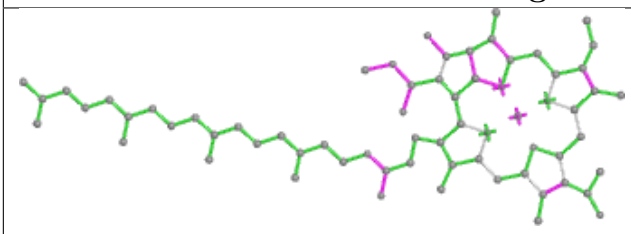

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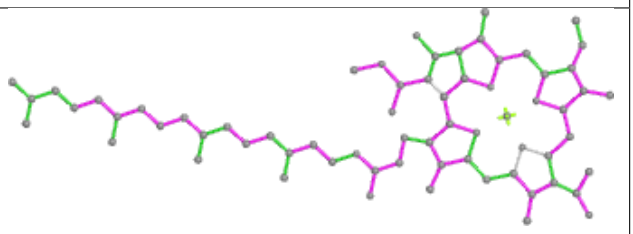
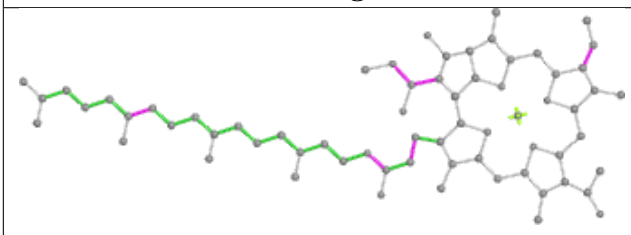


Bond angles



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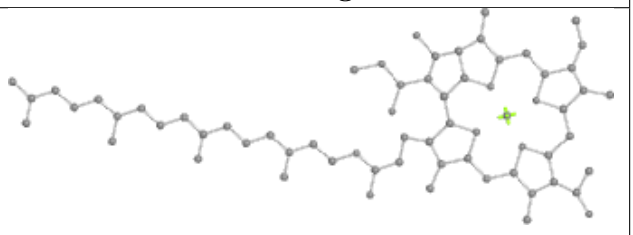
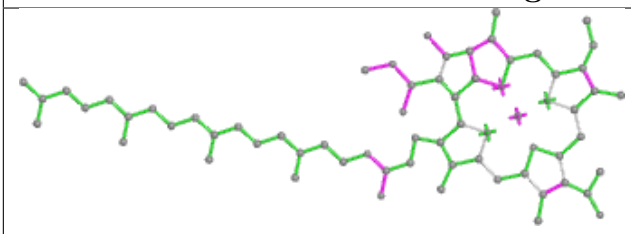
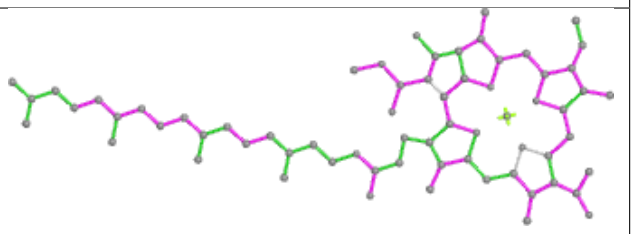


Rings

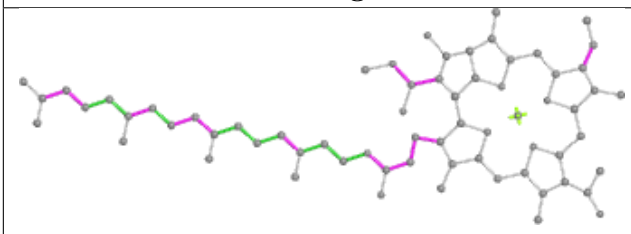
Ligand BCL D 101



Bond lengths



Bond angles



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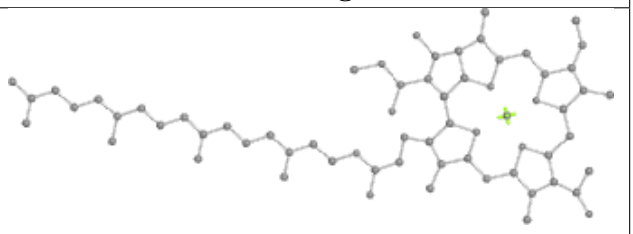

Rings

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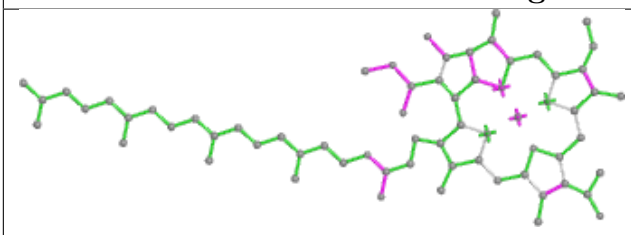

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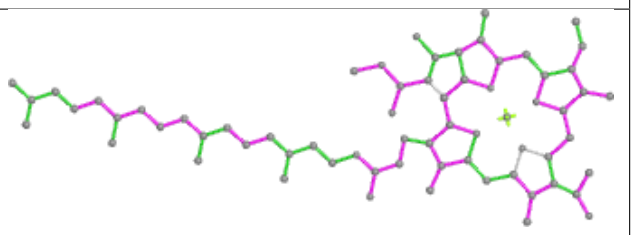

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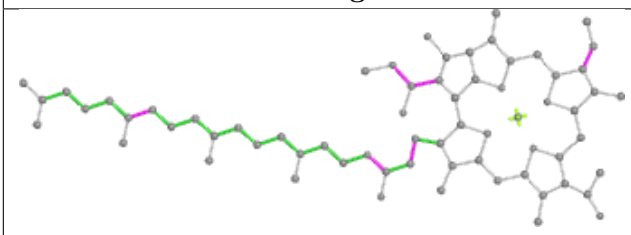

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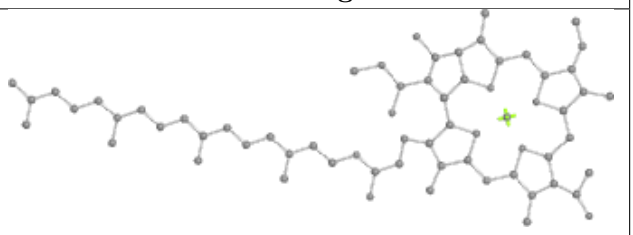
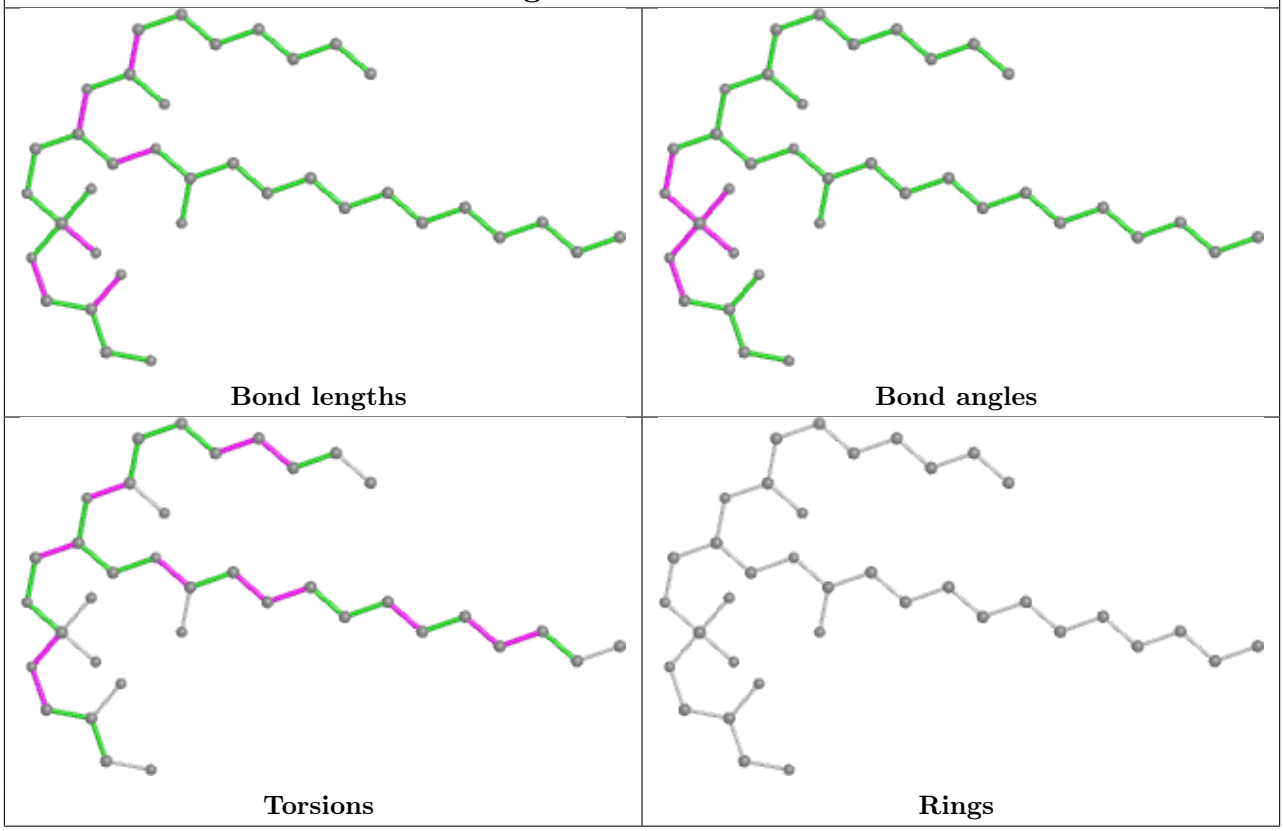


Rings

Ligand PGV P 103



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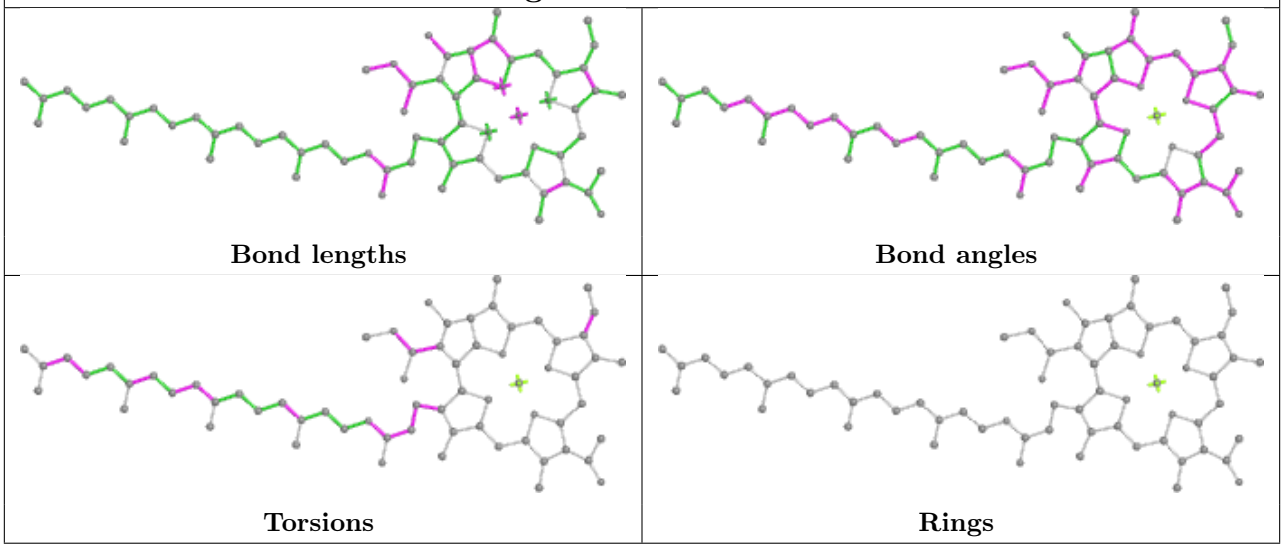
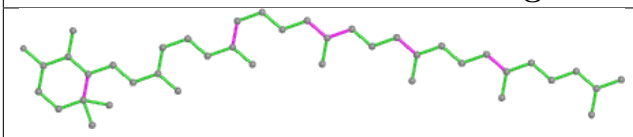


Ligand KGD 0 103



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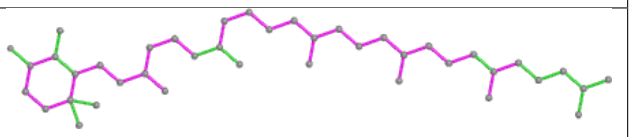
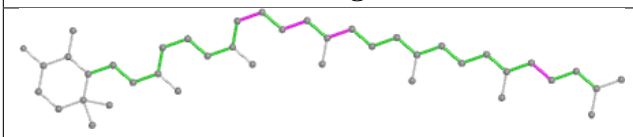


Bond angles



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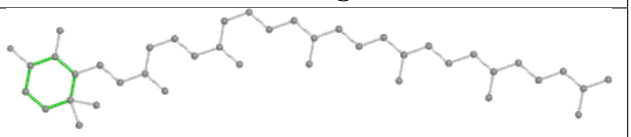
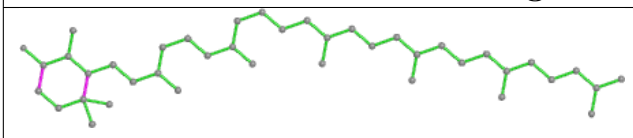


Rings

Ligand KGD I 102



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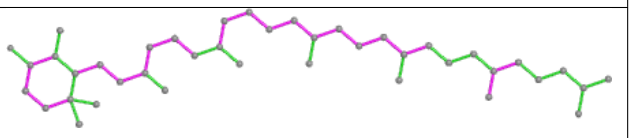
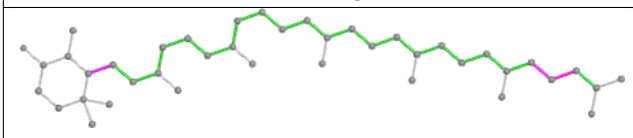


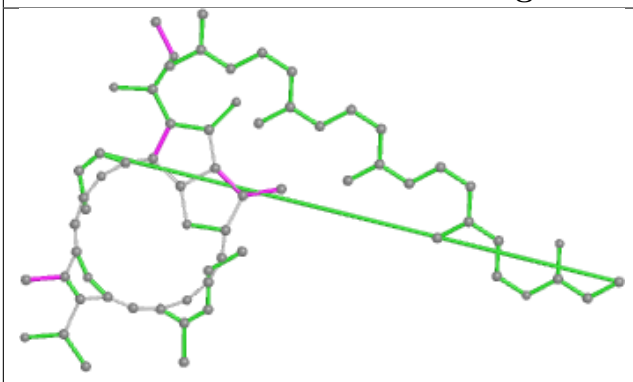
Bond angles



Torsions

Rings

Ligand BPH L 1005



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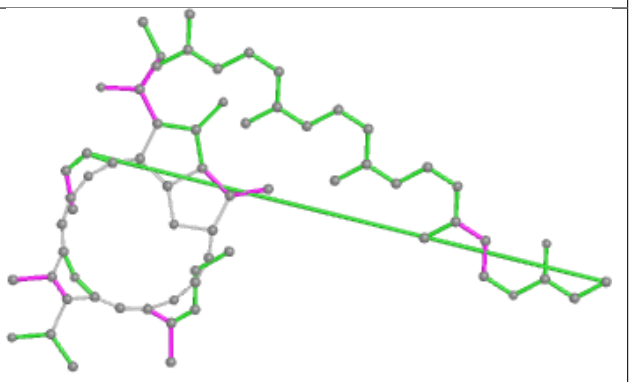
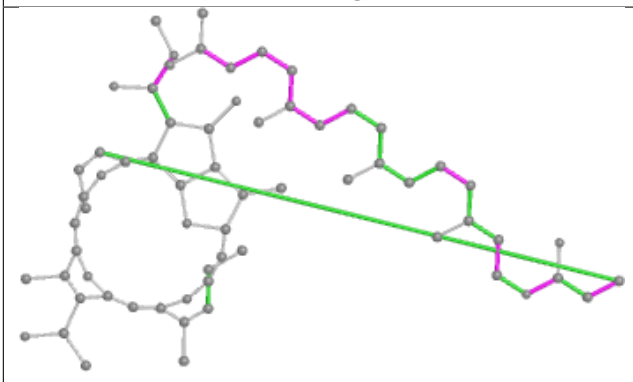
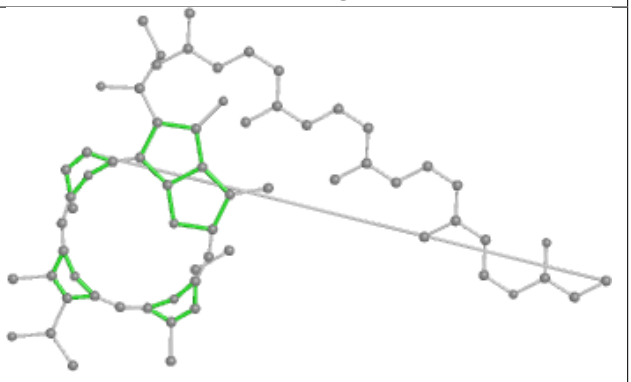


Bond angles

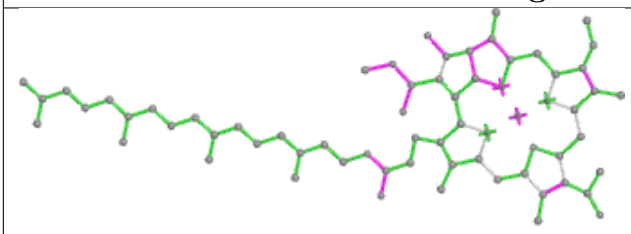


Torsions



Rings

Ligand BCL J 101



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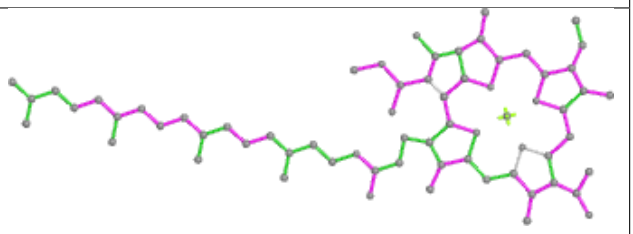
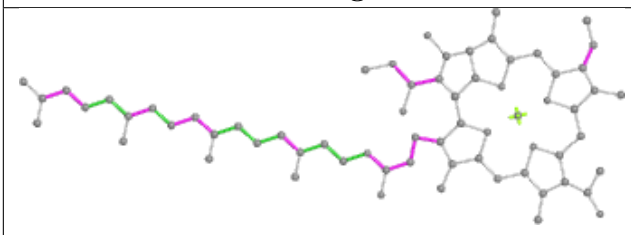
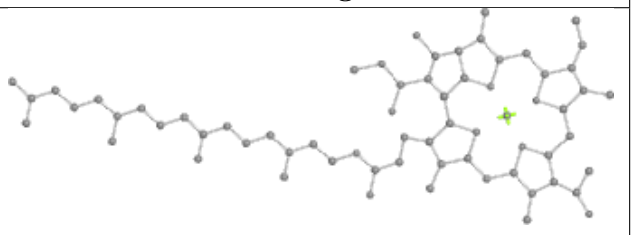


Bond angles

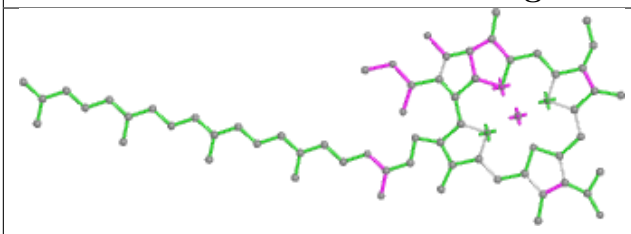


Torsions



Rings

Ligand BCL A 101



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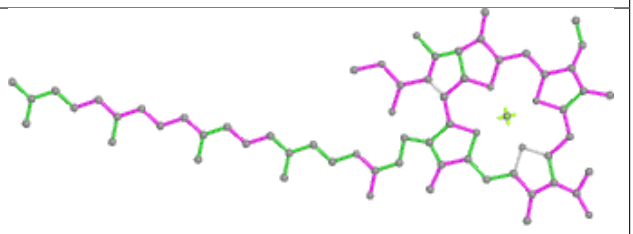
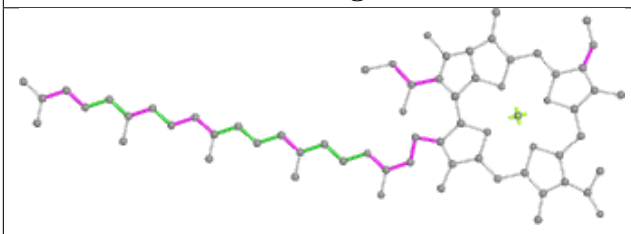
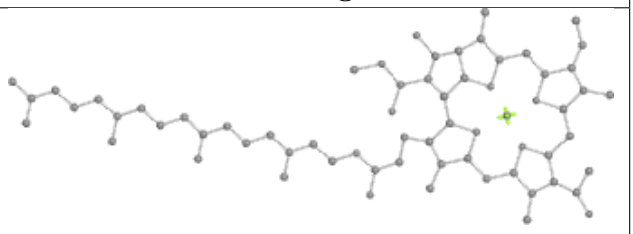


Bond angles

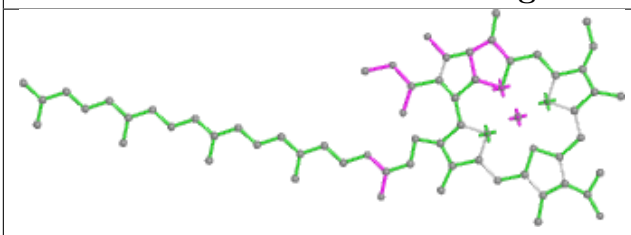


Torsions



Rings

Ligand BCL L 1001



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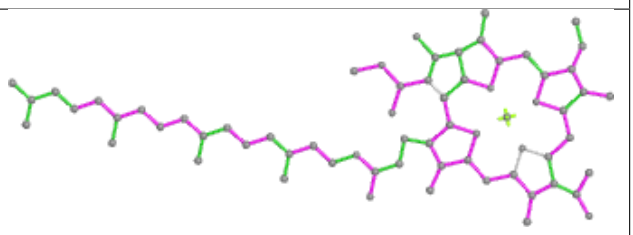
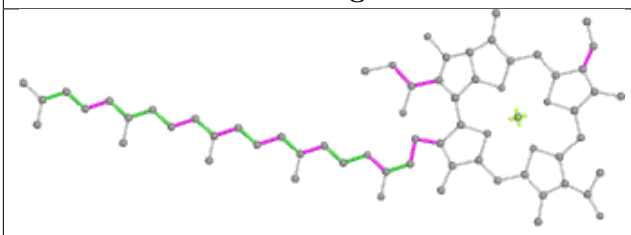


Bond angles



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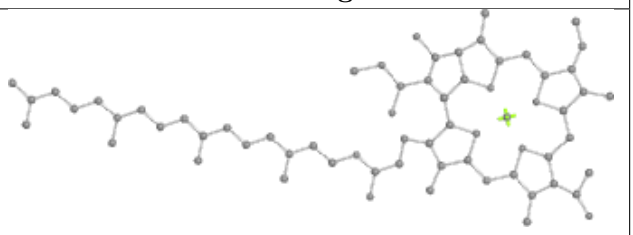
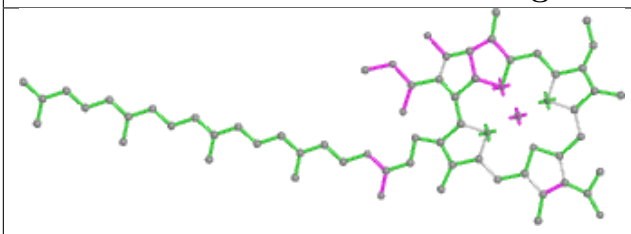


Rings

Ligand BCL I 101



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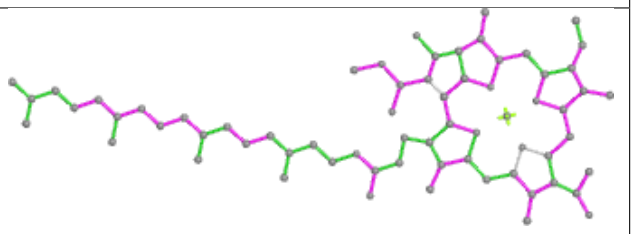
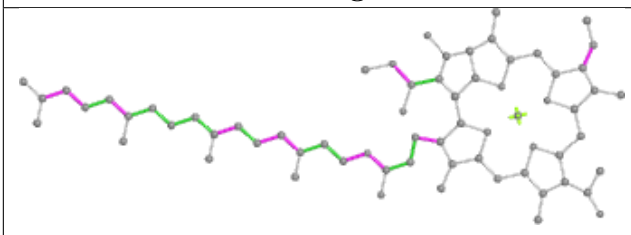
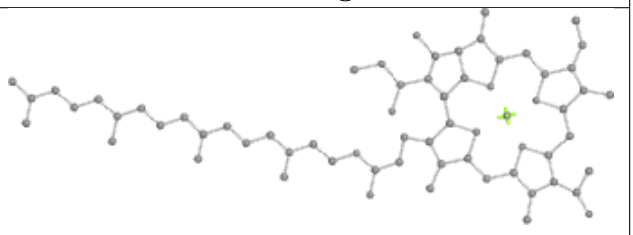


Bond angles

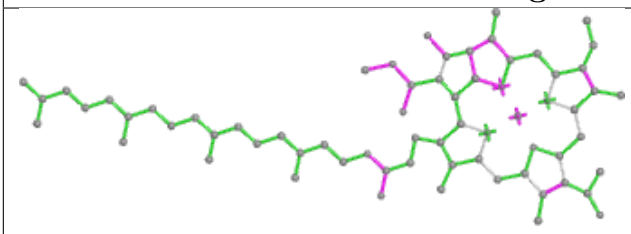


Torsions



Rings

Ligand BCL 1 101



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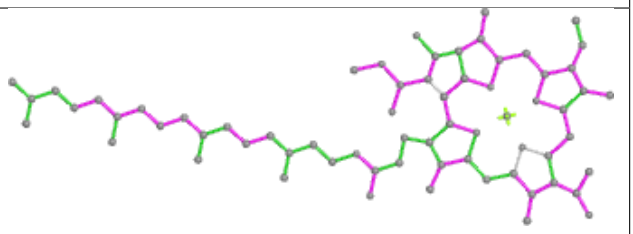
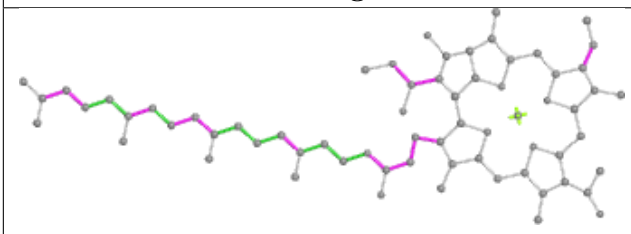
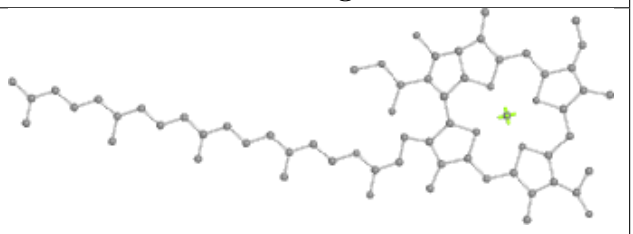


Bond angles

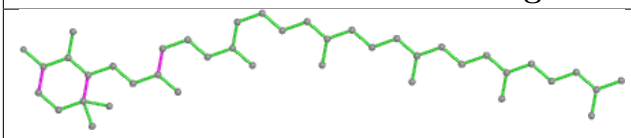


Torsions



Rings

Ligand KGD 0 104



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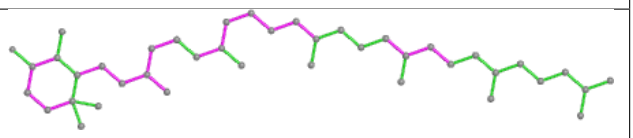
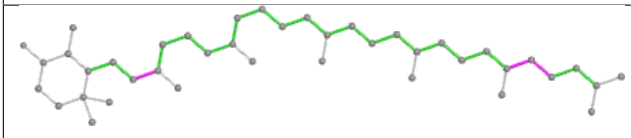
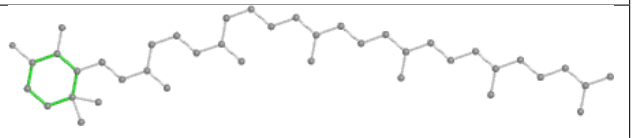


Bond angles

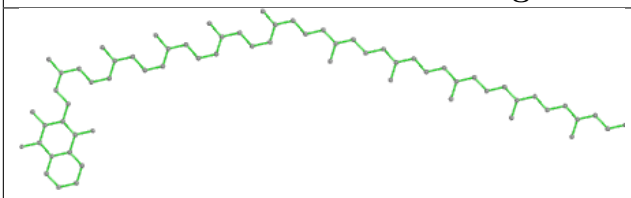


Torsions



Rings

Ligand MQE L 1004



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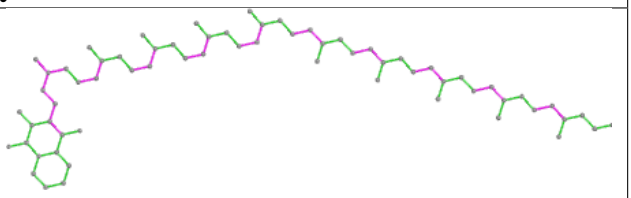
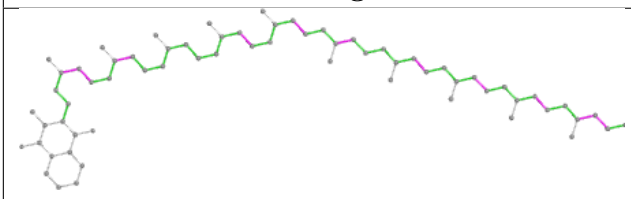
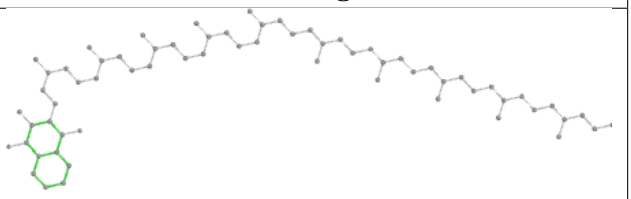


Bond angles

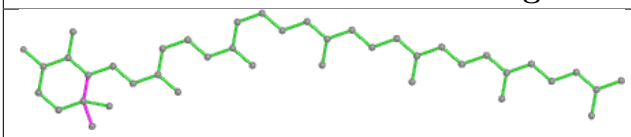


Torsions

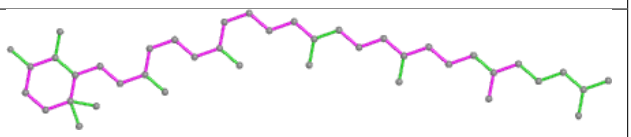


Rings

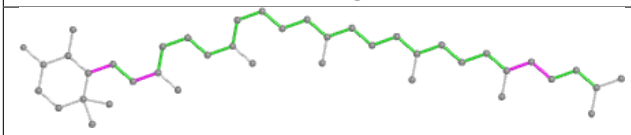
Ligand KGD S 104



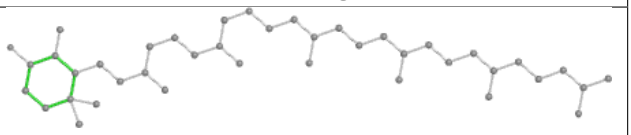
Bond lengths



Bond angles

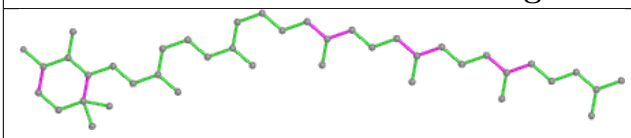


Torsions

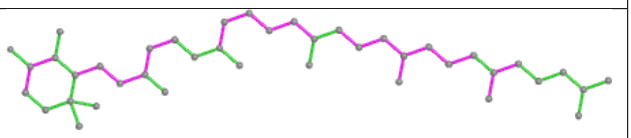


Rings

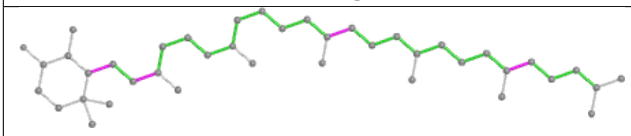
Ligand KGD 6 103



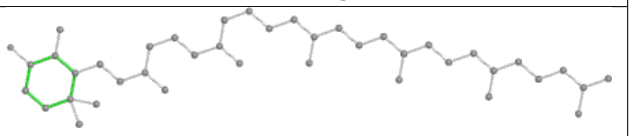
Bond lengths



Bond angles

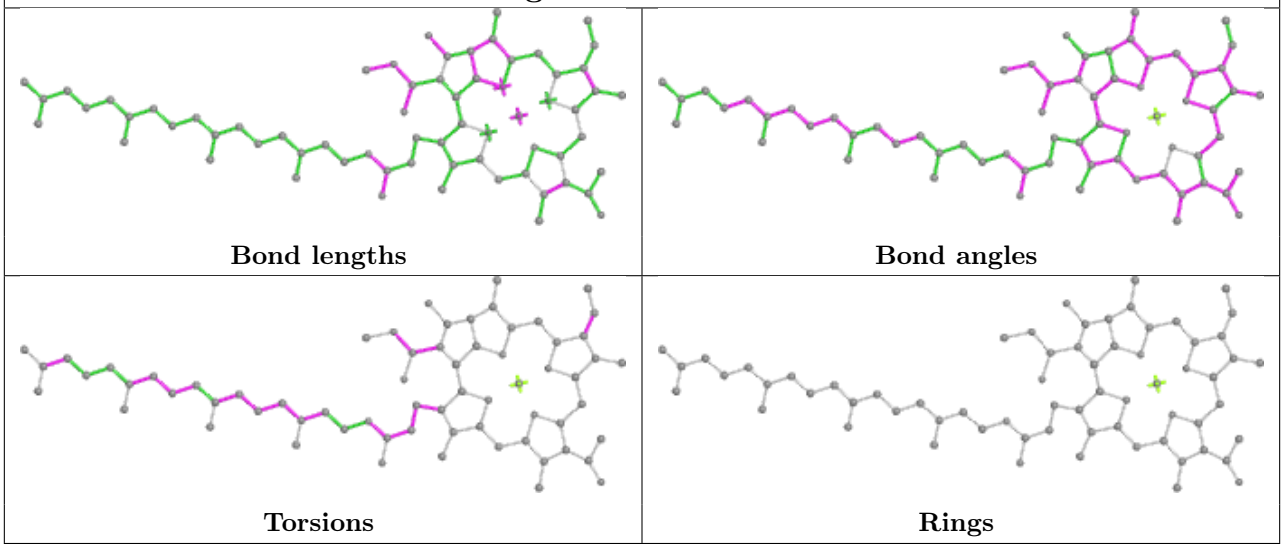


Torsions

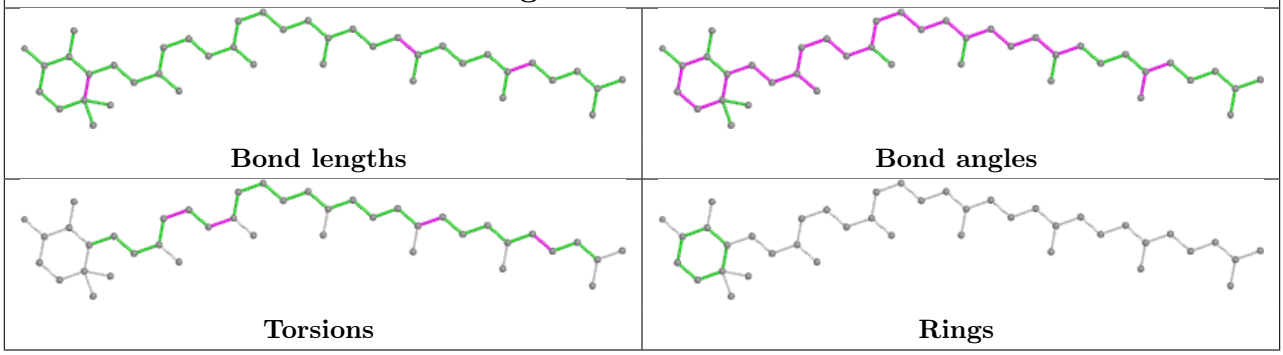


Rings

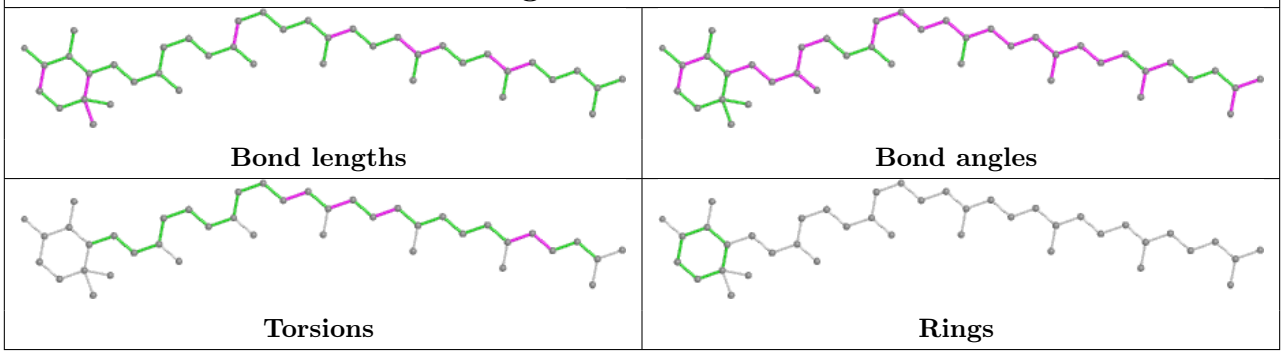
Ligand BCL X 101



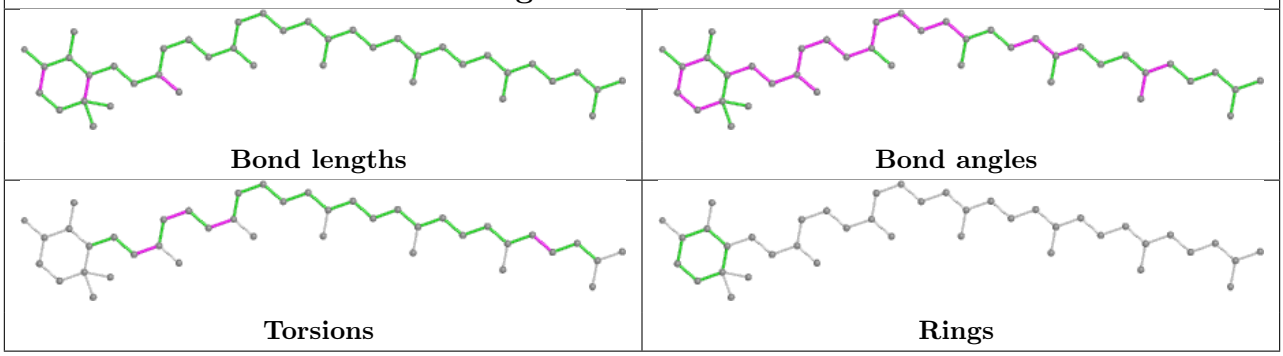
Ligand KGD N 103



Ligand KGD B 102



Ligand KGD W 101



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.

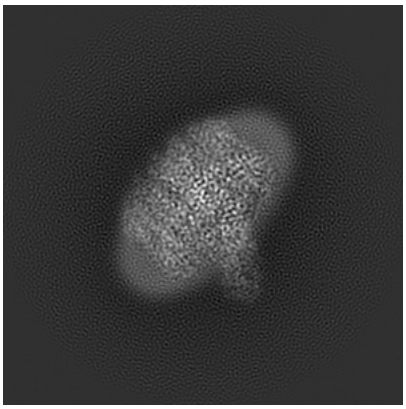
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34838. These allow visual inspection of the internal detail of the map and identification of artifacts.

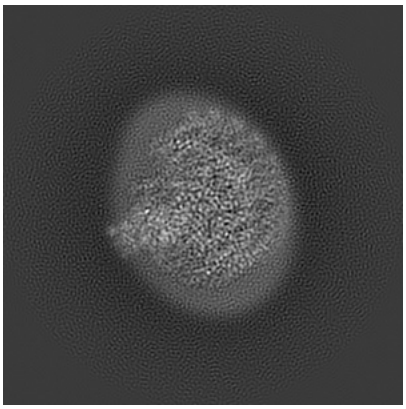
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

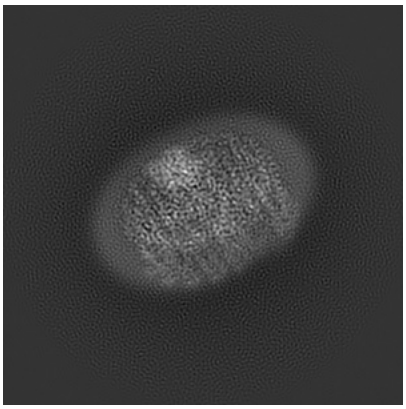
6.1.1 Primary map



X

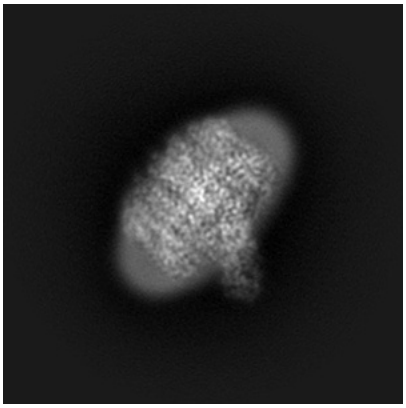


Y

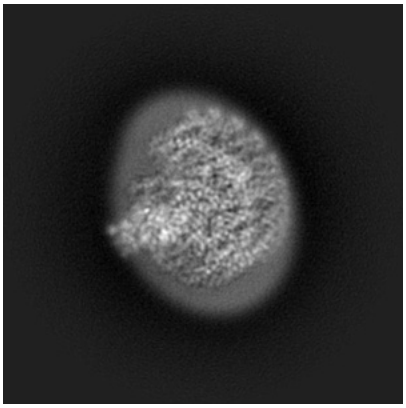


Z

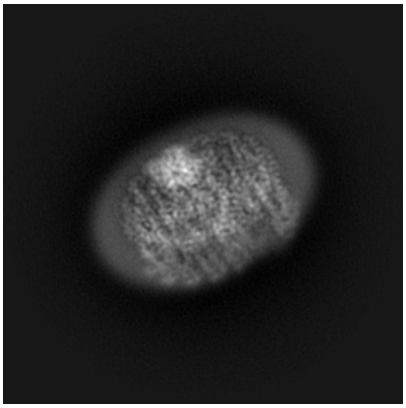
6.1.2 Raw map



X



Y

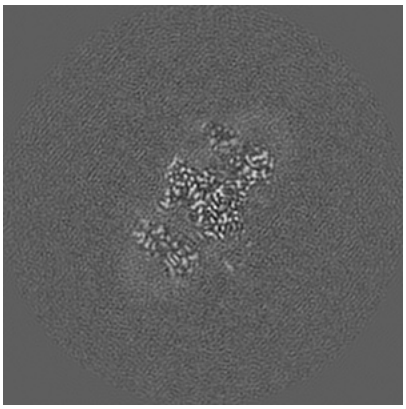


Z

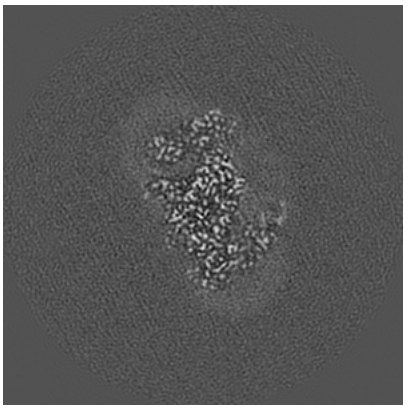
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

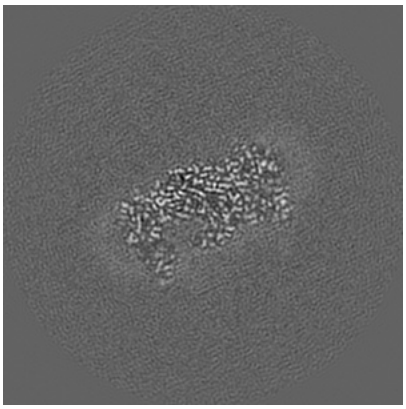
6.2.1 Primary map



X Index: 128

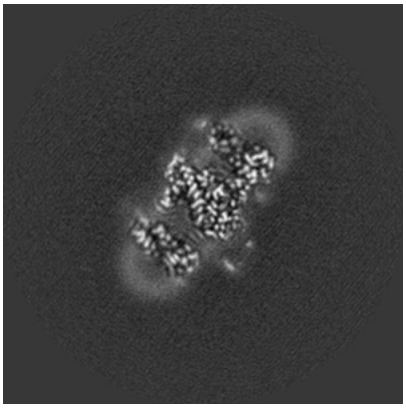


Y Index: 128

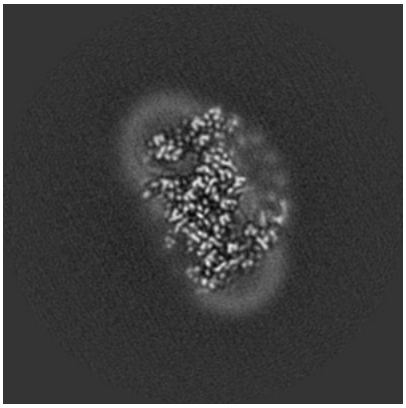


Z Index: 128

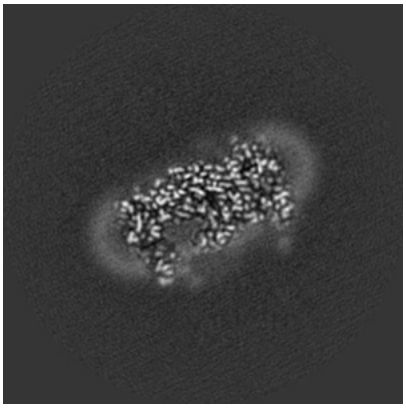
6.2.2 Raw map



X Index: 128



Y Index: 128

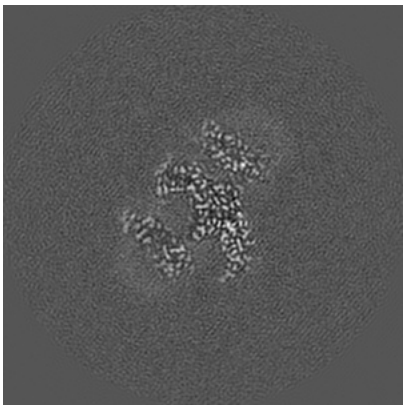


Z Index: 128

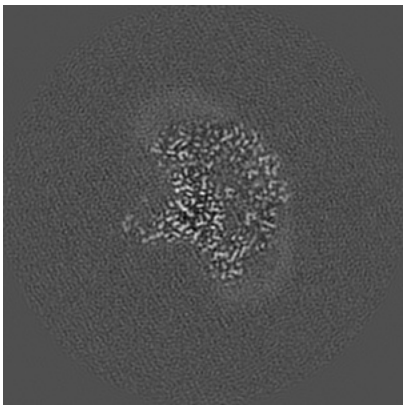
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

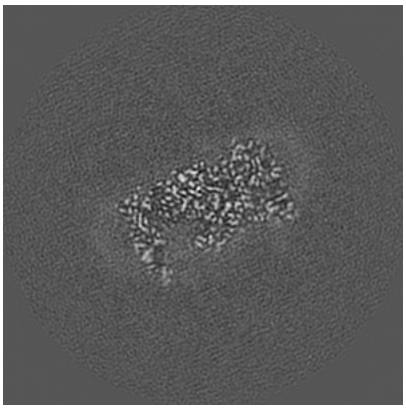
6.3.1 Primary map



X Index: 119

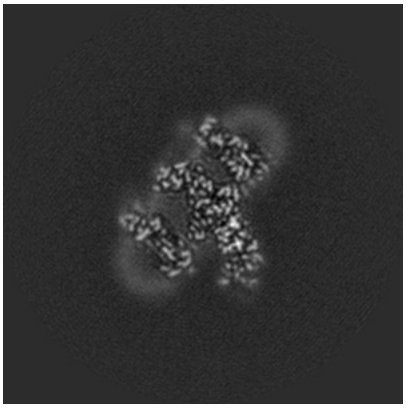


Y Index: 140

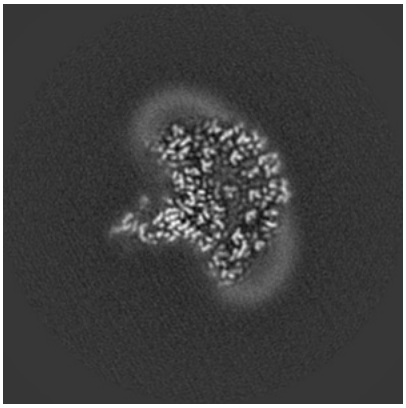


Z Index: 130

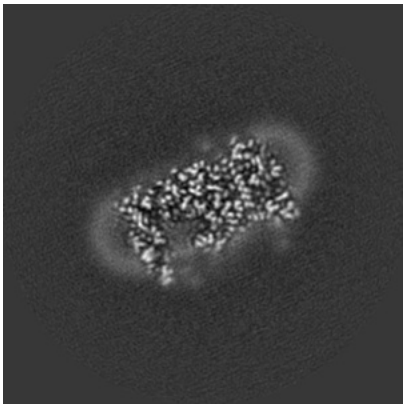
6.3.2 Raw map



X Index: 117



Y Index: 141

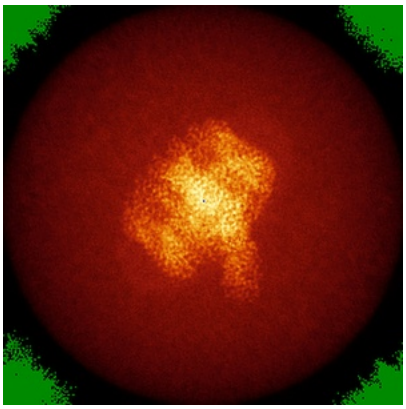


Z Index: 130

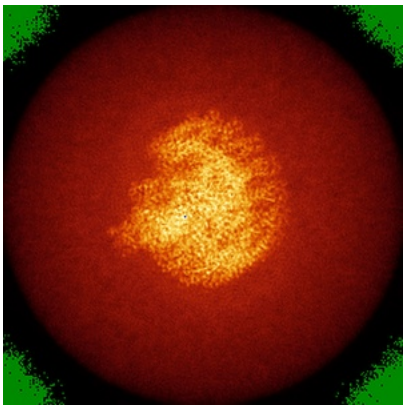
The images above show the largest variance slices of the map in three orthogonal directions.

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

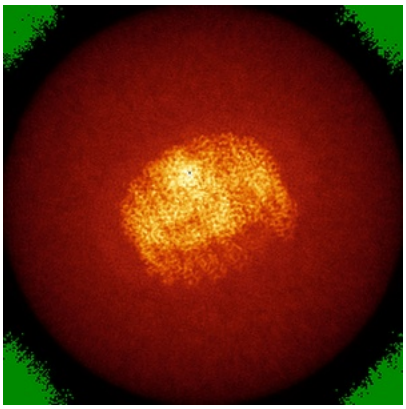
6.4.1 Primary map



X

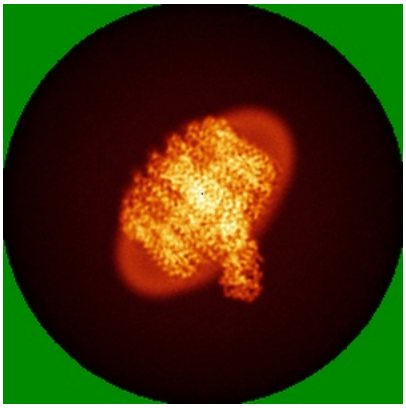


Y

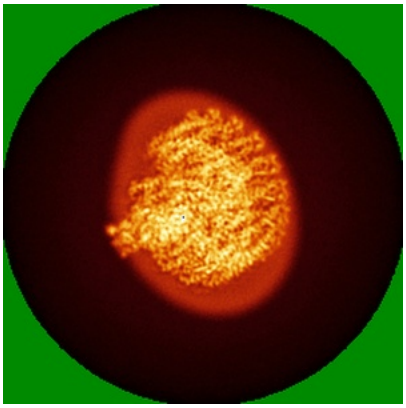


Z

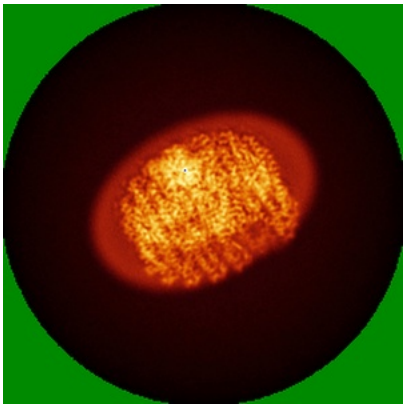
6.4.2 Raw map



X



Y

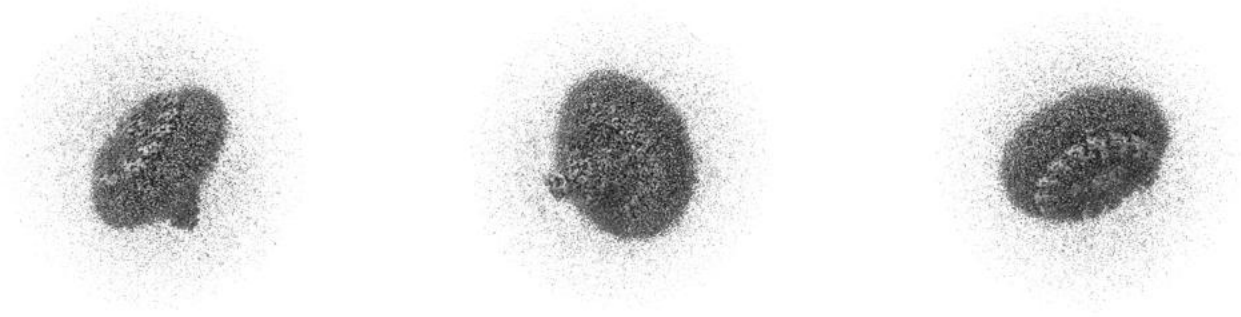


Z

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)

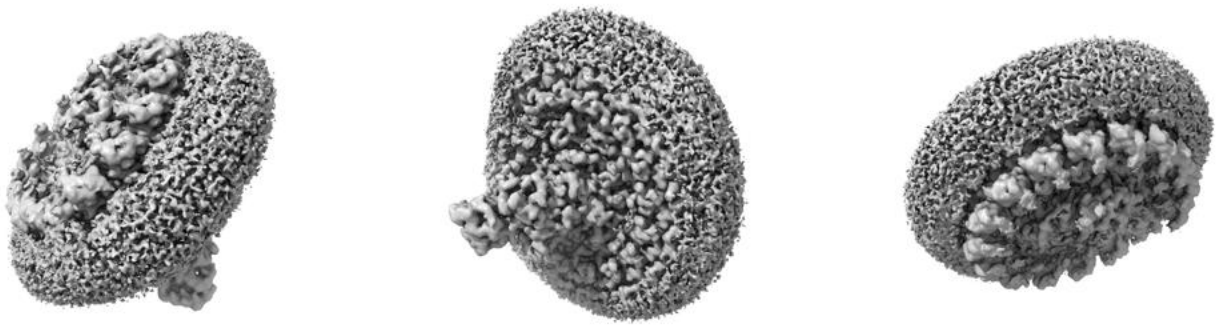
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

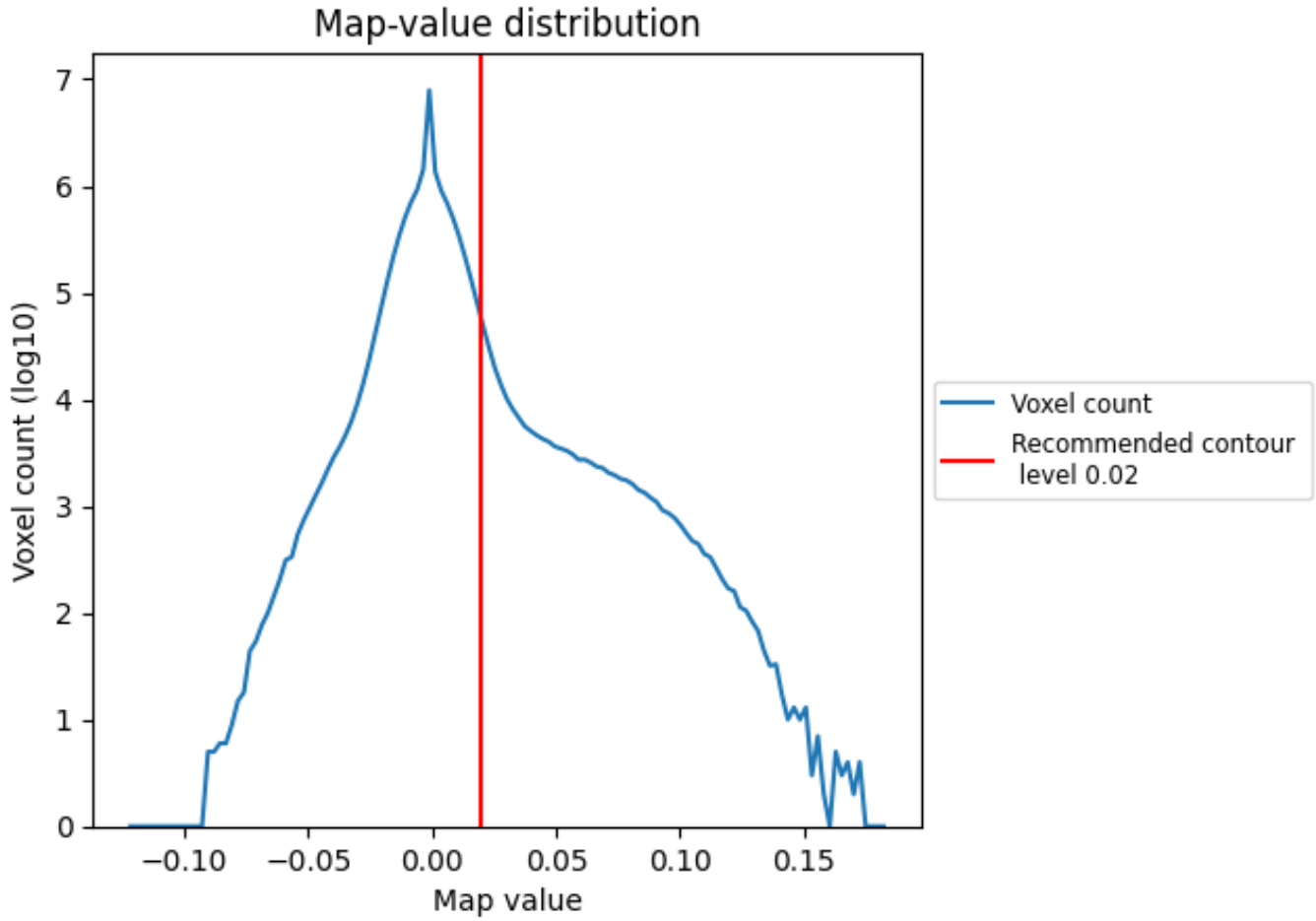
6.6 Mask visualisation (i)

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

7 Map analysis

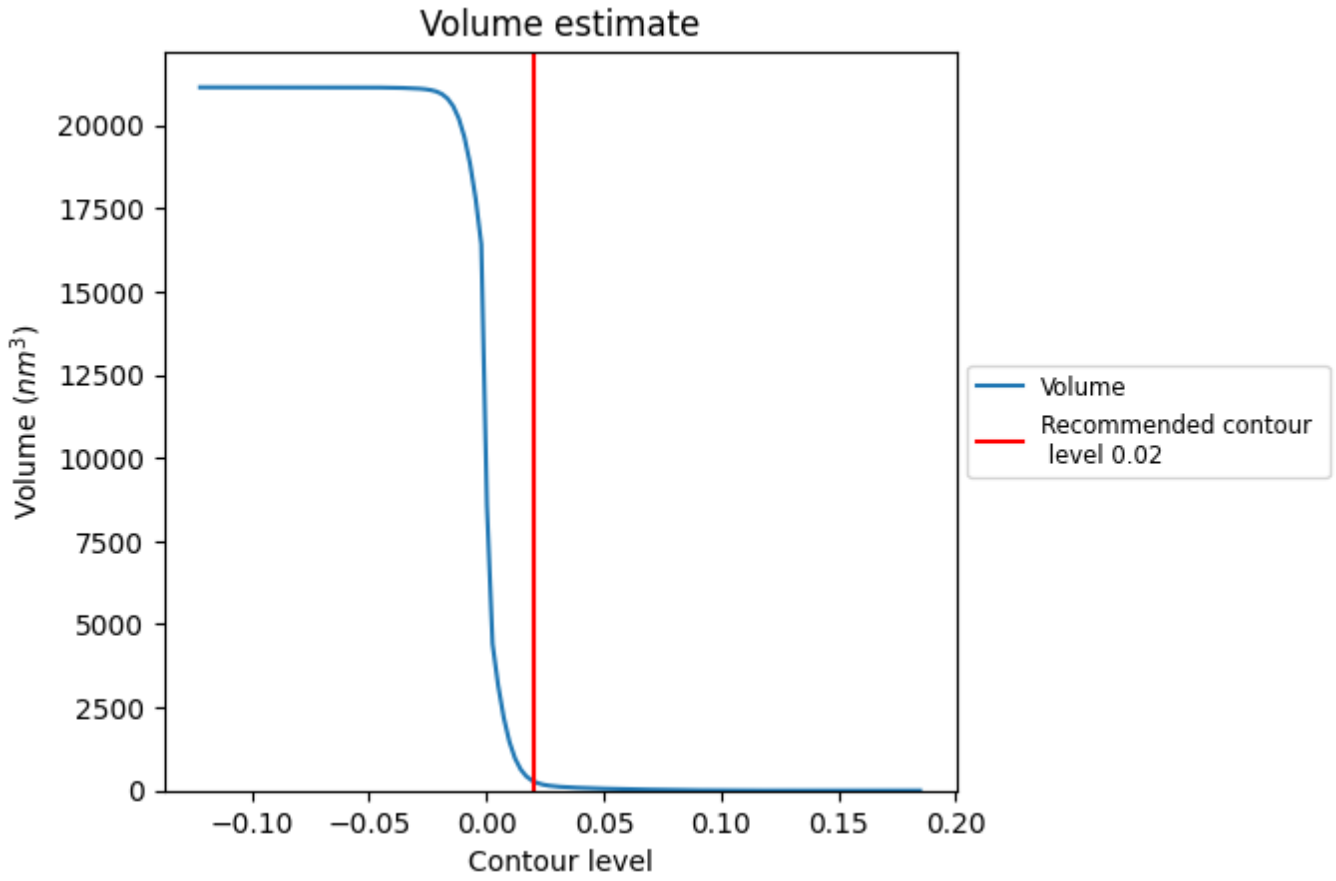
This section contains the results of statistical analysis of the map.

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.

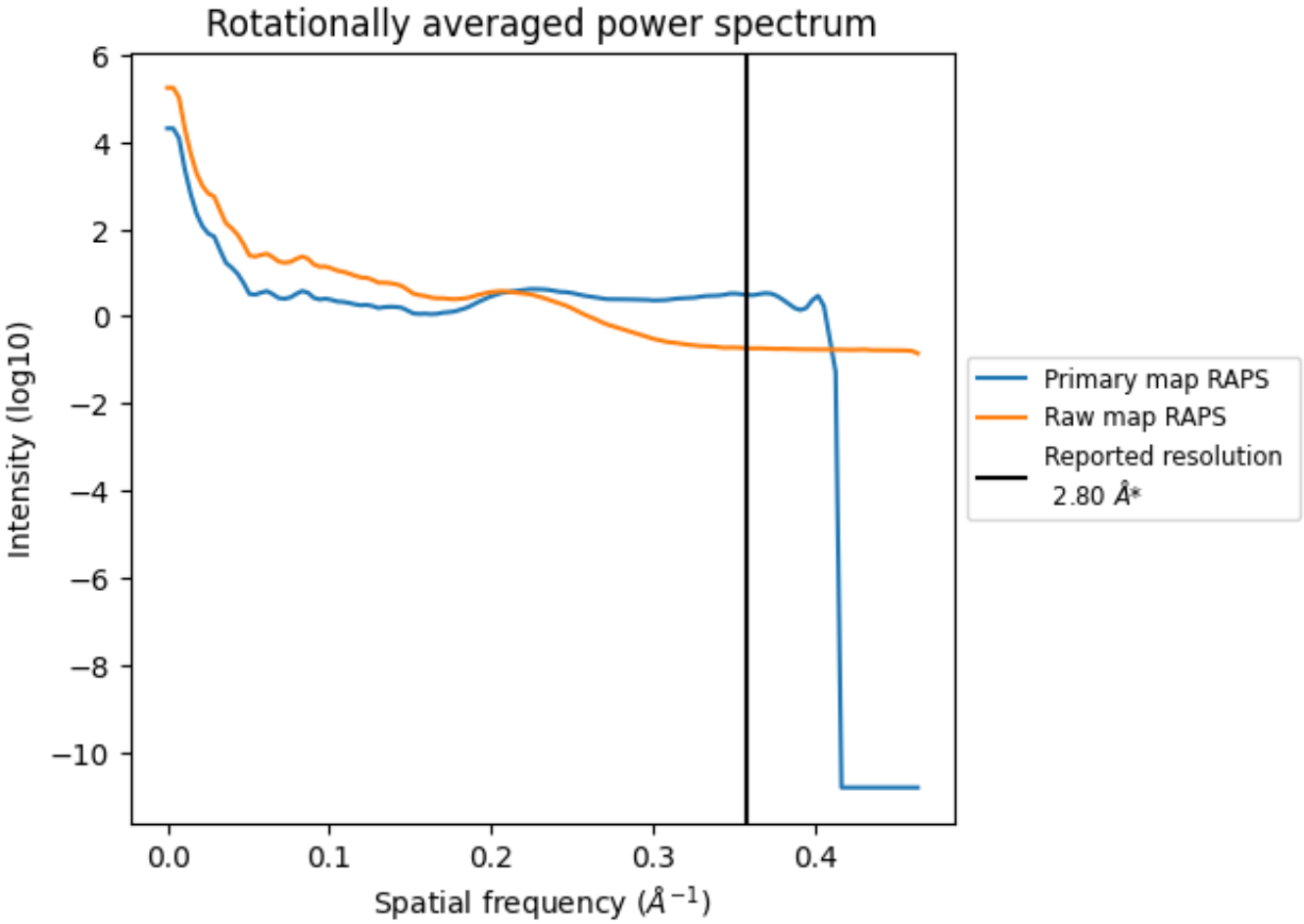
7.2 Volume estimate



The volume at the recommended contour level is 284 nm^3; this corresponds to an approximate mass of 257 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)

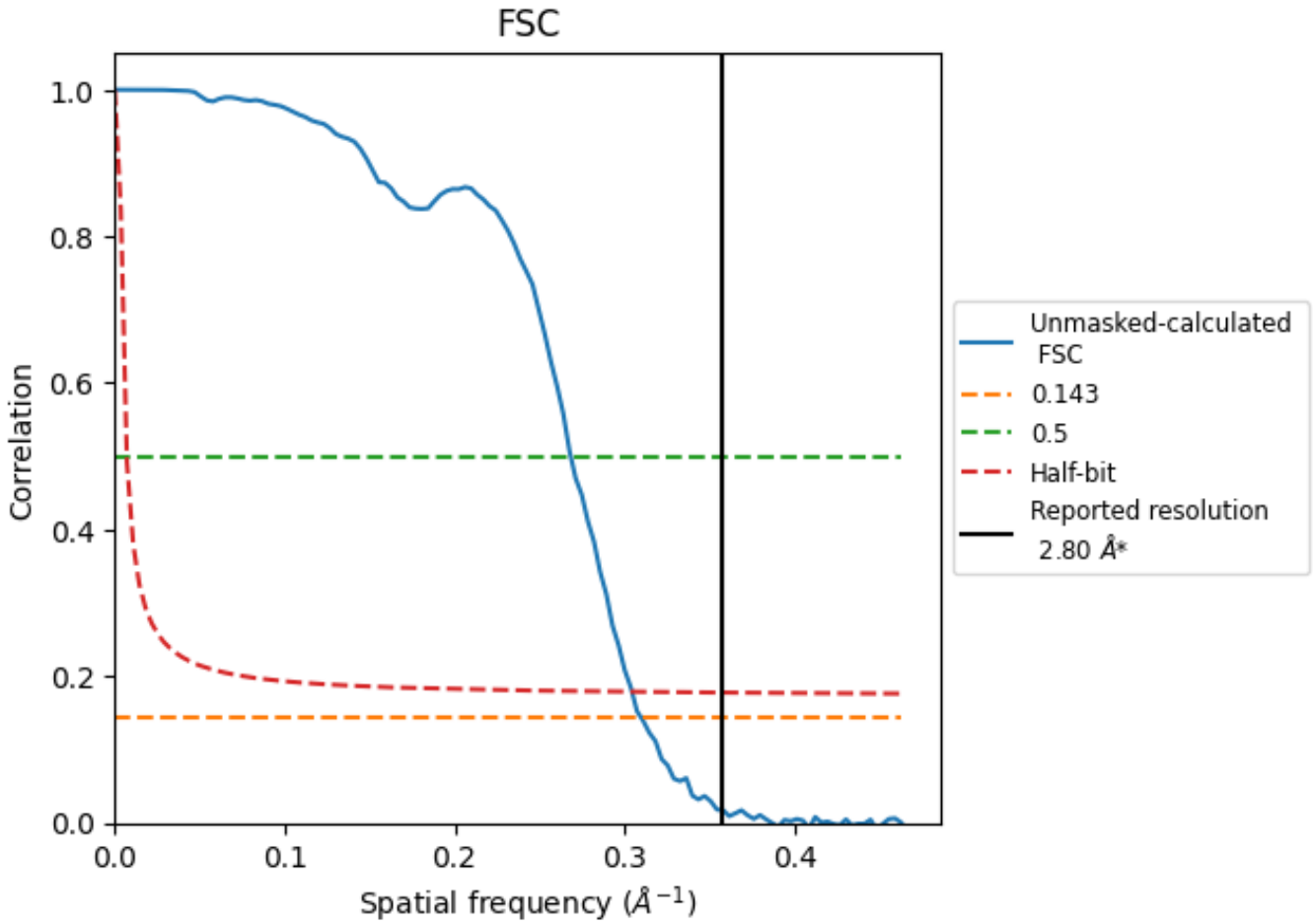


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates (i)

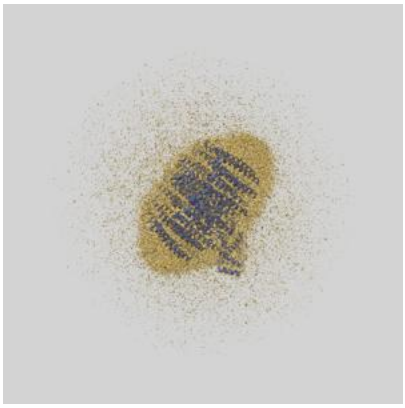
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.23	3.73	3.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.8 by more than 10 %

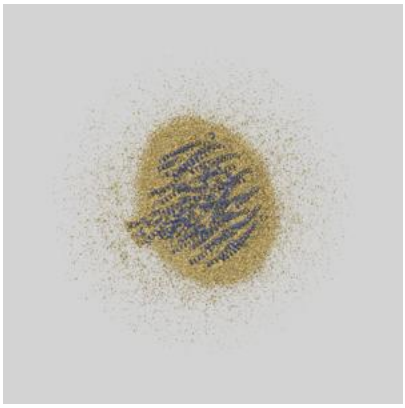
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34838 and PDB model 8HJU. Per-residue inclusion information can be found in section 3 on page 16.

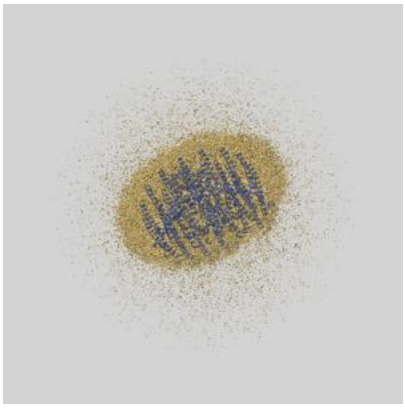
9.1 Map-model overlay



X



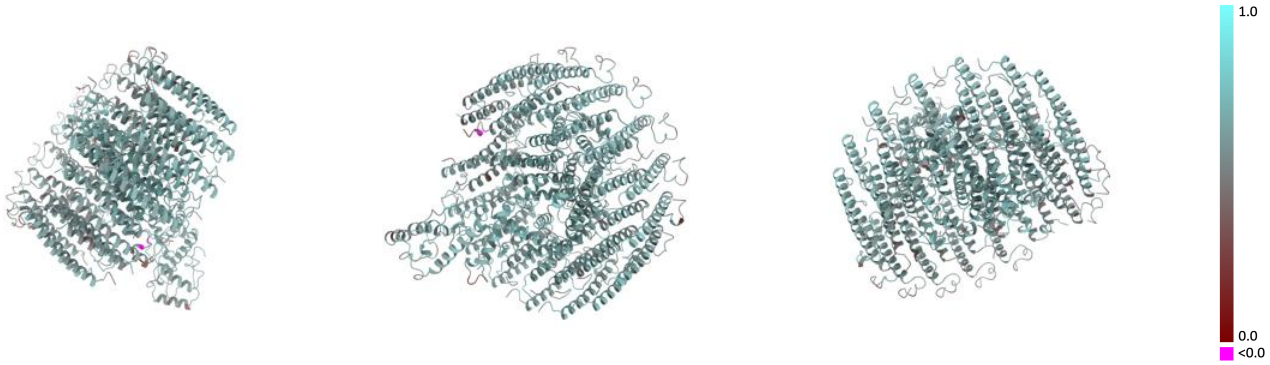
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

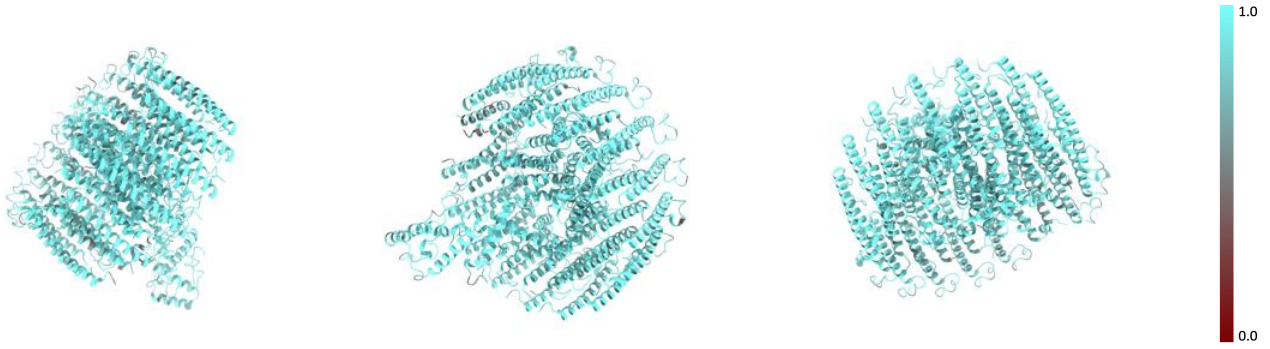
9.2 Q-score mapped to coordinate model (i)



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.

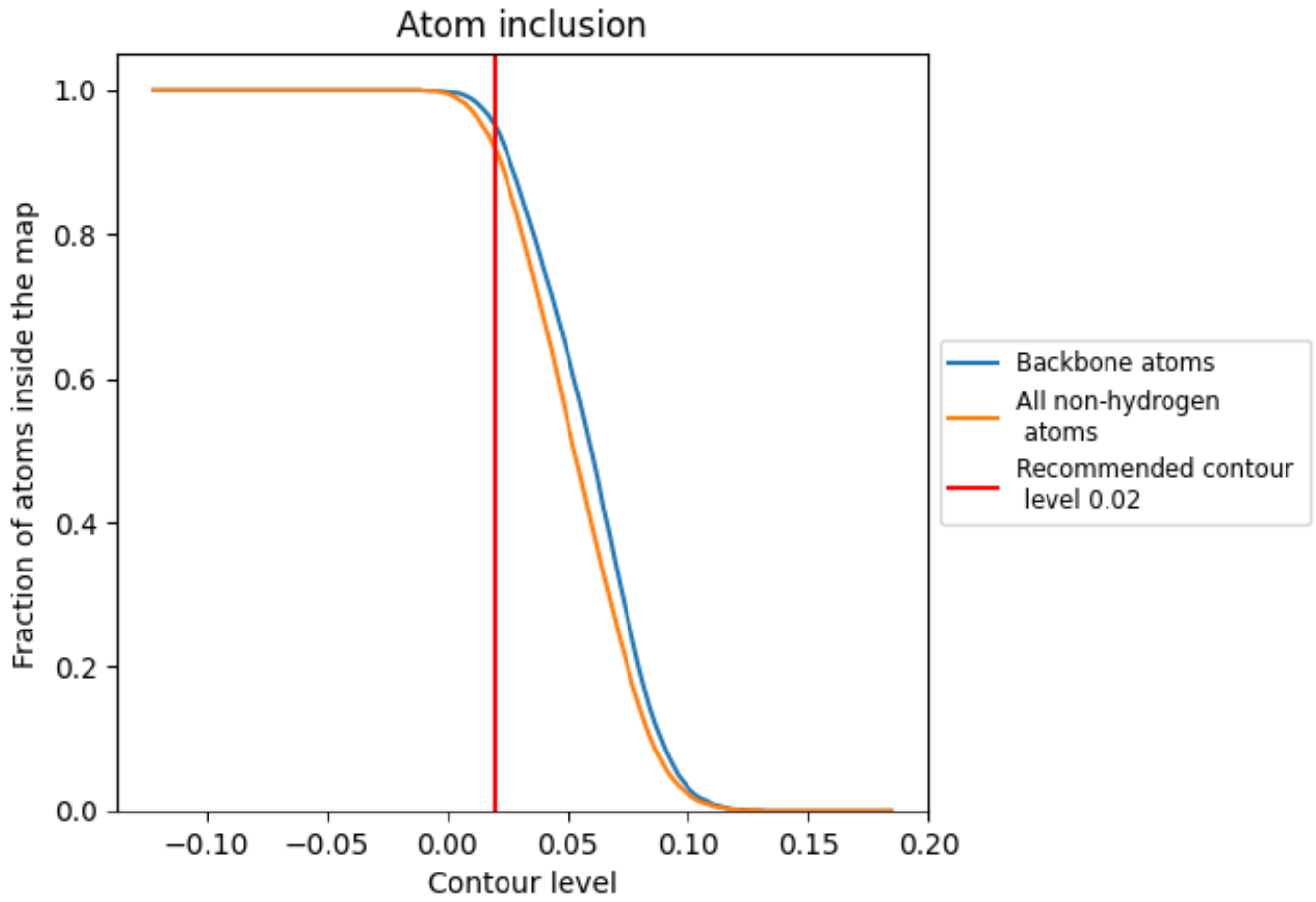
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9170	0.6030
0	0.9030	0.5860
1	0.8810	0.5640
2	0.8020	0.5290
3	0.9390	0.6030
4	0.8910	0.5770
5	0.9090	0.5960
6	0.8950	0.5820
7	0.9130	0.5860
8	0.8930	0.5820
9	0.9310	0.6120
A	0.9310	0.6030
B	0.9140	0.6030
C	0.9220	0.6010
D	0.9140	0.5840
E	0.9100	0.6000
F	0.9210	0.5980
G	0.8920	0.5870
H	0.9230	0.5910
I	0.8920	0.5910
J	0.9450	0.6150
K	0.8820	0.5900
L	0.9510	0.6370
M	0.9630	0.6490
N	0.9500	0.6190
O	0.9080	0.5950
P	0.9340	0.6200
Q	0.9200	0.6030
R	0.9210	0.5940
S	0.9170	0.6110
T	0.9140	0.5900
U	0.9060	0.5880
V	0.8360	0.5070
W	0.8610	0.5530
X	0.7420	0.5380

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Chain	Atom inclusion	Q-score
Y	0.9380	0.6150
Z	0.9310	0.6160