Full wwPDB EM Validation Report ⓘ

Apr 27, 2025 – 12:16 AM JST

PDB ID	:	8YDM / pdb_00008ydm
EMDB ID	:	EMD-39177
Title	:	Cryo-EM structure of CaRC-LH complex from Chloroflexus aurantiacus
Authors	:	Guoqiang, H.; Shishang, D.
Deposited on	:	2024-02-20
Resolution	:	3.05 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:

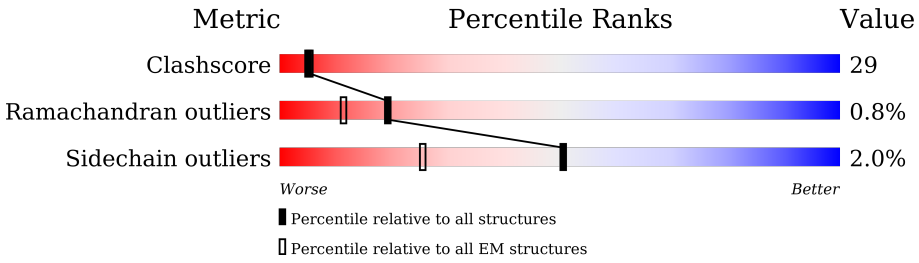
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.05 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	57	26% 42% 19% 5% · 32%
1	D	57	7% 40% 21% · 37%
1	F	57	9% 40% 23% · 33%
1	H	57	11% 44% 19% 37%
1	J	57	12% 44% 19% 37%
1	O	57	· 28% 21% 7% 5% 39%
1	Q	57	9% 46% 16% · 37%
2	B	53	42% 36% 36% 6% · 19%

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Mol	Chain	Length	Quality of chain
2	E	53	26% 72% 23% 6%
2	G	53	17% 64% 25% 8%
2	I	53	17% 49% 42% 6%
2	K	53	25% 51% 40% 6%
2	P	53	17% 36% 45% 9% 6%
2	R	53	30% 68% 26% 6%
3	C	414	20% 76% 22%
4	L	311	8% 66% 30%
5	M	307	65% 30%
6	N	64	22% 80% 8% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGV	C	505	-	-	X	-
12	BPH	L	403	X	-	-	-
12	BPH	M	401	X	-	-	-
7	BCL	M	402	-	-	X	-
7	BCL	O	103	-	-	X	-
8	U4Z	A	102	-	X	-	-
8	U4Z	D	102	-	X	-	-
8	U4Z	D	104	-	X	-	-
8	U4Z	G	101	-	X	-	-
8	U4Z	I	101	-	X	-	-
8	U4Z	I	102	-	X	-	-
8	U4Z	R	101	-	X	-	-
9	HEM	C	504	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15637 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 Light-harvesting protein B-808/866 alpha chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	39	Total	C	N	O	0	0
			314	210	51	53		
1	D	36	Total	C	N	O	0	0
			289	196	45	48		
1	F	38	Total	C	N	O	0	0
			307	207	50	50		
1	H	36	Total	C	N	O	0	0
			293	200	47	46		
1	J	36	Total	C	N	O	0	0
			289	196	45	48		
1	O	35	Total	C	N	O	0	0
			283	193	44	46		
1	Q	36	Total	C	N	O	0	0
			289	196	45	48		

- Molecule 2 is a protein called Light-harvesting protein B-808/866 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	43	Total	C	N	O	0	0
			370	257	60	53		
2	E	50	Total	C	N	O	0	0
			424	290	67	67		
2	G	49	Total	C	N	O	0	0
			416	286	66	64		
2	I	50	Total	C	N	O	0	0
			423	290	67	66		
2	K	50	Total	C	N	O	0	0
			424	290	67	67		
2	P	50	Total	C	N	O	0	0
			424	290	67	67		
2	R	50	Total	C	N	O	0	0
			424	290	67	67		

- Molecule 3 is a protein called Cytochrome c-554.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	407	Total	C	N	O	S	0	0
			3155	1999	552	589	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	306	Total	C	N	O	S	0	0
			2463	1649	393	412	9		

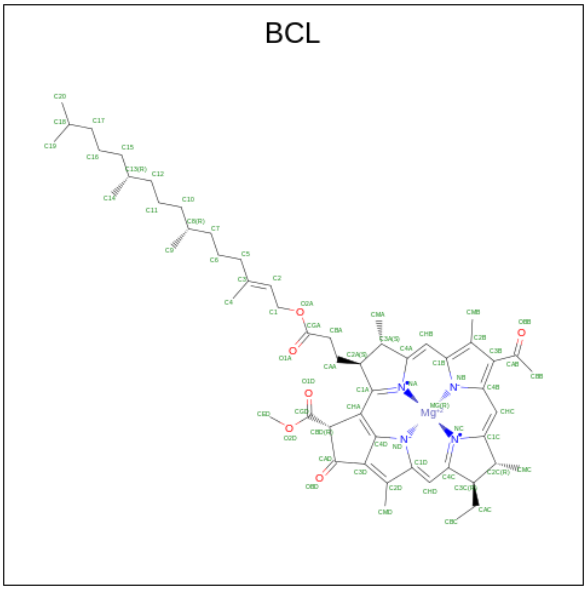
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	295	Total	C	N	O	S	0	0
			2404	1621	379	394	10		

- Molecule 6 is a protein called hypothetical protein chain N.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	56	Total	C	N	O	S	0	0
			421	273	74	72	2		

- Molecule 7 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	Mg	N	O	0
			53	42	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	A	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
7	D	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	E	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	F	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
7	G	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	H	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
7	I	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
7	I	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
7	J	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	K	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
7	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	O	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			47	36	1	4	6	

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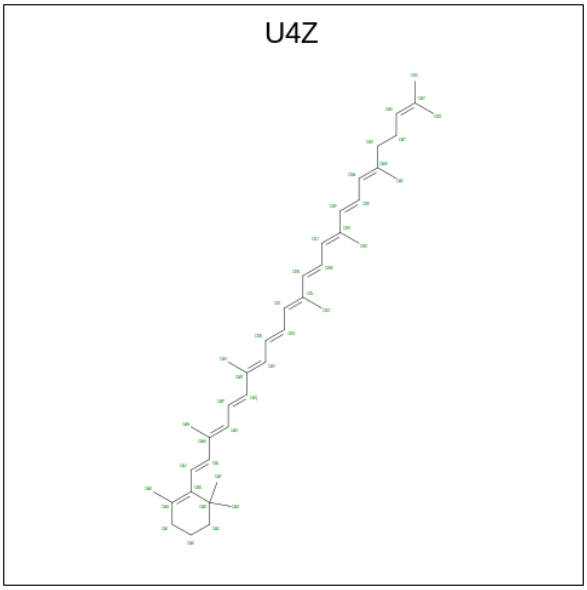
Mol	Chain	Residues	Atoms					AltConf
7	R	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
7	R	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 8 is gamma-Carotene (CCD ID: U4Z) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	C	0
			40	40	
8	B	1	Total	C	0
			40	40	
8	D	1	Total	C	0
			40	40	
8	D	1	Total	C	0
			40	40	
8	G	1	Total	C	0
			40	40	
8	I	1	Total	C	0
			40	40	
8	I	1	Total	C	0
			40	40	
8	K	1	Total	C	0
			40	40	
8	K	1	Total	C	0
			40	40	

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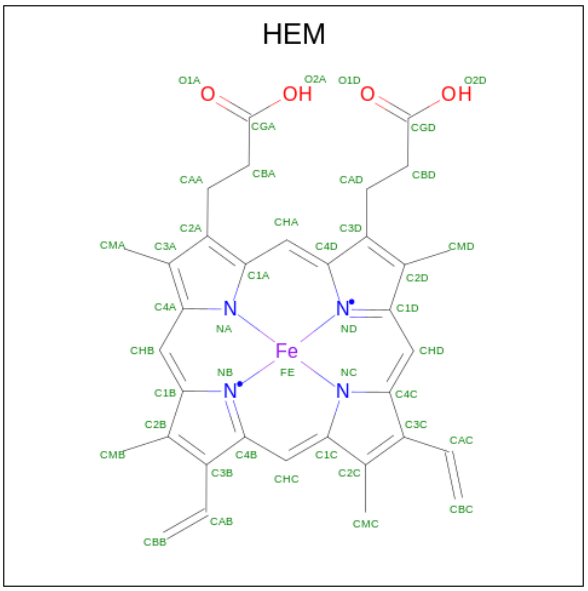
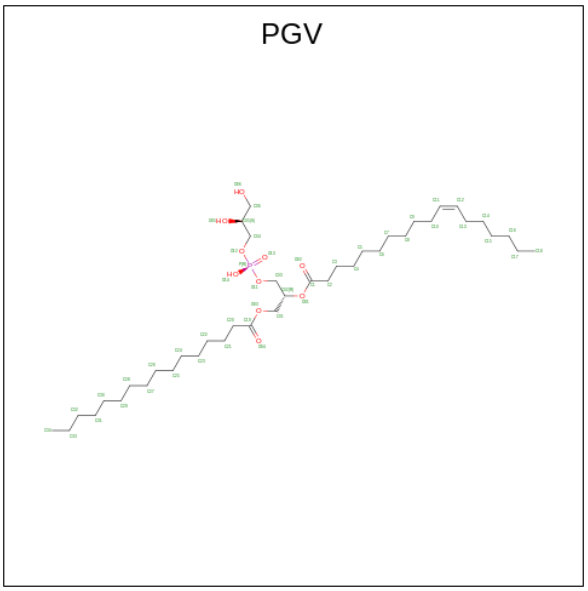
Mol	Chain	Residues	Atoms	AltConf
8	O	1	Total C 40 40	0
8	P	1	Total C 40 40	0
8	Q	1	Total C 40 40	0
8	R	1	Total C 40 40	0

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



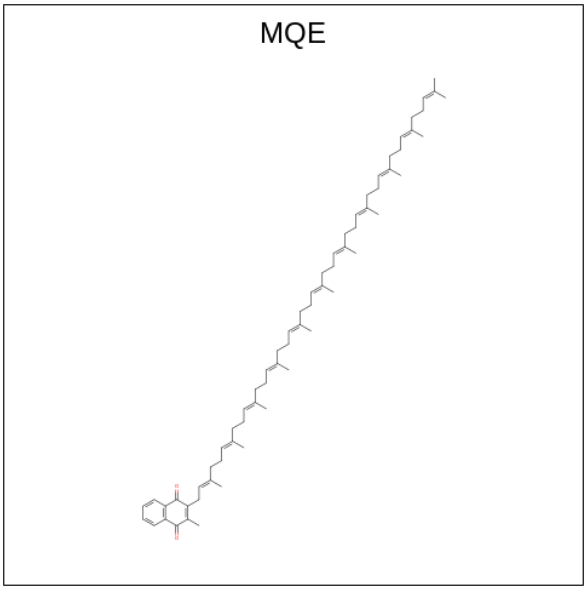
Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total C Fe N O 43 34 1 4 4	0
9	C	1	Total C Fe N O 43 34 1 4 4	0
9	C	1	Total C Fe N O 43 34 1 4 4	0
9	C	1	Total C Fe N O 43 34 1 4 4	0

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



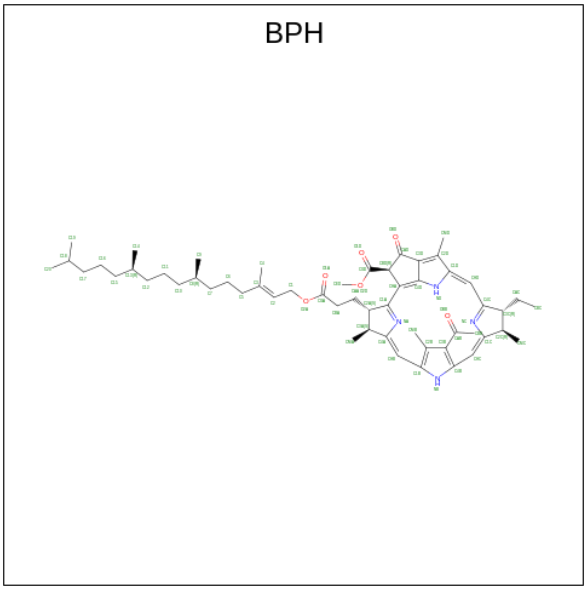
Mol	Chain	Residues	Atoms				AltConf
10	C	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 11 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 (CCD ID: MQE) (formula: $C_{66}H_{96}O_2$).



Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			63	61	2	
11	M	1	Total	C	O	0
			63	61	2	

- Molecule 12 is BACTERIOPHEOPHYTIN A (CCD ID: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms	AltConf
12	L	1	Total C N O 65 55 4 6	0
12	M	1	Total C N O 65 55 4 6	0
12	M	1	Total C N O 46 36 4 6	0

- Molecule 13 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

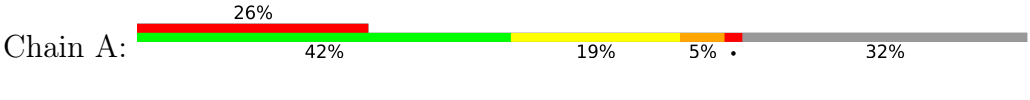
Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total Mn 1 1	0

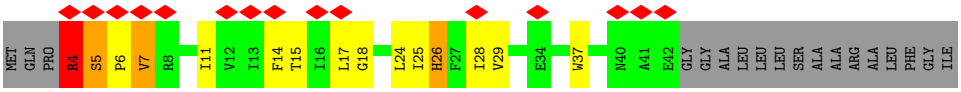
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Light-harvesting protein B-808/866 alpha chain

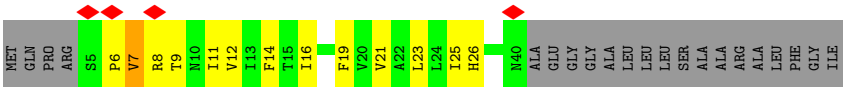
Chain A:





• Molecule 1: Light-harvesting protein B-808/866 alpha chain

Chain D:

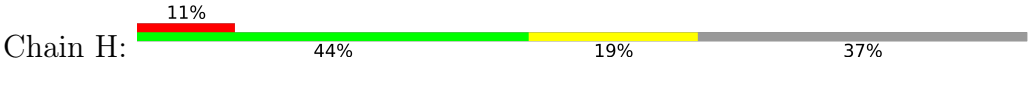


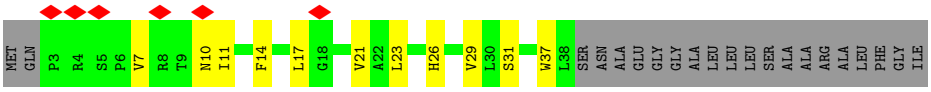
• Molecule 1: Light-harvesting protein B-808/866 alpha chain

Chain F:

• Molecule 1: Light-harvesting protein B-808/866 alpha chain

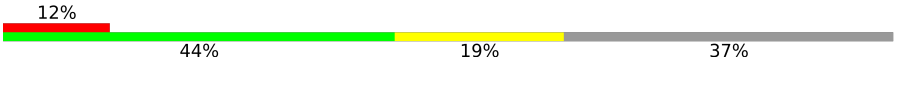
Chain H:

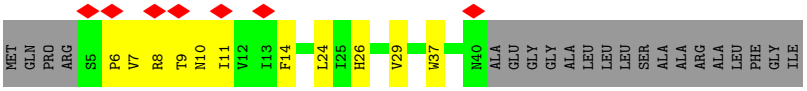




• Molecule 1: Light-harvesting protein B-808/866 alpha chain

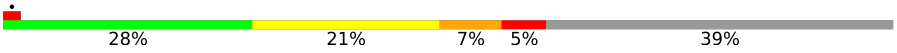
Chain J:

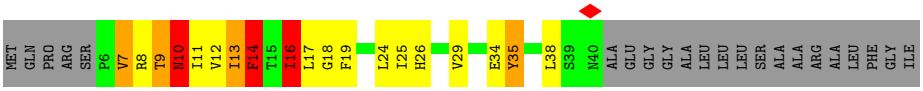




• Molecule 1: Light-harvesting protein B-808/866 alpha chain

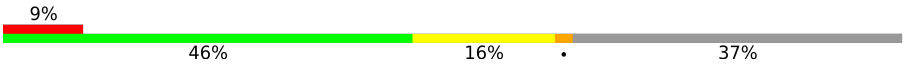
Chain O:

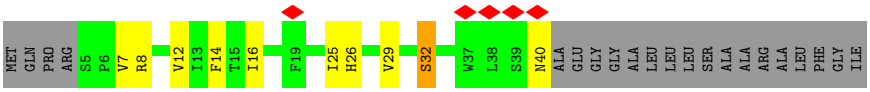




• Molecule 1: Light-harvesting protein B-808/866 alpha chain

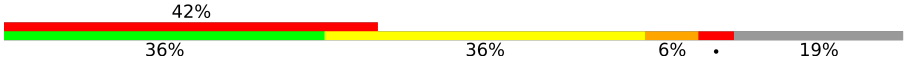
Chain Q:

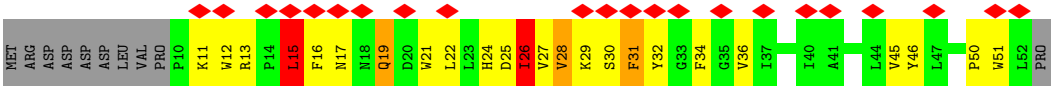




• Molecule 2: Light-harvesting protein B-808/866 beta chain

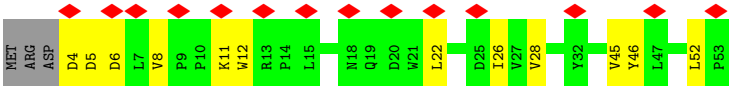
Chain B:





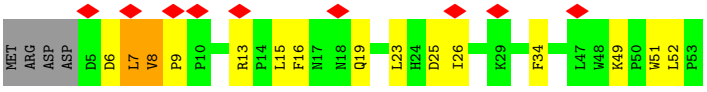
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain E:



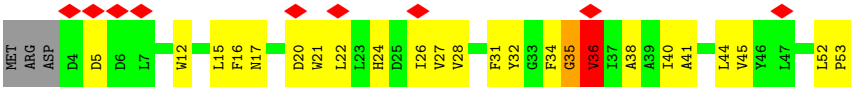
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain G:



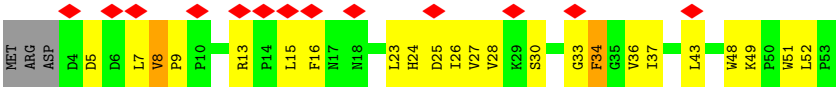
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain I:



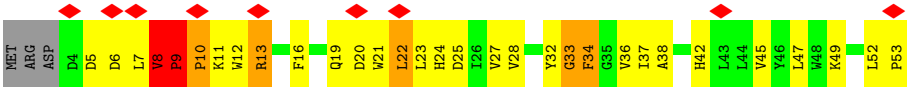
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain K:



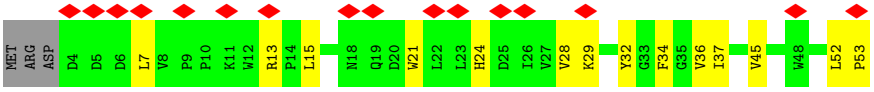
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain P:



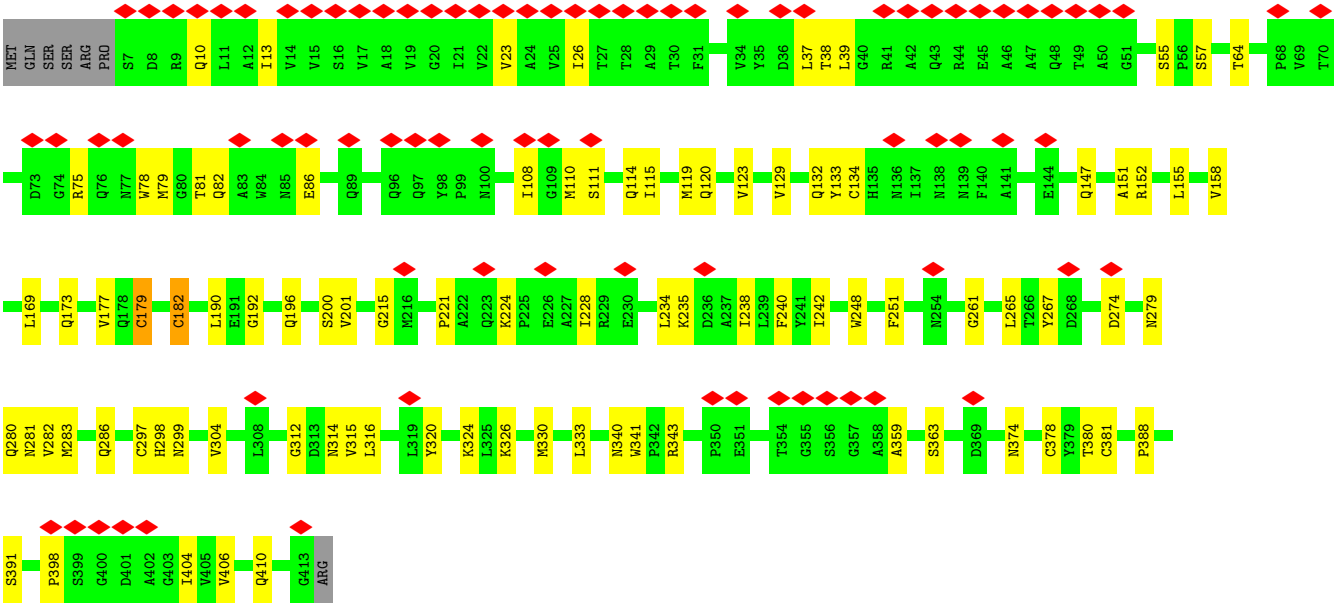
• Molecule 2: Light-harvesting protein B-808/866 beta chain

Chain R:



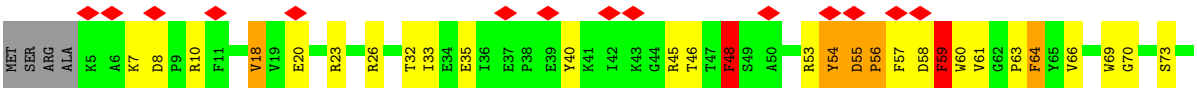
• Molecule 3: Cytochrome c-554

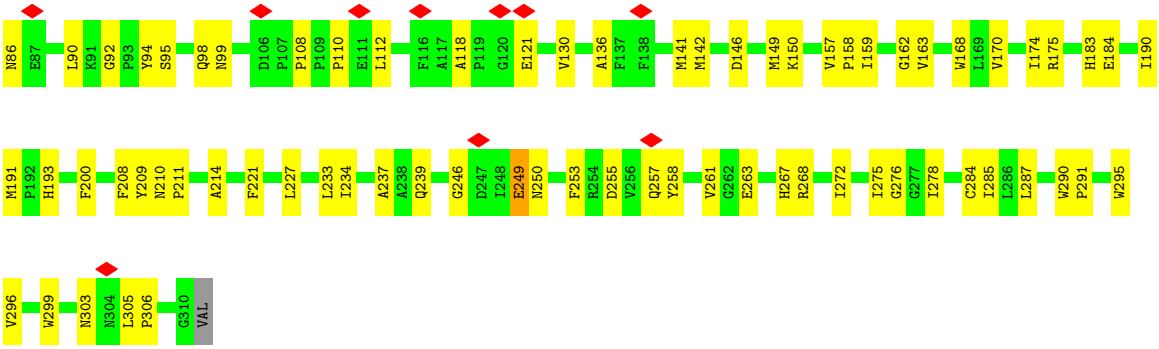
Chain C:



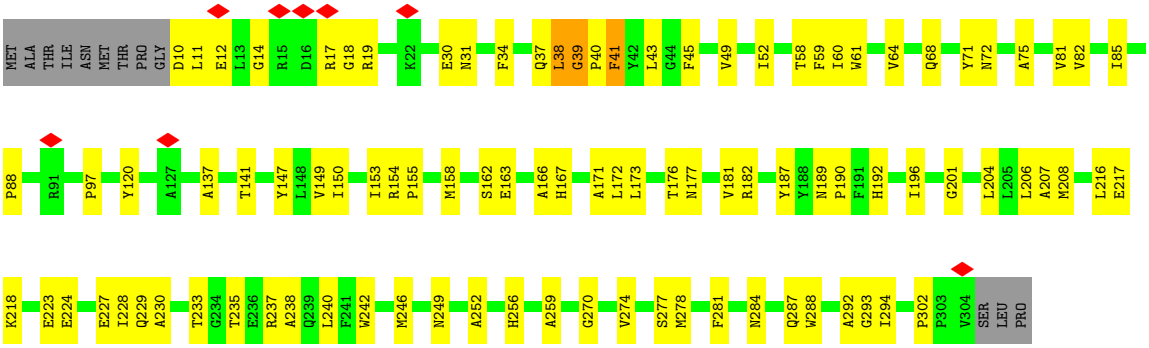
• Molecule 4: Reaction center protein L chain

Chain L:

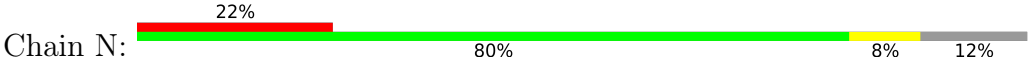


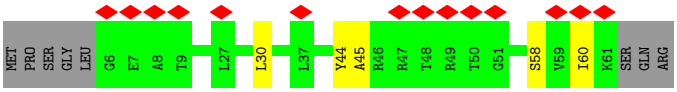


• Molecule 5: Reaction center protein M chain



• Molecule 6: hypothetical protein chain N





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36181	Depositor
Resolution determination method	Not provided	
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.807	Depositor
Minimum map value	-1.198	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	269.856, 269.856, 269.856	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8433, 0.8433, 0.8433	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPH, U4Z, MN, MQE, PGV, BCL, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.49	1/322 (0.3%)	0.84	3/441 (0.7%)
1	D	0.18	0/297	0.69	1/408 (0.2%)
1	F	0.27	0/316	0.81	0/433
1	H	0.15	0/302	0.55	0/414
1	J	0.21	0/297	0.67	0/408
1	O	1.70	8/291 (2.7%)	1.48	8/399 (2.0%)
1	Q	0.17	0/297	0.49	0/408
2	B	0.70	0/387	1.03	2/530 (0.4%)
2	E	0.23	0/443	0.51	0/609
2	G	0.23	0/435	0.62	0/598
2	I	0.81	0/442	0.80	2/609 (0.3%)
2	K	0.22	0/443	0.67	1/609 (0.2%)
2	P	0.97	2/443 (0.5%)	1.33	8/609 (1.3%)
2	R	0.18	0/443	0.51	0/609
3	C	0.25	1/3238 (0.0%)	0.53	1/4435 (0.0%)
4	L	0.53	7/2561 (0.3%)	0.77	10/3492 (0.3%)
5	M	0.46	5/2504 (0.2%)	0.50	2/3428 (0.1%)
6	N	0.17	0/429	0.47	0/585
All	All	0.50	24/13890 (0.2%)	0.70	38/19024 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	250	ASN	C-O	-8.37	1.13	1.24
1	O	9	THR	CA-C	-7.67	1.42	1.52
1	O	14	PHE	C-N	-7.19	1.25	1.33
1	O	35	TYR	C-O	-6.61	1.15	1.24
4	L	59	PHE	CA-C	-6.57	1.44	1.52
5	M	39	GLY	CA-C	-6.39	1.42	1.51
1	O	14	PHE	C-O	-6.35	1.16	1.24
1	O	35	TYR	CA-CB	-6.31	1.42	1.53
5	M	39	GLY	C-O	-6.01	1.15	1.24
5	M	41	PHE	C-O	-5.75	1.17	1.24
1	O	9	THR	C-O	-5.72	1.17	1.24
1	A	26	HIS	C-O	-5.66	1.17	1.24
5	M	37	GLN	C-O	-5.59	1.17	1.24
2	P	32	TYR	C-O	-5.48	1.17	1.24
4	L	64	PHE	C-O	-5.43	1.17	1.23
1	O	16	ILE	C-O	-5.43	1.16	1.24
2	P	34	PHE	C-N	-5.41	1.26	1.33
4	L	48	PHE	C-O	-5.31	1.17	1.24
1	O	35	TYR	CB-CG	-5.28	1.40	1.51
4	L	63	PRO	N-CA	-5.26	1.40	1.47
5	M	41	PHE	N-CA	-5.14	1.39	1.46
4	L	58	ASP	CA-C	-5.13	1.46	1.53
3	C	119	MET	C-O	-5.03	1.18	1.24
4	L	63	PRO	CA-C	-5.03	1.45	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	9	PRO	N-CA-C	13.54	127.22	110.70
2	P	8	VAL	CA-C-N	12.53	133.29	120.38
2	P	8	VAL	C-N-CA	12.53	133.29	120.38
1	O	18	GLY	N-CA-C	-12.01	84.72	113.18
4	L	55	ASP	CA-C-N	-11.45	105.53	119.84
4	L	55	ASP	C-N-CA	-11.45	105.53	119.84
4	L	55	ASP	CB-CA-C	-10.51	92.66	109.37
1	O	7	VAL	N-CA-C	9.53	126.03	113.07
4	L	55	ASP	N-CA-C	8.78	122.12	110.36
5	M	37	GLN	N-CA-C	8.62	123.28	109.24
2	K	34	PHE	N-CA-C	-8.47	101.27	111.69
1	A	4	ARG	CA-C-N	7.81	140.86	121.80
1	A	4	ARG	C-N-CA	7.81	140.86	121.80
2	I	35	GLY	N-CA-C	-7.78	94.74	113.18
2	P	32	TYR	CB-CA-C	-7.71	96.36	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	54	TYR	N-CA-C	7.67	119.98	107.32
4	L	55	ASP	N-CA-CB	-7.59	100.93	109.74
4	L	64	PHE	N-CA-C	7.37	122.35	109.96
1	A	7	VAL	N-CA-C	-7.34	106.74	113.71
1	O	10	ASN	N-CA-C	7.07	121.17	112.54
2	P	34	PHE	CA-C-O	7.03	127.88	120.42
2	P	34	PHE	CB-CA-C	-6.38	100.00	110.85
4	L	56	PRO	CA-C-N	6.30	133.57	121.54
4	L	56	PRO	C-N-CA	6.30	133.57	121.54
1	O	14	PHE	CA-C-O	6.13	127.26	120.82
2	B	26	ILE	N-CA-C	-6.09	104.58	110.42
1	O	16	ILE	CB-CA-C	-5.91	100.50	111.79
2	B	15	LEU	N-CA-C	-5.89	98.25	110.80
4	L	54	TYR	O-C-N	5.84	130.06	123.28
3	C	182	CYS	N-CA-CB	5.84	118.78	110.67
5	M	38	LEU	N-CA-C	-5.58	98.11	107.99
1	O	35	TYR	N-CA-C	5.34	119.42	113.01
1	D	7	VAL	N-CA-C	-5.26	107.27	113.42
2	P	33	GLY	CA-C-N	5.26	127.76	120.29
2	P	33	GLY	C-N-CA	5.26	127.76	120.29
1	O	13	ILE	CA-C-N	5.24	127.25	120.44
1	O	13	ILE	C-N-CA	5.24	127.25	120.44
2	I	36	VAL	N-CA-C	5.22	120.20	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	22	LEU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	314	0	324	46	0
1	D	289	0	300	40	0
1	F	307	0	321	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	293	0	310	21	0
1	J	289	0	300	16	0
1	O	283	0	296	60	0
1	Q	289	0	300	16	0
2	B	370	0	372	43	0
2	E	424	0	417	21	0
2	G	416	0	413	24	0
2	I	423	0	417	36	0
2	K	424	0	417	43	0
2	P	424	0	417	62	0
2	R	424	0	417	21	0
3	C	3155	0	3058	121	0
4	L	2463	0	2355	94	0
5	M	2404	0	2309	102	0
6	N	421	0	452	7	0
7	A	149	0	118	46	0
7	D	95	0	72	16	0
7	E	46	0	35	20	0
7	F	47	0	34	11	0
7	G	94	0	71	18	0
7	H	42	0	31	8	0
7	I	90	0	70	20	0
7	J	47	0	35	1	0
7	K	98	0	76	30	0
7	L	66	0	73	18	0
7	M	132	0	147	35	0
7	O	94	0	70	57	0
7	P	48	0	37	15	0
7	Q	47	0	35	9	0
7	R	90	0	68	22	0
8	A	40	0	0	17	0
8	B	40	0	0	2	0
8	D	80	0	0	31	0
8	G	40	0	0	2	0
8	I	80	0	0	18	0
8	K	80	0	0	13	0
8	O	40	0	0	11	0
8	P	40	0	0	14	0
8	Q	40	0	0	6	0
8	R	40	0	0	3	0
9	C	172	0	120	71	0
10	C	45	0	60	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	L	63	0	0	1	0
11	M	63	0	0	0	0
12	L	65	0	76	12	0
12	M	111	0	113	25	0
13	M	1	0	0	0	0
All	All	15637	0	14536	864	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 29.

All (864) 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)
3:C:378:CYS:SG	9:C:504:HEM:HAB	1.42	1.58
1:O:7:VAL:HG12	7:O:103:BCL:CAB	1.32	1.57
8:A:102:U4Z:CAF	2:B:26:ILE:CG2	1.82	1.56
1:A:15:THR:CG2	8:A:102:U4Z:CAO	1.82	1.56
3:C:381:CYS:SG	9:C:504:HEM:C3C	2.06	1.47
1:D:23:LEU:HD22	8:D:104:U4Z:CAZ	1.52	1.37
7:O:103:BCL:C2D	2:P:28:VAL:HG12	1.56	1.34
8:A:102:U4Z:CAF	2:B:26:ILE:HG21	1.46	1.33
3:C:381:CYS:SG	9:C:504:HEM:C2C	2.21	1.32
8:D:102:U4Z:CAG	2:E:26:ILE:HD11	1.61	1.29
1:A:15:THR:HG22	8:A:102:U4Z:CAO	1.51	1.26
2:R:34:PHE:CD2	7:R:102:BCL:C1	2.18	1.25
2:P:53:PRO:O	8:P:101:U4Z:CBC	1.86	1.24
3:C:378:CYS:SG	9:C:504:HEM:CAB	2.25	1.24
1:D:14:PHE:CZ	7:E:101:BCL:CBC	2.20	1.24
1:D:14:PHE:CZ	7:E:101:BCL:HBC3	1.74	1.22
1:O:7:VAL:CB	7:O:103:BCL:OBB	1.88	1.21
1:D:14:PHE:CE1	7:E:101:BCL:CBC	2.24	1.21
2:B:22:LEU:HD21	2:E:11:LYS:NZ	1.56	1.19
1:O:7:VAL:HG12	7:O:103:BCL:C3B	1.72	1.18
1:O:7:VAL:CG1	7:O:103:BCL:CAB	2.20	1.18
2:P:53:PRO:C	8:P:101:U4Z:CBC	2.17	1.17
1:O:7:VAL:CA	7:O:103:BCL:OBB	1.93	1.17
8:A:102:U4Z:CAF	2:B:26:ILE:HG22	1.54	1.17
2:K:8:VAL:CG1	2:K:13:ARG:HD2	1.75	1.16
2:E:5:ASP:OD1	2:E:8:VAL:HB	1.41	1.16
2:G:8:VAL:HG22	2:G:9:PRO:CD	1.74	1.15
1:D:23:LEU:CD2	8:D:104:U4Z:CAZ	2.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:8:VAL:HG12	2:K:13:ARG:HD2	1.21	1.11
1:H:14:PHE:CG	7:I:104:BCL:HBC2	1.84	1.11
2:G:8:VAL:CG2	2:G:9:PRO:HD2	1.80	1.11
3:C:179:CYS:CB	9:C:502:HEM:HAB	1.81	1.11
3:C:179:CYS:CA	9:C:502:HEM:HAB	1.80	1.10
1:A:15:THR:HG21	8:A:102:U4Z:CAO	1.71	1.10
4:L:208:PHE:CE1	7:L:402:BCL:HBB2	1.86	1.10
1:D:14:PHE:CD1	7:E:101:BCL:HBC2	1.88	1.09
1:D:14:PHE:CE1	7:E:101:BCL:HBC2	1.85	1.09
2:R:34:PHE:CE2	7:R:102:BCL:C1	2.35	1.08
8:K:101:U4Z:CAG	7:K:104:BCL:CAD	2.31	1.08
2:P:9:PRO:HB2	2:P:10:PRO:CD	1.82	1.08
1:A:29:VAL:HG11	7:A:101:BCL:HBC1	1.34	1.07
4:L:208:PHE:CZ	7:L:402:BCL:HBB2	1.89	1.06
12:M:406:BPH:HHC	12:M:406:BPH:HBB3	1.34	1.05
1:O:7:VAL:CG1	7:O:103:BCL:CMB	2.33	1.05
3:C:182:CYS:SG	3:C:381:CYS:HB3	1.98	1.03
7:O:103:BCL:C2D	2:P:28:VAL:CG1	2.36	1.03
1:H:21:VAL:HG11	8:I:101:U4Z:CBJ	1.89	1.02
3:C:182:CYS:HB2	9:C:502:HEM:HAC	1.42	1.02
1:D:23:LEU:HD13	8:D:104:U4Z:CAZ	1.90	1.01
7:K:102:BCL:HMB1	8:O:102:U4Z:CAS	1.90	1.01
2:P:53:PRO:OXT	8:P:101:U4Z:CBC	2.09	1.01
8:D:102:U4Z:CAG	2:E:26:ILE:CD1	2.38	1.01
5:M:52:ILE:HD13	1:O:17:LEU:HD11	1.42	1.00
12:M:401:BPH:HHD	12:M:401:BPH:HBC3	1.43	1.00
3:C:179:CYS:HB3	9:C:502:HEM:CAB	1.91	1.00
3:C:179:CYS:HA	9:C:502:HEM:HAB	1.40	0.99
1:D:21:VAL:HG21	8:D:102:U4Z:CBK	1.93	0.99
3:C:330:MET:HE1	9:C:504:HEM:C4D	1.99	0.98
1:O:7:VAL:CG1	7:O:103:BCL:C3B	2.40	0.98
1:O:14:PHE:O	1:O:17:LEU:O	1.80	0.98
7:A:103:BCL:C1	2:B:34:PHE:CZ	2.47	0.98
1:H:14:PHE:CD1	7:I:104:BCL:HBC2	1.98	0.98
7:O:103:BCL:HMA1	2:P:16:PHE:CE2	1.98	0.98
2:B:22:LEU:HD21	2:E:11:LYS:HZ1	1.25	0.97
8:D:104:U4Z:CAE	7:I:104:BCL:HBB2	1.95	0.97
8:K:101:U4Z:CAG	7:K:104:BCL:C3D	2.42	0.97
4:L:208:PHE:CZ	7:L:402:BCL:CBB	2.48	0.96
4:L:208:PHE:HZ	7:L:402:BCL:CBB	1.78	0.95
3:C:330:MET:HE1	9:C:504:HEM:ND	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG22	8:A:102:U4Z:CAP	1.96	0.95
1:A:29:VAL:HG21	7:A:103:BCL:HHD	1.50	0.94
1:O:7:VAL:CG1	7:O:103:BCL:HMB2	1.97	0.93
7:K:102:BCL:HBB2	8:O:102:U4Z:CBC	1.98	0.93
1:O:7:VAL:CG1	7:O:103:BCL:C2B	2.46	0.92
7:M:402:BCL:H2	7:M:402:BCL:H71	1.46	0.92
1:D:21:VAL:HG11	8:D:102:U4Z:CBK	1.98	0.92
1:H:14:PHE:CD1	7:I:104:BCL:CBC	2.53	0.92
1:A:29:VAL:CG1	7:A:101:BCL:HBC1	1.99	0.91
3:C:151:ALA:HB3	9:C:501:HEM:HMD1	1.52	0.91
5:M:189:ASN:HB3	5:M:192:HIS:HB3	1.51	0.91
1:D:14:PHE:CG	7:E:101:BCL:HBC2	2.06	0.91
7:Q:101:BCL:OBD	7:R:102:BCL:HBD	1.69	0.91
1:O:7:VAL:HA	7:O:103:BCL:OBB	1.71	0.91
3:C:134:CYS:SG	9:C:501:HEM:HAC	2.11	0.90
1:O:7:VAL:CG1	7:O:103:BCL:OBB	2.15	0.90
1:O:7:VAL:HG12	7:O:103:BCL:OBB	1.71	0.90
1:O:7:VAL:HB	7:O:103:BCL:OBB	1.70	0.89
2:B:25:ASP:HA	2:B:28:VAL:HG13	1.52	0.89
1:D:23:LEU:CD1	8:D:104:U4Z:CAZ	2.51	0.89
1:D:11:ILE:HG22	7:E:101:BCL:CMC	2.03	0.88
1:F:26:HIS:CE1	7:F:101:BCL:HMD3	2.08	0.88
3:C:179:CYS:HB3	9:C:502:HEM:HAB	1.46	0.88
1:O:14:PHE:CE2	7:O:103:BCL:H3C	2.08	0.88
2:P:9:PRO:CB	2:P:10:PRO:CD	2.49	0.88
7:O:103:BCL:C3D	2:P:28:VAL:CG1	2.51	0.87
10:C:505:PGV:H202	5:M:82:VAL:CG1	2.04	0.87
1:A:18:GLY:HA3	8:A:102:U4Z:CBG	2.04	0.87
1:D:19:PHE:HE1	8:D:104:U4Z:CBK	1.87	0.86
1:A:7:VAL:HA	7:A:104:BCL:OBB	1.74	0.86
3:C:297:CYS:SG	9:C:503:HEM:CAC	2.64	0.85
7:D:103:BCL:HBC1	2:E:45:VAL:HG11	1.57	0.85
12:L:403:BPH:HMB3	12:L:403:BPH:HBB2	1.59	0.85
7:K:102:BCL:CMB	8:O:102:U4Z:CAS	2.55	0.85
1:D:14:PHE:CE2	7:E:101:BCL:CBC	2.60	0.85
7:A:103:BCL:HBC1	2:B:45:VAL:HG11	1.57	0.85
8:K:103:U4Z:CAG	8:P:101:U4Z:CAE	2.55	0.85
1:O:14:PHE:CE1	8:O:102:U4Z:CBG	2.60	0.84
2:K:8:VAL:HG22	2:K:9:PRO:HD2	1.59	0.84
9:C:504:HEM:HHD	9:C:504:HEM:HBC2	1.59	0.84
1:A:15:THR:HG23	8:A:102:U4Z:CAO	2.05	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:7:VAL:HG12	7:O:103:BCL:C2B	2.06	0.84
1:D:14:PHE:CZ	7:E:101:BCL:HBC2	2.00	0.83
1:F:21:VAL:O	1:F:25:ILE:HG13	1.77	0.83
2:R:45:VAL:HG11	7:R:102:BCL:HBC1	1.57	0.83
1:D:26:HIS:CE1	7:D:103:BCL:HMD3	2.14	0.83
7:F:101:BCL:HBB2	7:F:101:BCL:HMB3	1.61	0.83
7:M:402:BCL:CHD	7:M:402:BCL:HBC3	2.08	0.83
5:M:58:THR:OG1	7:M:405:BCL:H201	1.79	0.82
1:O:7:VAL:HG11	7:O:103:BCL:C2B	2.08	0.82
1:A:14:PHE:CG	7:A:104:BCL:HBC2	2.14	0.82
2:P:9:PRO:CB	2:P:10:PRO:HD3	2.08	0.82
7:G:103:BCL:HBB2	7:G:103:BCL:HMB3	1.62	0.82
3:C:152:ARG:HG2	9:C:501:HEM:O2D	1.79	0.81
1:D:21:VAL:HG13	7:D:103:BCL:CED	2.09	0.81
2:P:8:VAL:HG12	2:P:9:PRO:HD2	1.60	0.81
7:O:103:BCL:HMA1	2:P:16:PHE:CZ	2.16	0.81
1:A:29:VAL:HG11	7:A:101:BCL:CBC	2.10	0.81
7:A:103:BCL:C1	2:B:34:PHE:CE2	2.65	0.80
1:D:14:PHE:CE2	7:E:101:BCL:HBC2	2.16	0.80
7:O:103:BCL:C3D	2:P:28:VAL:HG12	2.11	0.80
1:D:11:ILE:HG22	7:E:101:BCL:HMC2	1.63	0.80
1:D:14:PHE:CD2	7:E:101:BCL:HBC2	2.17	0.80
2:K:7:LEU:O	2:K:7:LEU:HD23	1.82	0.79
3:C:182:CYS:SG	3:C:381:CYS:CB	2.70	0.79
1:O:11:ILE:HG12	7:O:103:BCL:HMC2	1.64	0.79
4:L:290:TRP:HB3	4:L:291:PRO:HD3	1.65	0.79
3:C:182:CYS:CB	9:C:502:HEM:HAC	2.13	0.79
5:M:52:ILE:HD13	1:O:17:LEU:CD1	2.12	0.79
2:B:22:LEU:CD2	2:E:11:LYS:NZ	2.44	0.78
2:P:53:PRO:OXT	8:P:101:U4Z:CAY	2.31	0.78
3:C:378:CYS:CB	9:C:504:HEM:HAB	2.13	0.78
2:G:8:VAL:HG22	2:G:9:PRO:HD2	0.85	0.78
3:C:182:CYS:HB2	9:C:502:HEM:CAC	2.14	0.78
1:H:23:LEU:HD12	8:K:103:U4Z:CAZ	2.13	0.77
1:O:14:PHE:HE1	8:O:102:U4Z:CBG	1.96	0.77
7:O:103:BCL:CHD	7:O:103:BCL:HBC3	2.14	0.77
2:B:22:LEU:HD21	2:E:11:LYS:CE	2.13	0.77
2:I:45:VAL:HG11	7:I:103:BCL:HBC1	1.64	0.77
1:F:29:VAL:HG21	7:F:101:BCL:HBC3	1.65	0.77
2:B:12:TRP:H	2:B:12:TRP:CD1	2.01	0.77
1:D:21:VAL:HG13	7:D:103:BCL:HED1	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:MET:SD	9:C:504:HEM:NC	2.58	0.76
2:P:9:PRO:HB2	2:P:10:PRO:HD2	1.67	0.76
5:M:196:ILE:HD13	7:M:402:BCL:CMD	2.16	0.76
10:C:505:PGV:O13	10:C:505:PGV:O05	2.04	0.76
5:M:38:LEU:HD12	5:M:38:LEU:N	2.00	0.76
1:A:26:HIS:CE1	7:A:103:BCL:HMD3	2.21	0.76
1:O:29:VAL:HG11	7:O:101:BCL:HBC1	1.67	0.75
2:K:24:HIS:CE1	7:K:104:BCL:C1A	2.69	0.75
4:L:246:GLY:O	4:L:249:GLU:HG3	1.86	0.75
1:O:17:LEU:HD12	1:O:17:LEU:N	2.01	0.75
7:O:103:BCL:C3D	2:P:28:VAL:HG11	2.14	0.75
1:O:8:ARG:HH22	2:P:19:GLN:NE2	1.84	0.75
1:O:7:VAL:HG11	7:O:103:BCL:HMB2	1.67	0.75
3:C:378:CYS:SG	9:C:504:HEM:CBB	2.75	0.74
2:P:20:ASP:O	2:P:24:HIS:HB3	1.87	0.74
1:O:7:VAL:HG11	7:O:103:BCL:CMB	2.15	0.74
7:M:405:BCL:HMB1	7:M:405:BCL:HBB3	1.70	0.74
7:O:103:BCL:HBC3	7:O:103:BCL:HHD	1.69	0.74
2:B:11:LYS:HG3	2:B:13:ARG:HB2	1.69	0.73
8:A:102:U4Z:CAC	7:E:101:BCL:HBB2	2.17	0.73
2:B:22:LEU:HD21	2:E:11:LYS:HZ2	1.53	0.73
7:O:103:BCL:C1D	2:P:28:VAL:HG12	2.19	0.73
10:C:505:PGV:C20	5:M:82:VAL:CG1	2.66	0.73
3:C:297:CYS:SG	9:C:503:HEM:HAC	2.27	0.73
4:L:208:PHE:HE1	7:L:402:BCL:HBB2	1.46	0.73
7:A:101:BCL:O1A	8:D:102:U4Z:CBE	2.37	0.73
1:D:19:PHE:CE1	8:D:104:U4Z:CBK	2.71	0.73
8:K:103:U4Z:CAG	8:P:101:U4Z:CAI	2.66	0.73
1:A:4:ARG:HD3	1:A:4:ARG:N	2.03	0.73
10:C:505:PGV:H202	5:M:82:VAL:HG11	1.71	0.73
1:O:19:PHE:HE1	8:Q:102:U4Z:CBK	2.01	0.72
3:C:179:CYS:CB	9:C:502:HEM:CAB	2.57	0.72
2:E:5:ASP:OD1	2:E:8:VAL:CB	2.30	0.72
1:D:14:PHE:CE2	7:E:101:BCL:HBC3	2.23	0.72
2:K:24:HIS:HE1	7:K:104:BCL:C1A	2.01	0.72
3:C:182:CYS:HB3	3:C:380:THR:HG22	1.71	0.72
7:M:402:BCL:HBB2	7:M:402:BCL:HMB3	1.72	0.72
7:G:103:BCL:HAA1	7:G:103:BCL:HED2	1.70	0.71
7:O:103:BCL:HMC1	2:P:27:VAL:HG11	1.72	0.71
2:G:34:PHE:CE1	7:G:102:BCL:HED1	2.25	0.71
2:K:8:VAL:HG12	2:K:13:ARG:CD	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:PHE:CE1	7:I:104:BCL:CBC	2.74	0.71
1:O:11:ILE:HG12	7:O:103:BCL:CMC	2.21	0.71
1:D:14:PHE:CE1	7:E:101:BCL:HBC1	2.22	0.70
12:L:403:BPH:C20	5:M:172:LEU:HD11	2.22	0.70
2:B:29:LYS:O	2:B:32:TYR:N	2.24	0.70
1:A:7:VAL:CA	7:A:104:BCL:OBB	2.38	0.70
3:C:265:LEU:O	5:M:182:ARG:NH1	2.24	0.70
7:M:402:BCL:H2	7:M:402:BCL:C7	2.18	0.70
1:Q:14:PHE:CZ	8:Q:102:U4Z:CAV	2.75	0.70
2:I:34:PHE:CE1	7:I:103:BCL:O2A	2.45	0.69
7:L:402:BCL:H111	12:M:401:BPH:CHB	2.22	0.69
2:K:24:HIS:CE1	7:K:104:BCL:NA	2.60	0.69
7:D:103:BCL:HBB2	7:D:103:BCL:HMB3	1.74	0.69
8:D:104:U4Z:CBG	1:F:18:GLY:HA3	2.22	0.69
2:K:33:GLY:HA2	2:K:36:VAL:HG12	1.74	0.69
1:F:8:ARG:NH2	2:G:19:GLN:OE1	2.25	0.69
5:M:154:ARG:NH1	5:M:277:SER:O	2.26	0.69
3:C:179:CYS:HA	9:C:502:HEM:CAB	2.20	0.68
2:I:16:PHE:CE2	7:I:104:BCL:HMA1	2.28	0.68
3:C:330:MET:SD	9:C:504:HEM:FE	1.84	0.68
10:C:505:PGV:C20	5:M:82:VAL:HG13	2.22	0.68
1:O:14:PHE:HE2	7:O:103:BCL:H3C	1.58	0.68
1:O:35:TYR:CE1	2:P:49:LYS:HD2	2.29	0.68
12:M:401:BPH:CBB	12:M:401:BPH:HMB1	2.24	0.68
3:C:298:HIS:HE1	3:C:324:LYS:HE2	1.57	0.67
1:D:23:LEU:CG	8:D:104:U4Z:CAZ	2.72	0.67
3:C:110:MET:HE2	3:C:404:ILE:HG23	1.76	0.67
12:L:403:BPH:HBB2	12:L:403:BPH:CMB	2.25	0.67
4:L:118:ALA:HB3	4:L:121:GLU:HG2	1.75	0.67
12:M:406:BPH:HHC	12:M:406:BPH:CBB	2.14	0.67
3:C:238:ILE:HD11	3:C:281:ASN:HB3	1.77	0.67
7:O:103:BCL:C1D	2:P:28:VAL:CG1	2.72	0.67
1:O:7:VAL:HG13	7:O:103:BCL:HMB2	1.77	0.66
1:O:13:ILE:HA	1:O:16:ILE:HD12	1.78	0.66
7:P:102:BCL:HBB2	7:P:102:BCL:HMB3	1.75	0.66
2:G:52:LEU:HD21	8:G:101:U4Z:CBE	2.24	0.66
1:A:7:VAL:CB	7:A:104:BCL:OBB	2.43	0.66
7:F:101:BCL:HBB2	7:F:101:BCL:CMB	2.24	0.66
3:C:177:VAL:HG21	9:C:504:HEM:HBC1	1.76	0.66
3:C:315:VAL:HG11	4:L:200:PHE:HB2	1.77	0.66
3:C:330:MET:CE	9:C:504:HEM:ND	2.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:196:ILE:HD13	7:M:402:BCL:HMD2	1.76	0.66
7:Q:101:BCL:HED2	2:R:37:ILE:CG2	2.26	0.65
2:R:52:LEU:CD1	8:R:101:U4Z:CBE	2.74	0.65
4:L:258:TYR:HE1	5:M:39:GLY:O	1.80	0.65
12:M:401:BPH:HAA1	12:M:401:BPH:HBD	1.79	0.65
5:M:150:ILE:HG12	5:M:274:VAL:HG11	1.79	0.65
1:Q:14:PHE:CD1	7:R:103:BCL:HBC2	2.31	0.65
2:B:12:TRP:H	2:B:12:TRP:HD1	1.45	0.65
9:C:503:HEM:CMA	5:M:181:VAL:CG1	2.75	0.65
2:K:24:HIS:CE1	7:K:104:BCL:HMA3	2.31	0.64
3:C:182:CYS:SG	3:C:381:CYS:CA	2.85	0.64
10:C:505:PGV:H152	4:L:211:PRO:HA	1.77	0.64
3:C:274:ASP:OD2	5:M:162:SER:HB2	1.98	0.64
2:G:16:PHE:HE2	7:G:103:BCL:CMA	2.10	0.64
3:C:120:GLN:HA	9:C:501:HEM:HBB2	1.79	0.64
2:G:16:PHE:CE2	7:G:103:BCL:HMA1	2.33	0.64
2:I:34:PHE:HZ	7:I:103:BCL:O1D	1.81	0.64
2:P:8:VAL:HG13	2:P:21:TRP:CG	2.32	0.64
3:C:169:LEU:HD13	3:C:326:LYS:HD3	1.79	0.64
9:C:504:HEM:HHD	9:C:504:HEM:CBC	2.26	0.64
2:G:16:PHE:HE2	7:G:103:BCL:HMA1	1.63	0.64
2:G:52:LEU:CD2	8:G:101:U4Z:CBE	2.76	0.63
3:C:330:MET:SD	9:C:504:HEM:NB	2.71	0.63
4:L:55:ASP:OD1	4:L:55:ASP:N	2.28	0.63
3:C:283:MET:HG2	9:C:503:HEM:NB	2.13	0.63
7:G:103:BCL:HMB3	7:G:103:BCL:CBB	2.28	0.63
7:M:402:BCL:HBC3	7:M:402:BCL:HHD	1.81	0.63
12:M:401:BPH:HHD	12:M:401:BPH:CBC	2.18	0.63
1:D:23:LEU:HA	8:D:104:U4Z:CAZ	2.29	0.63
1:D:21:VAL:CG2	8:D:102:U4Z:CBK	2.75	0.63
3:C:340:ASN:OD1	3:C:343:ARG:NH2	2.33	0.62
1:A:14:PHE:CD1	7:A:104:BCL:HBC2	2.34	0.62
1:A:7:VAL:HB	7:A:104:BCL:OBB	2.00	0.62
1:A:25:ILE:HG22	7:A:103:BCL:C2D	2.30	0.62
5:M:201:GLY:HA2	7:M:402:BCL:H42	1.81	0.62
1:Q:26:HIS:CE1	7:R:102:BCL:HMD3	2.34	0.62
3:C:152:ARG:CG	9:C:501:HEM:O2D	2.48	0.62
10:C:505:PGV:C20	5:M:82:VAL:HG11	2.30	0.62
1:J:14:PHE:CD1	7:K:104:BCL:HAC1	2.35	0.62
7:H:101:BCL:H3C	8:K:101:U4Z:CBK	2.30	0.62
1:O:14:PHE:CE2	7:O:103:BCL:C3C	2.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:103:BCL:C1	2:B:34:PHE:CE1	2.83	0.62
7:A:101:BCL:OBD	7:A:103:BCL:HBD	1.99	0.61
10:C:505:PGV:H201	5:M:82:VAL:HG13	1.81	0.61
1:O:7:VAL:HG12	7:O:103:BCL:CMB	2.17	0.61
2:P:9:PRO:CG	2:P:12:TRP:HB2	2.29	0.61
4:L:53:ARG:HB2	4:L:54:TYR:HD1	1.65	0.61
2:K:30:SER:O	2:K:34:PHE:HB2	2.00	0.61
1:H:11:ILE:HD13	2:I:27:VAL:HG21	1.82	0.61
7:O:101:BCL:HMD1	2:P:42:HIS:ND1	2.16	0.61
4:L:191:MET:HE3	5:M:294:ILE:HD12	1.82	0.61
5:M:270:GLY:O	7:M:405:BCL:HED3	2.00	0.61
7:O:103:BCL:HBC1	8:P:101:U4Z:CAK	2.31	0.61
10:C:505:PGV:C04	10:C:505:PGV:H031	2.29	0.61
1:H:14:PHE:CD2	7:I:104:BCL:HBC2	2.35	0.60
4:L:253:PHE:O	4:L:257:GLN:N	2.34	0.60
12:M:406:BPH:HBB3	12:M:406:BPH:CHC	2.22	0.60
1:O:16:ILE:HG22	1:O:16:ILE:O	2.01	0.60
2:K:26:ILE:HG21	8:K:103:U4Z:CAF	2.32	0.60
3:C:398:PRO:HD2	3:C:406:VAL:HG21	1.82	0.60
1:Q:29:VAL:HG11	7:Q:101:BCL:HBC1	1.82	0.60
4:L:8:ASP:OD1	4:L:10:ARG:NH1	2.35	0.60
4:L:255:ASP:OD2	5:M:19:ARG:NH1	2.34	0.60
5:M:137:ALA:O	5:M:141:THR:HG23	2.00	0.60
12:M:401:BPH:HMB1	12:M:401:BPH:HBB3	1.84	0.60
2:P:34:PHE:HD2	7:P:102:BCL:H11	1.65	0.60
2:P:53:PRO:OXT	8:P:101:U4Z:CAX	2.49	0.60
5:M:196:ILE:HD13	7:M:402:BCL:HMD1	1.83	0.59
7:D:103:BCL:HBB2	7:D:103:BCL:CMB	2.32	0.59
7:G:102:BCL:HBB2	8:I:101:U4Z:CBC	2.32	0.59
1:D:21:VAL:CG1	8:D:102:U4Z:CBK	2.79	0.59
7:G:102:BCL:HMA3	8:I:102:U4Z:CBO	2.31	0.59
2:K:52:LEU:HD22	8:K:101:U4Z:CBE	2.31	0.59
3:C:158:VAL:HG21	9:C:502:HEM:CBB	2.33	0.59
5:M:85:ILE:HB	5:M:167:HIS:HB2	1.85	0.59
7:Q:101:BCL:HED2	2:R:37:ILE:HG22	1.85	0.59
5:M:204:LEU:O	5:M:208:MET:HG3	2.02	0.59
5:M:233:THR:OG1	5:M:237:ARG:NH1	2.31	0.59
1:F:26:HIS:CE1	7:F:101:BCL:CMD	2.84	0.59
7:O:103:BCL:CMD	2:P:28:VAL:HG12	2.32	0.59
2:R:53:PRO:HG2	8:R:101:U4Z:CAX	2.33	0.59
3:C:151:ALA:CB	9:C:501:HEM:HMD1	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:HD1	2:B:50:PRO:HA	1.67	0.59
1:O:19:PHE:CE1	8:Q:102:U4Z:CBK	2.84	0.59
7:P:102:BCL:HBB2	7:P:102:BCL:CMB	2.33	0.59
3:C:82:GLN:O	3:C:86:GLU:HG2	2.02	0.59
4:L:285:ILE:HG13	7:L:402:BCL:O1D	2.03	0.58
5:M:166:ALA:HB3	5:M:171:ALA:HB1	1.85	0.58
1:A:17:LEU:HD23	8:A:102:U4Z:CBO	2.33	0.58
2:K:28:VAL:HG21	7:K:104:BCL:O1D	2.03	0.58
2:E:11:LYS:NZ	2:E:11:LYS:O	2.35	0.58
7:K:102:BCL:C1C	7:P:102:BCL:HBB3	2.33	0.58
1:F:23:LEU:HD23	8:I:101:U4Z:CAZ	2.33	0.58
1:A:25:ILE:HG21	7:A:103:BCL:C4D	2.34	0.58
2:K:8:VAL:HG21	2:K:16:PHE:HE1	1.69	0.58
3:C:155:LEU:HD23	9:C:502:HEM:HBB2	1.83	0.58
3:C:182:CYS:O	3:C:190:LEU:HD13	2.04	0.58
3:C:298:HIS:CE1	3:C:324:LYS:HE2	2.37	0.58
2:I:34:PHE:CD1	8:I:101:U4Z:CAV	2.87	0.58
2:E:22:LEU:O	2:E:26:ILE:HG23	2.03	0.58
2:P:9:PRO:HG2	2:P:12:TRP:HB2	1.85	0.58
2:K:37:ILE:HG22	7:K:102:BCL:HED2	1.86	0.58
2:B:28:VAL:HG23	2:B:28:VAL:O	2.04	0.57
7:H:101:BCL:O2D	2:I:34:PHE:CE2	2.57	0.57
1:J:8:ARG:HD3	2:K:23:LEU:HD11	1.85	0.57
5:M:284:ASN:HB3	5:M:287:GLN:HB3	1.86	0.57
10:C:505:PGV:H251	5:M:81:VAL:HG21	1.86	0.57
2:I:22:LEU:HD11	2:K:15:LEU:HD22	1.86	0.57
7:L:402:BCL:HBB1	5:M:176:THR:HG21	1.86	0.57
4:L:54:TYR:CD1	4:L:54:TYR:N	2.72	0.57
1:A:15:THR:HG21	8:A:102:U4Z:CAL	2.35	0.57
1:F:22:ALA:HB2	7:F:101:BCL:O1D	2.05	0.57
7:M:402:BCL:CMB	7:M:402:BCL:CBB	2.83	0.57
1:A:4:ARG:N	1:A:4:ARG:HH11	2.03	0.56
1:F:22:ALA:O	1:F:26:HIS:HD2	1.87	0.56
12:L:403:BPH:H9C1	12:L:403:BPH:C12	2.34	0.56
5:M:88:PRO:HB3	5:M:97:PRO:HG2	1.87	0.56
2:R:34:PHE:HD2	7:R:102:BCL:C1	2.05	0.56
5:M:270:GLY:HA2	7:M:405:BCL:CED	2.34	0.56
1:O:8:ARG:NH2	2:P:19:GLN:NE2	2.52	0.56
3:C:326:LYS:HD2	9:C:504:HEM:HAA2	1.86	0.56
8:O:102:U4Z:CAG	7:R:103:BCL:HAC1	2.35	0.56
2:P:45:VAL:HG11	7:P:102:BCL:HBC1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:CD1	2:E:12:TRP:HH2	2.19	0.56
2:K:24:HIS:O	2:K:24:HIS:ND1	2.38	0.56
7:F:101:BCL:CMB	7:F:101:BCL:CBB	2.83	0.56
4:L:200:PHE:HD1	7:L:402:BCL:HMD3	1.71	0.56
10:C:505:PGV:H202	5:M:82:VAL:HG13	1.83	0.56
2:G:8:VAL:CG2	2:G:9:PRO:CD	2.56	0.56
4:L:48:PHE:HD2	4:L:55:ASP:HB3	1.71	0.56
2:B:22:LEU:CD2	2:E:11:LYS:HZ2	2.12	0.56
3:C:378:CYS:HG	9:C:504:HEM:CAB	2.15	0.56
1:F:23:LEU:CD2	8:I:101:U4Z:CAZ	2.84	0.56
2:I:45:VAL:HG11	7:I:103:BCL:CBC	2.32	0.56
1:O:7:VAL:C	7:O:103:BCL:OBB	2.49	0.56
7:H:101:BCL:HED1	2:I:34:PHE:CD2	2.41	0.55
2:K:37:ILE:CG2	7:K:102:BCL:HED2	2.35	0.55
3:C:221:PRO:HA	3:C:224:LYS:HE3	1.88	0.55
8:D:102:U4Z:CAQ	8:D:102:U4Z:CAN	2.84	0.55
8:D:102:U4Z:CAX	8:D:102:U4Z:CAZ	2.83	0.55
2:G:34:PHE:CD1	7:G:102:BCL:HED1	2.40	0.55
1:H:14:PHE:CD1	7:I:104:BCL:HBC1	2.41	0.55
2:P:8:VAL:CG1	2:P:9:PRO:HD2	2.31	0.55
1:A:25:ILE:CG2	7:A:103:BCL:C1D	2.84	0.55
1:A:26:HIS:NE2	7:A:101:BCL:NC	2.54	0.55
3:C:388:PRO:O	3:C:391:SER:OG	2.22	0.55
10:C:505:PGV:C15	4:L:211:PRO:HA	2.36	0.55
3:C:297:CYS:SG	9:C:503:HEM:CBC	2.94	0.55
9:C:503:HEM:HMA1	5:M:181:VAL:HG11	1.88	0.55
7:H:101:BCL:HED1	2:I:34:PHE:HD2	1.72	0.55
6:N:60:ILE:HG12	6:N:60:ILE:O	2.05	0.55
2:K:51:TRP:CD1	2:K:52:LEU:HD12	2.42	0.55
4:L:190:ILE:O	4:L:193:HIS:ND1	2.38	0.55
1:A:25:ILE:CG2	7:A:103:BCL:C2D	2.85	0.55
7:A:101:BCL:HED1	2:B:34:PHE:CE1	2.42	0.55
9:C:503:HEM:CMA	5:M:181:VAL:HG13	2.37	0.55
3:C:341:TRP:CZ2	9:C:502:HEM:HMD3	2.42	0.55
7:D:103:BCL:O1A	7:D:103:BCL:H3A	2.07	0.55
5:M:190:PRO:HG3	5:M:288:TRP:CH2	2.42	0.55
1:A:14:PHE:CD2	7:A:104:BCL:HBC2	2.41	0.55
3:C:120:GLN:HA	9:C:501:HEM:CBB	2.37	0.55
4:L:26:ARG:HB3	5:M:230:ALA:HB1	1.89	0.55
7:O:103:BCL:HMA3	2:P:24:HIS:CE1	2.41	0.55
8:D:104:U4Z:CAF	8:D:104:U4Z:CAI	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:25:ILE:HG21	7:P:102:BCL:C1D	2.37	0.55
2:B:29:LYS:O	2:B:31:PHE:N	2.39	0.54
3:C:326:LYS:HD2	9:C:504:HEM:CAA	2.37	0.54
1:H:29:VAL:HG11	7:H:101:BCL:HBC1	1.89	0.54
8:I:101:U4Z:CAZ	8:I:101:U4Z:CAX	2.84	0.54
1:J:11:ILE:HD13	2:K:27:VAL:HG21	1.89	0.54
2:P:34:PHE:CD2	7:P:102:BCL:H11	2.42	0.54
1:D:14:PHE:CE1	8:D:102:U4Z:CBO	2.91	0.54
1:D:14:PHE:CD1	7:E:101:BCL:CBC	2.67	0.54
8:D:102:U4Z:CAF	8:D:102:U4Z:CAI	2.84	0.54
10:C:505:PGV:C04	10:C:505:PGV:C03	2.85	0.54
7:O:101:BCL:HED2	2:P:37:ILE:HG22	1.90	0.54
2:B:26:ILE:HD13	2:E:12:TRP:HH2	1.71	0.54
3:C:299:ASN:HB2	3:C:320:TYR:HE2	1.72	0.54
3:C:330:MET:HE1	9:C:504:HEM:C1D	2.41	0.54
7:L:402:BCL:HAA1	7:M:402:BCL:HBC1	1.89	0.54
7:D:101:BCL:CMB	1:F:25:ILE:HD13	2.37	0.54
4:L:268:ARG:O	4:L:272:ILE:HG13	2.07	0.54
12:M:401:BPH:CBB	12:M:401:BPH:CMB	2.84	0.54
8:A:102:U4Z:CAX	8:A:102:U4Z:CAZ	2.85	0.54
2:P:22:LEU:C	2:P:24:HIS:N	2.65	0.54
12:L:403:BPH:CMB	12:L:403:BPH:CBB	2.85	0.54
2:B:19:GLN:HA	2:B:22:LEU:HD12	1.88	0.54
1:O:14:PHE:CZ	8:O:102:U4Z:CAV	2.91	0.53
3:C:177:VAL:HG21	9:C:504:HEM:CBC	2.38	0.53
8:D:104:U4Z:CAF	2:G:23:LEU:HD12	2.37	0.53
1:F:22:ALA:CB	7:F:101:BCL:O1D	2.56	0.53
9:C:503:HEM:CMA	5:M:181:VAL:HG11	2.38	0.53
7:D:101:BCL:HBB3	1:F:25:ILE:HG23	1.90	0.53
7:G:103:BCL:CBB	7:G:103:BCL:CMB	2.85	0.53
3:C:177:VAL:CG2	9:C:504:HEM:HBC1	2.38	0.53
7:G:103:BCL:HAA1	7:G:103:BCL:CED	2.36	0.53
1:H:17:LEU:O	1:H:21:VAL:HG23	2.08	0.53
1:O:7:VAL:HG13	7:O:103:BCL:CMB	2.30	0.53
2:P:38:ALA:CB	7:P:102:BCL:C2	2.87	0.53
4:L:258:TYR:CE1	5:M:39:GLY:O	2.61	0.53
2:P:5:ASP:OD1	2:P:13:ARG:HG2	2.09	0.53
10:C:505:PGV:H102	5:M:81:VAL:HG11	1.90	0.53
1:Q:12:VAL:O	1:Q:16:ILE:HG13	2.08	0.53
3:C:108:ILE:O	3:C:410:GLN:NE2	2.39	0.53
12:L:403:BPH:C12	12:L:403:BPH:C9	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:175:ARG:NH1	4:L:184:GLU:OE1	2.39	0.52
1:A:28:ILE:HG23	3:C:39:LEU:HD12	1.90	0.52
12:L:403:BPH:H162	12:L:403:BPH:HMB2	1.91	0.52
5:M:252:ALA:O	5:M:256:HIS:ND1	2.39	0.52
1:O:7:VAL:CG1	7:O:103:BCL:HMB3	2.36	0.52
3:C:182:CYS:CB	3:C:380:THR:HG22	2.38	0.52
2:K:8:VAL:HG21	2:K:16:PHE:CE1	2.44	0.52
2:I:5:ASP:HB3	2:I:17:ASN:HA	1.91	0.52
5:M:60:ILE:O	5:M:64:VAL:HG23	2.10	0.52
7:M:402:BCL:HBB2	7:M:402:BCL:CMB	2.40	0.52
1:O:11:ILE:CG1	7:O:103:BCL:HMC2	2.36	0.52
1:Q:14:PHE:CE2	8:Q:102:U4Z:CAV	2.92	0.52
4:L:98:GLN:HE21	5:M:293:GLY:HA3	1.74	0.52
2:P:52:LEU:CD2	8:P:101:U4Z:CBE	2.87	0.52
1:J:9:THR:HG22	1:J:9:THR:O	2.10	0.52
1:A:15:THR:CG2	8:A:102:U4Z:CAP	2.67	0.52
9:C:503:HEM:HMA3	5:M:181:VAL:HG13	1.92	0.52
2:K:5:ASP:OD1	2:K:13:ARG:NE	2.43	0.52
4:L:46:THR:OG1	4:L:150:LYS:NZ	2.43	0.52
4:L:233:LEU:HD22	4:L:253:PHE:CD2	2.45	0.52
12:M:401:BPH:CMB	12:M:401:BPH:HBB2	2.40	0.52
2:R:24:HIS:CE1	7:R:103:BCL:C4D	2.92	0.52
2:G:34:PHE:CE1	7:G:102:BCL:CED	2.93	0.52
1:O:29:VAL:HG11	7:O:101:BCL:CBC	2.40	0.52
2:I:5:ASP:OD1	2:I:5:ASP:N	2.41	0.51
2:I:41:ALA:O	2:I:45:VAL:HG23	2.11	0.51
7:A:101:BCL:O2D	2:B:34:PHE:HE1	1.93	0.51
4:L:95:SER:O	4:L:99:ASN:N	2.43	0.51
5:M:14:GLY:HA3	5:M:18:GLY:HA2	1.90	0.51
2:I:16:PHE:HE2	7:I:104:BCL:HMA1	1.75	0.51
2:P:38:ALA:HB2	7:P:102:BCL:C2	2.39	0.51
3:C:169:LEU:HD11	3:C:330:MET:HE3	1.93	0.51
2:K:8:VAL:CG2	2:K:16:PHE:HE1	2.24	0.51
1:A:37:TRP:CZ3	7:A:101:BCL:HBC3	2.46	0.51
8:A:102:U4Z:CAU	2:B:34:PHE:CD2	2.94	0.51
5:M:120:TYR:CE1	5:M:137:ALA:HB1	2.46	0.51
1:O:17:LEU:CD1	1:O:17:LEU:N	2.72	0.51
5:M:41:PHE:HE2	5:M:43:LEU:HG	1.75	0.51
5:M:72:ASN:HB3	5:M:75:ALA:HB3	1.93	0.51
1:D:26:HIS:CE1	7:D:103:BCL:CMD	2.92	0.51
4:L:59:PHE:CD1	4:L:59:PHE:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:227:LEU:HG	5:M:259:ALA:HB1	1.91	0.51
3:C:169:LEU:HD12	9:C:504:HEM:O2D	2.11	0.51
1:H:26:HIS:HE1	7:H:101:BCL:NC	2.09	0.51
12:M:401:BPH:HMB1	12:M:401:BPH:HBB2	1.93	0.51
3:C:182:CYS:SG	3:C:381:CYS:N	2.85	0.50
2:I:28:VAL:O	2:I:32:TYR:CD2	2.64	0.50
8:A:102:U4Z:CAE	7:E:101:BCL:HBB2	2.41	0.50
2:P:53:PRO:OXT	8:P:101:U4Z:CAT	2.60	0.50
1:Q:14:PHE:CD1	7:R:103:BCL:CBC	2.94	0.50
4:L:211:PRO:HG3	4:L:299:TRP:CZ2	2.47	0.50
4:L:253:PHE:HD1	4:L:257:GLN:HB3	1.76	0.50
12:M:401:BPH:CBC	12:M:401:BPH:CHD	2.85	0.50
3:C:115:ILE:HG21	9:C:501:HEM:HAA1	1.91	0.50
3:C:129:VAL:HG21	3:C:133:TYR:HD2	1.76	0.50
5:M:154:ARG:HB3	5:M:155:PRO:HD3	1.94	0.50
7:Q:101:BCL:HED2	2:R:37:ILE:HG21	1.93	0.50
4:L:227:LEU:HD13	5:M:206:LEU:HB2	1.93	0.50
2:G:26:ILE:HD11	2:I:12:TRP:CH2	2.47	0.50
4:L:210:ASN:ND2	4:L:295:TRP:CZ2	2.80	0.50
2:K:8:VAL:HG22	2:K:9:PRO:CD	2.37	0.50
1:Q:14:PHE:CG	7:R:103:BCL:HBC2	2.46	0.50
3:C:298:HIS:CE1	9:C:503:HEM:C1D	3.00	0.49
2:B:15:LEU:C	2:B:15:LEU:CD2	2.84	0.49
7:F:101:BCL:HBD	7:G:102:BCL:OBD	2.12	0.49
7:G:102:BCL:C1A	8:I:102:U4Z:CBO	2.91	0.49
5:M:38:LEU:N	5:M:38:LEU:CD1	2.74	0.49
8:D:104:U4Z:CAS	8:D:104:U4Z:CBC	2.86	0.49
1:H:29:VAL:HG12	1:H:37:TRP:HZ3	1.77	0.49
7:A:103:BCL:CMC	3:C:38:THR:OG1	2.60	0.49
7:A:103:BCL:HMC1	3:C:38:THR:OG1	2.12	0.49
3:C:299:ASN:HB2	3:C:320:TYR:CE2	2.47	0.49
2:I:34:PHE:CE1	8:I:101:U4Z:CBG	2.95	0.49
1:Q:40:ASN:OD1	1:Q:40:ASN:N	2.46	0.49
2:G:7:LEU:O	2:G:7:LEU:HD13	2.11	0.49
2:I:16:PHE:HB3	2:I:21:TRP:HB2	1.94	0.49
12:L:403:BPH:H203	5:M:172:LEU:HD11	1.93	0.49
5:M:207:ALA:CB	12:M:401:BPH:HBC3	2.42	0.49
1:O:7:VAL:O	7:O:103:BCL:OBB	2.29	0.49
1:D:26:HIS:HB3	8:D:104:U4Z:CAX	2.43	0.49
2:I:24:HIS:HE1	7:I:104:BCL:O1D	1.96	0.49
2:R:52:LEU:HD11	8:R:101:U4Z:CBE	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:VAL:CG1	9:C:501:HEM:HBC2	2.43	0.49
12:M:401:BPH:HAA1	12:M:401:BPH:CBD	2.41	0.49
1:O:10:ASN:HB2	7:O:103:BCL:CBB	2.42	0.49
1:J:26:HIS:CE1	7:J:101:BCL:HMD3	2.48	0.49
5:M:10:ASP:N	5:M:10:ASP:OD1	2.45	0.49
12:M:406:BPH:ND	12:M:406:BPH:NC	2.60	0.49
7:K:102:BCL:CHC	7:P:102:BCL:HBB3	2.43	0.48
8:B:101:U4Z:CAK	8:B:101:U4Z:CAL	2.90	0.48
5:M:19:ARG:HB3	5:M:40:PRO:HB2	1.95	0.48
5:M:270:GLY:HA2	7:M:405:BCL:HED2	1.94	0.48
3:C:134:CYS:SG	3:C:147:GLN:HB3	2.53	0.48
7:G:103:BCL:HHC	7:G:103:BCL:OBB	2.14	0.48
2:K:24:HIS:CE1	7:K:104:BCL:CHA	2.97	0.48
5:M:41:PHE:CE2	5:M:43:LEU:HG	2.47	0.48
3:C:314:ASN:HA	4:L:183:HIS:NE2	2.29	0.48
4:L:94:TYR:O	4:L:99:ASN:ND2	2.46	0.48
2:P:53:PRO:C	8:P:101:U4Z:CAT	2.87	0.48
8:D:102:U4Z:CBG	8:D:102:U4Z:CAU	2.90	0.48
1:F:22:ALA:O	1:F:26:HIS:CD2	2.65	0.48
2:I:34:PHE:HE1	8:I:101:U4Z:CBG	2.26	0.48
5:M:196:ILE:HG21	7:M:402:BCL:C3D	2.44	0.48
7:M:402:BCL:HMB3	7:M:402:BCL:CBB	2.42	0.48
8:O:102:U4Z:CAL	8:O:102:U4Z:CAK	2.91	0.48
1:D:21:VAL:HG13	7:D:103:BCL:HED3	1.92	0.48
4:L:141:MET:HE1	4:L:162:GLY:HA2	1.95	0.48
7:A:104:BCL:HED2	2:B:28:VAL:HG21	1.96	0.48
8:K:101:U4Z:CAK	8:K:101:U4Z:CAL	2.90	0.48
4:L:268:ARG:NH2	5:M:217:GLU:OE1	2.42	0.48
1:D:21:VAL:CG1	7:D:103:BCL:HED1	2.40	0.48
1:H:14:PHE:CG	7:I:104:BCL:CBC	2.73	0.48
1:J:11:ILE:HA	7:K:104:BCL:HMC1	1.95	0.48
4:L:208:PHE:CZ	7:L:402:BCL:HBB3	2.45	0.48
2:P:8:VAL:HG13	2:P:21:TRP:CD2	2.48	0.48
2:P:8:VAL:CB	2:P:9:PRO:HD2	2.43	0.48
7:A:104:BCL:HMA1	2:B:16:PHE:CE1	2.48	0.47
3:C:155:LEU:HD23	9:C:502:HEM:CBB	2.43	0.47
2:I:26:ILE:HD12	7:K:104:BCL:O1A	2.14	0.47
3:C:251:PHE:HZ	5:M:302:PRO:HD2	1.79	0.47
8:I:101:U4Z:CAG	7:K:104:BCL:HBC2	2.44	0.47
7:A:101:BCL:HED1	2:B:34:PHE:CD1	2.49	0.47
4:L:261:VAL:HG23	5:M:34:PHE:HD1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:305:LEU:HD23	4:L:306:PRO:HD2	1.96	0.47
7:O:103:BCL:CMC	2:P:27:VAL:HG11	2.41	0.47
2:P:8:VAL:HG13	2:P:21:TRP:CB	2.44	0.47
4:L:221:PHE:HB3	12:M:406:BPH:HBB2	1.95	0.47
3:C:179:CYS:HB3	9:C:502:HEM:C3B	2.48	0.47
3:C:279:ASN:O	3:C:283:MET:HE2	2.13	0.47
5:M:224:GLU:O	5:M:228:ILE:HG13	2.14	0.47
7:M:405:BCL:HBB3	7:M:405:BCL:CMB	2.44	0.47
3:C:341:TRP:HZ2	9:C:502:HEM:C2D	2.33	0.47
4:L:61:VAL:HG12	4:L:61:VAL:O	2.13	0.47
5:M:64:VAL:O	5:M:68:GLN:HG3	2.15	0.47
7:Q:101:BCL:OBD	7:R:102:BCL:CBD	2.53	0.47
1:A:26:HIS:CE1	7:A:101:BCL:ND	2.83	0.47
2:B:11:LYS:HD3	2:B:12:TRP:CD1	2.50	0.47
2:B:12:TRP:CD1	2:B:12:TRP:N	2.73	0.47
3:C:283:MET:HG3	9:C:503:HEM:NC	2.30	0.47
7:D:103:BCL:O2D	7:D:103:BCL:H2A	2.14	0.47
1:F:3:PRO:HA	2:G:15:LEU:C	2.39	0.47
1:J:6:PRO:HG3	2:K:16:PHE:HA	1.97	0.47
5:M:147:TYR:HB2	7:M:405:BCL:H62	1.96	0.47
12:M:406:BPH:CBB	12:M:406:BPH:CHC	2.86	0.47
7:L:402:BCL:HAC2	5:M:187:TYR:OH	2.14	0.47
1:D:6:PRO:HB2	1:D:9:THR:HG22	1.95	0.47
5:M:149:VAL:HA	5:M:153:ILE:HB	1.96	0.47
4:L:60:TRP:HA	4:L:64:PHE:O	2.14	0.47
3:C:280:GLN:OE1	5:M:177:ASN:ND2	2.48	0.46
10:C:505:PGV:H151	4:L:214:ALA:HB3	1.97	0.46
2:I:52:LEU:HD23	8:I:102:U4Z:CBA	2.45	0.46
7:M:405:BCL:H11	12:M:406:BPH:CBB	2.46	0.46
1:Q:7:VAL:HG22	7:R:103:BCL:OBB	2.14	0.46
2:B:19:GLN:CA	2:B:22:LEU:HD12	2.45	0.46
2:I:34:PHE:CG	2:I:34:PHE:O	2.69	0.46
8:I:102:U4Z:CAN	8:I:102:U4Z:CAQ	2.90	0.46
5:M:242:TRP:CE3	5:M:246:MET:HE2	2.49	0.46
1:Q:29:VAL:CG1	7:Q:101:BCL:HBC1	2.45	0.46
1:A:29:VAL:CG1	7:A:101:BCL:CBC	2.82	0.46
3:C:64:THR:HG22	3:C:81:THR:HA	1.98	0.46
3:C:120:GLN:CA	9:C:501:HEM:HBB2	2.45	0.46
8:Q:102:U4Z:CAK	8:Q:102:U4Z:CAL	2.91	0.46
2:R:45:VAL:HG11	7:R:102:BCL:CBC	2.36	0.46
1:O:14:PHE:CD1	1:O:14:PHE:C	2.90	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ILE:HG21	9:C:501:HEM:HMA2	1.98	0.46
4:L:258:TYR:CG	4:L:258:TYR:O	2.68	0.46
7:M:402:BCL:H141	7:M:402:BCL:H161	1.48	0.46
1:A:7:VAL:HG23	7:A:104:BCL:C4B	2.45	0.46
3:C:78:TRP:CD1	3:C:79:MET:HG2	2.51	0.46
3:C:182:CYS:HB3	3:C:380:THR:CG2	2.42	0.46
5:M:274:VAL:CG2	7:M:405:BCL:OBD	2.64	0.46
2:P:6:ASP:OD1	2:P:7:LEU:N	2.49	0.46
2:R:13:ARG:HG2	2:R:13:ARG:HH11	1.80	0.46
7:G:103:BCL:HBC2	7:G:103:BCL:H2C	1.52	0.46
1:H:7:VAL:HB	7:I:104:BCL:OBB	2.15	0.46
4:L:48:PHE:CD2	4:L:55:ASP:HB3	2.50	0.46
2:P:19:GLN:HG3	2:R:15:LEU:HG	1.97	0.46
2:K:48:TRP:CE2	2:K:49:LYS:HE3	2.51	0.46
4:L:66:VAL:O	4:L:70:GLY:HA3	2.16	0.46
4:L:157:VAL:HB	4:L:158:PRO:HD3	1.98	0.46
4:L:208:PHE:HB3	5:M:173:LEU:HD23	1.97	0.46
2:E:12:TRP:CZ2	7:E:101:BCL:H3A	2.52	0.45
2:E:46:TYR:OH	2:E:52:LEU:O	2.31	0.45
7:M:402:BCL:H91	7:M:402:BCL:H111	1.58	0.45
1:A:14:PHE:CD1	7:A:104:BCL:CBC	2.98	0.45
3:C:330:MET:SD	9:C:504:HEM:ND	2.88	0.45
3:C:378:CYS:SG	9:C:504:HEM:HBB1	2.53	0.45
2:E:4:ASP:C	2:E:6:ASP:H	2.24	0.45
2:K:7:LEU:HD23	2:K:7:LEU:C	2.41	0.45
2:P:9:PRO:HG3	2:P:12:TRP:HB2	1.99	0.45
1:J:10:ASN:HB2	7:K:104:BCL:HHC	1.99	0.45
2:I:34:PHE:CD1	2:I:34:PHE:O	2.70	0.45
8:K:103:U4Z:CAK	8:K:103:U4Z:CAL	2.91	0.45
12:M:401:BPH:HBC3	12:M:401:BPH:CHD	2.21	0.45
1:O:35:TYR:HE1	2:P:49:LYS:HD2	1.80	0.45
2:P:8:VAL:HG13	2:P:21:TRP:HB2	1.98	0.45
1:A:15:THR:HG21	8:A:102:U4Z:CAM	2.37	0.45
3:C:115:ILE:HG22	9:C:501:HEM:CMA	2.47	0.45
1:F:23:LEU:HD22	1:F:27:PHE:CE2	2.52	0.45
1:A:26:HIS:NE2	7:A:101:BCL:ND	2.64	0.45
3:C:299:ASN:N	3:C:320:TYR:HE2	2.15	0.45
2:I:24:HIS:NE2	7:I:104:BCL:ND	2.65	0.45
5:M:204:LEU:HD13	12:M:401:BPH:ND	2.31	0.45
7:Q:101:BCL:CAD	7:R:102:BCL:HBD	2.46	0.45
1:F:23:LEU:HD22	1:F:27:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:402:BCL:H122	12:M:401:BPH:HBA1	1.99	0.45
7:M:405:BCL:CMB	7:M:405:BCL:CBB	2.94	0.45
1:O:38:LEU:HB3	1:Q:32:SER:HB2	1.97	0.45
3:C:115:ILE:CG2	9:C:501:HEM:HMA2	2.46	0.45
4:L:159:ILE:O	4:L:163:VAL:HG23	2.16	0.45
4:L:209:TYR:HD2	4:L:296:VAL:HG22	1.82	0.45
7:M:405:BCL:HMB1	7:M:405:BCL:CBB	2.44	0.45
1:O:7:VAL:HG12	7:O:103:BCL:HMB3	1.98	0.45
8:P:101:U4Z:CAK	8:P:101:U4Z:CAL	2.95	0.45
7:A:101:BCL:CED	2:B:34:PHE:HE1	2.30	0.45
2:B:21:TRP:CE3	2:B:21:TRP:O	2.70	0.45
1:J:11:ILE:CD1	2:K:23:LEU:HD12	2.47	0.45
4:L:86:ASN:O	4:L:90:LEU:HB2	2.17	0.45
4:L:208:PHE:HZ	7:L:402:BCL:HBB3	1.73	0.45
5:M:192:HIS:NE2	7:M:405:BCL:NC	2.65	0.45
12:M:401:BPH:H2	12:M:401:BPH:H6C2	1.61	0.45
1:O:10:ASN:OD1	7:O:103:BCL:HBB1	2.17	0.45
3:C:10:GLN:O	3:C:13:ILE:HG22	2.17	0.45
3:C:282:VAL:O	3:C:286:GLN:HG3	2.17	0.45
1:D:8:ARG:NH2	1:F:5:SER:OG	2.50	0.45
7:D:103:BCL:CMB	7:D:103:BCL:CBB	2.95	0.45
4:L:23:ARG:HH21	5:M:223:GLU:CD	2.24	0.45
1:J:7:VAL:O	7:K:104:BCL:OBB	2.35	0.44
7:L:402:BCL:H142	7:M:402:BCL:HMB3	1.98	0.44
3:C:78:TRP:HB3	3:C:132:GLN:HB2	1.98	0.44
3:C:235:LYS:NZ	10:C:505:PGV:O13	2.49	0.44
7:D:101:BCL:HMB2	1:F:25:ILE:HD13	1.98	0.44
1:F:34:GLU:OE2	2:G:49:LYS:HD3	2.17	0.44
1:J:11:ILE:HA	7:K:104:BCL:CMC	2.46	0.44
4:L:40:TYR:HD2	5:M:240:LEU:HD12	1.83	0.44
4:L:246:GLY:O	4:L:249:GLU:CG	2.63	0.44
9:C:504:HEM:CBC	9:C:504:HEM:CHD	2.95	0.44
8:D:104:U4Z:CBO	1:F:17:LEU:CD2	2.95	0.44
2:I:34:PHE:CG	8:I:101:U4Z:CAU	3.01	0.44
4:L:92:GLY:HA3	4:L:99:ASN:OD1	2.17	0.44
5:M:17:ARG:HG3	5:M:17:ARG:HH11	1.82	0.44
2:P:22:LEU:C	2:P:24:HIS:H	2.25	0.44
2:B:45:VAL:HG23	8:B:101:U4Z:CBK	2.48	0.44
7:M:402:BCL:H112	7:M:402:BCL:H142	1.68	0.44
2:P:33:GLY:O	2:P:36:VAL:HG12	2.17	0.44
1:A:5:SER:HB3	1:A:6:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:505:PGV:O03	10:C:505:PGV:C1	2.66	0.44
3:C:201:VAL:HG11	3:C:235:LYS:HG3	2.00	0.44
2:K:52:LEU:HD22	8:K:101:U4Z:CAZ	2.48	0.44
4:L:64:PHE:CE2	5:M:246:MET:C	2.96	0.44
2:B:17:ASN:ND2	2:B:19:GLN:HB3	2.32	0.44
3:C:23:VAL:HA	3:C:26:ILE:HG22	1.99	0.44
3:C:330:MET:HA	3:C:333:LEU:HB3	1.99	0.44
10:C:505:PGV:H252	10:C:505:PGV:H101	2.00	0.44
2:G:6:ASP:OD1	2:G:6:ASP:N	2.51	0.44
7:L:402:BCL:HAA1	7:M:402:BCL:CBC	2.48	0.44
2:R:34:PHE:CE2	7:R:102:BCL:O2A	2.68	0.44
2:I:35:GLY:O	2:I:38:ALA:N	2.49	0.44
2:K:52:LEU:HB3	8:K:101:U4Z:CAZ	2.48	0.44
4:L:54:TYR:CG	4:L:54:TYR:O	2.70	0.43
10:C:505:PGV:H131	10:C:505:PGV:H162	1.75	0.43
5:M:61:TRP:NE1	5:M:167:HIS:O	2.52	0.43
6:N:30:LEU:HD23	6:N:30:LEU:HA	1.87	0.43
3:C:312:GLY:O	3:C:316:LEU:HB2	2.18	0.43
4:L:32:THR:HG22	6:N:45:ALA:O	2.18	0.43
4:L:287:LEU:O	4:L:291:PRO:HD2	2.19	0.43
5:M:227:GLU:HA	5:M:230:ALA:O	2.18	0.43
3:C:196:GLN:O	3:C:200:SER:HB2	2.19	0.43
1:F:26:HIS:CG	7:F:101:BCL:HMD2	2.53	0.43
1:J:29:VAL:HG11	7:K:102:BCL:HBC1	1.98	0.43
4:L:110:PRO:HD3	4:L:183:HIS:CE1	2.54	0.43
12:L:403:BPH:H201	5:M:172:LEU:HD21	2.01	0.43
5:M:158:MET:HE1	5:M:163:GLU:OE2	2.19	0.43
5:M:278:MET:HE3	5:M:281:PHE:CE2	2.53	0.43
10:C:505:PGV:O02	10:C:505:PGV:C19	2.66	0.43
2:G:23:LEU:HD21	2:I:15:LEU:HD21	2.01	0.43
4:L:73:SER:HA	4:L:136:ALA:HA	2.00	0.43
5:M:227:GLU:OE1	5:M:235:THR:OG1	2.27	0.43
3:C:298:HIS:CE1	9:C:503:HEM:ND	2.80	0.43
4:L:32:THR:OG1	4:L:35:GLU:OE1	2.35	0.43
4:L:278:ILE:HG13	7:L:402:BCL:O1A	2.18	0.43
4:L:18:VAL:HA	5:M:218:LYS:O	2.18	0.43
12:L:403:BPH:H9C1	12:L:403:BPH:H122	2.00	0.43
5:M:11:LEU:HD23	5:M:11:LEU:HA	1.87	0.43
5:M:270:GLY:HA2	7:M:405:BCL:HED3	1.99	0.43
1:O:7:VAL:HA	7:O:103:BCL:CAB	2.45	0.43
2:G:13:ARG:HD3	2:G:13:ARG:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:TRP:CZ3	7:H:101:BCL:HBC3	2.54	0.43
2:K:23:LEU:O	2:K:27:VAL:HG23	2.19	0.43
2:K:34:PHE:CZ	7:K:102:BCL:HBA2	2.54	0.43
4:L:7:LYS:HB2	4:L:7:LYS:HE2	1.74	0.43
4:L:130:VAL:HG23	4:L:168:TRP:CZ2	2.54	0.43
4:L:239:GLN:NE2	6:N:60:ILE:HA	2.33	0.43
5:M:11:LEU:O	5:M:12:GLU:HG2	2.19	0.43
3:C:55:SER:OG	3:C:57:SER:OG	2.31	0.43
8:D:102:U4Z:CAF	2:E:26:ILE:HD11	2.49	0.43
7:K:102:BCL:NC	7:P:102:BCL:HBB3	2.33	0.43
3:C:215:GLY:O	3:C:267:TYR:OH	2.25	0.43
1:D:12:VAL:O	1:D:16:ILE:HG13	2.18	0.43
2:K:48:TRP:NE1	2:P:53:PRO:HG2	2.34	0.43
4:L:45:ARG:C	4:L:149:MET:HE3	2.44	0.43
3:C:298:HIS:HD2	9:C:503:HEM:NB	2.16	0.42
10:C:505:PGV:H042	4:L:303:ASN:OD1	2.19	0.42
5:M:196:ILE:CD1	7:M:402:BCL:HMD1	2.49	0.42
1:A:26:HIS:CE1	7:A:101:BCL:C4D	3.01	0.42
2:B:32:TYR:O	2:B:36:VAL:HG23	2.19	0.42
1:F:5:SER:OG	1:F:6:PRO:HD3	2.19	0.42
2:K:52:LEU:CD2	8:K:101:U4Z:CAZ	2.97	0.42
2:P:9:PRO:HG3	2:P:12:TRP:HD1	1.84	0.42
1:A:26:HIS:HE1	7:A:101:BCL:C4D	2.32	0.42
2:G:16:PHE:CE2	7:G:103:BCL:CMA	2.95	0.42
2:I:31:PHE:HE2	8:I:102:U4Z:CAL	2.33	0.42
1:J:37:TRP:CZ3	7:K:102:BCL:HBC3	2.54	0.42
2:K:16:PHE:CZ	7:K:104:BCL:HMA1	2.54	0.42
12:L:403:BPH:CHD	12:L:403:BPH:HBC2	2.48	0.42
7:P:102:BCL:CMB	7:P:102:BCL:CBB	2.98	0.42
2:R:52:LEU:HB3	2:R:53:PRO:HD2	2.00	0.42
1:F:35:TYR:OH	2:G:51:TRP:HB3	2.20	0.42
3:C:123:VAL:HG12	9:C:501:HEM:HBC2	2.01	0.42
3:C:304:VAL:HG22	9:C:503:HEM:O2A	2.19	0.42
8:I:101:U4Z:CAI	1:J:10:ASN:OD1	2.67	0.42
8:O:102:U4Z:CAC	7:R:103:BCL:C4B	2.97	0.42
1:A:25:ILE:HG21	7:A:103:BCL:C1D	2.49	0.42
10:C:505:PGV:H21	10:C:505:PGV:H51	1.31	0.42
8:D:104:U4Z:CAE	1:H:10:ASN:HD21	2.33	0.42
1:F:26:HIS:NE2	7:F:101:BCL:OBD	2.53	0.42
2:K:28:VAL:CG2	7:K:104:BCL:OBD	2.68	0.42
1:A:11:ILE:HD11	2:B:24:HIS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:ARG:HH12	3:C:147:GLN:NE2	2.17	0.42
10:C:505:PGV:H201	5:M:82:VAL:CG1	2.44	0.42
1:D:25:ILE:HG21	7:D:103:BCL:C1D	2.50	0.42
7:L:402:BCL:HMB1	7:L:402:BCL:OBB	2.20	0.42
2:P:47:LEU:HD23	2:P:47:LEU:HA	1.80	0.42
1:Q:25:ILE:HG21	7:R:102:BCL:C1D	2.49	0.42
2:R:32:TYR:O	2:R:36:VAL:HG23	2.20	0.42
7:A:101:BCL:CED	2:B:34:PHE:CE1	3.03	0.42
3:C:359:ALA:O	3:C:363:SER:OG	2.36	0.42
2:K:43:LEU:HD23	2:K:43:LEU:HA	1.86	0.42
5:M:249:ASN:ND2	6:N:44:TYR:OH	2.52	0.42
12:M:401:BPH:H111	12:M:401:BPH:H143	1.44	0.42
1:O:24:LEU:HD22	8:O:102:U4Z:CBD	2.50	0.42
1:A:29:VAL:HG21	7:A:103:BCL:CHD	2.36	0.42
2:B:29:LYS:C	2:B:31:PHE:N	2.77	0.42
4:L:209:TYR:CD2	4:L:296:VAL:HG22	2.55	0.42
2:E:52:LEU:HD23	2:E:52:LEU:HA	1.87	0.41
2:I:40:ILE:O	2:I:44:LEU:HG	2.20	0.41
1:J:29:VAL:HG12	1:J:37:TRP:HZ3	1.85	0.41
7:O:103:BCL:C4D	2:P:28:VAL:CG1	2.96	0.41
7:Q:101:BCL:CAD	7:R:102:BCL:CAD	2.98	0.41
3:C:374:ASN:O	9:C:502:HEM:HMD2	2.20	0.41
8:D:104:U4Z:CAE	1:H:10:ASN:ND2	2.83	0.41
4:L:98:GLN:NE2	5:M:292:ALA:O	2.53	0.41
4:L:108:PRO:HB3	4:L:112:LEU:HD23	2.02	0.41
12:M:401:BPH:H102	12:M:401:BPH:H6C1	1.60	0.41
1:O:29:VAL:HG21	7:P:102:BCL:HHD	2.02	0.41
2:E:28:VAL:HG22	7:E:101:BCL:C2D	2.51	0.41
7:H:101:BCL:O2D	2:I:34:PHE:HE2	2.03	0.41
8:I:102:U4Z:CAC	7:I:104:BCL:C3D	2.98	0.41
4:L:7:LYS:HG2	5:M:31:ASN:OD1	2.20	0.41
4:L:46:THR:HG23	4:L:146:ASP:OD2	2.20	0.41
5:M:216:LEU:CD1	5:M:238:ALA:HB2	2.50	0.41
7:O:103:BCL:C4D	8:P:101:U4Z:CAC	2.98	0.41
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.86	0.41
2:I:34:PHE:CB	8:I:101:U4Z:CAU	2.98	0.41
7:M:402:BCL:HHC	7:M:402:BCL:OBB	2.21	0.41
1:O:16:ILE:H	1:O:16:ILE:HG13	1.71	0.41
2:R:24:HIS:CE1	7:R:103:BCL:ND	2.88	0.41
3:C:111:SER:HB3	3:C:114:GLN:OE1	2.18	0.41
4:L:20:GLU:OE1	4:L:20:GLU:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:210:ASN:ND2	4:L:295:TRP:CE2	2.87	0.41
2:R:7:LEU:HD12	2:R:21:TRP:HZ3	1.86	0.41
3:C:381:CYS:O	3:C:388:PRO:HB3	2.20	0.41
1:J:24:LEU:HA	5:M:59:PHE:HZ	1.86	0.41
4:L:210:ASN:OD1	4:L:284:CYS:HB2	2.21	0.41
5:M:45:PHE:O	5:M:49:VAL:HG23	2.20	0.41
1:O:26:HIS:CE1	7:P:102:BCL:HMD3	2.55	0.41
2:B:46:TYR:HE1	2:B:51:TRP:HB3	1.86	0.41
3:C:238:ILE:O	3:C:242:ILE:HG13	2.20	0.41
10:C:505:PGV:O02	10:C:505:PGV:C01	2.67	0.41
1:H:14:PHE:CE1	7:I:104:BCL:HBC1	2.54	0.41
1:H:31:SER:HB2	5:M:71:TYR:O	2.21	0.41
2:I:52:LEU:HA	2:I:53:PRO:HD3	1.90	0.41
4:L:33:ILE:HD13	6:N:44:TYR:CZ	2.56	0.41
1:Q:14:PHE:CE1	8:Q:102:U4Z:CBG	3.04	0.41
4:L:237:ALA:HB3	4:L:249:GLU:OE1	2.21	0.41
2:P:52:LEU:HD12	2:P:53:PRO:HD2	2.03	0.41
1:D:7:VAL:HG22	7:E:101:BCL:OBB	2.20	0.41
1:H:7:VAL:CG1	2:I:20:ASP:OD2	2.68	0.41
4:L:53:ARG:HB2	4:L:54:TYR:CD1	2.51	0.41
4:L:233:LEU:HD22	4:L:253:PHE:CE2	2.56	0.41
4:L:263:GLU:O	4:L:267:HIS:ND1	2.53	0.41
4:L:275:ILE:HG13	4:L:276:GLY:N	2.35	0.41
4:L:290:TRP:HB3	4:L:291:PRO:CD	2.43	0.41
7:M:405:BCL:H2C	7:M:405:BCL:HBC2	1.64	0.41
2:R:24:HIS:HE1	7:R:103:BCL:C4D	2.32	0.41
2:K:34:PHE:HZ	7:K:102:BCL:CGA	2.33	0.41
2:K:34:PHE:CE1	7:K:102:BCL:HED1	2.55	0.41
4:L:69:TRP:CG	4:L:142:MET:HB2	2.56	0.41
1:O:12:VAL:O	1:O:16:ILE:HG13	2.21	0.41
1:Q:8:ARG:O	1:Q:12:VAL:HG23	2.21	0.41
2:R:28:VAL:HG12	2:R:29:LYS:HD3	2.03	0.41
3:C:374:ASN:O	9:C:502:HEM:CMD	2.69	0.40
8:D:104:U4Z:CAF	2:G:23:LEU:CD1	2.99	0.40
2:K:25:ASP:O	2:K:28:VAL:HG12	2.21	0.40
4:L:170:VAL:HA	4:L:174:ILE:HB	2.01	0.40
4:L:233:LEU:HD23	11:L:401:MQE:CCH	2.51	0.40
4:L:234:ILE:HG21	5:M:256:HIS:CE1	2.56	0.40
2:P:52:LEU:HA	2:P:53:PRO:HD3	1.86	0.40
2:P:53:PRO:O	8:P:101:U4Z:CAT	2.70	0.40
1:Q:26:HIS:CE1	7:R:102:BCL:CMD	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HG23	7:A:104:BCL:CHC	2.50	0.40
1:A:14:PHE:CE1	7:A:104:BCL:CBC	3.03	0.40
1:A:37:TRP:CH2	7:A:101:BCL:H2C	2.56	0.40
3:C:182:CYS:SG	3:C:380:THR:HG22	2.62	0.40
3:C:234:LEU:HD21	3:C:281:ASN:ND2	2.36	0.40
3:C:192:GLY:HA2	3:C:380:THR:OG1	2.21	0.40
8:O:102:U4Z:CBF	7:P:102:BCL:CMA	2.99	0.40
7:A:101:BCL:HBC3	7:A:101:BCL:H2C	1.88	0.40
3:C:228:ILE:HD13	3:C:240:PHE:CZ	2.57	0.40
3:C:248:TRP:NE1	3:C:261:GLY:O	2.51	0.40
2:I:24:HIS:CE1	7:I:104:BCL:CHA	3.04	0.40
12:L:403:BPH:ND	12:L:403:BPH:NC	2.70	0.40
5:M:49:VAL:HG22	1:O:16:ILE:HG21	2.02	0.40
5:M:229:GLN:HA	6:N:58:SER:HB3	2.04	0.40
7:O:101:BCL:HED2	2:P:37:ILE:CG2	2.49	0.40
7:O:103:BCL:C4D	2:P:28:VAL:HG11	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	37/57 (65%)	34 (92%)	2 (5%)	1 (3%)	4 17
1	D	34/57 (60%)	33 (97%)	1 (3%)	0	100 100
1	F	36/57 (63%)	33 (92%)	3 (8%)	0	100 100
1	H	34/57 (60%)	33 (97%)	1 (3%)	0	100 100
1	J	34/57 (60%)	34 (100%)	0	0	100 100
1	O	33/57 (58%)	31 (94%)	2 (6%)	0	100 100
1	Q	34/57 (60%)	31 (91%)	3 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	41/53 (77%)	32 (78%)	6 (15%)	3 (7%)	1 4
2	E	48/53 (91%)	46 (96%)	2 (4%)	0	100 100
2	G	47/53 (89%)	44 (94%)	3 (6%)	0	100 100
2	I	48/53 (91%)	43 (90%)	4 (8%)	1 (2%)	5 21
2	K	48/53 (91%)	41 (85%)	7 (15%)	0	100 100
2	P	48/53 (91%)	42 (88%)	2 (4%)	4 (8%)	0 3
2	R	48/53 (91%)	46 (96%)	2 (4%)	0	100 100
3	C	405/414 (98%)	378 (93%)	27 (7%)	0	100 100
4	L	304/311 (98%)	263 (86%)	37 (12%)	4 (1%)	10 32
5	M	293/307 (95%)	279 (95%)	14 (5%)	0	100 100
6	N	54/64 (84%)	49 (91%)	5 (9%)	0	100 100
All	All	1626/1866 (87%)	1492 (92%)	121 (7%)	13 (1%)	19 43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	SER
2	B	19	GLN
2	B	30	SER
4	L	56	PRO
4	L	57	PHE
2	P	9	PRO
2	P	10	PRO
2	I	36	VAL
4	L	48	PHE
2	P	11	LYS
2	P	13	ARG
2	B	15	LEU
4	L	18	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	36/47 (77%)	35 (97%)	1 (3%)	38 63
1	D	34/47 (72%)	34 (100%)	0	100 100
1	F	36/47 (77%)	34 (94%)	2 (6%)	17 43
1	H	34/47 (72%)	34 (100%)	0	100 100
1	J	34/47 (72%)	34 (100%)	0	100 100
1	O	33/47 (70%)	28 (85%)	5 (15%)	2 8
1	Q	34/47 (72%)	33 (97%)	1 (3%)	37 62
2	B	38/48 (79%)	33 (87%)	5 (13%)	3 12
2	E	45/48 (94%)	45 (100%)	0	100 100
2	G	44/48 (92%)	41 (93%)	3 (7%)	13 36
2	I	45/48 (94%)	44 (98%)	1 (2%)	47 68
2	K	45/48 (94%)	44 (98%)	1 (2%)	47 68
2	P	45/48 (94%)	42 (93%)	3 (7%)	13 37
2	R	45/48 (94%)	45 (100%)	0	100 100
3	C	334/341 (98%)	331 (99%)	3 (1%)	75 86
4	L	249/254 (98%)	247 (99%)	2 (1%)	79 88
5	M	239/249 (96%)	238 (100%)	1 (0%)	89 93
6	N	44/51 (86%)	44 (100%)	0	100 100
All	All	1414/1560 (91%)	1386 (98%)	28 (2%)	50 71

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
2	B	15	LEU
2	B	26	ILE
2	B	27	VAL
2	B	28	VAL
2	B	31	PHE
3	C	37	LEU
3	C	173	GLN
3	C	179	CYS
1	F	23	LEU
1	F	25	ILE
2	G	7	LEU
2	G	8	VAL
2	G	25	ASP

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Mol	Chain	Res	Type
2	I	36	VAL
2	K	8	VAL
4	L	59	PHE
4	L	249	GLU
5	M	30	GLU
1	O	9	THR
1	O	10	ASN
1	O	14	PHE
1	O	16	ILE
1	O	34	GLU
2	P	8	VAL
2	P	23	LEU
2	P	25	ASP
1	Q	32	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	17	ASN
2	B	18	ASN
3	C	85	ASN
3	C	138	ASN
3	C	171	ASN
3	C	173	GLN
3	C	178	GLN
3	C	199	ASN
3	C	317	ASN
1	H	10	ASN
1	H	26	HIS
4	L	205	ASN
2	P	19	GLN
1	Q	10	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 1 is monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	HEM	C	501	3	41,50,50	1.32	4 (9%)	45,82,82	1.95	9 (20%)
7	BCL	D	103	2	45,55,74	1.96	10 (22%)	55,92,115	2.32	17 (30%)
8	U4Z	G	101	-	40,40,40	3.11	17 (42%)	50,51,51	6.45	29 (58%)
7	BCL	D	101	1	46,56,74	2.02	13 (28%)	56,93,115	2.53	23 (41%)
7	BCL	P	102	-	46,56,74	1.90	9 (19%)	56,93,115	2.30	17 (30%)
7	BCL	I	103	2	44,54,74	2.04	13 (29%)	54,91,115	2.53	22 (40%)
8	U4Z	I	102	-	40,40,40	2.62	14 (35%)	50,51,51	6.56	35 (70%)
12	BPH	M	401	-	51,70,70	1.46	9 (17%)	52,101,101	3.63	20 (38%)
7	BCL	G	102	-	46,56,74	2.03	13 (28%)	56,93,115	2.51	23 (41%)
9	HEM	C	503	3	41,50,50	1.40	4 (9%)	45,82,82	2.24	11 (24%)
7	BCL	A	104	2	47,57,74	1.99	12 (25%)	57,94,115	2.32	22 (38%)
7	BCL	M	402	4	64,74,74	2.28	23 (35%)	78,115,115	3.08	32 (41%)
11	MQE	M	403	-	64,64,69	0.21	0	78,81,87	0.38	1 (1%)
7	BCL	A	101	1	51,61,74	1.94	13 (25%)	62,99,115	2.46	23 (37%)
7	BCL	L	402	4	64,74,74	1.65	11 (17%)	78,115,115	2.34	25 (32%)
7	BCL	F	101	2	45,55,74	1.93	11 (24%)	55,92,115	2.97	27 (49%)
7	BCL	O	103	2	45,55,74	2.26	11 (24%)	55,92,115	3.01	17 (30%)
9	HEM	C	502	3	41,50,50	1.30	3 (7%)	45,82,82	1.92	9 (20%)
8	U4Z	D	102	-	40,40,40	2.64	16 (40%)	50,51,51	6.94	33 (66%)
7	BCL	K	102	1	45,55,74	2.04	13 (28%)	55,92,115	2.50	23 (41%)
8	U4Z	P	101	-	40,40,40	0.29	0	50,51,51	0.51	1 (2%)
7	BCL	A	103	-	45,55,74	2.05	12 (26%)	55,92,115	2.52	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	PGV	C	505	-	44,44,50	1.71	12 (27%)	47,50,56	2.72	18 (38%)
8	U4Z	A	102	-	40,40,40	2.59	18 (45%)	50,51,51	7.98	33 (66%)
8	U4Z	Q	102	-	40,40,40	1.16	2 (5%)	50,51,51	1.88	14 (28%)
8	U4Z	B	101	-	40,40,40	0.66	1 (2%)	50,51,51	0.88	2 (4%)
12	BPH	M	406	-	32,51,70	1.18	4 (12%)	29,78,101	1.53	6 (20%)
7	BCL	O	101	1	45,55,74	2.03	13 (28%)	55,92,115	2.53	23 (41%)
7	BCL	G	103	2	44,54,74	2.16	14 (31%)	54,91,115	2.55	21 (38%)
7	BCL	R	103	2	41,51,74	2.04	10 (24%)	50,87,115	2.43	21 (42%)
8	U4Z	D	104	-	40,40,40	2.72	15 (37%)	50,51,51	6.54	30 (60%)
8	U4Z	R	101	-	40,40,40	3.03	17 (42%)	50,51,51	6.31	32 (64%)
7	BCL	Q	101	-	45,55,74	2.04	13 (28%)	55,92,115	2.53	22 (40%)
12	BPH	L	403	-	51,70,70	1.59	9 (17%)	52,101,101	2.08	13 (25%)
8	U4Z	K	101	-	40,40,40	0.55	1 (2%)	50,51,51	0.82	3 (6%)
7	BCL	R	102	2	45,55,74	2.04	13 (28%)	55,92,115	2.50	23 (41%)
9	HEM	C	504	-	41,50,50	2.27	4 (9%)	45,82,82	1.96	9 (20%)
7	BCL	I	104	2	42,52,74	2.00	10 (23%)	51,88,115	2.38	21 (41%)
7	BCL	E	101	2	44,54,74	2.02	11 (25%)	54,91,115	2.37	22 (40%)
7	BCL	J	101	2	45,55,74	2.04	12 (26%)	55,92,115	2.51	23 (41%)
8	U4Z	K	103	-	40,40,40	1.17	2 (5%)	50,51,51	1.88	14 (28%)
8	U4Z	O	102	-	40,40,40	1.16	2 (5%)	50,51,51	1.89	14 (28%)
7	BCL	H	101	-	40,50,74	2.10	12 (30%)	49,86,115	2.65	24 (48%)
8	U4Z	I	101	-	40,40,40	2.80	15 (37%)	50,51,51	9.47	31 (62%)
11	MQE	L	401	-	64,64,69	0.23	0	78,81,87	0.40	1 (1%)
7	BCL	M	405	5	64,74,74	1.73	14 (21%)	78,115,115	2.45	29 (37%)
7	BCL	K	104	2	49,59,74	2.07	10 (20%)	60,97,115	2.23	21 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEM	C	501	3	-	4/12/54/54	-
7	BCL	D	103	2	-	12/15/115/137	-
8	U4Z	G	101	-	-	13/36/53/53	0/1/1/1
7	BCL	D	101	1	-	10/16/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	P	102	-	-	6/16/116/137	-
7	BCL	I	103	2	-	7/13/113/137	-
8	U4Z	I	102	-	-	12/36/53/53	0/1/1/1
12	BPH	M	401	-	2/2/18/22	17/37/105/105	0/5/6/6
7	BCL	G	102	-	-	10/16/116/137	-
9	HEM	C	503	3	-	4/12/54/54	-
7	BCL	A	104	2	-	9/17/117/137	-
7	BCL	M	402	4	-	13/37/137/137	-
11	MQE	M	403	-	-	15/59/79/85	0/2/2/2
7	BCL	A	101	1	-	12/22/122/137	-
7	BCL	L	402	4	-	17/37/137/137	-
7	BCL	F	101	2	-	9/15/115/137	-
7	BCL	O	103	2	-	6/15/115/137	-
9	HEM	C	502	3	-	4/12/54/54	-
8	U4Z	D	102	-	-	16/36/53/53	0/1/1/1
7	BCL	K	102	1	-	10/15/115/137	-
8	U4Z	P	101	-	-	3/36/53/53	0/1/1/1
7	BCL	A	103	-	-	7/15/115/137	-
10	PGV	C	505	-	-	26/49/49/55	-
8	U4Z	A	102	-	-	18/36/53/53	0/1/1/1
8	U4Z	Q	102	-	-	5/36/53/53	0/1/1/1
8	U4Z	B	101	-	-	4/36/53/53	0/1/1/1
12	BPH	M	406	-	-	4/15/83/105	0/5/6/6
7	BCL	O	101	1	-	10/15/115/137	-
7	BCL	G	103	2	-	4/13/113/137	-
7	BCL	R	103	2	-	5/10/110/137	-
8	U4Z	D	104	-	-	18/36/53/53	0/1/1/1
8	U4Z	R	101	-	-	14/36/53/53	0/1/1/1
7	BCL	Q	101	-	-	10/15/115/137	-
12	BPH	L	403	-	2/2/18/22	14/37/105/105	0/5/6/6
8	U4Z	K	101	-	-	1/36/53/53	0/1/1/1
7	BCL	R	102	2	-	7/15/115/137	-
9	HEM	C	504	-	-	4/12/54/54	-
7	BCL	I	104	2	-	5/11/111/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	E	101	2	-	5/13/113/137	-
7	BCL	J	101	2	-	7/15/115/137	-
8	U4Z	K	103	-	-	5/36/53/53	0/1/1/1
8	U4Z	O	102	-	-	5/36/53/53	0/1/1/1
7	BCL	H	101	-	-	4/8/108/137	-
8	U4Z	I	101	-	-	15/36/53/53	0/1/1/1
11	MQE	L	401	-	-	13/59/79/85	0/2/2/2
7	BCL	M	405	5	-	12/37/137/137	-
7	BCL	K	104	2	-	6/19/119/137	-

All (465) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	504	HEM	C3C-CAC	11.59	1.71	1.47
8	R	101	U4Z	CAH-CAD	11.37	1.54	1.34
8	G	101	U4Z	CAH-CAD	11.15	1.53	1.34
8	I	101	U4Z	CAH-CAD	10.75	1.53	1.34
8	D	104	U4Z	CAH-CAD	10.12	1.52	1.34
8	I	102	U4Z	CAH-CAD	9.66	1.51	1.34
8	D	102	U4Z	CAH-CAD	9.51	1.50	1.34
8	A	102	U4Z	CAH-CAD	9.17	1.50	1.34
7	O	103	BCL	CMD-C2D	7.98	1.67	1.50
7	D	103	BCL	MG-ND	-6.64	1.92	2.05
12	L	403	BPH	CBD-CGD	-6.33	1.43	1.52
7	A	103	BCL	MG-ND	-6.20	1.93	2.05
7	J	101	BCL	MG-ND	-6.16	1.93	2.05
7	K	104	BCL	OBD-CAD	6.15	1.33	1.22
7	I	103	BCL	MG-ND	-6.15	1.93	2.05
7	P	102	BCL	MG-ND	-6.15	1.93	2.05
7	R	102	BCL	MG-ND	-6.14	1.93	2.05
7	R	103	BCL	MG-ND	-6.07	1.93	2.05
7	F	101	BCL	MG-ND	-6.07	1.93	2.05
7	M	405	BCL	MG-ND	-6.04	1.93	2.05
7	I	104	BCL	MG-ND	-6.03	1.93	2.05
7	E	101	BCL	MG-ND	-6.01	1.93	2.05
7	A	104	BCL	MG-ND	-5.96	1.94	2.05
7	O	101	BCL	MG-ND	-5.95	1.94	2.05
7	G	103	BCL	MG-ND	-5.93	1.94	2.05
7	O	103	BCL	MG-ND	-5.90	1.94	2.05
7	H	101	BCL	MG-ND	-5.90	1.94	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	102	BCL	MG-ND	-5.87	1.94	2.05
7	K	102	BCL	MG-ND	-5.86	1.94	2.05
7	K	104	BCL	MG-ND	-5.85	1.94	2.05
7	D	101	BCL	MG-ND	-5.84	1.94	2.05
7	Q	101	BCL	MG-ND	-5.82	1.94	2.05
7	A	101	BCL	MG-ND	-5.78	1.94	2.05
7	M	402	BCL	CAC-C3C	-5.58	1.43	1.54
8	G	101	U4Z	CBF-CBH	5.43	1.57	1.45
7	D	103	BCL	O2D-CGD	5.23	1.46	1.33
7	P	102	BCL	O2D-CGD	5.19	1.45	1.33
7	O	103	BCL	O2D-CGD	5.19	1.45	1.33
7	K	104	BCL	O2D-CGD	5.17	1.45	1.33
8	D	104	U4Z	CAL-CAM	5.15	1.57	1.45
8	R	101	U4Z	CAL-CAM	5.13	1.57	1.45
7	M	402	BCL	C1B-NB	5.11	1.39	1.35
8	G	101	U4Z	CAL-CAM	5.08	1.56	1.45
8	I	101	U4Z	CAL-CAM	5.06	1.56	1.45
7	L	402	BCL	MG-NA	5.02	2.18	2.06
7	M	405	BCL	CAC-C3C	-4.98	1.44	1.54
7	G	103	BCL	CBD-CGD	-4.98	1.36	1.52
7	L	402	BCL	C1B-NB	4.76	1.39	1.35
7	M	402	BCL	MG-NA	4.75	2.17	2.06
8	G	101	U4Z	CBN-CBL	4.74	1.56	1.45
7	M	402	BCL	C3B-CAB	-4.70	1.36	1.49
7	G	103	BCL	C4D-ND	-4.67	1.31	1.37
8	R	101	U4Z	CAQ-CAR	4.65	1.55	1.45
9	C	503	HEM	C4D-ND	-4.65	1.32	1.40
7	G	102	BCL	C4D-ND	-4.63	1.31	1.37
7	M	405	BCL	C4D-ND	-4.58	1.31	1.37
8	I	101	U4Z	CAQ-CAR	4.58	1.55	1.45
8	G	101	U4Z	CBE-CBA	4.57	1.57	1.43
7	R	103	BCL	OBD-CAD	4.57	1.30	1.22
7	O	103	BCL	C4D-ND	-4.55	1.31	1.37
8	G	101	U4Z	CAP-CAO	4.55	1.57	1.43
7	I	103	BCL	C4D-ND	-4.51	1.31	1.37
7	K	102	BCL	C4D-ND	-4.51	1.31	1.37
7	F	101	BCL	C4D-ND	-4.51	1.31	1.37
7	K	104	BCL	C4D-ND	-4.50	1.31	1.37
7	A	101	BCL	C4D-ND	-4.49	1.31	1.37
7	I	103	BCL	OBD-CAD	4.49	1.30	1.22
7	R	102	BCL	C4D-ND	-4.49	1.31	1.37
7	I	104	BCL	C4D-ND	-4.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	103	BCL	O2A-CGA	4.49	1.45	1.30
7	Q	101	BCL	C4D-ND	-4.48	1.31	1.37
7	D	103	BCL	C4D-ND	-4.46	1.31	1.37
7	R	102	BCL	OBD-CAD	4.46	1.30	1.22
7	A	104	BCL	C4D-ND	-4.46	1.31	1.37
7	R	103	BCL	C4D-ND	-4.44	1.31	1.37
7	K	104	BCL	CMC-C2C	-4.43	1.43	1.53
7	J	101	BCL	C4D-ND	-4.43	1.31	1.37
7	H	101	BCL	C4D-ND	-4.43	1.31	1.37
7	A	103	BCL	OBD-CAD	4.43	1.30	1.22
7	E	101	BCL	C4D-ND	-4.42	1.31	1.37
7	E	101	BCL	OBD-CAD	4.41	1.30	1.22
7	A	104	BCL	OBD-CAD	4.41	1.30	1.22
7	O	101	BCL	OBD-CAD	4.40	1.30	1.22
7	Q	101	BCL	OBD-CAD	4.39	1.30	1.22
7	J	101	BCL	OBD-CAD	4.39	1.30	1.22
7	A	103	BCL	C4D-ND	-4.38	1.31	1.37
7	G	102	BCL	OBD-CAD	4.38	1.30	1.22
7	P	102	BCL	C4D-ND	-4.38	1.31	1.37
7	K	102	BCL	OBD-CAD	4.37	1.30	1.22
7	D	101	BCL	OBD-CAD	4.36	1.30	1.22
7	D	101	BCL	C4D-ND	-4.35	1.31	1.37
7	O	101	BCL	C4D-ND	-4.34	1.31	1.37
7	A	101	BCL	OBD-CAD	4.33	1.29	1.22
7	H	101	BCL	OBD-CAD	4.32	1.29	1.22
8	R	101	U4Z	CBN-CBL	4.31	1.55	1.45
8	R	101	U4Z	CBF-CBH	4.31	1.55	1.45
7	K	104	BCL	O2A-CGA	4.30	1.45	1.33
8	D	104	U4Z	CAP-CAO	4.30	1.56	1.43
7	P	102	BCL	O2A-CGA	4.29	1.45	1.33
7	H	101	BCL	O1D-CGD	-4.29	1.10	1.21
7	I	104	BCL	OBD-CAD	4.28	1.29	1.22
8	G	101	U4Z	CAQ-CAR	4.28	1.55	1.45
8	G	101	U4Z	CBG-CBI	4.27	1.56	1.43
7	A	101	BCL	O1D-CGD	-4.26	1.10	1.21
9	C	504	HEM	C4D-ND	-4.26	1.33	1.40
7	D	101	BCL	O1D-CGD	-4.24	1.10	1.21
7	K	102	BCL	O1D-CGD	-4.23	1.10	1.21
10	C	505	PGV	O02-C1	-4.23	1.10	1.22
7	Q	101	BCL	O1D-CGD	-4.22	1.10	1.21
9	C	502	HEM	C4D-ND	-4.22	1.33	1.40
7	A	104	BCL	O1D-CGD	-4.19	1.10	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	104	U4Z	CBF-CBH	4.19	1.54	1.45
7	G	102	BCL	O1D-CGD	-4.18	1.10	1.21
8	R	101	U4Z	CAP-CAO	4.17	1.56	1.43
7	O	101	BCL	O1D-CGD	-4.16	1.10	1.21
7	A	103	BCL	O1D-CGD	-4.15	1.10	1.21
7	E	101	BCL	O1D-CGD	-4.14	1.10	1.21
7	R	102	BCL	O1D-CGD	-4.13	1.10	1.21
7	J	101	BCL	O1D-CGD	-4.13	1.10	1.21
9	C	501	HEM	C4D-ND	-4.12	1.33	1.40
7	I	103	BCL	O1D-CGD	-4.12	1.10	1.21
8	D	104	U4Z	CBB-CAV	4.12	1.56	1.43
8	I	102	U4Z	CAQ-CAR	4.11	1.54	1.45
7	I	104	BCL	O1D-CGD	-4.10	1.10	1.21
7	R	103	BCL	O1D-CGD	-4.09	1.11	1.21
8	D	102	U4Z	CBE-CBA	4.08	1.56	1.43
7	M	402	BCL	CAA-C2A	-4.08	1.46	1.54
8	D	102	U4Z	CBG-CBI	4.06	1.56	1.43
8	R	101	U4Z	CBG-CBI	4.05	1.56	1.43
7	D	103	BCL	O2A-CGA	4.05	1.45	1.33
8	R	101	U4Z	CBE-CBA	4.04	1.56	1.43
7	O	103	BCL	O2A-CGA	4.02	1.45	1.33
8	D	104	U4Z	CAQ-CAR	4.01	1.54	1.45
7	G	103	BCL	O2D-CGD	3.98	1.42	1.33
8	G	101	U4Z	CBM-CBJ	3.97	1.55	1.43
8	D	104	U4Z	CBN-CBL	3.95	1.54	1.45
8	I	102	U4Z	CBE-CBA	3.93	1.55	1.43
8	A	102	U4Z	CAP-CAO	3.92	1.55	1.43
8	I	102	U4Z	CBN-CBL	3.91	1.54	1.45
12	M	401	BPH	C3A-C2A	-3.90	1.51	1.54
7	M	402	BCL	C2A-C1A	-3.86	1.43	1.52
8	I	102	U4Z	CAP-CAO	3.85	1.55	1.43
8	I	102	U4Z	CAL-CAM	3.84	1.54	1.45
8	R	101	U4Z	CBB-CAV	3.84	1.55	1.43
8	D	102	U4Z	CBB-CAV	3.84	1.55	1.43
8	G	101	U4Z	CBB-CAV	3.83	1.55	1.43
7	M	402	BCL	CMA-C3A	-3.83	1.44	1.53
7	F	101	BCL	O2D-CGD	3.82	1.42	1.33
8	R	101	U4Z	CBM-CBJ	3.81	1.55	1.43
8	I	102	U4Z	CBG-CBI	3.79	1.55	1.43
8	I	101	U4Z	CBB-CAV	3.78	1.55	1.43
8	I	101	U4Z	CBF-CBH	3.78	1.54	1.45
12	L	403	BPH	O2A-CGA	3.78	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	BCL	CAC-C3C	-3.76	1.46	1.54
7	O	103	BCL	OBD-CAD	3.75	1.28	1.22
8	A	102	U4Z	CBM-CBJ	3.74	1.55	1.43
7	L	402	BCL	MG-NC	3.74	2.15	2.06
8	A	102	U4Z	CBG-CBI	3.72	1.55	1.43
7	D	103	BCL	OBD-CAD	3.70	1.28	1.22
8	G	101	U4Z	CBA-CAW	3.69	1.38	1.34
7	M	402	BCL	CMB-C2B	-3.69	1.44	1.51
8	D	102	U4Z	CAL-CAM	3.67	1.53	1.45
8	D	102	U4Z	CAP-CAO	3.65	1.54	1.43
8	D	104	U4Z	CBG-CBI	3.65	1.54	1.43
7	P	102	BCL	OBD-CAD	3.65	1.28	1.22
8	I	101	U4Z	CBG-CBI	3.63	1.54	1.43
8	I	102	U4Z	CBB-CAV	3.61	1.54	1.43
8	D	102	U4Z	CBF-CBH	3.61	1.53	1.45
8	A	102	U4Z	CAL-CAM	3.59	1.53	1.45
7	M	402	BCL	CMC-C2C	-3.56	1.45	1.53
7	M	402	BCL	C5-C3	-3.56	1.43	1.51
8	I	101	U4Z	CAP-CAO	3.55	1.54	1.43
8	A	102	U4Z	CBB-CAV	3.52	1.54	1.43
8	I	101	U4Z	CBA-CAW	-3.51	1.30	1.34
7	M	402	BCL	O2A-CGA	3.48	1.43	1.33
8	D	102	U4Z	CBM-CBJ	3.47	1.54	1.43
8	R	101	U4Z	CAJ-CAD	3.47	1.57	1.45
7	M	402	BCL	MG-NC	3.47	2.14	2.06
7	F	101	BCL	O2A-CGA	3.43	1.43	1.33
7	A	103	BCL	O2D-CED	3.43	1.53	1.45
7	I	104	BCL	O2D-CED	3.42	1.53	1.45
8	D	102	U4Z	CAV-CAR	-3.42	1.31	1.35
8	D	104	U4Z	CBM-CBJ	3.42	1.54	1.43
7	R	103	BCL	O2D-CED	3.42	1.53	1.45
7	M	402	BCL	OBB-CAB	-3.40	1.12	1.22
7	L	402	BCL	O2D-CGD	3.40	1.41	1.33
8	I	102	U4Z	CBM-CBJ	3.38	1.53	1.43
8	A	102	U4Z	CBF-CBH	3.37	1.53	1.45
7	G	102	BCL	O2D-CED	3.36	1.53	1.45
7	J	101	BCL	O2D-CED	3.36	1.53	1.45
7	M	405	BCL	O2A-CGA	3.36	1.43	1.33
7	A	104	BCL	O2D-CED	3.35	1.53	1.45
7	G	103	BCL	CAC-C3C	-3.35	1.47	1.54
7	H	101	BCL	C3A-C2A	3.34	1.57	1.54
8	A	102	U4Z	CBE-CBA	3.34	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	101	BCL	O2D-CED	3.33	1.53	1.45
7	O	101	BCL	O2D-CED	3.33	1.53	1.45
10	C	505	PGV	O01-C1	3.32	1.43	1.34
8	D	104	U4Z	CAJ-CAD	3.31	1.56	1.45
8	I	102	U4Z	CBF-CBH	3.31	1.53	1.45
7	I	103	BCL	O2D-CED	3.31	1.53	1.45
7	Q	101	BCL	O2D-CED	3.29	1.53	1.45
9	C	503	HEM	C1D-ND	-3.29	1.32	1.38
7	R	102	BCL	O2D-CED	3.28	1.53	1.45
7	K	102	BCL	O2D-CED	3.28	1.53	1.45
7	F	101	BCL	CAA-C2A	-3.28	1.48	1.54
7	A	101	BCL	O2D-CED	3.28	1.53	1.45
7	H	101	BCL	O2D-CED	3.27	1.53	1.45
7	D	101	BCL	O2D-CED	3.27	1.53	1.45
7	R	102	BCL	O2D-CGD	-3.25	1.25	1.33
12	M	401	BPH	O2A-CGA	3.24	1.42	1.33
7	D	101	BCL	O2A-CGA	-3.24	1.23	1.33
8	I	101	U4Z	CBM-CBJ	3.22	1.53	1.43
7	D	101	BCL	O2D-CGD	-3.22	1.25	1.33
7	J	101	BCL	O2D-CGD	-3.22	1.25	1.33
7	M	402	BCL	C2-C3	-3.21	1.25	1.33
8	G	101	U4Z	CAJ-CAD	3.21	1.56	1.45
8	K	103	U4Z	CAB-CAD	-3.21	1.49	1.53
8	I	101	U4Z	CAJ-CAD	3.20	1.56	1.45
7	I	104	BCL	O2D-CGD	-3.19	1.25	1.33
10	C	505	PGV	O12-C04	-3.19	1.32	1.44
7	G	102	BCL	O2D-CGD	-3.19	1.25	1.33
7	A	101	BCL	O2A-CGA	-3.19	1.24	1.33
7	H	101	BCL	O2D-CGD	-3.18	1.25	1.33
8	I	101	U4Z	CBK-CBH	3.17	1.57	1.50
7	I	103	BCL	O2D-CGD	-3.17	1.25	1.33
7	Q	101	BCL	O2D-CGD	-3.16	1.25	1.33
7	R	103	BCL	O2D-CGD	-3.16	1.25	1.33
7	G	102	BCL	O2A-CGA	-3.16	1.24	1.33
7	O	101	BCL	O2D-CGD	-3.15	1.25	1.33
7	K	102	BCL	O2D-CGD	-3.15	1.25	1.33
7	A	103	BCL	O2D-CGD	-3.14	1.25	1.33
8	I	102	U4Z	CAO-CAM	-3.13	1.31	1.35
8	I	102	U4Z	CAJ-CAD	3.13	1.56	1.45
8	A	102	U4Z	CBN-CBL	3.13	1.52	1.45
12	M	401	BPH	C3D-C2D	-3.13	1.33	1.39
8	A	102	U4Z	CAV-CAR	-3.13	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	101	BCL	O2D-CGD	-3.12	1.25	1.33
12	L	403	BPH	C3D-C2D	-3.11	1.33	1.39
8	D	102	U4Z	CAO-CAM	-3.11	1.31	1.35
7	K	102	BCL	O1A-CGA	-3.10	1.13	1.22
7	D	101	BCL	O1A-CGA	-3.10	1.13	1.22
7	Q	101	BCL	O1A-CGA	-3.10	1.13	1.22
8	B	101	U4Z	CAI-CAH	-3.09	1.44	1.51
7	A	104	BCL	O2D-CGD	-3.09	1.25	1.33
9	C	504	HEM	C1D-ND	-3.09	1.32	1.38
7	E	101	BCL	O2D-CGD	-3.08	1.25	1.33
8	Q	102	U4Z	CAB-CAD	-3.06	1.49	1.53
8	O	102	U4Z	CAB-CAD	-3.06	1.49	1.53
8	A	102	U4Z	CAQ-CAR	3.05	1.52	1.45
7	O	101	BCL	O1A-CGA	-3.05	1.13	1.22
9	C	502	HEM	C1D-ND	-3.04	1.32	1.38
12	M	401	BPH	O2D-CGD	3.04	1.40	1.33
7	A	101	BCL	O1A-CGA	-3.02	1.13	1.22
12	M	406	BPH	C3D-C2D	-3.02	1.34	1.39
8	G	101	U4Z	CAS-CAW	3.02	1.57	1.51
7	M	402	BCL	C3A-C4A	-3.00	1.42	1.51
8	A	102	U4Z	CAJ-CAD	3.00	1.55	1.45
7	G	102	BCL	O1A-CGA	-3.00	1.13	1.22
9	C	501	HEM	C1D-ND	-2.99	1.32	1.38
9	C	504	HEM	C1B-NB	-2.97	1.35	1.40
7	A	104	BCL	O2A-CGA	-2.97	1.24	1.33
8	D	102	U4Z	CAS-CAW	2.95	1.57	1.51
9	C	503	HEM	C1B-NB	-2.93	1.35	1.40
7	A	103	BCL	O1A-CGA	-2.92	1.13	1.22
9	C	501	HEM	C1B-NB	-2.92	1.35	1.40
8	O	102	U4Z	CAI-CAH	-2.90	1.45	1.51
8	D	102	U4Z	CBN-CBL	2.88	1.52	1.45
8	D	102	U4Z	CAQ-CAR	2.88	1.52	1.45
8	K	103	U4Z	CAI-CAH	-2.88	1.45	1.51
8	D	102	U4Z	CAJ-CAD	2.86	1.55	1.45
8	Q	102	U4Z	CAI-CAH	-2.86	1.45	1.51
7	J	101	BCL	O2A-CGA	-2.86	1.23	1.33
7	L	402	BCL	O2A-CGA	2.86	1.41	1.33
7	R	102	BCL	O2A-CGA	-2.86	1.23	1.33
7	A	103	BCL	O2A-CGA	-2.85	1.23	1.33
7	L	402	BCL	CAC-C3C	-2.85	1.48	1.54
7	O	101	BCL	O2A-CGA	-2.84	1.23	1.33
10	C	505	PGV	P-O14	-2.84	1.42	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	505	PGV	O01-C02	-2.84	1.39	1.46
7	R	102	BCL	O1A-CGA	-2.83	1.14	1.22
8	R	101	U4Z	CBK-CBH	2.83	1.56	1.50
7	A	103	BCL	C1D-C2D	-2.82	1.39	1.45
7	J	101	BCL	O1A-CGA	-2.82	1.14	1.22
7	I	103	BCL	C1D-C2D	-2.81	1.39	1.45
7	F	101	BCL	C1D-C2D	-2.81	1.39	1.45
7	L	402	BCL	CMA-C3A	-2.81	1.47	1.53
7	K	102	BCL	O2A-CGA	-2.79	1.24	1.33
7	Q	101	BCL	O2A-CGA	-2.78	1.24	1.33
7	D	103	BCL	C1D-C2D	-2.76	1.39	1.45
7	L	402	BCL	CMC-C2C	-2.75	1.47	1.53
7	J	101	BCL	C1D-C2D	-2.75	1.39	1.45
7	E	101	BCL	C3B-C2B	-2.74	1.34	1.39
7	A	104	BCL	O1A-CGA	-2.74	1.14	1.22
10	C	505	PGV	O04-C19	-2.74	1.14	1.22
7	K	104	BCL	C3B-C2B	-2.73	1.34	1.39
7	R	102	BCL	C1D-C2D	-2.73	1.39	1.45
9	C	502	HEM	C1B-NB	-2.72	1.35	1.40
7	R	103	BCL	C3B-C2B	-2.72	1.34	1.39
7	G	103	BCL	C3B-C2B	-2.72	1.34	1.39
7	M	405	BCL	CAA-C2A	-2.71	1.49	1.54
10	C	505	PGV	O03-C01	-2.70	1.39	1.45
7	P	102	BCL	C1D-C2D	-2.70	1.40	1.45
7	A	104	BCL	C3B-C2B	-2.69	1.34	1.39
7	O	103	BCL	C3B-C2B	-2.69	1.34	1.39
7	I	104	BCL	C3B-C2B	-2.64	1.34	1.39
7	M	405	BCL	C1D-C2D	-2.63	1.40	1.45
12	M	406	BPH	CMD-C2D	-2.62	1.45	1.51
7	D	101	BCL	C1D-C2D	-2.62	1.40	1.45
7	Q	101	BCL	C1D-C2D	-2.60	1.40	1.45
8	G	101	U4Z	CAT-CAX	2.59	1.58	1.50
7	H	101	BCL	C1D-C2D	-2.59	1.40	1.45
7	M	405	BCL	CMA-C3A	-2.58	1.47	1.53
7	L	402	BCL	CAA-C2A	-2.56	1.49	1.54
7	A	101	BCL	C1D-C2D	-2.55	1.40	1.45
7	M	402	BCL	O2D-CED	-2.55	1.39	1.45
7	G	102	BCL	C1D-C2D	-2.53	1.40	1.45
8	K	101	U4Z	CAI-CAH	-2.53	1.46	1.51
7	K	104	BCL	C1D-C2D	-2.52	1.40	1.45
7	O	101	BCL	C1D-C2D	-2.51	1.40	1.45
7	R	103	BCL	C1D-C2D	-2.51	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	103	BCL	O1A-CGA	-2.50	1.13	1.22
7	K	102	BCL	C1D-C2D	-2.50	1.40	1.45
7	A	104	BCL	C1D-C2D	-2.50	1.40	1.45
7	E	101	BCL	C1D-C2D	-2.50	1.40	1.45
10	C	505	PGV	O05-C05	-2.49	1.36	1.43
7	P	102	BCL	C3B-C2B	-2.49	1.35	1.39
8	D	102	U4Z	CBK-CBH	2.49	1.56	1.50
7	M	402	BCL	C4-C3	-2.48	1.44	1.50
7	J	101	BCL	C3B-C2B	-2.48	1.35	1.39
8	R	101	U4Z	CAU-CAR	2.47	1.56	1.50
7	M	402	BCL	CBD-CGD	-2.46	1.44	1.52
7	G	103	BCL	C3B-CAB	-2.45	1.42	1.49
8	A	102	U4Z	CBK-CBH	2.45	1.55	1.50
8	A	102	U4Z	CBD-CAY	2.44	1.56	1.50
10	C	505	PGV	C04-C05	-2.44	1.42	1.51
7	A	103	BCL	C3B-C2B	-2.44	1.35	1.39
7	I	104	BCL	C1D-C2D	-2.44	1.40	1.45
7	G	103	BCL	C1D-C2D	-2.43	1.40	1.45
7	K	102	BCL	C3B-C2B	-2.42	1.35	1.39
8	D	104	U4Z	CBE-CBA	2.42	1.51	1.43
8	R	101	U4Z	CAS-CAW	2.42	1.56	1.51
8	A	102	U4Z	CBO-CBL	2.42	1.55	1.50
12	L	403	BPH	CMC-C2C	-2.42	1.48	1.53
7	J	101	BCL	C3D-C4D	-2.41	1.38	1.44
7	D	103	BCL	C3B-C2B	-2.41	1.35	1.39
7	M	402	BCL	CHD-C1D	2.40	1.43	1.38
7	M	402	BCL	CAA-CBA	-2.40	1.45	1.52
7	M	402	BCL	C3A-C2A	-2.39	1.47	1.54
8	I	101	U4Z	CAK-CAH	2.39	1.54	1.50
7	O	103	BCL	C1D-C2D	-2.39	1.40	1.45
8	D	104	U4Z	CBA-CAW	-2.39	1.31	1.34
7	E	101	BCL	O1A-CGA	-2.39	1.14	1.22
7	M	405	BCL	O2D-CGD	2.39	1.39	1.33
7	Q	101	BCL	C3D-C4D	-2.39	1.38	1.44
12	L	403	BPH	O2D-CGD	2.38	1.39	1.33
7	M	405	BCL	O2D-CED	-2.37	1.39	1.45
7	I	103	BCL	C3B-C2B	-2.36	1.35	1.39
7	E	101	BCL	C3D-C4D	-2.36	1.38	1.44
7	M	402	BCL	O1D-CGD	-2.36	1.15	1.21
7	K	102	BCL	C3D-C4D	-2.36	1.38	1.44
7	G	102	BCL	C3B-C2B	-2.36	1.35	1.39
7	H	101	BCL	C3B-C2B	-2.36	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	103	BCL	C3D-C4D	-2.36	1.38	1.44
7	A	104	BCL	C3D-C4D	-2.35	1.38	1.44
7	P	102	BCL	C3D-C4D	-2.35	1.38	1.44
7	O	101	BCL	C3B-C2B	-2.35	1.35	1.39
7	R	102	BCL	C3B-C2B	-2.35	1.35	1.39
7	O	103	BCL	C3D-C4D	-2.34	1.38	1.44
7	O	101	BCL	C3D-C4D	-2.34	1.38	1.44
7	D	101	BCL	C3B-C2B	-2.34	1.35	1.39
7	F	101	BCL	C3B-C2B	-2.34	1.35	1.39
7	A	101	BCL	C3D-C4D	-2.33	1.38	1.44
7	F	101	BCL	C3D-C4D	-2.33	1.38	1.44
7	G	102	BCL	C3D-C4D	-2.33	1.38	1.44
7	R	103	BCL	C3D-C4D	-2.33	1.38	1.44
7	G	103	BCL	CMC-C2C	-2.32	1.48	1.53
7	Q	101	BCL	C3B-C2B	-2.32	1.35	1.39
12	M	401	BPH	CAA-C2A	-2.32	1.48	1.54
7	A	101	BCL	C3B-C2B	-2.32	1.35	1.39
7	K	104	BCL	C3D-C4D	-2.32	1.38	1.44
10	C	505	PGV	P-O13	-2.32	1.42	1.50
8	G	101	U4Z	CBK-CBH	2.31	1.55	1.50
7	R	102	BCL	C3D-C4D	-2.30	1.39	1.44
7	D	103	BCL	C3D-C4D	-2.30	1.39	1.44
7	D	101	BCL	C3D-C4D	-2.30	1.39	1.44
7	M	405	BCL	C3D-C4D	-2.29	1.39	1.44
7	I	104	BCL	C3D-C4D	-2.29	1.39	1.44
8	R	101	U4Z	CBD-CAY	2.27	1.56	1.50
10	C	505	PGV	C06-C05	-2.26	1.42	1.51
7	H	101	BCL	C3D-C4D	-2.26	1.39	1.44
8	D	104	U4Z	CAS-CAW	2.25	1.56	1.51
7	I	103	BCL	C3D-C4D	-2.24	1.39	1.44
8	R	101	U4Z	CBO-CBL	2.24	1.55	1.50
12	L	403	BPH	CMA-C3A	-2.23	1.49	1.53
10	C	505	PGV	C20-C19	-2.23	1.44	1.50
7	G	103	BCL	C3D-C4D	-2.22	1.39	1.44
8	D	104	U4Z	CBK-CBH	2.21	1.55	1.50
8	I	101	U4Z	CBN-CBL	2.20	1.50	1.45
8	D	102	U4Z	CBI-CBL	-2.19	1.32	1.35
8	G	101	U4Z	CAU-CAR	2.19	1.55	1.50
7	M	405	BCL	C3D-C2D	-2.18	1.33	1.39
7	G	103	BCL	CAA-C2A	-2.18	1.50	1.54
7	H	101	BCL	C2C-C3C	-2.17	1.48	1.54
7	L	402	BCL	C5-C3	-2.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	101	BCL	C2C-C3C	-2.16	1.48	1.54
12	M	401	BPH	CAC-C3C	-2.14	1.49	1.53
12	L	403	BPH	OBB-CAB	-2.14	1.16	1.22
7	M	405	BCL	OBD-CAD	2.14	1.26	1.22
7	G	102	BCL	C2C-C3C	-2.14	1.48	1.54
7	O	101	BCL	C2C-C3C	-2.13	1.48	1.54
12	M	401	BPH	CMC-C2C	-2.13	1.49	1.53
7	D	101	BCL	C2C-C3C	-2.13	1.48	1.54
8	A	102	U4Z	CAT-CAX	2.13	1.57	1.50
12	L	403	BPH	O1A-CGA	-2.12	1.16	1.22
8	I	102	U4Z	CBK-CBH	2.12	1.55	1.50
7	K	102	BCL	C2C-C3C	-2.11	1.48	1.54
8	R	101	U4Z	CAK-CAH	2.10	1.54	1.50
8	A	102	U4Z	CBI-CBL	-2.10	1.33	1.35
7	A	101	BCL	C3D-C2D	-2.10	1.33	1.39
7	M	405	BCL	C3B-C2B	-2.10	1.35	1.39
7	A	103	BCL	C2C-C3C	-2.10	1.48	1.54
7	Q	101	BCL	C2C-C3C	-2.09	1.48	1.54
7	O	103	BCL	C3D-C2D	-2.09	1.33	1.39
8	I	102	U4Z	CAU-CAR	2.09	1.55	1.50
7	F	101	BCL	C2C-C3C	-2.08	1.48	1.54
7	K	102	BCL	C3D-C2D	-2.08	1.33	1.39
7	P	102	BCL	C2C-C3C	-2.07	1.48	1.54
7	R	102	BCL	C2C-C3C	-2.07	1.48	1.54
8	I	101	U4Z	CBE-CBA	2.07	1.49	1.43
7	A	104	BCL	C3D-C2D	-2.07	1.33	1.39
7	O	101	BCL	C3D-C2D	-2.06	1.33	1.39
8	A	102	U4Z	CAO-CAM	-2.06	1.33	1.35
7	G	103	BCL	C3D-C2D	-2.06	1.33	1.39
7	D	103	BCL	C2C-C3C	-2.06	1.48	1.54
12	M	401	BPH	CBB-CAB	-2.05	1.43	1.49
12	M	406	BPH	CHA-CBD	-2.05	1.49	1.52
7	Q	101	BCL	C3D-C2D	-2.05	1.33	1.39
9	C	503	HEM	C1B-C2B	-2.05	1.40	1.44
7	G	103	BCL	OBD-CAD	2.05	1.26	1.22
8	I	101	U4Z	CAB-CAD	-2.05	1.51	1.53
8	G	101	U4Z	CBD-CAY	2.05	1.55	1.50
7	I	103	BCL	C2C-C3C	-2.05	1.48	1.54
12	M	401	BPH	OBB-CAB	-2.04	1.16	1.22
7	I	103	BCL	O2A-CGA	-2.04	1.23	1.30
7	D	103	BCL	C3D-C2D	-2.04	1.33	1.39
7	R	102	BCL	C3D-C2D	-2.04	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	103	BCL	C3D-C2D	-2.04	1.33	1.39
7	D	101	BCL	C3D-C2D	-2.03	1.33	1.39
7	E	101	BCL	C3D-C2D	-2.03	1.33	1.39
7	I	104	BCL	C3D-C2D	-2.03	1.33	1.39
7	I	103	BCL	C3D-C2D	-2.03	1.33	1.39
7	H	101	BCL	C3D-C2D	-2.02	1.33	1.39
7	L	402	BCL	C4B-NB	2.02	1.37	1.35
7	M	402	BCL	CBB-CAB	-2.02	1.43	1.49
7	G	102	BCL	C3D-C2D	-2.01	1.33	1.39
12	L	403	BPH	CMD-C2D	-2.01	1.46	1.51
7	M	405	BCL	CBD-CGD	-2.01	1.46	1.52
7	O	103	BCL	CMC-C2C	2.01	1.57	1.53
7	K	104	BCL	C3D-C2D	-2.01	1.33	1.39
7	J	101	BCL	C2C-C3C	-2.00	1.48	1.54
8	D	104	U4Z	CAN-CAM	2.00	1.55	1.50
7	F	101	BCL	C3D-C2D	-2.00	1.33	1.39
12	M	406	BPH	CMB-C2B	-2.00	1.46	1.51
9	C	501	HEM	C3C-C2C	-2.00	1.37	1.40

All (912) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	102	U4Z	CBD-CAY-CBC	-33.58	40.43	114.60
8	I	101	U4Z	CAU-CAR-CAV	-33.25	76.35	122.92
8	I	101	U4Z	CAU-CAR-CAQ	-24.65	79.24	118.08
8	I	101	U4Z	CBM-CBJ-CBH	-23.99	93.07	127.31
8	I	101	U4Z	CAQ-CAR-CAV	23.87	155.56	118.94
8	I	101	U4Z	CBG-CBI-CBL	23.68	161.11	127.31
8	I	102	U4Z	CBM-CBJ-CBH	-22.72	94.88	127.31
8	D	104	U4Z	CBM-CBJ-CBH	-21.95	95.98	127.31
8	A	102	U4Z	CBM-CBJ-CBH	-21.89	96.07	127.31
8	R	101	U4Z	CBM-CBJ-CBH	-21.76	96.25	127.31
8	D	102	U4Z	CBM-CBJ-CBH	-21.22	97.03	127.31
8	G	101	U4Z	CBG-CBI-CBL	20.72	156.88	127.31
8	D	102	U4Z	CBG-CBI-CBL	20.21	156.15	127.31
8	G	101	U4Z	CBM-CBJ-CBH	-18.97	100.24	127.31
8	R	101	U4Z	CBG-CBI-CBL	17.60	152.42	127.31
8	G	101	U4Z	CBG-CBB-CAV	16.48	157.22	123.47
12	M	401	BPH	O2D-CGD-CBD	15.63	130.80	111.00
8	A	102	U4Z	CBG-CBI-CBL	14.98	148.69	127.31
7	O	103	BCL	CMC-C2C-C1C	-14.40	73.07	111.77
8	R	101	U4Z	CBG-CBB-CAV	14.31	152.79	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	104	U4Z	CBG-CBI-CBL	14.03	147.33	127.31
8	I	102	U4Z	CBK-CBH-CBF	-13.84	96.27	118.08
8	D	104	U4Z	CBE-CBF-CBH	13.78	165.12	126.42
8	I	102	U4Z	CBG-CBI-CBL	13.66	146.81	127.31
8	D	102	U4Z	CBE-CBF-CBH	13.58	164.56	126.42
8	I	102	U4Z	CAJ-CAL-CAM	-13.36	106.05	126.23
8	D	104	U4Z	CBG-CBB-CAV	12.84	149.77	123.47
8	D	102	U4Z	CBG-CBB-CAV	12.81	149.72	123.47
8	A	102	U4Z	CBG-CBB-CAV	12.15	148.37	123.47
8	D	102	U4Z	CAI-CAH-CAD	-12.02	105.27	122.73
8	G	101	U4Z	CBD-CAY-CBC	-11.57	89.05	114.60
8	I	101	U4Z	CBK-CBH-CBF	-11.00	100.75	118.08
12	M	401	BPH	O2D-CGD-O1D	-10.89	102.54	123.84
8	I	101	U4Z	CAO-CAP-CAQ	10.59	156.26	123.22
8	G	101	U4Z	CAO-CAP-CAQ	10.56	156.19	123.22
8	D	102	U4Z	CAJ-CAL-CAM	-10.49	110.38	126.23
8	A	102	U4Z	CBM-CBN-CBL	10.49	155.88	126.42
8	D	104	U4Z	CAO-CAP-CAQ	10.27	155.27	123.22
8	A	102	U4Z	CAI-CAH-CAD	-10.17	107.96	122.73
8	D	104	U4Z	CBO-CBL-CBN	-10.16	102.07	118.08
8	D	102	U4Z	CBB-CAV-CAR	-9.89	113.20	127.31
8	D	102	U4Z	CAP-CAO-CAM	-9.88	113.21	127.31
8	I	102	U4Z	CAL-CAJ-CAD	9.80	154.72	127.20
8	A	102	U4Z	CBK-CBH-CBF	-9.77	102.69	118.08
8	A	102	U4Z	CBE-CBF-CBH	9.76	153.84	126.42
8	D	102	U4Z	CBM-CBN-CBL	9.72	153.74	126.42
8	I	102	U4Z	CBB-CAV-CAR	-9.53	113.70	127.31
8	G	101	U4Z	CBM-CBN-CBL	9.46	152.98	126.42
7	M	402	BCL	CAC-C3C-C4C	-9.40	91.72	112.58
8	R	101	U4Z	CAJ-CAL-CAM	-9.40	112.03	126.23
8	R	101	U4Z	CAO-CAP-CAQ	9.39	152.51	123.22
8	R	101	U4Z	CBE-CBF-CBH	9.35	152.67	126.42
8	D	102	U4Z	CBO-CBL-CBN	-9.33	103.38	118.08
8	D	104	U4Z	CBN-CBL-CBI	9.31	133.22	118.94
8	R	101	U4Z	CBM-CBN-CBL	9.26	152.44	126.42
8	D	102	U4Z	CBD-CAY-CBC	-9.24	94.19	114.60
8	D	104	U4Z	CAI-CAH-CAD	-9.18	109.40	122.73
8	R	101	U4Z	CAL-CAJ-CAD	9.17	152.95	127.20
8	D	104	U4Z	CAP-CAO-CAM	-9.12	114.30	127.31
8	A	102	U4Z	CAO-CAP-CAQ	9.09	151.58	123.22
8	A	102	U4Z	CAJ-CAL-CAM	-9.06	112.54	126.23
8	I	101	U4Z	CAL-CAJ-CAD	8.96	152.38	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	101	U4Z	CBK-CBH-CBF	-8.94	103.98	118.08
8	I	102	U4Z	CAP-CAO-CAM	-8.92	114.57	127.31
8	I	101	U4Z	CBD-CAY-CBC	-8.78	95.21	114.60
10	C	505	PGV	O01-C1-C2	8.77	130.40	111.50
8	I	102	U4Z	CBK-CBH-CBJ	8.73	135.15	122.92
8	I	101	U4Z	CBK-CBH-CBJ	8.68	135.08	122.92
8	D	102	U4Z	CAL-CAJ-CAD	8.67	151.56	127.20
8	G	101	U4Z	CAL-CAJ-CAD	8.61	151.38	127.20
8	R	101	U4Z	CBD-CAY-CBC	-8.61	95.59	114.60
8	D	104	U4Z	CAL-CAJ-CAD	8.44	150.90	127.20
7	L	402	BCL	O2D-CGD-CBD	8.42	126.23	111.27
8	I	101	U4Z	CBO-CBL-CBN	-8.41	104.83	118.08
8	I	102	U4Z	CBD-CAY-CBC	-8.39	96.07	114.60
8	D	104	U4Z	CBD-CAY-CBC	-8.32	96.22	114.60
8	D	102	U4Z	CAO-CAP-CAQ	8.16	148.68	123.22
8	A	102	U4Z	CBO-CBL-CBN	-8.12	105.29	118.08
8	I	102	U4Z	CBM-CBN-CBL	8.02	148.94	126.42
8	I	102	U4Z	CBO-CBL-CBN	-7.98	105.50	118.08
8	G	101	U4Z	CBK-CBH-CBF	-7.96	105.53	118.08
8	G	101	U4Z	CBE-CBF-CBH	7.96	148.77	126.42
8	G	101	U4Z	CAZ-CAW-CAS	-7.93	101.93	115.27
8	I	101	U4Z	CAP-CAO-CAM	-7.89	116.04	127.31
8	D	104	U4Z	CBK-CBH-CBF	-7.87	105.67	118.08
8	A	102	U4Z	CAB-CAD-CAH	-7.68	111.79	122.61
8	A	102	U4Z	CBD-CAY-CAX	-7.67	100.47	122.65
8	A	102	U4Z	CBK-CBH-CBJ	7.62	133.59	122.92
8	I	102	U4Z	CBN-CBL-CBI	7.60	130.60	118.94
8	D	104	U4Z	CBK-CBH-CBJ	7.60	133.56	122.92
8	I	102	U4Z	CAO-CAP-CAQ	7.57	146.83	123.22
8	I	101	U4Z	CAI-CAH-CAD	-7.54	111.78	122.73
7	P	102	BCL	CMD-C2D-C1D	7.47	137.88	124.71
7	D	103	BCL	CMD-C2D-C1D	7.44	137.83	124.71
8	I	101	U4Z	CAJ-CAL-CAM	-7.34	115.14	126.23
7	O	103	BCL	CAC-C3C-C4C	-7.31	96.36	112.58
8	G	101	U4Z	CBO-CBL-CBN	-7.30	106.57	118.08
8	A	102	U4Z	CBB-CAV-CAR	-7.30	116.89	127.31
7	G	103	BCL	CMD-C2D-C1D	7.24	137.46	124.71
7	F	101	BCL	O2D-CGD-O1D	-7.21	109.75	123.84
8	I	101	U4Z	CBM-CBN-CBL	7.17	146.56	126.42
8	I	102	U4Z	CBE-CBF-CBH	7.16	146.53	126.42
7	G	103	BCL	CAC-C3C-C4C	-7.11	96.80	112.58
8	R	101	U4Z	CBO-CBL-CBN	-7.10	106.90	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	402	BCL	CMD-C2D-C1D	7.08	137.19	124.71
8	I	101	U4Z	CBE-CBF-CBH	6.99	146.06	126.42
7	F	101	BCL	O2D-CGD-CBD	6.97	123.65	111.27
8	I	102	U4Z	CBG-CBB-CAV	6.93	137.68	123.47
8	D	102	U4Z	CBK-CBH-CBJ	6.92	132.62	122.92
7	M	402	BCL	O2D-CGD-O1D	-6.92	110.31	123.84
8	I	101	U4Z	CBO-CBL-CBI	6.90	132.59	122.92
8	D	104	U4Z	CAB-CAD-CAH	-6.88	112.93	122.61
8	R	101	U4Z	CBK-CBH-CBJ	6.87	132.54	122.92
9	C	503	HEM	CHC-C4B-NB	6.85	131.87	124.43
8	A	102	U4Z	CAL-CAJ-CAD	6.77	146.21	127.20
8	D	104	U4Z	CBM-CBN-CBL	6.75	145.37	126.42
7	M	402	BCL	CBC-CAC-C3C	-6.67	98.62	113.47
12	M	401	BPH	CMC-C2C-C1C	-6.63	99.86	114.38
12	M	401	BPH	CBC-CAC-C3C	-6.51	100.65	113.77
8	G	101	U4Z	CBN-CBL-CBI	6.51	128.93	118.94
7	M	405	BCL	O2D-CGD-CBD	6.40	122.63	111.27
7	M	405	BCL	CBC-CAC-C3C	-6.35	99.34	113.47
8	A	102	U4Z	CBC-CAY-CAX	6.32	140.91	122.65
7	F	101	BCL	CBC-CAC-C3C	-6.32	99.40	113.47
8	D	104	U4Z	CAT-CAX-CAY	-6.24	106.41	127.75
8	I	102	U4Z	CAK-CAH-CAD	-6.23	117.53	124.53
8	I	102	U4Z	CBF-CBH-CBJ	6.22	128.49	118.94
8	A	102	U4Z	CBN-CBL-CBI	6.17	128.42	118.94
8	D	102	U4Z	CBK-CBH-CBF	-6.17	108.36	118.08
8	D	102	U4Z	CBN-CBL-CBI	6.12	128.33	118.94
8	I	101	U4Z	CBG-CBB-CAV	6.10	135.97	123.47
8	A	102	U4Z	CAP-CAQ-CAR	-6.07	109.37	126.42
7	M	402	BCL	C2A-C1A-CHA	5.99	134.33	123.86
12	L	403	BPH	O2D-CGD-CBD	5.98	118.57	111.00
7	M	402	BCL	CAA-C2A-C3A	-5.98	96.41	112.78
8	D	102	U4Z	CAB-CAD-CAH	-5.98	114.20	122.61
7	M	405	BCL	CMD-C2D-C1D	5.98	135.24	124.71
8	G	101	U4Z	CAJ-CAL-CAM	-5.95	117.24	126.23
8	D	104	U4Z	CAL-CAM-CAO	5.92	128.02	118.94
8	D	104	U4Z	CAZ-CAW-CAS	-5.91	105.33	115.27
7	J	101	BCL	O2D-CGD-CBD	5.79	121.56	111.27
7	O	101	BCL	C1D-ND-C4D	-5.76	102.25	106.33
7	R	102	BCL	O2D-CGD-CBD	5.75	121.49	111.27
7	A	103	BCL	O2D-CGD-CBD	5.75	121.48	111.27
7	I	103	BCL	O2D-CGD-CBD	5.74	121.46	111.27
7	G	102	BCL	CMB-C2B-C1B	-5.72	119.67	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	401	BPH	CMD-C2D-C3D	-5.72	113.98	124.68
7	L	402	BCL	CMD-C2D-C1D	5.71	134.78	124.71
7	A	101	BCL	C1D-ND-C4D	-5.71	102.28	106.33
7	A	101	BCL	CMB-C2B-C1B	-5.69	119.72	128.46
10	C	505	PGV	C02-O01-C1	5.69	131.79	117.79
7	D	101	BCL	C1D-ND-C4D	-5.68	102.30	106.33
7	O	101	BCL	CMB-C2B-C1B	-5.68	119.74	128.46
8	D	104	U4Z	CAN-CAM-CAO	-5.68	114.97	122.92
8	D	104	U4Z	CAK-CAH-CAD	-5.68	118.15	124.53
7	R	103	BCL	C1D-ND-C4D	-5.68	102.30	106.33
8	R	101	U4Z	CBB-CBG-CBI	-5.66	111.87	123.47
7	Q	101	BCL	C1D-ND-C4D	-5.66	102.32	106.33
7	H	101	BCL	C1D-ND-C4D	-5.66	102.32	106.33
7	G	102	BCL	C1D-ND-C4D	-5.65	102.32	106.33
7	K	102	BCL	CMB-C2B-C1B	-5.65	119.78	128.46
7	H	101	BCL	CMB-C2B-C1B	-5.63	119.81	128.46
7	D	101	BCL	CMB-C2B-C1B	-5.62	119.83	128.46
7	K	102	BCL	C1D-ND-C4D	-5.62	102.34	106.33
8	D	104	U4Z	CAP-CAQ-CAR	-5.61	110.65	126.42
7	Q	101	BCL	CMB-C2B-C1B	-5.61	119.84	128.46
7	J	101	BCL	CMB-C2B-C1B	-5.61	119.85	128.46
7	E	101	BCL	C1D-ND-C4D	-5.57	102.38	106.33
12	L	403	BPH	CMA-C3A-C4A	-5.54	102.24	114.38
7	O	103	BCL	C1D-ND-C4D	-5.54	102.40	106.33
9	C	504	HEM	C4D-ND-C1D	5.53	110.79	105.07
7	R	102	BCL	CMB-C2B-C1B	-5.52	119.98	128.46
7	A	103	BCL	CMB-C2B-C1B	-5.51	120.00	128.46
7	A	104	BCL	C1D-ND-C4D	-5.50	102.43	106.33
7	I	103	BCL	CMB-C2B-C1B	-5.50	120.02	128.46
7	I	104	BCL	C1D-ND-C4D	-5.48	102.44	106.33
8	I	102	U4Z	CAT-CAX-CAY	-5.47	109.06	127.75
9	C	503	HEM	C4D-ND-C1D	5.44	110.70	105.07
7	M	405	BCL	C1D-ND-C4D	-5.40	102.50	106.33
7	G	103	BCL	C1D-ND-C4D	-5.38	102.51	106.33
7	M	402	BCL	C1-C2-C3	-5.38	116.73	126.04
7	D	101	BCL	C2D-C1D-ND	5.37	114.06	110.10
7	A	103	BCL	C1D-ND-C4D	-5.37	102.52	106.33
8	K	103	U4Z	CBF-CBH-CBJ	-5.37	110.71	118.94
7	D	103	BCL	C1D-ND-C4D	-5.36	102.53	106.33
7	J	101	BCL	C1D-ND-C4D	-5.35	102.53	106.33
7	F	101	BCL	CBA-CAA-C2A	-5.35	98.07	113.86
7	K	104	BCL	C1D-ND-C4D	-5.35	102.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	101	BCL	CMD-C2D-C1D	5.35	134.13	124.71
8	O	102	U4Z	CBF-CBH-CBJ	-5.33	110.76	118.94
8	I	102	U4Z	CAJ-CAD-CAH	-5.33	108.55	121.46
7	M	402	BCL	CHD-C1D-ND	-5.32	119.57	124.45
7	Q	101	BCL	C2D-C1D-ND	5.31	114.02	110.10
7	H	101	BCL	C2D-C1D-ND	5.29	114.00	110.10
7	P	102	BCL	C1D-ND-C4D	-5.28	102.58	106.33
8	Q	102	U4Z	CBF-CBH-CBJ	-5.28	110.84	118.94
7	G	103	BCL	CAC-C3C-C2C	-5.28	101.07	114.26
7	R	102	BCL	C1D-ND-C4D	-5.27	102.59	106.33
12	L	403	BPH	O2A-CGA-CBA	5.26	128.43	111.91
9	C	501	HEM	CHB-C1B-NB	5.25	130.87	124.38
7	A	101	BCL	C2D-C1D-ND	5.24	113.97	110.10
7	M	405	BCL	C2D-C1D-ND	5.23	113.96	110.10
7	O	101	BCL	C2D-C1D-ND	5.22	113.95	110.10
7	D	103	BCL	C2D-C1D-ND	5.20	113.93	110.10
7	A	103	BCL	C2D-C1D-ND	5.19	113.93	110.10
7	F	101	BCL	C1D-ND-C4D	-5.18	102.65	106.33
7	F	101	BCL	CMC-C2C-C3C	-5.18	92.94	113.83
8	G	101	U4Z	CAU-CAR-CAV	-5.18	115.67	122.92
7	P	102	BCL	C2D-C1D-ND	5.16	113.91	110.10
7	K	102	BCL	O2D-CGD-O1D	-5.15	113.76	123.84
7	R	103	BCL	CAC-C3C-C2C	-5.15	101.39	114.26
9	C	502	HEM	CHB-C1B-NB	5.15	130.75	124.38
7	I	103	BCL	C1D-ND-C4D	-5.14	102.68	106.33
7	I	104	BCL	CAC-C3C-C2C	-5.14	101.41	114.26
7	R	102	BCL	C2D-C1D-ND	5.14	113.89	110.10
7	G	102	BCL	C2D-C1D-ND	5.13	113.89	110.10
7	E	101	BCL	CAC-C3C-C2C	-5.13	101.44	114.26
7	D	101	BCL	O2D-CGD-O1D	-5.13	113.81	123.84
7	A	104	BCL	CAC-C3C-C2C	-5.13	101.45	114.26
7	O	101	BCL	O2D-CGD-O1D	-5.13	113.82	123.84
7	K	102	BCL	C2D-C1D-ND	5.12	113.88	110.10
7	R	103	BCL	O2D-CGD-O1D	-5.12	113.84	123.84
7	E	101	BCL	O2D-CGD-O1D	-5.11	113.84	123.84
7	G	102	BCL	O2D-CGD-O1D	-5.11	113.84	123.84
7	Q	101	BCL	O2D-CGD-O1D	-5.11	113.85	123.84
7	I	103	BCL	C2D-C1D-ND	5.10	113.86	110.10
7	A	101	BCL	O2D-CGD-O1D	-5.10	113.86	123.84
7	O	103	BCL	O2D-CGD-CBD	5.10	120.33	111.27
7	J	101	BCL	C2D-C1D-ND	5.09	113.86	110.10
10	C	505	PGV	C23-C22-C21	-5.09	88.57	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	503	HEM	CHB-C1B-NB	5.09	130.67	124.38
7	R	103	BCL	C2D-C1D-ND	5.07	113.84	110.10
9	C	504	HEM	CHC-C4B-NB	5.07	129.93	124.43
7	A	104	BCL	O2D-CGD-O1D	-5.06	113.94	123.84
7	H	101	BCL	O2D-CGD-O1D	-5.06	113.94	123.84
7	F	101	BCL	C2D-C1D-ND	5.06	113.83	110.10
8	R	101	U4Z	CBB-CAV-CAR	-5.05	120.10	127.31
7	K	104	BCL	CMD-C2D-C1D	5.04	133.59	124.71
8	R	101	U4Z	CAP-CAQ-CAR	-5.02	112.32	126.42
8	R	101	U4Z	CAP-CAO-CAM	-5.02	120.15	127.31
7	I	104	BCL	O2D-CGD-O1D	-5.02	114.03	123.84
7	O	101	BCL	O2D-CGD-CBD	4.99	120.14	111.27
7	E	101	BCL	C2D-C1D-ND	4.99	113.78	110.10
7	K	104	BCL	O2D-CGD-CBD	4.99	120.13	111.27
7	Q	101	BCL	O2D-CGD-CBD	4.99	120.13	111.27
7	M	402	BCL	C4D-CHA-C1A	4.98	127.31	121.25
9	C	502	HEM	C4D-ND-C1D	4.98	110.22	105.07
7	G	102	BCL	O2D-CGD-CBD	4.98	120.11	111.27
12	L	403	BPH	C1-O2A-CGA	4.98	129.50	116.44
7	D	101	BCL	CAC-C3C-C2C	-4.97	101.83	114.26
7	K	102	BCL	O2D-CGD-CBD	4.97	120.09	111.27
7	K	102	BCL	CAC-C3C-C2C	-4.96	101.86	114.26
8	R	101	U4Z	CAZ-CAW-CAS	-4.96	106.92	115.27
7	H	101	BCL	O2D-CGD-CBD	4.96	120.08	111.27
7	D	101	BCL	O2D-CGD-CBD	4.96	120.08	111.27
7	L	402	BCL	CHD-C1D-ND	-4.95	119.90	124.45
7	D	103	BCL	O2D-CGD-CBD	4.95	120.07	111.27
7	A	104	BCL	C2D-C1D-ND	4.95	113.75	110.10
7	A	101	BCL	CAC-C3C-C2C	-4.94	101.91	114.26
7	O	101	BCL	CAC-C3C-C2C	-4.92	101.95	114.26
8	R	101	U4Z	CBN-CBL-CBI	4.92	126.50	118.94
7	J	101	BCL	O2D-CGD-O1D	-4.92	114.22	123.84
7	Q	101	BCL	CAC-C3C-C2C	-4.92	101.97	114.26
7	H	101	BCL	CAC-C3C-C2C	-4.91	101.99	114.26
7	L	402	BCL	CMC-C2C-C1C	-4.91	98.58	111.77
7	I	103	BCL	O2D-CGD-O1D	-4.91	114.24	123.84
12	M	401	BPH	CAC-C3C-C2C	4.90	126.51	114.26
7	A	101	BCL	O2D-CGD-CBD	4.90	119.97	111.27
7	A	103	BCL	O2D-CGD-O1D	-4.90	114.27	123.84
7	L	402	BCL	C4D-CHA-C1A	4.89	127.20	121.25
7	G	102	BCL	CAC-C3C-C2C	-4.89	102.04	114.26
7	A	103	BCL	C1C-NC-C4C	-4.89	104.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	102	BCL	O2D-CGD-CBD	4.89	119.95	111.27
7	I	104	BCL	C2D-C1D-ND	4.88	113.70	110.10
8	G	101	U4Z	CAQ-CAR-CAV	4.88	126.43	118.94
9	C	502	HEM	CHC-C4B-NB	4.88	129.73	124.43
7	O	103	BCL	C2D-C1D-ND	4.88	113.70	110.10
7	R	102	BCL	O2D-CGD-O1D	-4.87	114.32	123.84
7	D	103	BCL	C1C-NC-C4C	-4.85	104.53	106.71
8	R	101	U4Z	CAT-CAX-CAY	-4.85	111.19	127.75
7	M	402	BCL	CAA-CBA-CGA	-4.84	99.11	113.25
7	I	103	BCL	C1C-NC-C4C	-4.82	104.54	106.71
7	K	104	BCL	C2D-C1D-ND	4.82	113.66	110.10
7	M	402	BCL	OBB-CAB-C3B	-4.82	111.44	119.99
8	G	101	U4Z	CBD-CAY-CAX	4.80	136.52	122.65
7	M	405	BCL	C1C-NC-C4C	-4.79	104.55	106.71
7	G	103	BCL	C2D-C1D-ND	4.79	113.63	110.10
8	G	101	U4Z	CBF-CBH-CBJ	4.78	126.27	118.94
7	R	103	BCL	O2D-CGD-CBD	4.77	119.74	111.27
7	E	101	BCL	O2D-CGD-CBD	4.76	119.73	111.27
12	M	401	BPH	CGD-CBD-CAD	-4.76	95.33	110.73
7	I	104	BCL	O2D-CGD-CBD	4.74	119.70	111.27
9	C	501	HEM	CHC-C4B-NB	4.72	129.56	124.43
7	A	104	BCL	O2D-CGD-CBD	4.70	119.61	111.27
7	P	102	BCL	C1C-NC-C4C	-4.69	104.60	106.71
10	C	505	PGV	O01-C1-O02	-4.69	112.38	123.70
9	C	504	HEM	CHB-C1B-NB	4.66	130.14	124.38
7	Q	101	BCL	C1C-NC-C4C	-4.65	104.61	106.71
7	M	405	BCL	O2D-CGD-O1D	-4.63	114.78	123.84
7	M	405	BCL	CMB-C2B-C1B	-4.62	121.36	128.46
8	I	101	U4Z	CAT-CAX-CAY	-4.62	111.97	127.75
7	J	101	BCL	CAC-C3C-C2C	-4.61	102.73	114.26
7	F	101	BCL	CAA-C2A-C1A	4.60	127.05	111.97
7	A	103	BCL	CAC-C3C-C2C	-4.59	102.80	114.26
7	R	102	BCL	CAC-C3C-C2C	-4.58	102.81	114.26
7	F	101	BCL	C1C-NC-C4C	-4.58	104.65	106.71
8	G	101	U4Z	CAE-CAI-CAH	4.58	122.25	114.08
7	I	103	BCL	CAC-C3C-C2C	-4.57	102.83	114.26
7	J	101	BCL	C1C-NC-C4C	-4.57	104.65	106.71
8	D	102	U4Z	CAP-CAQ-CAR	-4.56	113.61	126.42
9	C	501	HEM	C4D-ND-C1D	4.56	109.78	105.07
7	R	102	BCL	C1C-NC-C4C	-4.56	104.66	106.71
8	G	101	U4Z	CAP-CAQ-CAR	-4.54	113.68	126.42
10	C	505	PGV	O11-P-O13	4.53	126.76	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	101	U4Z	CBA-CBE-CBF	-4.53	109.09	123.22
8	O	102	U4Z	CBG-CBI-CBL	-4.50	120.89	127.31
7	M	402	BCL	CMD-C2D-C3D	-4.48	117.30	127.61
8	K	103	U4Z	CBG-CBI-CBL	-4.47	120.93	127.31
10	C	505	PGV	C04-C05-C06	-4.46	95.80	111.67
8	A	102	U4Z	CAZ-CAW-CAS	-4.46	107.77	115.27
8	Q	102	U4Z	CBG-CBI-CBL	-4.46	120.95	127.31
8	A	102	U4Z	CAK-CAH-CAD	-4.42	119.57	124.53
7	M	402	BCL	C11-C10-C8	-4.41	101.67	115.92
9	C	503	HEM	CBA-CAA-C2A	-4.38	105.14	112.62
8	I	102	U4Z	CAQ-CAR-CAV	4.33	125.59	118.94
7	M	405	BCL	CAA-CBA-CGA	-4.33	100.60	113.25
7	E	101	BCL	CMB-C2B-C1B	-4.33	121.81	128.46
7	A	104	BCL	CMB-C2B-C1B	-4.32	121.82	128.46
9	C	501	HEM	CBA-CAA-C2A	-4.32	105.25	112.62
7	R	103	BCL	CMB-C2B-C1B	-4.31	121.83	128.46
8	A	102	U4Z	CBJ-CBM-CBN	-4.31	109.77	123.22
7	O	101	BCL	C1C-NC-C4C	-4.29	104.78	106.71
7	M	402	BCL	C16-C15-C13	-4.28	102.09	115.92
7	I	104	BCL	CMB-C2B-C1B	-4.27	121.91	128.46
8	D	104	U4Z	CAJ-CAL-CAM	-4.27	119.79	126.23
7	M	402	BCL	C7-C6-C5	-4.25	101.81	113.36
7	G	102	BCL	C1C-NC-C4C	-4.25	104.80	106.71
7	L	402	BCL	O2A-CGA-CBA	4.24	125.22	111.91
7	A	101	BCL	C1C-NC-C4C	-4.24	104.80	106.71
7	D	101	BCL	C1C-NC-C4C	-4.24	104.80	106.71
8	D	104	U4Z	CBD-CAY-CAX	4.23	134.89	122.65
7	H	101	BCL	C1C-NC-C4C	-4.21	104.81	106.71
8	D	102	U4Z	CBC-CAY-CAX	4.20	134.77	122.65
7	M	402	BCL	O1D-CGD-CBD	4.18	133.03	124.48
7	D	103	BCL	CHD-C1D-ND	-4.17	120.62	124.45
7	L	402	BCL	O2D-CGD-O1D	-4.16	115.70	123.84
8	I	101	U4Z	CAK-CAH-CAD	-4.15	119.87	124.53
10	C	505	PGV	C24-C23-C22	-4.15	93.38	114.42
7	A	103	BCL	CHD-C1D-ND	-4.12	120.67	124.45
8	G	101	U4Z	CBB-CBG-CBI	-4.10	115.07	123.47
7	R	102	BCL	CHD-C1D-ND	-4.10	120.69	124.45
12	M	401	BPH	CMB-C2B-C3B	4.10	132.35	124.68
8	R	101	U4Z	CAK-CAH-CAD	-4.08	119.95	124.53
7	R	103	BCL	CHD-C1D-ND	-4.08	120.71	124.45
7	K	102	BCL	C1C-NC-C4C	-4.06	104.88	106.71
8	G	101	U4Z	CBC-CAY-CAX	4.05	134.36	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	103	BCL	CHD-C1D-ND	-4.05	120.73	124.45
7	L	402	BCL	C4B-C3B-CAB	4.05	134.94	127.13
7	E	101	BCL	CHD-C1D-ND	-4.04	120.74	124.45
7	P	102	BCL	CHD-C1D-ND	-4.04	120.74	124.45
7	M	402	BCL	OBB-CAB-CBB	4.04	129.25	120.17
7	F	101	BCL	CHD-C1D-ND	-4.03	120.75	124.45
8	G	101	U4Z	CAB-CAD-CAH	-4.02	116.95	122.61
7	A	104	BCL	CHD-C1D-ND	-4.01	120.77	124.45
7	O	103	BCL	CHD-C1D-ND	-4.00	120.78	124.45
7	O	103	BCL	CMC-C2C-C3C	-4.00	97.68	113.83
7	J	101	BCL	CHD-C1D-ND	-4.00	120.78	124.45
7	D	101	BCL	CHD-C1D-ND	-3.97	120.81	124.45
7	I	104	BCL	CHD-C1D-ND	-3.96	120.82	124.45
7	M	405	BCL	CHD-C1D-ND	-3.94	120.83	124.45
8	A	102	U4Z	CAK-CAH-CAI	3.94	121.18	113.62
7	G	103	BCL	CHD-C1D-ND	-3.93	120.84	124.45
12	M	401	BPH	O2A-CGA-CBA	3.93	124.23	111.91
7	A	103	BCL	OBB-CAB-CBB	-3.91	111.37	120.17
7	K	104	BCL	CHD-C1D-ND	-3.91	120.86	124.45
7	O	101	BCL	CHD-C1D-ND	-3.89	120.88	124.45
7	R	103	BCL	OBB-CAB-CBB	-3.89	111.42	120.17
7	I	104	BCL	OBB-CAB-CBB	-3.88	111.43	120.17
7	K	104	BCL	C1-C2-C3	-3.88	120.47	126.75
7	H	101	BCL	CHD-C1D-ND	-3.87	120.89	124.45
7	G	102	BCL	OBB-CAB-CBB	-3.87	111.46	120.17
7	I	103	BCL	OBB-CAB-CBB	-3.86	111.48	120.17
7	A	104	BCL	OBB-CAB-CBB	-3.86	111.49	120.17
7	E	101	BCL	OBB-CAB-CBB	-3.86	111.49	120.17
7	J	101	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
7	K	102	BCL	OBB-CAB-CBB	-3.85	111.50	120.17
8	I	102	U4Z	CAZ-CAW-CAS	-3.85	108.80	115.27
7	R	102	BCL	OBB-CAB-CBB	-3.84	111.52	120.17
7	A	101	BCL	OBB-CAB-CBB	-3.84	111.52	120.17
8	D	102	U4Z	CBO-CBL-CBI	3.83	128.29	122.92
7	M	405	BCL	C1-O2A-CGA	3.83	126.49	116.44
7	O	101	BCL	OBB-CAB-CBB	-3.82	111.56	120.17
7	D	101	BCL	OBB-CAB-CBB	-3.82	111.58	120.17
10	C	505	PGV	C03-C02-C01	-3.82	102.76	111.79
7	G	102	BCL	CHD-C1D-ND	-3.82	120.95	124.45
7	Q	101	BCL	CHD-C1D-ND	-3.81	120.95	124.45
7	Q	101	BCL	OBB-CAB-CBB	-3.80	111.61	120.17
8	O	102	U4Z	CAP-CAO-CAM	-3.79	121.90	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	102	U4Z	CBJ-CBM-CBN	-3.78	111.42	123.22
8	A	102	U4Z	CAP-CAO-CAM	-3.78	121.92	127.31
7	F	101	BCL	CMB-C2B-C1B	-3.77	122.67	128.46
7	H	101	BCL	OBB-CAB-CBB	-3.77	111.69	120.17
8	G	101	U4Z	CBK-CBH-CBJ	3.76	128.19	122.92
7	M	402	BCL	C3A-C2A-C1A	3.76	106.97	101.34
7	A	101	BCL	CHD-C1D-ND	-3.76	121.00	124.45
8	K	103	U4Z	CAP-CAO-CAM	-3.76	121.95	127.31
8	Q	102	U4Z	CAP-CAO-CAM	-3.70	122.02	127.31
8	G	101	U4Z	CBB-CAV-CAR	3.70	132.59	127.31
12	M	406	BPH	CMD-C2D-C3D	3.70	131.59	124.68
7	M	402	BCL	C11-C12-C13	-3.69	103.98	115.92
7	M	405	BCL	C4-C3-C5	3.69	121.48	115.27
8	Q	102	U4Z	CAJ-CAL-CAM	-3.69	120.66	126.23
7	L	402	BCL	CAA-C2A-C3A	-3.68	102.70	112.78
7	M	405	BCL	O2A-CGA-CBA	3.66	123.39	111.91
8	K	103	U4Z	CAJ-CAL-CAM	-3.66	120.71	126.23
7	M	405	BCL	C4D-CHA-C1A	3.65	125.70	121.25
8	I	101	U4Z	CBC-CAY-CAX	3.65	133.19	122.65
7	K	102	BCL	CHD-C1D-ND	-3.64	121.11	124.45
8	G	101	U4Z	CAS-CAW-CBA	3.64	132.99	121.98
8	O	102	U4Z	CAJ-CAL-CAM	-3.64	120.74	126.23
12	M	401	BPH	CAC-C3C-C4C	-3.62	105.64	113.73
8	D	102	U4Z	CAK-CAH-CAI	3.59	120.52	113.62
7	G	103	BCL	O2D-CGD-O1D	3.59	130.86	123.84
7	M	402	BCL	C1D-ND-C4D	-3.59	103.78	106.33
7	H	101	BCL	CMB-C2B-C3B	3.59	131.39	124.68
7	O	101	BCL	CMB-C2B-C3B	3.59	131.39	124.68
7	G	102	BCL	CMB-C2B-C3B	3.59	131.39	124.68
8	A	102	U4Z	CAB-CAD-CAJ	3.58	125.92	115.78
12	M	406	BPH	O2D-CGD-CBD	3.58	115.53	111.00
7	A	101	BCL	CMB-C2B-C3B	3.57	131.36	124.68
7	K	102	BCL	CMB-C2B-C3B	3.56	131.34	124.68
7	L	402	BCL	CBC-CAC-C3C	-3.56	105.54	113.47
9	C	503	HEM	C4B-CHC-C1C	-3.55	117.87	122.56
8	R	101	U4Z	CBA-CBE-CBF	-3.55	112.14	123.22
8	I	102	U4Z	CAF-CAB-CAD	3.54	116.04	110.30
10	C	505	PGV	O03-C19-O04	-3.54	114.66	123.59
7	Q	101	BCL	CMB-C2B-C3B	3.54	131.30	124.68
7	D	101	BCL	CMB-C2B-C3B	3.54	131.29	124.68
8	R	101	U4Z	CBJ-CBM-CBN	-3.53	112.21	123.22
8	I	102	U4Z	CAN-CAM-CAO	-3.52	118.00	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	102	U4Z	CAB-CAD-CAJ	3.51	125.70	115.78
7	J	101	BCL	CMB-C2B-C3B	3.50	131.23	124.68
8	I	101	U4Z	CAB-CAD-CAH	-3.49	117.69	122.61
7	M	402	BCL	C6-C5-C3	-3.49	104.31	113.45
7	M	402	BCL	O2A-CGA-CBA	3.47	122.81	111.91
8	I	101	U4Z	CAK-CAH-CAI	3.47	120.28	113.62
8	I	102	U4Z	CAI-CAH-CAD	-3.46	117.71	122.73
9	C	502	HEM	CHB-C1B-C2B	-3.43	117.22	126.72
7	A	103	BCL	CMB-C2B-C3B	3.43	131.10	124.68
7	M	402	BCL	CMA-C3A-C4A	-3.42	102.58	111.77
8	I	102	U4Z	CBC-CAY-CAX	3.42	132.53	122.65
7	A	101	BCL	C6-C5-C3	-3.42	109.03	114.62
7	A	104	BCL	C4D-CHA-C1A	3.41	125.40	121.25
8	D	102	U4Z	CAU-CAR-CAV	-3.41	118.14	122.92
7	I	103	BCL	CMB-C2B-C3B	3.41	131.06	124.68
8	D	102	U4Z	CAQ-CAR-CAV	3.40	124.16	118.94
9	C	501	HEM	CHB-C1B-C2B	-3.40	117.32	126.72
8	I	101	U4Z	CBF-CBH-CBJ	3.40	124.15	118.94
7	M	402	BCL	O2A-CGA-O1A	-3.39	115.03	123.59
7	O	101	BCL	C4D-CHA-C1A	3.39	125.38	121.25
12	M	401	BPH	CMA-C3A-C4A	-3.38	106.97	114.38
7	K	104	BCL	C4D-CHA-C1A	3.38	125.36	121.25
7	G	102	BCL	O2A-CGA-O1A	-3.38	115.07	123.59
7	R	102	BCL	CMB-C2B-C3B	3.37	130.99	124.68
7	I	104	BCL	C4D-CHA-C1A	3.37	125.35	121.25
7	R	103	BCL	C4D-CHA-C1A	3.37	125.35	121.25
7	E	101	BCL	C4D-CHA-C1A	3.37	125.35	121.25
7	A	101	BCL	O2A-CGA-O1A	-3.36	115.10	123.59
7	A	104	BCL	C4B-CHC-C1C	-3.36	123.46	130.12
12	M	401	BPH	C1-C2-C3	-3.36	120.24	126.04
8	G	101	U4Z	CAI-CAH-CAD	-3.35	117.87	122.73
8	R	101	U4Z	CBD-CAY-CAX	3.34	132.30	122.65
7	K	104	BCL	C3A-C2A-C1A	3.33	106.33	101.34
12	L	403	BPH	CMC-C2C-C1C	-3.33	107.07	114.38
7	P	102	BCL	CMD-C2D-C3D	-3.33	119.95	127.61
7	G	103	BCL	C4D-CHA-C1A	3.33	125.30	121.25
10	C	505	PGV	O06-C06-C05	-3.32	94.28	110.20
7	D	103	BCL	CMD-C2D-C3D	-3.32	119.98	127.61
7	O	103	BCL	C4D-CHA-C1A	3.32	125.28	121.25
7	D	101	BCL	O2A-CGA-O1A	-3.31	115.23	123.59
7	K	102	BCL	C4D-CHA-C1A	3.31	125.27	121.25
8	A	102	U4Z	CBB-CBG-CBI	-3.30	116.71	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Q	101	BCL	C4D-CHA-C1A	3.29	125.25	121.25
7	I	104	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
7	R	103	BCL	C4B-CHC-C1C	-3.28	123.62	130.12
7	D	101	BCL	C4D-CHA-C1A	3.28	125.24	121.25
7	G	103	BCL	C4B-CHC-C1C	-3.28	123.63	130.12
8	R	101	U4Z	CBC-CAY-CAX	3.27	132.11	122.65
7	H	101	BCL	C4D-CHA-C1A	3.27	125.23	121.25
7	E	101	BCL	C4B-CHC-C1C	-3.27	123.64	130.12
7	G	102	BCL	C4D-CHA-C1A	3.27	125.23	121.25
8	R	101	U4Z	CAK-CAH-CAI	3.27	119.89	113.62
7	K	104	BCL	C4B-CHC-C1C	-3.27	123.65	130.12
7	L	402	BCL	CMD-C2D-C3D	-3.26	120.12	127.61
7	O	103	BCL	C4B-CHC-C1C	-3.26	123.67	130.12
7	L	402	BCL	C1D-ND-C4D	-3.25	104.02	106.33
7	L	402	BCL	O1D-CGD-CBD	-3.25	117.83	124.48
8	I	102	U4Z	CAU-CAR-CAV	-3.25	118.37	122.92
7	G	103	BCL	CMD-C2D-C3D	-3.25	120.14	127.61
7	D	103	BCL	C4D-CHA-C1A	3.23	125.18	121.25
9	C	503	HEM	CHC-C4B-C3B	-3.23	119.62	124.57
7	J	101	BCL	C4D-CHA-C1A	3.23	125.18	121.25
7	F	101	BCL	C4D-CHA-C1A	3.22	125.17	121.25
7	J	101	BCL	C4B-CHC-C1C	-3.22	123.74	130.12
10	C	505	PGV	C22-C21-C20	-3.22	101.62	113.19
7	A	101	BCL	C4D-CHA-C1A	3.22	125.17	121.25
7	L	402	BCL	O2A-CGA-O1A	-3.22	115.47	123.59
7	I	103	BCL	C4D-CHA-C1A	3.21	125.16	121.25
7	P	102	BCL	C4D-CHA-C1A	3.20	125.15	121.25
7	K	104	BCL	CMC-C2C-C1C	-3.20	103.17	111.77
7	D	103	BCL	C4B-CHC-C1C	-3.20	123.78	130.12
7	O	103	BCL	CAC-C3C-C2C	-3.19	106.28	114.26
7	R	102	BCL	C4B-CHC-C1C	-3.19	123.80	130.12
7	P	102	BCL	C4B-CHC-C1C	-3.18	123.81	130.12
7	A	103	BCL	C4D-CHA-C1A	3.18	125.12	121.25
7	F	101	BCL	C4B-CHC-C1C	-3.18	123.82	130.12
7	I	103	BCL	C4B-CHC-C1C	-3.17	123.85	130.12
8	K	103	U4Z	CBK-CBH-CBF	3.15	123.04	118.08
7	A	103	BCL	C4B-CHC-C1C	-3.15	123.89	130.12
7	A	104	BCL	CHA-C1A-NA	-3.14	119.20	126.40
7	R	102	BCL	C4D-CHA-C1A	3.14	125.07	121.25
12	L	403	BPH	O2A-CGA-O1A	-3.14	115.67	123.59
7	I	104	BCL	CHA-C1A-NA	-3.14	119.22	126.40
7	K	104	BCL	CHA-C1A-NA	-3.12	119.26	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	101	U4Z	CAG-CAB-CAD	-3.12	105.24	110.30
8	A	102	U4Z	CBF-CBH-CBJ	3.11	123.72	118.94
8	I	102	U4Z	CAP-CAQ-CAR	-3.11	117.67	126.42
7	G	103	BCL	CHA-C1A-NA	-3.10	119.30	126.40
8	O	102	U4Z	CBK-CBH-CBF	3.10	122.96	118.08
7	O	103	BCL	CMD-C2D-C1D	3.10	130.17	124.71
8	I	101	U4Z	CBD-CAY-CAX	3.09	131.58	122.65
9	C	501	HEM	CAD-CBD-CGD	-3.09	106.96	113.60
7	L	402	BCL	C6-C7-C8	-3.08	105.96	115.92
7	E	101	BCL	CHA-C1A-NA	-3.08	119.34	126.40
7	M	402	BCL	CHA-C1A-NA	-3.08	119.35	126.40
7	R	103	BCL	CHA-C1A-NA	-3.08	119.35	126.40
12	M	401	BPH	OBD-CAD-CBD	-3.07	121.32	125.82
7	K	104	BCL	C2A-C1A-CHA	3.06	129.21	123.86
7	H	101	BCL	CMA-C3A-C2A	-3.06	108.96	116.10
8	Q	102	U4Z	CBK-CBH-CBF	3.05	122.88	118.08
8	D	102	U4Z	CAL-CAM-CAO	3.05	123.62	118.94
8	G	101	U4Z	CAS-CAT-CAX	3.05	121.90	111.88
7	O	103	BCL	CHA-C1A-NA	-3.04	119.43	126.40
7	G	103	BCL	CMC-C2C-C3C	-3.04	101.58	113.83
7	K	104	BCL	C2A-C3A-C4A	-3.04	96.96	101.87
9	C	503	HEM	CHB-C1B-C2B	-3.03	118.33	126.72
7	M	405	BCL	CHA-C1A-NA	-3.03	119.47	126.40
8	I	102	U4Z	CBD-CAY-CAX	3.03	131.39	122.65
7	L	402	BCL	C4-C3-C2	-3.02	115.94	123.68
7	F	101	BCL	CGD-CBD-CAD	-3.01	101.00	110.73
9	C	504	HEM	CHB-C1B-C2B	-3.00	118.42	126.72
8	R	101	U4Z	CAB-CAD-CAH	-2.99	118.39	122.61
7	L	402	BCL	CMB-C2B-C1B	-2.99	123.86	128.46
8	D	102	U4Z	CAK-CAH-CAD	-2.99	121.17	124.53
11	L	401	MQE	CAY-CAX-CBQ	-2.98	115.31	118.50
7	L	402	BCL	CHA-C1A-NA	-2.97	119.59	126.40
7	M	402	BCL	CAC-C3C-C2C	-2.97	106.85	114.26
7	F	101	BCL	CAA-C2A-C3A	2.97	120.90	112.78
7	O	101	BCL	CHA-C1A-NA	-2.97	119.61	126.40
9	C	501	HEM	CHA-C4D-ND	2.95	128.03	124.38
8	R	101	U4Z	CBF-CBH-CBJ	2.95	123.47	118.94
10	C	505	PGV	C7-C6-C5	-2.95	99.46	114.42
7	Q	101	BCL	CHA-C1A-NA	-2.95	119.65	126.40
8	Q	102	U4Z	CAL-CAJ-CAD	-2.94	118.94	127.20
8	K	103	U4Z	CAL-CAJ-CAD	-2.94	118.95	127.20
7	M	402	BCL	O2D-CGD-CBD	2.93	116.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	403	MQE	CAY-CAX-CBQ	-2.93	115.37	118.50
8	O	102	U4Z	CAL-CAJ-CAD	-2.93	118.98	127.20
12	L	403	BPH	O2D-CGD-O1D	-2.93	118.12	123.84
8	I	102	U4Z	CBB-CBG-CBI	2.93	129.47	123.47
7	K	102	BCL	CHA-C1A-NA	-2.92	119.70	126.40
7	M	405	BCL	C3D-C2D-C1D	-2.92	101.84	105.83
9	C	503	HEM	CBD-CAD-C3D	-2.92	104.52	112.63
7	O	101	BCL	CMC-C2C-C3C	-2.91	102.08	113.83
7	A	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	M	405	BCL	CMB-C2B-C3B	2.91	130.12	124.68
7	D	101	BCL	CHA-C1A-NA	-2.91	119.73	126.40
7	F	101	BCL	O2A-CGA-CBA	2.91	123.73	112.23
7	G	102	BCL	CHA-C1A-NA	-2.91	119.74	126.40
7	H	101	BCL	CHA-C1A-NA	-2.91	119.74	126.40
7	H	101	BCL	CMC-C2C-C3C	-2.91	102.10	113.83
8	A	102	U4Z	CAG-CAB-CAD	-2.91	105.58	110.30
8	O	102	U4Z	CBG-CBB-CAV	-2.90	117.52	123.47
8	Q	102	U4Z	CBG-CBB-CAV	-2.90	117.53	123.47
8	D	102	U4Z	CBD-CAY-CAX	2.90	131.04	122.65
8	R	101	U4Z	CAE-CAI-CAH	2.90	119.26	114.08
7	Q	101	BCL	CMC-C2C-C3C	-2.90	102.12	113.83
9	C	504	HEM	CHA-C4D-ND	2.90	127.96	124.38
7	D	101	BCL	CMC-C2C-C3C	-2.89	102.17	113.83
7	G	102	BCL	CMC-C2C-C3C	-2.88	102.22	113.83
7	K	102	BCL	CMC-C2C-C3C	-2.87	102.24	113.83
12	M	401	BPH	CMA-C3A-C2A	-2.87	102.45	113.99
7	A	101	BCL	CMC-C2C-C3C	-2.86	102.28	113.83
8	A	102	U4Z	CBA-CBE-CBF	-2.86	114.29	123.22
7	I	103	BCL	O2A-CGA-O1A	-2.86	116.17	123.30
9	C	504	HEM	CHC-C4B-C3B	-2.86	120.20	124.57
7	R	102	BCL	CMC-C2C-C3C	-2.86	102.31	113.83
7	L	402	BCL	C4A-NA-C1A	2.85	107.99	106.71
7	Q	101	BCL	C3D-C2D-C1D	-2.85	101.94	105.83
7	A	103	BCL	CMC-C2C-C3C	-2.85	102.33	113.83
8	K	103	U4Z	CBG-CBB-CAV	-2.85	117.64	123.47
7	H	101	BCL	C4B-CHC-C1C	-2.85	124.48	130.12
7	J	101	BCL	CMC-C2C-C3C	-2.84	102.37	113.83
7	D	101	BCL	C4B-CHC-C1C	-2.84	124.50	130.12
7	I	103	BCL	CMC-C2C-C3C	-2.84	102.39	113.83
7	D	101	BCL	C3D-C2D-C1D	-2.83	101.96	105.83
12	M	401	BPH	O2A-CGA-O1A	-2.83	116.45	123.59
7	O	101	BCL	C3D-C2D-C1D	-2.83	101.97	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	101	BCL	C4B-CHC-C1C	-2.82	124.53	130.12
7	K	102	BCL	C3D-C2D-C1D	-2.82	101.99	105.83
8	K	101	U4Z	CAE-CAI-CAH	2.81	119.09	114.08
7	G	102	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
7	H	101	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
7	A	101	BCL	C3D-C2D-C1D	-2.81	102.00	105.83
12	L	403	BPH	O2A-C1-C2	-2.80	101.27	108.64
8	D	104	U4Z	CAB-CAD-CAJ	2.80	123.70	115.78
8	D	102	U4Z	CAN-CAM-CAO	-2.80	119.00	122.92
8	G	101	U4Z	CBJ-CBM-CBN	-2.79	114.50	123.22
7	M	405	BCL	C4B-CHC-C1C	-2.79	124.59	130.12
7	A	104	BCL	CMC-C2C-C3C	-2.78	102.62	113.83
7	I	104	BCL	CMC-C2C-C3C	-2.77	102.64	113.83
7	D	103	BCL	CHA-C1A-NA	-2.76	120.07	126.40
7	I	103	BCL	CHA-C1A-NA	-2.76	120.08	126.40
7	Q	101	BCL	C4B-CHC-C1C	-2.76	124.65	130.12
7	G	102	BCL	C4B-CHC-C1C	-2.76	124.66	130.12
7	A	101	BCL	C4B-CHC-C1C	-2.76	124.66	130.12
7	E	101	BCL	CMC-C2C-C3C	-2.75	102.72	113.83
12	L	403	BPH	C9-C8-C10	-2.75	101.32	111.29
7	R	102	BCL	CHA-C1A-NA	-2.75	120.10	126.40
7	P	102	BCL	CHA-C1A-NA	-2.75	120.10	126.40
7	R	103	BCL	CMC-C2C-C3C	-2.75	102.73	113.83
7	J	101	BCL	CHA-C1A-NA	-2.75	120.11	126.40
7	A	103	BCL	CHA-C1A-NA	-2.74	120.12	126.40
7	F	101	BCL	CHA-C1A-NA	-2.74	120.12	126.40
7	R	103	BCL	C3D-C2D-C1D	-2.73	102.10	105.83
7	M	402	BCL	C4-C3-C5	2.73	119.86	115.27
7	O	103	BCL	C3D-C2D-C1D	-2.73	102.11	105.83
7	M	405	BCL	CMA-C3A-C4A	-2.72	104.46	111.77
8	R	101	U4Z	CAI-CAH-CAD	-2.72	118.79	122.73
7	E	101	BCL	C3D-C2D-C1D	-2.71	102.13	105.83
10	C	505	PGV	C01-O03-C19	2.71	127.14	117.12
7	K	102	BCL	C4B-CHC-C1C	-2.71	124.76	130.12
7	P	102	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
7	M	405	BCL	CGD-CBD-CAD	-2.70	101.99	110.73
7	A	104	BCL	C3D-C2D-C1D	-2.70	102.15	105.83
7	I	104	BCL	C3D-C2D-C1D	-2.69	102.16	105.83
7	M	405	BCL	CED-O2D-CGD	2.69	122.01	115.94
7	R	102	BCL	C3D-C2D-C1D	-2.68	102.17	105.83
7	D	103	BCL	C3D-C2D-C1D	-2.67	102.18	105.83
12	L	403	BPH	CGD-CBD-CAD	-2.67	102.10	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	403	BPH	CAC-C3C-C4C	-2.67	107.78	113.73
7	A	103	BCL	CMA-C3A-C4A	-2.66	104.61	111.77
7	A	103	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
7	F	101	BCL	C3D-C2D-C1D	-2.66	102.20	105.83
7	J	101	BCL	C3D-C2D-C1D	-2.65	102.21	105.83
7	G	103	BCL	C3D-C2D-C1D	-2.65	102.22	105.83
8	I	101	U4Z	CAC-CAB-CAD	2.65	114.55	110.48
9	C	502	HEM	CHA-C4D-ND	2.64	127.64	124.38
7	J	101	BCL	CMA-C3A-C4A	-2.64	104.68	111.77
7	K	104	BCL	C3D-C2D-C1D	-2.64	102.23	105.83
8	K	103	U4Z	CAZ-CAW-CAS	2.63	119.70	115.27
8	Q	102	U4Z	CAZ-CAW-CAS	2.63	119.70	115.27
8	R	101	U4Z	CBO-CBL-CBI	2.63	126.61	122.92
7	G	103	BCL	OBB-CAB-CBB	2.63	126.08	120.17
7	P	102	BCL	O2A-CGA-CBA	2.62	120.14	111.91
7	I	103	BCL	C3D-C2D-C1D	-2.62	102.25	105.83
7	K	104	BCL	O2A-CGA-CBA	2.62	120.14	111.91
7	I	103	BCL	CMA-C3A-C4A	-2.62	104.73	111.77
7	R	102	BCL	CMA-C3A-C4A	-2.59	104.81	111.77
12	L	403	BPH	C4-C3-C5	2.59	119.62	115.27
8	O	102	U4Z	CAZ-CAW-CAS	2.58	119.62	115.27
8	A	102	U4Z	CAL-CAM-CAO	-2.58	114.98	118.94
8	I	102	U4Z	CAE-CAI-CAH	2.58	118.68	114.08
7	A	104	BCL	O2A-CGA-O1A	-2.57	117.10	123.59
7	O	101	BCL	O2A-CGA-O1A	-2.57	115.09	123.14
12	M	401	BPH	C4-C3-C5	2.56	119.58	115.27
7	M	405	BCL	C2A-C1A-CHA	2.56	128.34	123.86
7	K	104	BCL	C3C-C2C-C1C	2.56	106.00	101.87
10	C	505	PGV	O03-C19-C20	2.55	119.91	111.91
12	M	406	BPH	O2D-CGD-O1D	-2.55	118.86	123.84
7	K	102	BCL	O2A-CGA-O1A	-2.54	115.17	123.14
9	C	504	HEM	C4B-CHC-C1C	-2.54	119.20	122.56
8	I	102	U4Z	CAB-CAD-CAH	-2.54	119.03	122.61
7	Q	101	BCL	O2A-CGA-O1A	-2.54	115.18	123.14
9	C	504	HEM	C4B-C3B-C2B	-2.54	105.10	107.11
7	G	103	BCL	C3C-C2C-C1C	2.51	105.92	101.87
7	F	101	BCL	OBB-CAB-CBB	2.51	125.81	120.17
7	E	101	BCL	CMB-C2B-C3B	2.50	129.36	124.68
7	R	102	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
8	D	102	U4Z	CAC-CAE-CAI	-2.50	105.79	111.38
10	C	505	PGV	C9-C8-C7	-2.50	101.73	114.42
7	M	402	BCL	CMA-C3A-C2A	-2.50	103.75	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	102	BCL	C2A-C3A-C4A	-2.50	97.83	101.87
10	C	505	PGV	O03-C01-C02	-2.50	101.17	108.43
7	A	104	BCL	C3C-C2C-C1C	2.49	105.89	101.87
7	M	402	BCL	CMC-C2C-C3C	-2.49	103.80	113.83
7	O	103	BCL	C3C-C2C-C1C	2.49	105.88	101.87
7	O	103	BCL	C1C-NC-C4C	-2.48	105.59	106.71
7	D	103	BCL	C2A-C3A-C4A	-2.48	97.86	101.87
10	C	505	PGV	C6-C5-C4	-2.47	101.89	114.42
7	A	103	BCL	C2A-C3A-C4A	-2.47	97.88	101.87
7	I	104	BCL	C3C-C2C-C1C	2.47	105.85	101.87
8	P	101	U4Z	CAE-CAI-CAH	2.46	118.47	114.08
7	A	104	BCL	CMB-C2B-C3B	2.46	129.28	124.68
7	I	103	BCL	C2A-C3A-C4A	-2.46	97.89	101.87
7	R	103	BCL	C3C-C2C-C1C	2.46	105.84	101.87
7	J	101	BCL	C2A-C3A-C4A	-2.46	97.90	101.87
8	D	102	U4Z	CAT-CAX-CAY	-2.46	119.35	127.75
9	C	502	HEM	CHC-C4B-C3B	-2.46	120.81	124.57
7	K	104	BCL	C5-C3-C4	2.46	120.03	114.60
7	E	101	BCL	O2A-CGA-O1A	-2.45	117.18	123.30
7	R	103	BCL	CMB-C2B-C3B	2.45	129.27	124.68
8	K	101	U4Z	CAT-CAS-CAW	2.45	121.03	112.98
7	A	101	BCL	CMA-C3A-C4A	-2.43	105.23	111.77
7	F	101	BCL	C2A-C3A-C4A	-2.43	97.94	101.87
12	M	406	BPH	CBC-CAC-C3C	-2.43	108.87	113.77
8	Q	102	U4Z	CBB-CAV-CAR	-2.43	123.84	127.31
8	O	102	U4Z	CBB-CAV-CAR	-2.43	123.85	127.31
7	E	101	BCL	C3C-C2C-C1C	2.43	105.79	101.87
7	I	104	BCL	CMB-C2B-C3B	2.43	129.22	124.68
8	I	101	U4Z	CBJ-CBM-CBN	-2.42	115.67	123.22
8	B	101	U4Z	CAE-CAI-CAH	2.41	118.38	114.08
7	E	101	BCL	C1C-NC-C4C	-2.41	105.62	106.71
7	R	103	BCL	C1C-NC-C4C	-2.41	105.62	106.71
7	M	405	BCL	CAC-C3C-C2C	-2.41	108.24	114.26
8	A	102	U4Z	CBO-CBL-CBI	2.41	126.29	122.92
7	D	103	BCL	O2D-CGD-O1D	-2.41	119.13	123.84
7	O	103	BCL	O2D-CGD-O1D	-2.40	119.14	123.84
7	K	104	BCL	O2D-CGD-O1D	-2.40	119.14	123.84
7	R	103	BCL	CMD-C2D-C1D	2.40	128.94	124.71
7	O	101	BCL	CMA-C3A-C4A	-2.40	105.33	111.77
7	D	101	BCL	CMA-C3A-C4A	-2.39	105.34	111.77
8	D	104	U4Z	CBB-CAV-CAR	2.39	130.72	127.31
7	A	104	BCL	CMD-C2D-C1D	2.39	128.93	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	103	BCL	CMB-C2B-C1B	-2.39	124.79	128.46
7	K	102	BCL	CMA-C3A-C4A	-2.39	105.35	111.77
8	D	102	U4Z	CAS-CAW-CBA	2.39	129.20	121.98
9	C	501	HEM	C4B-C3B-C2B	-2.39	105.22	107.11
7	I	104	BCL	CMD-C2D-C1D	2.38	128.91	124.71
8	K	103	U4Z	CBB-CAV-CAR	-2.38	123.91	127.31
7	G	103	BCL	C1C-NC-C4C	-2.38	105.64	106.71
7	G	102	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
7	H	101	BCL	CMA-C3A-C4A	-2.37	105.40	111.77
8	O	102	U4Z	CBK-CBH-CBJ	2.37	126.24	122.92
7	Q	101	BCL	CMA-C3A-C4A	-2.37	105.41	111.77
8	Q	102	U4Z	CBK-CBH-CBJ	2.36	126.23	122.92
9	C	504	HEM	CMC-C2C-C3C	2.36	129.09	124.68
7	I	104	BCL	CMA-C3A-C4A	-2.35	105.45	111.77
8	K	103	U4Z	CBK-CBH-CBJ	2.35	126.22	122.92
7	J	101	BCL	CHC-C1C-NC	2.35	127.76	124.51
7	P	102	BCL	O2D-CGD-O1D	-2.35	119.25	123.84
9	C	503	HEM	CMA-C3A-C4A	-2.34	124.86	128.46
7	K	104	BCL	C1C-NC-C4C	-2.34	105.65	106.71
7	A	104	BCL	CMA-C3A-C4A	-2.34	105.48	111.77
8	I	101	U4Z	CBN-CBL-CBI	2.34	122.54	118.94
7	R	103	BCL	CMA-C3A-C4A	-2.34	105.49	111.77
7	E	101	BCL	CMA-C3A-C4A	-2.33	105.50	111.77
8	D	104	U4Z	CBB-CBG-CBI	-2.33	118.69	123.47
7	E	101	BCL	CMD-C2D-C1D	2.33	128.83	124.71
8	D	102	U4Z	CAZ-CAW-CAS	-2.33	111.36	115.27
9	C	502	HEM	C4B-CHC-C1C	-2.32	119.49	122.56
7	M	405	BCL	CHC-C1C-NC	2.31	127.71	124.51
9	C	503	HEM	CHA-C4D-ND	2.31	127.23	124.38
7	H	101	BCL	CMD-C2D-C1D	2.30	128.77	124.71
7	M	405	BCL	O2A-CGA-O1A	-2.30	117.79	123.59
12	M	401	BPH	C16-C15-C13	-2.30	108.50	115.92
8	A	102	U4Z	CAJ-CAD-CAH	-2.30	115.90	121.46
7	R	102	BCL	CHC-C1C-NC	2.29	127.69	124.51
7	K	102	BCL	C3C-C4C-CHD	-2.29	118.49	123.39
12	M	401	BPH	CAA-C2A-C3A	2.29	119.05	112.78
7	L	402	BCL	C5-C3-C2	2.29	125.74	121.12
7	G	103	BCL	OBB-CAB-C3B	-2.28	115.94	119.99
7	A	104	BCL	C1C-NC-C4C	-2.28	105.68	106.71
7	Q	101	BCL	CMD-C2D-C1D	2.28	128.73	124.71
7	P	102	BCL	CHC-C1C-NC	2.28	127.66	124.51
7	I	104	BCL	C1C-NC-C4C	-2.28	105.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	101	BCL	CHC-C1C-NC	2.27	127.65	124.51
7	D	101	BCL	CMD-C2D-C1D	2.26	128.70	124.71
12	M	401	BPH	CBA-CAA-C2A	2.26	120.42	113.81
7	M	402	BCL	C17-C16-C15	-2.26	102.86	113.24
7	J	101	BCL	O2A-CGA-O1A	-2.26	116.06	123.14
7	R	102	BCL	O2A-CGA-O1A	-2.26	116.07	123.14
8	Q	102	U4Z	CBA-CBE-CBF	2.26	130.26	123.22
9	C	502	HEM	C4B-C3B-C2B	-2.26	105.32	107.11
9	C	501	HEM	CHC-C4B-C3B	-2.25	121.12	124.57
8	O	102	U4Z	CBA-CBE-CBF	2.25	130.25	123.22
7	A	103	BCL	CHC-C1C-NC	2.25	127.63	124.51
7	A	101	BCL	C3C-C4C-CHD	-2.25	118.58	123.39
7	D	103	BCL	CHC-C1C-NC	2.25	127.62	124.51
7	I	103	BCL	CHC-C1C-NC	2.25	127.62	124.51
8	K	103	U4Z	CBA-CBE-CBF	2.25	130.24	123.22
7	A	103	BCL	O2A-CGA-O1A	-2.25	116.10	123.14
7	D	103	BCL	C3C-C2C-C1C	2.24	105.49	101.87
12	M	406	BPH	CMA-C3A-C4A	-2.24	109.47	114.38
7	Q	101	BCL	C3C-C4C-CHD	-2.23	118.63	123.39
7	A	103	BCL	C3C-C2C-C1C	2.23	105.47	101.87
7	G	103	BCL	CBC-CAC-C3C	2.22	118.42	113.47
7	G	102	BCL	C3C-C4C-CHD	-2.22	118.64	123.39
7	D	101	BCL	C3C-C4C-CHD	-2.22	118.65	123.39
10	C	505	PGV	O14-P-O13	-2.22	101.27	112.24
8	O	102	U4Z	CBJ-CBM-CBN	-2.22	116.29	123.22
7	M	405	BCL	CAA-C2A-C1A	2.22	119.24	111.97
7	R	102	BCL	C3C-C2C-C1C	2.21	105.45	101.87
7	J	101	BCL	C3C-C2C-C1C	2.21	105.44	101.87
7	F	101	BCL	C3C-C2C-C1C	2.21	105.44	101.87
7	K	102	BCL	CMD-C2D-C1D	2.21	128.60	124.71
8	K	103	U4Z	CBJ-CBM-CBN	-2.20	116.34	123.22
7	A	101	BCL	CGD-CBD-CAD	-2.20	103.62	110.73
7	A	101	BCL	CMD-C2D-C1D	2.20	128.58	124.71
7	G	102	BCL	CMD-C2D-C1D	2.19	128.58	124.71
8	Q	102	U4Z	CBJ-CBM-CBN	-2.19	116.37	123.22
8	D	104	U4Z	CAK-CAH-CAI	2.19	117.83	113.62
7	H	101	BCL	C3C-C4C-CHD	-2.18	118.73	123.39
8	O	102	U4Z	CAN-CAM-CAO	2.18	125.98	122.92
8	I	102	U4Z	CBJ-CBM-CBN	-2.18	116.42	123.22
7	D	101	BCL	CGD-CBD-CAD	-2.17	103.69	110.73
7	O	101	BCL	CMD-C2D-C1D	2.17	128.53	124.71
7	H	101	BCL	CGD-CBD-CAD	-2.17	103.72	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	502	HEM	CAD-CBD-CGD	-2.17	108.94	113.60
7	G	102	BCL	CGD-CBD-CAD	-2.16	103.72	110.73
7	O	101	BCL	C3C-C4C-CHD	-2.16	118.77	123.39
7	J	101	BCL	C2A-C1A-CHA	2.16	127.64	123.86
8	D	104	U4Z	CBC-CAY-CAX	2.16	128.89	122.65
7	Q	101	BCL	CGD-CBD-CAD	-2.16	103.75	110.73
7	A	103	BCL	C2A-C1A-CHA	2.16	127.63	123.86
7	I	103	BCL	C3C-C2C-C1C	2.15	105.35	101.87
7	D	103	BCL	C2A-C1A-CHA	2.15	127.62	123.86
7	A	103	BCL	CED-O2D-CGD	-2.15	111.07	115.94
7	G	102	BCL	CBB-CAB-C3B	2.15	126.72	120.34
7	O	101	BCL	CGD-CBD-CAD	-2.15	103.78	110.73
7	K	102	BCL	CBB-CAB-C3B	2.14	126.70	120.34
7	K	102	BCL	CGD-CBD-CAD	-2.14	103.80	110.73
7	A	101	BCL	CBB-CAB-C3B	2.14	126.70	120.34
7	I	103	BCL	C2A-C1A-CHA	2.14	127.60	123.86
7	L	402	BCL	C1C-NC-C4C	2.14	107.67	106.71
8	I	101	U4Z	CAP-CAQ-CAR	-2.14	120.41	126.42
7	D	101	BCL	CBB-CAB-C3B	2.14	126.69	120.34
7	I	103	BCL	CED-O2D-CGD	-2.14	111.10	115.94
7	P	102	BCL	C2A-C1A-CHA	2.14	127.59	123.86
7	P	102	BCL	C3C-C2C-C1C	2.13	105.31	101.87
8	R	101	U4Z	CAN-CAM-CAO	-2.13	119.94	122.92
7	L	402	BCL	CAA-C2A-C1A	-2.13	104.99	111.97
12	M	406	BPH	CMC-C2C-C1C	-2.13	109.71	114.38
8	A	102	U4Z	CAF-CAB-CAD	2.13	113.75	110.30
7	M	405	BCL	C16-C15-C13	-2.12	109.05	115.92
7	O	101	BCL	CBB-CAB-C3B	2.12	126.65	120.34
8	G	101	U4Z	CAT-CAX-CAY	-2.12	120.50	127.75
8	Q	102	U4Z	CAN-CAM-CAO	2.12	125.89	122.92
8	I	102	U4Z	CBA-CBE-CBF	-2.11	116.62	123.22
7	R	102	BCL	C2A-C1A-CHA	2.11	127.55	123.86
7	R	102	BCL	CED-O2D-CGD	-2.11	111.16	115.94
7	F	101	BCL	C2A-C1A-CHA	2.11	127.55	123.86
7	F	101	BCL	O2A-CGA-O1A	-2.11	116.53	123.14
7	A	104	BCL	CED-O2D-CGD	-2.11	111.17	115.94
7	F	101	BCL	CAC-C3C-C2C	2.10	119.51	114.26
8	K	103	U4Z	CAN-CAM-CAO	2.10	125.87	122.92
7	H	101	BCL	CBB-CAB-C3B	2.10	126.57	120.34
7	K	102	BCL	CED-O2D-CGD	-2.10	111.19	115.94
7	O	101	BCL	CHC-C1C-NC	2.10	127.41	124.51
7	H	101	BCL	CHC-C1C-NC	2.09	127.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	104	BCL	CED-O2D-CGD	-2.09	111.20	115.94
7	Q	101	BCL	CBB-CAB-C3B	2.09	126.55	120.34
7	J	101	BCL	CED-O2D-CGD	-2.09	111.21	115.94
7	H	101	BCL	CED-O2D-CGD	-2.09	111.21	115.94
7	D	101	BCL	CHC-C1C-NC	2.09	127.40	124.51
7	A	101	BCL	CED-O2D-CGD	-2.09	111.21	115.94
7	O	101	BCL	CED-O2D-CGD	-2.09	111.21	115.94
7	A	104	BCL	CHC-C1C-NC	2.09	127.40	124.51
7	J	101	BCL	CAA-CBA-CGA	-2.08	107.17	113.25
8	K	103	U4Z	CAI-CAH-CAD	-2.08	119.72	122.73
7	L	402	BCL	C2A-C1A-CHA	2.07	127.49	123.86
8	O	102	U4Z	CAI-CAH-CAD	-2.07	119.72	122.73
7	R	102	BCL	CAA-CBA-CGA	-2.07	107.19	113.25
7	K	104	BCL	CMC-C2C-C3C	-2.07	105.48	113.83
7	Q	101	BCL	CED-O2D-CGD	-2.07	111.26	115.94
9	C	503	HEM	C3D-C4D-ND	-2.06	107.87	110.17
8	D	104	U4Z	CBJ-CBM-CBN	-2.06	116.80	123.22
7	H	101	BCL	C2A-C3A-C4A	-2.06	99.16	101.78
7	M	405	BCL	C11-C12-C13	-2.06	109.27	115.92
7	G	102	BCL	CED-O2D-CGD	-2.06	111.29	115.94
7	E	101	BCL	CED-O2D-CGD	-2.05	111.29	115.94
8	D	104	U4Z	CAS-CAW-CBA	2.05	128.19	121.98
8	R	101	U4Z	CAU-CAR-CAV	-2.05	120.05	122.92
7	R	103	BCL	CED-O2D-CGD	-2.05	111.30	115.94
12	M	401	BPH	C4-C3-C2	-2.05	118.42	123.68
7	M	402	BCL	OBD-CAD-C3D	-2.05	123.59	128.52
8	I	102	U4Z	CAG-CAB-CAF	-2.05	102.25	108.53
7	M	405	BCL	CMD-C2D-C3D	-2.05	122.91	127.61
7	D	101	BCL	CED-O2D-CGD	-2.04	111.31	115.94
7	L	402	BCL	CMB-C2B-C3B	2.04	128.50	124.68
7	A	103	BCL	CAA-CBA-CGA	-2.04	107.28	113.25
7	O	103	BCL	O2A-CGA-CBA	2.04	120.28	112.23
8	B	101	U4Z	CAT-CAS-CAW	2.03	119.66	112.98
7	K	102	BCL	CHC-C1C-NC	2.03	127.32	124.51
7	G	102	BCL	CHC-C1C-NC	2.02	127.31	124.51
7	I	104	BCL	CGD-CBD-CAD	-2.02	104.20	110.73
7	K	104	BCL	CHC-C1C-NC	2.01	127.30	124.51
7	A	104	BCL	CGD-CBD-CAD	-2.01	104.21	110.73
12	L	403	BPH	O1A-CGA-CBA	-2.01	115.88	123.73
7	R	103	BCL	CGD-CBD-CAD	-2.01	104.22	110.73
8	Q	102	U4Z	CAI-CAH-CAD	-2.01	119.81	122.73
7	E	101	BCL	CHC-C1C-NC	2.01	127.29	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	101	BCL	CMB-C2B-C3B	2.01	128.44	124.68
7	I	104	BCL	CHC-C1C-NC	2.01	127.29	124.51
7	E	101	BCL	CGD-CBD-CAD	-2.01	104.22	110.73
7	G	103	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
8	D	102	U4Z	CAS-CAT-CAX	2.01	118.48	111.88
8	K	101	U4Z	CAC-CAE-CAI	2.01	115.86	111.38
7	D	103	BCL	O2A-CGA-CBA	2.00	120.15	112.23
7	L	402	BCL	O2A-C1-C2	-2.00	103.37	108.64
7	G	103	BCL	CHC-C1C-NC	2.00	127.28	124.51
7	R	103	BCL	CHC-C1C-NC	2.00	127.28	124.51

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	L	403	BPH	C8
12	L	403	BPH	C13
12	M	401	BPH	C8
12	M	401	BPH	C13

All (437) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	101	BCL	CHA-CBD-CGD-O1D
7	A	103	BCL	CBA-CGA-O2A-C1
7	A	103	BCL	O1A-CGA-O2A-C1
7	A	103	BCL	C4C-C3C-CAC-CBC
7	A	104	BCL	C4C-C3C-CAC-CBC
7	D	101	BCL	CHA-CBD-CGD-O1D
7	D	103	BCL	C1A-C2A-CAA-CBA
7	D	103	BCL	C3A-C2A-CAA-CBA
7	D	103	BCL	CBA-CGA-O2A-C1
7	D	103	BCL	C2C-C3C-CAC-CBC
7	D	103	BCL	C4C-C3C-CAC-CBC
7	D	103	BCL	CHA-CBD-CGD-O1D
7	D	103	BCL	CHA-CBD-CGD-O2D
7	E	101	BCL	C4C-C3C-CAC-CBC
7	F	101	BCL	C2A-CAA-CBA-CGA
7	F	101	BCL	C2C-C3C-CAC-CBC
7	F	101	BCL	C4C-C3C-CAC-CBC
7	G	102	BCL	CHA-CBD-CGD-O1D
7	G	103	BCL	C2C-C3C-CAC-CBC
7	G	103	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
7	G	103	BCL	CBD-CGD-O2D-CED
7	H	101	BCL	CHA-CBD-CGD-O1D
7	I	103	BCL	C4C-C3C-CAC-CBC
7	I	104	BCL	C4C-C3C-CAC-CBC
7	J	101	BCL	CBA-CGA-O2A-C1
7	J	101	BCL	O1A-CGA-O2A-C1
7	J	101	BCL	C4C-C3C-CAC-CBC
7	K	102	BCL	CHA-CBD-CGD-O1D
7	K	104	BCL	C2C-C3C-CAC-CBC
7	K	104	BCL	CHA-CBD-CGD-O1D
7	K	104	BCL	CHA-CBD-CGD-O2D
7	M	402	BCL	C4C-C3C-CAC-CBC
7	M	402	BCL	CBD-CGD-O2D-CED
7	O	101	BCL	CHA-CBD-CGD-O1D
7	P	102	BCL	C4C-C3C-CAC-CBC
7	Q	101	BCL	CHA-CBD-CGD-O1D
7	R	102	BCL	CBA-CGA-O2A-C1
7	R	102	BCL	O1A-CGA-O2A-C1
7	R	102	BCL	C4C-C3C-CAC-CBC
7	R	103	BCL	C1A-C2A-CAA-CBA
7	R	103	BCL	C4C-C3C-CAC-CBC
8	A	102	U4Z	CAH-CAD-CAJ-CAL
8	A	102	U4Z	CAJ-CAL-CAM-CAN
8	A	102	U4Z	CAJ-CAL-CAM-CAO
8	A	102	U4Z	CBE-CBF-CBH-CBJ
8	A	102	U4Z	CBE-CBF-CBH-CBK
8	B	101	U4Z	CAS-CAW-CBA-CBE
8	B	101	U4Z	CAZ-CAW-CBA-CBE
8	D	102	U4Z	CAB-CAD-CAJ-CAL
8	D	102	U4Z	CAP-CAQ-CAR-CAV
8	D	102	U4Z	CAT-CAS-CAW-CAZ
8	D	104	U4Z	CAB-CAD-CAJ-CAL
8	D	104	U4Z	CAH-CAD-CAJ-CAL
8	D	104	U4Z	CAP-CAQ-CAR-CAV
8	D	104	U4Z	CAR-CAV-CBB-CBG
8	D	104	U4Z	CBI-CBL-CBN-CBM
8	G	101	U4Z	CAJ-CAL-CAM-CAN
8	G	101	U4Z	CAM-CAO-CAP-CAQ
8	G	101	U4Z	CBI-CBL-CBN-CBM
8	G	101	U4Z	CBO-CBL-CBN-CBM
8	I	101	U4Z	CAH-CAD-CAJ-CAL
8	I	101	U4Z	CAP-CAQ-CAR-CAU

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Mol	Chain	Res	Type	Atoms
8	I	101	U4Z	CAT-CAS-CAW-CAZ
8	I	101	U4Z	CAT-CAS-CAW-CBA
8	I	101	U4Z	CBE-CBF-CBH-CBJ
8	I	101	U4Z	CBE-CBF-CBH-CBK
8	I	101	U4Z	CBI-CBL-CBN-CBM
8	I	101	U4Z	CBO-CBL-CBN-CBM
8	I	102	U4Z	CAJ-CAL-CAM-CAN
8	I	102	U4Z	CAJ-CAL-CAM-CAO
8	I	102	U4Z	CAW-CAS-CAT-CAX
8	I	102	U4Z	CAT-CAS-CAW-CAZ
8	I	102	U4Z	CAT-CAS-CAW-CBA
8	I	102	U4Z	CAR-CAV-CBB-CBG
8	K	103	U4Z	CAJ-CAL-CAM-CAN
8	O	102	U4Z	CAJ-CAL-CAM-CAN
8	P	101	U4Z	CAS-CAW-CBA-CBE
8	P	101	U4Z	CAZ-CAW-CBA-CBE
8	Q	102	U4Z	CAJ-CAL-CAM-CAN
8	R	101	U4Z	CAB-CAD-CAJ-CAL
8	R	101	U4Z	CAM-CAO-CAP-CAQ
8	R	101	U4Z	CAW-CAS-CAT-CAX
8	R	101	U4Z	CBH-CBJ-CBM-CBN
8	R	101	U4Z	CBO-CBL-CBN-CBM
9	C	501	HEM	C2B-C3B-CAB-CBB
9	C	502	HEM	C2B-C3B-CAB-CBB
9	C	503	HEM	C2B-C3B-CAB-CBB
9	C	503	HEM	C4B-C3B-CAB-CBB
9	C	504	HEM	C2B-C3B-CAB-CBB
9	C	504	HEM	C4B-C3B-CAB-CBB
10	C	505	PGV	C03-O11-P-O13
10	C	505	PGV	O12-C04-C05-O05
11	L	401	MQE	CAM-CAG-CAW-CBH
11	L	401	MQE	CAM-CAG-CAW-CBY
11	M	403	MQE	CAM-CAG-CAW-CBH
11	M	403	MQE	CAM-CAG-CAW-CBY
11	M	403	MQE	CAV-CAH-CAO-CBI
11	M	403	MQE	CBB-CAN-CAS-CBH
12	L	403	BPH	C4C-C3C-CAC-CBC
12	L	403	BPH	C3A-C2A-CAA-CBA
12	L	403	BPH	C1A-C2A-CAA-CBA
12	L	403	BPH	C11-C12-C13-C14
12	M	401	BPH	CBD-CGD-O2D-CED
12	M	401	BPH	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
12	M	401	BPH	C2C-C3C-CAC-CBC
12	M	401	BPH	C3A-C2A-CAA-CBA
12	M	401	BPH	C2A-CAA-CBA-CGA
12	M	401	BPH	C11-C10-C8-C9
7	G	103	BCL	O1D-CGD-O2D-CED
7	M	402	BCL	O1D-CGD-O2D-CED
7	A	101	BCL	O1A-CGA-O2A-C1
7	D	101	BCL	O1A-CGA-O2A-C1
7	G	102	BCL	O1A-CGA-O2A-C1
7	P	102	BCL	O1A-CGA-O2A-C1
7	D	103	BCL	O1A-CGA-O2A-C1
7	K	102	BCL	O1A-CGA-O2A-C1
7	O	101	BCL	O1A-CGA-O2A-C1
7	Q	101	BCL	O1A-CGA-O2A-C1
12	M	401	BPH	O1D-CGD-O2D-CED
7	P	102	BCL	CBA-CGA-O2A-C1
7	O	103	BCL	CBD-CGD-O2D-CED
12	M	406	BPH	CBD-CGD-O2D-CED
10	C	505	PGV	O02-C1-O01-C02
7	K	102	BCL	CBA-CGA-O2A-C1
7	O	101	BCL	CBA-CGA-O2A-C1
7	Q	101	BCL	CBA-CGA-O2A-C1
7	M	405	BCL	C3-C5-C6-C7
12	M	401	BPH	C3-C5-C6-C7
7	D	103	BCL	CBD-CGD-O2D-CED
7	M	405	BCL	C4-C3-C5-C6
8	A	102	U4Z	CAT-CAS-CAW-CAZ
8	A	102	U4Z	CAT-CAS-CAW-CBA
7	A	101	BCL	CBD-CGD-O2D-CED
7	D	101	BCL	CBD-CGD-O2D-CED
7	G	102	BCL	CBD-CGD-O2D-CED
7	H	101	BCL	CBD-CGD-O2D-CED
7	K	102	BCL	CBD-CGD-O2D-CED
7	O	101	BCL	CBD-CGD-O2D-CED
7	Q	101	BCL	CBD-CGD-O2D-CED
7	A	101	BCL	O1D-CGD-O2D-CED
7	D	101	BCL	O1D-CGD-O2D-CED
7	G	102	BCL	O1D-CGD-O2D-CED
7	H	101	BCL	O1D-CGD-O2D-CED
7	K	102	BCL	O1D-CGD-O2D-CED
7	O	101	BCL	O1D-CGD-O2D-CED
7	Q	101	BCL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
7	A	101	BCL	CBA-CGA-O2A-C1
7	D	101	BCL	CBA-CGA-O2A-C1
7	G	102	BCL	CBA-CGA-O2A-C1
8	A	102	U4Z	CAM-CAO-CAP-CAQ
8	D	102	U4Z	CAM-CAO-CAP-CAQ
8	D	102	U4Z	CAW-CBA-CBE-CBF
8	D	102	U4Z	CBB-CBG-CBI-CBL
8	D	104	U4Z	CAM-CAO-CAP-CAQ
8	D	104	U4Z	CAW-CBA-CBE-CBF
8	G	101	U4Z	CAR-CAV-CBB-CBG
8	G	101	U4Z	CBB-CBG-CBI-CBL
8	I	102	U4Z	CBB-CBG-CBI-CBL
7	F	101	BCL	CBD-CGD-O2D-CED
7	A	104	BCL	O1D-CGD-O2D-CED
7	E	101	BCL	O1D-CGD-O2D-CED
7	I	104	BCL	O1D-CGD-O2D-CED
7	R	103	BCL	O1D-CGD-O2D-CED
7	A	104	BCL	CBD-CGD-O2D-CED
7	E	101	BCL	CBD-CGD-O2D-CED
7	I	104	BCL	CBD-CGD-O2D-CED
7	R	103	BCL	CBD-CGD-O2D-CED
7	L	402	BCL	C4-C3-C5-C6
8	K	103	U4Z	CAT-CAS-CAW-CAZ
8	O	102	U4Z	CAT-CAS-CAW-CAZ
8	Q	102	U4Z	CAT-CAS-CAW-CAZ
11	L	401	MQE	CAS-CAN-CBB-CCA
7	L	402	BCL	C2-C3-C5-C6
8	D	102	U4Z	CAT-CAS-CAW-CBA
8	K	103	U4Z	CAT-CAS-CAW-CBA
8	O	102	U4Z	CAT-CAS-CAW-CBA
8	Q	102	U4Z	CAT-CAS-CAW-CBA
11	L	401	MQE	CAS-CAN-CBB-CBL
8	D	104	U4Z	CAW-CAS-CAT-CAX
8	P	101	U4Z	CAW-CAS-CAT-CAX
11	M	403	MQE	CAT-CAF-CAK-CBE
10	C	505	PGV	C2-C1-O01-C02
8	I	101	U4Z	CAW-CBA-CBE-CBF
8	R	101	U4Z	CAR-CAV-CBB-CBG
8	R	101	U4Z	CAW-CBA-CBE-CBF
7	M	405	BCL	C2-C3-C5-C6
7	L	402	BCL	C14-C13-C15-C16
7	M	402	BCL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
8	A	102	U4Z	CAP-CAQ-CAR-CAU
8	D	102	U4Z	CAP-CAQ-CAR-CAU
8	D	104	U4Z	CAJ-CAL-CAM-CAN
8	D	104	U4Z	CAP-CAQ-CAR-CAU
8	D	104	U4Z	CBO-CBL-CBN-CBM
8	R	101	U4Z	CBE-CBF-CBH-CBK
8	A	102	U4Z	CAP-CAQ-CAR-CAV
8	D	104	U4Z	CAJ-CAL-CAM-CAO
8	G	101	U4Z	CAJ-CAL-CAM-CAO
8	R	101	U4Z	CBE-CBF-CBH-CBJ
8	R	101	U4Z	CBI-CBL-CBN-CBM
7	M	405	BCL	CBA-CGA-O2A-C1
7	L	402	BCL	C8-C10-C11-C12
7	M	402	BCL	C8-C10-C11-C12
12	L	403	BPH	C5-C6-C7-C8
7	A	103	BCL	CBD-CGD-O2D-CED
7	I	103	BCL	CBD-CGD-O2D-CED
7	J	101	BCL	CBD-CGD-O2D-CED
7	R	102	BCL	CBD-CGD-O2D-CED
7	O	103	BCL	O1D-CGD-O2D-CED
10	C	505	PGV	C13-C14-C15-C16
9	C	504	HEM	C3D-CAD-CBD-CGD
12	L	403	BPH	C10-C11-C12-C13
8	A	102	U4Z	CBB-CBG-CBI-CBL
8	D	104	U4Z	CBB-CBG-CBI-CBL
8	R	101	U4Z	CBB-CBG-CBI-CBL
7	G	102	BCL	C2A-CAA-CBA-CGA
7	L	402	BCL	C2A-CAA-CBA-CGA
12	M	406	BPH	O1D-CGD-O2D-CED
11	L	401	MQE	CAP-CAC-CAI-CBD
11	L	401	MQE	CAV-CAH-CAO-CBI
11	L	401	MQE	CAZ-CAU-CBA-CBN
11	M	403	MQE	CAP-CAC-CAI-CBD
11	M	403	MQE	CAQ-CAD-CAJ-CBC
11	M	403	MQE	CAW-CAG-CAM-CBG
12	M	401	BPH	C13-C15-C16-C17
10	C	505	PGV	C2-C3-C4-C5
7	M	405	BCL	O1A-CGA-O2A-C1
10	C	505	PGV	C03-O11-P-O12
7	D	103	BCL	O1D-CGD-O2D-CED
11	M	403	MQE	CAO-CAH-CAV-CBX
7	A	101	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
7	D	101	BCL	C2A-CAA-CBA-CGA
7	K	102	BCL	C2A-CAA-CBA-CGA
7	O	101	BCL	C2A-CAA-CBA-CGA
7	Q	101	BCL	C2A-CAA-CBA-CGA
7	K	104	BCL	CBA-CGA-O2A-C1
8	A	102	U4Z	CAR-CAV-CBB-CBG
7	F	101	BCL	O1D-CGD-O2D-CED
10	C	505	PGV	C6-C7-C8-C9
10	C	505	PGV	C21-C22-C23-C24
7	L	402	BCL	C11-C10-C8-C9
8	G	101	U4Z	CBE-CBF-CBH-CBK
8	I	102	U4Z	CAP-CAQ-CAR-CAU
10	C	505	PGV	C04-C05-C06-O06
8	G	101	U4Z	CBE-CBF-CBH-CBJ
8	I	101	U4Z	CAP-CAQ-CAR-CAV
8	I	102	U4Z	CAP-CAQ-CAR-CAV
10	C	505	PGV	C3-C4-C5-C6
7	I	103	BCL	O1D-CGD-O2D-CED
7	R	102	BCL	O1D-CGD-O2D-CED
7	A	103	BCL	O1D-CGD-O2D-CED
7	J	101	BCL	O1D-CGD-O2D-CED
7	A	101	BCL	C3A-C2A-CAA-CBA
7	D	101	BCL	C3A-C2A-CAA-CBA
7	G	102	BCL	C3A-C2A-CAA-CBA
7	K	102	BCL	C3A-C2A-CAA-CBA
7	O	101	BCL	C3A-C2A-CAA-CBA
7	Q	101	BCL	C3A-C2A-CAA-CBA
8	D	102	U4Z	CAR-CAV-CBB-CBG
8	G	101	U4Z	CAW-CBA-CBE-CBF
11	M	403	MQE	CAL-CAE-CAR-CBV
12	L	403	BPH	CBA-CGA-O2A-C1
7	K	104	BCL	O1A-CGA-O2A-C1
12	M	401	BPH	C16-C17-C18-C20
7	M	402	BCL	C13-C15-C16-C17
12	L	403	BPH	O1A-CGA-O2A-C1
7	M	402	BCL	C3-C5-C6-C7
8	D	102	U4Z	CAH-CAD-CAJ-CAL
8	I	101	U4Z	CAB-CAD-CAJ-CAL
8	I	102	U4Z	CAB-CAD-CAJ-CAL
8	R	101	U4Z	CAH-CAD-CAJ-CAL
7	L	402	BCL	C11-C10-C8-C7
11	M	403	MQE	CAL-CAE-CAR-CBD

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Mol	Chain	Res	Type	Atoms
12	M	401	BPH	C6-C7-C8-C10
12	M	401	BPH	C16-C17-C18-C19
10	C	505	PGV	C4-C5-C6-C7
9	C	501	HEM	C4B-C3B-CAB-CBB
9	C	502	HEM	C4B-C3B-CAB-CBB
10	C	505	PGV	C14-C15-C16-C17
10	C	505	PGV	C23-C24-C25-C26
7	M	405	BCL	C10-C11-C12-C13
11	M	403	MQE	CAO-CAH-CAV-CBF
7	A	103	BCL	C2A-CAA-CBA-CGA
7	I	103	BCL	C2A-CAA-CBA-CGA
7	J	101	BCL	C2A-CAA-CBA-CGA
7	R	102	BCL	C2A-CAA-CBA-CGA
8	D	102	U4Z	CAJ-CAL-CAM-CAN
12	L	403	BPH	C8-C10-C11-C12
8	K	103	U4Z	CAJ-CAL-CAM-CAO
8	O	102	U4Z	CAJ-CAL-CAM-CAO
8	Q	102	U4Z	CAJ-CAL-CAM-CAO
7	A	101	BCL	C1A-C2A-CAA-CBA
7	A	104	BCL	C1A-C2A-CAA-CBA
7	D	101	BCL	C1A-C2A-CAA-CBA
7	E	101	BCL	C1A-C2A-CAA-CBA
7	F	101	BCL	C1A-C2A-CAA-CBA
7	G	102	BCL	C1A-C2A-CAA-CBA
7	I	104	BCL	C1A-C2A-CAA-CBA
7	K	102	BCL	C1A-C2A-CAA-CBA
7	M	402	BCL	C1A-C2A-CAA-CBA
7	O	101	BCL	C1A-C2A-CAA-CBA
7	O	103	BCL	C1A-C2A-CAA-CBA
7	Q	101	BCL	C1A-C2A-CAA-CBA
12	L	403	BPH	C13-C15-C16-C17
7	A	104	BCL	C2C-C3C-CAC-CBC
7	E	101	BCL	C2C-C3C-CAC-CBC
7	I	104	BCL	C2C-C3C-CAC-CBC
7	R	103	BCL	C2C-C3C-CAC-CBC
9	C	504	HEM	C2A-CAA-CBA-CGA
10	C	505	PGV	C15-C16-C17-C18
7	O	103	BCL	CBA-CGA-O2A-C1
7	A	104	BCL	O2A-C1-C2-C3
8	I	102	U4Z	CAM-CAO-CAP-CAQ
8	D	104	U4Z	CAT-CAS-CAW-CAZ
12	M	406	BPH	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	M	406	BPH	CHA-CBD-CGD-O2D
7	M	402	BCL	C4-C3-C5-C6
11	L	401	MQE	CAJ-CAD-CAQ-CBU
11	L	401	MQE	CAL-CAE-CAR-CBV
12	M	401	BPH	C5-C6-C7-C8
7	L	402	BCL	C6-C7-C8-C10
7	L	402	BCL	C11-C12-C13-C15
11	L	401	MQE	CAL-CAE-CAR-CBD
7	L	402	BCL	C11-C12-C13-C14
8	A	102	U4Z	CBO-CBL-CBN-CBM
8	D	102	U4Z	CBO-CBL-CBN-CBM
8	R	101	U4Z	CAJ-CAL-CAM-CAN
8	A	102	U4Z	CBI-CBL-CBN-CBM
8	D	102	U4Z	CAJ-CAL-CAM-CAO
8	D	102	U4Z	CBI-CBL-CBN-CBM
11	L	401	MQE	CBM-CBJ-CBO-CCB
8	B	101	U4Z	CAT-CAS-CAW-CAZ
7	M	402	BCL	C2-C3-C5-C6
8	D	104	U4Z	CAT-CAS-CAW-CBA
11	L	401	MQE	CAJ-CAD-CAQ-CBE
7	M	402	BCL	C3A-C2A-CAA-CBA
8	D	102	U4Z	CBH-CBJ-CBM-CBN
8	I	101	U4Z	CBB-CBG-CBI-CBL
7	L	402	BCL	C15-C16-C17-C18
10	C	505	PGV	C20-C21-C22-C23
7	A	101	BCL	C3-C5-C6-C7
12	M	401	BPH	C10-C11-C12-C13
10	C	505	PGV	C19-C20-C21-C22
10	C	505	PGV	O12-C04-C05-C06
12	L	403	BPH	C6-C7-C8-C9
7	A	101	BCL	C4C-C3C-CAC-CBC
7	D	101	BCL	C4C-C3C-CAC-CBC
7	G	102	BCL	C4C-C3C-CAC-CBC
7	H	101	BCL	C4C-C3C-CAC-CBC
7	K	102	BCL	C4C-C3C-CAC-CBC
7	O	101	BCL	C4C-C3C-CAC-CBC
7	O	103	BCL	C4C-C3C-CAC-CBC
7	Q	101	BCL	C4C-C3C-CAC-CBC
7	M	402	BCL	C6-C7-C8-C10
12	L	403	BPH	C6-C7-C8-C10
12	L	403	BPH	C11-C12-C13-C15
12	M	401	BPH	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
10	C	505	PGV	C22-C23-C24-C25
7	F	101	BCL	CAD-CBD-CGD-O2D
8	K	101	U4Z	CAZ-CAW-CBA-CBE
10	C	505	PGV	C01-C02-O01-C1
10	C	505	PGV	O01-C02-C03-O11
7	L	402	BCL	C13-C15-C16-C17
7	L	402	BCL	CHA-CBD-CGD-O1D
7	L	402	BCL	CHA-CBD-CGD-O2D
8	R	101	U4Z	CAJ-CAL-CAM-CAO
7	K	104	BCL	C1A-C2A-CAA-CBA
8	A	102	U4Z	CBH-CBJ-CBM-CBN
10	C	505	PGV	C05-C04-O12-P
10	C	505	PGV	C03-O11-P-O14
7	F	101	BCL	CAD-CBD-CGD-O1D
7	L	402	BCL	C6-C7-C8-C9
8	A	102	U4Z	CBA-CBE-CBF-CBH
8	D	102	U4Z	CBA-CBE-CBF-CBH
8	D	104	U4Z	CBA-CBE-CBF-CBH
8	G	101	U4Z	CAO-CAP-CAQ-CAR
8	I	101	U4Z	CAO-CAP-CAQ-CAR
8	K	103	U4Z	CBA-CBE-CBF-CBH
8	O	102	U4Z	CBA-CBE-CBF-CBH
8	Q	102	U4Z	CBA-CBE-CBF-CBH
7	A	104	BCL	C2-C1-O2A-CGA
7	M	402	BCL	C2-C1-O2A-CGA
7	O	103	BCL	O1A-CGA-O2A-C1
8	B	101	U4Z	CAT-CAS-CAW-CBA
7	M	405	BCL	C6-C7-C8-C10
7	M	405	BCL	C6-C7-C8-C9
8	D	104	U4Z	CBE-CBF-CBH-CBK
9	C	502	HEM	CAD-CBD-CGD-O2D
8	I	101	U4Z	CAR-CAV-CBB-CBG
11	L	401	MQE	CAR-CAE-CAL-CBF
9	C	501	HEM	CAA-CBA-CGA-O1A
7	I	103	BCL	CAA-CBA-CGA-O2A
9	C	502	HEM	CAD-CBD-CGD-O1D
7	P	102	BCL	C2A-CAA-CBA-CGA
7	I	103	BCL	CAA-CBA-CGA-O1A
7	M	405	BCL	C11-C10-C8-C9
7	M	405	BCL	C16-C17-C18-C19
8	G	101	U4Z	CAU-CAR-CAV-CBB
8	I	101	U4Z	CAU-CAR-CAV-CBB

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Mol	Chain	Res	Type	Atoms
9	C	501	HEM	CAA-CBA-CGA-O2A
9	C	503	HEM	CAA-CBA-CGA-O1A
7	L	402	BCL	C12-C13-C15-C16
8	G	101	U4Z	CAQ-CAR-CAV-CBB
7	A	104	BCL	O1A-CGA-O2A-C1
12	M	401	BPH	C1A-C2A-CAA-CBA
8	I	102	U4Z	CAW-CBA-CBE-CBF
10	C	505	PGV	C24-C25-C26-C27
9	C	503	HEM	CAA-CBA-CGA-O2A
11	M	403	MQE	CAR-CAE-CAL-CBF
7	A	101	BCL	C2-C3-C5-C6
10	C	505	PGV	C9-C10-C11-C12
11	M	403	MQE	CAI-CAC-CAP-CBT
7	M	405	BCL	CAD-CBD-CGD-O2D
7	A	104	BCL	CBA-CGA-O2A-C1
8	D	104	U4Z	CAS-CAT-CAX-CAY
12	L	403	BPH	O2A-C1-C2-C3
7	A	103	BCL	CHA-CBD-CGD-O1D
7	F	101	BCL	CHA-CBD-CGD-O1D
7	I	103	BCL	CHA-CBD-CGD-O1D
7	J	101	BCL	CHA-CBD-CGD-O1D
7	P	102	BCL	CHA-CBD-CGD-O1D
7	R	102	BCL	CHA-CBD-CGD-O1D
7	D	103	BCL	CAA-CBA-CGA-O2A
8	A	102	U4Z	CAS-CAT-CAX-CAY
8	A	102	U4Z	CAB-CAD-CAJ-CAL
7	M	405	BCL	CAA-CBA-CGA-O2A
10	C	505	PGV	C7-C8-C9-C10
7	A	101	BCL	CAA-CBA-CGA-O2A
7	D	101	BCL	CAA-CBA-CGA-O2A
7	G	102	BCL	CAA-CBA-CGA-O2A
7	K	102	BCL	CAA-CBA-CGA-O2A
7	L	402	BCL	C16-C17-C18-C20
7	P	102	BCL	C2C-C3C-CAC-CBC
7	O	101	BCL	CAA-CBA-CGA-O2A
7	Q	101	BCL	CAA-CBA-CGA-O2A
7	D	103	BCL	CAA-CBA-CGA-O1A
11	M	403	MQE	CAZ-CAU-CBA-CBN
12	M	401	BPH	C15-C16-C17-C18

There are no ring outliers.

46 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	501	HEM	14	0
7	D	103	BCL	13	0
8	G	101	U4Z	2	0
7	D	101	BCL	3	0
7	P	102	BCL	15	0
7	I	103	BCL	4	0
8	I	102	U4Z	6	0
12	M	401	BPH	18	0
7	G	102	BCL	7	0
9	C	503	HEM	14	0
7	A	104	BCL	13	0
7	M	402	BCL	21	0
7	A	101	BCL	19	0
7	L	402	BCL	18	0
7	F	101	BCL	11	0
7	O	103	BCL	52	0
9	C	502	HEM	18	0
8	D	102	U4Z	13	0
7	K	102	BCL	13	0
8	P	101	U4Z	14	0
7	A	103	BCL	15	0
10	C	505	PGV	24	0
8	A	102	U4Z	17	0
8	Q	102	U4Z	6	0
8	B	101	U4Z	2	0
12	M	406	BPH	7	0
7	O	101	BCL	5	0
7	G	103	BCL	11	0
7	R	103	BCL	9	0
8	D	104	U4Z	18	0
8	R	101	U4Z	3	0
7	Q	101	BCL	9	0
12	L	403	BPH	12	0
8	K	101	U4Z	8	0
7	R	102	BCL	13	0
9	C	504	HEM	25	0
7	I	104	BCL	16	0
7	E	101	BCL	20	0
7	J	101	BCL	1	0
8	K	103	U4Z	5	0
8	O	102	U4Z	11	0
7	H	101	BCL	8	0
8	I	101	U4Z	12	0

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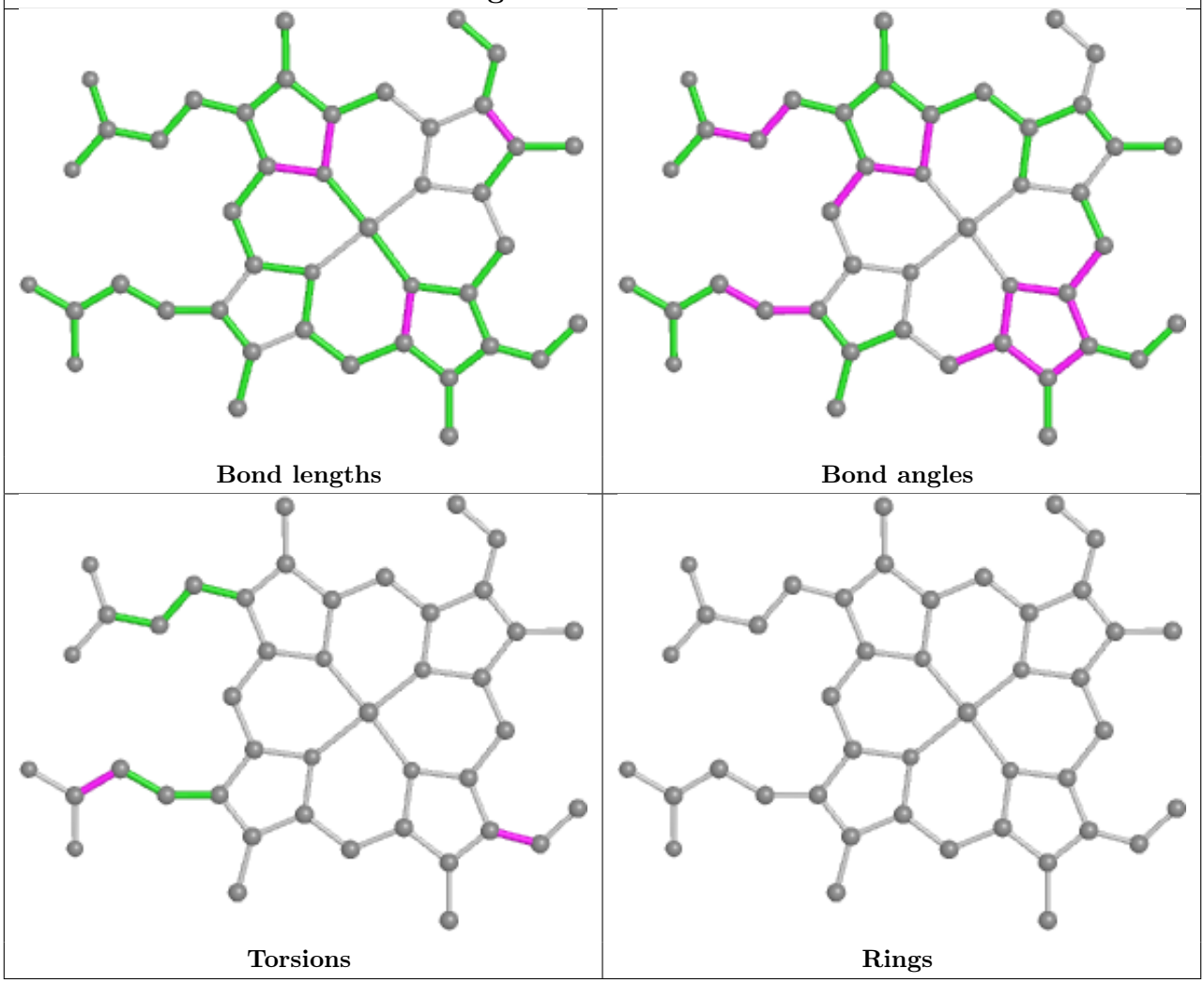
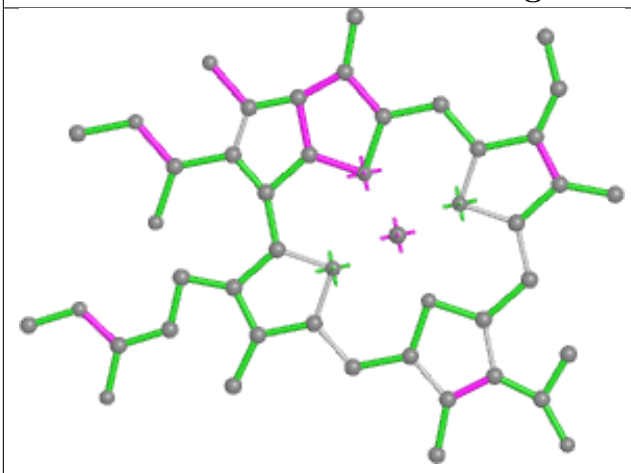
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	401	MQE	1	0
7	M	405	BCL	14	0
7	K	104	BCL	17	0

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.

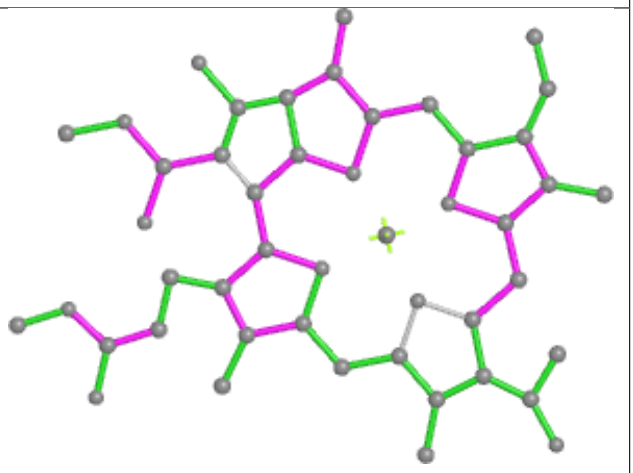
Ligand HEM C 501



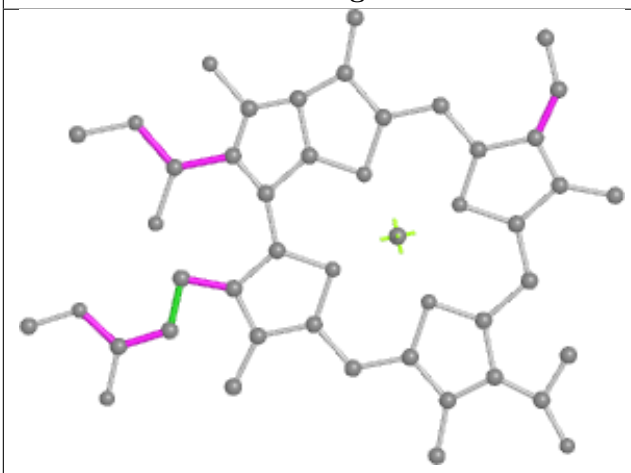
Ligand BCL D 103



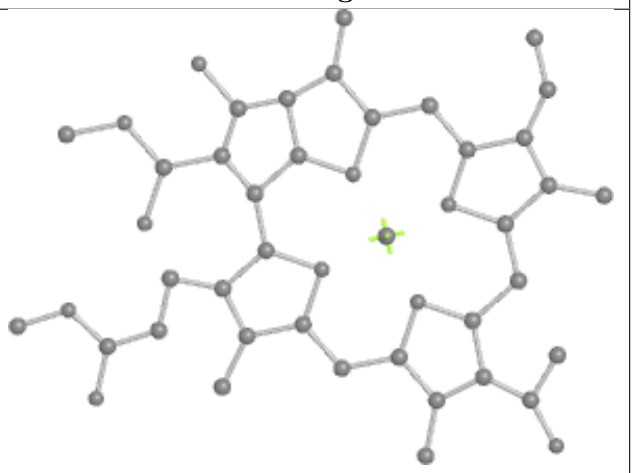
Bond lengths



Bond angles

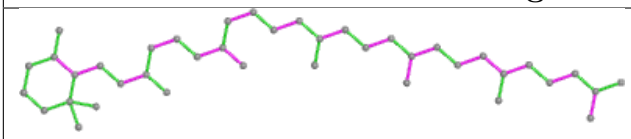


Torsions

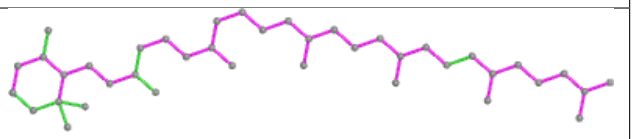


Rings

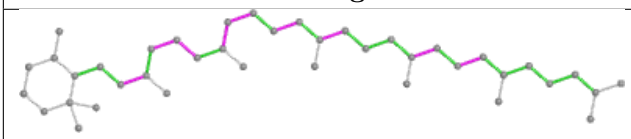
Ligand U4Z G 101



Bond lengths



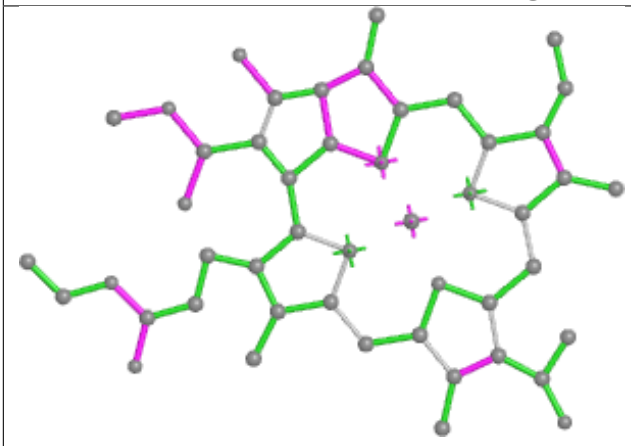
Bond angles



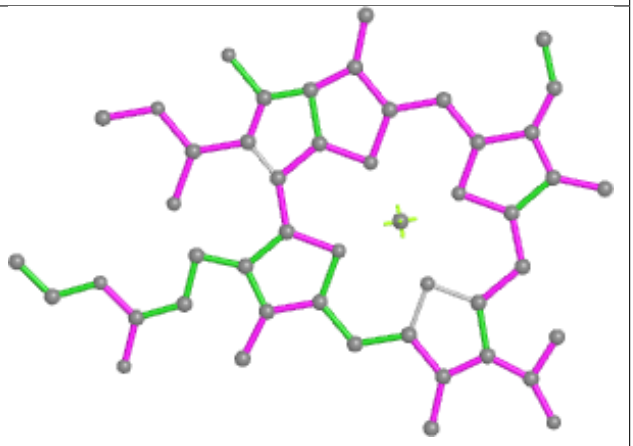
Torsions

Rings

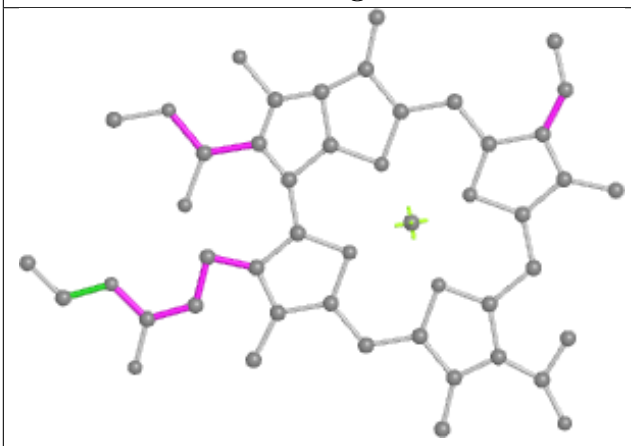
Ligand BCL D 101



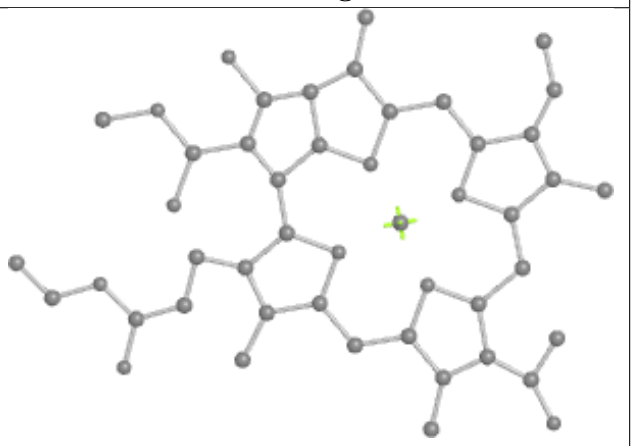
Bond lengths



Bond angles

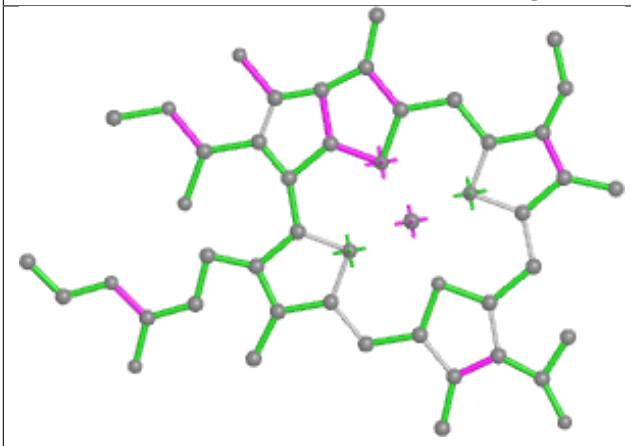


Torsions

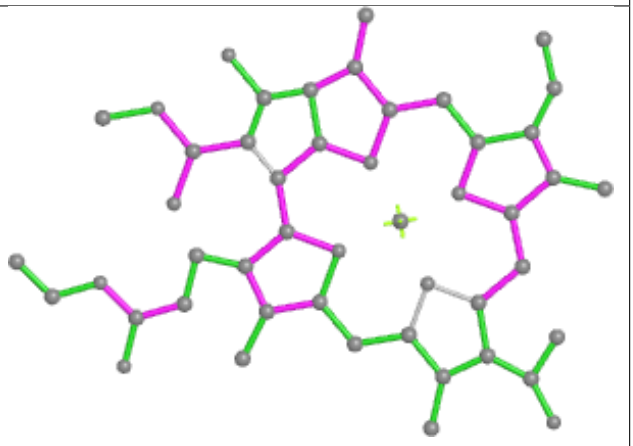


Rings

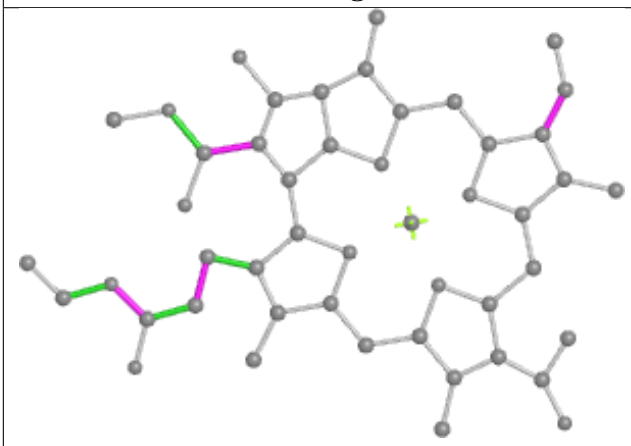
Ligand BCL P 102



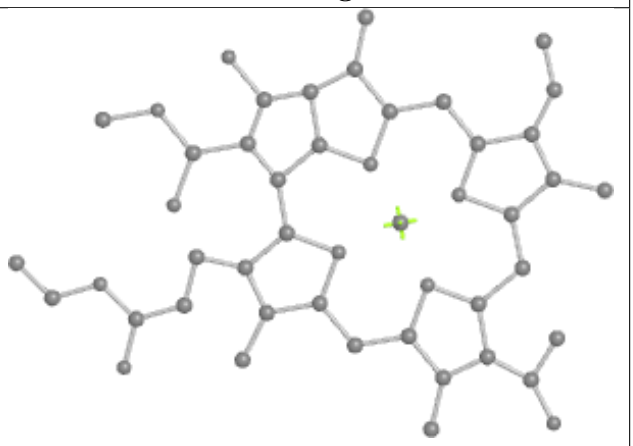
Bond lengths



Bond angles

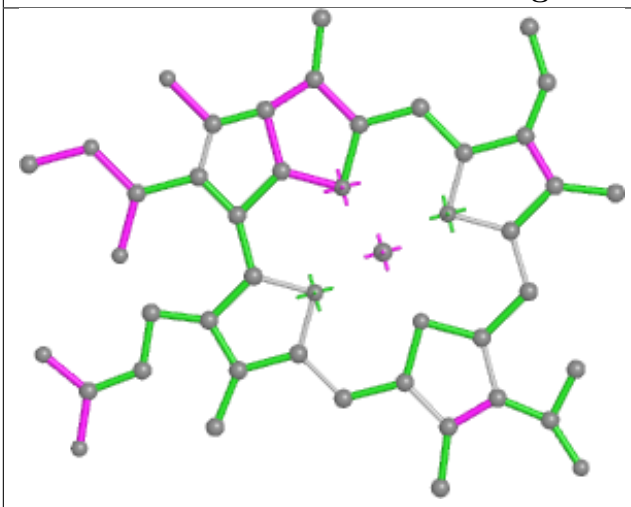


Torsions

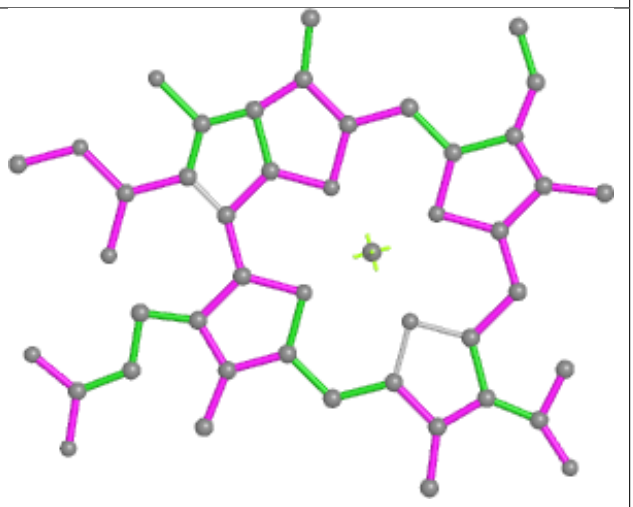


Rings

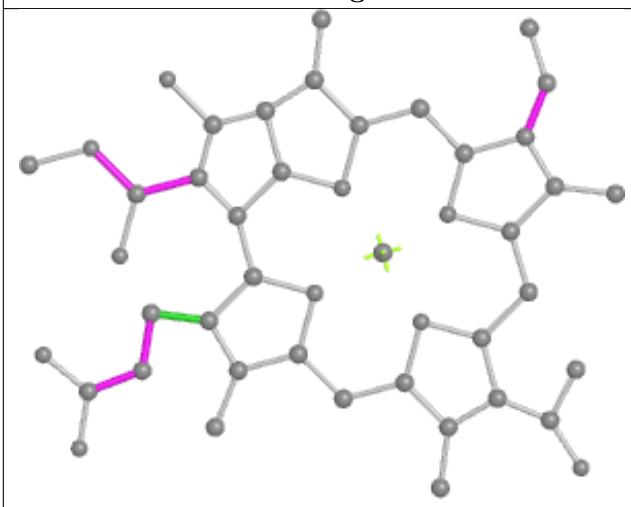
Ligand BCL I 103



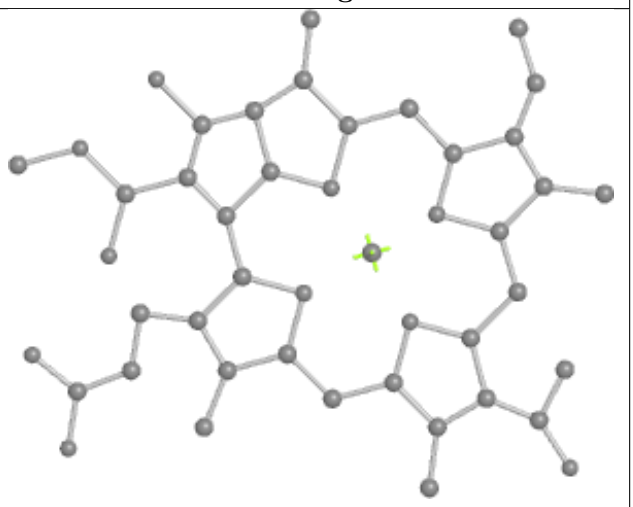
Bond lengths



Bond angles

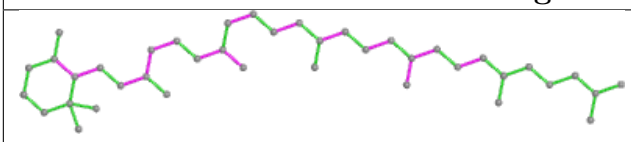


Torsions

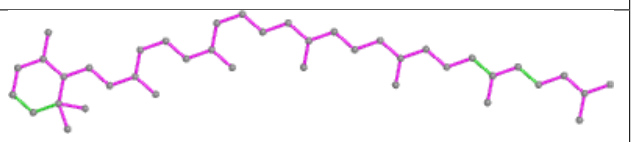


Rings

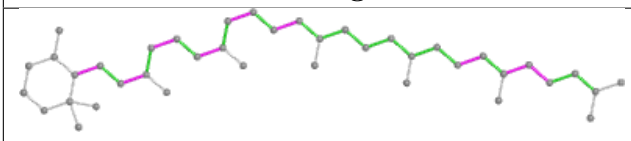
Ligand U4Z I 102



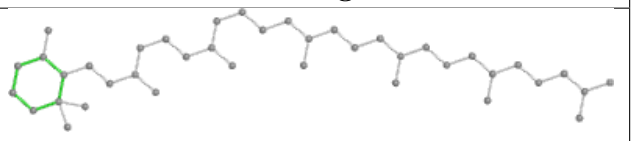
Bond lengths



Bond angles

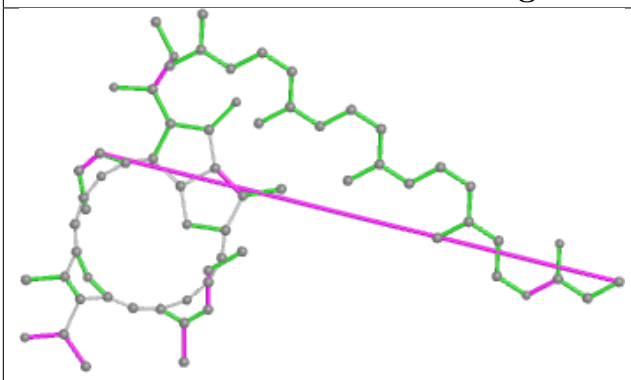


Torsions



Rings

Ligand BPH M 401



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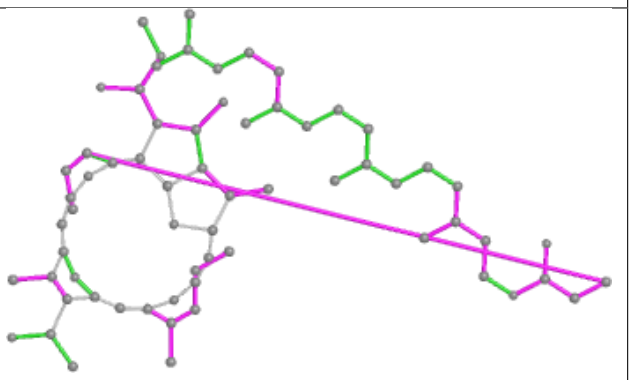
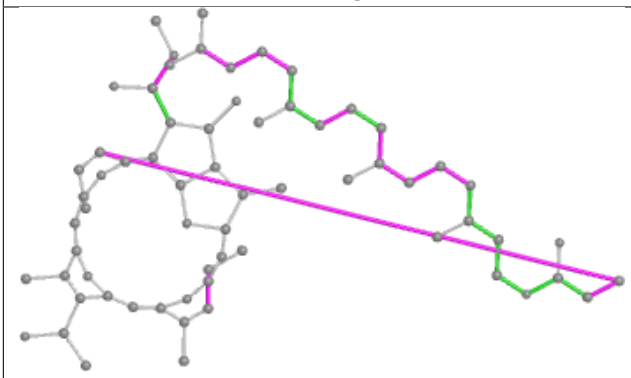
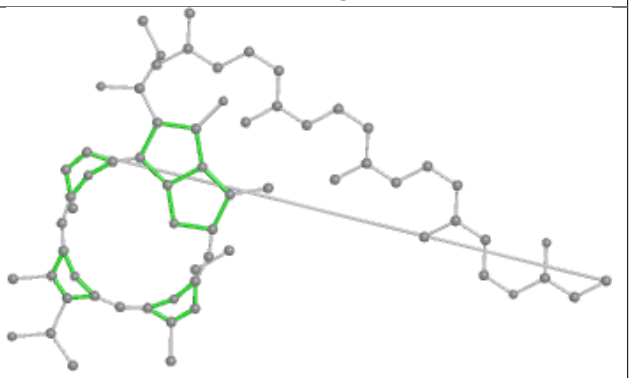


Bond angles

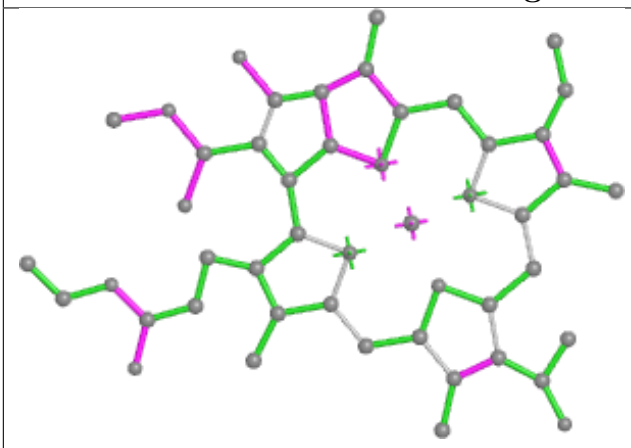


Torsions

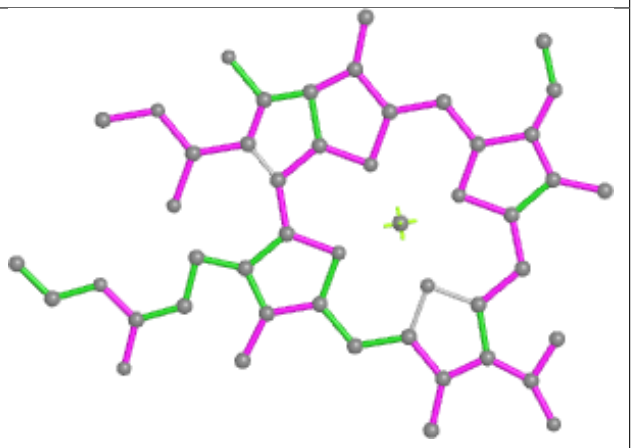


Rings

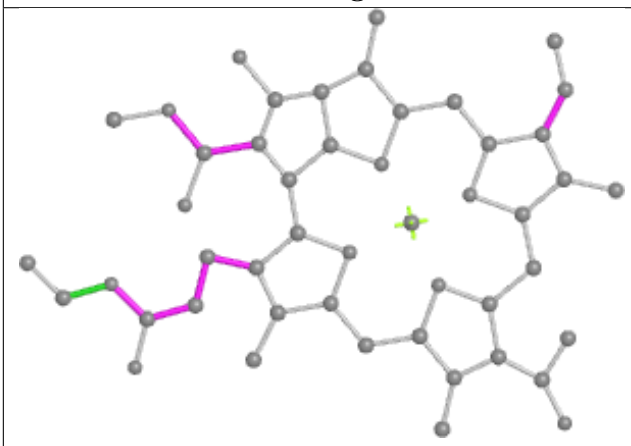
Ligand BCL G 102



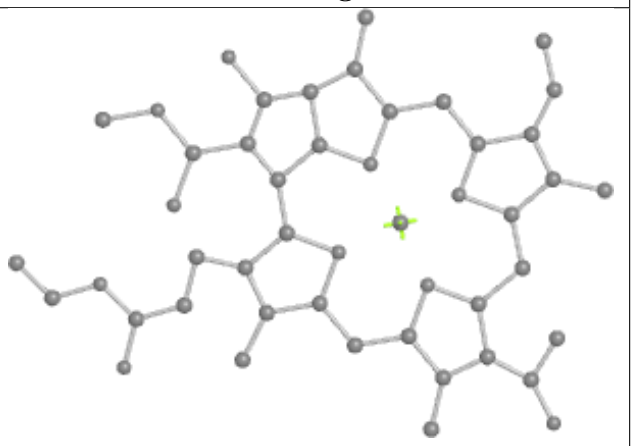
Bond lengths



Bond angles

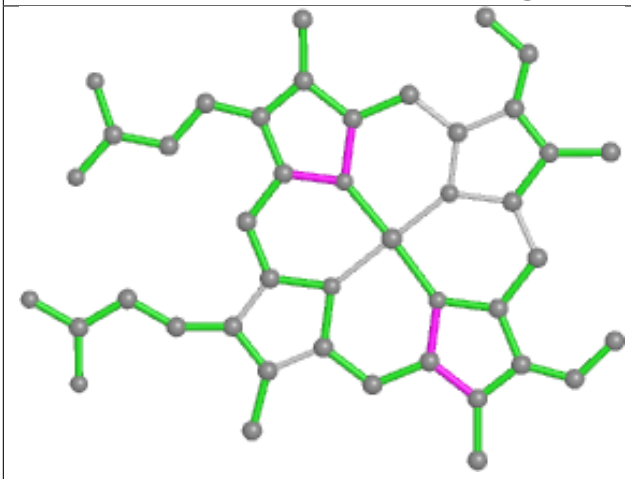


Torsions

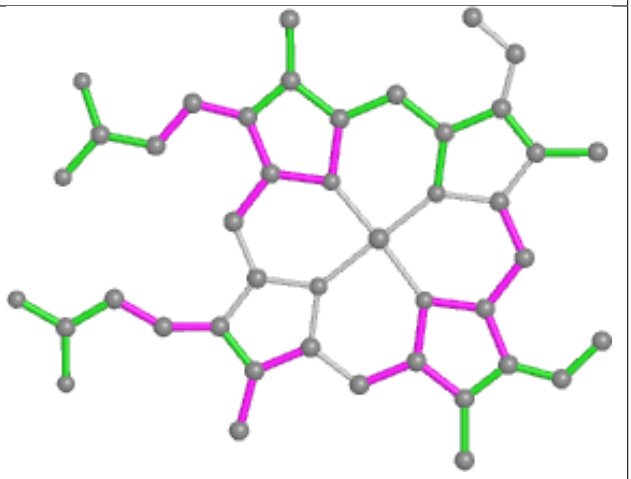


Rings

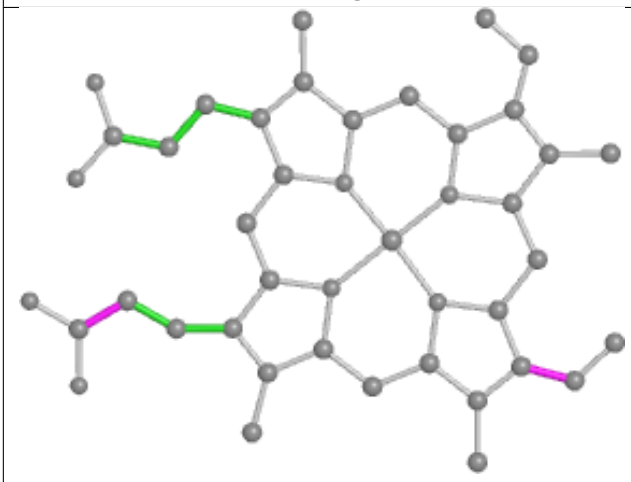
Ligand HEM C 503



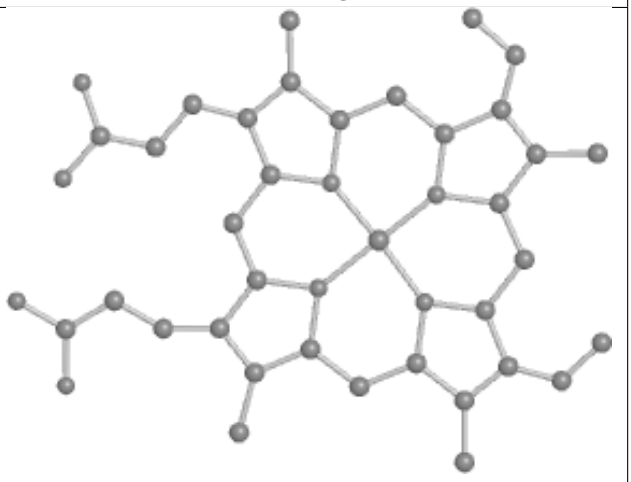
Bond lengths



Bond angles

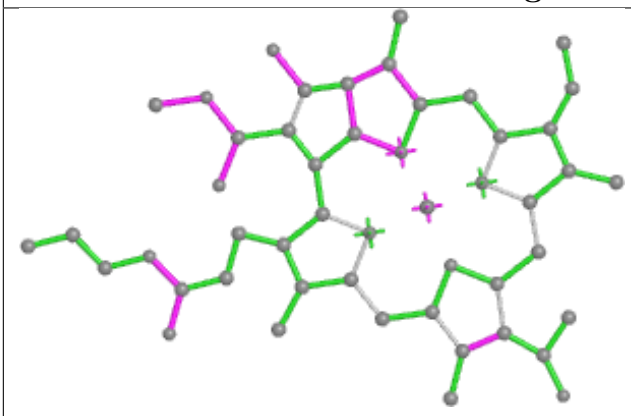


Torsions



Rings

Ligand BCL A 104



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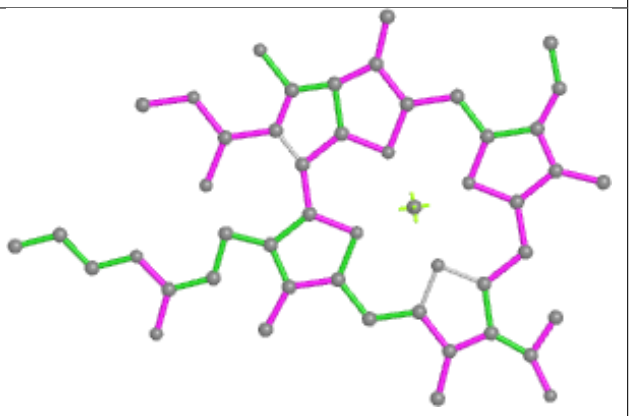
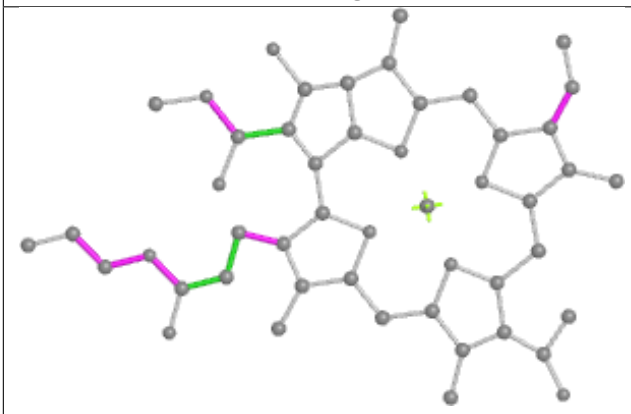
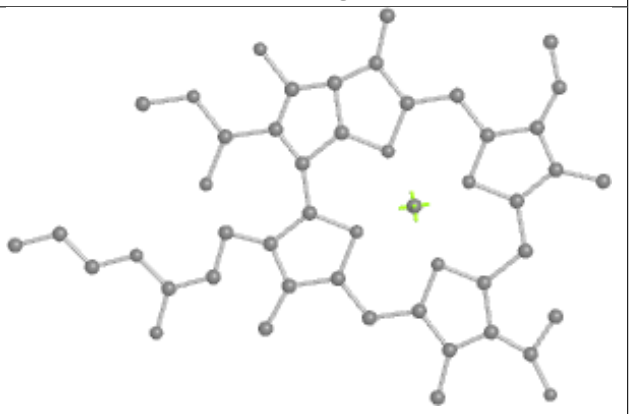


Bond angles

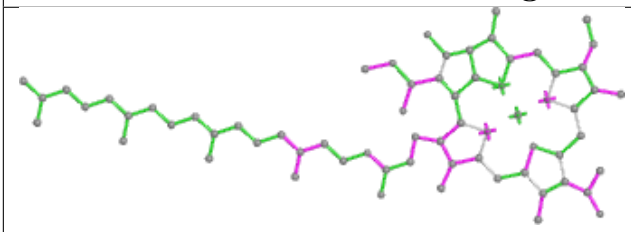


Torsions



Rings

Ligand BCL M 402



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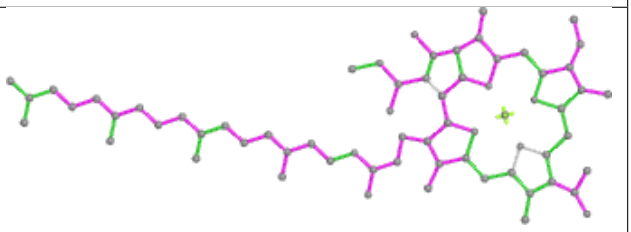
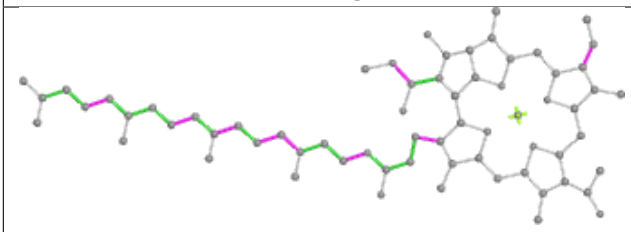
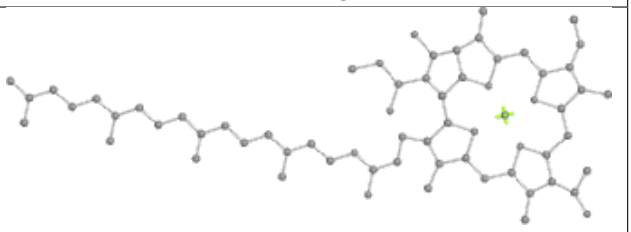


Bond angles

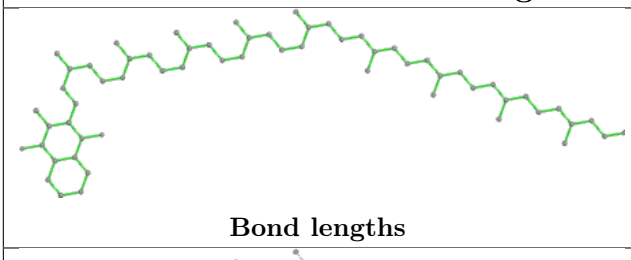


Torsions

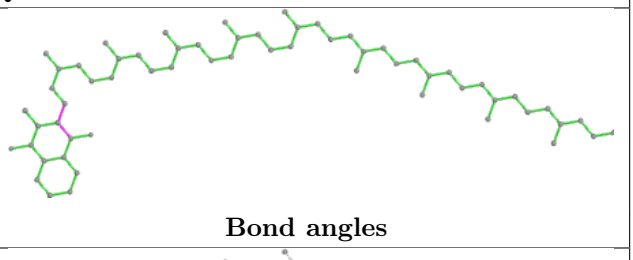


Rings

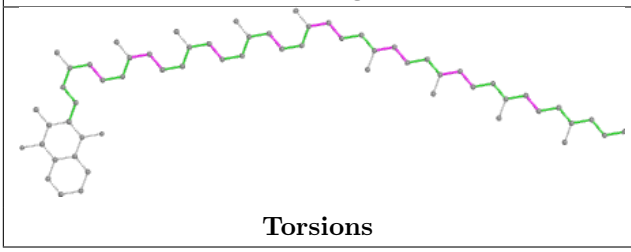
Ligand MQE M 403



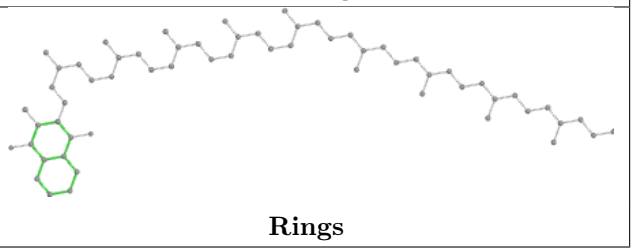
Bond lengths



Bond angles

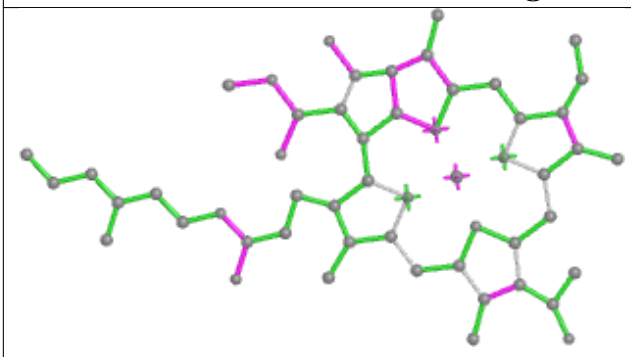


Torsions

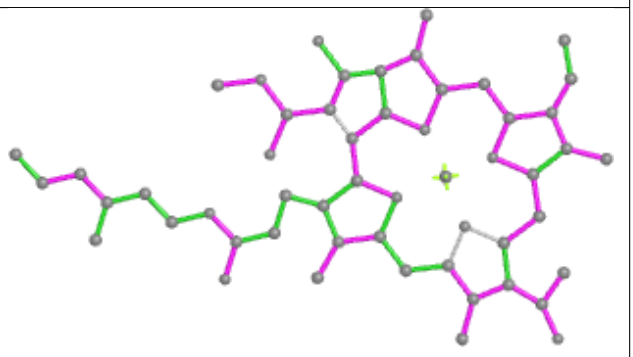


Rings

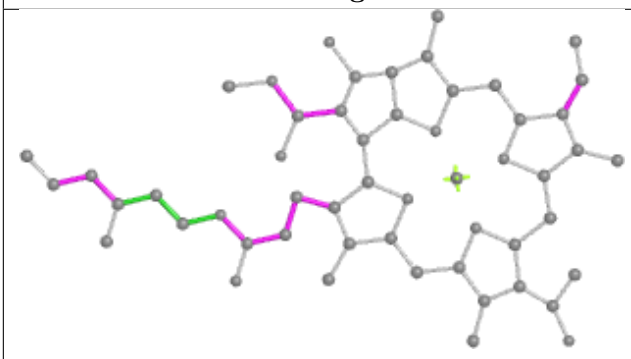
Ligand BCL A 101



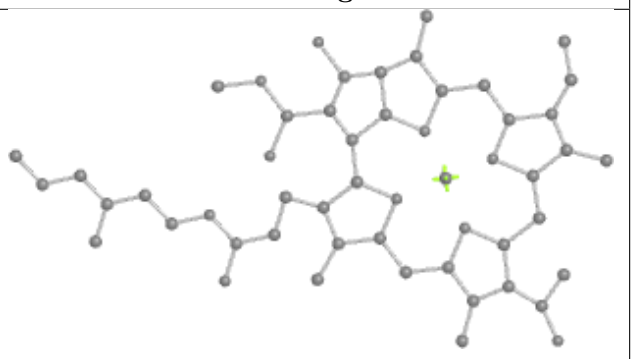
Bond lengths



Bond angles

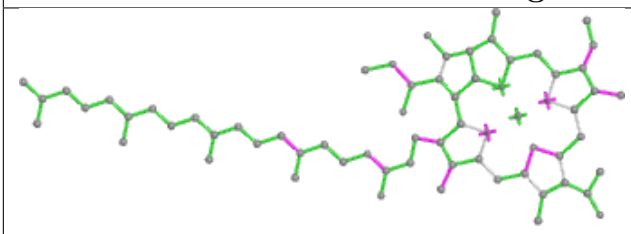


Torsions



Rings

Ligand BCL L 402



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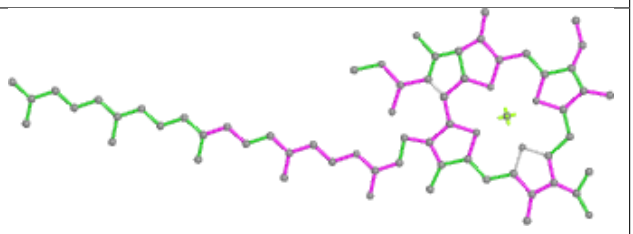
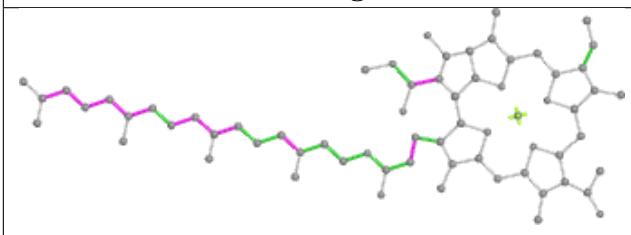
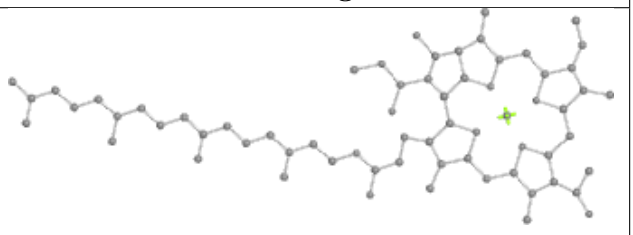


Bond angles

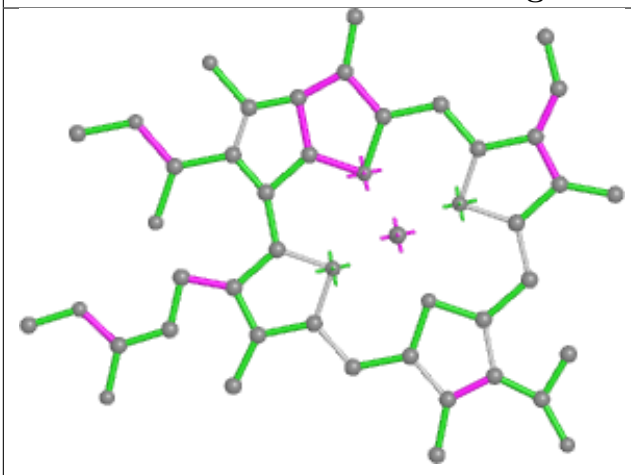


Torsions

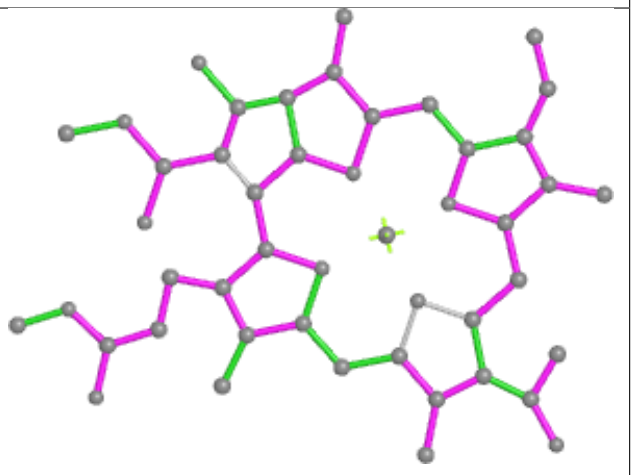


Rings

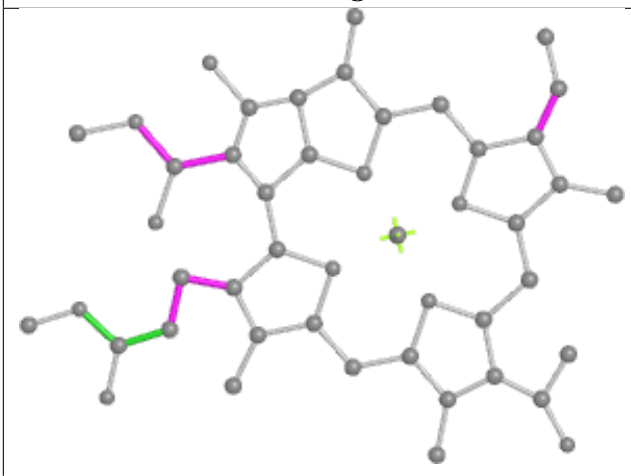
Ligand BCL F 101



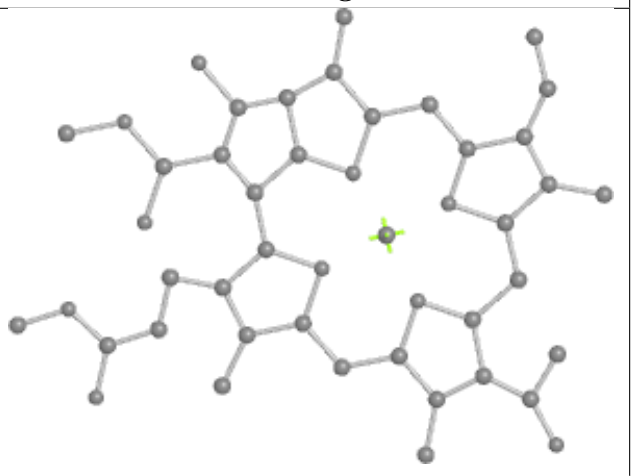
Bond lengths



Bond angles

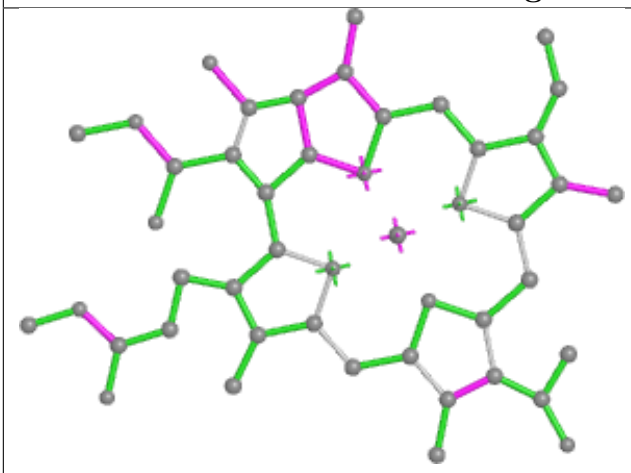


Torsions



Rings

Ligand BCL O 103



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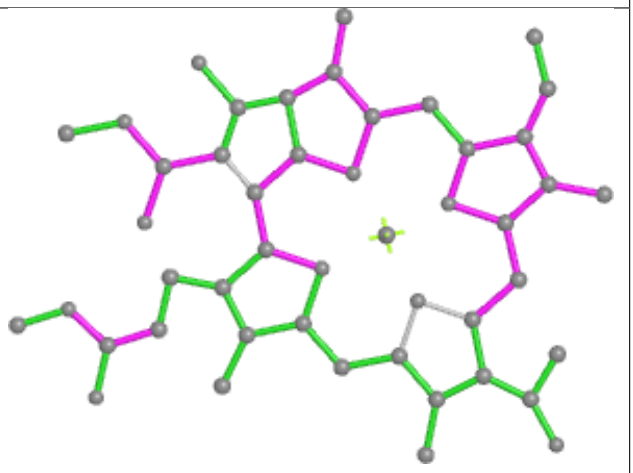
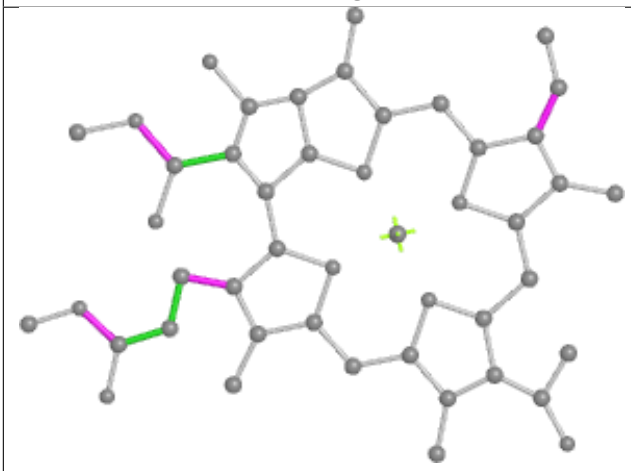
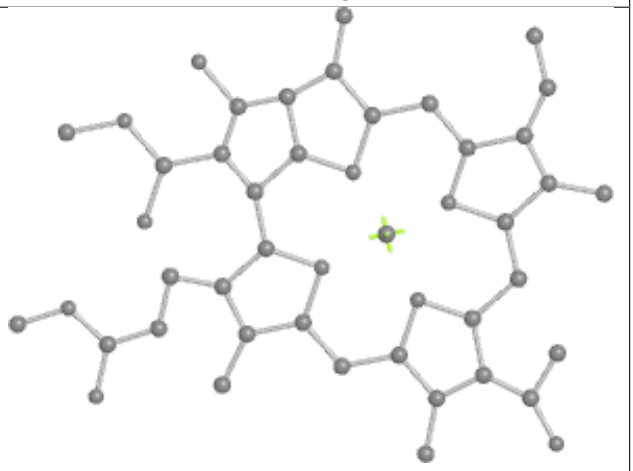


Bond angles

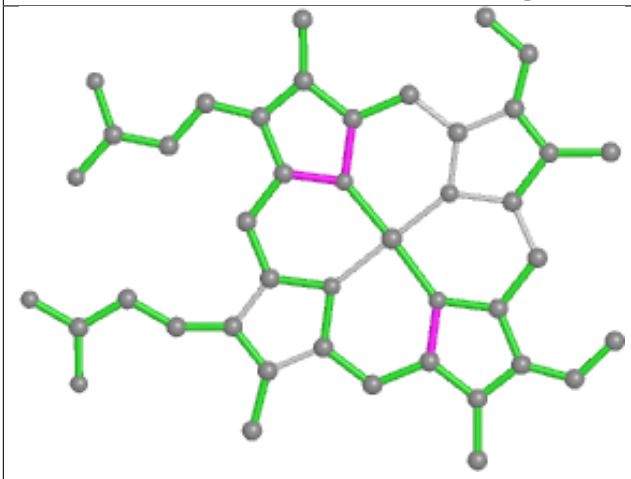


Torsions

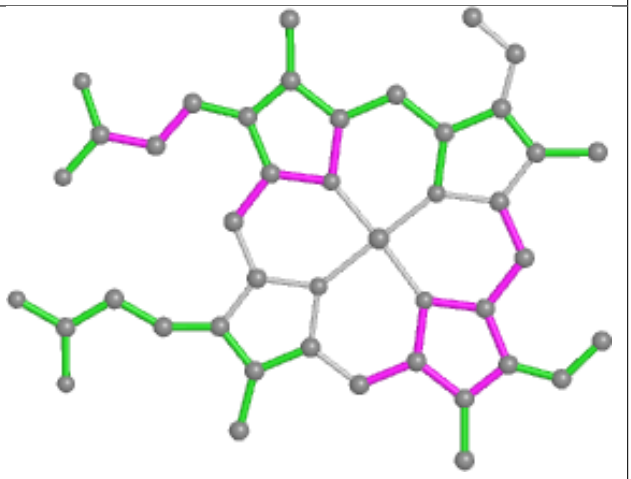


Rings

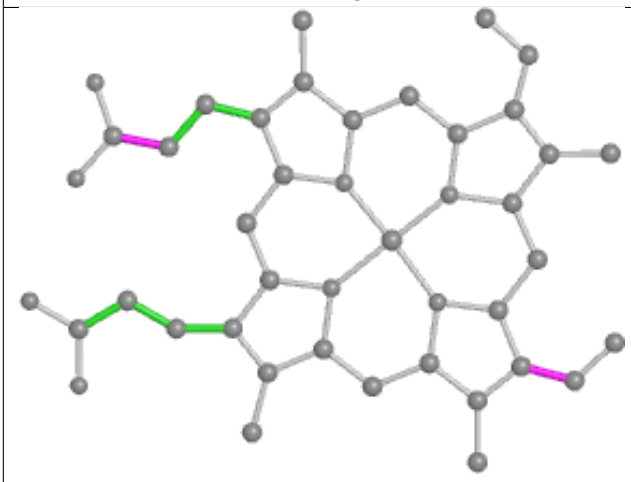
Ligand HEM C 502



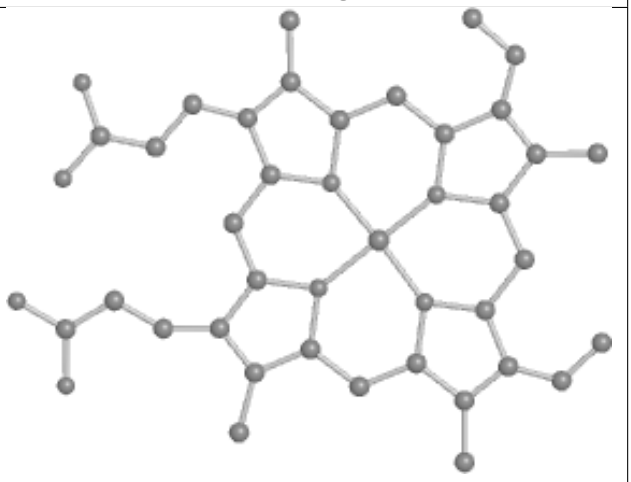
Bond lengths



Bond angles

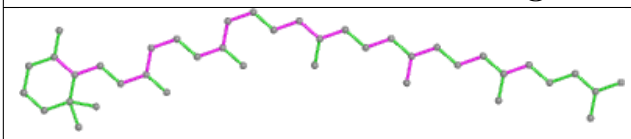


Torsions

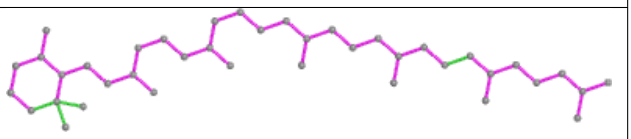


Rings

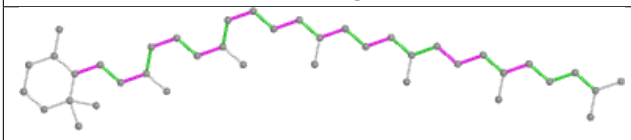
Ligand U4Z D 102



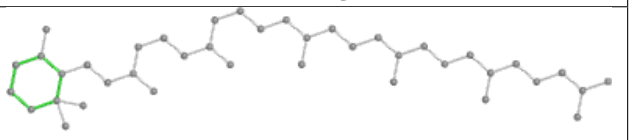
Bond lengths



Bond angles

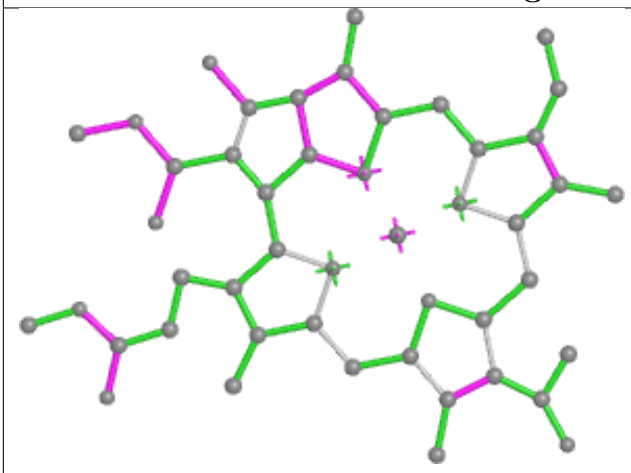


Torsions

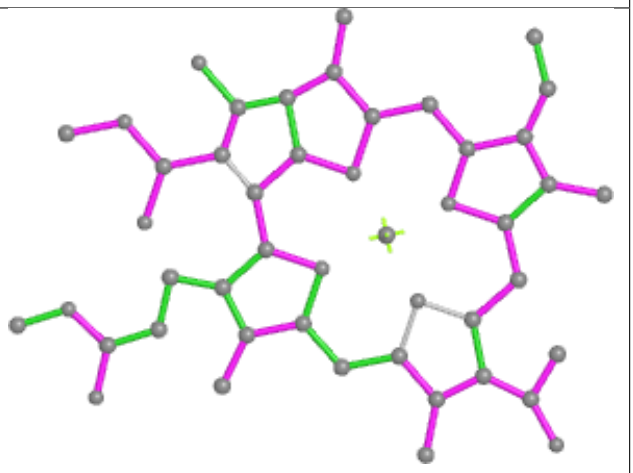


Rings

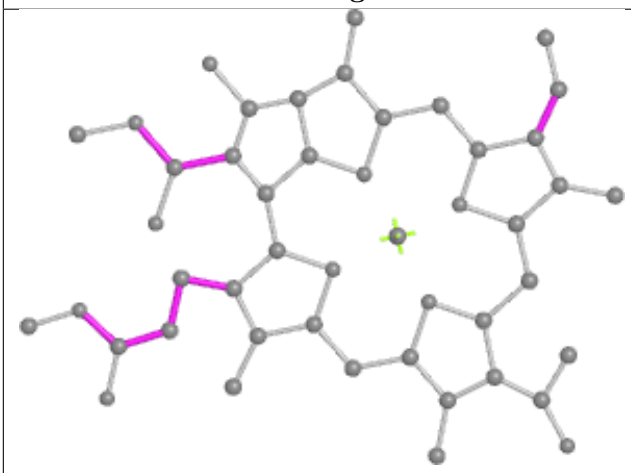
Ligand BCL K 102



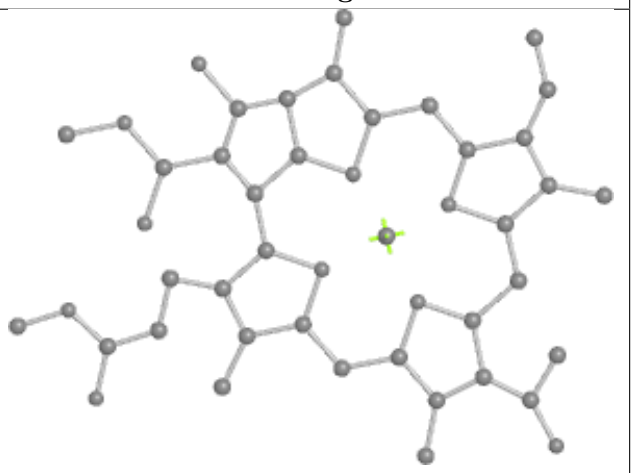
Bond lengths



Bond angles

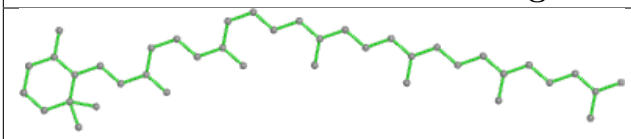


Torsions

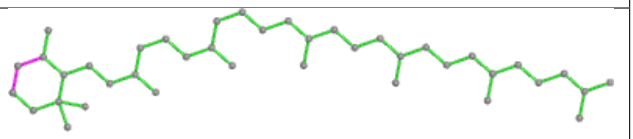


Rings

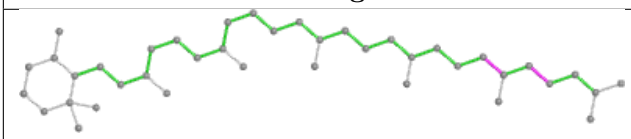
Ligand U4Z P 101



Bond lengths



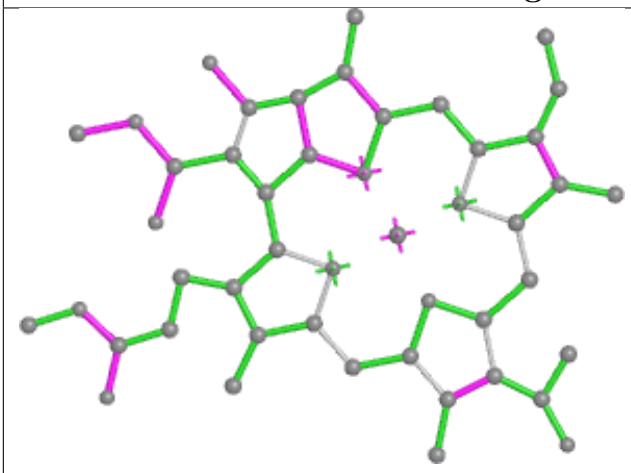
Bond angles



Torsions

Rings

Ligand BCL A 103



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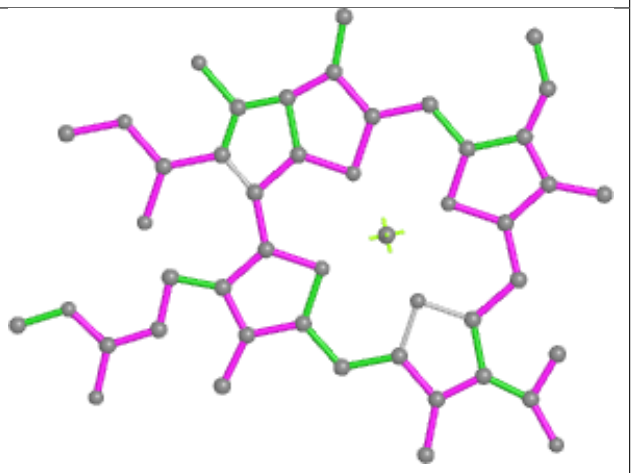
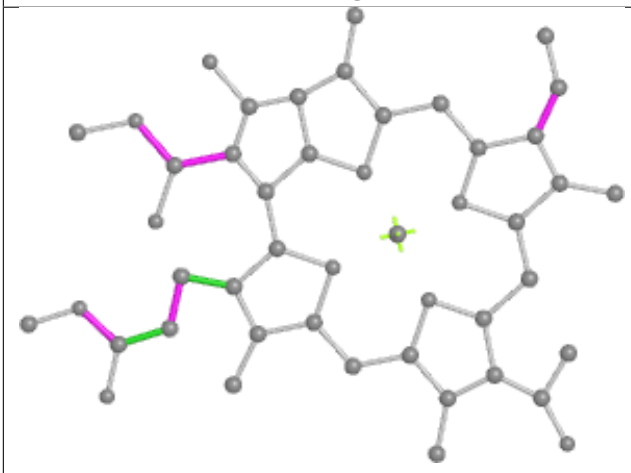
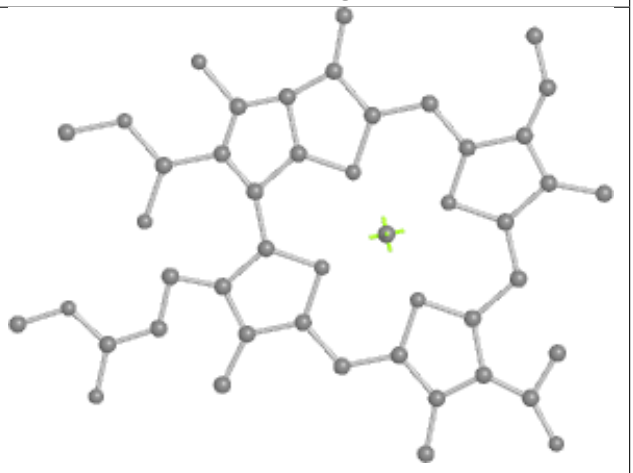


Bond angles

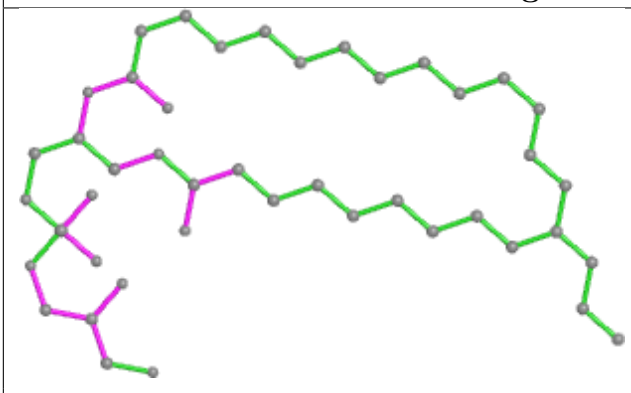


Torsions

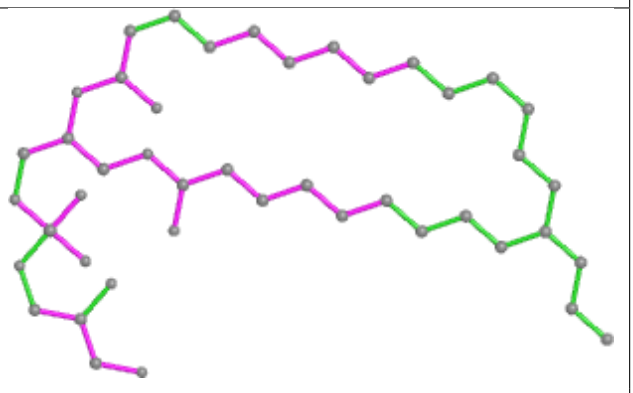


Rings

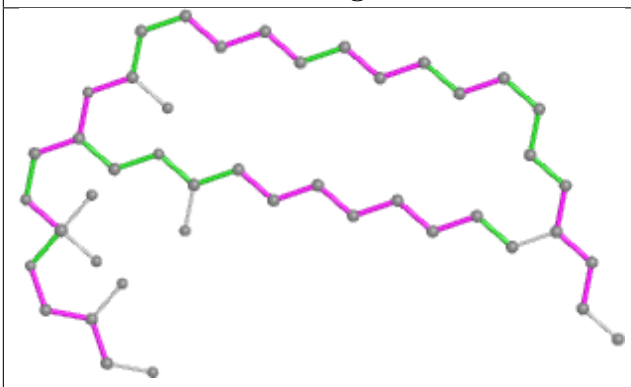
Ligand PGV C 505



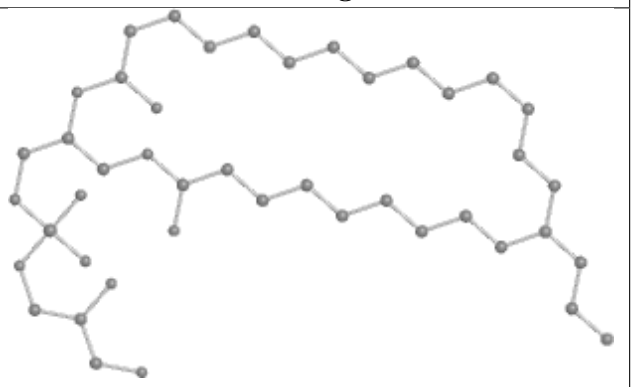
Bond lengths



Bond angles

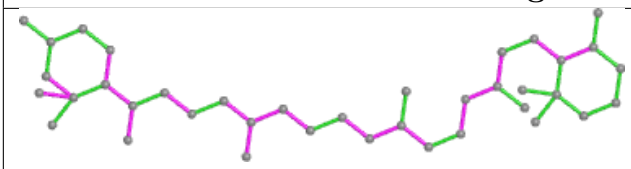


Torsions



Rings

Ligand U4Z A 102



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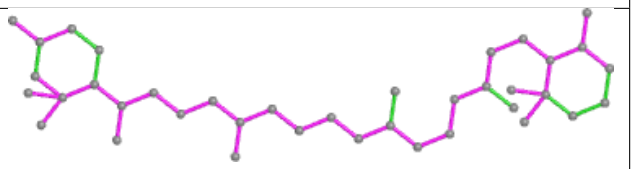
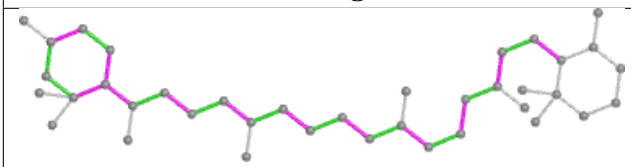


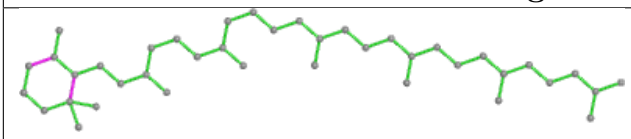
Bond angles



Torsions

Rings

Ligand U4Z Q 102



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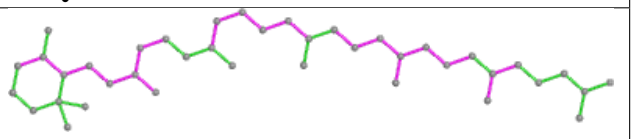
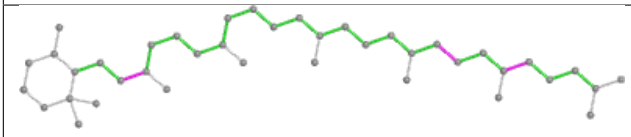


Bond angles



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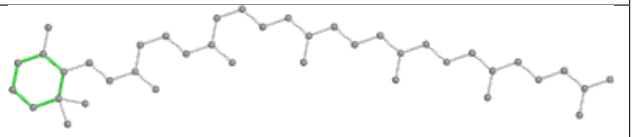
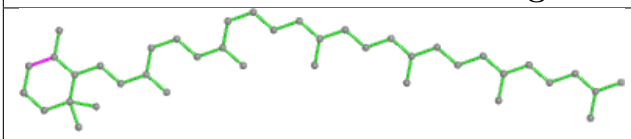


Rings

Ligand U4Z B 101



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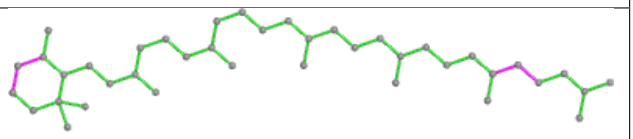
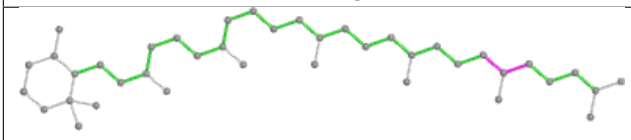


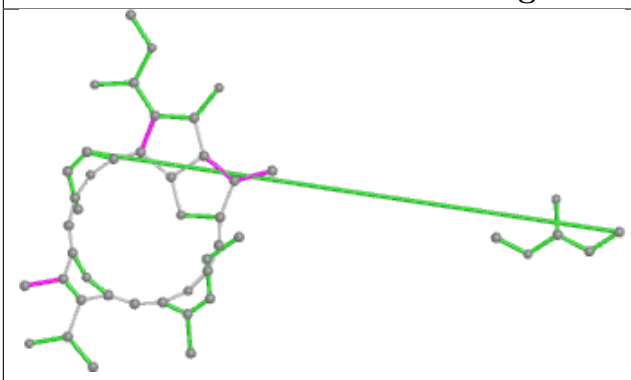
Bond angles



Torsions

Rings

Ligand BPH M 406



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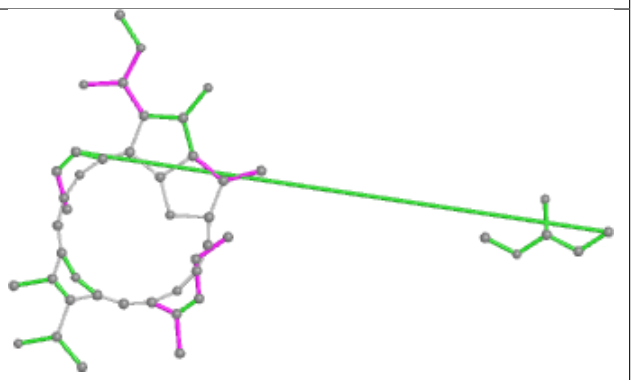
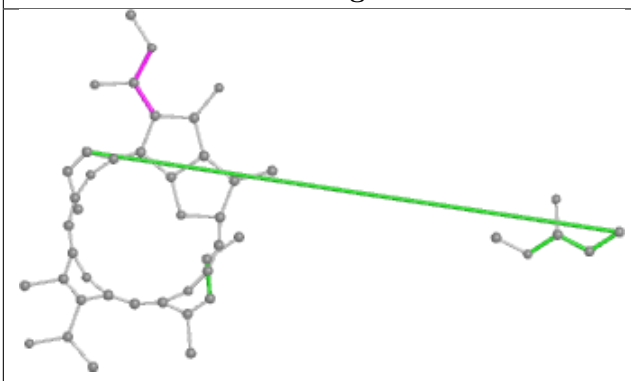


Bond angles



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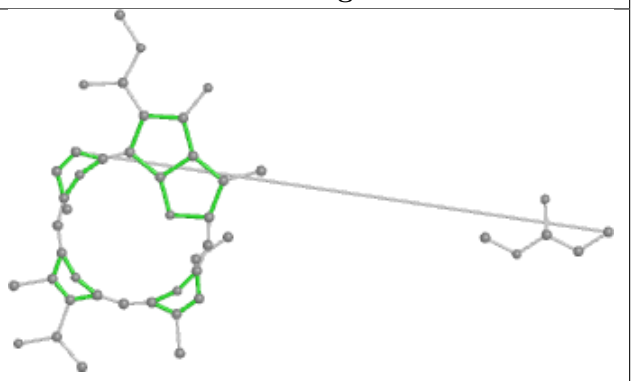
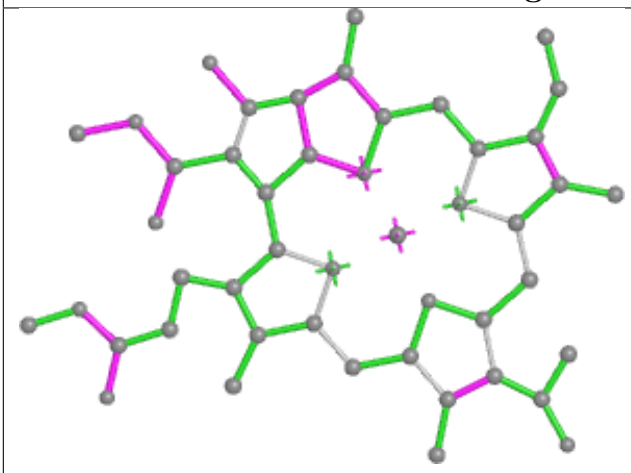


Rings

Ligand BCL O 101



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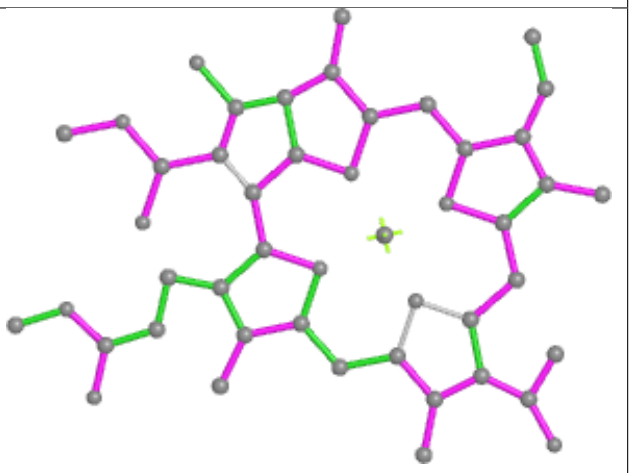
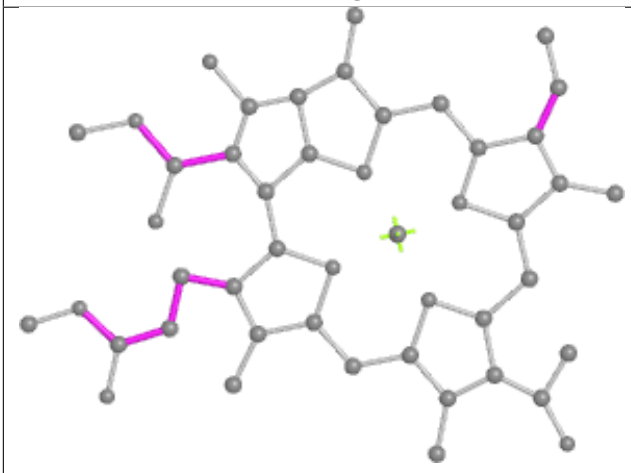


Bond angles



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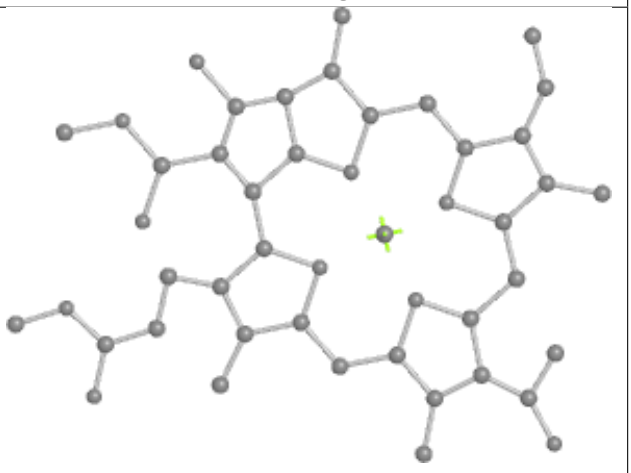
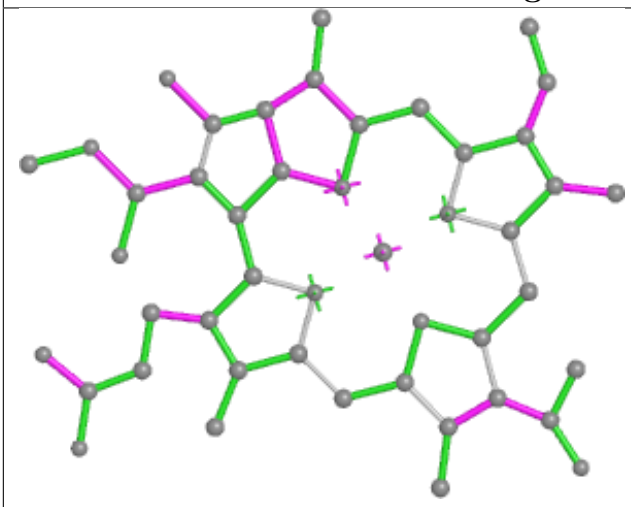
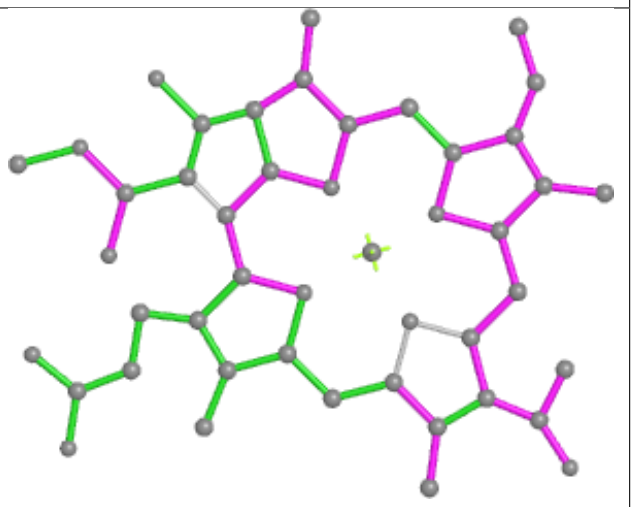


Rings

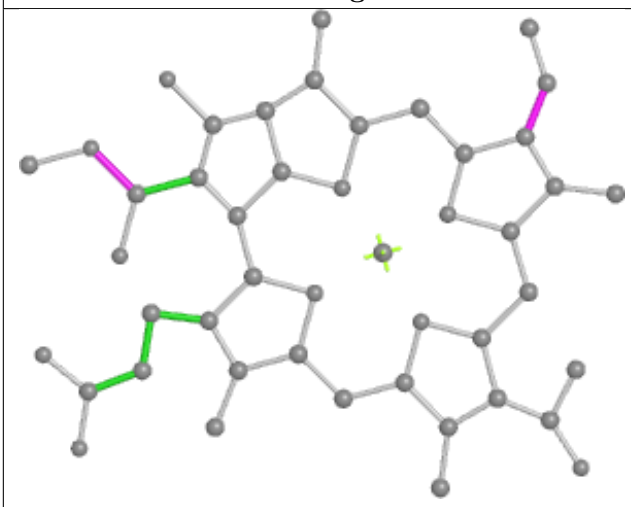
Ligand BCL G 103



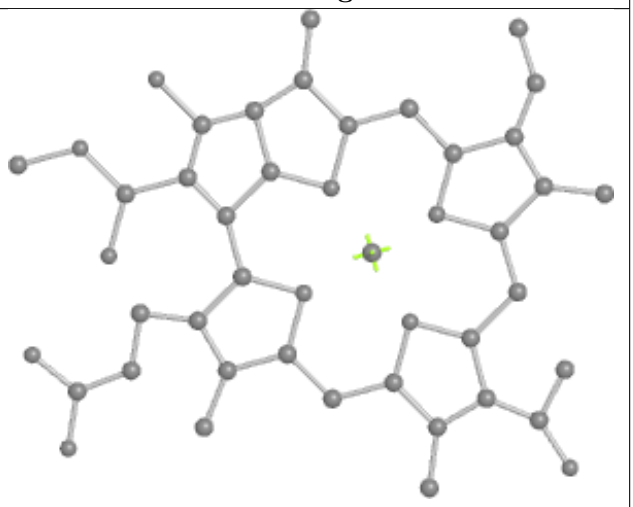
Bond lengths



Bond angles

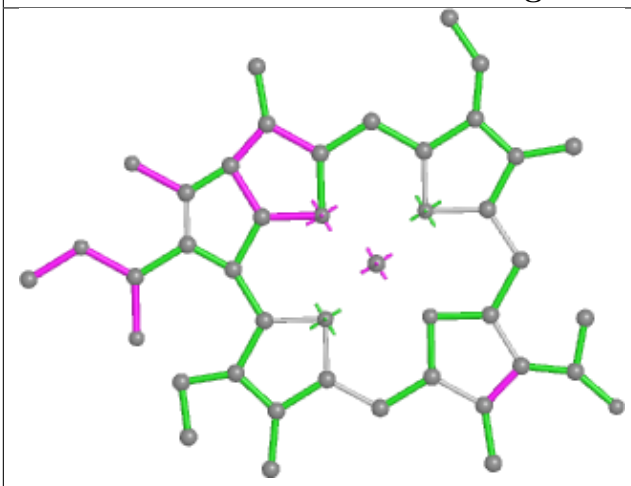


Torsions

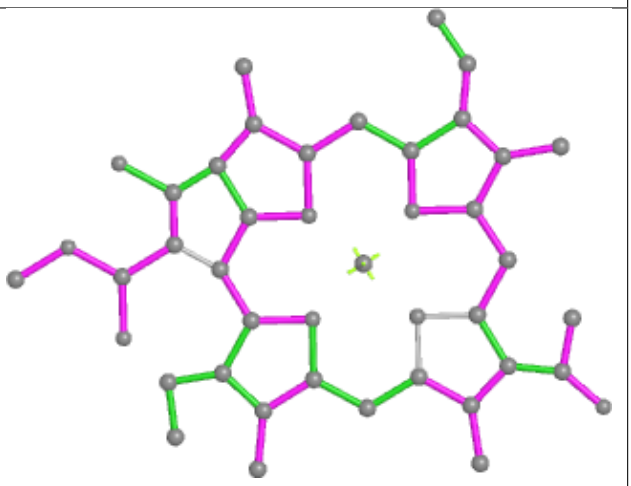


Rings

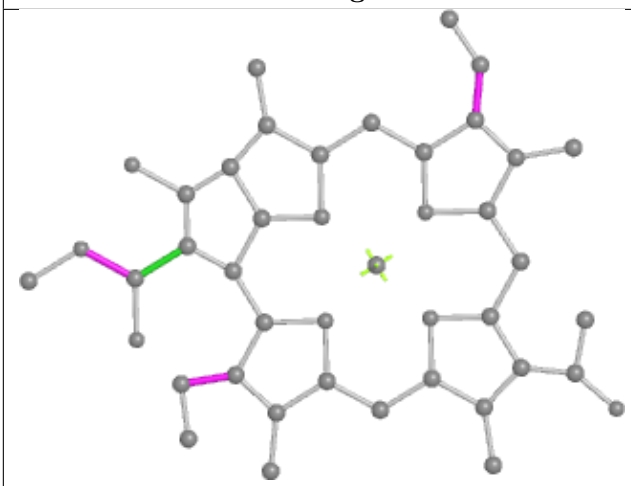
Ligand BCL R 103



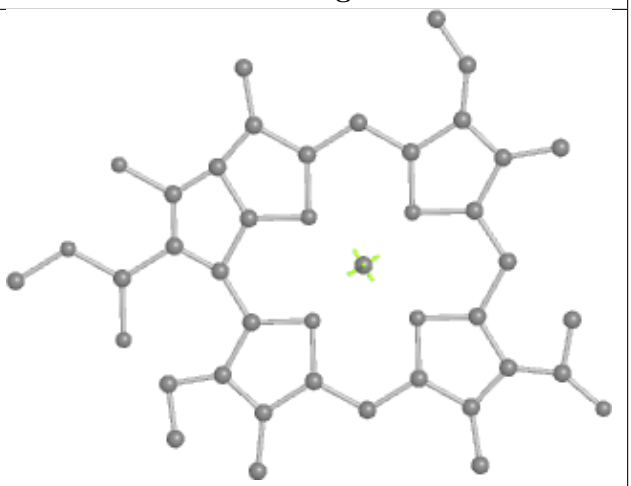
Bond lengths



Bond angles

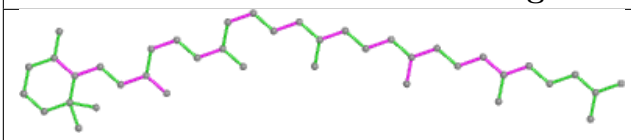


Torsions



Rings

Ligand U4Z D 104



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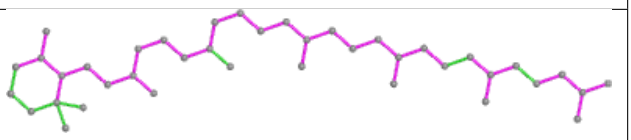
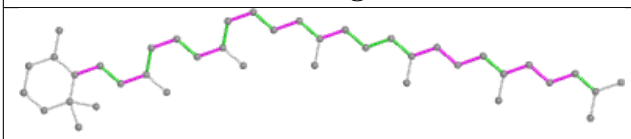
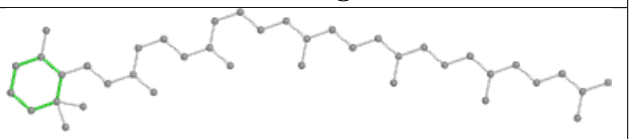


Bond angles

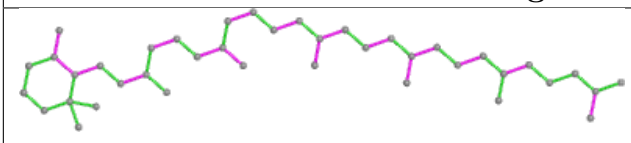


Torsions



Rings

Ligand U4Z R 101



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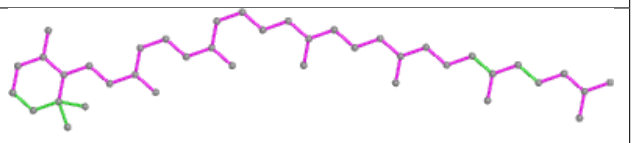
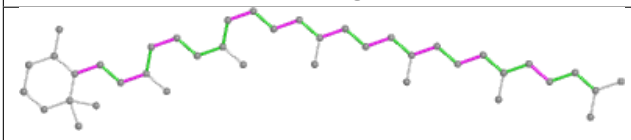


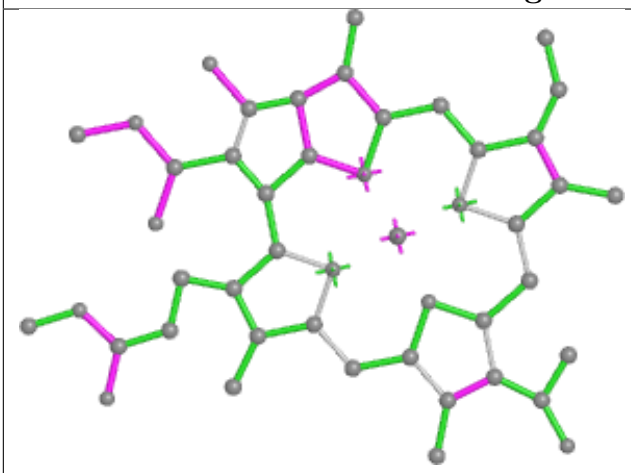
Bond angles



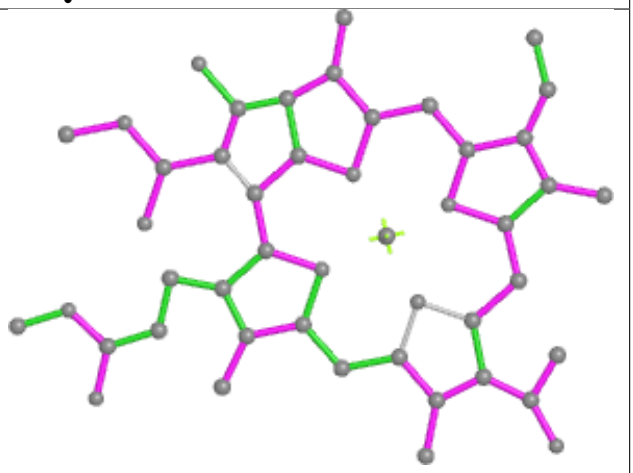
Torsions

Rings

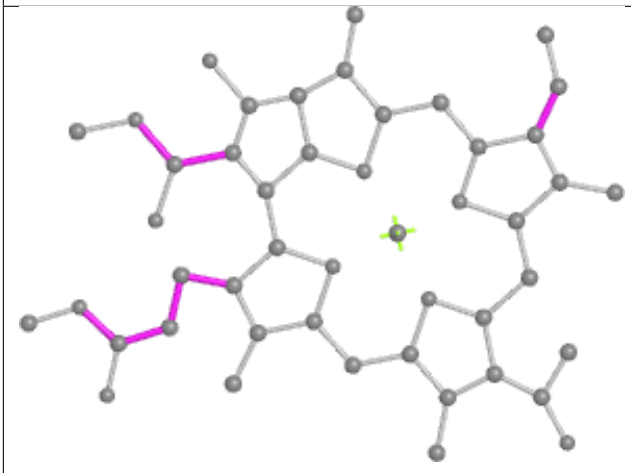
Ligand BCL Q 101



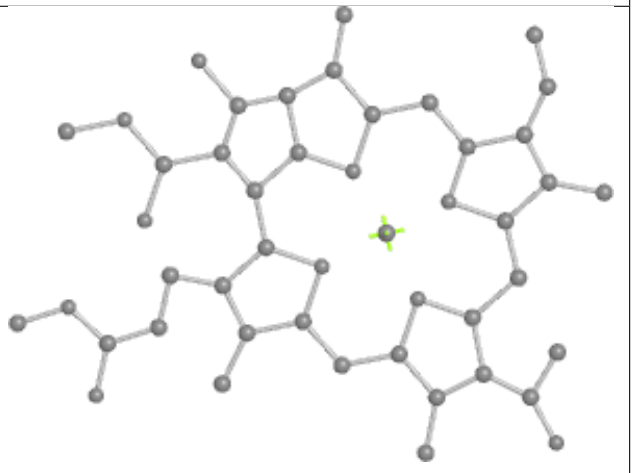
Bond lengths



Bond angles

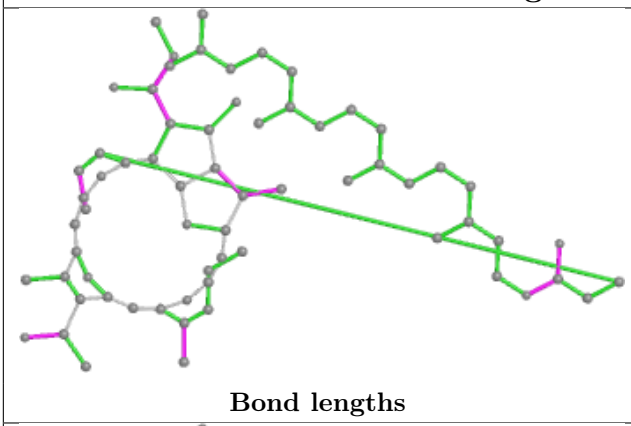


Torsions

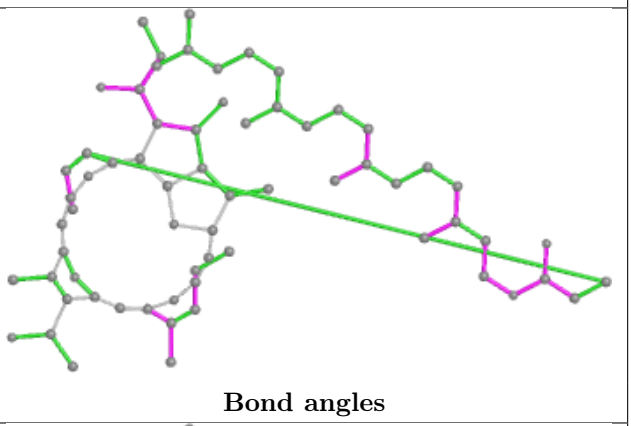


Rings

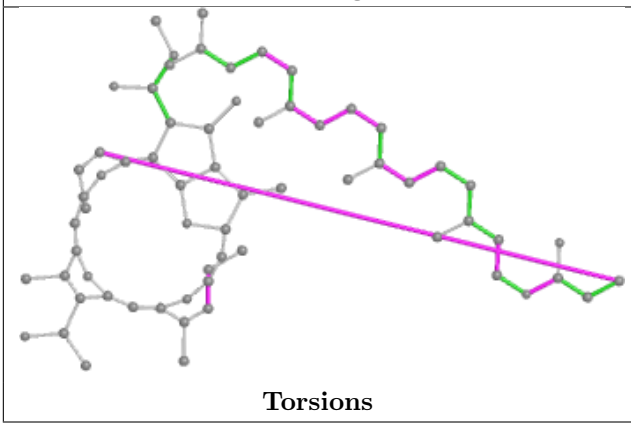
Ligand BPH L 403



Bond lengths



Bond angles



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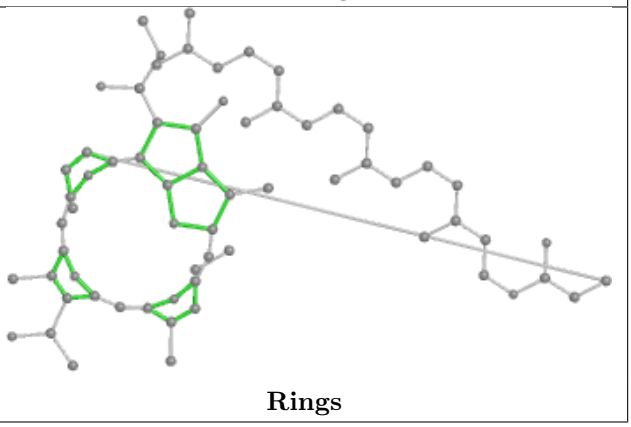
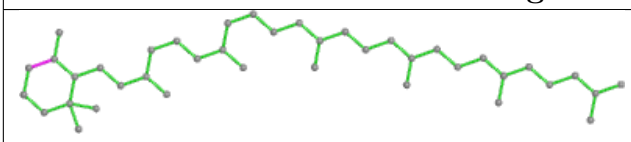
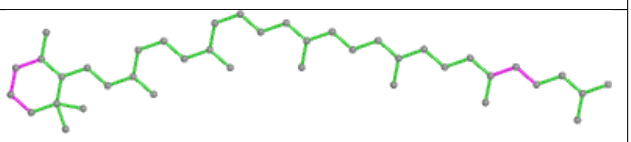


Rings

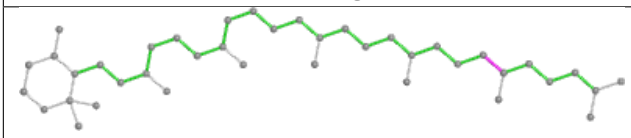
Ligand U4Z K 101



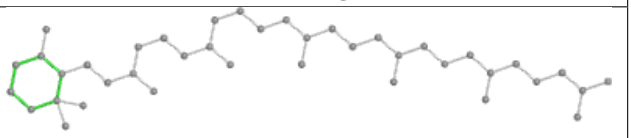
Bond lengths



Bond angles

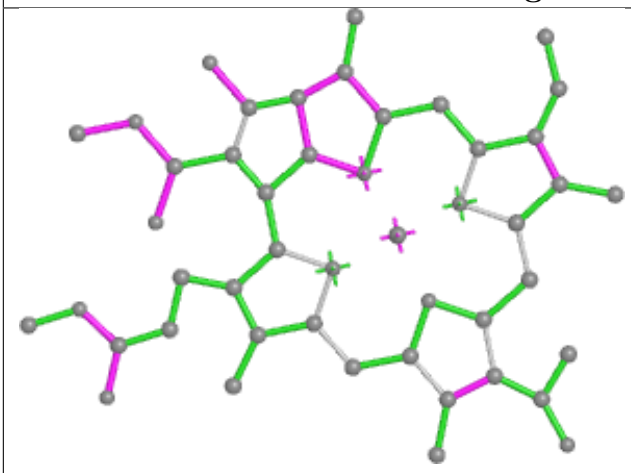


Torsions

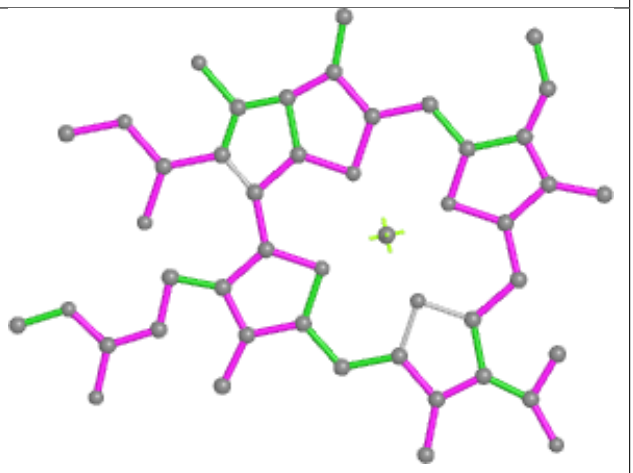


Rings

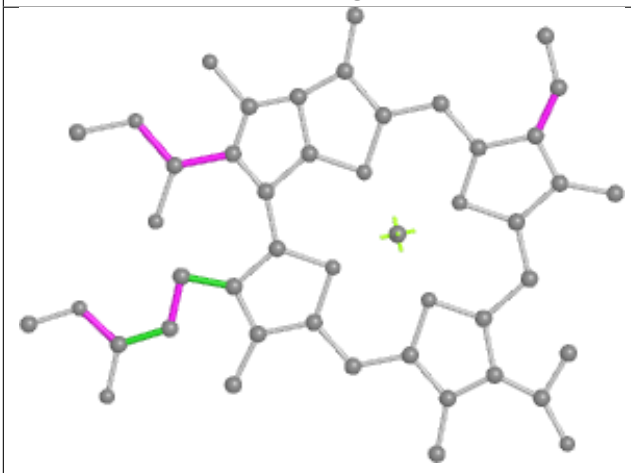
Ligand BCL R 102



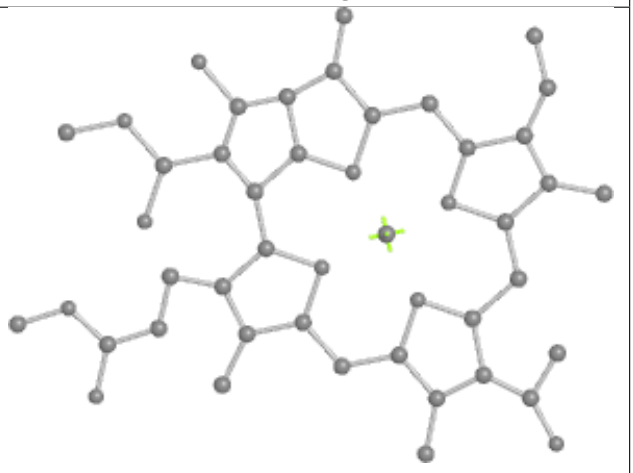
Bond lengths



Bond angles

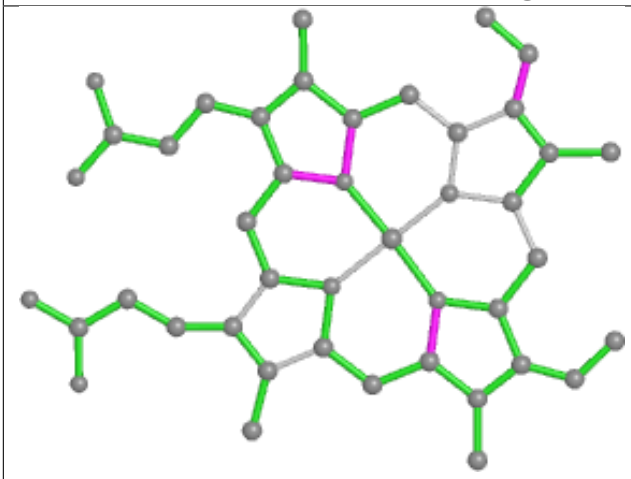


Torsions

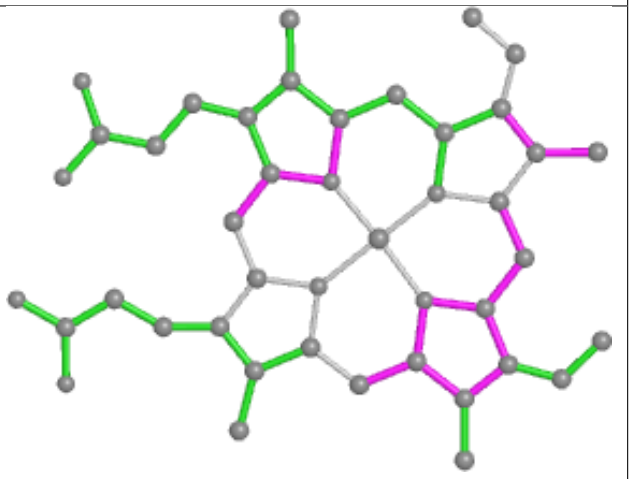


Rings

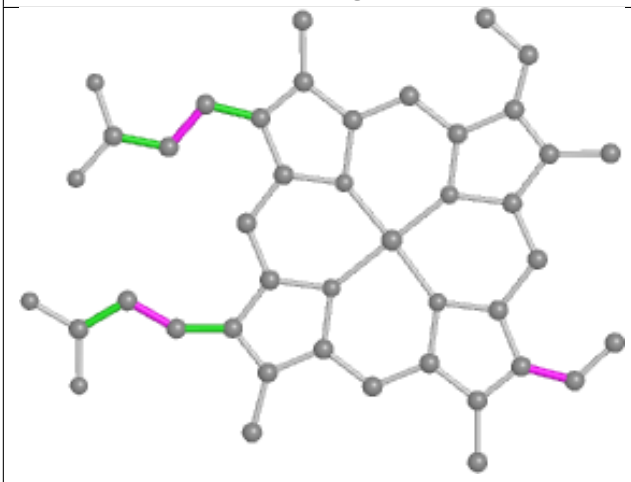
Ligand HEM C 504



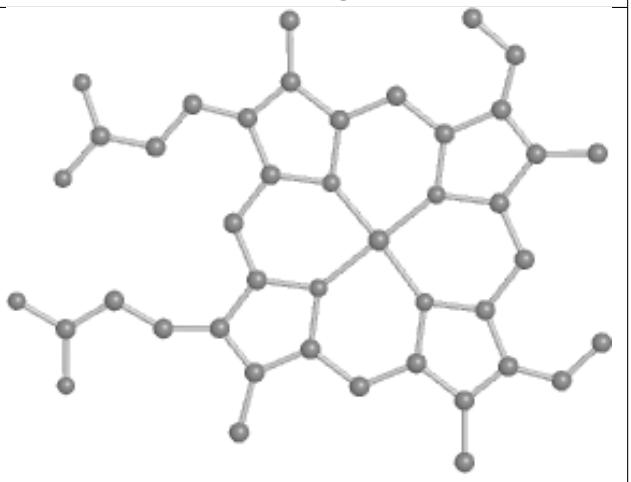
Bond lengths



Bond angles

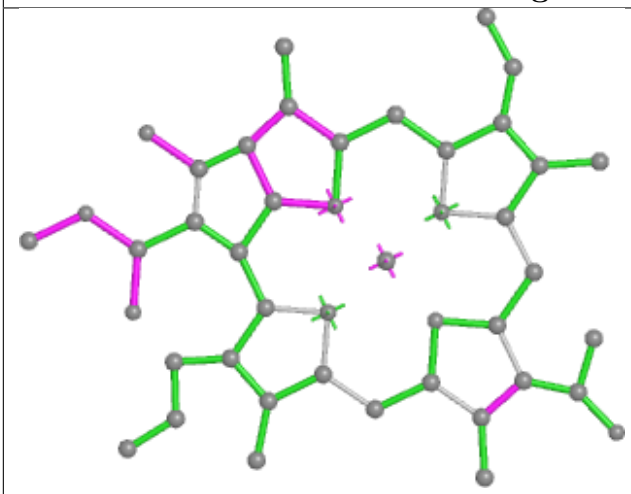


Torsions

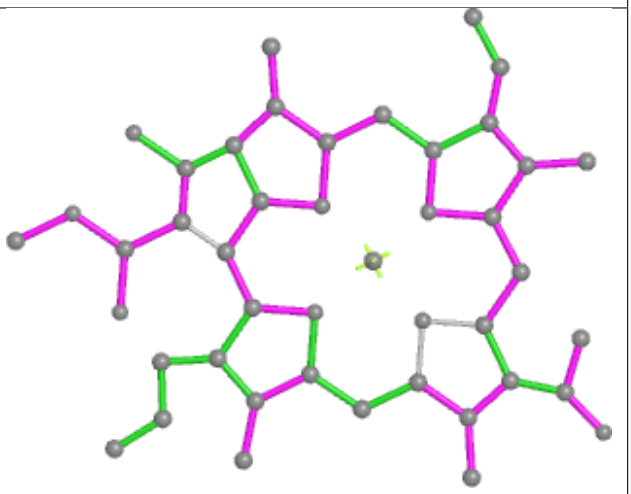


Rings

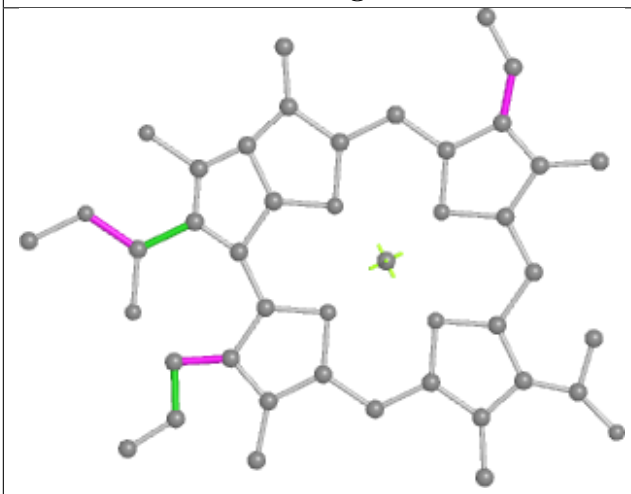
Ligand BCL I 104



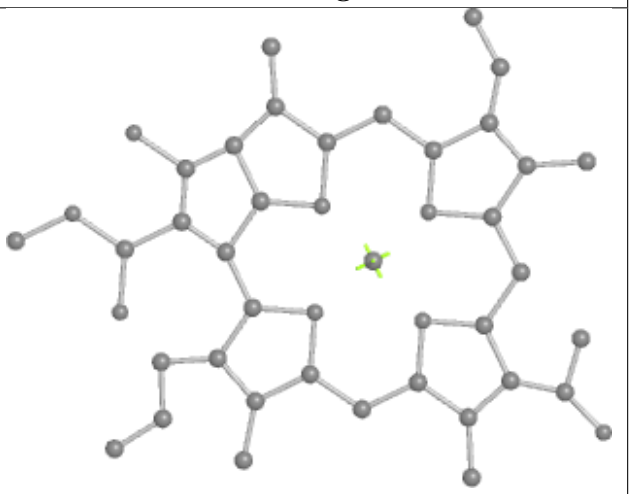
Bond lengths



Bond angles

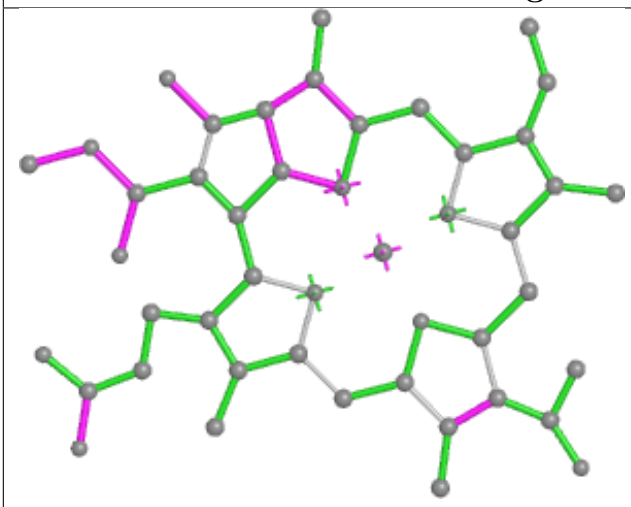


Torsions

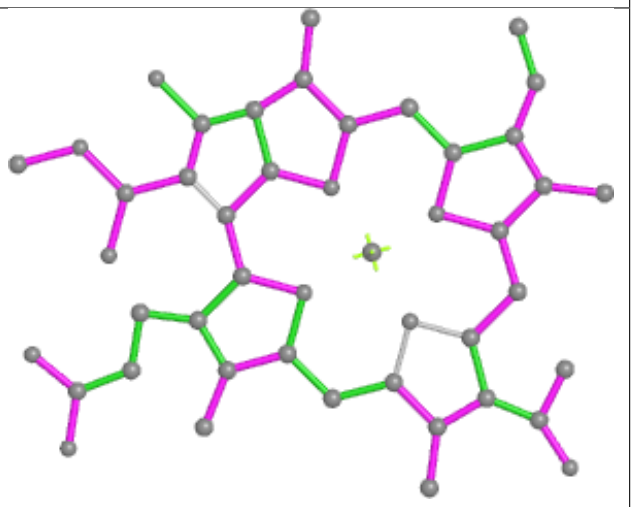


Rings

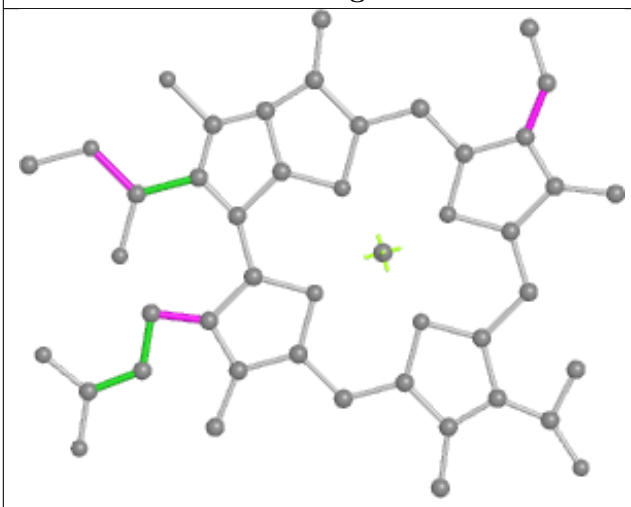
Ligand BCL E 101



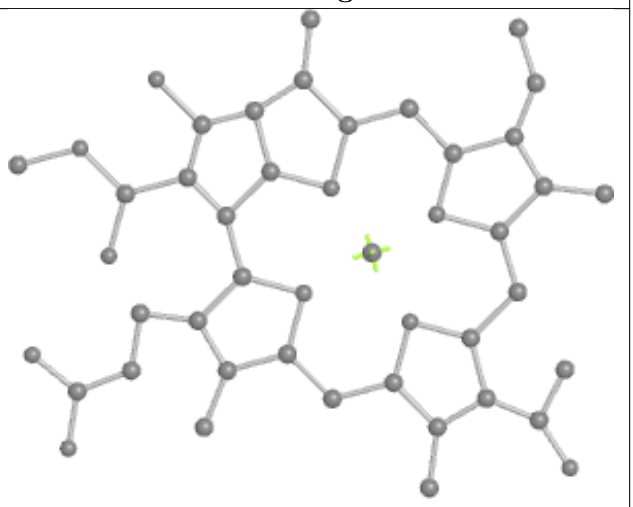
Bond lengths



Bond angles

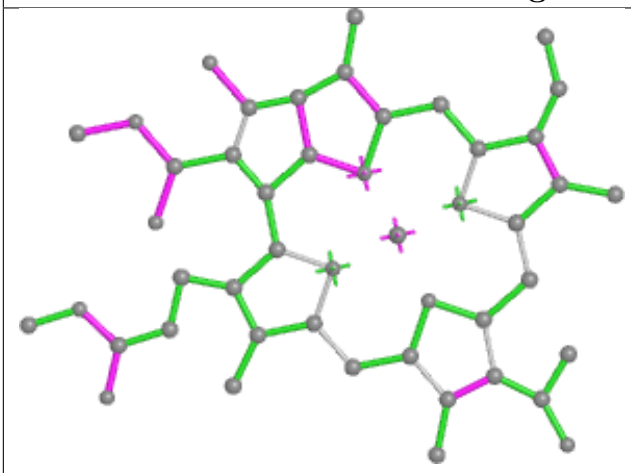


Torsions

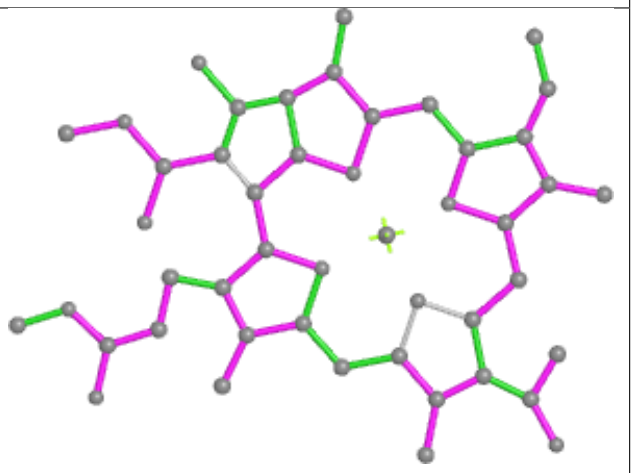


Rings

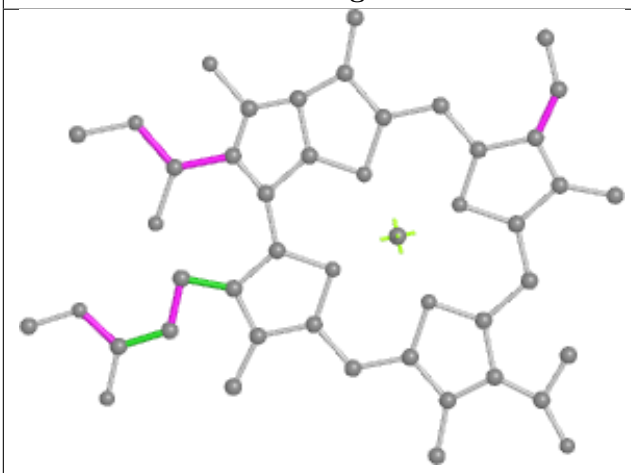
Ligand BCL J 101



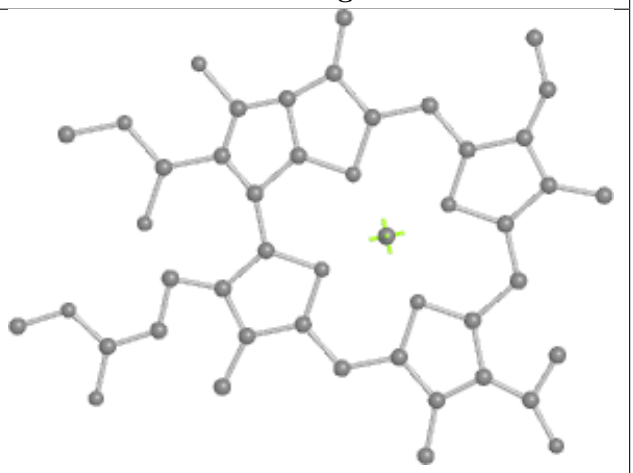
Bond lengths



Bond angles

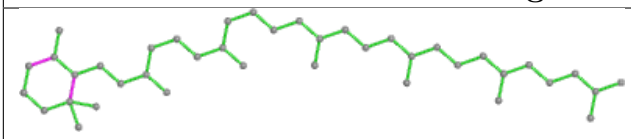


Torsions

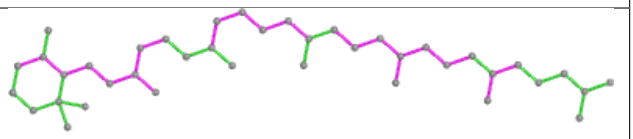


Rings

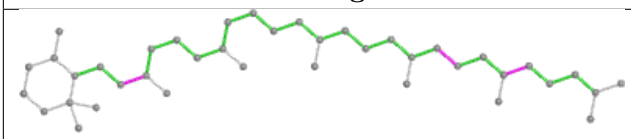
Ligand U4Z K 103



Bond lengths



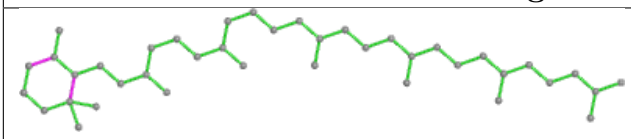
Bond angles



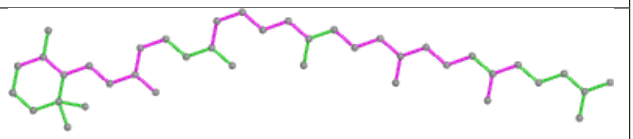
Torsions

Rings

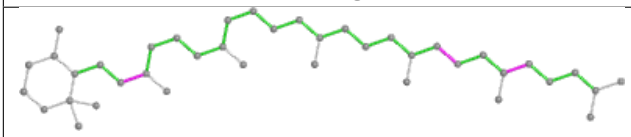
Ligand U4Z O 102



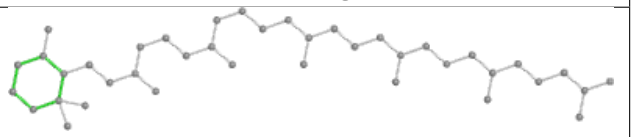
Bond lengths



Bond angles

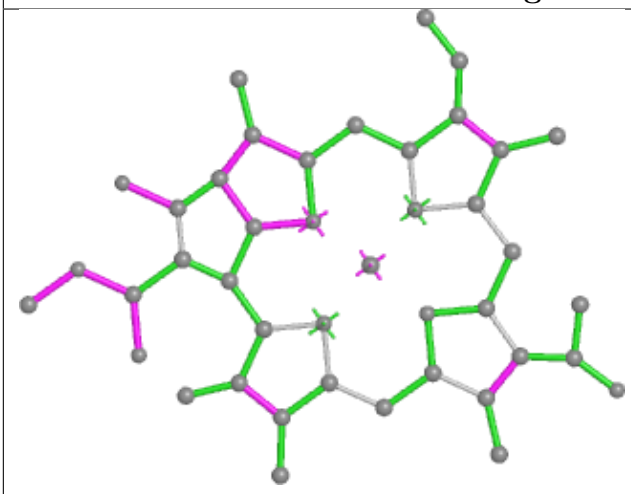


Torsions

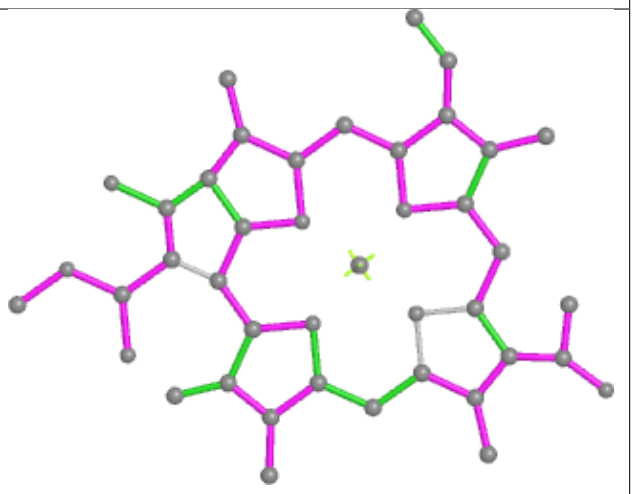


Rings

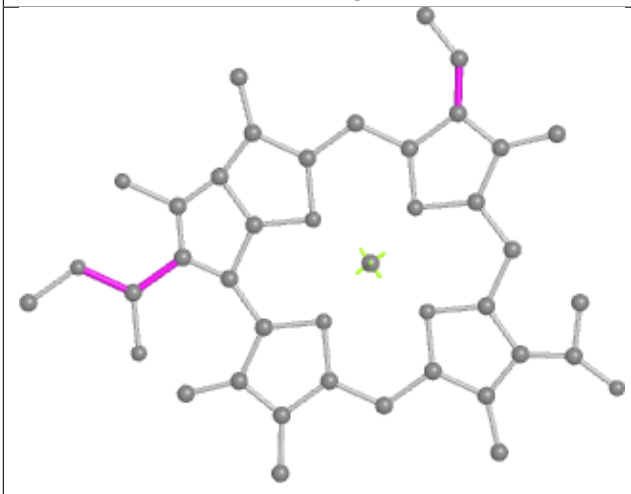
Ligand BCL H 101



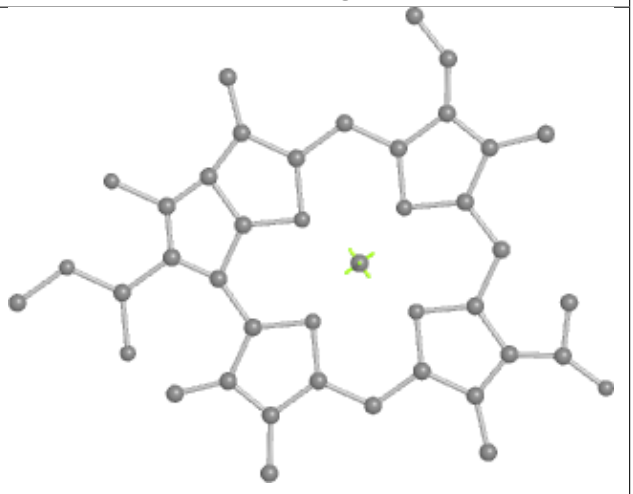
Bond lengths



Bond angles

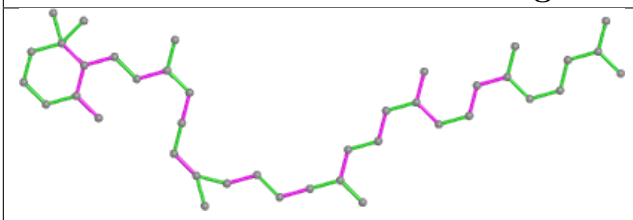


Torsions

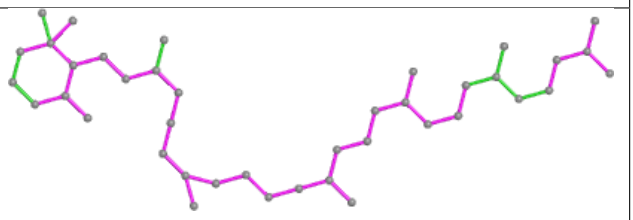


Rings

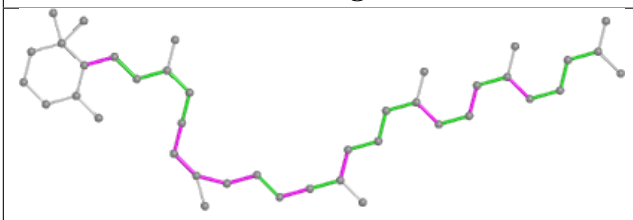
Ligand U4Z I 101



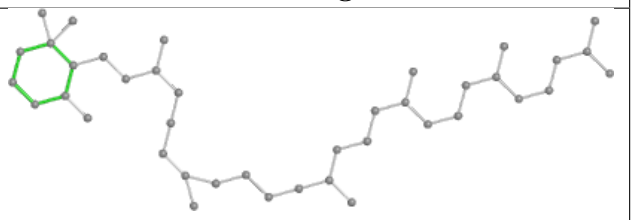
Bond lengths



Bond angles

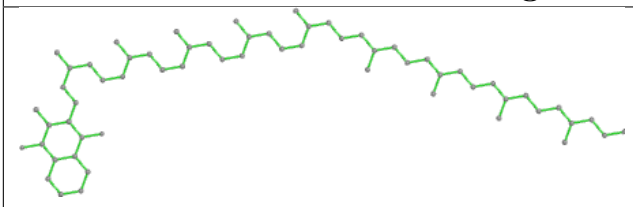


Torsions

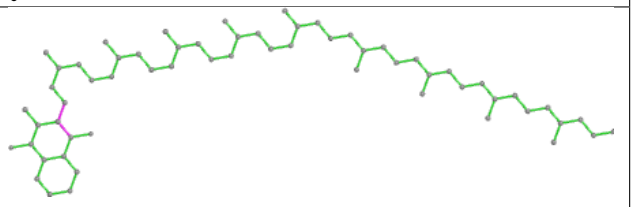


Rings

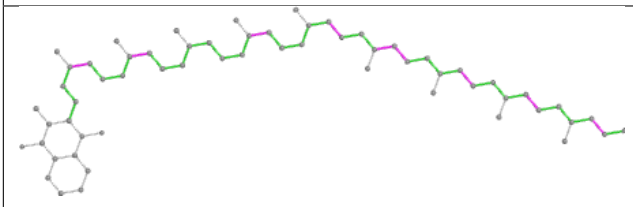
Ligand MQE L 401



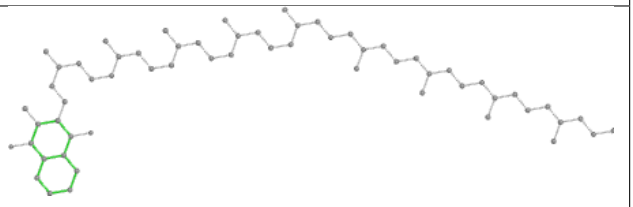
Bond lengths



Bond angles

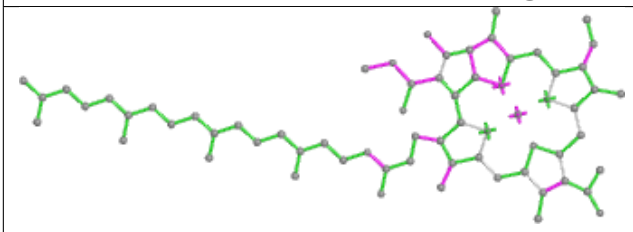


Torsions

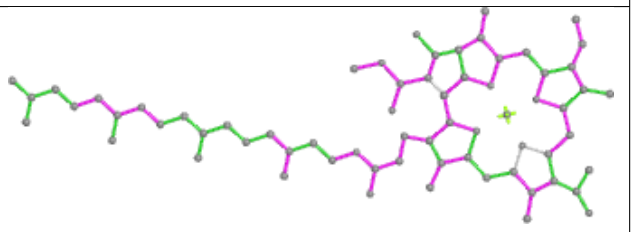


Rings

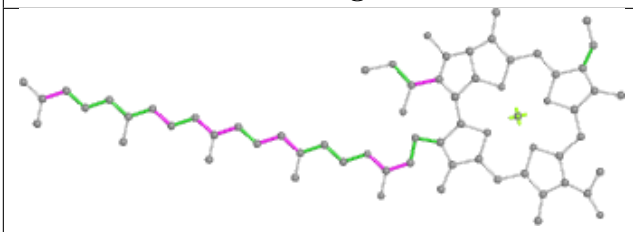
Ligand BCL M 405



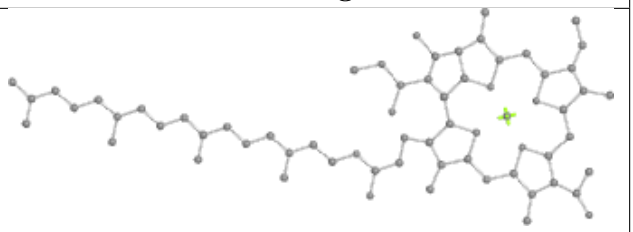
Bond lengths



Bond angles

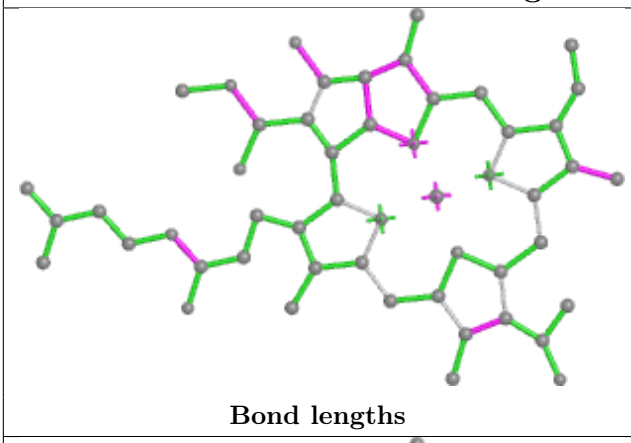


Torsions

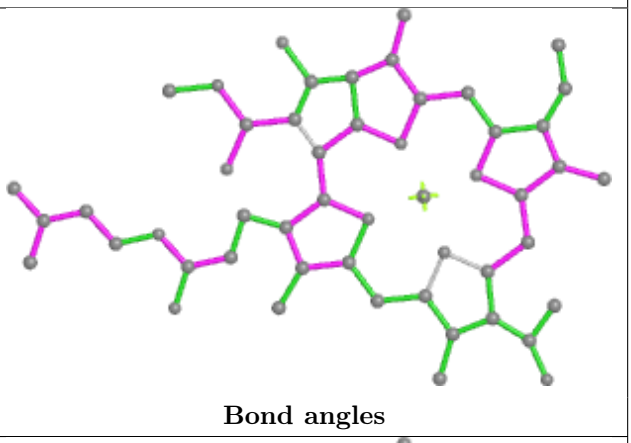


Rings

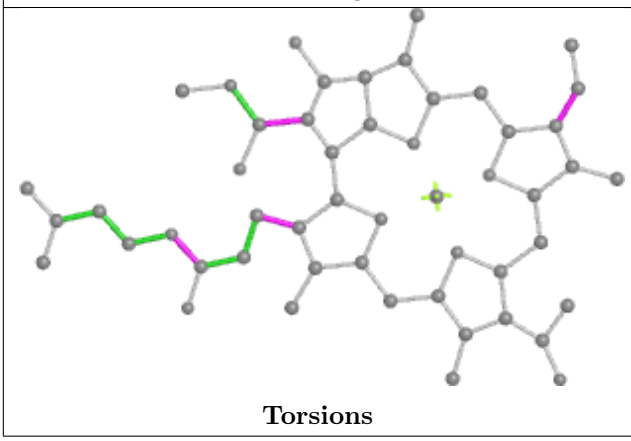
Ligand BCL K 104



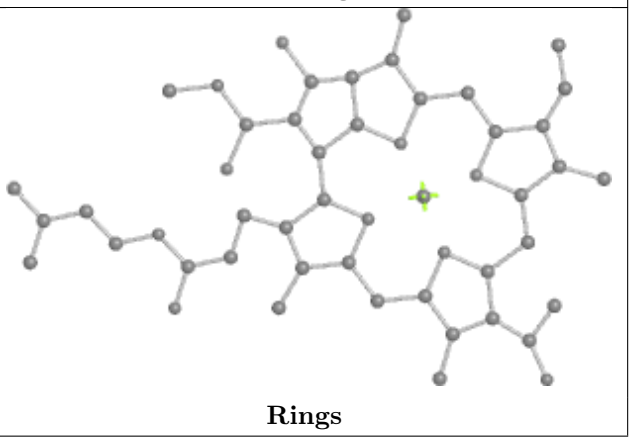
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

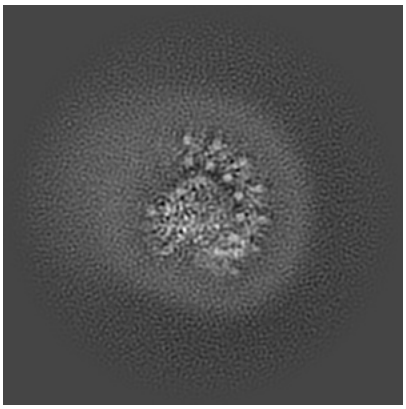
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39177. These allow visual inspection of the internal detail of the map and identification of artifacts.

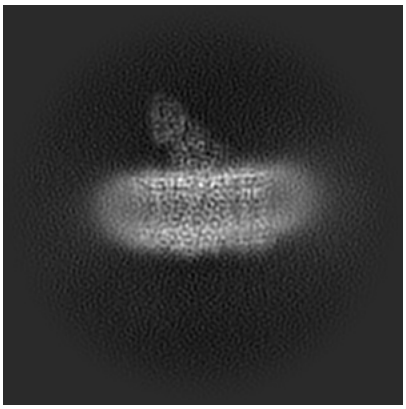
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

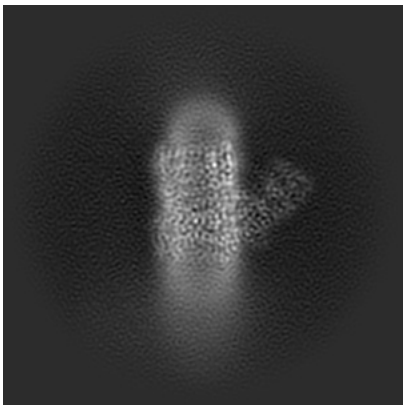
6.1.1 Primary map



X

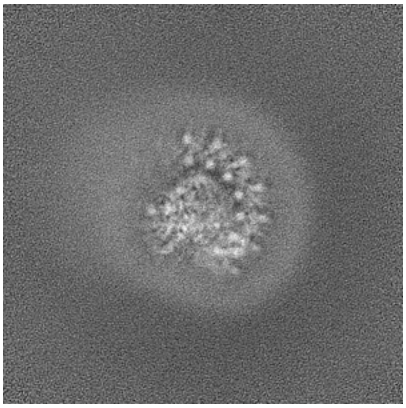


Y

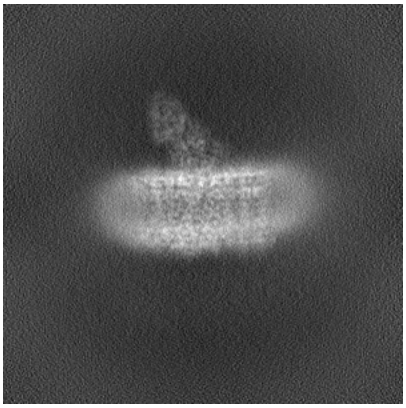


Z

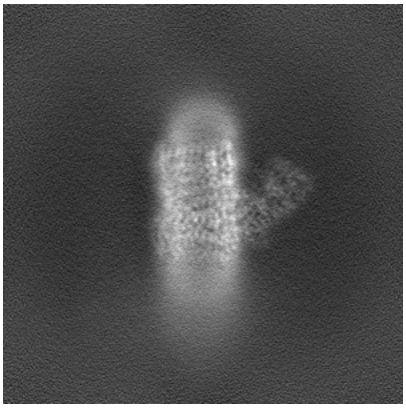
6.1.2 Raw map



X



Y

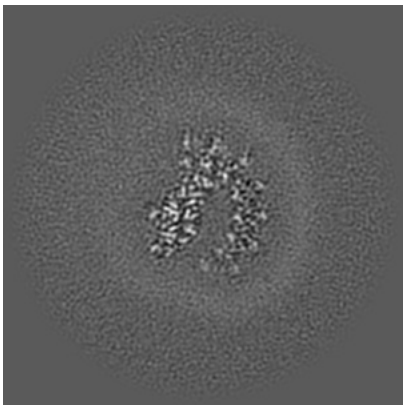


Z

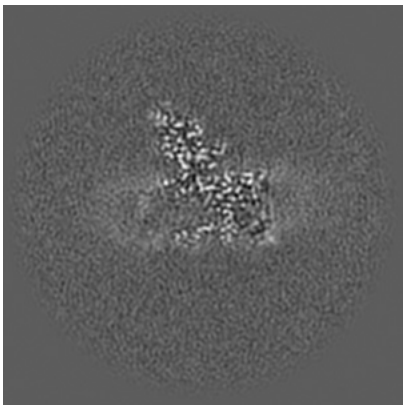
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

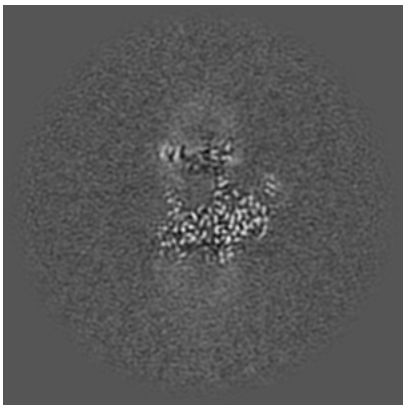
6.2.1 Primary map



X Index: 160

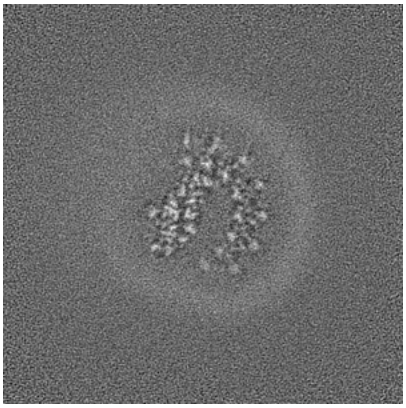


Y Index: 160

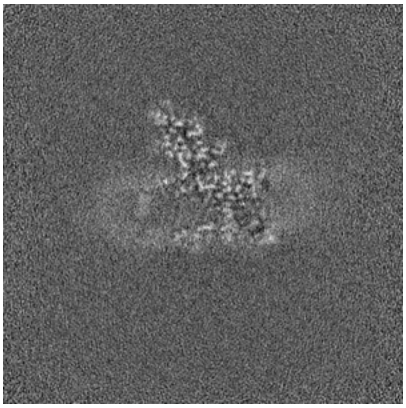


Z Index: 160

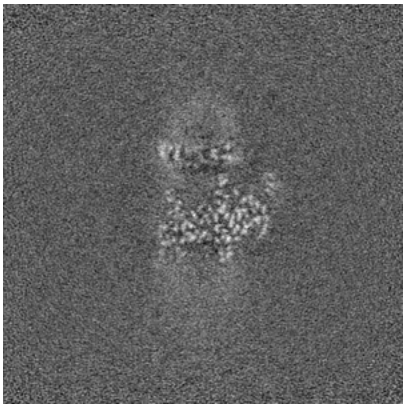
6.2.2 Raw map



X Index: 160



Y Index: 160

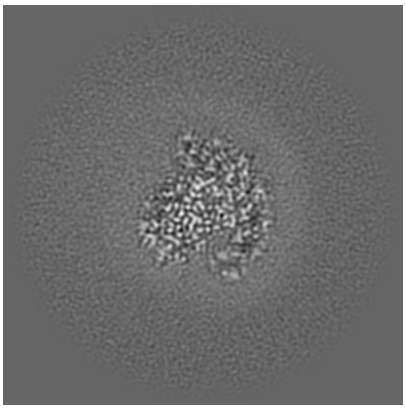


Z Index: 160

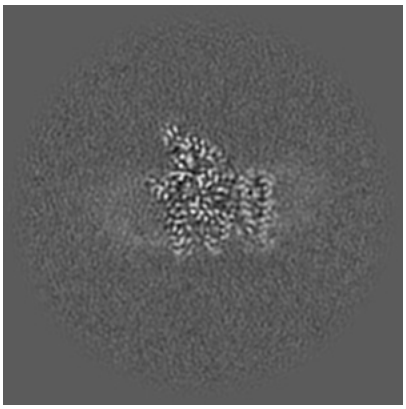
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

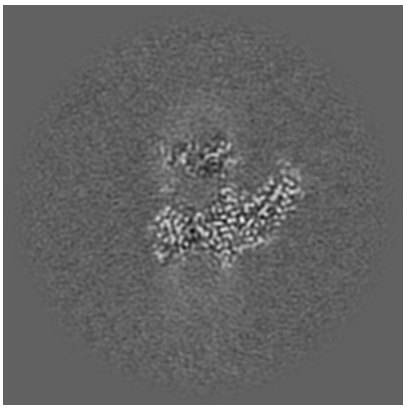
6.3.1 Primary map



X Index: 176

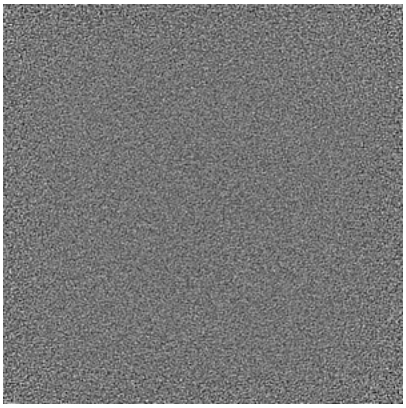


Y Index: 147

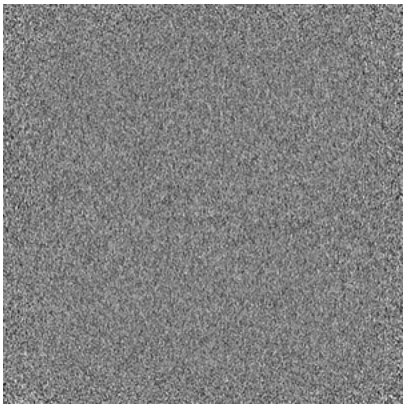


Z Index: 142

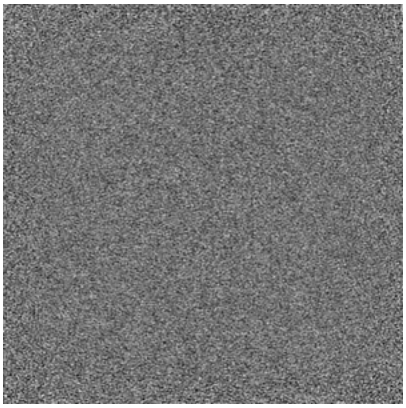
6.3.2 Raw map



X Index: 0



Y Index: 0

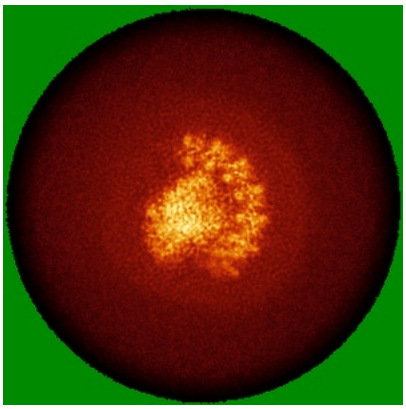


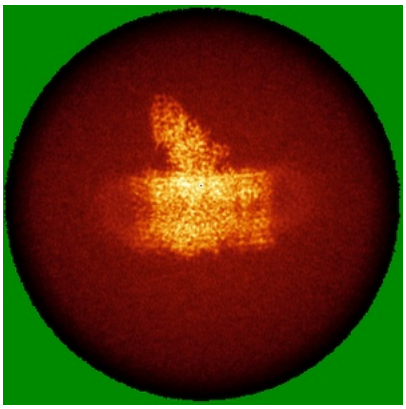
Z Index: 319

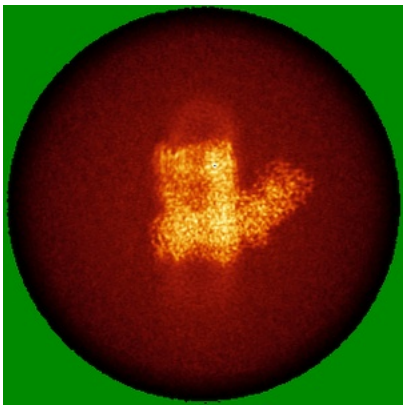
The images above show the largest variance slices of the map in three orthogonal directions.

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

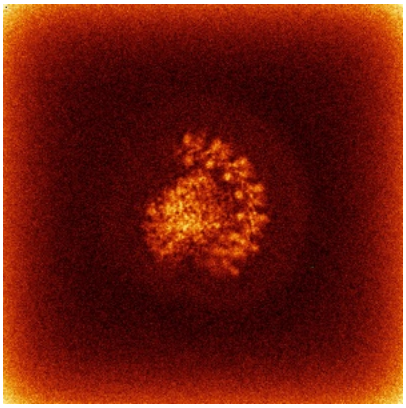
6.4.1 Primary map

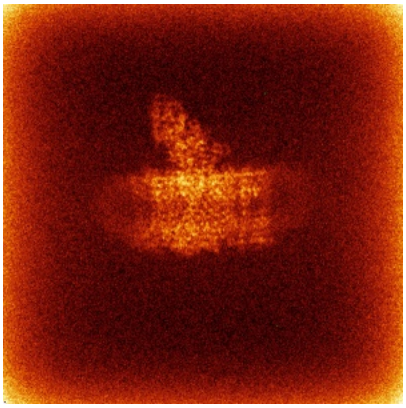

X

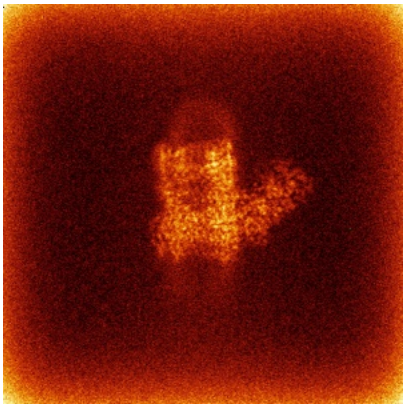

Y


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 0.4. 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.

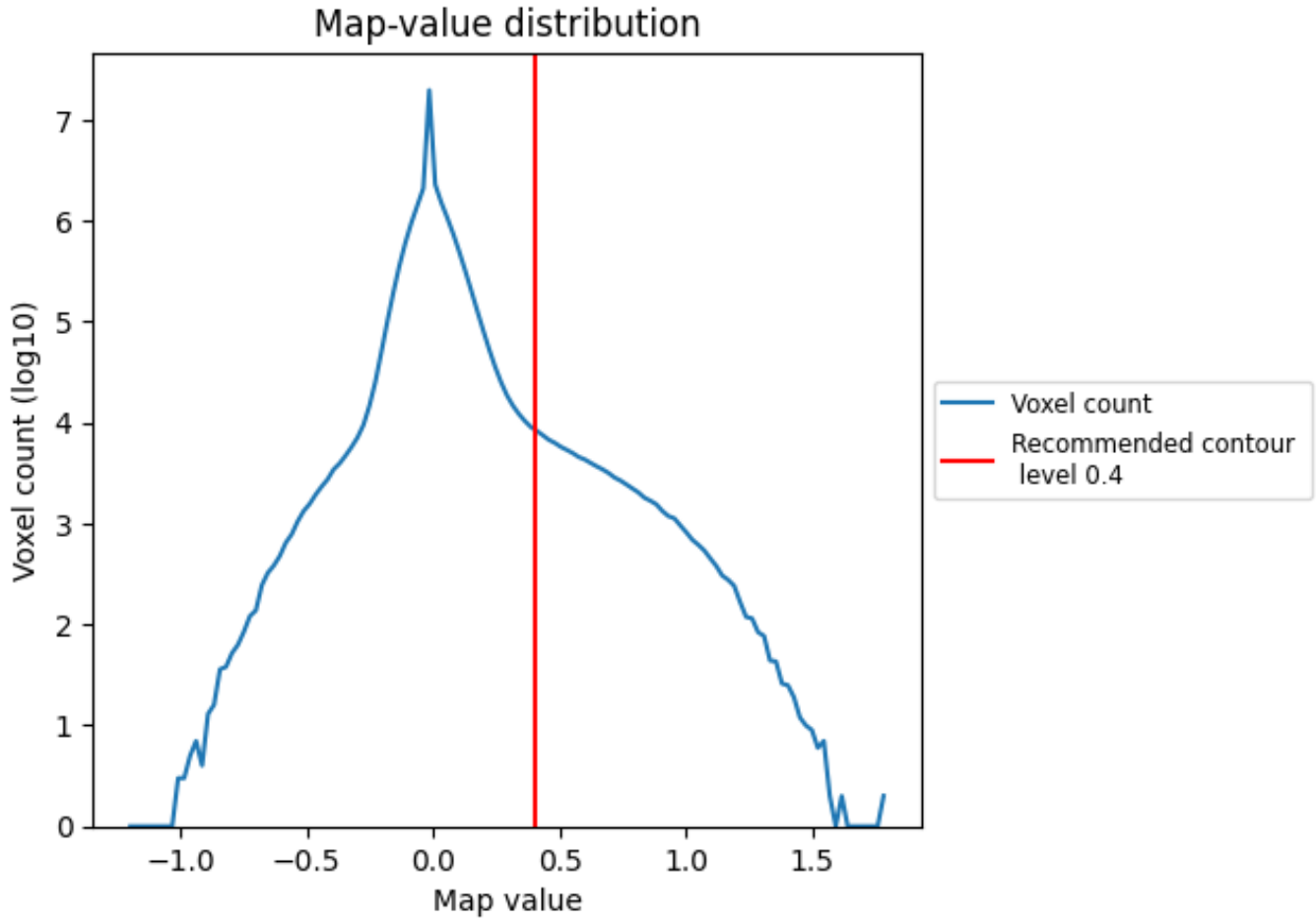
6.6 Mask visualisation (i)

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

7 Map analysis

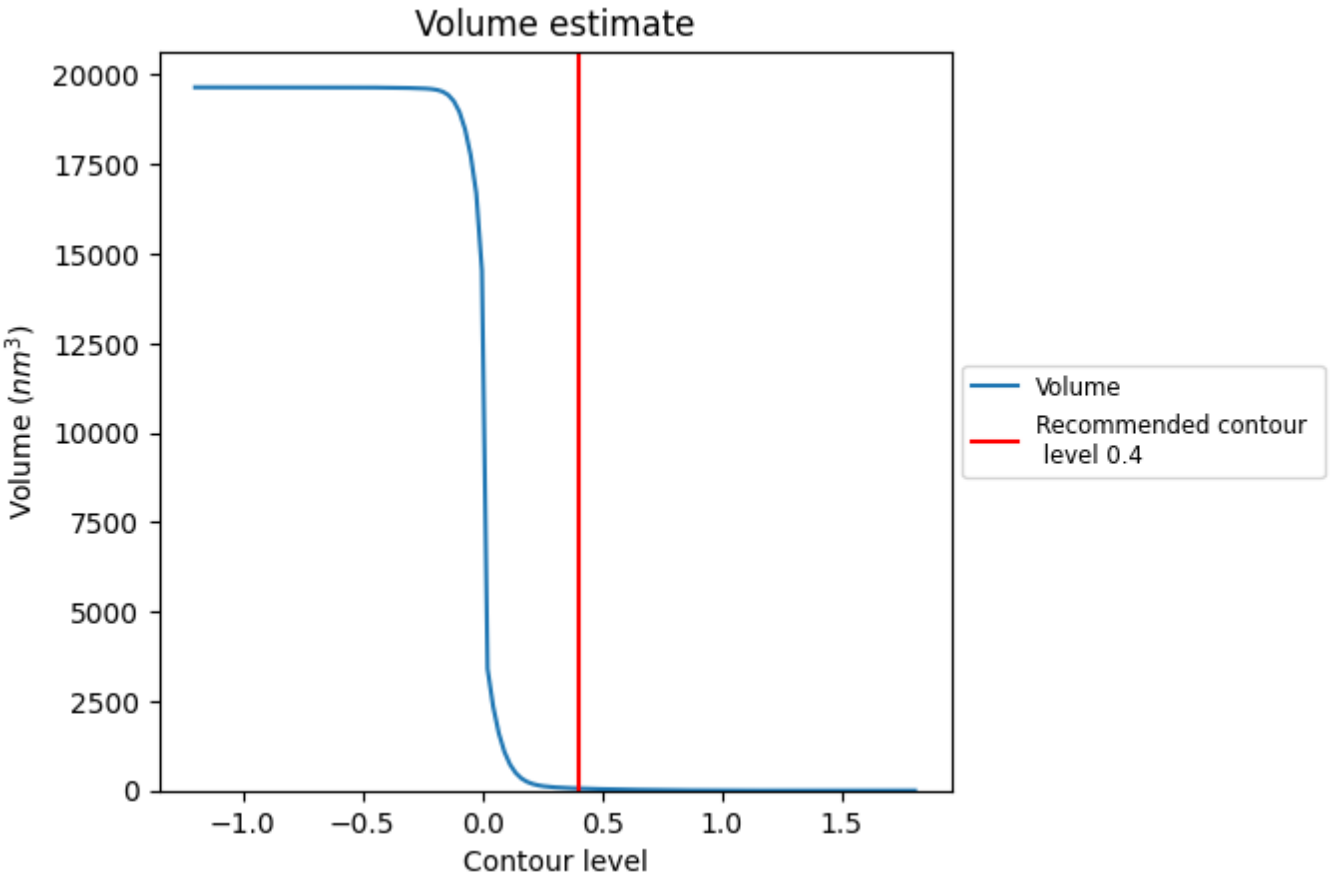
This section contains the results of statistical analysis of the map.

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.

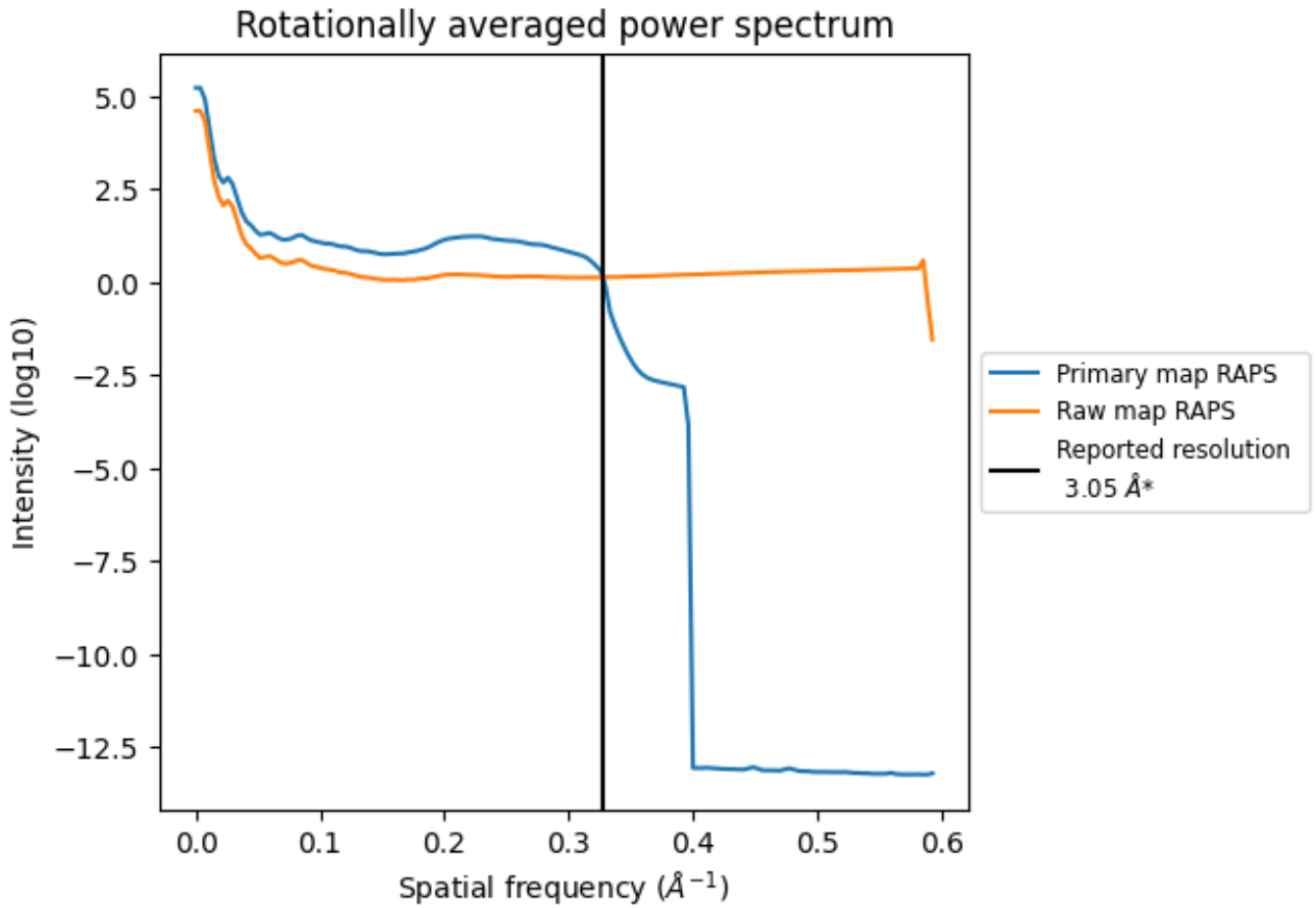
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 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)

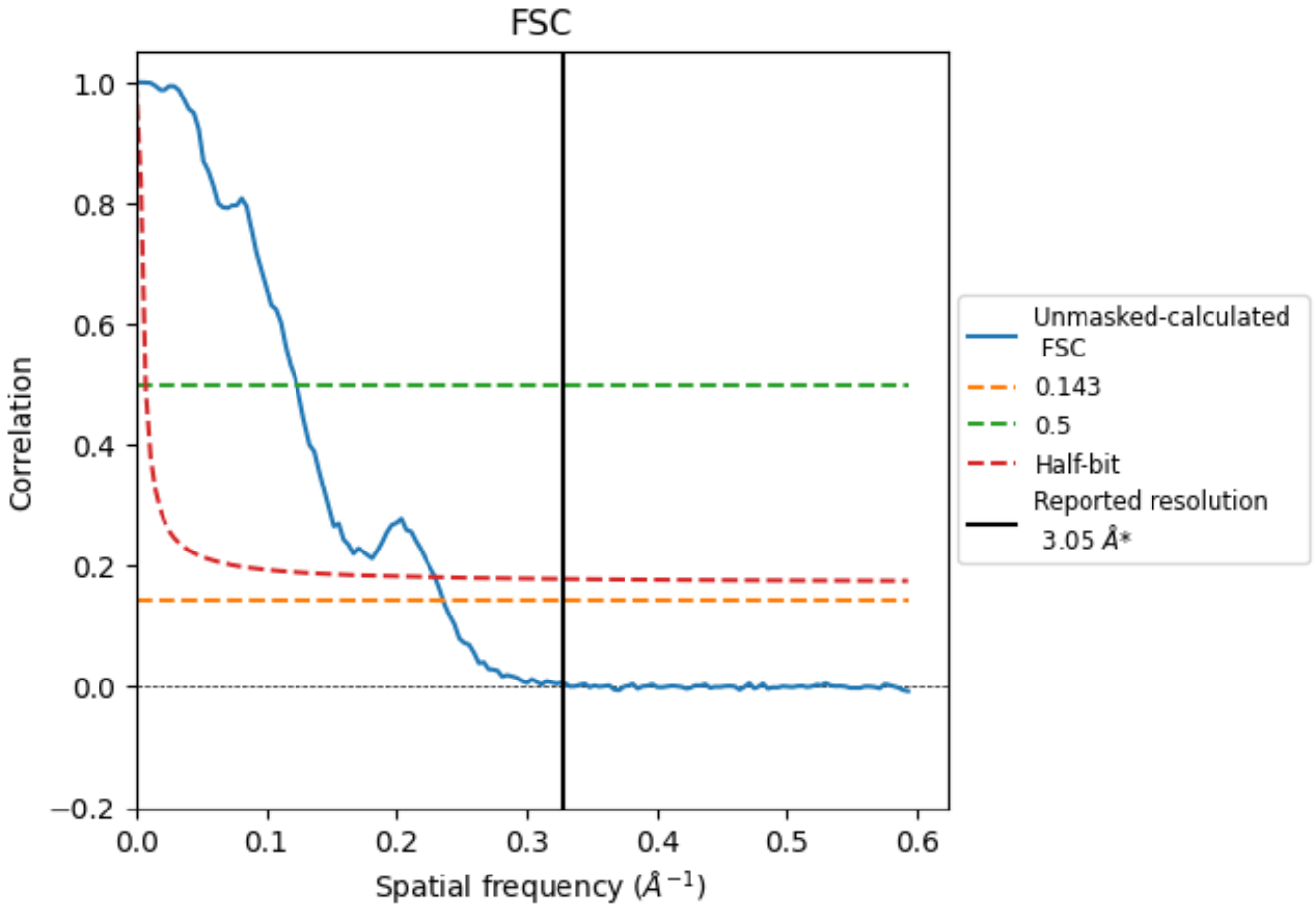


*Reported resolution corresponds to spatial frequency of 0.328 $Å^{-1}$

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 0.328 Å^{-1}

8.2 Resolution estimates (i)

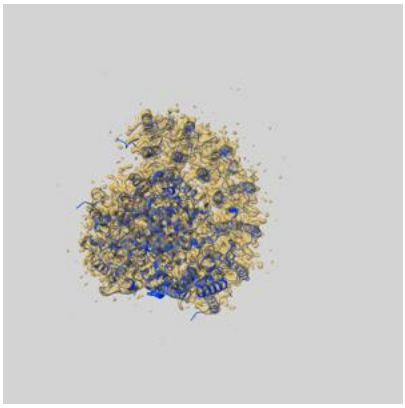
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	8.11	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

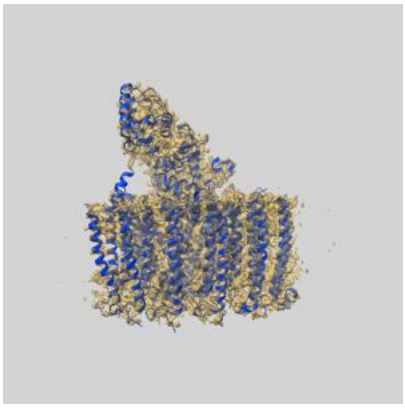
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39177 and PDB model 8YDM. Per-residue inclusion information can be found in section 3 on page 11.

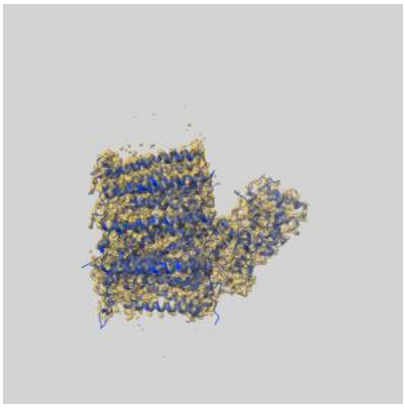
9.1 Map-model overlay



X



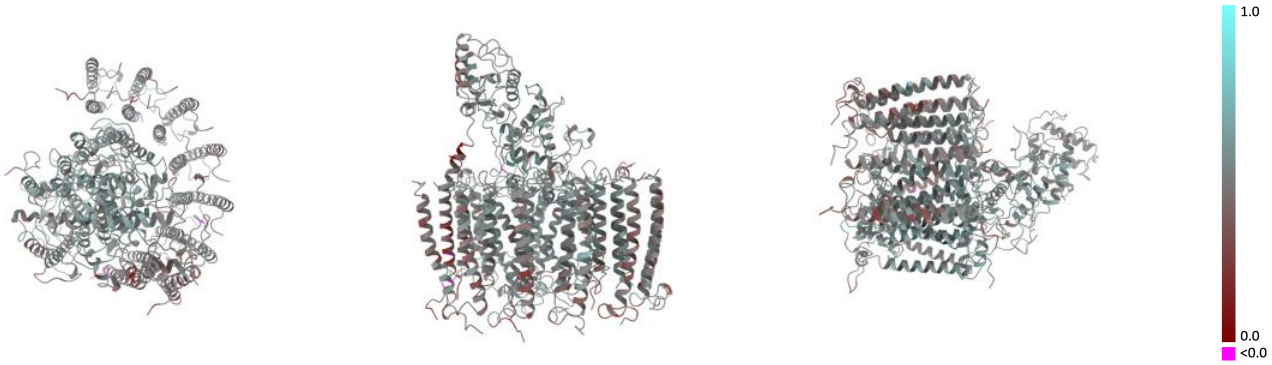
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

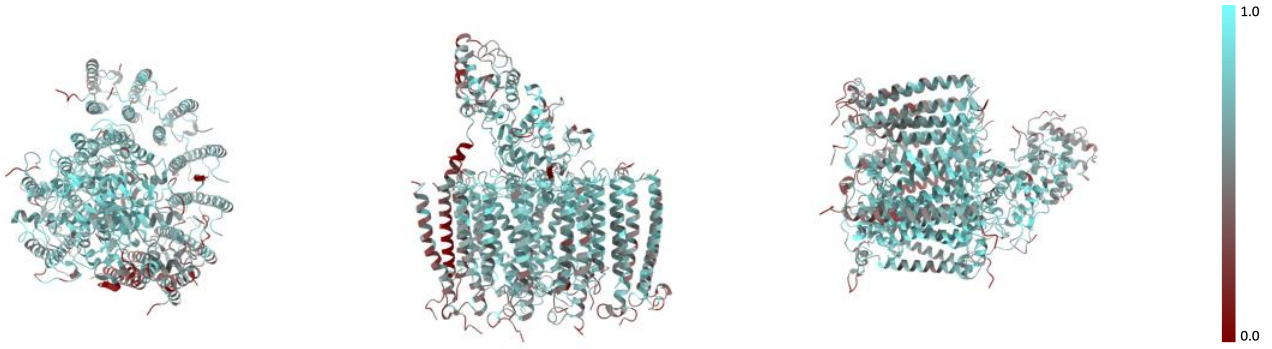
9.2 Q-score mapped to coordinate model (i)



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.

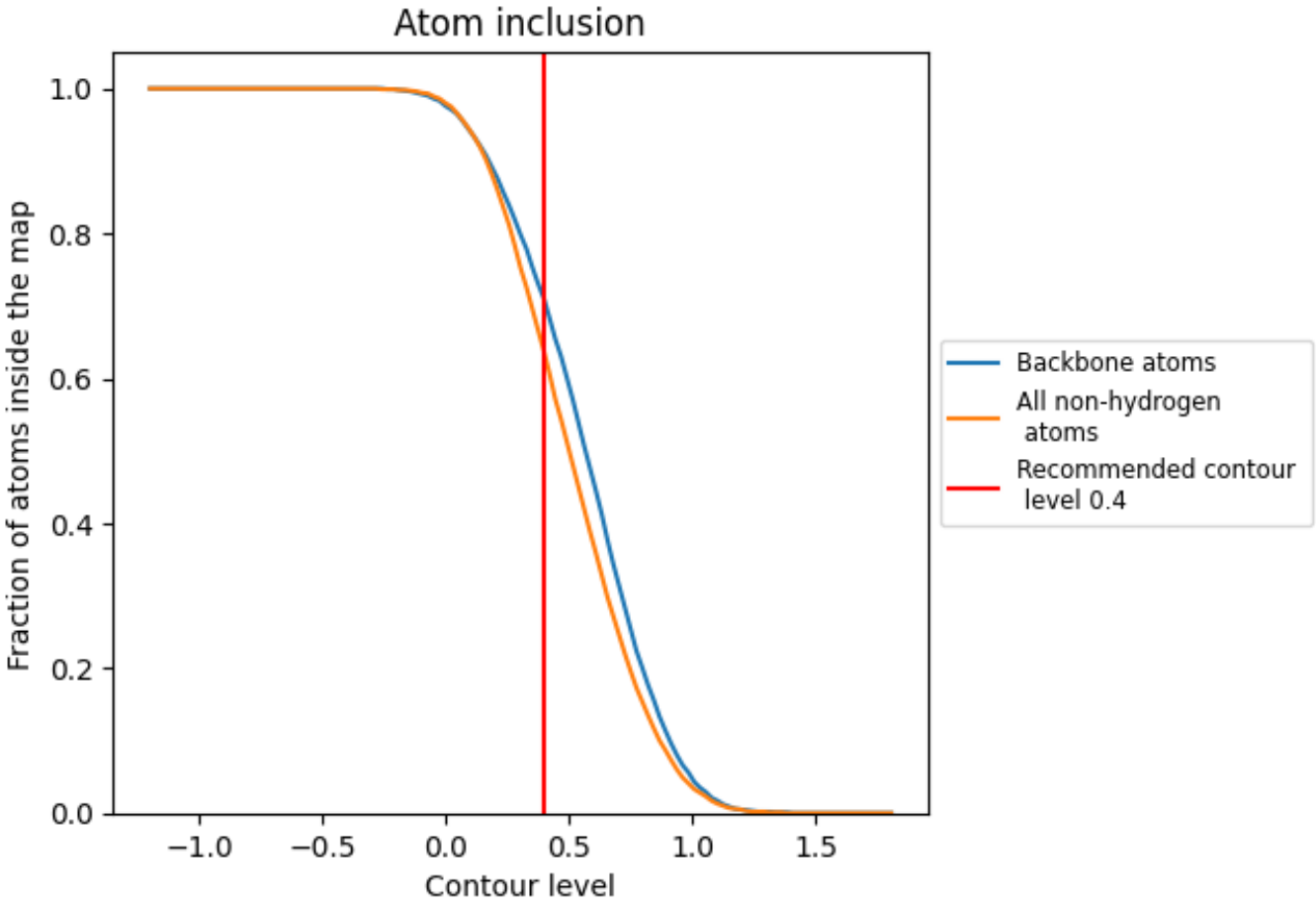
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 64% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.4910
A	0.4580	0.4510
B	0.4070	0.4200
C	0.6130	0.4930
D	0.6250	0.5080
E	0.5680	0.4420
F	0.6280	0.4750
G	0.6180	0.4770
H	0.6280	0.4940
I	0.5780	0.4760
J	0.6520	0.4740
K	0.5460	0.4280
L	0.7040	0.5010
M	0.7640	0.5430
N	0.5760	0.4960
O	0.6430	0.4910
P	0.6230	0.4680
Q	0.5330	0.4680
R	0.5060	0.4450