Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 11:26 am GMT

PDB ID	:	7NHP
EMDB ID	:	EMD-12336
Title	:	Structure of PSII-I (PSII with Psb27, Psb28, and Psb34)
Authors	:	Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.; Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on	:	2021-02-11
Resolution	:	2.72 Å(reported)

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

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

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

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

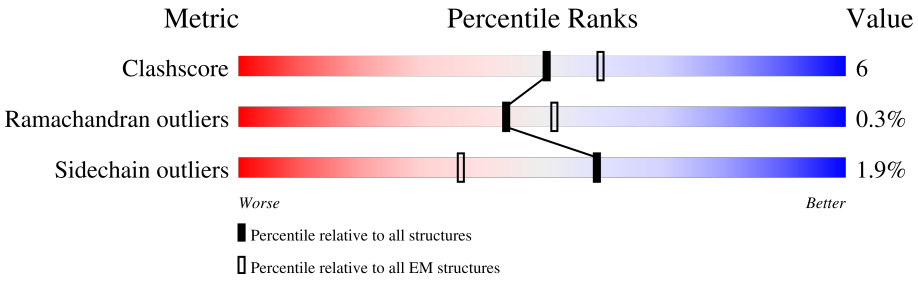
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	360	8% 84% 9% 7%
2	B	510	91% 6%
3	C	461	7% 80% 13% 6%
4	D	352	89% 7%
5	E	84	14% 85% 7% 8%
6	F	45	13% 82% 16%
7	H	66	94% 5%
8	I	38	58% 11% 32%

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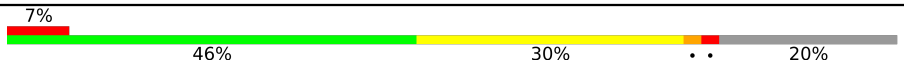
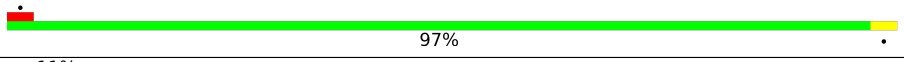
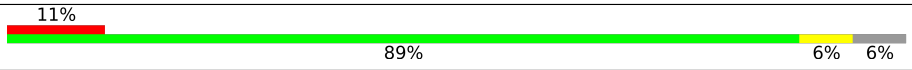
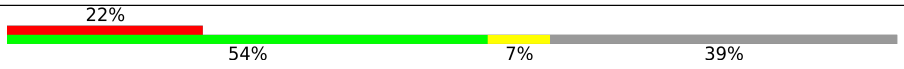
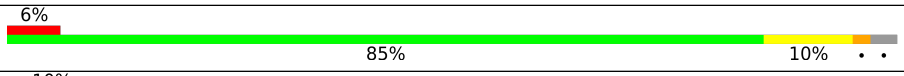
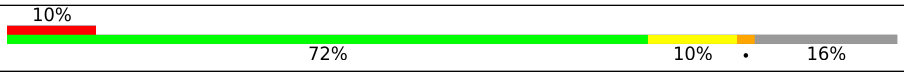
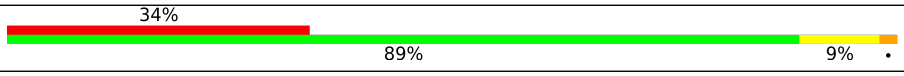
Mol	Chain	Length	Quality of chain
9	K	46	
10	L	37	
11	M	36	
12	T	32	
13	X	41	
14	y	46	
15	Z	62	
16	1	134	
17	2	116	
18	3	56	

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
21	PHO	A	403	X	-	-	-
21	PHO	D	407	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	408	X	-	-	-
22	CLA	D	409	X	-	-	-
23	BCR	K	101	-	-	X	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 21839 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 Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	335	2627	1720	432	460	15	0	0

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	496	3909	2569	649	678	13	0	0

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	432	3345	2197	561	575	12	0	0

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	341	2717	1800	444	461	12	0	0

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	77	635	417	103	115	0	0

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	38	307	207	50	49	1	0	0

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	26	Total	C	N	O	S	0	0
			211	150	27	33	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			293	204	43	46		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

- Molecule 11 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

- Molecule 12 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total	C	N	O	S	0	0
			241	170	34	35	2		

- Molecule 13 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

- Molecule 15 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	60	Total	C	N	O	S	0	0
			463	318	70	74	1		

- Molecule 16 is a protein called Photosystem II lipoprotein Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	113	Total	C	N	O	S	0	0
			893	556	161	173	3		

- Molecule 17 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	112	Total	C	N	O	S	0	0
			897	562	156	173	6		

- Molecule 18 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	56	Total	C	N	O	S	0	0
			419	269	74	75	1		

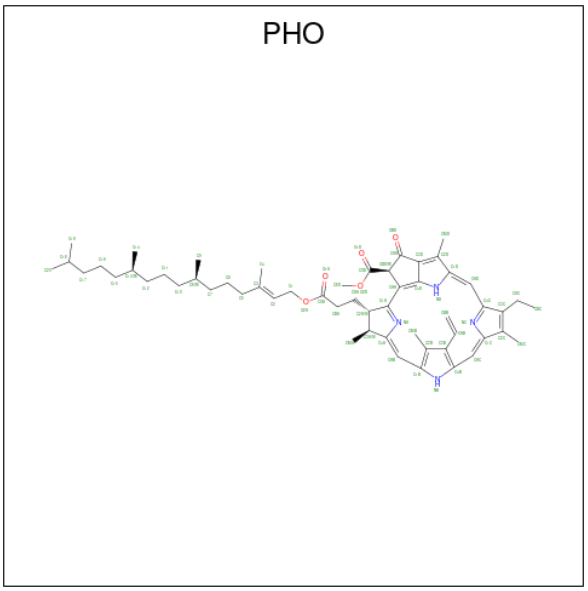
- Molecule 19 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mn	0
			1	1	

- Molecule 20 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

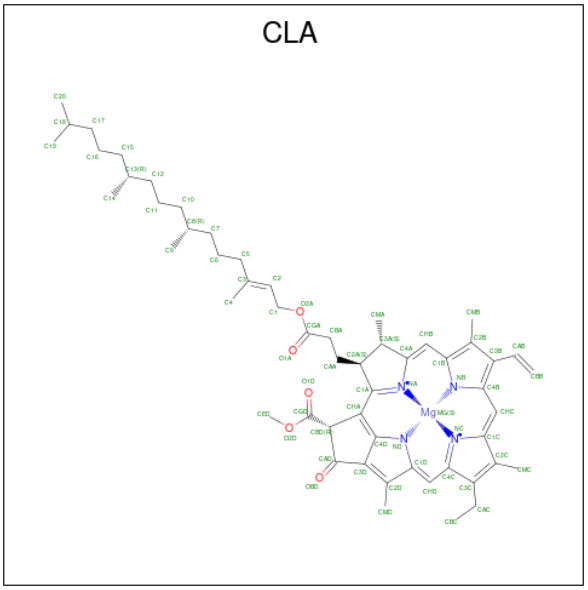
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total 64	C 55	N 4	O 5	0
21	D	1	Total 64	C 55	N 4	O 5	0

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 260	C 220	Mg 4	N 16	O 20	0
22	A	1	Total 260	C 220	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 260	C 220	Mg 4	N 16	O 20	0
22	A	1	Total 260	C 220	Mg 4	N 16	O 20	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	B	1	Total 1040	C 880	Mg 16	N 64	O 80	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
22	C	1	Total 845	C 715	Mg 13	N 52	O 65	0

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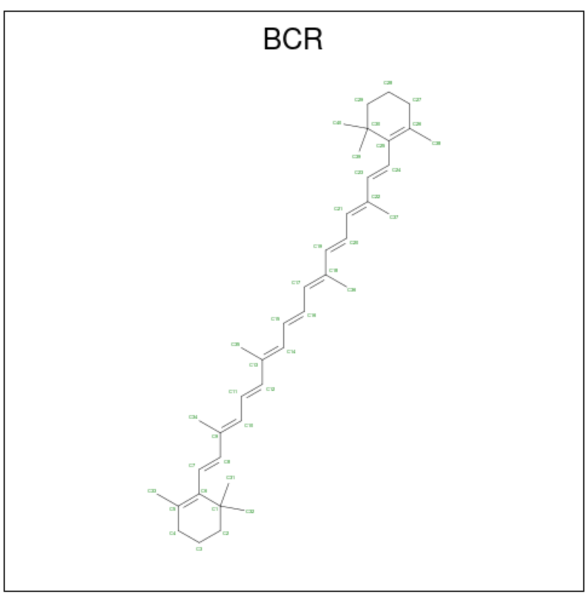
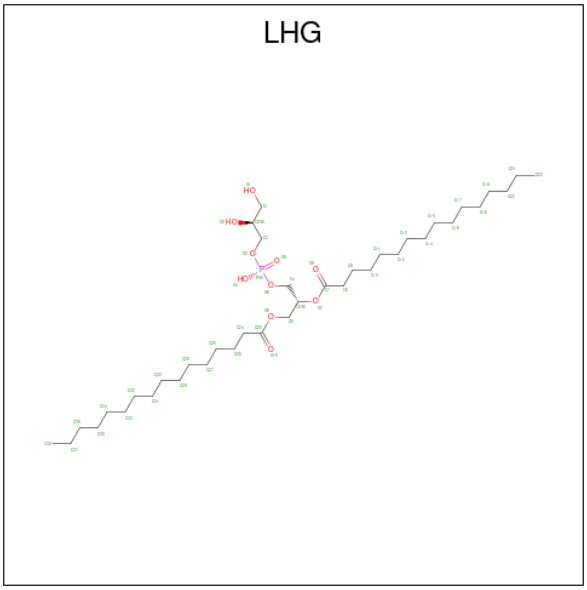
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	C	1	845	715	13	52	65	0
22	D	1	130	110	2	8	10	0
22	D	1	130	110	2	8	10	0

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



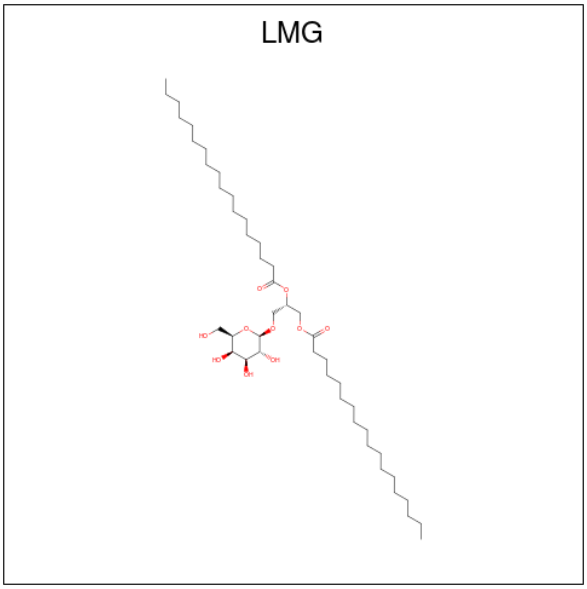
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 120 120	0
23	B	1	Total C 120 120	0
23	B	1	Total C 120 120	0
23	C	1	Total C 120 120	0
23	C	1	Total C 120 120	0
23	C	1	Total C 120 120	0
23	D	1	Total C 40 40	0
23	H	1	Total C 40 40	0
23	K	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 49 38 10 1	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

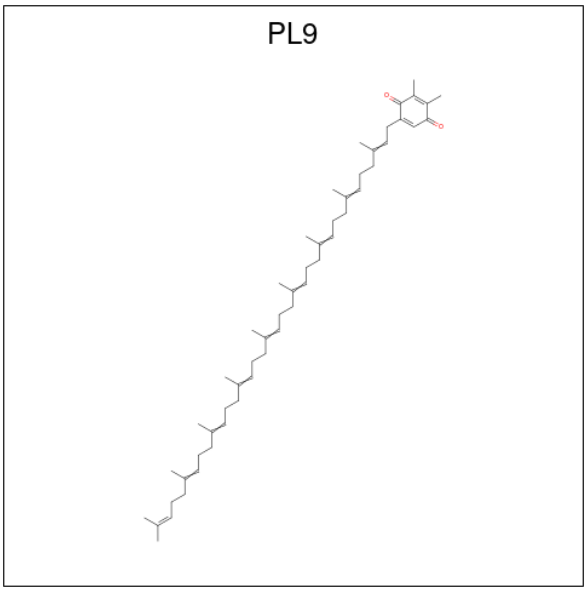


Mol	Chain	Residues	Atoms	AltConf
25	C	1	Total C O 110 90 20	0
25	C	1	Total C O 110 90 20	0
25	D	1	Total C O 220 180 40	0
25	D	1	Total C O 220 180 40	0
25	D	1	Total C O 220 180 40	0
25	D	1	Total C O 220 180 40	0
25	I	1	Total C O 55 45 10	0

- Molecule 26 is FE (III) ION (three-letter code: FE) (formula: Fe).

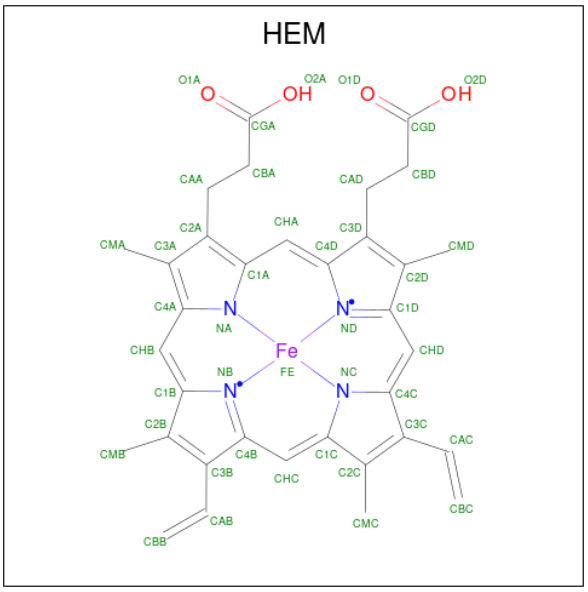
Mol	Chain	Residues	Atoms	AltConf
26	D	1	Total Fe 1 1	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			55	53	2	

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



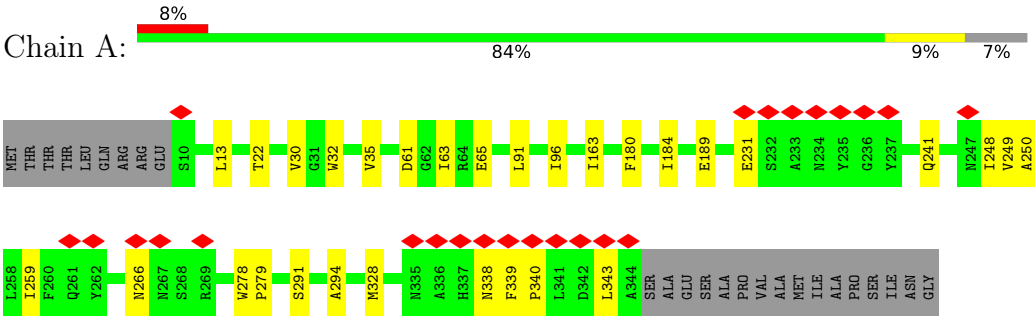
Mol	Chain	Residues	Atoms					AltConf
28	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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.

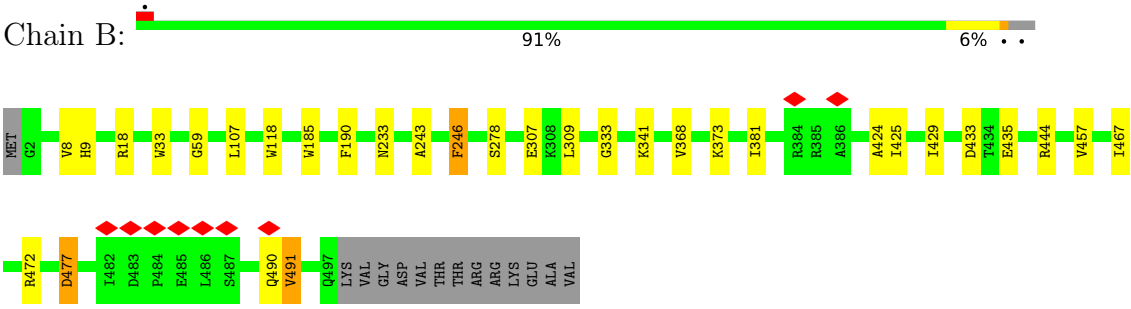
• Molecule 1: Photosystem II protein D1 1

Chain A:



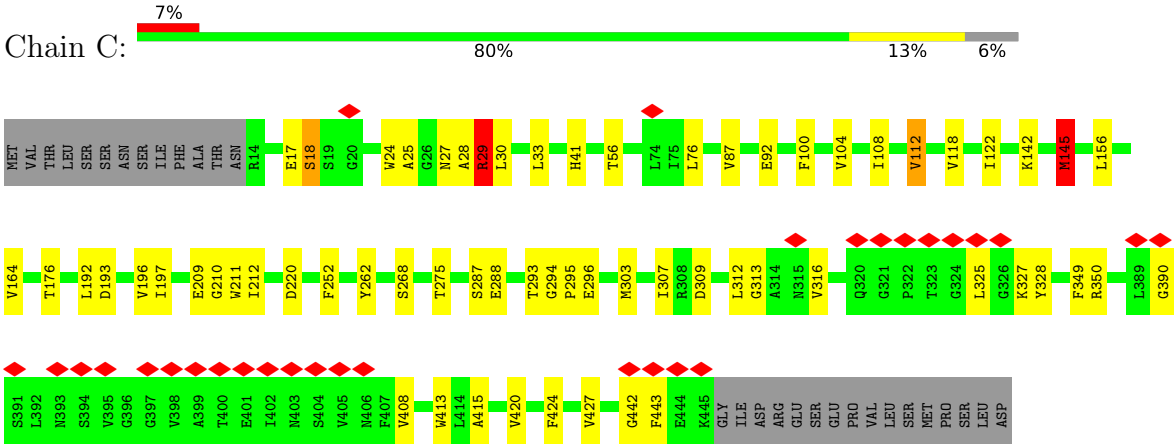
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



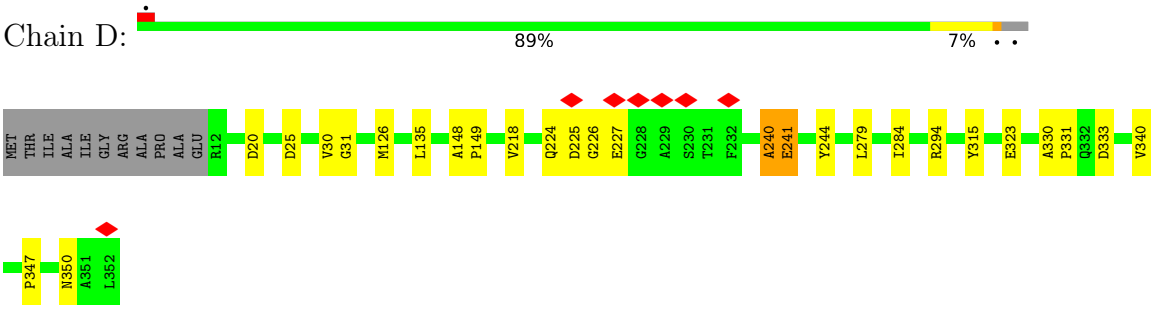
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



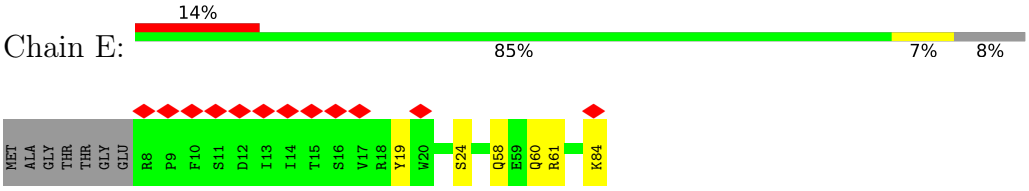
• Molecule 4: Photosystem II D2 protein

Chain D:



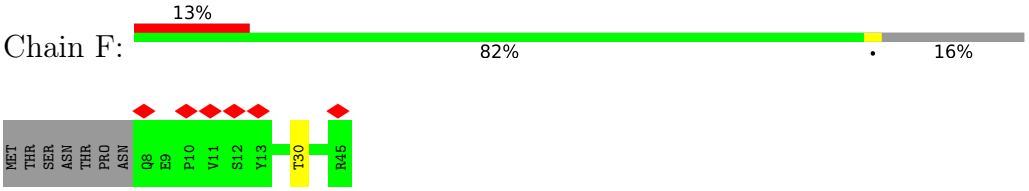
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



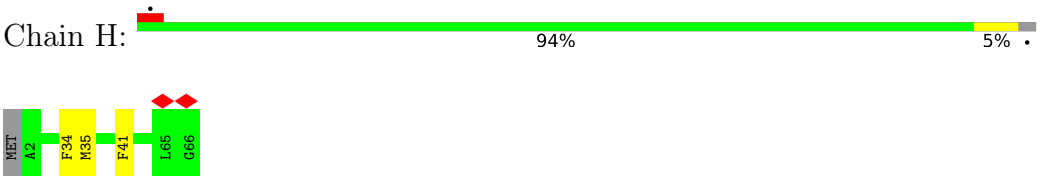
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



• Molecule 7: Photosystem II reaction center protein H

Chain H:

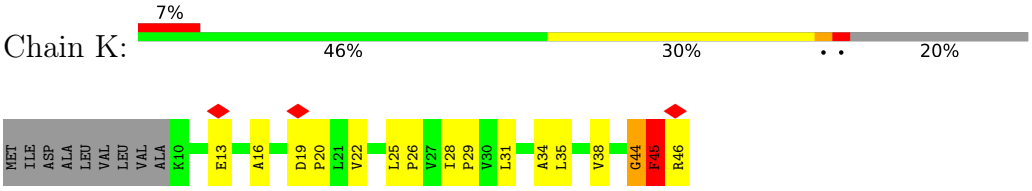


• Molecule 8: Photosystem II reaction center protein I

Chain I:

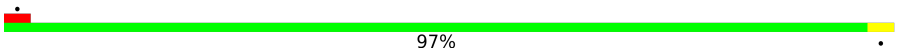
• Molecule 9: Photosystem II reaction center protein K

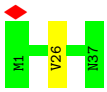
Chain K:



• Molecule 10: Photosystem II reaction center protein L

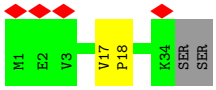
Chain L:





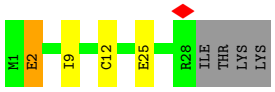
• Molecule 11: Photosystem II reaction center protein M

Chain M:



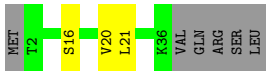
• Molecule 12: Photosystem II reaction center protein T

Chain T:



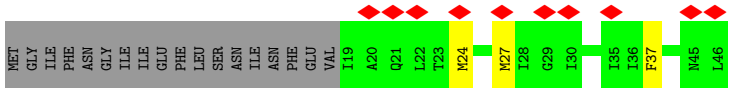
• Molecule 13: Photosystem II reaction center X protein

Chain X:



• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:

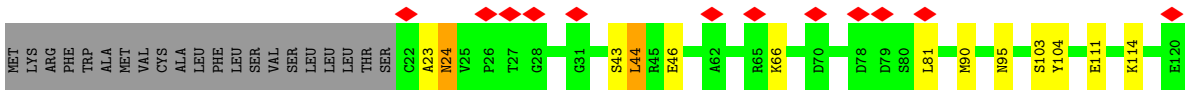


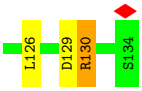
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:

• Molecule 16: Photosystem II lipoprotein Psb27

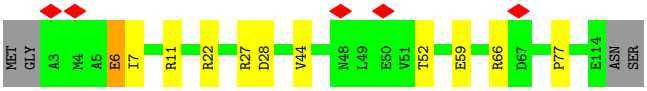
Chain 1:





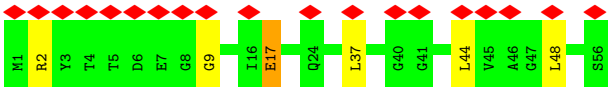
• Molecule 17: Photosystem II reaction center Psb28 protein

Chain 2:



• Molecule 18: Tsl0063 protein

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.062	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, HEM, BCR, LMG, MN, CL, PL9, PHO, FE, LHG

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	0.44	0/2712	0.76	3/3700 (0.1%)
2	B	0.45	0/4049	0.77	2/5519 (0.0%)
3	C	0.45	0/3456	0.79	7/4706 (0.1%)
4	D	0.42	0/2812	0.74	1/3832 (0.0%)
5	E	0.43	0/654	0.74	1/891 (0.1%)
6	F	0.48	0/317	0.76	0/433
7	H	0.43	0/524	0.82	0/713
8	I	0.57	0/216	0.87	0/292
9	K	0.44	0/303	0.80	1/416 (0.2%)
10	L	0.47	0/311	0.79	0/422
11	M	0.44	0/270	0.68	0/367
12	T	0.50	0/250	0.81	0/338
13	X	0.43	0/257	0.92	2/348 (0.6%)
14	y	0.56	0/209	0.97	0/279
15	Z	0.44	0/474	0.77	0/649
16	1	0.44	0/907	0.81	1/1220 (0.1%)
17	2	0.45	0/914	0.87	1/1231 (0.1%)
18	3	0.45	0/426	0.83	0/578
All	All	0.45	0/19061	0.78	19/25934 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
3	C	0	2
4	D	0	3
9	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	1	0	2
17	2	0	1
18	3	0	2
All	All	0	19

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	21	LEU	CB-CG-CD2	-8.09	97.25	111.00
3	C	145	MET	CB-CG-SD	8.00	136.40	112.40
17	2	22	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	C	420	VAL	CG1-CB-CG2	-6.59	100.36	110.90
3	C	29	ARG	NE-CZ-NH2	6.26	123.43	120.30
13	X	21	LEU	CB-CG-CD1	5.92	121.06	111.00
3	C	427	VAL	CG1-CB-CG2	-5.89	101.47	110.90
16	1	104	TYR	CA-CB-CG	5.84	124.49	113.40
1	A	328	MET	CG-SD-CE	5.78	109.45	100.20
1	A	328	MET	CB-CG-SD	5.76	129.67	112.40
5	E	19	TYR	CA-CB-CG	5.62	124.07	113.40
1	A	257	ARG	NE-CZ-NH1	5.55	123.08	120.30
4	D	294	ARG	NE-CZ-NH1	5.51	123.05	120.30
3	C	29	ARG	NE-CZ-NH1	-5.41	117.60	120.30
9	K	45	PHE	N-CA-C	-5.29	96.72	111.00
2	B	472	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	C	164	VAL	CG1-CB-CG2	-5.11	102.73	110.90
3	C	192	LEU	CB-CG-CD2	-5.06	102.40	111.00
2	B	491	VAL	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	1	24	ASN	Sidechain
16	1	95	ASN	Sidechain
17	2	27	ARG	Peptide
18	3	17	GLU	Sidechain
18	3	9	GLY	Peptide
1	A	189	GLU	Sidechain
1	A	266	ASN	Sidechain
1	A	338	ASN	Sidechain

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Mol	Chain	Res	Type	Group
1	A	343	LEU	Peptide
2	B	477	ASP	Sidechain
2	B	490	GLN	Peptide,Mainchain
3	C	220	ASP	Sidechain
3	C	424	PHE	Sidechain
4	D	225	ASP	Sidechain
4	D	241	GLU	Peptide
4	D	333	ASP	Sidechain
9	K	44	GLY	Peptide,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	2627	0	2524	19	0
2	B	3909	0	3763	24	0
3	C	3345	0	3273	66	0
4	D	2717	0	2621	18	0
5	E	635	0	625	4	0
6	F	307	0	312	1	0
7	H	511	0	532	3	0
8	I	211	0	227	4	0
9	K	293	0	305	25	0
10	L	304	0	316	2	0
11	M	267	0	289	1	0
12	T	241	0	244	2	0
13	X	254	0	282	1	0
14	y	208	0	237	0	0
15	Z	463	0	495	5	0
16	1	893	0	896	6	0
17	2	897	0	859	3	0
18	3	419	0	438	2	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	64	0	73	1	0
21	D	64	0	73	0	0
22	A	260	0	281	9	0
22	B	1040	0	1127	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	C	845	0	918	44	0
22	D	130	0	140	8	0
23	A	40	0	56	2	0
23	B	120	0	168	5	0
23	C	120	0	168	20	0
23	D	40	0	56	0	0
23	H	40	0	56	18	0
23	K	40	0	56	24	0
24	A	49	0	74	0	0
25	C	110	0	172	0	0
25	D	220	0	344	3	0
25	I	55	0	86	0	0
26	D	1	0	0	0	0
27	D	55	0	80	4	0
28	E	43	0	30	0	0
All	All	21839	0	22196	258	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 6.

All (258) 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)
23:C:515:BCR:H353	23:K:101:BCR:C33	1.74	1.18
3:C:122:ILE:HD11	22:C:512:CLA:H92	1.17	1.09
23:C:515:BCR:H353	23:K:101:BCR:H332	1.39	1.05
3:C:30:LEU:HD21	22:C:512:CLA:H2A	1.39	1.03
3:C:122:ILE:CD1	22:C:512:CLA:H92	1.88	1.03
9:K:34:ALA:HB1	23:K:101:BCR:H20C	1.42	1.00
23:C:515:BCR:C35	23:K:101:BCR:H332	1.95	0.95
3:C:27:ASN:OD1	22:C:510:CLA:H11	1.65	0.94
23:C:515:BCR:C13	23:K:101:BCR:H332	1.98	0.94
3:C:122:ILE:HD11	22:C:512:CLA:C9	1.97	0.93
22:B:609:CLA:C1B	23:H:101:BCR:H333	1.98	0.92
3:C:27:ASN:HB2	22:C:510:CLA:CBA	1.98	0.92
9:K:31:LEU:HD22	23:K:101:BCR:H363	1.51	0.90
22:B:609:CLA:C2B	23:H:101:BCR:H333	2.01	0.90
3:C:29:ARG:NH1	9:K:46:ARG:NH1	2.19	0.90
3:C:108:ILE:HD11	23:C:515:BCR:H332	1.52	0.89
3:C:29:ARG:NH1	9:K:46:ARG:CZ	2.40	0.85
22:B:609:CLA:C3B	23:H:101:BCR:H333	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:LEU:HD21	22:C:505:CLA:OBD	1.83	0.78
3:C:30:LEU:CD2	22:C:512:CLA:H2A	2.13	0.78
3:C:87:VAL:HG23	3:C:92:GLU:O	1.83	0.78
3:C:27:ASN:HB2	22:C:510:CLA:CGA	2.14	0.77
22:B:613:CLA:HBB1	22:B:613:CLA:HMB1	1.66	0.77
3:C:108:ILE:HD11	23:C:515:BCR:C33	2.16	0.76
23:C:515:BCR:C11	23:K:101:BCR:HC41	2.17	0.74
3:C:27:ASN:HB2	22:C:510:CLA:HBA2	1.69	0.74
22:A:405:CLA:HMA2	25:D:402:LMG:H271	1.71	0.73
22:C:503:CLA:HBB1	22:C:503:CLA:HMB1	1.69	0.73
3:C:108:ILE:HD13	15:Z:51:VAL:HG21	1.71	0.72
1:A:248:ILE:HG23	1:A:250:ALA:H	1.55	0.72
22:D:409:CLA:H201	23:H:101:BCR:H372	1.73	0.70
23:C:515:BCR:H353	23:K:101:BCR:H333	1.73	0.69
9:K:13:GLU:HA	9:K:16:ALA:HB2	1.73	0.68
22:B:609:CLA:C4B	23:H:101:BCR:H333	2.24	0.68
22:B:609:CLA:C2B	23:H:101:BCR:C33	2.72	0.68
3:C:312:LEU:HD12	3:C:313:GLY:N	2.09	0.68
3:C:309:ASP:OD1	3:C:328:TYR:OH	2.08	0.67
3:C:288:GLU:OE2	3:C:288:GLU:N	2.28	0.67
3:C:27:ASN:OD1	22:C:510:CLA:C1	2.43	0.67
3:C:29:ARG:HH12	9:K:46:ARG:CZ	2.07	0.67
3:C:316:VAL:HB	3:C:328:TYR:CD2	2.30	0.66
22:C:503:CLA:HMA1	23:C:516:BCR:H401	1.78	0.66
15:Z:36:SER:HA	15:Z:39:LEU:HD21	1.79	0.65
3:C:142:LYS:HA	3:C:145:MET:SD	2.36	0.65
22:B:612:CLA:H162	22:B:612:CLA:H101	1.77	0.65
22:B:608:CLA:O2D	22:B:608:CLA:H2A	1.96	0.65
22:B:616:CLA:HMA2	23:B:619:BCR:H362	1.77	0.65
3:C:29:ARG:HH12	9:K:46:ARG:NH1	1.95	0.64
2:B:307:GLU:N	2:B:307:GLU:OE2	2.29	0.64
3:C:25:ALA:HA	22:C:510:CLA:O1A	1.98	0.64
22:B:609:CLA:C3B	23:H:101:BCR:C33	2.76	0.63
22:B:606:CLA:HMB1	22:B:606:CLA:HBB1	1.79	0.63
16:1:129:ASP:OD1	16:1:130:ARG:N	2.32	0.62
22:B:605:CLA:HMA1	22:B:606:CLA:HBA2	1.83	0.61
22:B:603:CLA:HBB1	22:B:603:CLA:HMB1	1.83	0.61
2:B:467:ILE:HD13	4:D:126:MET:CE	2.30	0.61
3:C:28:ALA:HB2	22:C:510:CLA:HAA2	1.82	0.60
3:C:309:ASP:OD1	3:C:328:TYR:CZ	2.55	0.60
1:A:231:GLU:OE1	1:A:231:GLU:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:604:CLA:HMA2	22:B:604:CLA:HBA2	1.82	0.60
1:A:35:VAL:HG22	23:A:408:BCR:HC42	1.83	0.59
9:K:34:ALA:CB	23:K:101:BCR:H20C	2.27	0.59
9:K:34:ALA:HB1	23:K:101:BCR:C20	2.25	0.59
22:B:607:CLA:H101	22:B:607:CLA:H142	1.84	0.59
9:K:35:LEU:HD22	23:K:101:BCR:H351	1.85	0.59
3:C:193:ASP:O	3:C:196:VAL:HG22	2.04	0.58
3:C:118:VAL:HG12	22:C:512:CLA:H91	1.84	0.58
2:B:467:ILE:HD13	4:D:126:MET:HE3	1.86	0.58
22:B:611:CLA:HMB2	22:B:612:CLA:NB	2.20	0.57
16:1:44:LEU:O	16:1:44:LEU:HD12	2.04	0.57
2:B:18:ARG:HE	2:B:118:TRP:HB3	1.71	0.56
22:B:601:CLA:HBB2	7:H:41:PHE:CD1	2.41	0.56
4:D:30:VAL:HG13	4:D:31:GLY:H	1.70	0.56
5:E:84:LYS:OXT	5:E:84:LYS:HG2	2.06	0.56
1:A:63:ILE:HG13	1:A:65:GLU:HG2	1.87	0.56
22:B:609:CLA:NB	23:H:101:BCR:H333	2.21	0.56
3:C:197:ILE:HG23	23:C:516:BCR:H382	1.88	0.55
2:B:467:ILE:CD1	4:D:126:MET:HE1	2.35	0.55
2:B:368:VAL:HB	2:B:381:ILE:HD12	1.89	0.55
27:D:406:PL9:H352	10:L:26:VAL:CG1	2.37	0.55
3:C:27:ASN:CB	22:C:510:CLA:HBA2	2.37	0.55
22:B:612:CLA:H101	22:B:612:CLA:C16	2.37	0.54
3:C:196:VAL:HG23	3:C:197:ILE:HG12	1.89	0.54
1:A:249:VAL:HG21	4:D:25:ASP:OD2	2.08	0.54
4:D:30:VAL:HG13	4:D:31:GLY:N	2.22	0.54
16:1:43:SER:O	16:1:46:GLU:HG3	2.07	0.54
3:C:145:MET:HG3	22:C:509:CLA:HBC1	1.90	0.54
8:I:19:PHE:CZ	8:I:23:PHE:HE2	2.26	0.54
23:K:101:BCR:C8	23:K:101:BCR:H311	2.38	0.53
22:C:513:CLA:HBA1	22:C:513:CLA:HMA2	1.89	0.53
2:B:467:ILE:CD1	4:D:126:MET:CE	2.86	0.53
1:A:91:LEU:HD11	1:A:163:ILE:HA	1.90	0.53
3:C:29:ARG:CZ	9:K:46:ARG:NH2	2.71	0.53
1:A:180:PHE:O	1:A:184:ILE:HG13	2.09	0.53
22:A:405:CLA:H2A	22:A:405:CLA:CGD	2.39	0.53
3:C:122:ILE:HD11	22:C:512:CLA:C8	2.38	0.52
23:C:515:BCR:C11	23:K:101:BCR:C4	2.87	0.52
22:A:407:CLA:H72	22:A:407:CLA:H41	1.91	0.52
8:I:4:LEU:HA	8:I:7:THR:HG22	1.90	0.52
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:THR:HG22	3:C:176:THR:O	2.10	0.52
23:C:515:BCR:C10	23:K:101:BCR:HC41	2.40	0.51
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.92	0.51
22:B:603:CLA:HMB1	22:B:603:CLA:CBB	2.40	0.51
15:Z:10:ALA:O	15:Z:14:ILE:HG12	2.10	0.51
3:C:17:GLU:OE1	9:K:46:ARG:OXT	2.28	0.51
23:C:515:BCR:C12	23:K:101:BCR:H332	2.38	0.51
3:C:390:GLY:HA3	3:C:408:VAL:HG13	1.92	0.51
23:B:618:BCR:H331	23:B:618:BCR:C8	2.40	0.51
15:Z:23:VAL:HG23	15:Z:24:PRO:HD3	1.92	0.51
2:B:333:GLY:HA2	2:B:444:ARG:HH11	1.75	0.50
1:A:61:ASP:OD2	1:A:63:ILE:HG12	2.11	0.50
16:1:126:LEU:O	16:1:129:ASP:OD1	2.28	0.50
3:C:275:THR:HG23	3:C:415:ALA:HB1	1.93	0.50
4:D:240:ALA:O	4:D:241:GLU:HB2	2.12	0.50
23:H:101:BCR:C8	23:H:101:BCR:H311	2.38	0.50
2:B:243:ALA:HA	2:B:246:PHE:CE1	2.46	0.49
3:C:28:ALA:N	22:C:510:CLA:HBA1	2.27	0.49
2:B:424:ALA:HB2	2:B:429:ILE:HD11	1.94	0.49
22:B:611:CLA:HHC	22:B:611:CLA:HBB1	1.94	0.49
18:3:44:LEU:O	18:3:48:LEU:HG	2.13	0.49
1:A:248:ILE:HG12	1:A:249:VAL:H	1.76	0.49
3:C:209:GLU:HG3	3:C:210:GLY:H	1.78	0.49
22:C:512:CLA:H151	22:C:512:CLA:H101	1.92	0.49
27:D:406:PL9:H352	10:L:26:VAL:HG12	1.93	0.49
3:C:112:VAL:HG23	23:C:518:BCR:H362	1.93	0.49
22:C:504:CLA:H43	22:C:505:CLA:H52	1.96	0.48
3:C:327:LYS:HG2	3:C:328:TYR:CD2	2.49	0.48
1:A:291:SER:O	1:A:294:ALA:HB3	2.13	0.48
23:H:101:BCR:H392	23:H:101:BCR:C23	2.43	0.48
22:C:517:CLA:H141	22:C:517:CLA:H171	1.96	0.47
27:D:406:PL9:C33	27:D:406:PL9:H301	2.44	0.47
11:M:17:VAL:HB	11:M:18:PRO:HD3	1.95	0.47
22:D:409:CLA:H201	23:H:101:BCR:C37	2.43	0.47
5:E:58:GLN:O	5:E:61:ARG:NH2	2.47	0.47
9:K:13:GLU:OE2	9:K:13:GLU:N	2.47	0.47
16:1:111:GLU:HA	16:1:114:LYS:HG3	1.96	0.47
3:C:413:TRP:HB3	22:C:506:CLA:HMB2	1.97	0.47
3:C:112:VAL:CG2	23:C:518:BCR:H362	2.45	0.47
3:C:293:THR:HG22	3:C:295:PRO:HD2	1.96	0.47
12:T:2:GLU:H	12:T:2:GLU:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:404:LMG:H422	6:F:30:THR:HG21	1.97	0.47
3:C:30:LEU:HD12	22:C:511:CLA:CBB	2.45	0.46
9:K:25:LEU:O	9:K:28:ILE:HD12	2.15	0.46
2:B:309:LEU:HD23	2:B:309:LEU:O	2.16	0.46
22:B:608:CLA:HHC	22:B:608:CLA:HBB1	1.97	0.46
22:B:613:CLA:OBD	22:B:614:CLA:HHC	2.15	0.46
23:H:101:BCR:H392	23:H:101:BCR:H23C	1.97	0.46
9:K:28:ILE:N	9:K:29:PRO:CD	2.78	0.46
22:C:514:CLA:HHC	22:C:514:CLA:HBB1	1.97	0.46
9:K:31:LEU:CD2	23:K:101:BCR:H363	2.35	0.46
4:D:279:LEU:HD13	22:D:408:CLA:HBA1	1.98	0.46
9:K:35:LEU:O	9:K:38:VAL:HG22	2.15	0.46
3:C:29:ARG:NH1	9:K:46:ARG:NH2	2.63	0.46
22:C:511:CLA:HMA2	22:C:517:CLA:HMB2	1.97	0.46
1:A:96:ILE:CG2	8:I:4:LEU:HD21	2.46	0.45
3:C:211:TRP:CE3	3:C:212:ILE:HG12	2.52	0.45
22:C:512:CLA:H202	15:Z:23:VAL:HG21	1.97	0.45
22:A:405:CLA:HED1	27:D:406:PL9:H372	1.98	0.45
4:D:218:VAL:HG13	4:D:244:TYR:CD2	2.52	0.45
23:K:101:BCR:H392	23:K:101:BCR:C23	2.47	0.45
9:K:38:VAL:HG13	23:K:101:BCR:H21C	1.98	0.45
23:C:515:BCR:C12	23:K:101:BCR:HC41	2.46	0.45
22:B:608:CLA:OBD	22:B:610:CLA:HBB1	2.17	0.45
3:C:252:PHE:CZ	22:C:509:CLA:HBB2	2.52	0.45
23:K:101:BCR:H351	23:K:101:BCR:H15C	1.81	0.45
22:A:406:CLA:HBC2	22:A:406:CLA:HMC1	1.99	0.45
22:B:611:CLA:H93	25:D:403:LMG:H371	1.99	0.45
22:C:503:CLA:HMA1	23:C:516:BCR:H292	1.97	0.45
1:A:22:THR:HG22	1:A:22:THR:O	2.16	0.45
3:C:33:LEU:HD12	22:C:512:CLA:HED3	1.99	0.45
5:E:60:GLN:C	5:E:61:ARG:HD2	2.37	0.44
2:B:107:LEU:HD21	22:B:615:CLA:H42	1.99	0.44
22:C:503:CLA:CMA	23:C:516:BCR:H292	2.47	0.44
22:C:511:CLA:H93	22:C:513:CLA:HBA2	1.98	0.44
4:D:323:GLU:OE1	4:D:347:PRO:HG2	2.18	0.44
16:1:129:ASP:OD1	16:1:129:ASP:C	2.56	0.44
3:C:17:GLU:O	3:C:18:SER:CB	2.65	0.44
4:D:226:GLY:O	4:D:227:GLU:HB2	2.17	0.44
3:C:30:LEU:HD21	22:C:512:CLA:C2A	2.28	0.44
23:B:618:BCR:H15C	23:B:618:BCR:H351	1.90	0.44
23:C:515:BCR:C35	23:K:101:BCR:C33	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2:52:THR:HG22	17:2:66:ARG:HH12	1.82	0.44
2:B:33:TRP:CH2	22:B:604:CLA:HMB2	2.52	0.43
17:2:6:GLU:OE1	17:2:7:ILE:N	2.51	0.43
22:A:406:CLA:O2A	22:A:406:CLA:H52	2.16	0.43
3:C:30:LEU:CD1	22:C:511:CLA:CBB	2.96	0.43
3:C:100:PHE:O	3:C:104:VAL:HG22	2.18	0.43
3:C:293:THR:HG22	3:C:294:GLY:H	1.83	0.43
22:C:510:CLA:CBB	22:C:517:CLA:HMA1	2.49	0.43
23:B:619:BCR:H20C	23:B:619:BCR:H361	1.87	0.43
22:D:408:CLA:HBC3	22:D:408:CLA:HHD	2.00	0.43
22:D:409:CLA:CBB	22:D:409:CLA:HMB1	2.48	0.43
2:B:433:ASP:OD2	2:B:435:GLU:HG3	2.18	0.43
22:C:517:CLA:H141	22:C:517:CLA:C17	2.49	0.43
23:H:101:BCR:H382	23:H:101:BCR:H24C	1.74	0.43
22:B:601:CLA:H3A	23:H:101:BCR:H393	2.00	0.43
22:B:608:CLA:O2D	22:B:608:CLA:C2A	2.66	0.43
17:2:44:VAL:HG13	17:2:77:PRO:HB2	2.00	0.43
2:B:341:LYS:HG3	2:B:429:ILE:HG22	2.01	0.43
3:C:287:SER:N	3:C:288:GLU:OE2	2.52	0.43
3:C:293:THR:HG22	3:C:294:GLY:N	2.34	0.42
2:B:233:ASN:HB2	18:3:17:GLU:OE2	2.18	0.42
4:D:227:GLU:N	4:D:227:GLU:OE2	2.51	0.42
7:H:35:MET:HG3	23:H:101:BCR:H322	2.01	0.42
23:H:101:BCR:HC7	23:H:101:BCR:H331	1.40	0.42
3:C:303:MET:SD	3:C:307:ILE:HD11	2.59	0.42
2:B:185:TRP:CZ3	22:B:601:CLA:H122	2.54	0.42
1:A:30:VAL:O	1:A:30:VAL:HG13	2.19	0.42
9:K:19:ASP:HB3	9:K:20:PRO:HD3	2.02	0.42
1:A:255:PHE:O	1:A:259:ILE:HG22	2.19	0.42
2:B:368:VAL:HG22	2:B:425:ILE:HG21	2.01	0.42
3:C:156:LEU:HD12	22:C:509:CLA:HED1	2.02	0.42
3:C:296:GLU:HB2	3:C:349:PHE:CZ	2.54	0.42
3:C:312:LEU:HD12	3:C:313:GLY:CA	2.49	0.42
2:B:457:VAL:HG21	4:D:284:ILE:HG23	2.01	0.42
23:B:617:BCR:H20C	23:B:617:BCR:H361	1.92	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD1	2.55	0.42
13:X:16:SER:O	13:X:20:VAL:HG12	2.20	0.42
3:C:262:TYR:CD2	22:C:509:CLA:HBB1	2.55	0.42
23:K:101:BCR:H382	23:K:101:BCR:H24C	1.74	0.42
4:D:340:VAL:HG23	4:D:340:VAL:O	2.20	0.41
22:D:409:CLA:C20	23:H:101:BCR:C37	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:25:LEU:HB2	9:K:26:PRO:HD3	2.01	0.41
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.50	0.41
1:A:339:PHE:O	1:A:339:PHE:CD2	2.73	0.41
4:D:330:ALA:HB3	4:D:331:PRO:HD3	2.02	0.41
12:T:9:ILE:HA	12:T:12:CYS:SG	2.60	0.41
22:A:407:CLA:HHC	22:A:407:CLA:HBB1	2.01	0.41
2:B:59:GLY:O	22:B:607:CLA:H2A	2.20	0.41
22:B:609:CLA:HAC1	7:H:34:PHE:CE1	2.56	0.41
22:B:603:CLA:HBC3	22:B:603:CLA:HHD	2.01	0.41
1:A:32:TRP:O	8:I:19:PHE:HD1	2.03	0.41
2:B:190:PHE:CE1	22:B:601:CLA:C3B	3.04	0.41
22:B:601:CLA:HBD	22:B:601:CLA:H43	2.02	0.41
9:K:25:LEU:HA	9:K:28:ILE:CD1	2.51	0.41
1:A:248:ILE:CG1	1:A:249:VAL:H	2.34	0.41
9:K:22:VAL:HA	9:K:25:LEU:HG	2.03	0.41
22:B:608:CLA:OBD	22:B:610:CLA:CBB	2.68	0.41
3:C:41:HIS:HB3	22:C:513:CLA:OBD	2.21	0.41
9:K:44:GLY:O	9:K:45:PHE:HB2	2.21	0.41
22:A:405:CLA:HHB	22:A:405:CLA:HMA1	1.85	0.41
3:C:122:ILE:HD11	22:C:512:CLA:H61	2.03	0.41
3:C:442:GLY:O	3:C:443:PHE:HB2	2.21	0.41
22:A:405:CLA:CGD	22:A:405:CLA:C2A	2.98	0.40
23:A:408:BCR:C4	23:A:408:BCR:H323	2.51	0.40
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	2.02	0.40
22:C:504:CLA:O1A	22:C:505:CLA:H43	2.21	0.40
21:A:403:PHO:O2A	21:A:403:PHO:H43	2.21	0.40
22:D:409:CLA:HMB1	22:D:409:CLA:HBB1	2.03	0.40
23:C:515:BCR:H10C	23:K:101:BCR:HC41	2.03	0.40
9:K:38:VAL:CG1	23:K:101:BCR:H21C	2.50	0.40
1:A:339:PHE:O	1:A:339:PHE:CG	2.75	0.40
2:B:467:ILE:HD11	4:D:126:MET:HE1	2.04	0.40
5:E:61:ARG:HD2	5:E:61:ARG:N	2.35	0.40
22:B:610:CLA:HBB1	22:B:610:CLA:HHC	2.04	0.40
22:C:510:CLA:CGD	22:C:510:CLA:HAA1	2.51	0.40
22:D:409:CLA:C20	23:H:101:BCR:H372	2.47	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	333/360 (92%)	312 (94%)	19 (6%)	2 (1%)	25	48
2	B	494/510 (97%)	469 (95%)	24 (5%)	1 (0%)	47	72
3	C	430/461 (93%)	396 (92%)	33 (8%)	1 (0%)	47	72
4	D	339/352 (96%)	316 (93%)	22 (6%)	1 (0%)	41	65
5	E	75/84 (89%)	72 (96%)	3 (4%)	0	100	100
6	F	36/45 (80%)	34 (94%)	2 (6%)	0	100	100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
8	I	24/38 (63%)	24 (100%)	0	0	100	100
9	K	35/46 (76%)	30 (86%)	4 (11%)	1 (3%)	4	10
10	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	M	32/36 (89%)	32 (100%)	0	0	100	100
12	T	26/32 (81%)	24 (92%)	2 (8%)	0	100	100
13	X	33/41 (80%)	33 (100%)	0	0	100	100
14	y	26/46 (56%)	23 (88%)	3 (12%)	0	100	100
15	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100	100
16	1	111/134 (83%)	104 (94%)	6 (5%)	1 (1%)	17	38
17	2	110/116 (95%)	101 (92%)	8 (7%)	1 (1%)	17	38
18	3	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	2314/2522 (92%)	2171 (94%)	135 (6%)	8 (0%)	44	65

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491	VAL
4	D	240	ALA
9	K	45	PHE
17	2	28	ASP

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Mol	Chain	Res	Type
1	A	13	LEU
3	C	18	SER
1	A	340	PRO
16	1	23	ALA

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	271/291 (93%)	270 (100%)	1 (0%)	91 96
2	B	395/407 (97%)	391 (99%)	4 (1%)	76 90
3	C	335/362 (92%)	327 (98%)	8 (2%)	49 76
4	D	276/283 (98%)	271 (98%)	5 (2%)	59 82
5	E	69/73 (94%)	68 (99%)	1 (1%)	67 85
6	F	32/39 (82%)	32 (100%)	0	100 100
7	H	54/55 (98%)	54 (100%)	0	100 100
8	I	24/35 (69%)	24 (100%)	0	100 100
9	K	30/37 (81%)	30 (100%)	0	100 100
10	L	35/35 (100%)	35 (100%)	0	100 100
11	M	31/33 (94%)	31 (100%)	0	100 100
12	T	25/29 (86%)	23 (92%)	2 (8%)	12 26
13	X	28/34 (82%)	28 (100%)	0	100 100
14	y	21/37 (57%)	18 (86%)	3 (14%)	3 7
15	Z	50/52 (96%)	49 (98%)	1 (2%)	55 80
16	1	96/115 (84%)	89 (93%)	7 (7%)	14 31
17	2	94/97 (97%)	91 (97%)	3 (3%)	39 67
18	3	42/42 (100%)	40 (95%)	2 (5%)	25 51
All	All	1908/2056 (93%)	1871 (98%)	37 (2%)	59 81

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
2	B	246	PHE
2	B	278	SER
2	B	373	LYS
2	B	477	ASP
3	C	24	TRP
3	C	29	ARG
3	C	56	THR
3	C	112	VAL
3	C	145	MET
3	C	268	SER
3	C	325	LEU
3	C	350	ARG
4	D	20	ASP
4	D	135	LEU
4	D	224	GLN
4	D	315	TYR
4	D	350	ASN
5	E	24	SER
12	T	2	GLU
12	T	25	GLU
14	y	24	MET
14	y	27	MET
14	y	37	PHE
15	Z	39	LEU
16	1	24	ASN
16	1	44	LEU
16	1	66	LYS
16	1	81	LEU
16	1	90	MET
16	1	103	SER
16	1	130	ARG
17	2	6	GLU
17	2	11	ARG
17	2	59	GLU
18	3	2	ARG
18	3	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
2	B	9	HIS

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Mol	Chain	Res	Type
2	B	14	ASN
10	L	6	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	$\#\|Z\| > 2$
23	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.59	9 (16%)
23	BCR	B	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	A	406	-	65,73,73	1.57	10 (15%)	76,113,113	1.98	23 (30%)
25	LMG	D	403	-	55,55,55	0.92	2 (3%)	63,63,63	1.14	5 (7%)
22	CLA	B	605	-	65,73,73	1.68	10 (15%)	76,113,113	2.07	21 (27%)
22	CLA	B	607	-	65,73,73	1.67	13 (20%)	76,113,113	2.05	21 (27%)
22	CLA	C	504	-	65,73,73	1.56	10 (15%)	76,113,113	1.96	18 (23%)
22	CLA	C	512	-	65,73,73	1.85	9 (13%)	76,113,113	2.52	23 (30%)
23	BCR	D	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	C	506	-	65,73,73	1.63	14 (21%)	76,113,113	1.98	15 (19%)
25	LMG	I	101	-	55,55,55	0.99	2 (3%)	63,63,63	1.06	4 (6%)
22	CLA	A	405	-	65,73,73	1.65	8 (12%)	76,113,113	1.93	21 (27%)
23	BCR	C	518	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	5 (8%)
21	PHO	D	407	-	51,69,69	1.08	6 (11%)	47,99,99	1.41	7 (14%)
23	BCR	C	516	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	4 (7%)
22	CLA	B	612	-	65,73,73	1.67	9 (13%)	76,113,113	2.51	27 (35%)
22	CLA	D	408	-	65,73,73	1.75	12 (18%)	76,113,113	1.86	20 (26%)
23	BCR	H	101	-	41,41,41	3.44	14 (34%)	56,56,56	4.30	30 (53%)
22	CLA	B	610	-	65,73,73	1.58	9 (13%)	76,113,113	2.47	22 (28%)
22	CLA	C	508	-	65,73,73	1.78	8 (12%)	76,113,113	2.25	22 (28%)
25	LMG	C	501	-	55,55,55	1.11	3 (5%)	63,63,63	1.00	3 (4%)
23	BCR	B	617	-	41,41,41	0.99	2 (4%)	56,56,56	1.17	3 (5%)
22	CLA	C	513	-	65,73,73	1.67	13 (20%)	76,113,113	2.34	28 (36%)
22	CLA	C	514	-	65,73,73	1.77	13 (20%)	76,113,113	2.14	17 (22%)
23	BCR	B	619	-	41,41,41	0.95	2 (4%)	56,56,56	1.17	5 (8%)
24	LHG	A	409	-	48,48,48	0.79	1 (2%)	51,54,54	0.89	1 (1%)
22	CLA	B	611	-	65,73,73	1.68	10 (15%)	76,113,113	2.36	22 (28%)
22	CLA	D	409	-	65,73,73	1.61	9 (13%)	76,113,113	1.72	16 (21%)
22	CLA	B	608	-	65,73,73	1.65	11 (16%)	76,113,113	2.46	25 (32%)
25	LMG	D	404	-	55,55,55	0.93	0	63,63,63	1.14	3 (4%)
22	CLA	B	606	-	65,73,73	1.55	5 (7%)	76,113,113	1.82	21 (27%)
21	PHO	A	403	-	51,69,69	1.03	4 (7%)	47,99,99	1.15	5 (10%)
27	PL9	D	406	-	55,55,55	1.16	1 (1%)	68,69,69	1.55	8 (11%)
22	CLA	B	613	-	65,73,73	1.62	9 (13%)	76,113,113	2.23	17 (22%)
22	CLA	C	505	-	65,73,73	1.66	11 (16%)	76,113,113	2.32	24 (31%)
22	CLA	B	604	-	65,73,73	1.60	9 (13%)	76,113,113	2.26	25 (32%)
22	CLA	C	507	-	65,73,73	1.80	10 (15%)	76,113,113	2.54	21 (27%)
23	BCR	K	101	-	41,41,41	3.43	14 (34%)	56,56,56	4.27	29 (51%)
25	LMG	D	405	-	55,55,55	0.97	0	63,63,63	1.11	3 (4%)
22	CLA	B	615	-	65,73,73	1.64	11 (16%)	76,113,113	2.36	17 (22%)
22	CLA	A	404	-	65,73,73	1.65	10 (15%)	76,113,113	1.96	22 (28%)
22	CLA	C	510	-	65,73,73	1.76	9 (13%)	76,113,113	2.55	15 (19%)
25	LMG	D	402	-	55,55,55	0.98	0	63,63,63	1.09	4 (6%)
22	CLA	B	603	-	65,73,73	1.59	12 (18%)	76,113,113	2.05	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	A	408	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	9 (16%)
25	LMG	C	502	-	55,55,55	1.03	0	63,63,63	1.05	4 (6%)
28	HEM	E	101	5	41,50,50	1.44	3 (7%)	45,82,82	1.22	4 (8%)
22	CLA	C	503	-	65,73,73	1.52	9 (13%)	76,113,113	2.05	16 (21%)
22	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	2.53	25 (32%)
22	CLA	B	616	-	65,73,73	1.80	8 (12%)	76,113,113	2.84	22 (28%)
22	CLA	C	509	-	65,73,73	1.62	11 (16%)	76,113,113	2.44	25 (32%)
22	CLA	B	601	-	65,73,73	1.47	8 (12%)	76,113,113	2.89	26 (34%)
22	CLA	B	602	-	65,73,73	1.58	8 (12%)	76,113,113	2.51	24 (31%)
22	CLA	C	517	-	65,73,73	1.73	9 (13%)	76,113,113	2.44	21 (27%)
22	CLA	C	511	-	65,73,73	1.67	11 (16%)	76,113,113	2.40	22 (28%)
22	CLA	B	609	-	65,73,73	1.88	12 (18%)	76,113,113	2.36	21 (27%)
22	CLA	A	407	-	65,73,73	1.77	9 (13%)	76,113,113	1.63	16 (21%)

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
23	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	BCR	B	618	-	-	3/29/63/63	0/2/2/2
22	CLA	A	406	-	1/1/15/20	10/37/115/115	-
25	LMG	D	403	-	-	14/50/70/70	0/1/1/1
22	CLA	B	605	-	-	10/37/115/115	-
22	CLA	B	607	-	2/2/15/20	12/37/115/115	-
22	CLA	C	504	-	1/1/15/20	9/37/115/115	-
22	CLA	C	512	-	1/1/15/20	10/37/115/115	-
23	BCR	D	410	-	-	6/29/63/63	0/2/2/2
22	CLA	C	506	-	1/1/15/20	11/37/115/115	-
25	LMG	I	101	-	-	8/50/70/70	0/1/1/1
22	CLA	A	405	-	1/1/15/20	12/37/115/115	-
23	BCR	C	518	-	-	12/29/63/63	0/2/2/2
21	PHO	D	407	-	1/1/17/22	7/37/103/103	0/5/6/6
23	BCR	C	516	-	-	8/29/63/63	0/2/2/2
22	CLA	B	612	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	D	408	-	1/1/15/20	12/37/115/115	-
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	610	-	2/2/15/20	11/37/115/115	-
22	CLA	C	508	-	-	7/37/115/115	-
25	LMG	C	501	-	-	12/50/70/70	0/1/1/1
23	BCR	B	617	-	-	6/29/63/63	0/2/2/2
22	CLA	C	513	-	2/2/15/20	10/37/115/115	-
22	CLA	C	514	-	2/2/15/20	10/37/115/115	-
23	BCR	B	619	-	-	4/29/63/63	0/2/2/2
24	LHG	A	409	-	-	15/53/53/53	-
22	CLA	B	611	-	1/1/15/20	11/37/115/115	-
22	CLA	D	409	-	1/1/15/20	3/37/115/115	-
22	CLA	B	608	-	2/2/15/20	9/37/115/115	-
25	LMG	D	404	-	-	8/50/70/70	0/1/1/1
22	CLA	B	606	-	2/2/15/20	11/37/115/115	-
21	PHO	A	403	-	1/1/17/22	6/37/103/103	0/5/6/6
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	B	613	-	1/1/15/20	11/37/115/115	-
22	CLA	C	505	-	1/1/15/20	15/37/115/115	-
22	CLA	B	604	-	2/2/15/20	11/37/115/115	-
22	CLA	C	507	-	1/1/15/20	4/37/115/115	-
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
25	LMG	D	405	-	-	13/50/70/70	0/1/1/1
22	CLA	B	615	-	1/1/15/20	8/37/115/115	-
22	CLA	A	404	-	1/1/15/20	6/37/115/115	-
22	CLA	C	510	-	2/2/15/20	12/37/115/115	-
25	LMG	D	402	-	-	7/50/70/70	0/1/1/1
22	CLA	B	603	-	2/2/15/20	12/37/115/115	-
23	BCR	A	408	-	-	7/29/63/63	0/2/2/2
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1
28	HEM	E	101	5	-	5/12/54/54	-
22	CLA	C	503	-	1/1/15/20	8/37/115/115	-
22	CLA	B	614	-	2/2/15/20	4/37/115/115	-
22	CLA	C	509	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	616	-	-	9/37/115/115	-
22	CLA	B	601	-	3/3/15/20	9/37/115/115	-
22	CLA	B	602	-	1/1/15/20	13/37/115/115	-
22	CLA	C	517	-	1/1/15/20	10/37/115/115	-
22	CLA	C	511	-	1/1/15/20	13/37/115/115	-
22	CLA	B	609	-	2/2/15/20	9/37/115/115	-
22	CLA	A	407	-	2/2/15/20	7/37/115/115	-

All (415) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C1-C6	-10.18	1.39	1.53
23	K	101	BCR	C1-C6	-9.95	1.40	1.53
22	B	616	CLA	C4B-NB	9.89	1.44	1.35
22	B	609	CLA	C4B-NB	9.83	1.44	1.35
23	K	101	BCR	C5-C6	-9.67	1.17	1.34
22	A	405	CLA	C4B-NB	9.54	1.43	1.35
22	A	407	CLA	C4B-NB	9.49	1.43	1.35
22	C	508	CLA	C4B-NB	9.40	1.43	1.35
22	C	512	CLA	C4B-NB	9.27	1.43	1.35
22	C	507	CLA	C4B-NB	9.23	1.43	1.35
22	C	510	CLA	C4B-NB	9.14	1.43	1.35
23	H	101	BCR	C5-C6	-9.08	1.18	1.34
22	C	511	CLA	C4B-NB	8.97	1.43	1.35
22	D	408	CLA	C4B-NB	8.93	1.43	1.35
22	B	614	CLA	C4B-NB	8.91	1.43	1.35
23	H	101	BCR	C33-C5	-8.81	1.36	1.50
22	A	404	CLA	C4B-NB	8.72	1.43	1.35
22	B	612	CLA	C4B-NB	8.62	1.42	1.35
23	K	101	BCR	C33-C5	-8.56	1.36	1.50
22	C	514	CLA	C4B-NB	8.55	1.42	1.35
23	K	101	BCR	C30-C25	-8.48	1.42	1.53
22	C	517	CLA	C4B-NB	8.47	1.42	1.35
23	H	101	BCR	C30-C25	-8.44	1.42	1.53
22	C	505	CLA	C4B-NB	8.39	1.42	1.35
22	B	606	CLA	C4B-NB	8.34	1.42	1.35
22	B	605	CLA	C4B-NB	8.34	1.42	1.35
22	B	611	CLA	C4B-NB	8.31	1.42	1.35
22	B	615	CLA	C4B-NB	8.25	1.42	1.35
22	A	406	CLA	C4B-NB	8.25	1.42	1.35
22	B	607	CLA	C4B-NB	8.08	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	C4B-NB	8.02	1.42	1.35
22	B	604	CLA	C4B-NB	8.02	1.42	1.35
22	D	409	CLA	C4B-NB	7.94	1.42	1.35
22	B	602	CLA	C4B-NB	7.78	1.42	1.35
22	C	506	CLA	C4B-NB	7.74	1.42	1.35
22	B	608	CLA	C4B-NB	7.67	1.42	1.35
22	B	603	CLA	C4B-NB	7.63	1.42	1.35
22	C	503	CLA	C4B-NB	7.48	1.41	1.35
22	C	509	CLA	C4B-NB	7.44	1.41	1.35
22	C	504	CLA	C4B-NB	7.39	1.41	1.35
22	B	613	CLA	C4B-NB	7.33	1.41	1.35
22	B	610	CLA	C4B-NB	7.24	1.41	1.35
22	B	601	CLA	C4B-NB	6.65	1.41	1.35
23	H	101	BCR	C31-C1	-5.92	1.42	1.53
23	K	101	BCR	C31-C1	-5.76	1.42	1.53
23	H	101	BCR	C39-C30	-5.53	1.42	1.53
23	K	101	BCR	C39-C30	-5.46	1.43	1.53
28	E	101	HEM	C3C-C2C	-4.51	1.34	1.40
22	C	512	CLA	C3D-C4D	4.31	1.53	1.44
22	C	507	CLA	C3D-CAD	4.26	1.59	1.45
22	C	512	CLA	C3D-CAD	4.22	1.59	1.45
22	B	609	CLA	C3D-C4D	4.18	1.53	1.44
22	C	517	CLA	C3D-CAD	4.18	1.59	1.45
22	B	609	CLA	C3D-CAD	4.10	1.59	1.45
22	C	507	CLA	C3D-C4D	4.09	1.53	1.44
22	B	616	CLA	C3D-C4D	4.06	1.53	1.44
23	D	410	BCR	C1-C6	-4.01	1.48	1.53
22	C	508	CLA	C3D-CAD	3.89	1.58	1.45
22	B	614	CLA	C3D-C4D	3.88	1.52	1.44
22	B	614	CLA	C3D-CAD	3.87	1.58	1.45
22	B	613	CLA	C3D-CAD	3.86	1.58	1.45
22	B	616	CLA	CMD-C2D	-3.86	1.42	1.50
22	C	510	CLA	C3D-C4D	3.85	1.52	1.44
22	A	406	CLA	CHC-C1C	3.79	1.44	1.35
22	C	509	CLA	CMD-C2D	-3.77	1.42	1.50
22	B	612	CLA	C3B-C2B	-3.76	1.35	1.40
22	C	510	CLA	C3D-CAD	3.72	1.57	1.45
23	K	101	BCR	C32-C1	-3.72	1.46	1.53
22	D	409	CLA	C1D-ND	3.72	1.42	1.37
22	C	514	CLA	C3D-CAD	3.70	1.57	1.45
22	B	611	CLA	C3D-CAD	3.69	1.57	1.45
22	B	613	CLA	C3D-C4D	3.69	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	517	CLA	C3D-C4D	3.67	1.52	1.44
22	C	508	CLA	C3D-C4D	3.67	1.52	1.44
22	A	407	CLA	CHC-C1C	3.63	1.44	1.35
22	C	517	CLA	C1D-C2D	3.59	1.52	1.45
23	C	516	BCR	C30-C25	-3.56	1.48	1.53
22	C	514	CLA	C3D-C4D	3.54	1.52	1.44
22	B	611	CLA	C3D-C4D	3.52	1.52	1.44
22	C	505	CLA	CHC-C1C	3.50	1.44	1.35
22	A	405	CLA	CHC-C1C	3.50	1.43	1.35
22	B	615	CLA	C1D-ND	3.50	1.42	1.37
22	B	605	CLA	C1D-ND	3.50	1.42	1.37
22	B	610	CLA	C1D-ND	3.50	1.42	1.37
22	C	508	CLA	CHC-C1C	3.49	1.43	1.35
22	C	503	CLA	C4D-ND	-3.49	1.32	1.37
22	C	506	CLA	CMD-C2D	-3.49	1.43	1.50
22	C	510	CLA	CHC-C1C	3.48	1.43	1.35
22	B	608	CLA	C3D-CAD	3.48	1.56	1.45
23	H	101	BCR	C32-C1	-3.45	1.47	1.53
22	A	407	CLA	C1D-ND	3.45	1.42	1.37
22	C	513	CLA	CMB-C2B	-3.44	1.44	1.51
22	C	514	CLA	C1D-ND	3.43	1.42	1.37
22	B	602	CLA	C3D-C4D	3.43	1.51	1.44
22	D	408	CLA	CHC-C1C	3.42	1.43	1.35
23	C	518	BCR	C1-C6	-3.40	1.49	1.53
28	E	101	HEM	C3C-CAC	3.38	1.54	1.47
22	B	607	CLA	CMD-C2D	-3.35	1.43	1.50
22	C	514	CLA	CHC-C1C	3.33	1.43	1.35
22	B	609	CLA	CHC-C1C	3.33	1.43	1.35
22	C	512	CLA	C1D-C2D	3.33	1.51	1.45
22	B	605	CLA	C4D-ND	-3.33	1.33	1.37
22	D	408	CLA	C3D-CAD	3.32	1.56	1.45
22	B	604	CLA	CHC-C1C	3.32	1.43	1.35
22	B	603	CLA	CHC-C1C	3.32	1.43	1.35
22	C	505	CLA	CMD-C2D	-3.31	1.43	1.50
22	B	612	CLA	CMD-C2D	-3.29	1.43	1.50
22	B	610	CLA	C3D-C4D	3.28	1.51	1.44
22	B	607	CLA	CMB-C2B	-3.27	1.44	1.51
22	B	606	CLA	CHC-C1C	3.27	1.43	1.35
22	B	616	CLA	C3B-C2B	-3.26	1.35	1.40
22	C	511	CLA	CHC-C1C	3.25	1.43	1.35
22	B	616	CLA	CHC-C1C	3.25	1.43	1.35
22	D	409	CLA	C4D-ND	-3.25	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	403	LMG	O7-C8	-3.24	1.38	1.46
22	C	504	CLA	C4D-ND	-3.22	1.33	1.37
22	B	602	CLA	CMD-C2D	-3.21	1.44	1.50
23	A	408	BCR	C30-C25	-3.20	1.49	1.53
22	C	513	CLA	CMD-C2D	-3.20	1.44	1.50
22	B	611	CLA	C3B-C2B	-3.20	1.35	1.40
22	C	511	CLA	C3D-C4D	3.18	1.51	1.44
22	B	611	CLA	CMB-C2B	-3.17	1.45	1.51
22	B	609	CLA	CMD-C2D	-3.17	1.44	1.50
22	A	407	CLA	C4D-ND	-3.16	1.33	1.37
22	C	507	CLA	CHC-C1C	3.14	1.43	1.35
22	C	504	CLA	C1D-ND	3.13	1.41	1.37
23	H	101	BCR	C26-C25	-3.12	1.29	1.34
22	B	601	CLA	CMD-C2D	-3.12	1.44	1.50
23	C	515	BCR	C30-C25	-3.11	1.49	1.53
22	B	615	CLA	CMD-C2D	-3.10	1.44	1.50
22	C	512	CLA	C1D-ND	3.10	1.41	1.37
22	C	511	CLA	C1D-ND	3.09	1.41	1.37
22	C	508	CLA	CMB-C2B	-3.08	1.45	1.51
22	C	512	CLA	CHC-C1C	3.07	1.42	1.35
22	B	610	CLA	CMD-C2D	-3.06	1.44	1.50
22	C	506	CLA	C4D-ND	-3.06	1.33	1.37
23	K	101	BCR	C26-C25	-3.05	1.29	1.34
22	B	603	CLA	C4D-ND	-3.04	1.33	1.37
22	B	615	CLA	C3D-C4D	3.04	1.51	1.44
22	C	517	CLA	CHC-C1C	3.04	1.42	1.35
22	D	409	CLA	CHC-C1C	3.03	1.42	1.35
22	B	601	CLA	CHC-C1C	3.03	1.42	1.35
22	C	517	CLA	C1D-ND	3.03	1.41	1.37
22	A	406	CLA	C1D-ND	3.00	1.41	1.37
22	C	510	CLA	CMD-C2D	-3.00	1.44	1.50
22	B	612	CLA	CHC-C1C	3.00	1.42	1.35
22	B	608	CLA	CHC-C1C	2.98	1.42	1.35
23	H	101	BCR	C38-C26	-2.98	1.46	1.50
22	B	610	CLA	CHC-C1C	2.98	1.42	1.35
22	B	602	CLA	CHC-C1C	2.98	1.42	1.35
22	A	404	CLA	CHC-C1C	2.98	1.42	1.35
22	A	407	CLA	C3B-C2B	-2.97	1.36	1.40
22	C	507	CLA	CMD-C2D	-2.97	1.44	1.50
23	K	101	BCR	C38-C26	-2.97	1.46	1.50
22	C	510	CLA	C3B-C2B	-2.96	1.36	1.40
22	C	509	CLA	CHC-C1C	2.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	C1D-ND	2.96	1.41	1.37
23	B	618	BCR	C1-C6	-2.95	1.49	1.53
22	B	615	CLA	CHC-C1C	2.94	1.42	1.35
22	A	407	CLA	CMB-C2B	-2.94	1.45	1.51
22	B	604	CLA	CMD-C2D	-2.94	1.44	1.50
22	A	404	CLA	C3D-CAD	2.93	1.55	1.45
22	B	603	CLA	CMD-C2D	-2.93	1.44	1.50
22	B	604	CLA	CMB-C2B	-2.93	1.45	1.51
22	B	614	CLA	C1D-ND	2.93	1.41	1.37
23	C	515	BCR	C1-C6	-2.92	1.49	1.53
22	B	607	CLA	CHC-C1C	2.92	1.42	1.35
22	C	509	CLA	C3B-CAB	-2.92	1.42	1.47
22	B	607	CLA	C1D-ND	2.92	1.41	1.37
22	C	504	CLA	CHC-C1C	2.92	1.42	1.35
22	C	513	CLA	C3B-CAB	-2.91	1.42	1.47
22	C	504	CLA	CMD-C2D	-2.91	1.44	1.50
22	B	605	CLA	CHC-C1C	2.91	1.42	1.35
22	C	507	CLA	C1D-C2D	2.90	1.51	1.45
23	H	101	BCR	C40-C30	-2.90	1.48	1.53
21	A	403	PHO	CAC-C3C	-2.90	1.47	1.52
22	B	609	CLA	C1B-NB	2.90	1.37	1.35
23	B	619	BCR	C1-C6	-2.88	1.49	1.53
22	B	606	CLA	C4D-ND	-2.88	1.33	1.37
22	C	513	CLA	MG-ND	-2.88	2.00	2.05
22	B	613	CLA	CMD-C2D	-2.87	1.44	1.50
22	B	611	CLA	CHC-C1C	2.87	1.42	1.35
22	C	509	CLA	MG-ND	-2.87	2.00	2.05
22	B	607	CLA	MG-ND	-2.86	2.00	2.05
22	B	616	CLA	CMB-C2B	-2.85	1.45	1.51
23	C	518	BCR	C30-C25	-2.85	1.49	1.53
22	B	604	CLA	C3D-C4D	2.84	1.50	1.44
22	C	503	CLA	C1D-ND	2.84	1.41	1.37
22	B	605	CLA	CMB-C2B	-2.84	1.45	1.51
22	B	604	CLA	C4D-ND	-2.83	1.33	1.37
22	B	612	CLA	C1D-ND	2.83	1.41	1.37
22	B	613	CLA	CHC-C1C	2.83	1.42	1.35
22	C	506	CLA	CHC-C1C	2.82	1.42	1.35
22	B	605	CLA	C3B-C2B	-2.81	1.36	1.40
22	B	614	CLA	CMD-C2D	-2.81	1.44	1.50
22	B	614	CLA	C1D-C2D	2.81	1.50	1.45
22	C	506	CLA	CMB-C2B	-2.81	1.45	1.51
22	C	509	CLA	CMB-C2B	-2.81	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	CMD-C2D	-2.81	1.44	1.50
22	B	605	CLA	CMD-C2D	-2.80	1.44	1.50
22	B	608	CLA	CMD-C2D	-2.80	1.44	1.50
22	B	616	CLA	C3D-CAD	2.80	1.54	1.45
22	C	513	CLA	C3D-C4D	2.79	1.50	1.44
27	D	406	PL9	C6-C1	-2.79	1.43	1.48
22	A	404	CLA	CMB-C2B	-2.79	1.45	1.51
22	B	606	CLA	CMD-C2D	-2.78	1.44	1.50
23	A	408	BCR	C1-C6	-2.78	1.49	1.53
22	D	408	CLA	C3B-C2B	-2.78	1.36	1.40
22	B	614	CLA	CMB-C2B	-2.78	1.45	1.51
22	C	509	CLA	C4D-ND	-2.77	1.33	1.37
22	B	601	CLA	C3B-C2B	-2.76	1.36	1.40
22	B	612	CLA	C3D-C4D	2.76	1.50	1.44
22	C	512	CLA	CMD-C2D	-2.76	1.45	1.50
22	B	608	CLA	C3D-C4D	2.75	1.50	1.44
22	B	608	CLA	C1D-ND	2.75	1.41	1.37
22	C	514	CLA	C1D-C2D	2.75	1.50	1.45
22	B	610	CLA	C3B-C2B	-2.75	1.36	1.40
21	D	407	PHO	CAC-C3C	-2.75	1.47	1.52
22	C	503	CLA	CHC-C1C	2.74	1.42	1.35
22	C	513	CLA	C2A-C1A	2.74	1.58	1.52
22	B	607	CLA	C4D-ND	-2.73	1.33	1.37
25	C	501	LMG	C7-C8	2.72	1.59	1.50
22	C	503	CLA	CMB-C2B	-2.72	1.46	1.51
22	C	513	CLA	C3B-C2B	-2.72	1.36	1.40
22	B	613	CLA	CMB-C2B	-2.72	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.71	1.46	1.51
22	D	408	CLA	C3D-C4D	2.69	1.50	1.44
22	C	506	CLA	MG-ND	-2.69	2.00	2.05
22	B	601	CLA	CMB-C2B	-2.69	1.46	1.51
22	C	514	CLA	CMD-C2D	-2.68	1.45	1.50
22	B	615	CLA	C3B-C2B	-2.68	1.36	1.40
23	D	410	BCR	C30-C25	-2.68	1.50	1.53
22	C	505	CLA	C1D-ND	2.67	1.41	1.37
22	C	509	CLA	C3D-C2D	-2.67	1.31	1.39
22	A	404	CLA	C3D-C4D	2.66	1.50	1.44
23	K	101	BCR	C40-C30	-2.66	1.48	1.53
22	B	614	CLA	CHC-C1C	2.66	1.41	1.35
22	B	611	CLA	CMD-C2D	-2.66	1.45	1.50
22	B	608	CLA	CMA-C3A	-2.65	1.47	1.53
22	C	511	CLA	CMD-C2D	-2.65	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C1D-ND	2.64	1.41	1.37
22	B	602	CLA	CMB-C2B	-2.64	1.46	1.51
22	C	513	CLA	CHC-C1C	2.63	1.41	1.35
22	C	505	CLA	C3B-C2B	-2.62	1.36	1.40
22	A	405	CLA	CMD-C2D	-2.62	1.45	1.50
22	B	615	CLA	CMB-C2B	-2.61	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.61	1.46	1.51
22	A	404	CLA	C3B-C2B	-2.60	1.36	1.40
22	D	409	CLA	C3B-C2B	-2.60	1.36	1.40
22	D	409	CLA	CMB-C2B	-2.60	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.59	1.45	1.50
22	C	504	CLA	C3D-C4D	2.58	1.50	1.44
22	C	504	CLA	CMB-C2B	-2.57	1.46	1.51
22	D	408	CLA	CMB-C2B	-2.57	1.46	1.51
22	C	505	CLA	C3D-C4D	2.57	1.50	1.44
22	C	517	CLA	CMB-C2B	-2.56	1.46	1.51
22	C	511	CLA	C3B-C2B	-2.56	1.36	1.40
25	C	501	LMG	C4-C5	2.55	1.58	1.53
22	C	510	CLA	CMB-C2B	-2.55	1.46	1.51
24	A	409	LHG	P-O6	2.54	1.69	1.59
22	C	509	CLA	C3B-C2B	-2.54	1.36	1.40
23	B	618	BCR	C30-C25	-2.53	1.50	1.53
23	K	101	BCR	C2-C3	-2.52	1.46	1.52
22	D	408	CLA	MG-NC	2.51	2.12	2.06
22	B	605	CLA	C3D-C4D	2.51	1.49	1.44
22	B	604	CLA	C1D-ND	2.51	1.40	1.37
22	B	605	CLA	CMC-C2C	-2.50	1.45	1.50
22	B	607	CLA	C3B-C2B	-2.50	1.36	1.40
28	E	101	HEM	CAB-C3B	2.50	1.54	1.47
22	A	404	CLA	C1D-C2D	2.50	1.50	1.45
22	B	603	CLA	C3D-C4D	2.49	1.49	1.44
22	B	601	CLA	C3B-CAB	-2.49	1.42	1.47
22	B	612	CLA	C3B-CAB	-2.47	1.42	1.47
22	B	611	CLA	C1D-C2D	2.47	1.50	1.45
22	C	507	CLA	C1D-ND	2.46	1.40	1.37
22	B	613	CLA	C3B-C2B	-2.46	1.37	1.40
22	C	509	CLA	C3D-C4D	2.46	1.49	1.44
22	A	407	CLA	CMD-C2D	-2.46	1.45	1.50
21	D	407	PHO	CMB-C2B	-2.45	1.45	1.51
22	C	508	CLA	C1D-ND	2.45	1.40	1.37
22	A	406	CLA	CMD-C2D	-2.44	1.45	1.50
22	A	404	CLA	C1D-ND	2.44	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C1D-C2D	2.44	1.50	1.45
22	A	406	CLA	CMC-C2C	-2.43	1.45	1.50
22	B	603	CLA	C3B-C2B	-2.43	1.37	1.40
22	B	610	CLA	C3B-CAB	-2.42	1.43	1.47
23	B	617	BCR	C30-C25	-2.42	1.50	1.53
22	B	601	CLA	C3D-C4D	2.42	1.49	1.44
22	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	511	CLA	C4D-ND	-2.42	1.34	1.37
23	H	101	BCR	C29-C28	-2.41	1.46	1.52
22	C	513	CLA	C4D-ND	-2.39	1.34	1.37
22	D	408	CLA	C1D-C2D	2.39	1.50	1.45
22	D	409	CLA	CMD-C2D	-2.37	1.45	1.50
22	D	408	CLA	CMD-C2D	-2.36	1.45	1.50
22	B	613	CLA	C1D-ND	2.36	1.40	1.37
23	B	619	BCR	C30-C25	-2.36	1.50	1.53
22	B	607	CLA	MG-NA	2.36	2.11	2.06
22	C	507	CLA	CMB-C2B	-2.35	1.46	1.51
22	C	517	CLA	CMD-C2D	-2.35	1.45	1.50
22	C	507	CLA	C3B-C2B	-2.35	1.37	1.40
22	C	512	CLA	CMB-C2B	-2.34	1.46	1.51
23	C	516	BCR	C1-C6	-2.34	1.50	1.53
23	B	617	BCR	C1-C6	-2.34	1.50	1.53
22	A	406	CLA	C3D-C4D	2.34	1.49	1.44
23	H	101	BCR	C36-C18	-2.34	1.46	1.50
22	D	408	CLA	C1D-ND	2.33	1.40	1.37
22	B	604	CLA	C3B-C2B	-2.33	1.37	1.40
22	B	608	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	609	CLA	C1D-ND	2.32	1.40	1.37
23	K	101	BCR	C29-C28	-2.32	1.46	1.52
22	B	611	CLA	C1D-ND	2.32	1.40	1.37
22	A	406	CLA	C3B-C2B	-2.30	1.37	1.40
21	D	407	PHO	C3B-C2B	-2.30	1.37	1.40
22	C	514	CLA	C3B-C2B	-2.30	1.37	1.40
22	B	608	CLA	C3B-C2B	-2.30	1.37	1.40
22	C	507	CLA	C1B-NB	2.30	1.37	1.35
25	I	101	LMG	C7-C8	2.29	1.57	1.50
22	C	505	CLA	C3D-C2D	-2.29	1.32	1.39
22	B	603	CLA	CMB-C2B	-2.29	1.46	1.51
22	C	503	CLA	C3D-C4D	2.28	1.49	1.44
22	C	514	CLA	C1B-NB	2.28	1.37	1.35
22	C	503	CLA	C3B-CAB	-2.28	1.43	1.47
22	B	615	CLA	C4D-ND	-2.27	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	CMC-C2C	-2.27	1.46	1.50
25	D	403	LMG	C3-C2	2.26	1.58	1.52
22	B	607	CLA	C3D-C2D	-2.26	1.32	1.39
22	B	605	CLA	C3D-C2D	-2.26	1.32	1.39
22	C	506	CLA	C3D-C4D	2.24	1.49	1.44
22	C	510	CLA	C1D-C2D	2.24	1.49	1.45
22	C	512	CLA	C3B-C2B	-2.24	1.37	1.40
22	C	514	CLA	CBD-CGD	-2.24	1.45	1.52
21	D	407	PHO	CMD-C2D	-2.24	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.23	1.47	1.51
22	B	609	CLA	MG-NC	2.22	2.11	2.06
22	A	404	CLA	C3B-CAB	-2.22	1.43	1.47
22	B	612	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	613	CLA	C3B-CAB	-2.22	1.43	1.47
21	D	407	PHO	CMC-C2C	-2.22	1.46	1.51
22	A	406	CLA	C1D-C2D	2.21	1.49	1.45
21	A	403	PHO	C3B-C2B	-2.21	1.37	1.40
22	B	603	CLA	C3B-CAB	-2.21	1.43	1.47
22	B	609	CLA	C3B-CAB	-2.21	1.43	1.47
22	B	616	CLA	CMC-C2C	-2.21	1.46	1.50
22	C	506	CLA	C1D-ND	2.20	1.40	1.37
22	C	504	CLA	CMC-C2C	-2.20	1.46	1.50
22	C	506	CLA	C3B-C2B	-2.20	1.37	1.40
22	A	407	CLA	MG-ND	-2.19	2.01	2.05
22	A	405	CLA	C3D-C4D	2.19	1.49	1.44
22	B	610	CLA	CMB-C2B	-2.19	1.47	1.51
22	B	602	CLA	CMC-C2C	-2.19	1.46	1.50
22	C	505	CLA	CMB-C2B	-2.19	1.47	1.51
21	A	403	PHO	CMC-C2C	-2.18	1.46	1.51
22	C	506	CLA	MG-NA	2.18	2.11	2.06
22	C	511	CLA	C3D-C2D	-2.18	1.33	1.39
22	B	611	CLA	C3B-CAB	-2.18	1.43	1.47
22	B	607	CLA	CMC-C2C	-2.17	1.46	1.50
22	B	603	CLA	C2A-C1A	2.17	1.57	1.52
22	C	514	CLA	MG-NC	2.16	2.11	2.06
22	C	506	CLA	MG-NC	2.16	2.11	2.06
22	C	506	CLA	O2D-CGD	2.16	1.38	1.33
22	B	610	CLA	C4D-ND	-2.16	1.34	1.37
22	B	609	CLA	C3B-C2B	-2.16	1.37	1.40
22	A	405	CLA	C3B-C2B	-2.15	1.37	1.40
22	D	408	CLA	C4C-C3C	2.15	1.48	1.45
22	B	615	CLA	C3D-C2D	-2.15	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	408	CLA	MG-NA	2.15	2.11	2.06
22	A	406	CLA	CMB-C2B	-2.14	1.47	1.51
22	C	504	CLA	C3B-CAB	-2.14	1.43	1.47
22	C	510	CLA	CBD-CGD	-2.14	1.45	1.52
22	B	607	CLA	C3D-C4D	2.14	1.49	1.44
22	A	407	CLA	MG-NA	2.14	2.11	2.06
22	B	608	CLA	C3B-CAB	-2.14	1.43	1.47
23	H	101	BCR	C35-C13	-2.12	1.46	1.50
22	A	404	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	603	CLA	CMC-C2C	-2.11	1.46	1.50
22	B	609	CLA	CMB-C2B	-2.10	1.47	1.51
22	A	406	CLA	C4D-ND	-2.10	1.34	1.37
22	B	615	CLA	CMC-C2C	-2.10	1.46	1.50
22	B	614	CLA	C3B-C2B	-2.10	1.37	1.40
22	B	604	CLA	C2A-C1A	2.10	1.57	1.52
22	C	517	CLA	C3B-C2B	-2.09	1.37	1.40
22	C	513	CLA	MG-NA	2.09	2.11	2.06
22	D	409	CLA	C3B-CAB	-2.09	1.43	1.47
22	C	513	CLA	MG-NC	2.09	2.11	2.06
21	A	403	PHO	CMB-C2B	-2.09	1.46	1.51
22	C	513	CLA	C1D-ND	2.08	1.40	1.37
22	C	511	CLA	C2A-C1A	2.08	1.56	1.52
25	I	101	LMG	C4-C5	2.07	1.57	1.53
22	B	615	CLA	C2A-C1A	2.07	1.56	1.52
21	D	407	PHO	CBD-CGD	-2.06	1.49	1.52
23	H	101	BCR	C2-C3	-2.06	1.47	1.52
22	C	503	CLA	CMC-C2C	-2.06	1.46	1.50
23	K	101	BCR	C35-C13	-2.06	1.46	1.50
22	D	409	CLA	CMC-C2C	-2.06	1.46	1.50
22	C	514	CLA	C3B-CAB	-2.06	1.43	1.47
22	C	506	CLA	C3B-CAB	-2.05	1.43	1.47
22	B	601	CLA	C3D-C2D	-2.05	1.33	1.39
22	C	508	CLA	C3B-C2B	-2.04	1.37	1.40
25	C	501	LMG	C9-C8	2.04	1.56	1.50
22	C	505	CLA	MG-NC	2.04	2.11	2.06
22	C	505	CLA	C3B-CAB	-2.04	1.43	1.47
22	C	514	CLA	CMB-C2B	-2.03	1.47	1.51
22	C	509	CLA	O2D-CGD	2.03	1.38	1.33
23	C	516	BCR	C38-C26	-2.03	1.47	1.50
22	A	405	CLA	CMC-C2C	-2.03	1.46	1.50
23	K	101	BCR	C36-C18	-2.02	1.46	1.50
22	C	505	CLA	C4D-ND	-2.02	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C2A-C1A	2.02	1.56	1.52
22	C	504	CLA	MG-ND	-2.02	2.01	2.05
22	B	603	CLA	C3D-C2D	-2.01	1.33	1.39
22	C	511	CLA	CMC-C2C	-2.01	1.46	1.50
22	A	405	CLA	CMA-C3A	-2.01	1.48	1.53
22	C	506	CLA	C3D-C2D	-2.00	1.33	1.39
22	B	607	CLA	C3B-CAB	-2.00	1.43	1.47

All (897) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	601	CLA	C4A-NA-C1A	14.35	113.16	106.71
23	H	101	BCR	C33-C5-C6	-13.58	109.28	124.53
22	C	510	CLA	C4A-NA-C1A	13.10	112.60	106.71
22	B	616	CLA	C4A-NA-C1A	12.90	112.50	106.71
23	K	101	BCR	C33-C5-C6	-12.66	110.31	124.53
23	H	101	BCR	C38-C26-C25	-12.44	110.56	124.53
23	K	101	BCR	C38-C26-C25	-12.43	110.57	124.53
22	C	511	CLA	C4A-NA-C1A	12.33	112.25	106.71
22	B	616	CLA	C4D-C3D-CAD	12.11	122.37	108.10
22	B	615	CLA	C4A-NA-C1A	11.72	111.98	106.71
22	B	603	CLA	C4A-NA-C1A	11.22	111.75	106.71
22	B	602	CLA	C4A-NA-C1A	11.14	111.71	106.71
22	B	610	CLA	C4A-NA-C1A	11.12	111.71	106.71
22	B	614	CLA	C4A-NA-C1A	11.04	111.67	106.71
22	C	507	CLA	C4A-NA-C1A	10.58	111.46	106.71
23	K	101	BCR	C1-C6-C5	-10.30	108.10	122.61
22	C	505	CLA	C4A-NA-C1A	10.24	111.31	106.71
22	C	512	CLA	C4A-NA-C1A	10.22	111.30	106.71
22	C	517	CLA	C4A-NA-C1A	9.98	111.19	106.71
22	C	509	CLA	C4A-NA-C1A	9.94	111.17	106.71
22	B	605	CLA	C4A-NA-C1A	9.91	111.16	106.71
22	C	512	CLA	C4D-C3D-CAD	9.84	119.69	108.10
22	B	604	CLA	C4A-NA-C1A	9.83	111.13	106.71
22	B	608	CLA	C4A-NA-C1A	9.81	111.12	106.71
22	B	609	CLA	C4A-NA-C1A	9.63	111.03	106.71
23	H	101	BCR	C1-C6-C5	-9.60	109.10	122.61
22	C	507	CLA	C4D-C3D-CAD	9.37	119.14	108.10
22	B	612	CLA	C4A-NA-C1A	9.36	110.91	106.71
22	C	510	CLA	C4D-C3D-CAD	9.34	119.10	108.10
22	C	504	CLA	C4A-NA-C1A	9.24	110.86	106.71
22	B	611	CLA	C4A-NA-C1A	9.21	110.85	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	609	CLA	C4D-C3D-CAD	9.12	118.85	108.10
22	C	509	CLA	C4D-C3D-CAD	8.95	118.64	108.10
22	B	610	CLA	C4D-C3D-CAD	8.94	118.64	108.10
22	C	503	CLA	C4A-NA-C1A	8.89	110.70	106.71
22	B	612	CLA	C4D-C3D-CAD	8.84	118.52	108.10
22	B	614	CLA	C4D-C3D-CAD	8.77	118.43	108.10
22	B	613	CLA	C4A-NA-C1A	8.71	110.62	106.71
22	B	601	CLA	CMA-C3A-C4A	-8.58	88.70	111.77
22	C	513	CLA	C4A-NA-C1A	8.56	110.55	106.71
22	C	514	CLA	C4A-NA-C1A	8.53	110.54	106.71
23	H	101	BCR	C29-C30-C25	8.51	123.58	110.48
22	B	602	CLA	C4D-C3D-CAD	8.48	118.09	108.10
23	K	101	BCR	C29-C30-C25	8.41	123.43	110.48
23	K	101	BCR	C31-C1-C6	-8.37	96.73	110.30
22	C	505	CLA	C4D-C3D-CAD	8.36	117.94	108.10
22	B	615	CLA	C4D-C3D-CAD	8.11	117.66	108.10
23	H	101	BCR	C2-C1-C6	7.97	122.75	110.48
23	K	101	BCR	C2-C1-C6	7.83	122.54	110.48
22	C	517	CLA	C4D-C3D-CAD	7.83	117.33	108.10
22	C	506	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	C	508	CLA	C4A-NA-C1A	7.77	110.20	106.71
22	C	513	CLA	C4D-C3D-CAD	7.73	117.20	108.10
22	C	511	CLA	C4D-C3D-CAD	7.60	117.06	108.10
22	B	607	CLA	C4A-NA-C1A	7.45	110.06	106.71
22	A	404	CLA	C4A-NA-C1A	7.40	110.03	106.71
22	B	601	CLA	C4D-C3D-CAD	7.38	116.79	108.10
23	H	101	BCR	C30-C25-C26	-7.37	112.23	122.61
23	K	101	BCR	C30-C25-C26	-7.31	112.31	122.61
27	D	406	PL9	C7-C3-C4	7.31	122.82	116.88
22	D	409	CLA	C4A-NA-C1A	7.31	109.99	106.71
22	B	611	CLA	C4D-C3D-CAD	7.30	116.70	108.10
23	H	101	BCR	C31-C1-C6	-7.26	98.52	110.30
23	H	101	BCR	C24-C23-C22	-7.24	115.29	126.23
22	B	604	CLA	C4D-C3D-CAD	7.12	116.48	108.10
22	C	514	CLA	C4D-C3D-CAD	7.01	116.36	108.10
22	C	508	CLA	C4D-C3D-CAD	6.98	116.32	108.10
22	A	405	CLA	C4A-NA-C1A	6.84	109.78	106.71
22	B	613	CLA	C4D-C3D-CAD	6.75	116.05	108.10
22	C	503	CLA	CMA-C3A-C4A	6.73	129.86	111.77
22	B	608	CLA	C4D-C3D-CAD	6.62	115.89	108.10
22	B	606	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	B	609	CLA	C3D-C2D-C1D	6.43	114.60	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	C6-C7-C8	-6.40	95.23	115.92
22	B	607	CLA	C4D-C3D-CAD	6.38	115.61	108.10
22	A	406	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	C	504	CLA	C4D-C3D-CAD	6.08	115.27	108.10
22	B	601	CLA	CAA-C2A-C1A	6.05	131.81	111.97
22	C	507	CLA	C3D-C2D-C1D	6.05	114.08	105.83
22	C	512	CLA	C3D-C2D-C1D	6.04	114.08	105.83
23	K	101	BCR	C24-C23-C22	-6.04	117.11	126.23
22	B	616	CLA	C1D-ND-C4D	-5.91	102.13	106.33
22	C	509	CLA	O2D-CGD-CBD	5.90	121.75	111.27
22	C	514	CLA	C6-C7-C8	-5.86	96.98	115.92
22	B	601	CLA	CAA-C2A-C3A	5.82	128.71	112.78
22	B	611	CLA	C6-C7-C8	-5.77	97.26	115.92
22	C	510	CLA	C3D-C2D-C1D	5.73	113.65	105.83
22	B	608	CLA	C2A-C3A-C4A	5.64	110.99	101.87
22	B	605	CLA	C4D-C3D-CAD	5.63	114.74	108.10
22	C	506	CLA	C4D-C3D-CAD	5.61	114.70	108.10
22	C	517	CLA	C3D-C2D-C1D	5.57	113.44	105.83
22	B	616	CLA	C3D-C2D-C1D	5.52	113.37	105.83
22	B	603	CLA	C4D-C3D-CAD	5.50	114.58	108.10
23	H	101	BCR	C4-C5-C6	5.50	130.72	122.73
22	C	513	CLA	CMB-C2B-C1B	-5.47	120.05	128.46
22	B	602	CLA	OBD-CAD-C3D	5.44	141.60	128.52
22	B	613	CLA	C3D-C2D-C1D	5.41	113.22	105.83
22	B	614	CLA	C3D-C2D-C1D	5.39	113.18	105.83
22	B	610	CLA	OBD-CAD-C3D	5.32	141.33	128.52
23	C	515	BCR	C35-C13-C14	-5.32	115.47	122.92
22	C	517	CLA	C3D-C4D-ND	5.25	118.74	110.24
23	K	101	BCR	C2-C3-C4	-5.22	99.71	111.38
22	B	606	CLA	C4D-C3D-CAD	5.15	114.16	108.10
23	K	101	BCR	C4-C5-C6	5.14	130.20	122.73
22	B	612	CLA	C1D-ND-C4D	-5.14	102.69	106.33
22	C	514	CLA	C3D-C2D-C1D	5.09	112.78	105.83
22	B	608	CLA	CHB-C4A-NA	5.08	131.53	124.51
22	C	503	CLA	CMA-C3A-C2A	-5.07	93.37	113.83
22	C	512	CLA	C3D-C4D-ND	5.04	118.40	110.24
22	C	507	CLA	C3D-C4D-ND	5.01	118.35	110.24
23	K	101	BCR	C38-C26-C27	4.98	123.17	113.62
23	H	101	BCR	C38-C26-C27	4.97	123.17	113.62
22	D	408	CLA	C2D-C1D-ND	-4.97	106.44	110.10
23	K	101	BCR	C1-C6-C7	4.96	129.81	115.78
22	C	514	CLA	C2D-C1D-ND	-4.95	106.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	H	101	BCR	C1-C6-C7	4.95	129.77	115.78
22	B	612	CLA	OBD-CAD-C3D	4.94	140.40	128.52
22	C	517	CLA	C6-C7-C8	-4.92	100.01	115.92
22	B	611	CLA	C3D-C2D-C1D	4.91	112.53	105.83
23	H	101	BCR	C2-C3-C4	-4.89	100.44	111.38
22	B	611	CLA	CBA-CAA-C2A	4.87	128.25	113.86
22	B	609	CLA	C2D-C1D-ND	-4.85	106.53	110.10
22	C	508	CLA	CMB-C2B-C1B	-4.84	121.03	128.46
22	C	510	CLA	CHB-C4A-NA	4.83	131.19	124.51
22	B	601	CLA	CHB-C4A-NA	4.83	131.19	124.51
22	C	517	CLA	C2D-C1D-ND	-4.82	106.55	110.10
22	B	608	CLA	C3D-C2D-C1D	4.82	112.41	105.83
22	B	608	CLA	CMA-C3A-C2A	4.82	133.26	113.83
22	A	407	CLA	C4A-NA-C1A	4.77	108.85	106.71
22	C	509	CLA	O2D-CGD-O1D	-4.76	114.53	123.84
22	B	615	CLA	OBD-CAD-C3D	4.72	139.88	128.52
22	B	602	CLA	CAA-CBA-CGA	-4.68	99.57	113.25
22	B	615	CLA	C2A-C1A-CHA	4.67	132.03	123.86
22	B	614	CLA	C3D-C4D-ND	4.66	117.77	110.24
22	C	510	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	A	408	BCR	C1-C6-C5	-4.62	116.11	122.61
22	B	601	CLA	C4D-CHA-C1A	-4.62	115.63	121.25
22	B	608	CLA	C3D-C4D-ND	4.60	117.68	110.24
22	B	616	CLA	OBD-CAD-C3D	4.58	139.53	128.52
22	B	612	CLA	CMA-C3A-C2A	4.57	132.26	113.83
22	B	614	CLA	C11-C10-C8	4.55	130.64	115.92
22	B	612	CLA	C1B-CHB-C4A	-4.55	121.10	130.12
22	C	508	CLA	C3D-C4D-ND	4.54	117.59	110.24
22	D	408	CLA	C3D-C2D-C1D	4.51	111.98	105.83
22	A	407	CLA	CAA-C2A-C1A	4.50	126.73	111.97
22	C	513	CLA	CMA-C3A-C2A	4.50	131.97	113.83
22	D	408	CLA	CAC-C3C-C4C	4.49	130.64	124.81
22	C	503	CLA	C6-C7-C8	-4.49	101.40	115.92
22	B	609	CLA	C3D-C4D-ND	4.48	117.49	110.24
22	B	606	CLA	CMA-C3A-C2A	-4.48	95.77	113.83
22	B	613	CLA	C3A-C2A-C1A	4.47	108.04	101.34
22	B	602	CLA	C2A-C1A-CHA	4.46	131.65	123.86
22	B	613	CLA	CAA-C2A-C1A	4.43	126.50	111.97
23	H	101	BCR	C30-C25-C24	4.42	128.29	115.78
23	C	515	BCR	C35-C13-C12	4.42	125.03	118.08
22	C	508	CLA	C3D-C2D-C1D	4.40	111.84	105.83
22	C	505	CLA	CGD-CBD-CAD	4.40	124.98	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	611	CLA	C3D-C4D-ND	4.40	117.35	110.24
22	A	406	CLA	C6-C7-C8	-4.39	101.72	115.92
22	B	608	CLA	CAC-C3C-C4C	4.39	130.50	124.81
22	B	603	CLA	C2A-C1A-CHA	4.38	131.51	123.86
23	K	101	BCR	C30-C25-C24	4.38	128.16	115.78
22	C	511	CLA	OBD-CAD-C3D	4.38	139.05	128.52
22	B	602	CLA	C3A-C2A-C1A	4.36	107.86	101.34
22	B	607	CLA	C6-C7-C8	4.34	129.96	115.92
22	C	507	CLA	CBC-CAC-C3C	4.32	124.35	112.43
22	B	613	CLA	C2D-C1D-ND	-4.32	106.92	110.10
23	K	101	BCR	C32-C1-C31	4.31	121.76	108.53
22	B	616	CLA	C3D-C4D-ND	4.31	117.20	110.24
22	C	513	CLA	OBD-CAD-C3D	4.31	138.88	128.52
22	C	511	CLA	C2A-C1A-CHA	4.29	131.35	123.86
22	A	405	CLA	C4D-C3D-CAD	4.28	113.14	108.10
23	H	101	BCR	C40-C30-C25	-4.27	103.37	110.30
22	B	611	CLA	CAA-CBA-CGA	4.26	125.70	113.25
23	H	101	BCR	C32-C1-C31	4.26	121.59	108.53
22	B	601	CLA	C2A-C1A-CHA	4.22	131.23	123.86
22	C	507	CLA	C2D-C1D-ND	-4.20	107.01	110.10
22	C	509	CLA	OBD-CAD-C3D	4.18	138.59	128.52
22	C	507	CLA	C6-C7-C8	-4.17	102.42	115.92
22	B	607	CLA	CMA-C3A-C4A	4.16	122.95	111.77
23	K	101	BCR	C40-C30-C25	-4.13	103.59	110.30
23	H	101	BCR	C32-C1-C6	-4.12	103.62	110.30
22	A	405	CLA	C2A-C3A-C4A	4.11	108.50	101.87
22	A	406	CLA	C4D-C3D-CAD	4.09	112.92	108.10
22	C	506	CLA	OBD-CAD-C3D	4.08	138.34	128.52
22	A	404	CLA	C2D-C1D-ND	-4.07	107.11	110.10
22	C	505	CLA	C6-C7-C8	-4.07	102.77	115.92
22	C	507	CLA	CMA-C3A-C4A	4.07	122.71	111.77
22	A	406	CLA	C11-C10-C8	4.06	129.05	115.92
22	B	613	CLA	C3D-C4D-ND	4.06	116.80	110.24
22	B	615	CLA	C3A-C2A-C1A	4.05	107.41	101.34
22	C	517	CLA	CMA-C3A-C2A	4.05	130.17	113.83
22	C	507	CLA	CBA-CAA-C2A	4.05	125.82	113.86
22	C	511	CLA	C3A-C2A-C1A	4.05	107.40	101.34
22	B	604	CLA	CMA-C3A-C2A	4.04	130.12	113.83
22	C	508	CLA	CAC-C3C-C4C	4.04	130.05	124.81
22	B	606	CLA	CMA-C3A-C4A	4.02	122.59	111.77
22	C	509	CLA	C2A-C1A-CHA	4.02	130.89	123.86
22	C	508	CLA	CBA-CAA-C2A	4.02	125.72	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
22	B	604	CLA	C2A-C3A-C4A	3.99	108.32	101.87
22	C	511	CLA	CAA-C2A-C1A	3.98	125.02	111.97
22	B	613	CLA	CAA-CBA-CGA	-3.98	101.62	113.25
22	B	610	CLA	O2A-C1-C2	-3.98	98.18	108.64
22	D	408	CLA	CAA-C2A-C1A	3.97	124.98	111.97
22	C	506	CLA	O2D-CGD-O1D	-3.94	116.12	123.84
22	B	616	CLA	CHB-C4A-NA	3.94	129.96	124.51
22	B	607	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
22	C	514	CLA	C3D-C4D-ND	3.93	116.60	110.24
22	B	615	CLA	CAA-C2A-C1A	3.92	124.82	111.97
22	C	505	CLA	CMA-C3A-C4A	3.92	122.30	111.77
22	B	610	CLA	C3A-C2A-C1A	3.91	107.20	101.34
22	C	512	CLA	C2D-C1D-ND	-3.91	107.22	110.10
22	A	405	CLA	CHB-C4A-NA	3.90	129.91	124.51
22	B	616	CLA	CBA-CAA-C2A	3.88	125.33	113.86
22	C	503	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
22	B	604	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
22	B	607	CLA	O2D-CGD-CBD	3.85	118.11	111.27
22	C	517	CLA	CHB-C4A-NA	3.84	129.82	124.51
22	A	407	CLA	CMA-C3A-C2A	-3.84	98.34	113.83
22	C	506	CLA	O2D-CGD-CBD	3.84	118.08	111.27
22	B	604	CLA	CHB-C4A-NA	3.83	129.81	124.51
22	B	610	CLA	C6-C7-C8	-3.83	103.55	115.92
22	B	609	CLA	C6-C7-C8	3.82	128.27	115.92
22	C	513	CLA	C2A-C1A-CHA	3.82	130.54	123.86
24	A	409	LHG	O4-P-O5	3.82	131.11	112.24
22	B	608	CLA	CBA-CAA-C2A	3.82	125.13	113.86
22	A	406	CLA	CBA-CAA-C2A	3.81	125.11	113.86
22	B	613	CLA	CBA-CAA-C2A	3.80	125.09	113.86
22	C	503	CLA	C4D-C3D-CAD	3.77	112.54	108.10
22	C	513	CLA	C11-C10-C8	3.77	128.11	115.92
23	K	101	BCR	C39-C30-C25	-3.77	104.19	110.30
22	D	409	CLA	CMD-C2D-C1D	3.75	131.33	124.71
22	B	611	CLA	CMA-C3A-C4A	3.75	121.85	111.77
22	C	506	CLA	CBA-CAA-C2A	3.75	124.93	113.86
22	B	603	CLA	CAA-C2A-C1A	3.74	124.22	111.97
22	B	606	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
23	D	410	BCR	C33-C5-C6	-3.73	120.34	124.53
22	C	506	CLA	O2A-C1-C2	-3.73	98.84	108.64
22	B	601	CLA	OBD-CAD-C3D	3.72	137.48	128.52
22	B	608	CLA	C1B-CHB-C4A	-3.72	122.75	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	OBD-CAD-C3D	3.72	137.47	128.52
22	B	611	CLA	C2D-C1D-ND	-3.71	107.37	110.10
22	C	508	CLA	C1D-ND-C4D	-3.70	103.70	106.33
22	B	602	CLA	C11-C10-C8	3.70	127.89	115.92
22	B	602	CLA	O2A-C1-C2	3.70	118.36	108.64
22	B	602	CLA	CAA-C2A-C1A	3.70	124.09	111.97
27	D	406	PL9	C7-C3-C2	-3.69	118.45	123.30
22	B	614	CLA	C2D-C1D-ND	-3.68	107.39	110.10
22	C	503	CLA	C3A-C2A-C1A	3.68	106.85	101.34
22	B	607	CLA	OBD-CAD-C3D	3.68	137.37	128.52
22	C	505	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
22	C	507	CLA	C3A-C2A-C1A	3.67	106.84	101.34
22	C	509	CLA	C3B-C4B-NB	-3.66	104.47	109.21
22	D	409	CLA	CBA-CAA-C2A	3.66	124.67	113.86
22	B	607	CLA	C2A-C1A-CHA	3.65	130.25	123.86
22	C	509	CLA	C3A-C2A-C1A	3.65	106.81	101.34
22	C	504	CLA	OBD-CAD-C3D	3.65	137.30	128.52
22	C	504	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
22	B	608	CLA	C2D-C1D-ND	-3.64	107.42	110.10
22	D	408	CLA	C3D-C4D-ND	3.63	116.11	110.24
22	B	616	CLA	C11-C10-C8	3.63	127.65	115.92
22	C	513	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
22	C	517	CLA	C2A-C3A-C4A	3.62	107.71	101.87
22	A	404	CLA	C3D-C2D-C1D	3.61	110.76	105.83
22	B	614	CLA	O2D-CGD-CBD	3.60	117.66	111.27
22	C	504	CLA	CMA-C3A-C4A	3.59	121.42	111.77
22	C	510	CLA	CMA-C3A-C4A	3.59	121.42	111.77
23	K	101	BCR	C23-C24-C25	3.59	137.28	127.20
22	A	405	CLA	C3D-C4D-ND	3.58	116.02	110.24
25	D	404	LMG	O1-C1-C2	-3.58	102.72	108.30
22	C	512	CLA	C1D-ND-C4D	-3.57	103.80	106.33
22	C	513	CLA	CMB-C2B-C3B	3.57	131.36	124.68
22	B	614	CLA	CBA-CAA-C2A	3.57	124.40	113.86
22	A	404	CLA	C4D-C3D-CAD	3.57	112.30	108.10
22	B	605	CLA	CMA-C3A-C4A	3.56	121.35	111.77
22	C	512	CLA	CHB-C4A-NA	3.55	129.42	124.51
22	C	511	CLA	C6-C7-C8	3.54	127.38	115.92
22	A	407	CLA	CBA-CAA-C2A	3.54	124.33	113.86
23	H	101	BCR	C39-C30-C25	-3.54	104.56	110.30
22	B	605	CLA	C2A-C1A-CHA	3.53	130.04	123.86
22	B	612	CLA	CBA-CAA-C2A	3.53	124.29	113.86
22	C	512	CLA	OBD-CAD-C3D	3.53	137.01	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	614	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	C	510	CLA	CMA-C3A-C2A	3.50	127.96	113.83
22	B	611	CLA	O2A-C1-C2	3.50	117.84	108.64
22	C	507	CLA	CMA-C3A-C2A	-3.50	99.70	113.83
22	D	408	CLA	C4A-NA-C1A	3.50	108.28	106.71
22	B	612	CLA	CGD-CBD-CAD	3.49	122.05	110.73
23	C	516	BCR	C2-C1-C6	3.49	115.86	110.48
22	C	517	CLA	CHD-C1D-ND	-3.49	121.25	124.45
22	B	613	CLA	CMD-C2D-C1D	-3.48	118.58	124.71
22	D	408	CLA	CMD-C2D-C1D	-3.46	118.61	124.71
22	A	405	CLA	C1D-ND-C4D	-3.46	103.88	106.33
21	D	407	PHO	C6-C7-C8	3.46	127.09	115.92
22	B	605	CLA	OBD-CAD-C3D	3.45	136.83	128.52
22	C	508	CLA	CMA-C3A-C2A	-3.44	99.94	113.83
22	B	613	CLA	C2A-C1A-CHA	3.44	129.88	123.86
22	B	610	CLA	CMD-C2D-C3D	-3.44	119.71	127.61
22	B	601	CLA	C1D-ND-C4D	-3.43	103.89	106.33
28	E	101	HEM	CMC-C2C-C3C	3.43	131.10	124.68
22	B	601	CLA	C1-C2-C3	3.43	131.98	126.04
22	A	404	CLA	CAA-C2A-C1A	3.43	123.21	111.97
22	B	616	CLA	CMD-C2D-C3D	-3.43	119.73	127.61
22	B	610	CLA	CBC-CAC-C3C	3.42	121.87	112.43
27	D	406	PL9	C36-C34-C33	-3.42	114.19	121.12
22	D	408	CLA	C4D-C3D-CAD	3.41	112.11	108.10
22	B	612	CLA	O2A-C1-C2	-3.40	99.70	108.64
23	K	101	BCR	C3-C4-C5	3.40	120.14	114.08
22	A	406	CLA	C1-C2-C3	3.39	131.91	126.04
22	B	610	CLA	C2A-C1A-CHA	3.39	129.79	123.86
22	B	603	CLA	C3A-C2A-C1A	3.39	106.42	101.34
22	C	505	CLA	CHB-C4A-NA	3.39	129.20	124.51
22	C	508	CLA	CAA-C2A-C1A	3.39	123.08	111.97
22	C	511	CLA	CAC-C3C-C4C	3.38	129.19	124.81
22	C	503	CLA	O2D-CGD-O1D	-3.37	117.24	123.84
23	C	516	BCR	C35-C13-C14	-3.37	118.20	122.92
23	C	515	BCR	C11-C10-C9	-3.37	122.50	127.31
23	C	515	BCR	C2-C1-C6	3.36	115.66	110.48
22	B	615	CLA	CMD-C2D-C1D	3.36	130.64	124.71
22	B	610	CLA	CHB-C4A-NA	3.36	129.15	124.51
22	A	404	CLA	CMA-C3A-C4A	3.35	120.79	111.77
22	B	616	CLA	CMA-C3A-C2A	3.35	127.36	113.83
22	C	513	CLA	CBA-CAA-C2A	3.34	123.73	113.86
22	B	602	CLA	CBA-CAA-C2A	3.33	123.71	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	CMA-C3A-C4A	3.33	120.72	111.77
22	C	512	CLA	CMD-C2D-C3D	-3.33	119.96	127.61
27	D	406	PL9	C35-C34-C36	3.33	120.87	115.27
22	B	614	CLA	CAA-C2A-C3A	3.33	121.89	112.78
23	H	101	BCR	C28-C27-C26	3.32	120.01	114.08
22	C	512	CLA	CAA-C2A-C1A	3.32	122.84	111.97
25	D	405	LMG	C1-C2-C3	-3.32	103.09	110.00
22	B	605	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
22	B	610	CLA	CMD-C2D-C1D	3.31	130.54	124.71
22	B	611	CLA	C3A-C2A-C1A	3.30	106.29	101.34
22	A	404	CLA	C4-C3-C2	-3.29	115.23	123.68
22	A	405	CLA	CMA-C3A-C2A	3.29	127.11	113.83
22	B	602	CLA	C1-O2A-CGA	-3.29	107.82	116.44
23	K	101	BCR	C28-C27-C26	3.28	119.94	114.08
22	B	603	CLA	OBD-CAD-C3D	3.28	136.41	128.52
22	A	404	CLA	CBC-CAC-C3C	3.28	121.46	112.43
22	C	514	CLA	CAA-C2A-C1A	3.27	122.70	111.97
22	D	408	CLA	CMA-C3A-C2A	-3.27	100.64	113.83
22	C	505	CLA	OBD-CAD-C3D	3.27	136.38	128.52
22	C	512	CLA	C9-C8-C7	3.25	123.08	111.29
22	A	404	CLA	C3D-C4D-ND	3.25	115.50	110.24
22	B	610	CLA	CAA-C2A-C1A	3.25	122.62	111.97
23	H	101	BCR	C23-C24-C25	3.24	136.29	127.20
22	C	512	CLA	C3A-C2A-C1A	3.23	106.18	101.34
21	D	407	PHO	C11-C10-C8	3.23	126.35	115.92
22	C	513	CLA	C3B-C4B-NB	-3.23	105.04	109.21
23	B	619	BCR	C33-C5-C6	-3.23	120.91	124.53
22	C	510	CLA	C2D-C1D-ND	-3.23	107.73	110.10
22	C	511	CLA	CMD-C2D-C1D	3.22	130.39	124.71
22	C	513	CLA	C2D-C1D-ND	-3.22	107.73	110.10
22	C	517	CLA	O2A-C1-C2	-3.21	100.20	108.64
22	C	517	CLA	CHD-C1D-C2D	3.20	132.20	125.48
22	C	506	CLA	CMA-C3A-C4A	3.20	120.37	111.77
22	D	409	CLA	C4D-C3D-CAD	3.19	111.86	108.10
21	D	407	PHO	C9-C8-C10	3.19	122.85	111.29
22	B	605	CLA	CMD-C2D-C1D	3.19	130.33	124.71
22	D	408	CLA	C6-C7-C8	3.18	126.19	115.92
22	C	503	CLA	OBD-CAD-C3D	3.18	136.17	128.52
22	C	504	CLA	C11-C10-C8	3.18	126.19	115.92
22	A	406	CLA	C4-C3-C2	-3.18	115.53	123.68
22	B	614	CLA	C1D-ND-C4D	-3.17	104.08	106.33
22	C	514	CLA	C3A-C2A-C1A	3.17	106.09	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	514	CLA	C11-C10-C8	3.17	126.17	115.92
23	A	408	BCR	C8-C9-C10	3.17	123.80	118.94
25	C	501	LMG	C1-C2-C3	-3.16	103.42	110.00
22	B	611	CLA	O2A-CGA-O1A	-3.16	115.63	123.59
23	C	516	BCR	C27-C26-C25	3.15	127.31	122.73
22	B	612	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
22	A	407	CLA	CMD-C2D-C1D	3.14	130.24	124.71
22	B	604	CLA	C2A-C1A-CHA	3.13	129.34	123.86
22	A	406	CLA	CAA-C2A-C3A	3.13	121.35	112.78
22	B	602	CLA	C3D-C2D-C1D	3.13	110.10	105.83
25	C	502	LMG	O6-C1-O1	-3.13	102.57	109.97
22	C	510	CLA	C1D-ND-C4D	-3.12	104.12	106.33
22	B	603	CLA	CHB-C4A-NA	3.12	128.82	124.51
22	B	616	CLA	CMA-C3A-C4A	3.11	120.14	111.77
22	C	511	CLA	C9-C8-C7	3.11	122.55	111.29
22	B	605	CLA	C3A-C2A-C1A	3.11	105.99	101.34
23	H	101	BCR	C33-C5-C4	3.10	119.57	113.62
22	B	602	CLA	CMB-C2B-C1B	-3.10	123.71	128.46
22	C	510	CLA	O2A-CGA-O1A	-3.09	115.78	123.59
22	A	405	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
22	C	504	CLA	O2D-CGD-CBD	3.09	116.76	111.27
22	D	409	CLA	CAA-C2A-C3A	3.08	121.21	112.78
22	A	406	CLA	C3D-C4D-ND	3.07	115.21	110.24
22	B	606	CLA	CBA-CAA-C2A	3.07	122.92	113.86
22	B	604	CLA	CBA-CAA-C2A	3.07	122.91	113.86
22	A	405	CLA	O2A-C1-C2	-3.06	100.59	108.64
22	A	404	CLA	C5-C3-C2	3.06	127.31	121.12
22	A	407	CLA	C3B-C4B-NB	-3.06	105.26	109.21
22	B	609	CLA	CHB-C4A-NA	3.05	128.73	124.51
22	C	513	CLA	CGD-CBD-CAD	3.05	120.62	110.73
22	C	504	CLA	C3A-C2A-C1A	3.05	105.90	101.34
22	B	605	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
22	B	604	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
22	C	507	CLA	C1D-ND-C4D	-3.02	104.19	106.33
22	A	404	CLA	CBA-CAA-C2A	3.02	122.78	113.86
22	C	509	CLA	C4-C3-C5	3.02	120.35	115.27
22	A	406	CLA	CMA-C3A-C2A	-3.02	101.65	113.83
23	B	617	BCR	C2-C1-C6	3.01	115.12	110.48
22	A	404	CLA	O1D-CGD-CBD	3.01	130.64	124.48
22	B	615	CLA	O2A-C1-C2	-3.00	100.75	108.64
22	C	513	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	D	404	LMG	C6-C5-C4	-2.99	106.00	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	C9-C8-C7	2.99	122.11	111.29
22	B	614	CLA	CAA-C2A-C1A	2.98	121.75	111.97
22	A	405	CLA	CBA-CAA-C2A	2.98	122.66	113.86
22	B	606	CLA	CAA-C2A-C3A	2.97	120.92	112.78
22	C	508	CLA	C4-C3-C5	2.97	120.27	115.27
22	C	511	CLA	C1D-ND-C4D	-2.97	104.23	106.33
22	B	615	CLA	CHB-C4A-NA	2.97	128.62	124.51
22	B	609	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	D	410	BCR	C7-C8-C9	-2.96	121.76	126.23
22	B	616	CLA	O2A-C1-C2	-2.96	100.87	108.64
21	A	403	PHO	C9-C8-C10	2.95	121.99	111.29
22	D	409	CLA	CAA-C2A-C1A	2.95	121.66	111.97
22	C	503	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	B	601	CLA	C3B-C4B-NB	-2.94	105.40	109.21
22	B	609	CLA	CAA-C2A-C1A	2.94	121.61	111.97
22	C	511	CLA	CHB-C4A-NA	2.94	128.57	124.51
22	B	615	CLA	CMD-C2D-C3D	-2.94	120.86	127.61
22	C	517	CLA	CBA-CAA-C2A	2.93	122.52	113.86
22	B	601	CLA	C2A-C3A-C4A	2.93	106.60	101.87
22	C	509	CLA	C6-C5-C3	2.93	121.14	113.45
22	C	509	CLA	CBA-CAA-C2A	2.93	122.51	113.86
23	C	516	BCR	C36-C18-C17	-2.93	118.83	122.92
25	D	402	LMG	O6-C1-O1	-2.92	103.05	109.97
23	C	518	BCR	C40-C30-C25	2.92	115.03	110.30
22	B	602	CLA	C1-C2-C3	2.92	131.09	126.04
22	B	612	CLA	C3D-C4D-ND	2.91	114.95	110.24
22	B	614	CLA	C3A-C2A-C1A	2.91	105.69	101.34
22	B	604	CLA	CGD-CBD-CAD	2.91	120.15	110.73
22	B	614	CLA	CGD-CBD-CAD	-2.90	101.34	110.73
22	B	605	CLA	CBA-CAA-C2A	2.89	122.40	113.86
22	A	405	CLA	CMA-C3A-C4A	2.89	119.55	111.77
22	C	508	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	B	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	B	604	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
22	B	608	CLA	C9-C8-C7	2.88	121.73	111.29
22	C	504	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
22	B	606	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	K	101	BCR	C33-C5-C4	2.88	119.14	113.62
22	B	615	CLA	CBA-CAA-C2A	2.88	122.35	113.86
22	C	510	CLA	C4D-CHA-C1A	-2.87	117.75	121.25
22	C	512	CLA	CHD-C1D-ND	-2.87	121.81	124.45
22	C	508	CLA	C6-C5-C3	2.87	120.98	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	K	101	BCR	C20-C19-C18	-2.87	118.35	126.42
23	B	618	BCR	C35-C13-C14	-2.87	118.90	122.92
22	B	605	CLA	CAA-C2A-C1A	2.87	121.37	111.97
22	B	610	CLA	C3D-C2D-C1D	2.87	109.74	105.83
22	A	404	CLA	CAA-CBA-CGA	-2.84	104.95	113.25
22	B	608	CLA	CHD-C4C-C3C	2.84	129.01	124.84
23	K	101	BCR	C7-C8-C9	-2.83	121.95	126.23
22	A	404	CLA	C3A-C2A-C1A	2.83	105.58	101.34
22	B	611	CLA	C4-C3-C5	2.82	120.02	115.27
22	D	409	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
22	C	512	CLA	CAC-C3C-C4C	2.81	128.46	124.81
22	D	408	CLA	C9-C8-C10	2.81	121.48	111.29
22	D	408	CLA	CBA-CAA-C2A	2.81	122.17	113.86
22	B	612	CLA	CMA-C3A-C4A	2.81	119.33	111.77
22	B	612	CLA	C6-C5-C3	-2.81	106.09	113.45
23	H	101	BCR	C7-C8-C9	-2.80	122.00	126.23
22	B	616	CLA	C9-C8-C10	2.80	121.44	111.29
22	B	616	CLA	C2A-C3A-C4A	2.80	106.39	101.87
22	A	407	CLA	C4D-C3D-CAD	2.80	111.40	108.10
22	B	614	CLA	CHD-C1D-ND	-2.80	121.88	124.45
22	D	409	CLA	CMA-C3A-C2A	-2.80	102.55	113.83
22	B	609	CLA	OBD-CAD-C3D	2.79	135.25	128.52
22	B	613	CLA	CAA-C2A-C3A	2.79	120.42	112.78
22	A	405	CLA	CHD-C1D-ND	-2.79	121.89	124.45
23	K	101	BCR	C35-C13-C14	-2.79	119.02	122.92
22	B	608	CLA	CAA-CBA-CGA	2.79	121.40	113.25
22	B	613	CLA	O1D-CGD-CBD	2.79	130.18	124.48
22	C	509	CLA	CAA-C2A-C1A	2.78	121.10	111.97
23	H	101	BCR	C20-C19-C18	-2.78	118.60	126.42
22	C	508	CLA	C9-C8-C10	2.78	121.37	111.29
22	B	612	CLA	C3D-C2D-C1D	2.78	109.63	105.83
22	C	505	CLA	C3A-C2A-C1A	2.78	105.50	101.34
22	A	406	CLA	CHD-C1D-ND	-2.77	121.90	124.45
22	C	504	CLA	CBA-CAA-C2A	2.77	122.05	113.86
22	C	505	CLA	C2A-C1A-CHA	2.77	128.71	123.86
22	A	406	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
22	C	506	CLA	C9-C8-C10	2.76	121.29	111.29
22	B	608	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
25	D	403	LMG	C1-C2-C3	-2.75	104.26	110.00
22	C	517	CLA	CAA-C2A-C3A	2.75	120.31	112.78
22	B	607	CLA	CBC-CAC-C3C	2.75	120.02	112.43
22	C	505	CLA	CBA-CAA-C2A	2.75	121.98	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	602	CLA	C7-C6-C5	-2.75	105.89	113.36
22	B	614	CLA	CMD-C2D-C3D	-2.75	121.29	127.61
23	D	410	BCR	C38-C26-C25	-2.75	121.44	124.53
21	A	403	PHO	C9-C8-C7	2.74	121.23	111.29
22	C	504	CLA	C9-C8-C7	2.74	121.20	111.29
23	K	101	BCR	C15-C14-C13	-2.73	123.41	127.31
22	C	517	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
22	C	517	CLA	CMA-C3A-C4A	2.73	119.12	111.77
22	C	505	CLA	C1D-ND-C4D	-2.73	104.39	106.33
23	C	515	BCR	C34-C9-C10	-2.73	119.10	122.92
22	C	506	CLA	CAA-C2A-C1A	2.73	120.91	111.97
23	H	101	BCR	C35-C13-C14	-2.73	119.10	122.92
22	B	616	CLA	C6-C7-C8	2.72	124.72	115.92
23	K	101	BCR	C32-C1-C6	-2.72	105.88	110.30
22	B	606	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
22	B	606	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
22	B	606	CLA	CHD-C1D-ND	-2.72	121.96	124.45
22	A	405	CLA	C3D-C2D-C1D	2.71	109.53	105.83
22	C	506	CLA	CBC-CAC-C3C	2.71	119.91	112.43
22	A	404	CLA	C1-C2-C3	2.71	130.73	126.04
22	B	610	CLA	CBA-CAA-C2A	2.71	121.86	113.86
22	C	512	CLA	CBA-CAA-C2A	2.70	121.84	113.86
22	C	506	CLA	C2A-C1A-CHA	2.69	128.57	123.86
22	A	407	CLA	C2A-C1A-CHA	2.69	128.56	123.86
22	A	405	CLA	C9-C8-C7	2.69	121.03	111.29
22	C	509	CLA	O2A-C1-C2	-2.68	101.58	108.64
22	B	605	CLA	CMA-C3A-C2A	-2.68	103.02	113.83
22	C	513	CLA	CHA-C1A-NA	-2.68	120.26	126.40
22	C	507	CLA	C11-C10-C8	2.68	124.58	115.92
23	A	408	BCR	C35-C13-C14	-2.68	119.17	122.92
22	A	406	CLA	CAC-C3C-C4C	2.68	128.28	124.81
22	A	405	CLA	CHA-C1A-NA	-2.68	120.27	126.40
22	C	511	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
22	C	508	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	B	612	CLA	C11-C10-C8	2.67	124.55	115.92
22	A	404	CLA	C9-C8-C7	2.67	120.95	111.29
22	D	408	CLA	CAC-C3C-C2C	-2.66	122.98	127.53
22	B	604	CLA	O1D-CGD-CBD	2.66	129.93	124.48
22	C	513	CLA	C2A-C3A-C4A	2.66	106.16	101.87
23	B	618	BCR	C30-C25-C26	-2.66	118.87	122.61
23	B	618	BCR	C12-C13-C14	2.65	123.02	118.94
22	C	506	CLA	C11-C10-C8	2.65	124.50	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
22	B	604	CLA	C9-C8-C7	2.63	120.83	111.29
28	E	101	HEM	CMA-C3A-C4A	-2.63	124.42	128.46
22	B	614	CLA	C10-C8-C7	2.63	125.97	112.13
23	H	101	BCR	C15-C14-C13	-2.63	123.56	127.31
22	B	605	CLA	C9-C8-C7	2.63	120.80	111.29
23	H	101	BCR	C16-C15-C14	-2.62	118.10	123.47
21	A	403	PHO	C1B-NB-C4B	2.62	112.47	107.09
23	K	101	BCR	C16-C15-C14	-2.62	118.11	123.47
22	B	609	CLA	C3A-C2A-C1A	2.62	105.26	101.34
22	B	606	CLA	O1D-CGD-CBD	2.61	129.82	124.48
23	B	619	BCR	C30-C25-C26	-2.60	118.94	122.61
25	D	402	LMG	C3-C4-C5	-2.60	105.59	110.24
22	B	616	CLA	CAA-C2A-C1A	2.60	120.48	111.97
22	C	511	CLA	CMC-C2C-C1C	2.60	128.99	125.04
22	B	609	CLA	C3B-C4B-NB	-2.60	105.86	109.21
22	B	612	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	B	615	CLA	O1D-CGD-CBD	2.59	129.79	124.48
22	B	603	CLA	CMD-C2D-C1D	2.59	129.28	124.71
22	C	505	CLA	C1-C2-C3	2.59	130.52	126.04
22	B	608	CLA	C1D-ND-C4D	-2.59	104.50	106.33
22	C	506	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
22	B	604	CLA	C11-C10-C8	2.59	124.28	115.92
22	B	601	CLA	C9-C8-C7	2.58	120.64	111.29
22	C	507	CLA	O1D-CGD-CBD	2.58	129.76	124.48
22	A	406	CLA	CMB-C2B-C3B	2.58	129.50	124.68
22	B	605	CLA	C11-C10-C8	2.58	124.25	115.92
22	B	614	CLA	CMC-C2C-C1C	2.58	128.96	125.04
22	C	513	CLA	C3D-C2D-C1D	2.58	109.35	105.83
22	A	407	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
22	D	408	CLA	CAA-C2A-C3A	2.57	119.80	112.78
22	B	601	CLA	C9-C8-C10	2.57	120.58	111.29
22	C	514	CLA	CHB-C4A-NA	2.56	128.06	124.51
22	D	408	CLA	CMA-C3A-C4A	2.56	118.65	111.77
22	A	407	CLA	C9-C8-C7	2.56	120.56	111.29
22	B	611	CLA	CHD-C1D-ND	-2.56	122.10	124.45
28	E	101	HEM	C4B-CHC-C1C	2.55	125.93	122.56
25	I	101	LMG	C1-O6-C5	-2.55	108.68	113.69
22	C	509	CLA	C5-C3-C2	-2.55	115.96	121.12
22	A	406	CLA	C9-C8-C10	2.55	120.52	111.29
22	B	605	CLA	C1D-ND-C4D	-2.55	104.53	106.33
22	B	607	CLA	C9-C8-C7	2.54	120.51	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	512	CLA	C2A-C1A-CHA	2.54	128.30	123.86
22	B	607	CLA	CAA-C2A-C1A	2.54	120.30	111.97
22	C	513	CLA	CMA-C3A-C4A	2.54	118.60	111.77
22	C	508	CLA	CMA-C3A-C4A	2.54	118.60	111.77
22	A	405	CLA	CAA-C2A-C1A	2.54	120.30	111.97
22	B	603	CLA	C9-C8-C7	2.53	120.47	111.29
22	B	609	CLA	C10-C8-C7	2.53	125.44	112.13
22	B	611	CLA	C11-C10-C8	2.53	124.09	115.92
22	B	607	CLA	C3B-C4B-NB	-2.53	105.94	109.21
22	C	507	CLA	CAA-C2A-C1A	2.53	120.26	111.97
22	B	609	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
22	C	513	CLA	O2D-CGD-CBD	2.52	115.75	111.27
23	A	408	BCR	C34-C9-C8	-2.51	114.12	118.08
22	B	612	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
22	B	601	CLA	CMD-C2D-C1D	2.50	129.12	124.71
22	B	616	CLA	CAA-CBA-CGA	-2.50	105.94	113.25
23	B	619	BCR	C27-C26-C25	2.50	126.36	122.73
22	B	605	CLA	CBC-CAC-C3C	2.50	119.32	112.43
25	D	403	LMG	C3-C4-C5	-2.50	105.79	110.24
27	D	406	PL9	C8-C7-C3	2.49	119.01	111.98
22	A	407	CLA	CHA-C1A-NA	-2.49	120.70	126.40
22	B	603	CLA	C9-C8-C10	2.48	120.28	111.29
22	B	602	CLA	C9-C8-C10	2.48	120.28	111.29
23	K	101	BCR	C8-C9-C10	-2.48	115.13	118.94
22	C	508	CLA	CAA-CBA-CGA	-2.48	106.00	113.25
22	C	512	CLA	CHD-C1D-C2D	2.48	130.68	125.48
22	C	507	CLA	CHD-C1D-C2D	2.47	130.67	125.48
22	B	609	CLA	CBA-CAA-C2A	2.47	121.16	113.86
22	B	612	CLA	C9-C8-C7	2.47	120.25	111.29
22	B	614	CLA	CHD-C1D-C2D	2.47	130.66	125.48
22	C	507	CLA	CHD-C1D-ND	-2.47	122.19	124.45
22	C	511	CLA	O2A-C1-C2	-2.46	102.16	108.64
23	C	515	BCR	C1-C6-C5	-2.46	119.14	122.61
22	C	514	CLA	CMA-C3A-C4A	2.46	118.39	111.77
22	C	512	CLA	O2A-C1-C2	-2.46	102.17	108.64
22	C	508	CLA	C9-C8-C7	2.46	120.19	111.29
22	B	603	CLA	C3B-C4B-NB	-2.46	106.03	109.21
22	C	517	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
22	C	510	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
22	D	409	CLA	C1D-ND-C4D	-2.45	104.60	106.33
22	D	408	CLA	CBC-CAC-C3C	2.44	119.15	112.43
22	B	614	CLA	CHB-C4A-NA	2.43	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	608	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
23	H	101	BCR	C27-C26-C25	2.43	126.26	122.73
22	A	406	CLA	C3D-C2D-C1D	2.43	109.15	105.83
22	B	613	CLA	C4-C3-C5	2.43	119.36	115.27
23	K	101	BCR	C27-C26-C25	2.43	126.26	122.73
22	B	605	CLA	O2D-CGD-CBD	2.43	115.58	111.27
22	A	406	CLA	CAA-C2A-C1A	2.42	119.90	111.97
23	H	101	BCR	C8-C9-C10	-2.42	115.23	118.94
22	C	509	CLA	CMD-C2D-C3D	-2.42	122.06	127.61
22	B	609	CLA	CMA-C3A-C2A	-2.42	104.08	113.83
22	B	601	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
25	D	405	LMG	C8-O7-C10	2.41	123.72	117.79
22	C	511	CLA	CBA-CAA-C2A	2.41	120.97	113.86
22	B	616	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	C	513	CLA	CMC-C2C-C1C	2.40	128.70	125.04
22	C	517	CLA	C1D-ND-C4D	-2.40	104.63	106.33
22	D	409	CLA	CMC-C2C-C1C	2.40	128.69	125.04
22	B	611	CLA	O2A-CGA-CBA	2.40	119.44	111.91
22	C	508	CLA	C3A-C2A-C1A	2.40	104.93	101.34
21	D	407	PHO	C1B-NB-C4B	2.40	112.02	107.09
22	A	407	CLA	C3A-C2A-C1A	2.39	104.92	101.34
22	B	616	CLA	C1-O2A-CGA	2.39	122.72	116.44
22	C	513	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	B	601	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
22	B	606	CLA	C3B-C4B-NB	-2.38	106.13	109.21
22	B	604	CLA	CBC-CAC-C3C	2.38	119.00	112.43
22	B	607	CLA	C3A-C2A-C1A	2.38	104.91	101.34
22	C	510	CLA	C2A-C3A-C4A	2.38	105.72	101.87
22	A	407	CLA	C9-C8-C10	2.38	119.91	111.29
22	A	406	CLA	C5-C3-C2	2.38	125.92	121.12
23	C	518	BCR	C7-C8-C9	-2.38	122.65	126.23
22	A	405	CLA	CMB-C2B-C3B	2.37	129.12	124.68
22	C	514	CLA	C10-C8-C7	2.37	124.60	112.13
22	B	609	CLA	C11-C10-C8	2.37	123.58	115.92
22	B	607	CLA	CHA-C1A-NA	-2.37	120.97	126.40
22	B	604	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
23	B	618	BCR	C40-C30-C25	2.36	114.13	110.30
22	B	614	CLA	CMB-C2B-C3B	2.36	129.10	124.68
22	C	511	CLA	CHD-C1D-ND	-2.36	122.28	124.45
22	C	513	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
22	A	404	CLA	C2A-C1A-CHA	2.36	127.98	123.86
22	B	602	CLA	CMB-C2B-C3B	2.36	129.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	509	CLA	CHB-C4A-NA	2.36	127.77	124.51
22	B	608	CLA	CHD-C4C-NC	-2.36	120.49	124.20
22	C	504	CLA	CED-O2D-CGD	2.36	121.27	115.94
22	C	509	CLA	C3D-C2D-C1D	2.35	109.04	105.83
22	B	610	CLA	CMA-C3A-C4A	2.35	118.08	111.77
22	C	512	CLA	O1D-CGD-CBD	2.34	129.28	124.48
22	C	505	CLA	O2D-CGD-CBD	2.34	115.43	111.27
22	C	509	CLA	CMD-C2D-C1D	2.34	128.84	124.71
25	D	403	LMG	C1-O6-C5	-2.34	109.09	113.69
22	B	601	CLA	O2A-C1-C2	2.34	114.78	108.64
23	D	410	BCR	C2-C1-C6	2.34	114.08	110.48
22	B	606	CLA	CMC-C2C-C1C	2.34	128.59	125.04
22	B	611	CLA	CHD-C1D-C2D	2.33	130.38	125.48
22	C	514	CLA	C3B-C4B-NB	-2.33	106.19	109.21
22	B	602	CLA	O1D-CGD-CBD	2.33	129.25	124.48
22	B	604	CLA	CHA-C1A-NA	-2.33	121.06	126.40
22	B	601	CLA	C11-C10-C8	2.33	123.45	115.92
21	A	403	PHO	O2D-CGD-O1D	-2.33	119.29	123.84
23	C	515	BCR	C15-C14-C13	-2.33	123.99	127.31
22	C	508	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	B	606	CLA	CGD-CBD-CAD	2.32	118.26	110.73
22	A	404	CLA	CHD-C1D-C2D	2.32	130.35	125.48
22	D	409	CLA	C9-C8-C7	2.32	119.70	111.29
22	C	513	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
25	D	405	LMG	C1-O6-C5	-2.31	109.15	113.69
22	B	602	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
22	B	610	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	C	512	CLA	C11-C10-C8	2.31	123.39	115.92
22	B	605	CLA	C6-C7-C8	2.31	123.38	115.92
22	B	611	CLA	C9-C8-C10	2.31	119.65	111.29
23	B	618	BCR	C19-C18-C17	2.30	122.47	118.94
22	A	407	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	C	508	CLA	C2A-C1A-CHA	2.30	127.88	123.86
22	C	509	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
27	D	406	PL9	C22-C23-C24	-2.30	122.13	127.66
22	B	604	CLA	C10-C8-C7	2.29	124.19	112.13
22	B	604	CLA	CMD-C2D-C1D	2.29	128.76	124.71
22	B	609	CLA	C2A-C1A-CHA	2.29	127.87	123.86
22	B	616	CLA	C4D-CHA-C1A	-2.29	118.46	121.25
22	C	505	CLA	CMD-C2D-C3D	-2.29	122.34	127.61
22	B	605	CLA	C9-C8-C10	2.29	119.59	111.29
22	C	513	CLA	O2A-C1-C2	-2.29	102.61	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	613	CLA	C10-C8-C7	2.29	124.18	112.13
23	H	101	BCR	C15-C16-C17	-2.29	118.78	123.47
22	C	505	CLA	C4-C3-C5	-2.29	111.42	115.27
23	A	408	BCR	C23-C24-C25	-2.29	120.78	127.20
22	B	611	CLA	CHB-C4A-NA	2.29	127.67	124.51
22	A	404	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
22	B	610	CLA	C1-O2A-CGA	2.28	122.43	116.44
22	C	507	CLA	CAA-C2A-C3A	2.28	119.03	112.78
22	A	407	CLA	CMA-C3A-C4A	2.28	117.90	111.77
22	B	603	CLA	O1D-CGD-CBD	2.28	129.15	124.48
22	B	608	CLA	CAC-C3C-C2C	-2.28	123.63	127.53
22	B	601	CLA	C6-C5-C3	2.28	119.42	113.45
22	C	505	CLA	CMD-C2D-C1D	2.28	128.72	124.71
22	C	505	CLA	C3B-C4B-NB	-2.27	106.27	109.21
22	C	505	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	C	518	BCR	C27-C26-C25	2.27	126.03	122.73
22	B	612	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
22	B	608	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	C	514	CLA	C9-C8-C7	2.27	119.51	111.29
22	B	602	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	B	608	CLA	CHA-C1A-NA	-2.27	121.21	126.40
23	B	618	BCR	C27-C26-C25	2.26	126.01	122.73
25	D	404	LMG	C7-O1-C1	2.26	118.15	113.74
22	C	511	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
22	B	606	CLA	C9-C8-C10	2.26	119.46	111.29
23	B	618	BCR	C1-C6-C5	-2.26	119.44	122.61
22	A	406	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
22	B	615	CLA	C6-C7-C8	2.25	123.19	115.92
22	C	514	CLA	CHD-C1D-C2D	2.25	130.19	125.48
25	C	502	LMG	C3-C4-C5	-2.24	106.25	110.24
22	D	409	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	B	603	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
22	C	513	CLA	C10-C8-C7	2.23	123.88	112.13
23	B	617	BCR	C20-C21-C22	2.23	130.50	127.31
23	K	101	BCR	C15-C16-C17	-2.23	118.90	123.47
22	C	511	CLA	C11-C10-C8	2.23	123.13	115.92
25	I	101	LMG	O6-C1-O1	-2.23	104.70	109.97
22	C	504	CLA	C3B-C4B-NB	-2.23	106.33	109.21
22	A	405	CLA	O1D-CGD-CBD	2.23	129.04	124.48
22	C	504	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
22	B	607	CLA	C10-C8-C7	2.22	123.82	112.13
22	A	406	CLA	C2C-C1C-NC	-2.22	107.89	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	406	PL9	C20-C19-C21	2.22	119.00	115.27
22	C	504	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
22	B	608	CLA	C9-C8-C10	2.22	119.32	111.29
23	B	618	BCR	C2-C1-C6	2.22	113.89	110.48
23	A	408	BCR	C27-C26-C25	2.22	125.95	122.73
23	B	617	BCR	C30-C25-C26	-2.21	119.50	122.61
22	D	409	CLA	CHA-C1A-NA	-2.21	121.34	126.40
22	C	507	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
22	B	601	CLA	CHA-C1A-NA	-2.21	121.35	126.40
22	A	404	CLA	CMA-C3A-C2A	-2.21	104.93	113.83
22	C	505	CLA	O2A-C1-C2	2.20	114.43	108.64
22	C	505	CLA	C3D-C2D-C1D	2.20	108.84	105.83
22	A	405	CLA	C9-C8-C10	2.20	119.27	111.29
22	C	503	CLA	CBA-CAA-C2A	2.20	120.37	113.86
22	C	504	CLA	C10-C8-C7	2.20	123.71	112.13
22	C	509	CLA	CAA-C2A-C3A	2.20	118.81	112.78
22	B	612	CLA	C5-C3-C2	-2.20	116.66	121.12
22	A	406	CLA	C2D-C1D-ND	-2.20	108.48	110.10
23	A	408	BCR	C7-C8-C9	-2.20	122.91	126.23
22	C	509	CLA	C10-C8-C7	2.20	123.68	112.13
22	B	602	CLA	C9-C8-C7	2.19	119.23	111.29
22	D	408	CLA	C9-C8-C7	2.19	119.23	111.29
22	B	612	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
22	B	616	CLA	C10-C8-C7	2.19	123.64	112.13
22	B	613	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
22	B	603	CLA	CMC-C2C-C1C	2.19	128.37	125.04
25	D	402	LMG	C7-O1-C1	-2.19	109.47	113.74
22	C	503	CLA	CHD-C1D-ND	-2.19	122.45	124.45
22	B	614	CLA	CED-O2D-CGD	-2.18	111.00	115.94
22	B	614	CLA	CBC-CAC-C3C	2.18	118.45	112.43
22	C	511	CLA	CAC-C3C-C2C	-2.18	123.80	127.53
22	B	604	CLA	C6-C5-C3	2.18	119.17	113.45
22	D	408	CLA	CHD-C1D-C2D	2.18	130.05	125.48
27	D	406	PL9	O2-C1-C2	-2.18	116.79	121.78
22	C	512	CLA	CMA-C3A-C4A	2.17	117.62	111.77
22	B	602	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
22	B	607	CLA	CMB-C2B-C3B	2.17	128.74	124.68
22	C	509	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	C	507	CLA	C10-C8-C7	2.17	123.53	112.13
23	H	101	BCR	C19-C18-C17	2.16	122.25	118.94
22	C	504	CLA	CMB-C2B-C3B	2.16	128.71	124.68
22	C	511	CLA	CMD-C2D-C3D	-2.15	122.66	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	CMD-C2D-C1D	2.15	128.51	124.71
22	B	607	CLA	CHA-C4D-ND	2.15	137.00	132.50
22	C	508	CLA	C6-C7-C8	2.15	122.88	115.92
21	A	403	PHO	O1D-CGD-CBD	2.15	128.32	124.74
23	H	101	BCR	C16-C17-C18	-2.15	124.24	127.31
22	B	612	CLA	O1D-CGD-CBD	2.15	128.88	124.48
22	B	615	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
22	C	506	CLA	CHA-C1A-NA	-2.15	121.48	126.40
22	C	509	CLA	C9-C8-C7	2.14	119.06	111.29
22	C	512	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
22	C	510	CLA	C9-C8-C7	2.14	119.04	111.29
25	D	403	LMG	O6-C1-O1	-2.14	104.91	109.97
23	C	518	BCR	C2-C1-C6	2.14	113.78	110.48
22	A	406	CLA	C3A-C2A-C1A	2.14	104.54	101.34
25	C	502	LMG	O2-C2-C1	-2.14	104.86	110.05
22	B	609	CLA	CHD-C1D-C2D	2.14	129.96	125.48
22	B	603	CLA	C6-C7-C8	2.13	122.82	115.92
23	D	410	BCR	C34-C9-C8	-2.13	114.71	118.08
22	B	607	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
23	C	518	BCR	C39-C30-C25	-2.13	106.84	110.30
22	B	606	CLA	CED-O2D-CGD	2.13	120.76	115.94
22	D	408	CLA	C3B-C4B-NB	-2.13	106.45	109.21
22	C	505	CLA	C6-C5-C3	2.13	119.04	113.45
22	C	503	CLA	C9-C8-C10	2.13	119.00	111.29
22	B	601	CLA	CMB-C2B-C3B	2.13	128.66	124.68
22	B	603	CLA	CHA-C1A-NA	-2.13	121.53	126.40
22	C	509	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
22	B	606	CLA	C1D-ND-C4D	-2.13	104.83	106.33
25	C	501	LMG	C1-O6-C5	-2.12	109.52	113.69
22	D	409	CLA	C9-C8-C10	2.12	118.95	111.29
22	B	609	CLA	C9-C8-C7	2.12	118.95	111.29
23	A	408	BCR	C38-C26-C25	-2.11	122.16	124.53
22	C	514	CLA	CBA-CAA-C2A	2.11	120.10	113.86
23	D	410	BCR	C40-C30-C25	2.11	113.72	110.30
22	C	509	CLA	C11-C10-C8	2.11	122.74	115.92
23	C	515	BCR	C38-C26-C25	-2.11	122.16	124.53
22	B	606	CLA	OBD-CAD-C3D	2.11	133.59	128.52
22	B	601	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
25	I	101	LMG	O7-C10-O9	-2.11	118.61	123.70
22	C	510	CLA	C9-C8-C10	2.11	118.92	111.29
22	B	612	CLA	C1-O2A-CGA	2.11	121.97	116.44
22	B	608	CLA	CMB-C2B-C3B	2.11	128.62	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	611	CLA	C10-C8-C7	2.10	123.19	112.13
22	D	409	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
22	B	607	CLA	CBA-CAA-C2A	2.10	120.06	113.86
22	A	404	CLA	CHD-C1D-ND	-2.10	122.53	124.45
22	B	615	CLA	C10-C8-C7	2.10	123.16	112.13
22	B	610	CLA	C9-C8-C7	2.10	118.88	111.29
22	B	608	CLA	C6-C7-C8	2.09	122.69	115.92
22	B	610	CLA	CMA-C3A-C2A	-2.09	105.38	113.83
22	A	405	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	618	BCR	C31-C1-C6	-2.09	106.91	110.30
22	C	513	CLA	CAA-C2A-C1A	2.09	118.82	111.97
21	D	407	PHO	C3D-CAD-CBD	-2.09	104.85	107.61
22	C	503	CLA	O1D-CGD-CBD	2.09	128.75	124.48
22	B	610	CLA	C2D-C1D-ND	-2.09	108.57	110.10
22	B	602	CLA	C1D-ND-C4D	-2.08	104.85	106.33
22	D	408	CLA	C3A-C2A-C1A	2.08	104.46	101.34
22	C	517	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
22	C	512	CLA	C10-C8-C7	2.08	123.06	112.13
22	A	404	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	B	619	BCR	C37-C22-C23	2.07	121.34	118.08
21	D	407	PHO	O2D-CGD-O1D	-2.07	119.79	123.84
22	A	406	CLA	CHC-C1C-NC	2.07	127.34	124.20
22	B	612	CLA	C10-C8-C7	2.07	123.01	112.13
22	B	609	CLA	CMD-C2D-C1D	-2.07	121.07	124.71
22	C	517	CLA	C9-C8-C7	2.06	118.76	111.29
22	B	610	CLA	C1D-ND-C4D	-2.06	104.87	106.33
22	B	613	CLA	CMA-C3A-C2A	-2.06	105.52	113.83
22	B	611	CLA	C3B-C4B-NB	-2.06	106.55	109.21
22	C	507	CLA	C4D-CHA-C1A	-2.06	118.75	121.25
22	A	405	CLA	C6-C7-C8	2.05	122.56	115.92
22	B	605	CLA	CGD-CBD-CAD	2.05	117.39	110.73
22	B	615	CLA	C11-C10-C8	2.05	122.56	115.92
23	B	619	BCR	C8-C7-C6	-2.05	121.44	127.20
25	D	402	LMG	O7-C10-O9	-2.05	118.75	123.70
22	B	608	CLA	C3A-C2A-C1A	-2.05	98.27	101.34
22	B	605	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
22	B	601	CLA	CBA-CAA-C2A	2.05	119.91	113.86
23	C	515	BCR	C15-C16-C17	-2.05	119.28	123.47
22	B	614	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
22	B	607	CLA	CMD-C2D-C1D	2.04	128.32	124.71
28	E	101	HEM	O2A-CGA-CBA	2.04	120.59	114.03
22	C	505	CLA	C9-C8-C7	2.04	118.69	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	502	LMG	O3-C3-C2	-2.04	105.62	110.35
25	C	501	LMG	O2-C2-C1	-2.04	105.08	110.05
22	B	612	CLA	CAA-C2A-C3A	2.04	118.36	112.78
23	A	408	BCR	C12-C13-C14	2.04	122.07	118.94
22	C	503	CLA	C3B-C4B-NB	-2.04	106.58	109.21
22	C	505	CLA	C9-C8-C10	2.04	118.67	111.29
22	C	513	CLA	C9-C8-C7	2.04	118.67	111.29
22	A	407	CLA	CHA-C4D-ND	2.03	136.75	132.50
25	D	403	LMG	C6-C5-C4	-2.03	108.25	113.00
22	B	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
21	D	407	PHO	CMC-C2C-C3C	2.03	128.76	124.94
22	B	614	CLA	C7-C6-C5	-2.02	107.86	113.36
22	B	606	CLA	C3D-C4D-ND	2.02	113.51	110.24
22	C	517	CLA	C10-C8-C7	2.02	122.77	112.13
22	B	601	CLA	C3D-C2D-C1D	2.02	108.58	105.83
25	I	101	LMG	C3-C4-C5	-2.02	106.64	110.24
22	B	604	CLA	C3D-C2D-C1D	2.02	108.58	105.83
22	B	606	CLA	C9-C8-C7	2.01	118.59	111.29
22	C	503	CLA	C11-C10-C8	2.01	122.43	115.92
22	C	513	CLA	CMD-C2D-C1D	2.01	128.26	124.71
22	B	610	CLA	C3D-C4D-ND	2.01	113.49	110.24
22	C	504	CLA	CMD-C2D-C1D	2.01	128.25	124.71
22	C	514	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
22	B	611	CLA	C1-O2A-CGA	-2.01	111.18	116.44
22	C	511	CLA	C6-C5-C3	2.00	118.71	113.45
22	D	409	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (48) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	403	PHO	C8
21	D	407	PHO	C8
22	A	404	CLA	ND
22	A	405	CLA	C8
22	A	406	CLA	ND
22	A	407	CLA	C8
22	A	407	CLA	ND
22	B	601	CLA	C8
22	B	601	CLA	ND
22	B	601	CLA	C2A
22	B	602	CLA	ND
22	B	603	CLA	C8

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Mol	Chain	Res	Type	Atom
22	B	603	CLA	ND
22	B	604	CLA	C3A
22	B	604	CLA	ND
22	B	606	CLA	C8
22	B	606	CLA	ND
22	B	607	CLA	C8
22	B	607	CLA	ND
22	B	608	CLA	C8
22	B	608	CLA	C3A
22	B	609	CLA	C8
22	B	609	CLA	ND
22	B	610	CLA	C8
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	C8
22	B	613	CLA	ND
22	B	614	CLA	C8
22	B	614	CLA	ND
22	B	615	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND
22	C	505	CLA	C8
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	C8
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	C	513	CLA	C8
22	C	513	CLA	ND
22	C	514	CLA	C8
22	C	514	CLA	ND
22	C	517	CLA	ND
22	D	408	CLA	ND
22	D	409	CLA	C8

All (540) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	403	PHO	O2A-C1-C2-C3
22	A	404	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	A	404	CLA	C6-C7-C8-C9
22	A	405	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C1A-C2A-CAA-CBA
22	A	406	CLA	O2A-C1-C2-C3
22	A	407	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	O2A-C1-C2-C3
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	O2A-C1-C2-C3
22	B	603	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C3A-C2A-CAA-CBA
22	B	604	CLA	C6-C7-C8-C9
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C6-C7-C8-C9
22	B	607	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	C1A-C2A-CAA-CBA
22	B	608	CLA	C3A-C2A-CAA-CBA
22	B	608	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	C11-C10-C8-C9
22	B	609	CLA	C1A-C2A-CAA-CBA
22	B	609	CLA	C3A-C2A-CAA-CBA
22	B	609	CLA	C11-C10-C8-C7
22	B	610	CLA	C1A-C2A-CAA-CBA
22	B	610	CLA	C3A-C2A-CAA-CBA
22	B	611	CLA	C1A-C2A-CAA-CBA
22	B	611	CLA	C3A-C2A-CAA-CBA
22	B	612	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C3A-C2A-CAA-CBA
22	B	613	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	505	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C3A-C2A-CAA-CBA
22	C	505	CLA	O2A-C1-C2-C3
22	C	508	CLA	C1A-C2A-CAA-CBA
22	C	509	CLA	C3A-C2A-CAA-CBA
22	C	509	CLA	C2-C3-C5-C6
22	C	509	CLA	C4-C3-C5-C6
22	C	510	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C1A-C2A-CAA-CBA
22	C	511	CLA	C11-C10-C8-C7
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C6-C7-C8-C9
22	C	513	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	C1A-C2A-CAA-CBA
22	C	514	CLA	C3A-C2A-CAA-CBA
22	C	514	CLA	C11-C10-C8-C7
22	C	517	CLA	C3A-C2A-CAA-CBA
22	D	408	CLA	C1A-C2A-CAA-CBA
22	D	408	CLA	C3A-C2A-CAA-CBA
22	D	408	CLA	O2A-C1-C2-C3
22	D	408	CLA	C11-C10-C8-C9
22	D	409	CLA	C1A-C2A-CAA-CBA
23	A	408	BCR	C37-C22-C23-C24
23	B	617	BCR	C7-C8-C9-C10
23	B	617	BCR	C7-C8-C9-C34
23	B	618	BCR	C37-C22-C23-C24
23	B	619	BCR	C11-C12-C13-C14
23	B	619	BCR	C11-C12-C13-C35
23	C	515	BCR	C7-C8-C9-C10
23	C	515	BCR	C7-C8-C9-C34
23	C	515	BCR	C36-C18-C19-C20
23	C	516	BCR	C7-C8-C9-C10
23	C	516	BCR	C7-C8-C9-C34
23	C	516	BCR	C15-C16-C17-C18
23	C	516	BCR	C21-C22-C23-C24
23	C	516	BCR	C37-C22-C23-C24
23	C	516	BCR	C23-C24-C25-C30
23	C	518	BCR	C7-C8-C9-C10
23	C	518	BCR	C7-C8-C9-C34
23	C	518	BCR	C11-C12-C13-C14
23	C	518	BCR	C21-C22-C23-C24
23	C	518	BCR	C37-C22-C23-C24
23	C	518	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	D	410	BCR	C7-C8-C9-C10
23	D	410	BCR	C7-C8-C9-C34
23	H	101	BCR	C11-C12-C13-C14
23	H	101	BCR	C11-C12-C13-C35
23	K	101	BCR	C11-C12-C13-C14
23	K	101	BCR	C11-C12-C13-C35
24	A	409	LHG	C3-O3-P-O5
22	B	601	CLA	CBD-CGD-O2D-CED
22	D	408	CLA	C2C-C3C-CAC-CBC
22	D	408	CLA	C4C-C3C-CAC-CBC
22	C	513	CLA	C2A-CAA-CBA-CGA
22	B	611	CLA	CBA-CGA-O2A-C1
23	A	408	BCR	C19-C20-C21-C22
23	B	619	BCR	C9-C10-C11-C12
23	C	516	BCR	C13-C14-C15-C16
23	C	518	BCR	C13-C14-C15-C16
25	C	501	LMG	O6-C5-C6-O5
25	C	501	LMG	C4-C5-C6-O5
22	B	605	CLA	C4-C3-C5-C6
27	D	406	PL9	C35-C34-C36-C37
22	B	605	CLA	C2-C3-C5-C6
27	D	406	PL9	C33-C34-C36-C37
22	B	611	CLA	O1A-CGA-O2A-C1
24	A	409	LHG	C1-C2-C3-O3
22	A	405	CLA	CBA-CGA-O2A-C1
23	C	518	BCR	C9-C10-C11-C12
24	A	409	LHG	O2-C2-C3-O3
21	A	403	PHO	C6-C7-C8-C9
21	A	403	PHO	C11-C10-C8-C9
22	A	405	CLA	C6-C7-C8-C9
22	A	405	CLA	C11-C12-C13-C14
22	A	407	CLA	C6-C7-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	602	CLA	C6-C7-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	B	615	CLA	C6-C7-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	C	504	CLA	C6-C7-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	C	508	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C6-C7-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	B	604	CLA	C2A-CAA-CBA-CGA
22	C	517	CLA	C2A-CAA-CBA-CGA
23	B	617	BCR	C11-C12-C13-C35
23	C	518	BCR	C11-C12-C13-C35
23	C	518	BCR	C36-C18-C19-C20
23	D	410	BCR	C37-C22-C23-C24
23	H	101	BCR	C7-C8-C9-C34
23	H	101	BCR	C37-C22-C23-C24
23	K	101	BCR	C7-C8-C9-C34
23	K	101	BCR	C37-C22-C23-C24
23	A	408	BCR	C17-C18-C19-C20
23	B	617	BCR	C11-C12-C13-C14
23	H	101	BCR	C7-C8-C9-C10
23	H	101	BCR	C17-C18-C19-C20
23	K	101	BCR	C7-C8-C9-C10
23	K	101	BCR	C17-C18-C19-C20
22	C	509	CLA	C3-C5-C6-C7
22	B	613	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	CBD-CGD-O2D-CED
22	A	404	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C10-C8-C7
22	B	607	CLA	C6-C7-C8-C10
22	B	607	CLA	C11-C10-C8-C7
22	B	610	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C11-C10-C8-C7
22	B	614	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C10-C8-C7
22	B	616	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	C	513	CLA	C6-C7-C8-C10
22	C	517	CLA	C11-C10-C8-C7
22	A	405	CLA	O1A-CGA-O2A-C1
23	C	515	BCR	C9-C10-C11-C12
23	C	518	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	H	101	BCR	C9-C10-C11-C12
23	K	101	BCR	C9-C10-C11-C12
23	K	101	BCR	C19-C20-C21-C22
22	C	504	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	O1D-CGD-O2D-CED
21	D	407	PHO	C8-C10-C11-C12
22	A	406	CLA	C5-C6-C7-C8
22	B	605	CLA	C10-C11-C12-C13
22	A	406	CLA	C2C-C3C-CAC-CBC
22	B	612	CLA	CBA-CGA-O2A-C1
25	D	403	LMG	C41-C42-C43-C44
22	B	612	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	CBA-CGA-O2A-C1
23	B	617	BCR	C9-C10-C11-C12
23	H	101	BCR	C19-C20-C21-C22
22	C	503	CLA	CBD-CGD-O2D-CED
23	H	101	BCR	C11-C10-C9-C8
23	K	101	BCR	C11-C10-C9-C8
24	A	409	LHG	C24-C25-C26-C27
25	D	403	LMG	C11-C12-C13-C14
22	B	613	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	C14-C13-C15-C16
25	D	403	LMG	C10-C11-C12-C13
22	C	509	CLA	C2A-CAA-CBA-CGA
23	A	408	BCR	C36-C18-C19-C20
23	H	101	BCR	C36-C18-C19-C20
23	K	101	BCR	C36-C18-C19-C20
23	C	515	BCR	C17-C18-C19-C20
23	D	410	BCR	C21-C22-C23-C24
23	H	101	BCR	C21-C22-C23-C24
23	K	101	BCR	C21-C22-C23-C24
22	B	612	CLA	O1A-CGA-O2A-C1
25	D	403	LMG	C37-C38-C39-C40
25	I	101	LMG	C37-C38-C39-C40
22	B	602	CLA	CBA-CGA-O2A-C1
22	A	404	CLA	C3A-C2A-CAA-CBA
22	B	601	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
25	C	501	LMG	C28-C29-C30-C31
22	B	610	CLA	C4-C3-C5-C6
22	B	606	CLA	CBA-CGA-O2A-C1
21	A	403	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C2-C3-C5-C6
22	C	513	CLA	C2-C3-C5-C6
22	C	512	CLA	CBD-CGD-O2D-CED
24	A	409	LHG	C11-C12-C13-C14
24	A	409	LHG	C15-C16-C17-C18
22	C	509	CLA	O1A-CGA-O2A-C1
25	D	403	LMG	C36-C37-C38-C39
25	D	405	LMG	C34-C35-C36-C37
23	A	408	BCR	C23-C24-C25-C30
23	C	515	BCR	C23-C24-C25-C26
23	C	515	BCR	C23-C24-C25-C30
23	C	518	BCR	C23-C24-C25-C30
23	H	101	BCR	C1-C6-C7-C8
23	H	101	BCR	C5-C6-C7-C8
23	K	101	BCR	C1-C6-C7-C8
21	A	403	PHO	C4-C3-C5-C6
22	C	505	CLA	C4-C3-C5-C6
22	A	406	CLA	C6-C7-C8-C10
22	B	610	CLA	C2-C3-C5-C6
22	B	610	CLA	C11-C10-C8-C7
22	B	611	CLA	C6-C7-C8-C10
22	B	611	CLA	C11-C10-C8-C7
22	B	612	CLA	C6-C7-C8-C10
22	C	505	CLA	C2-C3-C5-C6
22	C	505	CLA	C11-C10-C8-C7
22	D	409	CLA	C11-C10-C8-C7
22	B	606	CLA	O1A-CGA-O2A-C1
24	A	409	LHG	C12-C13-C14-C15
22	A	405	CLA	C4-C3-C5-C6
22	C	513	CLA	C4-C3-C5-C6
22	C	517	CLA	C4-C3-C5-C6
27	D	406	PL9	C45-C44-C46-C47
22	A	407	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	B	611	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	A	404	CLA	C3-C5-C6-C7
22	C	512	CLA	C2A-CAA-CBA-CGA
22	C	514	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C8-C10-C11-C12
22	B	615	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	C	509	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	517	CLA	C1A-C2A-CAA-CBA
25	D	402	LMG	C11-C10-O7-C8
25	D	404	LMG	C33-C34-C35-C36
25	I	101	LMG	C40-C41-C42-C43
22	C	511	CLA	C4-C3-C5-C6
22	C	505	CLA	C10-C11-C12-C13
25	D	403	LMG	C19-C20-C21-C22
25	D	405	LMG	C8-C7-O1-C1
22	B	602	CLA	O1A-CGA-O2A-C1
23	A	408	BCR	C20-C21-C22-C37
22	C	512	CLA	C4-C3-C5-C6
22	C	512	CLA	C2-C3-C5-C6
25	C	501	LMG	C29-C30-C31-C32
22	C	504	CLA	CBA-CGA-O2A-C1
24	A	409	LHG	C17-C18-C19-C20
21	D	407	PHO	C11-C10-C8-C7
22	A	407	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	511	CLA	C2-C3-C5-C6
22	C	517	CLA	C2-C3-C5-C6
22	A	407	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	609	CLA	C2A-CAA-CBA-CGA
22	A	406	CLA	C4C-C3C-CAC-CBC
22	C	503	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	C4-C3-C5-C6
27	D	406	PL9	C43-C44-C46-C47
27	D	406	PL9	C47-C48-C49-C51
22	B	602	CLA	C3A-C2A-CAA-CBA
22	B	603	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
25	C	501	LMG	C7-C8-C9-O8
25	C	502	LMG	C41-C42-C43-C44
22	C	504	CLA	O1A-CGA-O2A-C1
22	B	609	CLA	CBA-CGA-O2A-C1
25	D	403	LMG	O7-C8-C9-O8
25	D	404	LMG	C32-C33-C34-C35
25	D	402	LMG	O9-C10-O7-C8
22	C	512	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	C2-C3-C5-C6
22	B	615	CLA	C10-C11-C12-C13
22	C	504	CLA	C11-C10-C8-C9
25	D	403	LMG	C20-C21-C22-C23
21	A	403	PHO	C3-C5-C6-C7
23	A	408	BCR	C23-C24-C25-C26
23	C	516	BCR	C23-C24-C25-C26
23	D	410	BCR	C5-C6-C7-C8
24	A	409	LHG	C25-C26-C27-C28
25	D	402	LMG	C17-C18-C19-C20
22	A	405	CLA	C8-C10-C11-C12
21	D	407	PHO	C6-C7-C8-C10
22	B	602	CLA	C12-C13-C15-C16
22	B	606	CLA	C12-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C7
22	C	503	CLA	C6-C7-C8-C10
22	C	507	CLA	C6-C7-C8-C10
22	C	511	CLA	C11-C12-C13-C15
22	C	514	CLA	C6-C7-C8-C10
22	C	517	CLA	C6-C7-C8-C10
22	D	408	CLA	C6-C7-C8-C10
22	B	603	CLA	O1D-CGD-O2D-CED
25	I	101	LMG	C18-C19-C20-C21
23	B	619	BCR	C11-C10-C9-C34
28	E	101	HEM	C2A-CAA-CBA-CGA
21	D	407	PHO	CAD-CBD-CGD-O2D
22	A	407	CLA	CAD-CBD-CGD-O2D
22	B	603	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	B	612	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	C	508	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	D	404	LMG	C7-C8-O7-C10
25	D	405	LMG	C7-C8-O7-C10
22	D	408	CLA	C8-C10-C11-C12
25	C	502	LMG	C40-C41-C42-C43
22	B	608	CLA	CHA-CBD-CGD-O2D
22	C	506	CLA	CHA-CBD-CGD-O1D
22	C	506	CLA	CHA-CBD-CGD-O2D
23	H	101	BCR	C20-C21-C22-C23
25	C	501	LMG	O7-C8-C9-O8
22	B	609	CLA	O1A-CGA-O2A-C1
25	D	405	LMG	C38-C39-C40-C41
24	A	409	LHG	C11-C10-C9-C8
22	C	517	CLA	C6-C7-C8-C9
22	C	514	CLA	C2-C1-O2A-CGA
22	B	605	CLA	CBA-CGA-O2A-C1
24	A	409	LHG	C5-C4-O6-P
22	D	408	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	O1A-CGA-O2A-C1
22	A	405	CLA	C11-C10-C8-C7
22	B	603	CLA	C6-C7-C8-C10
22	B	603	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C12-C13-C15
22	B	612	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	B	615	CLA	C6-C7-C8-C10
22	C	506	CLA	C11-C10-C8-C7
22	C	508	CLA	C6-C7-C8-C10
22	C	509	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	D	408	CLA	C12-C13-C15-C16
22	D	409	CLA	C6-C7-C8-C10
25	D	403	LMG	C38-C39-C40-C41
25	D	405	LMG	O1-C7-C8-O7
25	D	404	LMG	C8-C7-O1-C1
22	B	612	CLA	C8-C10-C11-C12
21	D	407	PHO	C14-C13-C15-C16
22	A	406	CLA	C11-C10-C8-C9
22	B	602	CLA	C14-C13-C15-C16
22	B	606	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C11-C10-C8-C9
27	D	406	PL9	C39-C41-C42-C43
25	C	502	LMG	C36-C37-C38-C39
25	C	501	LMG	C20-C21-C22-C23
25	D	405	LMG	O6-C5-C6-O5
22	B	611	CLA	C2-C1-O2A-CGA
25	I	101	LMG	C22-C23-C24-C25
23	D	410	BCR	C1-C6-C7-C8
22	B	610	CLA	C4C-C3C-CAC-CBC
22	C	511	CLA	C2A-CAA-CBA-CGA
23	K	101	BCR	C20-C21-C22-C23
25	D	405	LMG	O1-C7-C8-C9
22	B	602	CLA	C11-C10-C8-C7
22	B	613	CLA	C2-C3-C5-C6
22	B	615	CLA	C12-C13-C15-C16
22	A	406	CLA	C6-C7-C8-C9
22	B	612	CLA	C6-C7-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	511	CLA	C11-C10-C8-C9
25	D	402	LMG	C15-C16-C17-C18
25	D	402	LMG	C29-C28-O8-C9
27	D	406	PL9	C26-C27-C28-C29
22	A	406	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBA-CGA-O2A-C1
25	D	403	LMG	C33-C34-C35-C36
23	B	618	BCR	C19-C20-C21-C22
25	D	405	LMG	C14-C15-C16-C17
25	C	502	LMG	C38-C39-C40-C41
22	B	613	CLA	C4-C3-C5-C6
25	D	405	LMG	C24-C25-C26-C27
25	D	404	LMG	C22-C23-C24-C25
22	B	605	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C3A-C2A-CAA-CBA
22	B	616	CLA	C8-C10-C11-C12
22	C	506	CLA	C4C-C3C-CAC-CBC
24	A	409	LHG	C33-C34-C35-C36
25	D	405	LMG	C21-C22-C23-C24
25	C	501	LMG	C16-C17-C18-C19
22	A	405	CLA	C11-C10-C8-C9
22	B	608	CLA	C6-C7-C8-C9
22	B	604	CLA	C4C-C3C-CAC-CBC
28	E	101	HEM	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	611	CLA	O2A-C1-C2-C3
25	I	101	LMG	C24-C25-C26-C27
25	C	501	LMG	C7-C8-O7-C10
22	B	601	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
25	D	405	LMG	C12-C13-C14-C15
22	B	610	CLA	CAA-CBA-CGA-O2A
22	A	407	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C8-C10-C11-C12
28	E	101	HEM	CAD-CBD-CGD-O2D
23	B	617	BCR	C19-C20-C21-C22
22	B	601	CLA	C4-C3-C5-C6
22	C	505	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
23	H	101	BCR	C23-C24-C25-C26
23	K	101	BCR	C5-C6-C7-C8
22	C	513	CLA	C10-C11-C12-C13
25	C	501	LMG	C19-C20-C21-C22
22	B	608	CLA	CBD-CGD-O2D-CED
24	A	409	LHG	C27-C28-C29-C30
22	B	611	CLA	C13-C15-C16-C17
27	D	406	PL9	C29-C31-C32-C33
27	D	406	PL9	C34-C36-C37-C38
21	D	407	PHO	C12-C13-C15-C16
22	C	509	CLA	C13-C15-C16-C17
22	B	603	CLA	C11-C10-C8-C9
22	B	609	CLA	C6-C7-C8-C9
22	B	610	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C10-C8-C9
22	D	408	CLA	C14-C13-C15-C16
25	D	403	LMG	C31-C32-C33-C34
22	C	508	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	CAA-CBA-CGA-O2A
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	C	514	CLA	CAD-CBD-CGD-O2D
22	D	408	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	C	501	LMG	C9-C8-O7-C10
22	C	510	CLA	CAA-CBA-CGA-O2A
22	C	511	CLA	CAA-CBA-CGA-O2A
22	B	611	CLA	CBD-CGD-O2D-CED
25	C	502	LMG	C21-C22-C23-C24
21	D	407	PHO	C2C-C3C-CAC-CBC
22	A	404	CLA	C4C-C3C-CAC-CBC
22	B	613	CLA	O2A-C1-C2-C3
22	C	507	CLA	O2A-C1-C2-C3
22	C	513	CLA	O2A-C1-C2-C3
22	B	606	CLA	C2A-CAA-CBA-CGA
24	A	409	LHG	C35-C36-C37-C38
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
25	C	502	LMG	O8-C28-C29-C30
22	B	602	CLA	CAA-CBA-CGA-O2A
25	I	101	LMG	O7-C10-C11-C12
22	B	608	CLA	C2A-CAA-CBA-CGA
25	D	403	LMG	C21-C22-C23-C24
25	D	402	LMG	C20-C21-C22-C23
22	C	508	CLA	C11-C10-C8-C7
25	D	405	LMG	C42-C43-C44-C45
22	B	601	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C10-C8-C9
22	B	613	CLA	C11-C10-C8-C9
22	B	613	CLA	C14-C13-C15-C16
22	B	616	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
25	D	402	LMG	C35-C36-C37-C38
22	B	604	CLA	O1A-CGA-O2A-C1
28	E	101	HEM	CAA-CBA-CGA-O2A
22	B	604	CLA	C2C-C3C-CAC-CBC
25	D	404	LMG	C37-C38-C39-C40
25	D	403	LMG	C16-C17-C18-C19
25	C	501	LMG	C31-C32-C33-C34
22	C	510	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	CAA-CBA-CGA-O1A
23	B	618	BCR	C22-C23-C24-C25
22	A	406	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	CAA-CBA-CGA-O1A
25	C	502	LMG	O10-C28-C29-C30
23	K	101	BCR	C23-C24-C25-C26
25	D	404	LMG	C18-C19-C20-C21
22	B	607	CLA	C2A-CAA-CBA-CGA
22	C	513	CLA	O1D-CGD-O2D-CED
24	A	409	LHG	C7-C8-C9-C10
22	C	514	CLA	C4-C3-C5-C6
22	B	604	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	C3-C5-C6-C7
22	B	603	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C12-C13-C14
22	C	517	CLA	C11-C10-C8-C9
25	D	404	LMG	O8-C28-C29-C30
22	A	405	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
28	E	101	HEM	CAA-CBA-CGA-O1A
22	B	603	CLA	CAA-CBA-CGA-O2A
22	B	607	CLA	CAA-CBA-CGA-O2A
22	C	505	CLA	CAA-CBA-CGA-O2A
25	I	101	LMG	O8-C28-C29-C30
22	B	616	CLA	C5-C6-C7-C8
22	C	514	CLA	CAA-CBA-CGA-O2A
22	B	602	CLA	CAA-CBA-CGA-O1A
22	B	603	CLA	CAA-CBA-CGA-O1A
22	C	517	CLA	CAA-CBA-CGA-O2A
25	I	101	LMG	O9-C10-C11-C12
25	D	403	LMG	C12-C13-C14-C15
25	D	405	LMG	C23-C24-C25-C26

There are no ring outliers.

45 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	515	BCR	14	0
23	B	618	BCR	2	0
22	A	406	CLA	2	0

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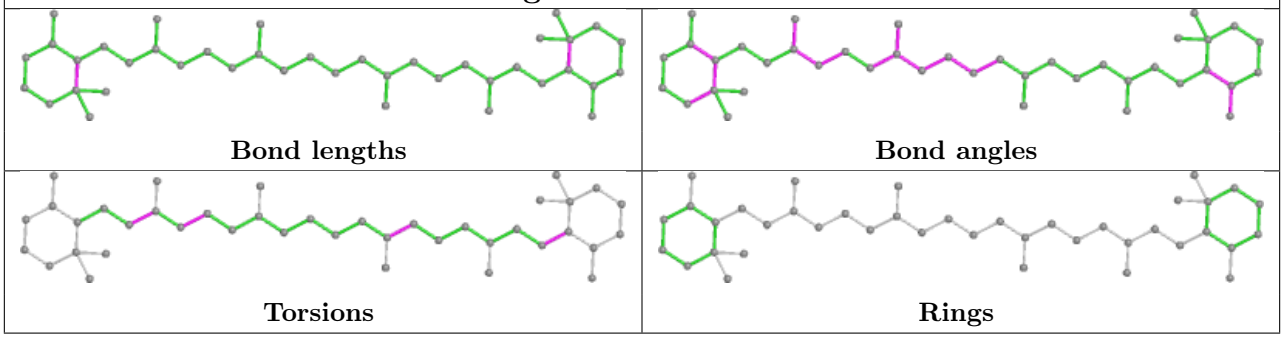
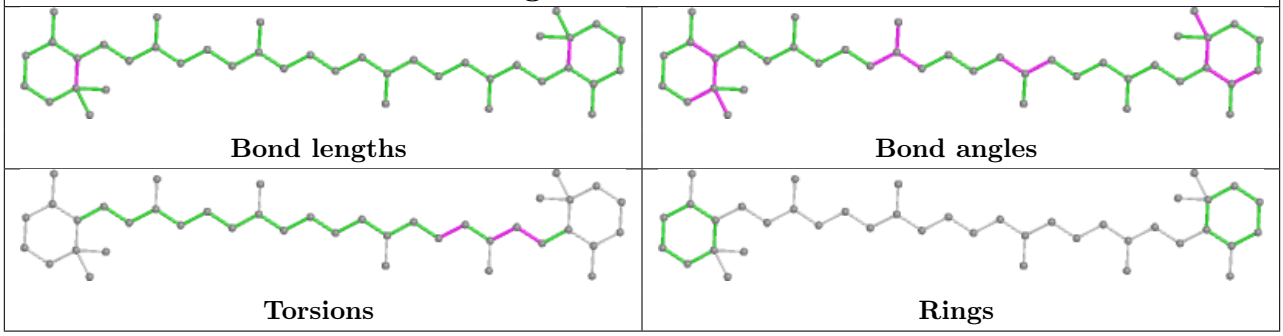
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	403	LMG	1	0
22	B	605	CLA	1	0
22	B	607	CLA	2	0
22	C	504	CLA	2	0
22	C	512	CLA	12	0
22	C	506	CLA	1	0
22	A	405	CLA	5	0
23	C	518	BCR	2	0
23	C	516	BCR	4	0
22	B	612	CLA	3	0
22	D	408	CLA	2	0
23	H	101	BCR	18	0
22	B	610	CLA	3	0
23	B	617	BCR	1	0
22	C	513	CLA	3	0
22	C	514	CLA	1	0
23	B	619	BCR	2	0
22	B	611	CLA	3	0
22	D	409	CLA	6	0
22	B	608	CLA	5	0
25	D	404	LMG	1	0
22	B	606	CLA	2	0
21	A	403	PHO	1	0
27	D	406	PL9	4	0
22	B	613	CLA	2	0
22	C	505	CLA	3	0
22	B	604	CLA	2	0
23	K	101	BCR	24	0
22	B	615	CLA	1	0
22	C	510	CLA	11	0
25	D	402	LMG	1	0
22	B	603	CLA	3	0
23	A	408	BCR	2	0
22	C	503	CLA	4	0
22	B	614	CLA	2	0
22	B	616	CLA	1	0
22	C	509	CLA	4	0
22	B	601	CLA	5	0
22	C	517	CLA	4	0
22	C	511	CLA	4	0
22	B	609	CLA	8	0
22	A	407	CLA	2	0

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

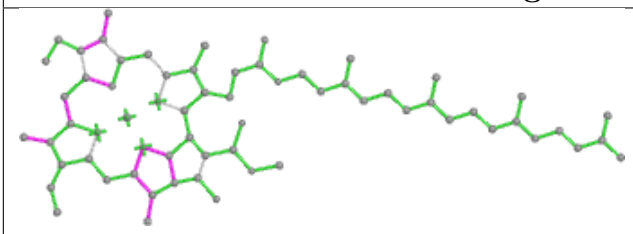
Ligand BCR C 515



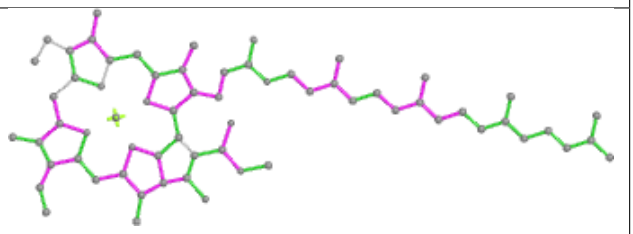
Ligand BCR B 618



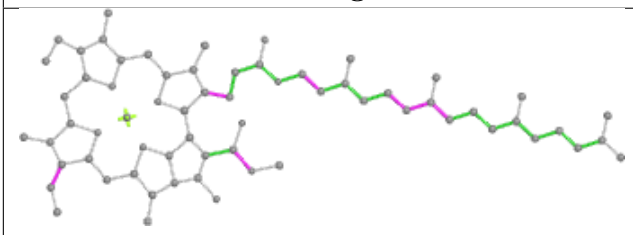
Ligand CLA A 406



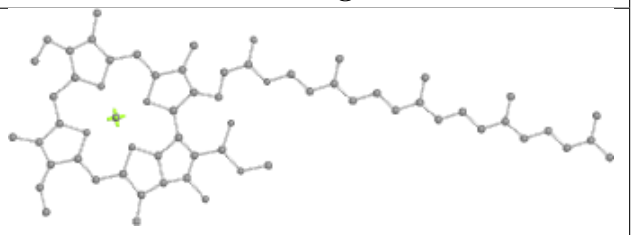
Bond lengths



Bond angles

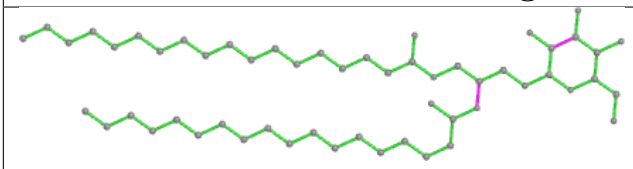


Torsions

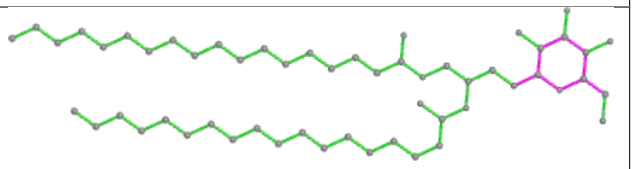


Rings

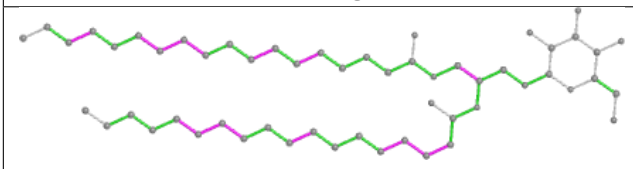
Ligand LMG D 403



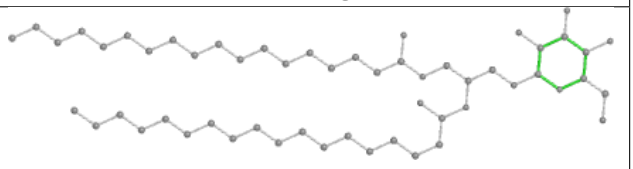
Bond lengths



Bond angles

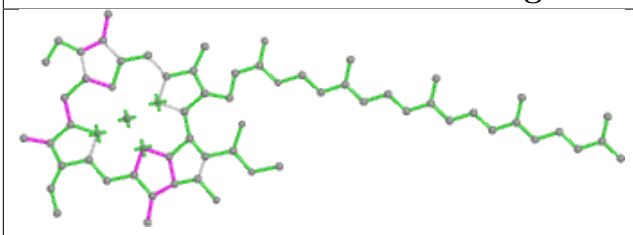


Torsions

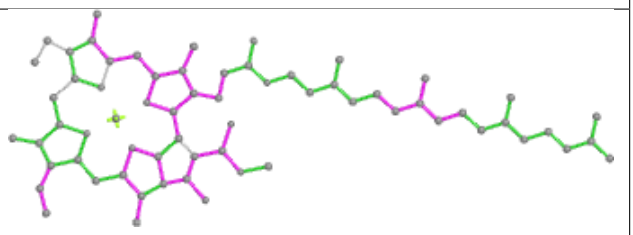


Rings

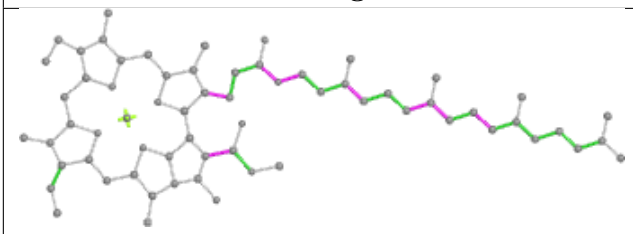
Ligand CLA B 605



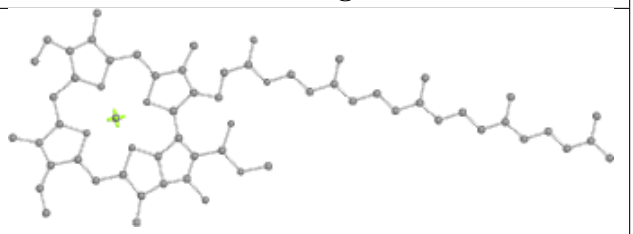
Bond lengths



Bond angles

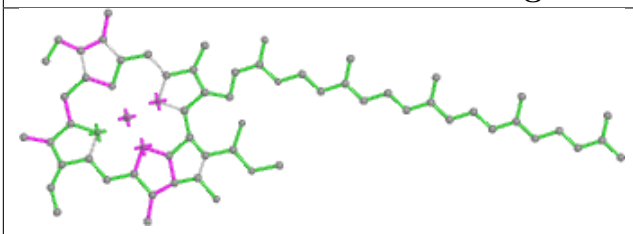


Torsions

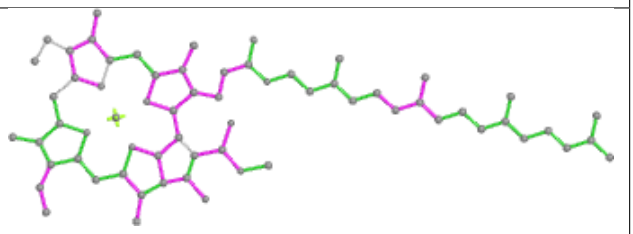


Rings

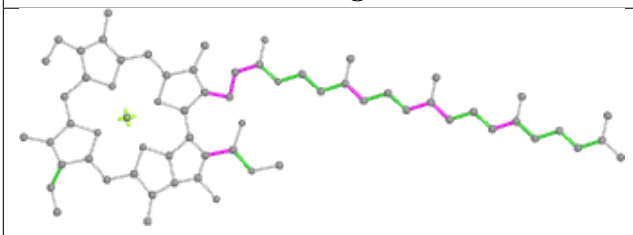
Ligand CLA B 607



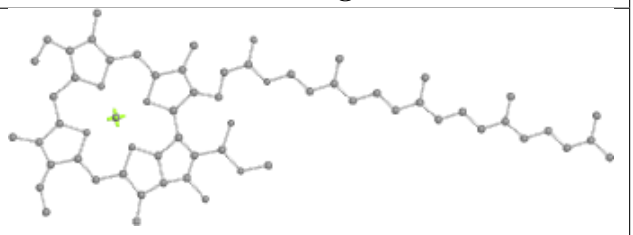
Bond lengths



Bond angles

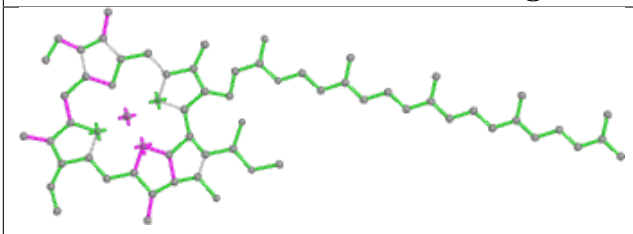


Torsions



Rings

Ligand CLA C 504



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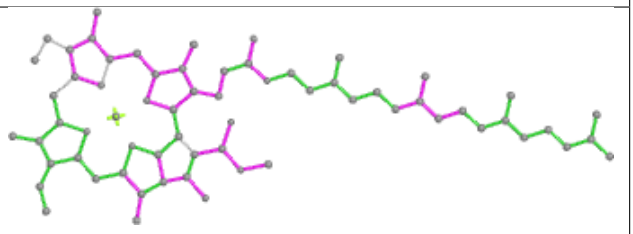
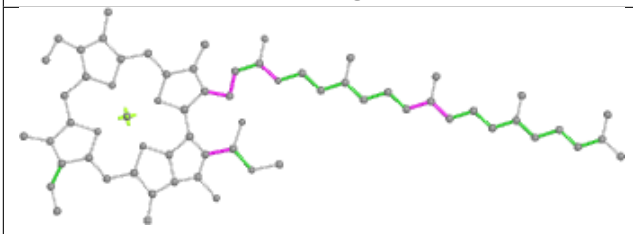
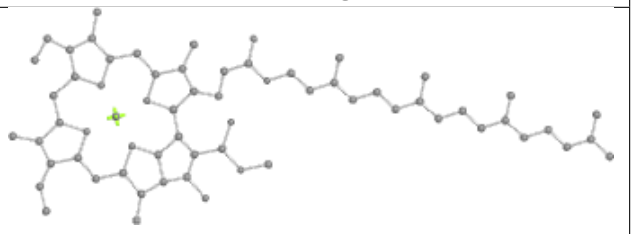


Bond angles

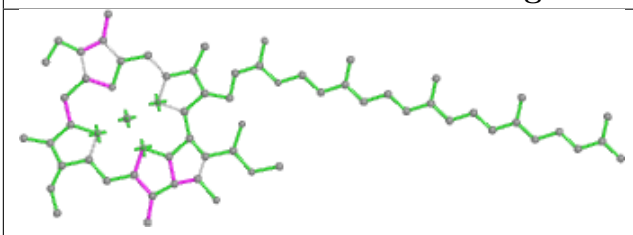


Torsions

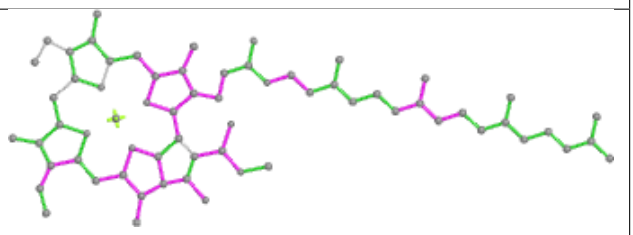


Rings

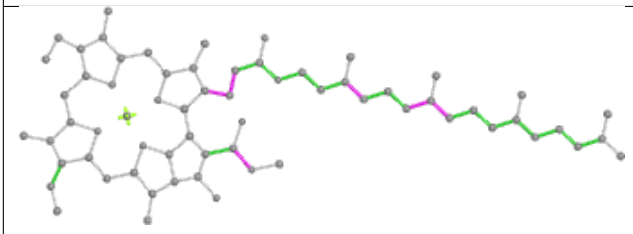
Ligand CLA C 512



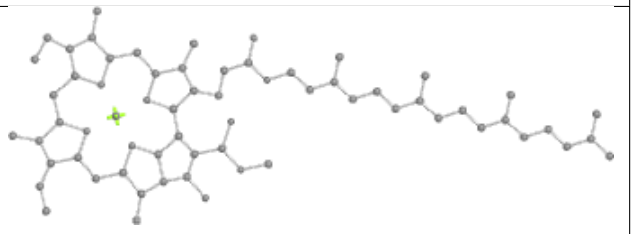
Bond lengths



Bond angles

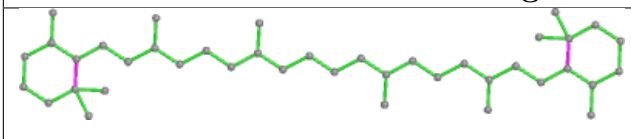


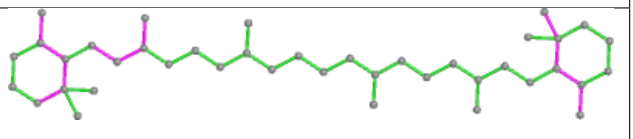
Torsions

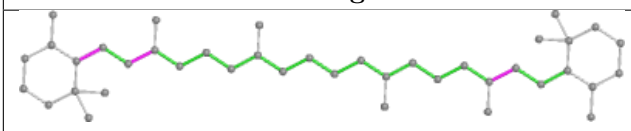


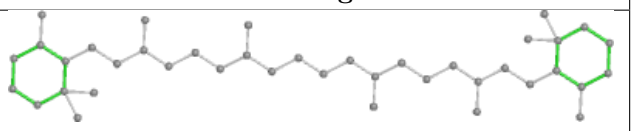
Rings

Ligand BCR D 410

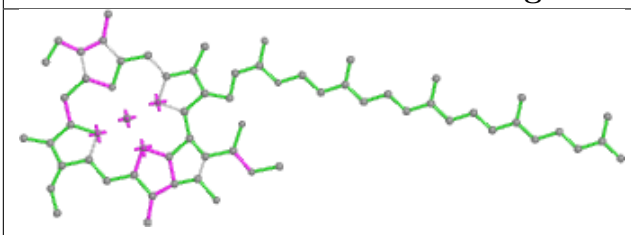

Bond lengths

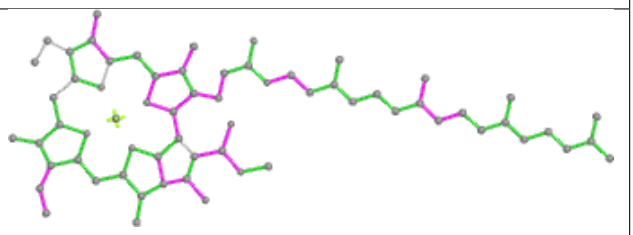

Bond angles

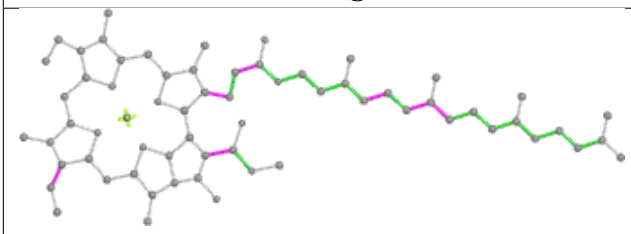

Torsions

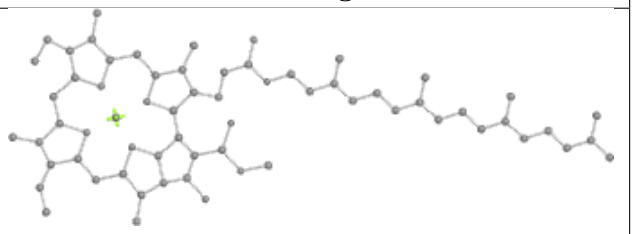

Rings

Ligand CLA C 506

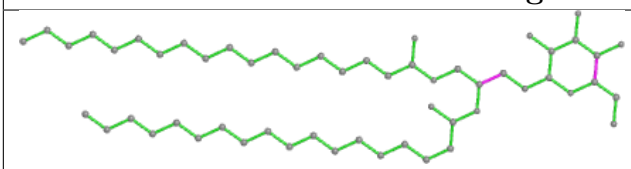

Bond lengths

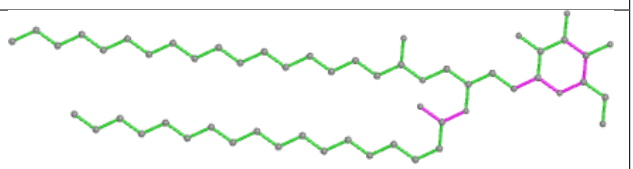

Bond angles

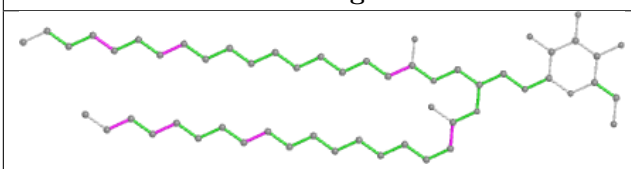

Torsions

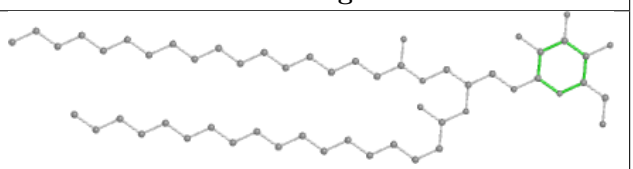

Rings

Ligand LMG I 101

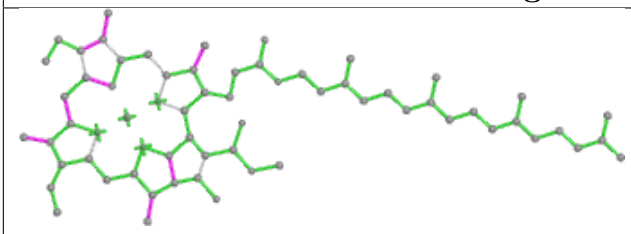

Bond lengths


Bond angles

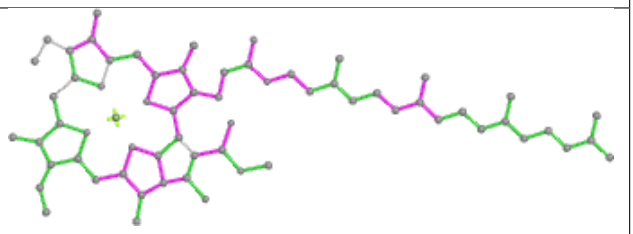

Torsions


Rings

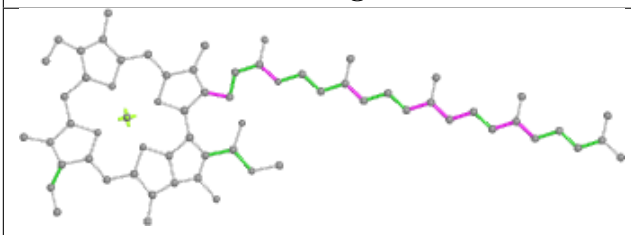
Ligand CLA A 405



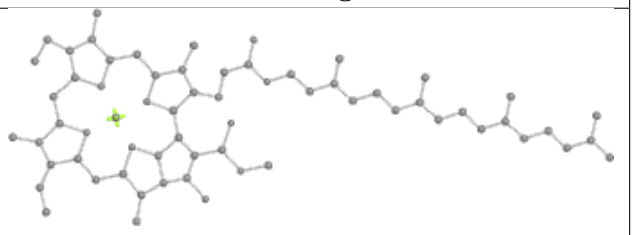
Bond lengths



Bond angles

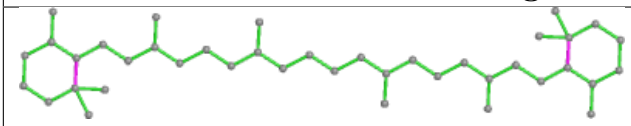


Torsions

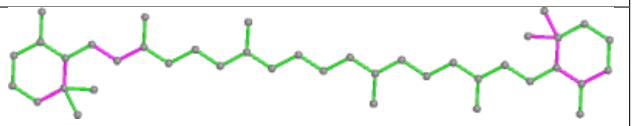


Rings

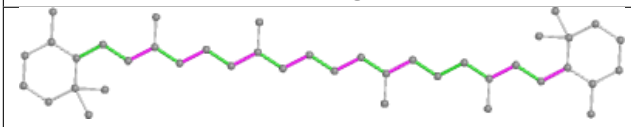
Ligand BCR C 518



Bond lengths



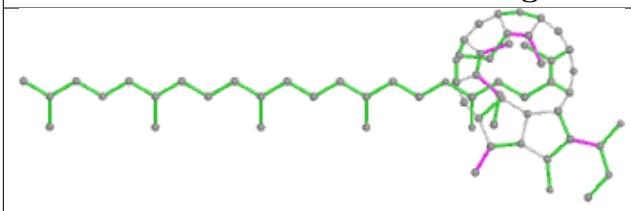
Bond angles



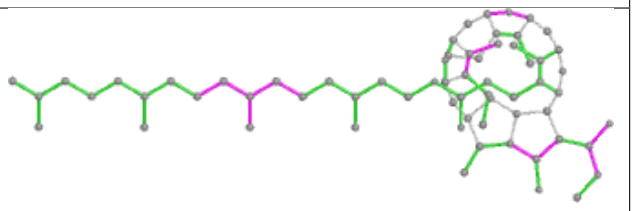
Torsions

Rings

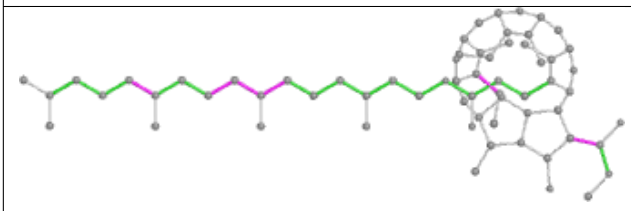
Ligand PHO D 407



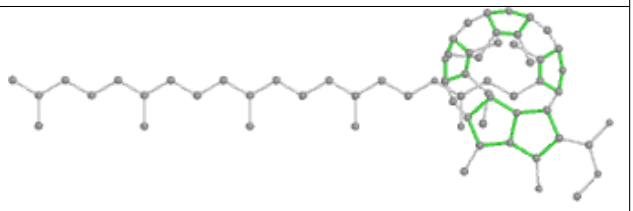
Bond lengths



Bond angles

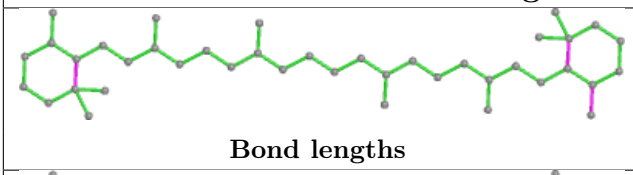


Torsions

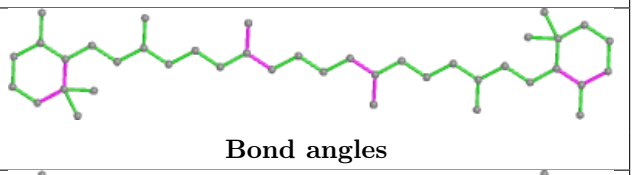


Rings

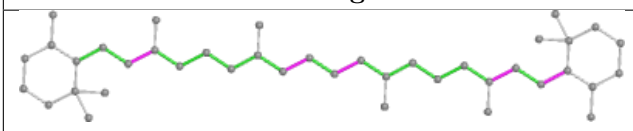
Ligand BCR C 516



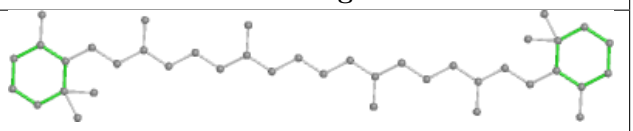
Bond lengths



Bond angles

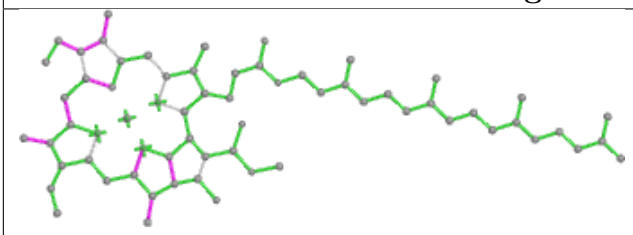


Torsions

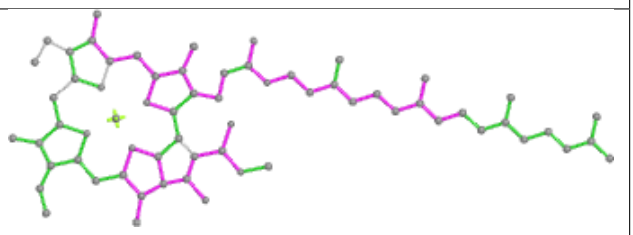


Rings

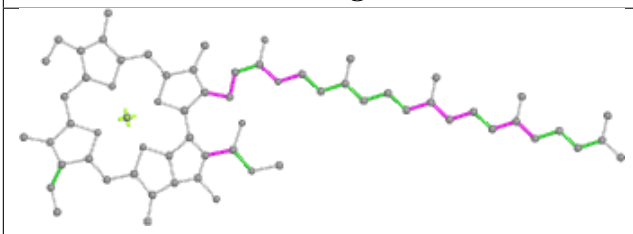
Ligand CLA B 612



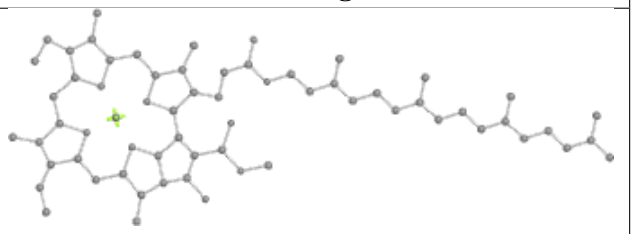
Bond lengths



Bond angles

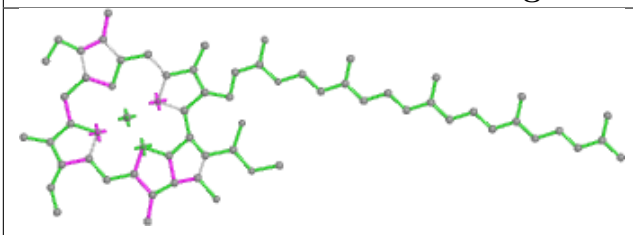


Torsions



Rings

Ligand CLA D 408



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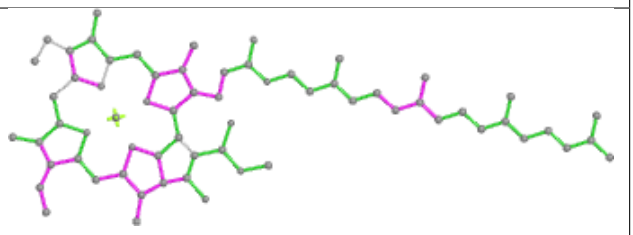
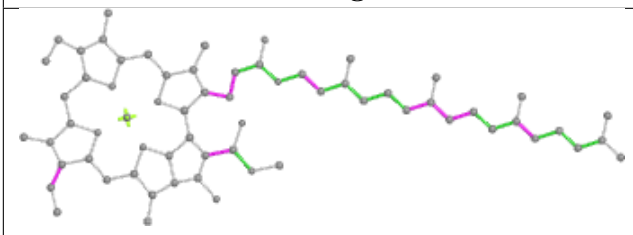
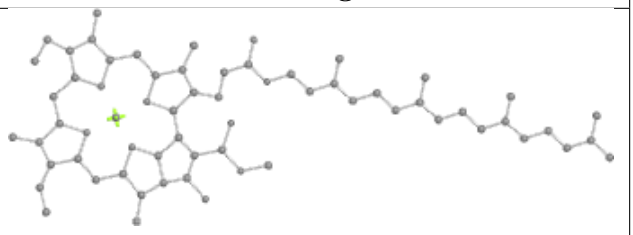


Bond angles

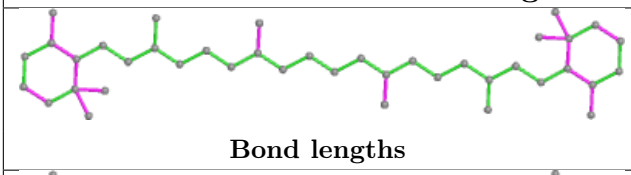


Torsions

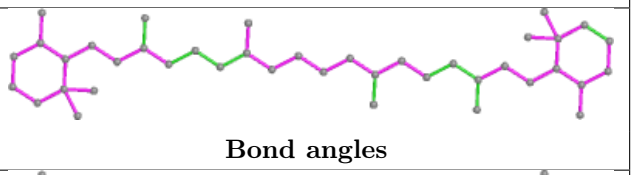


Rings

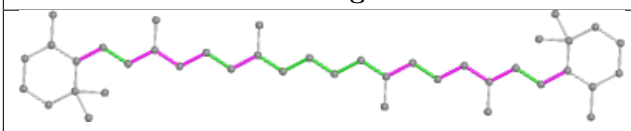
Ligand BCR H 101



Bond lengths



Bond angles



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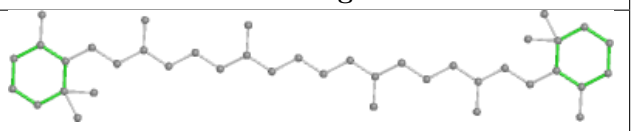
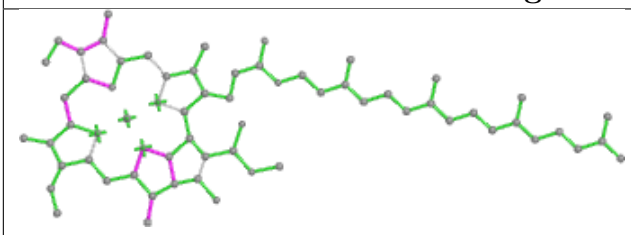
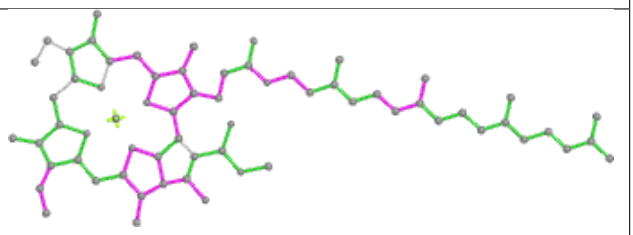


Rings

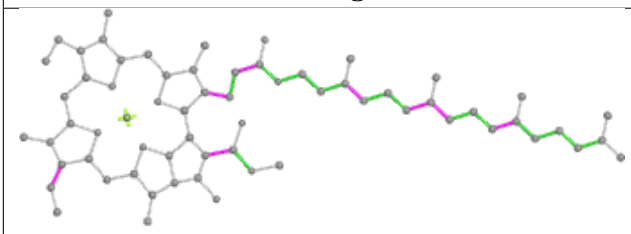
Ligand CLA B 610



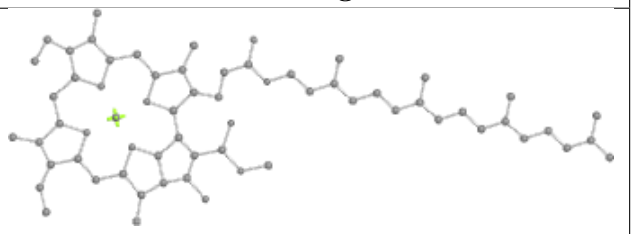
Bond lengths



Bond angles

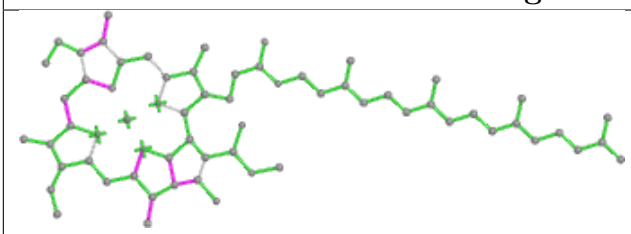


Torsions



Rings

Ligand CLA C 508



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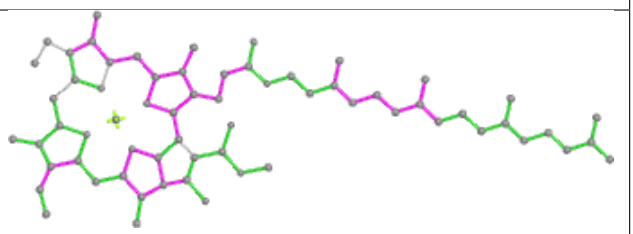
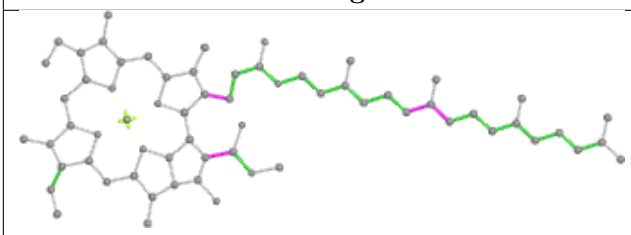


Bond angles



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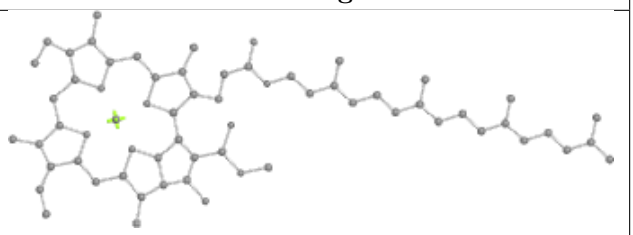
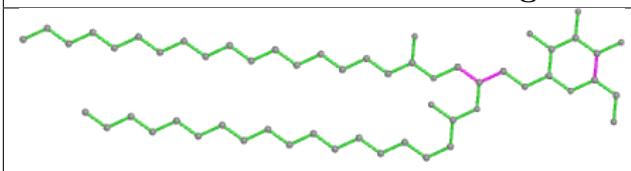
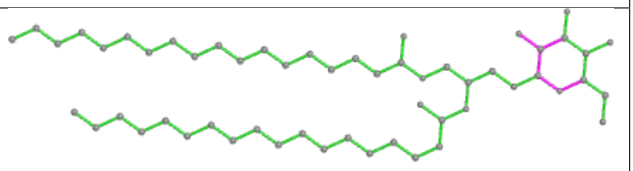


Rings

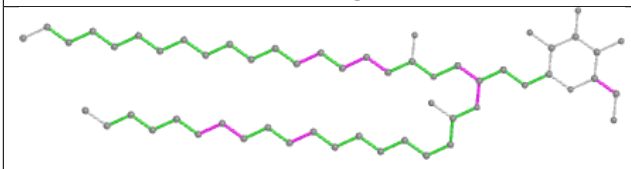
Ligand LMG C 501



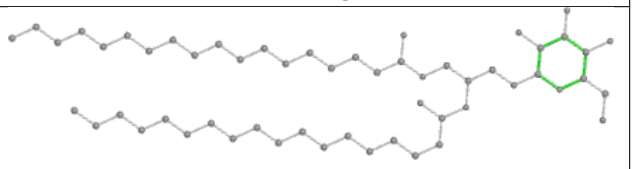
Bond lengths



Bond angles

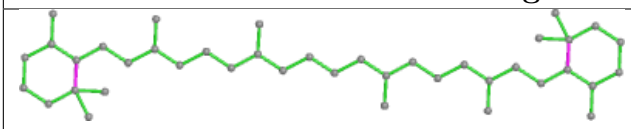


Torsions

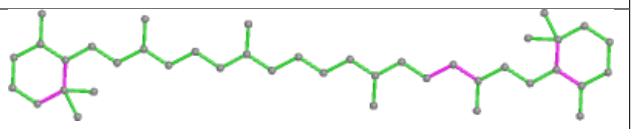


Rings

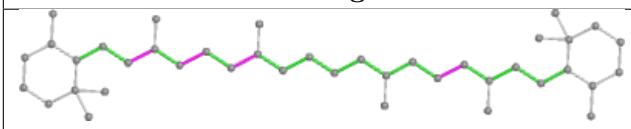
Ligand BCR B 617



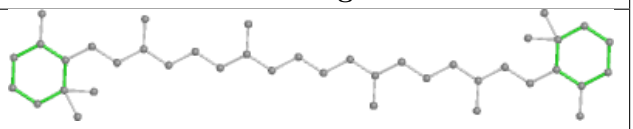
Bond lengths



Bond angles

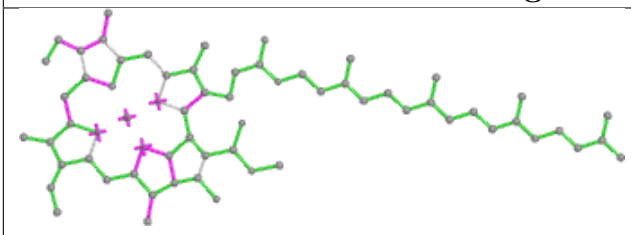


Torsions



Rings

Ligand CLA C 513



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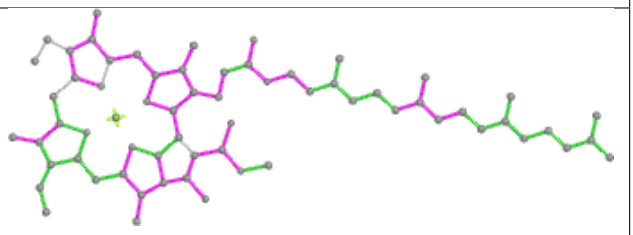
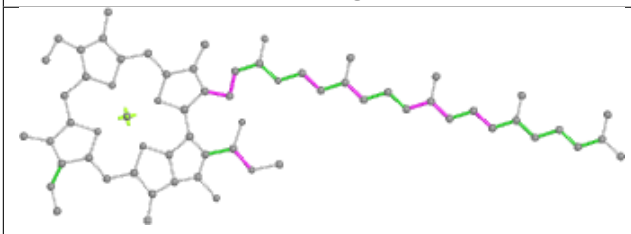
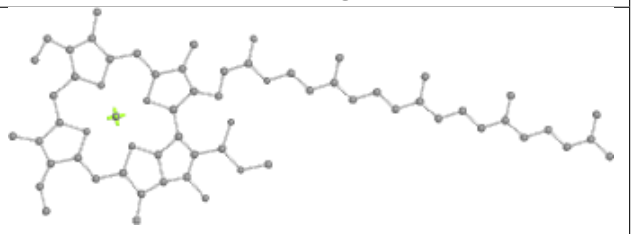


Bond angles

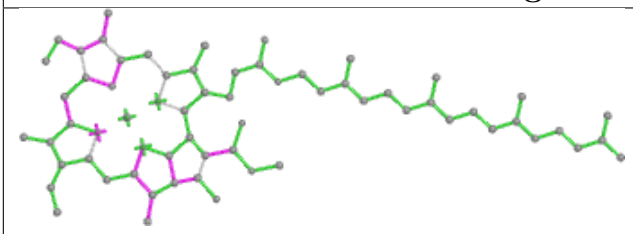


Torsions



Rings

Ligand CLA C 514



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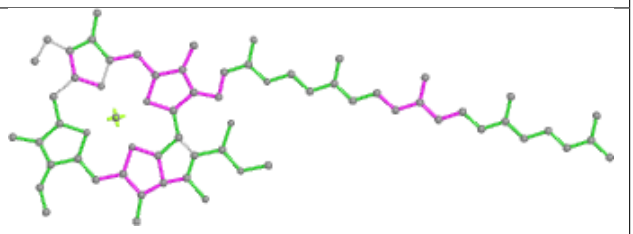
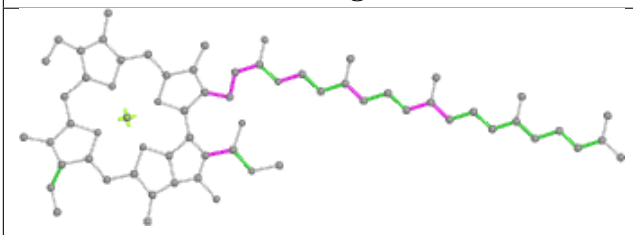
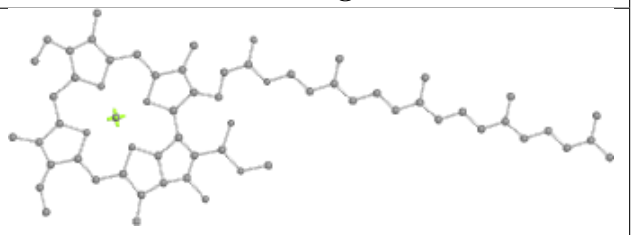


Bond angles

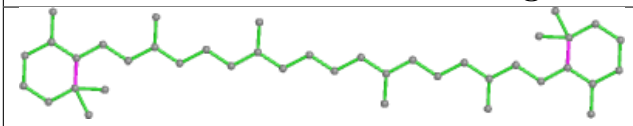


Torsions

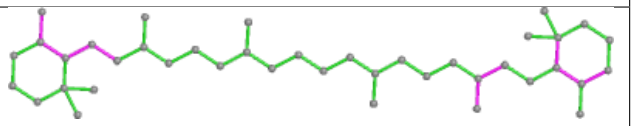


Rings

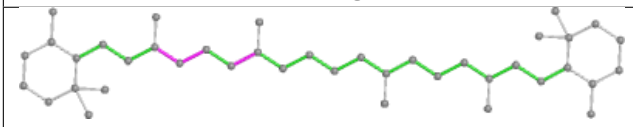
Ligand BCR B 619



Bond lengths



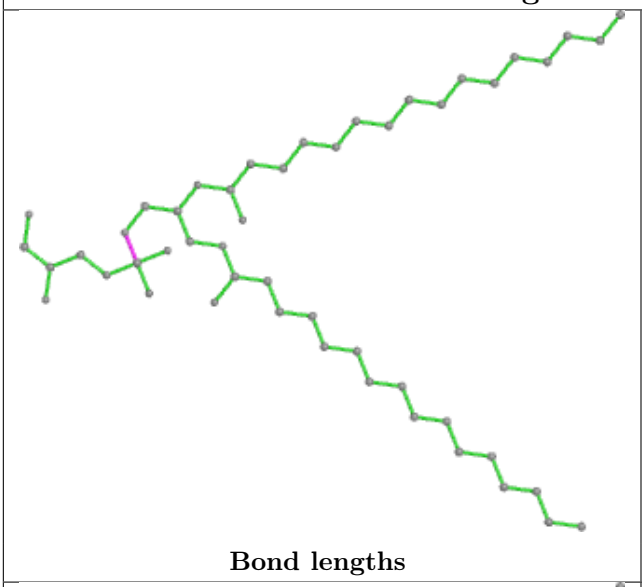
Bond angles



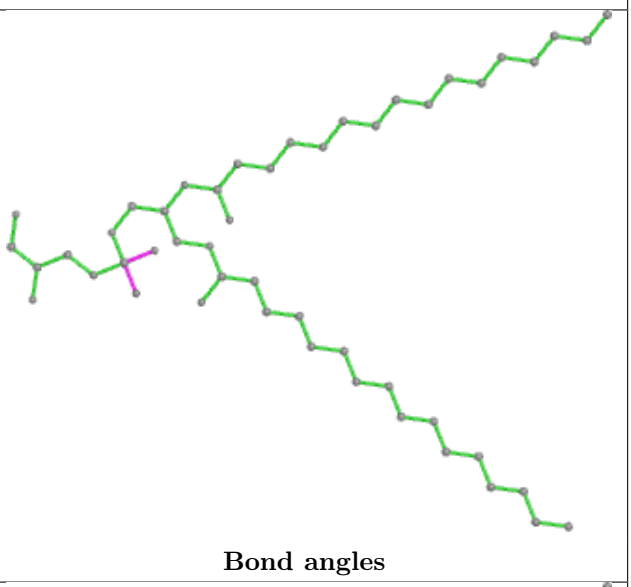
Torsions

Rings

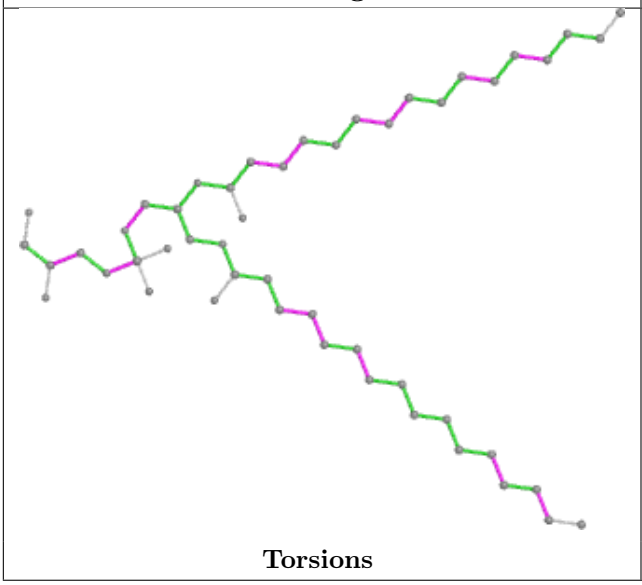
Ligand LHG A 409



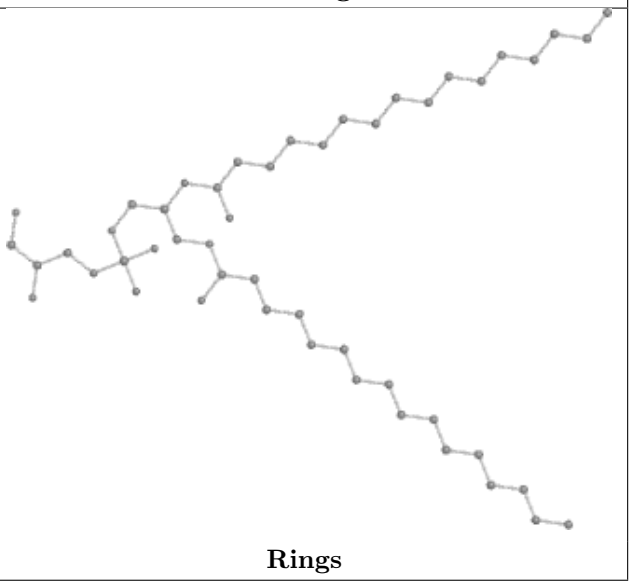
Bond lengths



Bond angles

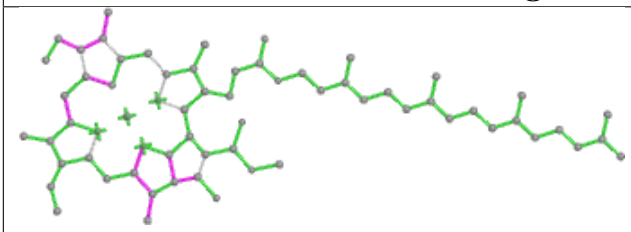


Torsions

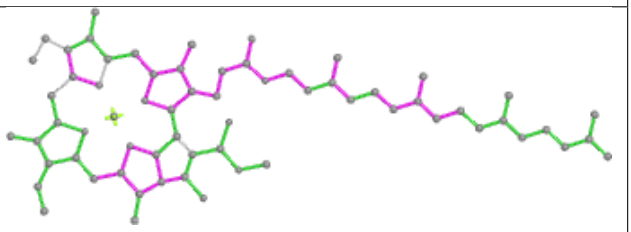


Rings

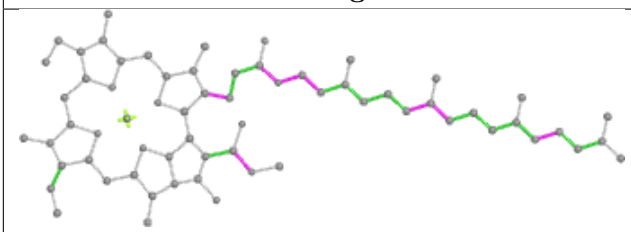
Ligand CLA B 611



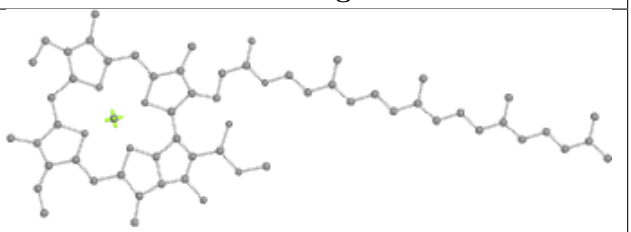
Bond lengths



Bond angles

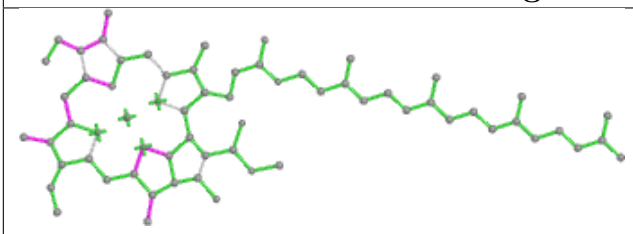


Torsions

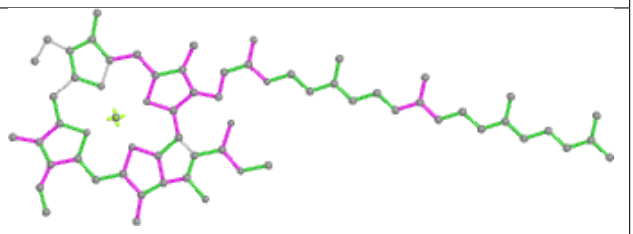


Rings

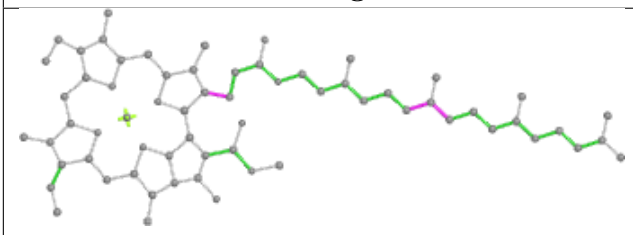
Ligand CLA D 409



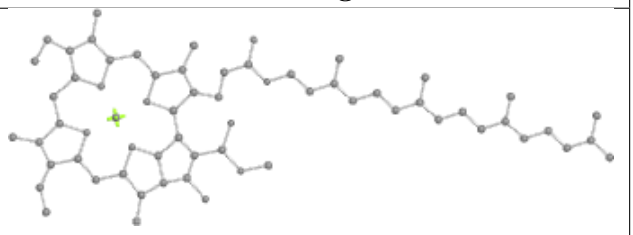
Bond lengths



Bond angles

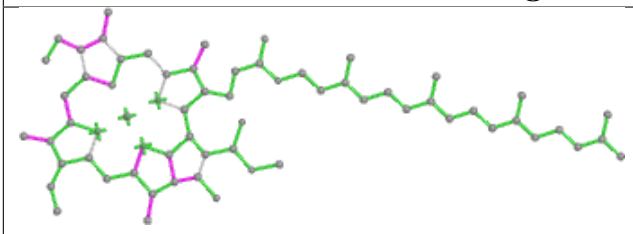


Torsions

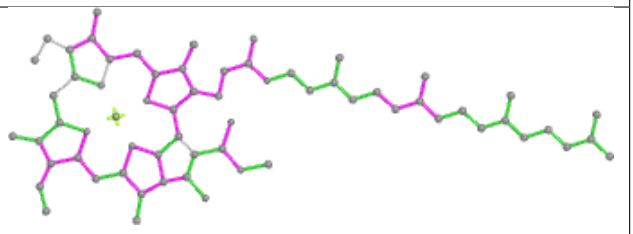


Rings

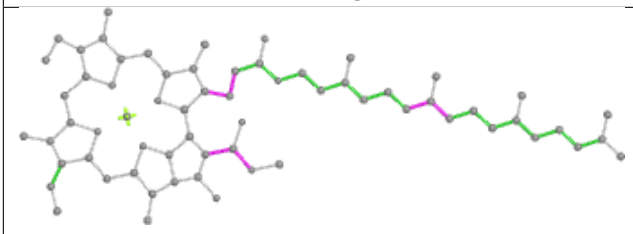
Ligand CLA B 608



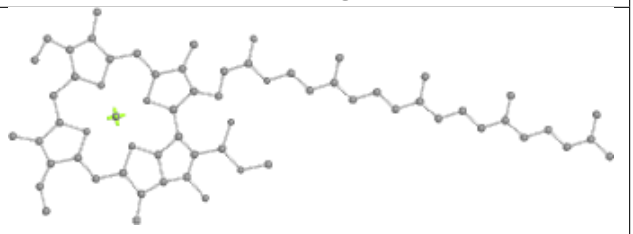
Bond lengths



Bond angles

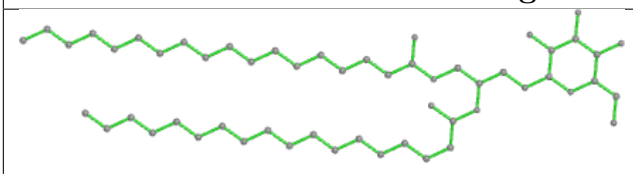


Torsions

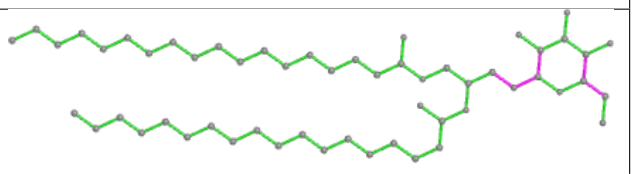


Rings

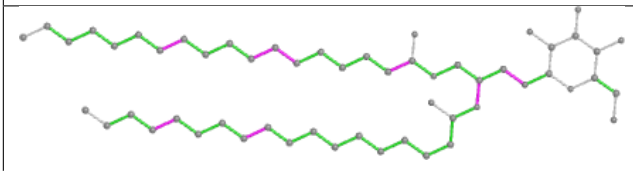
Ligand LMG D 404



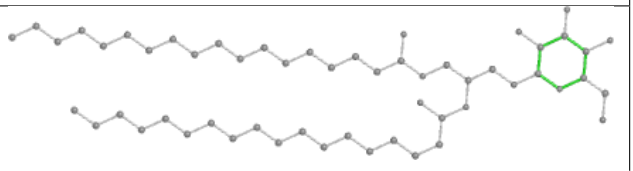
Bond lengths



Bond angles

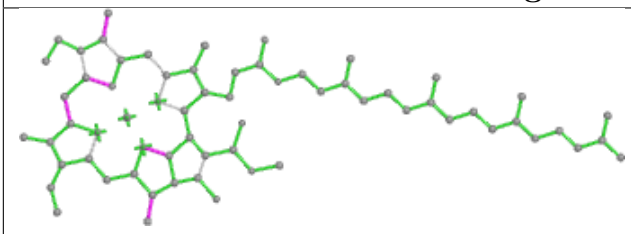


Torsions

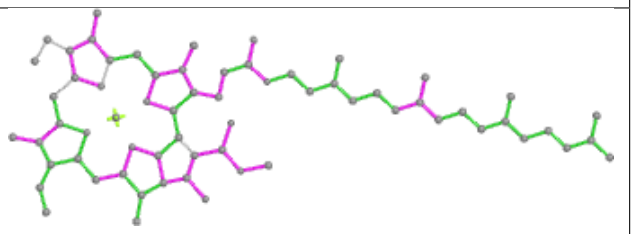


Rings

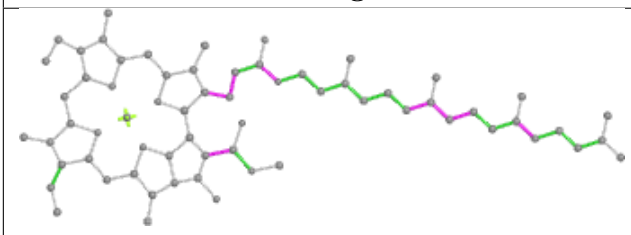
Ligand CLA B 606



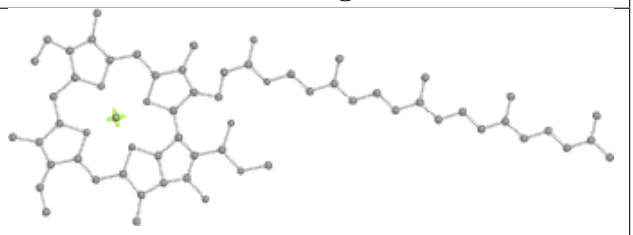
Bond lengths



Bond angles

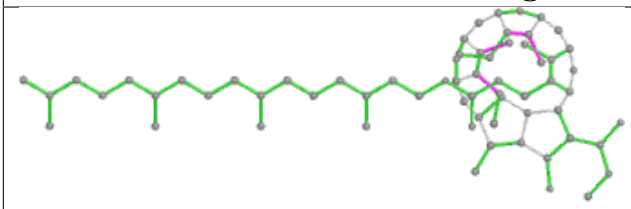


Torsions



Rings

Ligand PHO A 403



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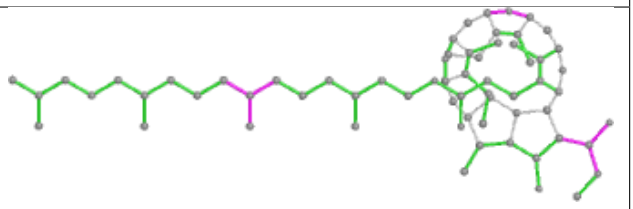
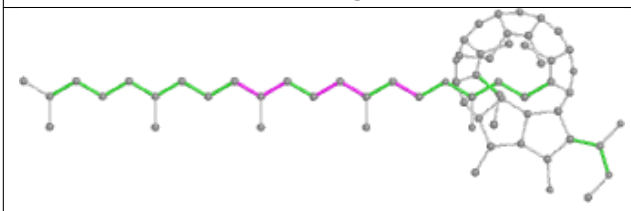
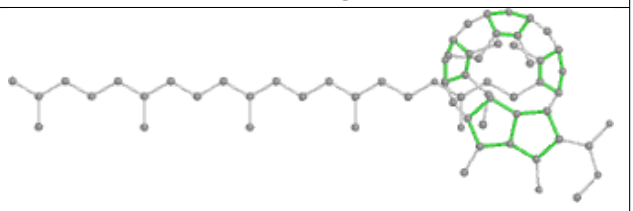


Bond angles

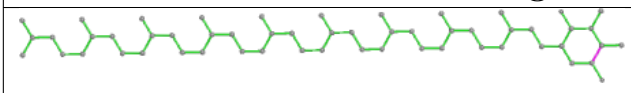


Torsions

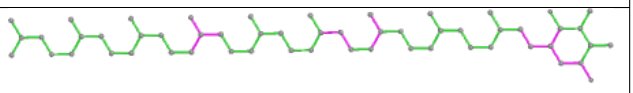


Rings

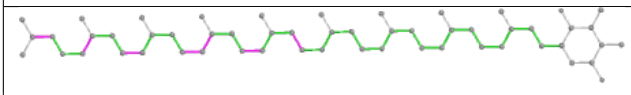
Ligand PL9 D 406



Bond lengths



Bond angles



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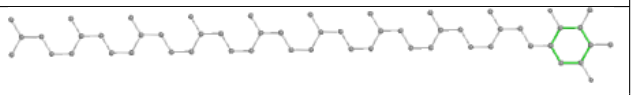
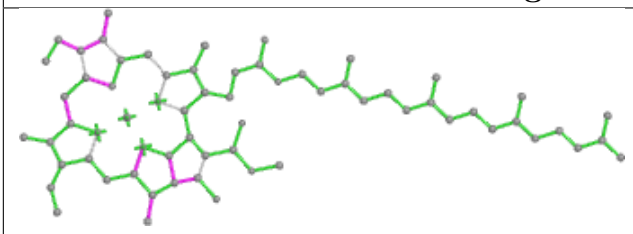


Rings

Ligand CLA B 613



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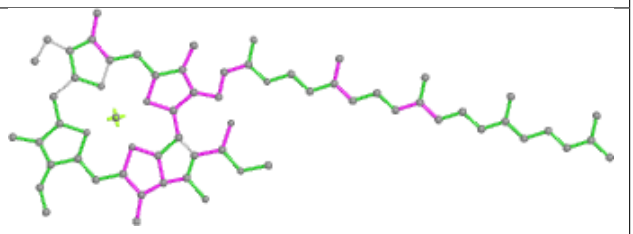
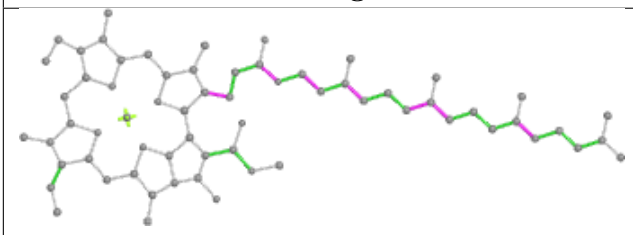
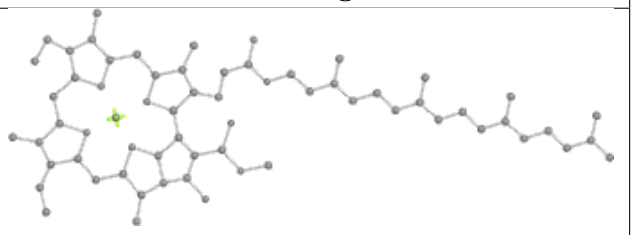


Bond angles

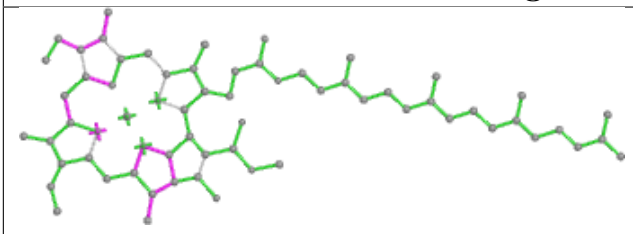


Torsions



Rings

Ligand CLA C 505



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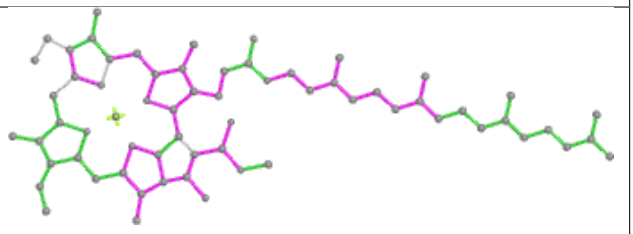
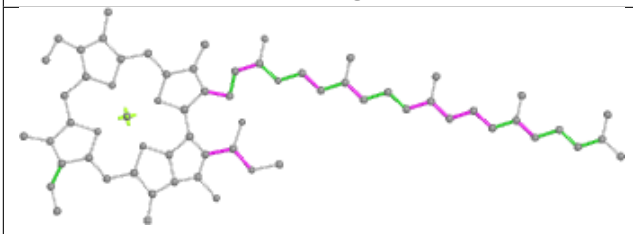


Bond angles



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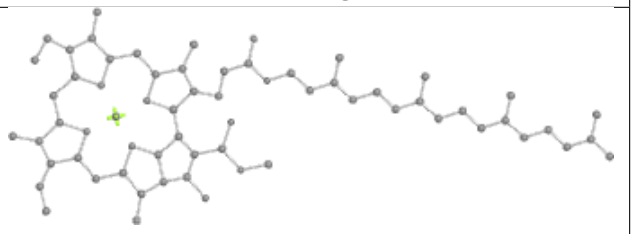
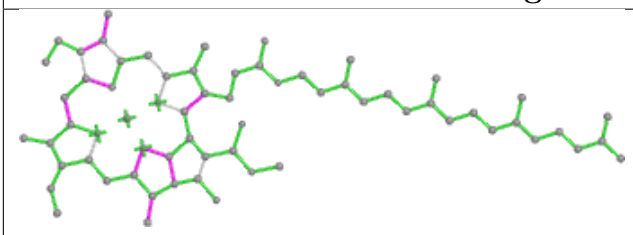
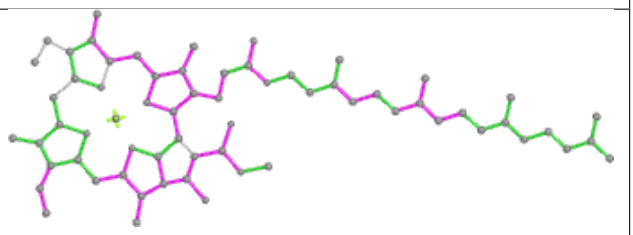


Rings

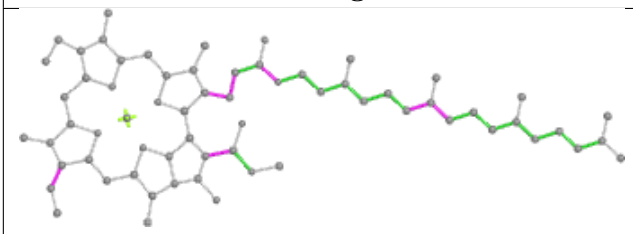
Ligand CLA B 604



Bond lengths



Bond angles



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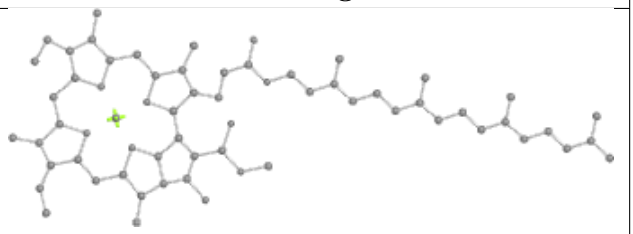
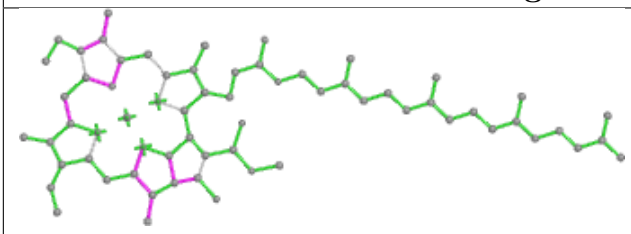


Rings

Ligand CLA C 507



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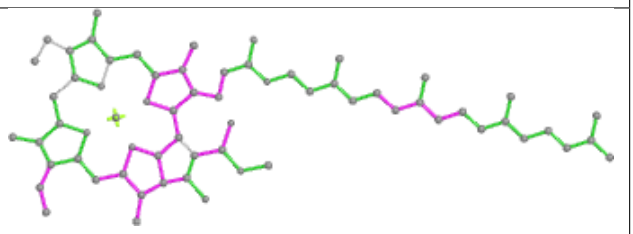
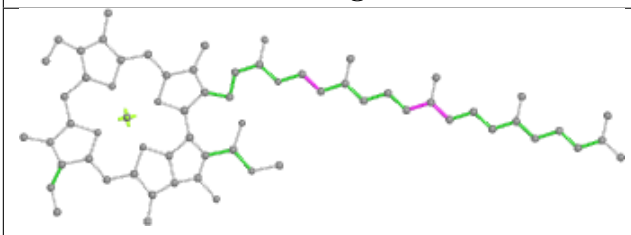
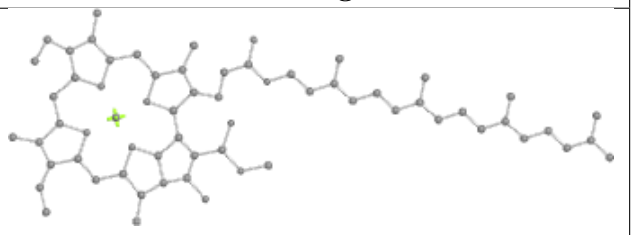


Bond angles

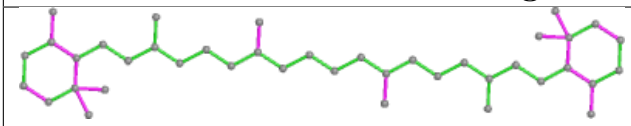


Torsions

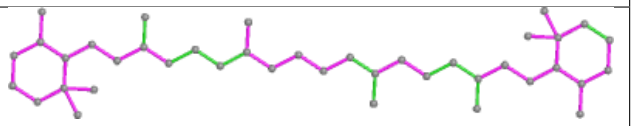


Rings

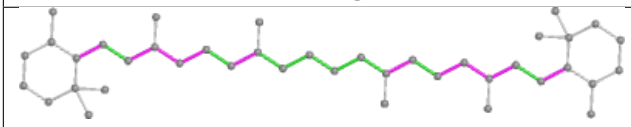
Ligand BCR K 101



Bond lengths



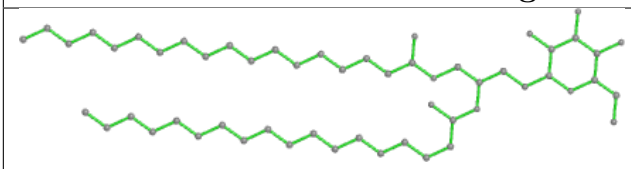
Bond angles



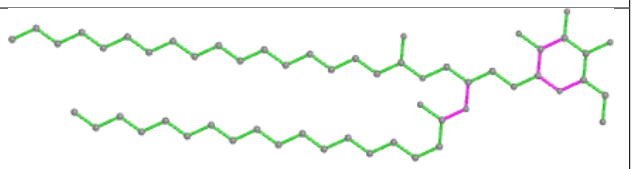
Torsions

Rings

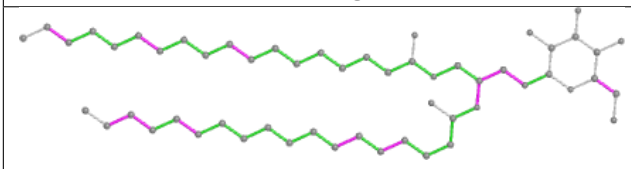
Ligand LMG D 405



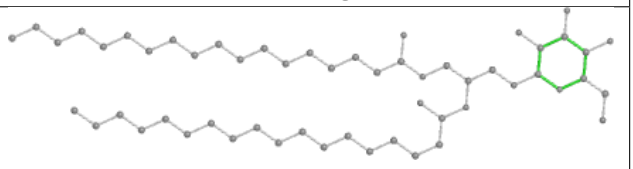
Bond lengths



Bond angles

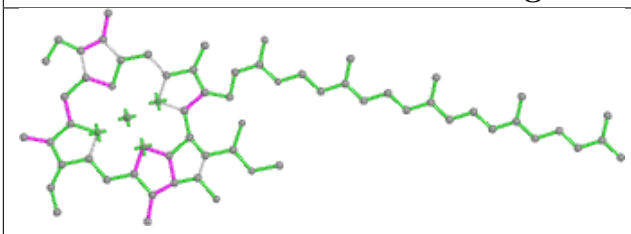


Torsions



Rings

Ligand CLA B 615



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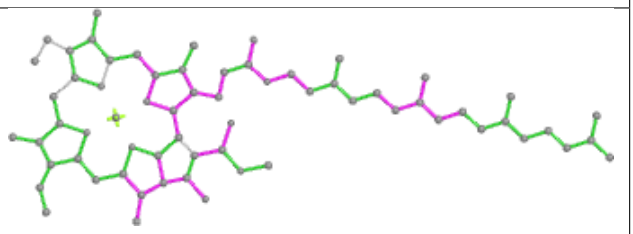
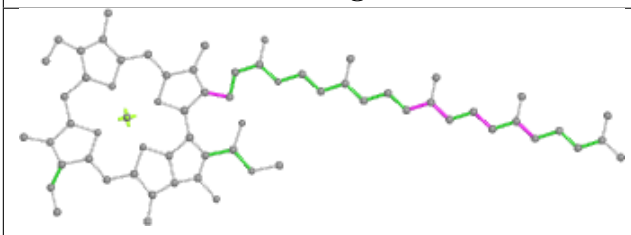


Bond angles



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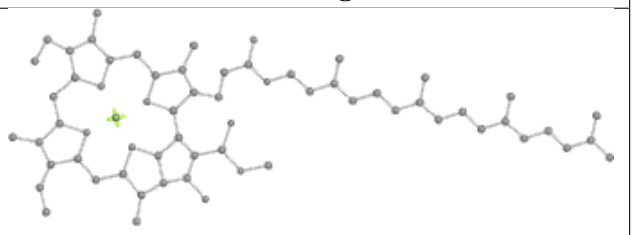
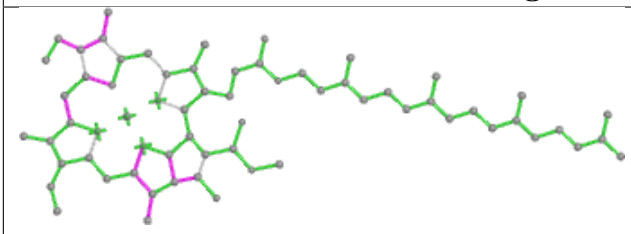
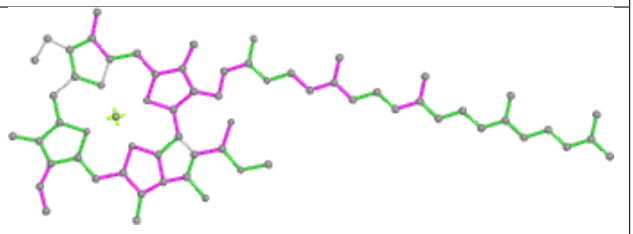


Rings

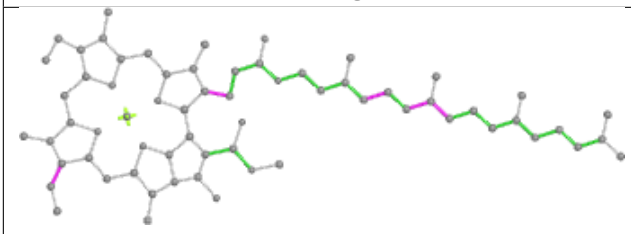
Ligand CLA A 404



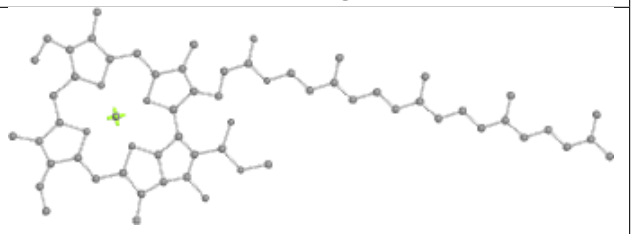
Bond lengths



Bond angles

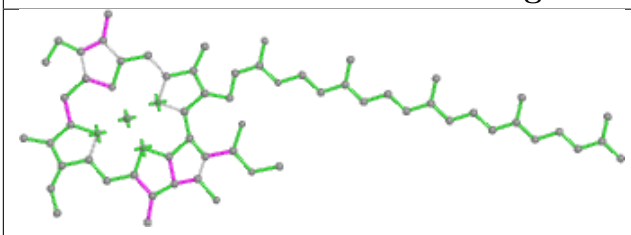


Torsions

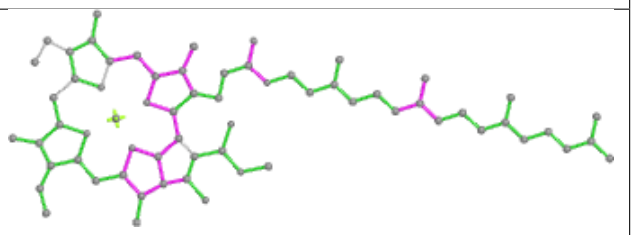


Rings

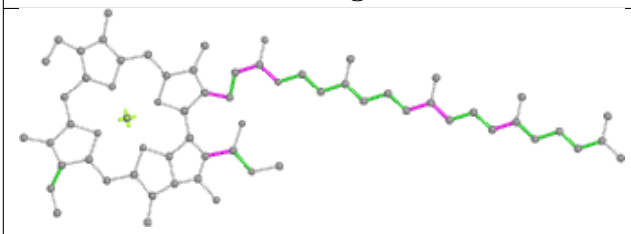
Ligand CLA C 510



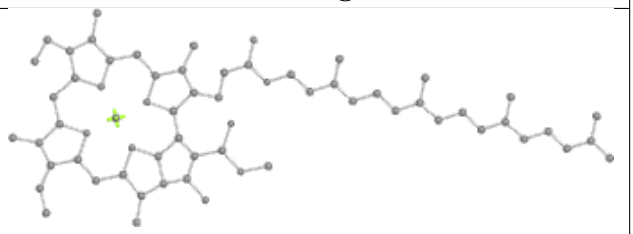
Bond lengths



Bond angles

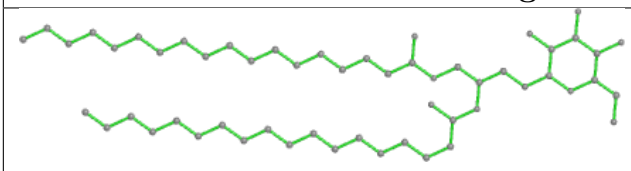


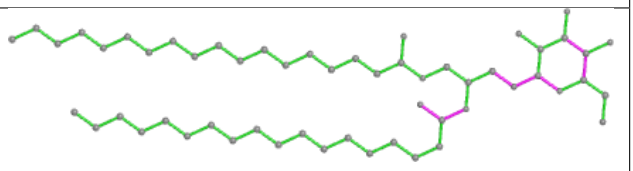
Torsions

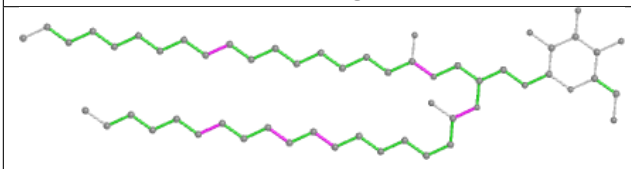


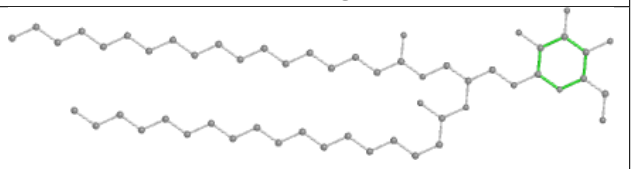
Rings

Ligand LMG D 402

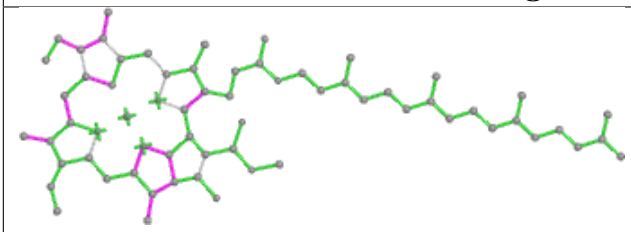

Bond lengths

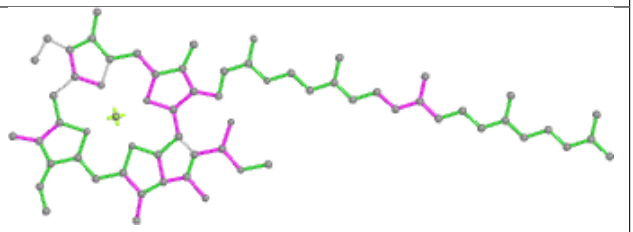

Bond angles

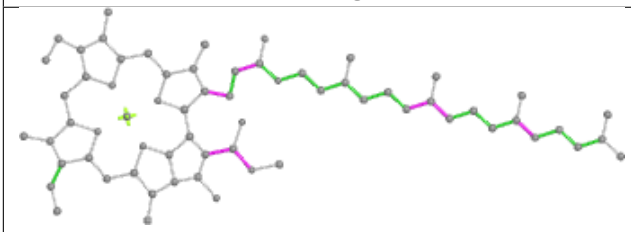

Torsions

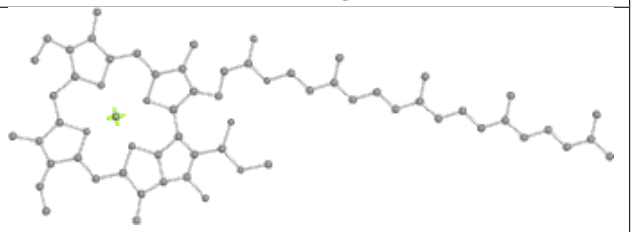

Rings

Ligand CLA B 603

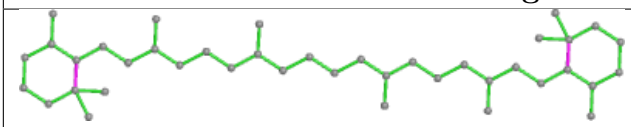

Bond lengths

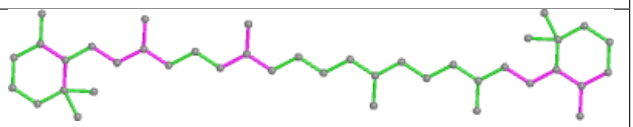

Bond angles

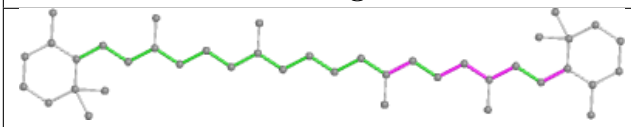

Torsions


Rings

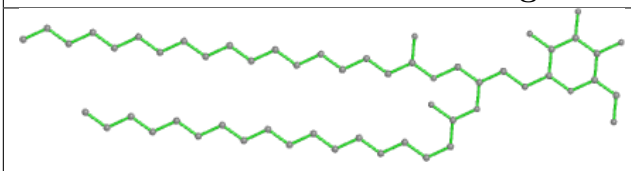
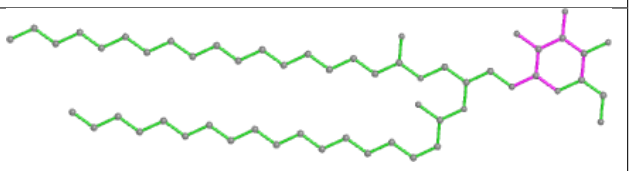
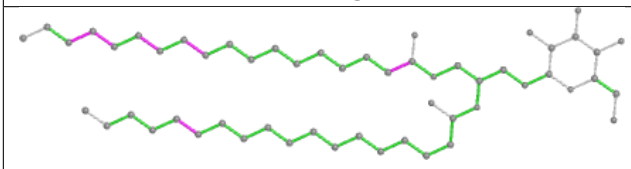
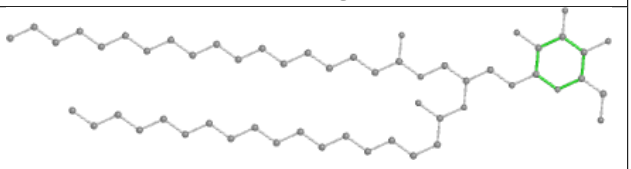
Ligand BCR A 408

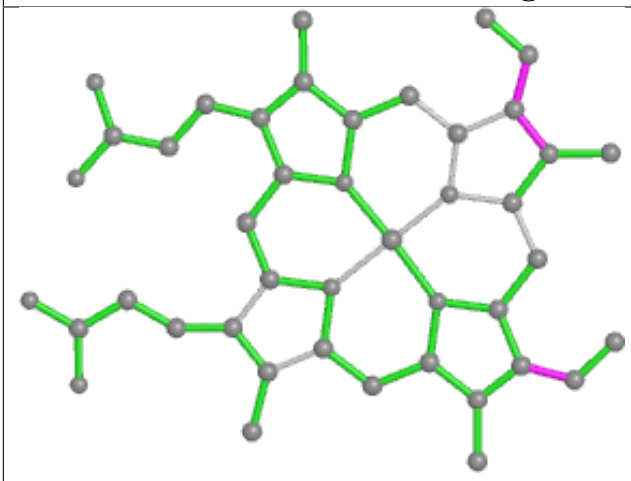
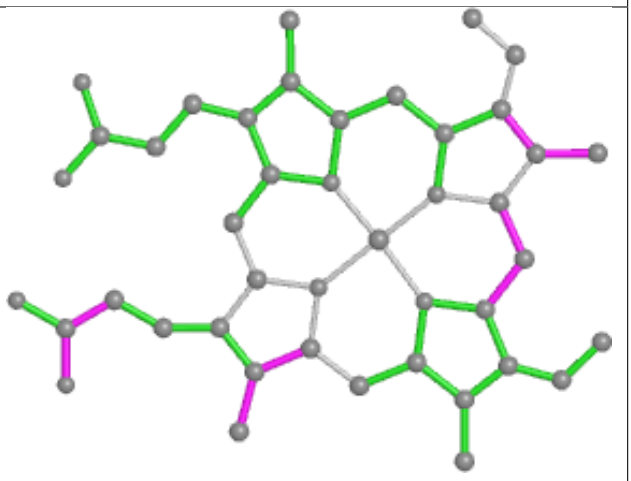
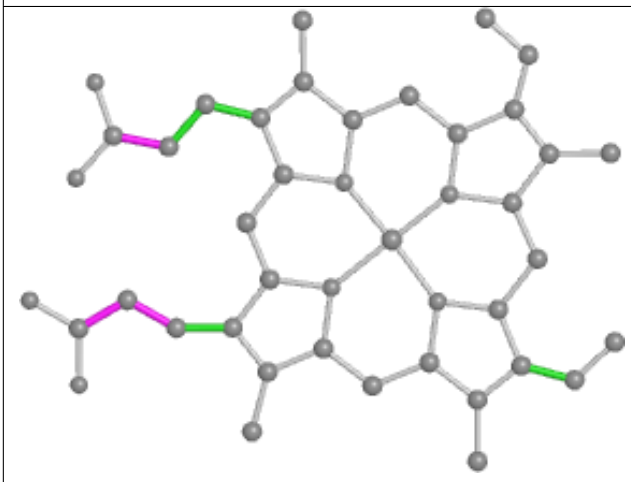
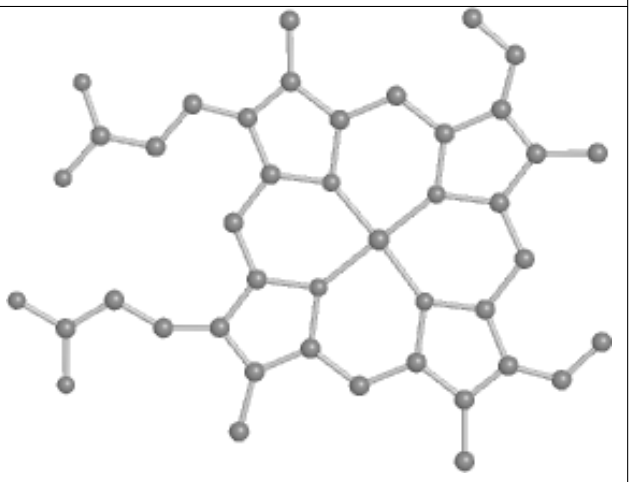

Bond lengths


Bond angles

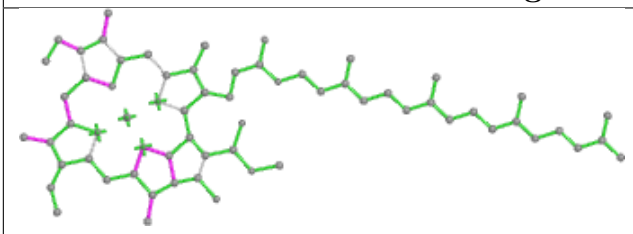

Torsions


Rings

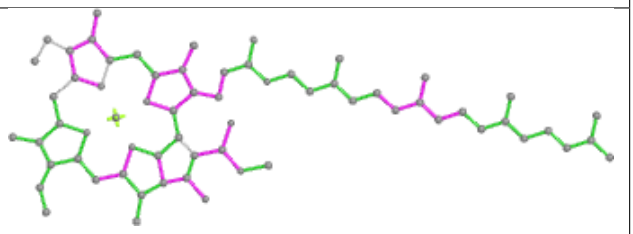
Ligand LMG C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEM E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

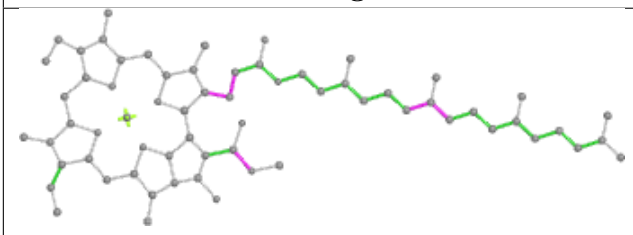
Ligand CLA C 503



Bond lengths



Bond angles



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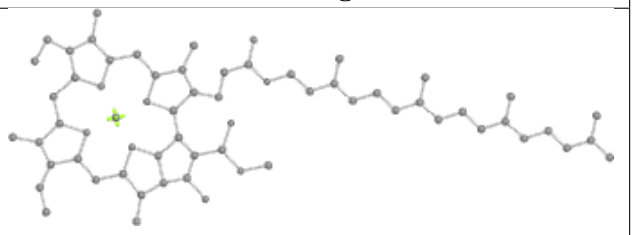
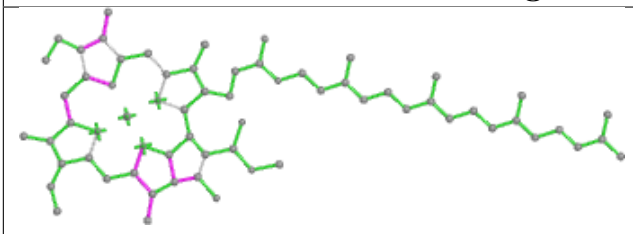
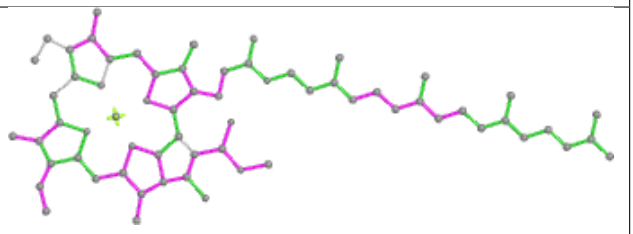


Rings

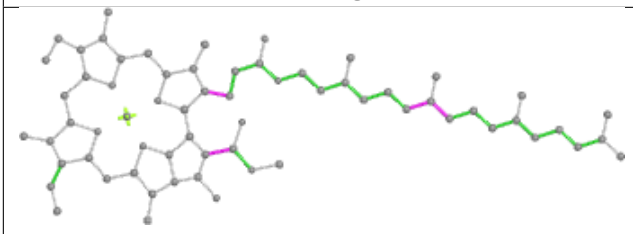
Ligand CLA B 614



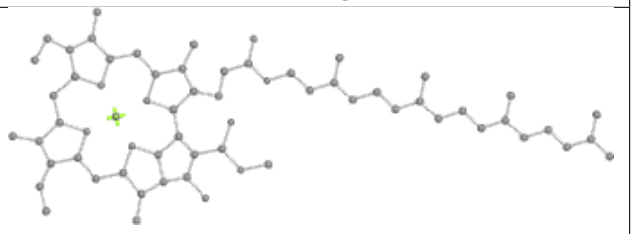
Bond lengths



Bond angles

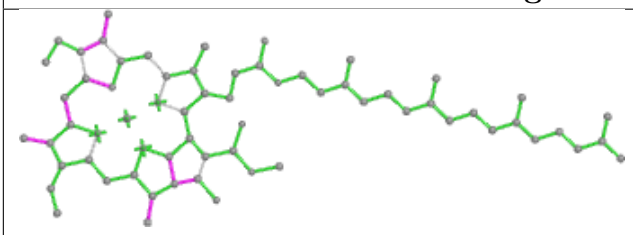


Torsions

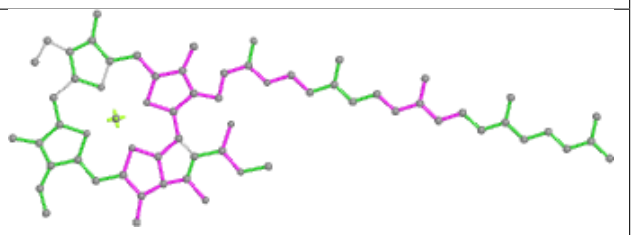


Rings

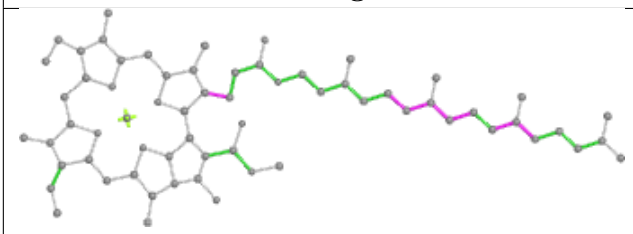
Ligand CLA B 616



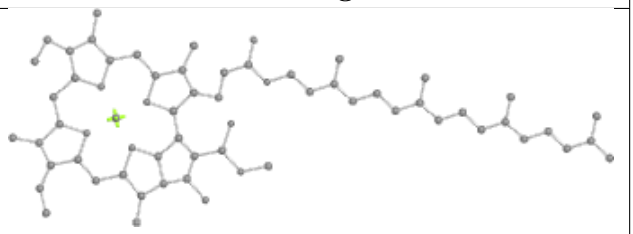
Bond lengths



Bond angles

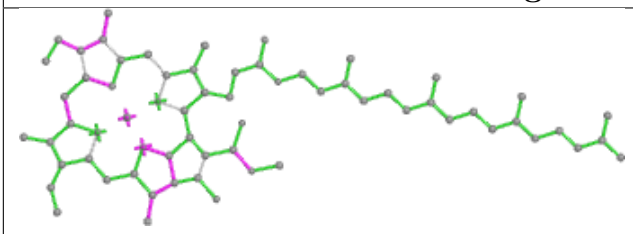


Torsions

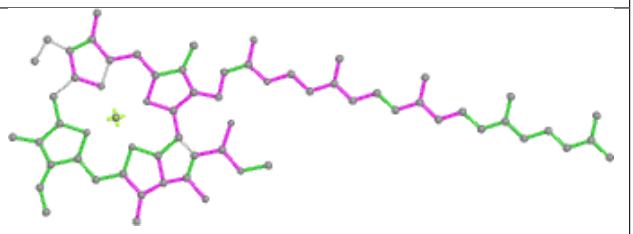


Rings

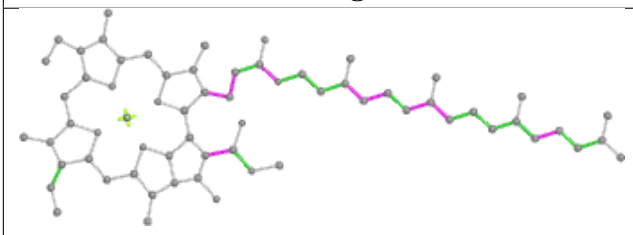
Ligand CLA C 509



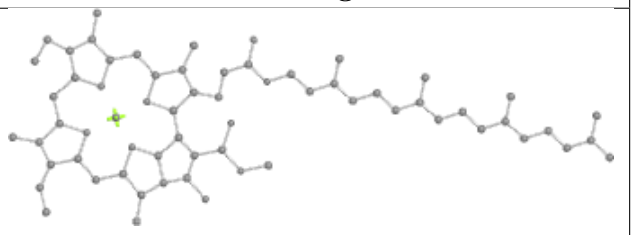
Bond lengths



Bond angles

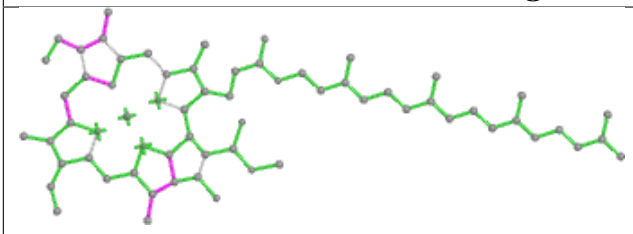


Torsions

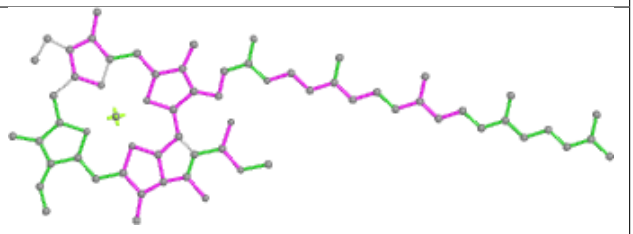


Rings

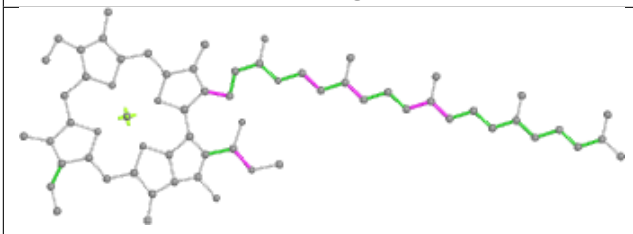
Ligand CLA B 601



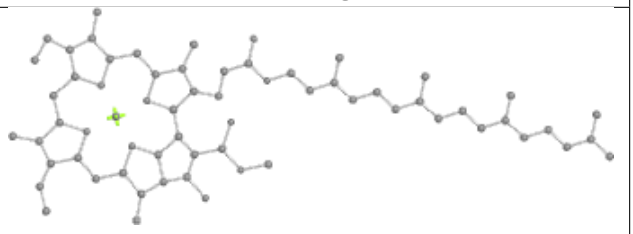
Bond lengths



Bond angles

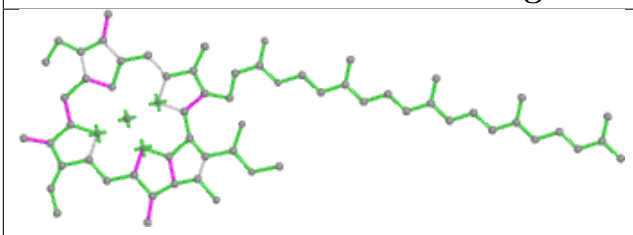


Torsions

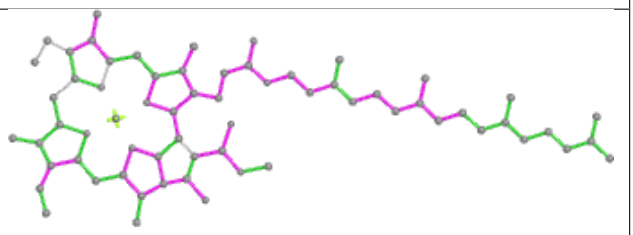


Rings

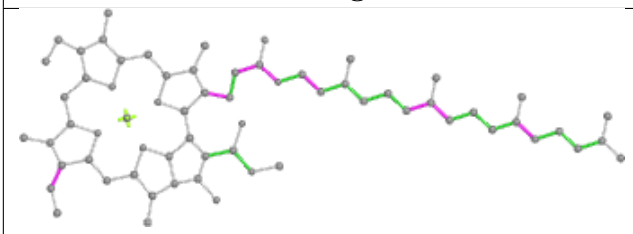
Ligand CLA B 602



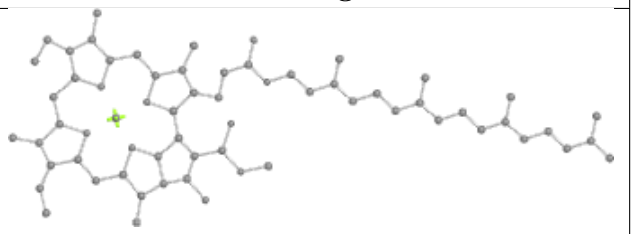
Bond lengths



Bond angles

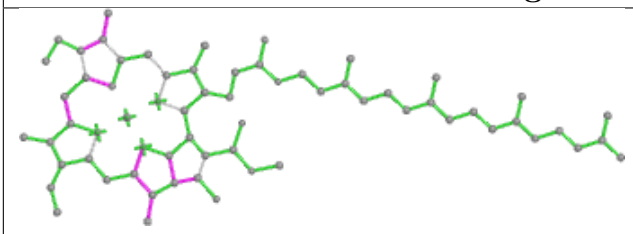


Torsions

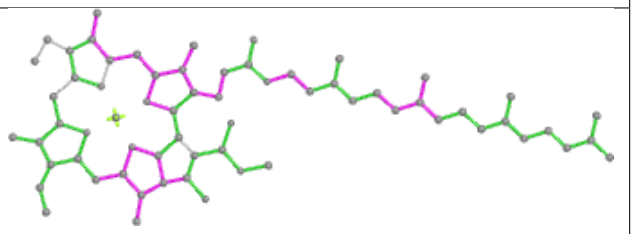


Rings

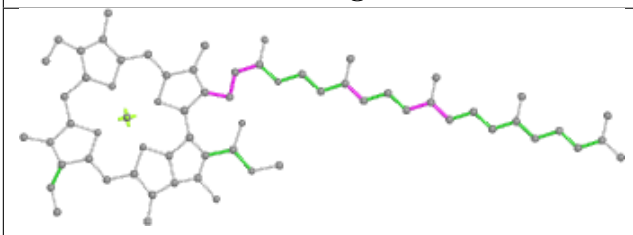
Ligand CLA C 517



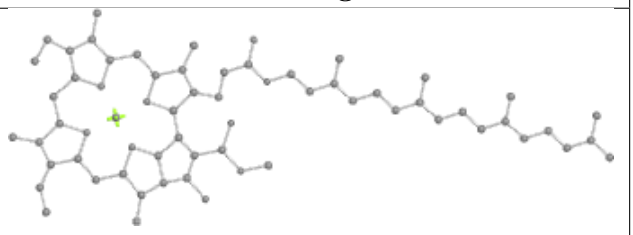
Bond lengths



Bond angles

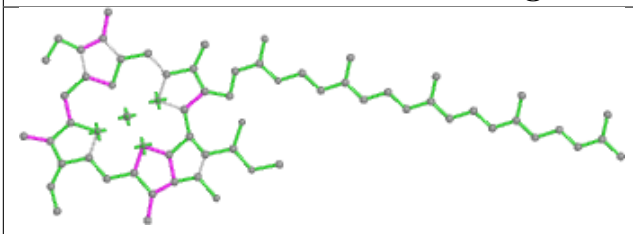


Torsions

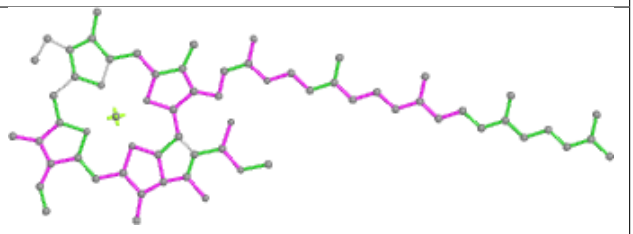


Rings

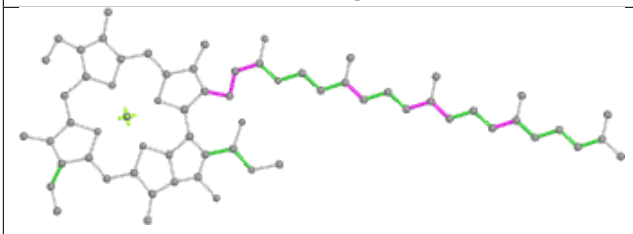
Ligand CLA C 511



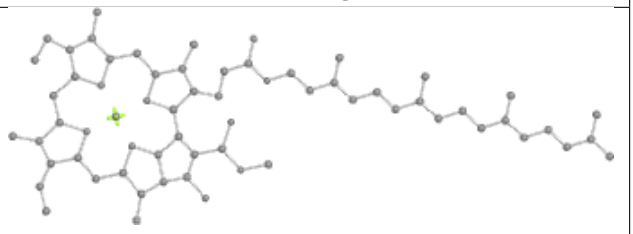
Bond lengths



Bond angles

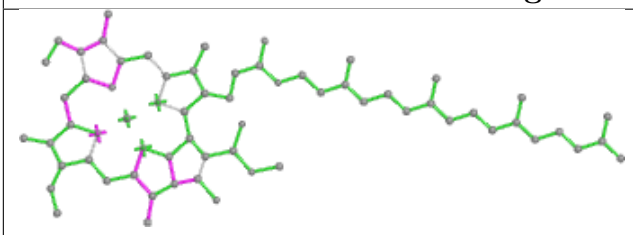


Torsions

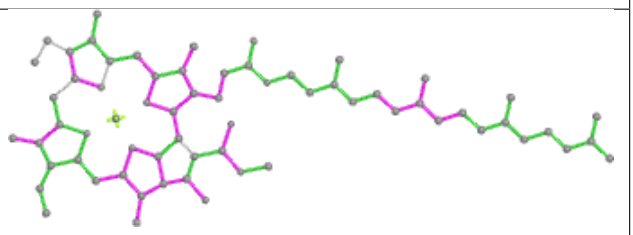


Rings

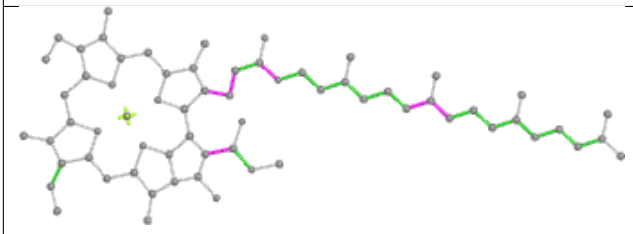
Ligand CLA B 609



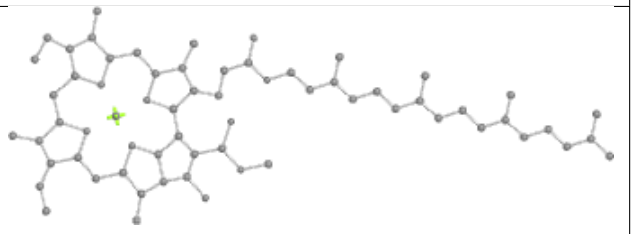
Bond lengths



Bond angles

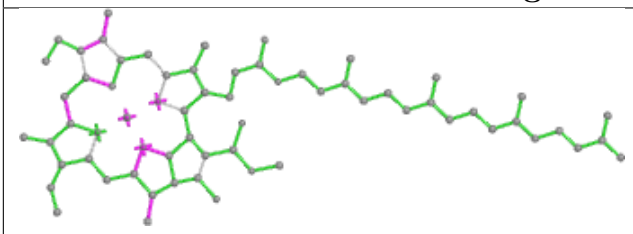


Torsions

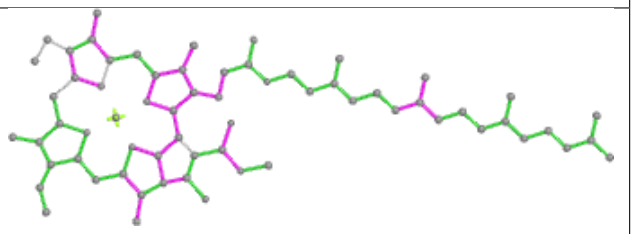


Rings

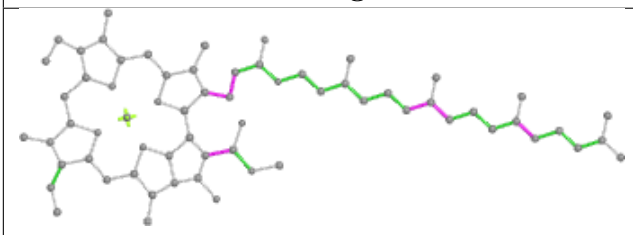
Ligand CLA A 407



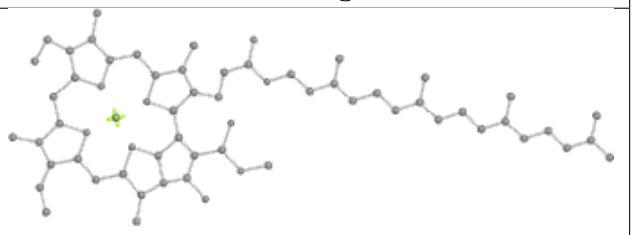
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

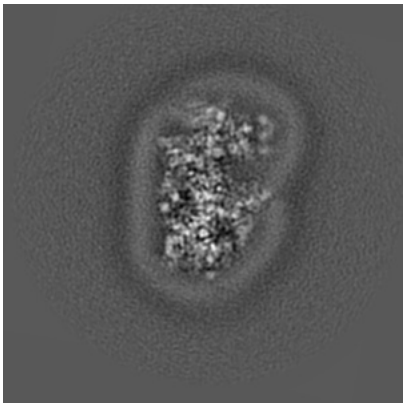
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12336. These allow visual inspection of the internal detail of the map and identification of artifacts.

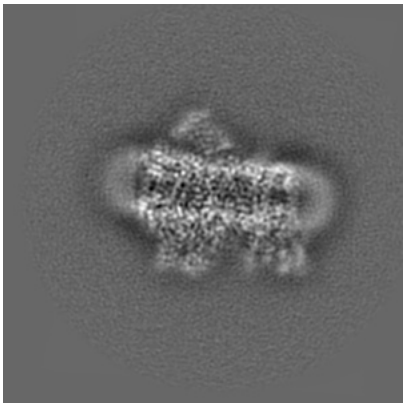
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

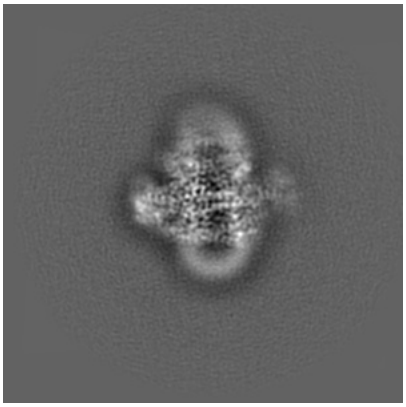
6.1.1 Primary map



X



Y

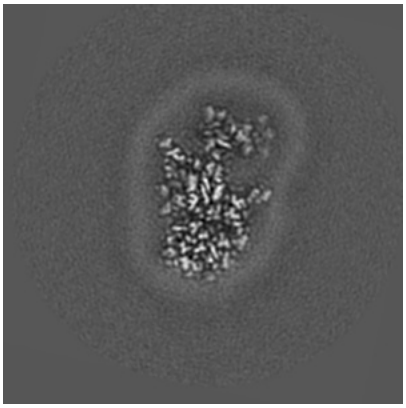


Z

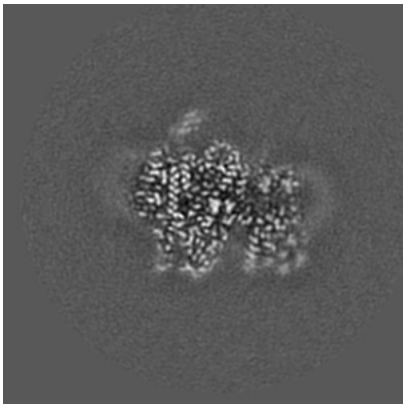
The images above show the map projected in three orthogonal directions.

6.2 Central slices

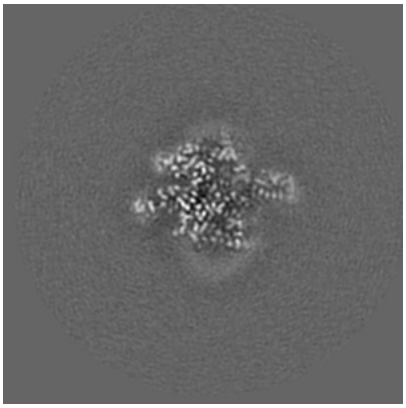
6.2.1 Primary map



X Index: 130



Y Index: 130

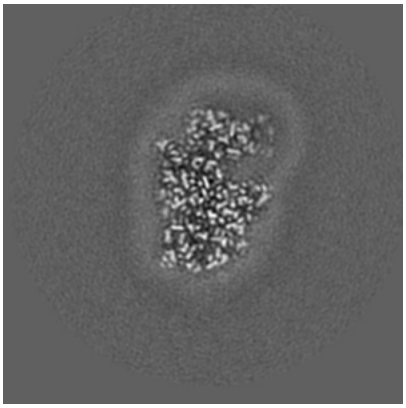


Z Index: 130

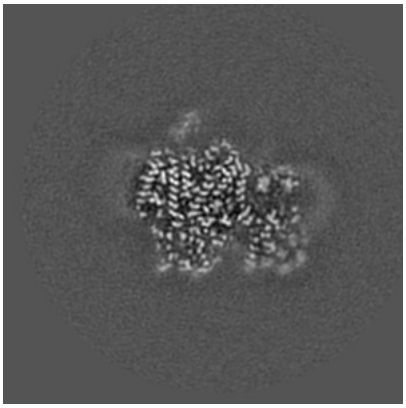
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

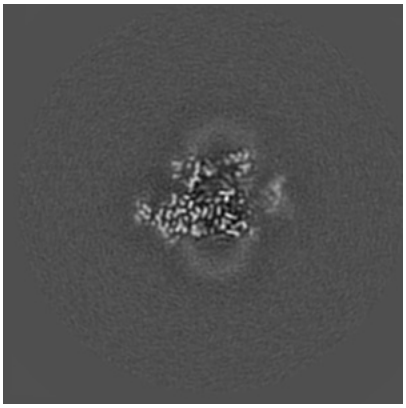
6.3.1 Primary map



X Index: 125



Y Index: 129



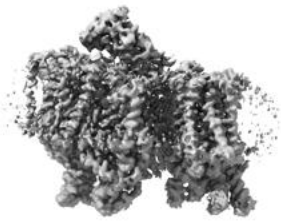
Z Index: 115

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

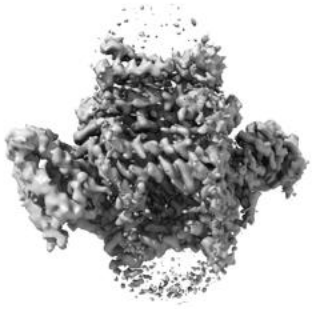
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

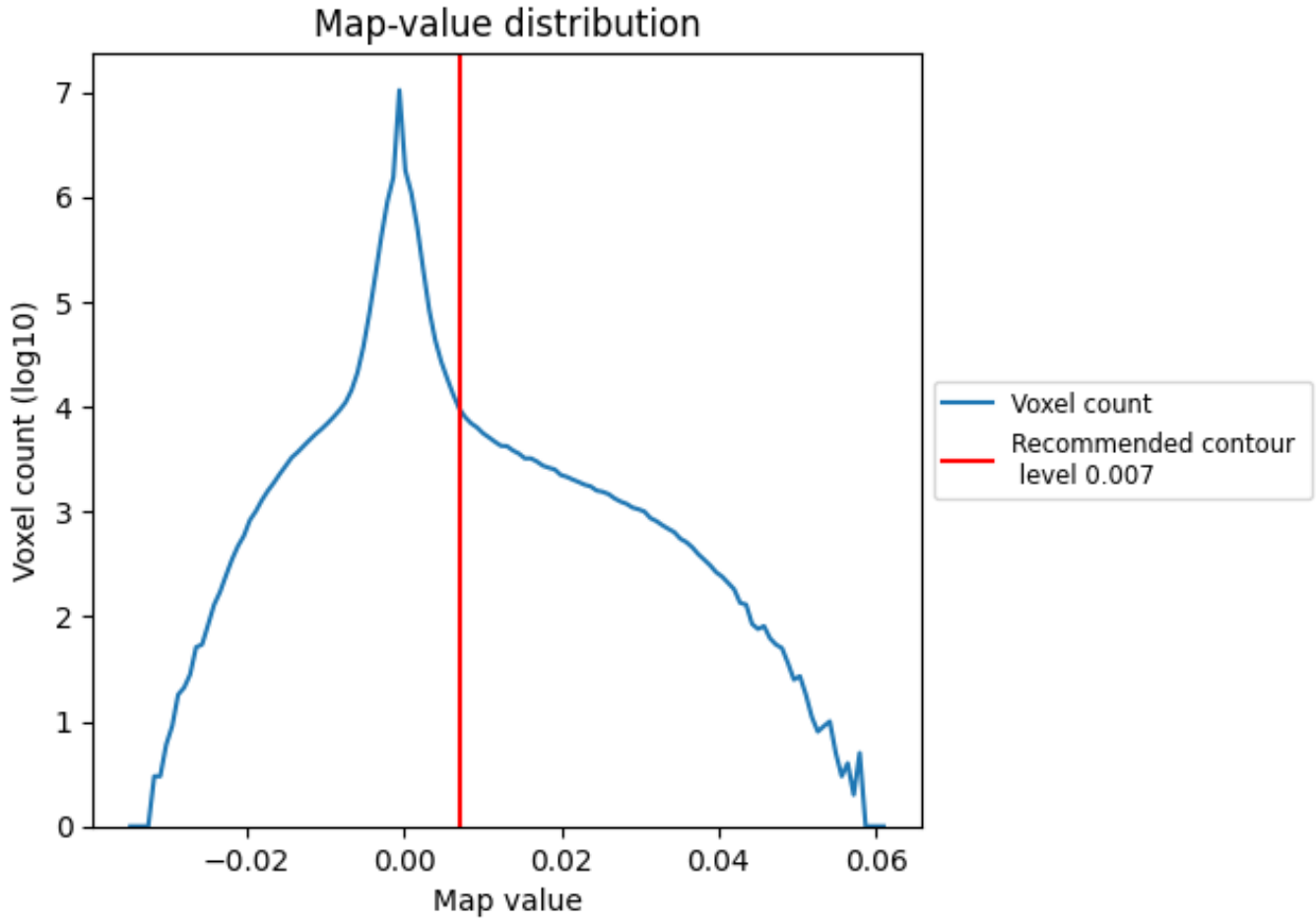
6.5 Mask visualisation (i)

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

7 Map analysis

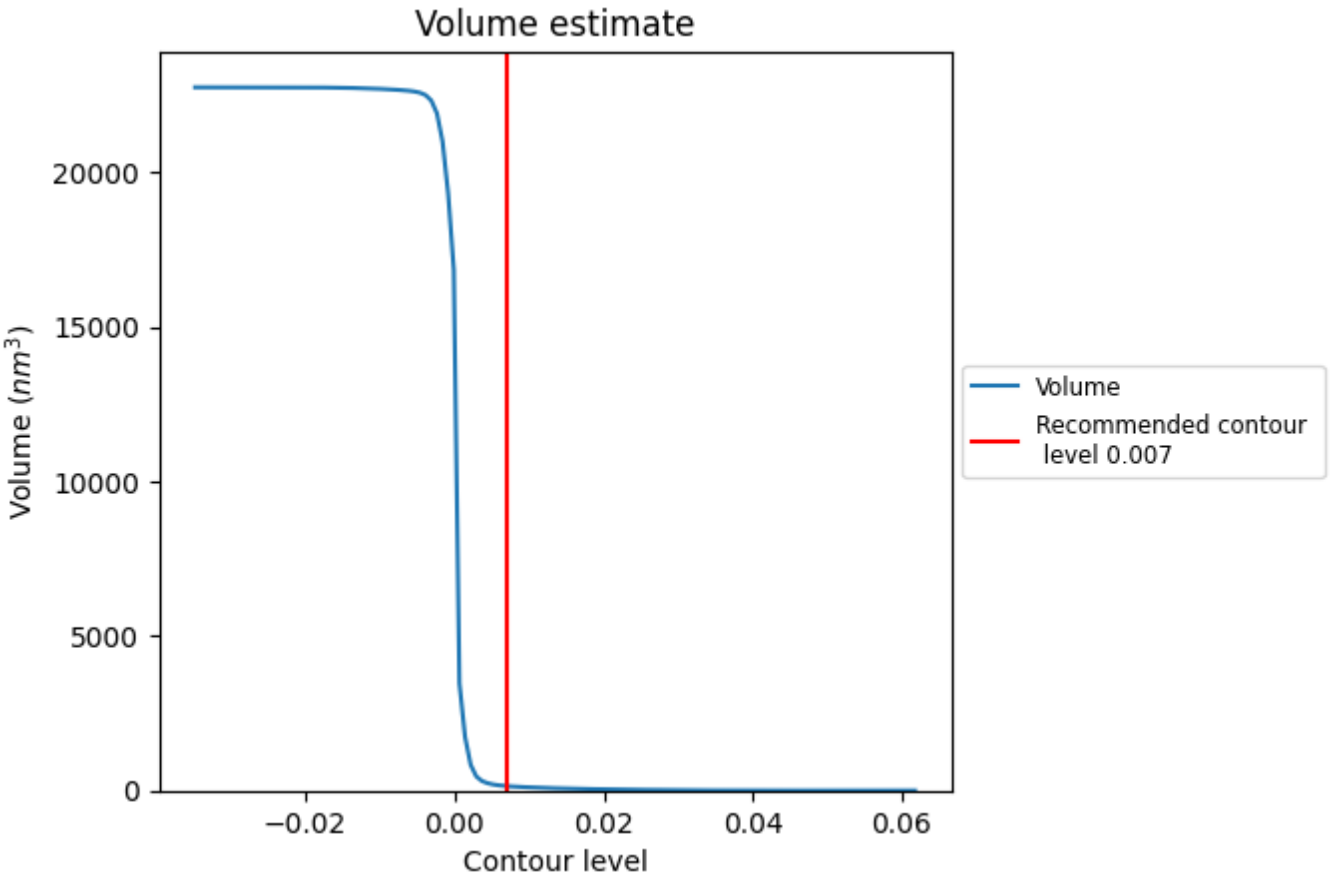
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

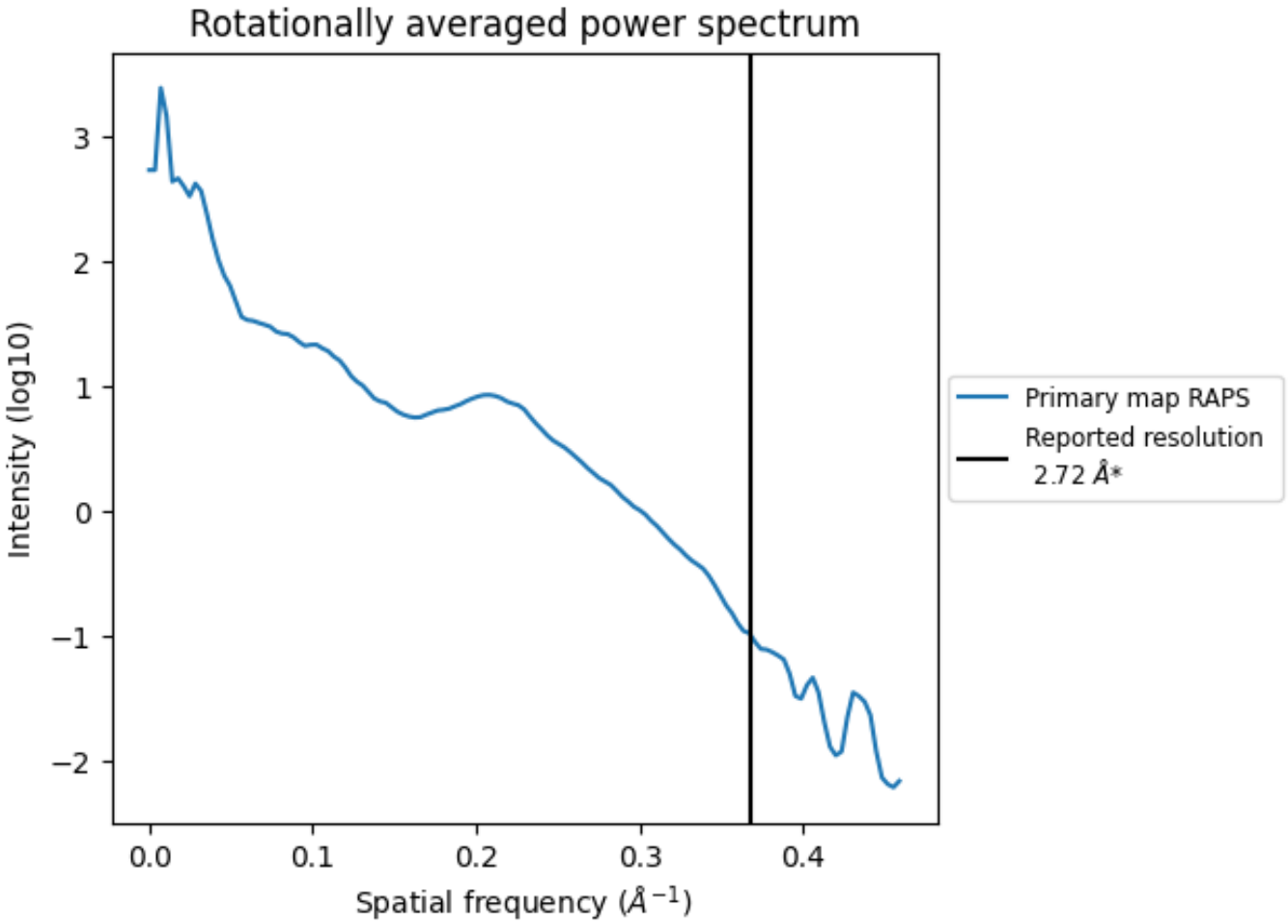
7.2 Volume estimate



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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 0.368 $Å^{-1}$

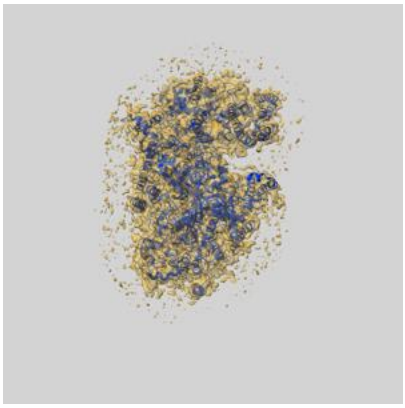
8 Fourier-Shell correlation (i)

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

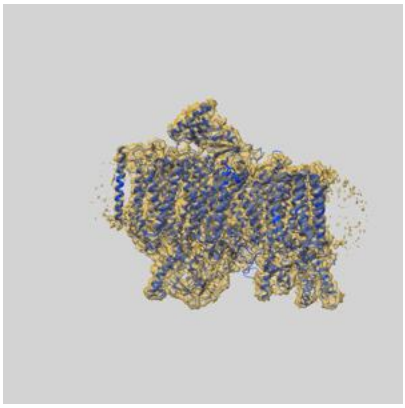
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12336 and PDB model 7NHP. Per-residue inclusion information can be found in section 3 on page 14.

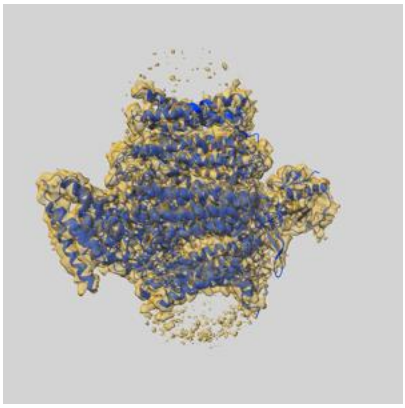
9.1 Map-model overlay



X



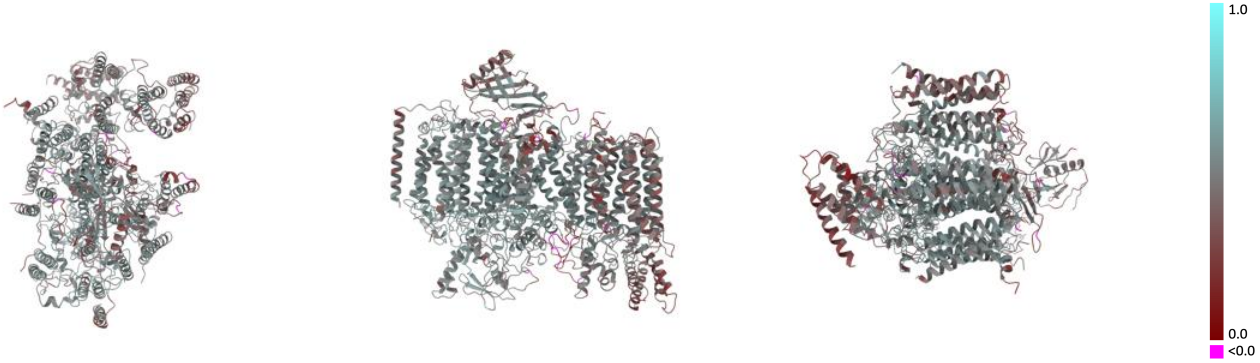
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 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.

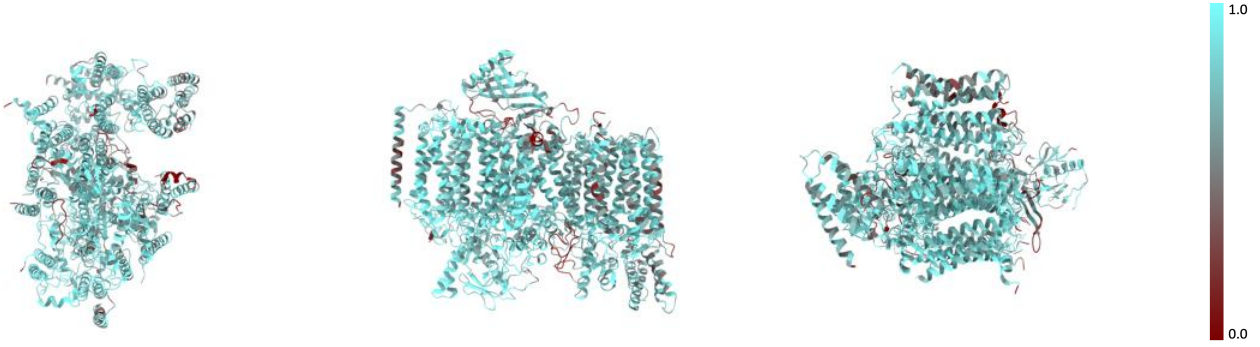
9.2 Q-score mapped to coordinate model (i)



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.

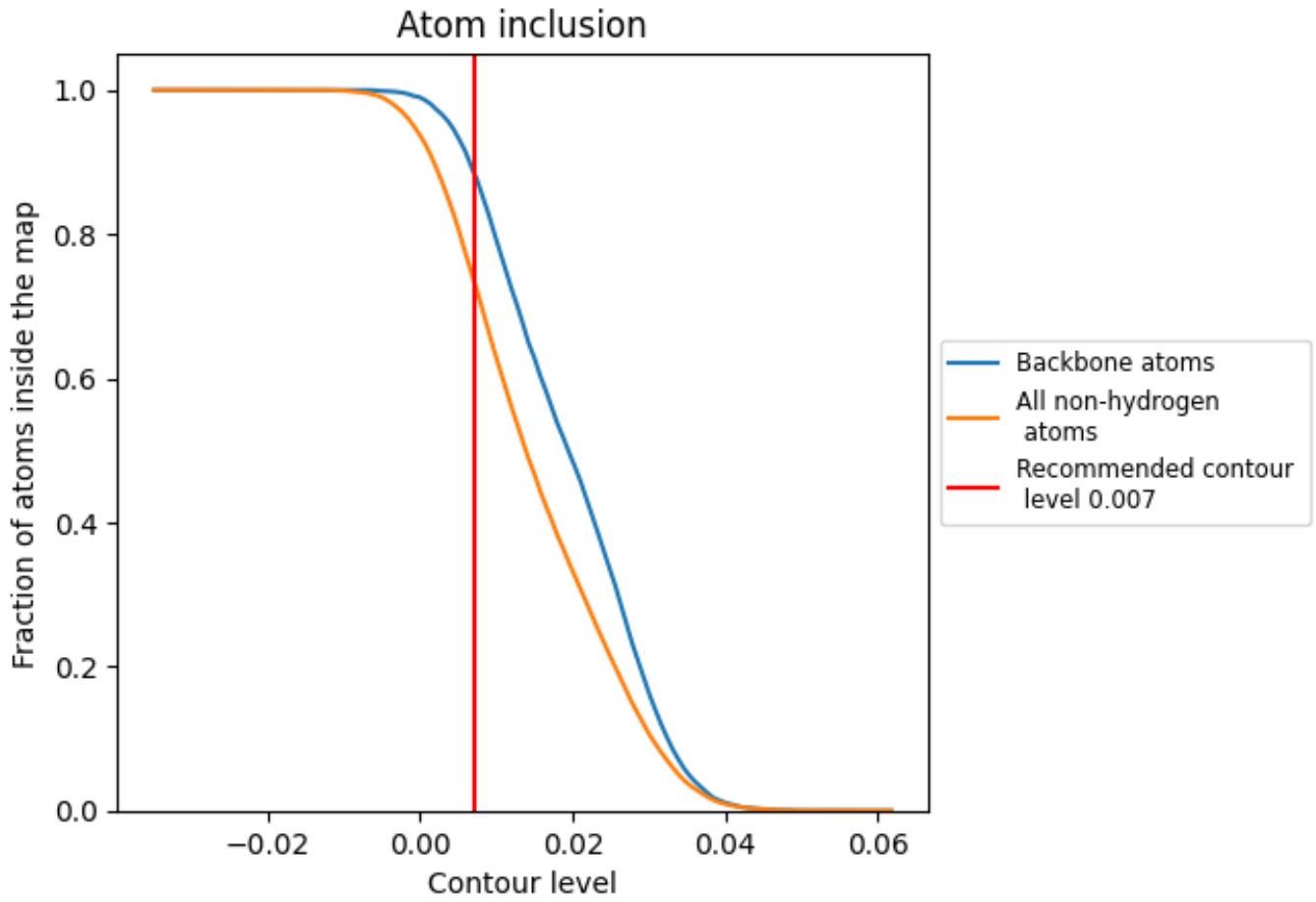
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7371	0.4690
1	0.6617	0.3400
2	0.7437	0.4250
3	0.5098	0.3840
A	0.7406	0.4840
B	0.8136	0.5100
C	0.6897	0.4410
D	0.7853	0.5250
E	0.7021	0.4240
F	0.6279	0.4010
H	0.8296	0.4890
I	0.6226	0.4120
K	0.6201	0.4340
L	0.7953	0.5040
M	0.6579	0.4600
T	0.7288	0.4740
X	0.7520	0.4890
Z	0.6245	0.3790
y	0.4755	0.3120