



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:01 PM UTC

PDB ID : 7DXA / pdb_00007dxa
EMDB ID : EMD-30902
Title : PSII intermediate Psb28-RC47
Authors : Sui, S.F.; Shen, J.R.; Han, G.Y.; Xiao, Y.N.; Huang, G.Q.
Deposited on : 2021-01-18
Resolution : 3.14 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

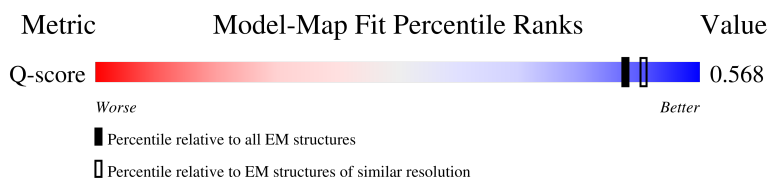
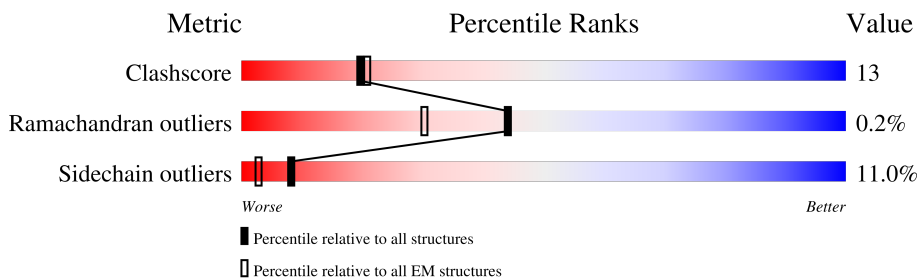
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.14 Å.

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



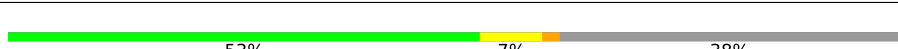
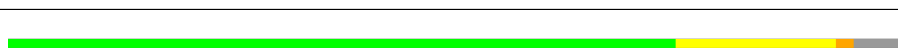
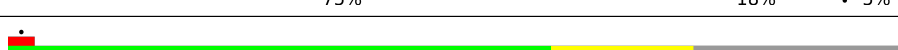
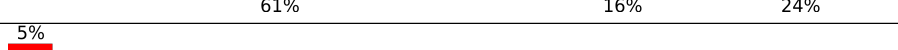
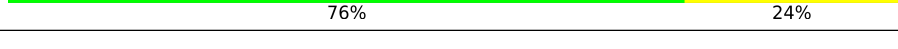
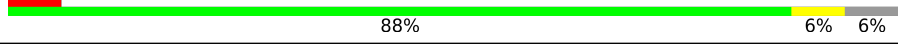
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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 $\leq 5\%$. 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	116	
2	B	56	
3	a	360	
4	b	505	

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Mol	Chain	Length	Quality of chain
5	d	342	
6	e	84	
7	f	45	
8	h	65	
9	i	38	
10	l	37	
11	m	36	
12	t	32	
13	x	40	
14	C	23	

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
16	CLA	a	402	X	-	-	-
16	CLA	b	602	X	-	-	-
16	CLA	b	603	X	-	-	-
16	CLA	b	604	X	-	-	-
16	CLA	b	605	X	-	-	-
16	CLA	b	606	X	-	X	-
16	CLA	b	607	X	-	-	-
16	CLA	b	610	X	-	-	-
16	CLA	b	612	X	-	-	-
16	CLA	b	613	X	-	-	-
16	CLA	b	614	X	-	-	-
16	CLA	b	615	X	-	-	-
16	CLA	b	616	X	-	-	-
16	CLA	d	401	X	-	-	-
16	CLA	d	404	X	-	-	-
19	CL	a	408	-	-	X	-

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 15162 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 reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	109	Total	C	N	O	S	0	0
			875	549	153	168	5		

- Molecule 2 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	50	Total	C	N	O	0	0
			365	237	65	63		

- Molecule 3 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	298	Total	C	N	O	S	0	0
			2311	1520	382	394	15		

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	494	Total	C	N	O	S	0	0
			3886	2554	646	673	13		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	339	Total	C	N	O	S	0	0
			2694	1787	439	456	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	63	Total	C	N	O	0	0
			509	334	81	94		

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	62	Total	C	N	O	S	0	0
			493	330	79	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	29	Total	C	N	O	S	0	0
			231	162	30	38	1		

- 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	31	Total	C	N	O	0	0
			244	165	36	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

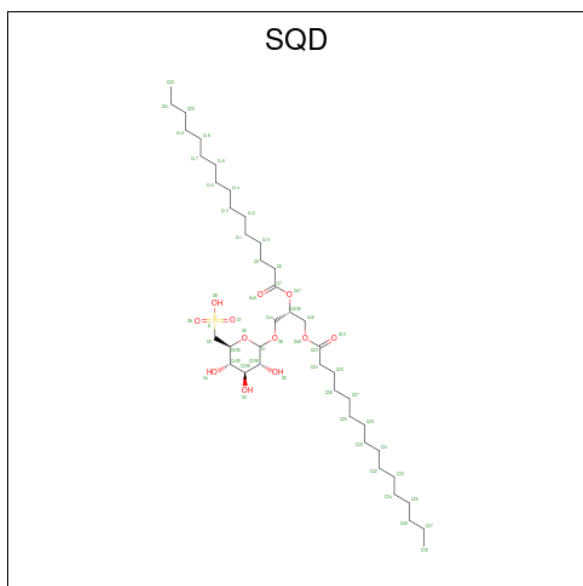
- Molecule 13 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	x	36	Total	C	N	O	0	0
			261	177	39	45		

- Molecule 14 is a protein called unidentified transmembrane protein.

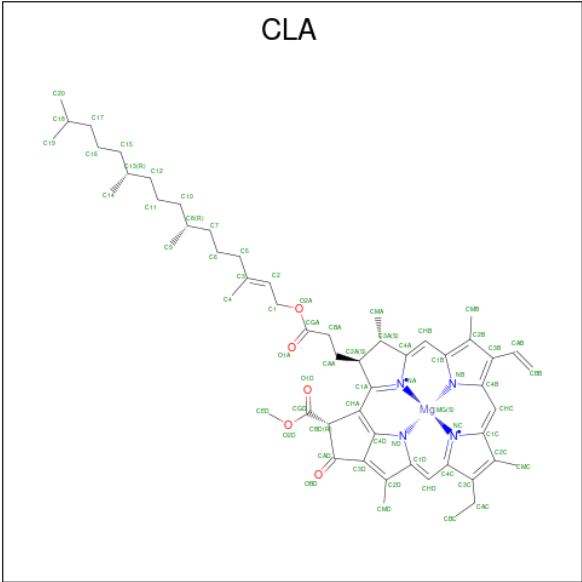
Mol	Chain	Residues	Atoms				AltConf	Trace
14	C	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
15	a	1	Total	C	O	S	0
			26	13	12	1	
15	l	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



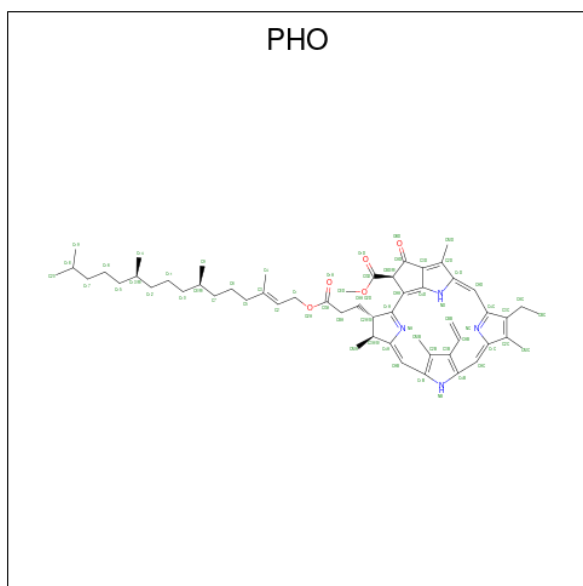
Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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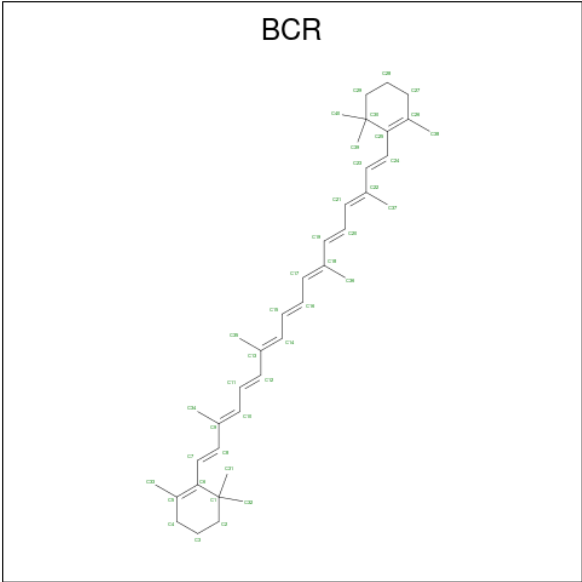
Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 17 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
17	a	1	Total	C	N	O	0
			64	55	4	5	
17	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

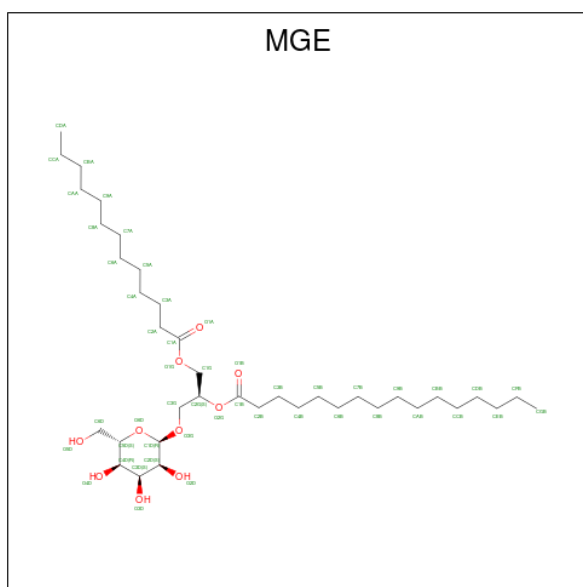


Mol	Chain	Residues	Atoms		AltConf
18	a	1	Total	C	0
			40	40	
18	b	1	Total	C	0
			40	40	
18	b	1	Total	C	0
			40	40	
18	b	1	Total	C	0
			40	40	
18	d	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
19	a	1	Total	Cl	0
			1	1	

- Molecule 20 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: C₃₈H₇₂O₁₀).

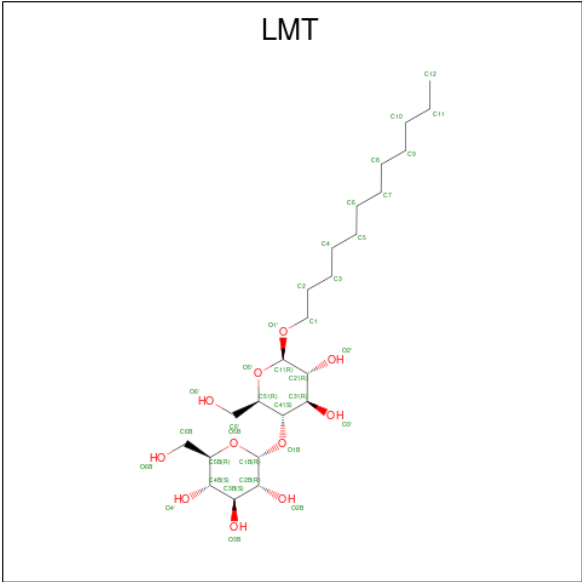


Mol	Chain	Residues	Atoms			AltConf
20	a	1	Total	C	O	0
			48	38	10	
20	b	1	Total	C	O	0
			48	38	10	
20	b	1	Total	C	O	0
			48	38	10	
20	d	1	Total	C	O	0
			47	37	10	
20	d	1	Total	C	O	0
			41	31	10	
20	d	1	Total	C	O	0
			48	38	10	
20	m	1	Total	C	O	0
			48	38	10	

- Molecule 21 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			AltConf
21	b	1	Total	C	O	0
			36	31	5	
21	x	1	Total	C	O	0
			17	16	1	

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

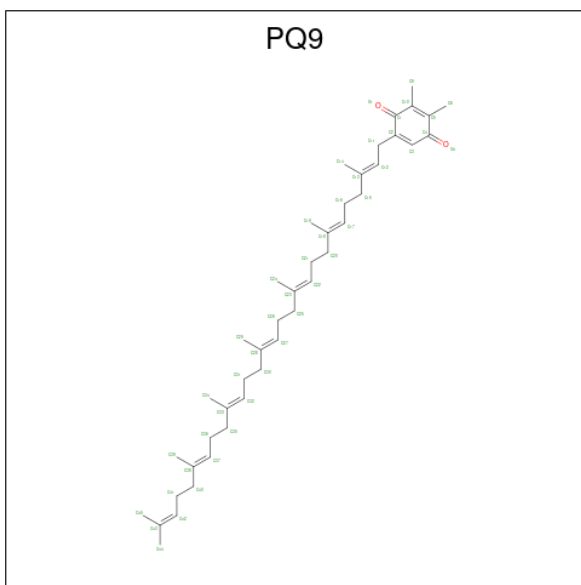


Mol	Chain	Residues	Atoms			AltConf
22	b	1	Total	C	O	0
			35	24	11	
22	d	1	Total	C	O	0
			35	24	11	
22	t	1	Total	C	O	0
			35	24	11	

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

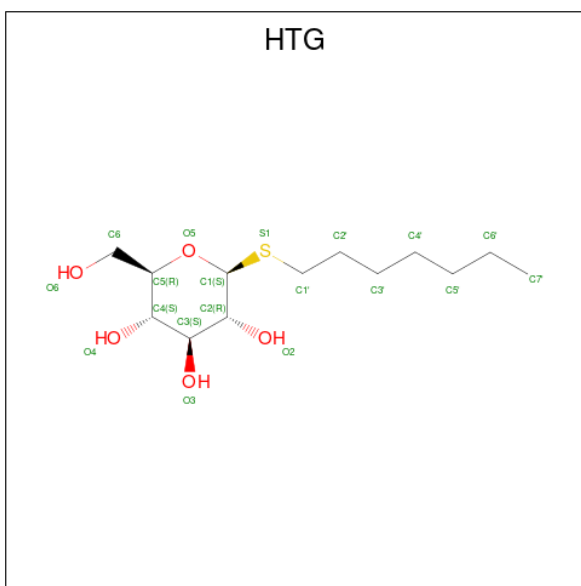
Mol	Chain	Residues	Atoms		AltConf
23	d	1	Total	Fe	0
			1	1	

- Molecule 24 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂).



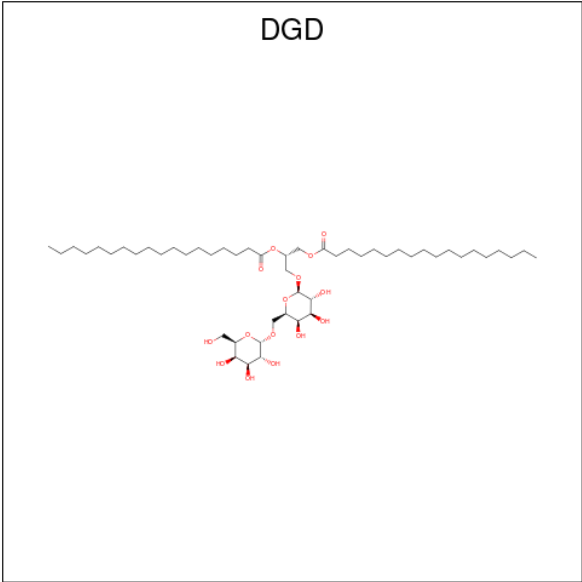
Mol	Chain	Residues	Atoms			AltConf
24	d	1	Total	C	O	0
			45	43	2	

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



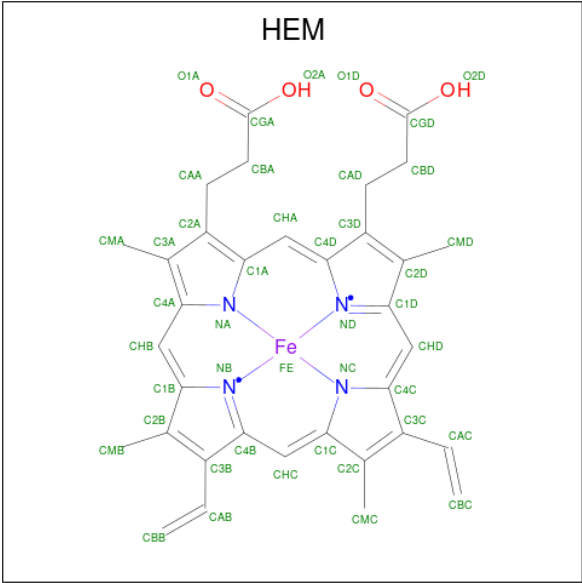
Mol	Chain	Residues	Atoms				AltConf
25	d	1	Total	C	O	S	0
			16	10	5	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
26	d	1	Total	C	O	0
			54	39	15	

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

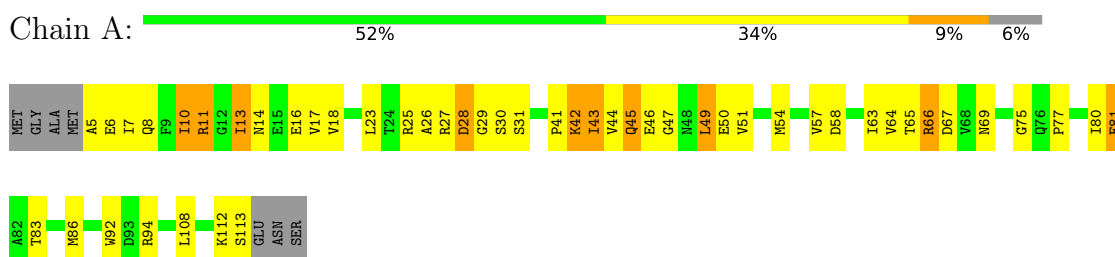


Mol	Chain	Residues	Atoms					AltConf
27	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

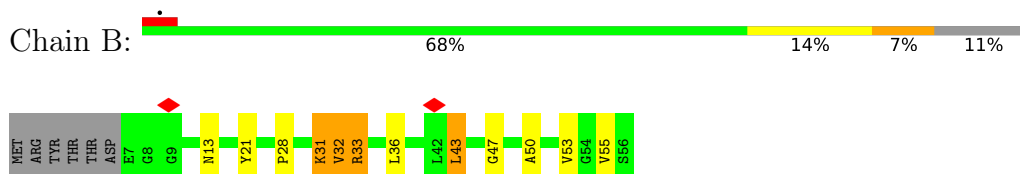
3 Residue-property plots

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.

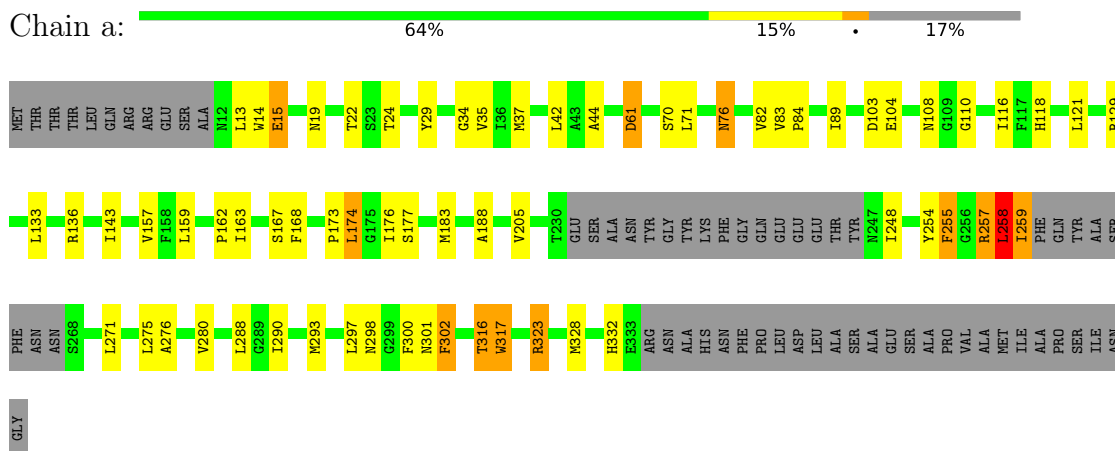
- Molecule 1: Photosystem II reaction center Psb28 protein



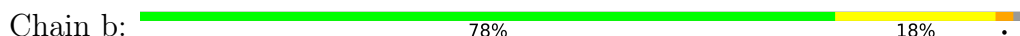
- Molecule 2: Tsl0063 protein

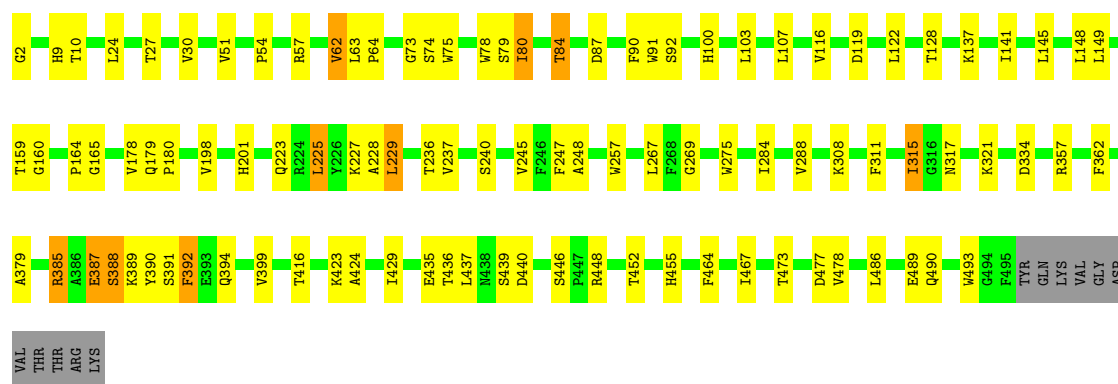


- Molecule 3: Photosystem II protein D1

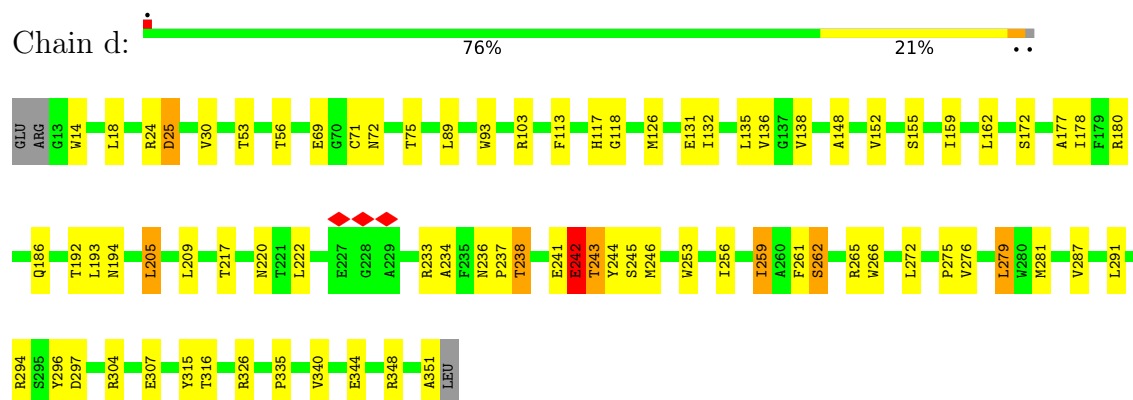


- Molecule 4: Photosystem II CP47 reaction center protein

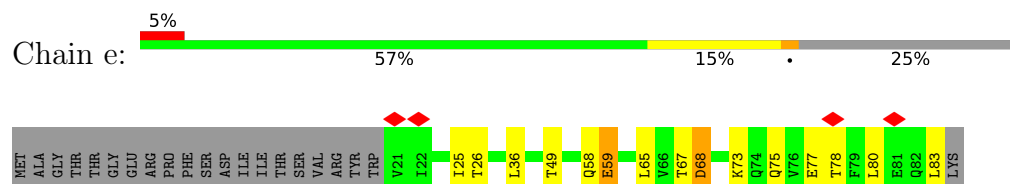




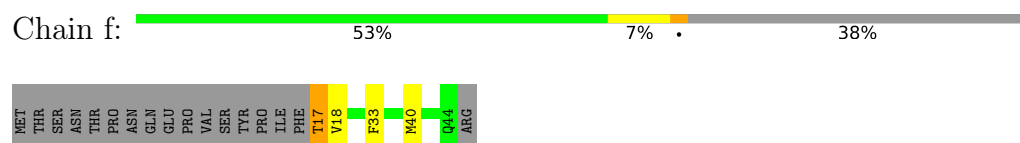
• Molecule 5: Photosystem II D2 protein



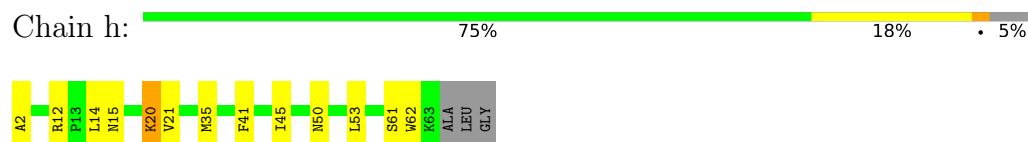
• Molecule 6: Cytochrome b559 subunit alpha



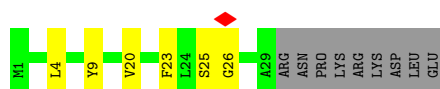
• Molecule 7: Cytochrome b559 subunit beta



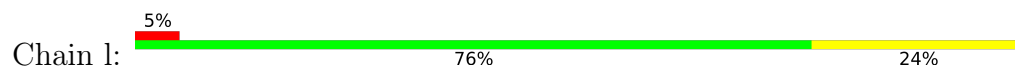
• Molecule 8: Photosystem II reaction center protein H



• Molecule 9: Photosystem II reaction center protein I



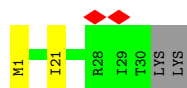
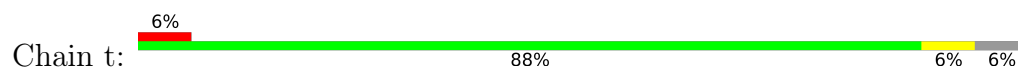
- Molecule 10: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein M



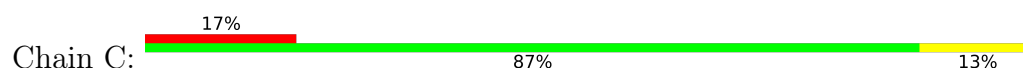
- Molecule 12: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein X



- Molecule 14: unidentified transmembrane protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241790	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.236	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQ9, SQD, DGD, CL, BCR, FE2, CLA, HEM, HTG, LMT, PHO, MGE, UNL

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	0.61	0/892	0.85	0/1202
2	B	0.38	0/371	0.71	0/505
3	a	0.49	0/2383	0.77	3/3249 (0.1%)
4	b	0.48	0/4025	0.72	2/5486 (0.0%)
5	d	0.51	0/2789	0.74	0/3803
6	e	0.36	0/523	0.79	3/714 (0.4%)
7	f	0.36	0/225	0.73	0/308
8	h	0.45	0/506	0.82	0/690
9	i	0.31	0/237	0.70	0/322
10	l	0.40	0/311	0.66	0/422
11	m	0.36	0/248	0.85	0/339
12	t	0.30	0/263	0.52	0/356
13	x	0.28	0/264	0.61	0/358
14	C	0.40	0/114	0.99	0/158
All	All	0.48	0/13151	0.75	8/17912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	d	0	1
6	e	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	b	435	GLU	CA-C-N	6.04	133.08	121.54
4	b	435	GLU	C-N-CA	6.04	133.08	121.54
6	e	67	THR	CA-C-N	5.66	129.75	121.31
6	e	67	THR	C-N-CA	5.66	129.75	121.31
3	a	258	LEU	CA-C-N	5.38	131.39	121.70
3	a	258	LEU	C-N-CA	5.38	131.39	121.70
3	a	110	GLY	N-CA-C	5.36	121.63	115.09
6	e	68	ASP	N-CA-C	5.17	117.59	110.35

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	d	93	TRP	Peptide
6	e	68	ASP	Peptide

5.2 Too-close contacts ⓘ

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	875	0	839	64	0
2	B	365	0	386	34	0
3	a	2311	0	2244	64	0
4	b	3886	0	3741	76	0
5	d	2694	0	2588	75	0
6	e	509	0	499	7	0
7	f	219	0	228	3	0
8	h	493	0	513	14	0
9	i	231	0	243	1	0
10	l	304	0	316	6	0
11	m	244	0	256	13	0
12	t	254	0	257	9	0
13	x	261	0	291	4	0
14	C	115	0	114	10	0
15	a	26	0	16	0	0
15	l	47	0	61	2	0
16	a	165	0	150	10	0
16	b	973	0	1017	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	d	176	0	172	18	0
17	a	128	0	148	11	0
18	a	40	0	56	4	0
18	b	120	0	168	21	0
18	d	40	0	56	4	0
18	h	40	0	56	4	0
19	a	1	0	0	2	0
20	a	48	0	72	0	0
20	b	96	0	144	3	0
20	d	136	0	193	14	0
20	m	48	0	72	2	0
21	b	36	0	0	0	0
21	x	17	0	0	1	0
22	b	35	0	46	0	0
22	d	35	0	46	1	0
22	t	35	0	46	1	0
23	d	1	0	0	0	0
24	d	45	0	64	6	0
25	d	16	0	17	6	0
26	d	54	0	66	1	0
27	e	43	0	30	0	0
All	All	15162	0	15211	381	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 13.

All (381) 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)
2:B:28:PRO:HA	2:B:31:LYS:CG	1.25	1.62
16:b:606:CLA:H71	18:b:619:BCR:C34	1.52	1.39
16:b:606:CLA:C7	18:b:619:BCR:H342	1.60	1.29
16:b:607:CLA:H191	20:d:409:MGE:C6A	1.63	1.29
2:B:28:PRO:HA	2:B:31:LYS:CD	1.71	1.20
5:d:14:TRP:CB	25:d:411:HTG:H61	1.73	1.19
2:B:28:PRO:CA	2:B:31:LYS:CG	2.20	1.19
16:b:607:CLA:H201	20:d:409:MGE:C6A	1.74	1.18
1:A:50:GLU:OE1	5:d:236:ASN:HB2	1.41	1.17
2:B:28:PRO:HA	2:B:31:LYS:HG2	1.20	1.13
5:d:14:TRP:HB3	25:d:411:HTG:C6	1.79	1.12
16:b:602:CLA:H43	8:h:45:ILE:HG22	1.33	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PRO:HA	2:B:31:LYS:HG3	1.27	1.06
5:d:14:TRP:HB3	25:d:411:HTG:H61	1.08	1.05
4:b:385:ARG:NH1	5:d:351:ALA:O	1.88	1.05
3:a:257:ARG:CZ	3:a:257:ARG:HA	1.88	1.03
1:A:16:GLU:OE1	1:A:42:LYS:NZ	1.93	1.01
2:B:28:PRO:O	2:B:32:VAL:HG12	1.61	1.01
16:b:607:CLA:C19	20:d:409:MGE:C6A	2.40	0.99
2:B:28:PRO:CA	2:B:31:LYS:CD	2.40	0.95
3:a:257:ARG:HH21	3:a:257:ARG:HG3	1.31	0.95
1:A:66:ARG:O	3:a:255:PHE:CE2	2.19	0.95
1:A:6:GLU:CD	1:A:14:ASN:HB3	1.90	0.95
16:b:607:CLA:C20	20:d:409:MGE:C6A	2.47	0.91
11:m:8:PHE:CE2	12:t:1:MET:HG3	2.06	0.91
1:A:66:ARG:O	3:a:255:PHE:HE2	1.53	0.91
5:d:241:GLU:OE2	5:d:244:TYR:OH	1.90	0.89
2:B:28:PRO:C	2:B:31:LYS:HG3	1.97	0.88
1:A:6:GLU:OE1	1:A:14:ASN:HB3	1.74	0.88
16:b:606:CLA:H2	18:b:619:BCR:H321	1.55	0.88
16:b:602:CLA:C4	8:h:45:ILE:HG22	2.04	0.87
2:B:50:ALA:HB3	14:C:36:ALA:CB	2.04	0.86
4:b:388:SER:HB3	4:b:394:GLN:HE22	1.40	0.86
11:m:8:PHE:HE2	12:t:1:MET:HG3	1.40	0.86
5:d:238:THR:HG21	5:d:242:GLU:OE2	1.75	0.85
1:A:5:ALA:N	1:A:58:ASP:HA	1.93	0.84
1:A:25:ARG:HE	1:A:29:GLY:HA2	1.42	0.83
3:a:332:HIS:HD2	19:a:408:CL:CL	1.98	0.83
16:b:606:CLA:H71	18:b:619:BCR:H342	0.83	0.83
2:B:28:PRO:HB3	2:B:31:LYS:HD2	1.59	0.82
16:b:602:CLA:H43	8:h:45:ILE:CG2	2.09	0.81
2:B:28:PRO:CA	2:B:31:LYS:HG3	1.95	0.81
5:d:14:TRP:CB	25:d:411:HTG:C6	2.50	0.80
16:b:607:CLA:C18	20:d:409:MGE:C6A	2.60	0.80
2:B:28:PRO:O	2:B:31:LYS:HG3	1.83	0.79
2:B:28:PRO:O	2:B:32:VAL:CG1	2.31	0.79
4:b:90:PHE:CE2	16:b:606:CLA:H162	2.18	0.78
5:d:238:THR:CG2	5:d:242:GLU:OE2	2.32	0.78
2:B:50:ALA:HB3	14:C:36:ALA:HB2	1.66	0.77
4:b:165:GLY:HA3	4:b:179:GLN:O	1.84	0.77
3:a:257:ARG:HA	3:a:257:ARG:NE	1.96	0.77
16:b:606:CLA:C5	18:b:619:BCR:H342	2.14	0.77
2:B:28:PRO:CB	2:B:31:LYS:CD	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:b:100:HIS:ND1	16:b:606:CLA:C4	2.48	0.76
1:A:6:GLU:OE2	1:A:14:ASN:CG	2.30	0.75
16:b:606:CLA:H71	18:b:619:BCR:C9	2.18	0.73
1:A:6:GLU:OE2	1:A:14:ASN:HB3	1.88	0.73
11:m:8:PHE:CE2	12:t:1:MET:HE2	2.24	0.73
2:B:28:PRO:CA	2:B:31:LYS:HG2	2.05	0.72
5:d:246:MET:CE	5:d:261:PHE:O	2.37	0.72
1:A:44:VAL:HG13	1:A:77:PRO:HB2	1.72	0.72
16:b:608:CLA:HBB1	5:d:126:MET:HE2	1.72	0.71
16:a:402:CLA:H202	17:a:404:PHO:H43	1.71	0.71
2:B:50:ALA:CB	14:C:36:ALA:HB2	2.19	0.71
4:b:62:VAL:HG13	16:b:605:CLA:HED3	1.73	0.71
2:B:28:PRO:CB	2:B:31:LYS:HD2	2.21	0.70
4:b:62:VAL:CG1	16:b:605:CLA:HED3	2.21	0.70
16:b:615:CLA:H2	16:b:616:CLA:HBB2	1.72	0.70
4:b:148:LEU:HD23	16:b:604:CLA:H191	1.73	0.69
16:b:606:CLA:H52	18:b:619:BCR:HC7	1.75	0.69
3:a:257:ARG:HE	5:d:136:VAL:CG2	2.06	0.69
1:A:69:ASN:ND2	1:A:81:GLU:OE1	2.26	0.69
2:B:50:ALA:HB3	14:C:36:ALA:HB1	1.75	0.69
2:B:28:PRO:HB3	2:B:31:LYS:CD	2.22	0.69
3:a:293:MET:HE1	3:a:298:ASN:HB3	1.75	0.69
11:m:8:PHE:CZ	12:t:1:MET:HE2	2.27	0.69
1:A:43:ILE:HD12	1:A:43:ILE:O	1.92	0.69
4:b:391:SER:CB	4:b:394:GLN:OE1	2.42	0.68
1:A:66:ARG:HD3	5:d:135:LEU:O	1.94	0.66
3:a:183:MET:SD	16:d:401:CLA:HAC1	2.35	0.66
3:a:257:ARG:HH21	3:a:257:ARG:CG	2.09	0.65
16:b:606:CLA:C6	18:b:619:BCR:H342	2.24	0.65
1:A:11:ARG:CB	1:A:11:ARG:HH21	2.10	0.65
2:B:43:LEU:HB3	14:C:43:ALA:HB2	1.79	0.65
1:A:6:GLU:OE2	1:A:14:ASN:CB	2.46	0.64
1:A:66:ARG:O	3:a:255:PHE:CZ	2.50	0.64
3:a:293:MET:HE1	3:a:298:ASN:CA	2.27	0.64
17:a:404:PHO:H162	16:d:401:CLA:H143	1.80	0.64
16:b:606:CLA:H2	18:b:619:BCR:C32	2.27	0.63
4:b:100:HIS:ND1	16:b:606:CLA:H42	2.14	0.62
1:A:66:ARG:CB	3:a:255:PHE:HZ	2.12	0.62
1:A:11:ARG:HH21	1:A:11:ARG:CG	2.12	0.62
4:b:100:HIS:CE1	16:b:606:CLA:H43	2.35	0.62
5:d:14:TRP:HB2	25:d:411:HTG:H61	1.74	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:89:ILE:HD11	3:a:108:ASN:HB3	1.80	0.62
4:b:247:PHE:HE1	16:b:602:CLA:H102	1.64	0.62
1:A:41:PRO:O	1:A:45:GLN:HG2	2.00	0.62
1:A:44:VAL:CG1	1:A:77:PRO:HB2	2.29	0.61
16:b:607:CLA:H2	20:b:620:MGE:H6A1	1.82	0.61
1:A:8:GLN:NE2	1:A:13:ILE:O	2.34	0.61
2:B:28:PRO:CA	2:B:31:LYS:HD2	2.27	0.61
5:d:186:GLN:HB2	16:d:404:CLA:HBC1	1.82	0.61
3:a:257:ARG:HE	5:d:136:VAL:HG22	1.67	0.60
4:b:149:LEU:HB2	16:b:604:CLA:H171	1.83	0.60
4:b:100:HIS:ND1	16:b:606:CLA:H43	2.17	0.60
1:A:5:ALA:N	1:A:58:ASP:CA	2.58	0.59
3:a:293:MET:HE1	3:a:298:ASN:HA	1.83	0.59
5:d:217:THR:HG21	5:d:253:TRP:HE1	1.66	0.59
4:b:64:PRO:HB3	4:b:267:LEU:HB3	1.83	0.59
1:A:51:VAL:HG12	3:a:255:PHE:HB2	1.85	0.59
16:a:402:CLA:HBC3	16:a:402:CLA:HMC3	1.83	0.59
1:A:81:GLU:O	1:A:81:GLU:HG2	2.02	0.59
18:d:407:BCR:H271	20:d:408:MGE:H231	1.85	0.58
16:a:402:CLA:C20	17:a:404:PHO:H43	2.33	0.58
3:a:76:ASN:OD1	3:a:76:ASN:N	2.37	0.58
3:a:257:ARG:NE	5:d:136:VAL:CG2	2.66	0.58
3:a:332:HIS:CD2	19:a:408:CL:CL	2.88	0.58
5:d:241:GLU:OE2	5:d:244:TYR:CZ	2.57	0.57
3:a:276:ALA:O	3:a:280:VAL:HG23	2.04	0.57
4:b:455:HIS:HE1	16:b:607:CLA:HBB2	1.69	0.57
1:A:41:PRO:O	1:A:45:GLN:CG	2.53	0.57
2:B:28:PRO:CB	2:B:31:LYS:HD3	2.33	0.57
3:a:29:TYR:O	3:a:129:ARG:NH1	2.38	0.57
3:a:29:TYR:OH	3:a:136:ARG:NH1	2.38	0.57
1:A:42:LYS:HA	1:A:45:GLN:HG3	1.86	0.57
3:a:293:MET:HE1	3:a:298:ASN:CB	2.34	0.57
6:e:77:GLU:HA	6:e:80:LEU:HB2	1.87	0.57
3:a:254:TYR:HA	5:d:237:PRO:HG2	1.87	0.56
1:A:46:GLU:HA	5:d:233:ARG:HD3	1.87	0.56
3:a:255:PHE:N	5:d:237:PRO:HG3	2.20	0.56
1:A:43:ILE:HD11	5:d:233:ARG:HH11	1.70	0.56
2:B:28:PRO:CA	2:B:31:LYS:HD3	2.34	0.56
4:b:9:HIS:ND1	16:b:613:CLA:O1A	2.38	0.56
15:l:101:SQD:H141	20:m:101:MGE:H7B1	1.86	0.56
2:B:36:LEU:HB3	14:C:50:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HB2	4:b:493:TRP:HB2	1.87	0.56
20:d:410:MGE:H9A2	12:t:21:ILE:HD11	1.88	0.56
4:b:247:PHE:CE1	16:b:602:CLA:H121	2.41	0.55
16:b:615:CLA:H2	16:b:616:CLA:CBB	2.36	0.55
1:A:66:ARG:CA	3:a:255:PHE:CZ	2.89	0.55
4:b:148:LEU:HD23	16:b:604:CLA:C19	2.35	0.55
4:b:311:PHE:O	4:b:317:ASN:ND2	2.40	0.55
1:A:66:ARG:HA	3:a:255:PHE:CZ	2.41	0.55
3:a:302:PHE:N	3:a:302:PHE:CD1	2.73	0.55
5:d:56:THR:HB	6:e:49:THR:HG23	1.88	0.55
4:b:229:LEU:HD21	16:b:609:CLA:H43	1.87	0.55
5:d:241:GLU:OE2	5:d:244:TYR:CE1	2.60	0.55
3:a:257:ARG:HG3	3:a:257:ARG:NH2	2.09	0.55
1:A:26:ALA:C	1:A:28:ASP:H	2.14	0.55
13:x:21:LEU:HD11	21:x:101:UNL:C38	2.37	0.55
1:A:49:LEU:O	5:d:233:ARG:NH1	2.38	0.54
16:a:402:CLA:HMC1	16:d:404:CLA:HAC2	1.88	0.54
10:l:12:LEU:H	11:m:29:THR:HG21	1.71	0.54
1:A:10:ILE:HD11	1:A:43:ILE:CD1	2.38	0.54
16:b:604:CLA:H43	16:b:605:CLA:H2	1.90	0.54
17:a:404:PHO:H72	16:d:401:CLA:H201	1.90	0.54
1:A:10:ILE:HG21	1:A:49:LEU:HB3	1.90	0.54
16:a:402:CLA:CMC	16:d:404:CLA:HAC2	2.37	0.54
3:a:44:ALA:HB2	3:a:118:HIS:HB2	1.90	0.54
3:a:84:PRO:HD3	3:a:173:PRO:HB3	1.90	0.54
3:a:257:ARG:HA	3:a:257:ARG:NH2	2.23	0.54
4:b:269:GLY:O	4:b:448:ARG:NH1	2.40	0.54
4:b:100:HIS:CE1	16:b:606:CLA:C4	2.91	0.54
4:b:164:PRO:HD3	16:b:606:CLA:O1D	2.08	0.53
15:l:101:SQD:H45	20:m:101:MGE:H4A1	1.90	0.53
16:b:607:CLA:HMC2	18:b:618:BCR:H323	1.88	0.53
4:b:486:LEU:HG	4:b:490:GLN:NE2	2.22	0.53
3:a:257:ARG:HD3	5:d:132:ILE:HG23	1.90	0.53
3:a:76:ASN:HD22	10:l:33:SER:HB3	1.74	0.53
16:b:606:CLA:C7	18:b:619:BCR:C34	2.43	0.53
16:b:613:CLA:HBB1	16:b:613:CLA:HMB1	1.90	0.53
4:b:9:HIS:CE1	16:b:613:CLA:O1A	2.62	0.53
4:b:149:LEU:HD22	16:b:604:CLA:H152	1.90	0.53
4:b:477:ASP:OD1	4:b:477:ASP:N	2.41	0.52
16:b:608:CLA:H191	5:d:89:LEU:HD13	1.91	0.52
3:a:176:ILE:CD1	16:d:401:CLA:HMA3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:a:403:CLA:CMC	16:d:404:CLA:H2	2.39	0.52
16:a:403:CLA:HMC1	16:d:404:CLA:H2	1.91	0.52
2:B:21:TYR:CE2	8:h:20:LYS:NZ	2.77	0.52
1:A:50:GLU:CD	5:d:236:ASN:HB2	2.27	0.52
4:b:464:PHE:HA	4:b:467:ILE:HD12	1.92	0.52
1:A:6:GLU:OE2	1:A:14:ASN:ND2	2.43	0.51
4:b:27:THR:HG22	4:b:107:LEU:HD13	1.91	0.51
4:b:388:SER:HA	5:d:344:GLU:OE1	2.10	0.51
20:b:622:MGE:H8B2	10:l:19:LEU:HD22	1.92	0.51
5:d:222:LEU:HD23	5:d:243:THR:O	2.10	0.51
8:h:61:SER:OG	8:h:62:TRP:N	2.44	0.51
16:b:610:CLA:H152	16:b:610:CLA:H203	1.92	0.51
13:x:2:THR:OG1	13:x:3:ILE:N	2.44	0.51
16:d:401:CLA:H42	24:d:406:PQ9:H22	1.91	0.51
3:a:257:ARG:NE	3:a:257:ARG:CA	2.73	0.51
4:b:91:TRP:CZ2	16:b:606:CLA:H18	2.45	0.51
5:d:262:SER:H	20:d:410:MGE:H2D	1.76	0.51
3:a:61:ASP:OD1	3:a:61:ASP:N	2.45	0.50
5:d:246:MET:HE1	24:d:406:PQ9:H93	1.93	0.50
16:b:604:CLA:HMC1	16:b:611:CLA:H191	1.92	0.50
3:a:183:MET:HG2	16:d:401:CLA:HBC1	1.94	0.50
4:b:2:GLY:N	10:l:9:PRO:O	2.44	0.50
1:A:11:ARG:CG	1:A:11:ARG:NH2	2.73	0.50
5:d:304:ARG:HH22	22:d:402:LMT:H3O1	1.58	0.49
1:A:8:GLN:HB2	1:A:13:ILE:O	2.12	0.49
3:a:34:GLY:HA2	3:a:37:MET:HB3	1.94	0.49
3:a:42:LEU:HD23	18:a:407:BCR:H12C	1.94	0.49
11:m:8:PHE:CE2	12:t:1:MET:CE	2.94	0.49
11:m:8:PHE:HD1	11:m:8:PHE:O	1.95	0.49
16:b:606:CLA:C7	18:b:619:BCR:C9	2.85	0.49
20:d:410:MGE:H8B2	20:d:410:MGE:H6A2	1.94	0.49
1:A:26:ALA:C	1:A:28:ASP:N	2.71	0.49
5:d:148:ALA:HB2	5:d:276:VAL:HG13	1.95	0.49
1:A:66:ARG:C	3:a:255:PHE:CE2	2.88	0.49
4:b:57:ARG:NH2	4:b:317:ASN:OD1	2.46	0.49
4:b:160:GLY:HA3	4:b:180:PRO:HB3	1.94	0.49
8:h:53:LEU:HA	13:x:6:SER:HB3	1.95	0.48
4:b:379:ALA:HA	4:b:390:TYR:HB3	1.95	0.48
1:A:44:VAL:HG12	1:A:44:VAL:O	2.12	0.48
4:b:24:LEU:HG	16:b:615:CLA:HED2	1.94	0.48
11:m:8:PHE:CD1	11:m:8:PHE:C	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:143:ILE:HG13	5:d:220:ASN:HD22	1.78	0.48
3:a:162:PRO:HB3	3:a:168:PHE:HA	1.95	0.48
3:a:129:ARG:NH2	5:d:256:ILE:O	2.47	0.48
16:a:402:CLA:H202	17:a:404:PHO:C4	2.42	0.48
5:d:296:TYR:OH	5:d:326:ARG:NH2	2.40	0.48
2:B:21:TYR:OH	8:h:20:LYS:NZ	2.46	0.48
4:b:145:LEU:HD22	16:b:604:CLA:H162	1.94	0.48
5:d:155:SER:HB2	5:d:287:VAL:HG23	1.95	0.48
4:b:78:TRP:HA	4:b:84:THR:HA	1.96	0.48
5:d:238:THR:HG21	5:d:242:GLU:CD	2.39	0.48
7:f:17:THR:OG1	7:f:18:VAL:N	2.44	0.48
5:d:205:LEU:HB3	16:d:401:CLA:H11	1.95	0.47
11:m:8:PHE:CD2	12:t:1:MET:HG3	2.48	0.47
17:a:405:PHO:HBC1	5:d:275:PRO:HB2	1.96	0.47
12:t:1:MET:N	22:t:101:LMT:O6'	2.44	0.47
18:a:407:BCR:H24C	18:a:407:BCR:H371	1.69	0.47
5:d:242:GLU:O	5:d:242:GLU:HG2	2.14	0.47
5:d:246:MET:CE	24:d:406:PQ9:H93	2.44	0.47
17:a:404:PHO:H193	16:d:401:CLA:H142	1.95	0.47
6:e:25:ILE:HG12	6:e:26:THR:HG22	1.96	0.47
1:A:11:ARG:NH2	1:A:11:ARG:HG2	2.29	0.47
1:A:43:ILE:CD1	5:d:233:ARG:HH11	2.28	0.47
3:a:82:VAL:HB	3:a:174:LEU:HD12	1.97	0.47
3:a:15:GLU:O	3:a:19:ASN:ND2	2.47	0.47
4:b:225:LEU:HA	4:b:228:ALA:HB3	1.97	0.47
4:b:275:TRP:CE2	4:b:315:ILE:HD13	2.50	0.47
5:d:265:ARG:NH2	20:d:409:MGE:O4D	2.48	0.47
9:i:25:SER:OG	9:i:26:GLY:N	2.47	0.47
1:A:66:ARG:CG	3:a:255:PHE:CZ	2.98	0.47
18:a:407:BCR:H341	18:a:407:BCR:H11C	1.65	0.47
4:b:391:SER:HB3	4:b:394:GLN:OE1	2.14	0.47
17:a:405:PHO:H61	5:d:118:GLY:HA2	1.97	0.47
5:d:113:PHE:O	5:d:117:HIS:ND1	2.48	0.46
1:A:51:VAL:HG12	3:a:255:PHE:CB	2.45	0.46
3:a:13:LEU:C	3:a:15:GLU:N	2.73	0.46
3:a:316:THR:OG1	3:a:317:TRP:N	2.48	0.46
4:b:9:HIS:CD2	16:b:612:CLA:HBB2	2.50	0.46
1:A:43:ILE:HD11	5:d:233:ARG:NH1	2.31	0.46
5:d:25:ASP:OD1	5:d:25:ASP:N	2.41	0.46
5:d:71:CYS:HB3	5:d:75:THR:HB	1.97	0.46
3:a:13:LEU:C	3:a:15:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:172:SER:HB2	5:d:177:ALA:HB1	1.97	0.46
1:A:44:VAL:HG13	1:A:77:PRO:CB	2.42	0.45
4:b:141:ILE:HD11	8:h:14:LEU:HD22	1.98	0.45
8:h:12:ARG:NH1	8:h:15:ASN:O	2.45	0.45
1:A:31:SER:HB3	4:b:490:GLN:HE22	1.81	0.45
16:b:606:CLA:C5	18:b:619:BCR:C34	2.92	0.45
5:d:103:ARG:HG2	6:e:73:LYS:HG2	1.98	0.45
16:d:404:CLA:H41	16:d:404:CLA:H61	1.64	0.45
2:B:33:ARG:O	14:C:50:ALA:HB1	2.16	0.45
4:b:391:SER:OG	4:b:392:PHE:N	2.48	0.45
5:d:297:ASP:OD1	5:d:297:ASP:N	2.49	0.45
2:B:47:GLY:O	14:C:36:ALA:HB1	2.17	0.45
4:b:73:GLY:HA2	4:b:79:SER:HA	1.97	0.45
5:d:89:LEU:HG	8:h:50:ASN:HD22	1.81	0.45
3:a:183:MET:CG	16:d:401:CLA:HBC1	2.47	0.45
4:b:79:SER:OG	4:b:80:ILE:N	2.49	0.45
4:b:237:VAL:HG11	16:b:610:CLA:H201	1.99	0.45
16:b:610:CLA:H203	16:b:610:CLA:C15	2.46	0.45
11:m:8:PHE:O	11:m:8:PHE:CD1	2.70	0.45
2:B:55:VAL:HB	4:b:159:THR:HG21	1.98	0.44
4:b:74:SER:HA	4:b:92:SER:HB2	1.99	0.44
1:A:67:ASP:OD2	1:A:83:THR:HB	2.17	0.44
2:B:31:LYS:HE3	2:B:31:LYS:HB2	1.55	0.44
4:b:74:SER:OG	4:b:75:TRP:N	2.49	0.44
5:d:296:TYR:O	5:d:315:TYR:OH	2.34	0.44
16:d:401:CLA:H203	16:d:401:CLA:H162	1.69	0.44
1:A:42:LYS:HE3	1:A:42:LYS:HB2	1.59	0.44
24:d:406:PQ9:H352	10:l:30:LEU:HD22	1.98	0.44
4:b:80:ILE:HD13	4:b:80:ILE:HA	1.84	0.44
5:d:53:THR:HG22	7:f:40:MET:HE1	1.99	0.44
4:b:455:HIS:HE1	16:b:607:CLA:CBB	2.30	0.44
3:a:259:ILE:H	3:a:259:ILE:HG13	1.48	0.43
18:b:619:BCR:H361	18:b:619:BCR:H20C	1.80	0.43
5:d:152:VAL:HG21	5:d:279:LEU:HD13	2.00	0.43
8:h:20:LYS:HZ3	8:h:20:LYS:HB2	1.83	0.43
4:b:122:LEU:HD21	16:b:615:CLA:HBC2	1.99	0.43
1:A:66:ARG:CA	3:a:255:PHE:HZ	2.30	0.43
3:a:14:TRP:O	3:a:14:TRP:CG	2.70	0.43
1:A:10:ILE:HD11	1:A:43:ILE:HD11	2.00	0.43
8:h:41:PHE:HB2	18:h:101:BCR:H16C	1.99	0.43
18:b:618:BCR:H24C	18:b:618:BCR:H371	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:m:8:PHE:HD1	11:m:8:PHE:C	2.26	0.43
1:A:69:ASN:HD22	1:A:81:GLU:CD	2.26	0.43
2:B:13:ASN:HB2	4:b:10:THR:HB	2.01	0.43
16:b:614:CLA:H62	16:b:614:CLA:H41	1.35	0.43
16:b:615:CLA:H92	16:b:615:CLA:H61	1.81	0.43
5:d:236:ASN:N	5:d:237:PRO:HD2	2.34	0.43
6:e:58:GLN:HG2	6:e:59:GLU:HG3	2.00	0.43
11:m:8:PHE:CE2	12:t:1:MET:CG	2.93	0.43
1:A:75:GLY:HA2	5:d:242:GLU:O	2.18	0.42
16:b:606:CLA:H52	18:b:619:BCR:H342	1.99	0.42
18:d:407:BCR:H15C	18:d:407:BCR:H351	1.89	0.42
18:a:407:BCR:H15C	18:a:407:BCR:H351	1.80	0.42
5:d:72:ASN:HA	20:d:408:MGE:H1D	2.01	0.42
5:d:262:SER:O	5:d:262:SER:OG	2.37	0.42
5:d:266:TRP:CD1	20:d:410:MGE:H1D	2.55	0.42
4:b:257:TRP:HB2	4:b:452:THR:HG21	2.01	0.42
6:e:75:GLN:O	6:e:78:THR:HB	2.19	0.42
4:b:236:THR:HB	4:b:473:THR:HG21	2.01	0.42
18:d:407:BCR:H11C	18:d:407:BCR:H341	1.93	0.42
16:a:402:CLA:H51	17:a:404:PHO:C4B	2.50	0.42
4:b:30:VAL:HG12	16:b:605:CLA:HHD	2.02	0.42
18:b:618:BCR:H20C	18:b:618:BCR:H361	1.83	0.42
20:b:622:MGE:H7A1	11:m:18:PRO:HB3	2.02	0.42
4:b:227:LYS:HE2	4:b:227:LYS:HB3	1.85	0.42
8:h:35:MET:HG2	18:h:101:BCR:H312	2.02	0.42
1:A:64:VAL:HG21	1:A:66:ARG:HH21	1.84	0.42
4:b:247:PHE:CE1	16:b:602:CLA:H102	2.50	0.42
16:b:608:CLA:H162	16:d:405:CLA:H3A	2.01	0.42
17:a:404:PHO:H61	17:a:404:PHO:H41	1.78	0.42
4:b:248:ALA:HA	16:b:603:CLA:H42	2.02	0.42
16:b:606:CLA:H72	18:b:619:BCR:H311	2.01	0.42
5:d:335:PRO:HB2	6:e:65:LEU:HD11	2.00	0.42
2:B:36:LEU:HB3	14:C:50:ALA:CB	2.50	0.42
4:b:57:ARG:NH1	4:b:334:ASP:OD1	2.53	0.42
5:d:14:TRP:HB3	25:d:411:HTG:O6	2.16	0.42
4:b:51:VAL:HG13	4:b:308:LYS:HB2	2.02	0.42
4:b:247:PHE:HD1	16:b:602:CLA:H142	1.84	0.41
16:b:607:CLA:H172	5:d:281:MET:HE2	2.01	0.41
4:b:119:ASP:OD1	8:h:2:ALA:N	2.53	0.41
4:b:424:ALA:HB2	4:b:429:ILE:HD11	2.02	0.41
5:d:246:MET:HE1	5:d:261:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:410:MGE:H4A2	10:l:22:LEU:HD22	2.02	0.41
3:a:258:LEU:H	3:a:258:LEU:HG	1.56	0.41
3:a:257:ARG:CG	3:a:257:ARG:NH2	2.73	0.41
4:b:247:PHE:CD1	16:b:602:CLA:H121	2.55	0.41
18:d:407:BCR:H363	7:f:33:PHE:HB3	2.03	0.41
1:A:66:ARG:CB	3:a:255:PHE:CZ	2.99	0.41
18:h:101:BCR:H15C	18:h:101:BCR:H351	1.83	0.41
5:d:24:ARG:HH12	13:x:35:ASP:HB3	1.84	0.41
24:d:406:PQ9:H193	20:d:410:MGE:H7B1	2.02	0.41
5:d:246:MET:HE3	5:d:261:PHE:O	2.19	0.41
2:B:50:ALA:HB1	14:C:36:ALA:HB2	1.99	0.41
3:a:188:ALA:HB2	3:a:328:MET:HB2	2.02	0.41
5:d:162:LEU:HD11	26:d:412:DGD:HA32	2.02	0.41
5:d:233:ARG:NH2	5:d:234:ALA:O	2.54	0.41
1:A:86:MET:HG2	1:A:92:TRP:HE3	1.85	0.41
16:a:402:CLA:HBB1	16:a:402:CLA:HMB1	2.02	0.41
4:b:388:SER:HB3	4:b:394:GLN:NE2	2.22	0.41
5:d:304:ARG:HE	5:d:304:ARG:HB3	1.62	0.41
24:d:406:PQ9:H191	24:d:406:PQ9:H211	1.87	0.41
1:A:113:SER:N	4:b:493:TRP:O	2.54	0.41
3:a:258:LEU:HB2	3:a:259:ILE:H	1.62	0.41
4:b:223:GLN:HG2	4:b:227:LYS:HE3	2.02	0.41
5:d:259:ILE:HA	5:d:259:ILE:HD12	1.85	0.40
16:d:404:CLA:HBB1	16:d:404:CLA:CHC	2.51	0.40
4:b:54:PRO:HD2	4:b:57:ARG:HB2	2.03	0.40
4:b:423:LYS:HA	4:b:423:LYS:HD2	1.92	0.40
17:a:405:PHO:H71	17:a:405:PHO:H112	1.77	0.40
16:b:603:CLA:HAB	16:b:605:CLA:H171	2.03	0.40
18:b:619:BCR:H24C	18:b:619:BCR:H371	1.77	0.40
5:d:159:ILE:HG21	5:d:287:VAL:HG22	2.03	0.40
1:A:66:ARG:HB3	3:a:255:PHE:HZ	1.85	0.40
3:a:323:ARG:HD3	3:a:323:ARG:HA	1.85	0.40
4:b:103:LEU:HD22	16:b:606:CLA:H41	2.04	0.40
4:b:103:LEU:HD22	16:b:606:CLA:H51	2.03	0.40
18:b:617:BCR:H11C	18:b:617:BCR:H341	1.88	0.40
1:A:17:VAL:HG21	1:A:41:PRO:HA	2.04	0.40
1:A:44:VAL:HG13	1:A:77:PRO:CG	2.52	0.40
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.78	0.40
3:a:257:ARG:CD	5:d:132:ILE:HG23	2.51	0.40
16:b:601:CLA:HMB2	18:h:101:BCR:H391	2.04	0.40
16:b:606:CLA:H72	18:b:619:BCR:C7	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	107/116 (92%)	91 (85%)	15 (14%)	1 (1%)	14	41
2	B	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
3	a	292/360 (81%)	272 (93%)	20 (7%)	0	100	100
4	b	464/505 (92%)	439 (95%)	24 (5%)	1 (0%)	43	70
5	d	337/342 (98%)	323 (96%)	13 (4%)	1 (0%)	36	64
6	e	61/84 (73%)	53 (87%)	8 (13%)	0	100	100
7	f	26/45 (58%)	26 (100%)	0	0	100	100
8	h	60/65 (92%)	57 (95%)	3 (5%)	0	100	100
9	i	27/38 (71%)	26 (96%)	1 (4%)	0	100	100
10	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	m	29/36 (81%)	27 (93%)	2 (7%)	0	100	100
12	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
13	x	34/40 (85%)	34 (100%)	0	0	100	100
14	C	21/23 (91%)	20 (95%)	1 (5%)	0	100	100
All	All	1569/1779 (88%)	1475 (94%)	91 (6%)	3 (0%)	44	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	d	242	GLU
1	A	47	GLY
4	b	387	GLU

5.3.2 Protein sidechains ⓘ

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	92/97 (95%)	70 (76%)	22 (24%)	1	3
2	B	36/42 (86%)	31 (86%)	5 (14%)	3	14
3	a	237/290 (82%)	200 (84%)	37 (16%)	2	11
4	b	392/403 (97%)	357 (91%)	35 (9%)	9	29
5	d	272/277 (98%)	245 (90%)	27 (10%)	7	26
6	e	55/73 (75%)	52 (94%)	3 (6%)	19	46
7	f	22/39 (56%)	21 (96%)	1 (4%)	24	52
8	h	53/54 (98%)	51 (96%)	2 (4%)	29	56
9	i	26/35 (74%)	22 (85%)	4 (15%)	2	11
10	l	35/35 (100%)	32 (91%)	3 (9%)	10	31
11	m	28/33 (85%)	26 (93%)	2 (7%)	13	37
12	t	26/29 (90%)	26 (100%)	0	100	100
13	x	29/33 (88%)	27 (93%)	2 (7%)	14	38
All	All	1303/1440 (90%)	1160 (89%)	143 (11%)	8	21

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	10	ILE
1	A	11	ARG
1	A	13	ILE
1	A	18	VAL
1	A	27	ARG
1	A	28	ASP
1	A	30	SER
1	A	42	LYS
1	A	43	ILE
1	A	45	GLN
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	54	MET
1	A	57	VAL
1	A	63	ILE
1	A	65	THR
1	A	66	ARG
1	A	80	ILE
1	A	81	GLU
1	A	94	ARG
1	A	108	LEU
1	A	112	LYS
2	B	31	LYS
2	B	32	VAL
2	B	33	ARG
2	B	43	LEU
2	B	53	VAL
3	a	15	GLU
3	a	22	THR
3	a	24	THR
3	a	35	VAL
3	a	61	ASP
3	a	70	SER
3	a	71	LEU
3	a	76	ASN
3	a	83	VAL
3	a	103	ASP
3	a	104	GLU
3	a	116	ILE
3	a	121	LEU
3	a	133	LEU
3	a	157	VAL
3	a	159	LEU
3	a	163	ILE
3	a	167	SER
3	a	174	LEU
3	a	177	SER
3	a	205	VAL
3	a	248	ILE
3	a	255	PHE
3	a	257	ARG
3	a	258	LEU
3	a	259	ILE
3	a	271	LEU

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Mol	Chain	Res	Type
3	a	275	LEU
3	a	288	LEU
3	a	290	ILE
3	a	297	LEU
3	a	300	PHE
3	a	301	ASN
3	a	302	PHE
3	a	316	THR
3	a	317	TRP
3	a	323	ARG
4	b	62	VAL
4	b	63	LEU
4	b	80	ILE
4	b	84	THR
4	b	87	ASP
4	b	116	VAL
4	b	128	THR
4	b	137	LYS
4	b	178	VAL
4	b	198	VAL
4	b	201	HIS
4	b	225	LEU
4	b	229	LEU
4	b	240	SER
4	b	245	VAL
4	b	284	ILE
4	b	288	VAL
4	b	315	ILE
4	b	321	LYS
4	b	357	ARG
4	b	362	PHE
4	b	385	ARG
4	b	387	GLU
4	b	388	SER
4	b	389	LYS
4	b	392	PHE
4	b	399	VAL
4	b	416	THR
4	b	436	THR
4	b	437	LEU
4	b	439	SER
4	b	440	ASP

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Mol	Chain	Res	Type
4	b	446	SER
4	b	478	VAL
4	b	489	GLU
5	d	18	LEU
5	d	25	ASP
5	d	30	VAL
5	d	69	GLU
5	d	131	GLU
5	d	138	VAL
5	d	178	ILE
5	d	180	ARG
5	d	192	THR
5	d	193	LEU
5	d	194	ASN
5	d	205	LEU
5	d	209	LEU
5	d	238	THR
5	d	242	GLU
5	d	243	THR
5	d	245	SER
5	d	259	ILE
5	d	262	SER
5	d	272	LEU
5	d	279	LEU
5	d	291	LEU
5	d	294	ARG
5	d	307	GLU
5	d	316	THR
5	d	340	VAL
5	d	348	ARG
6	e	36	LEU
6	e	59	GLU
6	e	83	LEU
7	f	17	THR
8	h	20	LYS
8	h	21	VAL
9	i	4	LEU
9	i	9	TYR
9	i	20	VAL
9	i	23	PHE
10	l	7	ARG
10	l	13	ASN

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Mol	Chain	Res	Type
10	l	32	SER
11	m	6	LEU
11	m	16	LEU
13	x	14	LEU
13	x	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	69	ASN
1	A	76	GLN
2	B	30	GLN
3	a	19	ASN
3	a	118	HIS
3	a	165	GLN
3	a	187	GLN
3	a	190	HIS
3	a	272	HIS
3	a	296	ASN
3	a	301	ASN
3	a	322	ASN
3	a	332	HIS
4	b	58	GLN
4	b	179	GLN
4	b	223	GLN
4	b	289	GLN
4	b	331	ASN
4	b	338	GLN
4	b	395	GLN
4	b	455	HIS
4	b	490	GLN
5	d	98	GLN
5	d	129	GLN
5	d	164	GLN
5	d	194	ASN
5	d	236	ASN
5	d	250	ASN
5	d	332	GLN
10	l	4	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 50 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 46 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
16	CLA	b	615	-	69,73,73	2.04	17 (24%)	82,113,113	2.38	28 (34%)
16	CLA	d	404	-	65,69,73	1.91	12 (18%)	77,108,113	3.86	38 (49%)
20	MGE	d	408	-	47,47,48	0.97	2 (4%)	55,55,56	1.21	5 (9%)
16	CLA	b	601	-	45,49,73	2.38	17 (37%)	54,84,113	4.55	28 (51%)
18	BCR	b	617	-	41,41,41	0.71	0	56,56,56	1.72	16 (28%)
16	CLA	b	602	-	69,73,73	2.14	18 (26%)	82,113,113	2.17	28 (34%)
16	CLA	b	611	-	69,73,73	2.06	16 (23%)	82,113,113	2.30	28 (34%)
22	LMT	d	402	-	36,36,36	0.41	0	47,47,47	0.87	0
18	BCR	d	407	-	41,41,41	0.68	0	56,56,56	1.62	13 (23%)
16	CLA	b	614	-	56,60,73	2.10	16 (28%)	65,97,113	3.09	36 (55%)
16	CLA	b	604	-	69,73,73	2.12	18 (26%)	82,113,113	2.46	28 (34%)
18	BCR	h	101	-	41,41,41	0.76	0	56,56,56	2.05	17 (30%)
22	LMT	t	101	-	36,36,36	0.46	0	47,47,47	1.11	4 (8%)
20	MGE	b	622	-	48,48,48	0.97	2 (4%)	56,56,56	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b	618	-	41,41,41	0.64	0	56,56,56	1.90	17 (30%)
15	SQD	l	101	-	45,47,54	1.25	3 (6%)	55,58,65	3.43	9 (16%)
18	BCR	b	619	-	41,41,41	0.72	1 (2%)	56,56,56	2.01	17 (30%)
25	HTG	d	411	-	16,16,19	1.08	2 (12%)	20,21,24	1.49	2 (10%)
16	CLA	b	603	-	69,73,73	2.06	19 (27%)	82,113,113	2.45	30 (36%)
16	CLA	a	403	-	54,58,73	2.06	12 (22%)	64,95,113	4.45	34 (53%)
20	MGE	d	410	-	48,48,48	0.98	3 (6%)	56,56,56	1.56	11 (19%)
16	CLA	b	607	-	69,73,73	2.31	18 (26%)	82,113,113	2.04	27 (32%)
20	MGE	m	101	-	48,48,48	1.01	3 (6%)	56,56,56	1.11	4 (7%)
22	LMT	b	623	-	36,36,36	0.44	0	47,47,47	0.85	1 (2%)
20	MGE	a	409	-	48,48,48	0.99	2 (4%)	56,56,56	1.05	4 (7%)
17	PHO	a	404	-	58,69,69	2.09	11 (18%)	55,99,99	1.93	14 (25%)
20	MGE	b	620	-	48,48,48	0.97	2 (4%)	56,56,56	1.38	5 (8%)
16	CLA	b	605	-	69,73,73	1.96	18 (26%)	82,113,113	2.43	28 (34%)
16	CLA	b	613	-	58,62,73	2.11	18 (31%)	68,99,113	2.46	25 (36%)
27	HEM	e	101	-	50,50,50	1.57	8 (16%)	67,82,82	1.66	11 (16%)
16	CLA	a	406	-	54,58,73	2.17	15 (27%)	64,95,113	4.43	34 (53%)
26	DGD	d	412	-	55,55,67	0.94	2 (3%)	69,69,81	1.18	7 (10%)
15	SQD	a	401	-	24,26,54	1.65	3 (12%)	34,37,65	4.44	11 (32%)
17	PHO	a	405	-	58,69,69	2.04	10 (17%)	55,99,99	1.97	14 (25%)
16	CLA	b	616	-	50,54,73	2.52	19 (38%)	59,90,113	2.69	27 (45%)
16	CLA	b	606	-	69,73,73	2.32	20 (28%)	82,113,113	2.43	30 (36%)
16	CLA	b	610	-	69,73,73	2.16	18 (26%)	82,113,113	2.44	26 (31%)
16	CLA	a	402	-	69,73,73	1.91	16 (23%)	82,113,113	2.28	30 (36%)
20	MGE	d	409	-	41,41,48	1.07	2 (4%)	49,49,56	1.46	9 (18%)
16	CLA	b	612	-	69,73,73	2.21	18 (26%)	82,113,113	2.50	29 (35%)
16	CLA	d	405	-	54,58,73	2.11	15 (27%)	64,95,113	4.19	32 (50%)
24	PQ9	d	406	-	45,45,45	0.77	1 (2%)	56,57,57	1.43	10 (17%)
18	BCR	a	407	-	41,41,41	0.72	0	56,56,56	2.39	19 (33%)
16	CLA	b	608	-	69,73,73	2.10	18 (26%)	82,113,113	2.10	25 (30%)
16	CLA	b	609	-	69,73,73	2.37	22 (31%)	82,113,113	1.98	24 (29%)
16	CLA	d	401	-	69,73,73	1.99	21 (30%)	82,113,113	2.20	24 (29%)

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
16	CLA	b	615	-	1/1/15/20	9/39/115/115	-
16	CLA	d	404	-	1/1/14/20	10/35/111/115	-
20	MGE	d	408	-	-	7/42/62/63	0/1/1/1
16	CLA	b	601	-	-	4/10/86/115	-
18	BCR	b	617	-	-	0/29/63/63	0/2/2/2
16	CLA	b	602	-	1/1/15/20	2/39/115/115	-
16	CLA	b	611	-	-	5/39/115/115	-
22	LMT	d	402	-	-	4/21/61/61	0/2/2/2
18	BCR	d	407	-	-	8/29/63/63	0/2/2/2
16	CLA	b	614	-	1/1/12/20	7/24/100/115	-
16	CLA	b	604	-	1/1/15/20	5/39/115/115	-
18	BCR	h	101	-	-	11/29/63/63	0/2/2/2
16	CLA	b	608	-	-	1/39/115/115	-
22	LMT	t	101	-	-	7/21/61/61	0/2/2/2
20	MGE	b	622	-	-	16/43/63/63	0/1/1/1
18	BCR	b	618	-	-	2/29/63/63	0/2/2/2
18	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	HTG	d	411	-	-	0/7/27/30	0/1/1/1
16	CLA	b	603	-	1/1/15/20	4/39/115/115	-
16	CLA	a	403	-	-	3/21/97/115	-
20	MGE	d	410	-	-	13/43/63/63	0/1/1/1
16	CLA	b	607	-	1/1/15/20	2/39/115/115	-
20	MGE	m	101	-	-	9/43/63/63	0/1/1/1
22	LMT	b	623	-	-	1/21/61/61	0/2/2/2
20	MGE	a	409	-	-	13/43/63/63	0/1/1/1
17	PHO	a	404	-	-	14/37/103/103	0/5/6/6
20	MGE	b	620	-	-	13/43/63/63	0/1/1/1
16	CLA	b	605	-	1/1/15/20	3/39/115/115	-
16	CLA	b	613	-	1/1/12/20	0/26/102/115	-
27	HEM	e	101	-	-	6/14/54/54	-
16	CLA	a	406	-	-	5/21/97/115	-
26	DGD	d	412	-	-	9/43/83/95	0/2/2/2
15	SQD	a	401	-	-	4/19/39/69	0/1/1/1
17	PHO	a	405	-	-	8/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	b	616	-	1/1/11/20	1/17/93/115	-
16	CLA	b	606	-	1/1/15/20	10/39/115/115	-
16	CLA	b	610	-	1/1/15/20	3/39/115/115	-
16	CLA	a	402	-	1/1/15/20	4/39/115/115	-
20	MGE	d	409	-	-	6/36/56/63	0/1/1/1
16	CLA	b	612	-	1/1/15/20	6/39/115/115	-
16	CLA	d	405	-	-	6/21/97/115	-
24	PQ9	d	406	-	-	9/41/61/61	0/1/1/1
18	BCR	a	407	-	-	9/29/63/63	0/2/2/2
15	SQD	l	101	-	-	14/42/62/69	0/1/1/1
16	CLA	b	609	-	-	2/39/115/115	-
16	CLA	d	401	-	1/1/15/20	3/39/115/115	-

All (438) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	612	CLA	MG-NA	10.40	2.31	2.06
16	b	606	CLA	MG-NA	10.30	2.30	2.06
17	a	405	PHO	C1B-C2B	9.51	1.49	1.39
17	a	404	PHO	C1B-C2B	8.93	1.49	1.39
16	b	615	CLA	MG-NA	8.37	2.26	2.06
16	b	611	CLA	MG-NA	8.35	2.26	2.06
16	a	406	CLA	C1D-ND	8.24	1.48	1.37
16	b	604	CLA	MG-NA	8.23	2.25	2.06
16	a	403	CLA	C1D-ND	8.05	1.48	1.37
16	b	608	CLA	MG-NA	7.71	2.24	2.06
16	d	404	CLA	C1D-ND	7.70	1.48	1.37
17	a	404	PHO	C3B-C4B	7.58	1.49	1.41
17	a	405	PHO	C3B-C4B	7.19	1.48	1.41
16	b	601	CLA	C1D-ND	7.16	1.47	1.37
16	d	405	CLA	C1D-ND	7.15	1.47	1.37
16	b	607	CLA	MG-NA	7.14	2.23	2.06
16	b	609	CLA	MG-NC	6.76	2.22	2.06
16	b	609	CLA	CHC-C1C	6.42	1.51	1.38
16	a	402	CLA	MG-NA	6.34	2.21	2.06
16	d	401	CLA	MG-NA	6.28	2.21	2.06
16	b	602	CLA	MG-NC	6.17	2.20	2.06
16	b	610	CLA	MG-NA	6.11	2.20	2.06
16	b	607	CLA	C3C-C2C	5.96	1.49	1.36
16	b	613	CLA	MG-NA	5.96	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	616	CLA	CHC-C1C	5.95	1.50	1.38
16	b	607	CLA	CHC-C1C	5.90	1.50	1.38
16	b	602	CLA	C3C-C2C	5.88	1.49	1.36
16	b	616	CLA	MG-NA	5.86	2.20	2.06
16	b	603	CLA	MG-NA	5.70	2.19	2.06
16	b	607	CLA	MG-NC	5.62	2.19	2.06
16	b	609	CLA	O2D-CGD	5.59	1.47	1.33
16	b	605	CLA	C1D-ND	-5.54	1.30	1.37
16	b	610	CLA	C3C-C2C	5.49	1.48	1.36
16	b	612	CLA	C3C-C2C	5.47	1.48	1.36
16	b	614	CLA	MG-NA	5.44	2.19	2.06
27	e	101	HEM	FE-NB	5.38	2.11	1.94
16	d	401	CLA	CHC-C1C	5.34	1.49	1.38
16	b	606	CLA	MG-NC	5.34	2.19	2.06
16	b	609	CLA	C3C-C2C	5.34	1.48	1.36
16	b	601	CLA	O2D-CGD	5.29	1.46	1.33
16	b	603	CLA	CHC-C1C	5.24	1.49	1.38
16	b	604	CLA	CHC-C1C	5.23	1.49	1.38
16	b	603	CLA	C3C-C2C	5.21	1.48	1.36
16	b	602	CLA	OBD-CAD	5.09	1.31	1.22
16	b	609	CLA	CHD-C1D	5.07	1.48	1.38
16	b	611	CLA	CHD-C1D	5.06	1.48	1.38
16	b	610	CLA	O2D-CGD	5.04	1.45	1.33
16	b	602	CLA	CHC-C1C	5.03	1.48	1.38
16	b	605	CLA	MG-NA	5.02	2.18	2.06
16	b	604	CLA	C3C-C2C	5.02	1.47	1.36
15	a	401	SQD	O47-C7	5.00	1.46	1.35
16	b	613	CLA	O2D-CGD	5.00	1.45	1.33
16	b	603	CLA	C1D-ND	-4.98	1.31	1.37
16	b	601	CLA	C3D-C4D	-4.97	1.33	1.44
16	b	605	CLA	O2D-CGD	4.96	1.45	1.33
16	b	605	CLA	CHC-C1C	4.95	1.48	1.38
16	a	402	CLA	OBD-CAD	4.92	1.31	1.22
16	b	615	CLA	C3C-C2C	4.91	1.47	1.36
15	a	401	SQD	O8-S	4.84	1.65	1.47
16	b	613	CLA	CHC-C1C	4.83	1.48	1.38
16	d	404	CLA	O2D-CGD	4.83	1.45	1.33
16	d	404	CLA	C3D-C4D	-4.82	1.33	1.44
15	l	101	SQD	O8-S	4.82	1.65	1.47
16	b	611	CLA	CHB-C1B	4.82	1.50	1.39
16	b	602	CLA	C1D-ND	-4.78	1.31	1.37
16	d	405	CLA	C3D-C4D	-4.77	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	616	CLA	C3C-C2C	4.76	1.47	1.36
16	b	610	CLA	CHD-C1D	4.76	1.47	1.38
16	b	605	CLA	C3C-C2C	4.74	1.47	1.36
16	b	614	CLA	CHD-C1D	4.73	1.47	1.38
16	b	616	CLA	C1D-ND	-4.71	1.31	1.37
16	b	616	CLA	O2D-CGD	4.70	1.44	1.33
16	b	602	CLA	CHD-C4C	4.70	1.49	1.39
16	a	403	CLA	C3D-C4D	-4.69	1.33	1.44
16	d	401	CLA	C3C-C2C	4.69	1.46	1.36
16	a	402	CLA	C3C-C2C	4.68	1.46	1.36
16	a	406	CLA	O2D-CGD	4.67	1.44	1.33
16	d	405	CLA	O2D-CGD	4.66	1.44	1.33
16	b	606	CLA	C3C-C2C	4.65	1.46	1.36
16	b	601	CLA	C3C-C2C	4.64	1.46	1.36
16	a	406	CLA	C3D-C4D	-4.58	1.33	1.44
16	b	610	CLA	MG-ND	-4.57	1.96	2.05
16	b	615	CLA	O2D-CGD	4.56	1.44	1.33
16	b	607	CLA	CHD-C1D	4.53	1.47	1.38
16	b	603	CLA	O2D-CGD	4.53	1.44	1.33
16	b	615	CLA	OBD-CAD	4.52	1.30	1.22
16	b	615	CLA	CHD-C4C	4.52	1.49	1.39
16	a	403	CLA	O2D-CGD	4.50	1.44	1.33
16	b	606	CLA	CHD-C1D	4.47	1.47	1.38
16	b	608	CLA	C4B-NB	-4.46	1.32	1.37
16	b	611	CLA	O2D-CGD	4.43	1.44	1.33
16	b	614	CLA	O2A-CGA	4.41	1.46	1.33
16	d	405	CLA	O2A-CGA	4.40	1.46	1.33
16	b	606	CLA	O2D-CGD	4.39	1.44	1.33
16	b	609	CLA	MG-NB	4.39	2.14	2.05
16	b	611	CLA	CHC-C1C	4.38	1.47	1.38
20	d	409	MGE	O2G-C1B	4.37	1.46	1.34
16	a	406	CLA	O2A-CGA	4.36	1.46	1.33
16	b	604	CLA	MG-ND	-4.33	1.97	2.05
20	m	101	MGE	O1G-C1A	4.33	1.46	1.33
16	b	616	CLA	CHD-C1D	4.32	1.46	1.38
20	a	409	MGE	O2G-C1B	4.31	1.46	1.34
16	b	608	CLA	CHC-C1C	4.31	1.47	1.38
16	b	613	CLA	C3C-C2C	4.30	1.46	1.36
16	b	602	CLA	CHD-C1D	4.26	1.46	1.38
16	d	401	CLA	CHD-C1D	4.25	1.46	1.38
15	l	101	SQD	O47-C7	4.25	1.46	1.34
16	b	613	CLA	O2A-CGA	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	612	CLA	CHC-C1C	4.24	1.47	1.38
16	b	608	CLA	C3C-C2C	4.22	1.45	1.36
20	m	101	MGE	O2G-C1B	4.22	1.46	1.34
20	b	620	MGE	O2G-C1B	4.22	1.46	1.34
16	b	614	CLA	CHB-C1B	4.22	1.48	1.39
16	a	402	CLA	C4B-NB	-4.22	1.32	1.37
20	a	409	MGE	O1G-C1A	4.21	1.45	1.33
26	d	412	DGD	O1G-C1A	4.21	1.45	1.33
27	e	101	HEM	FE-NC	4.20	2.09	1.95
20	b	620	MGE	O1G-C1A	4.18	1.45	1.33
20	d	408	MGE	O2G-C1B	4.16	1.46	1.34
20	d	409	MGE	O1G-C1A	4.16	1.45	1.33
16	b	608	CLA	OBD-CAD	4.14	1.29	1.22
20	d	410	MGE	O1G-C1A	4.13	1.45	1.33
26	d	412	DGD	O2G-C1B	4.13	1.45	1.34
16	b	612	CLA	C1B-C2B	4.11	1.52	1.43
16	b	616	CLA	O2A-CGA	4.11	1.45	1.33
15	l	101	SQD	O48-C23	4.09	1.45	1.33
20	b	622	MGE	O2G-C1B	4.07	1.45	1.34
16	b	607	CLA	O2D-CGD	4.07	1.43	1.33
16	a	403	CLA	O2A-CGA	4.06	1.45	1.33
16	d	405	CLA	C3C-C2C	4.05	1.45	1.36
16	b	606	CLA	CHC-C1C	4.05	1.46	1.38
16	b	604	CLA	CHD-C1D	4.04	1.46	1.38
16	b	610	CLA	OBD-CAD	4.04	1.29	1.22
16	b	616	CLA	MG-ND	4.02	2.13	2.05
16	a	406	CLA	C3C-C2C	4.01	1.45	1.36
20	d	408	MGE	O1G-C1A	4.01	1.45	1.33
16	b	606	CLA	CHB-C1B	4.00	1.48	1.39
16	b	604	CLA	O2D-CGD	4.00	1.43	1.33
16	b	610	CLA	CHC-C1C	4.00	1.46	1.38
16	b	609	CLA	MG-NA	3.99	2.15	2.06
16	b	602	CLA	CHB-C1B	3.99	1.48	1.39
16	d	401	CLA	CHD-C4C	3.99	1.48	1.39
20	b	622	MGE	O1G-C1A	3.98	1.44	1.33
16	b	611	CLA	C3C-C2C	3.98	1.45	1.36
16	b	610	CLA	C4C-C3C	3.97	1.51	1.45
16	d	404	CLA	O2A-CGA	3.97	1.44	1.33
16	b	616	CLA	CHB-C1B	3.97	1.48	1.39
16	d	404	CLA	C3C-C2C	3.95	1.45	1.36
16	b	614	CLA	CHD-C4C	3.94	1.48	1.39
16	b	607	CLA	MG-NB	3.92	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	614	CLA	O2D-CGD	3.91	1.42	1.33
16	b	612	CLA	O2D-CGD	3.91	1.42	1.33
16	a	402	CLA	MG-NB	-3.88	1.98	2.05
20	d	410	MGE	O2G-C1B	3.88	1.45	1.34
16	b	616	CLA	CHC-C4B	3.88	1.48	1.39
16	b	608	CLA	CHB-C1B	3.87	1.48	1.39
16	b	610	CLA	CHD-C4C	3.85	1.48	1.39
16	b	606	CLA	CHD-C4C	3.85	1.48	1.39
16	b	615	CLA	CHC-C1C	3.83	1.46	1.38
16	a	402	CLA	O2D-CGD	3.82	1.42	1.33
16	b	614	CLA	CHC-C4B	3.81	1.48	1.39
16	b	607	CLA	C3D-C2D	3.78	1.49	1.39
16	b	608	CLA	CHD-C1D	3.78	1.45	1.38
16	b	609	CLA	CHB-C1B	3.76	1.47	1.39
16	b	604	CLA	CHB-C1B	3.73	1.47	1.39
16	b	603	CLA	CHD-C1D	3.72	1.45	1.38
16	b	608	CLA	CHD-C4C	3.72	1.47	1.39
16	b	614	CLA	CHC-C1C	3.72	1.45	1.38
16	b	607	CLA	C1D-ND	-3.71	1.33	1.37
16	a	403	CLA	C3C-C2C	3.69	1.44	1.36
16	b	603	CLA	OBD-CAD	3.69	1.28	1.22
16	b	615	CLA	C3D-C2D	3.69	1.49	1.39
16	b	610	CLA	CHC-C4B	3.69	1.47	1.39
16	b	607	CLA	MG-ND	3.69	2.13	2.05
16	b	606	CLA	CHC-C4B	3.65	1.47	1.39
16	b	613	CLA	OBD-CAD	3.64	1.28	1.22
16	b	609	CLA	O2A-CGA	3.64	1.43	1.33
16	b	611	CLA	CHD-C4C	3.63	1.47	1.39
17	a	404	PHO	C4D-CHA	3.62	1.45	1.39
16	b	604	CLA	MG-NC	3.62	2.14	2.06
16	b	611	CLA	O2A-CGA	3.60	1.43	1.33
16	b	607	CLA	CHB-C1B	3.60	1.47	1.39
16	b	608	CLA	CHC-C4B	3.60	1.47	1.39
27	e	101	HEM	C1B-NB	-3.57	1.34	1.40
16	b	605	CLA	C1B-NB	-3.55	1.33	1.37
16	b	612	CLA	CHD-C1D	3.55	1.45	1.38
16	b	603	CLA	C1B-NB	-3.54	1.33	1.37
16	b	607	CLA	C1B-C2B	3.53	1.51	1.43
16	b	612	CLA	CHB-C1B	3.52	1.47	1.39
25	d	411	HTG	C1'-S1	-3.49	1.76	1.81
16	b	601	CLA	CHD-C1D	3.49	1.45	1.38
16	b	613	CLA	CHC-C4B	3.47	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	609	CLA	C3B-C4B	3.46	1.52	1.42
16	b	610	CLA	CHB-C1B	3.46	1.47	1.39
16	b	614	CLA	C3C-C2C	3.46	1.44	1.36
16	b	608	CLA	O2D-CGD	3.46	1.41	1.33
16	a	406	CLA	CHC-C1C	3.44	1.45	1.38
17	a	405	PHO	CAC-C3C	-3.44	1.45	1.51
16	b	608	CLA	C1B-NB	-3.40	1.33	1.37
16	b	601	CLA	CHC-C1C	3.40	1.45	1.38
16	b	609	CLA	C1B-C2B	3.39	1.51	1.43
16	b	610	CLA	MG-NC	3.39	2.14	2.06
16	b	602	CLA	O2A-CGA	3.37	1.43	1.33
17	a	405	PHO	C1D-C2D	3.36	1.43	1.39
16	b	601	CLA	OBD-CAD	3.36	1.28	1.22
16	b	609	CLA	OBD-CAD	3.35	1.28	1.22
17	a	404	PHO	C1D-C2D	3.34	1.43	1.39
16	b	601	CLA	CHD-C4C	3.34	1.46	1.39
16	a	406	CLA	OBD-CAD	3.33	1.28	1.22
16	b	603	CLA	C4B-NB	-3.33	1.33	1.37
16	b	602	CLA	C1B-C2B	3.33	1.50	1.43
16	b	607	CLA	CHC-C4B	3.33	1.46	1.39
16	b	606	CLA	C4D-CHA	3.32	1.49	1.38
16	a	402	CLA	CHD-C4C	3.32	1.46	1.39
16	d	404	CLA	CHC-C1C	3.31	1.45	1.38
17	a	404	PHO	CAC-C3C	-3.29	1.45	1.51
16	b	603	CLA	CHB-C1B	3.27	1.46	1.39
16	b	601	CLA	CHB-C4A	-3.27	1.29	1.37
16	b	613	CLA	CHD-C1D	3.26	1.44	1.38
16	b	609	CLA	CHC-C4B	3.26	1.46	1.39
16	b	603	CLA	CHD-C4C	3.23	1.46	1.39
16	b	609	CLA	CHD-C4C	3.23	1.46	1.39
16	b	612	CLA	CHC-C4B	3.22	1.46	1.39
16	d	401	CLA	CHB-C1B	3.21	1.46	1.39
16	b	612	CLA	O2A-CGA	3.20	1.42	1.33
16	d	405	CLA	CHC-C1C	3.20	1.44	1.38
16	b	610	CLA	C1B-NB	-3.20	1.33	1.37
16	d	401	CLA	C1D-ND	-3.19	1.33	1.37
16	b	614	CLA	MG-ND	-3.19	1.99	2.05
16	b	616	CLA	C3D-C2D	3.18	1.47	1.39
17	a	404	PHO	CMB-C2B	-3.17	1.45	1.51
16	b	608	CLA	C1D-ND	-3.17	1.33	1.37
16	d	404	CLA	OBD-CAD	3.16	1.27	1.22
16	b	607	CLA	C1B-NB	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	604	CLA	CHD-C4C	3.14	1.46	1.39
16	b	616	CLA	C4B-NB	-3.13	1.33	1.37
16	b	615	CLA	CHB-C1B	3.13	1.46	1.39
16	d	401	CLA	O2A-CGA	3.11	1.42	1.33
16	a	403	CLA	OBD-CAD	3.11	1.27	1.22
16	b	611	CLA	C3D-C2D	3.11	1.47	1.39
16	b	616	CLA	OBD-CAD	3.11	1.27	1.22
16	b	609	CLA	C3D-C2D	3.10	1.47	1.39
16	b	611	CLA	C4D-CHA	3.07	1.48	1.38
16	b	609	CLA	C4B-NB	-3.06	1.33	1.37
16	b	605	CLA	C3B-C4B	3.06	1.51	1.42
16	b	608	CLA	C3B-C4B	3.06	1.51	1.42
17	a	404	PHO	CMD-C2D	-3.04	1.45	1.51
16	b	615	CLA	CHD-C1D	3.02	1.44	1.38
16	b	604	CLA	C4B-NB	-3.02	1.33	1.37
16	d	405	CLA	OBD-CAD	3.02	1.27	1.22
16	b	612	CLA	C3D-C2D	3.02	1.47	1.39
17	a	405	PHO	C4D-ND	-3.01	1.34	1.38
16	b	607	CLA	CHD-C4C	3.01	1.46	1.39
16	b	603	CLA	C4D-CHA	3.00	1.48	1.38
27	e	101	HEM	C4D-ND	-3.00	1.35	1.40
16	d	401	CLA	OBD-CAD	2.99	1.27	1.22
16	b	606	CLA	C3D-C2D	2.98	1.47	1.39
16	b	603	CLA	C3D-C2D	2.97	1.47	1.39
17	a	404	PHO	CMC-C2C	-2.97	1.46	1.50
16	b	616	CLA	CHD-C4C	2.97	1.46	1.39
16	b	608	CLA	C4D-CHA	2.97	1.48	1.38
16	b	607	CLA	C4D-CHA	2.96	1.48	1.38
16	a	406	CLA	CHB-C4A	-2.95	1.30	1.37
16	a	402	CLA	C4D-CHA	2.94	1.48	1.38
16	b	612	CLA	C4B-NB	-2.94	1.34	1.37
17	a	405	PHO	CMD-C2D	-2.94	1.45	1.51
16	b	615	CLA	C4D-CHA	2.93	1.48	1.38
16	a	402	CLA	CHB-C1B	2.93	1.46	1.39
16	b	615	CLA	C1B-C2B	2.92	1.50	1.43
16	b	612	CLA	MG-NC	-2.92	1.99	2.06
16	b	612	CLA	C1B-NB	-2.91	1.34	1.37
16	b	609	CLA	C1D-ND	-2.90	1.34	1.37
16	b	607	CLA	C3B-C4B	2.90	1.51	1.42
16	b	609	CLA	C4D-CHA	2.90	1.48	1.38
16	b	605	CLA	O2A-CGA	2.89	1.41	1.33
16	b	602	CLA	CHC-C4B	2.88	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	d	401	CLA	MG-ND	-2.88	2.00	2.05
16	d	401	CLA	CHC-C4B	2.87	1.45	1.39
16	b	613	CLA	C3B-C4B	2.87	1.51	1.42
16	b	602	CLA	C1B-NB	-2.87	1.34	1.37
16	d	405	CLA	CHB-C4A	-2.87	1.30	1.37
16	b	601	CLA	C1D-C2D	2.86	1.51	1.45
16	b	613	CLA	CHD-C4C	2.86	1.45	1.39
16	b	605	CLA	CHB-C1B	2.86	1.45	1.39
16	a	402	CLA	O2A-CGA	2.86	1.41	1.33
17	a	405	PHO	C4D-CHA	2.85	1.43	1.39
16	a	406	CLA	CHC-C4B	2.85	1.45	1.39
16	b	613	CLA	C3D-C2D	2.85	1.46	1.39
16	b	616	CLA	C1C-C2C	2.85	1.50	1.44
16	a	402	CLA	CHC-C1C	2.85	1.44	1.38
16	b	616	CLA	C4D-CHA	2.83	1.48	1.38
16	a	403	CLA	CHC-C1C	2.82	1.44	1.38
16	a	403	CLA	CHB-C4A	-2.82	1.30	1.37
16	b	602	CLA	MG-NB	2.81	2.11	2.05
16	b	605	CLA	CHD-C1D	2.80	1.43	1.38
16	b	604	CLA	C3D-C2D	2.79	1.46	1.39
16	b	613	CLA	C1D-ND	-2.79	1.34	1.37
16	b	609	CLA	C4C-C3C	2.78	1.49	1.45
17	a	405	PHO	CMC-C2C	-2.77	1.46	1.50
16	b	602	CLA	C3B-C4B	2.77	1.50	1.42
16	b	613	CLA	C4D-CHA	2.76	1.47	1.38
16	b	606	CLA	O2A-CGA	2.74	1.41	1.33
16	b	605	CLA	OBD-CAD	2.73	1.27	1.22
16	d	405	CLA	CHD-C4C	2.73	1.45	1.39
16	b	602	CLA	C4C-C3C	2.73	1.49	1.45
16	b	616	CLA	C1C-NC	-2.73	1.33	1.37
16	a	402	CLA	CHD-C1D	2.72	1.43	1.38
16	b	605	CLA	CHD-C4C	2.72	1.45	1.39
16	b	610	CLA	C4D-CHA	2.71	1.47	1.38
16	b	615	CLA	MG-NC	2.71	2.12	2.06
16	b	603	CLA	O2A-CGA	2.70	1.41	1.33
16	d	405	CLA	CHD-C1D	2.70	1.43	1.38
15	a	401	SQD	O48-C23	2.70	1.46	1.33
17	a	404	PHO	C4D-ND	-2.68	1.34	1.38
16	d	401	CLA	C1-C2	2.68	1.56	1.49
16	b	606	CLA	OBD-CAD	2.66	1.27	1.22
16	b	607	CLA	O2A-CGA	2.65	1.41	1.33
16	b	601	CLA	C4B-NB	-2.65	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	601	CLA	C4C-C3C	2.65	1.49	1.45
16	b	606	CLA	C3B-C4B	2.64	1.50	1.42
16	b	615	CLA	CHC-C4B	2.64	1.45	1.39
16	d	404	CLA	CHC-C4B	2.63	1.45	1.39
16	b	608	CLA	O2A-CGA	2.63	1.41	1.33
16	b	604	CLA	C3B-C4B	2.62	1.50	1.42
16	d	404	CLA	CHB-C1B	2.62	1.45	1.39
16	b	604	CLA	C4D-CHA	2.62	1.47	1.38
16	d	401	CLA	C1B-C2B	2.61	1.49	1.43
16	b	615	CLA	O2A-CGA	2.61	1.41	1.33
16	b	613	CLA	C4C-C3C	2.61	1.49	1.45
16	b	614	CLA	MG-NC	2.60	2.12	2.06
16	a	402	CLA	C1B-C2B	2.59	1.49	1.43
16	b	605	CLA	CHC-C4B	2.59	1.45	1.39
16	b	608	CLA	C3D-C2D	2.59	1.46	1.39
16	a	402	CLA	CHC-C4B	2.58	1.45	1.39
16	b	606	CLA	MG-NB	2.58	2.10	2.05
16	d	404	CLA	CHB-C4A	-2.56	1.31	1.37
16	b	603	CLA	MG-ND	2.56	2.10	2.05
16	b	606	CLA	C1C-NC	-2.54	1.33	1.37
16	b	615	CLA	C1D-ND	-2.54	1.34	1.37
16	b	609	CLA	C1B-NB	-2.54	1.34	1.37
16	d	401	CLA	C1B-NB	-2.53	1.34	1.37
16	b	602	CLA	C4D-CHA	2.53	1.47	1.38
16	b	610	CLA	C3D-C2D	2.52	1.45	1.39
16	b	601	CLA	C3A-C2A	-2.52	1.52	1.54
16	b	602	CLA	C3D-C2D	2.52	1.45	1.39
16	b	606	CLA	MG-ND	2.52	2.10	2.05
17	a	405	PHO	CMB-C2B	-2.51	1.46	1.51
16	b	610	CLA	O2A-CGA	2.51	1.40	1.33
16	b	611	CLA	C1B-NB	-2.50	1.34	1.37
24	d	406	PQ9	C10-C5	2.49	1.47	1.35
16	b	612	CLA	OBD-CAD	2.49	1.26	1.22
16	b	604	CLA	MG-NB	2.49	2.10	2.05
16	b	611	CLA	C3B-C4B	2.48	1.49	1.42
16	b	605	CLA	C4D-CHA	2.47	1.46	1.38
16	b	610	CLA	C4B-NB	-2.47	1.34	1.37
16	b	603	CLA	CHC-C4B	2.46	1.44	1.39
17	a	404	PHO	C3B-C2B	-2.46	1.37	1.40
16	b	601	CLA	C3D-C2D	2.45	1.45	1.39
16	b	612	CLA	C3B-C4B	2.45	1.49	1.42
16	d	401	CLA	O2D-CGD	2.45	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	611	CLA	C1D-ND	-2.44	1.34	1.37
16	b	603	CLA	C3B-C4B	2.44	1.49	1.42
16	b	603	CLA	C1B-C2B	2.43	1.48	1.43
27	e	101	HEM	FE-ND	-2.42	1.87	1.94
16	b	605	CLA	C4B-NB	-2.41	1.34	1.37
16	a	403	CLA	CHD-C4C	2.40	1.44	1.39
16	b	606	CLA	C1C-C2C	2.39	1.49	1.44
16	b	604	CLA	C1C-NC	-2.39	1.34	1.37
27	e	101	HEM	C3C-C4C	-2.39	1.41	1.46
16	b	605	CLA	C1B-C2B	2.37	1.48	1.43
27	e	101	HEM	C1C-C2C	-2.37	1.40	1.45
16	b	612	CLA	C4D-CHA	2.37	1.46	1.38
16	a	406	CLA	CHD-C4C	2.37	1.44	1.39
16	b	605	CLA	MG-NB	2.37	2.10	2.05
16	d	405	CLA	CHB-C1B	2.35	1.44	1.39
16	b	612	CLA	CHD-C4C	2.35	1.44	1.39
16	d	405	CLA	C3D-C2D	2.34	1.45	1.39
16	d	405	CLA	CHC-C4B	2.33	1.44	1.39
16	b	614	CLA	C4D-CHA	2.32	1.46	1.38
16	b	613	CLA	C1B-C2B	2.31	1.48	1.43
16	b	615	CLA	C3B-C4B	2.31	1.49	1.42
16	b	615	CLA	C4C-C3C	2.31	1.49	1.45
16	d	404	CLA	C3B-C4B	2.30	1.49	1.42
16	b	616	CLA	C3B-C4B	2.30	1.49	1.42
16	b	614	CLA	C4C-C3C	2.29	1.48	1.45
16	b	613	CLA	C3D-C4D	-2.29	1.39	1.44
16	d	401	CLA	C4D-CHA	2.27	1.46	1.38
16	a	402	CLA	C3D-C2D	2.25	1.45	1.39
16	b	614	CLA	C4B-NB	-2.25	1.34	1.37
16	a	406	CLA	C3B-C4B	2.24	1.49	1.42
16	a	406	CLA	CHD-C1D	2.22	1.42	1.38
16	b	602	CLA	CBD-CAD	-2.22	1.46	1.56
16	b	608	CLA	C1B-C2B	2.22	1.48	1.43
16	b	609	CLA	MG-ND	2.21	2.10	2.05
16	b	604	CLA	O2A-CGA	2.21	1.39	1.33
16	b	603	CLA	MG-NC	-2.20	2.01	2.06
16	a	406	CLA	C1D-C2D	2.19	1.49	1.45
16	d	404	CLA	C1B-C2B	2.19	1.48	1.43
16	b	612	CLA	C1D-ND	-2.17	1.35	1.37
16	b	601	CLA	C1B-NB	-2.16	1.35	1.37
16	b	613	CLA	C1-C2	2.16	1.55	1.49
16	b	609	CLA	O2D-CED	-2.15	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	601	CLA	CHB-C1B	2.15	1.44	1.39
17	a	405	PHO	CAA-C2A	-2.15	1.49	1.54
16	a	406	CLA	CHB-C1B	2.15	1.44	1.39
16	d	401	CLA	CMD-C2D	2.14	1.55	1.50
16	d	401	CLA	C4B-NB	-2.14	1.35	1.37
16	b	604	CLA	C1B-C2B	2.14	1.48	1.43
16	b	606	CLA	C4C-C3C	2.13	1.48	1.45
27	e	101	HEM	C1D-ND	-2.13	1.34	1.38
16	b	608	CLA	CAA-C2A	2.13	1.58	1.54
16	b	611	CLA	C3D-C4D	-2.12	1.39	1.44
16	a	403	CLA	CHD-C1D	2.12	1.42	1.38
16	d	401	CLA	C4C-C3C	2.12	1.48	1.45
16	d	405	CLA	C1D-C2D	2.11	1.49	1.45
20	d	410	MGE	O3G-C1D	2.11	1.43	1.40
16	b	614	CLA	OBD-CAD	2.11	1.26	1.22
16	d	405	CLA	C1B-C2B	2.11	1.48	1.43
20	m	101	MGE	O3G-C1D	2.11	1.43	1.40
16	b	613	CLA	C1B-NB	-2.10	1.35	1.37
16	b	605	CLA	C1C-NC	-2.10	1.34	1.37
16	b	614	CLA	C3D-C2D	2.10	1.44	1.39
16	a	402	CLA	C1C-NC	-2.08	1.34	1.37
16	b	611	CLA	C1B-C2B	2.08	1.48	1.43
25	d	411	HTG	C1-S1	-2.07	1.77	1.80
16	a	406	CLA	C1B-NB	-2.07	1.35	1.37
17	a	404	PHO	CBD-CGD	-2.07	1.49	1.52
16	b	606	CLA	C3B-C2B	2.07	1.48	1.41
16	d	401	CLA	C3D-C2D	2.07	1.44	1.39
16	d	401	CLA	C3B-C4B	2.06	1.48	1.42
16	a	403	CLA	C3D-C2D	2.06	1.44	1.39
16	b	610	CLA	C3B-C4B	2.05	1.48	1.42
16	a	403	CLA	C1B-C2B	2.04	1.47	1.43
16	b	611	CLA	MG-NC	2.03	2.11	2.06
16	b	604	CLA	CHC-C4B	2.02	1.44	1.39
18	b	619	BCR	C30-C25	-2.02	1.51	1.53
16	b	616	CLA	MG-NC	2.01	2.11	2.06
16	b	601	CLA	CHC-C4B	2.01	1.43	1.39

All (867) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	406	CLA	C1D-ND-C4D	-19.10	92.91	106.31
16	a	403	CLA	C1D-ND-C4D	-17.90	93.75	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	404	CLA	C1D-ND-C4D	-16.80	94.53	106.31
16	d	405	CLA	C1D-ND-C4D	-16.75	94.56	106.31
15	a	401	SQD	O9-S-C6	-16.03	82.82	106.76
15	l	101	SQD	O9-S-C6	-15.82	83.13	106.76
16	b	601	CLA	C1D-ND-C4D	-15.26	95.61	106.31
16	b	606	CLA	C4A-NA-C1A	11.81	112.06	106.68
15	a	401	SQD	O8-S-O9	-11.76	81.97	111.40
15	l	101	SQD	O8-S-O9	-11.52	82.59	111.40
16	b	604	CLA	C4A-NA-C1A	9.76	111.13	106.68
16	a	403	CLA	C2C-C1C-NC	9.47	119.93	109.98
15	l	101	SQD	O9-S-O7	-9.47	83.02	113.82
16	d	404	CLA	C2C-C1C-NC	9.27	119.72	109.98
15	a	401	SQD	O9-S-O7	-9.13	84.14	113.82
16	b	601	CLA	C4A-NA-C1A	-9.08	102.54	106.68
16	b	601	CLA	CMD-C2D-C1D	9.01	140.60	124.73
16	a	403	CLA	CMD-C2D-C1D	9.00	140.58	124.73
16	b	601	CLA	C2B-C1B-NB	8.94	119.60	110.33
16	a	403	CLA	C2B-C1B-NB	8.73	119.38	110.33
16	b	601	CLA	C4D-CHA-C1A	-8.72	110.84	121.24
16	a	406	CLA	CMD-C2D-C1D	8.72	140.08	124.73
16	b	610	CLA	C4A-NA-C1A	8.67	110.64	106.68
16	d	405	CLA	C2C-C1C-NC	8.61	119.03	109.98
16	d	405	CLA	C2B-C1B-NB	8.51	119.15	110.33
16	b	614	CLA	C4A-NA-C1A	8.45	110.53	106.68
16	a	406	CLA	C2B-C1B-NB	8.41	119.05	110.33
16	b	612	CLA	CAC-C3C-C4C	8.40	135.72	124.79
16	d	404	CLA	CHD-C4C-C3C	-8.40	112.53	124.77
16	d	404	CLA	C2B-C1B-NB	8.21	118.84	110.33
16	a	406	CLA	C4A-NA-C1A	-8.10	102.98	106.68
16	b	601	CLA	C2C-C1C-NC	8.08	118.47	109.98
16	a	403	CLA	C3B-C4B-NB	8.05	117.71	110.53
15	l	101	SQD	O7-S-C6	7.93	118.59	106.76
16	b	611	CLA	C4A-NA-C1A	7.92	110.29	106.68
16	d	405	CLA	CMD-C2D-C1D	7.90	138.65	124.73
16	a	406	CLA	C2C-C1C-NC	7.82	118.19	109.98
16	a	406	CLA	C2D-C1D-ND	7.78	117.82	110.13
17	a	404	PHO	C4D-CHA-CBD	-7.75	104.74	108.45
16	b	612	CLA	C4A-NA-C1A	7.75	110.21	106.68
16	d	404	CLA	C3C-C4C-NC	7.73	120.34	110.43
16	d	404	CLA	CMD-C2D-C1D	7.64	138.19	124.73
16	a	406	CLA	C4D-CHA-C1A	-7.56	112.22	121.24
16	a	406	CLA	C3D-C4D-ND	7.47	122.14	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	601	CLA	C3D-C4D-ND	7.43	122.06	109.99
16	a	403	CLA	C2D-C1D-ND	7.35	117.41	110.13
15	a	401	SQD	O7-S-C6	7.33	117.70	106.76
18	a	407	BCR	C7-C8-C9	-7.27	115.48	126.23
16	d	405	CLA	C3D-C4D-ND	7.20	121.70	109.99
16	a	403	CLA	C3D-C4D-ND	7.16	121.63	109.99
16	a	406	CLA	C3C-C4C-NC	7.13	119.57	110.43
16	a	406	CLA	CHD-C4C-C3C	-7.11	114.41	124.77
16	b	614	CLA	C4D-CHA-C1A	-7.08	112.80	121.24
16	b	615	CLA	C4A-NA-C1A	6.96	109.85	106.68
16	b	601	CLA	CHD-C1D-ND	-6.95	115.02	124.80
16	b	605	CLA	CAC-C3C-C4C	6.93	133.80	124.79
15	a	401	SQD	O8-S-C6	6.92	119.33	105.97
16	a	402	CLA	CAC-C3C-C4C	6.92	133.79	124.79
16	b	614	CLA	C2D-C1D-ND	6.89	116.95	110.13
16	d	405	CLA	C2D-C1D-ND	6.87	116.92	110.13
16	b	616	CLA	CHD-C4C-C3C	-6.84	114.80	124.77
16	b	601	CLA	C3B-C2B-C1B	-6.84	99.11	107.17
17	a	405	PHO	C4D-CHA-CBD	-6.80	105.19	108.45
16	d	405	CLA	C4A-NA-C1A	-6.80	103.58	106.68
16	d	405	CLA	C3B-C4B-NB	6.77	116.57	110.53
16	b	614	CLA	C1D-ND-C4D	-6.76	101.57	106.31
16	d	405	CLA	C3C-C4C-NC	6.60	118.89	110.43
16	b	610	CLA	C2D-C1D-ND	6.58	116.64	110.13
16	d	404	CLA	C2D-C1D-ND	6.49	116.55	110.13
16	a	403	CLA	CHD-C4C-C3C	-6.46	115.36	124.77
16	b	605	CLA	C2C-C1C-NC	6.42	116.72	109.98
16	b	614	CLA	O2D-CGD-CBD	6.41	122.43	111.23
16	a	403	CLA	O2D-CGD-CBD	6.38	122.38	111.23
15	l	101	SQD	O8-S-C6	6.34	118.22	105.97
16	b	603	CLA	C2C-C1C-NC	6.32	116.62	109.98
16	b	616	CLA	O2D-CGD-CBD	6.30	122.24	111.23
16	b	613	CLA	C4A-NA-C1A	6.29	109.55	106.68
16	d	404	CLA	C3B-C4B-NB	6.24	116.10	110.53
16	d	404	CLA	O2D-CGD-CBD	6.24	122.13	111.23
16	a	403	CLA	C4A-NA-C1A	-6.23	103.83	106.68
16	a	403	CLA	C4D-CHA-C1A	-6.22	113.83	121.24
16	d	404	CLA	C3D-C4D-ND	6.20	120.06	109.99
16	a	403	CLA	C3C-C4C-NC	6.19	118.36	110.43
18	a	407	BCR	C11-C10-C9	-6.09	118.74	127.28
16	d	404	CLA	C4D-CHA-C1A	-6.03	114.05	121.24
16	b	612	CLA	CHD-C4C-C3C	-6.02	116.00	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	d	405	CLA	C4D-CHA-C1A	-5.97	114.13	121.24
16	a	403	CLA	C1C-C2C-C3C	-5.96	100.71	106.98
16	a	406	CLA	C3B-C2B-C1B	-5.94	100.17	107.17
16	d	405	CLA	O2D-CGD-CBD	5.89	121.53	111.23
16	a	402	CLA	C2D-C1D-ND	5.87	115.94	110.13
16	d	401	CLA	CHD-C4C-C3C	-5.86	116.24	124.77
16	a	403	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
16	d	405	CLA	C3B-C2B-C1B	-5.82	100.31	107.17
16	b	604	CLA	C2C-C1C-NC	5.76	116.03	109.98
16	a	406	CLA	C3D-C2D-C1D	-5.76	97.98	105.83
16	a	403	CLA	C3B-C2B-C1B	-5.76	100.39	107.17
16	d	404	CLA	C1C-C2C-C3C	-5.64	101.05	106.98
16	b	603	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
16	b	613	CLA	C2C-C1C-NC	5.62	115.89	109.98
16	d	405	CLA	CHD-C4C-C3C	-5.60	116.60	124.77
16	d	405	CLA	C3D-C2D-C1D	-5.60	98.18	105.83
16	b	601	CLA	C3B-C4B-NB	5.57	115.50	110.53
18	h	101	BCR	C7-C8-C9	-5.55	118.02	126.23
17	a	404	PHO	C2B-C1B-NB	-5.50	105.45	109.43
16	b	610	CLA	C2B-C1B-NB	5.50	116.03	110.33
16	b	616	CLA	C4A-NA-C1A	5.46	109.17	106.68
16	b	612	CLA	C4D-CHA-C1A	-5.46	114.74	121.24
16	b	601	CLA	C3C-C4C-NC	5.44	117.41	110.43
17	a	405	PHO	C2B-C1B-NB	-5.44	105.50	109.43
15	a	401	SQD	O47-C7-C8	5.42	120.76	111.09
16	b	613	CLA	CAC-C3C-C4C	5.42	131.84	124.79
16	a	406	CLA	O2D-CGD-CBD	5.40	120.67	111.23
16	b	603	CLA	C2B-C1B-NB	5.38	115.90	110.33
26	d	412	DGD	O2G-C1B-C2B	5.35	123.05	111.48
16	b	610	CLA	C1D-ND-C4D	-5.33	102.57	106.31
16	b	613	CLA	C1-C2-C3	-5.30	117.52	126.20
16	b	601	CLA	C1D-CHD-C4C	-5.29	114.79	126.02
25	d	411	HTG	C1'-S1-C1	5.28	111.86	100.45
16	d	404	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
16	b	615	CLA	C2B-C1B-NB	5.27	115.79	110.33
16	b	609	CLA	CAC-C3C-C4C	5.24	131.61	124.79
20	b	620	MGE	O2G-C1B-C2B	5.23	122.81	111.48
16	d	401	CLA	C2C-C1C-NC	5.23	115.47	109.98
16	a	402	CLA	C3B-C2B-C1B	-5.22	101.02	107.17
16	b	609	CLA	C2C-C1C-NC	5.19	115.44	109.98
16	b	615	CLA	C1C-C2C-C3C	-5.18	101.53	106.98
16	d	404	CLA	C3B-C2B-C1B	-5.18	101.06	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	603	CLA	C1C-C2C-C3C	-5.17	101.55	106.98
16	b	615	CLA	C2C-C1C-NC	5.08	115.32	109.98
20	d	410	MGE	O2G-C1B-C2B	5.07	122.46	111.48
16	d	405	CLA	CHD-C1D-ND	-5.06	117.68	124.80
18	a	407	BCR	C20-C21-C22	-5.05	120.19	127.28
27	e	101	HEM	CHD-C1D-ND	5.03	129.84	124.42
16	b	603	CLA	O2D-CGD-O1D	-5.02	114.09	123.85
18	d	407	BCR	C7-C8-C9	-5.00	118.84	126.23
16	b	604	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
16	b	608	CLA	O2D-CGD-CBD	4.98	119.94	111.23
16	b	608	CLA	C2C-C1C-NC	4.97	115.20	109.98
16	b	612	CLA	C3C-C4C-NC	4.96	116.79	110.43
16	b	601	CLA	C2D-C1D-ND	4.96	115.03	110.13
16	a	402	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
16	b	601	CLA	CHB-C1B-NB	-4.94	116.63	124.05
27	e	101	HEM	CHC-C4B-NB	4.94	129.74	124.42
16	d	404	CLA	C1D-CHD-C4C	-4.92	115.56	126.02
16	b	616	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
16	d	401	CLA	C2D-C1D-ND	4.92	114.99	110.13
16	b	603	CLA	CHD-C1D-ND	-4.90	117.90	124.80
16	b	613	CLA	C2D-C1D-ND	4.88	114.96	110.13
16	b	614	CLA	C1-C2-C3	-4.87	118.21	126.20
16	b	614	CLA	O2D-CGD-O1D	-4.86	114.39	123.85
16	b	603	CLA	C4-C3-C5	4.85	123.65	115.23
16	b	602	CLA	C2D-C1D-ND	4.85	114.92	110.13
16	b	613	CLA	CHD-C4C-C3C	-4.84	117.71	124.77
16	b	608	CLA	C1C-C2C-C3C	-4.84	101.89	106.98
16	b	615	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
16	b	603	CLA	C2D-C1D-ND	4.82	114.90	110.13
16	b	612	CLA	C4C-C3C-C2C	-4.82	99.88	106.89
16	b	607	CLA	CHD-C4C-C3C	-4.81	117.76	124.77
16	b	616	CLA	C2B-C1B-NB	4.81	115.31	110.33
16	b	610	CLA	C2C-C1C-NC	4.80	115.03	109.98
16	b	602	CLA	O2D-CGD-CBD	4.79	119.61	111.23
16	b	605	CLA	CHD-C4C-C3C	-4.79	117.79	124.77
16	b	605	CLA	C2D-C1D-ND	4.78	114.86	110.13
18	a	407	BCR	C24-C23-C22	-4.77	119.17	126.23
16	b	605	CLA	C4-C3-C5	4.77	123.50	115.23
16	b	604	CLA	CAC-C3C-C4C	4.76	130.98	124.79
16	d	405	CLA	C1C-C2C-C3C	-4.75	101.98	106.98
16	b	601	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
16	a	403	CLA	C1D-CHD-C4C	-4.71	116.00	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	603	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
16	b	616	CLA	C2D-C1D-ND	4.71	114.78	110.13
18	d	407	BCR	C24-C23-C22	-4.70	119.28	126.23
20	d	410	MGE	C1D-O6D-C5D	4.69	122.89	113.72
16	b	613	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
16	b	609	CLA	O2D-CGD-CBD	4.68	119.41	111.23
16	b	610	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
16	b	612	CLA	C2C-C1C-NC	4.64	114.86	109.98
16	b	615	CLA	CHC-C4B-NB	4.64	131.01	124.05
16	b	602	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
16	b	604	CLA	C2D-C1D-ND	4.63	114.71	110.13
16	b	606	CLA	CHD-C4C-C3C	-4.62	118.03	124.77
16	b	606	CLA	C2D-C1D-ND	4.62	114.70	110.13
16	a	402	CLA	C2C-C1C-NC	4.61	114.82	109.98
16	b	611	CLA	C1C-C2C-C3C	-4.60	102.14	106.98
16	b	604	CLA	CHD-C4C-C3C	-4.60	118.07	124.77
16	b	612	CLA	C2D-C1D-ND	4.58	114.66	110.13
16	b	605	CLA	O2D-CGD-CBD	4.58	119.23	111.23
16	b	608	CLA	CHD-C4C-C3C	-4.58	118.10	124.77
17	a	404	PHO	C2D-C1D-ND	-4.58	106.12	109.43
16	b	607	CLA	CAC-C3C-C4C	4.57	130.74	124.79
16	b	615	CLA	C1D-CHD-C4C	-4.56	116.33	126.02
16	d	401	CLA	C1D-CHD-C4C	-4.56	116.33	126.02
16	b	610	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
16	b	611	CLA	C2C-C1C-NC	4.54	114.75	109.98
16	a	406	CLA	C3B-C4B-NB	4.53	114.57	110.53
18	b	619	BCR	C20-C21-C22	-4.50	120.96	127.28
16	d	401	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
16	b	607	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
16	b	601	CLA	O2D-CGD-CBD	4.46	119.02	111.23
18	b	619	BCR	C7-C8-C9	-4.46	119.64	126.23
16	b	607	CLA	C4A-NA-C1A	4.44	108.70	106.68
16	b	602	CLA	O2D-CGD-O1D	-4.43	115.22	123.85
16	a	402	CLA	CHD-C4C-C3C	-4.42	118.32	124.77
16	a	403	CLA	CHD-C1D-ND	-4.42	118.58	124.80
16	b	608	CLA	C2D-C1D-ND	4.39	114.47	110.13
18	a	407	BCR	C1-C6-C5	-4.39	116.64	122.64
16	b	604	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
16	b	605	CLA	CMD-C2D-C1D	4.37	132.43	124.73
16	b	614	CLA	CHD-C4C-C3C	-4.34	118.45	124.77
16	b	611	CLA	C1-C2-C3	-4.32	119.12	126.20
16	b	615	CLA	C2D-C1D-ND	4.31	114.39	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	605	CLA	C3C-C4C-NC	4.28	115.92	110.43
16	b	611	CLA	CHD-C4C-C3C	-4.28	118.53	124.77
20	b	622	MGE	O2G-C1B-C2B	4.28	120.74	111.48
18	b	619	BCR	C27-C26-C25	-4.27	116.94	122.70
16	d	401	CLA	CHC-C4B-NB	4.27	130.45	124.05
16	a	406	CLA	C1D-CHD-C4C	-4.26	116.96	126.02
16	b	605	CLA	CHD-C1D-ND	-4.26	118.81	124.80
16	b	615	CLA	O2D-CGD-CBD	4.26	118.67	111.23
18	h	101	BCR	C16-C17-C18	-4.26	121.31	127.28
20	b	620	MGE	O1G-C1A-C2A	4.24	124.75	111.83
16	b	606	CLA	C2B-C1B-NB	4.23	114.71	110.33
16	b	605	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
16	b	601	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
18	b	618	BCR	C24-C23-C22	-4.20	120.02	126.23
16	b	607	CLA	C2C-C1C-NC	4.18	114.38	109.98
16	b	609	CLA	C4D-CHA-C1A	-4.18	116.26	121.24
16	a	406	CLA	CHD-C1D-ND	-4.17	118.93	124.80
16	a	406	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
16	b	614	CLA	C2C-C1C-NC	4.16	114.35	109.98
16	b	605	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
16	d	401	CLA	C3D-C2D-C1D	-4.13	100.20	105.83
16	d	405	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
16	b	616	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
16	b	611	CLA	CHA-C4D-ND	4.10	141.00	132.55
16	b	604	CLA	O2D-CGD-CBD	4.10	118.39	111.23
16	b	616	CLA	C2C-C1C-NC	4.09	114.28	109.98
16	b	615	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
18	a	407	BCR	C11-C12-C13	-4.09	115.15	126.36
16	b	610	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
16	b	607	CLA	C1D-ND-C4D	4.06	109.16	106.31
16	b	602	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
15	l	101	SQD	O47-C7-C8	4.06	120.26	111.48
16	b	603	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
18	b	619	BCR	C24-C23-C22	-4.05	120.24	126.23
16	b	615	CLA	O2D-CGD-O1D	-4.05	115.97	123.85
16	b	605	CLA	CMC-C2C-C1C	4.04	131.34	125.03
20	d	408	MGE	O2G-C1B-C2B	4.03	120.20	111.48
16	b	613	CLA	C2B-C1B-NB	4.03	114.50	110.33
16	b	611	CLA	C2D-C1D-ND	4.03	114.11	110.13
16	b	611	CLA	C4D-CHA-C1A	-4.03	116.44	121.24
16	b	604	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
16	b	614	CLA	C3D-C2D-C1D	-4.01	100.36	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	402	CLA	C1C-C2C-C3C	-4.01	102.77	106.98
16	b	608	CLA	O2D-CGD-O1D	-4.00	116.05	123.85
16	b	612	CLA	C1-C2-C3	-4.00	119.64	126.20
16	b	611	CLA	C4B-C3B-C2B	-4.00	102.33	107.30
16	b	606	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
16	b	602	CLA	C2C-C1C-NC	3.99	114.17	109.98
16	b	605	CLA	C4D-CHA-C1A	-3.98	116.49	121.24
16	b	606	CLA	C2C-C1C-NC	3.97	114.16	109.98
16	b	602	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
16	b	611	CLA	C3B-C4B-NB	3.96	114.06	110.53
16	b	615	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
16	b	606	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
16	b	616	CLA	C3C-C4C-NC	3.95	115.49	110.43
16	b	608	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
16	b	611	CLA	C2B-C1B-NB	3.94	114.41	110.33
16	a	406	CLA	C4C-C3C-C2C	-3.94	101.16	106.89
16	b	601	CLA	CAC-C3C-C4C	3.94	129.91	124.79
16	b	616	CLA	CAC-C3C-C4C	3.93	129.91	124.79
16	b	611	CLA	O2D-CGD-CBD	3.93	118.10	111.23
20	m	101	MGE	O2G-C1B-C2B	3.92	119.96	111.48
16	d	401	CLA	C2B-C1B-NB	3.91	114.38	110.33
18	h	101	BCR	C32-C1-C6	3.90	116.36	110.24
16	d	401	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
16	b	609	CLA	C3B-C2B-C1B	-3.87	102.61	107.17
16	b	612	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
20	d	409	MGE	O2G-C1B-C2B	3.86	119.83	111.48
16	b	602	CLA	C2B-C1B-NB	3.85	114.32	110.33
16	b	607	CLA	CHA-C4D-ND	3.84	140.46	132.55
18	b	619	BCR	C15-C14-C13	-3.83	121.91	127.28
18	b	619	BCR	C16-C17-C18	-3.83	121.91	127.28
16	b	612	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
16	b	610	CLA	C4D-CHA-C1A	-3.82	116.69	121.24
16	b	613	CLA	CMD-C2D-C1D	3.81	131.44	124.73
16	d	401	CLA	CHD-C4C-NC	3.81	130.14	124.23
16	b	603	CLA	CHC-C4B-NB	3.81	129.76	124.05
18	b	618	BCR	C20-C21-C22	-3.80	121.95	127.28
16	a	403	CLA	CMB-C2B-C1B	3.78	131.17	125.42
16	b	602	CLA	CHD-C4C-C3C	-3.77	119.27	124.77
16	b	604	CLA	C6-C5-C3	-3.77	104.28	113.47
16	b	608	CLA	C2B-C1B-NB	3.77	114.24	110.33
16	b	615	CLA	CAC-C3C-C4C	3.77	129.69	124.79
16	b	614	CLA	O2A-CGA-O1A	-3.76	114.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	610	CLA	O2D-CGD-CBD	3.75	117.79	111.23
16	b	603	CLA	CHD-C4C-NC	3.75	130.04	124.23
16	d	401	CLA	C4D-CHA-C1A	-3.74	116.78	121.24
16	b	614	CLA	CMD-C2D-C1D	3.74	131.31	124.73
18	b	618	BCR	C15-C14-C13	-3.73	122.04	127.28
16	b	610	CLA	CHD-C4C-C3C	-3.73	119.34	124.77
17	a	405	PHO	O1D-CGD-CBD	3.72	130.36	124.72
16	b	606	CLA	CHD-C1D-ND	-3.71	119.58	124.80
16	b	605	CLA	CHC-C4B-NB	3.71	129.61	124.05
16	b	611	CLA	CBC-CAC-C3C	-3.71	102.37	112.42
18	a	407	BCR	C21-C20-C19	3.70	133.93	123.20
16	b	602	CLA	CHD-C1D-ND	-3.70	119.59	124.80
16	a	402	CLA	C1D-ND-C4D	-3.70	103.72	106.31
16	b	604	CLA	CHC-C4B-NB	3.69	129.59	124.05
16	b	608	CLA	C4B-C3B-C2B	-3.69	102.72	107.30
18	h	101	BCR	C15-C14-C13	-3.68	122.11	127.28
16	a	402	CLA	CMB-C2B-C1B	3.68	131.02	125.42
20	d	409	MGE	C3G-C2G-C1G	-3.68	103.22	111.78
16	b	604	CLA	C3C-C4C-NC	3.67	115.13	110.43
16	b	606	CLA	C3B-C2B-C1B	-3.67	102.84	107.17
16	b	604	CLA	CMC-C2C-C1C	3.67	130.77	125.03
16	b	603	CLA	CHA-C4D-ND	3.65	140.08	132.55
16	b	602	CLA	CHA-C4D-ND	3.64	140.05	132.55
20	d	410	MGE	C2G-O2G-C1B	-3.63	109.10	117.80
16	b	616	CLA	O1D-CGD-CBD	-3.63	117.36	124.52
16	b	601	CLA	C4C-C3C-C2C	-3.63	101.61	106.89
16	b	609	CLA	C1-C2-C3	-3.62	120.26	126.20
16	b	608	CLA	C3B-C2B-C1B	-3.62	102.90	107.17
18	h	101	BCR	C11-C10-C9	-3.62	122.20	127.28
18	a	407	BCR	C15-C14-C13	-3.62	122.21	127.28
18	b	619	BCR	C11-C10-C9	-3.62	122.21	127.28
16	b	601	CLA	CHC-C1C-C2C	-3.61	116.68	126.95
16	b	614	CLA	C2B-C1B-NB	3.61	114.07	110.33
16	b	612	CLA	C3B-C2B-C1B	-3.61	102.91	107.17
24	d	406	PQ9	C39-C38-C40	3.61	121.49	115.23
16	b	604	CLA	CHA-C4D-ND	3.61	139.99	132.55
18	b	618	BCR	C3-C4-C5	-3.60	107.64	114.06
17	a	405	PHO	CMB-C2B-C3B	3.59	131.85	124.68
16	b	603	CLA	CAC-C3C-C4C	3.58	129.44	124.79
18	h	101	BCR	C8-C9-C10	3.57	124.62	119.01
16	b	614	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
16	a	406	CLA	C2A-C1A-CHA	-3.56	117.69	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	606	CLA	O2D-CGD-CBD	3.56	117.45	111.23
16	b	609	CLA	CHD-C4C-C3C	-3.56	119.59	124.77
16	b	615	CLA	CMC-C2C-C1C	3.56	130.59	125.03
16	b	611	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
16	b	616	CLA	CHD-C4C-NC	3.53	129.71	124.23
16	b	608	CLA	C4D-CHA-C1A	-3.53	117.03	121.24
16	a	403	CLA	CBC-CAC-C3C	-3.52	102.87	112.42
16	d	401	CLA	CBC-CAC-C3C	-3.51	102.90	112.42
16	d	405	CLA	C4C-C3C-C2C	-3.50	101.79	106.89
16	b	603	CLA	CMC-C2C-C1C	3.50	130.50	125.03
16	b	603	CLA	C3B-C4B-NB	3.49	113.65	110.53
16	b	616	CLA	CHD-C1D-ND	-3.49	119.89	124.80
16	a	403	CLA	CHC-C1C-C2C	-3.49	117.04	126.95
16	b	604	CLA	C3B-C2B-C1B	-3.49	103.06	107.17
16	b	611	CLA	C3D-C2D-C1D	-3.49	101.08	105.83
16	d	404	CLA	C4C-C3C-C2C	-3.48	101.82	106.89
16	b	604	CLA	C2B-C1B-NB	3.48	113.93	110.33
16	b	602	CLA	CMB-C2B-C3B	3.48	134.73	126.55
16	b	611	CLA	C1D-CHD-C4C	-3.47	118.63	126.02
16	d	404	CLA	C4A-NA-C1A	-3.47	105.09	106.68
16	d	404	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
16	b	608	CLA	CHA-C4D-ND	3.45	139.67	132.55
16	b	602	CLA	C1-C2-C3	-3.45	120.54	126.20
16	a	403	CLA	O2D-CGD-O1D	-3.44	117.15	123.85
20	a	409	MGE	O2G-C1B-C2B	3.44	118.92	111.48
20	d	409	MGE	C4D-C3D-C2D	3.43	116.86	110.83
16	b	602	CLA	C1D-CHD-C4C	-3.43	118.72	126.02
18	h	101	BCR	C28-C27-C26	-3.43	107.94	114.06
16	b	603	CLA	C4D-CHA-C1A	-3.43	117.16	121.24
20	b	622	MGE	O1G-C1A-C2A	3.42	122.27	111.83
16	b	609	CLA	C3C-C4C-NC	3.42	114.81	110.43
16	a	402	CLA	C7-C6-C5	-3.41	104.18	113.26
27	e	101	HEM	CHD-C1D-C2D	-3.40	119.67	125.03
16	a	402	CLA	C1D-CHD-C4C	-3.38	118.84	126.02
16	b	615	CLA	CHA-C4D-ND	3.37	139.51	132.55
16	b	609	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
16	b	614	CLA	CMB-C2B-C1B	3.37	130.54	125.42
18	h	101	BCR	C1-C6-C7	3.37	124.78	115.65
16	d	405	CLA	CMB-C2B-C1B	3.35	130.52	125.42
16	a	403	CLA	C4B-CHC-C1C	-3.35	118.38	126.25
16	b	601	CLA	CMD-C2D-C3D	-3.35	120.01	127.69
16	b	606	CLA	C4D-CHA-C1A	-3.35	117.25	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	a	407	BCR	C16-C17-C18	-3.34	122.59	127.28
16	b	606	CLA	O2D-CGD-O1D	-3.34	117.34	123.85
18	b	617	BCR	C27-C26-C25	-3.34	118.20	122.70
17	a	405	PHO	C6-C5-C3	3.33	121.59	113.47
16	a	402	CLA	C2B-C1B-NB	3.33	113.78	110.33
27	e	101	HEM	CHA-C4D-ND	3.33	128.49	124.37
16	b	614	CLA	C4-C3-C2	-3.33	115.08	123.63
20	a	409	MGE	C1D-O6D-C5D	3.32	120.20	113.72
16	b	614	CLA	C3B-C4B-NB	3.32	113.49	110.53
16	b	613	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
18	b	618	BCR	C1-C6-C5	-3.32	118.10	122.64
16	b	616	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
16	b	607	CLA	C4-C3-C5	3.31	120.98	115.23
16	b	605	CLA	C3B-C2B-C1B	-3.31	103.27	107.17
16	a	403	CLA	CHB-C4A-NA	3.31	129.18	124.40
18	b	618	BCR	C15-C16-C17	-3.30	116.77	123.52
18	b	617	BCR	C15-C14-C13	-3.29	122.67	127.28
16	b	609	CLA	C2D-C1D-ND	3.28	113.38	110.13
16	b	604	CLA	C4D-CHA-C1A	-3.28	117.33	121.24
16	b	615	CLA	CMD-C2D-C3D	3.28	135.22	127.69
18	b	617	BCR	C16-C17-C18	-3.28	122.67	127.28
16	b	612	CLA	CHC-C4B-NB	3.27	128.96	124.05
16	b	604	CLA	CMD-C2D-C1D	3.27	130.48	124.73
18	a	407	BCR	C36-C18-C19	3.26	123.07	118.09
16	b	606	CLA	CMD-C2D-C1D	3.25	130.45	124.73
16	b	607	CLA	C2D-C1D-ND	3.24	113.33	110.13
18	b	617	BCR	C11-C10-C9	-3.24	122.73	127.28
16	b	613	CLA	C4D-CHA-C1A	-3.23	117.39	121.24
16	d	405	CLA	CHB-C4A-NA	3.23	129.06	124.40
16	b	608	CLA	O2A-CGA-O1A	-3.23	115.55	123.63
16	d	404	CLA	O2A-CGA-CBA	3.23	121.68	111.83
16	b	610	CLA	C1D-CHD-C4C	-3.22	119.19	126.02
18	b	619	BCR	C38-C26-C27	3.21	120.43	113.60
16	b	613	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
16	b	601	CLA	CHA-C1A-NA	-3.21	119.13	126.39
20	d	409	MGE	O1G-C1A-C2A	3.20	121.60	111.83
18	a	407	BCR	C4-C5-C6	-3.20	118.38	122.70
16	b	610	CLA	CAA-CBA-CGA	-3.19	104.16	113.21
16	b	603	CLA	C5-C3-C2	-3.18	114.04	121.17
16	b	612	CLA	O2D-CGD-CBD	3.17	116.78	111.23
18	b	618	BCR	C4-C5-C6	-3.17	118.42	122.70
16	b	609	CLA	CHC-C4B-NB	3.17	128.80	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	614	CLA	CHC-C4B-NB	3.17	128.80	124.05
16	b	605	CLA	CHA-C4D-ND	3.15	139.04	132.55
16	d	404	CLA	CHC-C1C-C2C	-3.15	118.00	126.95
16	b	606	CLA	CMC-C2C-C3C	3.14	134.65	126.15
18	b	618	BCR	C16-C17-C18	-3.14	122.88	127.28
16	d	404	CLA	CAC-C3C-C4C	3.13	128.87	124.79
18	h	101	BCR	C20-C21-C22	-3.12	122.90	127.28
16	b	605	CLA	C4C-C3C-C2C	-3.12	102.36	106.89
16	d	401	CLA	CHA-C4D-ND	3.12	138.98	132.55
17	a	404	PHO	CBA-CAA-C2A	-3.12	104.60	113.78
16	b	616	CLA	O2A-CGA-CBA	3.11	123.88	112.14
16	b	613	CLA	C1-O2A-CGA	3.11	124.17	116.65
16	d	401	CLA	C1D-ND-C4D	-3.10	104.14	106.31
18	a	407	BCR	C20-C19-C18	3.10	134.86	126.36
16	b	605	CLA	C3A-C2A-C1A	-3.10	96.70	101.34
16	b	614	CLA	CHB-C4A-NA	3.09	128.86	124.40
16	b	615	CLA	C4-C3-C5	3.09	120.59	115.23
16	b	609	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
16	b	607	CLA	C2B-C1B-NB	3.08	113.53	110.33
16	b	614	CLA	C3B-C2B-C1B	-3.08	103.53	107.17
16	b	614	CLA	C1D-CHD-C4C	-3.08	119.47	126.02
16	d	404	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
16	b	605	CLA	CMB-C2B-C1B	3.08	130.11	125.42
16	a	402	CLA	CMD-C2D-C1D	3.08	130.15	124.73
27	e	101	HEM	CHD-C4C-NC	3.08	127.80	124.45
27	e	101	HEM	CHB-C1B-NB	3.07	128.17	124.37
16	d	405	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
16	b	611	CLA	CMC-C2C-C1C	3.07	129.83	125.03
16	b	607	CLA	C3B-C2B-C1B	-3.07	103.55	107.17
16	b	614	CLA	CAC-C3C-C4C	3.06	128.78	124.79
16	b	612	CLA	C4-C3-C5	3.06	120.55	115.23
16	b	607	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
16	b	614	CLA	CHA-C4D-ND	3.06	138.85	132.55
16	d	404	CLA	CHB-C4A-NA	3.05	128.80	124.40
16	b	608	CLA	CHD-C1D-ND	-3.05	120.51	124.80
16	b	606	CLA	O2A-CGA-O1A	-3.05	116.01	123.63
17	a	404	PHO	CBC-CAC-C3C	-3.04	108.52	112.87
16	b	610	CLA	CMB-C2B-C1B	3.04	130.05	125.42
17	a	405	PHO	C4-C3-C5	3.04	120.51	115.23
16	b	603	CLA	O2D-CGD-CBD	3.03	116.53	111.23
16	b	613	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
18	h	101	BCR	C24-C23-C22	-3.03	121.75	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	618	BCR	C11-C10-C9	-3.03	123.03	127.28
16	b	614	CLA	C1-O2A-CGA	3.02	123.97	116.65
16	b	614	CLA	CHD-C4C-NC	3.02	128.91	124.23
18	d	407	BCR	C11-C10-C9	-3.02	123.05	127.28
16	b	602	CLA	CMD-C2D-C3D	3.01	134.59	127.69
16	b	604	CLA	O2A-CGA-O1A	-3.00	116.11	123.63
15	l	101	SQD	O48-C23-C24	3.00	120.99	111.83
16	b	609	CLA	C2B-C1B-NB	3.00	113.44	110.33
16	b	613	CLA	C2A-C1A-CHA	-3.00	118.67	123.87
16	b	613	CLA	C3B-C2B-C1B	-3.00	103.64	107.17
16	b	607	CLA	CMD-C2D-C1D	3.00	130.00	124.73
16	b	606	CLA	CHD-C4C-NC	2.99	128.87	124.23
22	t	101	LMT	C2'-C3'-C4'	2.99	116.46	109.68
26	d	412	DGD	O1G-C1A-C2A	2.98	120.94	111.83
20	b	620	MGE	C1D-O6D-C5D	2.98	119.55	113.72
16	b	602	CLA	C4-C3-C5	2.98	120.41	115.23
16	a	402	CLA	CHD-C4C-NC	2.98	128.85	124.23
16	b	602	CLA	C4D-CHA-C1A	-2.98	117.69	121.24
16	b	605	CLA	CHC-C1C-NC	-2.97	119.84	124.31
16	a	402	CLA	C4D-CHA-C1A	-2.96	117.71	121.24
20	d	410	MGE	O1G-C1A-C2A	2.96	120.86	111.83
18	d	407	BCR	C16-C17-C18	-2.96	123.13	127.28
16	b	605	CLA	C2B-C1B-NB	2.96	113.39	110.33
16	a	403	CLA	C2A-C1A-CHA	-2.96	118.74	123.87
16	a	406	CLA	C4D-C3D-CAD	2.95	111.31	108.11
16	a	406	CLA	CHB-C4A-NA	2.95	128.66	124.40
27	e	101	HEM	C1B-NB-C4B	2.95	108.70	105.21
16	b	602	CLA	C2A-C3A-C4A	-2.95	97.11	101.87
16	b	616	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
16	b	608	CLA	CAC-C3C-C4C	2.94	128.62	124.79
16	b	615	CLA	CHD-C4C-NC	2.94	128.79	124.23
16	b	610	CLA	CHA-C4D-ND	2.93	138.60	132.55
16	b	612	CLA	C3B-C4B-NB	2.93	113.15	110.53
16	b	613	CLA	CHC-C4B-NB	2.93	128.44	124.05
16	b	613	CLA	CHD-C1D-ND	-2.92	120.69	124.80
16	b	607	CLA	CHD-C1D-ND	-2.92	120.69	124.80
16	a	402	CLA	CHC-C4B-NB	2.92	128.43	124.05
15	l	101	SQD	O8-S-O7	2.92	118.69	111.40
16	d	405	CLA	CAC-C3C-C4C	2.91	128.58	124.79
16	b	610	CLA	CHB-C4A-NA	2.91	128.60	124.40
16	a	406	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
15	a	401	SQD	C45-O47-C7	-2.90	112.72	117.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	b	619	BCR	C33-C5-C6	-2.90	121.32	124.48
18	h	101	BCR	C16-C15-C14	-2.89	117.60	123.52
16	d	405	CLA	CHB-C1B-C2B	-2.89	119.03	127.43
16	b	607	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
16	b	608	CLA	C3C-C4C-NC	2.89	114.13	110.43
17	a	405	PHO	O2D-CGD-O1D	-2.89	118.23	123.85
16	b	609	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
18	b	617	BCR	C8-C7-C6	-2.88	119.30	127.00
16	b	616	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
16	b	605	CLA	C2A-C1A-CHA	-2.88	118.88	123.87
16	b	607	CLA	CHD-C4C-NC	2.87	128.69	124.23
18	b	618	BCR	C30-C25-C26	-2.87	118.71	122.64
16	a	402	CLA	CAC-C3C-C2C	-2.87	122.28	127.56
16	a	403	CLA	O2A-CGA-CBA	2.87	120.58	111.83
16	b	606	CLA	C1-O2A-CGA	2.87	123.59	116.65
16	a	406	CLA	CHB-C1B-C2B	-2.86	119.11	127.43
16	b	606	CLA	C1D-ND-C4D	-2.86	104.30	106.31
16	b	602	CLA	CMA-C3A-C4A	-2.86	104.08	111.77
16	b	613	CLA	C3C-C4C-NC	2.86	114.09	110.43
15	a	401	SQD	O8-S-O7	2.86	118.55	111.40
20	b	620	MGE	O1G-C1A-O1A	-2.85	116.49	123.63
16	b	606	CLA	C3B-C4B-NB	2.85	113.08	110.53
18	b	617	BCR	C30-C25-C26	-2.85	118.74	122.64
16	d	405	CLA	CMC-C2C-C1C	2.85	129.49	125.03
16	b	605	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
16	b	608	CLA	C3B-C4B-NB	2.84	113.07	110.53
20	d	408	MGE	C1D-O6D-C5D	2.84	119.26	113.72
16	a	403	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
16	b	615	CLA	C3B-C4B-NB	2.83	113.06	110.53
16	b	602	CLA	O2A-CGA-O1A	-2.82	116.56	123.63
16	b	613	CLA	C3B-C4B-NB	2.82	113.05	110.53
18	a	407	BCR	C8-C9-C10	2.81	123.44	119.01
18	b	618	BCR	C8-C7-C6	-2.79	119.53	127.00
17	a	405	PHO	CAC-C3C-C2C	2.79	132.68	127.56
16	b	610	CLA	CHD-C4C-NC	2.79	128.55	124.23
16	b	610	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
16	b	610	CLA	CMD-C2D-C1D	2.78	129.63	124.73
16	b	607	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
17	a	405	PHO	C3B-C4B-NB	-2.78	105.65	107.46
16	b	607	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
16	a	406	CLA	CHC-C4B-NB	-2.77	119.89	124.05
20	d	408	MGE	O1G-C1A-C2A	2.77	120.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	614	CLA	C4-C3-C5	2.77	120.03	115.23
16	b	603	CLA	C1D-CHD-C4C	-2.77	120.14	126.02
16	d	404	CLA	C2A-C1A-CHA	-2.76	119.07	123.87
16	a	403	CLA	CMC-C2C-C1C	2.76	129.35	125.03
16	d	404	CLA	CMC-C2C-C1C	2.76	129.34	125.03
16	b	614	CLA	C4B-C3B-C2B	-2.76	103.88	107.30
16	a	402	CLA	CHA-C4D-ND	2.76	138.24	132.55
16	b	603	CLA	C2A-C1A-CHA	-2.75	119.09	123.87
16	b	616	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
16	a	406	CLA	C1-C2-C3	-2.74	122.32	126.76
16	b	609	CLA	C7-C6-C5	-2.74	105.96	113.26
16	b	609	CLA	CHD-C1D-ND	-2.74	120.95	124.80
18	b	618	BCR	C33-C5-C4	2.74	119.43	113.60
16	d	401	CLA	CMB-C2B-C1B	2.74	129.59	125.42
18	h	101	BCR	C7-C6-C5	-2.73	115.26	121.56
16	b	612	CLA	O2A-CGA-CBA	2.73	120.17	111.83
16	a	402	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
16	a	402	CLA	CHD-C1D-ND	-2.73	120.96	124.80
16	b	607	CLA	C4D-CHA-C1A	-2.73	117.99	121.24
16	b	611	CLA	C14-C13-C15	-2.73	101.56	111.27
16	b	607	CLA	O2D-CGD-CBD	2.72	115.99	111.23
26	d	412	DGD	C1E-O6E-C5E	2.72	119.04	113.72
18	b	617	BCR	C7-C8-C9	-2.72	122.21	126.23
18	h	101	BCR	C30-C25-C26	-2.72	118.92	122.64
16	b	615	CLA	CMB-C2B-C3B	2.72	132.94	126.55
16	a	402	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
18	b	617	BCR	C21-C20-C19	-2.71	115.36	123.20
16	b	604	CLA	CED-O2D-CGD	2.70	122.04	115.92
16	b	613	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
16	a	403	CLA	CMD-C2D-C3D	-2.70	121.50	127.69
16	b	616	CLA	CHA-C4D-ND	2.70	138.11	132.55
16	b	614	CLA	CBC-CAC-C3C	-2.69	105.12	112.42
16	d	405	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
20	d	410	MGE	O6D-C1D-O3G	2.69	116.39	110.04
16	a	406	CLA	O2A-CGA-CBA	2.68	120.02	111.83
16	b	605	CLA	C4A-NA-C1A	-2.68	105.45	106.68
16	d	401	CLA	C4A-NA-C1A	-2.68	105.45	106.68
24	d	406	PQ9	C29-C28-C27	-2.68	116.74	123.63
16	b	614	CLA	C4B-CHC-C1C	-2.68	119.94	126.25
16	d	405	CLA	O2A-CGA-CBA	2.68	120.00	111.83
16	b	603	CLA	C7-C6-C5	-2.68	106.13	113.26
16	a	406	CLA	CHC-C1C-C2C	-2.67	119.36	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	613	CLA	O2A-CGA-CBA	2.67	119.97	111.83
16	b	609	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
17	a	405	PHO	C4B-NB-C1B	2.66	112.70	108.82
16	b	603	CLA	C4B-C3B-C2B	-2.66	103.99	107.30
16	b	610	CLA	CHC-C4B-NB	2.66	128.04	124.05
16	a	406	CLA	CMC-C2C-C1C	2.66	129.18	125.03
16	b	609	CLA	CHA-C4D-ND	2.65	138.02	132.55
16	b	602	CLA	CHC-C4B-NB	2.64	128.01	124.05
24	d	406	PQ9	C19-C18-C20	2.64	119.81	115.23
18	b	617	BCR	C4-C5-C6	-2.64	119.14	122.70
16	d	404	CLA	C4D-C3D-CAD	2.64	110.97	108.11
16	d	404	CLA	CGD-CBD-CAD	-2.64	102.31	110.85
16	b	601	CLA	CMB-C2B-C1B	2.64	129.43	125.42
16	b	615	CLA	CHC-C4B-C3B	-2.64	115.93	127.37
16	b	614	CLA	O2A-CGA-CBA	2.62	119.83	111.83
16	b	608	CLA	C1D-CHD-C4C	-2.62	120.45	126.02
16	a	403	CLA	CHB-C1B-C2B	-2.62	119.83	127.43
16	b	614	CLA	CHD-C1D-ND	-2.61	121.12	124.80
18	d	407	BCR	C15-C14-C13	-2.61	123.61	127.28
20	m	101	MGE	O1G-C1A-C2A	2.61	119.80	111.83
24	d	406	PQ9	C11-C12-C13	-2.61	122.34	126.83
17	a	404	PHO	C3B-C4B-NB	-2.60	105.77	107.46
16	a	406	CLA	CMB-C2B-C1B	2.60	129.38	125.42
16	b	604	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
20	b	622	MGE	O1G-C1A-O1A	-2.60	117.12	123.63
18	b	618	BCR	C7-C8-C9	-2.60	122.39	126.23
18	b	617	BCR	C1-C6-C5	-2.59	119.09	122.64
15	a	401	SQD	C4-C3-C2	2.59	115.37	110.83
16	b	603	CLA	CMB-C2B-C3B	2.59	132.63	126.55
18	b	619	BCR	C32-C1-C6	-2.58	106.19	110.24
18	b	619	BCR	C1-C6-C5	-2.58	119.11	122.64
16	b	607	CLA	CBC-CAC-C3C	-2.58	105.43	112.42
16	b	615	CLA	CMA-C3A-C4A	-2.58	104.84	111.77
16	b	610	CLA	CHD-C1D-ND	-2.58	121.17	124.80
16	b	610	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
16	b	614	CLA	CED-O2D-CGD	2.57	121.74	115.92
17	a	404	PHO	C4-C3-C5	2.56	119.68	115.23
16	d	405	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
18	h	101	BCR	C34-C9-C10	-2.56	118.67	122.82
16	a	403	CLA	C1-C2-C3	-2.56	122.62	126.76
18	a	407	BCR	C28-C27-C26	-2.56	109.50	114.06
16	b	601	CLA	O1D-CGD-CBD	-2.55	119.49	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	d	407	BCR	C16-C15-C14	-2.55	118.31	123.52
17	a	405	PHO	CBC-CAC-C3C	-2.54	109.23	112.87
16	d	401	CLA	C1-O2A-CGA	2.54	122.80	116.65
16	b	616	CLA	CED-O2D-CGD	2.54	121.68	115.92
16	b	611	CLA	CMD-C2D-C1D	2.54	129.19	124.73
16	b	602	CLA	CHD-C4C-NC	2.54	128.16	124.23
16	b	616	CLA	C4D-CHA-C1A	-2.53	118.23	121.24
16	b	613	CLA	CHD-C4C-NC	2.53	128.15	124.23
16	b	616	CLA	CBC-CAC-C3C	-2.52	105.58	112.42
16	a	406	CLA	CMD-C2D-C3D	-2.52	121.92	127.69
16	b	611	CLA	CHD-C4C-NC	2.52	128.13	124.23
16	d	405	CLA	C4B-CHC-C1C	-2.52	120.33	126.25
16	b	606	CLA	CBC-CAC-C3C	-2.52	105.60	112.42
16	b	604	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
16	b	610	CLA	C3B-C4B-NB	2.51	112.77	110.53
20	a	409	MGE	O1G-C1A-C2A	2.51	119.48	111.83
20	d	409	MGE	C1D-O6D-C5D	2.50	118.61	113.72
16	a	403	CLA	C4D-C3D-CAD	2.50	110.83	108.11
16	b	602	CLA	O2A-CGA-CBA	2.50	119.47	111.83
16	b	609	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
22	b	623	LMT	C2'-C3'-C4'	2.50	115.36	109.68
16	a	403	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
16	b	603	CLA	CHC-C4B-C3B	-2.50	116.54	127.37
16	d	404	CLA	CMB-C2B-C1B	2.50	129.22	125.42
27	e	101	HEM	CAD-CBD-CGD	-2.50	107.05	113.67
20	d	409	MGE	C3D-C4D-C5D	2.50	114.76	110.23
16	d	404	CLA	CHD-C1D-ND	-2.49	121.29	124.80
16	d	404	CLA	CHB-C1B-C2B	-2.49	120.19	127.43
18	b	617	BCR	C40-C30-C25	-2.49	106.33	110.24
16	b	604	CLA	C7-C6-C5	-2.49	106.63	113.26
16	b	615	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
16	b	607	CLA	CGD-CBD-CAD	-2.49	102.80	110.85
16	d	401	CLA	C3C-C4C-NC	2.48	113.61	110.43
16	d	405	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
16	b	603	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
17	a	405	PHO	CAA-CBA-CGA	-2.47	106.19	113.21
20	b	622	MGE	C2G-O2G-C1B	-2.46	111.91	117.80
16	b	607	CLA	C7-C6-C5	-2.46	106.71	113.26
20	b	622	MGE	C3G-C2G-C1G	-2.45	106.06	111.78
20	d	408	MGE	O3G-C1D-C2D	2.45	112.00	108.27
16	b	602	CLA	C2A-C1A-CHA	-2.45	119.62	123.87
16	b	613	CLA	CHA-C4D-ND	2.45	137.60	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	612	CLA	C4B-CHC-C1C	-2.45	120.49	126.25
22	t	101	LMT	O1B-C1B-O5B	-2.44	104.27	110.69
18	b	618	BCR	C28-C27-C26	-2.44	109.71	114.06
18	b	619	BCR	C30-C25-C26	-2.44	119.31	122.64
16	b	608	CLA	CMD-C2D-C1D	2.43	129.01	124.73
16	b	602	CLA	C16-C17-C18	-2.42	105.12	115.94
16	b	606	CLA	CMB-C2B-C1B	2.42	129.10	125.42
20	d	408	MGE	C4D-C3D-C2D	2.42	115.07	110.83
16	d	404	CLA	C1-C2-C3	-2.41	122.25	126.20
16	a	402	CLA	C1-C2-C3	-2.41	122.25	126.20
20	d	410	MGE	C1D-C2D-C3D	-2.41	104.94	110.01
16	b	612	CLA	CED-O2D-CGD	2.41	121.37	115.92
16	b	607	CLA	CHC-C4B-NB	2.40	127.65	124.05
18	b	619	BCR	C33-C5-C4	2.40	118.72	113.60
22	t	101	LMT	C1'-C2'-C3'	2.40	115.05	110.01
16	b	607	CLA	C3B-C4B-NB	2.39	112.66	110.53
15	a	401	SQD	C3-C4-C5	2.38	114.55	110.23
16	b	601	CLA	CHD-C4C-C3C	-2.38	121.30	124.77
16	b	606	CLA	C4B-C3B-C2B	-2.38	104.34	107.30
22	t	101	LMT	O1B-C1B-C2B	2.38	113.95	108.09
20	m	101	MGE	C4D-C3D-C2D	2.38	115.01	110.83
16	b	612	CLA	CMB-C2B-C1B	2.38	129.04	125.42
18	a	407	BCR	C36-C18-C17	-2.38	118.97	122.82
17	a	405	PHO	C2D-C1D-ND	-2.37	107.72	109.43
16	d	404	CLA	C4B-CHC-C1C	-2.37	120.67	126.25
16	b	611	CLA	C7-C6-C5	-2.37	106.95	113.26
20	d	409	MGE	C3G-O3G-C1D	-2.37	108.72	113.80
16	b	607	CLA	C1-C2-C3	-2.36	122.34	126.20
18	h	101	BCR	C39-C30-C25	-2.35	106.55	110.24
16	b	607	CLA	C3C-C4C-NC	2.35	113.44	110.43
16	a	402	CLA	C3B-C4B-NB	2.35	112.63	110.53
18	b	617	BCR	C20-C21-C22	-2.35	123.99	127.28
16	d	405	CLA	C1-O2A-CGA	2.35	122.33	116.65
16	b	601	CLA	CHB-C4A-NA	-2.34	121.02	124.40
16	d	404	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
18	d	407	BCR	C21-C20-C19	-2.34	116.42	123.20
20	b	622	MGE	C4D-C3D-C2D	2.33	114.92	110.83
16	b	605	CLA	C4B-C3B-C2B	-2.33	104.41	107.30
16	b	616	CLA	C1-O2A-CGA	2.33	123.52	116.07
16	a	402	CLA	O2A-CGA-CBA	2.33	118.93	111.83
20	b	622	MGE	C1D-O6D-C5D	2.33	118.26	113.72
16	b	614	CLA	C2A-C1A-CHA	-2.33	119.83	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	605	CLA	C1-C2-C3	-2.32	122.39	126.20
16	b	605	CLA	C14-C13-C12	-2.32	103.00	111.27
16	d	401	CLA	CHC-C4B-C3B	-2.31	117.33	127.37
26	d	412	DGD	O2G-C1B-O1B	-2.31	118.30	123.70
16	b	609	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
18	d	407	BCR	C20-C21-C22	-2.31	124.05	127.28
16	b	611	CLA	CAC-C3C-C4C	2.31	127.79	124.79
16	b	616	CLA	CHC-C4B-NB	2.30	127.51	124.05
16	a	402	CLA	CMC-C2C-C3C	2.30	132.38	126.15
16	b	611	CLA	C3B-C2B-C1B	-2.30	104.46	107.17
16	b	616	CLA	CMB-C2B-C3B	2.30	131.96	126.55
16	b	609	CLA	C4B-C3B-C2B	-2.30	104.45	107.30
17	a	405	PHO	C6-C7-C8	2.29	123.59	115.97
16	b	615	CLA	C1-O2A-CGA	2.29	122.20	116.65
20	a	409	MGE	O6D-C5D-C4D	2.29	113.83	109.70
17	a	404	PHO	O2D-CGD-O1D	-2.29	119.39	123.85
18	b	619	BCR	C29-C28-C27	2.29	116.31	111.28
16	b	615	CLA	C11-C10-C8	-2.29	108.36	115.97
18	b	617	BCR	C38-C26-C27	2.29	118.47	113.60
18	b	617	BCR	C16-C15-C14	-2.28	118.84	123.52
18	d	407	BCR	C10-C11-C12	-2.28	116.59	123.20
16	b	608	CLA	CHD-C4C-NC	2.28	127.77	124.23
24	d	406	PQ9	C6-C5-C4	2.27	119.93	115.28
16	b	602	CLA	CED-O2D-CGD	2.27	121.07	115.92
18	d	407	BCR	C28-C27-C26	-2.27	110.01	114.06
16	d	404	CLA	C4-C3-C5	2.26	119.16	115.23
16	b	612	CLA	C2B-C1B-NB	2.26	112.67	110.33
16	b	614	CLA	C4D-C3D-CAD	2.26	110.56	108.11
18	b	618	BCR	C10-C11-C12	-2.26	116.64	123.20
16	b	606	CLA	O2A-CGA-CBA	2.26	118.72	111.83
16	b	612	CLA	C4B-C3B-C2B	-2.26	104.50	107.30
17	a	404	PHO	C5-C3-C2	-2.25	116.12	121.17
16	b	612	CLA	CMC-C2C-C1C	2.25	128.54	125.03
16	b	603	CLA	C3C-C4C-NC	2.24	113.30	110.43
15	l	101	SQD	C4-C3-C2	2.24	114.77	110.83
16	b	610	CLA	O2A-CGA-CBA	2.24	118.67	111.83
16	a	406	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
16	b	606	CLA	CHA-C4D-ND	2.24	137.16	132.55
16	b	614	CLA	C3D-C4D-ND	2.24	113.62	109.99
16	d	404	CLA	CHC-C4B-NB	-2.23	120.70	124.05
18	a	407	BCR	C33-C5-C4	2.23	118.35	113.60
16	b	611	CLA	CHD-C1D-ND	-2.23	121.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	614	CLA	CHC-C4B-C3B	-2.23	117.70	127.37
16	b	608	CLA	C6-C5-C3	-2.23	108.04	113.47
17	a	404	PHO	C6-C5-C3	2.21	118.86	113.47
27	e	101	HEM	C4C-CHD-C1D	-2.21	121.32	126.02
16	b	604	CLA	C3B-C4B-NB	2.21	112.50	110.53
16	b	612	CLA	CHC-C4B-C3B	-2.20	117.81	127.37
18	a	407	BCR	C10-C11-C12	2.20	129.56	123.20
16	b	611	CLA	C3C-C4C-NC	2.19	113.23	110.43
16	d	401	CLA	CGD-CBD-CAD	-2.19	103.77	110.85
18	b	618	BCR	C33-C5-C6	-2.18	122.10	124.48
16	b	604	CLA	CHC-C4B-C3B	-2.18	117.90	127.37
15	a	401	SQD	O6-C1-C2	2.18	111.58	108.27
16	a	403	CLA	CHB-C1B-NB	-2.18	120.78	124.05
20	b	620	MGE	O2G-C1B-O1B	-2.17	118.63	123.70
16	d	401	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
20	d	410	MGE	O6D-C5D-C6D	2.16	111.80	106.44
16	b	603	CLA	C1-C2-C3	-2.16	122.66	126.20
16	b	606	CLA	C4-C3-C5	2.16	118.97	115.23
18	b	617	BCR	C23-C24-C25	-2.16	121.24	127.00
16	a	406	CLA	CAC-C3C-C4C	2.16	127.59	124.79
16	d	401	CLA	C4C-C3C-C2C	-2.15	103.76	106.89
20	d	410	MGE	O1G-C1A-O1A	-2.15	118.25	123.63
16	b	611	CLA	C17-C16-C15	-2.15	103.65	113.28
20	d	409	MGE	O1G-C1A-O1A	-2.15	118.25	123.63
16	b	616	CLA	C3B-C4B-NB	2.15	112.45	110.53
18	b	619	BCR	C23-C24-C25	-2.15	121.26	127.00
16	b	611	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
16	b	606	CLA	C1-C2-C3	-2.14	122.68	126.20
16	b	602	CLA	C17-C16-C15	-2.14	103.67	113.28
16	b	606	CLA	CHC-C1C-C2C	-2.14	120.86	126.95
16	b	604	CLA	C1D-CHD-C4C	-2.14	121.47	126.02
16	b	615	CLA	CBB-CAB-C3B	-2.14	116.83	127.53
18	b	619	BCR	C15-C16-C17	-2.14	119.15	123.52
16	d	401	CLA	OBD-CAD-C3D	-2.13	123.44	128.42
16	d	401	CLA	CMD-C2D-C3D	2.13	132.57	127.69
24	d	406	PQ9	O4-C4-C5	-2.12	117.10	120.48
16	b	615	CLA	CBC-CAC-C3C	-2.12	106.67	112.42
16	b	608	CLA	C6-C7-C8	-2.12	108.91	115.97
27	e	101	HEM	C1A-CHA-C4D	-2.12	121.26	126.25
16	b	610	CLA	C4D-C3D-CAD	2.12	110.41	108.11
20	d	410	MGE	O2G-C1B-O1B	-2.12	118.75	123.70
16	b	610	CLA	C4B-C3B-C2B	-2.12	104.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	a	402	CLA	O2D-CGD-CBD	2.11	114.93	111.23
16	b	611	CLA	C16-C15-C13	2.11	122.97	115.97
18	d	407	BCR	C33-C5-C6	-2.11	122.18	124.48
20	d	409	MGE	O3D-C3D-C2D	-2.10	105.42	110.38
17	a	404	PHO	C4B-NB-C1B	2.10	111.88	108.82
16	a	402	CLA	C6-C5-C3	-2.10	108.36	113.47
24	d	406	PQ9	C24-C23-C25	2.10	118.87	115.23
16	b	609	CLA	CMB-C2B-C1B	2.09	128.60	125.42
16	b	612	CLA	CHA-C4D-ND	2.09	136.87	132.55
17	a	404	PHO	CMB-C2B-C3B	2.09	128.86	124.68
18	b	619	BCR	C4-C5-C6	-2.09	119.88	122.70
16	b	616	CLA	CHC-C1C-NC	-2.08	121.17	124.31
16	b	601	CLA	CMB-C2B-C3B	2.08	131.45	126.55
20	d	410	MGE	O6D-C5D-C4D	2.08	113.45	109.70
24	d	406	PQ9	C29-C28-C30	2.08	118.84	115.23
16	b	606	CLA	C3C-C4C-NC	2.08	113.09	110.43
16	b	612	CLA	CMD-C2D-C1D	2.07	128.38	124.73
16	b	602	CLA	CHB-C1B-C2B	-2.07	121.41	127.43
16	b	601	CLA	CHD-C1D-C2D	2.07	129.79	125.49
18	b	618	BCR	C1-C6-C7	2.07	121.26	115.65
16	d	405	CLA	CHC-C4B-NB	-2.07	120.95	124.05
16	b	606	CLA	C4C-C3C-C2C	-2.07	103.88	106.89
18	h	101	BCR	C20-C19-C18	-2.07	120.69	126.36
16	b	615	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
16	b	605	CLA	CAC-C3C-C2C	-2.07	123.76	127.56
16	d	404	CLA	CHB-C1B-NB	-2.07	120.95	124.05
16	b	604	CLA	O2A-CGA-CBA	2.06	118.13	111.83
24	d	406	PQ9	C3-C4-C5	2.06	121.45	119.00
16	d	404	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
16	b	608	CLA	C2A-C1A-CHA	-2.06	120.29	123.87
16	a	406	CLA	C4B-C3B-C2B	-2.05	104.75	107.30
16	b	609	CLA	CBB-CAB-C3B	-2.05	117.26	127.53
17	a	404	PHO	OBD-CAD-CBD	-2.05	122.81	125.82
18	d	407	BCR	C15-C16-C17	-2.05	119.32	123.52
16	a	403	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
24	d	406	PQ9	C14-C13-C15	2.05	118.78	115.23
16	b	603	CLA	CHC-C1C-NC	-2.05	121.22	124.31
16	a	402	CLA	C4C-C3C-C2C	-2.04	103.92	106.89
16	b	613	CLA	CHC-C4B-C3B	-2.04	118.51	127.37
16	b	606	CLA	C4B-CHC-C1C	-2.04	121.45	126.25
18	h	101	BCR	C1-C6-C5	-2.04	119.85	122.64
20	d	410	MGE	O3G-C3G-C2G	2.03	115.76	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	b	603	CLA	CBB-CAB-C3B	-2.03	117.38	127.53
18	a	407	BCR	C8-C7-C6	2.03	132.42	127.00
27	e	101	HEM	O2A-CGA-CBA	2.03	120.41	114.00
16	b	604	CLA	CBB-CAB-C3B	-2.03	117.41	127.53
16	a	402	CLA	CHC-C1C-C2C	-2.02	121.19	126.95
18	d	407	BCR	C35-C13-C12	2.02	121.18	118.09
16	b	612	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
26	d	412	DGD	O6D-C1D-C2D	-2.02	106.22	110.37
17	a	404	PHO	O1D-CGD-CBD	2.02	127.78	124.72
16	b	608	CLA	C1-O2A-CGA	2.02	121.53	116.65
16	b	608	CLA	CMC-C2C-C1C	2.02	128.18	125.03
16	d	405	CLA	CMA-C3A-C4A	-2.01	106.36	111.77
18	b	617	BCR	C11-C12-C13	-2.01	120.85	126.36
16	a	406	CLA	CAC-C3C-C2C	2.01	131.25	127.56
18	a	407	BCR	C29-C28-C27	-2.01	106.86	111.28
16	d	404	CLA	C6-C5-C3	-2.01	108.58	113.47
26	d	412	DGD	O6D-C5D-C6D	2.01	110.67	106.69
25	d	411	HTG	C1-O5-C5	2.01	116.16	112.56
16	a	402	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
20	m	101	MGE	C2G-O2G-C1B	-2.00	113.00	117.80
26	d	412	DGD	O1G-C1A-O1A	-2.00	118.62	123.63
16	b	612	CLA	C1D-ND-C4D	-2.00	104.91	106.31
16	b	609	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
20	b	622	MGE	C3G-O3G-C1D	-2.00	109.50	113.80
16	b	612	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	a	402	CLA	ND
16	b	602	CLA	ND
16	b	603	CLA	ND
16	b	604	CLA	ND
16	b	605	CLA	ND
16	b	606	CLA	ND
16	b	607	CLA	ND
16	b	610	CLA	ND
16	b	612	CLA	ND
16	b	613	CLA	ND
16	b	614	CLA	ND
16	b	615	CLA	ND
16	b	616	CLA	ND

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Mol	Chain	Res	Type	Atom
16	d	401	CLA	ND
16	d	404	CLA	C8

All (278) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	a	401	SQD	O5-C5-C6-S
15	a	401	SQD	C5-C6-S-O8
15	l	101	SQD	C5-C6-S-O7
15	l	101	SQD	C5-C6-S-O9
16	a	403	CLA	C2B-C3B-CAB-CBB
16	a	403	CLA	C4B-C3B-CAB-CBB
16	a	406	CLA	C1A-C2A-CAA-CBA
16	a	406	CLA	C3A-C2A-CAA-CBA
16	b	601	CLA	C4B-C3B-CAB-CBB
16	b	601	CLA	CBD-CGD-O2D-CED
16	b	605	CLA	C4-C3-C5-C6
16	b	614	CLA	CAD-CBD-CGD-O1D
16	b	614	CLA	CAD-CBD-CGD-O2D
16	b	614	CLA	C3-C5-C6-C7
17	a	405	PHO	CBD-CGD-O2D-CED
18	a	407	BCR	C7-C8-C9-C10
18	a	407	BCR	C7-C8-C9-C34
18	a	407	BCR	C11-C12-C13-C14
18	a	407	BCR	C17-C18-C19-C20
18	d	407	BCR	C21-C22-C23-C24
18	d	407	BCR	C37-C22-C23-C24
18	h	101	BCR	C5-C6-C7-C8
20	a	409	MGE	O2G-C2G-C3G-O3G
20	b	620	MGE	O2G-C2G-C3G-O3G
20	d	410	MGE	O6D-C1D-O3G-C3G
20	m	101	MGE	C2B-C1B-O2G-C2G
20	m	101	MGE	O1B-C1B-O2G-C2G
27	e	101	HEM	C2B-C3B-CAB-CBB
27	e	101	HEM	C4B-C3B-CAB-CBB
27	e	101	HEM	C2C-C3C-CAC-CBC
27	e	101	HEM	C4C-C3C-CAC-CBC
17	a	405	PHO	O1D-CGD-O2D-CED
15	a	401	SQD	C8-C7-O47-C45
16	a	406	CLA	O1A-CGA-O2A-C1
16	a	406	CLA	CBA-CGA-O2A-C1
16	d	405	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
16	d	404	CLA	C4-C3-C5-C6
17	a	404	PHO	C4-C3-C5-C6
16	b	605	CLA	C2-C3-C5-C6
17	a	404	PHO	C2-C3-C5-C6
16	b	601	CLA	O1D-CGD-O2D-CED
16	b	604	CLA	C3-C5-C6-C7
15	a	401	SQD	O49-C7-O47-C45
16	b	614	CLA	C2-C3-C5-C6
24	d	406	PQ9	C13-C15-C16-C17
24	d	406	PQ9	C23-C25-C26-C27
24	d	406	PQ9	C38-C40-C41-C42
22	t	101	LMT	O5'-C5'-C6'-O6'
16	b	614	CLA	C4-C3-C5-C6
17	a	405	PHO	C4-C3-C5-C6
24	d	406	PQ9	C39-C38-C40-C41
16	d	404	CLA	C2-C3-C5-C6
17	a	405	PHO	C2-C3-C5-C6
24	d	406	PQ9	C37-C38-C40-C41
16	d	405	CLA	O1D-CGD-O2D-CED
18	a	407	BCR	C11-C12-C13-C35
18	a	407	BCR	C36-C18-C19-C20
18	d	407	BCR	C7-C8-C9-C34
18	h	101	BCR	C7-C8-C9-C34
18	h	101	BCR	C7-C8-C9-C10
20	m	101	MGE	C1A-C2A-C3A-C4A
16	b	604	CLA	C13-C15-C16-C17
22	t	101	LMT	C4'-C5'-C6'-O6'
20	d	410	MGE	C1A-C2A-C3A-C4A
16	b	606	CLA	C11-C12-C13-C15
18	h	101	BCR	C9-C10-C11-C12
22	t	101	LMT	O5'-C1'-O1'-C1
16	d	404	CLA	C8-C10-C11-C12
16	d	404	CLA	C10-C11-C12-C13
20	b	622	MGE	C2B-C1B-O2G-C2G
16	b	603	CLA	C5-C6-C7-C8
17	a	405	PHO	C5-C6-C7-C8
20	b	622	MGE	O1B-C1B-O2G-C2G
16	a	402	CLA	C15-C16-C17-C18
20	d	410	MGE	C2D-C1D-O3G-C3G
22	t	101	LMT	C2'-C1'-O1'-C1
16	b	606	CLA	C13-C15-C16-C17
18	d	407	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
16	b	615	CLA	C10-C11-C12-C13
17	a	404	PHO	C16-C17-C18-C20
16	b	606	CLA	C16-C17-C18-C19
17	a	404	PHO	C16-C17-C18-C19
20	m	101	MGE	C5B-C6B-C7B-C8B
20	d	410	MGE	C2B-C1B-O2G-C2G
16	b	606	CLA	C6-C7-C8-C10
15	l	101	SQD	C23-C24-C25-C26
15	l	101	SQD	C14-C15-C16-C17
20	d	408	MGE	C5B-C6B-C7B-C8B
16	b	611	CLA	O1D-CGD-O2D-CED
20	a	409	MGE	C5B-C6B-C7B-C8B
16	b	601	CLA	C2B-C3B-CAB-CBB
18	d	407	BCR	C1-C6-C7-C8
18	d	407	BCR	C5-C6-C7-C8
18	d	407	BCR	C23-C24-C25-C26
18	d	407	BCR	C23-C24-C25-C30
18	h	101	BCR	C1-C6-C7-C8
18	h	101	BCR	C23-C24-C25-C26
18	h	101	BCR	C23-C24-C25-C30
16	b	608	CLA	C13-C15-C16-C17
20	b	620	MGE	C4A-C5A-C6A-C7A
16	a	402	CLA	C2C-C3C-CAC-CBC
15	l	101	SQD	C8-C7-O47-C45
18	h	101	BCR	C36-C18-C19-C20
20	d	410	MGE	C5B-C6B-C7B-C8B
16	b	606	CLA	C16-C17-C18-C20
16	b	612	CLA	C13-C15-C16-C17
20	d	410	MGE	O1B-C1B-O2G-C2G
16	d	401	CLA	C2C-C3C-CAC-CBC
20	b	622	MGE	C1A-C2A-C3A-C4A
16	d	404	CLA	C5-C6-C7-C8
16	b	603	CLA	CBD-CGD-O2D-CED
15	l	101	SQD	O47-C45-C46-O48
16	b	611	CLA	C13-C15-C16-C17
20	d	408	MGE	O6D-C5D-C6D-O5D
26	d	412	DGD	O6E-C5E-C6E-O5E
16	b	602	CLA	C16-C17-C18-C19
15	l	101	SQD	O49-C7-O47-C45
20	b	622	MGE	C9B-CAB-CBB-CCB
20	b	620	MGE	C3B-C4B-C5B-C6B
22	d	402	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
20	a	409	MGE	C2A-C1A-O1G-C1G
20	a	409	MGE	C6B-C7B-C8B-C9B
20	a	409	MGE	C2B-C3B-C4B-C5B
17	a	404	PHO	C6-C7-C8-C10
16	b	606	CLA	C2A-CAA-CBA-CGA
17	a	404	PHO	C6-C7-C8-C9
15	l	101	SQD	C44-C45-C46-O48
20	b	620	MGE	C1G-C2G-C3G-O3G
20	m	101	MGE	C3A-C4A-C5A-C6A
16	b	602	CLA	C16-C17-C18-C20
26	d	412	DGD	C4B-C5B-C6B-C7B
20	a	409	MGE	O1A-C1A-O1G-C1G
22	b	623	LMT	C4'-C5'-C6'-O6'
20	d	410	MGE	O6D-C5D-C6D-O5D
20	m	101	MGE	C4A-C5A-C6A-C7A
16	b	614	CLA	O1D-CGD-O2D-CED
20	b	622	MGE	CAB-CBB-CCB-CDB
15	l	101	SQD	C18-C19-C20-C21
16	b	612	CLA	C3-C5-C6-C7
20	a	409	MGE	C1B-C2B-C3B-C4B
16	b	615	CLA	C16-C17-C18-C20
16	b	611	CLA	C14-C13-C15-C16
20	m	101	MGE	C4B-C5B-C6B-C7B
17	a	405	PHO	C15-C16-C17-C18
16	b	609	CLA	C4B-C3B-CAB-CBB
16	b	606	CLA	C12-C13-C15-C16
16	b	611	CLA	C12-C13-C15-C16
16	b	615	CLA	C5-C6-C7-C8
18	h	101	BCR	C37-C22-C23-C24
20	a	409	MGE	C1G-C2G-C3G-O3G
20	b	620	MGE	O1G-C1G-C2G-C3G
20	d	410	MGE	C2B-C3B-C4B-C5B
20	a	409	MGE	C1A-C2A-C3A-C4A
16	a	402	CLA	C4C-C3C-CAC-CBC
16	b	615	CLA	O1D-CGD-O2D-CED
16	d	405	CLA	C2B-C3B-CAB-CBB
18	a	407	BCR	C23-C24-C25-C26
18	a	407	BCR	C23-C24-C25-C30
20	b	620	MGE	C8B-C9B-CAB-CBB
16	d	401	CLA	C4C-C3C-CAC-CBC
20	b	622	MGE	C7A-C8A-C9A-CAA
20	d	409	MGE	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
16	b	606	CLA	C11-C12-C13-C14
16	b	610	CLA	C11-C12-C13-C14
20	b	622	MGE	C2A-C3A-C4A-C5A
22	t	101	LMT	C5-C6-C7-C8
16	b	615	CLA	C16-C17-C18-C19
16	a	402	CLA	C16-C17-C18-C20
17	a	404	PHO	C8-C10-C11-C12
16	b	604	CLA	C6-C7-C8-C10
17	a	405	PHO	C11-C10-C8-C7
26	d	412	DGD	C3B-C4B-C5B-C6B
17	a	404	PHO	C15-C16-C17-C18
20	d	410	MGE	O2G-C1B-C2B-C3B
15	l	101	SQD	C7-C8-C9-C10
20	b	622	MGE	C2A-C1A-O1G-C1G
20	a	409	MGE	C7B-C8B-C9B-CAB
17	a	404	PHO	C3-C5-C6-C7
20	d	408	MGE	C4B-C5B-C6B-C7B
22	d	402	LMT	C5-C6-C7-C8
20	b	622	MGE	C3B-C4B-C5B-C6B
20	d	410	MGE	C9A-CAA-CBA-CCA
16	d	405	CLA	C4B-C3B-CAB-CBB
20	b	622	MGE	O1A-C1A-O1G-C1G
20	a	409	MGE	C2A-C3A-C4A-C5A
16	b	604	CLA	C6-C7-C8-C9
16	b	606	CLA	C14-C13-C15-C16
18	b	618	BCR	C19-C20-C21-C22
17	a	405	PHO	C8-C10-C11-C12
15	l	101	SQD	O5-C5-C6-S
16	d	404	CLA	O1D-CGD-O2D-CED
16	b	615	CLA	C13-C15-C16-C17
20	b	622	MGE	C1B-C2B-C3B-C4B
16	b	605	CLA	CAD-CBD-CGD-O1D
16	b	607	CLA	CAD-CBD-CGD-O1D
16	b	616	CLA	CHA-CBD-CGD-O1D
18	b	618	BCR	C13-C14-C15-C16
20	b	620	MGE	C9B-CAB-CBB-CCB
17	a	404	PHO	C5-C6-C7-C8
20	a	409	MGE	O6D-C5D-C6D-O5D
20	b	620	MGE	C1A-C2A-C3A-C4A
16	b	606	CLA	C15-C16-C17-C18
24	d	406	PQ9	C19-C18-C20-C21
18	a	407	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	d	402	LMT	O5B-C5B-C6B-O6B
20	b	620	MGE	CAA-CBA-CCA-CDA
20	b	620	MGE	C1B-C2B-C3B-C4B
26	d	412	DGD	C6B-C7B-C8B-C9B
20	b	620	MGE	O1G-C1G-C2G-O2G
16	b	607	CLA	C3-C5-C6-C7
16	d	404	CLA	CAA-CBA-CGA-O2A
18	h	101	BCR	C17-C18-C19-C20
20	d	410	MGE	C2G-C3G-O3G-C1D
26	d	412	DGD	C3A-C4A-C5A-C6A
26	d	412	DGD	C2B-C3B-C4B-C5B
15	l	101	SQD	C12-C13-C14-C15
16	b	615	CLA	C14-C13-C15-C16
16	d	404	CLA	C6-C7-C8-C9
20	d	409	MGE	C2B-C3B-C4B-C5B
26	d	412	DGD	CAA-CBA-CCA-CDA
26	d	412	DGD	C5B-C6B-C7B-C8B
20	b	622	MGE	C7B-C8B-C9B-CAB
20	d	409	MGE	C8B-C9B-CAB-CBB
24	d	406	PQ9	C17-C18-C20-C21
16	b	612	CLA	CBA-CGA-O2A-C1
22	d	402	LMT	C6-C7-C8-C9
20	b	622	MGE	O2G-C2G-C3G-O3G
20	d	409	MGE	CAB-CBB-CCB-CDB
20	d	409	MGE	C9B-CAB-CBB-CCB
20	d	408	MGE	C3A-C4A-C5A-C6A
20	m	101	MGE	O1G-C1A-C2A-C3A
16	b	612	CLA	C10-C11-C12-C13
22	t	101	LMT	C6-C7-C8-C9
16	a	403	CLA	C1A-C2A-CAA-CBA
16	d	404	CLA	C14-C13-C15-C16
16	b	615	CLA	C12-C13-C15-C16
16	b	610	CLA	C16-C17-C18-C20
20	a	409	MGE	C7A-C8A-C9A-CAA
27	e	101	HEM	CAA-CBA-CGA-O1A
24	d	406	PQ9	C24-C23-C25-C26
16	a	406	CLA	CBD-CGD-O2D-CED
16	d	401	CLA	C15-C16-C17-C18
27	e	101	HEM	CAA-CBA-CGA-O2A
16	d	405	CLA	O1A-CGA-O2A-C1
22	t	101	LMT	C4-C5-C6-C7
26	d	412	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
20	d	410	MGE	O1B-C1B-C2B-C3B
16	b	610	CLA	C2A-CAA-CBA-CGA
16	b	615	CLA	C3A-C2A-CAA-CBA
17	a	404	PHO	CBA-CGA-O2A-C1
20	d	408	MGE	CBB-CCB-CDB-CEB
15	l	101	SQD	O48-C23-C24-C25
16	b	609	CLA	C2B-C3B-CAB-CBB
20	b	620	MGE	O2G-C1B-C2B-C3B
16	b	614	CLA	C2-C1-O2A-CGA
17	a	404	PHO	O1A-CGA-O2A-C1
17	a	404	PHO	C2A-CAA-CBA-CGA
20	d	408	MGE	O1G-C1A-C2A-C3A
16	d	404	CLA	C12-C13-C15-C16
16	d	405	CLA	CBA-CGA-O2A-C1
16	b	603	CLA	C13-C15-C16-C17
18	h	101	BCR	C21-C22-C23-C24
16	b	603	CLA	C2A-CAA-CBA-CGA
16	b	612	CLA	C11-C10-C8-C7
17	a	404	PHO	C3A-C2A-CAA-CBA
24	d	406	PQ9	C22-C23-C25-C26
20	d	408	MGE	O1A-C1A-C2A-C3A
16	b	604	CLA	C16-C17-C18-C19
16	b	611	CLA	C16-C17-C18-C20
20	b	620	MGE	O1B-C1B-C2B-C3B
20	d	410	MGE	C9B-CAB-CBB-CCB
20	b	622	MGE	O2G-C1B-C2B-C3B
20	m	101	MGE	C2G-C3G-O3G-C1D
20	d	409	MGE	C6B-C7B-C8B-C9B
20	b	622	MGE	C1G-C2G-C3G-O3G
15	l	101	SQD	O10-C23-C24-C25
16	b	612	CLA	CAD-CBD-CGD-O2D
20	b	622	MGE	C6B-C7B-C8B-C9B

There are no ring outliers.

41 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	615	CLA	5	0
16	d	404	CLA	7	0
20	d	408	MGE	2	0
16	b	601	CLA	1	0
18	b	617	BCR	1	0

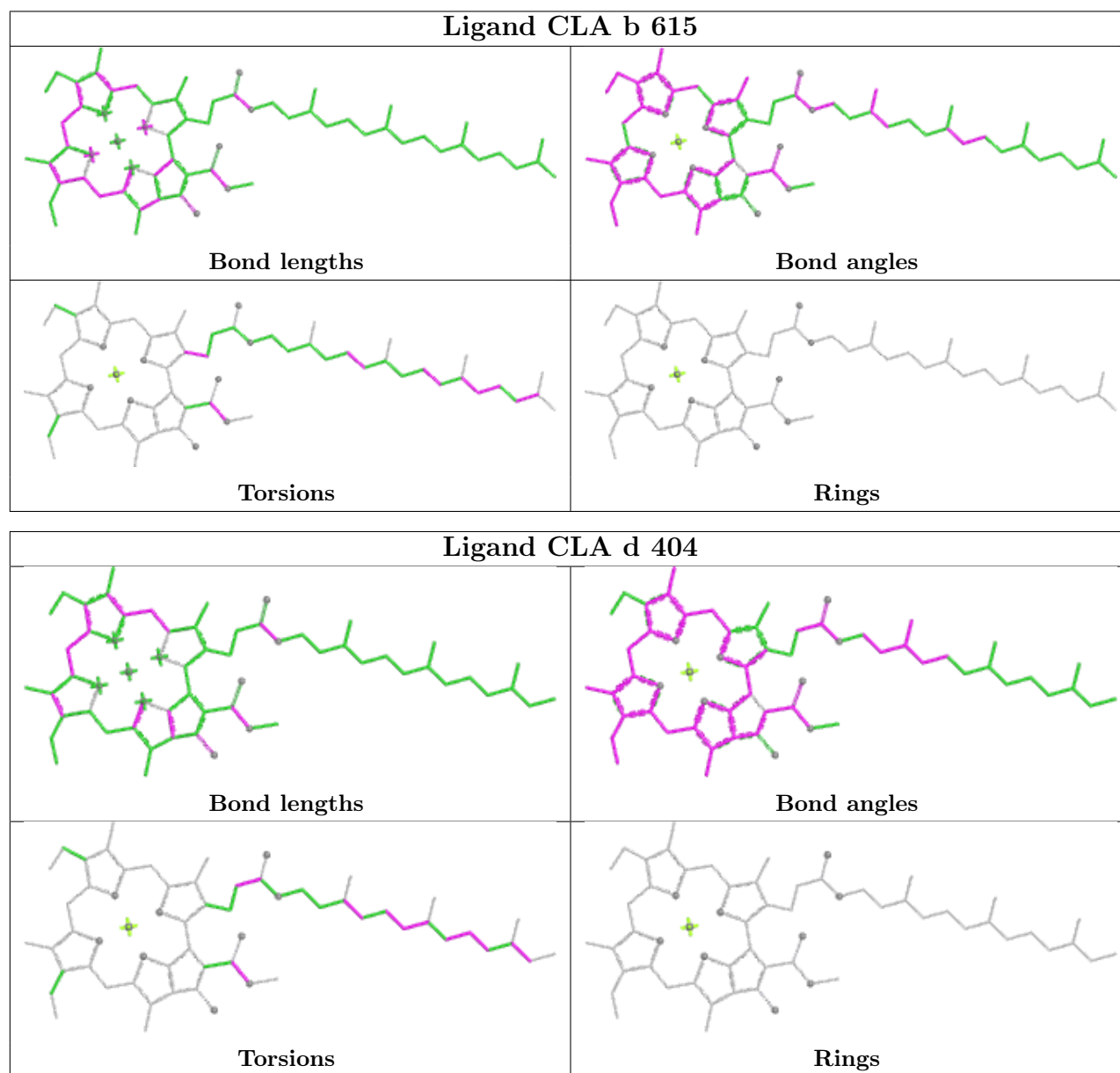
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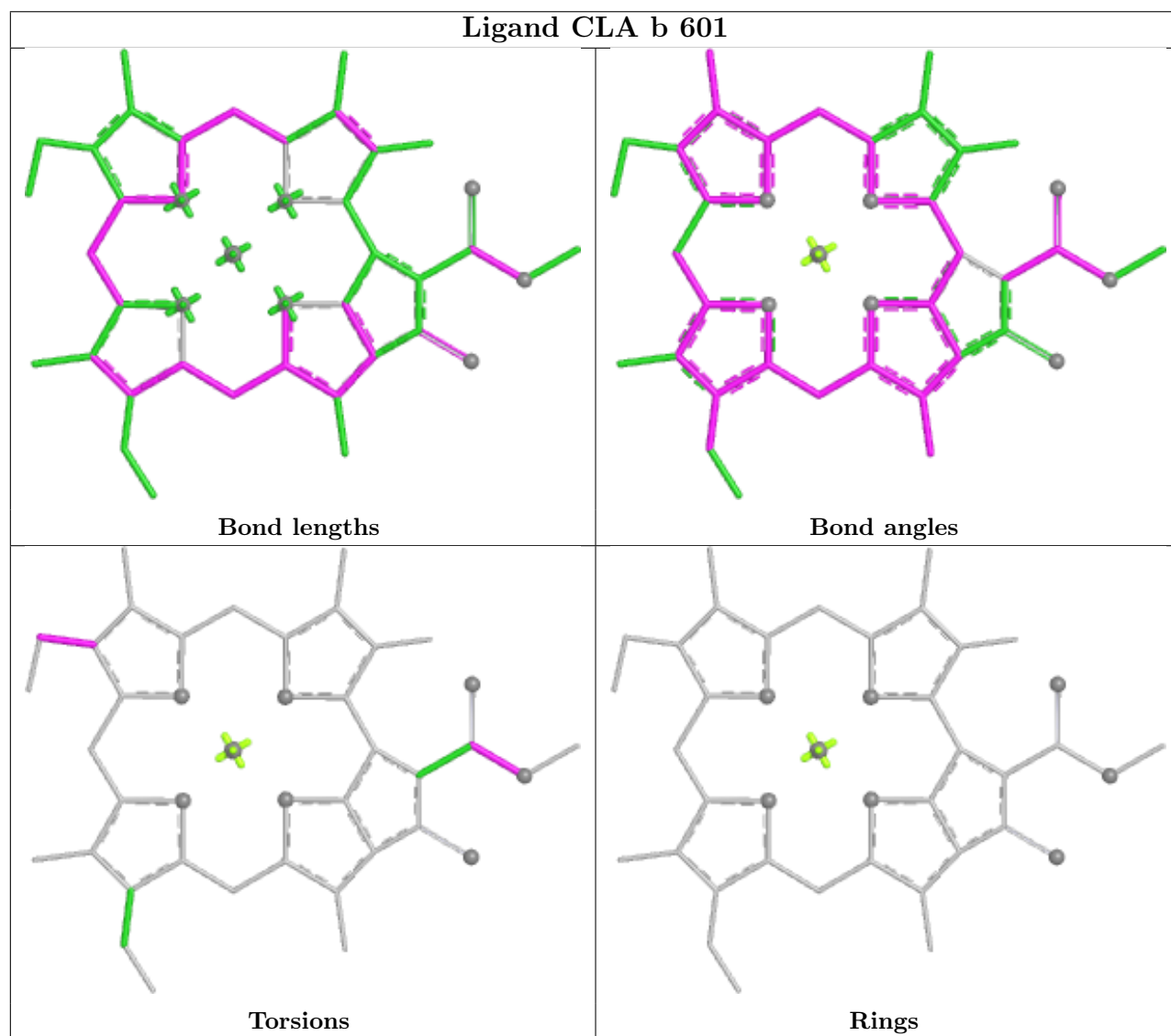
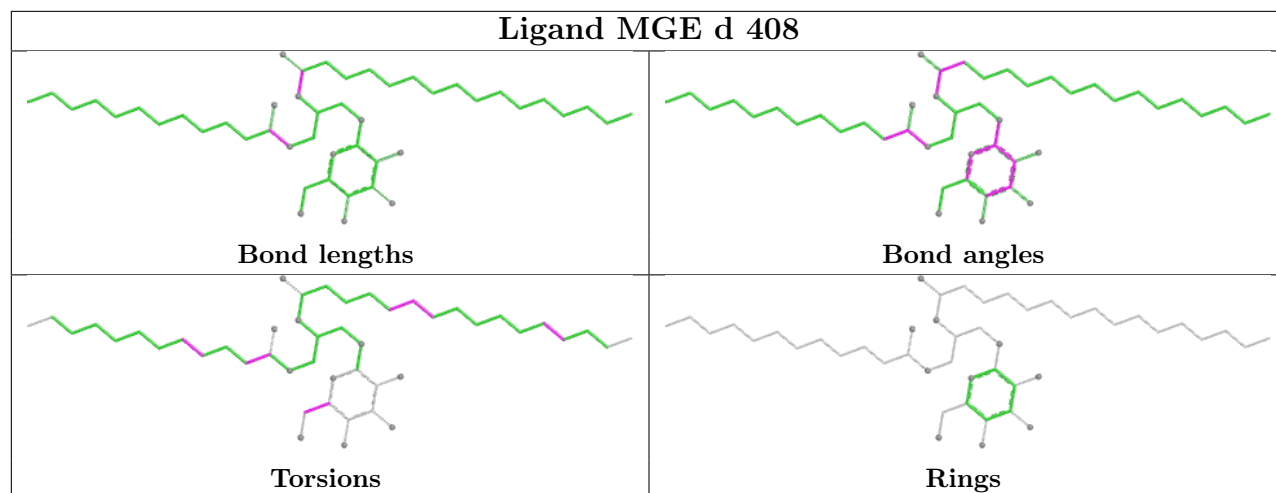
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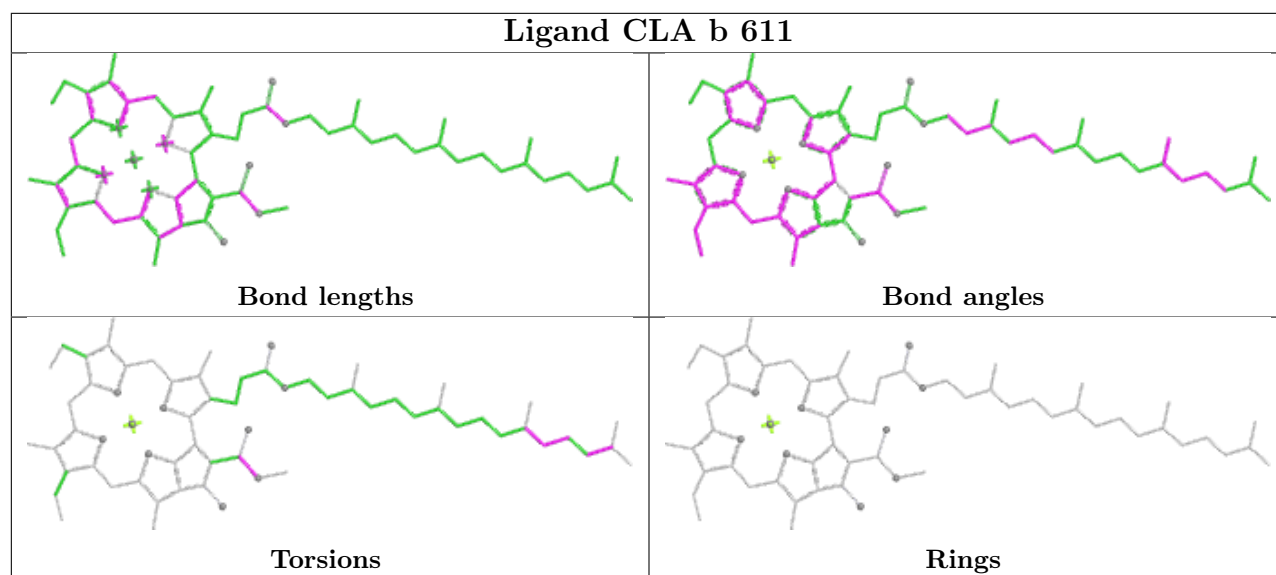
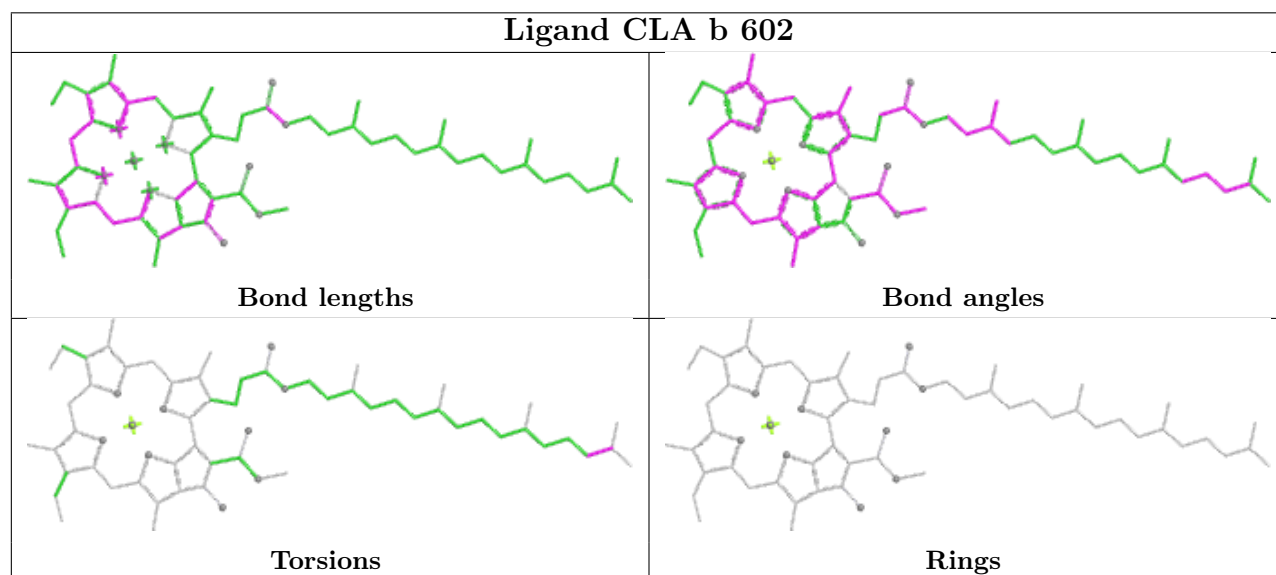
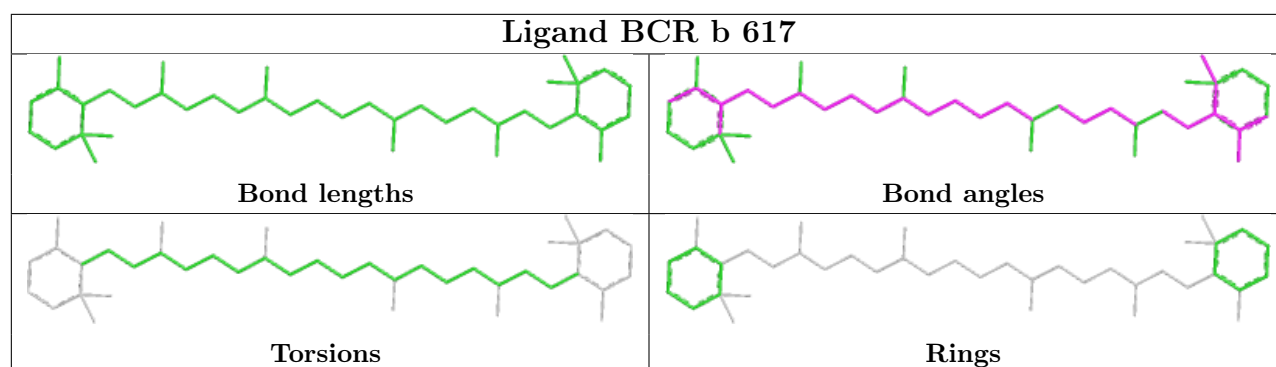
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	602	CLA	8	0
16	b	611	CLA	1	0
22	d	402	LMT	1	0
18	d	407	BCR	4	0
16	b	614	CLA	1	0
16	b	604	CLA	7	0
18	h	101	BCR	4	0
22	t	101	LMT	1	0
20	b	622	MGE	2	0
18	b	618	BCR	3	0
15	l	101	SQD	2	0
18	b	619	BCR	17	0
25	d	411	HTG	6	0
16	b	603	CLA	2	0
16	a	403	CLA	2	0
20	d	410	MGE	6	0
16	b	607	CLA	10	0
20	m	101	MGE	2	0
17	a	404	PHO	8	0
20	b	620	MGE	1	0
16	b	605	CLA	5	0
16	b	613	CLA	3	0
26	d	412	DGD	1	0
17	a	405	PHO	3	0
16	b	616	CLA	2	0
16	b	606	CLA	25	0
16	b	610	CLA	3	0
16	a	402	CLA	8	0
20	d	409	MGE	6	0
16	b	612	CLA	1	0
16	d	405	CLA	1	0
24	d	406	PQ9	6	0
18	a	407	BCR	4	0
16	b	608	CLA	3	0
16	b	609	CLA	1	0
16	d	401	CLA	10	0

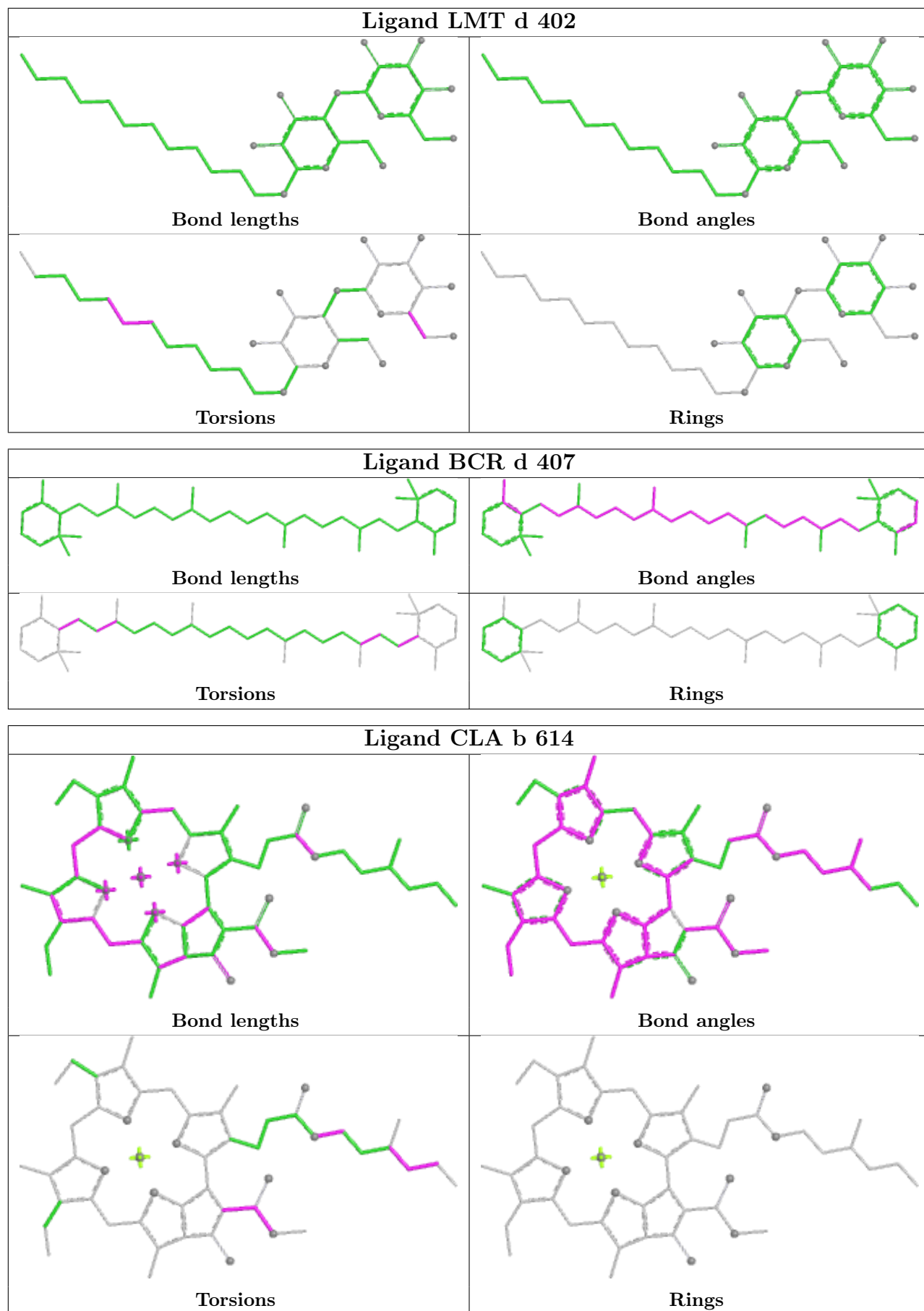
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

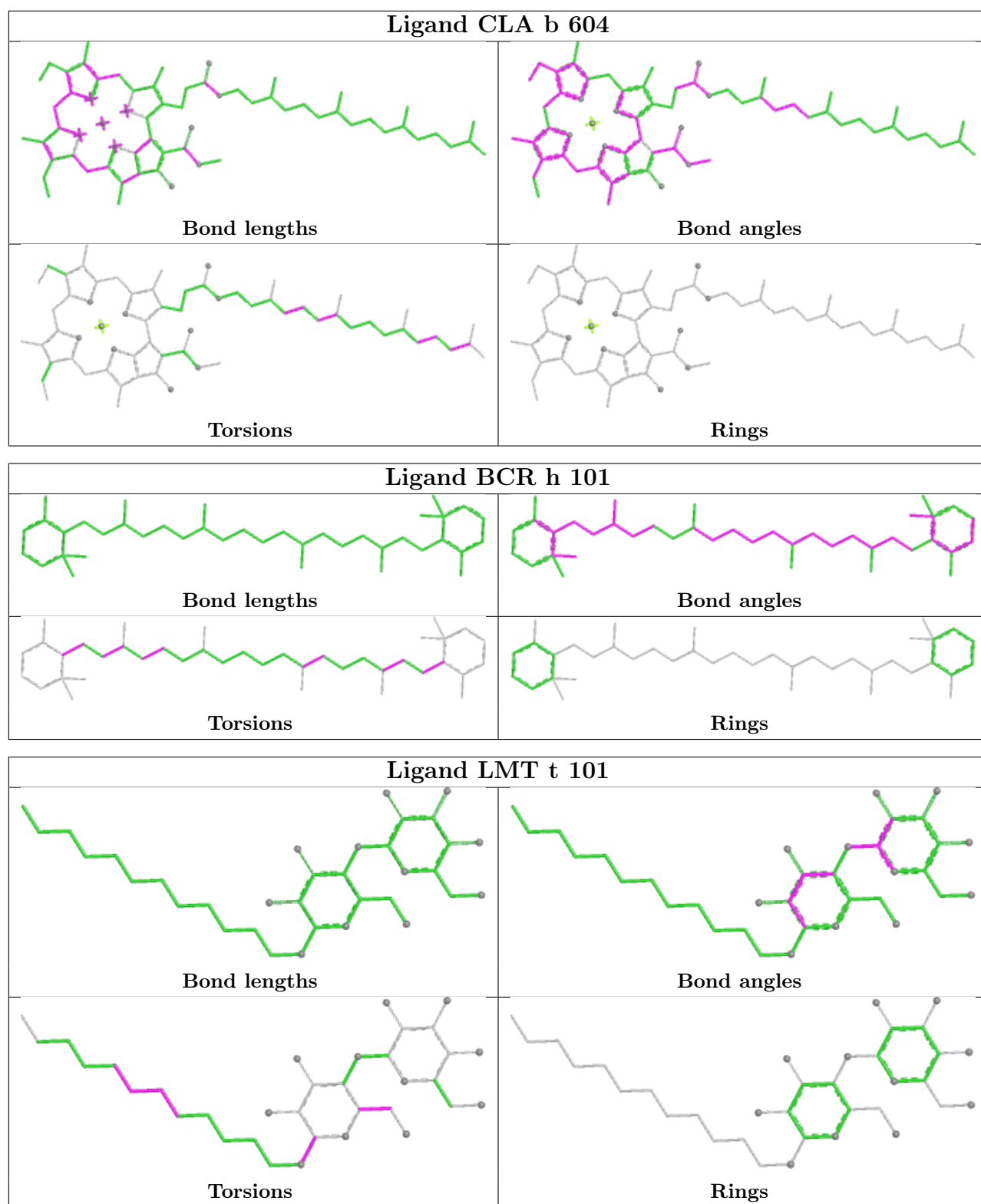
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

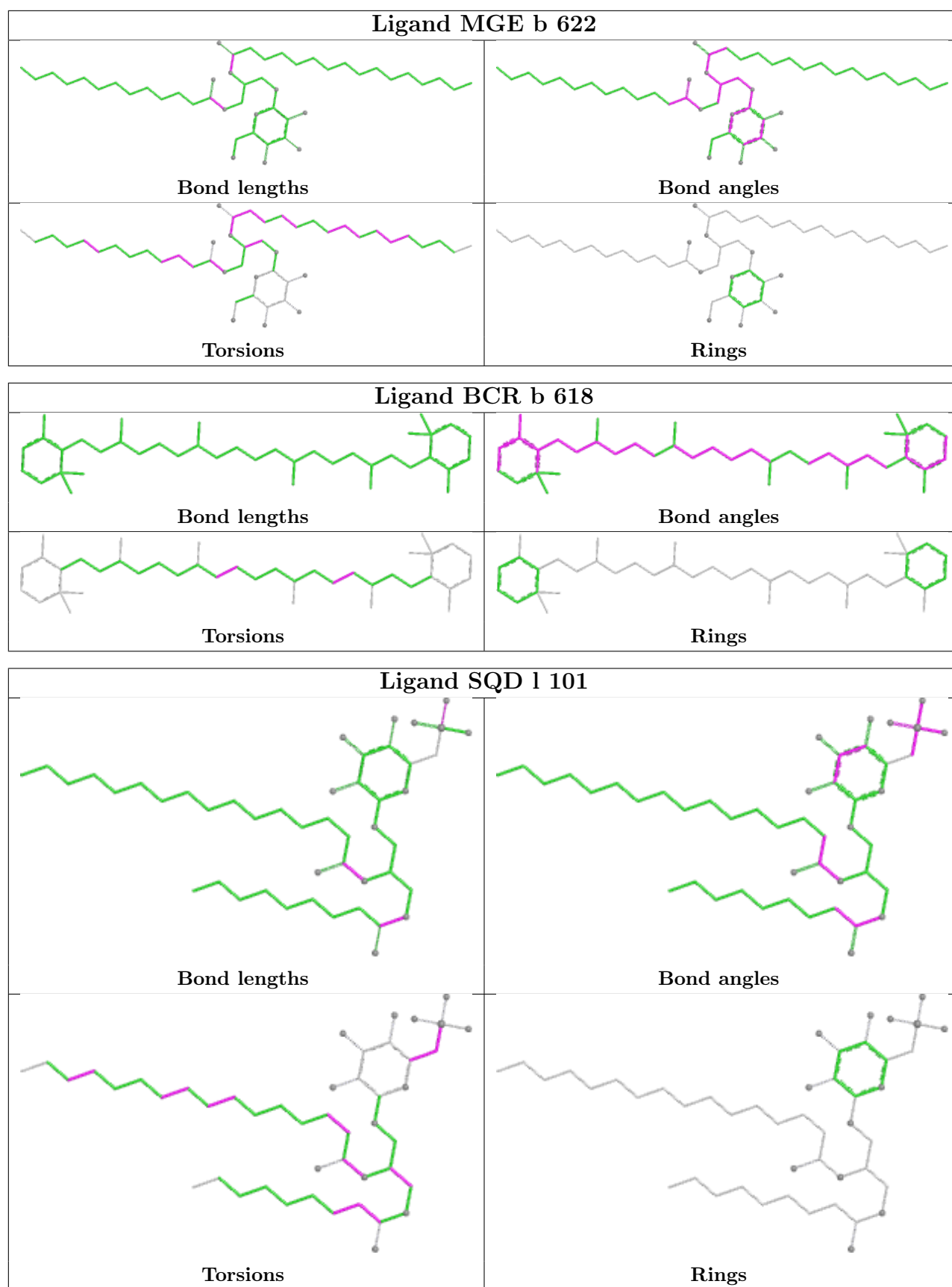


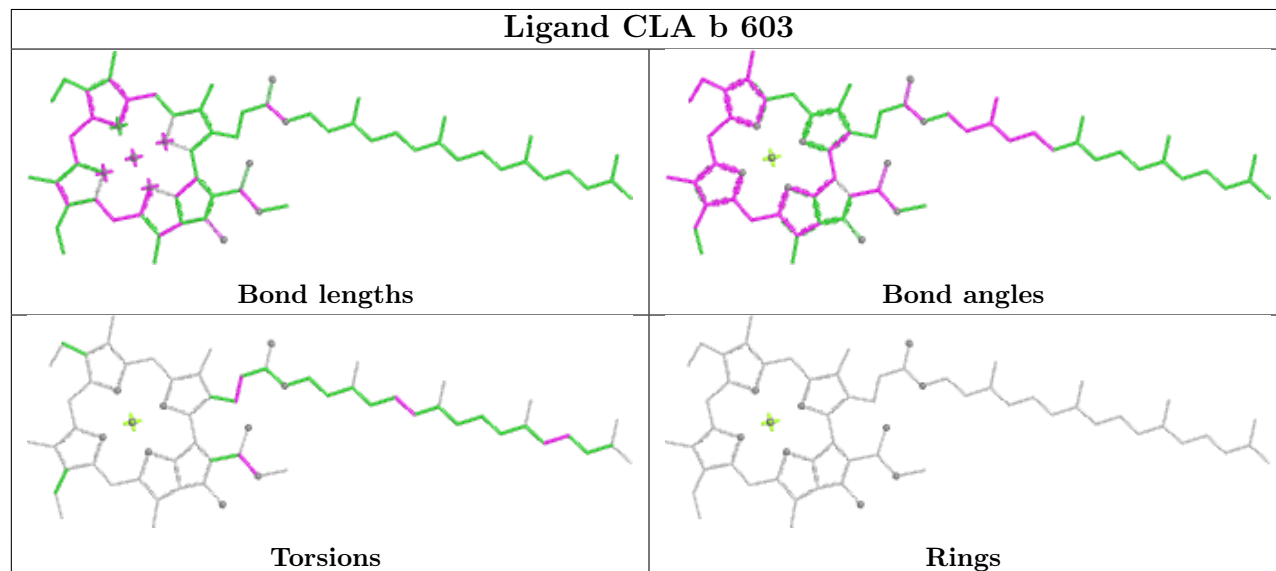
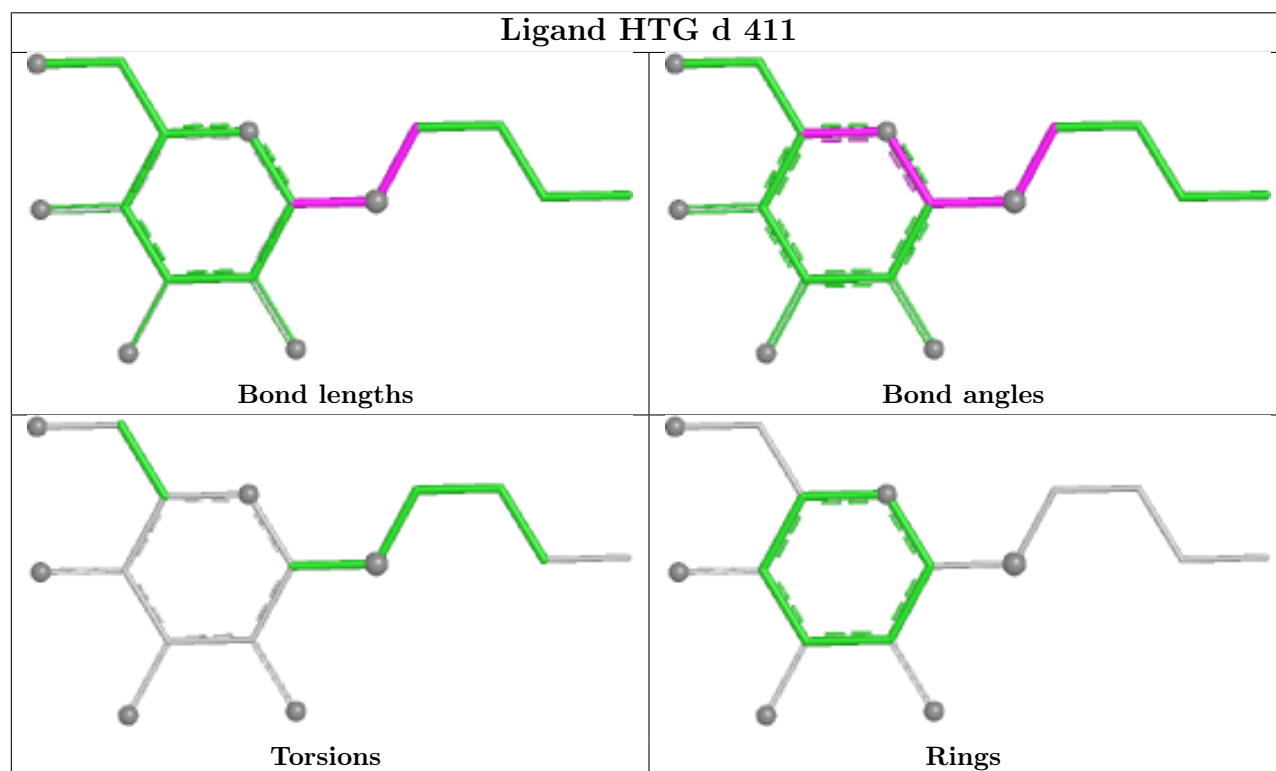
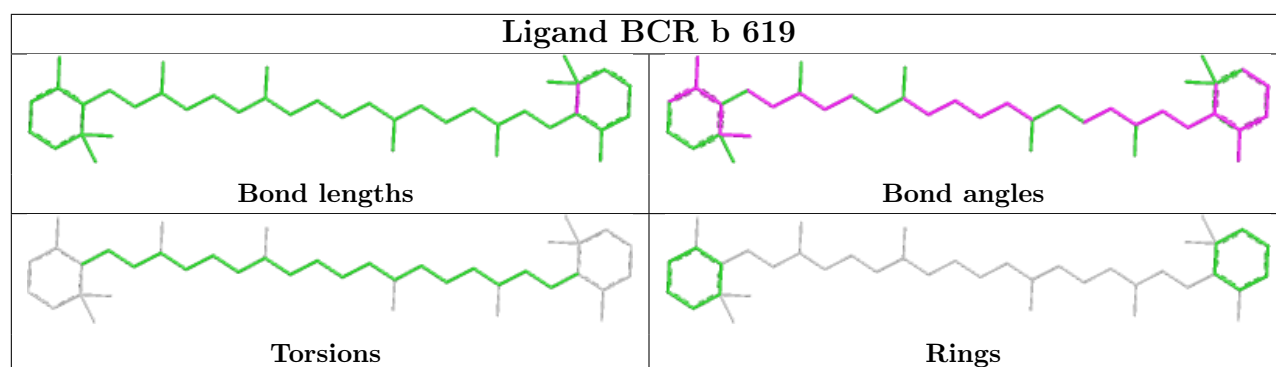




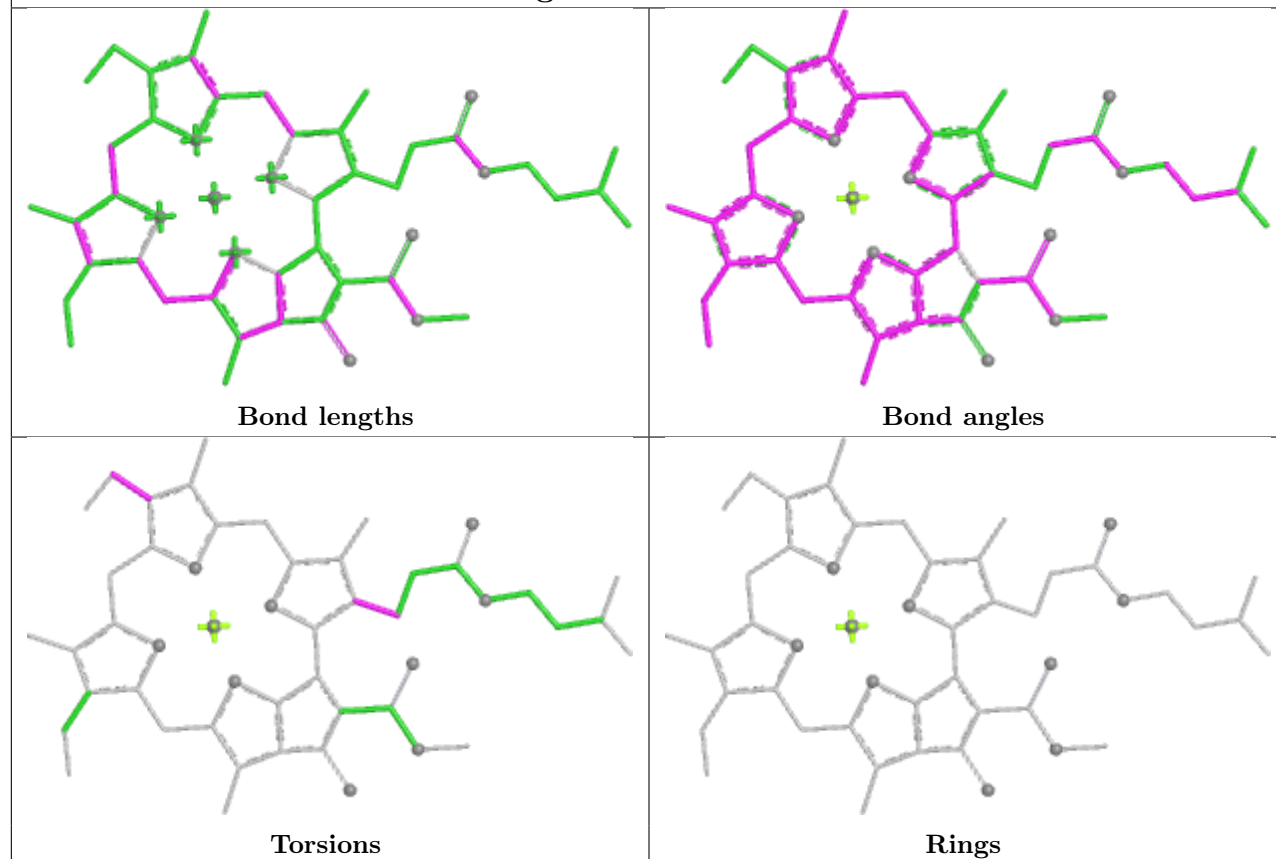




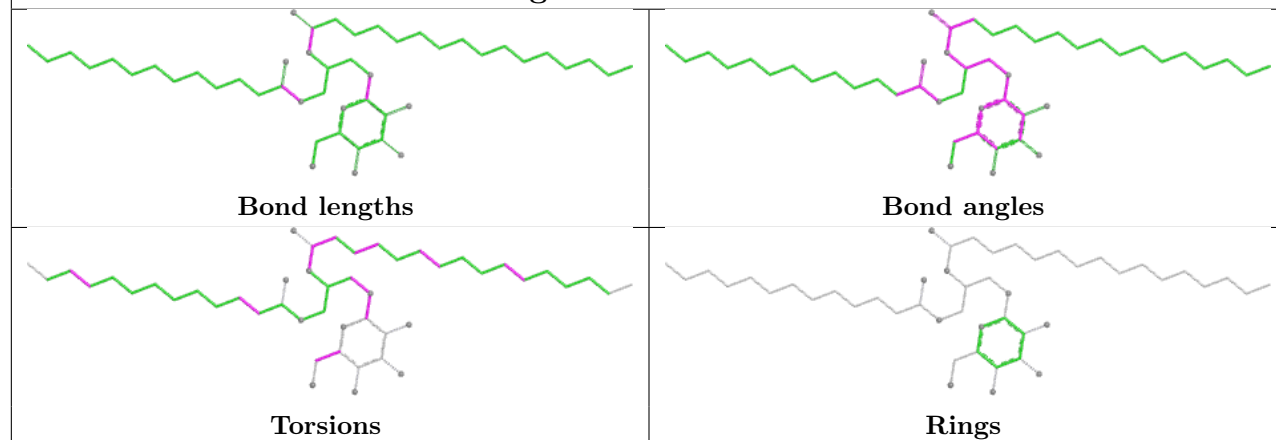


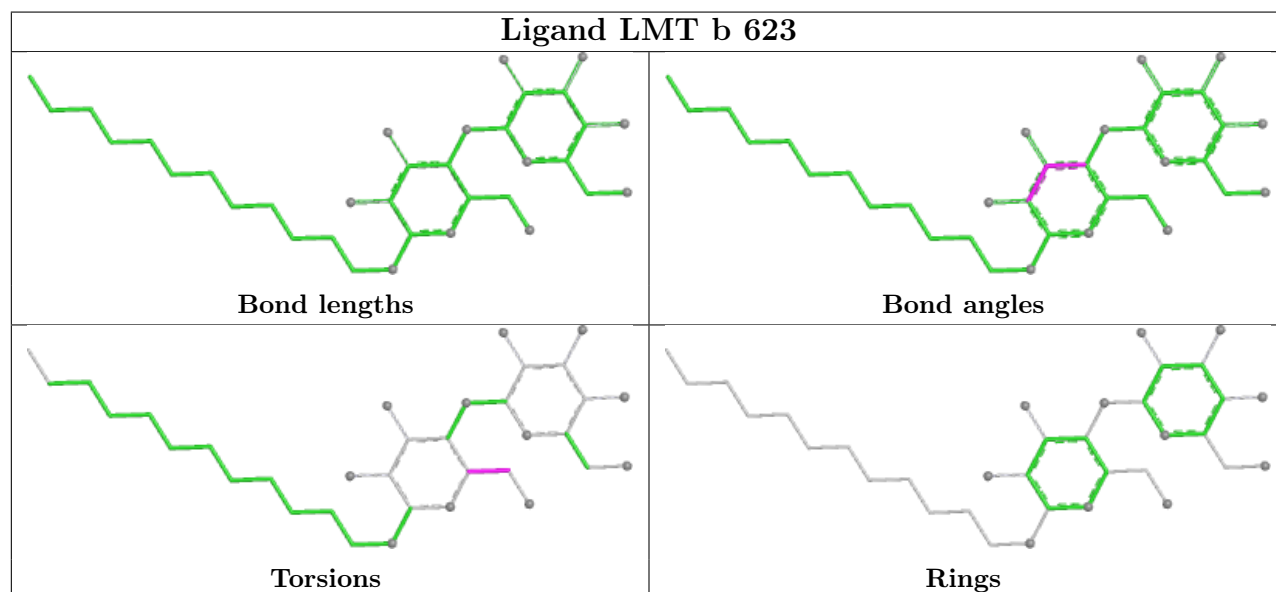
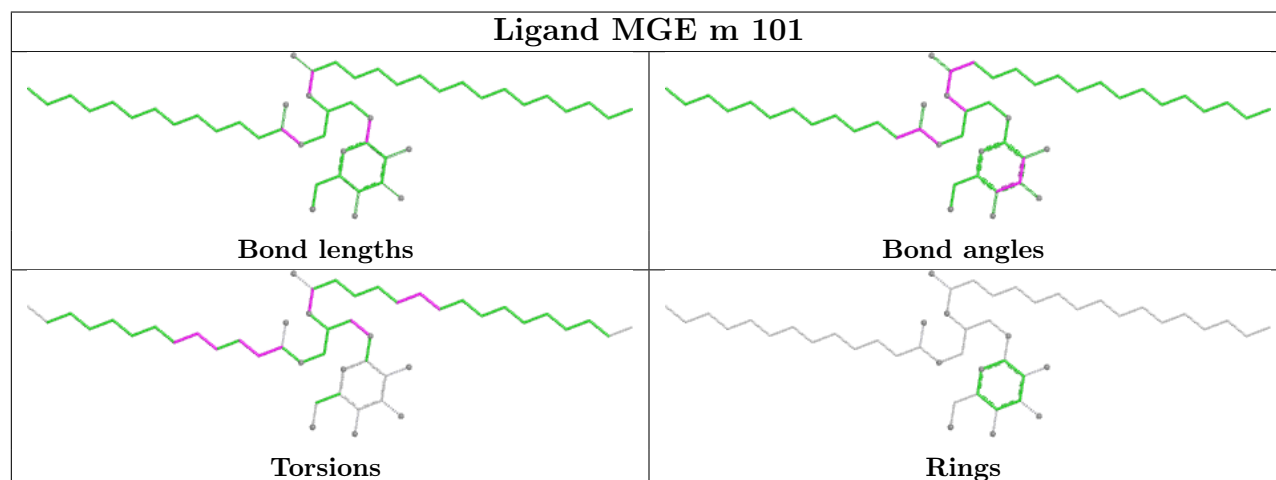
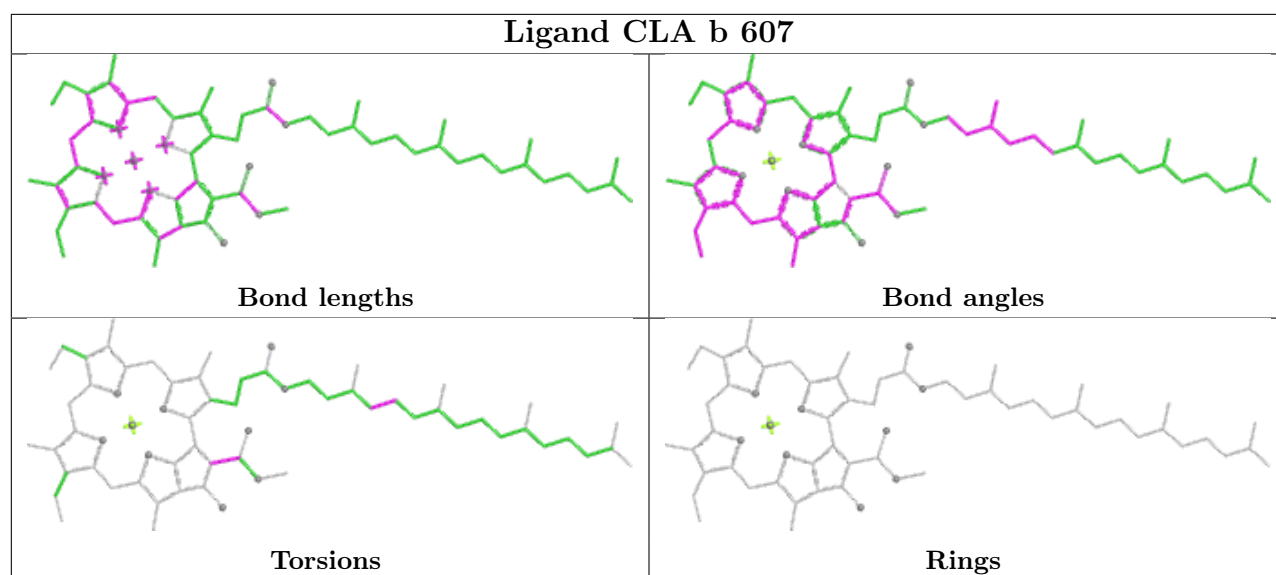


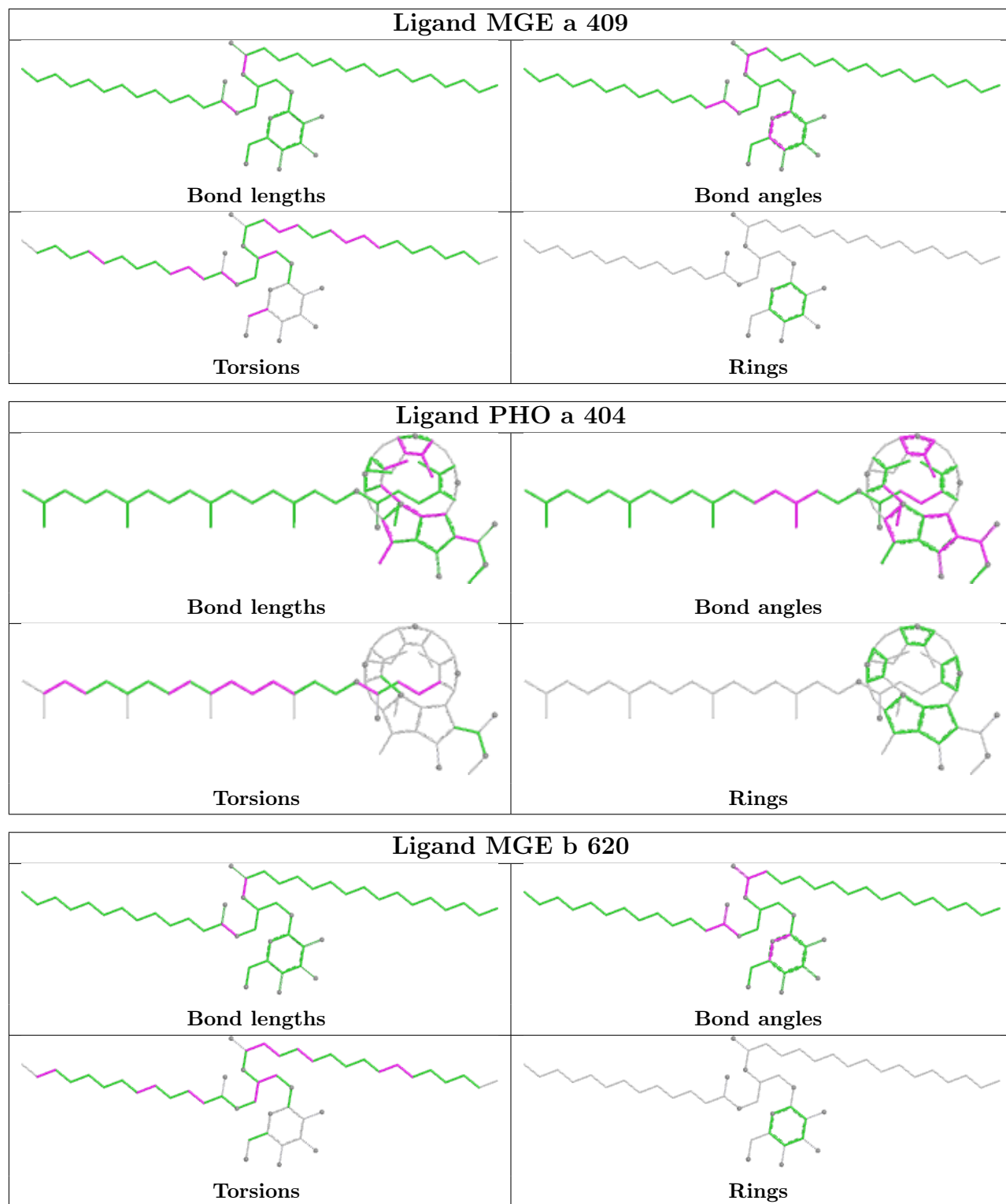
Ligand CLA a 403

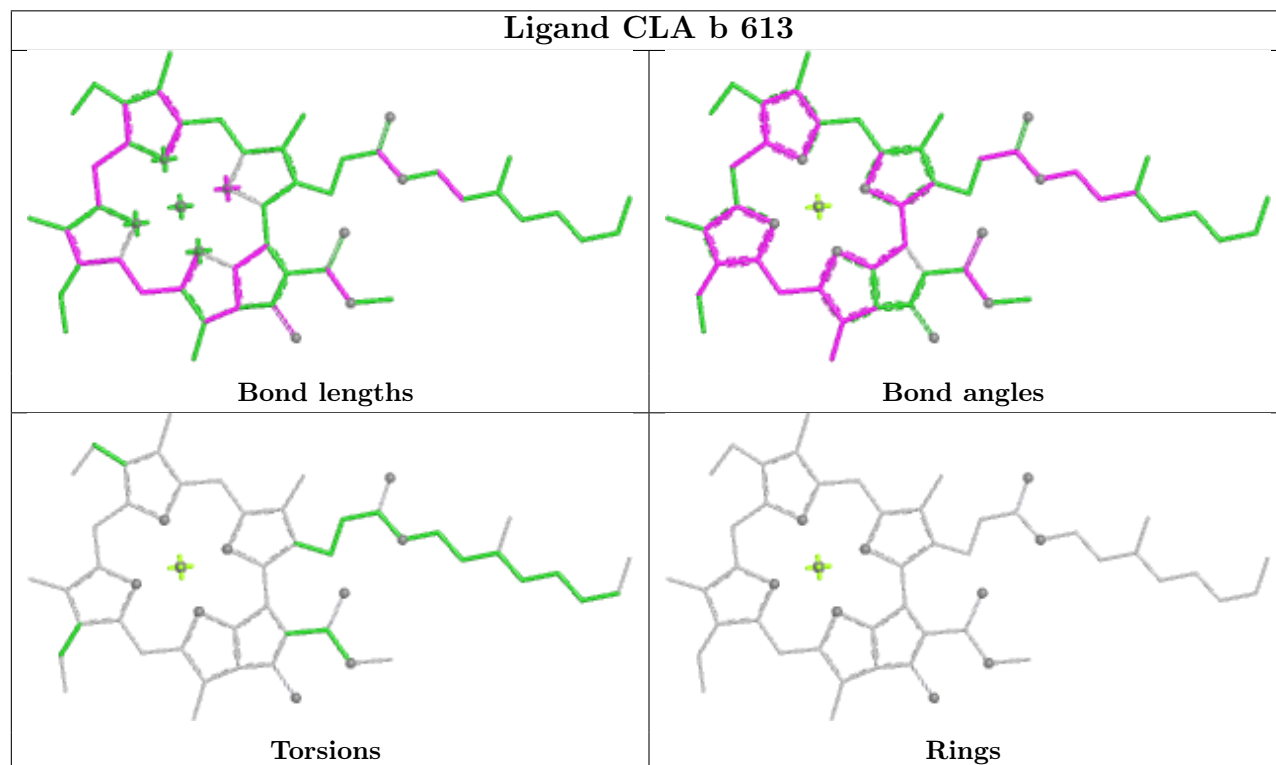
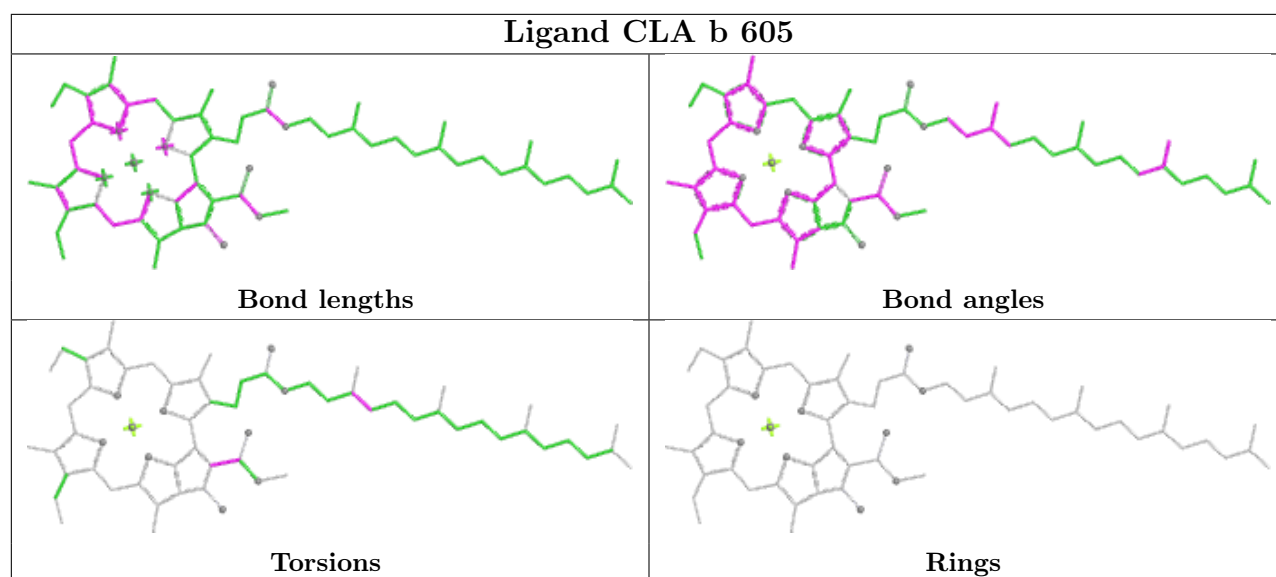


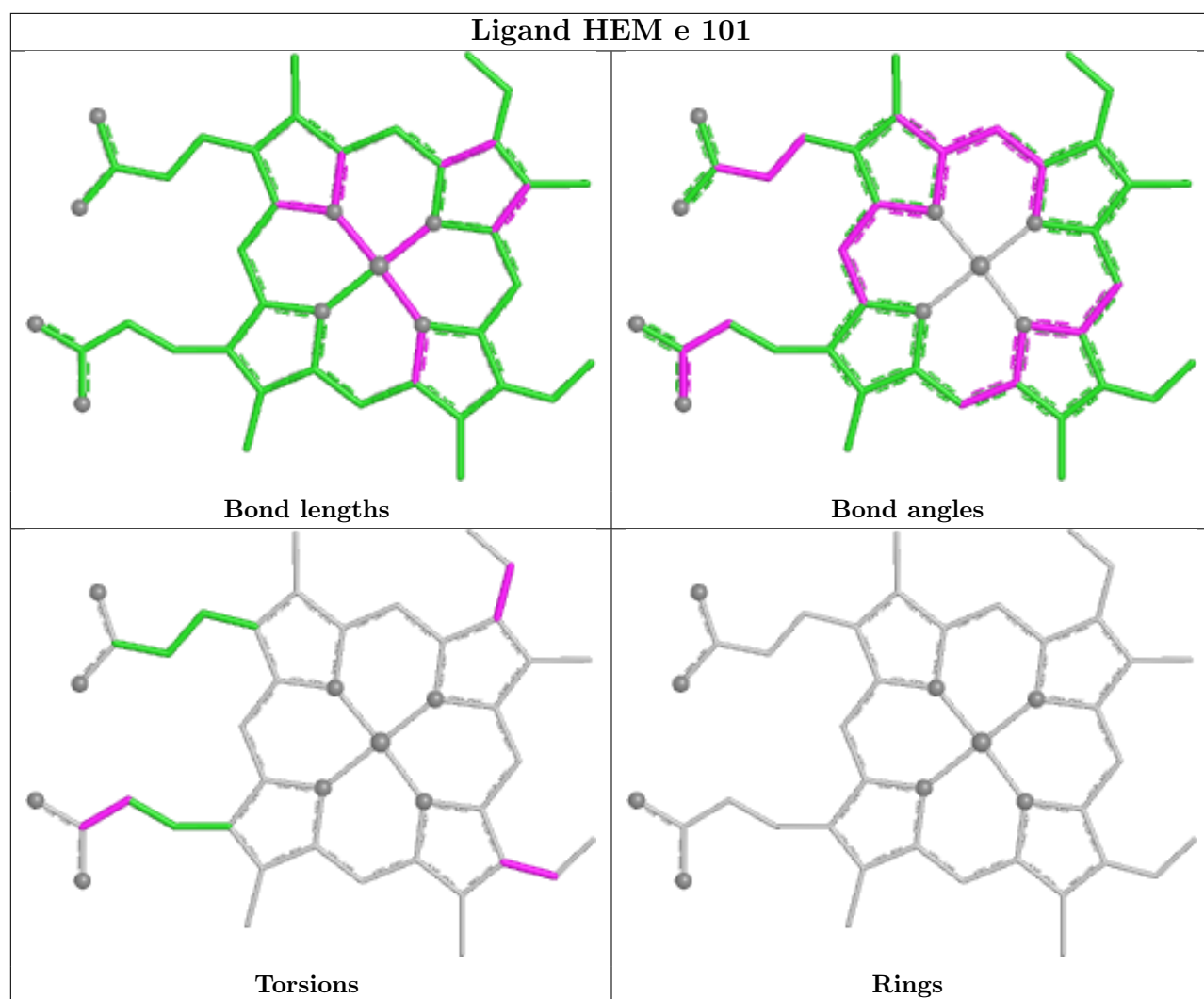
Ligand MGE d 410



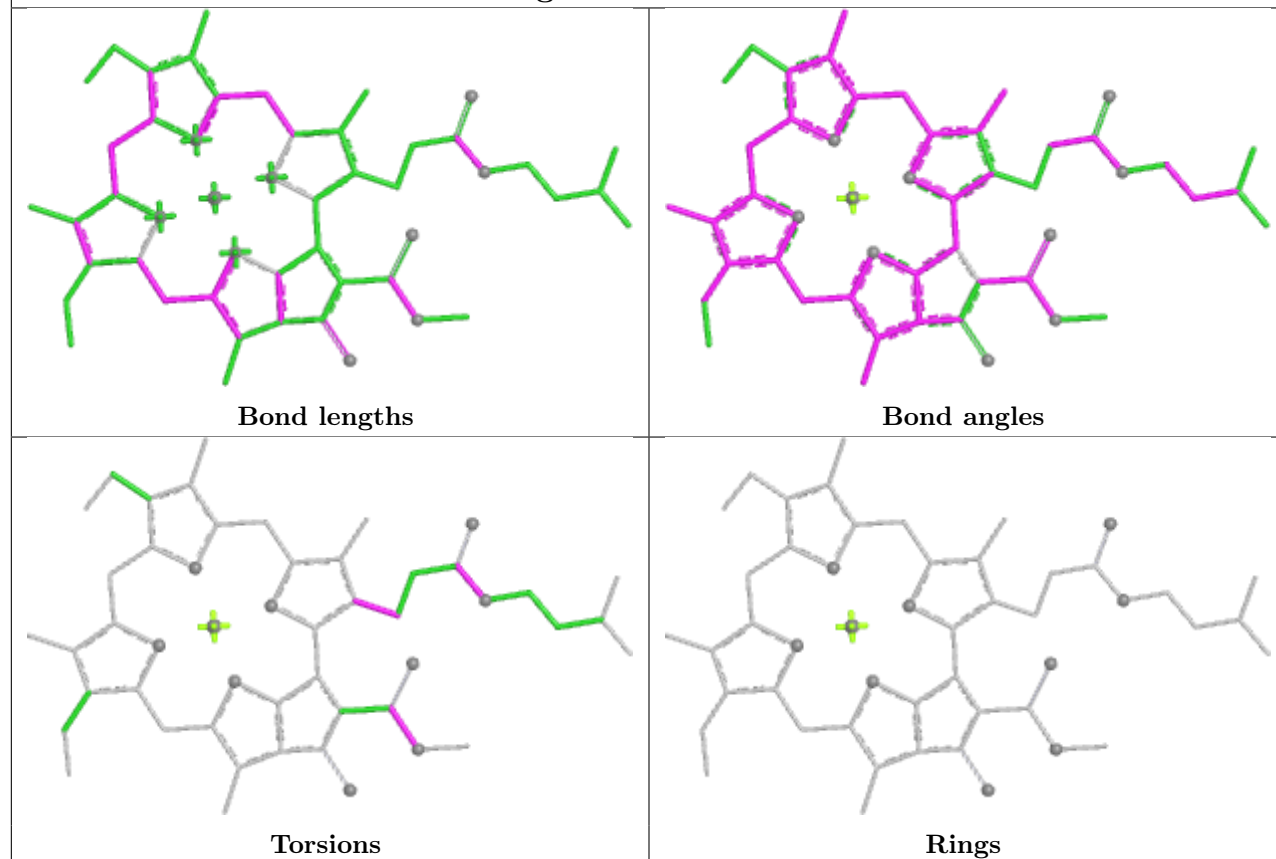




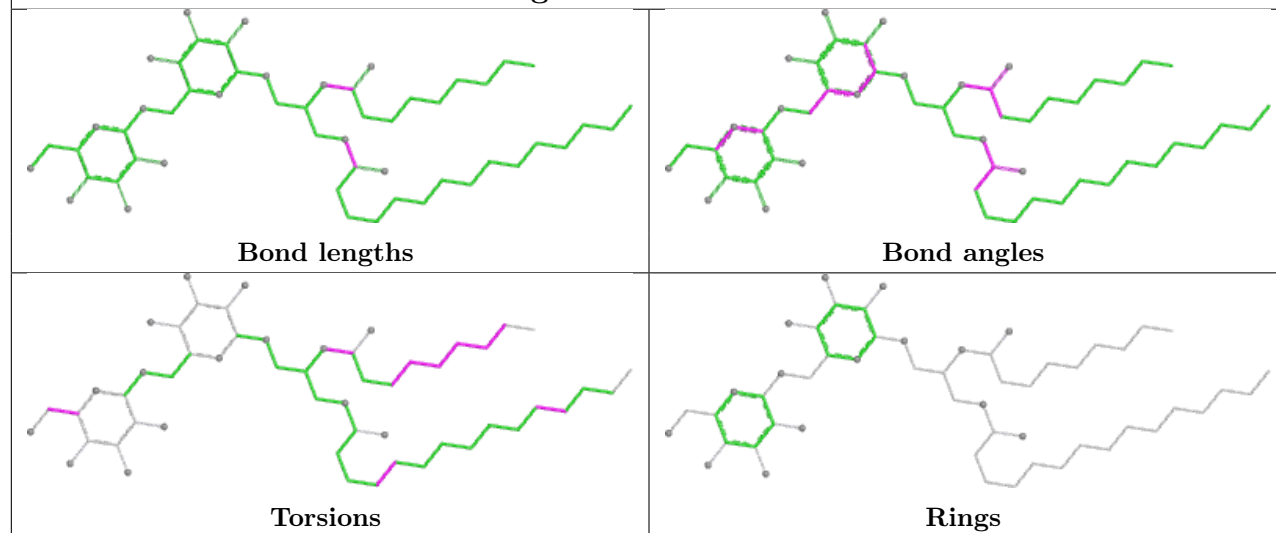


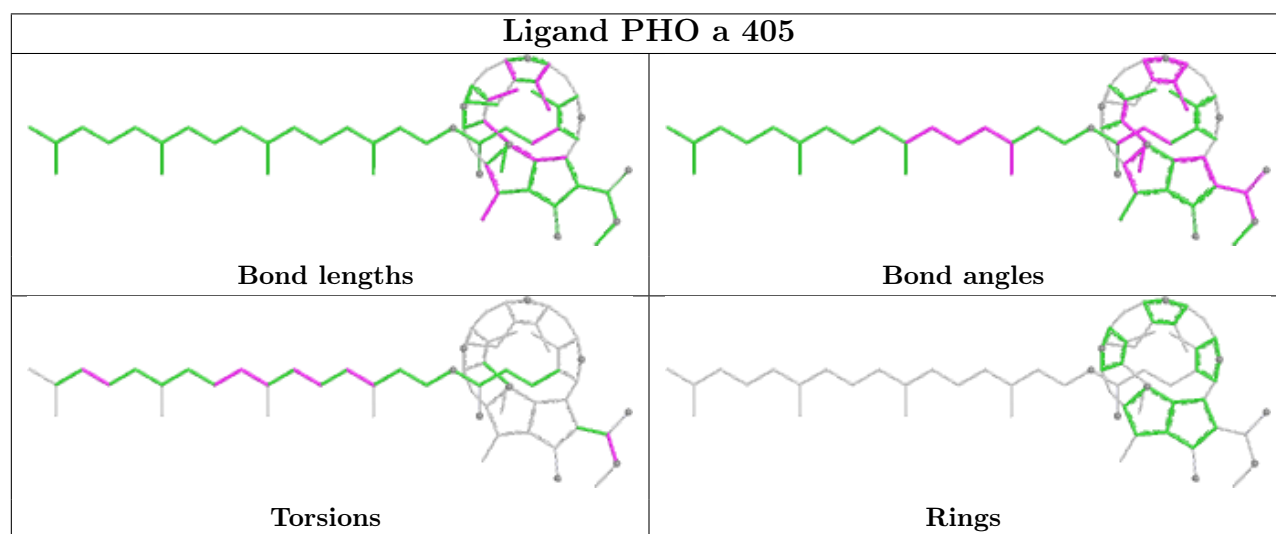
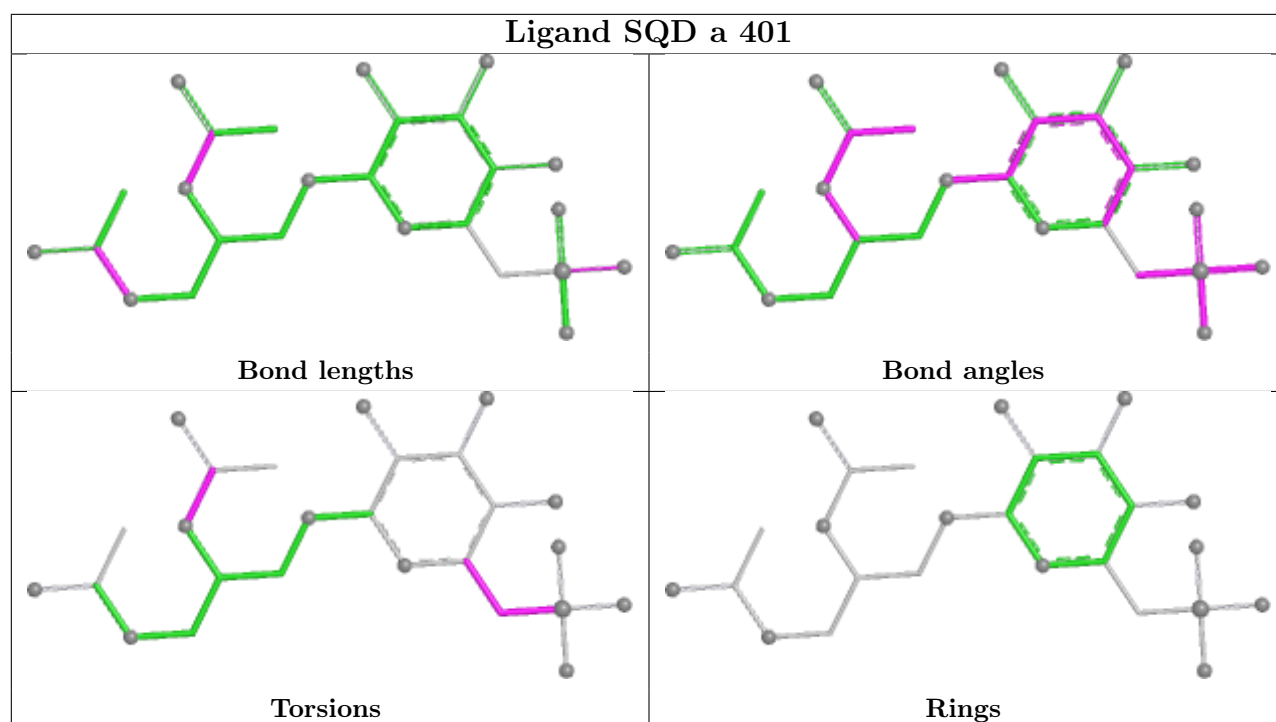


Ligand CLA a 406

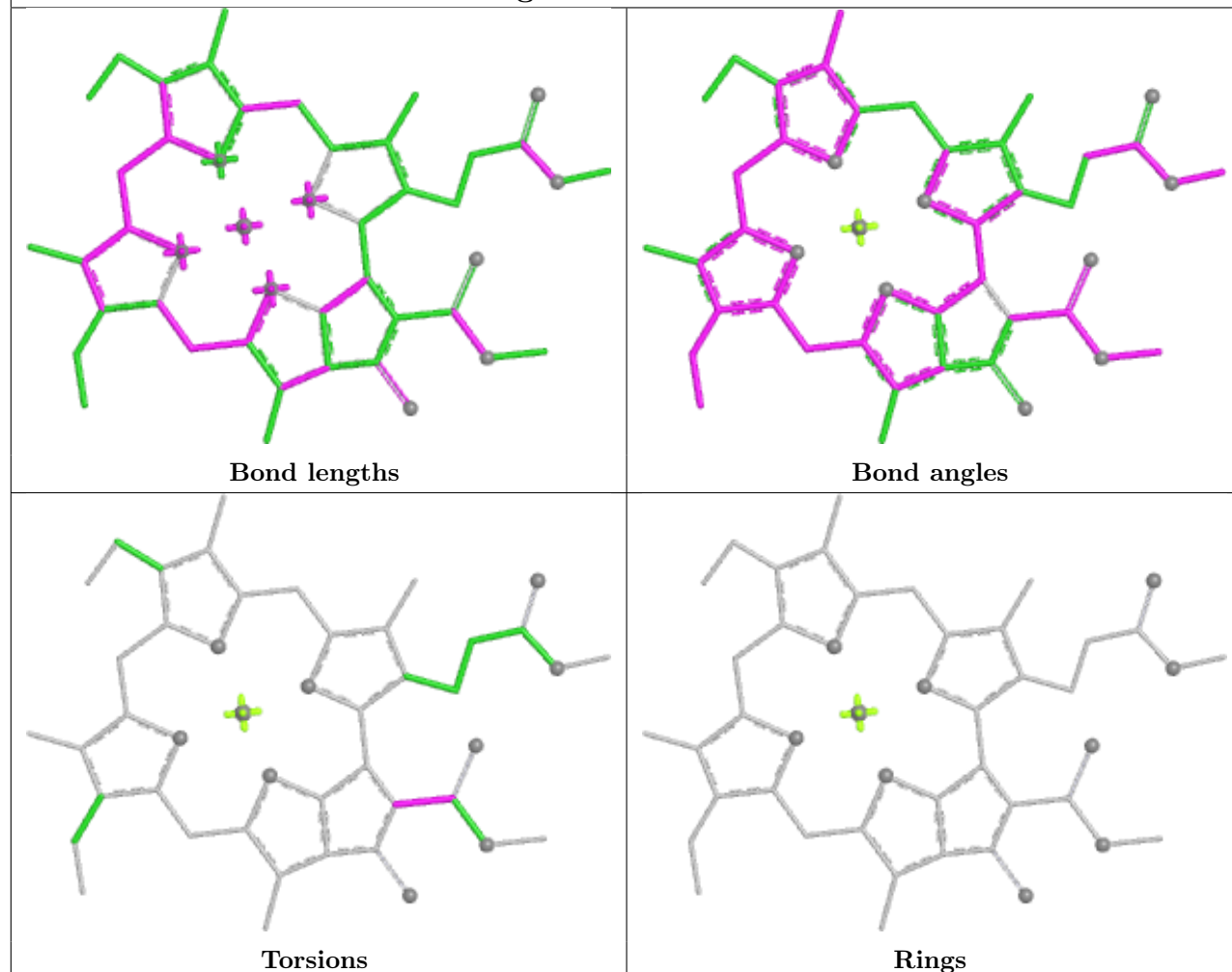


Ligand DGD d 412

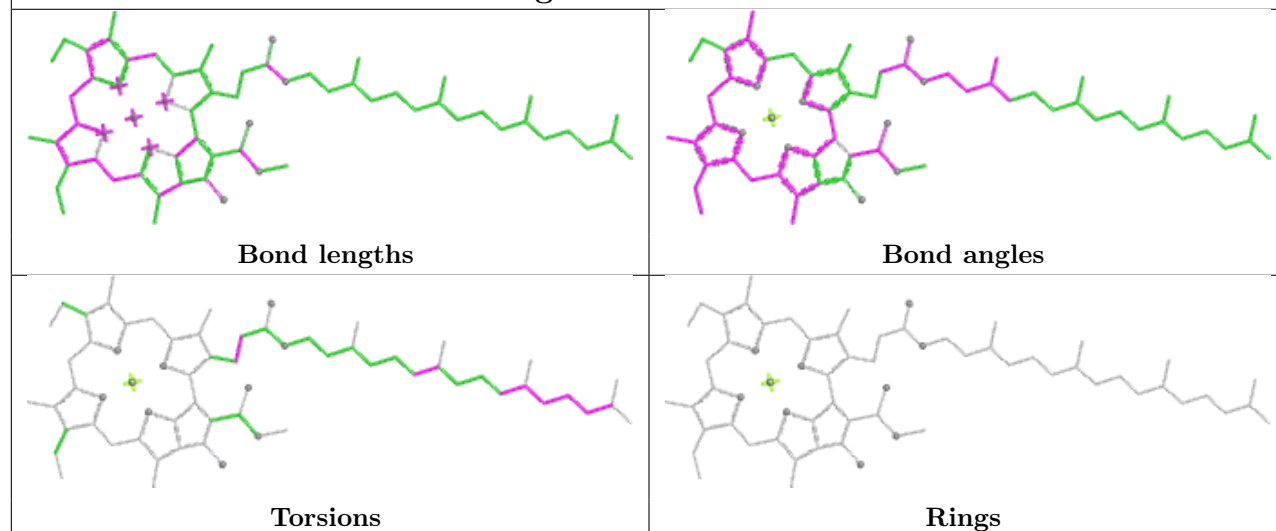


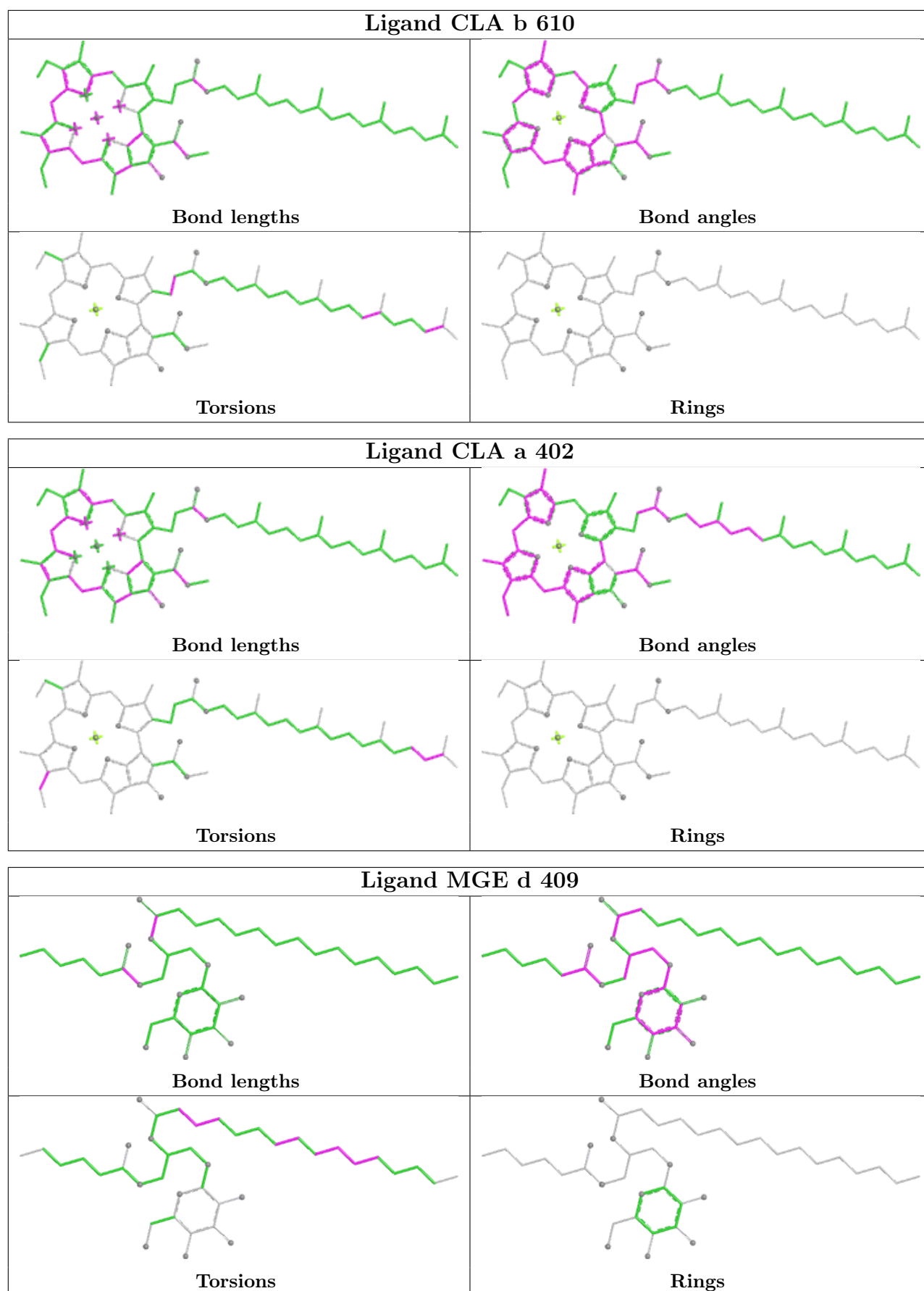


Ligand CLA b 616

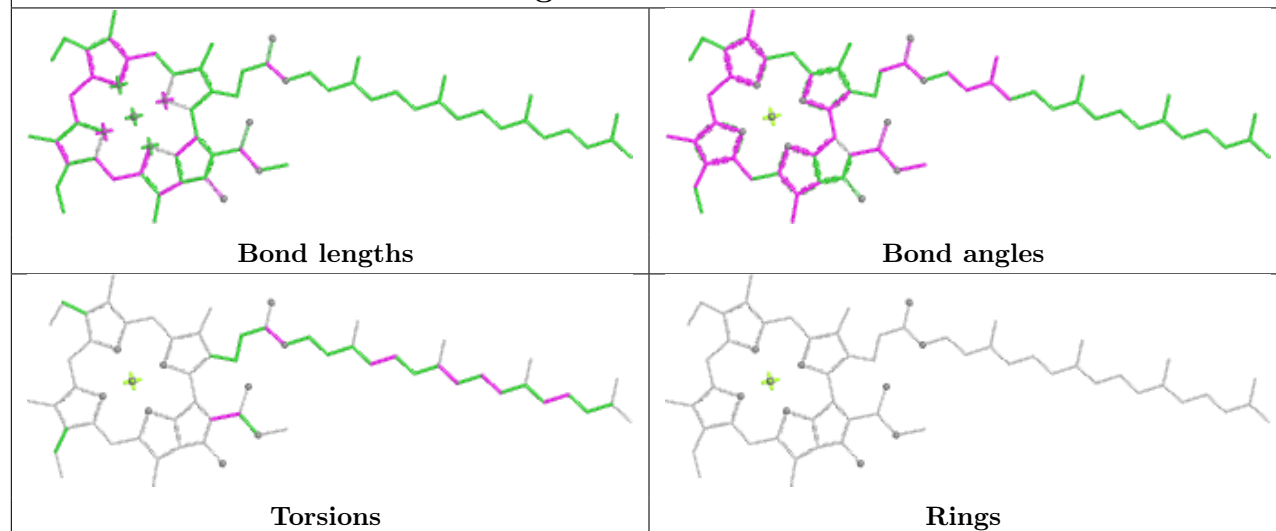


Ligand CLA b 606

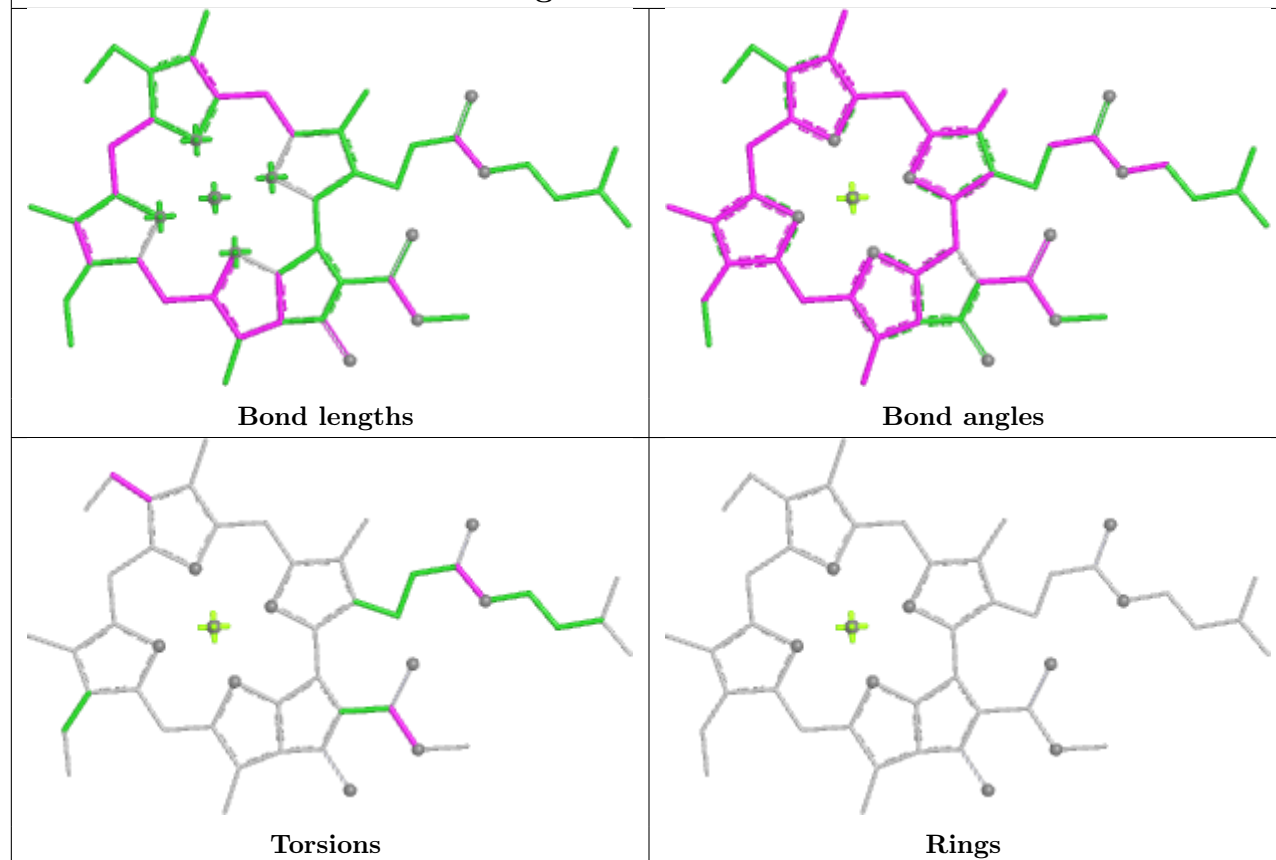


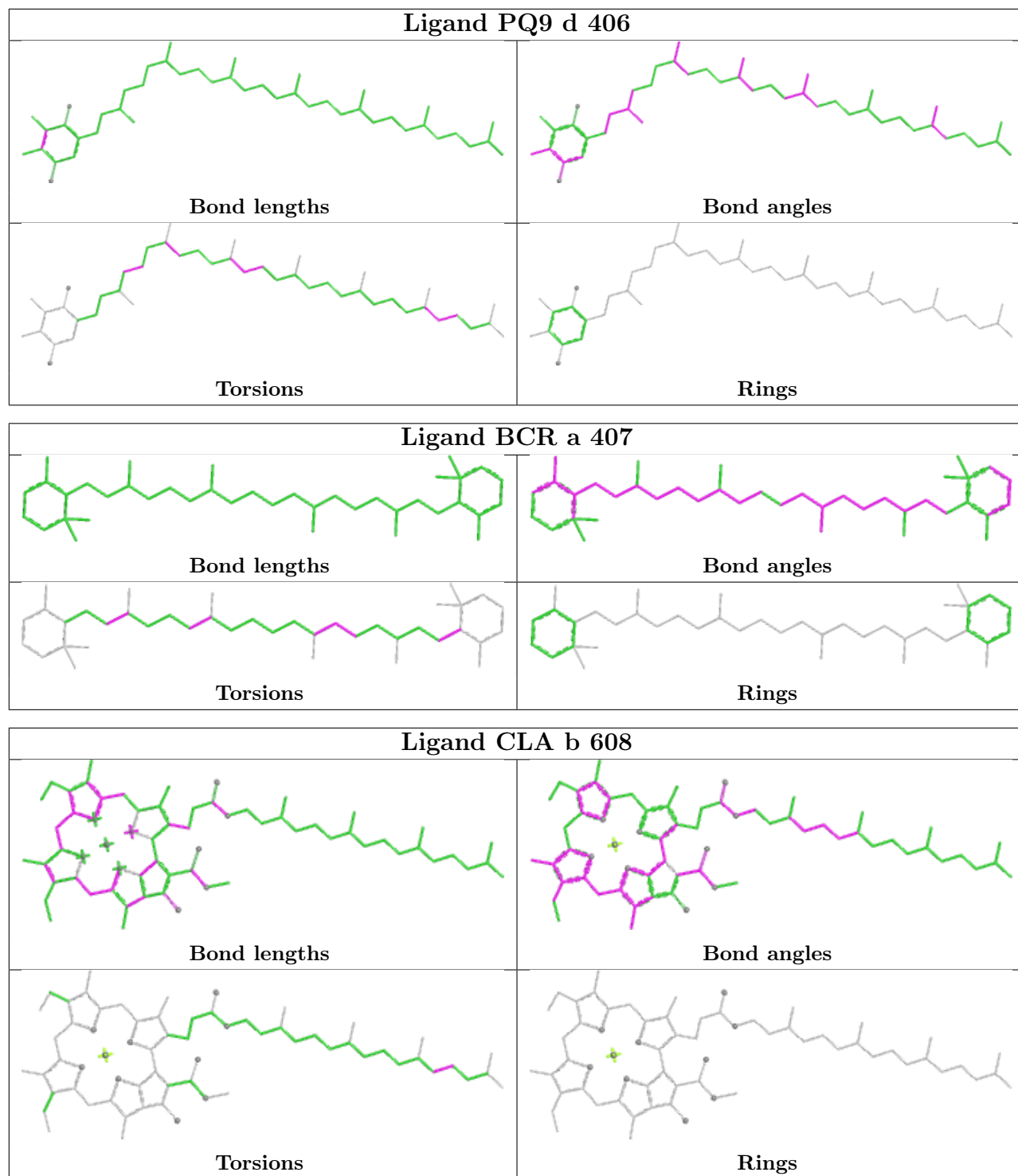


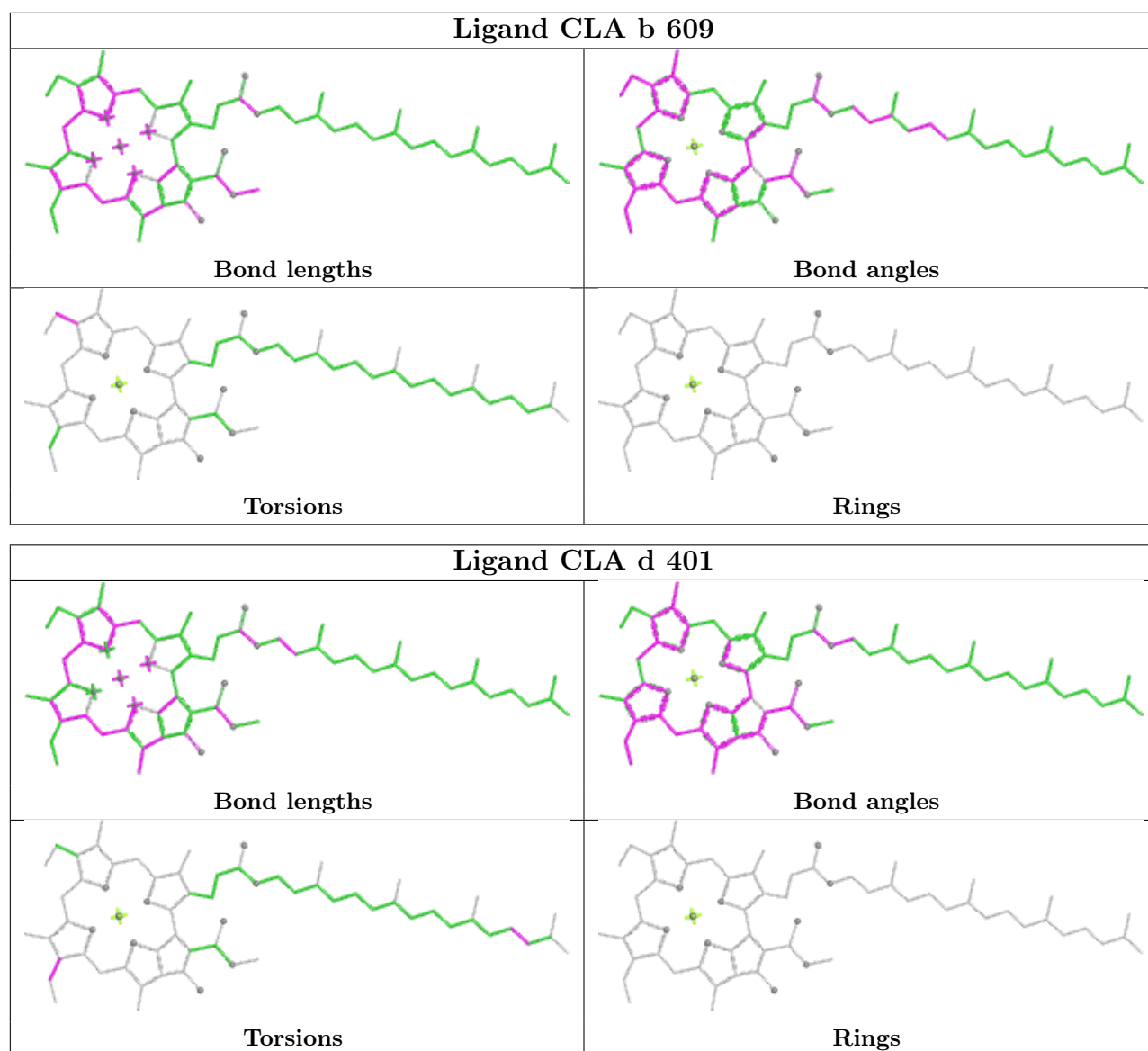
Ligand CLA b 612



Ligand CLA d 405







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.

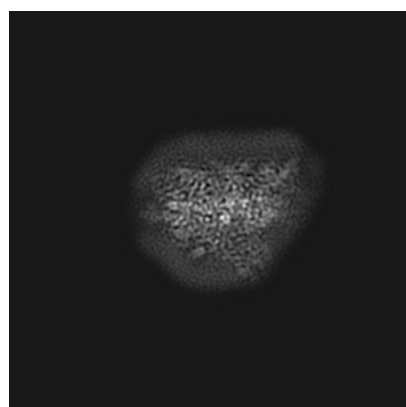
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30902. These allow visual inspection of the internal detail of the map and identification of artifacts.

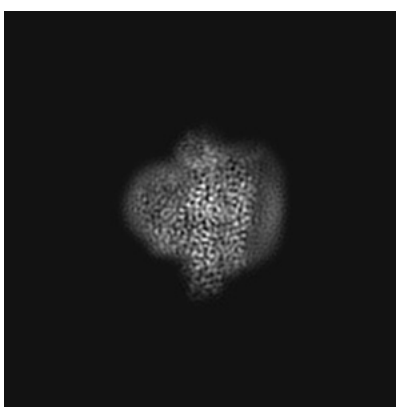
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

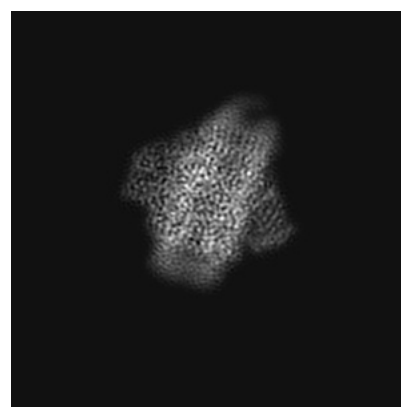
6.1.1 Primary map



X



Y

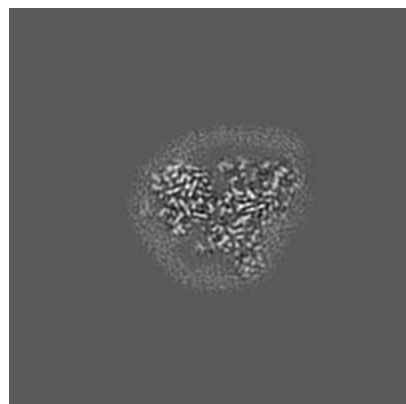


Z

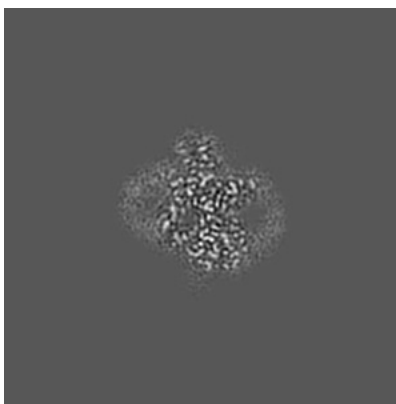
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

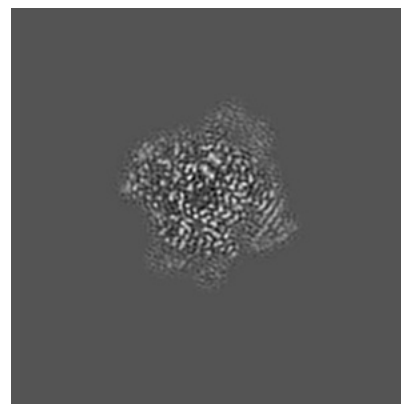
6.2.1 Primary map



X Index: 100



Y Index: 100

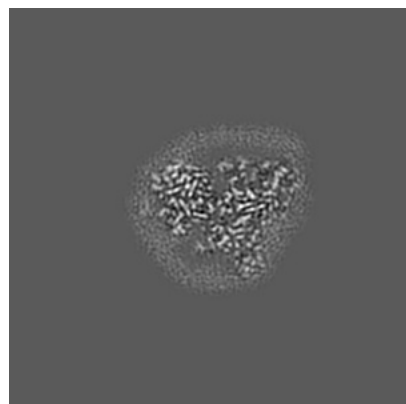


Z Index: 100

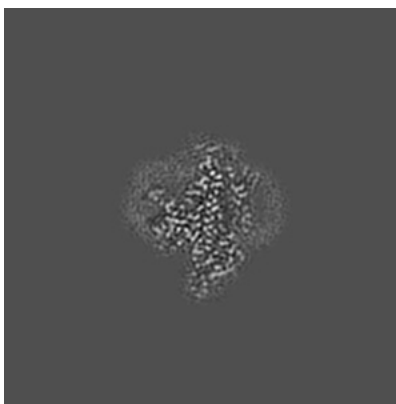
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

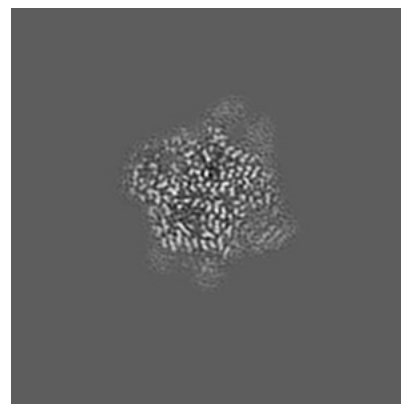
6.3.1 Primary map



X Index: 100



Y Index: 110

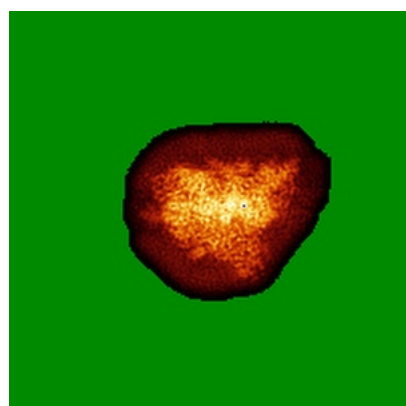


Z Index: 103

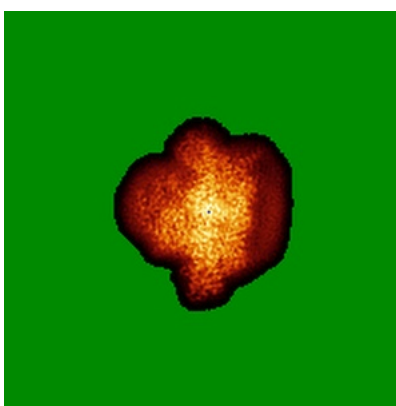
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

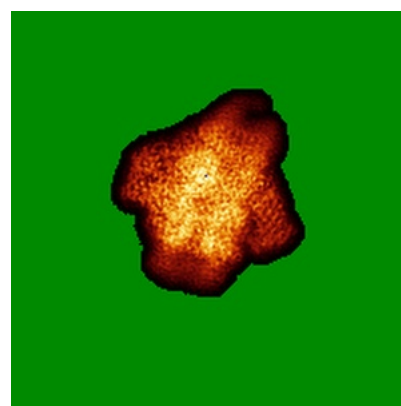
6.4.1 Primary map



X



Y

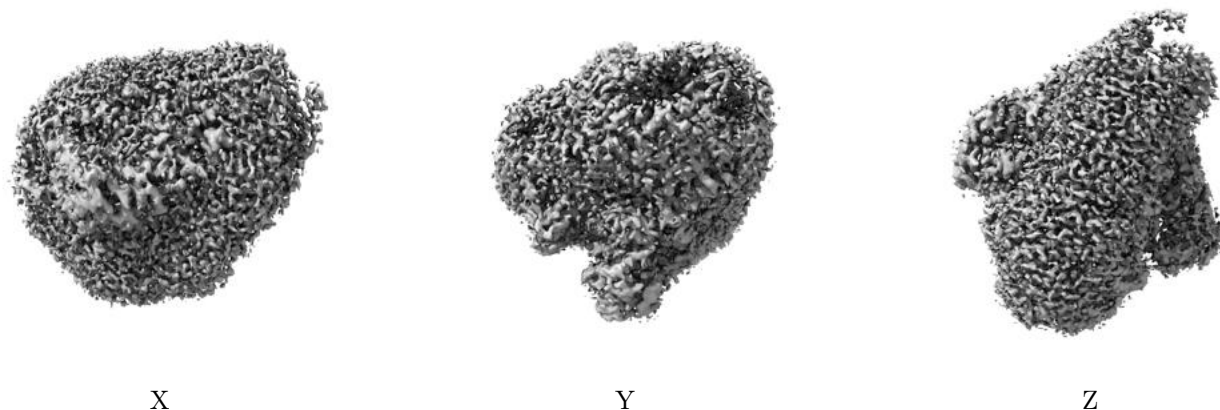


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

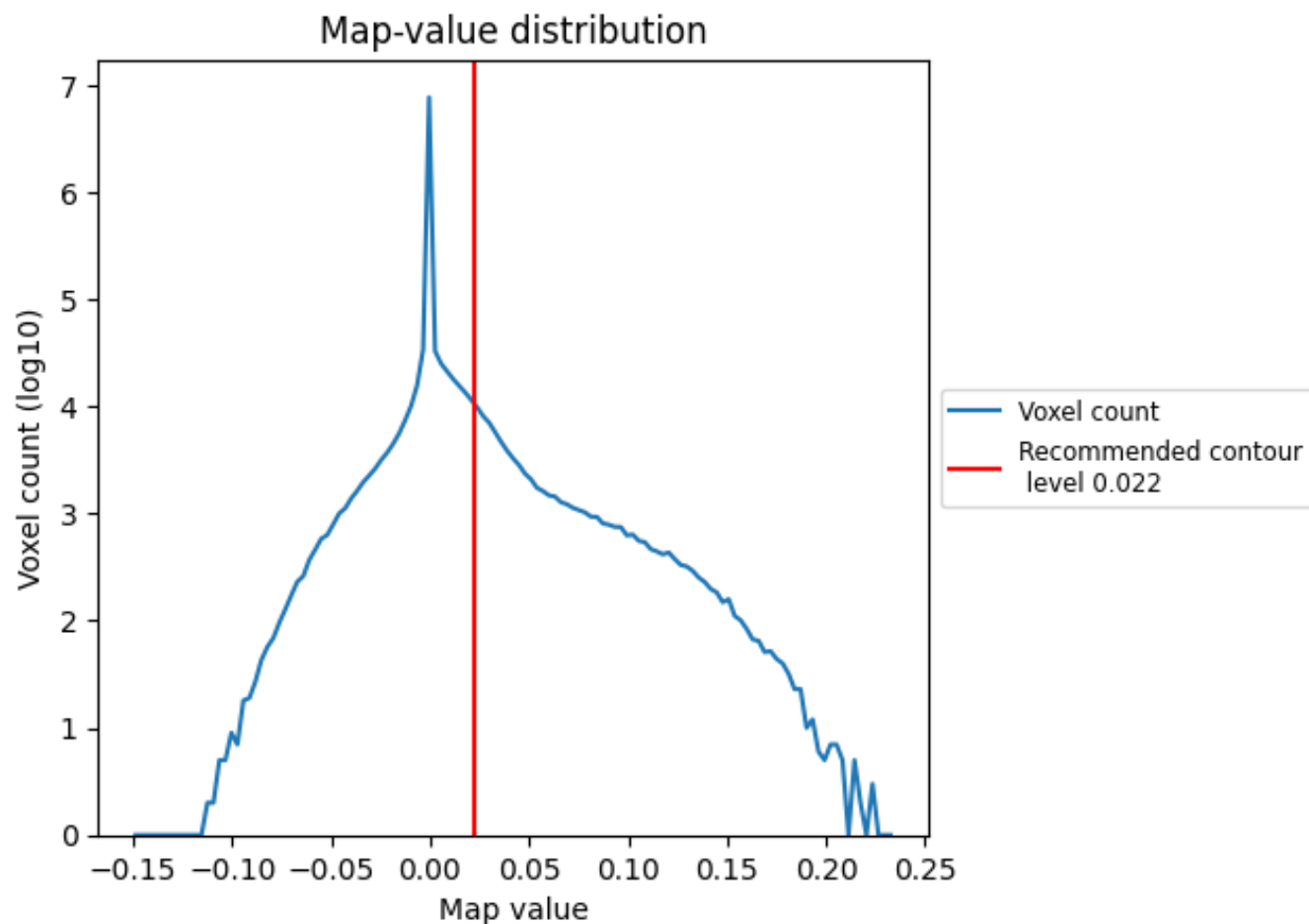
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

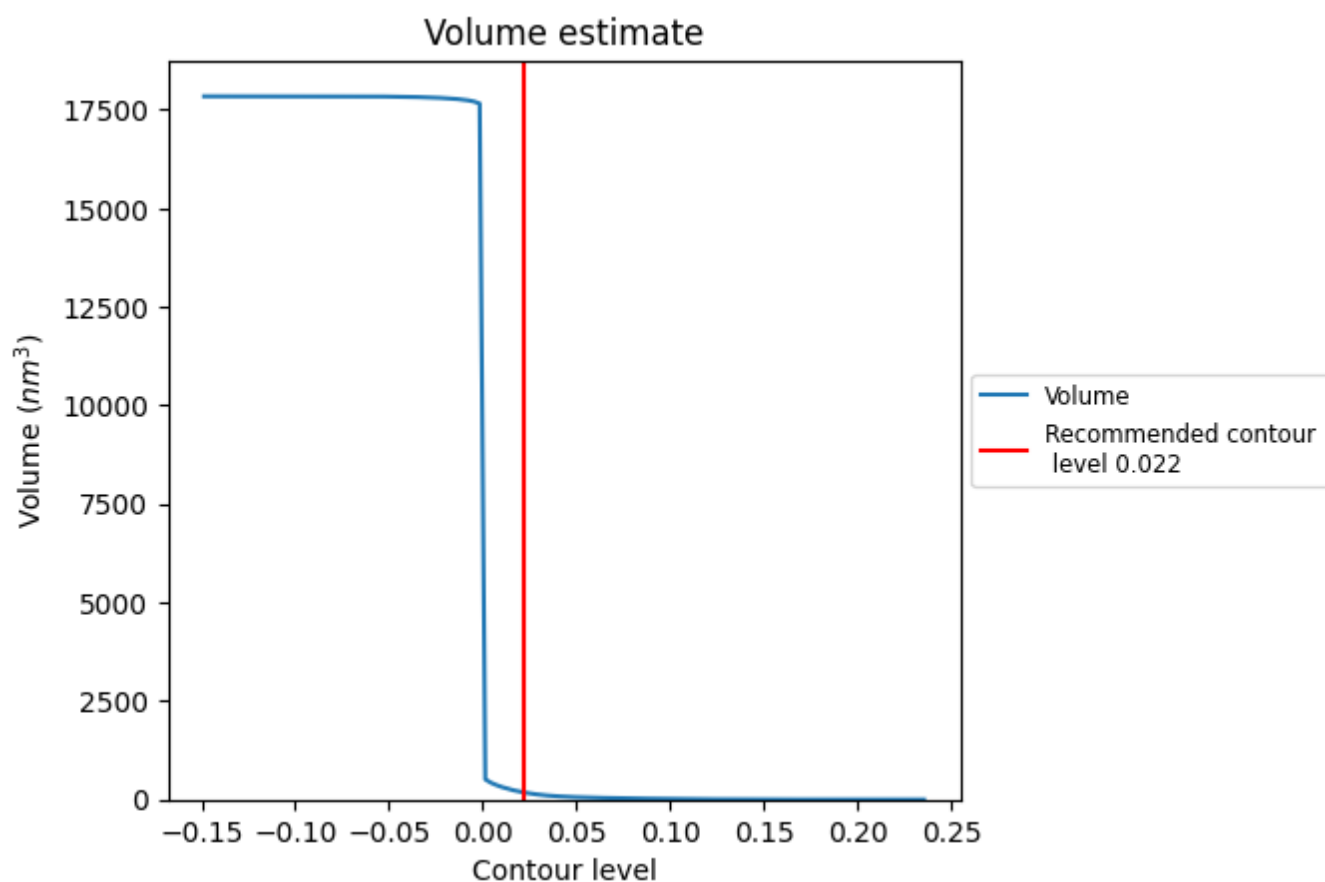
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

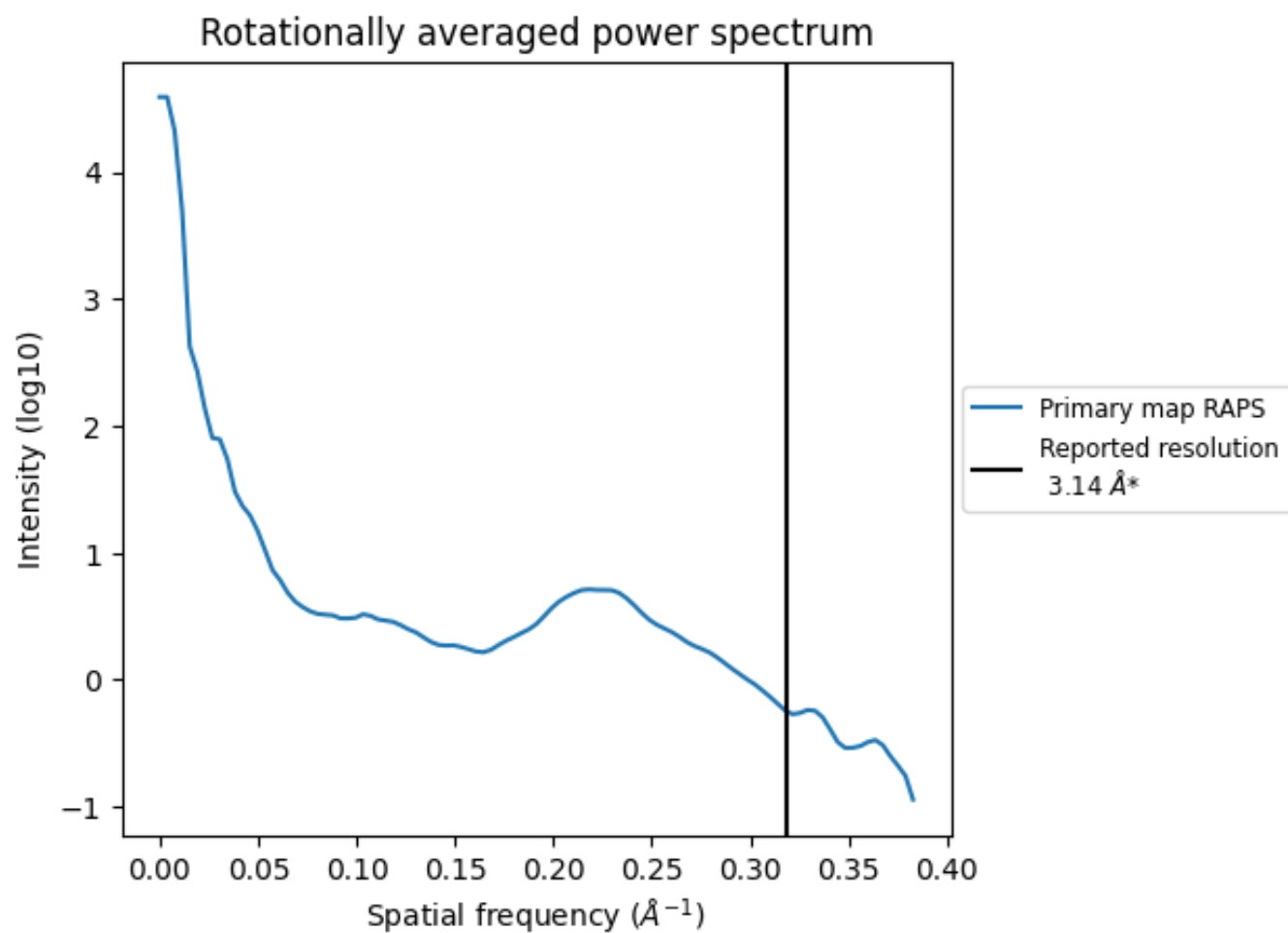
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 163 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.318 Å⁻¹

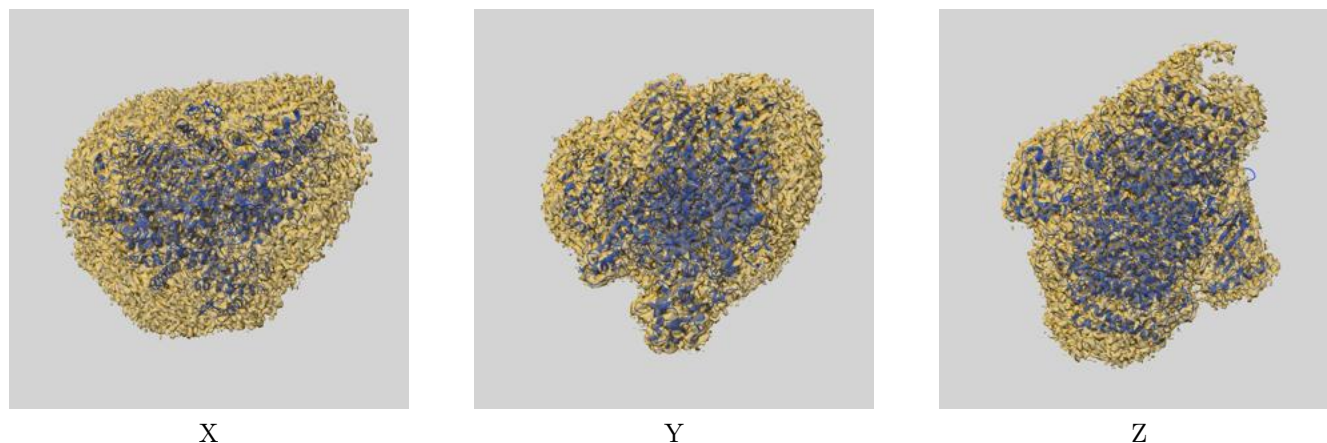
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

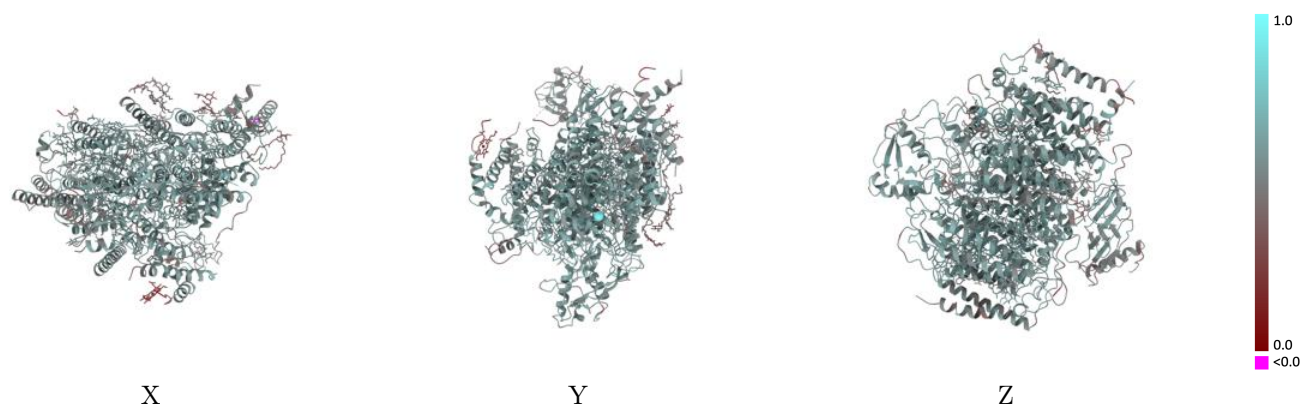
This section contains information regarding the fit between EMDB map EMD-30902 and PDB model 7DXA. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



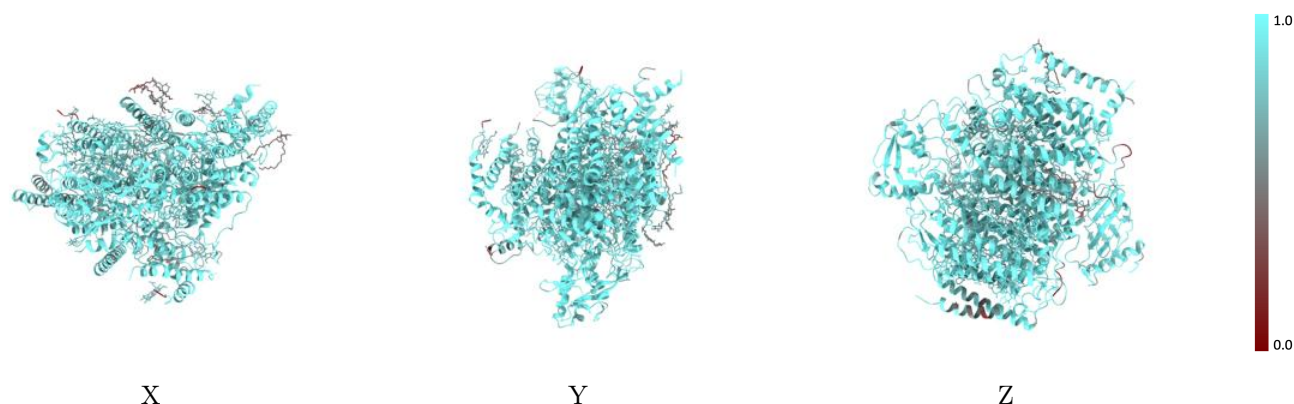
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



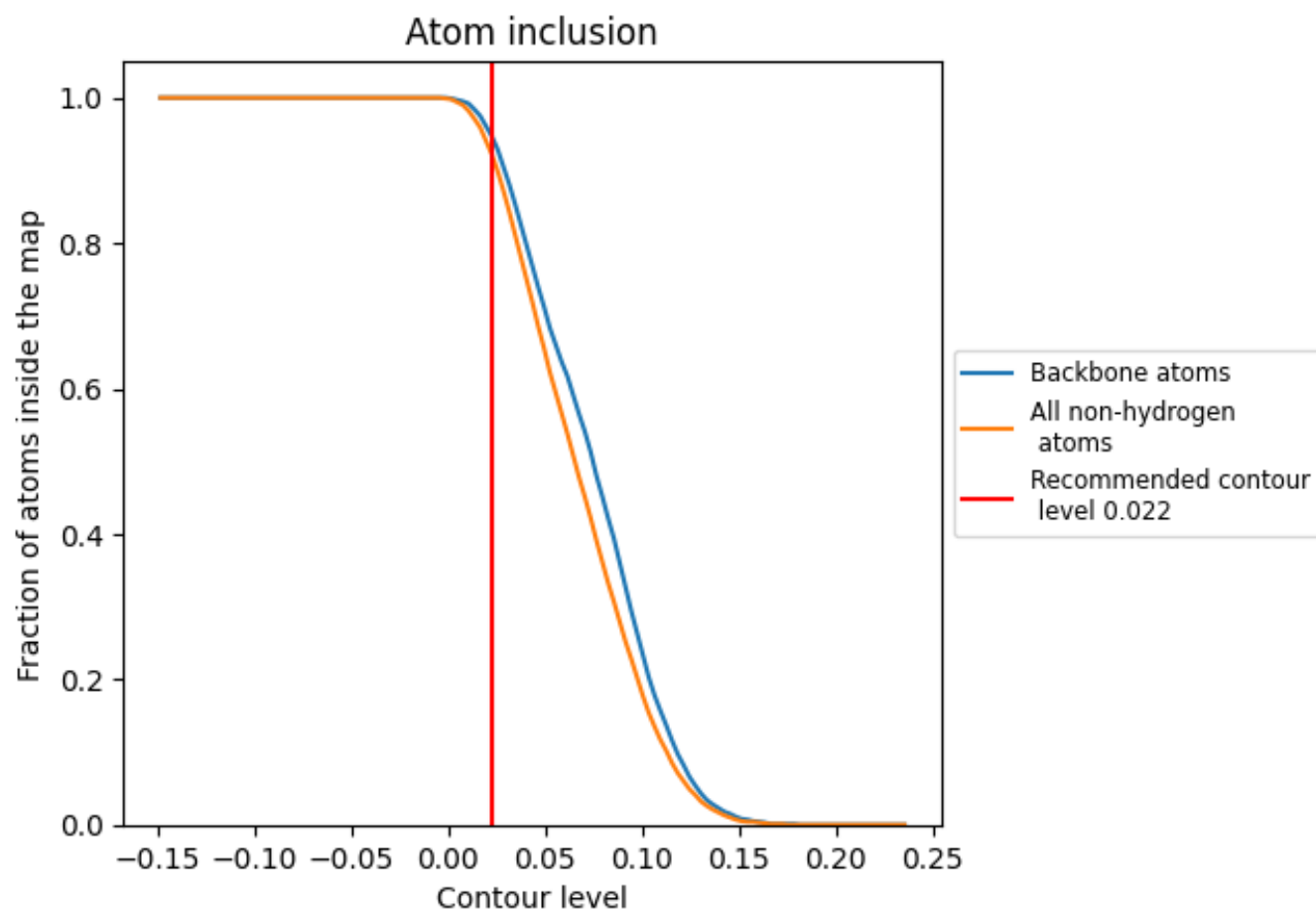
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5680
A	0.9200	0.5280
B	0.8660	0.5290
C	0.7300	0.4980
a	0.9400	0.5640
b	0.9440	0.5840
d	0.9500	0.5940
e	0.8070	0.4830
f	0.9540	0.5290
h	0.9660	0.5830
i	0.8440	0.4770
l	0.8350	0.5560
m	0.7870	0.5070
t	0.7920	0.5400
x	0.8810	0.5480

