



Full wwPDB EM Validation Report ⓘ

Sep 14, 2026 – 10:54 AM JST

PDB ID : 9WFZ / pdb_00009wfz
EMDB ID : EMD-65941
Title : Cryo-EM structure of PSII PsbA3-S264V from *Thermosynechococcus vestitus* BP-1 (local refinement)
Authors : Fan, S.B.; Nakajima, Y.; Shen, J.R.
Deposited on : 2025-08-22
Resolution : 2.08 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

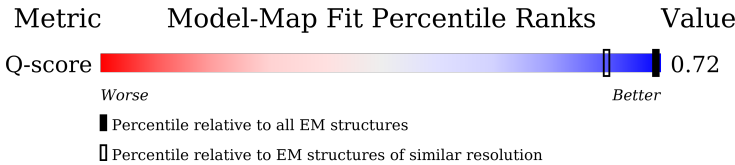
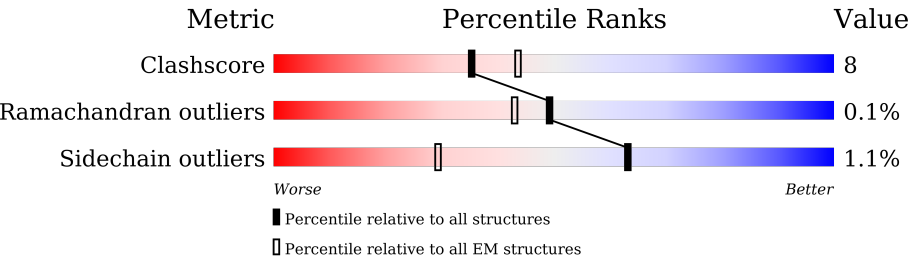
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.08 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	1976 (1.58 - 2.58)

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	I	38	92% 5%
2	K	46	61% 20% 20%
3	T	32	72% 19% 9%
4	V	163	73% 6% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	Y	46	
6	A	360	
7	B	510	
7	b	510	
8	C	461	
9	D	352	
10	E	84	
11	F	45	
12	J	40	
13	L	37	
14	M	36	
15	O	272	
16	U	134	
17	X	41	
18	Z	62	

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
22	HEC	V	201	X	-	-	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 17446 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 protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	36	Total	C	N	O	S	0	0
			261	176	41	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	K	37	Total	C	N	O	0	0
			275	193	42	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	29	Total	C	N	O	S	0	0
			232	164	32	34	2		

- Molecule 4 is a protein called Photosystem II extrinsic protein V.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	130	Total	C	N	O	S	0	0
			931	603	161	163	4		

- Molecule 5 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	29	Total	C	N	O	S	0	0
			177	118	30	28	1		

- Molecule 6 is a protein called Photosystem II protein D1 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	327	Total	C	N	O	S	0	2
			2516	1661	411	430	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	VAL	SER	variant	UNP Q8DIV4

- Molecule 7 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	212	Total	C	N	O	S	1	7
			1517	1000	248	267	2		
7	b	42	Total	C	N	O		0	6
			237	153	39	45			

- Molecule 8 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	350	Total	C	N	O	S	0	9
			2514	1632	436	436	10		

- Molecule 9 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	333	Total	C	N	O	S	1	2
			2603	1728	427	436	12		

- Molecule 10 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	61	Total	C	N	O	0	0
			474	321	77	76		

- Molecule 11 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	32	Total	C	N	O	S	0	0
			258	179	42	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	31	Total	C	N	O	S	0	0
			225	156	32	36	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	L	26	Total	C	N	O	1	1
			212	149	30	33		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	19	Total	C	N	O	S	0	3
			103	67	18	17	1		

- Molecule 15 is a protein called Photosystem II extrinsic protein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	188	Total	C	N	O	S	1	7
			1275	811	223	237	4		

- Molecule 16 is a protein called Photosystem II extrinsic protein U.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	94	Total	C	N	O	0	0
			683	445	120	118		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	X	23	Total	C	N	O	0	6
			110	73	18	19		

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	47	Total	C	N	O	S	0	4
			270	183	43	43	1		

- Molecule 19 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

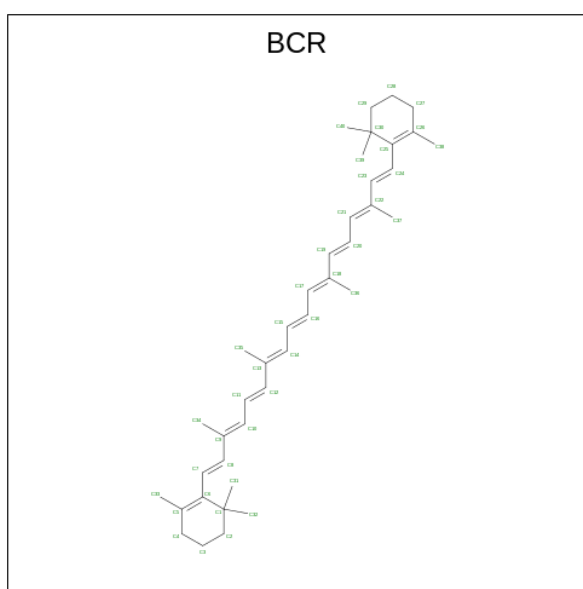
Mol	Chain	Residues	Atoms		AltConf
19	I	1	Total	C	0
			6	6	
19	K	1	Total	C	0
			13	13	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
19	T	1	Total C 5 5	0
19	A	1	Total C 8 8	0
19	D	1	Total C 7 7	0
19	X	1	Total C 9 9	0

- Molecule 20 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



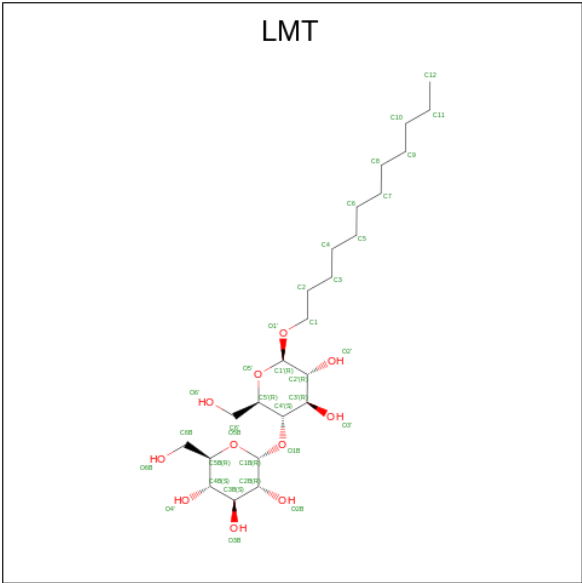
Mol	Chain	Residues	Atoms	AltConf
20	I	1	Total C 19 19	0
20	K	1	Total C 40 40	0
20	K	1	Total C 40 40	0
20	K	1	Total C 4 4	0
20	T	1	Total C 16 16	0
20	A	1	Total C 40 40	0
20	A	1	Total C 1 1	0

Continued on next page...

Continued from previous page...

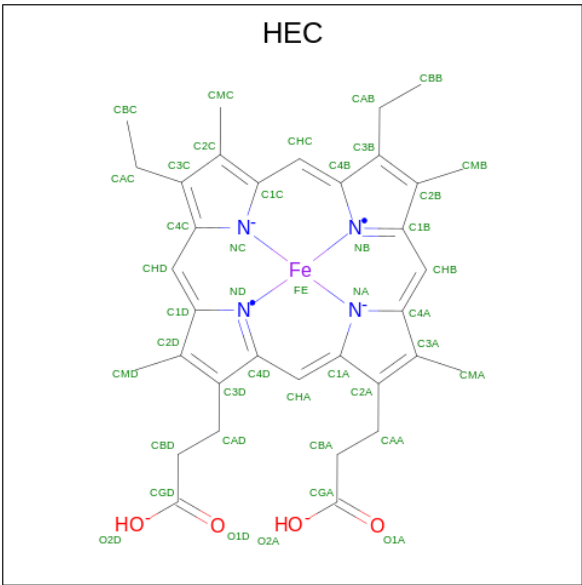
Mol	Chain	Residues	Atoms		AltConf
20	D	1	Total	C	0
			40	40	

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



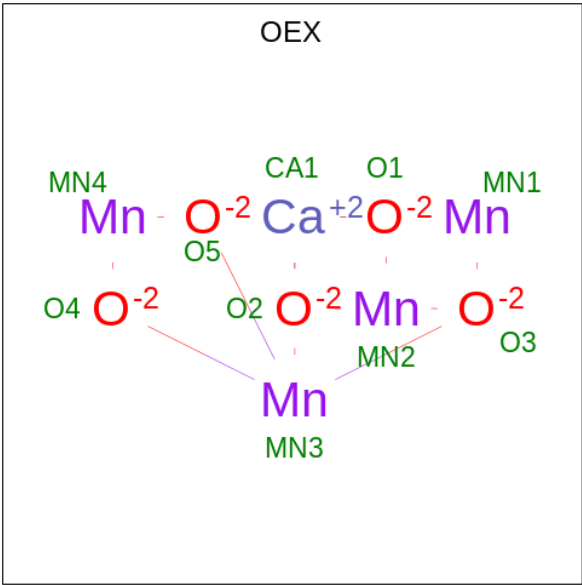
Mol	Chain	Residues	Atoms			AltConf
21	T	1	Total	C	O	0
			15	10	5	
21	J	1	Total	C	O	0
			24	18	6	
21	M	1	Total	O		0
			2	2		

- Molecule 22 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄).



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

- Molecule 23 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

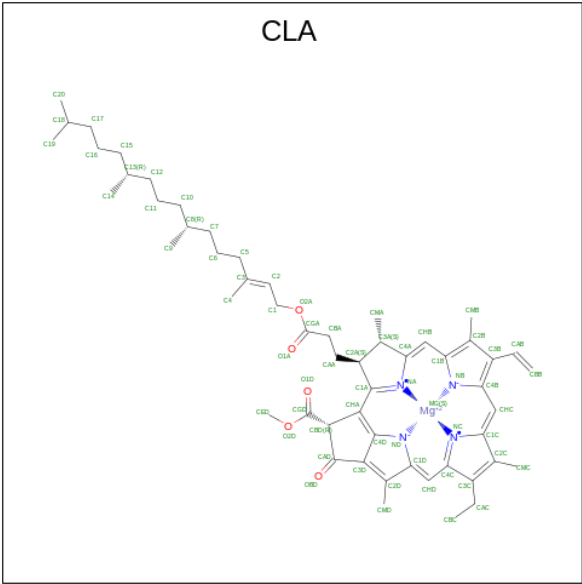
- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	Fe	0
			1	1	

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
25	A	2	Total	Cl	0
			2	2	

- Molecule 26 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



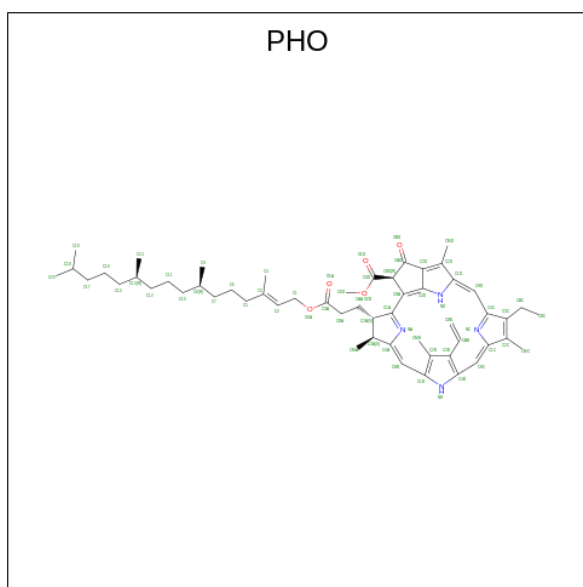
Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
26	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	B	1	Total	C	O			0
			25	23	2			
26	B	1	Total	C	O			0
			3	2	1			
26	C	1	Total	C	N	O		0
			30	26	1	3		
26	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

Continued on next page...

Continued from previous page...

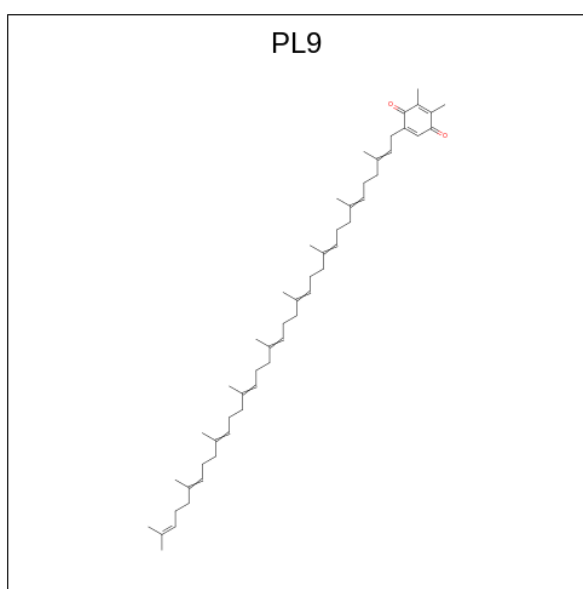
Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Mg	N	O	0
			54	45	1	3	5	
26	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			21	16	1	2	2	
26	C	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	C	1	Total	C	O			0
			4	2	2			
26	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C				0
			4	4				
26	D	1	Total	C				0
			10	10				
26	D	1	Total	C				0
			1	1				
26	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
26	D	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

- Molecule 27 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



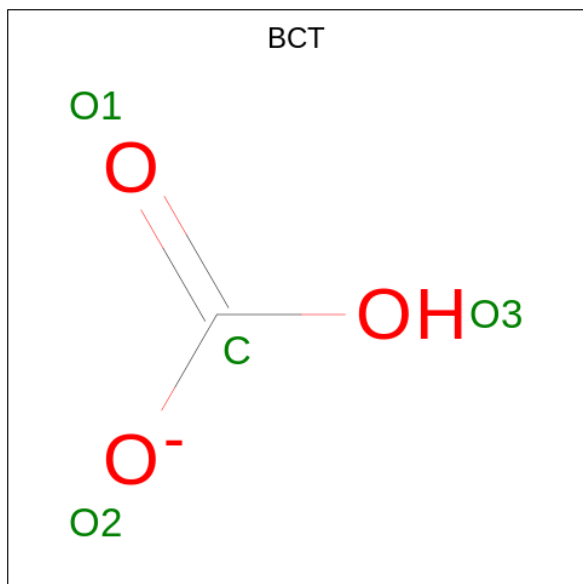
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			55	53	2	

Continued on next page...

Continued from previous page...

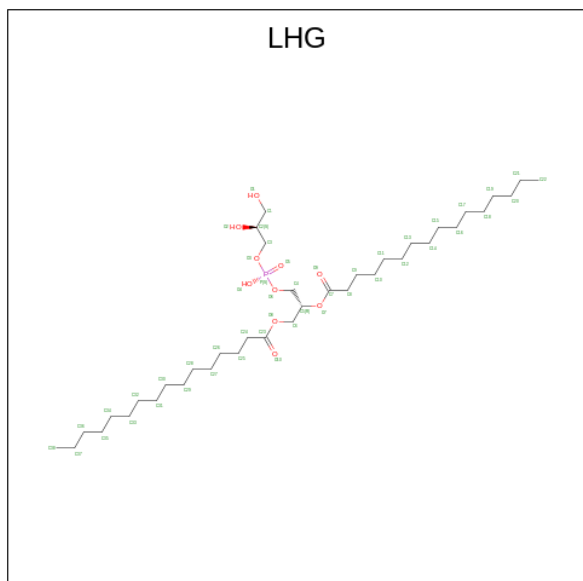
Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			55	53	2	

- Molecule 29 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



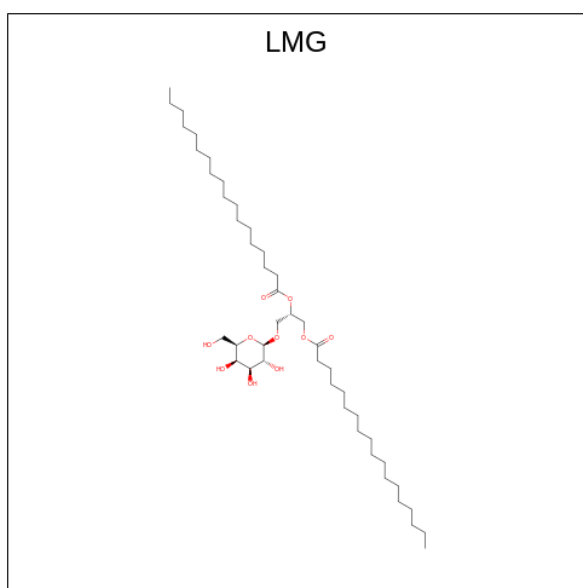
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	1
			4	1	3	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $\text{C}_{38}\text{H}_{75}\text{O}_{10}\text{P}$).



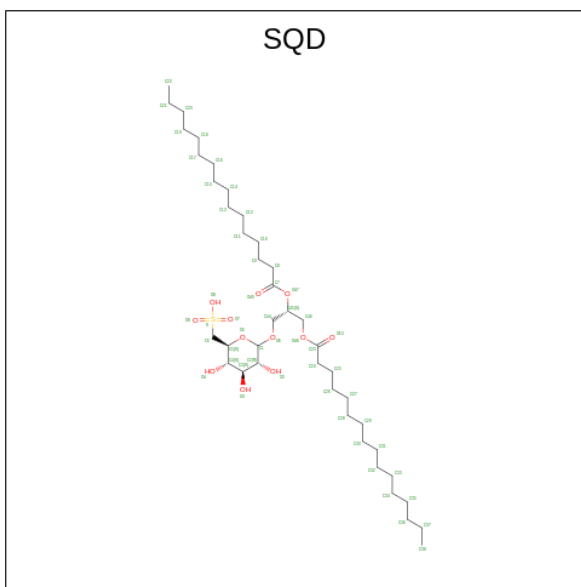
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	P	0
			39	28	10	1	
30	A	1	Total	C	O	P	0
			31	22	8	1	
30	D	1	Total	C	O	P	0
			49	38	10	1	
30	D	1	Total	C	O	P	0
			42	31	10	1	
30	L	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



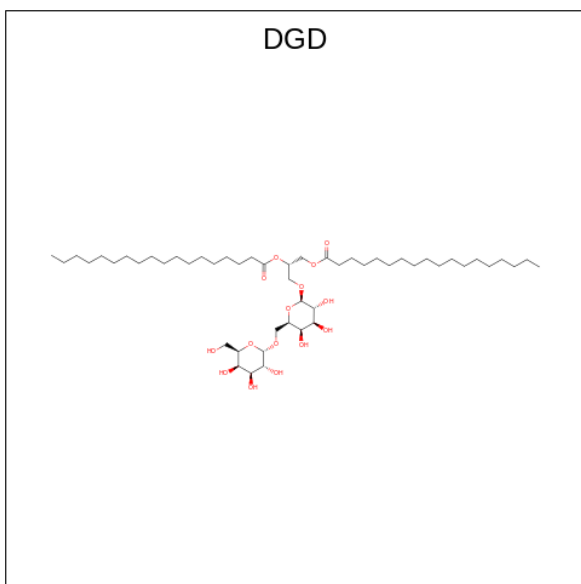
Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			31	22	9	
31	C	1	Total	C	O	0
			47	37	10	
31	D	1	Total	C	O	0
			38	28	10	

- Molecule 32 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
32	C	1	Total	C	O	S	0
			32	19	12	1	
32	F	1	Total	C	O	S	0
			23	11	11	1	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



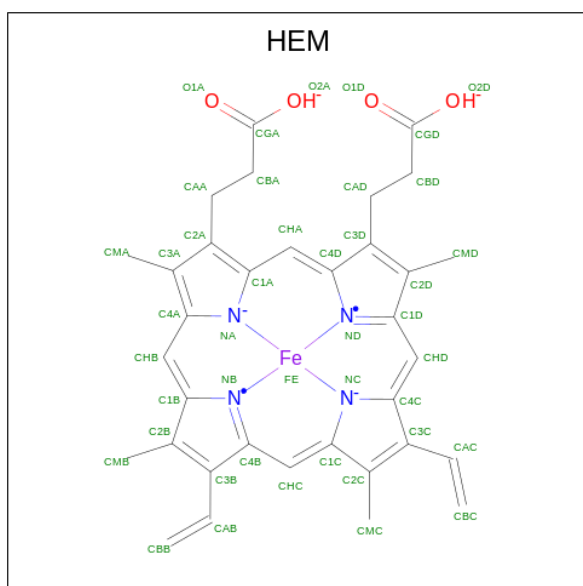
Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			52	37	15	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
33	C	1	Total	C	O	0
			50	35	15	
33	C	1	Total	C	O	0
			53	38	15	
33	D	1	Total	C	O	0
			54	40	14	

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



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	I	4	Total	O	0
			4	4	
35	K	2	Total	O	0
			2	2	
35	T	4	Total	O	0
			4	4	
35	V	10	Total	O	0
			10	10	
35	A	105	Total	O	2
			106	106	

Continued on next page...

Continued from previous page...

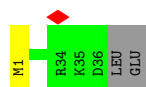
Mol	Chain	Residues	Atoms		AltConf
35	B	68	Total 68	O 68	0
35	C	85	Total 87	O 87	2
35	D	87	Total 88	O 88	1
35	E	6	Total 6	O 6	0
35	F	1	Total 1	O 1	0
35	J	3	Total 3	O 3	0
35	L	9	Total 9	O 9	0
35	M	4	Total 4	O 4	0
35	O	39	Total 39	O 39	1
35	U	7	Total 7	O 7	0
35	X	1	Total 1	O 1	0
35	b	5	Total 5	O 5	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

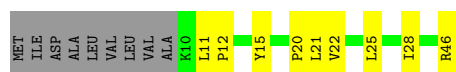
- Molecule 1: Photosystem II reaction center protein I

Chain I: 



- Molecule 2: Photosystem II reaction center protein K

Chain K: 



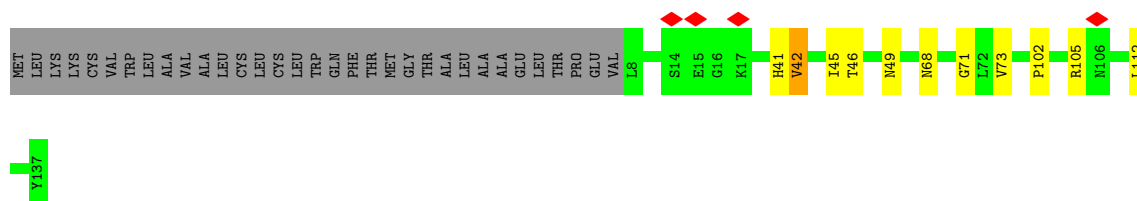
- Molecule 3: Photosystem II reaction center protein T

Chain T: 



- Molecule 4: Photosystem II extrinsic protein V

Chain V: 

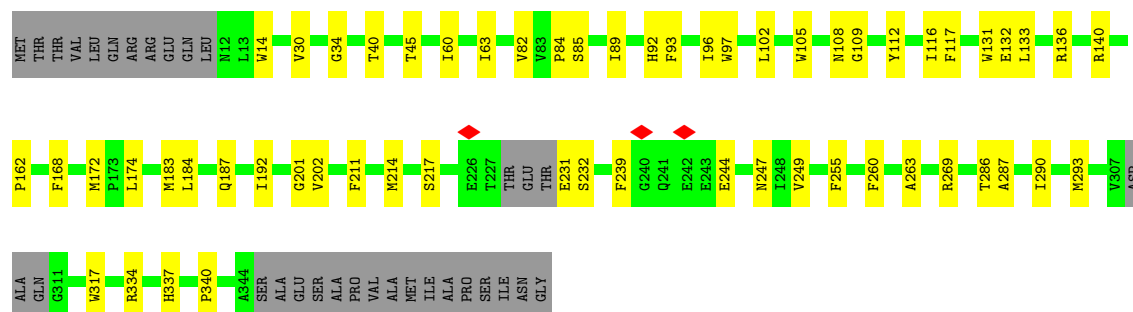
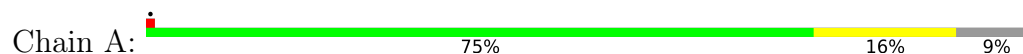


- Molecule 5: Photosystem II reaction center protein Psb30

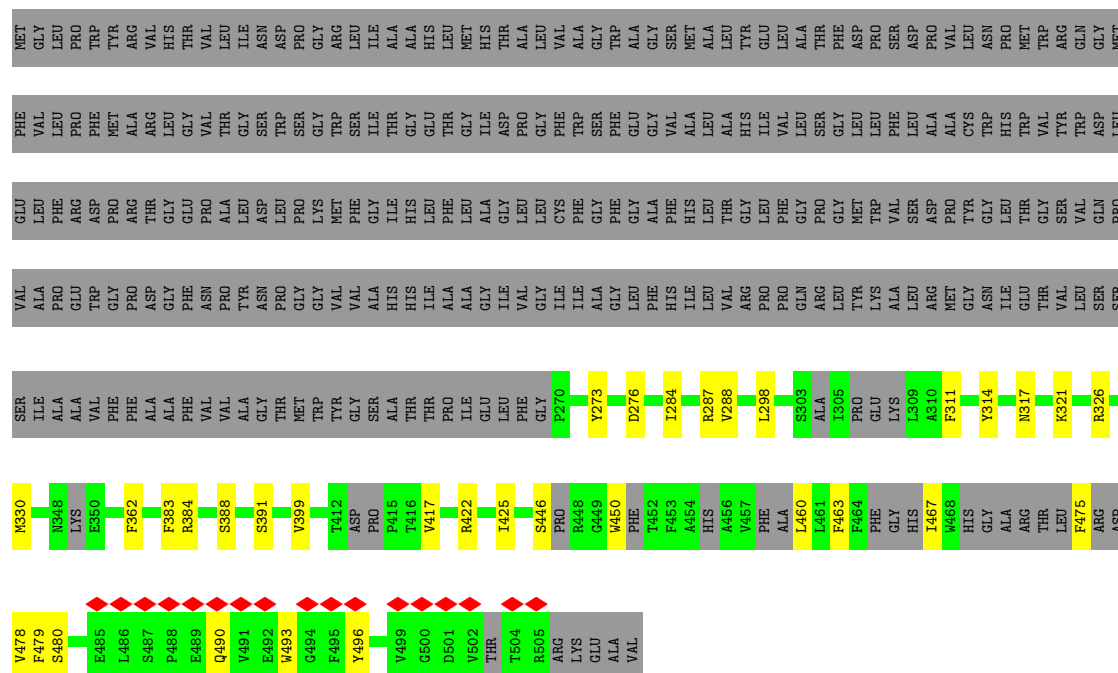
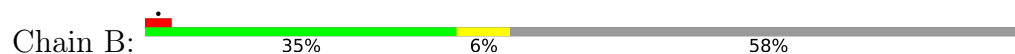
Chain Y: 



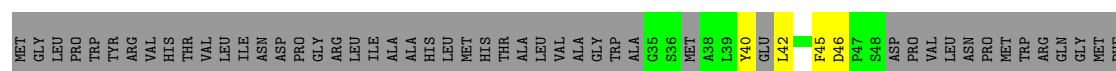
- Molecule 6: Photosystem II protein D1 3

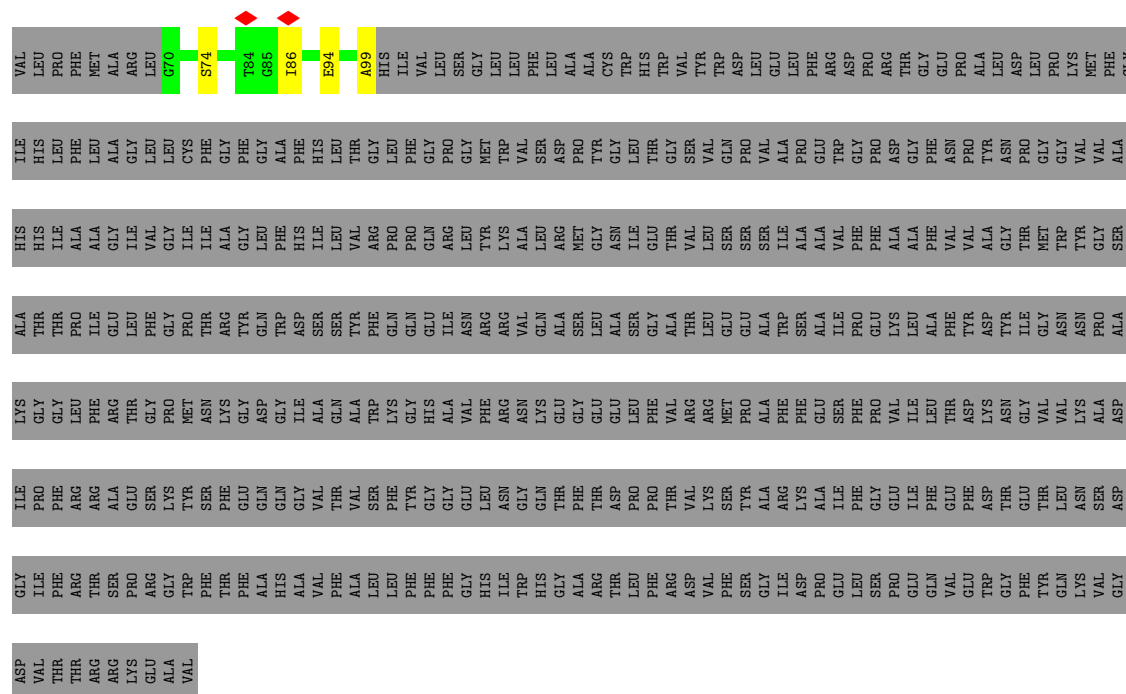


- Molecule 7: Photosystem II CP47 reaction center protein



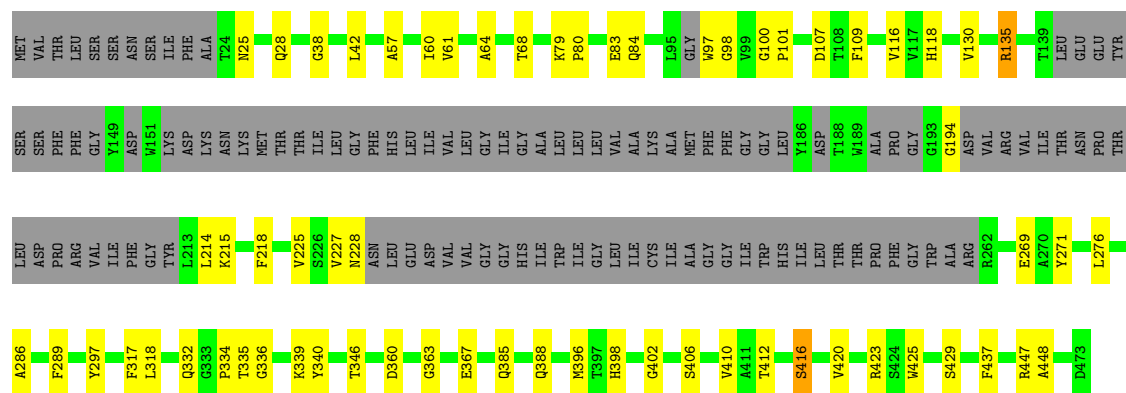
- Molecule 7: Photosystem II CP47 reaction center protein





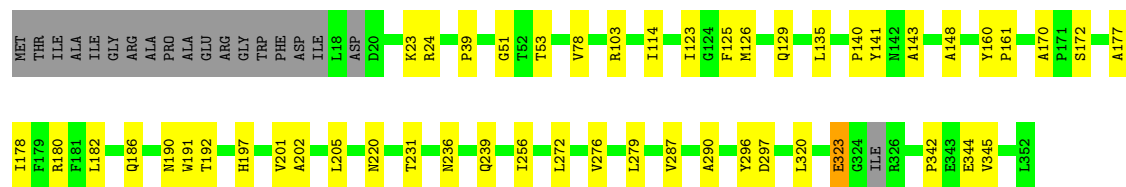
• Molecule 8: Photosystem II CP43 reaction center protein

Chain C: 62% 13% 24%



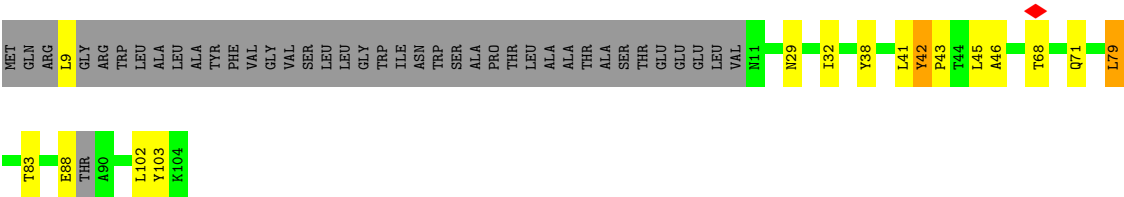
• Molecule 9: Photosystem II D2 protein

Chain D: 80% 14% 5%

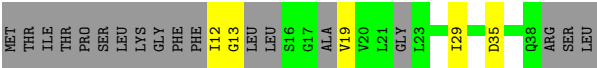


• Molecule 10: Cytochrome b559 subunit alpha

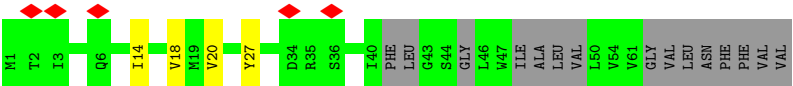
Chain E: 61% 12% 27%



• Molecule 17: Photosystem II reaction center protein X



• Molecule 18: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	93573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.350	Depositor
Minimum map value	-0.726	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.129	Depositor
Map size (Å)	290.56, 290.56, 290.56	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5675, 0.5675, 0.5675	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, OEX, CL, FE2, PHO, LMT, HEM, LHG, UNL, DGD, CLA, BCT, LMG, HEC, SQD, BCR

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	I	0.11	0/267	0.26	0/363
2	K	0.16	0/285	0.37	0/395
3	T	0.13	0/239	0.28	0/324
4	V	0.26	0/951	0.40	0/1301
5	Y	0.14	0/178	0.25	0/243
6	A	0.16	0/2595	0.34	0/3542
7	B	0.12	0/1539	0.30	0/2048
7	b	0.13	0/233	0.32	0/306
8	C	0.12	0/2569	0.28	0/3472
9	D	0.14	0/2691	0.31	0/3666
10	E	0.22	0/485	0.41	0/657
11	F	0.25	0/266	0.34	0/363
12	J	0.12	0/230	0.26	0/312
13	L	0.11	0/218	0.21	0/294
14	M	0.14	0/99	0.25	0/129
15	O	0.12	0/1285	0.28	0/1734
16	U	0.27	0/692	0.48	1/941 (0.1%)
17	X	0.16	0/101	0.31	0/127
18	Z	0.11	0/269	0.25	0/364
All	All	0.16	0/15192	0.32	1/20581 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	U	42	TYR	CB-CA-C	5.60	116.76	108.87

There are no chirality outliers.

There are no planarity outliers.

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	I	261	0	251	1	0
2	K	275	0	272	5	0
3	T	232	0	224	5	0
4	V	931	0	910	6	0
5	Y	177	0	164	4	0
6	A	2516	0	2407	51	0
7	B	1517	0	1323	24	0
7	b	237	0	178	7	0
8	C	2514	0	2328	48	0
9	D	2603	0	2504	42	0
10	E	474	0	451	8	0
11	F	258	0	268	5	0
12	J	225	0	235	2	0
13	L	212	0	229	1	0
14	M	103	0	98	1	0
15	O	1275	0	1172	18	0
16	U	683	0	664	11	0
17	X	110	0	90	7	0
18	Z	270	0	224	3	0
19	A	8	0	0	0	0
19	D	7	0	0	0	0
19	I	6	0	0	0	0
19	K	13	0	0	0	0
19	T	5	0	0	0	0
19	X	9	0	0	0	0
20	A	41	0	56	0	0
20	D	40	0	56	2	0
20	I	19	0	26	0	0
20	K	84	0	117	8	0
20	T	16	0	22	1	0
21	J	24	0	35	1	0
21	M	2	0	0	0	0
21	T	15	0	14	0	0
22	V	43	0	32	0	0
23	A	10	0	0	1	0
24	A	1	0	0	0	0
25	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	237	0	236	16	0
26	B	28	0	41	1	0
26	C	530	0	526	29	0
26	D	124	0	122	7	0
27	A	64	0	74	1	0
27	D	64	0	74	5	0
28	A	55	0	80	7	0
28	D	55	0	80	2	0
29	A	4	0	0	0	0
30	A	70	0	84	4	0
30	D	91	0	128	3	0
30	L	39	0	51	1	0
31	B	31	0	28	0	0
31	C	47	0	64	3	0
31	D	38	0	46	0	0
32	C	32	0	28	1	0
32	F	23	0	16	0	0
33	C	155	0	184	6	0
33	D	54	0	66	3	0
34	E	43	0	30	2	0
35	A	106	0	0	3	0
35	B	68	0	0	0	0
35	C	87	0	0	0	0
35	D	88	0	0	0	0
35	E	6	0	0	0	0
35	F	1	0	0	0	0
35	I	4	0	0	0	0
35	J	3	0	0	0	0
35	K	2	0	0	0	0
35	L	9	0	0	0	0
35	M	4	0	0	0	0
35	O	39	0	0	0	0
35	T	4	0	0	0	0
35	U	7	0	0	0	0
35	V	10	0	0	0	0
35	X	1	0	0	0	0
35	b	5	0	0	0	0
All	All	17446	0	16308	262	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 8.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:19:PHE:CD2	3:T:19:PHE:CZ	2.39	1.02
8:C:271:TYR:CE1	8:C:271:TYR:CE2	2.39	1.01
7:B:463:PHE:CG	7:B:463:PHE:CE1	2.40	1.00
8:C:109:PHE:CD1	8:C:109:PHE:CB	2.51	0.94
7:B:478:VAL:C	7:B:479:PHE:CA	2.41	0.94
7:B:479:PHE:C	7:B:480:SER:CA	2.42	0.93
17:X:12:ILE:C	17:X:13:GLY:CA	2.42	0.93
7:B:479:PHE:CA	7:B:479:PHE:CG	2.52	0.92
8:C:97:TRP:C	8:C:98:GLY:CA	2.42	0.92
6:A:14:TRP:CG	6:A:14:TRP:CA	2.53	0.91
8:C:100:GLY:C	8:C:101:PRO:CA	2.43	0.91
8:C:227:VAL:C	8:C:228:ASN:CA	2.44	0.90
26:C:509:CLA:C17	26:C:509:CLA:C19	2.50	0.90
7:b:45:PHE:C	7:b:46:ASP:CA	2.45	0.90
26:C:509:CLA:C17	26:C:509:CLA:C15	2.51	0.88
26:D:403:CLA:C17	26:D:403:CLA:C15	2.50	0.88
8:C:227:VAL:CG1	8:C:227:VAL:CA	2.53	0.86
7:B:467:ILE:CG1	7:B:467:ILE:CG2	2.53	0.86
17:X:19:VAL:CB	17:X:19:VAL:C	2.53	0.81
17:X:12:ILE:C	17:X:12:ILE:CB	2.53	0.81
7:b:46:ASP:CA	7:b:46:ASP:CG	2.54	0.81
7:b:99:ALA:CB	7:b:99:ALA:N	2.45	0.80
15:O:19:CYS:CB	15:O:19:CYS:N	2.44	0.80
26:A:412:CLA:HHC	26:A:412:CLA:HBB1	1.63	0.80
28:A:410:PL9:H261	30:A:415:LHG:H202	1.67	0.77
16:U:29:ASN:HD21	16:U:88:GLU:H	1.34	0.76
6:A:40:THR:HG23	26:A:408:CLA:HBB1	1.67	0.76
15:O:189:ARG:HG3	15:O:189:ARG:HH11	1.52	0.74
17:X:29:ILE:N	17:X:29:ILE:C	2.45	0.74
8:C:100:GLY:C	8:C:100:GLY:N	2.45	0.74
10:E:23:HIS:HB3	10:E:27:ILE:HD12	1.69	0.73
7:B:287:ARG:N	7:B:287:ARG:C	2.47	0.73
7:b:45:PHE:C	7:b:45:PHE:N	2.46	0.73
9:D:279:LEU:HD22	27:D:401:PHO:HBC3	1.72	0.71
9:D:192:THR:HG23	26:D:405:CLA:HBC2	1.71	0.71
8:C:107:ASP:OD1	8:C:107:ASP:CB	2.38	0.71
7:b:40:TYR:O	7:b:40:TYR:CA	2.40	0.70
8:C:214:LEU:O	8:C:215:LYS:N	2.25	0.70
8:C:194:GLY:O	8:C:194:GLY:CA	2.41	0.69
6:A:231:GLU:O	6:A:232:SER:N	2.25	0.69
15:O:51:LEU:HB3	15:O:65:PHE:HB3	1.75	0.69
15:O:213:GLY:O	15:O:214:THR:N	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:244:GLU:HB3	35:A:520:HOH:O	1.92	0.68
9:D:236:ASN:H	9:D:239:GLN:HE21	1.43	0.66
20:K:102:BCR:H382	26:C:511:CLA:HMB1	1.79	0.65
20:K:101:BCR:H10C	5:Y:28:ILE:HG23	1.78	0.65
31:C:502:LMG:H382	33:C:513:DGD:HB52	1.81	0.62
6:A:192:ILE:HG13	6:A:293:MET:HE1	1.82	0.61
8:C:318:LEU:HD12	8:C:340:TYR:HB3	1.82	0.61
9:D:186:GLN:HB2	26:D:405:CLA:HBC1	1.82	0.60
6:A:183:MET:HB3	26:A:405:CLA:HBC2	1.84	0.60
6:A:84:PRO:HA	6:A:112:TYR:CG	2.37	0.59
8:C:429:SER:HB3	33:C:514:DGD:HBT2	1.84	0.59
15:O:88:ASN:ND2	15:O:92:SER:O	2.34	0.59
9:D:123:ILE:HG12	26:D:403:CLA:HAB	1.85	0.59
30:A:414:LHG:O2	8:C:447:ARG:NE	2.35	0.59
8:C:83:GLU:OE2	8:C:398:HIS:NE2	2.36	0.58
26:C:509:CLA:HMB1	26:C:511:CLA:HBB1	1.85	0.58
20:K:102:BCR:H282	26:C:511:CLA:H72	1.84	0.58
9:D:23:LYS:HE2	9:D:135:LEU:HD21	1.85	0.58
9:D:172:SER:HB2	9:D:177:ALA:HB1	1.85	0.58
7:b:42:LEU:HD13	7:b:94:GLU:HG3	1.85	0.58
6:A:184:LEU:HD21	9:D:186:GLN:HG2	1.86	0.58
17:X:12:ILE:C	17:X:12:ILE:CG2	2.77	0.58
8:C:385:GLN:H	8:C:388:GLN:HE21	1.52	0.58
27:D:401:PHO:H3A	26:D:405:CLA:H142	1.86	0.57
34:E:101:HEM:HAC	11:F:27:ALA:HB1	1.86	0.57
8:C:218:PHE:HE2	31:C:502:LMG:H111	1.69	0.57
9:D:141:TYR:OH	30:D:412:LHG:O5	2.23	0.57
15:O:189:ARG:HG3	15:O:189:ARG:NH1	2.20	0.56
10:E:23:HIS:HA	10:E:26:THR:OG1	2.06	0.56
30:A:414:LHG:H152	30:A:414:LHG:H332	1.88	0.56
4:V:68:ASN:ND2	4:V:71:GLY:H	2.04	0.56
6:A:131:TRP:CH2	26:C:506:CLA:HAA2	2.41	0.56
6:A:334:ARG:NH2	35:A:511:HOH:O	2.39	0.56
8:C:130:VAL:HG22	26:C:511:CLA:H91	1.88	0.56
6:A:92:HIS:NE2	8:C:360:ASP:OD2	2.31	0.55
9:D:24:ARG:NH2	17:X:35:ASP:O	2.40	0.55
8:C:269:GLU:HG2	8:C:448:ALA:HB2	1.88	0.55
16:U:29:ASN:ND2	16:U:88:GLU:H	2.03	0.55
8:C:225:VAL:HG13	8:C:289:PHE:HA	1.89	0.55
33:C:514:DGD:HA21	21:J:101:LMT:H51	1.89	0.55
17:X:19:VAL:C	17:X:19:VAL:CG1	2.80	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:A:410:PL9:H252	27:D:401:PHO:HBA1	1.88	0.54
15:O:92:SER:HB3	15:O:131:PRO:HA	1.89	0.54
9:D:148:ALA:HB2	9:D:276:VAL:HG13	1.90	0.54
3:T:2:GLU:HG2	14:M:3:VAL:HG11	1.90	0.54
6:A:214:MET:HB3	28:A:410:PL9:H103	1.90	0.54
15:O:10:ILE:C	15:O:10:ILE:CG2	2.81	0.53
9:D:236:ASN:O	9:D:239:GLN:HG2	2.08	0.53
2:K:25:LEU:O	2:K:28:ILE:HG12	2.08	0.53
4:V:42:VAL:HG23	8:C:416:SER:HB3	1.91	0.53
28:A:410:PL9:H48	9:D:39:PRO:HG3	1.88	0.53
3:T:18:PHE:HB2	20:T:102:BCR:H21C	1.90	0.53
8:C:64:ALA:O	8:C:68:THR:OG1	2.24	0.53
9:D:103:ARG:HG3	10:E:73:LYS:HG3	1.90	0.53
6:A:132:GLU:O	6:A:136:ARG:HG2	2.09	0.53
7:B:314:TYR:OH	15:O:176:GLN:NE2	2.37	0.53
26:C:503:CLA:CBD	26:C:503:CLA:O2D	2.56	0.53
33:C:514:DGD:HB81	26:C:516:CLA:H52	1.91	0.53
8:C:385:GLN:H	8:C:388:GLN:NE2	2.06	0.53
7:b:74:SER:OG	7:b:94:GLU:OE2	2.25	0.53
6:A:162:PRO:HB3	6:A:168:PHE:HA	1.91	0.53
10:E:8:ARG:HB3	10:E:13:ILE:HD11	1.91	0.52
33:C:515:DGD:HB32	26:C:516:CLA:H43	1.90	0.52
6:A:93:PHE:HZ	26:A:408:CLA:HAA1	1.74	0.52
7:B:383:PHE:CZ	15:O:167:GLY:HA2	2.45	0.52
8:C:42:LEU:HD21	26:C:511:CLA:H2A	1.90	0.52
8:C:286:ALA:HB2	26:C:504:CLA:HMD1	1.91	0.52
6:A:133:LEU:HD23	9:D:256:ILE:HG12	1.90	0.52
6:A:290:ILE:HG13	26:A:405:CLA:HED2	1.92	0.52
26:C:508:CLA:HBC3	26:C:510:CLA:H71	1.90	0.52
18:Z:14:ILE:O	18:Z:18:VAL:HG13	2.10	0.52
2:K:11:LEU:HD11	2:K:22:VAL:HG21	1.91	0.52
6:A:337:HIS:NE2	23:A:401:OEX:O3	2.38	0.51
4:V:41:HIS:HA	4:V:45:ILE:O	2.10	0.51
9:D:53:THR:HG22	11:F:40:MET:HE1	1.93	0.51
10:E:18:ARG:O	10:E:22:ILE:HG13	2.11	0.51
8:C:79:LYS:HD2	8:C:84:GLN:HG3	1.92	0.51
8:C:437:PHE:HA	26:C:508:CLA:HMC2	1.93	0.51
8:C:276:LEU:HD21	26:C:508:CLA:HAB	1.92	0.51
20:K:101:BCR:H371	12:J:18:GLY:HA3	1.92	0.50
6:A:85:SER:HA	6:A:109:GLY:HA3	1.93	0.50
9:D:320:LEU:HA	9:D:323:GLU:OE2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:201:GLY:HA3	6:A:286:THR:HB	1.94	0.49
8:C:406:SER:HA	8:C:420:VAL:HG23	1.95	0.49
2:K:21:LEU:O	2:K:25:LEU:HG	2.13	0.49
7:B:490:GLN:HA	7:B:496:TYR:HE2	1.78	0.49
33:D:413:DGD:O2G	33:D:413:DGD:O1B	2.31	0.49
6:A:60:ILE:HD12	6:A:84:PRO:HD2	1.95	0.48
26:A:406:CLA:HMD3	9:D:182:LEU:HD11	1.94	0.48
15:O:39:ARG:HA	15:O:85:LEU:H	1.78	0.48
30:D:409:LHG:HC62	13:L:15:THR:HG23	1.95	0.48
8:C:28:GLN:NE2	32:C:501:SQD:O7	2.32	0.48
33:D:413:DGD:O1B	33:D:413:DGD:C2G	2.62	0.48
7:B:284:ILE:O	7:B:288:VAL:HG23	2.14	0.48
7:B:321:LYS:HE3	7:B:321:LYS:HB3	1.59	0.48
5:Y:39:LEU:HD22	5:Y:44:GLY:HA3	1.95	0.47
6:A:202:VAL:HG11	26:A:406:CLA:C3D	2.44	0.47
8:C:334:PRO:HA	15:O:153:THR:OG1	2.15	0.47
34:E:101:HEM:CAC	11:F:27:ALA:HB1	2.45	0.47
6:A:244:GLU:CB	35:A:520:HOH:O	2.55	0.47
8:C:79:LYS:HG2	8:C:80:PRO:HD2	1.96	0.47
2:K:20:PRO:HB3	5:Y:21:GLN:HG3	1.97	0.47
9:D:78:VAL:HG11	9:D:114:ILE:HD12	1.97	0.47
33:D:413:DGD:O1B	33:D:413:DGD:HG2	2.14	0.47
6:A:260:PHE:CZ	6:A:263:ALA:HB2	2.50	0.47
26:A:405:CLA:HBB1	26:D:405:CLA:NC	2.30	0.46
9:D:161:PRO:HB3	9:D:170:ALA:HB2	1.98	0.46
9:D:126:MET:HE3	9:D:143:ALA:O	2.16	0.46
7:B:422:ARG:O	7:B:425:ILE:HG12	2.14	0.46
8:C:38:GLY:HA3	26:C:511:CLA:HMD2	1.98	0.46
27:A:407:PHO:HAB	9:D:205:LEU:HD13	1.97	0.46
30:D:412:LHG:HC91	30:L:101:LHG:HC81	1.98	0.46
6:A:317:TRP:CZ3	9:D:180:ARG:HD2	2.51	0.46
6:A:340:PRO:HG3	16:U:103:TYR:CG	2.51	0.46
15:O:118:LEU:HD13	15:O:233:VAL:HG11	1.97	0.46
7:B:493:TRP:HB3	10:E:5:THR:HG23	1.98	0.46
9:D:201:VAL:HG22	26:D:405:CLA:C1B	2.46	0.46
15:O:40:ILE:HD11	15:O:85:LEU:HD13	1.98	0.46
9:D:178:ILE:O	9:D:182:LEU:HG	2.17	0.45
26:A:405:CLA:H72	26:A:405:CLA:H111	1.77	0.45
5:Y:39:LEU:HA	5:Y:39:LEU:HD23	1.78	0.45
9:D:51:GLY:HA3	9:D:78:VAL:HG22	1.98	0.45
20:K:102:BCR:H24C	20:K:102:BCR:H371	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:211:PHE:CD1	28:A:410:PL9:H112	2.51	0.45
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.98	0.45
28:A:410:PL9:HC8	28:A:410:PL9:HC2	1.67	0.45
6:A:96:ILE:HG12	6:A:105:TRP:CE2	2.52	0.45
8:C:61:VAL:HG12	8:C:118:HIS:O	2.16	0.45
8:C:297:TYR:O	8:C:423:ARG:NH2	2.48	0.45
3:T:10:PHE:O	3:T:14:ILE:HG12	2.15	0.45
6:A:184:LEU:HD23	26:A:405:CLA:HBC1	1.98	0.45
4:V:102:PRO:HA	4:V:105:ARG:HG3	1.99	0.45
7:B:384:ARG:HD3	16:U:102:LEU:HD11	1.99	0.44
26:C:506:CLA:H2	26:C:506:CLA:H61	1.73	0.44
20:D:407:BCR:H15C	20:D:407:BCR:H351	1.77	0.44
15:O:81:ILE:HD11	15:O:102:ASP:HA	1.99	0.44
16:U:68:THR:H	16:U:71:GLN:HE21	1.65	0.44
6:A:140:ARG:NH1	30:A:414:LHG:O5	2.34	0.44
8:C:135:ARG:HG3	18:Z:27:TYR:CD1	2.53	0.44
26:C:505:CLA:H8	26:C:505:CLA:H51	1.80	0.44
6:A:187:GLN:HB2	26:A:405:CLA:HAC2	1.99	0.44
6:A:183:MET:HA	26:A:405:CLA:HMD1	2.00	0.44
8:C:410:VAL:HG23	8:C:412:THR:H	1.83	0.44
6:A:63:ILE:HB	8:C:335:THR:HG21	1.99	0.44
26:C:506:CLA:HAA1	26:C:506:CLA:HBD	2.00	0.44
9:D:190:ASN:HB2	9:D:296:TYR:CD2	2.53	0.44
20:K:102:BCR:H15C	20:K:102:BCR:H351	1.80	0.43
16:U:45:LEU:HD21	16:U:71:GLN:HB3	2.00	0.43
4:V:46:THR:HB	4:V:49:ASN:O	2.19	0.43
6:A:45:THR:HG23	26:A:412:CLA:H201	1.99	0.43
7:B:311:PHE:O	7:B:317:ASN:ND2	2.49	0.43
7:B:330:MET:HE3	7:B:446:SER:N	2.33	0.43
26:C:511:CLA:H18	18:Z:20:VAL:HG12	2.00	0.43
8:C:60:ILE:HG22	26:C:505:CLA:HHD	2.01	0.43
9:D:320:LEU:HD23	9:D:323:GLU:OE2	2.18	0.43
1:I:1:MET:HB3	6:A:97:TRP:HA	2.00	0.43
6:A:30:VAL:O	6:A:34:GLY:HA3	2.18	0.43
26:C:504:CLA:HBB2	26:C:510:CLA:C15	2.48	0.43
6:A:14:TRP:CG	6:A:14:TRP:C	2.97	0.43
20:K:101:BCR:H15C	20:K:101:BCR:H351	1.85	0.42
7:B:460:LEU:HD22	9:D:287:VAL:HG21	2.01	0.42
8:C:317:PHE:HE2	8:C:396:MET:HE1	1.85	0.42
9:D:191:TRP:CZ2	9:D:197:HIS:HB2	2.53	0.42
12:J:15:THR:O	12:J:19:MET:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:104:BCR:HC42	8:C:116:VAL:HG11	2.01	0.42
16:U:32:ILE:HG13	16:U:46:ALA:HB1	2.00	0.42
6:A:214:MET:HE2	6:A:255:PHE:CE1	2.54	0.42
6:A:116:ILE:HG13	6:A:117:PHE:N	2.34	0.42
26:C:504:CLA:HBA2	26:C:505:CLA:H171	2.00	0.42
15:O:110[B]:MET:HE2	15:O:116:ILE:HD11	2.01	0.42
15:O:146:PHE:HE2	15:O:197:ILE:HB	1.84	0.42
16:U:68:THR:H	16:U:71:GLN:NE2	2.17	0.42
16:U:42:TYR:HA	16:U:43:PRO:HA	1.69	0.42
26:C:505:CLA:H112	26:C:505:CLA:H72	1.87	0.42
26:C:509:CLA:C2	26:C:509:CLA:H72	2.50	0.42
6:A:102:LEU:HD23	6:A:102:LEU:HA	1.89	0.42
26:A:412:CLA:HED1	28:D:408:PL9:H362	2.01	0.42
9:D:129:GLN:NE2	27:D:401:PHO:OBD	2.53	0.42
9:D:342:PRO:O	9:D:345:VAL:HG22	2.18	0.42
7:B:298:LEU:HD23	7:B:298:LEU:HA	1.84	0.41
15:O:127:ALA:HA	15:O:144:GLY:HA3	2.02	0.41
6:A:82:VAL:HB	6:A:174:LEU:HB2	2.01	0.41
8:C:363:GLY:O	8:C:367:GLU:HG2	2.19	0.41
9:D:202:ALA:HB2	28:D:408:PL9:H353	2.01	0.41
16:U:79:LEU:HD12	16:U:79:LEU:HA	1.90	0.41
6:A:269:ARG:HH11	9:D:231:THR:HB	1.84	0.41
6:A:247:ASN:HD21	6:A:249:VAL:HB	1.86	0.41
9:D:160:TYR:HA	9:D:290:ALA:HB2	2.03	0.41
9:D:161:PRO:HG3	9:D:170:ALA:HB2	2.02	0.41
6:A:287:ALA:HA	26:A:405:CLA:HED3	2.02	0.41
7:B:273:TYR:HA	7:B:276:ASP:HB2	2.02	0.41
7:B:326:ARG:NH2	9:D:297:ASP:OD2	2.47	0.41
8:C:339:LYS:HD2	8:C:340:TYR:CZ	2.55	0.41
6:A:140:ARG:HB2	9:D:220:ASN:HA	2.01	0.41
6:A:217:SER:HA	9:D:272:LEU:HD12	2.03	0.41
10:E:23:HIS:HB3	10:E:27:ILE:CD1	2.46	0.41
3:T:28:ARG:O	6:A:239:PHE:HB3	2.21	0.41
7:B:450:TRP:NE1	26:B:601:CLA:HBA1	2.36	0.41
8:C:57:ALA:O	8:C:61:VAL:HG23	2.21	0.41
9:D:125:PHE:CE2	27:D:401:PHO:HBD	2.56	0.41
4:V:73:VAL:HG22	4:V:112:LEU:HB3	2.03	0.41
6:A:89:ILE:HD11	6:A:108:ASN:HB3	2.03	0.41
7:B:399:VAL:HG12	7:B:417:VAL:HG22	2.02	0.41
8:C:402:GLY:HA3	8:C:420:VAL:HG22	2.03	0.41
6:A:260:PHE:CE2	6:A:263:ALA:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:475:PHE:CD1	9:D:140:PRO:HG3	2.56	0.40
8:C:332:GLN:HE21	8:C:336:GLY:HA2	1.87	0.40
10:E:8:ARG:O	11:F:19:ARG:NH2	2.39	0.40
6:A:172:MET:HE1	26:A:412:CLA:CHC	2.51	0.40
28:A:410:PL9:H353	11:F:26:LEU:HG	2.03	0.40
7:B:383:PHE:N	9:D:344:GLU:O	2.52	0.40
8:C:218:PHE:CE2	31:C:502:LMG:H111	2.53	0.40
26:C:504:CLA:HBB2	26:C:510:CLA:H151	2.02	0.40
6:A:247:ASN:HD22	6:A:247:ASN:C	2.29	0.40
8:C:425:TRP:HE3	33:C:514:DGD:HBT1	1.85	0.40
26:C:507:CLA:O1A	26:C:509:CLA:H61	2.22	0.40
26:C:510:CLA:H143	26:C:510:CLA:H111	1.92	0.40
2:K:12:PRO:HB2	2:K:15:TYR:HD1	1.86	0.40
26:C:516:CLA:H41	26:C:516:CLA:H62	1.61	0.40
20:D:407:BCR:H11C	20:D:407:BCR:H341	1.86	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	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
2	K	35/46 (76%)	35 (100%)	0	0	100	100
3	T	27/32 (84%)	27 (100%)	0	0	100	100
4	V	128/163 (78%)	126 (98%)	2 (2%)	0	100	100
5	Y	27/46 (59%)	27 (100%)	0	0	100	100
6	A	319/360 (89%)	315 (99%)	4 (1%)	0	100	100
7	B	180/510 (35%)	177 (98%)	3 (2%)	0	100	100
7	b	28/510 (6%)	27 (96%)	0	1 (4%)	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	C	328/461 (71%)	321 (98%)	7 (2%)	0	100	100
9	D	329/352 (94%)	323 (98%)	6 (2%)	0	100	100
10	E	50/84 (60%)	49 (98%)	1 (2%)	0	100	100
11	F	29/45 (64%)	29 (100%)	0	0	100	100
12	J	27/40 (68%)	27 (100%)	0	0	100	100
13	L	24/37 (65%)	24 (100%)	0	0	100	100
14	M	12/36 (33%)	12 (100%)	0	0	100	100
15	O	168/272 (62%)	163 (97%)	5 (3%)	0	100	100
16	U	89/134 (66%)	88 (99%)	1 (1%)	0	100	100
17	X	12/41 (29%)	12 (100%)	0	0	100	100
18	Z	36/62 (58%)	36 (100%)	0	0	100	100
All	All	1882/3269 (58%)	1851 (98%)	30 (2%)	1 (0%)	49	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	b	86	ILE

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	I	25/35 (71%)	25 (100%)	0	100	100
2	K	25/37 (68%)	24 (96%)	1 (4%)	28	28
3	T	22/29 (76%)	22 (100%)	0	100	100
4	V	88/138 (64%)	87 (99%)	1 (1%)	65	73
5	Y	11/37 (30%)	11 (100%)	0	100	100
6	A	253/291 (87%)	253 (100%)	0	100	100
7	B	131/407 (32%)	128 (98%)	3 (2%)	44	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	b	18/407 (4%)	18 (100%)	0	100	100
8	C	228/362 (63%)	224 (98%)	4 (2%)	51	58
9	D	259/283 (92%)	258 (100%)	1 (0%)	84	89
10	E	45/73 (62%)	44 (98%)	1 (2%)	45	51
11	F	26/39 (67%)	25 (96%)	1 (4%)	29	30
12	J	22/28 (79%)	22 (100%)	0	100	100
13	L	24/35 (69%)	24 (100%)	0	100	100
14	M	9/33 (27%)	9 (100%)	0	100	100
15	O	118/228 (52%)	118 (100%)	0	100	100
16	U	62/112 (55%)	59 (95%)	3 (5%)	23	22
17	X	6/34 (18%)	6 (100%)	0	100	100
18	Z	16/52 (31%)	16 (100%)	0	100	100
All	All	1388/2660 (52%)	1373 (99%)	15 (1%)	63	73

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	46	ARG
4	V	42	VAL
7	B	362	PHE
7	B	388	SER
7	B	391	SER
8	C	25	ASN
8	C	135	ARG
8	C	346	THR
8	C	416	SER
9	D	323	GLU
10	E	32	ILE
11	F	23	VAL
16	U	9	LEU
16	U	79	LEU
16	U	83	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
4	V	68	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	A	25	ASN
6	A	165	GLN
6	A	234	ASN
6	A	247	ASN
6	A	261	GLN
6	A	304	HIS
6	A	338	ASN
7	B	282	GLN
7	B	289	GLN
7	B	343	HIS
8	C	25	ASN
8	C	28	GLN
8	C	74	HIS
8	C	311	GLN
8	C	327	ASN
8	C	378	ASN
8	C	388	GLN
9	D	239	GLN
10	E	82	GLN
15	O	17	ASN
15	O	46	GLN
15	O	80	GLN
15	O	147	ASN
15	O	228	HIS
15	O	231	HIS
15	O	236	GLN
16	U	29	ASN
16	U	71	GLN

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 64 ligands modelled in this entry, 6 are unknown, 2 are modelled with single atom and 3 are monoatomic - leaving 53 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
26	CLA	D	406	9	48,52,73	2.39	19 (39%)	56,87,113	3.28	27 (48%)
26	CLA	D	405	9	69,73,73	2.01	20 (28%)	83,113,113	2.82	29 (34%)
26	CLA	A	408	6	55,59,73	2.31	20 (36%)	66,96,113	3.16	31 (46%)
26	CLA	C	510	8	69,73,73	2.07	20 (28%)	83,113,113	2.78	30 (36%)
26	CLA	B	602	-	1,1,73	0.01	0	-		
23	OEX	A	401	35,6,8	0,14,14	-	-	-		
21	LMT	J	101	-	24,24,36	0.15	0	29,29,47	0.32	0
26	CLA	C	506	8	59,63,73	2.22	20 (33%)	71,101,113	3.00	30 (42%)
26	CLA	B	601	-	24,24,73	0.95	1 (4%)	28,28,113	1.26	3 (10%)
20	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.88	16 (28%)
33	DGD	C	515	-	54,54,67	0.91	2 (3%)	68,68,81	1.06	4 (5%)
32	SQD	C	501	-	31,32,54	1.28	3 (9%)	40,43,65	1.42	6 (15%)
30	LHG	A	415	-	30,30,48	1.00	2 (6%)	33,35,54	1.10	1 (3%)
26	CLA	C	512	-	0,1,73	-	-	-		
20	BCR	K	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.76	15 (26%)
20	BCR	D	407	-	41,41,41	1.07	1 (2%)	56,56,56	1.99	10 (17%)
26	CLA	C	503	-	25,28,73	1.04	1 (4%)	28,35,113	2.18	4 (14%)
28	PL9	D	408	-	55,55,55	0.59	1 (1%)	68,69,69	1.76	20 (29%)
30	LHG	L	101	-	38,38,48	1.04	2 (5%)	41,44,54	1.13	3 (7%)
30	LHG	A	414	-	38,38,48	1.05	2 (5%)	41,44,54	1.12	3 (7%)
26	CLA	C	505	8	53,59,73	2.07	12 (22%)	60,86,113	3.18	19 (31%)
30	LHG	D	412	-	41,41,48	1.01	2 (4%)	44,47,54	1.08	3 (6%)
31	LMG	D	410	-	38,38,55	1.06	2 (5%)	46,46,63	1.12	4 (8%)
34	HEM	E	101	11,10	50,50,50	1.54	7 (14%)	66,82,82	1.71	12 (18%)
27	PHO	A	407	-	58,69,69	2.75	15 (25%)	56,99,99	2.82	17 (30%)
27	PHO	D	401	-	58,69,69	2.78	15 (25%)	56,99,99	2.80	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	516	35	69,73,73	2.07	21 (30%)	83,113,113	2.83	30 (36%)
20	BCR	I	102	-	19,19,41	0.58	0	26,26,56	1.65	8 (30%)
33	DGD	C	513	-	53,53,67	0.92	2 (3%)	67,67,81	1.05	3 (4%)
22	HEC	V	201	4	50,50,50	1.75	6 (12%)	68,82,82	1.41	6 (8%)
30	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	1.04	3 (5%)
29	BCT	A	413[A]	24	2,3,3	0.70	0	2,3,3	0.64	0
26	CLA	A	412	35	69,73,73	2.07	20 (28%)	83,113,113	2.80	28 (33%)
26	CLA	C	507	35	17,23,73	2.23	6 (35%)	18,34,113	2.91	5 (27%)
26	CLA	C	508	8	64,68,73	2.14	20 (31%)	77,107,113	2.92	28 (36%)
26	CLA	D	403	-	7,7,73	0.28	0	6,6,113	1.59	2 (33%)
26	CLA	C	509	8	63,67,73	2.18	20 (31%)	75,105,113	2.88	28 (37%)
20	BCR	T	102	-	16,16,41	1.42	1 (6%)	22,22,56	2.22	7 (31%)
20	BCR	K	104	-	3,3,41	0.21	0	2,2,56	0.65	0
31	LMG	C	502	-	47,47,55	0.97	2 (4%)	55,55,63	1.16	4 (7%)
28	PL9	A	410	-	55,55,55	0.61	1 (1%)	68,69,69	1.82	20 (29%)
33	DGD	D	413	-	53,53,67	0.68	1 (1%)	64,64,81	0.77	1 (1%)
21	LMT	T	103	-	12,12,36	0.17	0	11,11,47	0.58	0
26	CLA	C	511	8	69,73,73	2.06	20 (28%)	83,113,113	2.81	29 (34%)
33	DGD	C	514	-	51,51,67	0.95	2 (3%)	65,65,81	1.14	5 (7%)
26	CLA	A	406	35	60,64,73	2.23	21 (35%)	72,102,113	3.00	29 (40%)
31	LMG	B	603	-	29,29,55	1.52	3 (10%)	33,34,63	1.22	2 (6%)
26	CLA	A	405	6	69,73,73	2.03	19 (27%)	83,113,113	2.82	32 (38%)
26	CLA	C	504	8	54,58,73	2.32	20 (37%)	65,95,113	3.11	27 (41%)
32	SQD	F	101	-	22,23,54	1.03	2 (9%)	30,33,65	1.07	3 (10%)
26	CLA	D	402	-	3,3,73	0.03	0	3,3,113	0.08	0
20	BCR	A	409	-	41,41,41	1.07	1 (2%)	56,56,56	1.72	13 (23%)

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
26	CLA	D	406	9	-	0/13/90/115	-
26	CLA	D	405	9	-	4/39/115/115	-
26	CLA	A	408	6	-	5/23/99/115	-
26	CLA	C	510	8	-	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMT	J	101	-	-	0/15/35/61	0/1/1/2
26	CLA	C	506	8	-	10/27/103/115	-
26	CLA	B	601	-	-	4/26/26/115	-
20	BCR	K	102	-	-	0/29/63/63	0/2/2/2
33	DGD	C	515	-	-	2/42/82/95	0/2/2/2
32	SQD	C	501	-	-	7/27/47/69	0/1/1/1
30	LHG	A	415	-	-	8/33/33/53	-
20	BCR	K	101	-	-	7/29/63/63	0/2/2/2
20	BCR	D	407	-	-	8/29/63/63	0/2/2/2
26	CLA	C	503	-	-	6/24/40/115	0/1/1/9
28	PL9	D	408	-	-	10/53/73/73	0/1/1/1
30	LHG	L	101	-	-	11/43/43/53	-
30	LHG	A	414	-	-	13/43/43/53	-
26	CLA	C	505	8	-	5/37/89/115	0/6/6/9
30	LHG	D	412	-	-	23/46/46/53	-
31	LMG	D	410	-	-	3/33/53/70	0/1/1/1
34	HEM	E	101	11,10	-	9/14/54/54	-
27	PHO	A	407	-	-	6/37/103/103	0/5/6/6
27	PHO	D	401	-	-	0/37/103/103	0/5/6/6
26	CLA	C	516	35	-	13/39/115/115	-
20	BCR	I	102	-	-	2/11/28/63	0/1/1/2
33	DGD	C	513	-	-	9/41/81/95	0/2/2/2
22	HEC	V	201	4	1/1/3/7	4/14/54/54	-
30	LHG	D	409	-	-	9/53/53/53	-
26	CLA	A	412	35	-	7/39/115/115	-
26	CLA	C	507	35	-	1/7/31/115	0/3/3/9
26	CLA	C	508	8	-	8/33/109/115	-
26	CLA	D	403	-	-	2/2/1/115	-
26	CLA	C	509	8	-	8/31/107/115	-
20	BCR	T	102	-	-	2/8/25/63	0/1/1/2
20	BCR	K	104	-	-	1/1/1/63	-
31	LMG	C	502	-	-	6/42/62/70	0/1/1/1
28	PL9	A	410	-	-	11/53/73/73	0/1/1/1
33	DGD	D	413	-	-	3/38/74/95	0/2/2/2
21	LMT	T	103	-	-	0/10/10/61	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	511	8	-	5/39/115/115	-
33	DGD	C	514	-	-	7/39/79/95	0/2/2/2
26	CLA	A	406	35	-	5/29/105/115	-
31	LMG	B	603	-	-	1/21/38/70	0/1/1/1
26	CLA	A	405	6	-	6/39/115/115	-
26	CLA	C	504	8	-	3/21/97/115	-
32	SQD	F	101	-	-	3/15/35/69	0/1/1/1
20	BCR	A	409	-	-	2/29/63/63	0/2/2/2

All (359) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	401	PHO	C1D-C2D	8.91	1.49	1.39
27	A	407	PHO	C1D-C2D	8.81	1.49	1.39
27	A	407	PHO	C1B-C2B	8.74	1.49	1.39
27	D	401	PHO	C1B-C2B	8.66	1.49	1.39
22	V	201	HEC	C3D-C2D	7.98	1.53	1.36
26	C	505	CLA	C2C-C3C	7.09	1.48	1.33
27	D	401	PHO	C3B-C4B	6.90	1.49	1.41
27	A	407	PHO	C3B-C4B	6.62	1.49	1.41
27	D	401	PHO	C3B-C2B	6.47	1.49	1.40
27	A	407	PHO	C3B-C2B	6.29	1.49	1.40
27	A	407	PHO	C4D-CHA	6.23	1.49	1.39
27	D	401	PHO	C4D-CHA	6.12	1.49	1.39
27	D	401	PHO	C3C-C2C	5.73	1.48	1.36
27	A	407	PHO	C3C-C2C	5.71	1.48	1.36
31	B	603	LMG	O7-C10	5.65	1.45	1.33
20	K	102	BCR	C23-C22	-5.45	1.34	1.45
26	A	406	CLA	C3C-C2C	5.44	1.48	1.36
26	A	412	CLA	C3C-C2C	5.43	1.48	1.36
20	K	101	BCR	C23-C22	-5.41	1.34	1.45
26	A	408	CLA	C3C-C2C	5.40	1.48	1.36
26	C	511	CLA	C3C-C2C	5.39	1.48	1.36
26	C	509	CLA	C3C-C2C	5.37	1.48	1.36
26	C	516	CLA	C3C-C2C	5.35	1.48	1.36
26	C	510	CLA	C3C-C2C	5.33	1.48	1.36
26	D	406	CLA	C3C-C2C	5.32	1.48	1.36
20	A	409	BCR	C23-C22	-5.32	1.34	1.45
26	C	508	CLA	C3C-C2C	5.31	1.48	1.36
20	D	407	BCR	C23-C22	-5.28	1.34	1.45
26	C	504	CLA	C3C-C2C	5.28	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	102	BCR	C23-C22	-5.28	1.34	1.45
26	C	506	CLA	C3C-C2C	5.28	1.47	1.36
26	A	405	CLA	C3C-C2C	5.24	1.47	1.36
26	D	405	CLA	C3C-C2C	5.23	1.47	1.36
26	A	412	CLA	C1D-ND	5.22	1.44	1.37
27	A	407	PHO	C3D-C2D	5.21	1.48	1.39
26	D	406	CLA	C1D-ND	5.21	1.44	1.37
34	E	101	HEM	FE-NB	5.18	2.10	1.94
26	C	504	CLA	O2D-CGD	5.17	1.45	1.33
26	C	509	CLA	O2D-CGD	5.16	1.45	1.33
26	A	406	CLA	C1D-ND	5.15	1.44	1.37
26	C	511	CLA	C1D-ND	5.15	1.44	1.37
26	A	412	CLA	O2D-CGD	5.14	1.45	1.33
26	A	406	CLA	O2D-CGD	5.13	1.45	1.33
26	C	510	CLA	O2D-CGD	5.12	1.45	1.33
26	C	508	CLA	O2D-CGD	5.12	1.45	1.33
26	C	511	CLA	O2D-CGD	5.12	1.45	1.33
27	D	401	PHO	C3D-C2D	5.12	1.48	1.39
26	C	506	CLA	O2D-CGD	5.11	1.45	1.33
26	A	408	CLA	O2D-CGD	5.11	1.45	1.33
27	D	401	PHO	O2D-CGD	5.09	1.45	1.33
26	C	516	CLA	O2D-CGD	5.09	1.45	1.33
26	C	516	CLA	C1D-ND	5.09	1.44	1.37
26	C	510	CLA	C1D-ND	5.07	1.44	1.37
26	C	509	CLA	C1D-ND	5.06	1.44	1.37
27	A	407	PHO	O2D-CGD	5.06	1.45	1.33
26	D	406	CLA	O2D-CGD	5.06	1.45	1.33
26	A	405	CLA	O2D-CGD	5.05	1.45	1.33
26	A	408	CLA	C1D-ND	5.04	1.44	1.37
26	C	508	CLA	C1D-ND	5.04	1.44	1.37
26	D	405	CLA	O2D-CGD	5.03	1.45	1.33
26	C	504	CLA	C1D-ND	5.01	1.43	1.37
26	C	506	CLA	C1D-ND	5.00	1.43	1.37
26	A	405	CLA	C1D-ND	4.99	1.43	1.37
26	C	507	CLA	C4B-C3B	4.98	1.49	1.37
26	C	505	CLA	O2D-CGD	4.90	1.45	1.33
26	A	406	CLA	CHC-C1C	4.81	1.48	1.38
26	C	509	CLA	CHC-C1C	4.75	1.48	1.38
26	A	408	CLA	CHC-C1C	4.75	1.48	1.38
26	C	510	CLA	CHC-C1C	4.75	1.48	1.38
26	D	405	CLA	C1D-ND	4.72	1.43	1.37
26	C	511	CLA	CHC-C1C	4.70	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	505	CLA	C1D-ND	4.69	1.44	1.37
26	C	508	CLA	CHC-C1C	4.64	1.47	1.38
26	A	405	CLA	CHC-C1C	4.63	1.47	1.38
26	D	405	CLA	CHC-C1C	4.62	1.47	1.38
26	C	516	CLA	CHC-C1C	4.62	1.47	1.38
26	C	506	CLA	CHC-C1C	4.58	1.47	1.38
26	C	504	CLA	CHC-C1C	4.57	1.47	1.38
26	D	406	CLA	CHC-C1C	4.56	1.47	1.38
27	D	401	PHO	OBD-CAD	4.50	1.28	1.22
26	A	412	CLA	CHC-C1C	4.48	1.47	1.38
26	A	406	CLA	CHD-C1D	4.45	1.47	1.38
26	C	509	CLA	CHD-C1D	4.45	1.47	1.38
26	C	510	CLA	CHD-C1D	4.45	1.47	1.38
26	C	509	CLA	O2A-CGA	4.45	1.46	1.33
26	D	406	CLA	CHD-C1D	4.44	1.47	1.38
26	C	516	CLA	CHD-C1D	4.41	1.47	1.38
26	A	412	CLA	CHD-C1D	4.41	1.47	1.38
26	A	405	CLA	CHD-C1D	4.40	1.46	1.38
26	C	508	CLA	CHD-C1D	4.37	1.46	1.38
26	A	412	CLA	O2A-CGA	4.36	1.46	1.33
26	A	408	CLA	CHD-C1D	4.35	1.46	1.38
27	A	407	PHO	OBD-CAD	4.35	1.28	1.22
26	A	408	CLA	O2A-CGA	4.32	1.46	1.33
26	B	601	CLA	O2A-CGA	4.32	1.46	1.33
26	C	506	CLA	CHD-C1D	4.31	1.46	1.38
26	C	511	CLA	CHD-C1D	4.31	1.46	1.38
26	C	503	CLA	O2A-CGA	4.31	1.45	1.33
26	C	504	CLA	CHD-C1D	4.31	1.46	1.38
26	A	406	CLA	O2A-CGA	4.28	1.45	1.33
26	C	508	CLA	O2A-CGA	4.28	1.45	1.33
26	C	516	CLA	O2A-CGA	4.27	1.45	1.33
26	C	505	CLA	CHD-C1D	4.26	1.46	1.38
31	C	502	LMG	O8-C28	4.26	1.45	1.33
26	C	504	CLA	O2A-CGA	4.26	1.45	1.33
26	C	505	CLA	O2A-CGA	4.25	1.45	1.33
31	B	603	LMG	O8-C28	4.24	1.45	1.33
30	D	412	LHG	O8-C23	4.23	1.45	1.33
26	C	506	CLA	O2A-CGA	4.22	1.45	1.33
30	A	414	LHG	O8-C23	4.22	1.45	1.33
26	C	510	CLA	O2A-CGA	4.21	1.45	1.33
31	D	410	LMG	O8-C28	4.21	1.45	1.33
22	V	201	HEC	FE-ND	4.19	2.07	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	101	LHG	O8-C23	4.18	1.45	1.33
26	A	405	CLA	O2A-CGA	4.18	1.45	1.33
33	C	514	DGD	O1G-C1A	4.17	1.45	1.33
26	D	405	CLA	O2A-CGA	4.17	1.45	1.33
32	C	501	SQD	O48-C23	4.16	1.45	1.33
26	A	406	CLA	CHD-C4C	4.15	1.48	1.39
31	C	502	LMG	O7-C10	4.15	1.46	1.34
33	C	515	DGD	O1G-C1A	4.15	1.45	1.33
33	D	413	DGD	O1G-C1A	4.14	1.45	1.33
27	D	401	PHO	O2A-CGA	4.14	1.45	1.33
30	A	414	LHG	O7-C7	4.14	1.46	1.34
26	C	511	CLA	O2A-CGA	4.12	1.45	1.33
26	C	510	CLA	CHD-C4C	4.12	1.48	1.39
27	A	407	PHO	O2A-CGA	4.11	1.45	1.33
26	A	408	CLA	CHD-C4C	4.11	1.48	1.39
30	A	415	LHG	O7-C7	4.11	1.45	1.34
30	D	409	LHG	O8-C23	4.10	1.45	1.33
33	C	513	DGD	O1G-C1A	4.10	1.45	1.33
26	D	406	CLA	CHD-C4C	4.10	1.48	1.39
30	L	101	LHG	O7-C7	4.09	1.45	1.34
26	D	405	CLA	CHD-C1D	4.08	1.46	1.38
31	D	410	LMG	O7-C10	4.08	1.45	1.34
26	C	516	CLA	CHD-C4C	4.08	1.48	1.39
33	C	515	DGD	O2G-C1B	4.08	1.45	1.34
33	C	513	DGD	O2G-C1B	4.05	1.45	1.34
26	C	508	CLA	CHD-C4C	4.05	1.48	1.39
33	C	514	DGD	O2G-C1B	4.04	1.45	1.34
26	C	507	CLA	O2A-CGA	4.04	1.45	1.33
26	C	509	CLA	CHD-C4C	4.04	1.48	1.39
26	A	412	CLA	CHD-C4C	4.03	1.48	1.39
26	C	505	CLA	CHD-C4C	4.03	1.48	1.39
26	C	506	CLA	CHD-C4C	4.02	1.48	1.39
26	A	405	CLA	CHD-C4C	4.02	1.48	1.39
26	C	511	CLA	CHD-C4C	4.00	1.48	1.39
34	E	101	HEM	FE-NC	4.00	2.08	1.95
26	C	504	CLA	CHD-C4C	4.00	1.48	1.39
30	D	412	LHG	O7-C7	3.99	1.45	1.34
30	D	409	LHG	O7-C7	3.98	1.45	1.34
32	C	501	SQD	O47-C7	3.98	1.45	1.34
26	D	405	CLA	CHD-C4C	3.95	1.48	1.39
26	C	508	CLA	C3D-C2D	3.84	1.49	1.39
26	C	516	CLA	C3D-C2D	3.83	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	504	CLA	C3D-C2D	3.82	1.49	1.39
26	A	412	CLA	C3D-C2D	3.79	1.49	1.39
26	D	406	CLA	C3D-C2D	3.79	1.49	1.39
26	A	408	CLA	C3D-C2D	3.77	1.49	1.39
26	C	505	CLA	C3D-C2D	3.77	1.49	1.39
26	C	509	CLA	C3D-C2D	3.75	1.49	1.39
26	A	406	CLA	C3D-C2D	3.72	1.49	1.39
26	C	511	CLA	C3D-C2D	3.72	1.49	1.39
26	A	406	CLA	CHC-C4B	3.70	1.47	1.39
26	C	506	CLA	OBD-CAD	3.69	1.28	1.22
26	C	505	CLA	OBD-CAD	3.69	1.28	1.22
26	A	408	CLA	CHC-C4B	3.69	1.47	1.39
26	C	510	CLA	C3D-C2D	3.69	1.49	1.39
26	C	516	CLA	CHC-C4B	3.67	1.47	1.39
26	C	516	CLA	OBD-CAD	3.67	1.28	1.22
26	C	511	CLA	CHC-C4B	3.66	1.47	1.39
26	C	509	CLA	OBD-CAD	3.65	1.28	1.22
26	A	408	CLA	OBD-CAD	3.65	1.28	1.22
26	C	504	CLA	OBD-CAD	3.64	1.28	1.22
26	C	506	CLA	CHC-C4B	3.63	1.47	1.39
34	E	101	HEM	C4D-ND	-3.63	1.34	1.40
26	C	508	CLA	OBD-CAD	3.62	1.28	1.22
26	C	510	CLA	CHC-C4B	3.62	1.47	1.39
26	A	405	CLA	CHC-C4B	3.62	1.47	1.39
26	A	412	CLA	CHC-C4B	3.62	1.47	1.39
26	C	509	CLA	CHC-C4B	3.61	1.47	1.39
26	C	508	CLA	CHC-C4B	3.61	1.47	1.39
26	D	406	CLA	CHC-C4B	3.61	1.47	1.39
26	C	510	CLA	OBD-CAD	3.61	1.28	1.22
26	A	406	CLA	OBD-CAD	3.60	1.28	1.22
26	D	405	CLA	CHC-C4B	3.60	1.47	1.39
26	A	405	CLA	OBD-CAD	3.59	1.28	1.22
26	C	511	CLA	CHB-C1B	3.58	1.47	1.39
26	C	504	CLA	CHB-C1B	3.57	1.47	1.39
26	D	405	CLA	C3D-C2D	3.57	1.48	1.39
26	C	504	CLA	CHC-C4B	3.57	1.47	1.39
26	A	405	CLA	C3D-C2D	3.56	1.48	1.39
26	C	511	CLA	OBD-CAD	3.56	1.28	1.22
26	C	509	CLA	CHB-C1B	3.56	1.47	1.39
26	D	406	CLA	OBD-CAD	3.55	1.28	1.22
26	D	405	CLA	OBD-CAD	3.54	1.28	1.22
26	C	505	CLA	C4C-C3C	3.54	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	412	CLA	OBD-CAD	3.52	1.28	1.22
26	C	510	CLA	CHB-C1B	3.51	1.47	1.39
26	A	412	CLA	C1B-NB	-3.51	1.33	1.37
26	C	516	CLA	CHB-C1B	3.50	1.47	1.39
26	A	405	CLA	C1B-NB	-3.49	1.33	1.37
26	C	509	CLA	C1B-NB	-3.49	1.33	1.37
26	D	405	CLA	CHB-C1B	3.48	1.47	1.39
26	C	506	CLA	C1B-NB	-3.48	1.33	1.37
26	C	507	CLA	C2A-C3A	-3.48	1.52	1.57
26	A	412	CLA	CHB-C1B	3.47	1.47	1.39
26	C	510	CLA	C1B-NB	-3.47	1.33	1.37
26	C	506	CLA	CHB-C1B	3.47	1.47	1.39
26	D	406	CLA	CHB-C1B	3.46	1.47	1.39
22	V	201	HEC	FE-NB	3.45	2.05	1.94
26	A	406	CLA	CHB-C1B	3.43	1.47	1.39
26	C	508	CLA	CHB-C1B	3.43	1.47	1.39
26	C	506	CLA	C3D-C2D	3.42	1.48	1.39
26	A	408	CLA	CHB-C1B	3.40	1.47	1.39
26	C	504	CLA	C1B-NB	-3.39	1.33	1.37
34	E	101	HEM	C1B-NB	-3.39	1.34	1.40
26	C	508	CLA	C1B-NB	-3.36	1.33	1.37
26	C	507	CLA	CHB-C1B	3.34	1.46	1.39
26	D	405	CLA	C1B-NB	-3.34	1.33	1.37
26	A	408	CLA	C1B-NB	-3.34	1.33	1.37
26	C	516	CLA	C1B-NB	-3.32	1.33	1.37
26	A	406	CLA	C1B-NB	-3.32	1.33	1.37
26	C	509	CLA	C4B-NB	-3.28	1.33	1.37
31	B	603	LMG	O7-C8	-3.27	1.42	1.46
26	D	406	CLA	C1B-NB	-3.24	1.33	1.37
26	A	405	CLA	CHB-C1B	3.23	1.46	1.39
26	C	508	CLA	C4B-NB	-3.22	1.33	1.37
26	C	510	CLA	C4B-NB	-3.19	1.33	1.37
26	A	406	CLA	C4B-NB	-3.17	1.33	1.37
26	C	511	CLA	C1B-NB	-3.16	1.33	1.37
26	C	504	CLA	C4B-NB	-3.15	1.33	1.37
26	A	412	CLA	C3B-C4B	3.13	1.50	1.42
26	A	408	CLA	C4B-NB	-3.09	1.34	1.37
26	C	516	CLA	C4B-NB	-3.08	1.34	1.37
26	C	511	CLA	C4B-NB	-3.08	1.34	1.37
26	C	506	CLA	C4B-NB	-3.08	1.34	1.37
26	D	406	CLA	C4B-NB	-3.04	1.34	1.37
26	D	405	CLA	C4B-NB	-3.04	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	201	HEC	FE-NA	3.02	2.05	1.95
26	A	412	CLA	C4B-NB	-3.01	1.34	1.37
26	C	505	CLA	C2A-C3A	-2.97	1.52	1.55
26	D	406	CLA	C3B-C4B	2.95	1.49	1.42
26	C	516	CLA	C3B-C4B	2.94	1.49	1.42
26	A	405	CLA	C3B-C4B	2.94	1.49	1.42
26	C	507	CLA	C1B-NB	-2.93	1.33	1.37
32	F	101	SQD	C6-S	-2.92	1.66	1.77
26	C	506	CLA	C3B-C4B	2.92	1.49	1.42
26	A	405	CLA	C4B-NB	-2.89	1.34	1.37
26	A	406	CLA	C3B-C4B	2.88	1.49	1.42
26	A	408	CLA	C3B-C4B	2.83	1.49	1.42
26	C	508	CLA	C3B-C4B	2.83	1.49	1.42
32	C	501	SQD	C6-S	-2.82	1.67	1.77
26	C	511	CLA	C3B-C4B	2.79	1.49	1.42
26	C	504	CLA	C3B-C4B	2.73	1.49	1.42
22	V	201	HEC	FE-NC	2.72	2.04	1.95
26	C	510	CLA	C3B-C4B	2.66	1.49	1.42
26	C	509	CLA	C3B-C4B	2.65	1.49	1.42
26	D	405	CLA	C3B-C4B	2.64	1.48	1.42
28	A	410	PL9	C6-C5	2.60	1.48	1.35
26	C	511	CLA	C4D-CHA	2.56	1.47	1.38
28	D	408	PL9	C6-C5	2.55	1.48	1.35
26	C	505	CLA	C4D-CHA	2.54	1.47	1.38
26	C	504	CLA	C4D-CHA	2.54	1.47	1.38
26	D	405	CLA	C1B-C2B	2.54	1.49	1.43
26	C	509	CLA	C4D-CHA	2.54	1.47	1.38
32	F	101	SQD	O48-C23	2.54	1.45	1.33
26	D	406	CLA	C4D-CHA	2.53	1.47	1.38
26	C	511	CLA	C1B-C2B	2.53	1.49	1.43
26	C	516	CLA	C4D-CHA	2.53	1.47	1.38
26	C	504	CLA	C1B-C2B	2.53	1.49	1.43
27	D	401	PHO	CHA-CBD	-2.52	1.48	1.51
30	A	415	LHG	O8-C23	2.52	1.45	1.33
26	C	506	CLA	C1B-C2B	2.52	1.49	1.43
26	C	508	CLA	C4D-CHA	2.51	1.47	1.38
26	C	510	CLA	C1B-C2B	2.51	1.49	1.43
26	C	510	CLA	C4D-CHA	2.51	1.47	1.38
27	D	401	PHO	C3A-C2A	-2.51	1.52	1.54
26	D	405	CLA	C3D-C4D	-2.50	1.38	1.44
26	C	516	CLA	C1B-C2B	2.50	1.49	1.43
34	E	101	HEM	C1C-C2C	-2.50	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	412	CLA	C1B-C2B	2.49	1.49	1.43
26	A	408	CLA	C4D-CHA	2.49	1.47	1.38
26	A	412	CLA	C4D-CHA	2.49	1.47	1.38
26	C	509	CLA	C1B-C2B	2.48	1.49	1.43
26	C	508	CLA	C1B-C2B	2.46	1.49	1.43
26	D	406	CLA	C1B-C2B	2.46	1.49	1.43
26	A	405	CLA	C4D-CHA	2.45	1.47	1.38
26	C	507	CLA	C1B-C2B	2.45	1.49	1.43
26	C	510	CLA	C3D-C4D	-2.45	1.38	1.44
26	C	506	CLA	C3D-C4D	-2.45	1.38	1.44
26	C	506	CLA	C4D-CHA	2.44	1.47	1.38
26	A	406	CLA	C3D-C4D	-2.44	1.38	1.44
26	D	406	CLA	C4C-C3C	2.43	1.49	1.45
27	D	401	PHO	C4B-NB	-2.43	1.34	1.38
26	A	406	CLA	C4D-CHA	2.43	1.47	1.38
26	C	516	CLA	C4C-C3C	2.41	1.49	1.45
26	A	406	CLA	C1B-C2B	2.39	1.48	1.43
26	C	508	CLA	C4C-C3C	2.39	1.49	1.45
26	A	405	CLA	C3D-C4D	-2.38	1.38	1.44
26	A	408	CLA	C3D-C4D	-2.38	1.38	1.44
26	D	405	CLA	C4D-CHA	2.38	1.46	1.38
27	A	407	PHO	C4B-NB	-2.37	1.34	1.38
26	C	509	CLA	C1C-C2C	2.37	1.49	1.44
26	C	509	CLA	C3D-C4D	-2.37	1.38	1.44
26	C	511	CLA	C1C-C2C	2.37	1.49	1.44
26	A	412	CLA	C3D-C4D	-2.37	1.38	1.44
26	C	506	CLA	C4C-C3C	2.37	1.49	1.45
26	C	504	CLA	C3D-C4D	-2.37	1.38	1.44
26	A	408	CLA	C1B-C2B	2.37	1.48	1.43
26	A	406	CLA	C4C-C3C	2.36	1.49	1.45
26	C	508	CLA	C3D-C4D	-2.36	1.38	1.44
26	A	406	CLA	C1C-C2C	2.36	1.49	1.44
26	D	406	CLA	C3D-C4D	-2.34	1.38	1.44
26	A	405	CLA	C1B-C2B	2.33	1.48	1.43
26	C	511	CLA	C3D-C4D	-2.33	1.38	1.44
26	D	405	CLA	C1C-C2C	2.33	1.49	1.44
26	C	511	CLA	C4C-C3C	2.33	1.49	1.45
26	A	408	CLA	C1C-C2C	2.32	1.49	1.44
26	C	506	CLA	C1C-C2C	2.32	1.49	1.44
26	C	509	CLA	C4C-C3C	2.32	1.49	1.45
26	C	509	CLA	C3B-C2B	2.31	1.49	1.41
26	A	408	CLA	C4C-C3C	2.31	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	504	CLA	C4C-C3C	2.30	1.49	1.45
27	A	407	PHO	C1B-NB	-2.30	1.34	1.38
26	C	508	CLA	C3B-C2B	2.28	1.48	1.41
26	A	405	CLA	C1C-C2C	2.27	1.49	1.44
26	C	516	CLA	C3D-C4D	-2.26	1.39	1.44
26	D	406	CLA	C1C-C2C	2.26	1.48	1.44
26	C	516	CLA	C1C-C2C	2.25	1.48	1.44
27	D	401	PHO	C1B-NB	-2.25	1.34	1.38
26	A	405	CLA	C4C-C3C	2.25	1.48	1.45
26	A	412	CLA	C4C-C3C	2.25	1.48	1.45
26	C	508	CLA	C1C-C2C	2.23	1.48	1.44
26	C	510	CLA	C1C-C2C	2.23	1.48	1.44
26	C	510	CLA	C4C-C3C	2.23	1.48	1.45
26	C	516	CLA	C3B-C2B	2.22	1.48	1.41
26	C	506	CLA	C3B-C2B	2.22	1.48	1.41
26	D	406	CLA	C3B-C2B	2.21	1.48	1.41
26	C	505	CLA	C3D-C4D	-2.20	1.39	1.44
27	A	407	PHO	C3A-C2A	-2.20	1.52	1.54
34	E	101	HEM	C1D-ND	-2.19	1.34	1.38
26	A	412	CLA	C3B-C2B	2.18	1.48	1.41
26	C	510	CLA	C3B-C2B	2.17	1.48	1.41
27	A	407	PHO	CHA-CBD	-2.15	1.49	1.51
26	A	406	CLA	C3B-C2B	2.14	1.48	1.41
26	A	408	CLA	C3B-C2B	2.14	1.48	1.41
26	C	504	CLA	C1C-C2C	2.13	1.48	1.44
27	A	407	PHO	C1D-ND	-2.12	1.34	1.38
26	D	405	CLA	C3B-C2B	2.11	1.48	1.41
26	A	406	CLA	C1D-C2D	2.11	1.49	1.45
27	D	401	PHO	C1D-ND	-2.10	1.34	1.38
34	E	101	HEM	C3C-C4C	-2.09	1.42	1.46
26	C	511	CLA	C3B-C2B	2.06	1.48	1.41
22	V	201	HEC	CMB-C2B	2.06	1.55	1.50
26	D	405	CLA	C4C-C3C	2.06	1.48	1.45
26	C	504	CLA	C3B-C2B	2.04	1.48	1.41
26	A	412	CLA	C1C-C2C	2.03	1.48	1.44
26	C	516	CLA	C1D-C2D	2.02	1.49	1.45

All (615) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	C1C-C2C-C3C	-12.60	103.04	112.33
27	A	407	PHO	C2D-C1D-ND	11.11	117.20	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	401	PHO	C2D-C1D-ND	11.08	117.18	109.53
26	A	406	CLA	C1D-ND-C4D	-9.45	99.62	106.33
26	A	408	CLA	C1D-ND-C4D	-9.39	99.67	106.33
26	C	516	CLA	C1D-ND-C4D	-9.34	99.70	106.33
26	C	508	CLA	C1D-ND-C4D	-9.32	99.71	106.33
26	D	405	CLA	C1D-ND-C4D	-9.28	99.74	106.33
26	C	503	CLA	C3A-C4A-CHB	-9.25	115.75	130.50
26	C	504	CLA	C1D-ND-C4D	-9.20	99.80	106.33
26	C	511	CLA	C1D-ND-C4D	-9.18	99.81	106.33
26	D	406	CLA	C1D-ND-C4D	-9.18	99.81	106.33
26	A	412	CLA	C1D-ND-C4D	-9.18	99.81	106.33
26	A	405	CLA	C1D-ND-C4D	-8.97	99.96	106.33
26	C	506	CLA	C1D-ND-C4D	-8.88	100.03	106.33
26	C	509	CLA	C1D-ND-C4D	-8.78	100.10	106.33
26	C	510	CLA	C1D-ND-C4D	-8.71	100.15	106.33
26	C	505	CLA	C1D-ND-C4D	-8.56	99.59	106.41
26	A	405	CLA	C2B-C1B-NB	8.28	115.78	110.23
26	C	508	CLA	C2B-C1B-NB	8.02	115.61	110.23
26	A	408	CLA	C2B-C1B-NB	8.01	115.60	110.23
26	C	505	CLA	C2D-C1D-ND	8.01	116.00	110.10
27	A	407	PHO	O2D-CGD-CBD	7.94	121.06	111.00
26	C	516	CLA	C2B-C1B-NB	7.93	115.55	110.23
26	C	509	CLA	C2B-C1B-NB	7.83	115.48	110.23
26	C	507	CLA	C2B-C1B-NB	7.80	115.46	110.23
26	D	406	CLA	C2B-C1B-NB	7.79	115.46	110.23
26	A	406	CLA	C2B-C1B-NB	7.76	115.44	110.23
26	C	516	CLA	C2D-C1D-ND	7.72	115.79	110.10
26	C	504	CLA	C2D-C1D-ND	7.70	115.78	110.10
26	C	510	CLA	C2B-C1B-NB	7.67	115.38	110.23
26	A	412	CLA	C2B-C1B-NB	7.66	115.37	110.23
26	C	508	CLA	C2D-C1D-ND	7.66	115.75	110.10
26	A	408	CLA	C2D-C1D-ND	7.65	115.75	110.10
26	C	511	CLA	C2D-C1D-ND	7.63	115.73	110.10
26	C	506	CLA	C2B-C1B-NB	7.63	115.35	110.23
26	A	412	CLA	C2D-C1D-ND	7.55	115.67	110.10
26	D	405	CLA	C2B-C1B-NB	7.50	115.26	110.23
26	D	405	CLA	C2D-C1D-ND	7.49	115.62	110.10
26	C	511	CLA	C2B-C1B-NB	7.47	115.24	110.23
26	A	406	CLA	C2D-C1D-ND	7.39	115.55	110.10
26	D	406	CLA	C2D-C1D-ND	7.39	115.55	110.10
27	D	401	PHO	O2D-CGD-CBD	7.32	120.27	111.00
26	C	504	CLA	C2B-C1B-NB	7.25	115.09	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	506	CLA	CMD-C2D-C1D	7.12	137.25	124.71
26	C	509	CLA	C2D-C1D-ND	7.10	115.33	110.10
26	A	405	CLA	C2D-C1D-ND	7.04	115.29	110.10
26	A	405	CLA	CMD-C2D-C1D	7.03	137.10	124.71
26	C	510	CLA	CMD-C2D-C1D	6.98	137.01	124.71
26	A	406	CLA	CMD-C2D-C1D	6.97	136.99	124.71
26	C	510	CLA	C2D-C1D-ND	6.92	115.20	110.10
26	C	511	CLA	CMD-C2D-C1D	6.78	136.67	124.71
26	A	412	CLA	CMD-C2D-C1D	6.74	136.59	124.71
26	D	405	CLA	CMD-C2D-C1D	6.73	136.58	124.71
26	C	505	CLA	CMD-C2D-C1D	6.72	136.55	124.71
26	C	509	CLA	CMD-C2D-C1D	6.70	136.53	124.71
26	C	506	CLA	C2D-C1D-ND	6.69	115.04	110.10
26	A	406	CLA	CHD-C1D-ND	-6.67	118.32	124.45
26	A	408	CLA	CMD-C2D-C1D	6.66	136.46	124.71
27	D	401	PHO	C4D-ND-C1D	-6.64	102.07	108.83
26	D	406	CLA	CMD-C2D-C1D	6.62	136.38	124.71
26	C	516	CLA	CMD-C2D-C1D	6.61	136.35	124.71
27	A	407	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
27	A	407	PHO	C4D-ND-C1D	-6.57	102.15	108.83
26	A	408	CLA	CHD-C1D-ND	-6.56	118.42	124.45
26	C	507	CLA	C1B-C2B-C3B	-6.50	100.89	107.02
26	C	505	CLA	CHD-C1D-ND	-6.49	118.49	124.45
27	D	401	PHO	C2B-C1B-NB	6.48	114.00	109.53
22	V	201	HEC	C1D-ND-C4D	6.42	111.70	105.07
26	A	412	CLA	CHD-C1D-ND	-6.37	118.60	124.45
26	A	405	CLA	CHD-C1D-ND	-6.35	118.62	124.45
26	C	516	CLA	CHD-C1D-ND	-6.35	118.62	124.45
26	C	508	CLA	CHD-C1D-ND	-6.34	118.63	124.45
27	A	407	PHO	C2B-C1B-NB	6.30	113.88	109.53
26	C	508	CLA	CMD-C2D-C1D	6.29	135.80	124.71
27	D	401	PHO	C1C-C2C-C3C	-6.26	103.41	108.61
26	A	405	CLA	C4A-NA-C1A	-6.23	103.90	106.71
26	D	406	CLA	CHD-C1D-ND	-6.20	118.76	124.45
26	C	511	CLA	CHD-C1D-ND	-6.19	118.77	124.45
26	C	504	CLA	CMD-C2D-C1D	6.17	135.59	124.71
26	D	405	CLA	CHD-C1D-ND	-6.16	118.79	124.45
26	C	510	CLA	CHD-C1D-ND	-6.08	118.87	124.45
26	C	509	CLA	CHD-C1D-ND	-6.07	118.87	124.45
26	C	504	CLA	CHD-C1D-ND	-5.94	119.00	124.45
26	D	405	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
26	C	506	CLA	CHD-C1D-ND	-5.78	119.14	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	511	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
26	C	504	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
26	C	506	CLA	O2D-CGD-CBD	5.61	121.24	111.27
26	C	506	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
26	A	405	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
26	C	516	CLA	O2D-CGD-CBD	5.54	121.11	111.27
26	D	405	CLA	C4A-NA-C1A	-5.51	104.23	106.71
26	C	510	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
26	A	408	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
26	C	509	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
26	C	508	CLA	O2D-CGD-CBD	5.46	120.98	111.27
26	C	505	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
26	C	508	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
26	C	506	CLA	C4A-NA-C1A	-5.41	104.27	106.71
26	A	412	CLA	C2C-C1C-NC	5.41	115.04	109.97
26	C	506	CLA	C2C-C1C-NC	5.40	115.03	109.97
26	A	412	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
26	C	504	CLA	C2C-C1C-NC	5.35	114.99	109.97
26	D	406	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
26	C	505	CLA	O2D-CGD-CBD	5.31	120.70	111.27
26	A	406	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
20	K	101	BCR	C33-C5-C6	-5.28	118.60	124.53
26	C	516	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
26	D	406	CLA	C2C-C1C-NC	5.23	114.87	109.97
20	D	407	BCR	C24-C23-C22	-5.21	118.37	126.23
26	C	516	CLA	C2C-C1C-NC	5.18	114.83	109.97
26	C	510	CLA	C2C-C1C-NC	5.14	114.79	109.97
20	T	102	BCR	C24-C23-C22	-5.14	118.47	126.23
26	A	406	CLA	C4A-NA-C1A	-5.13	104.40	106.71
28	A	410	PL9	C7-C3-C4	5.12	121.04	116.88
26	C	510	CLA	O2D-CGD-CBD	5.12	120.37	111.27
26	D	405	CLA	C2C-C1C-NC	5.12	114.76	109.97
20	T	102	BCR	C20-C21-C22	-5.11	119.90	127.24
26	A	405	CLA	C2C-C1C-NC	5.10	114.75	109.97
20	D	407	BCR	C15-C14-C13	-5.09	120.04	127.31
26	A	408	CLA	C4A-NA-C1A	-5.09	104.42	106.71
26	C	508	CLA	C4A-NA-C1A	-5.06	104.43	106.71
27	D	401	PHO	C3D-C4D-ND	5.06	114.61	107.72
26	C	511	CLA	C2C-C1C-NC	5.04	114.69	109.97
26	C	509	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
26	D	406	CLA	C4A-NA-C1A	-5.03	104.44	106.71
26	A	406	CLA	O2D-CGD-CBD	5.02	120.18	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	509	CLA	C2C-C1C-NC	5.01	114.67	109.97
26	A	412	CLA	O2D-CGD-CBD	5.00	120.15	111.27
27	A	407	PHO	C3D-C4D-ND	5.00	114.53	107.72
26	C	504	CLA	O2D-CGD-CBD	4.99	120.13	111.27
26	C	508	CLA	C2C-C1C-NC	4.99	114.64	109.97
26	C	510	CLA	C4A-NA-C1A	-4.96	104.48	106.71
26	C	509	CLA	O2D-CGD-CBD	4.95	120.06	111.27
26	A	408	CLA	C2C-C1C-NC	4.93	114.59	109.97
31	C	502	LMG	O7-C10-C11	4.93	122.13	111.50
26	C	509	CLA	C4A-NA-C1A	-4.93	104.49	106.71
26	A	408	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
34	E	101	HEM	CHC-C4B-NB	4.91	129.75	124.42
26	C	516	CLA	C4A-NA-C1A	-4.90	104.50	106.71
26	A	406	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
26	C	508	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
26	C	511	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
20	D	407	BCR	C7-C8-C9	-4.88	118.86	126.23
26	C	510	CLA	C3B-C2B-C1B	-4.88	101.28	107.16
26	D	405	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
26	C	516	CLA	C3B-C2B-C1B	-4.84	101.32	107.16
26	C	511	CLA	C4A-NA-C1A	-4.84	104.53	106.71
26	A	405	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
26	A	406	CLA	C2C-C1C-NC	4.82	114.49	109.97
26	A	408	CLA	O2D-CGD-CBD	4.81	119.81	111.27
26	D	406	CLA	O2D-CGD-CBD	4.81	119.81	111.27
26	C	506	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
26	D	406	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
31	B	603	LMG	O7-C10-O9	-4.72	119.56	125.57
26	A	406	CLA	C3D-C4D-ND	4.68	117.81	110.24
26	C	505	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
26	C	504	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
26	C	511	CLA	O2D-CGD-CBD	4.63	119.50	111.27
26	C	508	CLA	C3D-C4D-ND	4.60	117.69	110.24
26	A	408	CLA	C3D-C4D-ND	4.59	117.66	110.24
26	C	511	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
26	A	412	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
26	D	406	CLA	C3D-C4D-ND	4.54	117.58	110.24
26	C	516	CLA	C3D-C4D-ND	4.54	117.58	110.24
26	D	405	CLA	C3D-C4D-ND	4.50	117.52	110.24
26	C	508	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
26	C	516	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
26	A	408	CLA	C3D-C2D-C1D	-4.48	99.71	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	C3D-C4D-ND	4.48	117.48	110.24
26	C	504	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
26	A	412	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
26	C	504	CLA	C4A-NA-C1A	-4.47	104.69	106.71
26	C	504	CLA	C3D-C4D-ND	4.45	117.44	110.24
26	D	405	CLA	O2D-CGD-CBD	4.45	119.17	111.27
26	A	412	CLA	C3D-C4D-ND	4.45	117.43	110.24
26	A	405	CLA	C3D-C4D-ND	4.42	117.39	110.24
20	K	102	BCR	C20-C21-C22	-4.42	121.00	127.31
26	D	406	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	A	406	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
26	C	511	CLA	C3D-C4D-ND	4.38	117.32	110.24
26	C	506	CLA	C3D-C4D-ND	4.38	117.32	110.24
26	C	509	CLA	C3D-C4D-ND	4.36	117.29	110.24
26	C	510	CLA	C3D-C4D-ND	4.35	117.28	110.24
26	C	511	CLA	C1-C2-C3	-4.35	118.52	126.04
26	A	412	CLA	C4A-NA-C1A	-4.32	104.76	106.71
26	D	405	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
26	C	509	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
26	C	510	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
20	A	409	BCR	C15-C14-C13	-4.21	121.30	127.31
26	A	405	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
33	C	514	DGD	O2G-C1B-C2B	4.19	120.53	111.50
30	L	101	LHG	O7-C7-C8	4.19	120.52	111.50
28	A	410	PL9	C7-C3-C2	-4.15	117.84	123.30
20	K	102	BCR	C15-C14-C13	-4.13	121.41	127.31
33	C	515	DGD	O2G-C1B-C2B	4.08	120.29	111.50
26	C	504	CLA	C1-C2-C3	-4.08	120.16	126.75
20	T	102	BCR	C28-C27-C26	-4.06	106.83	114.08
34	E	101	HEM	C1B-NB-C4B	4.05	109.26	105.07
30	A	414	LHG	O7-C7-C8	4.03	120.20	111.50
20	K	102	BCR	C24-C23-C22	-4.03	120.15	126.23
27	D	401	PHO	C1-C2-C3	-4.03	119.08	126.04
20	D	407	BCR	C33-C5-C6	-4.02	120.01	124.53
31	D	410	LMG	O7-C10-C11	4.00	120.11	111.50
26	A	412	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
26	C	506	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
26	A	405	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
20	K	102	BCR	C7-C8-C9	-3.96	120.25	126.23
33	C	513	DGD	O2G-C1B-C2B	3.95	120.01	111.50
30	A	415	LHG	O7-C7-C8	3.93	119.96	111.50
26	C	505	CLA	C2A-C1A-NA	3.93	117.23	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	408	PL9	C7-C8-C9	-3.90	120.30	126.79
34	E	101	HEM	C4C-NC-C1C	3.90	109.17	105.35
30	D	412	LHG	O7-C7-C8	3.89	119.89	111.50
20	D	407	BCR	C20-C21-C22	-3.89	121.76	127.31
26	C	505	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
20	D	407	BCR	C16-C17-C18	-3.86	121.80	127.31
26	C	504	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
26	D	405	CLA	C3C-C4C-NC	3.85	114.89	110.57
30	D	409	LHG	O7-C7-C8	3.82	119.73	111.50
26	C	506	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
26	C	510	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
26	C	506	CLA	C3C-C4C-NC	3.79	114.82	110.57
32	C	501	SQD	O47-C7-C8	3.79	119.66	111.50
26	C	516	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
26	C	506	CLA	C1-C2-C3	-3.77	119.53	126.04
26	C	504	CLA	C3C-C4C-NC	3.77	114.80	110.57
26	C	509	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
26	D	405	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
26	C	510	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
26	C	511	CLA	C3C-C4C-NC	3.72	114.75	110.57
26	A	412	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
26	C	506	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
26	C	511	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
26	A	405	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
26	C	516	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
20	K	101	BCR	C16-C17-C18	-3.69	122.05	127.31
34	E	101	HEM	CHD-C4C-NC	3.68	128.42	124.44
26	A	408	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	K	102	BCR	C16-C17-C18	-3.66	122.08	127.31
20	K	102	BCR	C11-C10-C9	-3.65	122.10	127.31
26	D	406	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
26	A	406	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
28	A	410	PL9	C7-C8-C9	-3.63	120.75	126.79
26	C	509	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
26	D	406	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
26	D	405	CLA	C1D-CHD-C4C	-3.61	118.28	126.06
20	K	101	BCR	C15-C14-C13	-3.60	122.18	127.31
20	A	409	BCR	C16-C17-C18	-3.59	122.19	127.31
26	C	509	CLA	C3C-C4C-NC	3.56	114.57	110.57
20	I	102	BCR	C33-C5-C6	-3.56	120.53	124.53
26	A	406	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
26	C	504	CLA	C1C-C2C-C3C	-3.56	103.22	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	508	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
26	C	511	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
26	C	508	CLA	C3C-C4C-NC	3.55	114.55	110.57
20	D	407	BCR	C11-C10-C9	-3.54	122.26	127.31
26	B	601	CLA	O2A-CGA-CBA	3.54	120.66	111.38
26	A	408	CLA	C1-C2-C3	-3.54	119.93	126.04
26	A	405	CLA	C3C-C4C-NC	3.51	114.51	110.57
26	C	508	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
26	A	408	CLA	C1D-CHD-C4C	-3.51	118.50	126.06
20	D	407	BCR	C38-C26-C25	-3.49	120.60	124.53
26	D	406	CLA	C3C-C4C-NC	3.48	114.47	110.57
26	C	510	CLA	C1-C2-C3	-3.47	120.04	126.04
26	C	508	CLA	C3B-C4B-NB	3.46	113.73	110.52
26	C	510	CLA	C3C-C4C-NC	3.46	114.45	110.57
26	A	412	CLA	C1-C2-C3	-3.45	120.08	126.04
26	A	408	CLA	C3C-C4C-NC	3.44	114.43	110.57
26	C	516	CLA	C3C-C4C-NC	3.44	114.42	110.57
26	D	405	CLA	C1-C2-C3	-3.41	120.14	126.04
34	E	101	HEM	CAD-CBD-CGD	3.39	120.89	113.60
26	A	412	CLA	C3B-C4B-NB	3.31	113.58	110.52
26	C	505	CLA	CMA-C3A-C4A	-3.30	109.63	113.67
26	C	503	CLA	C1-C2-C3	-3.30	120.33	126.04
26	A	406	CLA	C3C-C4C-NC	3.30	114.27	110.57
26	C	510	CLA	C3B-C4B-NB	3.30	113.58	110.52
28	D	408	PL9	C37-C38-C39	-3.30	119.72	127.66
32	C	501	SQD	O8-S-C6	3.29	110.99	105.74
26	A	405	CLA	O2D-CGD-CBD	3.27	117.08	111.27
26	C	516	CLA	C1-C2-C3	-3.26	120.41	126.04
26	A	412	CLA	C3C-C4C-NC	3.25	114.21	110.57
26	C	509	CLA	C3B-C4B-NB	3.24	113.52	110.52
34	E	101	HEM	CHB-C1B-NB	3.22	128.35	124.37
26	A	408	CLA	C4-C3-C5	3.22	119.67	115.98
26	C	508	CLA	C1-C2-C3	-3.21	120.49	126.04
26	C	516	CLA	C3B-C4B-NB	3.20	113.48	110.52
20	A	409	BCR	C38-C26-C25	-3.18	120.96	124.53
26	A	405	CLA	C1-C2-C3	-3.17	120.56	126.04
26	D	406	CLA	C3B-C4B-NB	3.16	113.44	110.52
26	C	504	CLA	C3B-C4B-NB	3.15	113.44	110.52
26	C	504	CLA	CMB-C2B-C1B	3.15	130.16	125.37
26	C	511	CLA	CMB-C2B-C1B	3.14	130.15	125.37
34	E	101	HEM	CHD-C1D-ND	3.12	127.80	124.42
26	D	405	CLA	C3B-C4B-NB	3.12	113.41	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	505	CLA	C1-C2-C3	-3.10	120.68	126.04
28	D	408	PL9	C15-C14-C16	3.10	120.48	115.27
26	D	406	CLA	CAC-C3C-C4C	3.09	128.82	124.81
34	E	101	HEM	C4D-ND-C1D	3.09	108.27	105.07
28	D	408	PL9	C20-C19-C21	3.09	120.47	115.27
27	A	407	PHO	C4-C3-C5	3.09	120.47	115.27
26	A	412	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
27	D	401	PHO	C1A-C2A-C3A	-3.07	99.92	102.84
28	A	410	PL9	C37-C38-C39	-3.05	120.31	127.66
26	C	507	CLA	C2A-C3A-C4A	-3.05	99.29	101.57
26	C	506	CLA	C3B-C4B-NB	3.04	113.34	110.52
28	D	408	PL9	C10-C9-C11	3.04	120.39	115.27
20	A	409	BCR	C20-C21-C22	-3.03	122.98	127.31
26	C	506	CLA	CAC-C3C-C4C	3.03	128.74	124.81
34	E	101	HEM	CHA-C4D-ND	3.03	128.11	124.37
20	A	409	BCR	C11-C10-C9	-3.03	122.99	127.31
26	C	504	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
28	A	410	PL9	C10-C9-C11	3.02	120.34	115.27
28	A	410	PL9	C32-C33-C34	-3.01	120.41	127.66
20	K	101	BCR	C38-C26-C25	-3.01	121.15	124.53
26	A	406	CLA	C1-C2-C3	-3.01	120.84	126.04
26	C	516	CLA	CAC-C3C-C4C	3.00	128.71	124.81
26	A	405	CLA	CAC-C3C-C4C	3.00	128.71	124.81
26	C	511	CLA	C4-C3-C5	3.00	120.31	115.27
26	C	504	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
26	C	505	CLA	CBC-CAC-C3C	-2.99	106.15	113.82
26	D	406	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
28	D	408	PL9	C12-C13-C14	-2.97	120.50	127.66
27	A	407	PHO	C1A-C2A-C3A	-2.97	100.01	102.84
26	D	405	CLA	CHD-C4C-NC	2.97	128.88	124.20
26	A	408	CLA	C3B-C4B-NB	2.97	113.27	110.52
28	A	410	PL9	C17-C18-C19	-2.97	120.52	127.66
26	A	405	CLA	C3B-C4B-NB	2.96	113.26	110.52
26	C	507	CLA	CMB-C2B-C3B	2.96	129.41	122.52
26	C	509	CLA	C4-C3-C5	2.94	120.22	115.27
26	A	412	CLA	CHD-C4C-NC	2.93	128.83	124.20
26	C	508	CLA	CAC-C3C-C4C	2.92	128.60	124.81
26	C	510	CLA	CHD-C4C-NC	2.92	128.80	124.20
26	A	408	CLA	CHD-C4C-NC	2.92	128.80	124.20
26	A	405	CLA	CHD-C4C-NC	2.92	128.80	124.20
26	D	405	CLA	C4-C3-C5	2.91	120.17	115.27
26	C	510	CLA	CHC-C1C-C2C	-2.90	118.66	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	516	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
26	A	405	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
26	C	506	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
26	C	511	CLA	CHD-C4C-NC	2.88	128.75	124.20
26	C	511	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
26	D	405	CLA	CMB-C2B-C1B	2.88	129.76	125.37
26	C	508	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
26	C	506	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
33	C	515	DGD	O1G-C1A-C2A	2.87	120.90	111.91
26	C	508	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
28	A	410	PL9	C42-C43-C44	-2.85	120.79	127.66
26	D	403	CLA	CMB-C2B-C3B	2.85	129.82	112.35
30	A	414	LHG	O8-C23-C24	2.85	120.86	111.91
26	A	406	CLA	CHD-C4C-NC	2.84	128.68	124.20
26	C	504	CLA	CHD-C4C-NC	2.83	128.67	124.20
26	C	507	CLA	CMB-C2B-C1B	2.83	129.69	125.37
20	K	101	BCR	C10-C11-C12	-2.83	114.38	123.22
26	C	509	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
26	C	511	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
28	A	410	PL9	C30-C29-C31	2.83	120.03	115.27
26	C	509	CLA	CHD-C4C-NC	2.82	128.65	124.20
26	C	511	CLA	CAC-C3C-C4C	2.82	128.47	124.81
26	A	406	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
27	D	401	PHO	CMB-C2B-C3B	2.82	129.95	124.68
28	D	408	PL9	C25-C24-C26	2.82	120.01	115.27
26	A	408	CLA	CHC-C1C-C2C	-2.81	118.93	126.73
26	C	509	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
20	A	409	BCR	C24-C23-C22	-2.80	122.01	126.23
28	D	408	PL9	C45-C44-C46	2.80	119.98	115.27
26	A	405	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
26	D	405	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
26	D	406	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
28	D	408	PL9	C17-C18-C19	-2.79	120.94	127.66
28	D	408	PL9	C53-C6-C1	2.79	120.69	114.99
26	C	503	CLA	O2A-CGA-CBA	2.79	120.66	111.91
26	C	511	CLA	C3B-C4B-NB	2.79	113.10	110.52
26	A	412	CLA	CAA-C2A-C3A	-2.78	105.16	112.78
20	A	409	BCR	C33-C5-C6	-2.78	121.41	124.53
26	C	509	CLA	CAC-C3C-C4C	2.78	128.41	124.81
26	B	601	CLA	C1-C2-C3	-2.78	121.24	126.04
26	A	406	CLA	C3B-C4B-NB	2.77	113.09	110.52
26	C	505	CLA	O2A-CGA-CBA	2.77	120.61	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	516	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
26	C	504	CLA	CAC-C3C-C4C	2.77	128.41	124.81
26	C	508	CLA	CHD-C4C-NC	2.77	128.57	124.20
26	C	511	CLA	O2A-CGA-CBA	2.76	120.58	111.91
26	C	510	CLA	O2A-CGA-CBA	2.76	120.57	111.91
26	C	508	CLA	C4-C3-C5	2.76	119.91	115.27
28	D	408	PL9	C27-C28-C29	-2.76	121.02	127.66
33	C	514	DGD	O1G-C1A-C2A	2.75	120.55	111.91
26	C	509	CLA	O2A-CGA-CBA	2.74	120.52	111.91
26	C	506	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	K	102	BCR	C3-C4-C5	-2.74	109.19	114.08
28	D	408	PL9	C30-C29-C31	2.74	119.87	115.27
26	C	505	CLA	CAC-C3C-C4C	2.74	128.58	125.27
31	B	603	LMG	O8-C28-C29	2.73	120.48	111.91
26	D	406	CLA	CHD-C4C-NC	2.73	128.51	124.20
27	A	407	PHO	O1D-CGD-CBD	-2.73	120.19	124.74
26	A	408	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
32	C	501	SQD	O48-C23-C24	2.73	120.47	111.91
26	A	405	CLA	CMB-C2B-C1B	2.72	129.51	125.37
33	D	413	DGD	O1G-C1A-C2A	2.72	120.44	111.91
26	A	406	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
20	T	102	BCR	C38-C26-C25	-2.72	121.48	124.53
26	D	405	CLA	O2A-CGA-CBA	2.72	120.43	111.91
28	A	410	PL9	C45-C44-C46	2.71	119.84	115.27
26	D	405	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
20	K	102	BCR	C10-C11-C12	-2.70	114.79	123.22
26	A	405	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
26	C	516	CLA	CHD-C4C-NC	2.69	128.44	124.20
26	D	405	CLA	CMC-C2C-C1C	2.68	129.12	125.04
26	C	510	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
28	D	408	PL9	C22-C23-C24	-2.67	121.23	127.66
28	A	410	PL9	C22-C23-C24	-2.66	121.26	127.66
30	D	412	LHG	O8-C23-C24	2.66	120.25	111.91
26	C	508	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	D	401	PHO	C4-C3-C5	2.65	119.74	115.27
26	A	405	CLA	CMC-C2C-C1C	2.65	129.07	125.04
20	K	101	BCR	C8-C7-C6	-2.65	119.77	127.20
26	C	516	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
22	V	201	HEC	C4A-NA-C1A	2.64	107.94	105.35
20	A	409	BCR	C3-C4-C5	-2.64	109.36	114.08
20	A	409	BCR	C7-C8-C9	-2.64	122.25	126.23
26	C	506	CLA	O2D-CGD-O1D	-2.64	118.68	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	410	PL9	C53-C6-C1	2.63	120.38	114.99
20	I	102	BCR	C11-C10-C9	-2.63	123.55	127.31
26	D	405	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
28	D	408	PL9	C35-C34-C36	2.63	119.70	115.27
26	A	412	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
26	A	406	CLA	CAC-C3C-C4C	2.63	128.22	124.81
26	A	405	CLA	O2A-CGA-CBA	2.63	120.16	111.91
26	C	506	CLA	O2A-CGA-CBA	2.63	120.15	111.91
26	A	408	CLA	CAC-C3C-C4C	2.62	128.21	124.81
26	C	505	CLA	C4-C3-C5	2.62	119.68	115.27
26	B	601	CLA	C4-C3-C5	2.62	119.68	115.27
26	A	406	CLA	O2A-CGA-CBA	2.62	120.12	111.91
22	V	201	HEC	C2A-C1A-NA	-2.61	107.78	110.32
26	A	408	CLA	O2A-CGA-CBA	2.61	120.11	111.91
26	A	408	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
28	A	410	PL9	C20-C19-C21	2.61	119.67	115.27
20	I	102	BCR	C3-C4-C5	-2.60	109.43	114.08
27	A	407	PHO	O2D-CGD-O1D	-2.60	118.75	123.84
26	A	412	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
30	D	409	LHG	O8-C23-C24	2.60	120.06	111.91
26	C	508	CLA	O2A-CGA-CBA	2.59	120.05	111.91
20	T	102	BCR	C38-C26-C27	2.59	118.60	113.62
20	K	102	BCR	C33-C5-C6	-2.59	121.62	124.53
26	C	504	CLA	O2A-CGA-CBA	2.58	120.01	111.91
26	C	505	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
27	A	407	PHO	C1-C2-C3	-2.57	121.59	126.04
26	C	504	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
26	A	412	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
26	C	510	CLA	CAC-C3C-C4C	2.57	128.14	124.81
26	D	406	CLA	CMB-C2B-C1B	2.57	129.28	125.37
26	A	406	CLA	C4-C3-C5	2.56	119.58	115.27
31	D	410	LMG	C8-O7-C10	-2.56	111.49	117.79
28	A	410	PL9	C40-C39-C41	2.56	119.58	115.27
26	A	408	CLA	CMB-C2B-C1B	2.55	129.26	125.37
26	C	510	CLA	C4-C3-C5	2.55	119.56	115.27
22	V	201	HEC	C4C-NC-C1C	2.54	107.83	105.35
27	A	407	PHO	CMB-C2B-C3B	2.54	129.43	124.68
28	D	408	PL9	C32-C33-C34	-2.54	121.55	127.66
30	L	101	LHG	O8-C23-C24	2.54	119.86	111.91
22	V	201	HEC	C4B-NB-C1B	2.53	107.69	105.07
26	A	412	CLA	CMB-C2B-C1B	2.53	129.23	125.37
26	A	406	CLA	CMB-C2B-C1B	2.53	129.23	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	102	BCR	C15-C16-C17	-2.53	118.30	123.47
31	C	502	LMG	O8-C28-C29	2.53	119.83	111.91
26	C	506	CLA	CMB-C2B-C1B	2.52	129.21	125.37
33	C	513	DGD	C2G-O2G-C1B	-2.52	111.58	117.79
26	C	516	CLA	C4-C3-C5	2.52	119.52	115.27
26	C	510	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
26	D	403	CLA	C2B-C3B-CAB	2.51	129.53	112.84
26	C	509	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
28	A	410	PL9	C25-C24-C26	2.51	119.49	115.27
26	A	412	CLA	O2A-CGA-CBA	2.50	119.77	111.91
28	A	410	PL9	C35-C34-C36	2.50	119.47	115.27
26	C	516	CLA	CMB-C2B-C1B	2.50	129.17	125.37
26	D	405	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
20	T	102	BCR	C29-C30-C25	2.49	114.32	110.48
30	D	409	LHG	C5-O7-C7	-2.49	111.66	117.79
27	D	401	PHO	O2D-CGD-O1D	-2.49	118.98	123.84
28	A	410	PL9	C15-C14-C16	2.48	119.45	115.27
20	K	101	BCR	C16-C15-C14	-2.48	118.39	123.47
32	F	101	SQD	O7-S-C6	2.46	109.87	106.94
28	D	408	PL9	C42-C43-C44	-2.46	121.73	127.66
30	L	101	LHG	C5-O7-C7	-2.46	111.73	117.79
26	C	506	CLA	CMC-C2C-C1C	2.46	128.78	125.04
26	A	405	CLA	C4-C3-C5	2.46	119.41	115.27
26	A	408	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
26	C	511	CLA	CMC-C2C-C1C	2.45	128.78	125.04
26	C	516	CLA	O2A-CGA-CBA	2.45	119.60	111.91
20	I	102	BCR	C7-C8-C9	-2.45	122.53	126.23
26	A	406	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
26	C	508	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
26	A	412	CLA	C4-C3-C5	2.43	119.37	115.27
20	K	101	BCR	C21-C20-C19	-2.42	115.67	123.22
26	C	509	CLA	CMC-C2C-C1C	2.42	128.72	125.04
32	C	501	SQD	O9-S-C6	2.41	109.81	106.94
26	D	405	CLA	CAC-C3C-C4C	2.41	127.94	124.81
26	D	405	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
26	A	408	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
28	D	408	PL9	C51-C49-C50	2.40	119.91	114.60
28	A	410	PL9	C27-C28-C29	-2.40	121.88	127.66
20	K	101	BCR	C37-C22-C23	2.40	121.86	118.08
26	D	406	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
30	D	412	LHG	C5-O7-C7	-2.40	111.89	117.79
26	C	510	CLA	CMC-C2C-C1C	2.39	128.69	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	401	PHO	O1D-CGD-CBD	-2.39	120.75	124.74
26	C	516	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
26	A	406	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
20	K	102	BCR	C29-C30-C25	2.39	114.15	110.48
26	A	408	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
26	C	506	CLA	C4-C3-C5	2.38	119.27	115.27
26	C	510	CLA	CMB-C2B-C1B	2.38	128.99	125.37
27	D	401	PHO	CMA-C3A-C4A	-2.37	109.18	114.38
27	D	401	PHO	O2A-CGA-CBA	2.37	119.35	111.91
28	D	408	PL9	C7-C3-C4	2.37	118.80	116.88
26	C	503	CLA	C4-C3-C5	2.37	119.25	115.27
28	A	410	PL9	C51-C49-C50	2.37	119.83	114.60
26	C	510	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
26	A	408	CLA	CMC-C2C-C1C	2.36	128.63	125.04
33	C	514	DGD	C2G-O2G-C1B	-2.36	111.98	117.79
28	D	408	PL9	C40-C39-C41	2.36	119.23	115.27
20	K	101	BCR	C23-C24-C25	-2.35	120.60	127.20
33	C	513	DGD	O1G-C1A-C2A	2.35	119.27	111.91
20	I	102	BCR	C8-C7-C6	-2.35	120.61	127.20
20	K	102	BCR	C2-C1-C6	2.31	114.04	110.48
27	A	407	PHO	CMA-C3A-C4A	-2.31	109.31	114.38
32	C	501	SQD	C45-O47-C7	-2.31	112.10	117.79
26	A	406	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
26	A	406	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
26	C	506	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
26	C	506	CLA	CBC-CAC-C3C	-2.29	106.11	112.43
26	D	406	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
26	C	508	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
33	C	515	DGD	C2G-O2G-C1B	-2.28	112.17	117.79
26	A	405	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
32	F	101	SQD	O8-S-C6	2.28	109.37	105.74
34	E	101	HEM	CHA-C1A-NA	2.28	128.04	123.85
26	C	510	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
20	D	407	BCR	C28-C27-C26	-2.27	110.02	114.08
20	I	102	BCR	C10-C11-C12	-2.27	116.12	123.22
26	C	504	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
20	T	102	BCR	C37-C22-C21	-2.26	119.75	122.92
27	A	407	PHO	C4A-C3A-C2A	-2.26	100.69	102.84
26	D	405	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
26	C	510	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
28	D	408	PL9	C7-C3-C2	-2.26	120.33	123.30
26	D	406	CLA	CBC-CAC-C3C	-2.25	106.22	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	506	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	A	412	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
20	K	102	BCR	C21-C20-C19	-2.23	116.25	123.22
20	K	102	BCR	C28-C27-C26	-2.23	110.10	114.08
31	D	410	LMG	O6-C5-C4	2.22	113.73	109.69
26	A	412	CLA	CAC-C3C-C4C	2.22	127.70	124.81
26	C	516	CLA	CMC-C2C-C1C	2.22	128.42	125.04
26	C	509	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
20	A	409	BCR	C2-C1-C6	2.22	113.90	110.48
31	C	502	LMG	O7-C10-O9	-2.22	118.34	123.70
26	C	509	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
26	D	406	CLA	CMC-C2C-C1C	2.21	128.40	125.04
20	A	409	BCR	C15-C16-C17	-2.20	118.97	123.47
27	D	401	PHO	C6-C5-C3	-2.19	107.71	113.45
28	A	410	PL9	C47-C48-C49	-2.19	120.26	127.75
20	K	101	BCR	C24-C23-C22	-2.19	122.93	126.23
26	A	406	CLA	CMC-C2C-C1C	2.18	128.37	125.04
26	C	511	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
26	C	504	CLA	C2A-C1A-CHA	-2.18	120.06	123.86
33	C	514	DGD	O1G-C1A-O1A	-2.16	118.14	123.59
27	A	407	PHO	C6-C5-C3	-2.16	107.79	113.45
26	C	506	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
26	C	508	CLA	CMC-C2C-C1C	2.15	128.31	125.04
34	E	101	HEM	C4A-NA-C1A	2.15	107.45	105.35
31	D	410	LMG	O8-C28-C29	2.14	118.63	111.91
31	C	502	LMG	C8-O7-C10	-2.14	112.52	117.79
26	C	516	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
20	K	101	BCR	C34-C9-C8	2.12	121.42	118.08
20	K	101	BCR	C28-C27-C26	-2.12	110.30	114.08
26	C	504	CLA	C5-C3-C4	2.10	119.25	114.60
26	C	511	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
26	A	405	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
20	K	101	BCR	C11-C10-C9	-2.09	124.32	127.31
20	K	102	BCR	C36-C18-C19	2.09	121.37	118.08
26	A	408	CLA	CHB-C4A-NA	2.08	127.39	124.51
26	A	405	CLA	CED-O2D-CGD	2.08	120.65	115.94
26	C	516	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
26	A	405	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
20	D	407	BCR	C3-C4-C5	-2.08	110.36	114.08
32	F	101	SQD	O9-S-C6	2.07	109.40	106.94
26	C	505	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
34	E	101	HEM	O2A-CGA-CBA	2.07	120.67	114.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	I	102	BCR	C35-C13-C12	2.06	120.50	118.51
20	K	101	BCR	C33-C5-C4	2.06	117.58	113.62
20	I	102	BCR	C34-C9-C8	2.05	121.30	118.08
33	C	514	DGD	C1D-C2D-C3D	2.04	114.25	110.00
26	A	405	CLA	CHB-C4A-NA	2.04	127.33	124.51
26	C	509	CLA	CHB-C4A-NA	2.04	127.33	124.51
26	C	511	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
26	C	511	CLA	C4-C3-C2	-2.04	118.45	123.68
27	A	407	PHO	C6-C7-C8	-2.03	109.34	115.92
26	A	405	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
26	A	408	CLA	CHB-C1B-C2B	-2.03	121.51	127.24
27	A	407	PHO	O2A-CGA-CBA	2.03	118.27	111.91
26	C	516	CLA	CHB-C4A-NA	2.02	127.31	124.51
20	K	102	BCR	C38-C26-C25	-2.02	122.25	124.53
32	C	501	SQD	O6-C1-C2	2.02	111.46	108.30
26	C	509	CLA	CHB-C1B-NB	-2.02	122.12	124.26
33	C	515	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
30	A	414	LHG	O8-C23-O10	-2.02	118.50	123.59
20	A	409	BCR	C21-C20-C19	-2.02	116.93	123.22
26	D	406	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
26	C	508	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
26	C	510	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
26	D	406	CLA	CHB-C4A-NA	2.01	127.29	124.51
20	A	409	BCR	C10-C11-C12	-2.00	116.96	123.22
22	V	201	HEC	CAD-C3D-C4D	2.00	128.15	124.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	V	201	HEC	NA

All (266) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	I	102	BCR	C1-C6-C7-C8
20	K	101	BCR	C5-C6-C7-C8
20	K	101	BCR	C7-C8-C9-C34
20	D	407	BCR	C1-C6-C7-C8
20	D	407	BCR	C7-C8-C9-C34
20	D	407	BCR	C21-C22-C23-C24
20	D	407	BCR	C37-C22-C23-C24
26	A	408	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	408	CLA	C4B-C3B-CAB-CBB
26	A	408	CLA	C4-C3-C5-C6
26	A	412	CLA	CHA-CBD-CGD-O1D
26	A	412	CLA	CHA-CBD-CGD-O2D
26	C	503	CLA	C2A-C1A-CHA-CBD
26	C	508	CLA	CHA-CBD-CGD-O1D
26	C	508	CLA	CHA-CBD-CGD-O2D
26	C	511	CLA	C2B-C3B-CAB-CBB
26	C	511	CLA	C4B-C3B-CAB-CBB
26	C	516	CLA	C2-C3-C5-C6
26	C	516	CLA	C4-C3-C5-C6
26	D	403	CLA	CMB-C2B-C3B-CAB
26	D	405	CLA	C2B-C3B-CAB-CBB
26	D	405	CLA	C4B-C3B-CAB-CBB
30	A	414	LHG	C3-O3-P-O4
30	A	414	LHG	C4-O6-P-O4
30	A	414	LHG	C4-O6-P-O5
30	A	415	LHG	C4-O6-P-O5
30	D	409	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O5
30	D	412	LHG	C3-O3-P-O4
30	D	412	LHG	C3-O3-P-O5
30	D	412	LHG	C3-O3-P-O6
30	D	412	LHG	C4-O6-P-O4
30	D	412	LHG	O7-C5-C6-O8
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C3-O3-P-O5
30	L	101	LHG	C4-O6-P-O4
30	L	101	LHG	C4-O6-P-O5
31	C	502	LMG	C11-C10-O7-C8
34	E	101	HEM	C2B-C3B-CAB-CBB
34	E	101	HEM	C2C-C3C-CAC-CBC
34	E	101	HEM	C4C-C3C-CAC-CBC
30	D	412	LHG	O10-C23-O8-C6
26	A	405	CLA	CBD-CGD-O2D-CED
31	C	502	LMG	O9-C10-O7-C8
26	C	506	CLA	C3-C5-C6-C7
26	C	516	CLA	C3-C5-C6-C7
26	C	509	CLA	CBA-CGA-O2A-C1
30	D	412	LHG	C24-C23-O8-C6
26	C	509	CLA	C3-C5-C6-C7
26	C	509	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	508	CLA	CBD-CGD-O2D-CED
28	A	410	PL9	C24-C26-C27-C28
28	D	408	PL9	C9-C11-C12-C13
30	A	414	LHG	C24-C23-O8-C6
30	D	412	LHG	C1-C2-C3-O3
26	A	405	CLA	O1D-CGD-O2D-CED
30	D	412	LHG	O2-C2-C3-O3
32	F	101	SQD	O47-C45-C46-O48
26	C	516	CLA	C8-C10-C11-C12
26	C	509	CLA	C2-C1-O2A-CGA
26	D	403	CLA	C2B-C3B-CAB-CBB
31	D	410	LMG	O6-C5-C6-O5
30	A	414	LHG	O10-C23-O8-C6
33	C	513	DGD	O6E-C1E-O5D-C6D
28	A	410	PL9	C9-C11-C12-C13
28	A	410	PL9	C14-C16-C17-C18
28	D	408	PL9	C39-C41-C42-C43
33	C	513	DGD	O6D-C5D-C6D-O5D
30	A	414	LHG	C3-O3-P-O6
30	A	414	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O3
30	D	412	LHG	C4-O6-P-O3
30	L	101	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O3
30	D	409	LHG	C24-C23-O8-C6
26	A	405	CLA	C2A-CAA-CBA-CGA
26	C	506	CLA	CBA-CGA-O2A-C1
32	F	101	SQD	C44-C45-C46-O48
30	A	415	LHG	C24-C23-O8-C6
33	D	413	DGD	CBB-CCB-CDB-CEB
31	B	603	LMG	C28-C29-C30-C31
33	C	513	DGD	C2E-C1E-O5D-C6D
33	C	514	DGD	C2E-C1E-O5D-C6D
30	A	415	LHG	O10-C23-O8-C6
30	D	409	LHG	O10-C23-O8-C6
26	C	510	CLA	C4-C3-C5-C6
27	A	407	PHO	C4-C3-C5-C6
26	C	507	CLA	C2A-CAA-CBA-CGA
33	C	513	DGD	C4D-C5D-C6D-O5D
20	D	407	BCR	C7-C8-C9-C10
30	A	415	LHG	C10-C11-C12-C13
33	C	514	DGD	O6E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
30	D	412	LHG	C13-C14-C15-C16
30	D	412	LHG	C12-C13-C14-C15
27	A	407	PHO	C2-C3-C5-C6
26	C	506	CLA	O1A-CGA-O2A-C1
20	I	102	BCR	C5-C6-C7-C8
20	K	101	BCR	C1-C6-C7-C8
20	D	407	BCR	C5-C6-C7-C8
26	C	516	CLA	CBA-CGA-O2A-C1
28	D	408	PL9	C30-C29-C31-C32
26	C	510	CLA	C2-C3-C5-C6
26	C	508	CLA	O1D-CGD-O2D-CED
26	B	601	CLA	C3-C5-C6-C7
30	D	412	LHG	C7-C8-C9-C10
34	E	101	HEM	C4B-C3B-CAB-CBB
26	A	412	CLA	C15-C16-C17-C18
26	C	503	CLA	C2A-CAA-CBA-CGA
26	C	516	CLA	O1A-CGA-O2A-C1
26	A	412	CLA	C1A-C2A-CAA-CBA
26	B	601	CLA	CBA-CGA-O2A-C1
30	L	101	LHG	O6-C4-C5-C6
22	V	201	HEC	C3D-CAD-CBD-CGD
26	C	516	CLA	C13-C15-C16-C17
33	C	513	DGD	O6E-C5E-C6E-O5E
26	C	511	CLA	CBA-CGA-O2A-C1
30	L	101	LHG	O2-C2-C3-O3
26	B	601	CLA	O1A-CGA-O2A-C1
28	A	410	PL9	C12-C11-C9-C10
28	D	408	PL9	C28-C29-C31-C32
26	C	511	CLA	O1A-CGA-O2A-C1
20	K	101	BCR	C37-C22-C23-C24
26	C	503	CLA	CBA-CGA-O2A-C1
30	A	414	LHG	C4-C5-C6-O8
30	D	412	LHG	C4-C5-C6-O8
30	L	101	LHG	C17-C18-C19-C20
26	C	509	CLA	C5-C6-C7-C8
26	A	412	CLA	C2C-C3C-CAC-CBC
28	A	410	PL9	C12-C11-C9-C8
20	D	407	BCR	C23-C24-C25-C26
33	C	514	DGD	C3B-C4B-C5B-C6B
20	K	101	BCR	C7-C8-C9-C10
30	D	409	LHG	O6-C4-C5-C6
26	C	516	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	510	CLA	C8-C10-C11-C12
30	D	412	LHG	C28-C29-C30-C31
27	A	407	PHO	CAD-CBD-CGD-O2D
31	C	502	LMG	C29-C28-O8-C9
22	V	201	HEC	C2B-C3B-CAB-CBB
32	C	501	SQD	O6-C44-C45-C46
26	C	504	CLA	CHA-CBD-CGD-O1D
26	C	504	CLA	CHA-CBD-CGD-O2D
26	C	509	CLA	CHA-CBD-CGD-O1D
26	C	516	CLA	CHA-CBD-CGD-O1D
26	C	503	CLA	O1A-CGA-O2A-C1
30	A	414	LHG	O7-C5-C6-O8
32	C	501	SQD	O6-C44-C45-O47
26	C	509	CLA	C8-C10-C11-C12
26	A	406	CLA	C1A-C2A-CAA-CBA
26	C	503	CLA	C1A-C2A-CAA-CBA
30	D	412	LHG	C29-C30-C31-C32
30	D	409	LHG	C3-O3-P-O6
28	D	408	PL9	C45-C44-C46-C47
31	C	502	LMG	O10-C28-O8-C9
26	A	406	CLA	C4B-C3B-CAB-CBB
30	D	412	LHG	C4-O6-P-O5
33	C	513	DGD	CBB-CCB-CDB-CEB
30	D	412	LHG	C25-C26-C27-C28
26	C	504	CLA	CAD-CBD-CGD-O1D
26	C	516	CLA	CAD-CBD-CGD-O1D
32	C	501	SQD	O5-C5-C6-S
30	L	101	LHG	O6-C4-C5-O7
26	A	412	CLA	C2A-CAA-CBA-CGA
20	K	104	BCR	C3-C4-C5-C33
28	D	408	PL9	C15-C14-C16-C17
26	C	516	CLA	C14-C13-C15-C16
26	C	516	CLA	C5-C6-C7-C8
26	A	406	CLA	C2B-C3B-CAB-CBB
26	C	509	CLA	C6-C7-C8-C10
26	A	405	CLA	C2-C1-O2A-CGA
26	A	408	CLA	C2-C1-O2A-CGA
26	C	505	CLA	C2-C1-O2A-CGA
26	C	508	CLA	C2-C1-O2A-CGA
30	D	409	LHG	O6-C4-C5-O7
26	C	506	CLA	C4-C3-C5-C6
20	T	102	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	T	102	BCR	C23-C24-C25-C30
20	D	407	BCR	C23-C24-C25-C30
26	C	508	CLA	O1A-CGA-O2A-C1
34	E	101	HEM	C2A-CAA-CBA-CGA
30	A	415	LHG	C4-O6-P-O3
30	A	415	LHG	C3-O3-P-O5
26	C	508	CLA	C5-C6-C7-C8
26	A	405	CLA	C3-C5-C6-C7
26	C	508	CLA	CBA-CGA-O2A-C1
20	K	101	BCR	C21-C22-C23-C24
26	C	506	CLA	C2-C3-C5-C6
33	C	514	DGD	C1A-C2A-C3A-C4A
33	C	515	DGD	O6D-C1D-O3G-C3G
26	C	506	CLA	C2-C1-O2A-CGA
26	D	405	CLA	C2-C1-O2A-CGA
33	C	515	DGD	C2D-C1D-O3G-C3G
31	C	502	LMG	C37-C38-C39-C40
26	C	506	CLA	C2A-CAA-CBA-CGA
33	C	513	DGD	C2A-C3A-C4A-C5A
28	D	408	PL9	C13-C14-C16-C17
28	D	408	PL9	C43-C44-C46-C47
28	A	410	PL9	C4-C3-C7-C8
30	L	101	LHG	C1-C2-C3-O3
26	C	505	CLA	C3-C5-C6-C7
32	C	501	SQD	O49-C7-O47-C45
26	A	412	CLA	C4C-C3C-CAC-CBC
34	E	101	HEM	CAD-CBD-CGD-O1D
32	C	501	SQD	C7-C8-C9-C10
30	D	412	LHG	C16-C17-C18-C19
33	D	413	DGD	C6A-C7A-C8A-C9A
22	V	201	HEC	C4B-C3B-CAB-CBB
34	E	101	HEM	CAD-CBD-CGD-O2D
28	A	410	PL9	C30-C29-C31-C32
26	C	503	CLA	C2-C1-O2A-CGA
27	A	407	PHO	C2-C1-O2A-CGA
26	C	510	CLA	O1A-CGA-O2A-C1
30	A	414	LHG	C28-C29-C30-C31
20	K	101	BCR	C23-C24-C25-C30
20	A	409	BCR	C1-C6-C7-C8
20	A	409	BCR	C23-C24-C25-C30
30	D	412	LHG	C30-C31-C32-C33
32	C	501	SQD	C45-C44-O6-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	514	DGD	C5D-C6D-O5D-C1E
26	C	510	CLA	CBA-CGA-O2A-C1
28	D	408	PL9	C40-C39-C41-C42
28	D	408	PL9	C18-C19-C21-C22
33	C	514	DGD	C8B-C9B-CAB-CBB
27	A	407	PHO	C3A-C2A-CAA-CBA
33	C	513	DGD	O2G-C1B-C2B-C3B
26	C	505	CLA	CAD-CBD-CGD-O2D
26	B	601	CLA	C2-C1-O2A-CGA
28	A	410	PL9	C45-C44-C46-C47
28	A	410	PL9	C28-C29-C31-C32
30	A	415	LHG	O7-C7-C8-C9
30	D	412	LHG	O8-C23-C24-C25
30	D	412	LHG	C27-C28-C29-C30
33	C	514	DGD	CBB-CCB-CDB-CEB
26	D	405	CLA	C8-C10-C11-C12
31	D	410	LMG	O7-C10-C11-C12
26	A	406	CLA	CHA-CBD-CGD-O1D
26	A	406	CLA	CHA-CBD-CGD-O2D
26	C	505	CLA	CHA-CBD-CGD-O2D
26	C	516	CLA	CHA-CBD-CGD-O2D
34	E	101	HEM	CAA-CBA-CGA-O1A
30	D	409	LHG	O7-C5-C6-O8
26	C	505	CLA	C5-C6-C7-C8
34	E	101	HEM	CAA-CBA-CGA-O2A
22	V	201	HEC	C2C-C3C-CAC-CBC
27	A	407	PHO	CHA-CBD-CGD-O1D
26	C	506	CLA	CAA-CBA-CGA-O2A
28	A	410	PL9	C41-C42-C43-C44
28	A	410	PL9	C43-C44-C46-C47
30	D	412	LHG	O10-C23-C24-C25
32	C	501	SQD	C8-C7-O47-C45
30	A	415	LHG	O9-C7-C8-C9
26	C	506	CLA	CAA-CBA-CGA-O1A
33	C	513	DGD	O1B-C1B-C2B-C3B
26	C	511	CLA	C3-C5-C6-C7
31	D	410	LMG	O9-C10-C11-C12
26	A	408	CLA	C2-C3-C5-C6
26	C	506	CLA	CAD-CBD-CGD-O1D
30	A	414	LHG	C30-C31-C32-C33
26	C	510	CLA	CAA-CBA-CGA-O2A
31	C	502	LMG	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	A	405	CLA	C4-C3-C5-C6
30	A	414	LHG	O8-C23-C24-C25
26	C	510	CLA	CAA-CBA-CGA-O1A
32	F	101	SQD	O6-C44-C45-O47
30	A	414	LHG	O10-C23-C24-C25
33	D	413	DGD	CDA-CEA-CFA-CGA

There are no ring outliers.

40 monomers are involved in 92 short contacts:

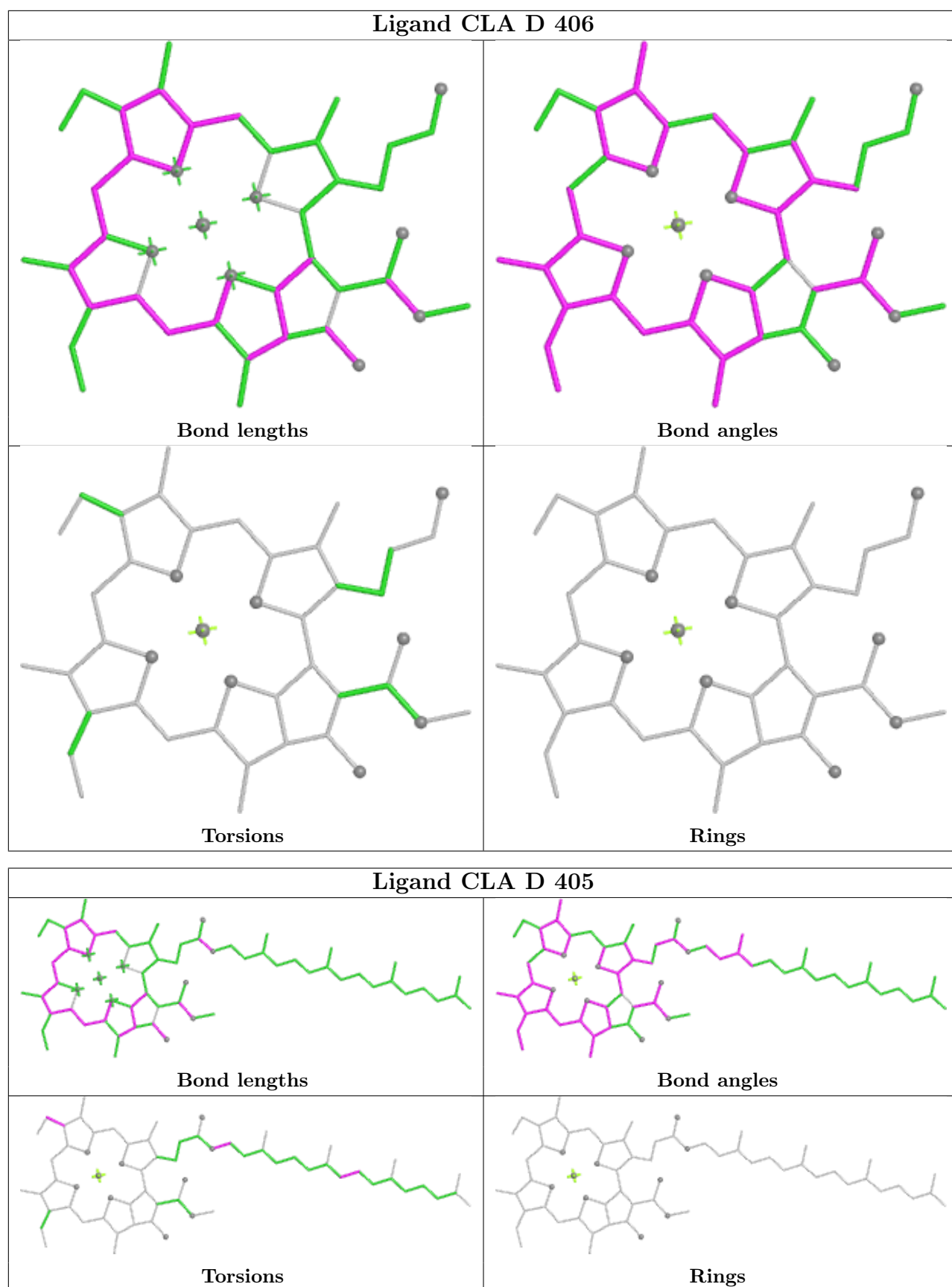
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	405	CLA	5	0
26	A	408	CLA	2	0
26	C	510	CLA	4	0
23	A	401	OEX	1	0
21	J	101	LMT	1	0
26	C	506	CLA	3	0
26	B	601	CLA	1	0
20	K	102	BCR	4	0
33	C	515	DGD	1	0
32	C	501	SQD	1	0
30	A	415	LHG	1	0
20	K	101	BCR	3	0
20	D	407	BCR	2	0
26	C	503	CLA	1	0
28	D	408	PL9	2	0
30	L	101	LHG	1	0
30	A	414	LHG	3	0
26	C	505	CLA	4	0
30	D	412	LHG	2	0
34	E	101	HEM	2	0
27	A	407	PHO	1	0
27	D	401	PHO	5	0
26	C	516	CLA	3	0
33	C	513	DGD	1	0
30	D	409	LHG	1	0
26	A	412	CLA	4	0
26	C	507	CLA	1	0
26	C	508	CLA	3	0
26	D	403	CLA	2	0
26	C	509	CLA	5	0
20	T	102	BCR	1	0

Continued on next page...

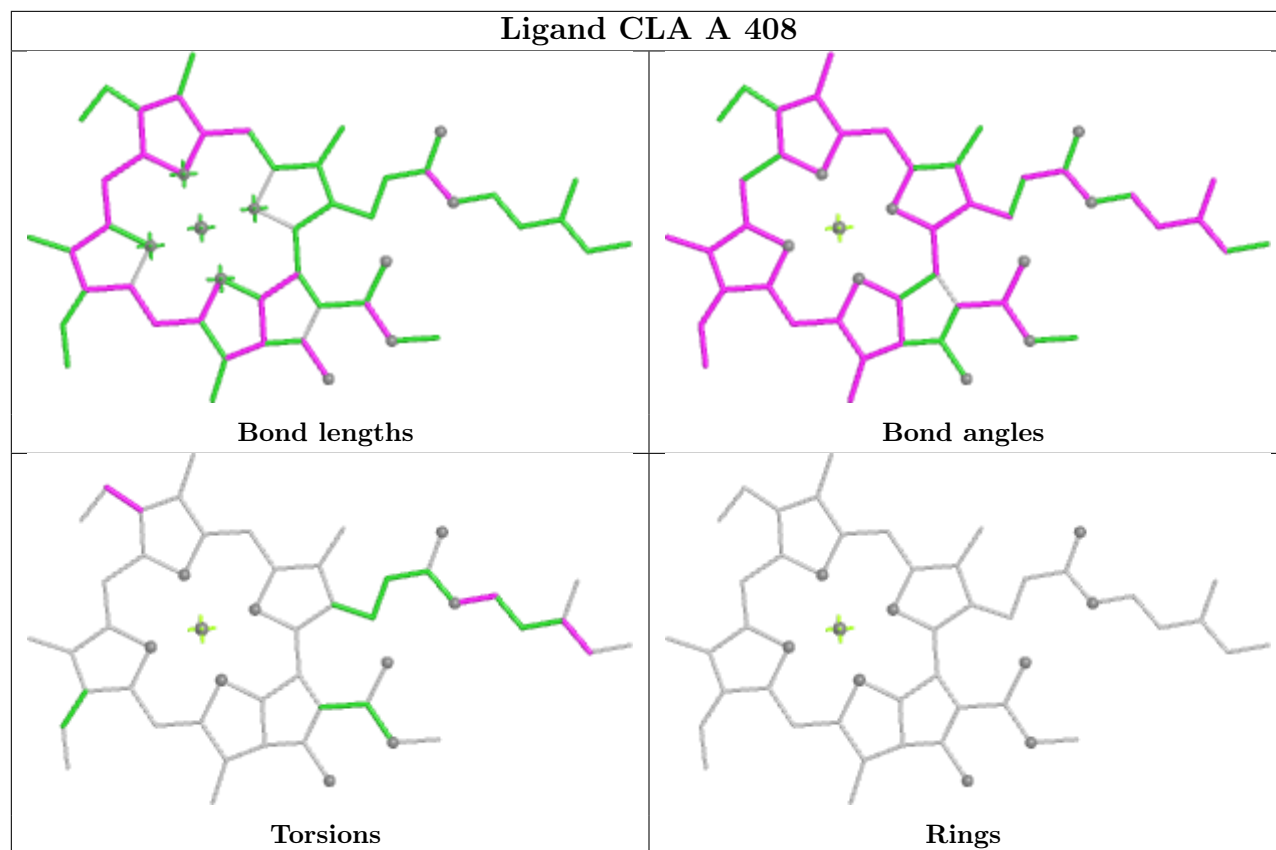
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	K	104	BCR	1	0
31	C	502	LMG	3	0
28	A	410	PL9	7	0
33	D	413	DGD	3	0
26	C	511	CLA	7	0
33	C	514	DGD	4	0
26	A	406	CLA	2	0
26	A	405	CLA	8	0
26	C	504	CLA	4	0

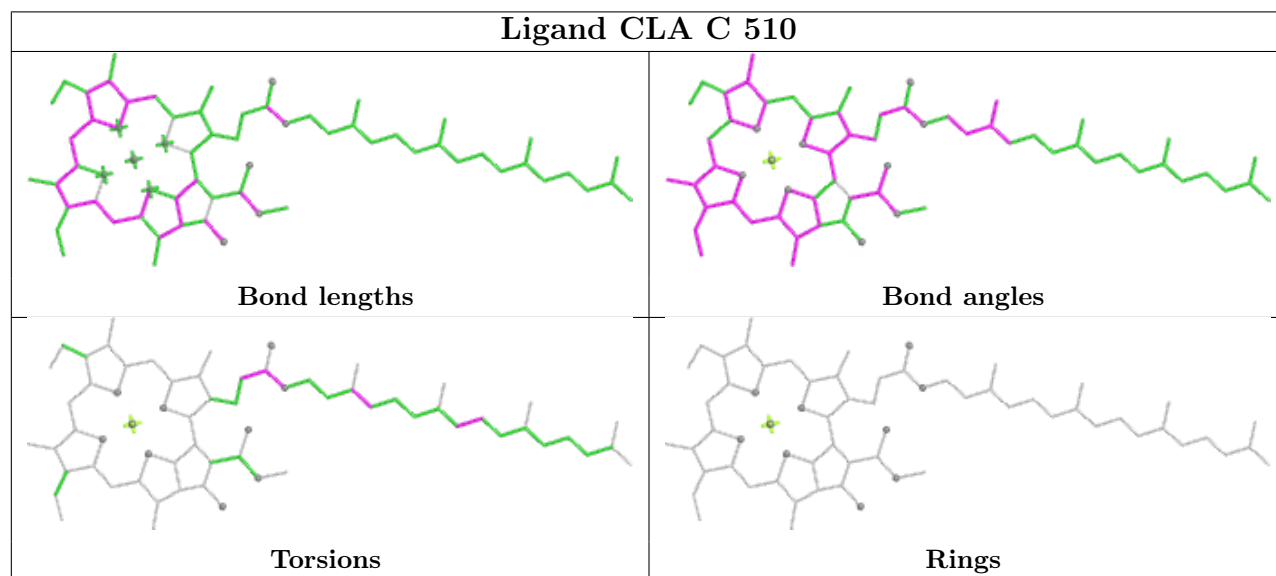
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

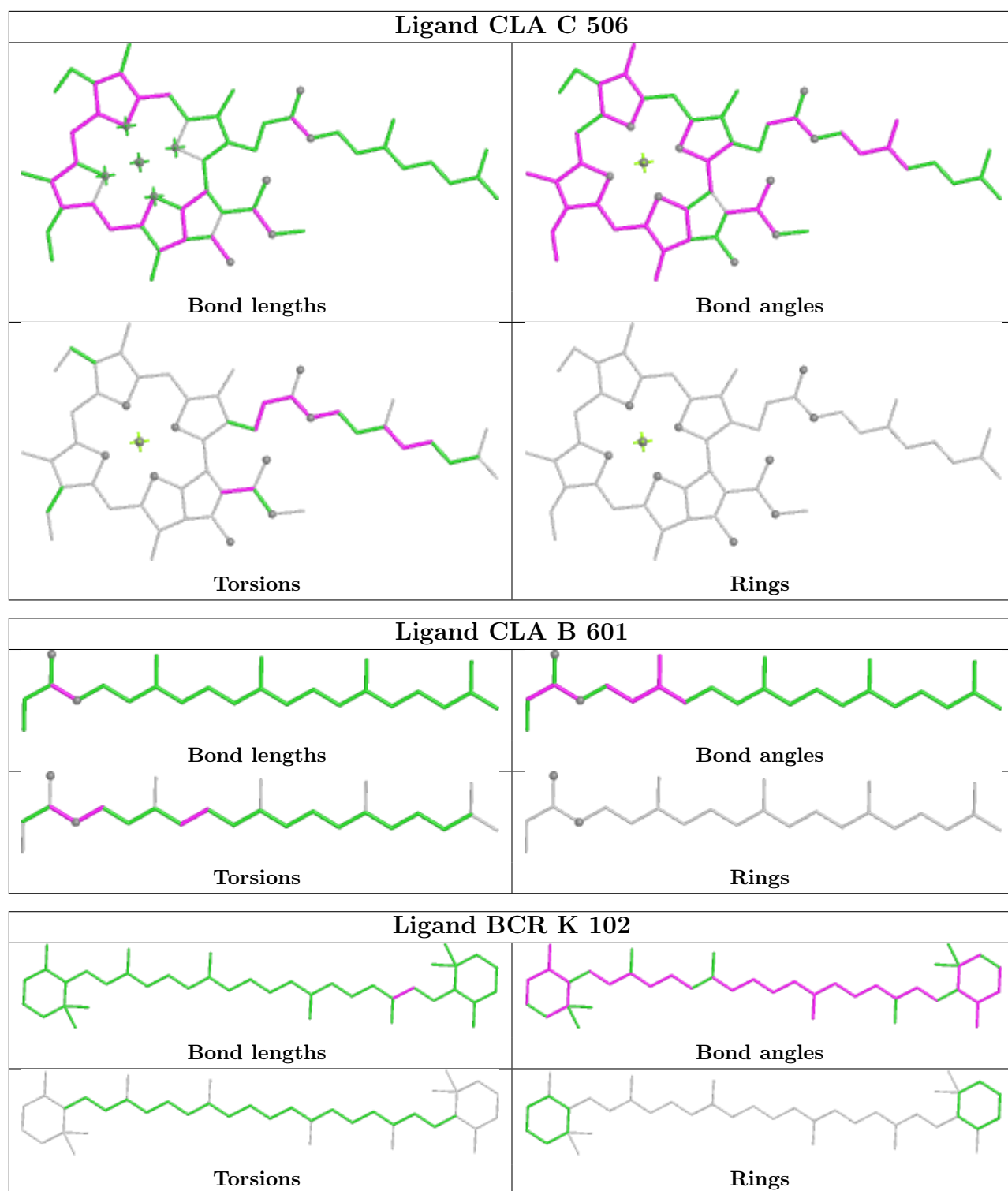


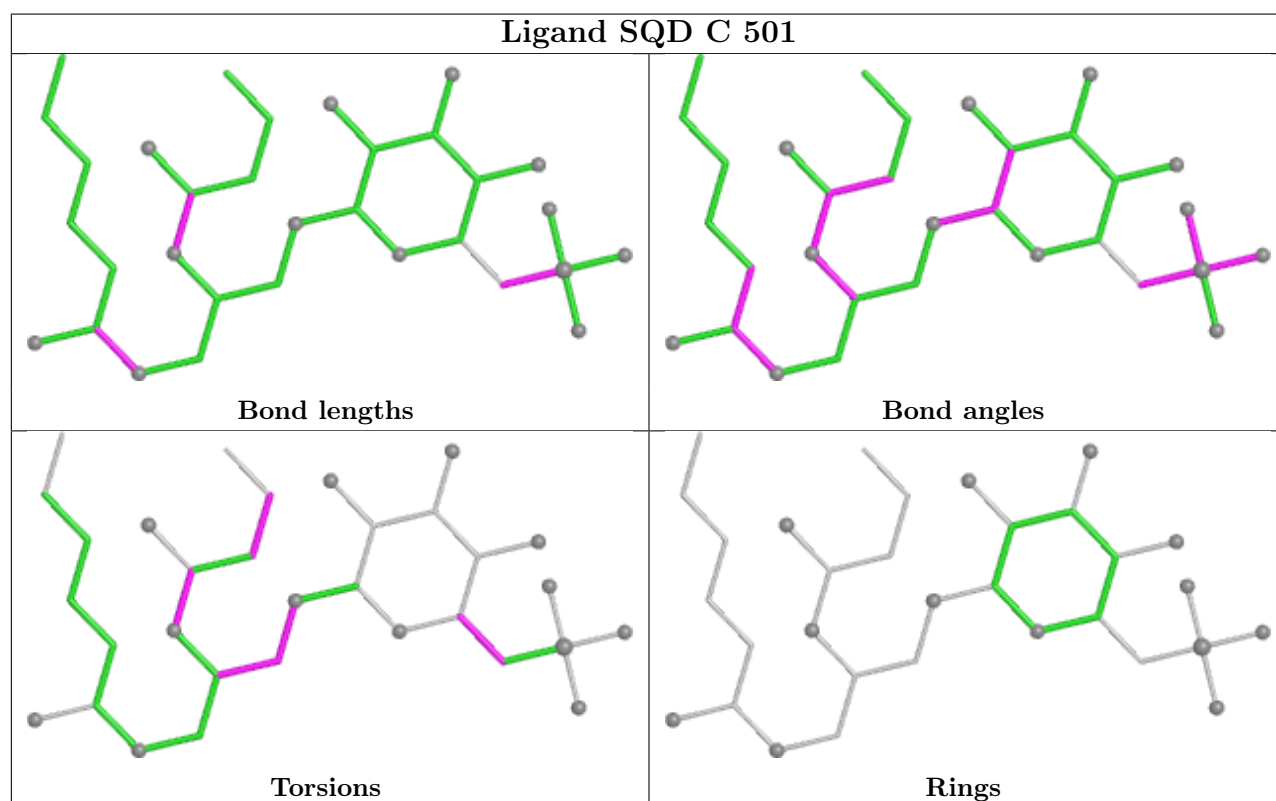
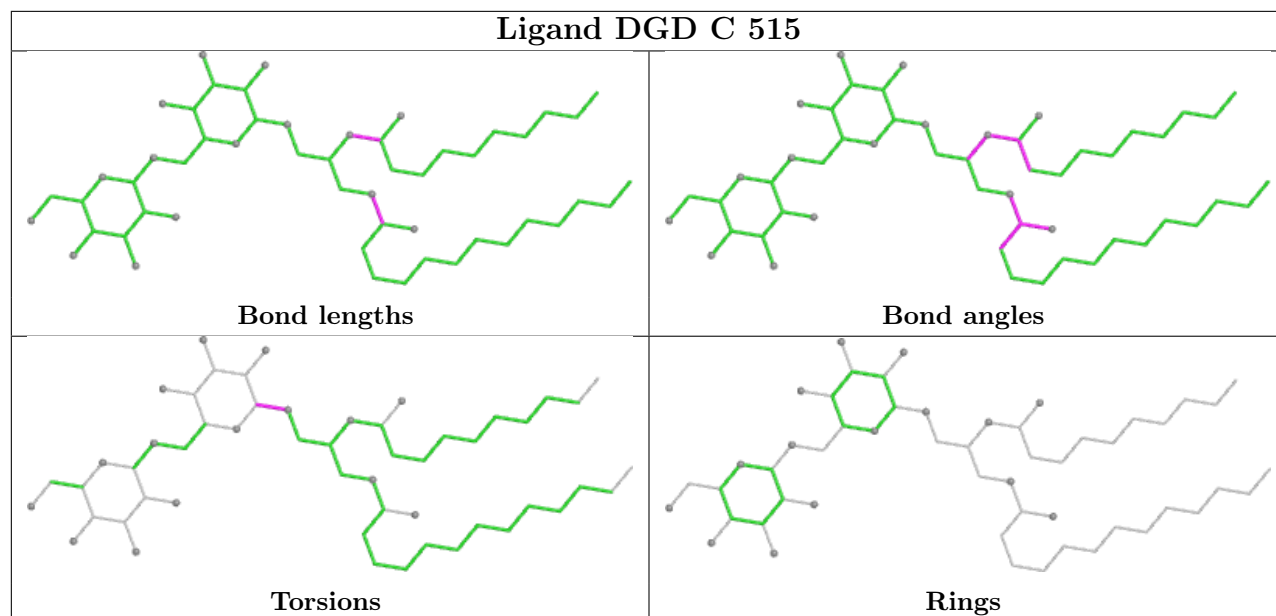
Ligand CLA A 408

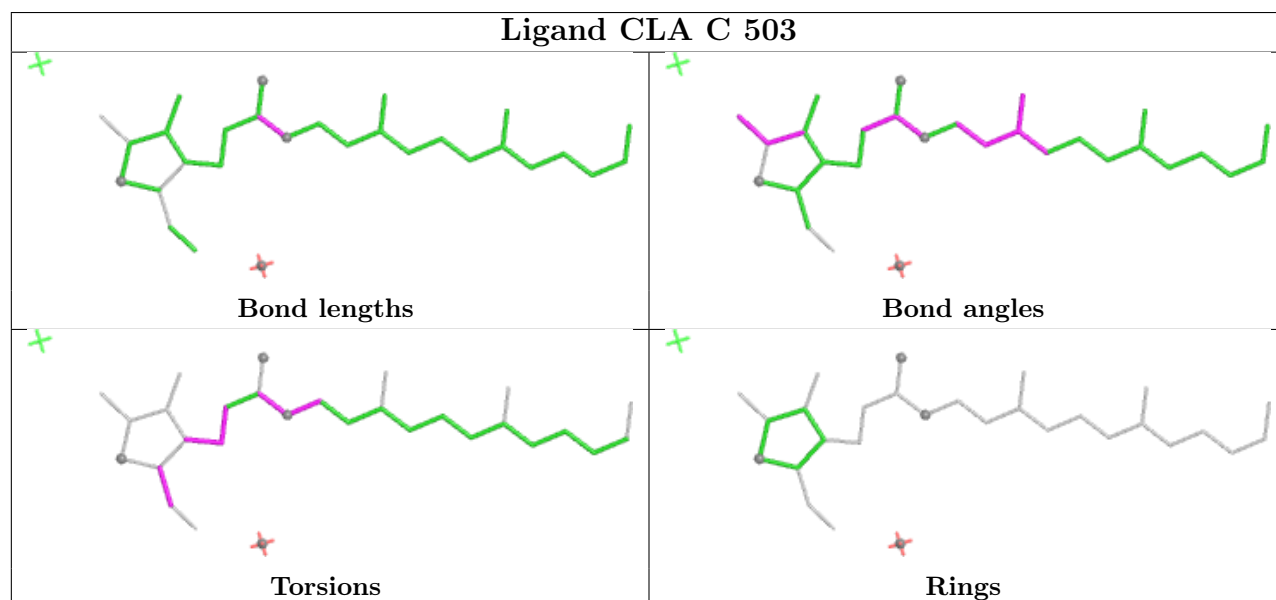
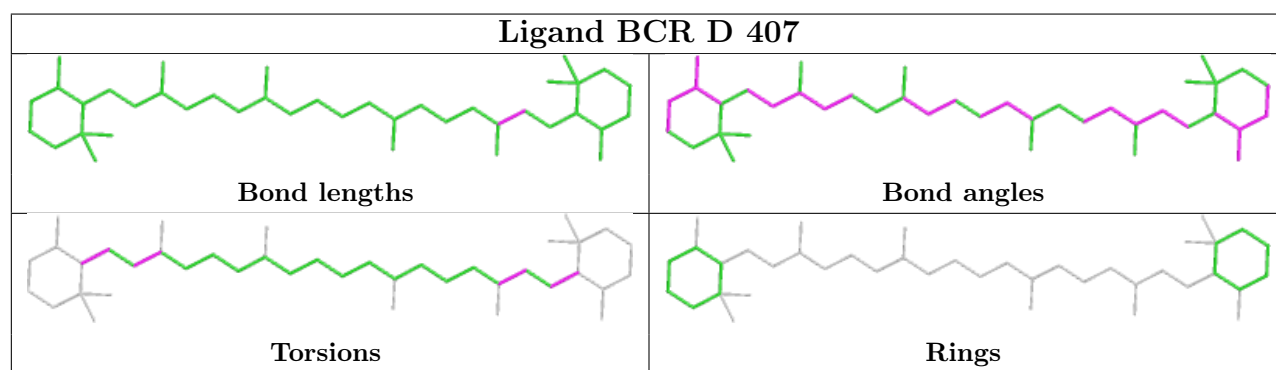
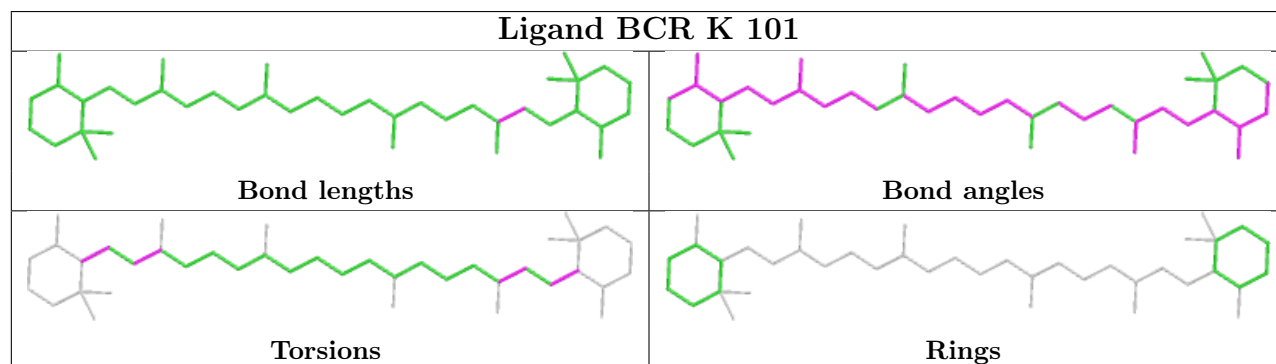
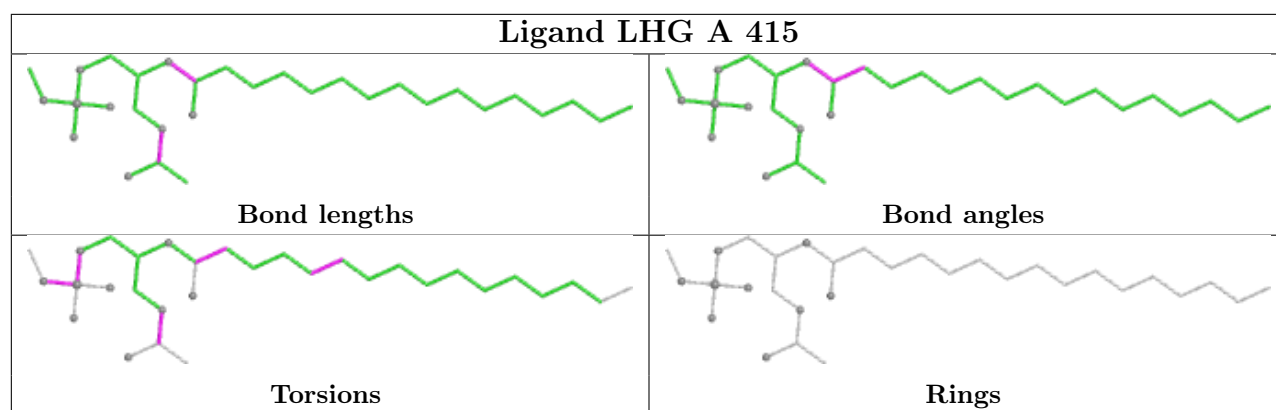


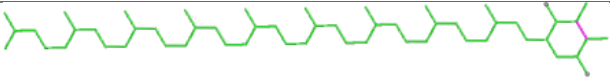
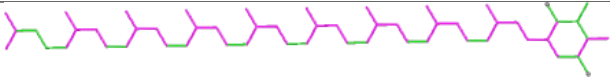
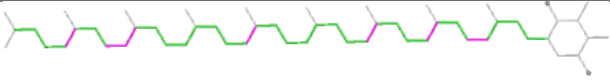
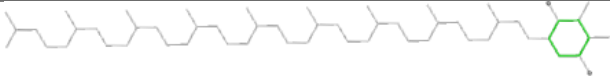
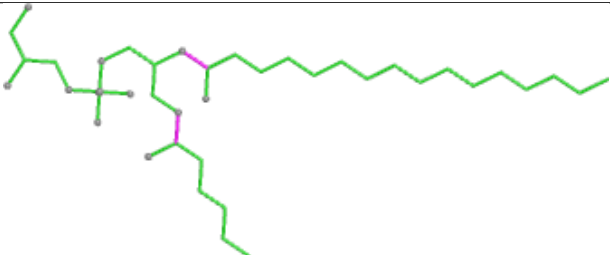
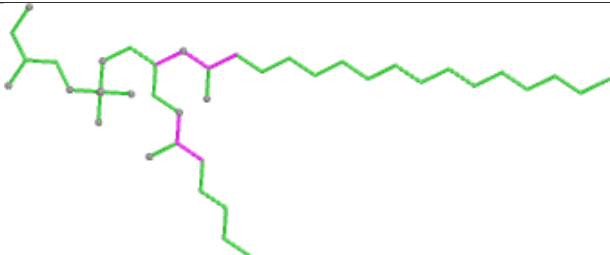
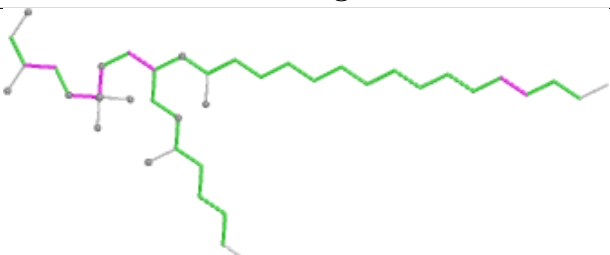
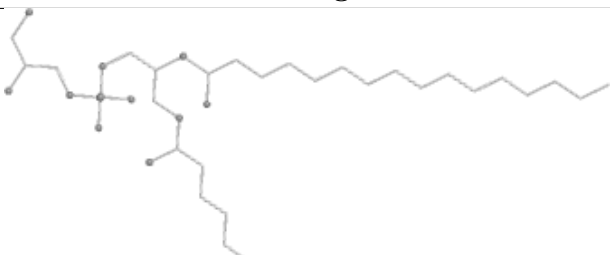
Ligand CLA C 510

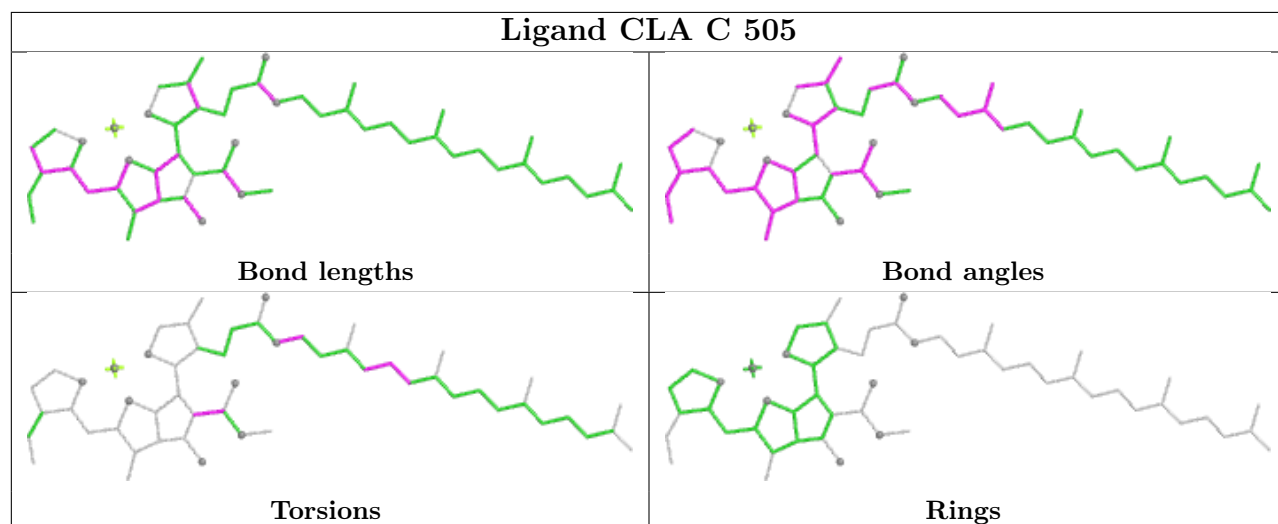
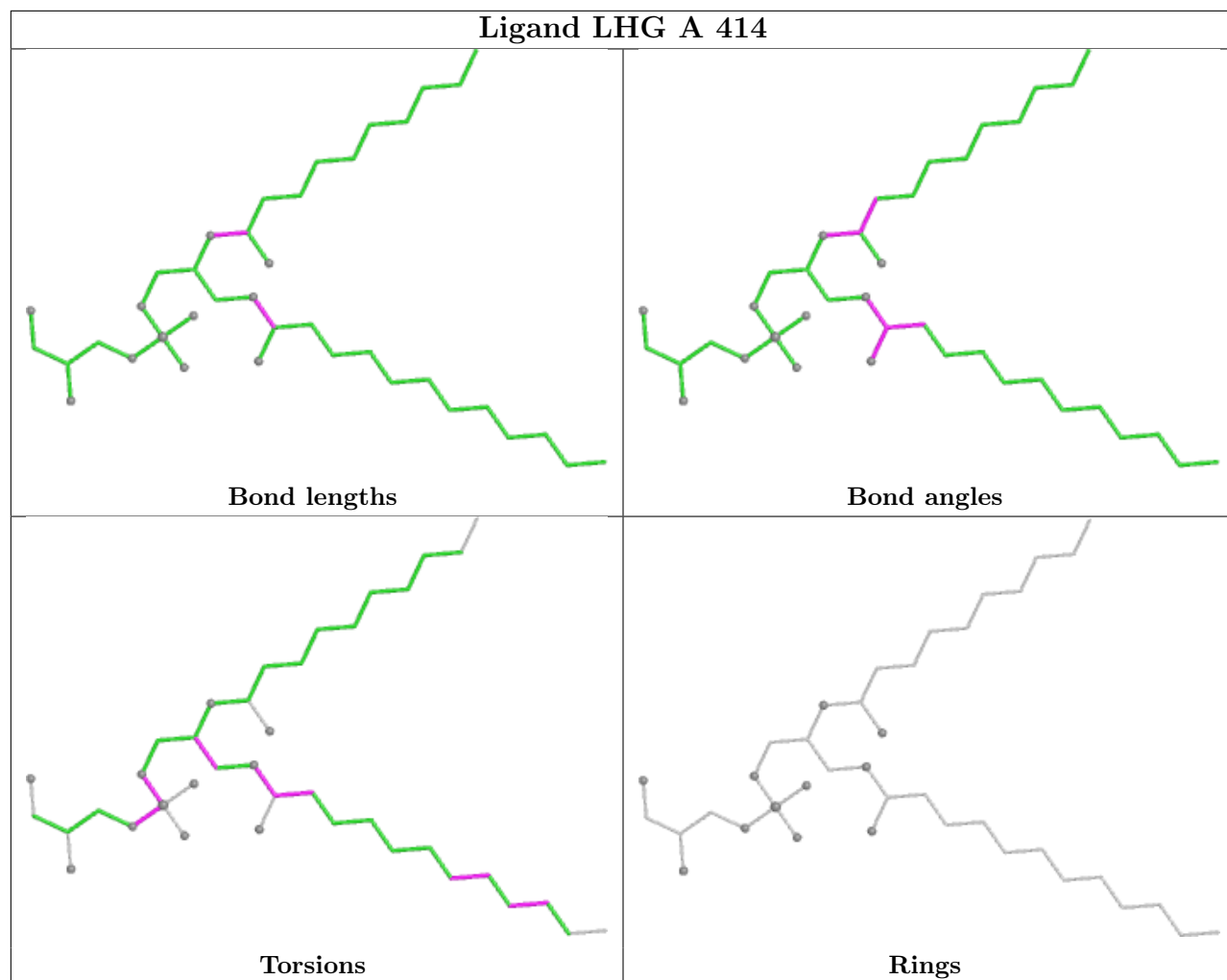


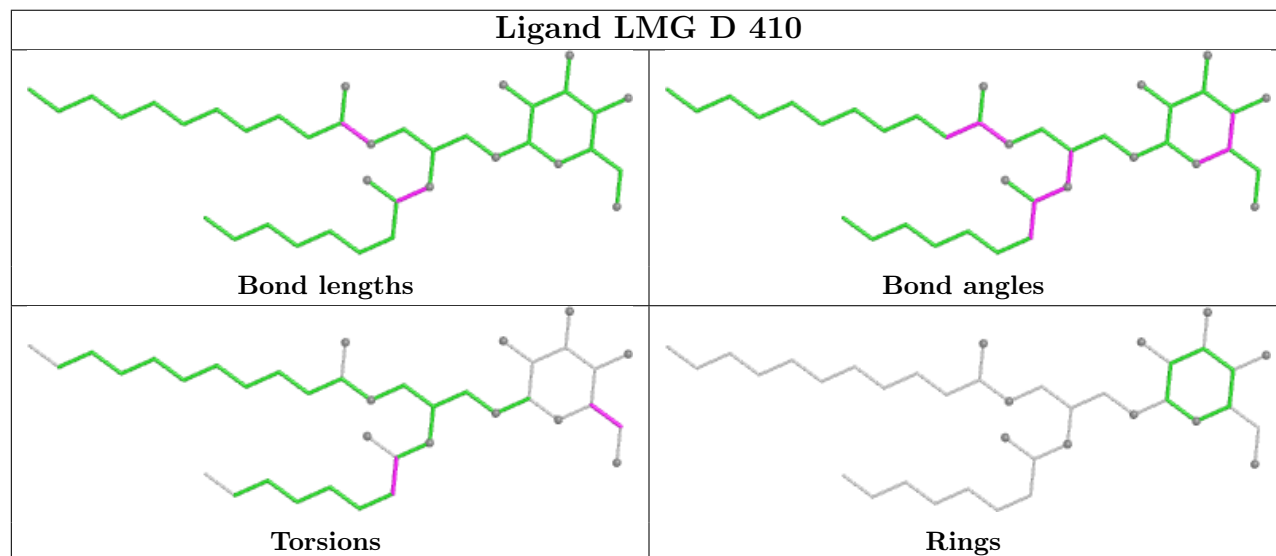
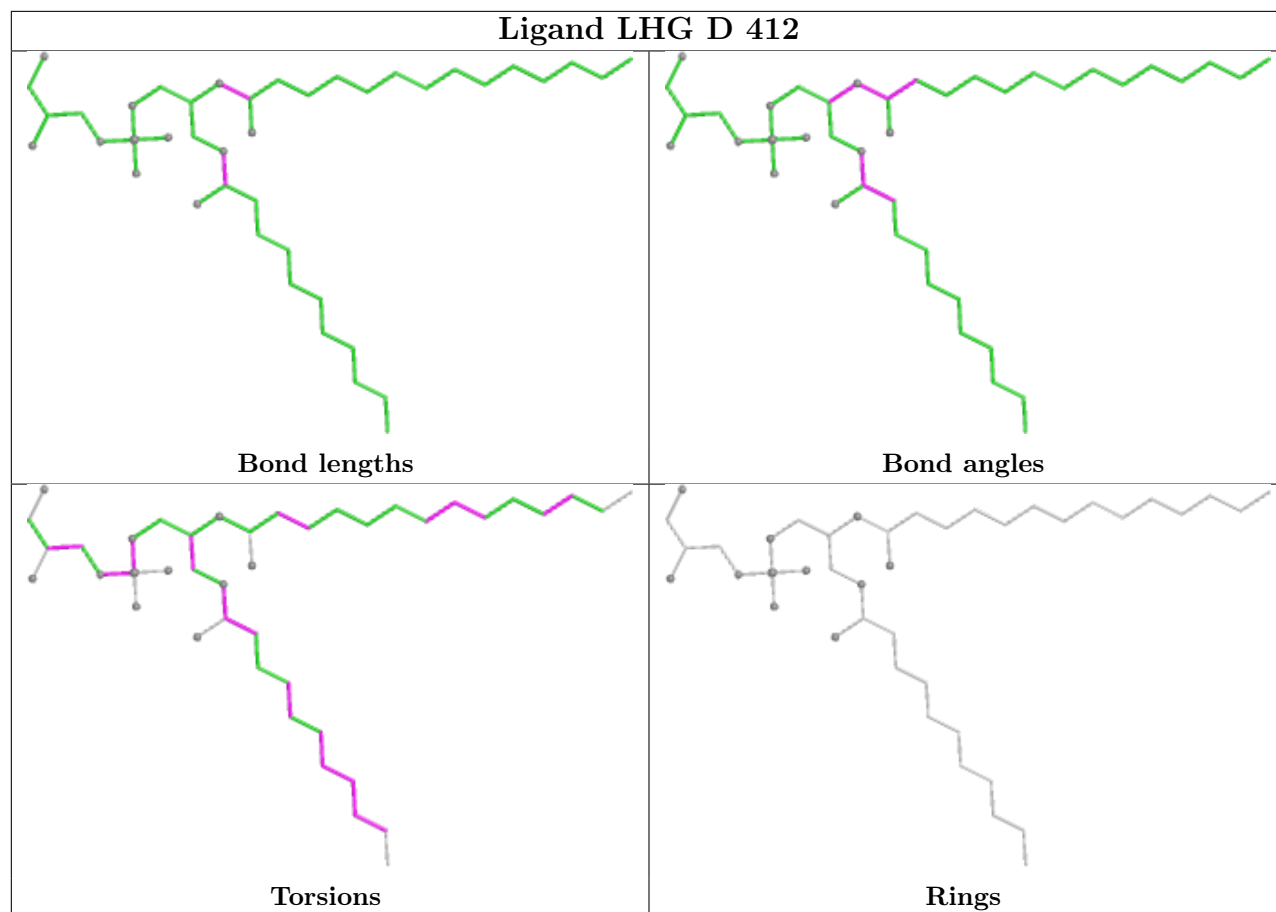


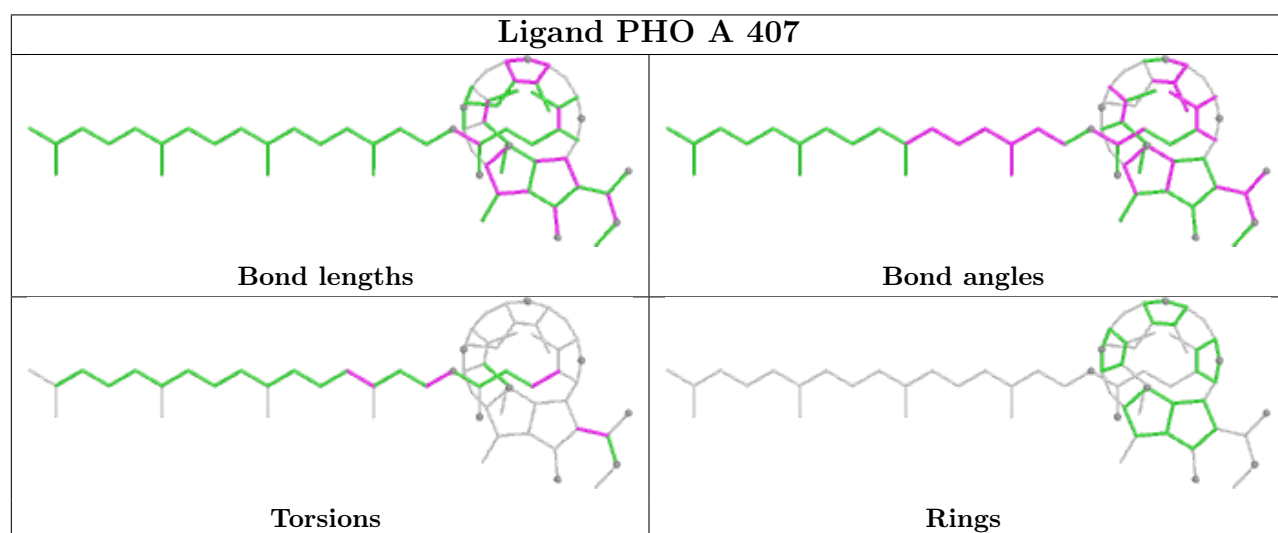
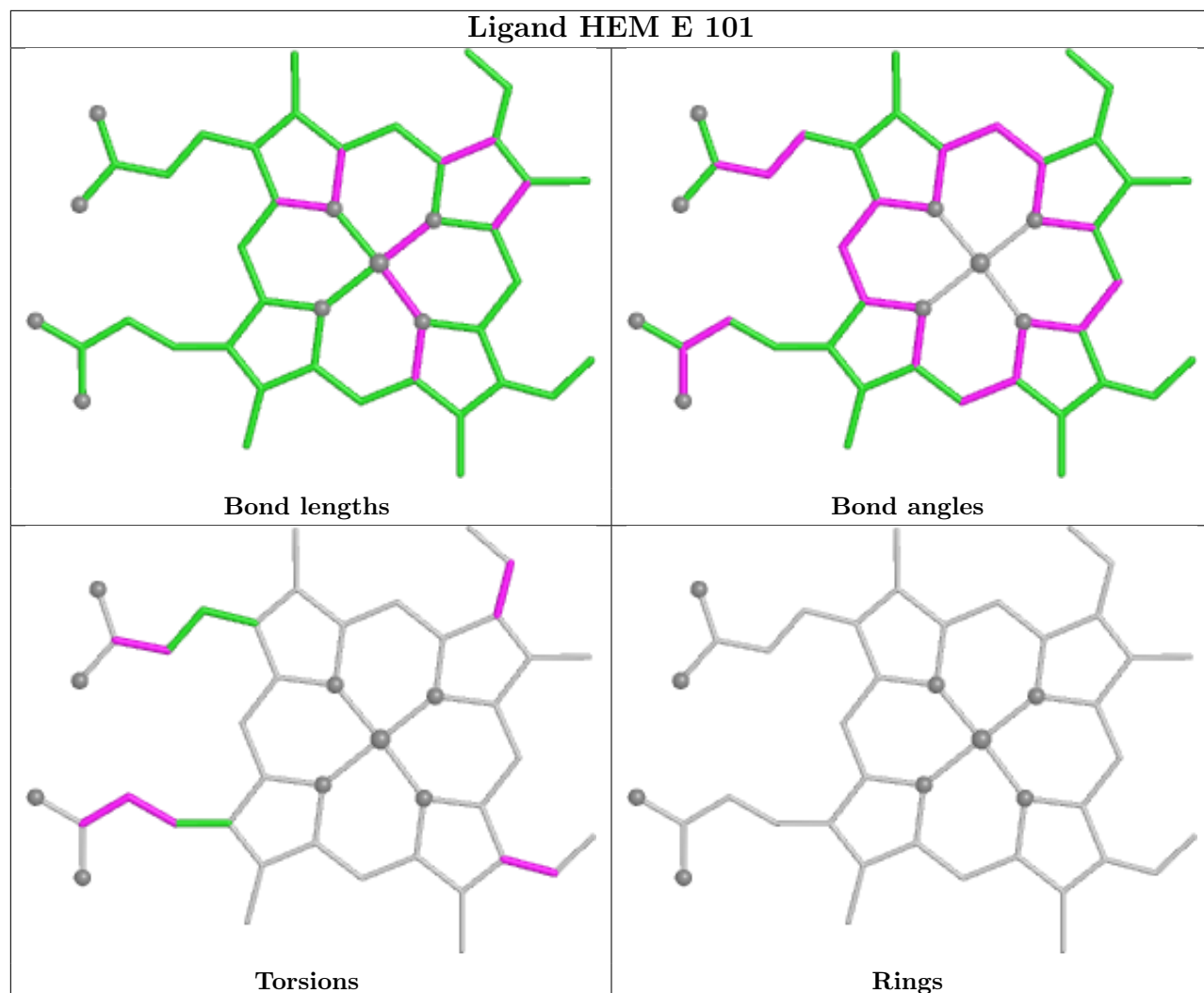


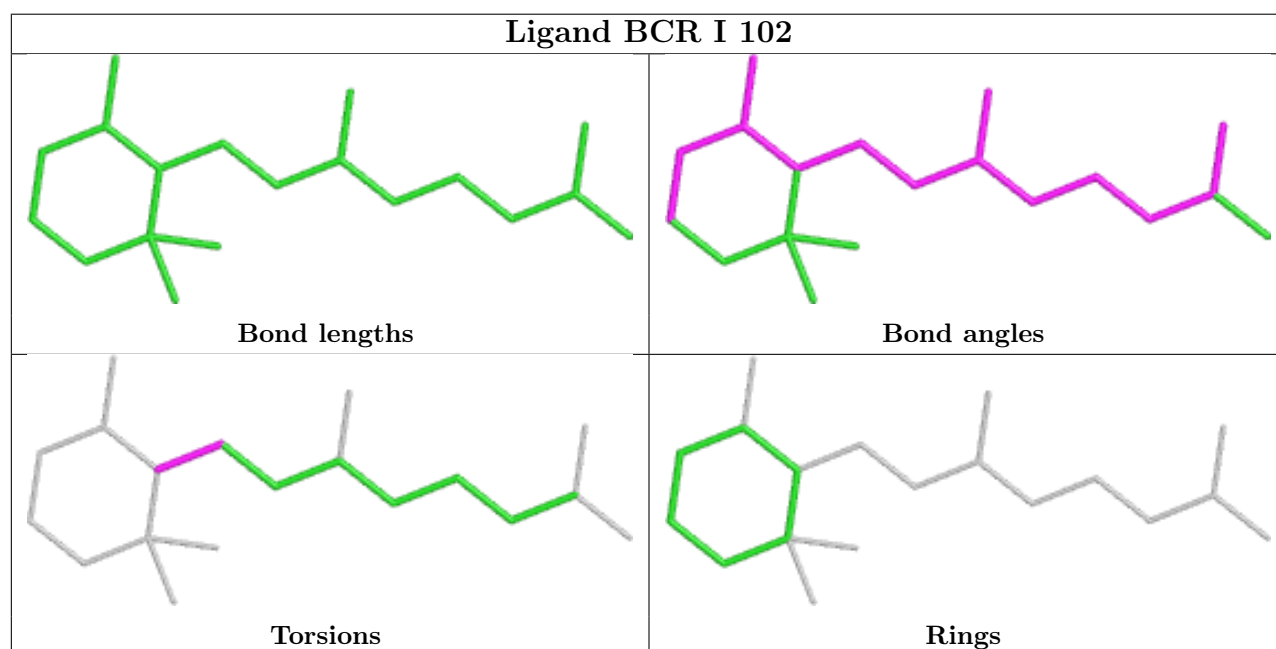
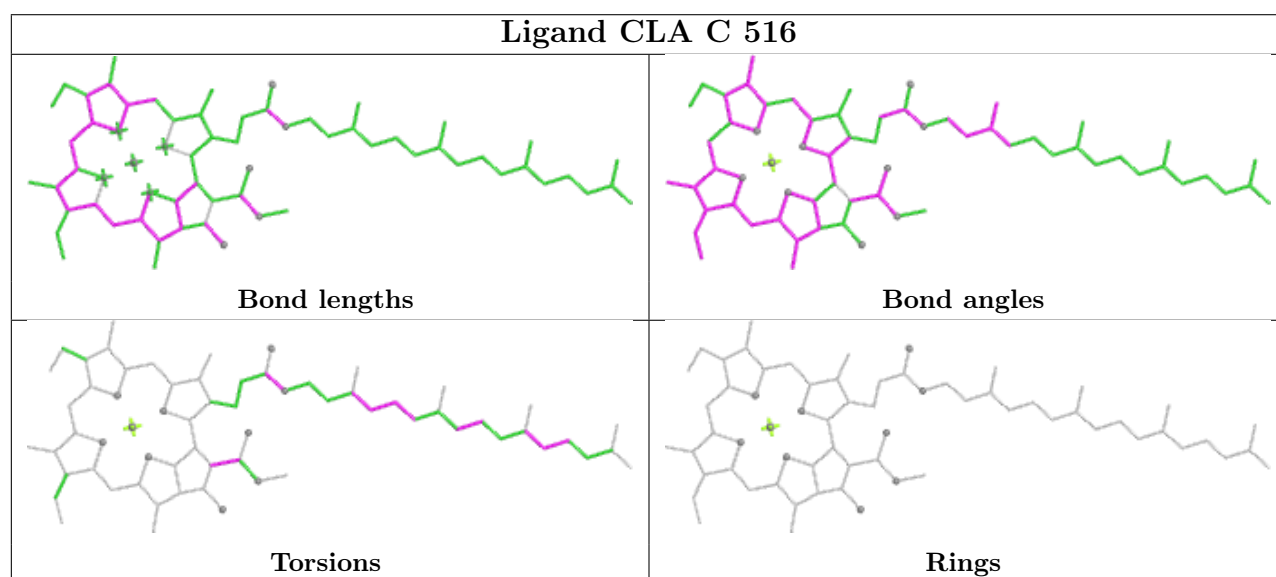
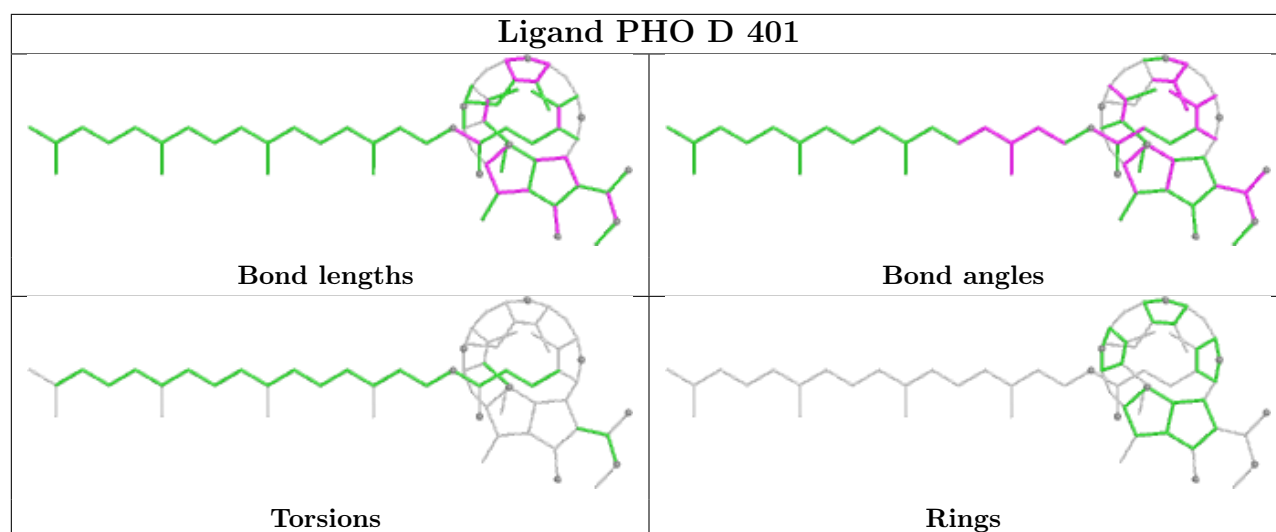


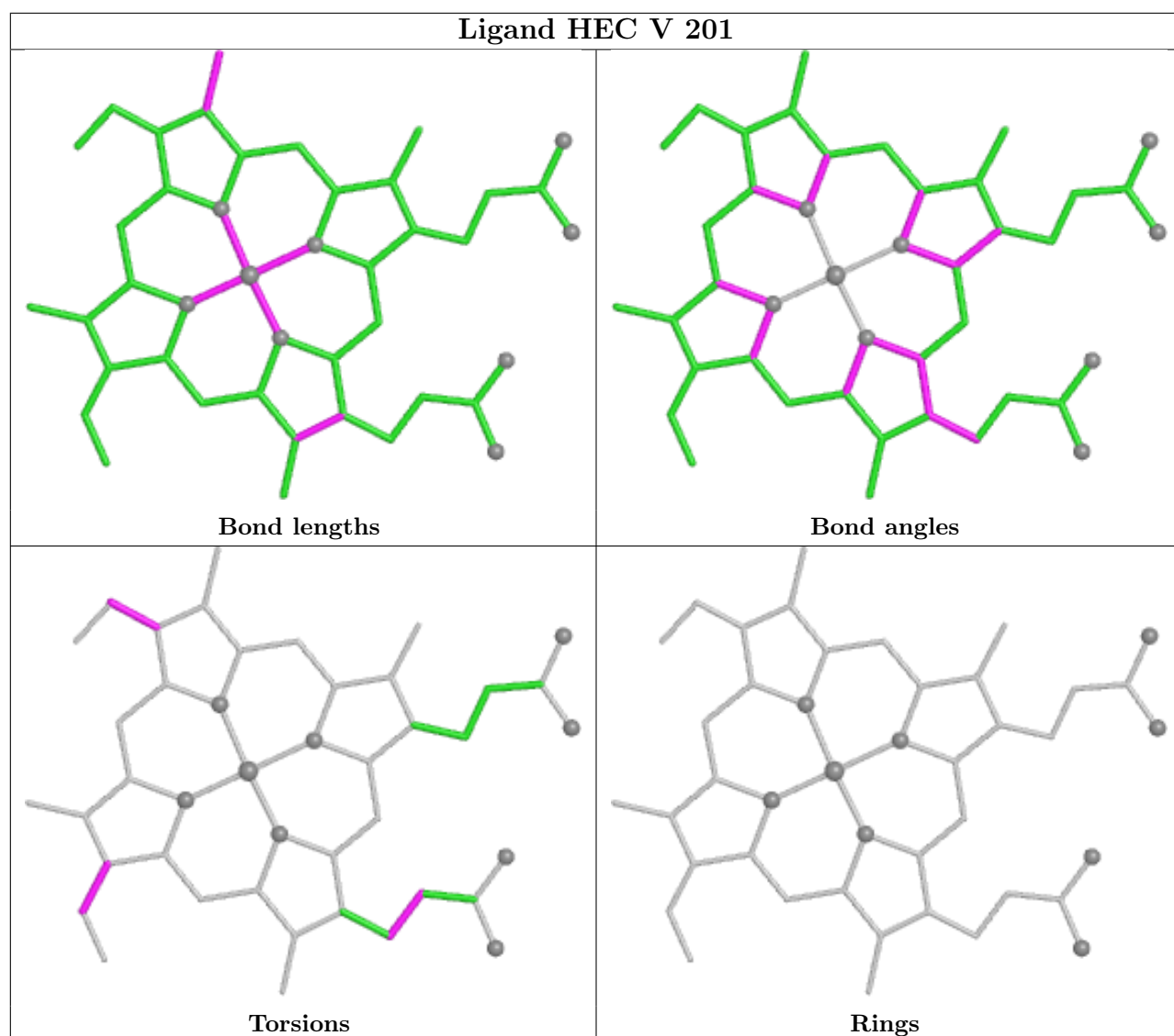
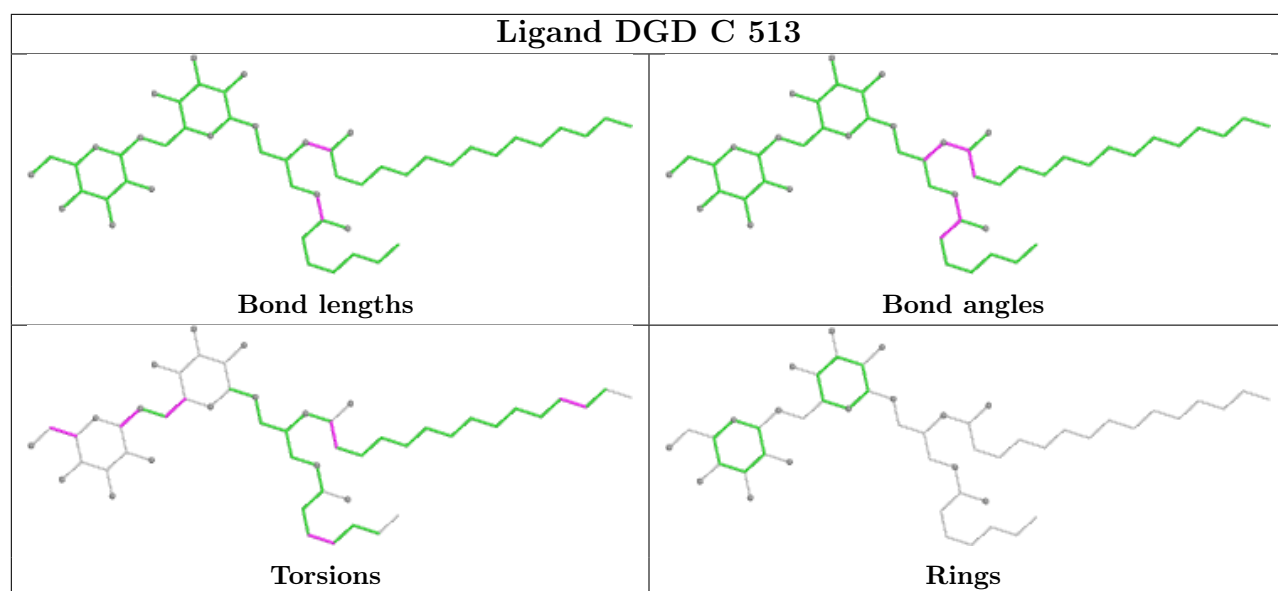
Ligand PL9 D 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LHG L 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

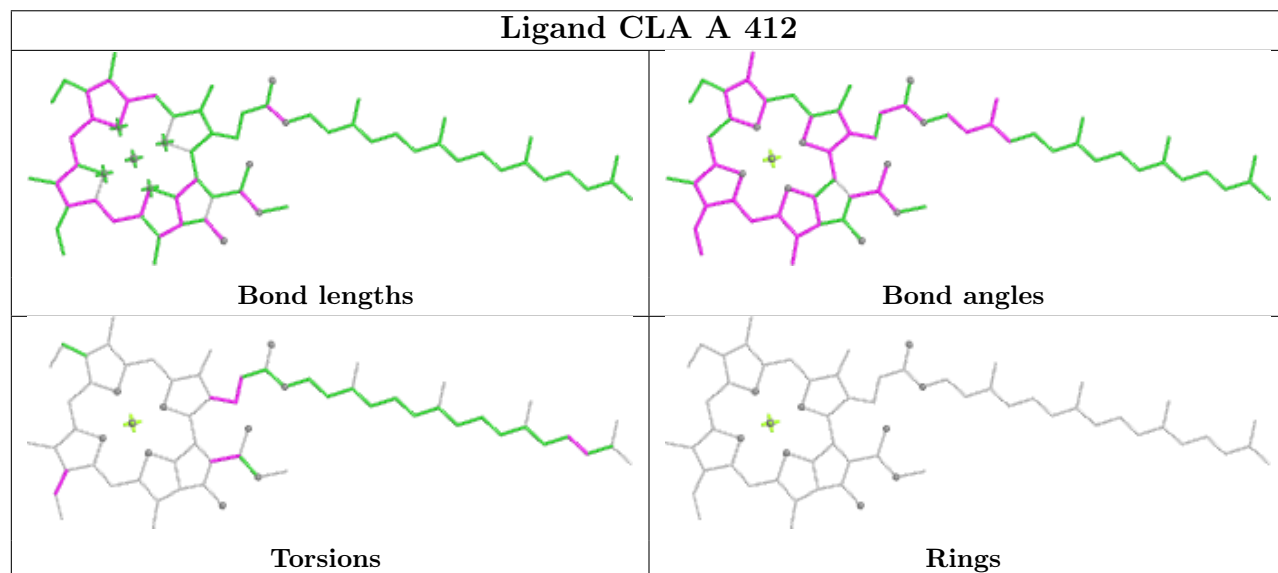
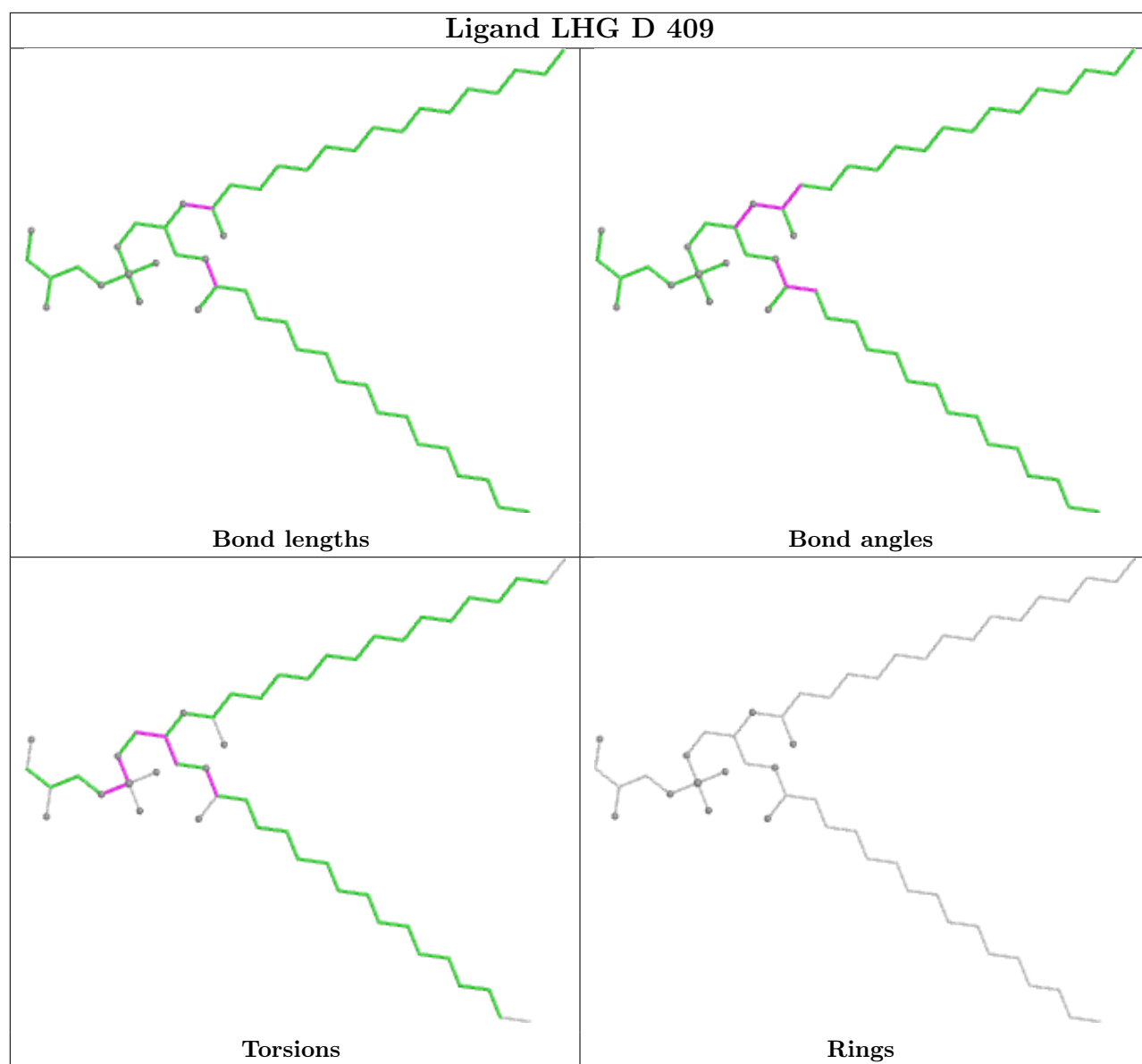


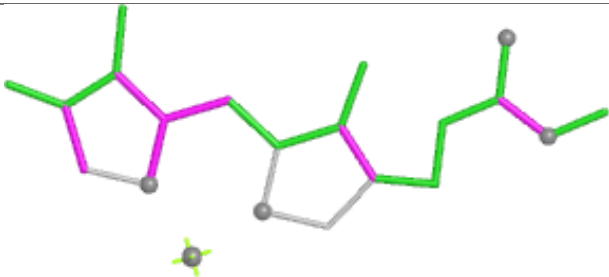
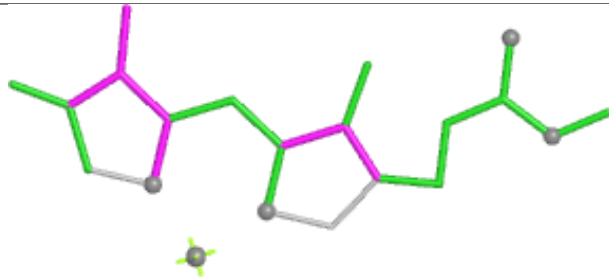
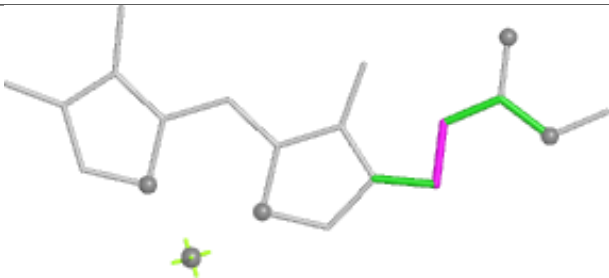
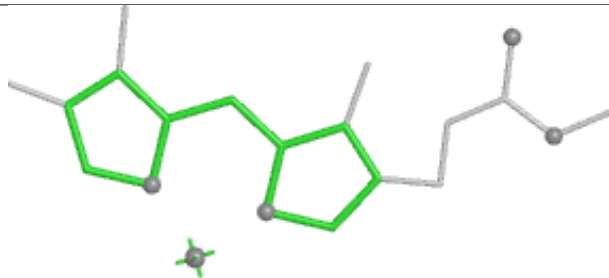


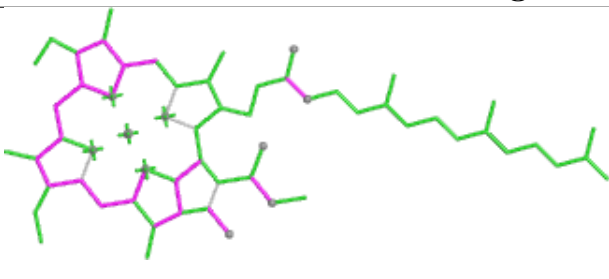
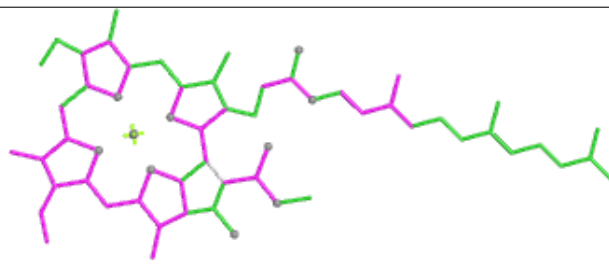
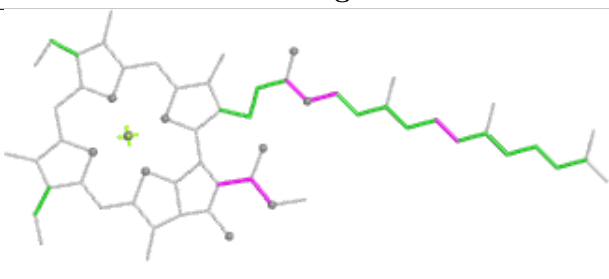
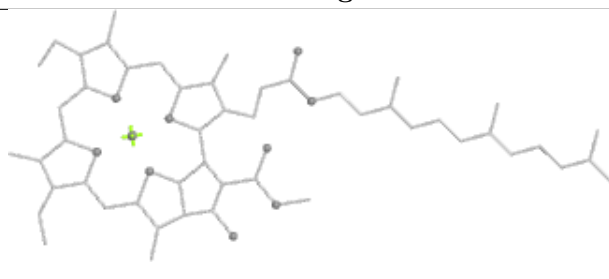




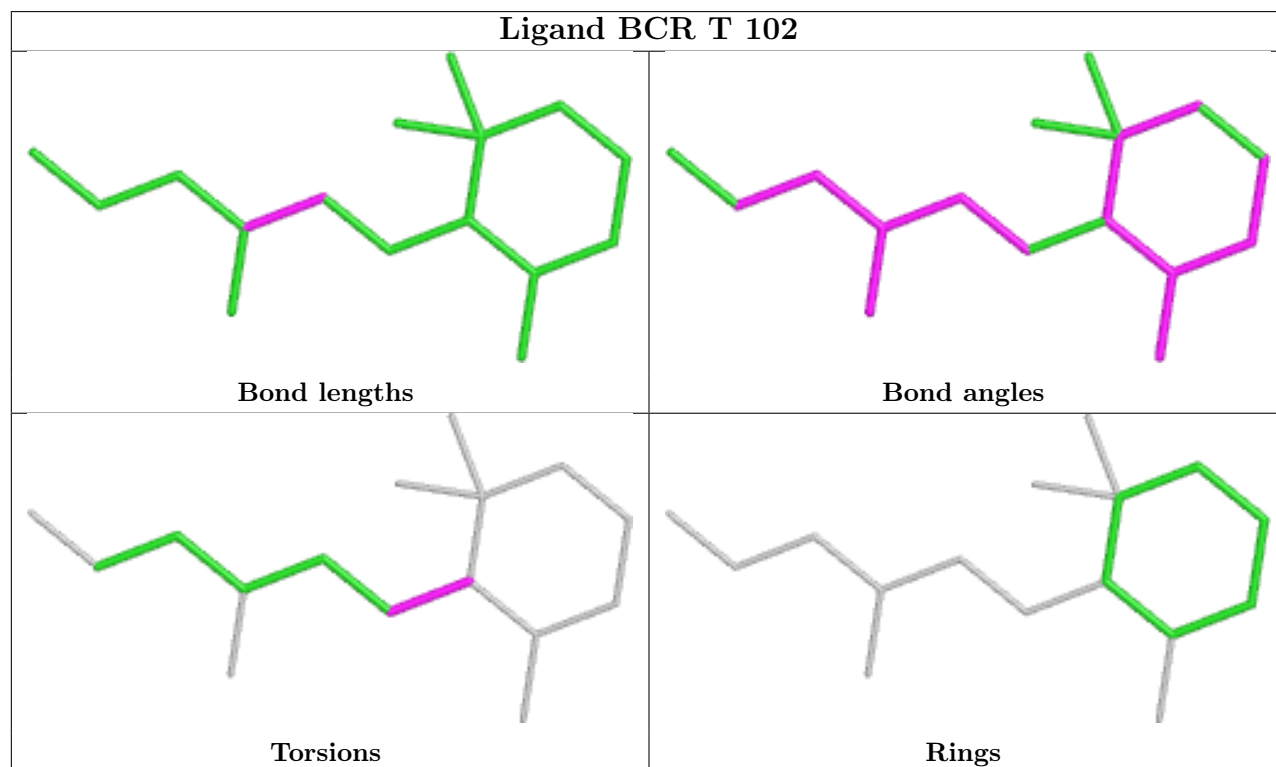
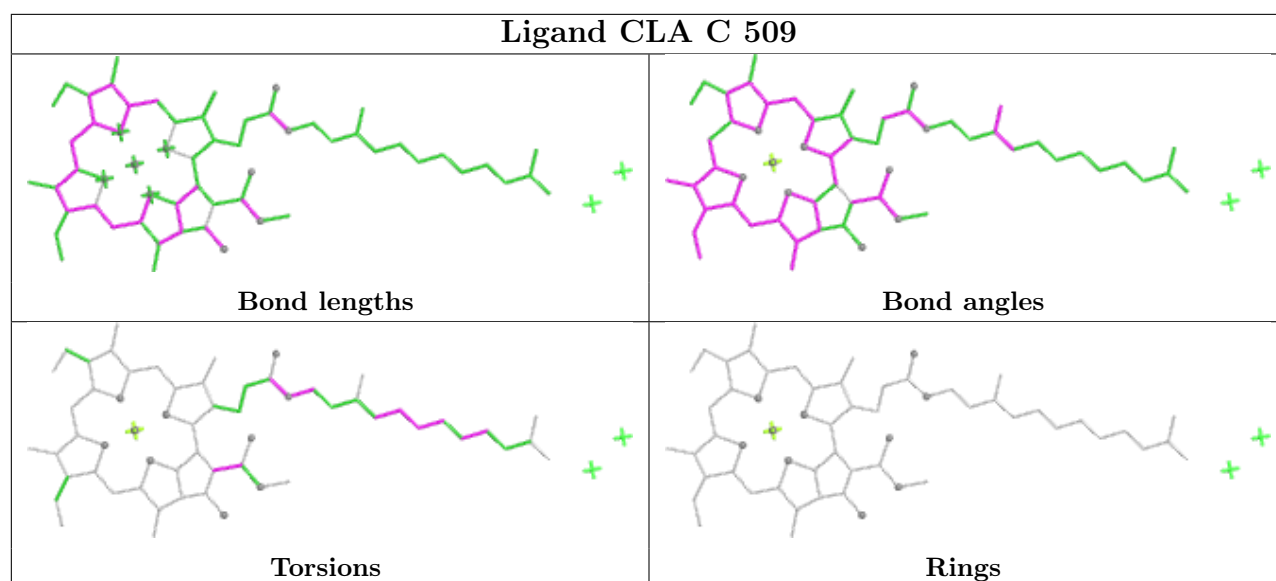


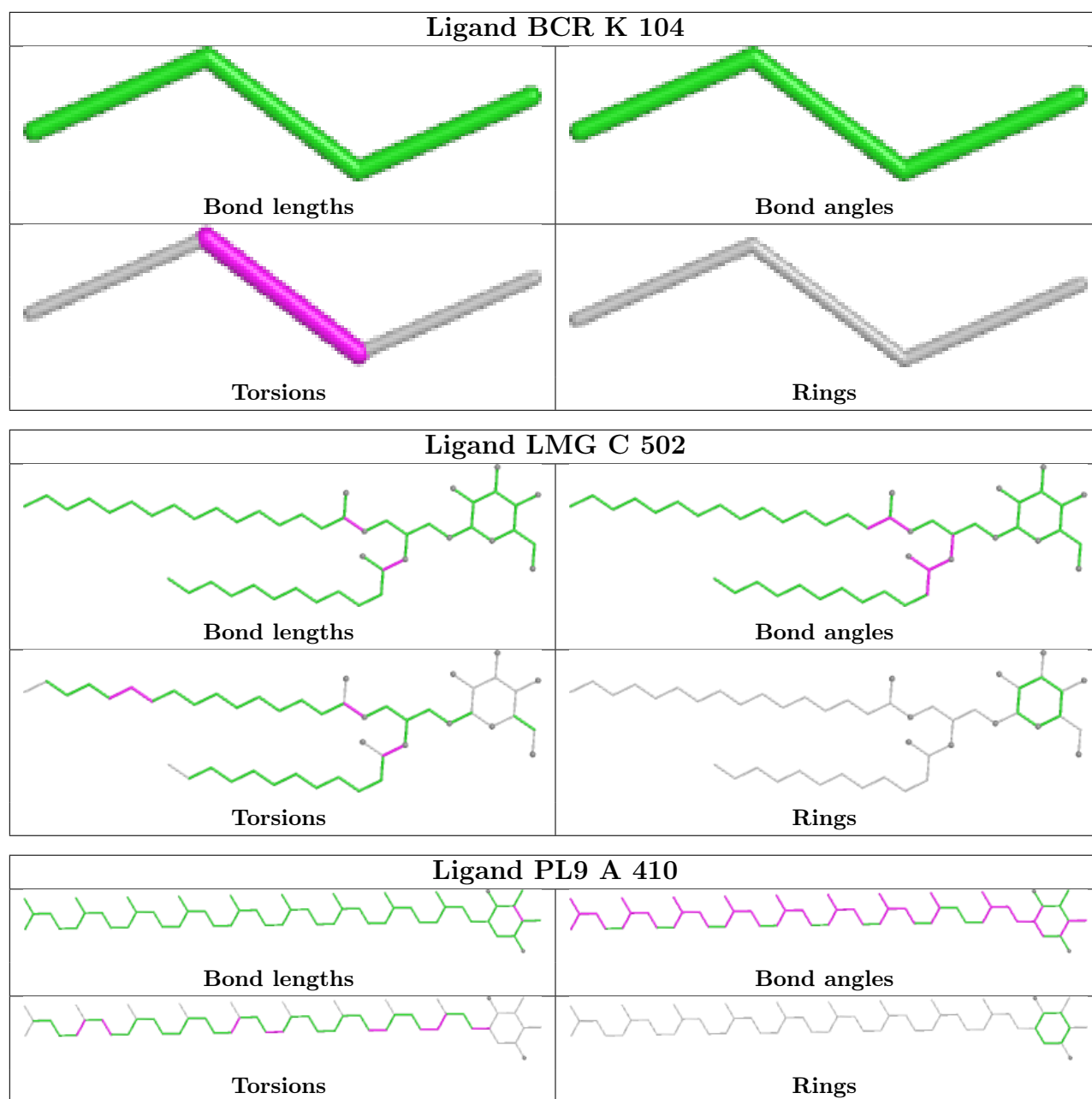


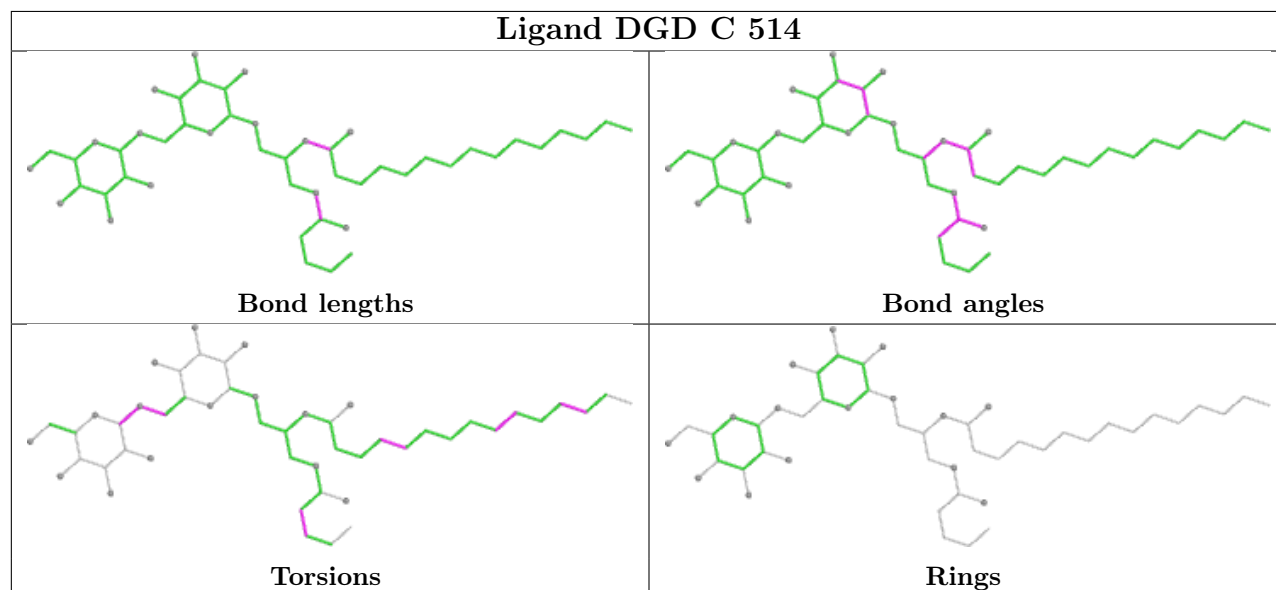
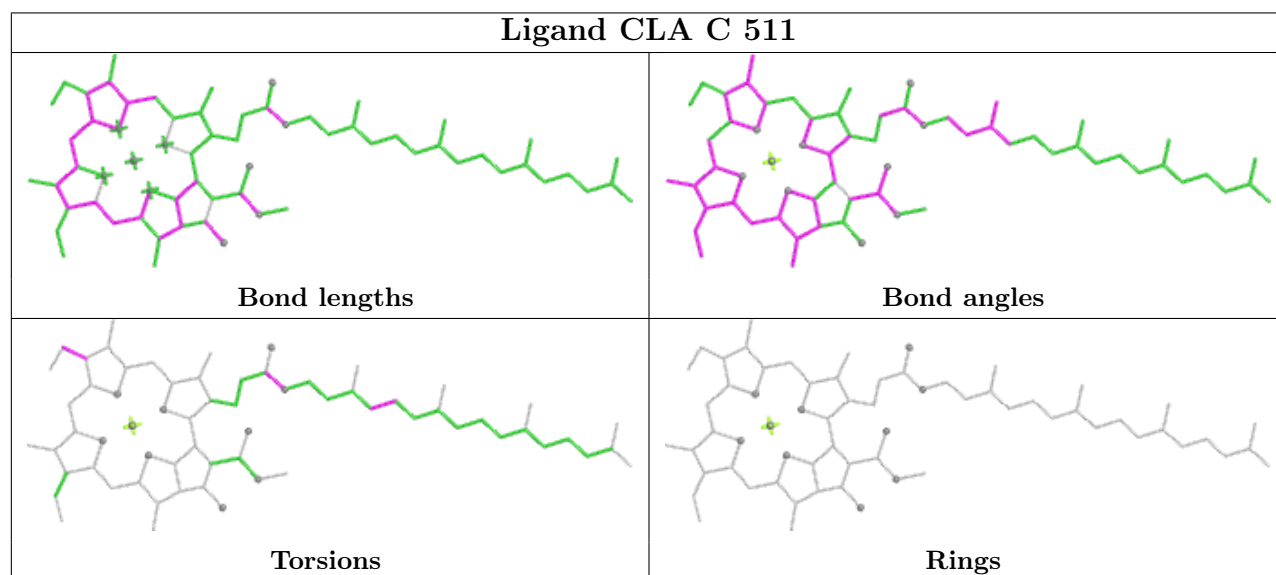
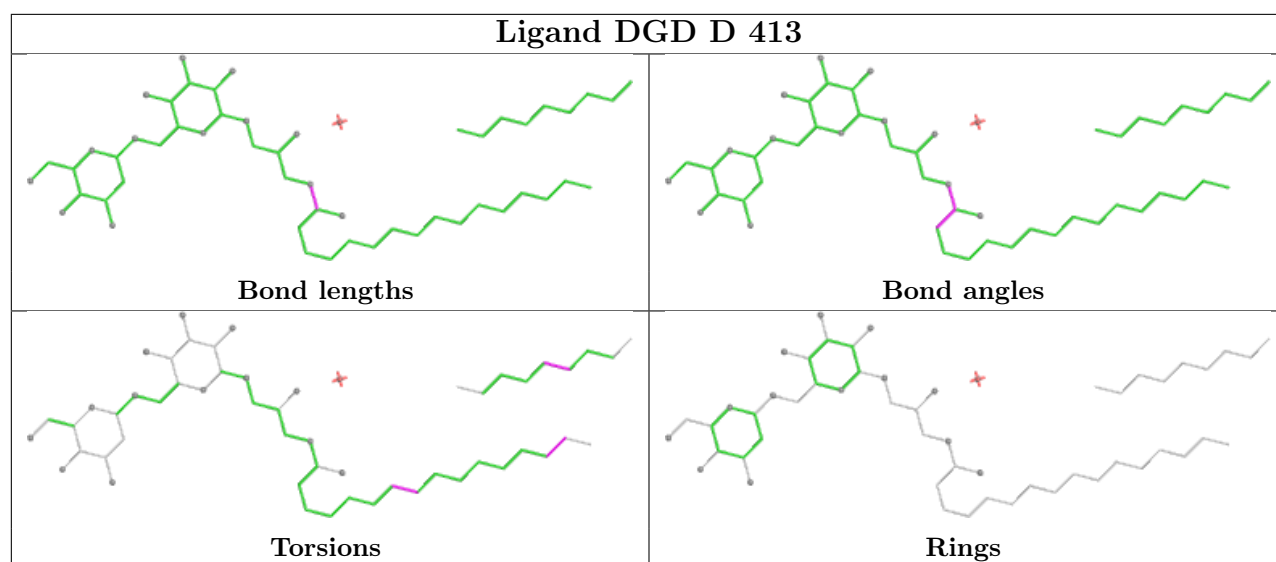
Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

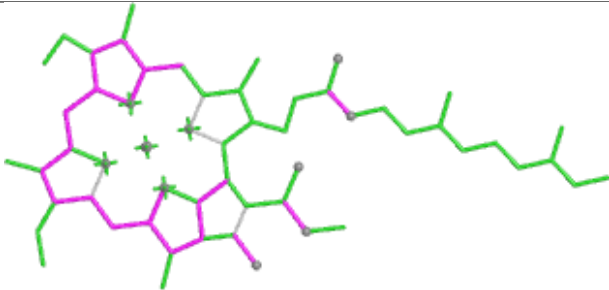
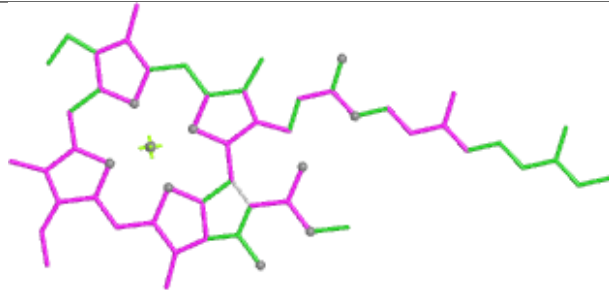
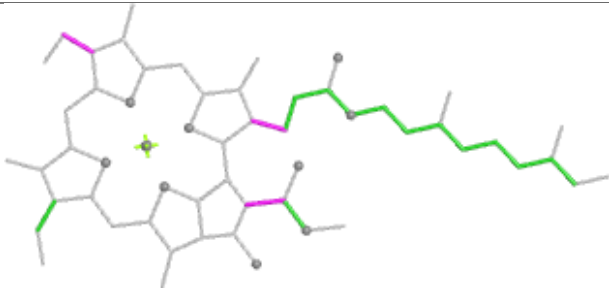
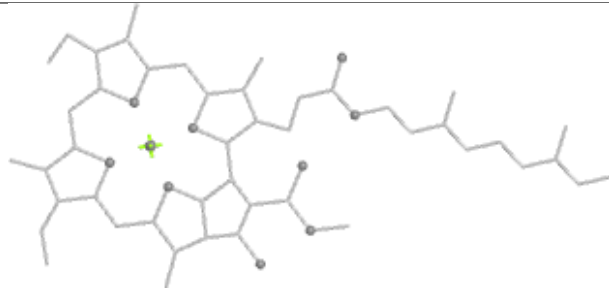
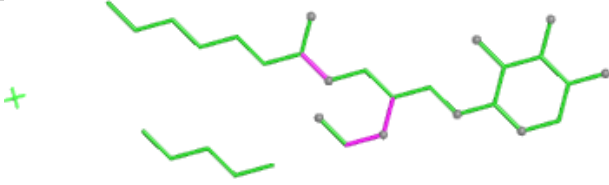
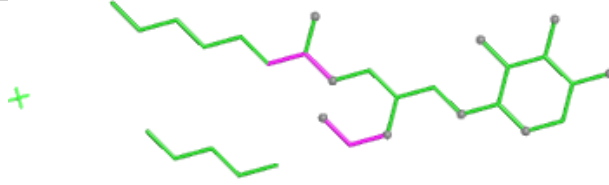
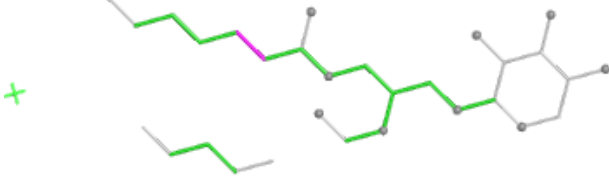
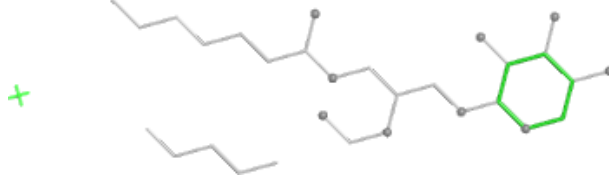
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

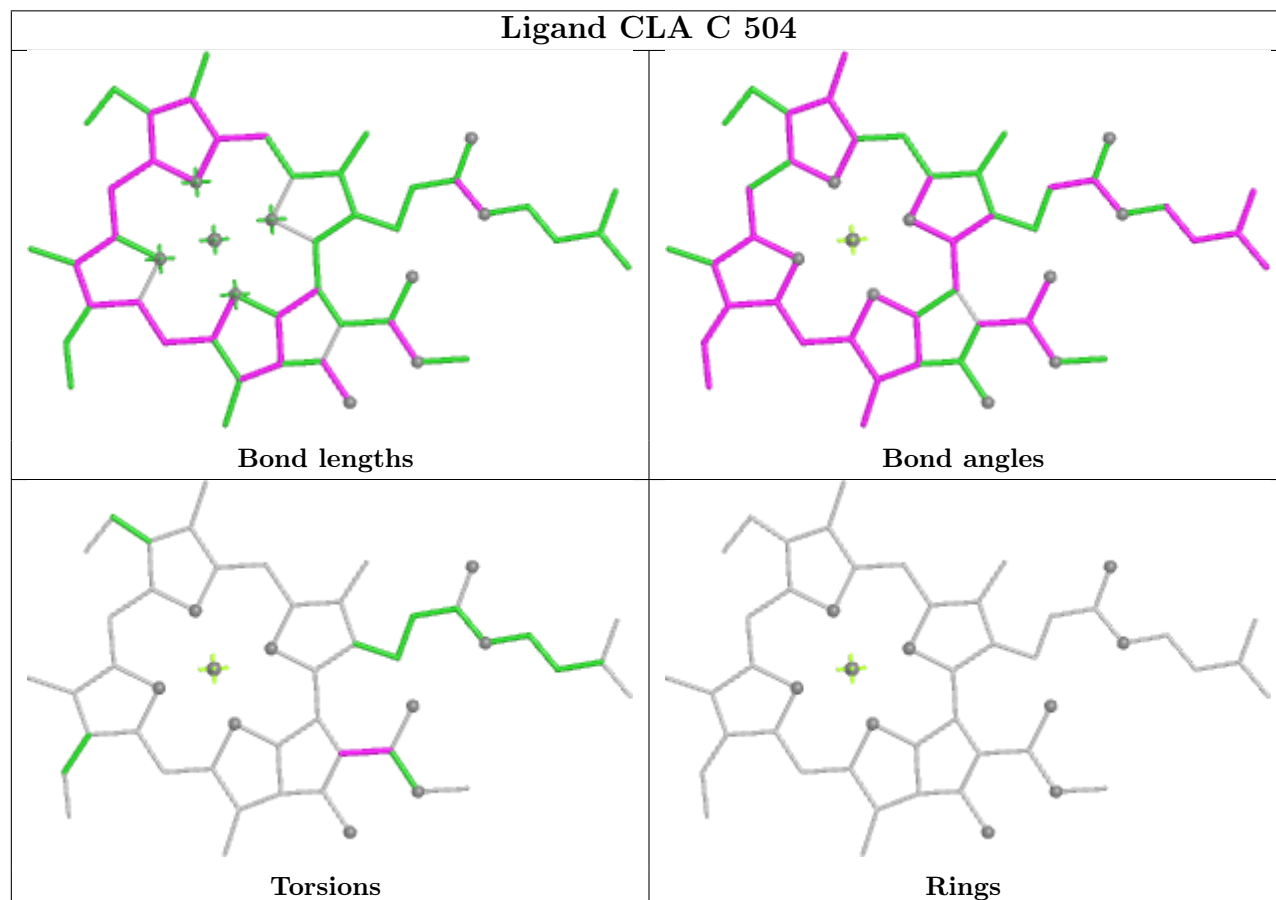
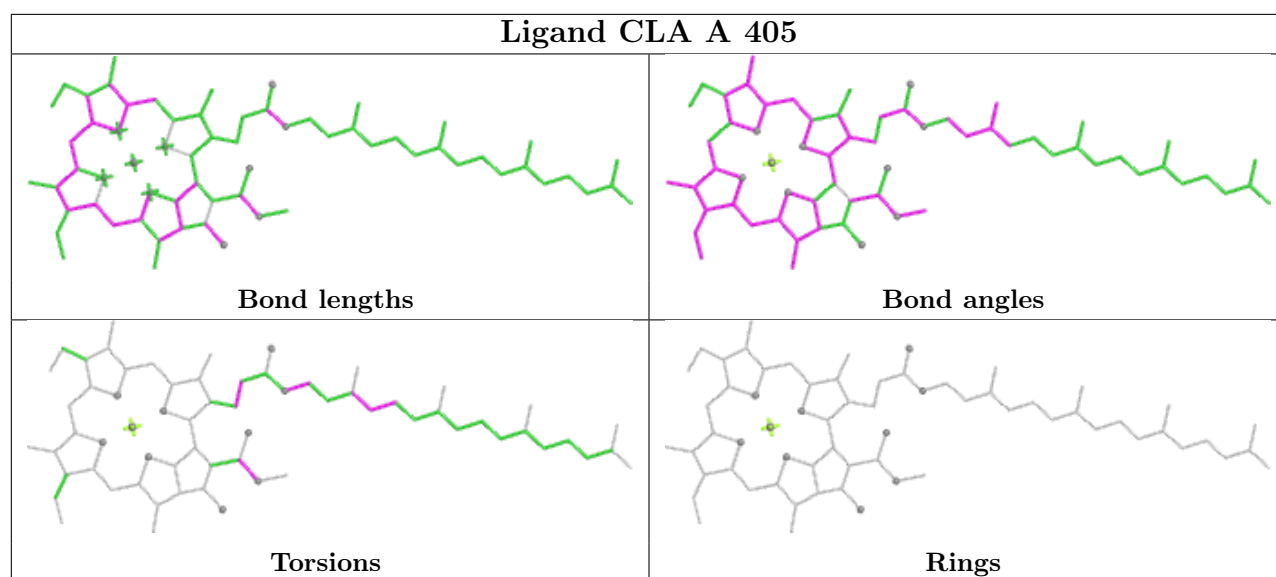
Ligand CLA D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

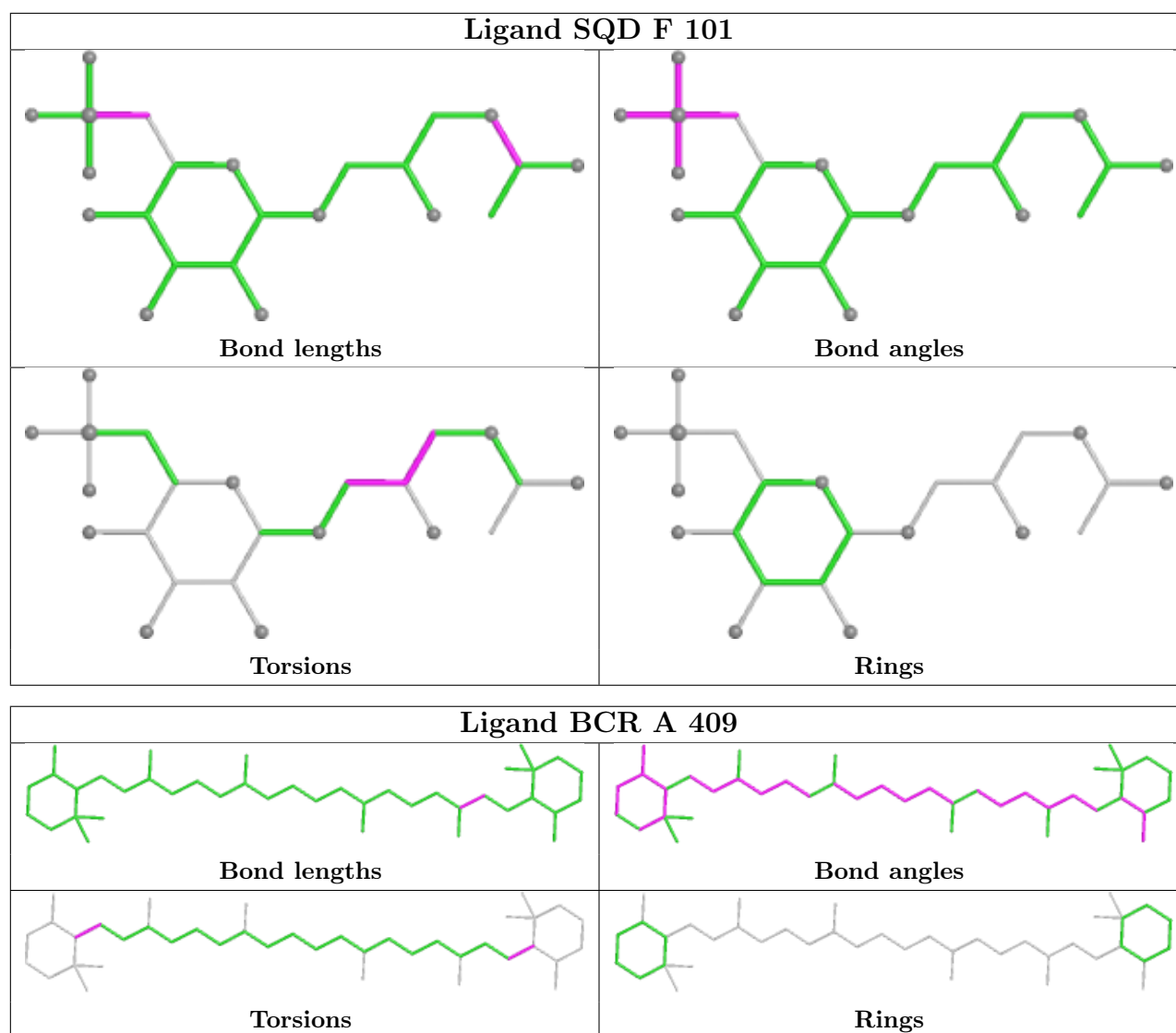






Ligand CLA A 406			
			
Bond lengths	Bond angles		
			
Torsions	Rings		
Ligand LMG B 603			
			
Bond lengths	Bond angles		
			
Torsions	Rings		





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	50:PRO	C	61:ARG	N	16.06

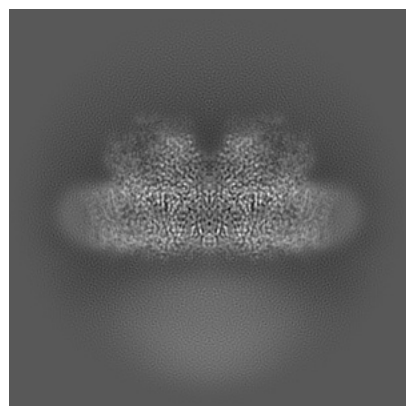
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65941. These allow visual inspection of the internal detail of the map and identification of artifacts.

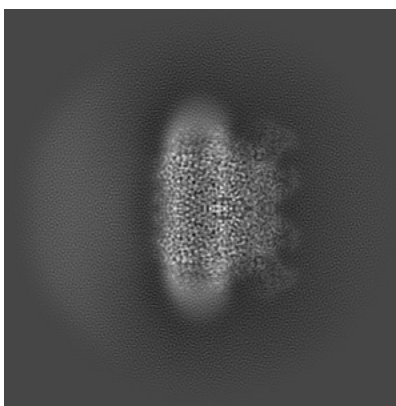
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

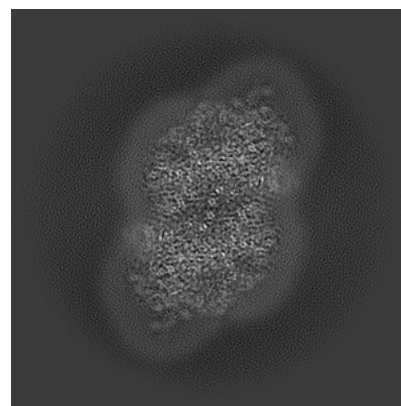
6.1.1 Primary map



X

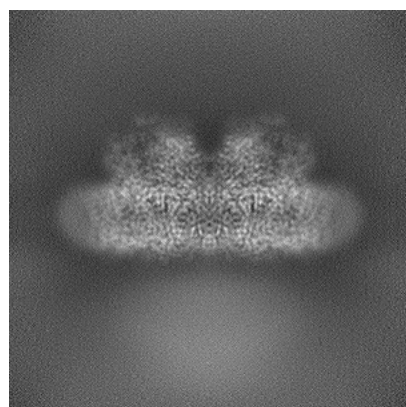


Y

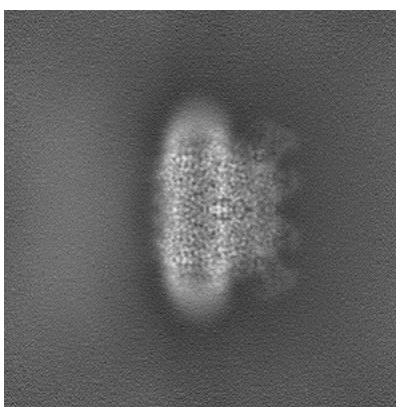


Z

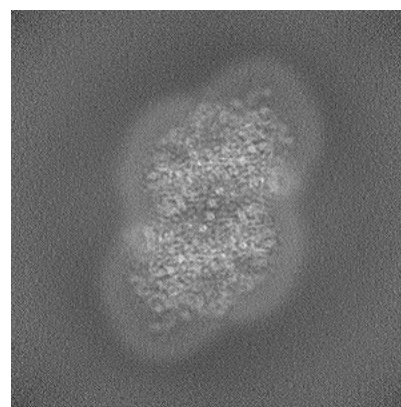
6.1.2 Raw map



X



Y

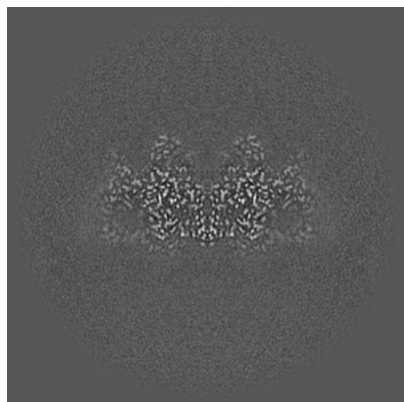


Z

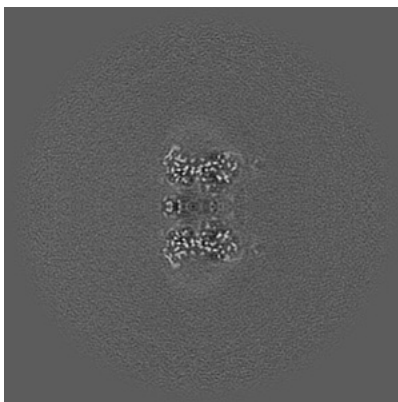
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

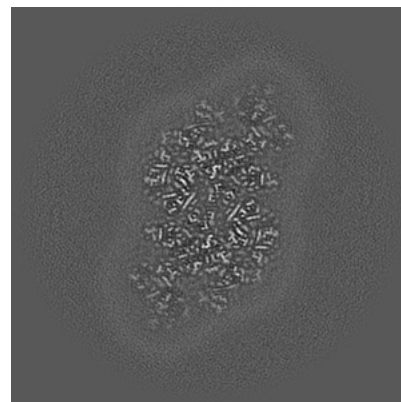
6.2.1 Primary map



X Index: 256

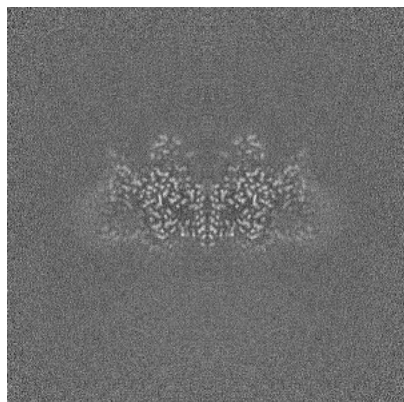


Y Index: 256

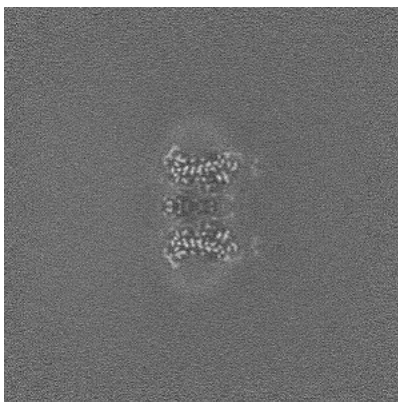


Z Index: 256

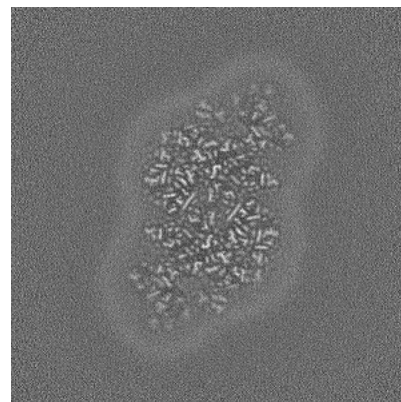
6.2.2 Raw map



X Index: 256



Y Index: 256

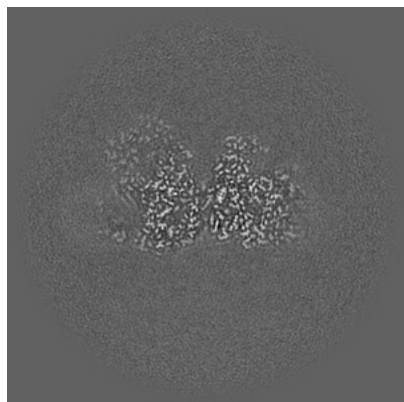


Z Index: 256

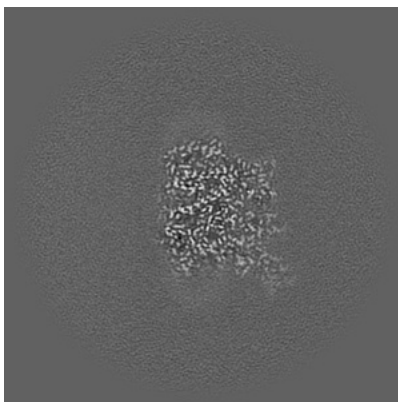
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

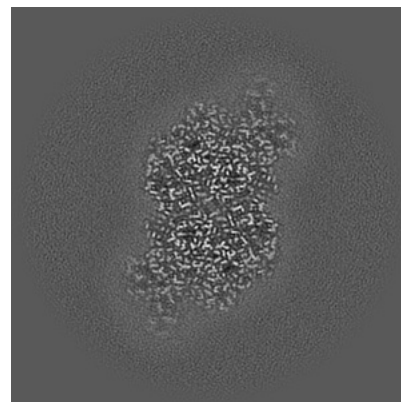
6.3.1 Primary map



X Index: 230

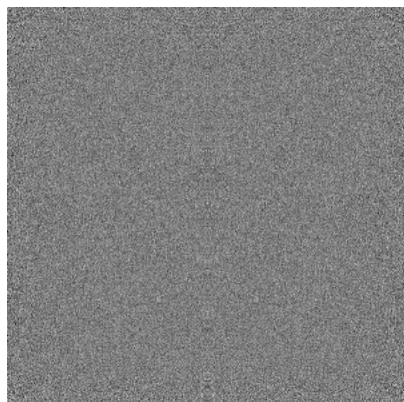


Y Index: 209

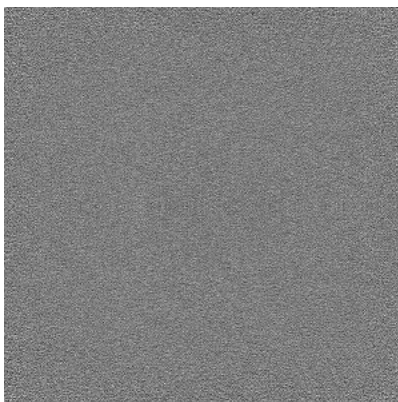


Z Index: 275

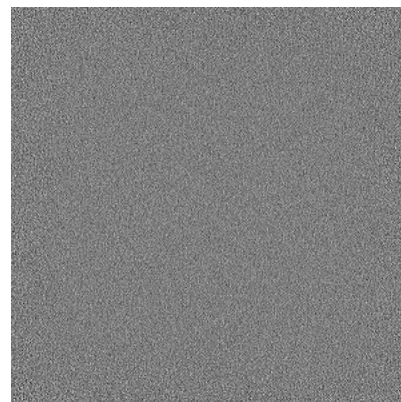
6.3.2 Raw map



X Index: 0



Y Index: 0

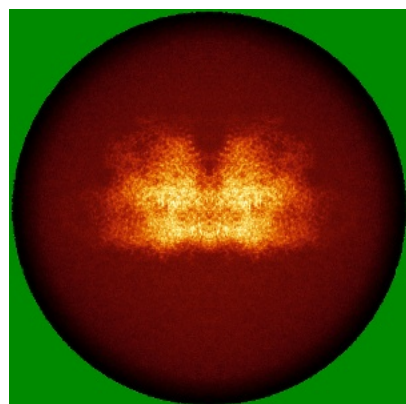


Z Index: 0

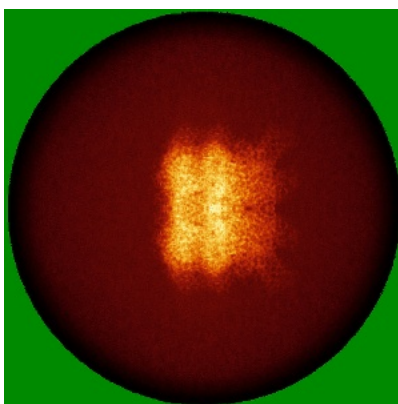
The images above show the largest variance slices of the map in three orthogonal directions.

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

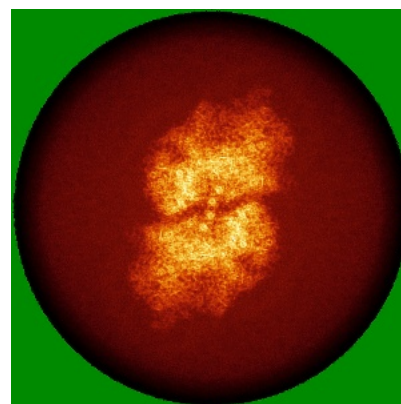
6.4.1 Primary map



X

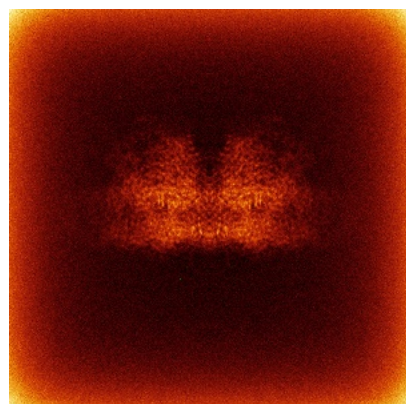


Y

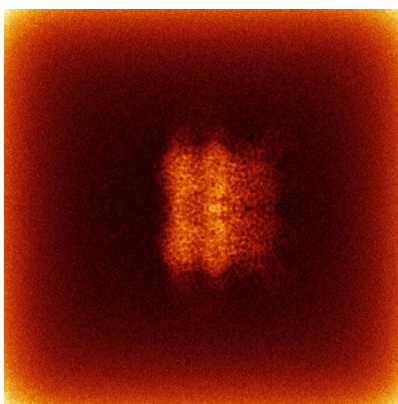


Z

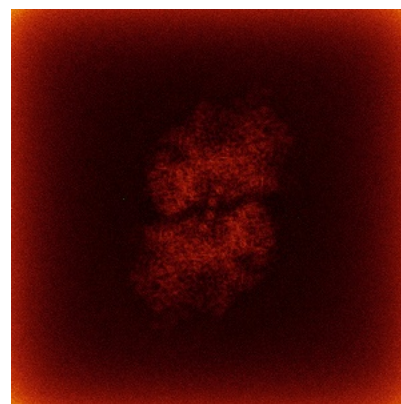
6.4.2 Raw map



X



Y

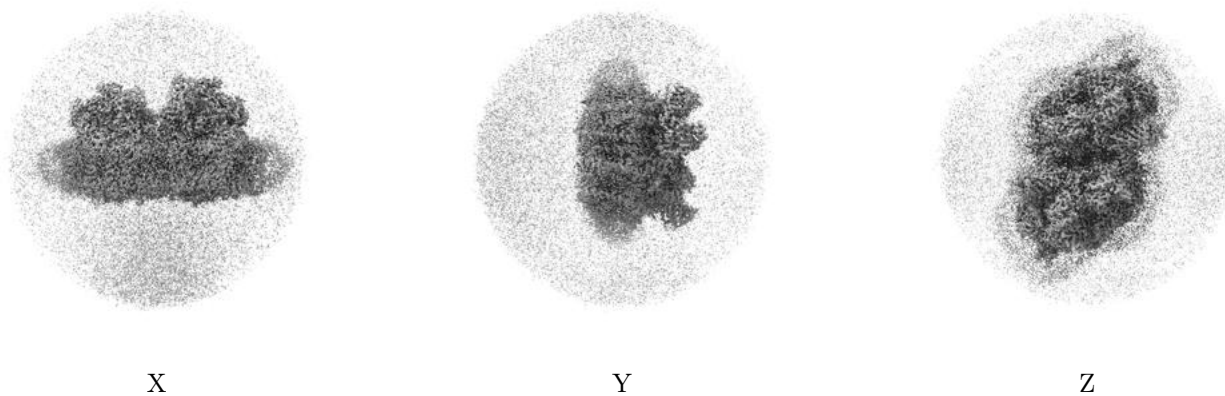


Z

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

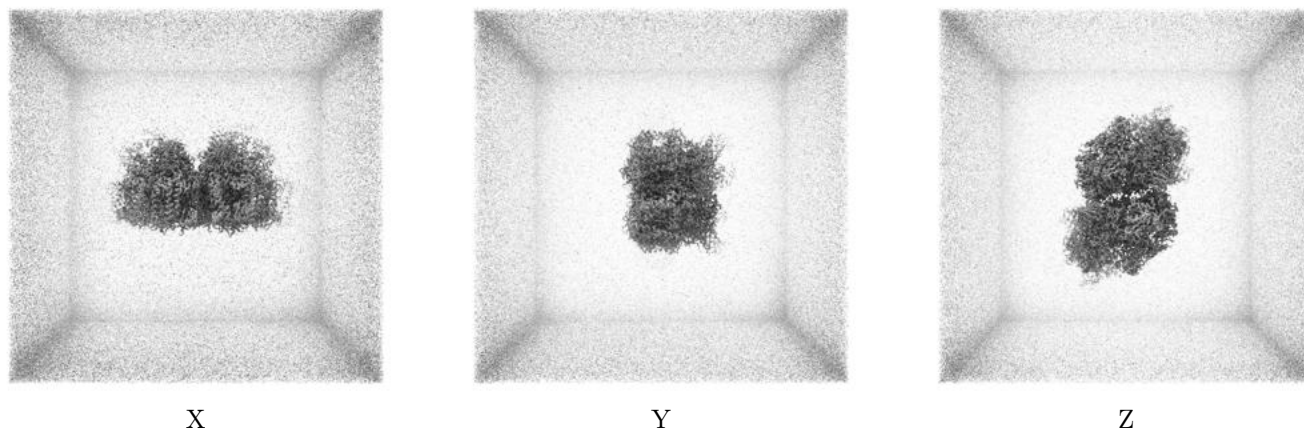
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.129. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

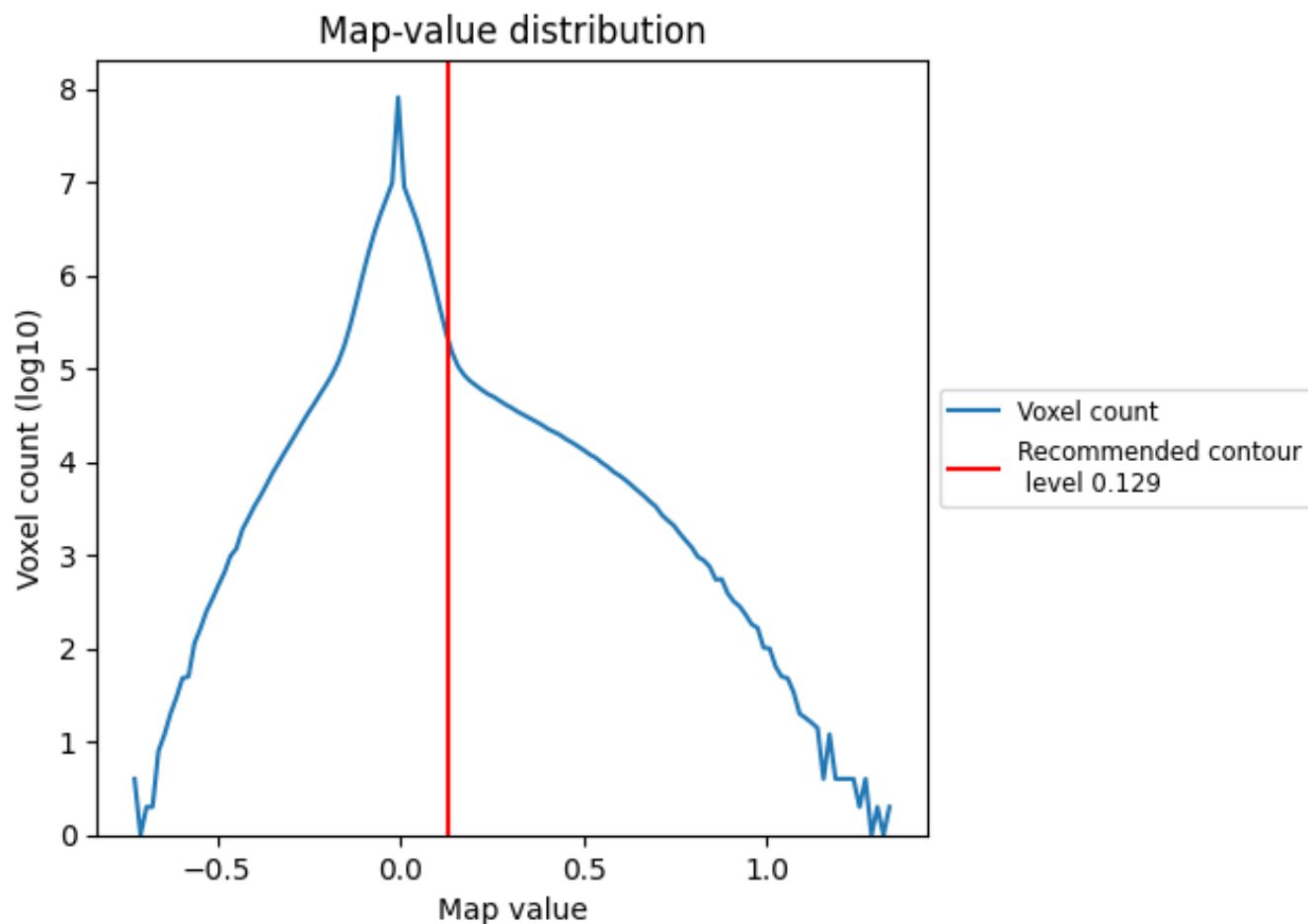
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

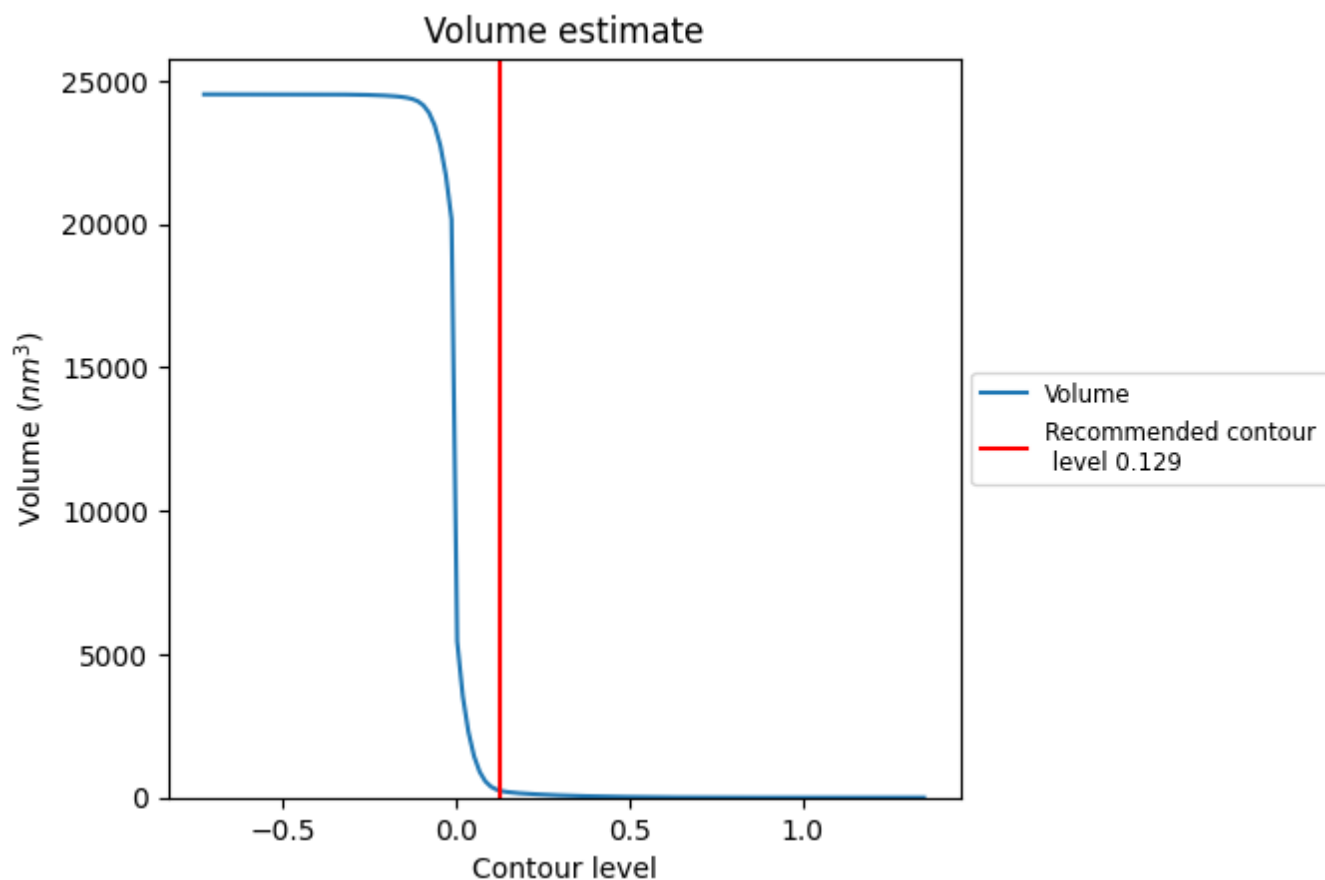
This section contains the results of statistical analysis of the map.

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.

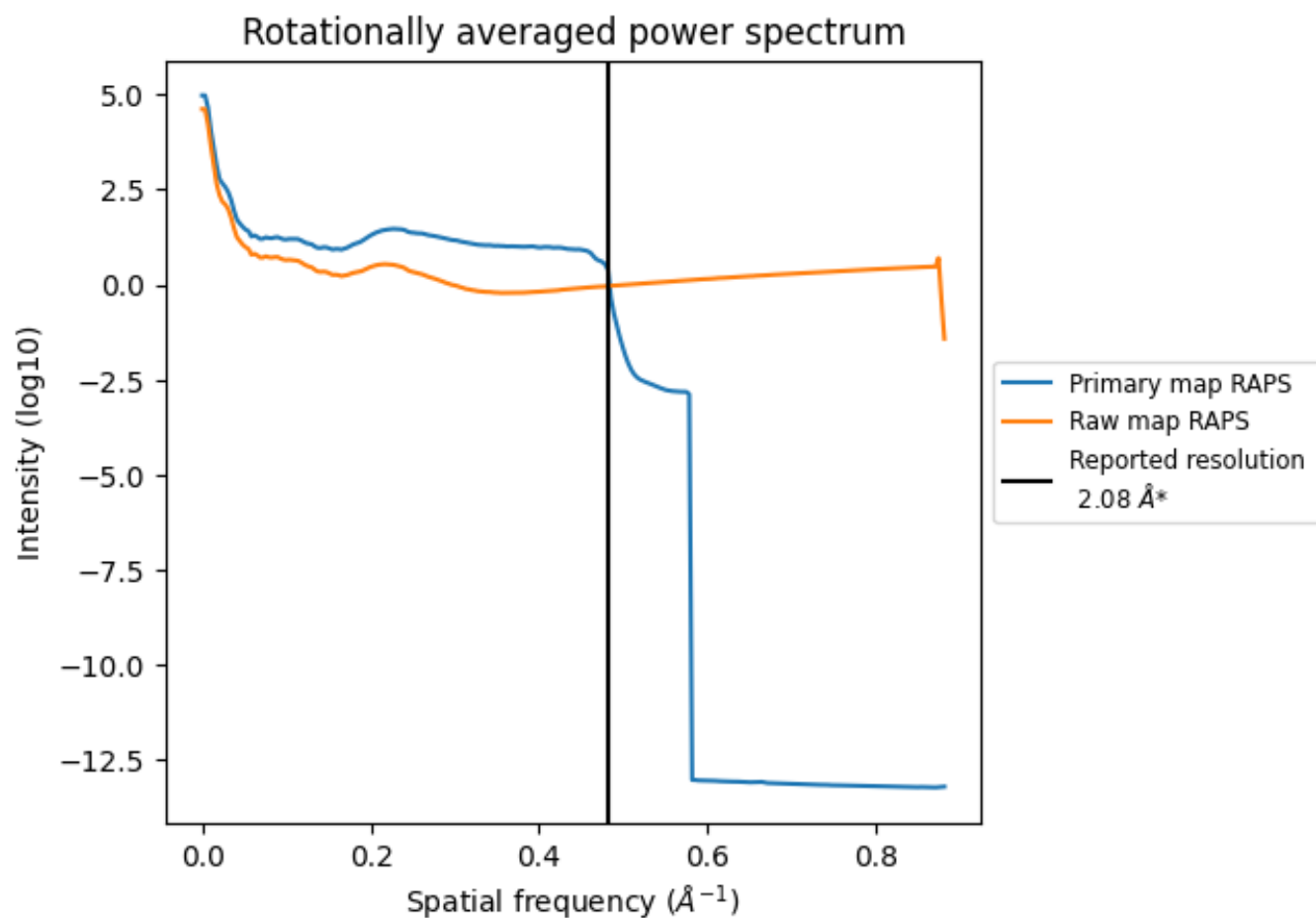
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 240 nm^3 ; this corresponds to an approximate mass of 216 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 ⓘ

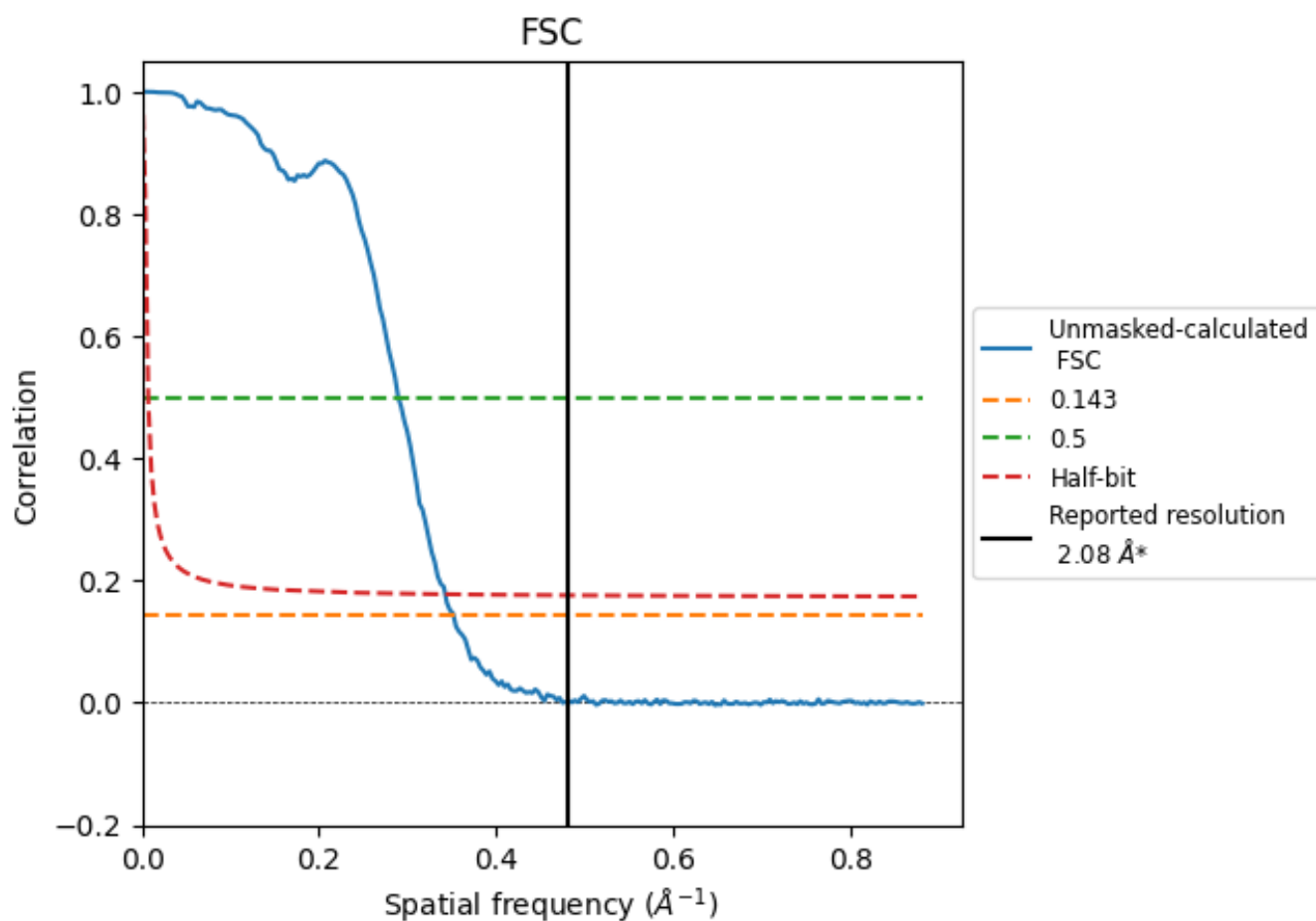


*Reported resolution corresponds to spatial frequency of 0.481 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.481 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.08	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.84	3.46	2.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.84 differs from the reported value 2.08 by more than 10 %

9 Map-model fit [i](#)

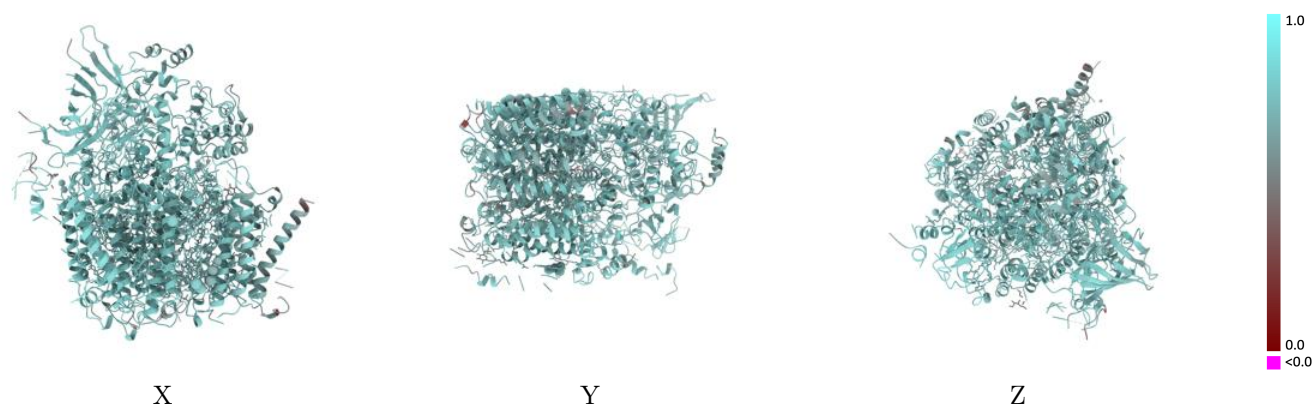
This section contains information regarding the fit between EMDB map EMD-65941 and PDB model 9WFZ. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



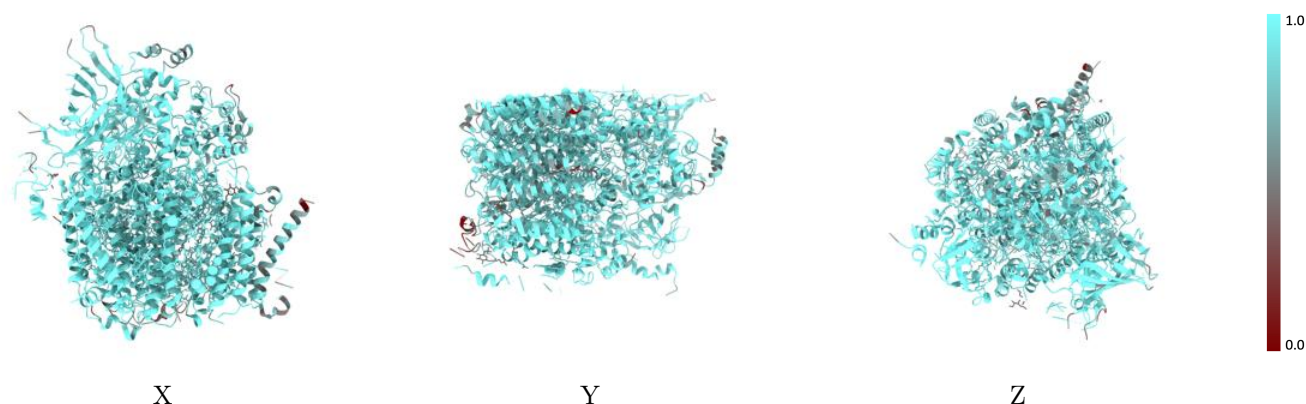
The images above show the 3D surface view of the map at the recommended contour level 0.129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



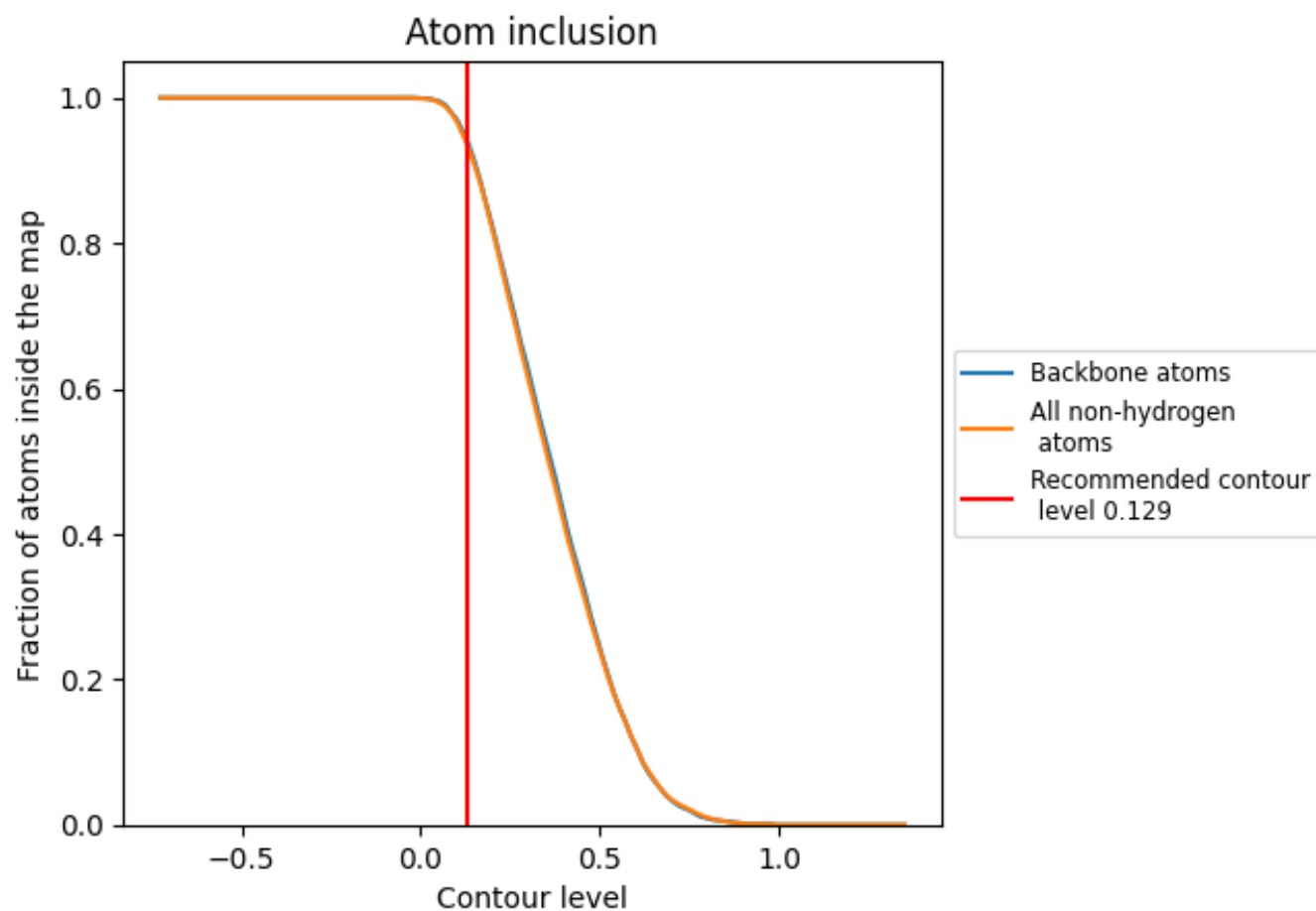
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.129).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.7200
A	 0.9620	 0.7420
B	 0.9240	 0.7250
C	 0.9610	 0.7240
D	 0.9810	 0.7440
E	 0.8930	 0.6830
F	 0.8800	 0.6860
I	 0.9650	 0.7140
J	 0.8780	 0.6860
K	 0.8700	 0.6780
L	 0.9960	 0.7580
M	 0.9910	 0.7370
O	 0.9270	 0.7120
T	 0.9400	 0.7230
U	 0.8780	 0.6910
V	 0.8670	 0.6860
X	 0.9330	 0.6770
Y	 0.7680	 0.6400
Z	 0.6750	 0.5920
b	 0.9570	 0.7060

