



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 AM UTC

PDB ID : 3KZI / pdb_00003kzi
Title : Crystal Structure of Monomeric Form of Cyanobacterial Photosystem II
Authors : Gabdulkhakov, A.; Guskov, A.; Broser, M.; Kern, J.; Zouni, A.; Saenger, W.
Deposited on : 2009-12-08
Resolution : 3.60 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

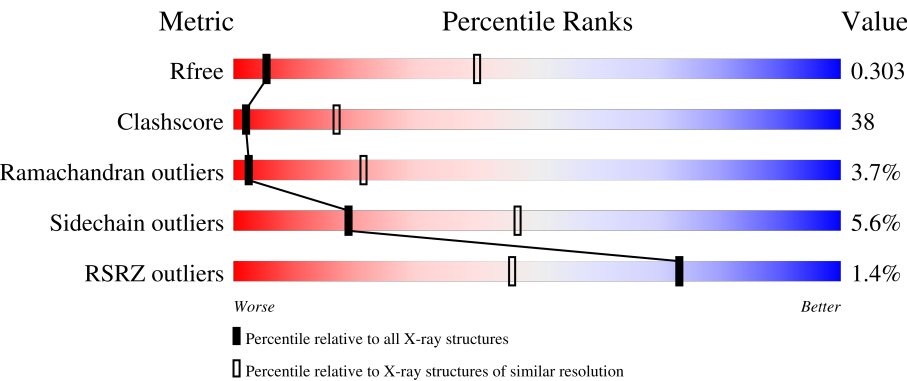
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	2% 41% 50% 6% • •
2	B	510	2% 49% 40% 6% • 5%
3	C	461	% 37% 53% 7% •
4	D	352	3% 48% 41% 8% •
5	E	83	24% 54% 12% • 7%

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Mol	Chain	Length	Quality of chain
6	F	44	
7	H	65	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	36	
13	O	246	
14	T	32	
15	U	104	
16	V	137	
17	y	46	
18	X	40	
19	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
21	CLA	A	362	X	-	-	-
21	CLA	A	363	X	-	-	-
21	CLA	A	364	X	-	-	-
21	CLA	A	366	X	-	-	-
21	CLA	B	511	X	-	-	-
21	CLA	B	512	X	-	-	-
21	CLA	B	513	X	-	X	-
21	CLA	B	514	X	-	-	-
21	CLA	B	515	X	-	-	-
21	CLA	B	516	X	-	-	-
21	CLA	B	517	X	-	-	-
21	CLA	B	518	X	-	-	-
21	CLA	B	519	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	520	X	-	-	-
21	CLA	B	521	X	-	-	-
21	CLA	B	522	X	-	-	-
21	CLA	B	523	X	-	-	-
21	CLA	B	524	X	-	-	-
21	CLA	B	525	X	-	-	-
21	CLA	B	526	X	-	-	-
21	CLA	C	477	X	-	-	-
21	CLA	C	478	X	-	-	-
21	CLA	C	479	X	-	-	-
21	CLA	C	480	X	-	-	-
21	CLA	C	481	X	-	-	-
21	CLA	C	482	X	-	-	-
21	CLA	C	483	X	-	-	-
21	CLA	C	484	X	-	-	-
21	CLA	C	485	X	-	-	-
21	CLA	C	486	X	-	X	-
21	CLA	C	487	X	-	-	-
21	CLA	C	488	X	-	-	-
21	CLA	D	354	X	-	-	-
21	CLA	D	356	X	-	-	-
21	CLA	K	483	X	-	-	-
22	PHO	A	365	X	-	-	-
22	PHO	D	355	X	-	-	-
23	MES	A	367	-	-	X	-
27	LMG	A	373	-	-	X	-
27	LMG	D	360	-	-	X	-
28	DGD	B	528	-	-	X	-
28	DGD	C	492	X	-	-	-
28	DGD	C	493	X	-	X	-
32	PL9	D	357	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 24678 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	485	Total	C	N	O	S	0	0	0
			3812	2505	635	659	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	448	Total	C	N	O	S	0	0	0
			3455	2262	580	600	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

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

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

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	S	0	0	0
			774	491	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

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

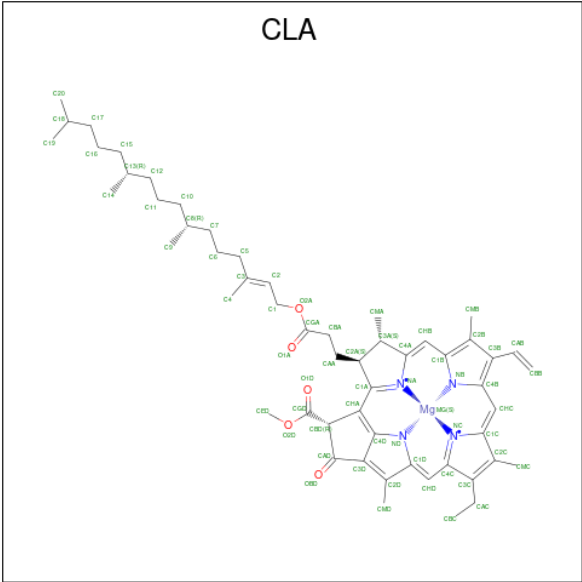
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



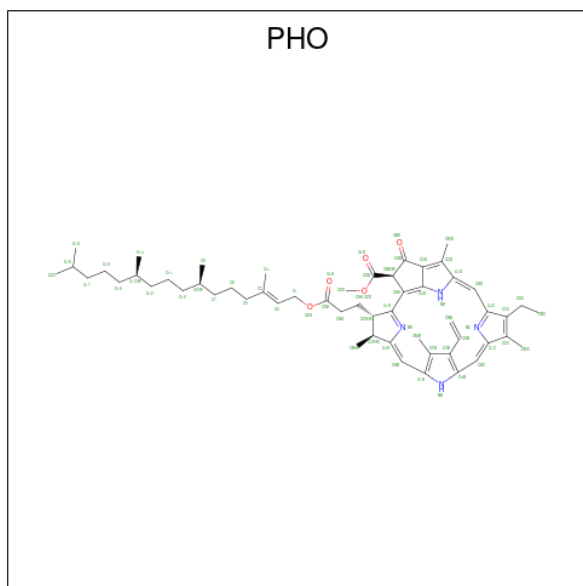
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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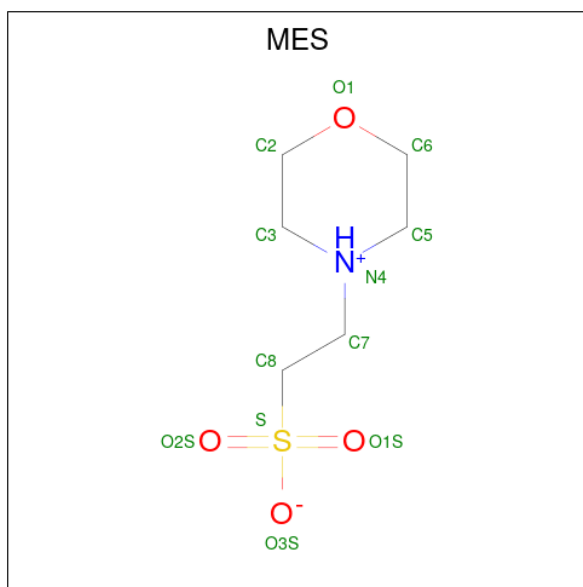
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	K	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

- Molecule 22 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



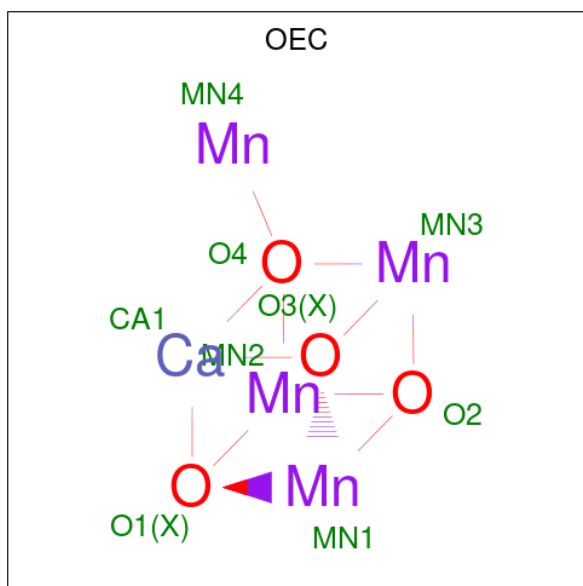
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 23 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



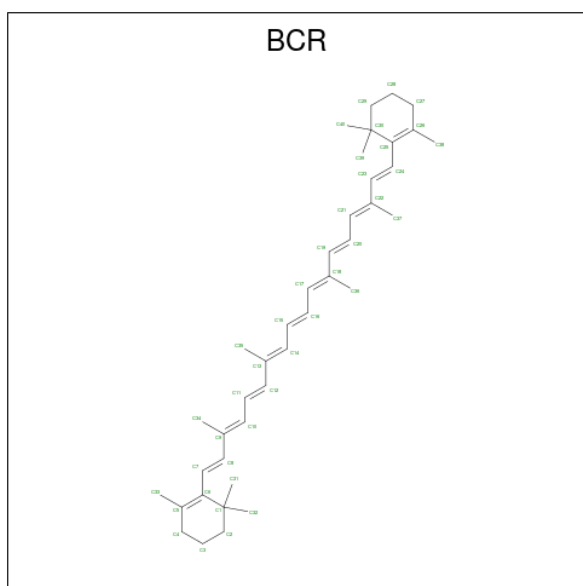
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 24 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



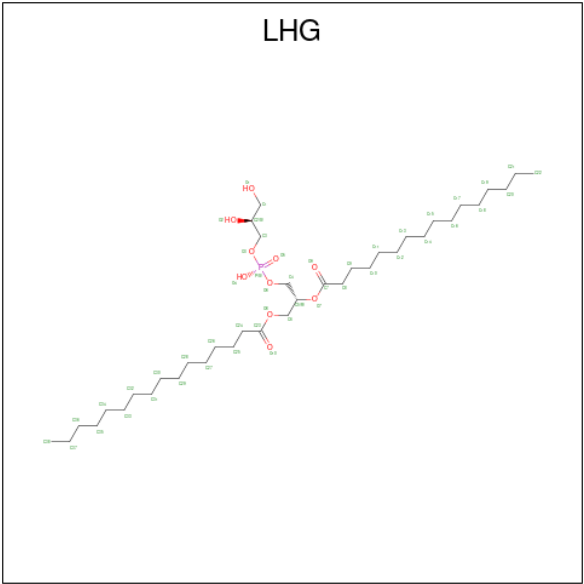
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	1	Total	Ca Mn	0	0
			5	1 4		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



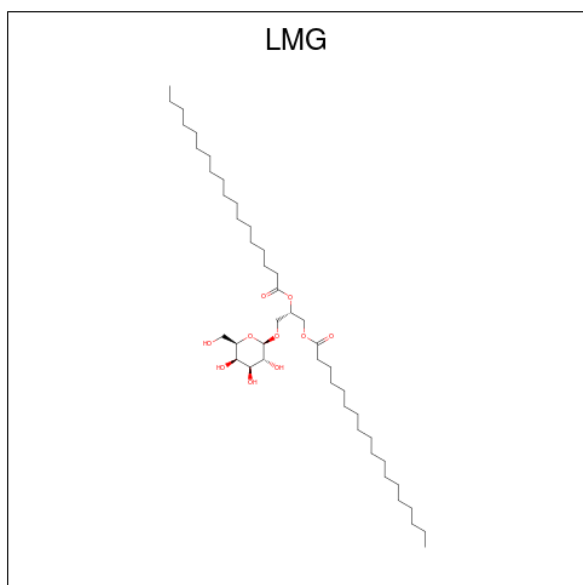
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	X	1	Total C 40 40	0	0
25	Z	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



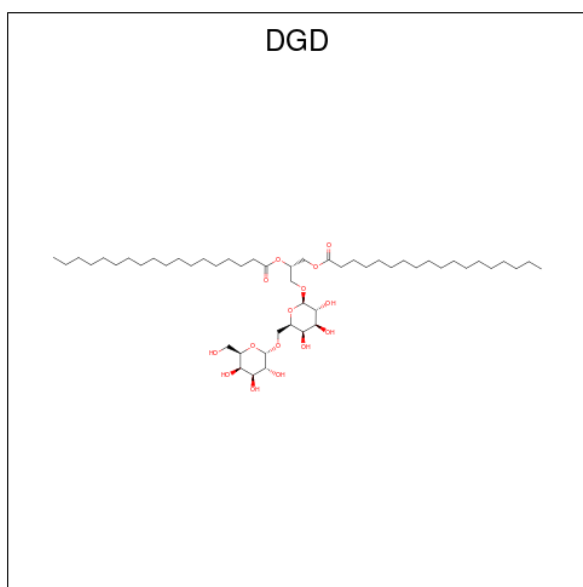
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



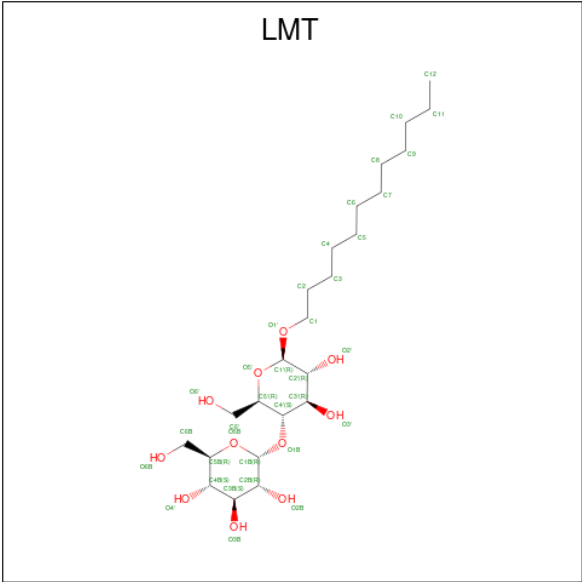
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	J	1	Total	C	O	0	0
			48	38	10		
27	M	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



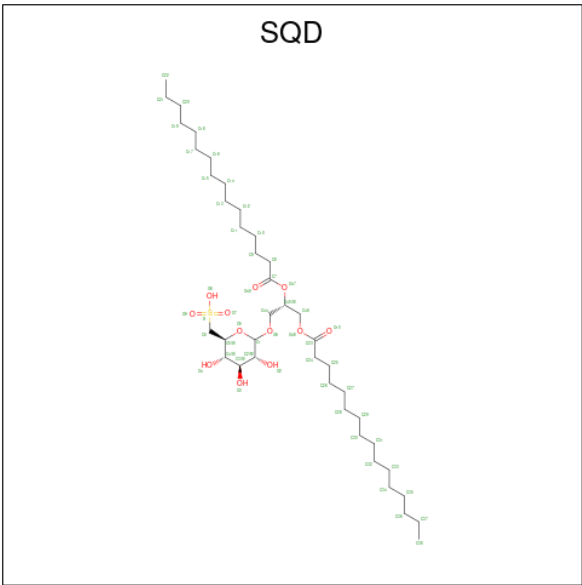
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			52	37	15		
28	B	1	Total	C	O	0	0
			66	51	15		
28	B	1	Total	C	O	0	0
			58	43	15		
28	C	1	Total	C	O	0	0
			56	41	15		
28	C	1	Total	C	O	0	0
			53	38	15		
28	C	1	Total	C	O	0	0
			62	47	15		
28	C	1	Total	C	O	0	0
			66	51	15		
28	D	1	Total	C	O	0	0
			63	48	15		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



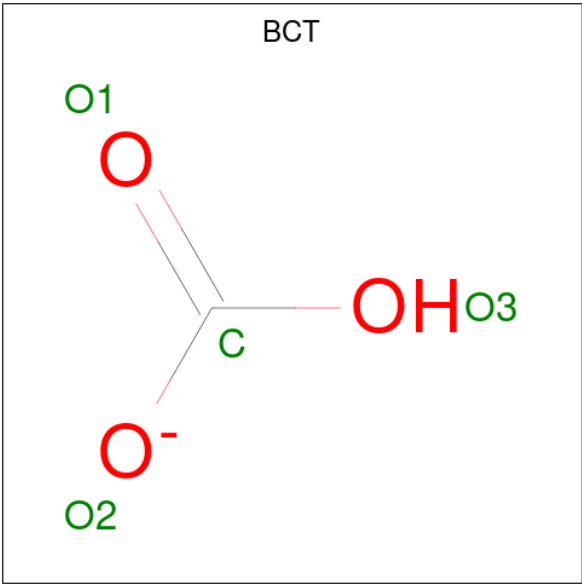
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			31	20	11		
29	I	1	Total	C	O	0	0
			35	24	11		
29	O	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



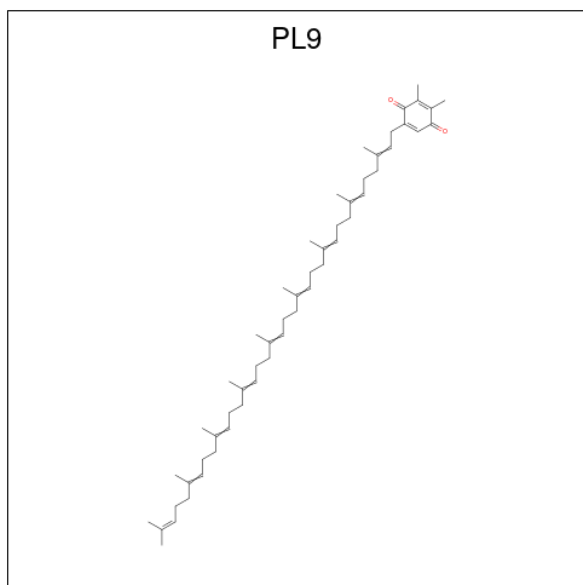
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	C	1	Total	C	O	S	0	0
			51	38	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	L	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



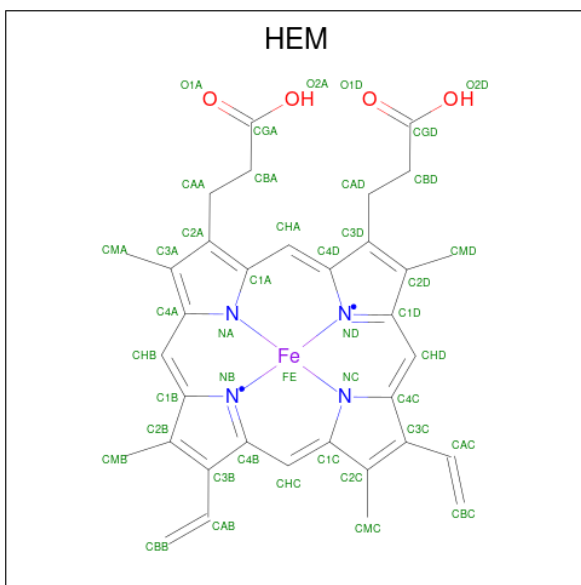
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 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: $C_{53}H_{80}O_2$).



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

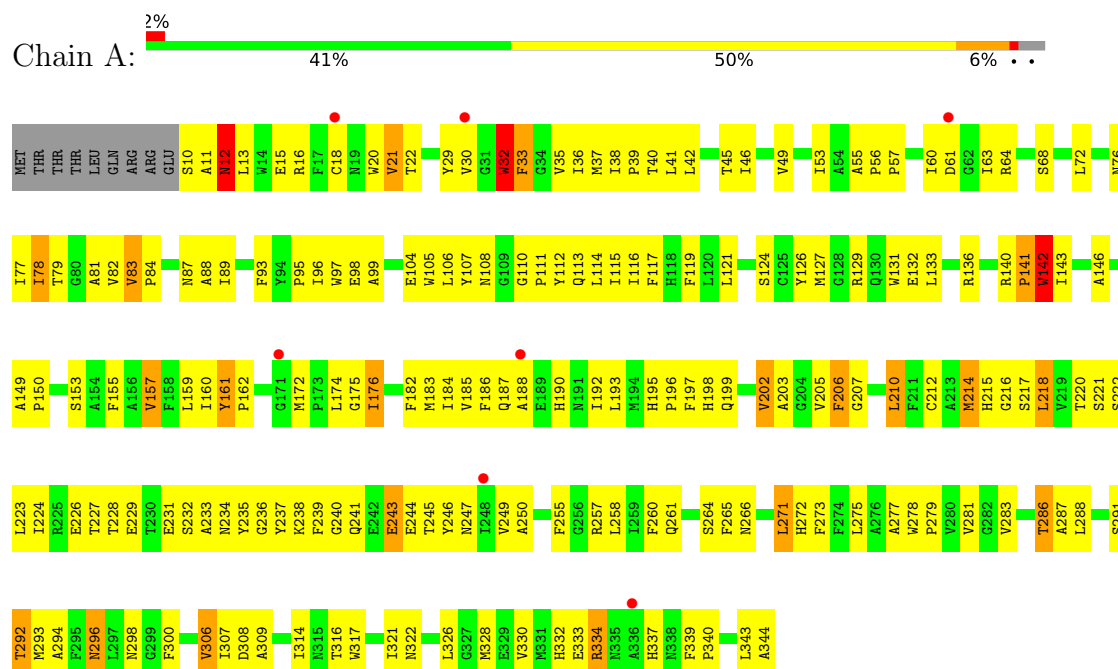
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	F	1	Total Ca 1 1	0	0
34	K	1	Total Ca 1 1	0	0
34	O	1	Total Ca 1 1	0	0

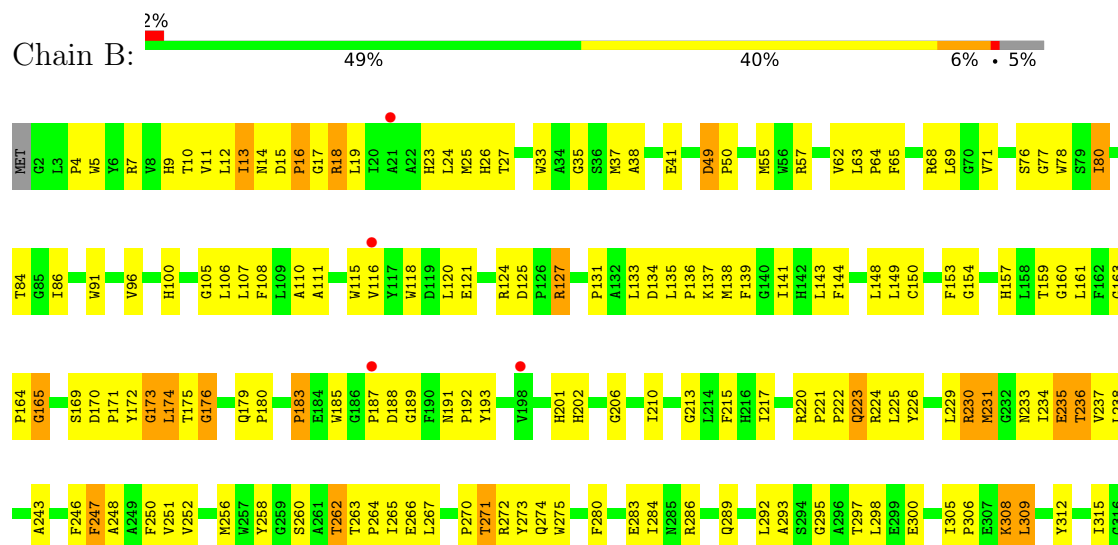
3 Residue-property plots

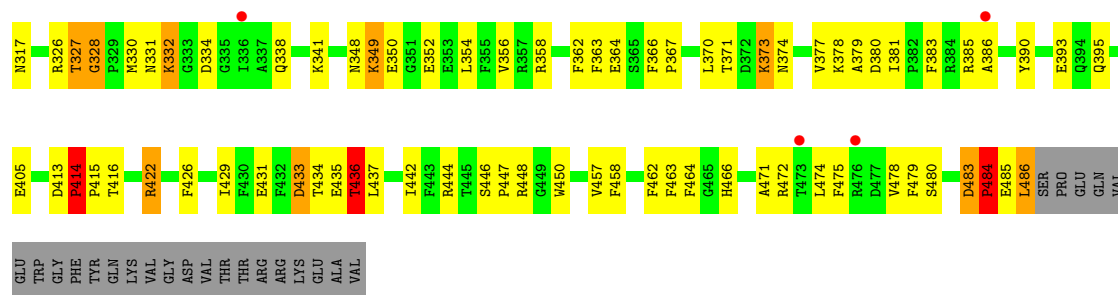
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 Q(B) protein 1

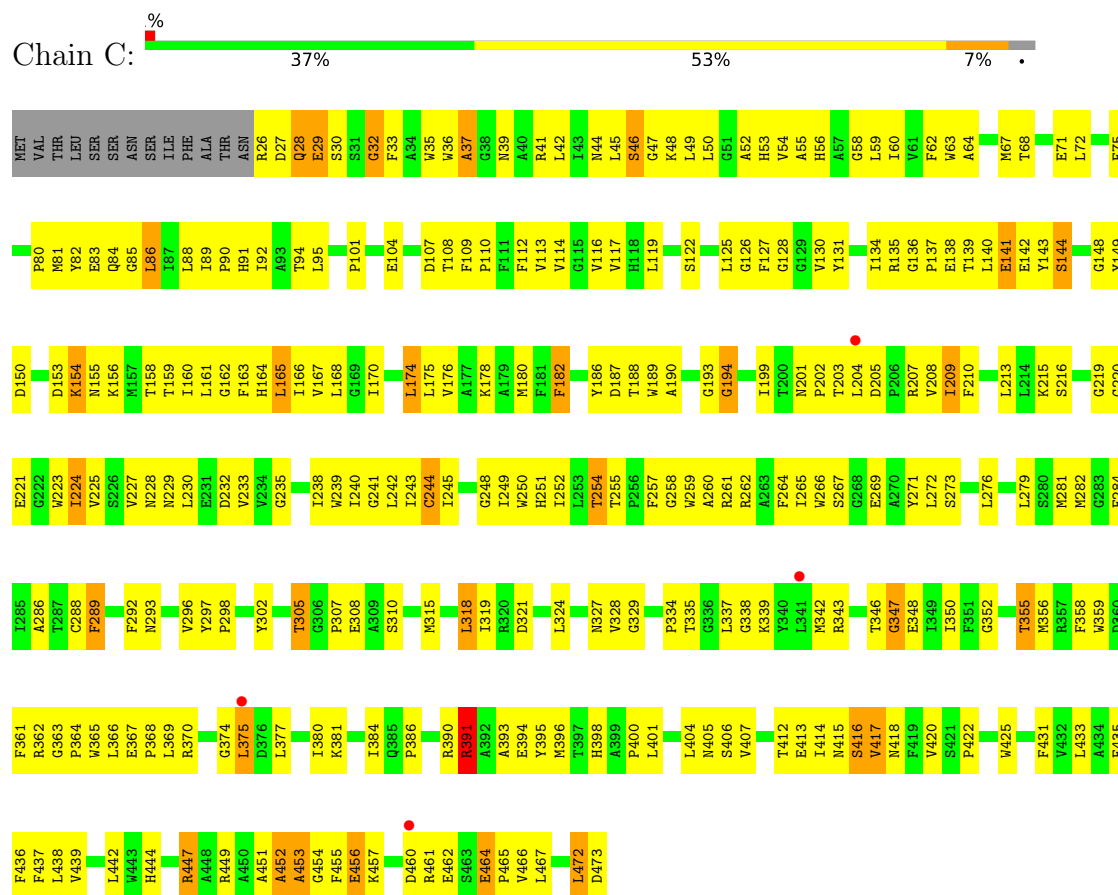


• Molecule 2: Photosystem II core light harvesting protein

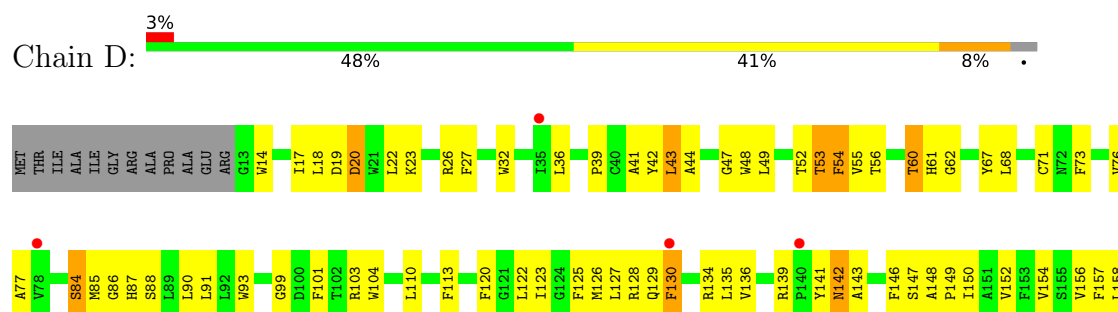


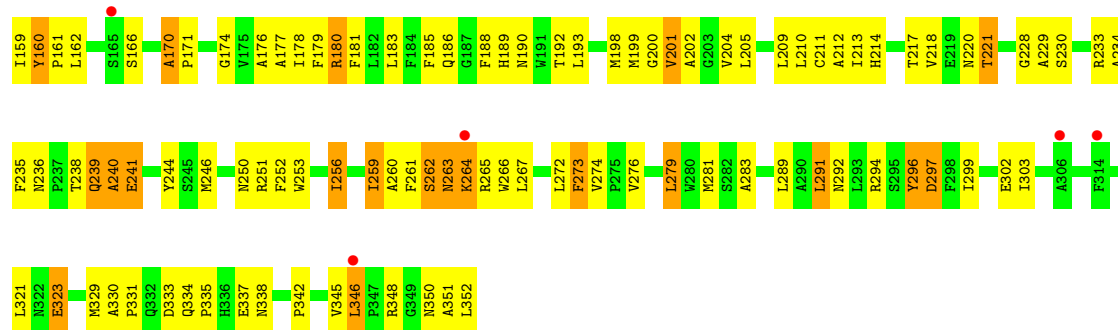


- Molecule 3: Photosystem II CP43 protein



- Molecule 4: Photosystem II D2 protein

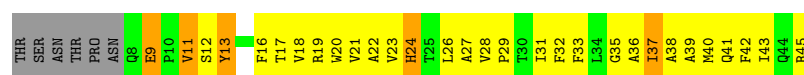




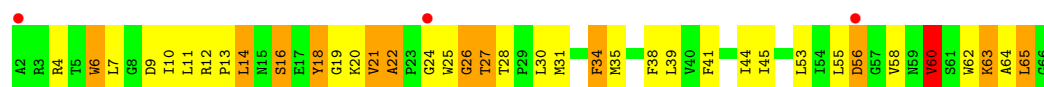
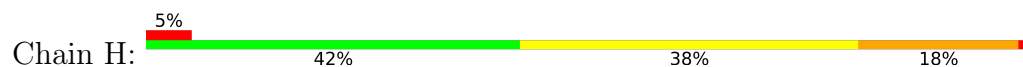
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta



• Molecule 7: Photosystem II reaction center protein H



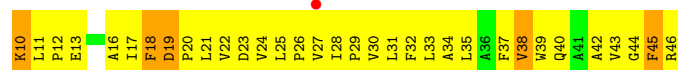
• Molecule 8: Photosystem II reaction center protein I



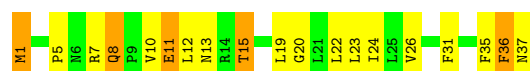
• Molecule 9: Photosystem II reaction center protein J



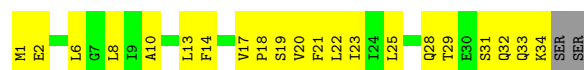
• Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



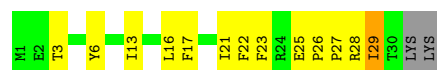
- Molecule 12: Photosystem II reaction center protein M



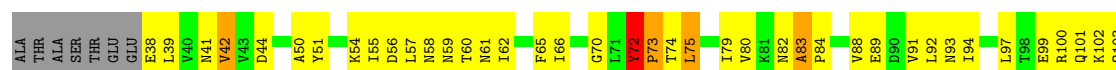
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein





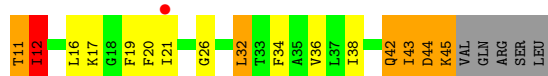
• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein ycf12



• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.89Å 224.69Å 337.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.60 29.87 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.2 (29.87-3.60) 99.1 (29.87-3.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.297 , 0.308 0.296 , 0.303	Depositor DCC
R_{free} test set	1054 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	153.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24678	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.55	0/2713	1.06	19/3700 (0.5%)
2	B	0.54	0/3947	1.03	26/5379 (0.5%)
3	C	0.50	0/3567	1.00	13/4856 (0.3%)
4	D	0.58	0/2801	1.01	12/3818 (0.3%)
5	E	0.50	0/654	1.17	9/891 (1.0%)
6	F	0.80	0/317	0.99	0/433
7	H	0.48	0/520	0.93	2/709 (0.3%)
8	I	0.54	0/293	1.08	2/395 (0.5%)
9	J	0.48	0/255	1.17	2/346 (0.6%)
10	K	0.50	0/303	0.96	1/416 (0.2%)
11	L	0.50	0/311	1.02	1/422 (0.2%)
12	M	0.54	0/270	0.91	0/367
13	O	0.53	0/1876	1.03	13/2548 (0.5%)
14	T	0.56	0/265	0.97	0/359
15	U	0.55	0/785	1.10	6/1064 (0.6%)
16	V	0.51	0/1081	0.95	4/1468 (0.3%)
17	y	0.66	0/202	1.23	1/272 (0.4%)
18	X	0.48	0/257	0.90	0/348
19	Z	0.48	0/490	1.12	4/669 (0.6%)
All	All	0.54	0/20907	1.03	115/28460 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	34	ASP	N-CA-C	-9.30	101.71	113.43
17	y	22	LEU	N-CA-C	-9.06	101.48	112.54
3	C	182	PHE	N-CA-C	8.82	123.87	113.20
13	O	102	THR	N-CA-C	8.79	120.94	111.36
5	E	57	ALA	N-CA-C	-8.68	99.34	110.53
15	U	51	TYR	N-CA-C	-8.63	97.72	110.23
3	C	439	VAL	N-CA-C	-8.45	102.63	110.82
2	B	483	ASP	CA-C-N	8.38	130.31	119.84
2	B	483	ASP	C-N-CA	8.38	130.31	119.84
9	J	36	LEU	N-CA-C	-8.34	103.24	113.41
15	U	74	THR	N-CA-C	8.15	119.86	110.97
3	C	318	LEU	N-CA-C	-8.07	102.56	111.36
13	O	103	SER	N-CA-C	7.89	121.67	110.23
8	I	2	GLU	N-CA-C	-7.63	103.42	112.89
5	E	24	SER	N-CA-C	-7.57	103.30	112.54
2	B	328	GLY	CA-C-N	7.55	127.46	120.21
2	B	328	GLY	C-N-CA	7.55	127.46	120.21
5	E	70	PHE	N-CA-C	7.46	119.05	111.07
2	B	327	THR	N-CA-C	7.42	119.54	110.41
3	C	347	GLY	N-CA-C	7.33	123.41	114.69
4	D	54	PHE	N-CA-C	7.16	121.89	112.72
2	B	236	THR	N-CA-C	-7.08	105.18	114.31
10	K	38	VAL	N-CA-C	-6.99	103.70	110.42
4	D	296	TYR	N-CA-C	6.96	118.66	111.14
2	B	363	PHE	N-CA-C	6.87	119.89	108.96
9	J	39	SER	N-CA-C	-6.86	104.01	114.16
3	C	254	THR	N-CA-C	6.82	117.58	108.38
4	D	156	VAL	N-CA-C	6.75	117.36	110.82
15	U	72	TYR	N-CA-C	6.71	124.64	109.81
5	E	67	THR	N-CA-C	6.62	122.17	113.30
19	Z	37	LYS	N-CA-C	-6.60	104.95	112.87
13	O	200	LEU	CA-C-N	6.60	128.09	119.84
13	O	200	LEU	C-N-CA	6.60	128.09	119.84
1	A	87	ASN	N-CA-C	-6.58	105.07	113.23
3	C	37	ALA	N-CA-C	-6.56	103.38	112.30
15	U	62	ILE	N-CA-C	6.53	118.07	110.62
16	V	104	ASN	CA-C-N	6.43	126.19	119.76
16	V	104	ASN	C-N-CA	6.43	126.19	119.76
1	A	36	ILE	N-CA-C	-6.42	106.29	111.81
4	D	272	LEU	N-CA-C	-6.30	103.72	111.40
2	B	37	MET	N-CA-C	-6.29	104.52	111.82
4	D	142	ASN	N-CA-C	-6.27	105.46	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	381	ILE	CA-C-N	6.22	126.19	119.78
2	B	381	ILE	C-N-CA	6.22	126.19	119.78
2	B	332	LYS	N-CA-C	-6.20	105.68	113.18
13	O	40	GLY	N-CA-C	-6.13	107.24	115.21
1	A	142	TRP	N-CA-C	6.12	123.83	110.80
13	O	249	ASP	N-CA-C	-6.01	105.59	113.17
2	B	484	PRO	N-CA-C	6.00	124.82	112.47
4	D	147	SER	N-CA-C	-5.94	104.89	111.36
4	D	273	PHE	N-CA-C	5.92	118.24	111.02
1	A	32	TRP	N-CA-C	-5.91	104.42	111.69
13	O	196	SER	N-CA-C	5.91	116.04	108.24
3	C	32	GLY	N-CA-C	-5.89	99.23	113.18
2	B	163	GLY	CA-C-N	5.84	127.14	119.84
2	B	163	GLY	C-N-CA	5.84	127.14	119.84
2	B	174	LEU	N-CA-C	-5.79	108.02	114.62
1	A	78	ILE	N-CA-C	5.79	116.57	110.72
5	E	8	ARG	CA-C-N	5.74	127.02	119.84
5	E	8	ARG	C-N-CA	5.74	127.02	119.84
16	V	75	ASN	CA-C-N	5.73	125.44	119.82
16	V	75	ASN	C-N-CA	5.73	125.44	119.82
3	C	224	ILE	CB-CA-C	-5.64	104.64	112.04
13	O	128	ASP	N-CA-C	5.62	119.23	112.93
3	C	302	TYR	N-CA-C	-5.60	101.36	109.31
4	D	297	ASP	N-CA-C	5.59	117.91	109.41
1	A	261	GLN	N-CA-C	5.57	122.66	110.80
2	B	80	ILE	N-CA-C	5.55	116.94	110.62
2	B	49	ASP	CA-C-N	5.53	126.01	120.04
2	B	49	ASP	C-N-CA	5.53	126.01	120.04
5	E	26	THR	N-CA-C	5.51	116.97	111.07
5	E	23	HIS	N-CA-C	5.50	119.25	112.54
7	H	34	PHE	N-CA-C	-5.50	105.28	111.28
1	A	146	ALA	N-CA-C	-5.50	105.37	111.36
1	A	339	PHE	CA-C-N	5.49	126.71	119.84
1	A	339	PHE	C-N-CA	5.49	126.71	119.84
1	A	88	ALA	N-CA-C	-5.49	105.45	111.82
4	D	170	ALA	N-CA-C	-5.46	103.04	110.36
5	E	13	ILE	N-CA-C	5.42	115.62	110.42
7	H	22	ALA	N-CA-C	-5.41	102.28	110.39
4	D	181	PHE	N-CA-C	-5.40	105.48	111.36
2	B	247	PHE	N-CA-C	-5.39	105.31	111.14
1	A	83	VAL	CA-C-N	5.37	125.31	119.78
1	A	83	VAL	C-N-CA	5.37	125.31	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	228	ASN	N-CA-C	5.37	119.61	112.30
2	B	77	GLY	N-CA-C	5.34	120.04	113.79
15	U	70	GLY	N-CA-C	5.34	122.16	114.10
8	I	17	LEU	N-CA-C	-5.33	105.11	111.03
11	L	36	PHE	N-CA-C	-5.32	106.29	112.89
13	O	205	GLU	N-CA-C	5.29	120.01	113.50
2	B	19	LEU	N-CA-C	-5.28	105.20	111.69
1	A	56	PRO	CA-C-N	5.25	125.26	119.90
1	A	56	PRO	C-N-CA	5.25	125.26	119.90
3	C	464	GLU	CA-C-N	5.23	126.38	119.84
3	C	464	GLU	C-N-CA	5.23	126.38	119.84
19	Z	35	ARG	N-CA-C	-5.21	105.67	112.23
3	C	391	ARG	N-CA-C	-5.18	105.54	111.14
1	A	33	PHE	N-CA-C	-5.17	105.82	111.82
2	B	57	ARG	N-CA-C	-5.17	107.14	113.50
2	B	237	VAL	N-CA-C	-5.17	104.59	111.05
13	O	181	ASN	N-CA-C	5.14	119.40	113.18
13	O	194	TYR	N-CA-C	5.14	117.75	110.50
2	B	165	GLY	N-CA-C	-5.14	105.87	111.21
15	U	75	LEU	N-CA-C	5.12	116.67	111.14
2	B	120	LEU	N-CA-C	-5.12	103.28	110.50
19	Z	33	TRP	N-CA-C	-5.11	106.13	112.47
13	O	81	GLU	CA-C-N	5.09	124.75	119.56
13	O	81	GLU	C-N-CA	5.09	124.75	119.56
1	A	266	ASN	N-CA-C	-5.07	107.03	114.39
2	B	317	ASN	N-CA-C	-5.07	105.89	113.89
1	A	296	ASN	N-CA-C	5.05	118.70	112.24
1	A	195	HIS	CA-C-N	5.01	124.45	119.24
1	A	195	HIS	C-N-CA	5.01	124.45	119.24
4	D	235	PHE	N-CA-C	5.01	117.13	109.07
4	D	299	ILE	N-CA-C	5.00	115.72	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	258	0
2	B	3812	0	3683	274	0
3	C	3455	0	3378	387	0
4	D	2706	0	2608	244	0
5	E	635	0	625	82	0
6	F	307	0	312	52	0
7	H	507	0	521	69	0
8	I	286	0	308	25	0
9	J	249	0	262	52	0
10	K	293	0	305	63	0
11	L	304	0	316	29	0
12	M	267	0	289	34	0
13	O	1845	0	1801	127	0
14	T	256	0	262	26	0
15	U	774	0	773	51	0
16	V	1060	0	1068	51	0
17	y	201	0	226	32	0
18	X	254	0	282	30	0
19	Z	479	0	516	69	0
20	A	1	0	0	0	0
21	A	260	0	288	48	0
21	B	1040	0	1152	131	0
21	C	780	0	864	134	0
21	D	130	0	144	18	0
21	K	65	0	72	12	0
22	A	64	0	74	6	0
22	D	64	0	74	15	0
23	A	12	0	13	13	0
24	A	5	0	0	0	0
25	A	40	0	56	9	0
25	B	120	0	168	8	0
25	C	80	0	112	24	0
25	D	40	0	56	8	0
25	J	80	0	112	19	0
25	X	40	0	56	5	0
25	Z	40	0	56	5	0
26	A	39	0	51	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	37	0	44	5	0
27	A	51	0	72	40	0
27	B	49	0	68	6	0
27	C	45	0	60	6	0
27	D	94	0	127	36	0
27	I	43	0	56	0	0
27	J	48	0	66	4	0
27	M	42	0	54	3	0
28	A	52	0	62	1	0
28	B	124	0	170	41	0
28	C	237	0	311	77	0
28	D	63	0	87	0	0
29	A	35	0	46	0	0
29	B	35	0	46	2	0
29	D	66	0	81	3	0
29	I	35	0	46	2	0
29	O	35	0	46	1	0
29	T	35	0	46	1	0
30	C	51	0	68	5	0
30	D	43	0	49	9	0
30	F	45	0	53	0	0
30	L	47	0	60	2	0
31	D	4	0	0	0	0
32	D	55	0	80	30	0
33	F	43	0	30	6	0
33	V	43	0	30	5	0
34	F	1	0	0	0	0
34	K	1	0	0	0	0
34	O	1	0	0	0	0
All	All	24678	0	25265	1891	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 38.

All (1891) 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)
30:C:475:SQD:C3	30:C:475:SQD:C4	1.74	1.58
16:V:63:CYS:SG	33:V:164:HEM:HAB	1.65	1.35
27:A:373:LMG:H112	4:D:266:TRP:CH2	1.77	1.19
1:A:271:LEU:HD11	23:A:367:MES:C8	1.73	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:533:DGD:HAH1	12:M:17:VAL:HG21	1.21	1.14
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.25	1.13
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.18	1.13
2:B:327:THR:HA	21:B:517:CLA:O1A	1.49	1.12
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.23	1.11
1:A:271:LEU:CD1	23:A:367:MES:H82	1.80	1.11
3:C:174:LEU:HD22	21:C:478:CLA:H161	1.21	1.10
10:K:10:LYS:O	10:K:10:LYS:HG2	1.44	1.10
3:C:293:ASN:HA	28:C:491:DGD:O2E	1.53	1.09
27:A:373:LMG:H332	12:M:22:LEU:HD21	1.27	1.08
3:C:174:LEU:CD2	21:C:478:CLA:H161	1.84	1.07
17:y:35:ILE:HG22	19:Z:21:ILE:HG23	1.37	1.06
21:B:518:CLA:H42	4:D:127:LEU:HD11	1.07	1.05
5:E:15:THR:HG22	9:J:7:ARG:CG	1.85	1.05
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.31	1.05
28:B:528:DGD:O1B	28:B:528:DGD:HG12	1.57	1.04
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.20	1.04
5:E:15:THR:CG2	9:J:7:ARG:HG2	1.86	1.04
3:C:254:THR:HG22	3:C:255:THR:H	1.18	1.04
13:O:178:ARG:HH11	13:O:178:ARG:HG3	1.18	1.04
1:A:214:MET:HE2	1:A:214:MET:HA	1.40	1.03
28:B:528:DGD:O2D	4:D:87:HIS:HB2	1.58	1.03
27:D:360:LMG:O6	11:L:15:THR:HG21	1.62	1.00
27:A:373:LMG:H112	4:D:266:TRP:HH2	0.85	1.00
2:B:250:PHE:HD1	28:B:528:DGD:HB92	1.22	1.00
2:B:149:LEU:HG	21:B:513:CLA:HBC1	1.41	1.00
27:A:373:LMG:H372	12:M:18:PRO:CB	1.91	0.98
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.00	0.96
27:A:373:LMG:C37	12:M:18:PRO:HB3	1.93	0.96
27:A:373:LMG:H372	12:M:18:PRO:HB3	0.97	0.96
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.49	0.95
13:O:230:VAL:HG12	13:O:231:ASP:H	1.30	0.94
14:T:29:ILE:H	14:T:29:ILE:HD12	1.33	0.94
3:C:286:ALA:HB2	21:C:478:CLA:HMD1	1.50	0.93
15:U:83:ALA:HB1	15:U:84:PRO:CD	1.98	0.93
25:C:489:BCR:H312	19:Z:9:LEU:HD11	1.51	0.93
1:A:11:ALA:O	1:A:12:ASN:HB2	1.67	0.93
27:A:373:LMG:C11	4:D:266:TRP:HH2	1.80	0.92
2:B:332:LYS:HE3	28:B:533:DGD:O4D	1.68	0.92
11:L:1:MET:HG2	11:L:1:MET:O	1.70	0.92
3:C:407:VAL:HA	28:C:493:DGD:O2E	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:517:CLA:H202	4:D:281:MET:SD	2.11	0.91
4:D:186:GLN:HB2	21:D:354:CLA:HBC1	1.52	0.91
3:C:225:VAL:HG21	28:C:491:DGD:HG11	1.52	0.90
1:A:286:THR:HG23	21:A:362:CLA:HED3	1.50	0.90
27:D:360:LMG:O7	11:L:19:LEU:HD21	1.71	0.89
27:D:360:LMG:H212	14:T:17:PHE:HZ	1.36	0.89
21:B:524:CLA:H18	28:B:533:DGD:HAS1	1.53	0.89
5:E:15:THR:CG2	9:J:7:ARG:CG	2.48	0.89
28:B:528:DGD:HO2D	4:D:87:HIS:CG	1.90	0.89
3:C:224:ILE:O	3:C:227:VAL:HG23	1.73	0.89
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.55	0.88
2:B:434:THR:HG23	13:O:204:LYS:HE3	1.54	0.88
21:B:514:CLA:H11	21:B:522:CLA:H152	1.54	0.88
1:A:214:MET:HE1	4:D:142:ASN:ND2	1.89	0.88
7:H:35:MET:HE2	25:X:107:BCR:HC21	1.55	0.88
28:C:493:DGD:HE62	9:J:40:LEU:HD21	1.54	0.88
2:B:271:THR:HG22	2:B:273:TYR:H	1.39	0.88
5:E:15:THR:HG21	9:J:7:ARG:HG2	1.56	0.87
3:C:305:THR:HG22	3:C:308:GLU:H	1.40	0.87
13:O:218:LEU:HD22	15:U:119:THR:HG21	1.57	0.87
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.56	0.87
13:O:69:LEU:HD12	13:O:70:CYS:H	1.39	0.87
27:A:373:LMG:H231	27:D:360:LMG:H202	1.54	0.87
4:D:23:LYS:HZ1	30:D:361:SQD:H462	1.38	0.87
3:C:155:ASN:HD21	3:C:255:THR:HB	1.40	0.87
28:B:528:DGD:HBE1	4:D:159:ILE:HG23	1.57	0.87
1:A:193:LEU:HD11	21:A:362:CLA:HMC2	1.56	0.86
3:C:447:ARG:HG2	3:C:447:ARG:HH11	1.40	0.86
2:B:250:PHE:HD1	28:B:528:DGD:C9B	1.88	0.86
16:V:30:THR:HB	16:V:31:PRO:HD2	1.54	0.86
4:D:259:ILE:HG12	27:D:360:LMG:H301	1.57	0.86
11:L:5:PRO:HA	11:L:7:ARG:HH22	1.40	0.86
25:C:489:BCR:H353	25:J:112:BCR:H321	1.56	0.85
13:O:178:ARG:HH11	13:O:178:ARG:CG	1.88	0.85
4:D:129:GLN:NE2	4:D:143:ALA:HA	1.92	0.85
21:B:513:CLA:HBB1	21:B:515:CLA:H171	1.59	0.85
7:H:12:ARG:O	7:H:12:ARG:HD3	1.76	0.85
11:L:8:GLN:N	11:L:8:GLN:HE21	1.75	0.85
5:E:18:ARG:HD2	5:E:22:ILE:HD11	1.60	0.84
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.57	0.84
2:B:250:PHE:CD1	28:B:528:DGD:HB92	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:11:TRP:CH2	17:y:36:ILE:HD11	2.12	0.84
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.60	0.83
1:A:39:PRO:HG3	25:A:369:BCR:HC8	1.58	0.83
28:B:533:DGD:HG31	12:M:6:LEU:HD12	1.59	0.83
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.39	0.83
2:B:124:ARG:HE	2:B:131:PRO:HD3	1.43	0.83
27:D:360:LMG:H221	14:T:13:ILE:HG21	1.60	0.83
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.61	0.83
21:C:478:CLA:H12	21:C:479:CLA:H42	1.61	0.82
28:B:528:DGD:O2D	4:D:87:HIS:CB	2.27	0.82
7:H:31:MET:HE3	7:H:35:MET:HE1	1.62	0.82
1:A:214:MET:HB3	23:A:367:MES:H61	1.59	0.82
4:D:135:LEU:HD23	30:D:361:SQD:O2	1.78	0.82
21:B:518:CLA:CBB	4:D:123:ILE:HG12	2.10	0.81
1:A:192:ILE:HA	1:A:293:MET:HE1	1.61	0.81
3:C:407:VAL:HG22	28:C:493:DGD:O2E	1.81	0.81
3:C:28:GLN:OE1	3:C:28:GLN:HA	1.78	0.81
27:D:360:LMG:H341	14:T:21:ILE:HD11	1.62	0.81
2:B:247:PHE:HE1	21:B:512:CLA:H8	1.46	0.81
3:C:254:THR:HG22	3:C:255:THR:N	1.96	0.81
4:D:23:LYS:NZ	30:D:361:SQD:H462	1.97	0.80
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.63	0.80
17:y:39:LEU:HB3	17:y:46:LEU:HD21	1.64	0.80
4:D:323:GLU:HG2	13:O:194:TYR:OH	1.81	0.80
5:E:84:LYS:HB2	5:E:84:LYS:NZ	1.97	0.80
3:C:135:ARG:HE	19:Z:33:TRP:NE1	1.80	0.80
27:A:373:LMG:C20	32:D:357:PL9:H212	2.13	0.79
25:C:489:BCR:HC22	10:K:18:PHE:HD1	1.46	0.79
1:A:214:MET:HE1	4:D:142:ASN:HD21	1.45	0.79
3:C:473:ASP:HB2	14:T:26:PRO:CB	2.11	0.79
30:C:475:SQD:C3	30:C:475:SQD:C5	2.60	0.79
28:B:533:DGD:HAH1	12:M:17:VAL:CG2	2.08	0.79
10:K:10:LYS:O	10:K:10:LYS:CG	2.30	0.78
13:O:230:VAL:HG12	13:O:231:ASP:N	1.98	0.78
2:B:434:THR:CG2	13:O:204:LYS:HE3	2.12	0.78
21:C:484:CLA:H141	21:K:483:CLA:H162	1.64	0.78
19:Z:32:ASP:CG	19:Z:33:TRP:H	1.90	0.78
2:B:483:ASP:CG	2:B:484:PRO:HD2	2.07	0.78
3:C:437:PHE:HA	21:C:484:CLA:HMC2	1.66	0.78
1:A:190:HIS:HB3	1:A:293:MET:HE2	1.64	0.78
19:Z:36:SER:HA	19:Z:39:LEU:HG	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:HIS:HA	23:A:367:MES:H51	1.63	0.78
2:B:383:PHE:O	13:O:192:SER:HA	1.84	0.78
3:C:110:PRO:HG3	27:C:494:LMG:H141	1.65	0.78
21:C:480:CLA:H143	21:C:484:CLA:H152	1.66	0.77
2:B:348:ASN:HB3	2:B:354:LEU:HD21	1.65	0.77
1:A:218:LEU:HD22	23:A:367:MES:H52	1.66	0.77
3:C:233:VAL:HA	25:C:490:BCR:H281	1.65	0.77
4:D:152:VAL:HG11	21:D:354:CLA:H11	1.67	0.77
13:O:31:LEU:HB2	13:O:36:ILE:HD11	1.67	0.77
1:A:271:LEU:HD21	23:A:367:MES:HN4	1.50	0.77
27:D:360:LMG:H201	11:L:22:LEU:HD11	1.66	0.77
17:y:34:MET:HE1	17:y:38:LEU:HD21	1.65	0.77
27:A:373:LMG:H332	12:M:22:LEU:CD2	2.12	0.77
3:C:284:PHE:HB3	28:C:491:DGD:HA52	1.66	0.77
3:C:135:ARG:HE	19:Z:33:TRP:HE1	1.30	0.76
3:C:315:MET:HE1	3:C:369:LEU:HD12	1.66	0.76
2:B:134:ASP:OD2	2:B:137:LYS:HE3	1.86	0.76
1:A:131:TRP:CH2	21:C:481:CLA:HBA2	2.20	0.76
4:D:192:THR:HG23	21:D:354:CLA:HBC2	1.68	0.76
1:A:214:MET:HE3	22:D:355:PHO:HMD2	1.68	0.76
5:E:35:TRP:CD2	6:F:39:ALA:HB2	2.20	0.76
2:B:271:THR:HG22	2:B:273:TYR:N	1.98	0.76
3:C:209:ILE:HG23	25:C:490:BCR:H382	1.65	0.76
19:Z:49:ALA:O	19:Z:53:VAL:HG23	1.86	0.76
11:L:5:PRO:HA	11:L:7:ARG:NH2	2.00	0.75
1:A:46:ILE:HD13	28:A:375:DGD:HBE2	1.68	0.75
1:A:93:PHE:CZ	21:A:366:CLA:HBA1	2.20	0.75
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.14	0.75
30:C:475:SQD:H251	26:C:476:LHG:H102	1.66	0.75
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.66	0.75
3:C:391:ARG:NH1	3:C:391:ARG:HB2	2.02	0.75
21:C:477:CLA:HMB2	25:C:490:BCR:H403	1.67	0.75
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.67	0.75
8:I:4:LEU:HD22	29:I:274:LMT:H52	1.69	0.75
4:D:279:LEU:HG	22:D:355:PHO:HBC3	1.67	0.75
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.68	0.75
13:O:35:ASP:C	13:O:36:ILE:HD12	2.12	0.74
21:B:523:CLA:HED3	21:B:523:CLA:H2	1.68	0.74
16:V:63:CYS:SG	33:V:164:HEM:CAB	2.61	0.74
21:B:518:CLA:H42	4:D:127:LEU:CD1	2.03	0.74
18:X:12:ILE:O	18:X:12:ILE:HG23	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:MET:CB	23:A:367:MES:H61	2.16	0.74
27:A:373:LMG:H192	32:D:357:PL9:H221	1.69	0.74
3:C:135:ARG:NE	19:Z:33:TRP:HE1	1.85	0.74
3:C:223:TRP:CZ2	28:C:474:DGD:HA62	2.23	0.74
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.17	0.74
19:Z:32:ASP:HB2	19:Z:35:ARG:HG2	1.67	0.74
4:D:244:TYR:OH	4:D:264:LYS:HE3	1.88	0.74
5:E:18:ARG:HB3	5:E:18:ARG:HH11	1.52	0.74
27:A:373:LMG:C33	12:M:22:LEU:HD21	2.14	0.74
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.68	0.74
3:C:418:ASN:HB2	28:C:493:DGD:O4E	1.88	0.73
2:B:234:ILE:HD11	21:B:520:CLA:H191	1.70	0.73
3:C:29:GLU:HB3	10:K:46:ARG:NH1	2.03	0.73
3:C:135:ARG:HB2	19:Z:27:TYR:HB3	1.69	0.73
3:C:155:ASN:HA	3:C:158:THR:HG22	1.69	0.73
4:D:41:ALA:HB2	22:D:355:PHO:H43	1.70	0.73
21:B:518:CLA:H102	21:B:518:CLA:H142	1.69	0.73
5:E:81:GLU:C	5:E:83:LEU:H	1.96	0.73
10:K:21:LEU:HD13	17:y:24:MET:HE2	1.70	0.73
1:A:214:MET:HA	1:A:214:MET:CE	2.17	0.73
1:A:41:LEU:O	1:A:45:THR:HG22	1.89	0.73
5:E:15:THR:HG22	9:J:7:ARG:HG3	1.71	0.73
30:C:475:SQD:C4	30:C:475:SQD:C2	2.66	0.73
18:X:34:PHE:O	18:X:38:ILE:HG12	1.88	0.73
1:A:42:LEU:HD12	25:A:369:BCR:C11	2.18	0.73
3:C:85:GLY:O	21:C:480:CLA:HED1	1.89	0.73
3:C:241:GLY:O	3:C:245:ILE:HG13	1.88	0.73
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.23	0.73
5:E:17:VAL:O	5:E:21:VAL:HG23	1.88	0.73
4:D:85:MET:HE1	5:E:69:ARG:HA	1.71	0.72
27:A:373:LMG:H202	32:D:357:PL9:H212	1.70	0.72
3:C:225:VAL:CG2	28:C:491:DGD:HG11	2.20	0.72
1:A:35:VAL:HA	25:A:369:BCR:H333	1.70	0.72
3:C:407:VAL:HA	28:C:493:DGD:HO2E	1.52	0.72
3:C:168:LEU:HD13	21:C:483:CLA:H43	1.71	0.72
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.70	0.72
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.72	0.72
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.55	0.72
3:C:305:THR:CG2	3:C:308:GLU:H	2.02	0.72
7:H:63:LYS:C	7:H:65:LEU:H	1.98	0.72
3:C:240:ILE:O	3:C:244:CYS:HB2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:THR:CG2	3:C:255:THR:H	2.00	0.72
3:C:415:ASN:O	3:C:416:SER:HB3	1.89	0.72
25:C:489:BCR:H11C	25:J:112:BCR:H322	1.69	0.71
3:C:91:HIS:CD2	21:C:478:CLA:HBA1	2.25	0.71
21:B:511:CLA:H152	21:B:511:CLA:HMD2	1.72	0.71
3:C:404:LEU:HG	28:C:493:DGD:O1A	1.90	0.71
27:D:360:LMG:H192	11:L:22:LEU:HD21	1.71	0.71
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.04	0.71
2:B:135:LEU:HD23	2:B:138:MET:HE3	1.71	0.71
2:B:327:THR:CA	21:B:517:CLA:O1A	2.36	0.71
13:O:206:GLU:CD	13:O:206:GLU:H	1.97	0.71
1:A:40:THR:HG21	1:A:121:LEU:HD23	1.73	0.71
21:A:366:CLA:HMC2	25:A:369:BCR:H12C	1.72	0.71
21:B:513:CLA:H161	7:H:38:PHE:HE2	1.54	0.71
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.19	0.71
3:C:391:ARG:HB2	3:C:391:ARG:HH11	1.56	0.71
1:A:93:PHE:HZ	21:A:366:CLA:HBA1	1.54	0.71
2:B:250:PHE:CD1	28:B:528:DGD:C9B	2.72	0.71
4:D:44:ALA:HB3	22:D:355:PHO:H92	1.72	0.71
4:D:129:GLN:HE22	4:D:143:ALA:HA	1.55	0.71
1:A:22:THR:HG21	8:I:30:ARG:HD3	1.72	0.71
3:C:348:GLU:OE2	13:O:37:VAL:HA	1.91	0.70
3:C:187:ASP:HB2	3:C:230:LEU:HD12	1.74	0.70
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.02	0.70
3:C:116:VAL:HG12	25:C:489:BCR:H332	1.72	0.70
2:B:224:ARG:HG2	7:H:24:GLY:O	1.91	0.70
13:O:33:TYR:O	13:O:37:VAL:HG23	1.92	0.70
13:O:77:LEU:HD23	13:O:93:PRO:HA	1.74	0.70
13:O:69:LEU:HD12	13:O:70:CYS:N	2.05	0.70
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.26	0.70
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.73	0.70
2:B:222:PRO:HG3	7:H:27:THR:H	1.57	0.70
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.27	0.70
2:B:135:LEU:HA	2:B:138:MET:HE3	1.74	0.70
3:C:52:ALA:HA	21:C:486:CLA:HMB3	1.73	0.70
16:V:115:ALA:CB	16:V:122:ARG:HD2	2.22	0.70
3:C:219:GLY:HA2	28:C:491:DGD:O3D	1.92	0.70
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.74	0.70
28:B:533:DGD:CDA	12:M:17:VAL:HG21	2.12	0.69
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.06	0.69
3:C:54:VAL:HG13	21:C:487:CLA:HED1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:ILE:HG12	27:D:360:LMG:C30	2.21	0.69
15:U:38:GLU:HG2	15:U:39:LEU:N	2.05	0.69
2:B:65:PHE:O	21:B:515:CLA:HBA1	1.92	0.69
21:B:521:CLA:H193	21:B:523:CLA:H92	1.74	0.69
2:B:137:LYS:HD2	7:H:14:LEU:O	1.93	0.69
2:B:284:ILE:HG12	2:B:309:LEU:CD1	2.22	0.69
4:D:39:PRO:O	4:D:43:LEU:HD22	1.93	0.69
21:B:513:CLA:H161	7:H:38:PHE:CE2	2.28	0.69
3:C:404:LEU:HD21	28:C:493:DGD:HA31	1.73	0.69
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.27	0.69
1:A:119:PHE:HZ	21:A:362:CLA:H101	1.58	0.69
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.74	0.69
3:C:284:PHE:CB	28:C:491:DGD:HA52	2.23	0.69
21:C:478:CLA:O1A	21:C:479:CLA:H11	1.92	0.69
4:D:41:ALA:CB	22:D:355:PHO:H43	2.23	0.69
9:J:22:ILE:HG21	27:J:492:LMG:H202	1.75	0.69
19:Z:30:PRO:HG3	19:Z:33:TRP:HZ3	1.58	0.69
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.74	0.69
3:C:60:ILE:HG21	21:C:479:CLA:H191	1.75	0.69
3:C:158:THR:O	3:C:251:HIS:HB3	1.92	0.69
27:J:492:LMG:O8	27:J:492:LMG:O9	2.11	0.69
19:Z:28:ALA:O	19:Z:30:PRO:HD3	1.93	0.69
3:C:68:THR:OG1	21:C:479:CLA:HED1	1.92	0.69
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.76	0.68
2:B:264:PRO:HG2	2:B:267:LEU:HD12	1.75	0.68
21:B:524:CLA:OBD	11:L:10:VAL:HG21	1.93	0.68
5:E:81:GLU:O	5:E:83:LEU:N	2.24	0.68
3:C:130:VAL:HG13	21:C:486:CLA:H92	1.74	0.68
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.68
19:Z:32:ASP:HB3	19:Z:35:ARG:NH1	2.07	0.68
1:A:121:LEU:HD21	21:A:366:CLA:HMB3	1.75	0.68
21:B:521:CLA:H52	21:B:524:CLA:HBC3	1.74	0.68
27:A:373:LMG:HC92	2:B:5:TRP:HE1	1.59	0.68
28:C:493:DGD:HD3	9:J:32:ALA:O	1.93	0.68
25:D:358:BCR:H403	9:J:25:VAL:HG21	1.75	0.68
2:B:188:ASP:HA	7:H:58:VAL:HG23	1.76	0.68
16:V:29:LEU:HD13	16:V:151:ILE:HD11	1.75	0.68
3:C:166:ILE:O	3:C:170:ILE:HG13	1.94	0.68
10:K:19:ASP:N	10:K:20:PRO:HD2	2.09	0.68
1:A:192:ILE:CA	1:A:293:MET:HE1	2.23	0.68
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:ASN:HA	28:C:493:DGD:HG12	1.75	0.68
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.29	0.68
10:K:21:LEU:CD1	17:y:24:MET:HE2	2.24	0.68
1:A:271:LEU:HD11	23:A:367:MES:H82	0.83	0.68
1:A:307:ILE:HG13	6:F:45:ARG:HD2	1.76	0.68
2:B:133:LEU:HB3	2:B:138:MET:CE	2.24	0.68
2:B:328:GLY:O	21:B:517:CLA:HBA1	1.94	0.67
2:B:332:LYS:HE3	28:B:533:DGD:C4D	2.24	0.67
2:B:464:PHE:HD2	21:B:521:CLA:HAC2	1.58	0.67
4:D:152:VAL:CG1	21:D:354:CLA:H11	2.24	0.67
6:F:18:VAL:HG13	6:F:19:ARG:H	1.59	0.67
3:C:30:SER:HB2	10:K:46:ARG:O	1.94	0.67
3:C:472:LEU:HD12	3:C:473:ASP:H	1.59	0.67
3:C:113:VAL:HG12	27:C:494:LMG:H192	1.76	0.67
4:D:27:PHE:CD2	6:F:19:ARG:HD3	2.29	0.67
5:E:78:THR:O	5:E:81:GLU:HB2	1.94	0.67
1:A:39:PRO:HB2	21:A:366:CLA:HBB1	1.75	0.67
1:A:183:MET:HG2	21:A:363:CLA:HBC1	1.77	0.67
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.59	0.67
28:B:533:DGD:HA81	12:M:14:PHE:HA	1.75	0.67
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.77	0.67
4:D:87:HIS:HD2	4:D:162:LEU:HD23	1.58	0.67
4:D:180:ARG:HH11	4:D:180:ARG:CG	2.08	0.67
2:B:135:LEU:HD23	2:B:138:MET:CE	2.25	0.67
2:B:462:PHE:HA	21:B:521:CLA:HMC2	1.75	0.67
21:C:479:CLA:H171	21:K:483:CLA:HBB2	1.77	0.67
28:C:492:DGD:O3D	25:J:115:BCR:H382	1.94	0.67
1:A:45:THR:HB	22:A:365:PHO:H8	1.77	0.67
1:A:278:TRP:HA	28:C:493:DGD:HAG1	1.76	0.67
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.78	0.67
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.66
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.26	0.66
25:C:489:BCR:HC22	10:K:18:PHE:CD1	2.31	0.66
5:E:84:LYS:HB2	5:E:84:LYS:HZ2	1.60	0.66
2:B:483:ASP:OD2	2:B:484:PRO:HD2	1.94	0.66
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.77	0.66
3:C:155:ASN:HD21	3:C:255:THR:CB	2.07	0.66
3:C:377:LEU:O	3:C:381:LYS:HB2	1.95	0.66
28:C:493:DGD:HBF1	27:D:359:LMG:H211	1.77	0.66
2:B:62:VAL:CG1	21:B:515:CLA:HED3	2.26	0.66
3:C:305:THR:HG22	3:C:308:GLU:CB	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.48	0.66
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.77	0.66
4:D:267:LEU:HD23	4:D:267:LEU:C	2.20	0.66
9:J:11:TRP:CZ3	17:y:36:ILE:HD11	2.31	0.66
27:A:373:LMG:C11	4:D:266:TRP:CH2	2.66	0.66
2:B:271:THR:CG2	2:B:273:TYR:H	2.08	0.66
3:C:44:ASN:C	3:C:45:LEU:HD12	2.20	0.66
5:E:15:THR:HG22	9:J:7:ARG:CB	2.25	0.66
19:Z:33:TRP:O	19:Z:37:LYS:HB2	1.95	0.66
1:A:119:PHE:CZ	21:A:362:CLA:H101	2.30	0.66
28:C:492:DGD:HB52	25:J:115:BCR:H352	1.78	0.66
4:D:209:LEU:HD23	4:D:209:LEU:C	2.22	0.65
2:B:385:ARG:HD3	13:O:191:ALA:O	1.96	0.65
3:C:437:PHE:HZ	21:K:483:CLA:HMB3	1.62	0.65
4:D:192:THR:CG2	21:D:354:CLA:HBC2	2.26	0.65
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.62	0.65
2:B:271:THR:HB	2:B:274:GLN:HG3	1.78	0.65
27:D:360:LMG:O9	27:D:360:LMG:C7	2.43	0.65
3:C:437:PHE:HA	21:C:484:CLA:CMC	2.26	0.65
21:C:486:CLA:H151	19:Z:24:PRO:HG3	1.79	0.65
21:B:517:CLA:H141	21:B:517:CLA:H172	1.79	0.65
3:C:453:ALA:O	8:I:34:ARG:HB2	1.97	0.65
3:C:165:LEU:HD21	21:C:482:CLA:HHC	1.78	0.65
3:C:220:GLY:N	28:C:491:DGD:O3D	2.29	0.65
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.78	0.65
15:U:83:ALA:CB	15:U:84:PRO:HD2	2.14	0.65
2:B:86:ILE:HD12	2:B:86:ILE:O	1.97	0.65
1:A:64:ARG:NH1	13:O:98:THR:HG21	2.12	0.65
3:C:89:ILE:N	3:C:90:PRO:HD2	2.11	0.65
21:B:513:CLA:H3A	21:B:513:CLA:O2A	1.97	0.64
16:V:143:GLY:O	16:V:147:VAL:HG23	1.97	0.64
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.79	0.64
2:B:442:ILE:HD11	13:O:200:LEU:HD23	1.76	0.64
32:D:357:PL9:H262	32:D:357:PL9:C30	2.27	0.64
3:C:141:GLU:CD	3:C:141:GLU:H	2.05	0.64
3:C:437:PHE:CZ	21:K:483:CLA:HMB3	2.33	0.64
21:D:356:CLA:H42	18:X:26:GLY:HA3	1.79	0.64
2:B:7:ARG:HA	21:B:521:CLA:HBA1	1.78	0.64
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.32	0.64
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.78	0.64
2:B:250:PHE:HB3	28:B:528:DGD:HB82	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:7:ARG:O	11:L:7:ARG:HD2	1.97	0.64
2:B:331:ASN:HB3	2:B:437:LEU:HD12	1.79	0.64
21:C:483:CLA:OBD	21:C:485:CLA:H152	1.96	0.64
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.63	0.64
13:O:120:THR:HG22	13:O:154:SER:OG	1.96	0.64
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.78	0.64
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.62	0.64
5:E:36:LEU:O	5:E:40:THR:HG23	1.98	0.64
2:B:284:ILE:HG23	2:B:305:ILE:HD12	1.80	0.63
19:Z:55:GLY:HA2	25:Z:116:BCR:H312	1.80	0.63
1:A:32:TRP:HA	1:A:32:TRP:CE3	2.32	0.63
1:A:57:PRO:HG3	1:A:68:SER:CB	2.28	0.63
3:C:318:LEU:HD23	3:C:318:LEU:C	2.24	0.63
14:T:29:ILE:H	14:T:29:ILE:CD1	1.95	0.63
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.80	0.63
2:B:297:THR:OG1	2:B:300:GLU:HG3	1.98	0.63
2:B:486:LEU:O	2:B:486:LEU:HD13	1.98	0.63
3:C:37:ALA:C	21:C:484:CLA:HBA1	2.23	0.63
3:C:310:SER:OG	3:C:355:THR:HG23	1.98	0.63
32:D:357:PL9:H262	32:D:357:PL9:H302	1.80	0.63
6:F:19:ARG:NH2	33:F:85:HEM:O2D	2.32	0.63
17:y:41:VAL:C	17:y:43:ARG:H	2.06	0.63
5:E:26:THR:O	5:E:29:ALA:HB3	1.98	0.63
2:B:247:PHE:HB2	21:B:518:CLA:HBC1	1.80	0.63
1:A:300:PHE:CZ	3:C:404:LEU:HD23	2.33	0.62
21:B:513:CLA:H3A	21:B:513:CLA:CGA	2.29	0.62
21:B:517:CLA:H11	28:B:533:DGD:HB32	1.79	0.62
3:C:407:VAL:CA	28:C:493:DGD:O2E	2.45	0.62
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.32	0.62
4:D:246:MET:HE3	4:D:262:SER:HA	1.82	0.62
1:A:22:THR:HG21	8:I:30:ARG:CD	2.29	0.62
27:A:373:LMG:H201	32:D:357:PL9:H212	1.80	0.62
3:C:135:ARG:NE	19:Z:33:TRP:NE1	2.47	0.62
3:C:293:ASN:CA	28:C:491:DGD:O2E	2.40	0.62
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.82	0.62
11:L:7:ARG:C	11:L:8:GLN:HE21	2.06	0.62
1:A:18:CYS:O	1:A:22:THR:HG22	2.00	0.62
13:O:117:GLY:O	13:O:159:VAL:HG12	1.98	0.62
5:E:23:HIS:HA	5:E:26:THR:OG1	2.00	0.62
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.34	0.62
13:O:36:ILE:HG23	13:O:41:LEU:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ASP:OD2	3:C:110:PRO:HD3	1.99	0.62
21:C:486:CLA:H141	19:Z:20:VAL:O	2.00	0.62
13:O:234:THR:OG1	13:O:236:GLU:HG2	2.00	0.62
15:U:54:LYS:HB2	15:U:113:THR:HG23	1.82	0.62
1:A:228:THR:HG22	1:A:229:GLU:H	1.65	0.62
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.80	0.62
28:B:528:DGD:HE5	28:B:528:DGD:HD61	1.82	0.62
3:C:418:ASN:HA	28:C:493:DGD:HE2	1.81	0.62
10:K:18:PHE:HD2	10:K:18:PHE:N	1.97	0.62
1:A:42:LEU:HD12	25:A:369:BCR:H11C	1.81	0.62
2:B:371:THR:HG22	2:B:377:VAL:HA	1.81	0.62
5:E:10:PHE:CE2	6:F:19:ARG:NH1	2.67	0.62
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.81	0.61
3:C:44:ASN:O	3:C:45:LEU:HD12	1.99	0.61
3:C:119:LEU:HG	25:C:489:BCR:H10C	1.82	0.61
5:E:18:ARG:O	5:E:22:ILE:HG13	2.00	0.61
2:B:69:LEU:HD11	21:B:513:CLA:OBD	2.00	0.61
3:C:80:PRO:HD2	16:V:129:LYS:HZ1	1.65	0.61
26:C:476:LHG:H171	28:C:492:DGD:HBG2	1.82	0.61
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.30	0.61
5:E:64:PRO:HB3	5:E:84:LYS:HE2	1.82	0.61
17:y:42:ARG:HG2	17:y:42:ARG:HH11	1.66	0.61
19:Z:32:ASP:CB	19:Z:35:ARG:HG2	2.30	0.61
1:A:218:LEU:CD2	23:A:367:MES:H52	2.30	0.61
2:B:69:LEU:HD12	21:B:515:CLA:HBA2	1.82	0.61
3:C:41:ARG:NH1	21:C:486:CLA:OBD	2.33	0.61
28:C:492:DGD:HB42	28:C:493:DGD:HA21	1.81	0.61
15:U:66:ILE:O	15:U:66:ILE:HG22	1.98	0.61
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.81	0.61
3:C:113:VAL:HG11	27:C:494:LMG:H172	1.81	0.61
3:C:461:ARG:HH11	3:C:461:ARG:HG3	1.65	0.61
4:D:342:PRO:O	4:D:345:VAL:HG12	2.01	0.61
2:B:264:PRO:CG	2:B:267:LEU:HD12	2.31	0.61
27:B:531:LMG:HC2	4:D:141:TYR:OH	2.00	0.61
3:C:224:ILE:HD11	21:C:477:CLA:H93	1.81	0.61
3:C:248:GLY:O	3:C:252:ILE:HG12	2.00	0.61
3:C:374:GLY:O	3:C:375:LEU:C	2.44	0.61
6:F:31:ILE:HD12	6:F:31:ILE:N	2.16	0.61
14:T:29:ILE:HD12	14:T:29:ILE:N	2.10	0.61
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.15	0.61
15:U:94:ILE:O	15:U:97:LEU:HG	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:517:CLA:HBC3	25:B:529:BCR:H10C	1.83	0.61
3:C:52:ALA:HA	21:C:486:CLA:CMB	2.31	0.61
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.82	0.61
3:C:405:ASN:HB2	28:C:493:DGD:HG32	1.82	0.61
7:H:12:ARG:HD3	7:H:12:ARG:C	2.24	0.61
1:A:53:ILE:HD11	32:D:357:PL9:H501	1.82	0.61
3:C:114:VAL:HG22	27:C:494:LMG:H211	1.83	0.61
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.61
5:E:15:THR:CG2	9:J:8:ILE:H	2.13	0.61
5:E:79:PHE:O	5:E:84:LYS:HB3	2.01	0.61
7:H:19:GLY:O	7:H:21:VAL:HG13	1.99	0.61
13:O:39:THR:OG1	13:O:41:LEU:HB2	2.01	0.61
1:A:214:MET:HE3	22:D:355:PHO:CMD	2.31	0.61
27:A:373:LMG:H331	11:L:24:ILE:HD11	1.81	0.61
10:K:18:PHE:N	10:K:18:PHE:CD2	2.68	0.61
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.81	0.61
3:C:88:LEU:HB3	21:C:479:CLA:HED3	1.83	0.61
9:J:18:GLY:HA3	25:J:112:BCR:H371	1.82	0.61
21:B:518:CLA:HBB2	4:D:123:ILE:HG12	1.82	0.60
3:C:143:TYR:O	3:C:144:SER:HB2	2.00	0.60
3:C:180:MET:HE3	3:C:202:PRO:HD3	1.82	0.60
21:C:480:CLA:H93	28:C:492:DGD:HAT2	1.83	0.60
16:V:90:PRO:O	16:V:92:ARG:HD3	2.01	0.60
1:A:322:ASN:OD1	3:C:412:THR:HA	2.01	0.60
21:A:362:CLA:H111	22:A:365:PHO:H3A	1.83	0.60
27:A:373:LMG:H192	32:D:357:PL9:C22	2.31	0.60
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.36	0.60
6:F:38:ALA:O	6:F:41:GLN:HG2	2.01	0.60
10:K:10:LYS:O	10:K:11:LEU:C	2.43	0.60
13:O:86:ARG:HG3	13:O:86:ARG:HH11	1.66	0.60
15:U:97:LEU:O	15:U:102:LYS:HE2	2.01	0.60
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.82	0.60
10:K:17:ILE:HD12	10:K:17:ILE:N	2.17	0.60
2:B:124:ARG:NE	2:B:131:PRO:HD3	2.13	0.60
3:C:204:LEU:HD21	3:C:238:ILE:HG21	1.84	0.60
3:C:391:ARG:HD2	3:C:395:TYR:CE2	2.36	0.60
13:O:230:VAL:CG1	13:O:231:ASP:H	2.10	0.60
15:U:89:GLU:CD	15:U:89:GLU:H	2.09	0.60
1:A:153:SER:HB2	21:A:362:CLA:H43	1.83	0.60
7:H:58:VAL:HG13	7:H:58:VAL:O	2.00	0.60
1:A:343:LEU:O	1:A:344:ALA:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:GLY:HA2	25:D:358:BCR:H332	1.83	0.60
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.83	0.60
18:X:12:ILE:HG12	18:X:16:LEU:CD1	2.30	0.60
19:Z:33:TRP:O	19:Z:33:TRP:HD1	1.84	0.60
1:A:107:TYR:CD1	13:O:141:ARG:NH1	2.69	0.60
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.08	0.60
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.02	0.60
3:C:264:PHE:HE2	21:C:482:CLA:O1A	1.85	0.60
10:K:24:VAL:HG21	17:y:25:ILE:HG12	1.84	0.60
27:A:373:LMG:H311	11:L:20:GLY:HA2	1.82	0.60
3:C:178:LYS:HB2	21:C:478:CLA:H162	1.83	0.60
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.83	0.60
1:A:306:VAL:HG13	1:A:314:ILE:O	2.01	0.60
2:B:143:LEU:HA	21:B:520:CLA:HED1	1.83	0.60
2:B:238:LEU:HD13	21:B:522:CLA:C1D	2.32	0.60
5:E:18:ARG:HB3	5:E:18:ARG:NH1	2.17	0.60
2:B:213:GLY:O	2:B:217:ILE:HG13	2.02	0.60
3:C:39:ASN:OD1	21:C:485:CLA:HBB2	2.02	0.59
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.82	0.59
13:O:87:GLN:O	13:O:88:GLU:HB3	2.02	0.59
15:U:113:THR:O	15:U:114:VAL:HG23	2.02	0.59
1:A:22:THR:HG21	8:I:30:ARG:NE	2.16	0.59
21:B:517:CLA:H142	27:B:531:LMG:H382	1.84	0.59
5:E:15:THR:HG23	9:J:8:ILE:O	2.01	0.59
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.66	0.59
27:B:531:LMG:H201	27:B:531:LMG:H291	1.83	0.59
3:C:292:PHE:O	28:C:491:DGD:O2E	2.20	0.59
13:O:31:LEU:HD12	13:O:31:LEU:N	2.17	0.59
1:A:309:ALA:HB3	16:V:27:ALA:O	2.03	0.59
21:B:520:CLA:HHC	21:B:520:CLA:HBB1	1.83	0.59
3:C:233:VAL:HA	25:C:490:BCR:C28	2.32	0.59
17:y:19:ILE:HG23	17:y:20:ALA:H	1.68	0.59
2:B:172:TYR:O	2:B:174:LEU:HG	2.02	0.59
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.37	0.59
6:F:16:PHE:HE2	33:F:85:HEM:HMA2	1.66	0.59
2:B:149:LEU:CG	21:B:513:CLA:HBC1	2.26	0.59
4:D:261:PHE:HB2	32:D:357:PL9:H521	1.83	0.59
10:K:33:LEU:HD23	21:K:483:CLA:OBD	2.03	0.59
1:A:22:THR:HG21	8:I:30:ARG:HE	1.67	0.59
21:B:512:CLA:C4	7:H:45:ILE:HD11	2.33	0.59
6:F:27:ALA:HB1	33:F:85:HEM:HBC2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ALA:O	8:I:1:MET:HE3	2.02	0.59
5:E:56:TYR:O	16:V:27:ALA:HB2	2.02	0.59
2:B:133:LEU:HB3	2:B:138:MET:HE2	1.85	0.59
21:B:511:CLA:HHC	21:B:511:CLA:HBB1	1.84	0.59
3:C:418:ASN:CB	28:C:493:DGD:HE2	2.32	0.59
21:C:480:CLA:H42	28:C:493:DGD:HA32	1.84	0.59
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.01	0.59
2:B:458:PHE:HB3	21:B:514:CLA:HBC2	1.84	0.59
3:C:281:MET:HE1	21:C:481:CLA:HAC2	1.84	0.59
21:C:480:CLA:H43	28:C:492:DGD:HA91	1.85	0.59
6:F:23:VAL:O	6:F:27:ALA:HB2	2.03	0.59
3:C:112:PHE:O	3:C:116:VAL:HG13	2.03	0.58
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.37	0.58
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.68	0.58
3:C:369:LEU:HD21	3:C:384:ILE:HD13	1.85	0.58
21:C:481:CLA:H12	8:I:23:PHE:CD2	2.38	0.58
4:D:55:VAL:HG21	4:D:110:LEU:CD1	2.33	0.58
9:J:22:ILE:HG13	25:J:115:BCR:H10C	1.85	0.58
13:O:80:GLU:O	13:O:89:ALA:HB1	2.03	0.58
1:A:238:LYS:O	1:A:241:GLN:HG3	2.03	0.58
3:C:95:LEU:HD11	21:C:479:CLA:HBA2	1.83	0.58
3:C:380:ILE:HA	3:C:384:ILE:HD11	1.85	0.58
3:C:418:ASN:CA	28:C:493:DGD:HE2	2.34	0.58
27:D:360:LMG:O9	27:D:360:LMG:HC72	2.03	0.58
5:E:8:ARG:N	6:F:13:TYR:CE1	2.71	0.58
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.86	0.58
3:C:28:GLN:HB2	21:C:486:CLA:HED2	1.86	0.58
4:D:32:TRP:CG	30:D:361:SQD:H251	2.38	0.58
10:K:17:ILE:HD12	10:K:17:ILE:H	1.69	0.58
2:B:188:ASP:OD1	7:H:58:VAL:HA	2.04	0.58
21:C:477:CLA:H71	21:C:477:CLA:HMB3	1.86	0.58
5:E:15:THR:HG23	9:J:8:ILE:H	1.68	0.58
5:E:76:VAL:O	5:E:80:LEU:HD22	2.03	0.58
2:B:262:THR:HG21	21:B:513:CLA:HBA2	1.86	0.58
21:B:516:CLA:H161	21:B:526:CLA:H161	1.84	0.58
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.67	0.58
2:B:150:CYS:HA	21:B:513:CLA:HBC2	1.85	0.58
2:B:238:LEU:HB2	21:B:522:CLA:HMD3	1.84	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD13	21:D:354:CLA:HBA2	1.86	0.58
1:A:142:TRP:HB2	4:D:220:ASN:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:VAL:O	3:C:134:ILE:HG12	2.04	0.58
13:O:123:GLU:HG2	13:O:124:GLU:N	2.18	0.58
15:U:38:GLU:HG2	15:U:39:LEU:H	1.68	0.58
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.34	0.58
19:Z:14:ILE:O	19:Z:18:VAL:HG23	2.04	0.58
2:B:462:PHE:HA	21:B:521:CLA:CMC	2.33	0.58
3:C:122:SER:OG	25:C:489:BCR:H14C	2.04	0.58
3:C:305:THR:HG23	3:C:307:PRO:CD	2.32	0.58
4:D:239:GLN:O	4:D:240:ALA:HB3	2.03	0.58
1:A:203:ALA:HB1	28:C:493:DGD:HBV2	1.86	0.57
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.39	0.57
3:C:60:ILE:HG21	21:C:479:CLA:C19	2.34	0.57
32:D:357:PL9:H43	27:D:360:LMG:C25	2.34	0.57
9:J:14:ALA:HB1	25:J:112:BCR:C38	2.34	0.57
2:B:12:LEU:HD22	2:B:18:ARG:HB2	1.87	0.57
3:C:289:PHE:CD1	21:C:477:CLA:H12	2.38	0.57
3:C:447:ARG:HH11	3:C:447:ARG:CG	2.14	0.57
32:D:357:PL9:H23	32:D:357:PL9:H303	1.87	0.57
5:E:15:THR:O	9:J:8:ILE:HD12	2.03	0.57
19:Z:30:PRO:C	19:Z:32:ASP:H	2.12	0.57
2:B:55:MET:HE2	2:B:80:ILE:HD12	1.85	0.57
2:B:393:GLU:HG2	15:U:44:ASP:O	2.03	0.57
3:C:362:ARG:HG2	28:C:491:DGD:HE61	1.86	0.57
28:C:493:DGD:O3D	9:J:37:GLY:O	2.22	0.57
19:Z:32:ASP:C	19:Z:34:ASP:N	2.60	0.57
19:Z:55:GLY:CA	25:Z:116:BCR:H312	2.34	0.57
2:B:150:CYS:CA	21:B:513:CLA:HBC2	2.35	0.57
2:B:224:ARG:NE	7:H:25:TRP:NE1	2.52	0.57
3:C:281:MET:HE2	28:C:474:DGD:HAE1	1.85	0.57
4:D:252:PHE:O	4:D:256:ILE:HG22	2.05	0.57
4:D:279:LEU:CD1	21:D:354:CLA:HBA2	2.35	0.57
6:F:20:TRP:O	6:F:24:HIS:HB2	2.04	0.57
1:A:234:ASN:HB2	27:A:373:LMG:HC3	1.87	0.57
3:C:39:ASN:HB2	21:C:484:CLA:HBA2	1.85	0.57
4:D:122:LEU:HD21	22:D:355:PHO:H62	1.86	0.57
4:D:188:PHE:HE2	4:D:329:MET:CE	2.17	0.57
7:H:63:LYS:O	7:H:65:LEU:N	2.37	0.57
16:V:74:THR:O	16:V:75:ASN:HB2	2.04	0.57
17:y:19:ILE:HG23	17:y:20:ALA:N	2.19	0.57
2:B:10:THR:C	2:B:12:LEU:H	2.12	0.57
21:B:521:CLA:OBD	27:B:531:LMG:HC8	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:39:LEU:CB	17:y:46:LEU:HD21	2.32	0.57
1:A:214:MET:HB3	23:A:367:MES:C6	2.33	0.57
1:A:233:ALA:HB3	27:B:531:LMG:HC4	1.86	0.57
3:C:286:ALA:HB2	21:C:478:CLA:CMD	2.30	0.57
27:D:360:LMG:C20	11:L:22:LEU:HD11	2.34	0.57
12:M:29:THR:O	12:M:32:GLN:HG3	2.05	0.57
1:A:38:ILE:O	1:A:42:LEU:HG	2.05	0.57
1:A:244:GLU:HG3	1:A:246:TYR:H	1.70	0.57
2:B:230:ARG:O	2:B:233:ASN:HB3	2.05	0.57
2:B:262:THR:HG21	21:B:513:CLA:CBA	2.35	0.57
3:C:343:ARG:NH1	3:C:347:GLY:O	2.38	0.57
10:K:31:LEU:O	10:K:34:ALA:HB3	2.04	0.57
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.34	0.57
18:X:45:LYS:HD3	18:X:45:LYS:N	2.20	0.57
1:A:160:ILE:HD11	28:C:491:DGD:HA91	1.86	0.56
2:B:256:MET:HA	2:B:263:THR:HG21	1.87	0.56
28:B:528:DGD:HO2D	4:D:87:HIS:CB	2.09	0.56
3:C:193:GLY:O	3:C:194:GLY:C	2.48	0.56
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.88	0.56
4:D:113:PHE:CE2	25:D:358:BCR:HC41	2.40	0.56
4:D:152:VAL:HG21	4:D:279:LEU:CD1	2.35	0.56
10:K:26:PRO:O	10:K:29:PRO:HD2	2.05	0.56
1:A:13:LEU:H	1:A:13:LEU:HD12	1.69	0.56
1:A:183:MET:HE1	21:A:363:CLA:HMD2	1.87	0.56
27:A:373:LMG:H202	32:D:357:PL9:H201	1.86	0.56
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.87	0.56
2:B:191:ASN:HB2	7:H:58:VAL:CG2	2.35	0.56
2:B:192:PRO:HD2	7:H:60:VAL:HG12	1.88	0.56
3:C:305:THR:HG22	3:C:308:GLU:N	2.16	0.56
4:D:36:LEU:O	4:D:39:PRO:HD2	2.05	0.56
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.70	0.56
18:X:12:ILE:CG1	18:X:16:LEU:HD12	2.33	0.56
1:A:77:ILE:HG12	14:T:6:TYR:CD1	2.40	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.40	0.56
1:A:193:LEU:HD21	21:A:362:CLA:C2C	2.36	0.56
1:A:265:PHE:CD1	1:A:271:LEU:HA	2.41	0.56
27:A:373:LMG:C25	27:D:360:LMG:C22	2.83	0.56
17:y:33:PRO:O	17:y:36:ILE:HG13	2.05	0.56
19:Z:16:SER:O	19:Z:20:VAL:HG23	2.04	0.56
4:D:18:LEU:O	4:D:22:LEU:HG	2.05	0.56
13:O:178:ARG:CG	13:O:178:ARG:NH1	2.55	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.88	0.56
4:D:18:LEU:HD22	18:X:38:ILE:HD13	1.86	0.56
7:H:58:VAL:O	7:H:58:VAL:CG1	2.53	0.56
1:A:334:ARG:NH1	13:O:184:ASP:C	2.64	0.56
3:C:113:VAL:CG1	27:C:494:LMG:H192	2.36	0.56
2:B:224:ARG:HG3	7:H:25:TRP:CD1	2.41	0.56
4:D:157:PHE:CE1	4:D:171:PRO:HG2	2.41	0.56
13:O:31:LEU:HD12	13:O:31:LEU:H	1.71	0.56
4:D:267:LEU:HD23	4:D:267:LEU:O	2.06	0.56
13:O:88:GLU:OE2	13:O:90:GLU:HG2	2.06	0.56
1:A:292:THR:OG1	28:C:492:DGD:CEA	2.54	0.56
4:D:113:PHE:CZ	25:D:358:BCR:HC41	2.41	0.56
6:F:18:VAL:HG13	6:F:19:ARG:N	2.21	0.56
16:V:87:LEU:HD12	16:V:87:LEU:N	2.20	0.56
1:A:187:GLN:HB2	21:A:362:CLA:HAC2	1.88	0.55
18:X:16:LEU:HD13	18:X:16:LEU:C	2.31	0.55
19:Z:26:ALA:CB	19:Z:40:ILE:HD11	2.36	0.55
21:A:362:CLA:H202	21:A:363:CLA:H112	1.88	0.55
2:B:293:ALA:C	2:B:295:GLY:H	2.14	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CE2	2.41	0.55
3:C:167:VAL:CG1	21:C:487:CLA:H11	2.36	0.55
13:O:59:ASP:C	13:O:61:SER:H	2.14	0.55
19:Z:21:ILE:O	19:Z:25:VAL:HG22	2.07	0.55
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.88	0.55
3:C:107:ASP:OD2	3:C:109:PHE:HB3	2.06	0.55
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.88	0.55
15:U:72:TYR:O	15:U:73:PRO:C	2.48	0.55
1:A:37:MET:HG2	1:A:41:LEU:HD12	1.89	0.55
21:B:512:CLA:H203	28:B:528:DGD:HB91	1.88	0.55
25:J:112:BCR:HC31	10:K:21:LEU:HD21	1.89	0.55
1:A:217:SER:HA	1:A:220:THR:HG22	1.88	0.55
3:C:199:ILE:N	3:C:199:ILE:HD12	2.22	0.55
3:C:250:TRP:CD1	3:C:250:TRP:C	2.84	0.55
4:D:48:TRP:CE2	22:D:355:PHO:H161	2.42	0.55
5:E:30:LEU:HD12	33:F:85:HEM:HMC1	1.88	0.55
11:L:11:GLU:HG2	11:L:12:LEU:N	2.19	0.55
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.42	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.87	0.55
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.88	0.55
1:A:20:TRP:O	1:A:21:VAL:C	2.50	0.55
1:A:29:TYR:CD2	1:A:133:LEU:HD13	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ASN:HD21	7:H:60:VAL:HA	1.72	0.55
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.88	0.55
3:C:239:TRP:CE3	3:C:243:ILE:HD11	2.42	0.55
3:C:337:LEU:HD12	13:O:131:PRO:HG3	1.88	0.55
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.42	0.55
4:D:85:MET:CE	5:E:69:ARG:HA	2.36	0.55
7:H:63:LYS:C	7:H:65:LEU:N	2.65	0.55
16:V:59:PHE:HA	16:V:63:CYS:SG	2.47	0.55
3:C:64:ALA:HB2	21:C:479:CLA:HMD2	1.89	0.55
3:C:135:ARG:HG2	19:Z:33:TRP:CZ2	2.42	0.55
8:I:11:VAL:O	8:I:15:PHE:HD2	1.89	0.55
13:O:227:VAL:HG12	13:O:228:ALA:N	2.22	0.55
18:X:32:LEU:HD23	18:X:32:LEU:N	2.22	0.55
19:Z:29:SER:HB2	19:Z:31:GLN:HG3	1.88	0.55
2:B:100:HIS:CE1	21:B:516:CLA:H11	2.42	0.55
5:E:8:ARG:NE	5:E:13:ILE:HG12	2.22	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.89	0.55
19:Z:23:VAL:O	19:Z:26:ALA:HB3	2.06	0.55
26:A:371:LHG:HC2	4:D:229:ALA:HB1	1.87	0.55
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.70	0.55
3:C:223:TRP:CG	3:C:224:ILE:H	2.25	0.55
21:C:488:CLA:HMB2	25:Z:116:BCR:H402	1.89	0.55
19:Z:36:SER:OG	19:Z:39:LEU:HD12	2.07	0.55
2:B:25:MET:HE1	2:B:108:PHE:CE1	2.42	0.54
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.36	0.54
4:D:250:ASN:ND2	4:D:262:SER:HB3	2.22	0.54
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.07	0.54
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.88	0.54
1:A:131:TRP:CE3	1:A:132:GLU:N	2.75	0.54
21:B:520:CLA:H111	21:B:525:CLA:HAA1	1.88	0.54
3:C:55:ALA:HB1	25:C:489:BCR:H373	1.89	0.54
3:C:127:PHE:HE1	19:Z:23:VAL:HG21	1.72	0.54
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.90	0.54
5:E:55:TYR:O	5:E:84:LYS:HE3	2.07	0.54
13:O:141:ARG:HG2	13:O:141:ARG:HH11	1.71	0.54
13:O:154:SER:O	13:O:168:PHE:HA	2.07	0.54
27:A:373:LMG:C25	27:D:360:LMG:H222	2.37	0.54
2:B:23:HIS:C	21:B:525:CLA:HED1	2.33	0.54
2:B:169:SER:O	7:H:65:LEU:HD13	2.06	0.54
3:C:45:LEU:HD23	3:C:48:LYS:HD2	1.89	0.54
3:C:155:ASN:O	3:C:158:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:487:CLA:H172	21:C:487:CLA:CMA	2.37	0.54
4:D:152:VAL:HG11	21:D:354:CLA:C1	2.34	0.54
4:D:152:VAL:HG11	21:D:354:CLA:HBA1	1.88	0.54
30:L:213:SQD:H261	27:M:217:LMG:H191	1.90	0.54
15:U:66:ILE:O	15:U:66:ILE:CG2	2.56	0.54
1:A:197:PHE:CE2	28:C:492:DGD:CEA	2.90	0.54
21:C:477:CLA:H3A	21:C:477:CLA:O2A	2.08	0.54
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.07	0.54
19:Z:36:SER:HA	19:Z:39:LEU:CG	2.35	0.54
2:B:247:PHE:CE1	21:B:512:CLA:H8	2.33	0.54
21:B:518:CLA:H111	4:D:120:PHE:CE1	2.42	0.54
4:D:180:ARG:HG3	4:D:180:ARG:NH1	2.23	0.54
17:y:20:ALA:C	17:y:22:LEU:H	2.15	0.54
1:A:45:THR:OG1	21:A:363:CLA:H141	2.08	0.54
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.89	0.54
21:C:477:CLA:C3D	21:C:479:CLA:H2	2.38	0.54
15:U:100:ARG:O	15:U:103:GLN:HB3	2.07	0.54
21:B:519:CLA:HAC2	7:H:34:PHE:CE2	2.43	0.54
3:C:259:TRP:H	3:C:259:TRP:CD1	2.26	0.54
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.90	0.54
16:V:135:GLU:O	16:V:139:VAL:HG23	2.08	0.54
4:D:303:ILE:HD13	12:M:2:GLU:HG2	1.88	0.54
6:F:43:ILE:HG22	9:J:36:LEU:HD21	1.90	0.54
13:O:218:LEU:HD22	15:U:119:THR:CG2	2.35	0.54
21:A:364:CLA:H203	27:D:359:LMG:H402	1.89	0.54
2:B:474:LEU:O	4:D:134:ARG:NH1	2.41	0.54
21:B:511:CLA:HBB2	7:H:44:ILE:HG21	1.90	0.54
19:Z:35:ARG:O	19:Z:38:GLN:HB3	2.07	0.54
1:A:235:TYR:C	1:A:237:TYR:H	2.16	0.53
3:C:125:LEU:HD22	21:C:487:CLA:CED	2.37	0.53
7:H:12:ARG:N	7:H:13:PRO:HD2	2.23	0.53
3:C:80:PRO:HB2	3:C:83:GLU:HG3	1.90	0.53
4:D:86:GLY:O	4:D:166:SER:HB2	2.08	0.53
4:D:239:GLN:O	4:D:240:ALA:CB	2.55	0.53
5:E:15:THR:O	9:J:8:ILE:CD1	2.56	0.53
6:F:9:GLU:C	6:F:11:VAL:H	2.15	0.53
3:C:165:LEU:HD21	21:C:482:CLA:HBB1	1.89	0.53
3:C:418:ASN:HB2	28:C:493:DGD:HE2	1.89	0.53
28:C:492:DGD:HG11	27:J:492:LMG:H301	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.90	0.53
32:D:357:PL9:H352	11:L:26:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:GLU:HG2	2:B:235:GLU:O	2.08	0.53
21:B:521:CLA:H52	21:B:524:CLA:CBC	2.38	0.53
25:B:530:BCR:HC31	29:B:535:LMT:H72	1.90	0.53
3:C:174:LEU:HD12	21:C:487:CLA:H51	1.89	0.53
3:C:223:TRP:CH2	28:C:474:DGD:HA62	2.44	0.53
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.91	0.53
10:K:43:VAL:O	10:K:43:VAL:HG13	2.09	0.53
2:B:150:CYS:N	21:B:513:CLA:HBC2	2.23	0.53
2:B:471:ALA:HB2	4:D:130:PHE:CE2	2.44	0.53
9:J:15:THR:O	9:J:19:MET:HG3	2.08	0.53
1:A:160:ILE:HD11	28:C:491:DGD:HA81	1.90	0.53
21:B:512:CLA:H201	4:D:159:ILE:HG12	1.89	0.53
3:C:243:ILE:O	21:C:482:CLA:HMC1	2.09	0.53
3:C:407:VAL:CG2	28:C:493:DGD:O2E	2.55	0.53
3:C:416:SER:H	28:C:493:DGD:C3E	2.22	0.53
3:C:425:TRP:CZ2	21:C:480:CLA:HBA2	2.44	0.53
12:M:25:LEU:O	12:M:28:GLN:HG3	2.08	0.53
13:O:82:PRO:HB3	13:O:87:GLN:HG3	1.89	0.53
16:V:116:GLU:HG3	16:V:116:GLU:O	2.08	0.53
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.37	0.53
2:B:106:LEU:HD22	21:B:516:CLA:H193	1.90	0.53
3:C:54:VAL:HA	21:C:487:CLA:CED	2.39	0.53
3:C:404:LEU:CD2	28:C:493:DGD:HA31	2.37	0.53
19:Z:32:ASP:C	19:Z:34:ASP:H	2.17	0.53
21:A:363:CLA:H101	27:D:360:LMG:C25	2.39	0.53
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.91	0.53
7:H:55:LEU:O	7:H:58:VAL:HG12	2.09	0.53
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.09	0.53
3:C:53:HIS:HB3	21:C:487:CLA:OBD	2.09	0.53
25:C:489:BCR:C11	25:J:112:BCR:H322	2.38	0.53
4:D:18:LEU:HD22	18:X:38:ILE:CD1	2.38	0.53
32:D:357:PL9:C35	11:L:26:VAL:HB	2.38	0.53
13:O:190:LEU:HB2	13:O:214:LYS:HB2	1.90	0.53
33:V:164:HEM:HMA2	33:V:164:HEM:HBA1	1.90	0.53
1:A:107:TYR:HD1	13:O:141:ARG:NH1	2.05	0.53
21:B:515:CLA:H92	21:B:522:CLA:H18	1.91	0.53
4:D:238:THR:O	4:D:239:GLN:O	2.27	0.53
21:B:520:CLA:H121	21:B:520:CLA:O1D	2.09	0.52
3:C:449:ARG:HG2	21:C:481:CLA:HED3	1.91	0.52
28:C:493:DGD:O2D	9:J:32:ALA:HB1	2.10	0.52
25:D:358:BCR:H391	9:J:21:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:24:VAL:O	10:K:27:VAL:HG12	2.10	0.52
1:A:10:SER:C	1:A:12:ASN:H	2.16	0.52
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.07	0.52
1:A:278:TRP:HA	28:C:493:DGD:CIA	2.38	0.52
2:B:328:GLY:C	21:B:517:CLA:HBA1	2.34	0.52
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.90	0.52
3:C:239:TRP:HE3	3:C:243:ILE:HD11	1.74	0.52
3:C:391:ARG:HH11	3:C:391:ARG:CB	2.19	0.52
21:C:484:CLA:H43	21:C:486:CLA:HAC1	1.90	0.52
4:D:44:ALA:CB	22:D:355:PHO:H92	2.39	0.52
13:O:190:LEU:HD12	15:U:41:ASN:ND2	2.24	0.52
15:U:100:ARG:HH11	15:U:103:GLN:HG2	1.73	0.52
19:Z:3:ILE:O	19:Z:7:LEU:HG	2.09	0.52
3:C:216:SER:HB2	28:C:474:DGD:HG31	1.91	0.52
26:C:476:LHG:H142	25:J:115:BCR:HC21	1.89	0.52
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.91	0.52
4:D:337:GLU:O	4:D:338:ASN:C	2.51	0.52
1:A:114:LEU:HD23	1:A:114:LEU:C	2.34	0.52
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.40	0.52
2:B:7:ARG:HE	21:B:521:CLA:HED1	1.74	0.52
2:B:143:LEU:CA	21:B:520:CLA:HED1	2.39	0.52
2:B:464:PHE:CD2	21:B:521:CLA:HAC2	2.44	0.52
28:B:528:DGD:HE5	28:B:528:DGD:C6D	2.39	0.52
3:C:276:LEU:HD11	3:C:444:HIS:HD2	1.73	0.52
4:D:76:VAL:O	4:D:77:ALA:HB2	2.10	0.52
13:O:31:LEU:HB2	13:O:36:ILE:CD1	2.38	0.52
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.92	0.52
19:Z:55:GLY:N	25:Z:116:BCR:H312	2.23	0.52
1:A:218:LEU:HD23	23:A:367:MES:H72	1.90	0.52
21:C:480:CLA:H193	28:C:492:DGD:HBV1	1.91	0.52
17:y:36:ILE:C	17:y:36:ILE:HD12	2.35	0.52
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.45	0.52
1:A:334:ARG:NH1	13:O:183:LEU:O	2.42	0.52
1:A:334:ARG:HD2	13:O:183:LEU:HB2	1.92	0.52
2:B:191:ASN:ND2	7:H:60:VAL:HA	2.24	0.52
28:B:533:DGD:HAE1	12:M:17:VAL:HG21	1.92	0.52
3:C:405:ASN:CB	28:C:493:DGD:HG32	2.40	0.52
3:C:452:ALA:O	3:C:454:GLY:N	2.42	0.52
27:D:360:LMG:H212	14:T:17:PHE:CZ	2.28	0.52
13:O:240:THR:HA	13:O:264:VAL:HA	1.92	0.52
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:21:GLN:HA	17:y:23:THR:HG22	1.90	0.52
9:J:11:TRP:CG	10:K:42:ALA:HA	2.45	0.52
15:U:83:ALA:CB	15:U:84:PRO:CD	2.77	0.52
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.75	0.52
2:B:341:LYS:HD2	2:B:429:ILE:HG22	1.90	0.52
3:C:47:GLY:O	3:C:50:LEU:HB3	2.10	0.52
3:C:393:ALA:HB1	33:V:164:HEM:HBC1	1.91	0.52
3:C:447:ARG:HG2	3:C:447:ARG:NH1	2.16	0.52
4:D:221:THR:O	4:D:221:THR:HG23	2.10	0.52
5:E:61:ARG:HH22	16:V:153:GLY:HA3	1.74	0.52
13:O:141:ARG:NH1	13:O:141:ARG:HG2	2.24	0.52
15:U:66:ILE:HG13	15:U:72:TYR:CD1	2.44	0.52
19:Z:31:GLN:O	19:Z:32:ASP:HB3	2.10	0.52
1:A:49:VAL:O	1:A:53:ILE:HG13	2.10	0.52
3:C:271:TYR:CE1	21:C:483:CLA:HAC1	2.44	0.52
3:C:281:MET:CE	21:C:481:CLA:HAC2	2.40	0.52
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.91	0.52
7:H:25:TRP:O	7:H:26:GLY:C	2.53	0.52
11:L:1:MET:O	11:L:1:MET:CG	2.48	0.52
13:O:225:LEU:C	13:O:226:ASN:HD22	2.17	0.52
19:Z:29:SER:C	19:Z:31:GLN:H	2.17	0.52
19:Z:32:ASP:CG	19:Z:33:TRP:N	2.60	0.52
2:B:12:LEU:CD2	2:B:18:ARG:HB2	2.40	0.52
3:C:425:TRP:HB3	21:C:480:CLA:HMB3	1.91	0.52
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.52
1:A:228:THR:HG22	1:A:229:GLU:N	2.25	0.51
4:D:334:GLN:N	4:D:335:PRO:HD3	2.25	0.51
5:E:61:ARG:NH2	16:V:153:GLY:HA3	2.25	0.51
2:B:222:PRO:CG	7:H:27:THR:H	2.21	0.51
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.75	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.45	0.51
4:D:136:VAL:O	4:D:136:VAL:HG12	2.10	0.51
4:D:346:LEU:O	4:D:348:ARG:HG3	2.10	0.51
25:D:358:BCR:H391	25:J:115:BCR:H332	1.91	0.51
10:K:30:VAL:HA	21:K:483:CLA:H191	1.93	0.51
19:Z:32:ASP:OD1	19:Z:36:SER:HB2	2.11	0.51
1:A:202:VAL:HG11	21:A:364:CLA:OBD	2.09	0.51
3:C:346:THR:O	13:O:40:GLY:HA2	2.10	0.51
7:H:38:PHE:HB2	25:X:107:BCR:H10C	1.92	0.51
16:V:147:VAL:O	16:V:150:LYS:HB2	2.10	0.51
18:X:12:ILE:O	18:X:12:ILE:CG2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:ASP:HB3	13:O:202:GLN:HG3	1.92	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.45	0.51
3:C:95:LEU:CD1	21:C:479:CLA:HBA2	2.40	0.51
3:C:227:VAL:HG11	25:C:490:BCR:H282	1.93	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
1:A:10:SER:C	1:A:12:ASN:N	2.69	0.51
2:B:149:LEU:HD22	21:B:514:CLA:H161	1.92	0.51
21:C:477:CLA:H151	21:C:483:CLA:HMB3	1.93	0.51
5:E:9:PRO:O	5:E:10:PHE:C	2.53	0.51
1:A:78:ILE:O	1:A:176:ILE:HB	2.10	0.51
1:A:150:PRO:O	21:A:362:CLA:H43	2.11	0.51
1:A:183:MET:HB3	21:A:362:CLA:HBC2	1.92	0.51
21:A:363:CLA:HED2	4:D:198:MET:SD	2.50	0.51
3:C:128:GLY:HA3	21:C:488:CLA:C3C	2.40	0.51
3:C:269:GLU:OE1	3:C:447:ARG:HG2	2.10	0.51
5:E:15:THR:CG2	9:J:7:ARG:CB	2.85	0.51
25:J:112:BCR:C15	10:K:31:LEU:HB3	2.41	0.51
14:T:25:GLU:O	14:T:26:PRO:C	2.54	0.51
2:B:327:THR:HG22	21:B:517:CLA:H12	1.92	0.51
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.35	0.51
3:C:415:ASN:O	3:C:416:SER:CB	2.57	0.51
13:O:118:SER:HB3	13:O:157:PRO:HA	1.93	0.51
19:Z:47:TRP:O	19:Z:50:LEU:HB2	2.11	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.92	0.51
2:B:246:PHE:CD1	2:B:246:PHE:C	2.88	0.51
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.11	0.51
10:K:17:ILE:H	10:K:17:ILE:CD1	2.24	0.51
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.41	0.51
2:B:172:TYR:O	2:B:173:GLY:C	2.52	0.51
2:B:229:LEU:O	2:B:231:MET:N	2.43	0.51
3:C:158:THR:HG21	3:C:254:THR:O	2.10	0.51
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.91	0.51
18:X:17:LYS:O	18:X:21:ILE:HG13	2.10	0.51
27:A:373:LMG:O4	11:L:13:ASN:ND2	2.44	0.51
2:B:91:TRP:HE1	29:B:535:LMT:H41	1.75	0.51
10:K:25:LEU:HB2	10:K:26:PRO:HD3	1.93	0.51
16:V:30:THR:HB	16:V:31:PRO:CD	2.35	0.51
19:Z:36:SER:C	19:Z:38:GLN:N	2.69	0.51
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.46	0.50
19:Z:17:PHE:CE2	19:Z:21:ILE:HD11	2.45	0.50
1:A:227:THR:HA	1:A:231:GLU:OE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:364:CLA:HBB1	4:D:157:PHE:CE2	2.45	0.50
21:B:518:CLA:HBA1	30:D:361:SQD:H101	1.93	0.50
4:D:86:GLY:HA2	4:D:166:SER:HB3	1.93	0.50
19:Z:5:PHE:HA	19:Z:57:LEU:CD2	2.40	0.50
21:A:364:CLA:HED1	28:C:493:DGD:HBW2	1.93	0.50
2:B:125:ASP:OD2	2:B:127:ARG:HB3	2.11	0.50
3:C:81:MET:CE	3:C:89:ILE:HG22	2.41	0.50
3:C:137:PRO:HB2	3:C:139:THR:O	2.12	0.50
21:C:481:CLA:O1A	8:I:23:PHE:CZ	2.64	0.50
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.40	0.50
4:D:99:GLY:HA3	29:D:363:LMT:H2'	1.94	0.50
8:I:27:ASP:N	8:I:28:PRO:CD	2.74	0.50
13:O:271:PRO:HG2	13:O:272:ALA:H	1.76	0.50
1:A:190:HIS:CB	1:A:293:MET:HE2	2.38	0.50
1:A:214:MET:O	1:A:215:HIS:C	2.54	0.50
27:A:373:LMG:C25	27:D:360:LMG:H231	2.41	0.50
2:B:137:LYS:O	2:B:141:ILE:HG13	2.11	0.50
2:B:229:LEU:O	2:B:230:ARG:C	2.54	0.50
28:C:493:DGD:HG31	9:J:33:TYR:CZ	2.47	0.50
28:C:493:DGD:HB51	27:D:359:LMG:H121	1.94	0.50
1:A:215:HIS:O	1:A:216:GLY:C	2.53	0.50
1:A:283:VAL:O	1:A:286:THR:HG22	2.11	0.50
27:A:373:LMG:HC61	11:L:11:GLU:OE2	2.11	0.50
2:B:250:PHE:O	28:B:528:DGD:HB82	2.11	0.50
3:C:56:HIS:C	3:C:58:GLY:N	2.68	0.50
3:C:125:LEU:HA	21:C:488:CLA:HMC1	1.94	0.50
4:D:53:THR:HG22	4:D:67:TYR:CE2	2.47	0.50
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.92	0.50
7:H:62:TRP:O	7:H:63:LYS:O	2.30	0.50
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.93	0.50
3:C:155:ASN:CA	3:C:158:THR:HG22	2.39	0.50
3:C:159:THR:HG23	3:C:252:ILE:HD13	1.93	0.50
4:D:262:SER:OG	27:D:360:LMG:O3	2.28	0.50
32:D:357:PL9:H33	32:D:357:PL9:H301	1.93	0.50
29:D:363:LMT:O2'	18:X:21:ILE:HD12	2.11	0.50
13:O:94:THR:HB	13:O:135:GLN:O	2.12	0.50
2:B:55:MET:CE	2:B:80:ILE:HD12	2.42	0.50
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.93	0.50
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.93	0.50
21:B:512:CLA:HBD	21:B:512:CLA:H43	1.92	0.50
3:C:452:ALA:C	3:C:454:GLY:N	2.68	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:481:CLA:HAA2	21:C:481:CLA:HBD	1.92	0.50
21:C:486:CLA:H13	19:Z:20:VAL:HG13	1.93	0.50
4:D:135:LEU:HD23	30:D:361:SQD:HO2	1.77	0.50
4:D:180:ARG:CG	4:D:180:ARG:NH1	2.70	0.50
1:A:126:TYR:OH	22:A:365:PHO:O1D	2.23	0.50
1:A:243:GLU:H	1:A:243:GLU:CD	2.16	0.50
3:C:72:LEU:HD11	3:C:108:THR:HB	1.93	0.50
3:C:116:VAL:CG1	25:C:489:BCR:H332	2.40	0.50
3:C:405:ASN:HA	28:C:493:DGD:C1G	2.40	0.50
4:D:36:LEU:C	4:D:39:PRO:HD2	2.37	0.50
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.34	0.50
13:O:43:ASN:OD1	13:O:103:SER:HB2	2.12	0.50
1:A:249:VAL:HG11	2:B:486:LEU:HD23	1.92	0.50
2:B:26:HIS:CE1	21:B:522:CLA:HMA2	2.47	0.50
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.40	0.50
3:C:224:ILE:CD1	21:C:477:CLA:H93	2.42	0.50
19:Z:5:PHE:CE1	19:Z:54:VAL:HG13	2.46	0.50
1:A:106:LEU:HD11	25:A:369:BCR:H402	1.94	0.49
1:A:239:PHE:O	14:T:29:ILE:HA	2.12	0.49
28:B:533:DGD:HAW2	12:M:13:LEU:HD13	1.93	0.49
3:C:155:ASN:HA	3:C:158:THR:CG2	2.38	0.49
3:C:460:ASP:O	3:C:461:ARG:C	2.55	0.49
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.47	0.49
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.49
3:C:126:GLY:O	3:C:130:VAL:HG23	2.12	0.49
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.47	0.49
18:X:43:ILE:HG22	18:X:43:ILE:O	2.12	0.49
1:A:192:ILE:CB	1:A:293:MET:HE1	2.42	0.49
1:A:215:HIS:N	23:A:367:MES:H61	2.27	0.49
27:A:373:LMG:H202	32:D:357:PL9:C21	2.40	0.49
3:C:33:PHE:CE1	4:D:229:ALA:CB	2.96	0.49
3:C:264:PHE:CE1	21:C:483:CLA:HBB1	2.48	0.49
3:C:405:ASN:CA	28:C:493:DGD:HG12	2.42	0.49
3:C:449:ARG:HG2	21:C:481:CLA:CED	2.42	0.49
21:C:484:CLA:C4	21:C:486:CLA:HAC1	2.42	0.49
27:D:360:LMG:H192	11:L:22:LEU:CD2	2.42	0.49
2:B:256:MET:O	2:B:448:ARG:NH1	2.42	0.49
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.01	0.49
17:y:24:MET:O	17:y:25:ILE:C	2.55	0.49
19:Z:12:LEU:HB2	19:Z:50:LEU:HD22	1.93	0.49
21:A:363:CLA:H11	22:A:365:PHO:HMB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LEU:HD21	21:C:482:CLA:CHC	2.43	0.49
4:D:192:THR:HG23	21:D:354:CLA:CBC	2.39	0.49
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.49
2:B:134:ASP:OD2	2:B:137:LYS:HB2	2.12	0.49
2:B:183:PRO:HB2	2:B:185:TRP:CH2	2.46	0.49
2:B:286:ARG:HG2	2:B:286:ARG:NH1	2.26	0.49
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.95	0.49
5:E:30:LEU:CD1	6:F:28:VAL:HG13	2.41	0.49
7:H:53:LEU:HD12	18:X:19:PHE:CD1	2.47	0.49
13:O:59:ASP:HB3	13:O:62:GLN:HB3	1.93	0.49
13:O:159:VAL:HG13	13:O:159:VAL:O	2.13	0.49
19:Z:5:PHE:HA	19:Z:57:LEU:HD21	1.95	0.49
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.12	0.49
6:F:45:ARG:NH1	9:J:40:LEU:OXT	2.46	0.49
21:B:518:CLA:H161	21:B:519:CLA:H203	1.95	0.49
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.49
4:D:283:ALA:HA	21:D:354:CLA:CED	2.43	0.49
9:J:34:ALA:O	9:J:35:GLY:O	2.31	0.49
10:K:17:ILE:C	10:K:18:PHE:HD2	2.21	0.49
1:A:183:MET:HE1	21:A:363:CLA:CMD	2.43	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.13	0.49
3:C:89:ILE:N	3:C:90:PRO:CD	2.75	0.49
4:D:19:ASP:O	4:D:20:ASP:C	2.55	0.49
27:A:373:LMG:H192	32:D:357:PL9:C23	2.43	0.49
2:B:86:ILE:HD12	2:B:86:ILE:C	2.38	0.49
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.73	0.49
28:B:533:DGD:C3G	12:M:6:LEU:HD12	2.38	0.49
3:C:109:PHE:HB3	3:C:110:PRO:HD3	1.94	0.49
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.95	0.49
21:C:478:CLA:CGA	21:C:479:CLA:H11	2.43	0.49
21:C:481:CLA:HAA2	21:C:481:CLA:CBD	2.41	0.49
4:D:126:MET:CE	4:D:150:ILE:HG13	2.43	0.49
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.93	0.49
11:L:12:LEU:HD22	12:M:25:LEU:HD12	1.93	0.49
13:O:126:GLY:O	13:O:128:ASP:N	2.45	0.49
1:A:159:LEU:C	1:A:162:PRO:HD2	2.38	0.48
21:C:486:CLA:H111	10:K:32:PHE:HE1	1.77	0.48
10:K:30:VAL:HA	21:K:483:CLA:H201	1.94	0.48
16:V:95:ILE:O	16:V:99:VAL:HG23	2.12	0.48
1:A:13:LEU:H	1:A:13:LEU:CD1	2.27	0.48
2:B:435:GLU:O	2:B:436:THR:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:520:CLA:H11	21:B:522:CLA:H201	1.95	0.48
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.94	0.48
4:D:261:PHE:HB2	32:D:357:PL9:C52	2.43	0.48
5:E:28:PRO:O	5:E:32:ILE:HG13	2.13	0.48
9:J:14:ALA:HB1	25:J:112:BCR:H382	1.94	0.48
13:O:226:ASN:HD22	13:O:226:ASN:N	2.11	0.48
18:X:42:GLN:O	18:X:43:ILE:HG13	2.12	0.48
1:A:224:ILE:O	1:A:226:GLU:OE2	2.30	0.48
3:C:167:VAL:HG13	21:C:487:CLA:H11	1.96	0.48
3:C:315:MET:O	3:C:319:ILE:HG13	2.12	0.48
3:C:390:ARG:NH2	16:V:126:ILE:HD13	2.29	0.48
21:C:486:CLA:H161	19:Z:20:VAL:HG13	1.94	0.48
4:D:210:LEU:HD21	32:D:357:PL9:H13	1.95	0.48
6:F:31:ILE:N	6:F:31:ILE:CD1	2.76	0.48
13:O:223:ILE:HG12	13:O:224:SER:N	2.27	0.48
33:V:164:HEM:HBA1	33:V:164:HEM:CMA	2.42	0.48
17:y:21:GLN:O	17:y:21:GLN:HG2	2.13	0.48
18:X:32:LEU:O	18:X:36:VAL:HG23	2.13	0.48
2:B:35:GLY:O	2:B:38:ALA:HB3	2.13	0.48
2:B:118:TRP:CH2	11:L:5:PRO:HD2	2.48	0.48
4:D:60:THR:HG23	4:D:61:HIS:HD2	1.75	0.48
13:O:86:ARG:HG3	13:O:86:ARG:NH1	2.26	0.48
1:A:193:LEU:HD21	21:A:362:CLA:HMC2	1.96	0.48
21:A:364:CLA:HMA1	22:D:355:PHO:H203	1.96	0.48
2:B:154:GLY:O	2:B:159:THR:HG23	2.13	0.48
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.49	0.48
4:D:193:LEU:O	4:D:193:LEU:HG	2.14	0.48
27:D:360:LMG:C22	14:T:13:ILE:HG21	2.36	0.48
16:V:63:CYS:O	16:V:64:ALA:C	2.55	0.48
1:A:13:LEU:HD12	1:A:13:LEU:N	2.28	0.48
1:A:172:MET:HE1	21:A:363:CLA:CHC	2.43	0.48
1:A:199:GLN:NE2	21:A:364:CLA:HED2	2.29	0.48
21:A:366:CLA:C1	28:C:474:DGD:HB22	2.44	0.48
2:B:10:THR:C	2:B:12:LEU:N	2.71	0.48
28:B:528:DGD:HD3	4:D:87:HIS:ND1	2.29	0.48
3:C:91:HIS:NE2	21:C:478:CLA:HBA1	2.28	0.48
3:C:315:MET:CE	3:C:366:LEU:HD13	2.44	0.48
4:D:274:VAL:HA	32:D:357:PL9:H253	1.95	0.48
4:D:303:ILE:CD1	12:M:2:GLU:HG2	2.44	0.48
8:I:6:ILE:O	8:I:10:ILE:HG12	2.13	0.48
27:A:373:LMG:H312	12:M:22:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:516:CLA:H62	25:B:530:BCR:H342	1.95	0.48
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.38	0.48
2:B:25:MET:HE3	25:B:527:BCR:H23C	1.95	0.48
3:C:71:GLU:OE1	3:C:89:ILE:HG13	2.13	0.48
3:C:135:ARG:HB2	19:Z:27:TYR:CB	2.42	0.48
3:C:442:LEU:HD21	21:C:481:CLA:HMB2	1.96	0.48
21:C:480:CLA:C4	28:C:493:DGD:HA32	2.43	0.48
21:C:486:CLA:C4D	10:K:39:TRP:HH2	2.26	0.48
4:D:180:ARG:HH11	4:D:180:ARG:HG3	1.79	0.48
16:V:64:ALA:O	16:V:65:SER:C	2.56	0.48
21:B:523:CLA:H161	25:B:529:BCR:H312	1.96	0.48
3:C:154:LYS:HE2	3:C:261:ARG:HD2	1.94	0.48
3:C:413:GLU:HG3	3:C:414:ILE:H	1.78	0.48
4:D:26:ARG:HD3	6:F:18:VAL:HG21	1.95	0.48
4:D:201:VAL:O	4:D:205:LEU:HB2	2.13	0.48
10:K:11:LEU:HD12	10:K:19:ASP:HA	1.96	0.48
1:A:205:VAL:HG21	21:A:362:CLA:HMA2	1.96	0.48
2:B:9:HIS:HB2	21:B:521:CLA:O1A	2.13	0.48
21:B:512:CLA:H42	7:H:45:ILE:CD1	2.44	0.48
21:B:523:CLA:H61	21:B:523:CLA:H41	1.59	0.48
3:C:413:GLU:HG3	3:C:414:ILE:N	2.28	0.48
4:D:146:PHE:O	4:D:150:ILE:HG12	2.14	0.48
10:K:20:PRO:O	10:K:23:ASP:HB2	2.13	0.48
13:O:36:ILE:HD12	13:O:36:ILE:N	2.29	0.48
2:B:175:THR:O	2:B:176:GLY:O	2.31	0.47
2:B:221:PRO:HA	21:B:519:CLA:HED3	1.95	0.47
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.48	0.47
3:C:67:MET:HE1	21:C:480:CLA:C1D	2.43	0.47
3:C:457:LYS:HE3	4:D:228:GLY:O	2.13	0.47
30:C:475:SQD:O8	4:D:233:ARG:HG3	2.14	0.47
21:C:487:CLA:H172	21:C:487:CLA:HMA1	1.95	0.47
7:H:30:LEU:HD11	7:H:34:PHE:HE1	1.78	0.47
8:I:24:LEU:O	8:I:26:GLY:N	2.41	0.47
12:M:8:LEU:HD21	29:T:226:LMT:H81	1.95	0.47
1:A:111:PRO:O	1:A:115:ILE:HG13	2.14	0.47
1:A:287:ALA:HA	21:A:362:CLA:HED2	1.96	0.47
1:A:330:VAL:HG11	4:D:348:ARG:HG2	1.96	0.47
2:B:106:LEU:CD2	21:B:516:CLA:H193	2.44	0.47
3:C:30:SER:OG	4:D:233:ARG:NH2	2.47	0.47
3:C:55:ALA:C	25:C:489:BCR:H373	2.39	0.47
3:C:466:VAL:HG13	4:D:251:ARG:HD2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:487:CLA:H121	21:C:488:CLA:H202	1.96	0.47
4:D:93:TRP:HA	4:D:99:GLY:H	1.80	0.47
5:E:22:ILE:O	5:E:26:THR:HG23	2.14	0.47
6:F:33:PHE:C	6:F:35:GLY:H	2.22	0.47
7:H:39:LEU:C	7:H:39:LEU:HD23	2.39	0.47
13:O:79:LYS:HE2	13:O:89:ALA:HB3	1.95	0.47
1:A:281:VAL:HB	28:C:493:DGD:HAG3	1.96	0.47
21:B:517:CLA:H61	21:B:517:CLA:H41	1.67	0.47
3:C:94:THR:HG22	3:C:298:PRO:HD2	1.96	0.47
2:B:124:ARG:HG3	2:B:124:ARG:NH1	2.26	0.47
2:B:124:ARG:HD3	2:B:131:PRO:N	2.30	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.47	0.47
32:D:357:PL9:H301	32:D:357:PL9:C33	2.45	0.47
5:E:77:GLU:HA	5:E:80:LEU:HD23	1.95	0.47
16:V:45:ILE:HG12	16:V:46:THR:N	2.28	0.47
1:A:287:ALA:HA	21:A:362:CLA:CED	2.44	0.47
26:A:371:LHG:H341	21:C:480:CLA:H203	1.96	0.47
2:B:215:PHE:CD2	2:B:215:PHE:C	2.93	0.47
2:B:250:PHE:CB	28:B:528:DGD:HB82	2.45	0.47
2:B:265:ILE:HG13	2:B:266:GLU:N	2.30	0.47
2:B:373:LYS:HA	2:B:373:LYS:HD2	1.55	0.47
3:C:116:VAL:HG23	3:C:117:VAL:N	2.28	0.47
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.49	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.42	0.47
5:E:35:TRP:C	5:E:35:TRP:CD1	2.93	0.47
15:U:89:GLU:CD	15:U:89:GLU:N	2.73	0.47
19:Z:30:PRO:C	19:Z:32:ASP:N	2.72	0.47
1:A:124:SER:O	1:A:127:MET:HB3	2.15	0.47
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.96	0.47
1:A:243:GLU:HA	4:D:241:GLU:HA	1.97	0.47
2:B:258:TYR:CE2	28:B:528:DGD:O1B	2.67	0.47
2:B:274:GLN:NE2	7:H:62:TRP:NE1	2.63	0.47
2:B:348:ASN:O	2:B:349:LYS:C	2.57	0.47
21:B:515:CLA:HMA2	21:B:516:CLA:HMA2	1.97	0.47
3:C:29:GLU:HA	10:K:46:ARG:HH12	1.79	0.47
3:C:363:GLY:O	3:C:364:PRO:C	2.56	0.47
4:D:23:LYS:HZ1	30:D:361:SQD:C46	2.18	0.47
4:D:32:TRP:CZ3	30:D:361:SQD:H282	2.49	0.47
27:D:360:LMG:H361	14:T:21:ILE:HD11	1.97	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.83	0.47
9:J:14:ALA:C	25:J:112:BCR:H382	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:35:LEU:HA	10:K:38:VAL:HG23	1.96	0.47
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.96	0.47
1:A:22:THR:CG2	8:I:30:ARG:HD3	2.42	0.47
2:B:24:LEU:HD21	21:B:526:CLA:CAB	2.44	0.47
2:B:68:ARG:HH22	21:B:514:CLA:HED3	1.80	0.47
2:B:248:ALA:HA	21:B:513:CLA:H42	1.97	0.47
3:C:67:MET:HE1	21:C:480:CLA:CHD	2.45	0.47
3:C:288:CYS:SG	28:C:491:DGD:HA21	2.55	0.47
3:C:447:ARG:CG	3:C:447:ARG:NH1	2.74	0.47
4:D:122:LEU:CD2	22:D:355:PHO:H62	2.44	0.47
4:D:259:ILE:HG12	27:D:360:LMG:C29	2.44	0.47
5:E:81:GLU:C	5:E:83:LEU:N	2.64	0.47
8:I:30:ARG:O	8:I:31:ASN:HB3	2.14	0.47
11:L:24:ILE:HD12	11:L:24:ILE:N	2.29	0.47
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.49	0.47
2:B:201:HIS:CE1	21:B:513:CLA:HMB2	2.49	0.47
3:C:135:ARG:HB2	19:Z:27:TYR:CG	2.50	0.47
4:D:134:ARG:HA	4:D:134:ARG:HE	1.78	0.47
10:K:44:GLY:O	10:K:45:PHE:C	2.57	0.47
1:A:176:ILE:HG23	21:A:363:CLA:O1D	2.14	0.47
21:B:517:CLA:HBC3	25:B:529:BCR:HC8	1.97	0.47
3:C:407:VAL:CA	28:C:493:DGD:HO2E	2.26	0.47
16:V:83:GLU:CD	16:V:83:GLU:H	2.23	0.47
21:B:522:CLA:H12	21:B:525:CLA:HAA2	1.96	0.47
3:C:365:TRP:CB	3:C:391:ARG:HG2	2.45	0.47
4:D:202:ALA:HB3	32:D:357:PL9:C30	2.44	0.47
13:O:135:GLN:HG2	13:O:141:ARG:HG3	1.97	0.47
14:T:22:PHE:C	14:T:23:PHE:CD2	2.93	0.47
1:A:129:ARG:C	1:A:131:TRP:H	2.23	0.46
26:A:371:LHG:O4	4:D:230:SER:HA	2.14	0.46
5:E:8:ARG:HA	6:F:13:TYR:CE2	2.50	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	0.46
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.43	0.46
21:B:519:CLA:OBD	7:H:27:THR:HB	2.15	0.46
3:C:127:PHE:HA	21:C:486:CLA:H192	1.96	0.46
3:C:436:PHE:O	21:C:484:CLA:HAC1	2.14	0.46
29:D:536:LMT:H5'	30:D:361:SQD:H5	1.97	0.46
13:O:113:VAL:HA	13:O:119:LEU:HD23	1.97	0.46
16:V:68:VAL:O	16:V:68:VAL:HG13	2.15	0.46
18:X:12:ILE:HD13	18:X:12:ILE:C	2.40	0.46
19:Z:23:VAL:HB	19:Z:24:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TRP:CZ3	25:A:369:BCR:H371	2.49	0.46
28:B:528:DGD:O2D	4:D:87:HIS:CG	2.54	0.46
3:C:193:GLY:O	3:C:194:GLY:O	2.33	0.46
4:D:261:PHE:O	4:D:262:SER:HB3	2.14	0.46
16:V:148:GLU:OE1	16:V:148:GLU:HA	2.14	0.46
28:B:533:DGD:HA81	12:M:14:PHE:CA	2.42	0.46
3:C:208:VAL:O	3:C:209:ILE:C	2.57	0.46
4:D:27:PHE:CD2	6:F:19:ARG:CD	2.97	0.46
10:K:11:LEU:O	10:K:12:PRO:C	2.57	0.46
1:A:12:ASN:O	1:A:16:ARG:HG3	2.15	0.46
2:B:63:LEU:N	2:B:64:PRO:HD2	2.30	0.46
2:B:138:MET:SD	21:B:525:CLA:HAC1	2.55	0.46
2:B:234:ILE:C	2:B:236:THR:H	2.23	0.46
2:B:252:VAL:HG13	21:B:513:CLA:H12	1.97	0.46
3:C:265:ILE:HG13	21:C:481:CLA:HED1	1.97	0.46
4:D:128:ARG:O	4:D:129:GLN:C	2.59	0.46
4:D:274:VAL:HG13	32:D:357:PL9:H253	1.97	0.46
13:O:82:PRO:O	13:O:83:LYS:CB	2.64	0.46
16:V:102:MET:HE1	16:V:141:ILE:CD1	2.45	0.46
1:A:157:VAL:HG21	21:A:363:CLA:CMC	2.45	0.46
1:A:216:GLY:O	1:A:220:THR:HG22	2.16	0.46
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.46	0.46
3:C:213:LEU:HD21	25:C:490:BCR:C20	2.46	0.46
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.45	0.46
11:L:31:PHE:HB3	11:L:35:PHE:CE1	2.51	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
1:A:221:SER:HB2	4:D:139:ARG:O	2.16	0.46
3:C:390:ARG:CZ	16:V:126:ILE:HD13	2.46	0.46
9:J:15:THR:HA	25:J:112:BCR:C37	2.46	0.46
9:J:36:LEU:C	9:J:38:SER:H	2.23	0.46
17:y:42:ARG:HG2	17:y:42:ARG:NH1	2.30	0.46
19:Z:5:PHE:HE1	19:Z:54:VAL:HG13	1.80	0.46
1:A:45:THR:HG23	1:A:46:ILE:N	2.31	0.46
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.97	0.46
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.96	0.46
2:B:413:ASP:O	2:B:414:PRO:C	2.57	0.46
3:C:42:LEU:CD2	21:C:486:CLA:HED3	2.44	0.46
3:C:45:LEU:O	3:C:46:SER:C	2.58	0.46
3:C:189:TRP:O	3:C:190:ALA:C	2.58	0.46
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.44	0.46
3:C:276:LEU:HD21	21:C:484:CLA:CBB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:MET:HE1	3:C:356:MET:HE2	1.98	0.46
3:C:370:ARG:HD3	13:O:33:TYR:CE2	2.51	0.46
3:C:472:LEU:HD12	3:C:473:ASP:N	2.28	0.46
4:D:217:THR:O	4:D:221:THR:HB	2.15	0.46
7:H:35:MET:HG3	25:X:107:BCR:H323	1.98	0.46
12:M:18:PRO:O	12:M:21:PHE:HB3	2.16	0.46
16:V:54:GLU:OE1	16:V:54:GLU:HA	2.16	0.46
17:y:39:LEU:CD2	19:Z:25:VAL:HG12	2.46	0.46
1:A:96:ILE:C	1:A:98:GLU:H	2.23	0.46
1:A:121:LEU:HD11	21:C:481:CLA:H171	1.98	0.46
2:B:222:PRO:O	2:B:223:GLN:C	2.59	0.46
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.75	0.46
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.51	0.46
28:C:492:DGD:HBE2	28:C:493:DGD:HA92	1.97	0.46
5:E:36:LEU:HA	5:E:39:SER:HG	1.79	0.46
1:A:64:ARG:O	13:O:178:ARG:NH2	2.49	0.46
1:A:306:VAL:HG11	1:A:316:THR:HG23	1.97	0.46
3:C:39:ASN:HD21	21:C:486:CLA:C1C	2.29	0.46
3:C:49:LEU:O	3:C:53:HIS:ND1	2.43	0.46
3:C:142:GLU:C	3:C:144:SER:H	2.24	0.46
3:C:143:TYR:O	3:C:144:SER:CB	2.64	0.46
21:D:354:CLA:H101	22:D:355:PHO:H2	1.98	0.46
5:E:51:ARG:O	5:E:53:ASP:N	2.49	0.46
19:Z:36:SER:C	19:Z:38:GLN:H	2.24	0.46
1:A:32:TRP:HA	1:A:32:TRP:HE3	1.76	0.45
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.46	0.45
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.51	0.45
1:A:326:LEU:HD21	3:C:412:THR:HB	1.98	0.45
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.98	0.45
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.98	0.45
3:C:435:PHE:O	3:C:438:LEU:N	2.49	0.45
3:C:451:ALA:HA	3:C:456:GLU:CD	2.41	0.45
21:C:486:CLA:H8	25:C:489:BCR:H402	1.97	0.45
4:D:41:ALA:HB2	22:D:355:PHO:C4	2.44	0.45
27:D:359:LMG:O3	9:J:32:ALA:HA	2.16	0.45
7:H:11:LEU:C	7:H:13:PRO:HD2	2.41	0.45
1:A:131:TRP:CZ3	21:C:481:CLA:HBA2	2.51	0.45
21:A:366:CLA:H12	28:C:474:DGD:HB22	1.98	0.45
2:B:27:THR:CG2	2:B:107:LEU:HD13	2.45	0.45
2:B:110:ALA:CB	21:B:526:CLA:HMB2	2.47	0.45
21:B:519:CLA:C3D	7:H:31:MET:HB2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:VAL:HG23	3:C:329:GLY:N	2.31	0.45
5:E:64:PRO:HD3	5:E:84:LYS:HE2	1.98	0.45
10:K:18:PHE:O	10:K:22:VAL:HG23	2.16	0.45
1:A:39:PRO:HB2	21:A:366:CLA:CBB	2.44	0.45
1:A:202:VAL:O	1:A:206:PHE:HB2	2.17	0.45
2:B:15:ASP:O	2:B:17:GLY:N	2.50	0.45
2:B:68:ARG:HH12	21:B:514:CLA:CED	2.30	0.45
2:B:380:ASP:C	2:B:380:ASP:OD1	2.60	0.45
3:C:54:VAL:HG22	21:C:487:CLA:HED1	1.99	0.45
3:C:176:VAL:HG11	3:C:238:ILE:HG12	1.99	0.45
3:C:210:PHE:HZ	3:C:243:ILE:HD11	1.81	0.45
3:C:223:TRP:CH2	28:C:474:DGD:HA82	2.51	0.45
6:F:12:SER:O	6:F:13:TYR:HB2	2.16	0.45
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.45	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.80	0.45
1:A:255:PHE:HD2	1:A:264:SER:HG	1.63	0.45
2:B:68:ARG:HH12	21:B:514:CLA:HED1	1.81	0.45
21:B:518:CLA:H102	21:B:518:CLA:C14	2.41	0.45
28:B:528:DGD:C6D	28:B:528:DGD:C5E	2.94	0.45
3:C:276:LEU:CD1	3:C:444:HIS:HD2	2.30	0.45
4:D:14:TRP:CE3	18:X:38:ILE:HD12	2.52	0.45
6:F:23:VAL:O	6:F:23:VAL:HG22	2.17	0.45
6:F:33:PHE:C	6:F:35:GLY:N	2.74	0.45
13:O:190:LEU:HD12	15:U:41:ASN:CG	2.41	0.45
19:Z:35:ARG:HG3	19:Z:36:SER:N	2.30	0.45
1:A:309:ALA:HB2	5:E:52:PRO:C	2.42	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.97	0.45
21:B:515:CLA:H41	21:B:515:CLA:H61	1.51	0.45
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.45
3:C:245:ILE:O	3:C:249:ILE:HG12	2.16	0.45
3:C:258:GLY:CA	3:C:262:ARG:HH12	2.28	0.45
4:D:126:MET:HE3	4:D:150:ILE:HG13	1.99	0.45
5:E:10:PHE:CZ	6:F:19:ARG:HD2	2.51	0.45
9:J:14:ALA:HB1	25:J:112:BCR:C26	2.46	0.45
13:O:56:TYR:O	13:O:161:SER:HA	2.17	0.45
13:O:88:GLU:HG2	13:O:89:ALA:N	2.31	0.45
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.99	0.45
16:V:30:THR:O	16:V:34:LEU:HG	2.17	0.45
26:A:371:LHG:HC11	3:C:447:ARG:CZ	2.46	0.45
21:B:516:CLA:HBB1	21:B:516:CLA:HHC	1.99	0.45
21:B:517:CLA:C1	28:B:533:DGD:HB32	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HD13	21:C:483:CLA:C4	2.45	0.45
3:C:318:LEU:HD23	3:C:318:LEU:O	2.16	0.45
10:K:18:PHE:O	10:K:19:ASP:C	2.60	0.45
15:U:80:VAL:HG22	15:U:127:ARG:NH2	2.31	0.45
15:U:80:VAL:HG22	15:U:127:ARG:HH21	1.82	0.45
1:A:38:ILE:HB	25:A:369:BCR:H331	1.99	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CD2	2.52	0.45
7:H:21:VAL:HG23	7:H:22:ALA:O	2.16	0.45
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.98	0.45
21:A:363:CLA:H2	27:A:373:LMG:H242	1.99	0.45
2:B:62:VAL:HG11	21:B:515:CLA:HED3	1.99	0.45
2:B:463:PHE:C	2:B:463:PHE:CD2	2.94	0.45
3:C:258:GLY:C	3:C:262:ARG:NH1	2.74	0.45
4:D:56:THR:HB	5:E:49:THR:HG23	1.97	0.45
4:D:213:ILE:HG23	4:D:214:HIS:N	2.30	0.45
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.43	0.45
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.17	0.45
27:A:373:LMG:O10	27:A:373:LMG:O9	2.34	0.45
2:B:10:THR:O	2:B:13:ILE:HG13	2.16	0.45
2:B:422:ARG:HG2	2:B:422:ARG:HH11	1.82	0.45
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.29	0.45
3:C:258:GLY:HA3	3:C:262:ARG:HH12	1.81	0.45
13:O:69:LEU:HB3	13:O:107:ILE:CB	2.35	0.45
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.45
14:T:22:PHE:C	14:T:23:PHE:HD2	2.24	0.45
2:B:71:VAL:HG21	2:B:96:VAL:CG2	2.47	0.45
2:B:247:PHE:CD2	21:B:513:CLA:H111	2.52	0.45
3:C:163:PHE:CD1	3:C:252:ILE:HD11	2.52	0.45
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.99	0.45
21:C:479:CLA:H61	21:C:479:CLA:H41	1.58	0.45
4:D:67:TYR:CE1	4:D:76:VAL:HG11	2.51	0.45
15:U:100:ARG:NH1	15:U:103:GLN:HG2	2.31	0.45
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.52	0.45
27:A:373:LMG:H171	11:L:23:LEU:HD13	1.99	0.44
2:B:141:ILE:O	2:B:144:PHE:HB3	2.17	0.44
2:B:225:LEU:O	2:B:226:TYR:C	2.60	0.44
2:B:385:ARG:O	2:B:386:ALA:C	2.60	0.44
2:B:450:TRP:HB3	21:B:517:CLA:CMB	2.47	0.44
25:B:529:BCR:H361	25:B:529:BCR:H20C	1.80	0.44
3:C:68:THR:OG1	21:C:479:CLA:CED	2.63	0.44
3:C:110:PRO:O	3:C:114:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:337:LEU:CD1	13:O:131:PRO:HG3	2.47	0.44
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.47	0.44
13:O:173:ASN:ND2	13:O:220:LYS:HD3	2.32	0.44
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.52	0.44
4:D:122:LEU:CG	22:D:355:PHO:H62	2.47	0.44
5:E:34:GLY:HA2	6:F:32:PHE:CE2	2.53	0.44
7:H:9:ASP:O	7:H:12:ARG:HB3	2.17	0.44
7:H:28:THR:O	7:H:31:MET:HB3	2.18	0.44
8:I:4:LEU:O	8:I:8:VAL:HG23	2.17	0.44
2:B:148:LEU:HG	21:B:514:CLA:H193	1.99	0.44
3:C:334:PRO:HA	13:O:179:THR:OG1	2.17	0.44
3:C:436:PHE:HB3	21:K:483:CLA:H93	1.99	0.44
25:D:358:BCR:H331	25:D:358:BCR:C8	2.47	0.44
27:D:360:LMG:H221	14:T:13:ILE:CG2	2.38	0.44
6:F:36:ALA:O	6:F:38:ALA:N	2.50	0.44
7:H:16:SER:C	7:H:18:TYR:H	2.25	0.44
18:X:16:LEU:HD11	18:X:20:PHE:CE2	2.53	0.44
1:A:185:VAL:O	1:A:186:PHE:C	2.61	0.44
3:C:264:PHE:CE2	21:C:482:CLA:O1A	2.66	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
9:J:22:ILE:HG21	27:J:492:LMG:C20	2.45	0.44
10:K:17:ILE:N	10:K:17:ILE:CD1	2.81	0.44
13:O:116:ASP:OD2	13:O:116:ASP:C	2.58	0.44
15:U:89:GLU:C	15:U:91:VAL:N	2.76	0.44
1:A:182:PHE:O	1:A:186:PHE:HB2	2.18	0.44
2:B:71:VAL:HG21	2:B:96:VAL:HG21	1.99	0.44
21:B:512:CLA:C20	28:B:528:DGD:HB91	2.48	0.44
3:C:28:GLN:CB	21:C:486:CLA:HED2	2.47	0.44
3:C:276:LEU:HD21	21:C:484:CLA:HBB1	1.99	0.44
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.44
4:D:253:TRP:HB2	4:D:260:ALA:HB2	2.00	0.44
15:U:72:TYR:CB	15:U:73:PRO:CD	2.92	0.44
16:V:59:PHE:CD1	16:V:63:CYS:SG	3.08	0.44
16:V:81:ARG:HG2	16:V:81:ARG:HH11	1.83	0.44
1:A:60:ILE:HG23	1:A:61:ASP:N	2.32	0.44
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.16	0.44
4:D:333:ASP:C	4:D:335:PRO:HD3	2.43	0.44
5:E:15:THR:CG2	9:J:7:ARG:HB3	2.47	0.44
6:F:36:ALA:O	6:F:39:ALA:N	2.51	0.44
17:y:32:GLY:N	17:y:33:PRO:HD2	2.32	0.44
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:O	2:B:16:PRO:C	2.60	0.44
4:D:185:PHE:CE2	4:D:289:LEU:HD12	2.52	0.44
4:D:209:LEU:O	4:D:213:ILE:HG22	2.18	0.44
7:H:41:PHE:O	7:H:45:ILE:HG23	2.18	0.44
1:A:110:GLY:O	1:A:111:PRO:C	2.60	0.44
2:B:444:ARG:HH11	2:B:444:ARG:HG3	1.82	0.44
3:C:394:GLU:OE2	3:C:398:HIS:CD2	2.71	0.44
4:D:202:ALA:HB3	32:D:357:PL9:H302	2.00	0.44
32:D:357:PL9:C43	27:D:360:LMG:C25	2.95	0.44
13:O:120:THR:HG22	13:O:154:SER:CB	2.47	0.44
18:X:44:ASP:O	18:X:45:LYS:HB3	2.17	0.44
1:A:129:ARG:C	1:A:131:TRP:N	2.76	0.44
1:A:220:THR:O	1:A:223:LEU:HG	2.18	0.44
2:B:187:PRO:C	2:B:189:GLY:H	2.26	0.44
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.44
21:B:517:CLA:CBC	25:B:529:BCR:H10C	2.48	0.44
3:C:54:VAL:HA	21:C:487:CLA:HED1	2.00	0.44
3:C:82:TYR:HA	3:C:422:PRO:HG2	2.00	0.44
3:C:92:ILE:HD11	21:C:479:CLA:HED2	1.99	0.44
4:D:154:VAL:O	4:D:158:LEU:HB2	2.18	0.44
4:D:221:THR:CG2	4:D:244:TYR:HB2	2.48	0.44
25:D:358:BCR:C39	9:J:21:VAL:HG11	2.48	0.44
27:D:360:LMG:H111	27:D:360:LMG:H292	1.98	0.44
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.99	0.44
7:H:44:ILE:HG12	18:X:19:PHE:CZ	2.52	0.44
1:A:217:SER:O	1:A:220:THR:HG22	2.18	0.43
2:B:283:GLU:OE1	2:B:283:GLU:HA	2.17	0.43
2:B:447:PRO:O	2:B:448:ARG:C	2.60	0.43
21:C:487:CLA:HBB1	21:C:487:CLA:HHC	2.00	0.43
21:C:488:CLA:C1	21:C:488:CLA:HAA1	2.47	0.43
4:D:67:TYR:OH	27:D:359:LMG:H291	2.18	0.43
5:E:74:GLN:HG3	5:E:75:GLN:N	2.31	0.43
6:F:45:ARG:NH2	6:F:45:ARG:HB3	2.33	0.43
8:I:27:ASP:O	8:I:28:PRO:C	2.59	0.43
10:K:17:ILE:O	10:K:17:ILE:HG22	2.17	0.43
10:K:20:PRO:HB2	17:y:21:GLN:CB	2.48	0.43
13:O:59:ASP:C	13:O:61:SER:N	2.76	0.43
26:A:371:LHG:HC32	4:D:229:ALA:O	2.18	0.43
2:B:206:GLY:O	2:B:210:ILE:HG13	2.18	0.43
2:B:271:THR:CG2	2:B:273:TYR:HB2	2.48	0.43
2:B:484:PRO:O	2:B:485:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:518:CLA:C1	4:D:127:LEU:HD21	2.48	0.43
28:B:533:DGD:HA32	12:M:10:ALA:HB1	2.00	0.43
3:C:235:GLY:O	3:C:238:ILE:HB	2.18	0.43
4:D:101:PHE:O	4:D:104:TRP:HB3	2.18	0.43
21:D:356:CLA:C4	18:X:26:GLY:HA3	2.47	0.43
13:O:116:ASP:OD1	13:O:157:PRO:HB3	2.18	0.43
13:O:225:LEU:N	13:O:225:LEU:HD12	2.33	0.43
16:V:39:ASN:HD21	16:V:43:LYS:HB3	1.82	0.43
1:A:29:TYR:OH	1:A:132:GLU:OE2	2.26	0.43
1:A:198:HIS:O	1:A:202:VAL:HG12	2.18	0.43
2:B:164:PRO:HG2	2:B:165:GLY:H	1.82	0.43
2:B:434:THR:HG21	13:O:204:LYS:HE3	1.97	0.43
2:B:463:PHE:CE1	28:B:528:DGD:CFA	3.01	0.43
3:C:242:LEU:O	3:C:243:ILE:C	2.61	0.43
3:C:338:GLY:O	3:C:339:LYS:C	2.60	0.43
3:C:390:ARG:NE	16:V:126:ILE:CG2	2.82	0.43
3:C:416:SER:OG	16:V:68:VAL:HG23	2.17	0.43
4:D:238:THR:O	4:D:239:GLN:C	2.60	0.43
4:D:329:MET:O	4:D:330:ALA:C	2.61	0.43
5:E:72:ALA:O	5:E:76:VAL:HG23	2.18	0.43
10:K:20:PRO:O	17:y:21:GLN:HG3	2.18	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
19:Z:17:PHE:HE2	19:Z:21:ILE:HD11	1.84	0.43
1:A:210:LEU:C	1:A:210:LEU:CD2	2.92	0.43
2:B:327:THR:HG22	21:B:517:CLA:C1	2.49	0.43
2:B:348:ASN:OD1	2:B:352:GLU:HB2	2.18	0.43
21:B:514:CLA:H142	21:B:525:CLA:H52	2.01	0.43
28:B:533:DGD:HA32	12:M:10:ALA:CB	2.49	0.43
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.54	0.43
3:C:362:ARG:CG	28:C:491:DGD:HE61	2.48	0.43
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.54	0.43
4:D:176:ALA:C	4:D:178:ILE:H	2.26	0.43
10:K:18:PHE:CE1	19:Z:9:LEU:HG	2.53	0.43
10:K:30:VAL:N	21:K:483:CLA:H191	2.34	0.43
13:O:72:GLN:O	13:O:263:GLY:HA3	2.17	0.43
15:U:54:LYS:HD2	15:U:113:THR:CG2	2.49	0.43
1:A:309:ALA:HB3	5:E:53:ASP:HA	2.00	0.43
2:B:238:LEU:N	21:B:522:CLA:HMD1	2.33	0.43
2:B:247:PHE:HD2	21:B:513:CLA:H111	1.83	0.43
21:B:512:CLA:CAA	7:H:45:ILE:HD12	2.48	0.43
3:C:60:ILE:CG2	21:C:479:CLA:HMD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:LEU:HG	10:K:10:LYS:N	2.33	0.43
21:C:486:CLA:H122	10:K:32:PHE:CE1	2.53	0.43
5:E:38:VAL:CG2	6:F:36:ALA:HB1	2.47	0.43
13:O:70:CYS:O	13:O:265:PHE:HB2	2.18	0.43
19:Z:36:SER:HA	19:Z:39:LEU:CD1	2.48	0.43
1:A:12:ASN:O	1:A:13:LEU:C	2.60	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	1.99	0.43
3:C:160:ILE:HA	3:C:163:PHE:CD2	2.53	0.43
5:E:8:ARG:HA	6:F:13:TYR:CZ	2.52	0.43
19:Z:22:GLY:O	19:Z:23:VAL:C	2.61	0.43
1:A:42:LEU:HA	1:A:45:THR:HG22	2.00	0.43
1:A:187:GLN:HB2	21:A:362:CLA:CAC	2.48	0.43
27:A:373:LMG:H301	12:M:22:LEU:HD22	1.99	0.43
2:B:252:VAL:HG11	21:B:514:CLA:OBD	2.18	0.43
2:B:284:ILE:HG23	2:B:305:ILE:CD1	2.48	0.43
3:C:128:GLY:N	21:C:488:CLA:HAC2	2.33	0.43
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.00	0.43
4:D:253:TRP:HA	4:D:256:ILE:HG23	2.01	0.43
29:I:274:LMT:H6D	13:O:95:LYS:NZ	2.34	0.43
10:K:46:ARG:NH1	10:K:46:ARG:HB2	2.34	0.43
2:B:263:THR:HB	2:B:448:ARG:HH12	1.82	0.43
2:B:289:GLN:OE1	2:B:292:LEU:HD12	2.19	0.43
3:C:50:LEU:O	3:C:54:VAL:HG23	2.17	0.43
3:C:433:LEU:HD13	21:C:478:CLA:CHC	2.49	0.43
3:C:455:PHE:C	3:C:457:LYS:H	2.26	0.43
3:C:473:ASP:HA	14:T:27:PRO:HD2	2.01	0.43
4:D:263:ASN:O	4:D:265:ARG:N	2.52	0.43
4:D:291:LEU:O	4:D:292:ASN:HB2	2.18	0.43
13:O:109:GLY:HA3	13:O:122:VAL:O	2.18	0.43
13:O:171:GLU:HA	13:O:221:GLY:O	2.19	0.43
17:y:31:ALA:O	17:y:35:ILE:HG23	2.19	0.43
18:X:44:ASP:C	18:X:45:LYS:CD	2.92	0.43
2:B:33:TRP:NE1	21:B:517:CLA:HMC2	2.34	0.43
2:B:327:THR:O	2:B:444:ARG:NE	2.46	0.43
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.43
7:H:55:LEU:HB2	7:H:58:VAL:CG1	2.49	0.43
12:M:33:GLN:HG2	12:M:34:LYS:N	2.33	0.43
17:y:41:VAL:C	17:y:43:ARG:N	2.71	0.43
18:X:32:LEU:HD23	18:X:32:LEU:H	1.83	0.43
1:A:157:VAL:HG21	21:A:363:CLA:HMC1	2.00	0.43
3:C:33:PHE:CE1	4:D:229:ALA:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LYS:CD	3:C:138:GLU:HG3	2.49	0.43
3:C:55:ALA:HB1	25:C:489:BCR:C37	2.49	0.43
3:C:56:HIS:C	3:C:58:GLY:H	2.27	0.43
3:C:310:SER:HG	3:C:355:THR:HG23	1.84	0.43
3:C:453:ALA:C	8:I:34:ARG:HB2	2.44	0.43
28:C:492:DGD:HB41	9:J:29:PHE:CZ	2.54	0.43
4:D:199:MET:O	4:D:200:GLY:C	2.60	0.43
8:I:20:VAL:C	8:I:22:GLY:H	2.26	0.43
10:K:43:VAL:O	10:K:46:ARG:HG3	2.19	0.43
12:M:1:MET:HG2	12:M:2:GLU:H	1.84	0.43
16:V:103:LYS:O	16:V:122:ARG:HG2	2.19	0.43
17:y:20:ALA:HA	17:y:22:LEU:HD12	2.01	0.43
1:A:45:THR:CB	22:A:365:PHO:H8	2.48	0.42
1:A:247:ASN:HB3	1:A:250:ALA:HB3	2.00	0.42
1:A:286:THR:CG2	21:A:362:CLA:HED3	2.35	0.42
2:B:222:PRO:HG3	7:H:27:THR:N	2.28	0.42
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.42
2:B:413:ASP:OD1	2:B:416:THR:HB	2.19	0.42
3:C:63:TRP:O	3:C:64:ALA:C	2.62	0.42
21:C:484:CLA:H41	21:C:484:CLA:H62	1.64	0.42
21:C:487:CLA:H172	21:C:487:CLA:HMA3	2.00	0.42
4:D:125:PHE:O	4:D:128:ARG:HB3	2.19	0.42
5:E:34:GLY:O	5:E:37:PHE:HB3	2.19	0.42
9:J:12:ILE:O	9:J:16:VAL:HG23	2.19	0.42
15:U:91:VAL:HG13	15:U:92:LEU:N	2.33	0.42
1:A:55:ALA:HA	25:A:369:BCR:C27	2.50	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.55	0.42
28:B:528:DGD:HD61	28:B:528:DGD:C5E	2.48	0.42
3:C:164:HIS:CB	21:C:483:CLA:HED3	2.49	0.42
3:C:164:HIS:HB2	21:C:483:CLA:HED3	2.00	0.42
3:C:318:LEU:HG	3:C:328:VAL:CG1	2.48	0.42
4:D:279:LEU:HD22	21:D:354:CLA:HMA2	2.01	0.42
12:M:33:GLN:CG	12:M:34:LYS:N	2.82	0.42
18:X:44:ASP:C	18:X:45:LYS:HD3	2.44	0.42
1:A:239:PHE:HB3	14:T:28:ARG:O	2.19	0.42
1:A:291:SER:HB3	3:C:431:PHE:CE2	2.54	0.42
2:B:105:GLY:O	2:B:108:PHE:HB3	2.19	0.42
2:B:349:LYS:HG2	2:B:395:GLN:O	2.19	0.42
3:C:29:GLU:CB	10:K:46:ARG:NH1	2.80	0.42
3:C:101:PRO:O	3:C:104:GLU:HB2	2.19	0.42
3:C:155:ASN:C	3:C:158:THR:HG22	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.42
3:C:259:TRP:C	3:C:261:ARG:N	2.74	0.42
3:C:406:SER:HA	3:C:420:VAL:CG2	2.49	0.42
10:K:20:PRO:HB2	17:y:21:GLN:HB3	2.01	0.42
26:A:371:LHG:H351	21:K:483:CLA:H71	2.01	0.42
27:A:373:LMG:HC92	2:B:5:TRP:NE1	2.32	0.42
2:B:251:VAL:HB	21:B:513:CLA:C4	2.50	0.42
3:C:37:ALA:O	21:C:484:CLA:HBA1	2.19	0.42
3:C:202:PRO:HB2	3:C:235:GLY:HA2	2.01	0.42
21:C:483:CLA:H61	21:C:483:CLA:H41	1.92	0.42
5:E:60:GLN:HG2	5:E:62:SER:H	1.84	0.42
12:M:19:SER:O	12:M:23:ILE:HG13	2.18	0.42
13:O:59:ASP:O	13:O:61:SER:N	2.53	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.70	0.42
16:V:130:MET:SD	16:V:133:LEU:HD12	2.60	0.42
1:A:207:GLY:O	1:A:210:LEU:HB3	2.20	0.42
2:B:433:ASP:OD1	2:B:433:ASP:C	2.61	0.42
3:C:162:GLY:O	3:C:166:ILE:HG13	2.18	0.42
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.53	0.42
6:F:21:VAL:O	6:F:22:ALA:C	2.62	0.42
10:K:16:ALA:O	10:K:19:ASP:HB2	2.20	0.42
17:y:42:ARG:O	17:y:43:ARG:C	2.61	0.42
1:A:33:PHE:CE2	21:C:481:CLA:O1A	2.73	0.42
1:A:160:ILE:HD11	28:C:491:DGD:C9A	2.50	0.42
1:A:222:SER:O	1:A:246:TYR:HB2	2.19	0.42
2:B:330:MET:SD	2:B:446:SER:HB3	2.59	0.42
21:B:524:CLA:H41	21:B:524:CLA:H61	1.85	0.42
21:B:526:CLA:C1D	7:H:7:LEU:HD23	2.50	0.42
3:C:205:ASP:OD1	3:C:207:ARG:HB3	2.19	0.42
3:C:396:MET:HE1	16:V:73:LYS:O	2.19	0.42
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.72	0.42
21:C:477:CLA:C2D	21:C:479:CLA:H2	2.50	0.42
5:E:69:ARG:HG3	5:E:70:PHE:N	2.34	0.42
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.42
3:C:414:ILE:HG22	3:C:415:ASN:N	2.35	0.42
28:C:493:DGD:HBW1	27:D:359:LMG:H181	2.02	0.42
5:E:35:TRP:CG	6:F:39:ALA:HB2	2.55	0.42
11:L:36:PHE:O	11:L:37:ASN:C	2.61	0.42
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.55	0.42
1:A:39:PRO:CB	21:A:366:CLA:HBB1	2.45	0.42
1:A:273:PHE:CD1	26:A:371:LHG:H242	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:PRO:HB3	2:B:133:LEU:HD21	2.02	0.42
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.92	0.42
2:B:222:PRO:HB3	7:H:26:GLY:N	2.34	0.42
2:B:413:ASP:O	2:B:413:ASP:CG	2.63	0.42
3:C:365:TRP:HB3	3:C:391:ARG:HG2	2.02	0.42
26:C:476:LHG:H171	28:C:492:DGD:HBN1	2.00	0.42
4:D:52:THR:HG22	4:D:67:TYR:CE2	2.54	0.42
5:E:78:THR:HA	5:E:81:GLU:HG2	2.02	0.42
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.33	0.42
30:L:213:SQD:H82	27:M:217:LMG:H152	2.01	0.42
1:A:42:LEU:HA	1:A:45:THR:CG2	2.49	0.42
1:A:210:LEU:C	1:A:210:LEU:HD23	2.45	0.42
1:A:234:ASN:CB	27:A:373:LMG:HC3	2.48	0.42
1:A:317:TRP:O	1:A:321:ILE:HG13	2.20	0.42
2:B:191:ASN:HB2	7:H:58:VAL:HG22	2.00	0.42
2:B:448:ARG:HH11	2:B:448:ARG:HG3	1.84	0.42
3:C:84:GLN:C	3:C:86:LEU:HD13	2.45	0.42
3:C:125:LEU:HG	25:Z:116:BCR:C36	2.49	0.42
3:C:148:GLY:O	3:C:156:LYS:NZ	2.51	0.42
28:C:492:DGD:HB52	25:J:115:BCR:C35	2.47	0.42
5:E:15:THR:HG23	9:J:8:ILE:N	2.34	0.42
7:H:35:MET:HA	25:X:107:BCR:C32	2.50	0.42
8:I:7:THR:O	8:I:8:VAL:C	2.63	0.42
8:I:17:LEU:O	8:I:18:LEU:C	2.61	0.42
8:I:20:VAL:C	8:I:22:GLY:N	2.77	0.42
13:O:248:ASP:CG	13:O:250:ASP:H	2.27	0.42
29:O:274:LMT:H5'	29:O:274:LMT:H1B	1.92	0.42
15:U:41:ASN:O	15:U:42:VAL:C	2.62	0.42
22:A:365:PHO:HAC2	4:D:212:ALA:HB3	2.01	0.42
27:A:373:LMG:C31	12:M:22:LEU:HD21	2.50	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.54	0.42
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.42
2:B:472:ARG:HG2	2:B:472:ARG:HH11	1.84	0.42
3:C:140:LEU:HB2	3:C:148:GLY:HA2	2.02	0.42
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.01	0.42
3:C:461:ARG:HG3	3:C:461:ARG:NH1	2.32	0.42
4:D:261:PHE:N	32:D:357:PL9:O1	2.51	0.42
7:H:18:TYR:CG	7:H:19:GLY:N	2.85	0.42
10:K:30:VAL:CA	21:K:483:CLA:H191	2.50	0.42
16:V:153:GLY:O	16:V:154:ASP:C	2.62	0.42
27:A:373:LMG:C25	27:D:360:LMG:C21	2.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:373:LMG:C31	11:L:20:GLY:HA2	2.49	0.41
27:A:373:LMG:H131	4:D:273:PHE:CE2	2.55	0.41
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.01	0.41
2:B:280:PHE:O	2:B:284:ILE:HG13	2.20	0.41
28:B:533:DGD:HG11	12:M:6:LEU:HD12	2.02	0.41
21:C:486:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
4:D:204:VAL:HG22	4:D:279:LEU:HD21	2.01	0.41
6:F:9:GLU:C	6:F:11:VAL:N	2.78	0.41
6:F:45:ARG:CZ	9:J:40:LEU:OXT	2.68	0.41
9:J:15:THR:O	25:J:112:BCR:H372	2.19	0.41
13:O:227:VAL:CG1	13:O:228:ALA:N	2.82	0.41
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.55	0.41
1:A:104:GLU:OE2	13:O:99:ARG:HD3	2.20	0.41
1:A:131:TRP:CH2	21:C:481:CLA:CBA	2.99	0.41
1:A:228:THR:HB	1:A:231:GLU:HB3	2.01	0.41
3:C:405:ASN:HB2	28:C:493:DGD:O6D	2.20	0.41
3:C:417:VAL:C	28:C:493:DGD:O3E	2.62	0.41
21:C:478:CLA:O1A	21:C:479:CLA:HBD	2.19	0.41
4:D:122:LEU:HG	22:D:355:PHO:H62	2.02	0.41
7:H:27:THR:O	7:H:28:THR:C	2.63	0.41
17:y:36:ILE:O	17:y:39:LEU:HB2	2.20	0.41
1:A:236:GLY:HA3	4:D:265:ARG:NH1	2.35	0.41
1:A:332:HIS:HB3	4:D:321:LEU:HD21	2.01	0.41
2:B:260:SER:C	2:B:262:THR:H	2.28	0.41
2:B:260:SER:C	2:B:262:THR:N	2.76	0.41
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.28	0.41
3:C:125:LEU:HD22	21:C:487:CLA:HED3	2.00	0.41
3:C:315:MET:HE1	3:C:369:LEU:CD1	2.45	0.41
4:D:302:GLU:OE1	4:D:302:GLU:HA	2.20	0.41
14:T:16:LEU:O	14:T:17:PHE:C	2.63	0.41
15:U:50:ALA:HB1	15:U:113:THR:HG21	2.01	0.41
15:U:75:LEU:O	15:U:79:ILE:HG13	2.20	0.41
15:U:82:ASN:ND2	15:U:94:ILE:HG23	2.34	0.41
1:A:10:SER:OG	1:A:13:LEU:HD12	2.20	0.41
1:A:193:LEU:HD21	21:A:362:CLA:CMC	2.50	0.41
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.02	0.41
21:B:513:CLA:H203	21:B:519:CLA:H92	2.02	0.41
3:C:72:LEU:O	10:K:10:LYS:N	2.52	0.41
3:C:109:PHE:CD2	27:C:494:LMG:H112	2.55	0.41
3:C:264:PHE:HE2	21:C:482:CLA:CGA	2.33	0.41
3:C:292:PHE:CD2	28:C:491:DGD:HG31	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:456:GLU:N	3:C:456:GLU:OE1	2.53	0.41
4:D:176:ALA:C	4:D:178:ILE:N	2.78	0.41
4:D:189:HIS:O	4:D:190:ASN:C	2.63	0.41
4:D:274:VAL:HG13	32:D:357:PL9:H222	2.02	0.41
15:U:55:ILE:HG21	15:U:65:PHE:CE1	2.56	0.41
19:Z:5:PHE:CD2	19:Z:61:VAL:HG21	2.54	0.41
1:A:205:VAL:HG21	21:A:362:CLA:CMA	2.51	0.41
1:A:260:PHE:CD1	1:A:260:PHE:C	2.98	0.41
1:A:292:THR:C	1:A:294:ALA:H	2.28	0.41
21:B:521:CLA:HBB2	21:B:523:CLA:HMB3	2.01	0.41
27:B:531:LMG:C2	4:D:141:TYR:OH	2.67	0.41
3:C:55:ALA:CB	25:C:489:BCR:H373	2.51	0.41
26:C:476:LHG:H242	26:C:476:LHG:H121	2.02	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.71	0.41
4:D:259:ILE:HG21	27:D:360:LMG:H292	2.01	0.41
6:F:28:VAL:CB	6:F:29:PRO:HD3	2.46	0.41
7:H:31:MET:HE3	7:H:35:MET:CE	2.40	0.41
9:J:11:TRP:CE2	9:J:12:ILE:HG12	2.55	0.41
11:L:22:LEU:O	11:L:26:VAL:HG13	2.21	0.41
13:O:215:ARG:NE	15:U:39:LEU:HD22	2.34	0.41
1:A:190:HIS:HB3	1:A:293:MET:CE	2.43	0.41
1:A:296:ASN:HB2	3:C:400:PRO:O	2.20	0.41
1:A:307:ILE:HG13	6:F:45:ARG:CD	2.49	0.41
2:B:328:GLY:N	21:B:517:CLA:O1A	2.54	0.41
3:C:75:PHE:CD1	3:C:86:LEU:HD21	2.48	0.41
3:C:272:LEU:O	3:C:273:SER:C	2.63	0.41
3:C:464:GLU:O	3:C:467:LEU:HB2	2.19	0.41
4:D:161:PRO:CB	4:D:170:ALA:HB2	2.51	0.41
7:H:55:LEU:O	7:H:56:ASP:C	2.62	0.41
10:K:28:ILE:O	10:K:31:LEU:HB2	2.21	0.41
13:O:36:ILE:O	13:O:37:VAL:C	2.63	0.41
15:U:59:ASN:O	15:U:60:THR:C	2.64	0.41
16:V:121:LEU:C	16:V:123:SER:H	2.28	0.41
19:Z:24:PRO:C	19:Z:26:ALA:N	2.76	0.41
1:A:12:ASN:O	1:A:15:GLU:HB3	2.20	0.41
1:A:105:TRP:CZ3	1:A:111:PRO:HG3	2.55	0.41
1:A:155:PHE:CD1	28:C:491:DGD:HAE2	2.56	0.41
2:B:12:LEU:O	2:B:14:ASN:N	2.54	0.41
2:B:127:ARG:C	2:B:127:ARG:HD2	2.45	0.41
2:B:289:GLN:OE1	2:B:289:GLN:HA	2.21	0.41
2:B:479:PHE:O	2:B:480:SER:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:ASP:HB2	3:C:230:LEU:CD1	2.48	0.41
3:C:321:ASP:HA	3:C:324:LEU:HD23	2.01	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.50	0.41
13:O:136:MET:O	13:O:137:ALA:C	2.63	0.41
13:O:184:ASP:C	13:O:184:ASP:OD1	2.63	0.41
15:U:58:ASN:HD22	15:U:114:VAL:HG13	1.84	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.85	0.41
1:A:277:ALA:O	1:A:281:VAL:HG23	2.21	0.41
2:B:49:ASP:HA	2:B:50:PRO:HD2	1.88	0.41
2:B:160:GLY:O	2:B:161:LEU:C	2.63	0.41
2:B:220:ARG:NH1	7:H:20:LYS:O	2.51	0.41
3:C:259:TRP:O	3:C:260:ALA:C	2.62	0.41
21:C:480:CLA:HHC	21:C:480:CLA:HBB1	2.03	0.41
5:E:44:TYR:OH	6:F:43:ILE:HD13	2.21	0.41
6:F:24:HIS:HE1	33:F:85:HEM:ND	2.19	0.41
6:F:38:ALA:HB1	9:J:27:LEU:CD2	2.50	0.41
7:H:13:PRO:HG2	7:H:14:LEU:H	1.85	0.41
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.41
13:O:120:THR:HA	13:O:153:ALA:O	2.21	0.41
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.03	0.41
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.51	0.41
1:A:114:LEU:HD23	1:A:114:LEU:O	2.21	0.41
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.01	0.41
2:B:76:SER:HG	2:B:78:TRP:CD1	2.39	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.88	0.41
2:B:354:LEU:HD12	2:B:378:LYS:HB2	2.02	0.41
2:B:475:PHE:HB3	2:B:478:VAL:CG2	2.51	0.41
3:C:67:MET:HE1	21:C:480:CLA:C4C	2.51	0.41
3:C:175:LEU:HA	21:C:478:CLA:H141	2.02	0.41
3:C:199:ILE:N	3:C:199:ILE:CD1	2.83	0.41
25:C:489:BCR:H20C	25:C:489:BCR:H361	1.87	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:A:18:CYS:O	1:A:22:THR:CG2	2.69	0.41
1:A:131:TRP:CE3	1:A:132:GLU:CA	3.03	0.41
1:A:278:TRP:CH2	28:C:493:DGD:HBV1	2.56	0.41
21:A:364:CLA:H91	21:D:354:CLA:H203	2.02	0.41
2:B:191:ASN:OD1	2:B:193:TYR:N	2.52	0.41
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.86	0.41
3:C:267:SER:O	3:C:271:TYR:CD2	2.74	0.41
3:C:318:LEU:C	3:C:318:LEU:CD2	2.94	0.41
4:D:84:SER:HB2	4:D:85:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:64:PRO:HB3	5:E:84:LYS:CD	2.51	0.41
6:F:31:ILE:HG12	33:F:85:HEM:HMC2	2.03	0.41
6:F:37:ILE:O	6:F:37:ILE:HG22	2.20	0.41
7:H:10:ILE:H	7:H:10:ILE:HG13	1.70	0.41
13:O:73:PRO:HG2	13:O:102:THR:HB	2.03	0.41
13:O:147:THR:OG1	13:O:148:VAL:N	2.54	0.41
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.41
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.66	0.40
21:A:363:CLA:H92	32:D:357:PL9:H422	2.02	0.40
2:B:238:LEU:HD13	21:B:522:CLA:C2D	2.51	0.40
2:B:414:PRO:CB	2:B:415:PRO:HD3	2.40	0.40
2:B:457:VAL:O	2:B:458:PHE:C	2.62	0.40
3:C:64:ALA:HB2	21:C:479:CLA:C2D	2.51	0.40
3:C:216:SER:HA	28:C:474:DGD:HG12	2.03	0.40
3:C:271:TYR:CE1	21:C:483:CLA:CAC	3.04	0.40
3:C:307:PRO:HG3	3:C:358:PHE:CD1	2.56	0.40
3:C:308:GLU:HG3	3:C:361:PHE:CZ	2.56	0.40
3:C:327:ASN:HB3	13:O:125:ASP:OD1	2.21	0.40
3:C:369:LEU:CD2	3:C:384:ILE:HD13	2.51	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CE1	2.55	0.40
4:D:274:VAL:HG22	32:D:357:PL9:H253	2.03	0.40
10:K:28:ILE:O	10:K:29:PRO:C	2.61	0.40
12:M:10:ALA:O	12:M:14:PHE:HB2	2.21	0.40
12:M:31:SER:HA	27:M:217:LMG:HC72	2.03	0.40
15:U:91:VAL:C	15:U:93:ASN:N	2.78	0.40
17:y:20:ALA:O	17:y:23:THR:HG22	2.21	0.40
17:y:46:LEU:N	17:y:46:LEU:HD23	2.36	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:288:LEU:O	1:A:292:THR:HB	2.21	0.40
2:B:224:ARG:NE	7:H:25:TRP:HE1	2.19	0.40
2:B:472:ARG:HE	21:B:521:CLA:HED2	1.86	0.40
21:B:518:CLA:H11	4:D:127:LEU:HD21	2.04	0.40
21:B:525:CLA:H62	21:B:525:CLA:H41	1.72	0.40
3:C:116:VAL:CG2	3:C:117:VAL:N	2.84	0.40
3:C:188:THR:CG2	3:C:298:PRO:HB3	2.50	0.40
4:D:90:LEU:O	21:D:356:CLA:HED1	2.21	0.40
5:E:15:THR:HG22	9:J:8:ILE:H	1.83	0.40
5:E:84:LYS:HB2	5:E:84:LYS:HZ3	1.79	0.40
6:F:45:ARG:CB	6:F:45:ARG:HH21	2.35	0.40
25:J:115:BCR:H20C	25:J:115:BCR:H361	1.96	0.40
13:O:226:ASN:N	13:O:226:ASN:ND2	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:SER:HA	1:A:220:THR:CG2	2.51	0.40
27:A:373:LMG:C20	32:D:357:PL9:C21	2.92	0.40
21:B:513:CLA:CBB	21:B:515:CLA:H171	2.42	0.40
21:B:517:CLA:C2	28:B:533:DGD:HB52	2.52	0.40
3:C:59:LEU:HD11	25:C:489:BCR:H372	2.03	0.40
3:C:350:ILE:CG2	3:C:359:TRP:HB2	2.51	0.40
7:H:53:LEU:HD21	7:H:55:LEU:HD21	2.03	0.40
9:J:24:ILE:HG23	9:J:25:VAL:N	2.37	0.40
10:K:34:ALA:O	10:K:37:PHE:HB2	2.20	0.40
13:O:157:PRO:O	13:O:158:ASN:O	2.38	0.40
13:O:208:LEU:O	13:O:209:ALA:C	2.63	0.40
18:X:11:THR:OG1	25:X:107:BCR:H282	2.21	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
2:B:150:CYS:HA	21:B:513:CLA:CBC	2.52	0.40
2:B:272:ARG:HG3	2:B:273:TYR:N	2.36	0.40
21:B:522:CLA:H102	21:B:522:CLA:H13	1.86	0.40
3:C:127:PHE:CE1	19:Z:23:VAL:HG21	2.54	0.40
21:C:483:CLA:H121	25:C:490:BCR:H362	2.04	0.40
21:C:486:CLA:C14	19:Z:24:PRO:HG2	2.51	0.40
4:D:84:SER:HB3	5:E:68:ASP:HA	2.04	0.40
4:D:185:PHE:HE2	4:D:289:LEU:HD12	1.87	0.40
4:D:239:GLN:HB3	4:D:240:ALA:H	1.33	0.40
27:D:360:LMG:H361	14:T:21:ILE:CD1	2.51	0.40
5:E:30:LEU:CD2	6:F:28:VAL:HG13	2.51	0.40
21:K:483:CLA:HHC	21:K:483:CLA:HBB1	2.03	0.40
13:O:49:ASP:CG	13:O:50:ASP:N	2.79	0.40
1:A:72:LEU:HD23	14:T:3:THR:HG21	2.03	0.40
1:A:113:GLN:O	1:A:114:LEU:C	2.65	0.40
1:A:116:ILE:HG13	1:A:117:PHE:N	2.37	0.40
1:A:214:MET:HB2	23:A:367:MES:H61	1.99	0.40
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.86	0.40
1:A:244:GLU:CD	1:A:245:THR:H	2.27	0.40
2:B:153:PHE:O	2:B:157:HIS:HB3	2.22	0.40
2:B:262:THR:HG21	21:B:513:CLA:HBA1	2.03	0.40
2:B:483:ASP:CB	2:B:484:PRO:CD	2.97	0.40
3:C:141:GLU:HA	3:C:148:GLY:HA3	2.04	0.40
21:C:481:CLA:O1A	8:I:23:PHE:CE1	2.74	0.40
4:D:17:ILE:HG21	18:X:42:GLN:HG3	2.03	0.40
4:D:279:LEU:CD1	21:D:354:CLA:CBA	3.00	0.40
6:F:42:PHE:N	6:F:42:PHE:CD1	2.90	0.40
7:H:7:LEU:HG	7:H:11:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:215:ARG:HD2	15:U:39:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	5	31
2	B	483/510 (95%)	416 (86%)	54 (11%)	13 (3%)	4	27
3	C	446/461 (97%)	370 (83%)	60 (14%)	16 (4%)	2	22
4	D	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	4	27
5	E	75/83 (90%)	66 (88%)	5 (7%)	4 (5%)	1	14
6	F	36/44 (82%)	22 (61%)	9 (25%)	5 (14%)	0	3
7	H	63/65 (97%)	45 (71%)	9 (14%)	9 (14%)	0	3
8	I	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	1	13
9	J	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	1	12
10	K	35/37 (95%)	26 (74%)	7 (20%)	2 (6%)	1	13
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	201 (83%)	29 (12%)	11 (5%)	2	17
14	T	28/32 (88%)	25 (89%)	3 (11%)	0	100	100
15	U	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	2	19
16	V	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	18	51
17	y	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	2
18	X	33/40 (82%)	25 (76%)	5 (15%)	3 (9%)	0	6
19	Z	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2559/2714 (94%)	2121 (83%)	343 (13%)	95 (4%)	2	21

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	141	PRO
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
3	C	452	ALA
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
5	E	82	GLN
7	H	18	TYR
7	H	63	LYS
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
15	U	72	TYR
15	U	83	ALA
16	V	75	ASN
17	y	43	ARG
19	Z	32	ASP
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	209	ILE
3	C	456	GLU
4	D	234	ALA
4	D	264	LYS
6	F	37	ILE
7	H	26	GLY
9	J	38	SER
13	O	83	LYS
13	O	231	ASP

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Mol	Chain	Res	Type
15	U	73	PRO
17	y	25	ILE
18	X	43	ILE
2	B	13	ILE
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	375	LEU
3	C	453	ALA
4	D	263	ASN
5	E	9	PRO
6	F	17	THR
7	H	16	SER
7	H	64	ALA
10	K	13	GLU
10	K	45	PHE
13	O	60	SER
13	O	158	ASN
13	O	165	SER
19	Z	24	PRO
19	Z	28	ALA
2	B	173	GLY
2	B	231	MET
2	B	235	GLU
3	C	154	LYS
4	D	73	PHE
5	E	10	PHE
13	O	51	THR
17	y	24	MET
18	X	44	ASP
1	A	97	TRP
3	C	462	GLU
6	F	13	TYR
7	H	6	TRP
7	H	65	LEU
15	U	42	VAL
18	X	12	ILE
1	A	334	ARG
4	D	351	ALA

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Mol	Chain	Res	Type
7	H	14	LEU
1	A	21	VAL
2	B	16	PRO
13	O	159	VAL
3	C	201	ASN
6	F	9	GLU
6	F	11	VAL
17	y	35	ILE
5	E	52	PRO
7	H	60	VAL
8	I	32	PRO
13	O	232	GLY
1	A	176	ILE
4	D	160	TYR
13	O	127	ILE
13	O	152	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/280 (97%)	255 (94%)	16 (6%)	18	45
2	B	385/407 (95%)	368 (96%)	17 (4%)	25	52
3	C	348/362 (96%)	332 (95%)	16 (5%)	24	51
4	D	275/283 (97%)	257 (94%)	18 (6%)	15	43
5	E	69/72 (96%)	63 (91%)	6 (9%)	9	34
6	F	32/38 (84%)	31 (97%)	1 (3%)	35	59
7	H	53/54 (98%)	49 (92%)	4 (8%)	12	39
8	I	32/35 (91%)	30 (94%)	2 (6%)	16	44
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	53
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	30
11	L	35/35 (100%)	31 (89%)	4 (11%)	5	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	31/33 (94%)	30 (97%)	1 (3%)	34	58
13	O	202/208 (97%)	194 (96%)	8 (4%)	28	54
14	T	27/29 (93%)	26 (96%)	1 (4%)	30	56
15	U	84/89 (94%)	80 (95%)	4 (5%)	23	50
16	V	116/117 (99%)	112 (97%)	4 (3%)	32	57
17	y	20/37 (54%)	17 (85%)	3 (15%)	3	17
18	X	28/33 (85%)	23 (82%)	5 (18%)	2	11
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	32
All	All	2114/2222 (95%)	1995 (94%)	119 (6%)	19	47

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	202	VAL
1	A	206	PHE
1	A	210	LEU
1	A	214	MET
1	A	218	LEU
1	A	243	GLU
1	A	271	LEU
1	A	275	LEU
1	A	286	THR
1	A	292	THR
1	A	306	VAL
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	116	VAL
2	B	223	GLN
2	B	262	THR
2	B	271	THR
2	B	308	LYS
2	B	309	LEU
2	B	362	PHE

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Mol	Chain	Res	Type
2	B	373	LYS
2	B	374	ASN
2	B	414	PRO
2	B	422	ARG
2	B	433	ASP
2	B	436	THR
2	B	486	LEU
3	C	26	ARG
3	C	27	ASP
3	C	28	GLN
3	C	29	GLU
3	C	86	LEU
3	C	165	LEU
3	C	174	LEU
3	C	244	CYS
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	391	ARG
3	C	401	LEU
3	C	417	VAL
3	C	447	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	60	THR
4	D	84	SER
4	D	91	LEU
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	221	THR
4	D	236	ASN
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	323	GLU
4	D	346	LEU
5	E	9	PRO

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Mol	Chain	Res	Type
5	E	18	ARG
5	E	52	PRO
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
6	F	24	HIS
7	H	21	VAL
7	H	27	THR
7	H	56	ASP
7	H	60	VAL
8	I	32	PRO
8	I	33	LYS
9	J	7	ARG
10	K	10	LYS
10	K	18	PHE
10	K	19	ASP
11	L	1	MET
11	L	8	GLN
11	L	11	GLU
11	L	15	THR
12	M	20	VAL
13	O	31	LEU
13	O	87	GLN
13	O	88	GLU
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	32	GLU
16	V	45	ILE
16	V	63	CYS
16	V	116	GLU
17	y	25	ILE
17	y	28	ILE
17	y	46	LEU
18	X	11	THR

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Mol	Chain	Res	Type
18	X	12	ILE
18	X	32	LEU
18	X	42	GLN
18	X	45	LYS
19	Z	14	ILE
19	Z	25	VAL
19	Z	33	TRP
19	Z	58	ASN
19	Z	62	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	165	GLN
1	A	241	GLN
1	A	247	ASN
1	A	261	GLN
1	A	337	HIS
2	B	26	HIS
2	B	201	HIS
2	B	216	HIS
2	B	282	GLN
2	B	374	ASN
3	C	44	ASN
3	C	118	HIS
3	C	155	ASN
3	C	251	HIS
3	C	398	HIS
3	C	418	ASN
3	C	441	HIS
3	C	444	HIS
4	D	98	GLN
4	D	129	GLN
4	D	142	ASN
4	D	224	GLN
4	D	239	GLN
4	D	250	ASN
4	D	301	GLN
6	F	44	GLN
7	H	59	ASN
11	L	8	GLN

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Mol	Chain	Res	Type
12	M	33	GLN
13	O	87	GLN
13	O	106	GLN
13	O	135	GLN
13	O	150	ASN
13	O	173	ASN
13	O	222	GLN
13	O	226	ASN
15	U	82	ASN
16	V	104	ASN
18	X	42	GLN
19	Z	6	GLN
19	Z	31	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 87 ligands modelled in this entry, 4 are monoatomic - leaving 83 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	$\# Z > 2$
29	LMT	D	536	-	36,36,36	1.71	10 (27%)	47,47,47	1.61	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	C	482	-	69,73,73	2.86	23 (33%)	82,113,113	1.85	15 (18%)
23	MES	A	367	-	12,12,12	1.51	1 (8%)	15,16,16	1.06	0
25	BCR	D	358	-	41,41,41	1.76	7 (17%)	56,56,56	2.34	21 (37%)
25	BCR	B	529	-	41,41,41	2.18	7 (17%)	56,56,56	2.21	19 (33%)
28	DGD	C	492	-	63,63,67	1.43	11 (17%)	77,77,81	2.73	20 (25%)
25	BCR	B	530	-	41,41,41	2.56	9 (21%)	56,56,56	2.27	23 (41%)
29	LMT	O	274	-	36,36,36	2.01	12 (33%)	47,47,47	1.41	8 (17%)
27	LMG	M	217	-	42,42,55	2.02	8 (19%)	50,50,63	1.47	7 (14%)
21	CLA	A	362	-	69,73,73	2.15	19 (27%)	82,113,113	1.76	11 (13%)
33	HEM	V	164	16	50,50,50	2.72	25 (50%)	67,82,82	2.41	19 (28%)
21	CLA	B	516	-	69,73,73	2.55	19 (27%)	82,113,113	1.96	17 (20%)
21	CLA	C	479	-	69,73,73	2.47	19 (27%)	82,113,113	1.91	13 (15%)
30	SQD	C	475	-	49,51,54	2.71	27 (55%)	59,62,65	2.65	17 (28%)
28	DGD	A	375	-	53,53,67	2.09	13 (24%)	67,67,81	2.47	22 (32%)
29	LMT	T	226	-	36,36,36	1.80	9 (25%)	47,47,47	0.98	2 (4%)
21	CLA	C	486	3	69,73,73	2.95	25 (36%)	82,113,113	1.79	15 (18%)
21	CLA	B	525	-	69,73,73	2.46	19 (27%)	82,113,113	1.83	12 (14%)
25	BCR	B	527	-	41,41,41	1.83	7 (17%)	56,56,56	2.40	21 (37%)
32	PL9	D	357	-	55,55,55	3.24	22 (40%)	68,69,69	2.85	27 (39%)
27	LMG	D	360	-	48,48,55	0.57	1 (2%)	56,56,63	1.12	6 (10%)
21	CLA	A	364	-	69,73,73	2.33	20 (28%)	82,113,113	1.90	16 (19%)
21	CLA	C	480	-	69,73,73	2.42	19 (27%)	82,113,113	1.97	13 (15%)
21	CLA	C	488	-	69,73,73	2.55	21 (30%)	82,113,113	1.85	15 (18%)
22	PHO	D	355	-	58,69,69	3.74	16 (27%)	55,99,99	1.96	11 (20%)
21	CLA	K	483	-	69,73,73	2.24	17 (24%)	82,113,113	1.78	13 (15%)
21	CLA	B	511	-	69,73,73	2.82	28 (40%)	82,113,113	1.79	14 (17%)
31	BCT	D	353	20	3,3,3	0.53	0	2,3,3	0.36	0
21	CLA	B	512	-	69,73,73	2.15	17 (24%)	82,113,113	1.62	11 (13%)
27	LMG	C	494	-	45,45,55	1.98	8 (17%)	53,53,63	2.20	16 (30%)
29	LMT	D	363	-	32,32,36	1.83	7 (21%)	43,43,47	1.50	6 (13%)
30	SQD	D	361	-	41,43,54	2.64	19 (46%)	51,54,65	2.81	16 (31%)
21	CLA	B	517	-	69,73,73	2.69	22 (31%)	82,113,113	2.04	20 (24%)
21	CLA	C	487	-	69,73,73	2.79	25 (36%)	82,113,113	1.85	11 (13%)
27	LMG	A	373	-	51,51,55	0.56	1 (1%)	59,59,63	1.10	5 (8%)
27	LMG	J	492	-	48,48,55	2.03	10 (20%)	56,56,63	1.88	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	524	-	69,73,73	2.56	22 (31%)	82,113,113	1.85	15 (18%)
25	BCR	J	115	-	41,41,41	2.22	8 (19%)	56,56,56	3.32	17 (30%)
21	CLA	B	521	-	69,73,73	2.45	17 (24%)	82,113,113	1.92	20 (24%)
21	CLA	B	522	-	69,73,73	2.23	17 (24%)	82,113,113	1.70	11 (13%)
25	BCR	C	490	-	41,41,41	1.99	6 (14%)	56,56,56	2.26	24 (42%)
21	CLA	A	363	-	69,73,73	2.22	19 (27%)	82,113,113	1.90	14 (17%)
21	CLA	B	513	-	69,73,73	2.24	18 (26%)	82,113,113	1.88	14 (17%)
29	LMT	I	274	-	36,36,36	1.88	12 (33%)	47,47,47	1.34	7 (14%)
21	CLA	B	519	-	69,73,73	2.34	17 (24%)	82,113,113	1.83	15 (18%)
28	DGD	B	528	-	59,59,67	0.61	2 (3%)	73,73,81	1.07	8 (10%)
21	CLA	C	484	-	69,73,73	2.43	19 (27%)	82,113,113	1.82	14 (17%)
28	DGD	D	362	-	64,64,67	2.15	22 (34%)	78,78,81	2.47	21 (26%)
26	LHG	A	371	-	38,38,48	2.27	6 (15%)	41,44,54	1.41	4 (9%)
21	CLA	C	483	-	69,73,73	2.59	23 (33%)	82,113,113	1.79	13 (15%)
21	CLA	B	523	-	69,73,73	2.28	19 (27%)	82,113,113	1.67	13 (15%)
21	CLA	C	477	-	69,73,73	2.35	16 (23%)	82,113,113	1.91	16 (19%)
25	BCR	Z	116	-	41,41,41	2.02	8 (19%)	56,56,56	2.14	21 (37%)
29	LMT	B	535	-	36,36,36	1.88	9 (25%)	47,47,47	1.15	2 (4%)
28	DGD	B	533	-	67,67,67	1.55	15 (22%)	81,81,81	1.83	19 (23%)
25	BCR	C	489	-	41,41,41	1.92	7 (17%)	56,56,56	2.13	19 (33%)
27	LMG	B	531	-	49,49,55	1.74	6 (12%)	57,57,63	2.81	18 (31%)
21	CLA	C	481	-	69,73,73	2.73	22 (31%)	82,113,113	2.02	16 (19%)
21	CLA	B	518	-	69,73,73	2.55	19 (27%)	82,113,113	2.11	16 (19%)
21	CLA	B	515	-	69,73,73	2.40	19 (27%)	82,113,113	1.78	14 (17%)
27	LMG	I	220	-	43,43,55	2.09	12 (27%)	51,51,63	2.18	13 (25%)
25	BCR	A	369	-	41,41,41	1.97	6 (14%)	56,56,56	2.13	23 (41%)
21	CLA	C	478	-	69,73,73	2.28	17 (24%)	82,113,113	1.75	15 (18%)
21	CLA	B	514	-	69,73,73	2.33	16 (23%)	82,113,113	1.60	12 (14%)
21	CLA	D	354	-	69,73,73	2.56	18 (26%)	82,113,113	1.68	14 (17%)
25	BCR	J	112	-	41,41,41	1.93	7 (17%)	56,56,56	2.47	24 (42%)
21	CLA	C	485	-	69,73,73	2.47	20 (28%)	82,113,113	1.76	13 (15%)
21	CLA	B	526	-	69,73,73	2.65	22 (31%)	82,113,113	1.78	12 (14%)
22	PHO	A	365	-	58,69,69	4.00	16 (27%)	55,99,99	2.06	11 (20%)
28	DGD	C	474	-	57,57,67	2.11	15 (26%)	71,71,81	3.51	25 (35%)
25	BCR	X	107	-	41,41,41	1.55	5 (12%)	56,56,56	2.46	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HEM	F	85	5	50,50,50	2.91	21 (42%)	67,82,82	2.49	20 (29%)
29	LMT	A	376	-	36,36,36	2.00	10 (27%)	47,47,47	1.47	8 (17%)
21	CLA	D	356	-	69,73,73	2.38	20 (28%)	82,113,113	1.87	14 (17%)
28	DGD	C	493	-	67,67,67	1.51	16 (23%)	81,81,81	2.95	28 (34%)
30	SQD	L	213	-	45,47,54	2.70	25 (55%)	55,58,65	2.76	19 (34%)
21	CLA	A	366	-	69,73,73	2.34	20 (28%)	82,113,113	1.77	11 (13%)
26	LHG	C	476	-	36,36,48	2.44	6 (16%)	39,42,54	1.50	4 (10%)
27	LMG	D	359	-	46,46,55	1.80	6 (13%)	54,54,63	2.54	17 (31%)
30	SQD	F	224	-	43,45,54	2.74	22 (51%)	53,56,65	2.73	20 (37%)
21	CLA	B	520	-	69,73,73	2.29	19 (27%)	82,113,113	1.71	11 (13%)
28	DGD	C	491	-	54,54,67	1.67	9 (16%)	68,68,81	2.94	24 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	D	536	-	-	1/21/61/61	0/2/2/2
21	CLA	C	482	-	2/2/15/20	10/39/115/115	-
23	MES	A	367	-	-	3/6/14/14	0/1/1/1
25	BCR	D	358	-	-	3/29/63/63	0/2/2/2
25	BCR	B	529	-	-	0/29/63/63	0/2/2/2
28	DGD	C	492	-	1/1/13/13	8/51/91/95	0/2/2/2
25	BCR	B	530	-	-	4/29/63/63	0/2/2/2
29	LMT	O	274	-	-	3/21/61/61	0/2/2/2
27	LMG	M	217	-	-	3/37/57/70	0/1/1/1
21	CLA	A	362	-	2/2/15/20	9/39/115/115	-
33	HEM	V	164	16	-	10/14/54/54	-
21	CLA	B	516	-	2/2/15/20	10/39/115/115	-
21	CLA	C	479	-	2/2/15/20	12/39/115/115	-
30	SQD	C	475	-	-	22/46/66/69	0/1/1/1
28	DGD	A	375	-	-	6/41/81/95	0/2/2/2
29	LMT	T	226	-	-	1/21/61/61	0/2/2/2
21	CLA	C	486	3	2/2/15/20	6/39/115/115	-
21	CLA	B	525	-	2/2/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	527	-	-	4/29/63/63	0/2/2/2
32	PL9	D	357	-	-	17/53/73/73	0/1/1/1
27	LMG	D	360	-	-	20/43/63/70	0/1/1/1
21	CLA	A	364	-	2/2/15/20	11/39/115/115	-
21	CLA	C	480	-	2/2/15/20	14/39/115/115	-
21	CLA	C	488	-	2/2/15/20	7/39/115/115	-
22	PHO	D	355	-	1/1/17/22	16/37/103/103	0/5/6/6
21	CLA	K	483	-	2/2/15/20	6/39/115/115	-
21	CLA	B	511	-	2/2/15/20	16/39/115/115	-
21	CLA	B	512	-	2/2/15/20	7/39/115/115	-
27	LMG	C	494	-	-	3/40/60/70	0/1/1/1
29	LMT	D	363	-	-	1/17/57/61	0/2/2/2
30	SQD	D	361	-	-	16/38/58/69	0/1/1/1
21	CLA	B	517	-	2/2/15/20	8/39/115/115	-
21	CLA	C	487	-	2/2/15/20	8/39/115/115	-
27	LMG	A	373	-	-	20/46/66/70	0/1/1/1
27	LMG	J	492	-	-	5/43/63/70	0/1/1/1
21	CLA	B	524	-	2/2/15/20	12/39/115/115	-
25	BCR	J	115	-	-	3/29/63/63	0/2/2/2
21	CLA	B	521	-	2/2/15/20	9/39/115/115	-
21	CLA	B	522	-	2/2/15/20	14/39/115/115	-
25	BCR	C	490	-	-	3/29/63/63	0/2/2/2
21	CLA	A	363	-	2/2/15/20	9/39/115/115	-
21	CLA	B	513	-	2/2/15/20	10/39/115/115	-
29	LMT	I	274	-	-	2/21/61/61	0/2/2/2
21	CLA	B	519	-	2/2/15/20	7/39/115/115	-
28	DGD	B	528	-	-	18/47/87/95	0/2/2/2
21	CLA	C	484	-	2/2/15/20	12/39/115/115	-
28	DGD	D	362	-	-	10/52/92/95	0/2/2/2
26	LHG	A	371	-	-	16/43/43/53	-
21	CLA	C	483	-	2/2/15/20	10/39/115/115	-
21	CLA	B	523	-	2/2/15/20	11/39/115/115	-
21	CLA	C	477	-	2/2/15/20	10/39/115/115	-
25	BCR	Z	116	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	B	535	-	-	3/21/61/61	0/2/2/2
28	DGD	B	533	-	-	9/55/95/95	0/2/2/2
25	BCR	C	489	-	-	5/29/63/63	0/2/2/2
27	LMG	B	531	-	-	4/44/64/70	0/1/1/1
21	CLA	C	481	-	2/2/15/20	11/39/115/115	-
21	CLA	B	518	-	2/2/15/20	8/39/115/115	-
21	CLA	B	515	-	2/2/15/20	8/39/115/115	-
27	LMG	I	220	-	-	4/38/58/70	0/1/1/1
25	BCR	A	369	-	-	5/29/63/63	0/2/2/2
21	CLA	C	478	-	2/2/15/20	7/39/115/115	-
21	CLA	B	514	-	2/2/15/20	10/39/115/115	-
21	CLA	D	354	-	2/2/15/20	10/39/115/115	-
25	BCR	J	112	-	-	1/29/63/63	0/2/2/2
21	CLA	C	485	-	2/2/15/20	10/39/115/115	-
21	CLA	B	526	-	2/2/15/20	9/39/115/115	-
22	PHO	A	365	-	1/1/17/22	6/37/103/103	0/5/6/6
28	DGD	C	474	-	-	7/45/85/95	0/2/2/2
25	BCR	X	107	-	-	3/29/63/63	0/2/2/2
33	HEM	F	85	5	-	8/14/54/54	-
29	LMT	A	376	-	-	3/21/61/61	0/2/2/2
21	CLA	D	356	-	2/2/15/20	8/39/115/115	-
28	DGD	C	493	-	1/1/13/13	9/55/95/95	0/2/2/2
30	SQD	L	213	-	-	16/42/62/69	0/1/1/1
21	CLA	A	366	-	2/2/15/20	6/39/115/115	-
26	LHG	C	476	-	-	16/41/41/53	-
27	LMG	D	359	-	-	5/41/61/70	0/1/1/1
30	SQD	F	224	-	-	18/40/60/69	0/1/1/1
21	CLA	B	520	-	2/2/15/20	14/39/115/115	-
28	DGD	C	491	-	-	5/42/82/95	0/2/2/2

All (1199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C3A-C2A	-17.56	1.39	1.54
22	D	355	PHO	C3A-C2A	-17.49	1.39	1.54
32	D	357	PL9	C28-C29	11.74	1.60	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	365	PHO	C1D-C2D	11.48	1.52	1.39
21	C	486	CLA	MG-NA	11.31	2.33	2.06
21	B	524	CLA	C2-C3	11.25	1.58	1.33
22	A	365	PHO	C3B-C4B	11.03	1.52	1.41
21	C	482	CLA	C2-C3	10.97	1.58	1.33
21	B	521	CLA	C2-C3	10.89	1.58	1.33
21	B	517	CLA	C2-C3	10.77	1.57	1.33
22	D	355	PHO	C1D-C2D	10.70	1.51	1.39
21	B	518	CLA	C2-C3	10.63	1.57	1.33
21	C	487	CLA	C2-C3	10.59	1.57	1.33
21	B	514	CLA	C2-C3	10.13	1.56	1.33
21	C	477	CLA	C2-C3	10.09	1.56	1.33
32	D	357	PL9	C13-C14	10.06	1.56	1.33
21	B	526	CLA	C2-C3	10.04	1.56	1.33
21	B	515	CLA	C2-C3	10.03	1.56	1.33
27	B	531	LMG	O1-C1	-10.01	1.23	1.40
21	B	516	CLA	C2-C3	10.00	1.56	1.33
21	C	486	CLA	C2-C3	9.99	1.56	1.33
27	M	217	LMG	O1-C1	-9.98	1.23	1.40
27	I	220	LMG	O1-C1	-9.93	1.23	1.40
27	C	494	LMG	O1-C1	-9.90	1.23	1.40
27	J	492	LMG	O1-C1	-9.89	1.23	1.40
21	B	519	CLA	C2-C3	9.89	1.55	1.33
27	D	359	LMG	O1-C1	-9.88	1.23	1.40
21	C	479	CLA	C2-C3	9.88	1.55	1.33
21	C	481	CLA	C2-C3	9.80	1.55	1.33
21	B	525	CLA	C2-C3	9.76	1.55	1.33
21	D	354	CLA	MG-NA	9.67	2.29	2.06
21	C	480	CLA	C2-C3	9.55	1.55	1.33
21	B	511	CLA	C2-C3	9.52	1.55	1.33
21	B	520	CLA	C2-C3	9.49	1.54	1.33
21	C	483	CLA	C2-C3	9.41	1.54	1.33
22	D	355	PHO	C3B-C4B	9.38	1.51	1.41
21	C	481	CLA	MG-NA	9.27	2.28	2.06
21	A	364	CLA	C2-C3	9.27	1.54	1.33
21	D	356	CLA	C2-C3	9.22	1.54	1.33
21	B	522	CLA	C2-C3	9.11	1.54	1.33
21	C	485	CLA	C2-C3	9.10	1.54	1.33
21	B	523	CLA	C2-C3	9.08	1.54	1.33
26	C	476	LHG	P-O5	9.08	1.82	1.50
21	C	478	CLA	C2-C3	9.06	1.53	1.33
25	B	530	BCR	C30-C25	8.98	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	354	CLA	C2-C3	8.95	1.53	1.33
22	A	365	PHO	C2-C3	8.89	1.53	1.33
21	K	483	CLA	C2-C3	8.86	1.53	1.33
32	D	357	PL9	C2-C3	8.86	1.56	1.34
26	A	371	LHG	P-O5	8.78	1.81	1.50
21	C	488	CLA	C2-C3	8.78	1.53	1.33
21	C	484	CLA	C2-C3	8.76	1.53	1.33
21	A	366	CLA	C2-C3	8.68	1.53	1.33
22	A	365	PHO	CHA-CBD	8.63	1.61	1.51
30	C	475	SQD	C4-C3	8.59	1.74	1.52
21	B	513	CLA	C2-C3	8.53	1.52	1.33
21	A	363	CLA	C2-C3	8.49	1.52	1.33
22	D	355	PHO	C3B-C2B	8.45	1.51	1.40
21	B	512	CLA	C2-C3	8.36	1.52	1.33
30	F	224	SQD	C4-C3	8.01	1.73	1.52
21	B	518	CLA	O2A-CGA	7.81	1.56	1.33
21	C	488	CLA	MG-NA	7.80	2.24	2.06
22	A	365	PHO	C3B-C2B	7.80	1.50	1.40
30	D	361	SQD	C4-C3	7.79	1.72	1.52
33	F	85	HEM	O1D-CGD	7.53	1.46	1.22
25	B	529	BCR	C30-C25	7.49	1.63	1.53
33	V	164	HEM	O1D-CGD	7.45	1.46	1.22
22	D	355	PHO	C2-C3	7.32	1.49	1.33
25	C	489	BCR	C1-C6	7.31	1.63	1.53
25	B	530	BCR	C1-C6	7.28	1.63	1.53
30	L	213	SQD	C4-C3	7.22	1.71	1.52
33	F	85	HEM	C3B-C2B	7.21	1.51	1.37
28	A	375	DGD	O3G-C1D	7.17	1.52	1.40
21	A	362	CLA	C2-C3	7.15	1.49	1.33
25	J	112	BCR	C30-C25	7.06	1.62	1.53
25	J	115	BCR	C30-C25	6.95	1.62	1.53
21	B	511	CLA	C4C-C3C	6.80	1.56	1.45
26	C	476	LHG	P-O3	6.73	1.85	1.59
25	A	369	BCR	C30-C25	6.66	1.62	1.53
21	B	517	CLA	O2A-CGA	6.64	1.52	1.33
21	B	524	CLA	O2A-CGA	6.53	1.52	1.33
28	C	474	DGD	O5D-C1E	6.52	1.51	1.40
28	D	362	DGD	O5D-C1E	6.52	1.51	1.40
25	Z	116	BCR	C30-C25	6.46	1.62	1.53
21	B	511	CLA	O2D-CGD	6.38	1.48	1.33
21	C	487	CLA	O2A-CGA	6.37	1.51	1.33
32	D	357	PL9	C3-C4	-6.30	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	484	CLA	O2D-CGD	6.26	1.48	1.33
21	B	517	CLA	MG-NA	6.25	2.21	2.06
21	B	526	CLA	MG-NA	6.25	2.21	2.06
25	C	490	BCR	C1-C6	6.24	1.61	1.53
28	D	362	DGD	O3G-C1D	6.17	1.50	1.40
21	B	515	CLA	O2A-CGA	6.14	1.51	1.33
25	Z	116	BCR	C1-C6	6.13	1.61	1.53
21	C	482	CLA	O2D-CGD	6.08	1.48	1.33
21	C	487	CLA	MG-NA	6.01	2.20	2.06
25	J	115	BCR	C5-C6	5.99	1.44	1.34
25	C	490	BCR	C30-C25	5.97	1.61	1.53
21	B	511	CLA	O2A-CGA	5.91	1.50	1.33
26	A	371	LHG	P-O3	5.85	1.82	1.59
21	B	526	CLA	O2A-CGA	5.82	1.50	1.33
21	B	516	CLA	O2A-CGA	5.82	1.50	1.33
21	C	482	CLA	C1C-C2C	5.78	1.56	1.44
21	C	486	CLA	O2A-CGA	5.78	1.50	1.33
21	C	477	CLA	O2D-CGD	5.73	1.47	1.33
21	B	511	CLA	MG-NA	5.72	2.19	2.06
21	B	513	CLA	O2A-CGA	5.69	1.49	1.33
21	A	364	CLA	O2A-CGA	5.68	1.49	1.33
21	C	482	CLA	C4C-C3C	5.63	1.54	1.45
28	C	491	DGD	O5D-C1E	5.61	1.49	1.40
21	C	482	CLA	O2A-CGA	5.61	1.49	1.33
25	A	369	BCR	C1-C6	5.61	1.61	1.53
21	B	516	CLA	C3A-C2A	-5.60	1.39	1.54
21	C	477	CLA	O2A-CGA	5.58	1.49	1.33
21	B	517	CLA	C3A-C2A	-5.58	1.39	1.54
21	C	477	CLA	C3A-C2A	-5.58	1.39	1.54
21	B	513	CLA	C3A-C2A	-5.57	1.39	1.54
21	B	523	CLA	C3A-C2A	-5.57	1.39	1.54
21	D	356	CLA	C3A-C2A	-5.57	1.39	1.54
21	B	521	CLA	C3A-C2A	-5.57	1.39	1.54
21	B	512	CLA	C3A-C2A	-5.56	1.39	1.54
21	A	366	CLA	C3A-C2A	-5.56	1.39	1.54
21	C	478	CLA	C3A-C2A	-5.56	1.39	1.54
21	C	481	CLA	O2A-CGA	5.56	1.49	1.33
21	C	485	CLA	C3A-C2A	-5.56	1.39	1.54
21	C	484	CLA	C3A-C2A	-5.56	1.39	1.54
21	B	514	CLA	C3A-C2A	-5.56	1.39	1.54
21	A	362	CLA	C3A-C2A	-5.56	1.39	1.54
21	A	364	CLA	C3A-C2A	-5.55	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	488	CLA	C3A-C2A	-5.55	1.39	1.54
21	B	518	CLA	C3A-C2A	-5.55	1.39	1.54
21	B	522	CLA	C3A-C2A	-5.54	1.39	1.54
21	B	520	CLA	C3A-C2A	-5.53	1.39	1.54
21	C	482	CLA	C3A-C2A	-5.53	1.39	1.54
21	B	519	CLA	C3A-C2A	-5.53	1.39	1.54
21	C	480	CLA	C3A-C2A	-5.53	1.39	1.54
21	C	479	CLA	C3A-C2A	-5.53	1.39	1.54
21	B	515	CLA	C3A-C2A	-5.52	1.39	1.54
21	C	481	CLA	C3A-C2A	-5.52	1.39	1.54
21	B	524	CLA	C3A-C2A	-5.52	1.39	1.54
21	C	487	CLA	C3A-C2A	-5.52	1.39	1.54
21	K	483	CLA	C3A-C2A	-5.51	1.39	1.54
33	V	164	HEM	C3B-C2B	5.51	1.48	1.37
21	A	363	CLA	C3A-C2A	-5.51	1.39	1.54
21	B	525	CLA	C3A-C2A	-5.50	1.39	1.54
21	B	511	CLA	C3A-C2A	-5.50	1.39	1.54
21	C	486	CLA	C3A-C2A	-5.49	1.39	1.54
21	D	354	CLA	C3A-C2A	-5.49	1.39	1.54
21	B	526	CLA	C3A-C2A	-5.48	1.39	1.54
21	C	481	CLA	C1C-C2C	5.46	1.55	1.44
21	C	483	CLA	C3A-C2A	-5.46	1.39	1.54
21	B	525	CLA	O2A-CGA	5.46	1.49	1.33
21	B	520	CLA	C4C-C3C	5.46	1.54	1.45
32	D	357	PL9	C6-C1	-5.44	1.39	1.48
25	B	527	BCR	C1-C6	5.42	1.60	1.53
21	C	483	CLA	O2D-CGD	5.36	1.46	1.33
21	C	487	CLA	C4C-C3C	5.35	1.54	1.45
21	B	519	CLA	O2D-CGD	5.34	1.46	1.33
21	D	354	CLA	O2A-CGA	5.30	1.48	1.33
21	B	521	CLA	O2D-CGD	5.30	1.46	1.33
26	C	476	LHG	P-O6	5.29	1.80	1.59
33	F	85	HEM	FE-NB	5.29	2.11	1.94
21	C	479	CLA	O2A-CGA	5.29	1.48	1.33
30	D	361	SQD	O47-C7	5.26	1.49	1.34
25	J	115	BCR	C26-C25	5.24	1.43	1.34
21	B	526	CLA	O2D-CGD	5.22	1.46	1.33
28	C	474	DGD	O6D-C1D	5.21	1.55	1.41
22	D	355	PHO	CHA-CBD	5.20	1.57	1.51
21	C	485	CLA	C4C-C3C	5.18	1.53	1.45
21	C	486	CLA	C1C-C2C	5.17	1.55	1.44
33	F	85	HEM	C4D-ND	-5.11	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	516	CLA	O2D-CGD	5.11	1.45	1.33
21	C	485	CLA	O2D-CGD	5.10	1.45	1.33
21	C	478	CLA	O2A-CGA	5.10	1.48	1.33
21	B	525	CLA	O2D-CGD	5.09	1.45	1.33
21	C	483	CLA	MG-NA	5.08	2.18	2.06
25	B	527	BCR	C30-C25	5.05	1.60	1.53
21	C	486	CLA	O2D-CGD	5.04	1.45	1.33
30	L	213	SQD	O5-C5	5.04	1.56	1.44
21	D	356	CLA	O2A-CGA	5.02	1.48	1.33
28	D	362	DGD	O6D-C1D	5.01	1.54	1.41
21	B	516	CLA	C4C-C3C	5.01	1.53	1.45
28	C	491	DGD	O6D-C1D	5.01	1.54	1.41
21	C	483	CLA	C4C-C3C	5.01	1.53	1.45
21	B	522	CLA	O2D-CGD	5.01	1.45	1.33
21	C	486	CLA	C4C-C3C	4.99	1.53	1.45
25	B	529	BCR	C5-C6	4.98	1.42	1.34
21	B	525	CLA	MG-NA	4.98	2.18	2.06
21	C	488	CLA	O2A-CGA	4.96	1.47	1.33
33	F	85	HEM	C4A-C3A	4.96	1.54	1.43
29	T	226	LMT	C4B-C3B	-4.95	1.39	1.52
21	C	483	CLA	O2A-CGA	4.95	1.47	1.33
29	O	274	LMT	C4B-C3B	-4.94	1.39	1.52
25	B	529	BCR	C26-C25	4.93	1.42	1.34
28	C	491	DGD	O3G-C1D	4.91	1.48	1.40
29	A	376	LMT	C4B-C3B	-4.91	1.39	1.52
21	C	487	CLA	C1C-C2C	4.91	1.54	1.44
29	D	363	LMT	C4B-C3B	-4.91	1.39	1.52
21	B	514	CLA	O2A-CGA	4.90	1.47	1.33
29	D	536	LMT	C4B-C3B	-4.89	1.39	1.52
29	B	535	LMT	C4B-C3B	-4.89	1.39	1.52
30	L	213	SQD	O7-S	4.88	1.58	1.45
30	F	224	SQD	O47-C7	4.88	1.48	1.34
29	I	274	LMT	C4B-C3B	-4.87	1.39	1.52
21	C	488	CLA	O2D-CGD	4.86	1.45	1.33
21	B	521	CLA	C1D-C2D	4.85	1.54	1.45
28	B	533	DGD	O5D-C1E	4.84	1.48	1.40
21	D	356	CLA	C1C-C2C	4.84	1.54	1.44
21	B	515	CLA	C1C-C2C	4.82	1.54	1.44
21	C	487	CLA	O2D-CGD	4.81	1.45	1.33
21	B	524	CLA	C1C-C2C	4.81	1.54	1.44
21	B	512	CLA	O2A-CGA	4.81	1.47	1.33
33	F	85	HEM	C1C-C2C	4.81	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	485	CLA	C1C-C2C	4.80	1.54	1.44
21	B	526	CLA	C4C-C3C	4.80	1.53	1.45
25	D	358	BCR	C26-C25	4.80	1.42	1.34
21	B	521	CLA	C4C-C3C	4.79	1.53	1.45
21	C	488	CLA	C1C-C2C	4.79	1.54	1.44
21	C	484	CLA	O2A-CGA	4.79	1.47	1.33
21	K	483	CLA	O2A-CGA	4.79	1.47	1.33
29	A	376	LMT	O5B-C1B	4.79	1.54	1.41
33	F	85	HEM	CBC-CAC	4.78	1.53	1.30
30	F	224	SQD	O48-C23	4.77	1.47	1.33
21	D	354	CLA	C4C-C3C	4.77	1.53	1.45
33	V	164	HEM	CBC-CAC	4.76	1.53	1.30
26	A	371	LHG	P-O6	4.76	1.78	1.59
25	D	358	BCR	C30-C25	4.76	1.59	1.53
21	C	480	CLA	O2A-CGA	4.74	1.47	1.33
21	A	362	CLA	O2D-CGD	4.74	1.44	1.33
21	C	483	CLA	C1C-C2C	4.73	1.54	1.44
30	L	213	SQD	O47-C7	4.72	1.47	1.34
21	K	483	CLA	O2D-CGD	4.72	1.44	1.33
21	C	482	CLA	MG-NC	4.71	2.17	2.06
25	B	530	BCR	C26-C25	4.70	1.42	1.34
33	F	85	HEM	C3B-C4B	4.70	1.54	1.44
22	D	355	PHO	CMC-C2C	4.69	1.57	1.50
21	A	363	CLA	O2A-CGA	4.69	1.47	1.33
21	B	518	CLA	C4-C3	-4.69	1.39	1.50
21	C	479	CLA	C1D-C2D	4.68	1.54	1.45
22	A	365	PHO	O2D-CGD	4.67	1.44	1.33
21	B	520	CLA	C4-C3	-4.67	1.39	1.50
30	D	361	SQD	O7-S	4.66	1.58	1.45
21	D	354	CLA	C4-C3	-4.66	1.39	1.50
21	A	362	CLA	C4-C3	-4.66	1.39	1.50
21	C	481	CLA	CAA-CBA	-4.65	1.39	1.52
21	B	512	CLA	C4-C3	-4.65	1.39	1.50
21	B	517	CLA	C4-C3	-4.65	1.39	1.50
21	A	366	CLA	O2A-CGA	4.65	1.46	1.33
22	D	355	PHO	C4-C3	-4.65	1.39	1.50
21	B	516	CLA	C4-C3	-4.65	1.39	1.50
21	B	522	CLA	O2A-CGA	4.64	1.46	1.33
21	C	482	CLA	C4-C3	-4.64	1.39	1.50
22	A	365	PHO	C4-C3	-4.63	1.39	1.50
21	A	366	CLA	C4-C3	-4.63	1.39	1.50
21	B	519	CLA	C4-C3	-4.63	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	514	CLA	C4-C3	-4.62	1.39	1.50
21	D	356	CLA	C4-C3	-4.62	1.39	1.50
21	D	356	CLA	C4C-C3C	4.62	1.52	1.45
21	B	511	CLA	C3B-C2B	4.62	1.56	1.41
21	C	481	CLA	C4-C3	-4.62	1.39	1.50
21	B	513	CLA	C4-C3	-4.62	1.39	1.50
21	C	483	CLA	C4-C3	-4.61	1.39	1.50
21	B	515	CLA	C4-C3	-4.61	1.39	1.50
21	C	479	CLA	C4-C3	-4.61	1.39	1.50
21	A	366	CLA	C1C-C2C	4.61	1.53	1.44
21	C	484	CLA	C4-C3	-4.61	1.39	1.50
21	B	523	CLA	C4-C3	-4.61	1.39	1.50
21	B	524	CLA	C4-C3	-4.61	1.39	1.50
21	A	363	CLA	C4-C3	-4.60	1.39	1.50
21	C	484	CLA	C3B-C4B	4.60	1.56	1.42
21	B	511	CLA	C4-C3	-4.60	1.39	1.50
21	A	364	CLA	C4-C3	-4.60	1.39	1.50
21	C	485	CLA	C3B-C4B	4.60	1.56	1.42
21	C	477	CLA	C4-C3	-4.60	1.39	1.50
21	C	480	CLA	C4-C3	-4.60	1.39	1.50
21	C	486	CLA	C4-C3	-4.60	1.39	1.50
21	C	485	CLA	C1D-C2D	4.60	1.54	1.45
25	B	530	BCR	C5-C6	4.59	1.42	1.34
21	C	485	CLA	C4-C3	-4.59	1.39	1.50
21	K	483	CLA	C4-C3	-4.59	1.39	1.50
21	C	487	CLA	C4-C3	-4.59	1.39	1.50
21	B	522	CLA	C4-C3	-4.59	1.39	1.50
21	B	526	CLA	C4-C3	-4.59	1.39	1.50
21	C	488	CLA	C4-C3	-4.58	1.39	1.50
21	B	518	CLA	CAA-CBA	-4.58	1.39	1.52
21	C	478	CLA	O2D-CGD	4.58	1.44	1.33
21	C	478	CLA	C4-C3	-4.57	1.39	1.50
21	B	525	CLA	C4-C3	-4.57	1.39	1.50
21	B	517	CLA	CAA-CBA	-4.57	1.39	1.52
21	B	515	CLA	CAA-CBA	-4.56	1.39	1.52
21	C	484	CLA	CAA-CBA	-4.56	1.39	1.52
21	A	362	CLA	MG-NA	4.56	2.17	2.06
28	A	375	DGD	O6D-C1D	4.56	1.53	1.41
21	B	521	CLA	C4-C3	-4.56	1.39	1.50
21	B	519	CLA	CAA-CBA	-4.55	1.39	1.52
21	C	480	CLA	CAA-CBA	-4.54	1.39	1.52
25	C	489	BCR	C30-C25	4.54	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	480	CLA	O2D-CGD	4.54	1.44	1.33
21	C	478	CLA	CAA-CBA	-4.54	1.39	1.52
30	C	475	SQD	O47-C7	4.53	1.47	1.34
21	B	522	CLA	CAA-CBA	-4.53	1.39	1.52
21	B	520	CLA	CAA-CBA	-4.52	1.39	1.52
21	C	479	CLA	CAA-CBA	-4.52	1.39	1.52
21	C	488	CLA	CAA-CBA	-4.52	1.39	1.52
21	C	477	CLA	CAA-CBA	-4.52	1.39	1.52
21	B	514	CLA	C4C-C3C	4.52	1.52	1.45
21	C	480	CLA	C4C-C3C	4.52	1.52	1.45
21	C	479	CLA	C1C-C2C	4.51	1.53	1.44
28	A	375	DGD	O6D-C5D	4.51	1.55	1.44
22	A	365	PHO	CAA-CBA	-4.51	1.39	1.52
21	A	366	CLA	O2D-CGD	4.51	1.44	1.33
21	C	484	CLA	C1C-C2C	4.51	1.53	1.44
21	B	521	CLA	CAA-CBA	-4.51	1.39	1.52
21	B	512	CLA	CAA-CBA	-4.51	1.39	1.52
21	A	362	CLA	CAA-CBA	-4.50	1.39	1.52
21	K	483	CLA	CAA-CBA	-4.50	1.39	1.52
25	B	530	BCR	C2-C1	4.50	1.64	1.54
21	B	524	CLA	CAA-CBA	-4.50	1.39	1.52
25	J	115	BCR	C29-C30	4.49	1.64	1.54
33	V	164	HEM	C1C-C2C	4.49	1.54	1.45
21	D	356	CLA	CAA-CBA	-4.49	1.39	1.52
21	B	514	CLA	CAA-CBA	-4.49	1.39	1.52
21	B	523	CLA	CAA-CBA	-4.49	1.39	1.52
29	O	274	LMT	O5B-C1B	4.48	1.53	1.41
21	D	354	CLA	CAA-CBA	-4.48	1.39	1.52
21	C	486	CLA	CAA-CBA	-4.48	1.39	1.52
25	B	529	BCR	C1-C6	4.48	1.59	1.53
21	B	513	CLA	O2D-CGD	4.47	1.44	1.33
21	B	511	CLA	MG-NC	4.47	2.16	2.06
21	A	364	CLA	CAA-CBA	-4.47	1.39	1.52
25	J	112	BCR	C5-C6	4.47	1.42	1.34
21	A	366	CLA	CAA-CBA	-4.46	1.39	1.52
21	B	513	CLA	CAA-CBA	-4.46	1.39	1.52
21	B	516	CLA	CAA-CBA	-4.46	1.39	1.52
21	C	482	CLA	CAA-CBA	-4.46	1.39	1.52
30	F	224	SQD	O7-S	4.45	1.57	1.45
21	C	485	CLA	CAA-CBA	-4.45	1.39	1.52
22	D	355	PHO	CAA-CBA	-4.45	1.39	1.52
21	C	483	CLA	CAA-CBA	-4.44	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	363	LMT	O1'-C1'	4.44	1.47	1.40
21	B	526	CLA	CAA-CBA	-4.44	1.39	1.52
21	B	523	CLA	C1C-C2C	4.44	1.53	1.44
21	A	363	CLA	CAA-CBA	-4.44	1.39	1.52
21	B	516	CLA	MG-NC	4.43	2.16	2.06
21	B	520	CLA	O2D-CGD	4.43	1.44	1.33
21	B	521	CLA	O2A-CGA	4.42	1.46	1.33
21	B	525	CLA	CAA-CBA	-4.42	1.39	1.52
21	B	523	CLA	C3B-C4B	4.41	1.55	1.42
21	K	483	CLA	C1C-C2C	4.40	1.53	1.44
27	J	492	LMG	O7-C8	4.40	1.57	1.46
21	B	511	CLA	CAA-CBA	-4.40	1.39	1.52
21	C	487	CLA	CAA-CBA	-4.39	1.39	1.52
30	F	224	SQD	O5-C5	4.38	1.55	1.44
21	C	478	CLA	C1C-C2C	4.38	1.53	1.44
21	B	515	CLA	O2D-CGD	4.37	1.44	1.33
28	C	492	DGD	O6D-C1D	4.37	1.53	1.41
21	C	485	CLA	O2A-CGA	4.35	1.46	1.33
30	D	361	SQD	O5-C5	4.35	1.55	1.44
21	C	482	CLA	C1B-NB	4.35	1.43	1.37
21	C	481	CLA	C4C-C3C	4.34	1.52	1.45
21	B	523	CLA	O2A-CGA	4.34	1.46	1.33
21	C	482	CLA	C3B-C4B	4.33	1.55	1.42
21	A	366	CLA	MG-NC	4.33	2.16	2.06
21	B	517	CLA	C1C-C2C	4.33	1.53	1.44
33	F	85	HEM	FE-NC	4.33	2.09	1.95
21	C	478	CLA	C4C-C3C	4.33	1.52	1.45
21	K	483	CLA	C4C-C3C	4.33	1.52	1.45
21	A	363	CLA	C3B-C4B	4.33	1.55	1.42
21	B	517	CLA	C4C-C3C	4.33	1.52	1.45
21	C	482	CLA	C1D-C2D	4.32	1.53	1.45
25	B	530	BCR	C29-C30	4.31	1.64	1.54
21	D	354	CLA	C1C-C2C	4.31	1.53	1.44
21	B	525	CLA	C1C-C2C	4.31	1.53	1.44
28	C	474	DGD	O3G-C1D	4.29	1.47	1.40
28	C	493	DGD	O6D-C1D	4.28	1.52	1.41
25	C	490	BCR	C5-C6	4.28	1.41	1.34
33	V	164	HEM	C3C-C4C	4.25	1.53	1.46
21	B	519	CLA	C4C-C3C	4.25	1.52	1.45
30	L	213	SQD	O48-C23	4.24	1.45	1.33
21	B	519	CLA	O2A-CGA	4.24	1.45	1.33
23	A	367	MES	C8-S	4.23	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	364	CLA	C4C-C3C	4.23	1.52	1.45
30	C	475	SQD	O5-C5	4.23	1.54	1.44
21	B	523	CLA	O2D-CGD	4.23	1.43	1.33
21	B	512	CLA	O2D-CGD	4.22	1.43	1.33
21	B	517	CLA	O2D-CGD	4.22	1.43	1.33
21	B	517	CLA	C1D-C2D	4.22	1.53	1.45
21	B	522	CLA	C1C-C2C	4.21	1.53	1.44
21	A	364	CLA	O2D-CGD	4.21	1.43	1.33
21	B	518	CLA	C1C-C2C	4.19	1.53	1.44
21	B	519	CLA	C1D-C2D	4.18	1.53	1.45
22	A	365	PHO	O2A-CGA	4.18	1.45	1.33
21	C	480	CLA	C1C-C2C	4.18	1.53	1.44
21	C	479	CLA	O2D-CGD	4.17	1.43	1.33
21	B	524	CLA	O2D-CGD	4.17	1.43	1.33
21	B	517	CLA	C3B-C4B	4.15	1.54	1.42
26	A	371	LHG	O7-C7	4.15	1.46	1.34
28	A	375	DGD	O5D-C1E	4.15	1.47	1.40
25	D	358	BCR	C1-C6	4.15	1.59	1.53
28	C	474	DGD	O1G-C1A	4.15	1.45	1.33
21	B	524	CLA	C4C-C3C	4.14	1.52	1.45
21	B	518	CLA	O2D-CGD	4.14	1.43	1.33
21	C	479	CLA	C4C-C3C	4.13	1.52	1.45
21	C	487	CLA	MG-NC	4.13	2.16	2.06
21	A	363	CLA	C1C-C2C	4.12	1.52	1.44
21	B	524	CLA	C1D-C2D	4.11	1.53	1.45
25	X	107	BCR	C26-C25	4.10	1.41	1.34
33	V	164	HEM	C4D-ND	-4.10	1.33	1.40
21	C	477	CLA	C4C-C3C	4.09	1.52	1.45
25	Z	116	BCR	C26-C25	4.09	1.41	1.34
33	V	164	HEM	FE-NC	4.09	2.08	1.95
21	D	354	CLA	O2D-CGD	4.08	1.43	1.33
21	C	486	CLA	CHC-C1C	4.07	1.46	1.38
30	L	213	SQD	O6-C1	4.07	1.47	1.40
21	C	479	CLA	MG-NC	4.06	2.15	2.06
28	C	474	DGD	O6D-C5D	4.06	1.54	1.44
30	D	361	SQD	C1-C2	4.06	1.64	1.52
25	B	529	BCR	C29-C30	4.06	1.63	1.54
21	C	481	CLA	O2D-CGD	4.06	1.43	1.33
25	D	358	BCR	C29-C30	4.05	1.63	1.54
21	B	516	CLA	C1C-C2C	4.05	1.52	1.44
21	C	488	CLA	C4C-C3C	4.04	1.51	1.45
21	A	366	CLA	C3B-C4B	4.04	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	516	CLA	CBA-CGA	4.02	1.62	1.50
22	D	355	PHO	O2A-CGA	4.02	1.45	1.33
21	B	518	CLA	C1D-C2D	4.01	1.53	1.45
22	A	365	PHO	CMC-C2C	4.00	1.56	1.50
21	B	515	CLA	C3B-C4B	4.00	1.54	1.42
21	B	518	CLA	C4C-C3C	4.00	1.51	1.45
21	B	513	CLA	C3B-C4B	4.00	1.54	1.42
21	B	519	CLA	C1C-C2C	3.99	1.52	1.44
30	L	213	SQD	C1-C2	3.99	1.64	1.52
21	C	480	CLA	MG-NB	3.98	2.13	2.05
21	C	481	CLA	C1B-NB	3.98	1.43	1.37
21	B	526	CLA	C3B-C4B	3.97	1.54	1.42
21	C	483	CLA	MG-NC	3.96	2.15	2.06
21	C	483	CLA	C1D-C2D	3.96	1.53	1.45
21	A	362	CLA	C4C-C3C	3.95	1.51	1.45
21	C	481	CLA	C3B-C4B	3.94	1.54	1.42
33	V	164	HEM	O2D-CGD	3.94	1.43	1.30
21	A	366	CLA	C4C-C3C	3.94	1.51	1.45
30	C	475	SQD	C1-C2	3.94	1.64	1.52
21	B	526	CLA	C1D-C2D	3.94	1.53	1.45
21	B	520	CLA	O2A-CGA	3.94	1.44	1.33
21	C	478	CLA	C3B-C4B	3.94	1.54	1.42
21	C	486	CLA	MG-NB	3.93	2.13	2.05
21	B	514	CLA	C1C-C2C	3.93	1.52	1.44
28	C	474	DGD	O6E-C1E	3.93	1.51	1.41
21	B	520	CLA	C1C-C2C	3.91	1.52	1.44
21	C	485	CLA	MG-NA	3.91	2.15	2.06
21	D	356	CLA	O2D-CGD	3.89	1.42	1.33
29	B	535	LMT	O5B-C1B	3.89	1.51	1.41
21	B	513	CLA	C1C-C2C	3.89	1.52	1.44
21	B	526	CLA	C1B-NB	3.88	1.43	1.37
28	C	474	DGD	O2G-C1B	3.88	1.45	1.34
25	A	369	BCR	C26-C25	3.87	1.41	1.34
21	C	483	CLA	C3B-C4B	3.87	1.54	1.42
26	C	476	LHG	O8-C23	3.87	1.44	1.33
28	B	533	DGD	O6D-C1D	3.86	1.51	1.41
21	B	523	CLA	C4C-C3C	3.86	1.51	1.45
25	B	527	BCR	C26-C25	3.85	1.41	1.34
22	D	355	PHO	O2D-CGD	3.85	1.42	1.33
21	B	514	CLA	O2D-CGD	3.85	1.42	1.33
21	B	513	CLA	C4C-C3C	3.84	1.51	1.45
21	C	487	CLA	C5-C3	3.84	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	520	CLA	MG-NC	3.83	2.15	2.06
28	C	474	DGD	C3G-C2G	3.83	1.62	1.50
21	A	364	CLA	C1C-C2C	3.82	1.52	1.44
21	B	522	CLA	C4C-C3C	3.82	1.51	1.45
21	B	512	CLA	C1C-C2C	3.82	1.52	1.44
28	A	375	DGD	C3G-C2G	3.81	1.62	1.50
21	K	483	CLA	MG-NC	3.81	2.15	2.06
21	C	482	CLA	MG-NB	3.81	2.13	2.05
33	V	164	HEM	C4A-C3A	3.81	1.52	1.43
21	B	512	CLA	C4C-C3C	3.80	1.51	1.45
21	A	364	CLA	C1D-C2D	3.80	1.52	1.45
21	B	511	CLA	CMC-C2C	3.79	1.58	1.50
21	B	524	CLA	C3B-C4B	3.79	1.53	1.42
21	B	525	CLA	MG-NC	3.79	2.15	2.06
21	A	363	CLA	O2D-CGD	3.79	1.42	1.33
21	B	516	CLA	C5-C3	3.78	1.59	1.51
21	B	511	CLA	C1D-C2D	3.78	1.52	1.45
30	C	475	SQD	O7-S	3.78	1.55	1.45
28	B	533	DGD	O6E-C1E	3.78	1.51	1.41
21	C	484	CLA	C4C-C3C	3.78	1.51	1.45
21	C	486	CLA	C1D-C2D	3.77	1.52	1.45
21	B	524	CLA	C5-C3	3.77	1.59	1.51
25	J	112	BCR	C1-C6	3.77	1.58	1.53
21	C	488	CLA	C3B-C4B	3.77	1.53	1.42
25	A	369	BCR	C5-C6	3.76	1.40	1.34
21	C	484	CLA	MG-NC	3.76	2.15	2.06
30	C	475	SQD	O6-C1	3.75	1.46	1.40
25	C	489	BCR	C2-C1	3.75	1.62	1.54
21	C	485	CLA	MG-NC	3.74	2.15	2.06
21	B	522	CLA	C3B-C4B	3.74	1.53	1.42
21	B	525	CLA	C4C-C3C	3.72	1.51	1.45
21	C	481	CLA	C1D-C2D	3.72	1.52	1.45
21	B	511	CLA	CHB-C4A	3.72	1.47	1.37
25	J	115	BCR	C1-C6	3.71	1.58	1.53
21	C	480	CLA	C1B-NB	3.71	1.42	1.37
28	A	375	DGD	O6E-C5E	3.70	1.53	1.44
33	F	85	HEM	C3C-C4C	3.70	1.52	1.46
30	C	475	SQD	O48-C23	3.69	1.44	1.33
33	V	164	HEM	CAC-C3C	3.69	1.57	1.47
21	B	521	CLA	C1C-C2C	3.69	1.52	1.44
21	C	486	CLA	O1D-CGD	3.69	1.30	1.21
21	B	521	CLA	O1D-CGD	3.68	1.30	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	484	CLA	C1D-C2D	3.68	1.52	1.45
25	X	107	BCR	C29-C30	3.68	1.62	1.54
21	C	480	CLA	CMC-C2C	3.68	1.58	1.50
21	C	486	CLA	C3B-C4B	3.67	1.53	1.42
21	C	481	CLA	C3B-C2B	3.67	1.53	1.41
28	D	362	DGD	C2A-C1A	3.67	1.61	1.50
21	B	519	CLA	C3B-C4B	3.66	1.53	1.42
21	B	511	CLA	O1D-CGD	3.66	1.30	1.21
21	B	521	CLA	C5-C3	3.66	1.58	1.51
25	B	529	BCR	C2-C1	3.65	1.62	1.54
21	C	482	CLA	C3B-C2B	3.65	1.53	1.41
32	D	357	PL9	C12-C13	-3.65	1.39	1.50
32	D	357	PL9	C6-C5	3.64	1.53	1.35
21	B	512	CLA	C3B-C4B	3.64	1.53	1.42
21	C	480	CLA	C3B-C4B	3.64	1.53	1.42
21	C	478	CLA	C1D-C2D	3.63	1.52	1.45
25	C	490	BCR	C2-C1	3.63	1.62	1.54
21	B	521	CLA	MG-NC	3.62	2.14	2.06
21	C	482	CLA	O1D-CGD	3.62	1.30	1.21
21	C	477	CLA	C1C-C2C	3.62	1.51	1.44
21	D	356	CLA	MG-NC	3.61	2.14	2.06
21	B	525	CLA	C3B-C4B	3.60	1.53	1.42
32	D	357	PL9	C32-C33	-3.60	1.39	1.50
21	C	487	CLA	CMC-C2C	3.60	1.58	1.50
21	C	488	CLA	C1D-C2D	3.60	1.52	1.45
21	C	485	CLA	C1B-NB	3.59	1.42	1.37
21	C	488	CLA	O1D-CGD	3.59	1.30	1.21
28	C	493	DGD	O5D-C6D	-3.59	1.37	1.43
30	C	475	SQD	O3-C3	3.59	1.51	1.43
21	B	526	CLA	MG-NC	3.58	2.14	2.06
32	D	357	PL9	C37-C38	-3.58	1.39	1.50
26	A	371	LHG	O8-C23	3.57	1.43	1.33
21	K	483	CLA	C3B-C4B	3.56	1.53	1.42
25	J	112	BCR	C2-C1	3.55	1.62	1.54
21	D	356	CLA	C1D-C2D	3.55	1.52	1.45
33	F	85	HEM	CAC-C3C	3.55	1.56	1.47
21	A	362	CLA	C1C-C2C	3.55	1.51	1.44
33	F	85	HEM	O2D-CGD	3.55	1.42	1.30
21	B	514	CLA	C1D-C2D	3.54	1.52	1.45
21	C	487	CLA	CAA-C2A	3.54	1.60	1.54
32	D	357	PL9	C27-C28	-3.53	1.39	1.50
21	B	526	CLA	MG-NB	3.53	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	523	CLA	MG-NC	3.52	2.14	2.06
21	B	517	CLA	C5-C3	3.52	1.58	1.51
29	B	535	LMT	O5'-C1'	3.51	1.50	1.41
21	A	362	CLA	MG-NB	3.51	2.12	2.05
29	O	274	LMT	O1B-C4'	3.50	1.52	1.43
28	D	362	DGD	O2G-C1B	3.49	1.44	1.34
25	A	369	BCR	C2-C1	3.49	1.62	1.54
21	C	483	CLA	CMC-C2C	3.49	1.57	1.50
21	B	511	CLA	C1C-C2C	3.49	1.51	1.44
21	B	518	CLA	MG-NB	3.48	2.12	2.05
29	D	536	LMT	O5B-C1B	3.48	1.50	1.41
21	C	481	CLA	CMC-C2C	3.48	1.57	1.50
21	B	521	CLA	C3B-C4B	3.48	1.52	1.42
21	C	482	CLA	CBA-CGA	3.47	1.60	1.50
21	C	480	CLA	C1D-C2D	3.47	1.52	1.45
29	D	363	LMT	O5'-C1'	3.47	1.50	1.41
29	I	274	LMT	O5B-C1B	3.46	1.50	1.41
28	C	493	DGD	C5B-C4B	-3.46	1.34	1.51
25	J	112	BCR	C29-C30	3.46	1.62	1.54
21	A	364	CLA	C3B-C4B	3.46	1.52	1.42
21	C	482	CLA	CMC-C2C	3.45	1.57	1.50
25	Z	116	BCR	C5-C6	3.45	1.40	1.34
21	B	515	CLA	CMC-C2C	3.43	1.57	1.50
25	B	527	BCR	C5-C6	3.43	1.40	1.34
21	C	481	CLA	CHC-C1C	3.43	1.45	1.38
21	A	362	CLA	C3B-C4B	3.42	1.52	1.42
21	B	518	CLA	MG-NC	3.42	2.14	2.06
21	C	477	CLA	MG-NB	3.42	2.12	2.05
21	B	514	CLA	MG-NC	3.42	2.14	2.06
29	A	376	LMT	O1B-C1B	3.42	1.51	1.41
28	A	375	DGD	O6E-C1E	3.42	1.50	1.41
21	B	517	CLA	CHC-C1C	3.41	1.45	1.38
21	C	487	CLA	C3B-C2B	3.41	1.52	1.41
21	C	485	CLA	CMC-C2C	3.41	1.57	1.50
21	B	518	CLA	C3B-C4B	3.41	1.52	1.42
21	A	362	CLA	C1D-C2D	3.41	1.52	1.45
25	Z	116	BCR	C29-C30	3.40	1.61	1.54
29	B	535	LMT	O1'-C1'	3.40	1.45	1.40
33	V	164	HEM	CMC-C2C	3.40	1.57	1.50
33	V	164	HEM	O2A-CGA	-3.39	1.19	1.30
21	B	515	CLA	C1D-C2D	3.39	1.52	1.45
21	B	526	CLA	O1D-CGD	3.39	1.29	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	476	LHG	O7-C7	3.39	1.43	1.34
21	C	479	CLA	MG-NB	3.38	2.12	2.05
21	C	484	CLA	MG-NB	3.38	2.12	2.05
21	D	356	CLA	C3B-C4B	3.38	1.52	1.42
29	T	226	LMT	O5'-C1'	3.38	1.50	1.41
21	B	519	CLA	CMC-C2C	3.38	1.57	1.50
21	D	356	CLA	CMC-C2C	3.38	1.57	1.50
25	X	107	BCR	C1-C6	3.38	1.58	1.53
29	B	535	LMT	O1B-C1B	3.38	1.51	1.41
21	A	363	CLA	CMC-C2C	3.37	1.57	1.50
21	B	511	CLA	C1B-NB	3.37	1.42	1.37
21	B	523	CLA	C1D-C2D	3.37	1.52	1.45
30	D	361	SQD	O8-S	3.37	1.59	1.47
25	A	369	BCR	C29-C30	3.36	1.61	1.54
25	Z	116	BCR	C2-C1	3.36	1.61	1.54
21	B	516	CLA	C3B-C4B	3.35	1.52	1.42
21	A	366	CLA	O1D-CGD	3.35	1.29	1.21
21	D	354	CLA	MG-ND	-3.34	1.99	2.05
21	C	478	CLA	CMC-C2C	3.34	1.57	1.50
28	D	362	DGD	O1G-C1G	3.34	1.52	1.45
21	B	513	CLA	MG-NC	3.34	2.14	2.06
33	V	164	HEM	C4A-NA	-3.33	1.33	1.39
25	B	527	BCR	C2-C1	3.33	1.61	1.54
21	B	520	CLA	CMC-C2C	3.33	1.57	1.50
32	D	357	PL9	C2-C1	3.32	1.53	1.44
21	C	479	CLA	C3B-C2B	3.32	1.52	1.41
21	C	485	CLA	MG-NB	3.31	2.12	2.05
21	C	486	CLA	C1B-NB	3.30	1.42	1.37
21	B	511	CLA	CHB-C1B	3.30	1.46	1.39
30	D	361	SQD	O48-C23	3.29	1.42	1.33
21	C	487	CLA	O1D-CGD	3.29	1.29	1.21
21	C	482	CLA	CAC-C3C	3.29	1.59	1.51
21	B	511	CLA	CBA-CGA	3.28	1.60	1.50
28	C	493	DGD	O5D-C1E	3.28	1.45	1.40
25	B	527	BCR	C29-C30	3.28	1.61	1.54
21	C	486	CLA	CHD-C4C	3.28	1.46	1.39
21	B	525	CLA	C5-C3	3.27	1.58	1.51
29	A	376	LMT	O1B-C4'	3.27	1.52	1.43
30	C	475	SQD	C20-C19	-3.26	1.35	1.51
33	F	85	HEM	O2A-CGA	-3.26	1.20	1.30
29	O	274	LMT	O5'-C1'	3.26	1.50	1.41
25	C	489	BCR	C29-C30	3.26	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	116	BCR	C38-C26	3.25	1.56	1.50
21	C	484	CLA	C3B-C2B	3.25	1.52	1.41
21	B	515	CLA	MG-NC	3.25	2.14	2.06
33	V	164	HEM	FE-NB	3.25	2.04	1.94
21	B	512	CLA	C1D-C2D	3.25	1.51	1.45
21	C	477	CLA	MG-NC	3.24	2.14	2.06
33	F	85	HEM	FE-NA	3.24	2.05	1.95
21	C	477	CLA	C3B-C4B	3.24	1.52	1.42
28	C	491	DGD	C5B-C4B	-3.23	1.35	1.51
30	F	224	SQD	C8-C7	3.23	1.60	1.50
21	B	516	CLA	CMC-C2C	3.23	1.57	1.50
21	B	515	CLA	C5-C3	3.23	1.57	1.51
28	D	362	DGD	O6E-C1E	3.22	1.50	1.41
25	D	358	BCR	C2-C1	3.22	1.61	1.54
25	X	107	BCR	C2-C1	3.22	1.61	1.54
21	D	354	CLA	C3B-C4B	3.21	1.52	1.42
21	A	366	CLA	C3B-C2B	3.21	1.52	1.41
21	C	477	CLA	C1D-C2D	3.21	1.51	1.45
21	C	487	CLA	C3B-C4B	3.21	1.52	1.42
25	C	490	BCR	C29-C30	3.21	1.61	1.54
29	O	274	LMT	O1B-C1B	3.20	1.50	1.41
21	C	488	CLA	C3B-C2B	3.20	1.52	1.41
21	B	526	CLA	C3B-C2B	3.20	1.52	1.41
21	B	519	CLA	MG-NC	3.20	2.13	2.06
21	B	526	CLA	C1C-C2C	3.19	1.51	1.44
21	A	362	CLA	O1D-CGD	3.18	1.29	1.21
30	L	213	SQD	O5-C1	3.18	1.50	1.41
21	C	479	CLA	C3B-C4B	3.18	1.52	1.42
21	A	364	CLA	MG-NA	3.18	2.13	2.06
29	T	226	LMT	O1'-C1'	3.17	1.45	1.40
25	J	115	BCR	C2-C1	3.17	1.61	1.54
30	F	224	SQD	C1-C2	3.17	1.61	1.52
21	B	514	CLA	C3B-C4B	3.17	1.51	1.42
21	B	514	CLA	C3B-C2B	3.17	1.51	1.41
30	C	475	SQD	C19-C18	-3.16	1.36	1.51
30	C	475	SQD	C33-C32	-3.16	1.36	1.51
21	B	517	CLA	O1D-CGD	3.14	1.29	1.21
21	C	486	CLA	CHC-C4B	3.14	1.46	1.39
21	K	483	CLA	CMC-C2C	3.14	1.57	1.50
21	B	519	CLA	C3B-C2B	3.14	1.51	1.41
21	B	512	CLA	O1D-CGD	3.13	1.29	1.21
21	B	515	CLA	C4C-C3C	3.12	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	274	LMT	C3'-C4'	3.12	1.60	1.52
21	C	484	CLA	CHC-C1C	3.11	1.44	1.38
21	C	484	CLA	C1B-NB	3.11	1.41	1.37
30	L	213	SQD	O8-S	3.11	1.58	1.47
30	D	361	SQD	O6-C1	3.10	1.45	1.40
28	A	375	DGD	O1G-C1G	3.10	1.52	1.45
21	C	479	CLA	CMC-C2C	3.10	1.57	1.50
30	F	224	SQD	O5-C1	3.10	1.49	1.41
28	D	362	DGD	C1G-C2G	3.09	1.60	1.50
21	C	483	CLA	C5-C3	3.09	1.57	1.51
21	C	483	CLA	C3B-C2B	3.09	1.51	1.41
21	B	513	CLA	C1D-C2D	3.08	1.51	1.45
21	B	520	CLA	C1D-C2D	3.08	1.51	1.45
21	A	366	CLA	CMC-C2C	3.07	1.57	1.50
21	C	477	CLA	CMC-C2C	3.07	1.57	1.50
21	A	366	CLA	C1D-C2D	3.07	1.51	1.45
30	F	224	SQD	C14-C13	-3.07	1.36	1.51
21	B	525	CLA	C3B-C2B	3.06	1.51	1.41
30	D	361	SQD	C15-C14	-3.06	1.36	1.51
21	A	363	CLA	C1D-C2D	3.06	1.51	1.45
21	C	478	CLA	O1D-CGD	3.06	1.29	1.21
30	L	213	SQD	C12-C11	-3.05	1.36	1.51
30	C	475	SQD	C17-C16	-3.05	1.36	1.51
21	A	363	CLA	CBA-CGA	3.05	1.59	1.50
21	B	525	CLA	O1D-CGD	3.05	1.28	1.21
21	D	354	CLA	CMC-C2C	3.05	1.57	1.50
21	C	483	CLA	C1B-NB	3.05	1.41	1.37
30	D	361	SQD	C14-C13	-3.04	1.36	1.51
21	C	484	CLA	O1D-CGD	3.04	1.28	1.21
30	F	224	SQD	C24-C23	3.04	1.59	1.50
21	A	364	CLA	CMC-C2C	3.04	1.57	1.50
21	B	513	CLA	CMC-C2C	3.04	1.57	1.50
29	A	376	LMT	C4'-C5'	3.04	1.61	1.52
30	F	224	SQD	C13-C12	-3.04	1.36	1.51
21	C	488	CLA	CHC-C1C	3.04	1.44	1.38
21	B	513	CLA	O1D-CGD	3.03	1.28	1.21
30	C	475	SQD	C12-C11	-3.03	1.36	1.51
21	D	356	CLA	MG-NA	3.03	2.13	2.06
30	F	224	SQD	O3-C3	3.03	1.50	1.43
21	B	514	CLA	MG-ND	-3.03	1.99	2.05
30	D	361	SQD	C16-C15	-3.02	1.36	1.51
29	O	274	LMT	O1'-C1'	3.02	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	487	CLA	CBA-CGA	3.02	1.59	1.50
33	F	85	HEM	CMC-C2C	3.02	1.57	1.50
21	C	480	CLA	C3B-C2B	3.02	1.51	1.41
30	D	361	SQD	C12-C11	-3.01	1.36	1.51
27	C	494	LMG	O6-C1	3.01	1.49	1.41
21	A	362	CLA	O2A-CGA	3.01	1.42	1.33
29	I	274	LMT	C4'-C5'	3.01	1.61	1.52
28	B	533	DGD	O2G-C1B	3.01	1.42	1.34
30	D	361	SQD	C13-C12	-3.01	1.36	1.51
21	B	517	CLA	CMC-C2C	3.01	1.56	1.50
21	C	481	CLA	CAA-C2A	-3.00	1.48	1.54
30	F	224	SQD	C17-C16	-3.00	1.36	1.51
30	L	213	SQD	C16-C15	-2.99	1.36	1.51
21	C	486	CLA	C3B-C2B	2.98	1.51	1.41
21	C	479	CLA	O1D-CGD	2.98	1.28	1.21
21	C	477	CLA	O1D-CGD	2.98	1.28	1.21
21	B	518	CLA	O1D-CGD	2.98	1.28	1.21
30	F	224	SQD	C12-C11	-2.98	1.36	1.51
21	A	366	CLA	MG-NB	2.98	2.11	2.05
30	L	213	SQD	C17-C16	-2.98	1.37	1.51
21	C	481	CLA	O1D-CGD	2.97	1.28	1.21
21	B	514	CLA	CBA-CGA	2.97	1.59	1.50
21	B	516	CLA	C3B-C2B	2.97	1.51	1.41
28	D	362	DGD	O1G-C1A	2.97	1.42	1.33
30	F	224	SQD	O8-S	2.97	1.58	1.47
21	B	516	CLA	C1D-C2D	2.97	1.51	1.45
21	A	363	CLA	O1D-CGD	2.97	1.28	1.21
30	F	224	SQD	C15-C14	-2.96	1.37	1.51
30	C	475	SQD	C11-C10	-2.96	1.37	1.51
30	D	361	SQD	C11-C10	-2.95	1.37	1.51
21	C	488	CLA	C1B-NB	2.95	1.41	1.37
21	C	486	CLA	CHD-C1D	2.95	1.44	1.38
27	M	217	LMG	O7-C8	2.95	1.53	1.46
27	C	494	LMG	O7-C8	2.94	1.53	1.46
32	D	357	PL9	C33-C34	2.94	1.39	1.33
21	C	482	CLA	MG-NA	2.94	2.13	2.06
30	C	475	SQD	C32-C31	-2.94	1.37	1.51
21	C	478	CLA	MG-NC	2.93	2.13	2.06
30	D	361	SQD	O3-C3	2.92	1.50	1.43
21	B	522	CLA	MG-NC	2.92	2.13	2.06
30	C	475	SQD	C18-C17	-2.91	1.37	1.51
27	D	359	LMG	C16-C15	-2.91	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	C	474	DGD	C4E-C3E	2.91	1.59	1.52
21	C	479	CLA	MG-NA	2.91	2.13	2.06
21	B	516	CLA	O1D-CGD	2.91	1.28	1.21
21	B	523	CLA	MG-ND	-2.90	2.00	2.05
30	L	213	SQD	C11-C10	-2.90	1.37	1.51
28	A	375	DGD	C5B-C4B	-2.90	1.37	1.51
21	C	488	CLA	MG-NB	2.90	2.11	2.05
21	B	520	CLA	O1D-CGD	2.89	1.28	1.21
29	A	376	LMT	O5'-C1'	2.89	1.49	1.41
21	A	363	CLA	CAA-C2A	2.89	1.59	1.54
21	B	512	CLA	MG-NC	2.89	2.13	2.06
21	B	520	CLA	C3B-C2B	2.88	1.50	1.41
21	B	524	CLA	O1D-CGD	2.88	1.28	1.21
30	C	475	SQD	C16-C15	-2.87	1.37	1.51
21	B	524	CLA	CMC-C2C	2.86	1.56	1.50
21	D	354	CLA	C3B-C2B	2.86	1.50	1.41
21	B	515	CLA	C1B-NB	2.86	1.41	1.37
21	B	514	CLA	CMC-C2C	2.86	1.56	1.50
21	K	483	CLA	C1B-NB	2.86	1.41	1.37
21	C	483	CLA	O1D-CGD	2.85	1.28	1.21
25	C	489	BCR	C5-C6	2.85	1.39	1.34
21	C	487	CLA	C1B-NB	2.85	1.41	1.37
21	B	523	CLA	O1D-CGD	2.85	1.28	1.21
29	O	274	LMT	C4'-C5'	2.84	1.60	1.52
21	C	480	CLA	MG-NC	2.84	2.13	2.06
32	D	357	PL9	C8-C9	2.83	1.39	1.33
30	F	224	SQD	C16-C15	-2.83	1.37	1.51
27	I	220	LMG	O6-C1	2.83	1.49	1.41
21	B	522	CLA	CAC-C3C	2.83	1.58	1.51
21	B	525	CLA	C1D-C2D	2.82	1.50	1.45
21	C	487	CLA	C1D-C2D	2.82	1.50	1.45
33	V	164	HEM	C3B-C4B	2.81	1.50	1.44
28	C	474	DGD	C5B-C4B	-2.81	1.37	1.51
21	A	364	CLA	O1D-CGD	2.81	1.28	1.21
29	B	535	LMT	O1B-C4'	2.81	1.51	1.43
21	C	483	CLA	MG-NB	2.80	2.11	2.05
21	B	516	CLA	MG-ND	-2.80	2.00	2.05
30	L	213	SQD	C13-C12	-2.80	1.37	1.51
21	B	522	CLA	CMC-C2C	2.79	1.56	1.50
32	D	357	PL9	C18-C19	2.79	1.39	1.33
28	C	492	DGD	O5D-C6D	-2.79	1.38	1.43
21	B	512	CLA	C3B-C2B	2.79	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	213	SQD	C15-C14	-2.79	1.37	1.51
21	B	515	CLA	C3B-C2B	2.79	1.50	1.41
25	D	358	BCR	C5-C6	2.78	1.39	1.34
28	C	491	DGD	O2E-C2E	-2.78	1.36	1.43
32	D	357	PL9	C38-C39	2.78	1.39	1.33
32	D	357	PL9	C43-C44	2.78	1.39	1.33
21	A	364	CLA	MG-NC	2.77	2.12	2.06
21	D	354	CLA	C1D-ND	-2.77	1.34	1.37
21	A	363	CLA	C3B-C2B	2.77	1.50	1.41
29	A	376	LMT	O1'-C1'	2.77	1.44	1.40
30	L	213	SQD	C20-C19	-2.77	1.38	1.51
25	C	489	BCR	C26-C25	2.77	1.39	1.34
30	C	475	SQD	C8-C7	2.77	1.58	1.50
21	B	523	CLA	C1B-NB	2.77	1.41	1.37
21	K	483	CLA	C1D-C2D	2.77	1.50	1.45
29	T	226	LMT	C1B-C2B	2.77	1.60	1.52
29	D	363	LMT	O5B-C1B	2.76	1.48	1.41
30	F	224	SQD	O6-C1	2.76	1.44	1.40
21	C	479	CLA	C5-C3	2.76	1.57	1.51
33	V	164	HEM	FE-NA	2.75	2.04	1.95
30	C	475	SQD	C13-C12	-2.75	1.38	1.51
21	B	518	CLA	C3B-C2B	2.75	1.50	1.41
21	B	515	CLA	MG-NB	2.75	2.11	2.05
30	L	213	SQD	C14-C13	-2.74	1.38	1.51
25	J	112	BCR	C26-C25	2.74	1.39	1.34
21	B	526	CLA	CHB-C4A	2.74	1.44	1.37
21	C	487	CLA	CHB-C4A	2.74	1.44	1.37
21	B	517	CLA	MG-NB	2.74	2.11	2.05
27	C	494	LMG	C16-C15	-2.74	1.38	1.51
28	D	362	DGD	O2G-C2G	2.74	1.53	1.46
21	B	519	CLA	O1D-CGD	2.74	1.28	1.21
30	C	475	SQD	C15-C14	-2.73	1.38	1.51
27	M	217	LMG	O7-C10	2.73	1.42	1.34
21	B	520	CLA	C3B-C4B	2.72	1.50	1.42
33	V	164	HEM	C1A-C2A	-2.72	1.39	1.44
21	B	520	CLA	MG-NB	2.72	2.11	2.05
27	M	217	LMG	O6-C1	2.72	1.48	1.41
21	C	481	CLA	MG-NB	2.72	2.11	2.05
27	J	492	LMG	O6-C1	2.72	1.48	1.41
21	B	513	CLA	CBA-CGA	2.72	1.58	1.50
28	C	492	DGD	O2G-C1B	2.71	1.41	1.34
29	D	363	LMT	C4'-C5'	2.71	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	362	CLA	MG-NC	2.71	2.12	2.06
21	D	356	CLA	CBA-CGA	2.71	1.58	1.50
30	C	475	SQD	O8-S	2.70	1.57	1.47
33	F	85	HEM	CHC-C1C	2.70	1.43	1.38
21	B	518	CLA	O2A-C1	2.69	1.53	1.46
25	C	489	BCR	C19-C18	-2.69	1.40	1.46
21	C	485	CLA	C3B-C2B	2.69	1.50	1.41
27	C	494	LMG	O1-C7	2.69	1.48	1.43
21	A	363	CLA	C1D-ND	-2.69	1.34	1.37
21	B	518	CLA	CBA-CGA	2.69	1.58	1.50
29	I	274	LMT	O1'-C1'	2.69	1.44	1.40
33	V	164	HEM	C1D-C2D	2.68	1.50	1.44
30	C	475	SQD	O5-C1	2.68	1.48	1.41
25	X	107	BCR	C5-C6	2.68	1.39	1.34
33	F	85	HEM	C4D-C3D	2.68	1.49	1.45
21	A	364	CLA	CBA-CGA	2.68	1.58	1.50
21	B	524	CLA	MG-NA	2.67	2.12	2.06
28	A	375	DGD	C2A-C1A	2.67	1.58	1.50
27	I	220	LMG	C4-C5	2.67	1.58	1.53
28	C	493	DGD	C3G-C2G	2.67	1.59	1.50
25	B	530	BCR	C38-C26	2.66	1.55	1.50
30	L	213	SQD	C19-C18	-2.66	1.38	1.51
28	C	492	DGD	O5D-C1E	2.66	1.44	1.40
27	J	492	LMG	O7-C10	2.66	1.41	1.34
21	B	517	CLA	C6-C7	2.65	1.63	1.52
27	I	220	LMG	C16-C15	-2.65	1.38	1.51
21	A	363	CLA	MG-NB	2.65	2.11	2.05
33	V	164	HEM	FE-ND	2.65	2.03	1.94
29	T	226	LMT	O5B-C1B	2.65	1.48	1.41
21	C	480	CLA	O1D-CGD	2.65	1.27	1.21
21	B	524	CLA	CBA-CGA	2.65	1.58	1.50
21	D	356	CLA	O1D-CGD	2.65	1.27	1.21
21	C	478	CLA	C3B-C2B	2.65	1.50	1.41
27	I	220	LMG	O8-C28	2.65	1.41	1.33
21	C	482	CLA	CAA-C2A	2.64	1.58	1.54
30	C	475	SQD	C14-C13	-2.64	1.38	1.51
28	D	362	DGD	C3D-C2D	2.64	1.59	1.52
27	B	531	LMG	C16-C15	-2.64	1.38	1.51
21	B	517	CLA	O2A-C1	2.64	1.53	1.46
21	B	526	CLA	C5-C3	2.64	1.56	1.51
21	A	364	CLA	C3B-C2B	2.63	1.50	1.41
28	B	533	DGD	C4E-C3E	2.63	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	511	CLA	C3B-C4B	2.63	1.50	1.42
21	C	484	CLA	CAC-C3C	2.63	1.57	1.51
21	C	477	CLA	C3B-C2B	2.62	1.50	1.41
22	D	355	PHO	C4C-C3C	2.62	1.53	1.45
21	C	487	CLA	CAC-C3C	2.62	1.57	1.51
21	C	487	CLA	MG-NB	2.62	2.11	2.05
21	A	362	CLA	C3B-C2B	2.61	1.50	1.41
21	C	488	CLA	CAC-C3C	2.61	1.57	1.51
33	F	85	HEM	FE-ND	2.61	2.02	1.94
21	B	523	CLA	CMC-C2C	2.60	1.56	1.50
21	C	488	CLA	CMC-C2C	2.59	1.56	1.50
21	D	356	CLA	C5-C3	2.59	1.56	1.51
21	B	516	CLA	MG-NB	2.59	2.10	2.05
28	C	491	DGD	O6D-C5D	2.59	1.50	1.44
27	M	217	LMG	C16-C15	-2.58	1.38	1.51
21	B	525	CLA	CMC-C2C	2.58	1.56	1.50
29	D	536	LMT	O5'-C1'	2.58	1.48	1.41
25	B	529	BCR	C38-C26	2.58	1.55	1.50
21	D	354	CLA	O1D-CGD	2.58	1.27	1.21
21	B	525	CLA	C1B-NB	2.58	1.41	1.37
21	B	513	CLA	MG-NB	2.58	2.10	2.05
21	B	522	CLA	O1D-CGD	2.57	1.27	1.21
21	C	488	CLA	CHD-C4C	2.57	1.45	1.39
21	C	485	CLA	O1D-CGD	2.57	1.27	1.21
21	D	356	CLA	C3B-C2B	2.57	1.49	1.41
28	D	362	DGD	C1E-C2E	2.57	1.60	1.52
28	C	493	DGD	O3G-C1D	2.57	1.44	1.40
21	B	515	CLA	CHC-C1C	2.57	1.43	1.38
21	D	356	CLA	MG-NB	2.57	2.10	2.05
22	A	365	PHO	O1D-CGD	2.56	1.27	1.21
21	B	521	CLA	C3B-C2B	2.56	1.49	1.41
21	K	483	CLA	C3B-C2B	2.56	1.49	1.41
21	B	516	CLA	O2A-C1	2.56	1.53	1.46
30	F	224	SQD	C11-C10	-2.55	1.39	1.51
21	B	518	CLA	CMC-C2C	2.55	1.56	1.50
21	B	515	CLA	CBA-CGA	2.55	1.58	1.50
21	B	517	CLA	CHD-C1D	2.55	1.43	1.38
30	L	213	SQD	C8-C7	2.55	1.58	1.50
21	A	364	CLA	MG-ND	-2.55	2.00	2.05
22	A	365	PHO	C3D-CAD	-2.54	1.42	1.47
21	C	482	CLA	CMD-C2D	2.54	1.56	1.50
30	D	361	SQD	C8-C7	2.54	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	362	CLA	CMC-C2C	2.54	1.56	1.50
21	B	524	CLA	MG-NC	2.53	2.12	2.06
21	B	523	CLA	MG-NB	2.53	2.10	2.05
21	C	486	CLA	CBA-CGA	2.53	1.58	1.50
21	C	483	CLA	CAC-C3C	2.53	1.57	1.51
29	A	376	LMT	C1B-C2B	2.53	1.59	1.52
25	C	490	BCR	C26-C25	2.53	1.38	1.34
28	D	362	DGD	O6D-C5D	2.53	1.50	1.44
21	C	480	CLA	C5-C3	2.53	1.56	1.51
28	C	474	DGD	C4A-C3A	-2.52	1.39	1.51
28	C	492	DGD	C9A-C8A	-2.52	1.39	1.51
28	C	492	DGD	C4A-C3A	-2.52	1.39	1.51
21	B	523	CLA	CHC-C1C	2.52	1.43	1.38
28	B	533	DGD	C4A-C3A	-2.51	1.39	1.51
25	D	358	BCR	C19-C18	-2.51	1.40	1.46
33	V	164	HEM	C4D-C3D	2.51	1.49	1.45
27	B	531	LMG	C39-C38	-2.50	1.39	1.51
30	L	213	SQD	O3-C3	2.50	1.49	1.43
21	B	519	CLA	CMD-C2D	2.50	1.55	1.50
29	B	535	LMT	C10-C9	-2.50	1.39	1.51
27	C	494	LMG	C34-C33	-2.50	1.39	1.51
28	C	493	DGD	C4A-C3A	-2.50	1.39	1.51
21	A	366	CLA	C1B-NB	2.50	1.41	1.37
28	B	533	DGD	CEB-CDB	-2.50	1.39	1.51
33	V	164	HEM	C1B-C2B	-2.49	1.39	1.44
21	B	518	CLA	C5-C3	2.49	1.56	1.51
29	D	536	LMT	C10-C9	-2.49	1.39	1.51
28	C	493	DGD	CFB-CEB	-2.49	1.39	1.51
27	D	359	LMG	C34-C33	-2.49	1.39	1.51
28	C	493	DGD	CEB-CDB	-2.49	1.39	1.51
28	C	492	DGD	CFB-CEB	-2.48	1.39	1.51
29	T	226	LMT	C10-C9	-2.48	1.39	1.51
21	C	479	CLA	CMD-C2D	2.48	1.55	1.50
29	I	274	LMT	C10-C9	-2.48	1.39	1.51
29	D	536	LMT	C5-C4	-2.48	1.39	1.51
28	C	493	DGD	C9A-C8A	-2.48	1.39	1.51
21	A	366	CLA	CHC-C1C	2.48	1.43	1.38
21	D	354	CLA	C1D-C2D	2.48	1.50	1.45
28	C	474	DGD	C3E-C2E	2.48	1.58	1.52
27	I	220	LMG	C34-C33	-2.48	1.39	1.51
28	C	491	DGD	C4A-C3A	-2.47	1.39	1.51
28	C	493	DGD	C9B-C8B	-2.47	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	O	274	LMT	C10-C9	-2.47	1.39	1.51
21	A	366	CLA	MG-ND	-2.47	2.00	2.05
28	C	493	DGD	CDA-CCA	-2.47	1.39	1.51
29	B	535	LMT	C5-C4	-2.47	1.39	1.51
27	D	359	LMG	C39-C38	-2.47	1.39	1.51
28	B	533	DGD	C5B-C4B	-2.47	1.39	1.51
21	C	486	CLA	CMC-C2C	2.47	1.55	1.50
28	B	533	DGD	CDA-CCA	-2.47	1.39	1.51
27	B	531	LMG	C20-C19	-2.47	1.39	1.51
28	D	362	DGD	C3G-C2G	2.47	1.58	1.50
30	L	213	SQD	C18-C17	-2.47	1.39	1.51
27	J	492	LMG	C34-C33	-2.47	1.39	1.51
28	B	533	DGD	C9A-C8A	-2.47	1.39	1.51
30	C	475	SQD	C21-C20	-2.46	1.36	1.51
32	D	357	PL9	C5-C4	2.46	1.55	1.47
29	O	274	LMT	C5-C4	-2.46	1.39	1.51
27	B	531	LMG	C34-C33	-2.46	1.39	1.51
28	B	533	DGD	CFB-CEB	-2.46	1.39	1.51
21	B	525	CLA	MG-NB	2.46	2.10	2.05
28	D	362	DGD	CEB-CDB	-2.46	1.39	1.51
28	A	375	DGD	C4A-C3A	-2.46	1.39	1.51
21	B	511	CLA	CAA-C2A	2.46	1.58	1.54
28	C	492	DGD	CEB-CDB	-2.46	1.39	1.51
29	O	274	LMT	O5B-C5B	2.46	1.50	1.44
28	D	362	DGD	CFB-CEB	-2.46	1.39	1.51
29	A	376	LMT	C10-C9	-2.46	1.39	1.51
29	A	376	LMT	C5-C4	-2.45	1.39	1.51
33	F	85	HEM	C1B-C2B	-2.45	1.39	1.44
21	C	487	CLA	C2A-C1A	2.45	1.57	1.52
28	D	362	DGD	CDA-CCA	-2.45	1.39	1.51
27	M	217	LMG	C34-C33	-2.45	1.39	1.51
27	J	492	LMG	C39-C38	-2.45	1.39	1.51
32	D	357	PL9	C10-C9	2.45	1.56	1.50
28	C	474	DGD	C9B-C8B	-2.45	1.39	1.51
29	I	274	LMT	C5-C4	-2.45	1.39	1.51
27	C	494	LMG	C20-C19	-2.45	1.39	1.51
28	C	491	DGD	C9A-C8A	-2.45	1.39	1.51
21	B	524	CLA	C3B-C2B	2.44	1.49	1.41
28	C	474	DGD	C9A-C8A	-2.44	1.39	1.51
27	D	359	LMG	C20-C19	-2.44	1.39	1.51
32	D	357	PL9	C23-C24	2.44	1.38	1.33
29	T	226	LMT	C5-C4	-2.44	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	511	CLA	MG-NB	2.44	2.10	2.05
28	A	375	DGD	C9B-C8B	-2.44	1.39	1.51
28	C	492	DGD	C9B-C8B	-2.44	1.39	1.51
28	B	533	DGD	C9B-C8B	-2.44	1.39	1.51
30	D	361	SQD	C17-C16	-2.43	1.36	1.51
27	I	220	LMG	C20-C19	-2.43	1.39	1.51
28	D	362	DGD	C9A-C8A	-2.43	1.39	1.51
27	J	492	LMG	C20-C19	-2.43	1.39	1.51
21	B	514	CLA	O1D-CGD	2.43	1.27	1.21
28	B	533	DGD	C2B-C1B	2.42	1.57	1.50
27	M	217	LMG	C20-C19	-2.42	1.39	1.51
21	B	512	CLA	MG-NA	2.42	2.12	2.06
29	D	363	LMT	C5-C4	-2.42	1.39	1.51
21	A	362	CLA	CHC-C1C	2.42	1.43	1.38
29	D	363	LMT	O5'-C5'	2.42	1.50	1.44
21	B	524	CLA	MG-NB	2.41	2.10	2.05
28	D	362	DGD	C5B-C4B	-2.41	1.39	1.51
28	D	362	DGD	C4A-C3A	-2.41	1.39	1.51
28	D	362	DGD	C9B-C8B	-2.41	1.39	1.51
21	B	522	CLA	C1D-C2D	2.41	1.50	1.45
27	I	220	LMG	O6-C5	2.41	1.50	1.44
25	B	530	BCR	C7-C6	2.40	1.53	1.45
21	B	525	CLA	CBA-CGA	2.40	1.57	1.50
30	C	475	SQD	C34-C33	-2.40	1.36	1.51
27	D	359	LMG	O6-C1	2.39	1.48	1.41
29	I	274	LMT	C1B-C2B	2.39	1.59	1.52
21	B	513	CLA	C1D-ND	-2.39	1.34	1.37
29	I	274	LMT	C3B-C2B	2.39	1.58	1.52
21	B	511	CLA	CHD-C1D	2.38	1.43	1.38
21	C	483	CLA	CHC-C1C	2.38	1.43	1.38
21	C	488	CLA	CHC-C4B	2.37	1.44	1.39
25	B	527	BCR	C38-C26	2.37	1.54	1.50
21	K	483	CLA	MG-NB	2.37	2.10	2.05
32	D	357	PL9	C48-C49	2.36	1.39	1.32
28	C	491	DGD	C3G-C2G	2.36	1.58	1.50
22	D	355	PHO	C1C-C2C	2.36	1.53	1.45
28	C	492	DGD	C5B-C4B	-2.36	1.40	1.51
29	D	536	LMT	C4'-C5'	2.36	1.59	1.52
21	B	523	CLA	C3B-C2B	2.36	1.49	1.41
21	B	522	CLA	MG-ND	-2.36	2.01	2.05
21	A	364	CLA	C1D-ND	-2.36	1.34	1.37
21	C	481	CLA	CHC-C4B	2.35	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	517	CLA	CHD-C4C	2.35	1.44	1.39
21	B	513	CLA	C3B-C2B	2.34	1.49	1.41
26	C	476	LHG	C4-C5	2.34	1.58	1.50
25	Z	116	BCR	C23-C22	-2.34	1.40	1.46
27	B	531	LMG	O6-C1	2.34	1.47	1.41
21	B	511	CLA	CAC-C3C	2.34	1.57	1.51
21	B	524	CLA	CAC-C3C	2.33	1.57	1.51
29	I	274	LMT	O5'-C1'	2.33	1.47	1.41
33	F	85	HEM	C1D-C2D	2.33	1.49	1.44
21	B	521	CLA	CBA-CGA	2.33	1.57	1.50
21	B	511	CLA	C5-C3	2.33	1.56	1.51
32	D	357	PL9	C36-C37	-2.33	1.46	1.53
30	F	224	SQD	C18-C17	-2.33	1.37	1.51
29	D	536	LMT	C4B-C5B	2.32	1.58	1.53
21	B	521	CLA	CMD-C2D	2.32	1.55	1.50
21	C	486	CLA	MG-NC	2.32	2.11	2.06
21	B	524	CLA	CMD-C2D	2.32	1.55	1.50
28	C	493	DGD	C4E-C3E	2.32	1.58	1.52
21	A	362	CLA	CHD-C4C	2.31	1.44	1.39
21	D	354	CLA	CHD-C1D	2.31	1.42	1.38
29	O	274	LMT	O5'-C5'	2.31	1.50	1.44
21	B	522	CLA	C1D-ND	-2.30	1.34	1.37
30	D	361	SQD	O5-C1	2.30	1.47	1.41
30	L	213	SQD	C21-C20	-2.30	1.37	1.51
21	C	488	CLA	CMD-C2D	2.30	1.55	1.50
21	C	485	CLA	CHC-C1C	2.29	1.43	1.38
27	J	492	LMG	C16-C15	-2.29	1.40	1.51
28	C	493	DGD	O2E-C2E	-2.29	1.37	1.43
21	A	363	CLA	C4C-C3C	2.28	1.48	1.45
22	D	355	PHO	C1A-C2A	2.28	1.54	1.51
22	A	365	PHO	C1C-C2C	2.28	1.52	1.45
21	A	364	CLA	C3D-C2D	-2.28	1.32	1.39
28	C	493	DGD	C4D-C3D	-2.28	1.46	1.52
21	B	519	CLA	MG-ND	-2.27	2.01	2.05
22	A	365	PHO	CAC-C3C	2.27	1.56	1.51
21	B	511	CLA	MG-ND	-2.27	2.01	2.05
27	I	220	LMG	O1-C7	2.27	1.47	1.43
28	B	528	DGD	O5D-C1E	2.27	1.44	1.40
21	D	356	CLA	C1D-ND	-2.27	1.34	1.37
30	L	213	SQD	C44-C45	2.27	1.57	1.50
28	C	474	DGD	C2A-C1A	2.26	1.57	1.50
21	B	521	CLA	CMC-C2C	2.26	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	164	HEM	CAB-C3B	-2.26	1.41	1.47
21	C	478	CLA	CAC-C3C	2.25	1.56	1.51
21	C	486	CLA	C5-C3	2.25	1.55	1.51
27	I	220	LMG	O8-C9	2.25	1.50	1.45
21	B	524	CLA	C1B-NB	2.25	1.40	1.37
27	D	360	LMG	O1-C1	2.25	1.43	1.40
21	B	511	CLA	CBD-CHA	2.25	1.62	1.51
21	C	484	CLA	OBD-CAD	2.25	1.26	1.22
21	C	481	CLA	CHD-C4C	2.25	1.44	1.39
28	B	528	DGD	O3G-C1D	2.24	1.43	1.40
21	C	478	CLA	C5-C3	2.24	1.55	1.51
21	B	520	CLA	CAC-C3C	2.23	1.56	1.51
29	T	226	LMT	C4B-C5B	2.23	1.57	1.53
21	B	519	CLA	MG-NB	2.22	2.10	2.05
27	A	373	LMG	O1-C1	2.22	1.43	1.40
27	J	492	LMG	C11-C10	2.22	1.57	1.50
21	D	354	CLA	CHC-C1C	2.22	1.42	1.38
21	C	483	CLA	MG-ND	-2.21	2.01	2.05
21	A	366	CLA	MG-NA	2.21	2.11	2.06
30	L	213	SQD	C24-C23	2.21	1.57	1.50
25	J	115	BCR	C24-C23	2.21	1.39	1.33
27	J	492	LMG	C4-C5	2.21	1.57	1.53
21	K	483	CLA	MG-ND	-2.20	2.01	2.05
21	C	479	CLA	CBA-CGA	2.20	1.57	1.50
21	B	513	CLA	CHC-C1C	2.20	1.42	1.38
29	I	274	LMT	O5'-C5'	2.19	1.49	1.44
21	B	520	CLA	MG-ND	-2.19	2.01	2.05
25	B	530	BCR	C24-C23	2.19	1.39	1.33
21	C	483	CLA	CBA-CGA	2.19	1.57	1.50
21	C	478	CLA	C1B-NB	2.18	1.40	1.37
21	B	515	CLA	O1D-CGD	2.18	1.26	1.21
22	D	355	PHO	O1D-CGD	2.18	1.26	1.21
21	B	526	CLA	CMC-C2C	2.17	1.55	1.50
21	B	523	CLA	C5-C3	2.17	1.55	1.51
28	C	493	DGD	O6E-C5E	-2.17	1.39	1.44
21	B	512	CLA	CMC-C2C	2.17	1.55	1.50
21	C	477	CLA	CBA-CGA	2.17	1.57	1.50
21	B	511	CLA	CHD-C4C	2.16	1.44	1.39
29	B	535	LMT	C1B-C2B	2.16	1.58	1.52
21	C	482	CLA	CHD-C4C	2.16	1.44	1.39
21	B	524	CLA	CHC-C1C	2.14	1.42	1.38
21	B	512	CLA	MG-NB	2.14	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	V	164	HEM	CHB-C1B	-2.13	1.34	1.38
21	C	485	CLA	MG-ND	-2.13	2.01	2.05
21	A	363	CLA	MG-NC	2.12	2.11	2.06
21	C	487	CLA	CHB-C1B	2.12	1.44	1.39
30	F	224	SQD	C19-C18	-2.12	1.35	1.50
27	I	220	LMG	C7-C8	2.12	1.57	1.50
27	M	217	LMG	C11-C10	2.12	1.56	1.50
21	B	517	CLA	C3B-C2B	2.12	1.48	1.41
29	T	226	LMT	O5B-C5B	2.11	1.49	1.44
21	C	486	CLA	C4B-NB	2.11	1.40	1.37
21	A	362	CLA	C1D-ND	-2.10	1.35	1.37
21	C	484	CLA	CMD-C2D	2.10	1.55	1.50
21	B	526	CLA	CHD-C4C	2.10	1.44	1.39
29	D	536	LMT	C3'-C4'	2.10	1.58	1.52
28	B	533	DGD	O2G-C2G	2.10	1.51	1.46
30	C	475	SQD	C22-C21	-2.09	1.35	1.50
21	C	487	CLA	O2A-C1	2.09	1.51	1.46
27	C	494	LMG	C7-C8	2.09	1.57	1.50
21	B	512	CLA	MG-ND	-2.08	2.01	2.05
25	J	112	BCR	C19-C18	-2.08	1.41	1.46
21	C	485	CLA	CMD-C2D	2.08	1.55	1.50
32	D	357	PL9	C11-C9	2.08	1.55	1.51
21	B	522	CLA	C3B-C2B	2.08	1.48	1.41
22	A	365	PHO	C3D-C2D	-2.07	1.36	1.39
29	D	536	LMT	C1B-C2B	2.07	1.58	1.52
21	B	526	CLA	CMD-C2D	2.07	1.55	1.50
21	C	482	CLA	C4B-NB	2.07	1.40	1.37
30	C	475	SQD	C24-C23	2.07	1.56	1.50
28	D	362	DGD	C2B-C1B	2.07	1.56	1.50
33	V	164	HEM	CHC-C1C	2.07	1.42	1.38
21	B	526	CLA	CHB-C1B	2.07	1.44	1.39
30	F	224	SQD	C44-C45	2.07	1.57	1.50
21	B	520	CLA	C1D-ND	-2.06	1.35	1.37
21	K	483	CLA	O1D-CGD	2.06	1.26	1.21
21	C	481	CLA	CHD-C1D	2.06	1.42	1.38
29	D	536	LMT	O1B-C1B	2.06	1.47	1.41
21	C	481	CLA	CBD-CHA	2.06	1.61	1.51
30	L	213	SQD	C22-C21	-2.06	1.35	1.50
21	C	480	CLA	OBD-CAD	2.06	1.26	1.22
33	V	164	HEM	C1C-NC	-2.05	1.35	1.39
25	J	115	BCR	C4-C5	2.05	1.54	1.51
21	C	483	CLA	CMD-C2D	2.05	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	518	CLA	C1D-ND	-2.04	1.35	1.37
33	F	85	HEM	C4A-NA	-2.04	1.35	1.39
21	A	364	CLA	CBD-CHA	2.04	1.61	1.51
21	B	520	CLA	C1B-NB	2.03	1.40	1.37
21	D	356	CLA	CHC-C1C	2.03	1.42	1.38
21	A	363	CLA	CHC-C1C	2.03	1.42	1.38
21	B	517	CLA	CHC-C4B	2.03	1.44	1.39
29	O	274	LMT	C1B-C2B	2.03	1.58	1.52
21	B	511	CLA	C4B-NB	2.03	1.40	1.37
21	C	486	CLA	OBD-CAD	2.02	1.26	1.22
28	A	375	DGD	C1G-C2G	2.02	1.57	1.50
30	D	361	SQD	O6-C44	-2.02	1.40	1.43
21	C	480	CLA	CBA-CGA	2.02	1.56	1.50
21	A	366	CLA	C5-C3	2.02	1.55	1.51
26	A	371	LHG	C3-C2	2.01	1.57	1.51
28	C	492	DGD	CDA-CCA	-2.01	1.39	1.51
22	D	355	PHO	C3D-CAD	-2.01	1.43	1.47
29	I	274	LMT	O5B-C5B	2.01	1.49	1.44
28	B	533	DGD	C2A-C1A	2.01	1.56	1.50
27	I	220	LMG	C1-C2	2.00	1.58	1.52

All (1197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	474	DGD	O1G-C1G-C2G	12.52	144.47	108.40
25	J	115	BCR	C32-C1-C6	-10.90	93.14	110.24
28	C	492	DGD	O5D-C1E-C2E	10.88	124.80	108.27
33	F	85	HEM	CMA-C3A-C4A	10.64	141.62	125.42
28	C	491	DGD	O5D-C1E-C2E	10.63	124.41	108.27
21	B	518	CLA	C4A-NA-C1A	10.22	111.34	106.68
28	D	362	DGD	O5D-C1E-C2E	10.13	123.66	108.27
25	J	115	BCR	C32-C1-C31	-10.06	79.83	108.63
28	C	493	DGD	O5D-C1E-C2E	10.02	123.49	108.27
33	V	164	HEM	CMA-C3A-C4A	9.71	140.21	125.42
27	D	359	LMG	C8-O7-C10	9.69	140.99	117.80
21	C	487	CLA	C4A-NA-C1A	9.66	111.09	106.68
21	B	525	CLA	C4A-NA-C1A	9.57	111.05	106.68
27	C	494	LMG	C8-O7-C10	9.46	140.44	117.80
28	C	474	DGD	O5D-C1E-C2E	9.31	122.41	108.27
21	C	477	CLA	C4A-NA-C1A	9.22	110.89	106.68
30	L	213	SQD	O5-C1-O6	9.19	131.75	110.04
21	B	516	CLA	C4A-NA-C1A	9.17	110.86	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	356	CLA	C4A-NA-C1A	9.15	110.86	106.68
21	A	366	CLA	C4A-NA-C1A	9.07	110.82	106.68
27	B	531	LMG	C8-O7-C10	8.94	139.20	117.80
28	A	375	DGD	C2G-O2G-C1B	8.92	139.15	117.80
21	C	479	CLA	C4A-NA-C1A	8.91	110.74	106.68
30	F	224	SQD	O5-C1-O6	8.86	130.97	110.04
21	C	488	CLA	C4A-NA-C1A	8.82	110.70	106.68
21	C	482	CLA	C4A-NA-C1A	8.82	110.70	106.68
32	D	357	PL9	C7-C8-C9	-8.78	111.71	126.83
33	F	85	HEM	CMA-C3A-C2A	-8.74	107.09	125.62
28	C	493	DGD	O5D-C6D-C5D	8.74	129.11	109.42
28	C	474	DGD	O6D-C5D-C6D	8.70	123.95	106.69
28	C	491	DGD	C2G-O2G-C1B	8.70	138.62	117.80
21	B	526	CLA	C4A-NA-C1A	8.67	110.64	106.68
21	C	485	CLA	C4A-NA-C1A	8.59	110.60	106.68
21	B	511	CLA	C4A-NA-C1A	8.55	110.58	106.68
28	C	493	DGD	O6D-C5D-C6D	8.54	123.63	106.69
21	B	513	CLA	C4A-NA-C1A	8.54	110.58	106.68
21	C	483	CLA	C4A-NA-C1A	8.38	110.50	106.68
32	D	357	PL9	C7-C3-C4	8.37	123.80	116.91
21	K	483	CLA	C4A-NA-C1A	8.35	110.49	106.68
27	I	220	LMG	C8-O7-C10	8.28	137.60	117.80
30	D	361	SQD	O5-C1-O6	8.25	129.54	110.04
21	A	364	CLA	C4A-NA-C1A	8.23	110.44	106.68
30	C	475	SQD	O5-C1-O6	8.20	129.41	110.04
21	A	362	CLA	C4A-NA-C1A	8.19	110.42	106.68
21	C	480	CLA	C4A-NA-C1A	8.15	110.39	106.68
28	C	474	DGD	O5D-C6D-C5D	8.12	127.71	109.42
21	C	484	CLA	C4A-NA-C1A	8.08	110.37	106.68
21	B	520	CLA	C4A-NA-C1A	8.08	110.36	106.68
21	B	522	CLA	C4A-NA-C1A	7.99	110.32	106.68
33	V	164	HEM	CMA-C3A-C2A	-7.91	108.84	125.62
28	C	493	DGD	C2G-O2G-C1B	7.88	136.66	117.80
21	C	486	CLA	C4A-NA-C1A	7.77	110.22	106.68
21	C	478	CLA	C4A-NA-C1A	7.75	110.21	106.68
21	B	515	CLA	C4A-NA-C1A	7.72	110.20	106.68
21	B	521	CLA	C4A-NA-C1A	7.71	110.20	106.68
21	B	519	CLA	C4A-NA-C1A	7.53	110.12	106.68
28	C	491	DGD	O6D-C5D-C6D	7.49	121.54	106.69
21	B	512	CLA	C4A-NA-C1A	7.35	110.03	106.68
30	C	475	SQD	O6-C1-C2	7.34	119.43	108.27
21	B	523	CLA	C4A-NA-C1A	7.34	110.03	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	363	CLA	C4A-NA-C1A	7.34	110.03	106.68
21	B	517	CLA	C4A-NA-C1A	7.29	110.00	106.68
28	C	492	DGD	O6D-C5D-C6D	7.20	120.97	106.69
30	D	361	SQD	O6-C1-C2	7.15	119.13	108.27
30	D	361	SQD	O7-S-C6	7.14	117.42	106.76
25	J	115	BCR	C2-C1-C6	7.13	120.79	110.44
28	D	362	DGD	C3G-O3G-C1D	-7.11	98.55	113.80
22	D	355	PHO	O2D-CGD-CBD	7.03	118.67	110.95
21	B	524	CLA	C4A-NA-C1A	7.03	109.88	106.68
28	B	533	DGD	O2G-C1B-C2B	7.00	126.63	111.48
30	L	213	SQD	O6-C1-C2	6.99	118.89	108.27
25	J	115	BCR	C32-C1-C2	-6.93	82.33	108.95
25	X	107	BCR	C38-C26-C25	6.93	132.04	124.48
28	C	474	DGD	C6D-C5D-C4D	-6.92	97.53	112.07
22	A	365	PHO	O2D-CGD-CBD	6.90	118.53	110.95
27	J	492	LMG	O7-C10-C11	6.89	126.39	111.48
21	C	481	CLA	C4A-NA-C1A	6.88	109.82	106.68
28	C	474	DGD	O1G-C1A-C2A	6.77	132.49	111.83
30	C	475	SQD	O7-S-C6	6.75	116.83	106.76
25	D	358	BCR	C38-C26-C25	6.73	131.82	124.48
28	C	474	DGD	O2G-C1B-C2B	6.66	125.88	111.48
27	B	531	LMG	C13-C12-C11	-6.63	88.78	113.13
30	L	213	SQD	O7-S-C6	6.62	116.64	106.76
21	D	354	CLA	C4A-NA-C1A	6.57	109.68	106.68
30	F	224	SQD	O7-S-C6	6.55	116.53	106.76
25	J	112	BCR	C33-C5-C6	6.55	131.63	124.48
25	A	369	BCR	C38-C26-C25	6.45	131.52	124.48
28	C	491	DGD	O5D-C6D-C5D	6.44	123.95	109.42
28	D	362	DGD	O5D-C6D-C5D	6.43	123.92	109.42
25	B	529	BCR	C38-C26-C25	6.42	131.49	124.48
25	J	115	BCR	C38-C26-C25	6.42	131.49	124.48
22	A	365	PHO	C4D-CHA-CBD	-6.38	105.39	108.45
27	B	531	LMG	C19-C18-C17	-6.36	82.22	114.37
28	C	493	DGD	C6D-O5D-C1E	-6.35	100.17	113.80
26	C	476	LHG	C25-C24-C23	6.32	136.87	113.69
28	C	492	DGD	C6D-O5D-C1E	-6.30	100.28	113.80
25	J	115	BCR	C33-C5-C6	6.29	131.35	124.48
25	B	529	BCR	C33-C5-C6	6.29	131.35	124.48
28	C	474	DGD	O3G-C1D-C2D	-6.28	98.74	108.27
28	C	493	DGD	C6D-C5D-C4D	-6.28	98.89	112.07
25	B	527	BCR	C38-C26-C25	6.27	131.33	124.48
30	F	224	SQD	O6-C1-C2	6.27	117.79	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	217	LMG	O7-C10-C11	6.27	125.03	111.48
30	F	224	SQD	C10-C9-C8	6.17	135.81	113.13
30	D	361	SQD	C10-C9-C8	6.16	135.77	113.13
28	C	474	DGD	O6D-C1D-O3G	6.15	124.58	110.04
25	B	527	BCR	C33-C5-C6	6.15	131.19	124.48
21	C	481	CLA	CAA-C2A-C1A	-6.15	91.83	111.97
26	A	371	LHG	C25-C24-C23	6.14	136.21	113.69
30	C	475	SQD	C10-C9-C8	6.12	135.62	113.13
28	C	493	DGD	C4B-C3B-C2B	-6.11	90.68	113.13
30	D	361	SQD	C25-C24-C23	6.10	136.06	113.69
21	A	364	CLA	C4D-C3D-CAD	6.08	114.71	108.11
25	Z	116	BCR	C38-C26-C25	6.06	131.10	124.48
27	D	359	LMG	C13-C12-C11	-6.06	90.85	113.13
21	B	514	CLA	C4A-NA-C1A	6.06	109.44	106.68
25	D	358	BCR	C33-C5-C6	6.06	131.09	124.48
28	C	492	DGD	O5D-C6D-C5D	6.05	123.05	109.42
32	D	357	PL9	C32-C33-C34	-6.03	113.82	127.62
30	L	213	SQD	C10-C9-C8	6.01	135.21	113.13
30	F	224	SQD	C25-C24-C23	6.00	135.67	113.69
28	D	362	DGD	O3G-C3G-C2G	5.94	125.28	110.82
30	L	213	SQD	C25-C24-C23	5.90	135.31	113.69
28	D	362	DGD	O6D-C5D-C6D	5.86	118.32	106.69
21	C	481	CLA	CBA-CAA-C2A	5.86	131.24	113.79
27	B	531	LMG	C17-C16-C15	-5.80	85.05	114.37
25	C	490	BCR	C33-C5-C6	5.76	130.77	124.48
25	C	489	BCR	C38-C26-C25	5.73	130.74	124.48
21	C	481	CLA	CAA-CBA-CGA	-5.71	96.99	113.21
21	C	482	CLA	C4D-C3D-CAD	5.67	114.27	108.11
25	J	115	BCR	C31-C1-C6	5.66	119.12	110.24
28	C	491	DGD	C1G-O1G-C1A	5.64	137.74	117.12
28	C	493	DGD	C3G-O3G-C1D	-5.64	101.70	113.80
21	C	480	CLA	CBA-CAA-C2A	5.64	130.57	113.79
21	C	481	CLA	C4D-C3D-CAD	5.61	114.20	108.11
25	B	530	BCR	C38-C26-C25	5.57	130.56	124.48
30	C	475	SQD	C25-C24-C23	5.56	134.07	113.69
28	C	491	DGD	O1G-C1G-C2G	-5.54	92.41	108.40
28	C	492	DGD	C6A-C5A-C4A	-5.54	86.37	114.37
28	C	492	DGD	O2G-C1B-C2B	5.51	123.39	111.48
28	C	492	DGD	C4A-C3A-C2A	-5.48	92.99	113.13
21	B	524	CLA	O2D-CGD-CBD	5.48	120.81	111.23
27	D	359	LMG	C7-O1-C1	-5.46	102.08	113.80
25	B	527	BCR	C8-C7-C6	5.44	141.54	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	375	DGD	O3G-C1D-C2D	-5.44	100.01	108.27
28	C	491	DGD	C4B-C3B-C2B	-5.43	93.17	113.13
29	D	536	LMT	C1B-O1B-C4'	-5.41	105.14	117.98
28	A	375	DGD	C6D-O5D-C1E	-5.37	102.29	113.80
32	D	357	PL9	C12-C13-C14	-5.37	115.34	127.62
25	J	115	BCR	C23-C24-C25	5.33	141.25	127.00
25	Z	116	BCR	C33-C5-C6	5.32	130.28	124.48
25	X	107	BCR	C15-C14-C13	5.28	134.69	127.28
21	B	517	CLA	C4D-C3D-CAD	5.28	113.84	108.11
21	C	483	CLA	C4D-C3D-CAD	5.27	113.83	108.11
21	B	511	CLA	O2D-CGD-CBD	5.26	120.43	111.23
27	I	220	LMG	C13-C12-C11	-5.25	93.84	113.13
21	A	362	CLA	C4D-C3D-CAD	5.23	113.78	108.11
33	F	85	HEM	CAD-C3D-C2D	5.20	137.62	127.87
25	A	369	BCR	C24-C23-C22	5.19	133.92	126.23
21	C	480	CLA	CAA-C2A-C1A	-5.17	95.05	111.97
28	C	474	DGD	C1G-O1G-C1A	-5.16	98.27	117.12
28	C	491	DGD	C6D-C5D-C4D	-5.16	101.24	112.07
27	B	531	LMG	C7-O1-C1	-5.14	102.77	113.80
25	A	369	BCR	C33-C5-C6	5.14	130.09	124.48
28	C	474	DGD	C6D-O5D-C1E	-5.13	102.79	113.80
28	A	375	DGD	O5D-C1E-C2E	5.12	116.05	108.27
25	C	490	BCR	C38-C26-C25	5.12	130.07	124.48
28	C	492	DGD	C6D-C5D-C4D	-5.11	101.35	112.07
32	D	357	PL9	C22-C23-C24	-5.10	115.94	127.62
21	D	354	CLA	C4D-C3D-CAD	5.09	113.64	108.11
27	D	359	LMG	O1-C7-C8	5.09	123.20	110.82
28	A	375	DGD	C6D-C5D-C4D	-5.09	101.39	112.07
21	B	513	CLA	C4D-C3D-CAD	5.08	113.63	108.11
25	B	530	BCR	C33-C5-C6	5.08	130.02	124.48
25	J	112	BCR	C38-C26-C25	5.07	130.02	124.48
21	B	511	CLA	C4D-C3D-CAD	5.07	113.61	108.11
32	D	357	PL9	C42-C43-C44	-5.06	116.05	127.62
21	B	518	CLA	CAA-C2A-C1A	-5.04	95.46	111.97
21	C	479	CLA	O2D-CGD-CBD	5.04	120.03	111.23
21	C	486	CLA	C3B-C4B-NB	-5.03	106.04	110.53
21	D	356	CLA	C4D-C3D-CAD	5.03	113.57	108.11
28	A	375	DGD	C4B-C3B-C2B	-4.98	94.84	113.13
21	B	525	CLA	C4D-C3D-CAD	4.97	113.50	108.11
21	A	366	CLA	C4D-C3D-CAD	4.97	113.50	108.11
21	B	520	CLA	C4D-C3D-CAD	4.97	113.50	108.11
21	C	484	CLA	C3B-C4B-NB	-4.95	106.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	V	164	HEM	C4A-C3A-C2A	-4.94	101.16	106.82
28	C	493	DGD	C1D-O6D-C5D	-4.92	104.10	113.72
32	D	357	PL9	C11-C9-C8	-4.92	110.12	121.17
25	X	107	BCR	C33-C5-C6	4.91	129.85	124.48
21	K	483	CLA	C4D-C3D-CAD	4.91	113.44	108.11
22	D	355	PHO	C4A-C3A-C2A	4.90	107.50	102.84
28	D	362	DGD	C6D-O5D-C1E	-4.88	103.33	113.80
21	B	524	CLA	C4D-C3D-CAD	4.88	113.41	108.11
21	B	517	CLA	C3B-C4B-NB	-4.87	106.18	110.53
21	C	487	CLA	C4D-C3D-CAD	4.84	113.37	108.11
21	C	479	CLA	C4D-C3D-CAD	4.84	113.36	108.11
28	C	474	DGD	C3G-O3G-C1D	4.84	124.17	113.80
28	A	375	DGD	C3G-O3G-C1D	4.84	124.17	113.80
21	B	519	CLA	C4D-C3D-CAD	4.84	113.36	108.11
28	C	474	DGD	C1D-O6D-C5D	-4.83	104.28	113.72
22	A	365	PHO	C3D-C4D-ND	4.82	113.88	107.71
21	B	524	CLA	CBA-CAA-C2A	4.81	128.10	113.79
28	C	492	DGD	C1D-O6D-C5D	-4.81	104.33	113.72
21	B	518	CLA	C4D-C3D-CAD	4.80	113.31	108.11
27	B	531	LMG	O7-C8-C7	4.79	125.52	108.34
21	B	516	CLA	C2A-C1A-CHA	4.78	132.16	123.87
25	J	112	BCR	C2-C1-C6	4.77	117.37	110.44
21	C	477	CLA	C4D-C3D-CAD	4.76	113.27	108.11
21	K	483	CLA	O2D-CGD-CBD	4.75	119.54	111.23
21	B	523	CLA	C3B-C4B-NB	-4.75	106.29	110.53
21	A	363	CLA	C4D-C3D-CAD	4.75	113.27	108.11
21	C	483	CLA	C3B-C4B-NB	-4.75	106.29	110.53
25	B	530	BCR	C7-C8-C9	4.75	133.26	126.23
21	C	488	CLA	C3B-C4B-NB	-4.74	106.30	110.53
21	C	482	CLA	C3B-C4B-NB	-4.73	106.31	110.53
22	D	355	PHO	C4D-CHA-CBD	-4.73	106.19	108.45
21	C	480	CLA	C4D-C3D-CAD	4.71	113.22	108.11
22	A	365	PHO	C4A-C3A-C2A	4.70	107.31	102.84
30	L	213	SQD	C44-O6-C1	4.70	123.87	113.80
21	C	488	CLA	C3A-C2A-C1A	4.68	108.35	101.34
22	D	355	PHO	C3D-C4D-ND	4.67	113.69	107.71
25	J	115	BCR	C8-C7-C6	4.66	139.45	127.00
30	F	224	SQD	O8-S-C6	-4.66	96.97	105.97
27	B	531	LMG	C22-C21-C20	-4.66	90.81	114.37
21	B	514	CLA	C4D-C3D-CAD	4.66	113.17	108.11
27	B	531	LMG	C9-C8-C7	-4.65	100.95	111.78
25	J	115	BCR	C1-C6-C5	-4.64	116.29	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	494	LMG	C9-O8-C28	4.63	134.05	117.12
25	C	489	BCR	C24-C23-C22	4.61	133.06	126.23
28	C	492	DGD	C3G-O3G-C1D	-4.60	103.94	113.80
21	B	522	CLA	C3B-C4B-NB	-4.58	106.44	110.53
21	C	488	CLA	C4D-C3D-CAD	4.58	113.08	108.11
21	B	521	CLA	CBA-CAA-C2A	4.58	127.41	113.79
28	C	492	DGD	C8A-C7A-C6A	-4.57	91.25	114.37
28	C	474	DGD	O3G-C3G-C2G	-4.55	99.74	110.82
21	C	478	CLA	C4D-C3D-CAD	4.55	113.05	108.11
25	X	107	BCR	C12-C13-C14	-4.55	111.86	119.01
21	B	516	CLA	C4D-C3D-CAD	4.54	113.04	108.11
21	B	521	CLA	C4D-C3D-CAD	4.54	113.04	108.11
21	A	363	CLA	CBA-CAA-C2A	4.54	127.31	113.79
25	X	107	BCR	C29-C30-C25	4.54	117.03	110.44
33	V	164	HEM	CHA-C4D-C3D	-4.54	116.86	125.23
21	B	520	CLA	O2D-CGD-CBD	4.52	119.13	111.23
21	B	513	CLA	C3B-C4B-NB	-4.51	106.50	110.53
28	C	493	DGD	O6E-C1E-O5D	4.50	120.67	110.04
27	D	359	LMG	C9-C8-C7	4.49	122.27	111.78
21	C	485	CLA	C4D-C3D-CAD	4.49	112.99	108.11
33	F	85	HEM	C4A-C3A-C2A	-4.49	101.68	106.82
28	D	362	DGD	C1G-O1G-C1A	4.47	133.47	117.12
28	B	533	DGD	O6D-C5D-C6D	4.47	115.56	106.69
21	B	524	CLA	C3B-C4B-NB	-4.46	106.55	110.53
21	A	363	CLA	O2D-CGD-CBD	4.45	119.01	111.23
21	B	512	CLA	C4D-C3D-CAD	4.45	112.94	108.11
27	B	531	LMG	C15-C14-C13	-4.44	91.91	114.37
21	B	518	CLA	CBA-CAA-C2A	4.44	127.00	113.79
21	C	487	CLA	C2A-C1A-CHA	4.44	131.57	123.87
21	C	480	CLA	O2D-CGD-CBD	4.44	118.98	111.23
21	C	481	CLA	C3B-C4B-NB	-4.43	106.57	110.53
28	C	474	DGD	C3G-C2G-C1G	4.43	122.12	111.78
21	B	525	CLA	C3B-C4B-NB	-4.43	106.58	110.53
28	C	493	DGD	O6D-C5D-C4D	4.43	117.68	109.70
28	C	491	DGD	C4A-C3A-C2A	-4.43	96.86	113.13
32	D	357	PL9	C3-C4-C5	4.42	124.08	118.57
33	V	164	HEM	CHA-C4D-ND	4.41	129.82	124.37
21	A	366	CLA	C3B-C4B-NB	-4.40	106.60	110.53
21	C	477	CLA	C3A-C2A-C1A	4.40	107.93	101.34
25	J	112	BCR	C11-C10-C9	4.39	133.44	127.28
25	C	490	BCR	C24-C23-C22	4.39	132.72	126.23
21	C	479	CLA	C1-C2-C3	4.38	133.37	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	533	DGD	O5D-C1E-C2E	4.37	114.91	108.27
21	C	484	CLA	C4D-C3D-CAD	4.37	112.85	108.11
29	D	363	LMT	C1-O1'-C1'	4.36	121.13	113.68
29	D	363	LMT	C1B-O1B-C4'	-4.36	107.65	117.98
21	B	517	CLA	C11-C10-C8	4.36	130.44	115.97
21	B	515	CLA	C3B-C4B-NB	-4.35	106.65	110.53
33	V	164	HEM	C1B-NB-C4B	4.34	110.35	105.21
21	B	515	CLA	C4D-C3D-CAD	4.34	112.82	108.11
21	D	354	CLA	C3B-C4B-NB	-4.33	106.66	110.53
21	K	483	CLA	C3B-C4B-NB	-4.33	106.67	110.53
21	B	513	CLA	C2A-C1A-CHA	4.31	131.35	123.87
28	C	491	DGD	C6D-O5D-C1E	-4.31	104.55	113.80
21	C	485	CLA	C3B-C4B-NB	-4.31	106.69	110.53
32	D	357	PL9	C10-C9-C8	-4.30	112.59	123.63
21	B	526	CLA	C4D-C3D-CAD	4.29	112.77	108.11
27	D	359	LMG	O7-C8-C7	4.28	123.71	108.34
21	B	517	CLA	O2D-CGD-CBD	4.27	118.69	111.23
25	Z	116	BCR	C29-C30-C25	4.26	116.62	110.44
25	J	112	BCR	C7-C8-C9	4.25	132.52	126.23
28	A	375	DGD	O6D-C1D-O3G	4.24	120.06	110.04
27	C	494	LMG	C13-C12-C11	-4.23	97.57	113.13
21	C	487	CLA	C3B-C4B-NB	-4.23	106.75	110.53
32	D	357	PL9	C46-C47-C48	4.22	132.92	112.02
21	D	356	CLA	O2D-CGD-CBD	4.22	118.61	111.23
21	B	521	CLA	CAA-C2A-C1A	-4.22	98.15	111.97
21	B	526	CLA	C3B-C4B-NB	-4.22	106.77	110.53
28	C	474	DGD	C3A-C2A-C1A	-4.21	98.26	113.69
33	F	85	HEM	CHA-C4D-ND	4.21	129.58	124.37
21	A	364	CLA	C3B-C4B-NB	-4.21	106.78	110.53
27	B	531	LMG	C18-C17-C16	4.20	135.58	114.37
25	C	490	BCR	C29-C30-C25	4.19	116.53	110.44
32	D	357	PL9	C7-C3-C2	-4.19	118.45	123.39
27	D	359	LMG	O8-C9-C8	-4.19	96.31	108.40
30	L	213	SQD	O8-S-C6	-4.19	97.88	105.97
25	D	358	BCR	C24-C23-C22	4.19	132.43	126.23
33	F	85	HEM	CHA-C4D-C3D	-4.19	117.50	125.23
25	X	107	BCR	C8-C7-C6	4.19	138.18	127.00
25	J	112	BCR	C23-C24-C25	4.18	138.17	127.00
30	F	224	SQD	C11-C10-C9	4.18	135.49	114.37
21	B	522	CLA	C4D-C3D-CAD	4.18	112.64	108.11
21	B	523	CLA	C4D-C3D-CAD	4.18	112.64	108.11
25	X	107	BCR	C30-C25-C26	-4.16	116.95	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	376	LMT	O1B-C1B-C2B	4.16	118.33	108.09
21	C	486	CLA	C4D-C3D-CAD	4.15	112.61	108.11
21	D	354	CLA	O2D-CGD-CBD	4.13	118.45	111.23
25	D	358	BCR	C2-C1-C6	4.12	116.43	110.44
27	I	220	LMG	C9-C8-C7	-4.10	102.22	111.78
28	B	533	DGD	O6E-C1E-O5D	4.09	119.71	110.04
21	C	483	CLA	O2D-CGD-CBD	4.09	118.38	111.23
27	C	494	LMG	O1-C7-C8	-4.08	100.90	110.82
21	A	363	CLA	C3B-C4B-NB	-4.07	106.90	110.53
32	D	357	PL9	C20-C19-C21	4.06	122.28	115.23
21	B	518	CLA	O2D-CGD-CBD	4.06	118.32	111.23
25	J	115	BCR	C38-C26-C27	-4.05	104.96	113.60
28	B	533	DGD	O1G-C1A-C2A	4.05	124.19	111.83
21	D	356	CLA	C3B-C4B-NB	-4.05	106.92	110.53
21	B	525	CLA	C2A-C1A-CHA	4.03	130.86	123.87
25	B	527	BCR	C29-C30-C25	4.03	116.29	110.44
21	C	486	CLA	CBA-CAA-C2A	4.02	125.75	113.79
30	C	475	SQD	O48-C23-C24	4.02	124.08	111.83
21	B	516	CLA	C3A-C2A-C1A	4.02	107.35	101.34
21	B	512	CLA	C3B-C4B-NB	-4.01	106.95	110.53
21	A	362	CLA	C3B-C4B-NB	-4.01	106.95	110.53
21	C	487	CLA	C2A-C3A-C4A	4.00	108.33	101.87
21	C	480	CLA	C3A-C2A-C1A	4.00	107.33	101.34
21	C	485	CLA	C2A-C1A-CHA	3.99	130.80	123.87
32	D	357	PL9	C15-C14-C16	3.98	122.13	115.23
25	J	112	BCR	C29-C30-C25	3.98	116.22	110.44
21	B	525	CLA	O2D-CGD-CBD	3.98	118.18	111.23
21	C	480	CLA	C3B-C4B-NB	-3.98	106.98	110.53
25	X	107	BCR	C38-C26-C27	-3.95	105.17	113.60
21	A	363	CLA	C1-C2-C3	3.95	132.67	126.20
32	D	357	PL9	C30-C29-C31	3.95	122.08	115.23
21	B	516	CLA	C3B-C4B-NB	-3.94	107.02	110.53
30	F	224	SQD	O48-C23-C24	3.93	123.83	111.83
28	C	493	DGD	C6B-C5B-C4B	-3.93	94.49	114.37
21	A	366	CLA	O2D-CGD-CBD	3.93	118.10	111.23
25	B	529	BCR	C33-C5-C4	-3.92	105.23	113.60
33	V	164	HEM	CAD-C3D-C2D	3.92	135.21	127.87
21	C	486	CLA	C1-C2-C3	3.92	132.61	126.20
28	C	492	DGD	O2G-C2G-C1G	3.91	122.38	108.34
28	B	533	DGD	C3A-C2A-C1A	-3.91	99.36	113.69
21	B	526	CLA	C1-C2-C3	3.91	132.60	126.20
21	K	483	CLA	C1-C2-C3	3.90	132.59	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	364	CLA	C2A-C1A-CHA	3.90	130.64	123.87
28	D	362	DGD	C6D-C5D-C4D	-3.90	103.88	112.07
21	C	477	CLA	O2D-CGD-CBD	3.90	118.05	111.23
30	D	361	SQD	C44-O6-C1	3.90	122.15	113.80
21	C	480	CLA	CAA-CBA-CGA	-3.90	102.15	113.21
25	B	527	BCR	C2-C1-C6	3.89	116.09	110.44
25	B	530	BCR	C29-C30-C25	3.89	116.09	110.44
21	C	481	CLA	C3A-C2A-C1A	3.89	107.17	101.34
33	F	85	HEM	C4B-C3B-C2B	-3.89	103.70	107.28
27	M	217	LMG	C9-O8-C28	3.89	131.33	117.12
21	A	362	CLA	O2D-CGD-CBD	3.88	118.02	111.23
25	C	489	BCR	C33-C5-C6	3.88	128.72	124.48
25	D	358	BCR	C38-C26-C27	-3.88	105.33	113.60
25	B	530	BCR	C23-C24-C25	3.87	137.34	127.00
30	D	361	SQD	C11-C10-C9	3.87	133.93	114.37
21	C	487	CLA	O2D-CGD-CBD	3.87	117.99	111.23
27	I	220	LMG	O7-C8-C7	3.87	122.21	108.34
25	X	107	BCR	C2-C1-C6	3.86	116.05	110.44
27	B	531	LMG	C20-C19-C18	3.86	133.89	114.37
21	C	482	CLA	CBA-CAA-C2A	3.86	125.28	113.79
25	B	527	BCR	C16-C17-C18	3.86	132.69	127.28
21	B	514	CLA	C3B-C4B-NB	-3.86	107.09	110.53
21	C	478	CLA	O2D-CGD-CBD	3.85	117.96	111.23
21	B	518	CLA	C3A-C2A-C1A	3.85	107.10	101.34
25	D	358	BCR	C1-C6-C5	-3.84	117.39	122.64
25	J	115	BCR	C29-C30-C25	3.83	116.00	110.44
28	D	362	DGD	C3G-C2G-C1G	3.82	120.69	111.78
21	B	515	CLA	CBA-CAA-C2A	3.82	125.16	113.79
21	C	488	CLA	CAA-CBA-CGA	-3.81	102.38	113.21
21	C	478	CLA	C3B-C4B-NB	-3.80	107.13	110.53
32	D	357	PL9	C35-C34-C36	3.80	121.83	115.23
22	A	365	PHO	C1A-C2A-C3A	3.80	106.45	102.84
21	B	519	CLA	CBA-CAA-C2A	3.80	125.10	113.79
30	L	213	SQD	C11-C10-C9	3.80	133.57	114.37
28	D	362	DGD	C2G-O2G-C1B	3.80	126.88	117.80
21	B	521	CLA	C3B-C4B-NB	-3.79	107.15	110.53
21	B	517	CLA	C1-C2-C3	3.79	132.40	126.20
21	B	515	CLA	CAA-C2A-C1A	-3.78	99.59	111.97
21	A	366	CLA	C2A-C1A-CHA	3.77	130.42	123.87
27	A	373	LMG	O7-C10-C11	3.77	119.64	111.48
28	C	474	DGD	O6E-C1E-O5D	3.77	118.95	110.04
30	D	361	SQD	O8-S-C6	-3.77	98.69	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	528	DGD	O2G-C1B-C2B	3.77	119.63	111.48
21	C	477	CLA	C2A-C1A-CHA	3.76	130.40	123.87
25	J	112	BCR	C33-C5-C4	-3.76	105.58	113.60
28	A	375	DGD	O5D-C6D-C5D	3.75	117.87	109.42
29	D	536	LMT	O1'-C1-C2	-3.73	96.70	109.37
27	D	360	LMG	O7-C10-C11	3.73	119.55	111.48
25	Z	116	BCR	C23-C24-C25	3.73	136.96	127.00
21	B	513	CLA	C2A-C3A-C4A	3.73	107.89	101.87
21	B	519	CLA	C1-C2-C3	3.72	132.30	126.20
21	B	526	CLA	O2D-CGD-CBD	3.72	117.74	111.23
28	D	362	DGD	O2G-C1B-C2B	3.72	119.53	111.48
21	C	487	CLA	C1-C2-C3	3.71	132.28	126.20
30	C	475	SQD	C31-C30-C29	3.71	133.12	114.37
25	A	369	BCR	C38-C26-C27	-3.71	105.69	113.60
30	C	475	SQD	C11-C10-C9	3.71	133.11	114.37
30	C	475	SQD	C44-O6-C1	3.71	121.75	113.80
25	B	530	BCR	C2-C1-C6	3.71	115.82	110.44
25	C	489	BCR	C29-C30-C25	3.70	115.82	110.44
21	B	511	CLA	C2A-C3A-C4A	3.70	107.85	101.87
21	B	519	CLA	C3B-C4B-NB	-3.70	107.23	110.53
21	B	517	CLA	C3A-C2A-C1A	3.68	106.85	101.34
30	C	475	SQD	O8-S-C6	-3.67	98.88	105.97
21	B	513	CLA	C3A-C2A-C1A	3.67	106.84	101.34
29	O	274	LMT	C3B-C4B-C5B	3.66	116.88	110.23
25	C	489	BCR	C38-C26-C27	-3.66	105.78	113.60
25	D	358	BCR	C29-C30-C25	3.66	115.76	110.44
21	B	515	CLA	O2D-CGD-CBD	3.66	117.63	111.23
21	B	518	CLA	C2A-C3A-C4A	3.66	107.78	101.87
32	D	357	PL9	C25-C24-C26	3.66	121.58	115.23
25	B	529	BCR	C29-C30-C25	3.65	115.75	110.44
26	A	371	LHG	O8-C23-C24	3.65	122.97	111.83
21	B	518	CLA	C3B-C4B-NB	-3.65	107.27	110.53
21	C	477	CLA	C3B-C4B-NB	-3.64	107.28	110.53
27	I	220	LMG	C12-C11-C10	3.63	127.00	113.69
25	D	358	BCR	C33-C5-C4	-3.63	105.86	113.60
25	B	529	BCR	C38-C26-C27	-3.62	105.89	113.60
29	B	535	LMT	C3B-C4B-C5B	3.62	116.79	110.23
27	B	531	LMG	C38-C37-C36	3.61	132.64	114.37
25	C	490	BCR	C8-C7-C6	3.61	136.63	127.00
21	C	479	CLA	C3B-C4B-NB	-3.61	107.31	110.53
27	I	220	LMG	C15-C14-C13	-3.60	96.16	114.37
27	D	359	LMG	C9-O8-C28	3.60	130.28	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	112	BCR	C30-C25-C26	-3.60	117.72	122.64
25	J	115	BCR	C33-C5-C4	-3.59	105.94	113.60
21	B	512	CLA	O2D-CGD-CBD	3.59	117.50	111.23
29	A	376	LMT	C3B-C4B-C5B	3.59	116.73	110.23
28	C	492	DGD	C3G-C2G-C1G	-3.58	103.43	111.78
32	D	357	PL9	C20-C19-C18	-3.58	114.43	123.63
25	J	112	BCR	C8-C9-C10	-3.58	113.38	119.01
29	I	274	LMT	C3B-C4B-C5B	3.58	116.72	110.23
21	C	479	CLA	CBA-CAA-C2A	3.58	124.43	113.79
27	J	492	LMG	C38-C37-C36	3.57	132.44	114.37
21	A	364	CLA	CBA-CAA-C2A	3.57	124.42	113.79
33	F	85	HEM	CAD-C3D-C4D	-3.57	118.48	124.70
25	B	530	BCR	C33-C5-C4	-3.57	105.99	113.60
33	V	164	HEM	C3B-C4B-NB	-3.57	106.91	109.47
28	B	533	DGD	C1D-O6D-C5D	-3.56	106.76	113.72
25	Z	116	BCR	C8-C7-C6	3.55	136.49	127.00
28	C	492	DGD	O6D-C5D-C4D	3.55	116.10	109.70
25	D	358	BCR	C30-C25-C26	-3.55	117.78	122.64
30	F	224	SQD	C44-O6-C1	3.55	121.41	113.80
21	B	522	CLA	C3A-C2A-C1A	3.55	106.65	101.34
21	C	488	CLA	C2A-C1A-CHA	3.55	130.02	123.87
25	C	490	BCR	C33-C5-C4	-3.55	106.04	113.60
27	J	492	LMG	C8-O7-C10	3.54	126.27	117.80
27	C	494	LMG	O7-C8-C7	3.54	121.04	108.34
25	B	530	BCR	C30-C25-C26	-3.54	117.80	122.64
25	A	369	BCR	C30-C25-C26	-3.54	117.80	122.64
25	J	112	BCR	C1-C6-C5	-3.53	117.81	122.64
21	C	478	CLA	C3A-C2A-C1A	3.53	106.63	101.34
30	L	213	SQD	O48-C23-C24	3.53	122.59	111.83
25	C	490	BCR	C23-C22-C21	-3.53	113.46	119.01
21	B	513	CLA	O2D-CGD-CBD	3.53	117.39	111.23
21	B	519	CLA	C3A-C2A-C1A	3.52	106.61	101.34
26	C	476	LHG	O7-C7-C8	3.52	119.10	111.48
21	B	516	CLA	CBA-CAA-C2A	3.52	124.26	113.79
25	B	527	BCR	C33-C5-C4	-3.52	106.10	113.60
25	A	369	BCR	C29-C30-C25	3.50	115.53	110.44
21	B	526	CLA	C2A-C1A-CHA	3.50	129.95	123.87
21	B	520	CLA	C2A-C3A-C4A	3.50	107.53	101.87
27	D	359	LMG	C12-C11-C10	3.50	126.50	113.69
27	B	531	LMG	C12-C11-C10	3.48	126.46	113.69
21	B	517	CLA	C2A-C1A-CHA	3.48	129.91	123.87
28	A	375	DGD	O6D-C5D-C6D	3.48	113.59	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	362	CLA	C2A-C3A-C4A	3.48	107.49	101.87
27	D	360	LMG	C8-O7-C10	-3.48	109.47	117.80
29	D	536	LMT	C3B-C4B-C5B	3.48	116.54	110.23
30	D	361	SQD	O48-C23-C24	3.48	122.44	111.83
21	C	483	CLA	C2A-C1A-CHA	3.48	129.90	123.87
28	C	491	DGD	C3G-O3G-C1D	-3.47	106.35	113.80
27	C	494	LMG	C38-C37-C36	3.47	131.93	114.37
21	C	484	CLA	C1-C2-C3	3.47	131.89	126.20
21	B	525	CLA	C2A-C3A-C4A	3.47	107.48	101.87
21	C	485	CLA	C3A-C2A-C1A	3.47	106.54	101.34
21	B	526	CLA	C2A-C3A-C4A	3.47	107.47	101.87
22	A	365	PHO	C4D-ND-C1D	-3.47	104.72	108.87
21	C	484	CLA	C3A-C2A-C1A	3.46	106.53	101.34
28	B	528	DGD	C2G-O2G-C1B	-3.46	109.50	117.80
27	J	492	LMG	C12-C11-C10	-3.46	101.00	113.69
21	A	366	CLA	C3A-C2A-C1A	3.46	106.53	101.34
27	A	373	LMG	C8-O7-C10	-3.46	109.51	117.80
21	D	356	CLA	C2A-C3A-C4A	3.46	107.46	101.87
21	B	526	CLA	C3A-C2A-C1A	3.45	106.51	101.34
21	B	521	CLA	O2D-CGD-CBD	3.45	117.27	111.23
21	C	479	CLA	C2A-C3A-C4A	3.45	107.44	101.87
25	J	115	BCR	C30-C25-C26	-3.45	117.92	122.64
27	B	531	LMG	C16-C15-C14	3.45	131.80	114.37
25	X	107	BCR	C16-C17-C18	3.45	132.11	127.28
21	K	483	CLA	C3A-C2A-C1A	3.44	106.50	101.34
25	X	107	BCR	C35-C13-C12	3.44	123.34	118.09
21	D	354	CLA	C12-C11-C10	-3.44	97.88	113.28
21	B	524	CLA	CAA-C2A-C1A	-3.43	100.72	111.97
29	D	363	LMT	C3B-C4B-C5B	3.43	116.45	110.23
21	A	363	CLA	CAA-C2A-C1A	-3.43	100.73	111.97
21	C	481	CLA	O2D-CGD-CBD	3.42	117.21	111.23
29	O	274	LMT	O1'-C1-C2	-3.42	97.76	109.37
25	B	527	BCR	C38-C26-C27	-3.42	106.30	113.60
21	B	515	CLA	C3A-C2A-C1A	3.42	106.46	101.34
25	D	358	BCR	C23-C24-C25	3.41	136.11	127.00
29	B	535	LMT	C1-O1'-C1'	-3.41	107.86	113.68
21	B	518	CLA	CAA-CBA-CGA	-3.41	103.54	113.21
25	C	490	BCR	C2-C1-C6	3.39	115.37	110.44
21	C	486	CLA	CAA-C2A-C1A	-3.39	100.86	111.97
21	D	356	CLA	C2A-C1A-CHA	3.39	129.75	123.87
21	C	478	CLA	C2A-C3A-C4A	3.38	107.33	101.87
25	B	529	BCR	C8-C7-C6	3.38	136.03	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	527	BCR	C12-C13-C14	-3.38	113.69	119.01
21	C	484	CLA	O2D-CGD-CBD	3.38	117.14	111.23
21	C	488	CLA	C1-C2-C3	3.37	131.72	126.20
21	B	517	CLA	C2A-C3A-C4A	3.37	107.32	101.87
33	F	85	HEM	C1B-NB-C4B	3.37	109.20	105.21
21	B	519	CLA	O2D-CGD-CBD	3.37	117.12	111.23
33	V	164	HEM	CBA-CAA-C2A	3.37	121.85	112.53
25	Z	116	BCR	C16-C17-C18	3.37	132.00	127.28
25	C	489	BCR	C35-C13-C12	3.36	123.23	118.09
21	C	484	CLA	CBA-CAA-C2A	3.36	123.80	113.79
22	A	365	PHO	O1D-CGD-CBD	-3.36	119.63	124.72
21	D	356	CLA	CBA-CAA-C2A	3.35	123.77	113.79
21	A	364	CLA	C3A-C2A-C1A	3.35	106.35	101.34
21	A	364	CLA	C2A-C3A-C4A	3.34	107.27	101.87
21	C	484	CLA	CAA-C2A-C1A	-3.34	101.02	111.97
25	X	107	BCR	C23-C24-C25	3.34	135.93	127.00
21	C	477	CLA	CAA-C2A-C1A	-3.34	101.03	111.97
21	A	364	CLA	O2D-CGD-CBD	3.34	117.06	111.23
21	C	482	CLA	C2A-C3A-C4A	3.33	107.25	101.87
28	C	492	DGD	O6E-C1E-O5D	3.33	117.92	110.04
28	A	375	DGD	O2G-C2G-C3G	3.33	120.30	108.34
25	B	529	BCR	C23-C24-C25	3.32	135.88	127.00
21	B	524	CLA	C2A-C3A-C4A	3.32	107.24	101.87
25	Z	116	BCR	C33-C5-C4	-3.32	106.51	113.60
25	C	490	BCR	C38-C26-C27	-3.32	106.52	113.60
21	A	362	CLA	C3A-C2A-C1A	3.32	106.31	101.34
21	B	515	CLA	C2A-C3A-C4A	3.32	107.23	101.87
21	K	483	CLA	C2A-C3A-C4A	3.31	107.22	101.87
21	B	525	CLA	C3A-C2A-C1A	3.31	106.30	101.34
28	A	375	DGD	C3G-C2G-C1G	-3.31	104.07	111.78
25	X	107	BCR	C1-C6-C5	-3.31	118.12	122.64
21	B	516	CLA	C2A-C3A-C4A	3.30	107.20	101.87
21	B	519	CLA	C2A-C1A-CHA	3.30	129.59	123.87
25	D	358	BCR	C8-C7-C6	3.29	135.80	127.00
27	J	492	LMG	C14-C13-C12	-3.29	97.72	114.37
21	A	363	CLA	C3A-C2A-C1A	3.29	106.27	101.34
21	D	354	CLA	C2A-C3A-C4A	3.29	107.19	101.87
21	B	521	CLA	C2A-C3A-C4A	3.29	107.18	101.87
33	F	85	HEM	CBC-CAC-C3C	-3.29	111.09	127.53
27	B	531	LMG	O1-C7-C8	3.29	118.81	110.82
21	A	363	CLA	C2A-C3A-C4A	3.28	107.17	101.87
21	C	477	CLA	C2A-C3A-C4A	3.28	107.17	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	524	CLA	C1-C2-C3	3.28	131.57	126.20
29	T	226	LMT	C3B-C4B-C5B	3.28	116.18	110.23
21	C	482	CLA	CED-O2D-CGD	3.27	123.33	115.92
28	C	493	DGD	O1G-C1G-C2G	-3.27	98.97	108.40
25	C	489	BCR	C2-C1-C6	3.27	115.18	110.44
21	C	483	CLA	C1-C2-C3	3.26	131.55	126.20
21	B	522	CLA	CED-O2D-CGD	3.26	123.32	115.92
25	B	530	BCR	C24-C23-C22	3.26	131.06	126.23
21	C	479	CLA	O1D-CGD-CBD	-3.26	118.09	124.52
21	B	522	CLA	C2A-C1A-CHA	3.26	129.53	123.87
21	B	519	CLA	CAA-CBA-CGA	-3.25	103.97	113.21
25	B	529	BCR	C2-C1-C6	3.25	115.16	110.44
28	A	375	DGD	C6B-C5B-C4B	-3.24	97.98	114.37
21	C	481	CLA	C2A-C3A-C4A	3.24	107.11	101.87
21	B	514	CLA	C2A-C3A-C4A	3.24	107.10	101.87
21	A	366	CLA	C2A-C3A-C4A	3.24	107.10	101.87
21	C	484	CLA	CED-O2D-CGD	3.24	123.26	115.92
26	C	476	LHG	O8-C23-C24	3.24	121.71	111.83
28	C	474	DGD	O2G-C2G-C1G	3.24	119.96	108.34
25	X	107	BCR	C24-C23-C22	3.24	131.03	126.23
21	D	356	CLA	C3A-C2A-C1A	3.23	106.18	101.34
21	B	520	CLA	C3B-C4B-NB	-3.22	107.66	110.53
25	C	490	BCR	C30-C25-C26	-3.22	118.24	122.64
21	B	516	CLA	CED-O2D-CGD	3.21	123.20	115.92
28	C	474	DGD	O1G-C1A-O1A	-3.20	115.62	123.63
27	I	220	LMG	C17-C16-C15	-3.19	98.22	114.37
25	A	369	BCR	C33-C5-C4	-3.19	106.79	113.60
28	C	491	DGD	C3B-C2B-C1B	3.19	125.36	113.69
21	C	486	CLA	C3A-C2A-C1A	3.18	106.11	101.34
25	B	527	BCR	C35-C13-C12	3.18	122.95	118.09
25	B	530	BCR	C1-C6-C5	-3.18	118.29	122.64
21	C	478	CLA	CBA-CAA-C2A	3.18	123.26	113.79
21	B	521	CLA	C3A-C2A-C1A	3.18	106.09	101.34
21	C	485	CLA	C2A-C3A-C4A	3.17	107.00	101.87
25	B	527	BCR	C30-C25-C26	-3.17	118.30	122.64
21	C	486	CLA	C2A-C3A-C4A	3.17	106.99	101.87
29	O	274	LMT	C1-O1'-C1'	3.17	119.09	113.68
21	C	483	CLA	C2A-C3A-C4A	3.17	106.99	101.87
21	B	512	CLA	C2A-C3A-C4A	3.17	106.98	101.87
21	C	483	CLA	C3A-C2A-C1A	3.16	106.08	101.34
25	J	112	BCR	C24-C23-C22	3.16	130.91	126.23
25	B	530	BCR	C38-C26-C27	-3.16	106.86	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	116	BCR	C38-C26-C27	-3.16	106.87	113.60
21	B	524	CLA	O1D-CGD-CBD	-3.15	118.30	124.52
21	B	511	CLA	C3B-C4B-NB	-3.15	107.72	110.53
28	C	491	DGD	C6B-C5B-C4B	-3.15	98.44	114.37
25	C	489	BCR	C1-C6-C5	-3.15	118.33	122.64
25	J	112	BCR	C30-C25-C24	3.15	124.18	115.65
25	J	112	BCR	C38-C26-C27	-3.14	106.89	113.60
28	D	362	DGD	O6D-C5D-C4D	3.14	115.36	109.70
27	I	220	LMG	O8-C28-C29	3.14	121.42	111.83
21	B	514	CLA	CBA-CAA-C2A	3.14	123.13	113.79
25	Z	116	BCR	C2-C1-C6	3.14	115.00	110.44
25	B	527	BCR	C23-C24-C25	3.14	135.37	127.00
21	B	523	CLA	O2D-CGD-CBD	3.13	116.71	111.23
25	C	490	BCR	C1-C6-C5	-3.12	118.38	122.64
25	B	527	BCR	C1-C6-C5	-3.12	118.38	122.64
25	C	489	BCR	C30-C25-C26	-3.12	118.38	122.64
21	C	482	CLA	C3A-C2A-C1A	3.11	106.00	101.34
29	D	536	LMT	C4-C3-C2	-3.11	98.62	114.37
25	Z	116	BCR	C30-C25-C26	-3.11	118.38	122.64
21	B	516	CLA	C1-C2-C3	3.11	131.29	126.20
25	X	107	BCR	C33-C5-C4	-3.11	106.97	113.60
33	V	164	HEM	CAB-C3B-C2B	-3.11	118.33	128.43
21	B	520	CLA	C3A-C2A-C1A	3.11	105.99	101.34
21	K	483	CLA	C2A-C1A-CHA	3.10	129.25	123.87
28	C	492	DGD	C5A-C4A-C3A	3.10	130.04	114.37
27	D	359	LMG	C15-C14-C13	-3.10	98.70	114.37
30	D	361	SQD	C3-C4-C5	-3.10	104.62	110.23
21	B	519	CLA	C2A-C3A-C4A	3.10	106.87	101.87
30	C	475	SQD	C3-C4-C5	-3.10	104.62	110.23
28	A	375	DGD	O6D-C5D-C4D	-3.09	104.12	109.70
30	D	361	SQD	O9-S-C6	-3.09	102.15	106.76
25	C	489	BCR	C32-C1-C6	3.09	115.08	110.24
21	B	520	CLA	C1-C2-C3	3.08	131.25	126.20
21	C	479	CLA	CAA-C2A-C1A	-3.08	101.88	111.97
30	F	224	SQD	C45-O47-C7	3.08	125.16	117.80
21	B	518	CLA	C11-C10-C8	3.08	126.19	115.97
21	B	514	CLA	O2D-CGD-CBD	3.08	116.61	111.23
28	A	375	DGD	C3B-C2B-C1B	3.07	124.96	113.69
21	C	482	CLA	O2D-CGD-CBD	3.07	116.60	111.23
25	B	529	BCR	C1-C6-C5	-3.06	118.45	122.64
30	D	361	SQD	C45-O47-C7	3.06	125.11	117.80
27	B	531	LMG	C21-C20-C19	3.05	129.81	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	523	CLA	C3A-C2A-C1A	3.05	105.91	101.34
27	C	494	LMG	C31-C30-C29	-3.05	101.93	113.13
28	C	474	DGD	O1A-C1A-C2A	-3.05	111.86	123.78
21	C	485	CLA	CED-O2D-CGD	3.05	122.83	115.92
25	B	529	BCR	C21-C20-C19	3.05	132.02	123.20
21	B	512	CLA	C3A-C2A-C1A	3.04	105.90	101.34
21	B	511	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
32	D	357	PL9	C35-C34-C33	-3.03	115.84	123.63
21	B	516	CLA	CAA-CBA-CGA	-3.02	104.62	113.21
21	C	484	CLA	C2A-C3A-C4A	3.02	106.75	101.87
29	I	274	LMT	O1B-C4'-C3'	3.02	114.92	107.23
21	B	523	CLA	C4D-CHA-C1A	3.02	124.84	121.24
27	I	220	LMG	O8-C9-C8	3.02	117.09	108.40
21	B	522	CLA	C2A-C3A-C4A	3.01	106.73	101.87
28	C	493	DGD	O3G-C3G-C2G	3.01	118.14	110.82
29	D	536	LMT	C1-O1'-C1'	3.01	118.82	113.68
33	V	164	HEM	CBC-CAC-C3C	-3.00	112.52	127.53
21	A	363	CLA	C2A-C1A-CHA	3.00	129.07	123.87
25	D	358	BCR	C37-C22-C23	3.00	122.67	118.09
21	C	477	CLA	CED-O2D-CGD	3.00	122.71	115.92
28	C	491	DGD	O6E-C1E-O5D	3.00	117.12	110.04
30	C	475	SQD	C32-C31-C30	3.00	129.51	114.37
25	Z	116	BCR	C32-C1-C6	2.99	114.93	110.24
21	B	523	CLA	C2A-C1A-CHA	2.99	129.05	123.87
30	L	213	SQD	C31-C30-C29	2.98	133.51	113.36
21	C	477	CLA	CAA-CBA-CGA	-2.98	104.75	113.21
25	C	489	BCR	C23-C22-C21	-2.98	114.33	119.01
28	C	491	DGD	C1D-O6D-C5D	-2.98	107.91	113.72
21	C	486	CLA	CED-O2D-CGD	2.97	122.64	115.92
28	C	493	DGD	C3B-C2B-C1B	2.97	124.56	113.69
28	C	493	DGD	O3D-C3D-C2D	2.96	117.35	110.38
21	B	523	CLA	C2A-C3A-C4A	2.96	106.64	101.87
32	D	357	PL9	C15-C14-C13	-2.95	116.04	123.63
25	C	490	BCR	C20-C21-C22	2.95	131.42	127.28
30	F	224	SQD	C3-C4-C5	-2.95	104.88	110.23
25	C	489	BCR	C37-C22-C23	2.95	122.59	118.09
27	J	492	LMG	C9-C8-C7	-2.94	104.93	111.78
21	B	519	CLA	CED-O2D-CGD	2.93	122.56	115.92
29	I	274	LMT	O1'-C1-C2	-2.93	99.42	109.37
25	B	529	BCR	C30-C25-C26	-2.92	118.64	122.64
21	B	519	CLA	CAA-C2A-C1A	-2.92	102.40	111.97
21	B	521	CLA	C4B-C3B-C2B	-2.92	103.67	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	478	CLA	CAA-C2A-C1A	-2.91	102.42	111.97
25	J	112	BCR	C8-C7-C6	2.91	134.78	127.00
21	C	480	CLA	C2A-C3A-C4A	2.91	106.57	101.87
25	C	490	BCR	C15-C14-C13	2.91	131.36	127.28
21	B	523	CLA	C1-C2-C3	2.91	130.96	126.20
21	B	513	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
25	C	489	BCR	C33-C5-C4	-2.90	107.40	113.60
21	B	518	CLA	C3D-C4D-ND	2.90	114.70	109.99
21	C	485	CLA	O2D-CGD-CBD	2.90	116.30	111.23
32	D	357	PL9	O1-C4-C3	-2.90	117.67	120.73
21	B	515	CLA	C3D-C4D-ND	2.90	114.70	109.99
22	D	355	PHO	OBD-CAD-C3D	2.90	132.41	127.89
25	B	527	BCR	C19-C18-C17	-2.90	114.45	119.01
21	B	521	CLA	CAA-CBA-CGA	-2.89	104.99	113.21
27	J	492	LMG	O8-C9-C8	2.89	116.73	108.40
25	D	358	BCR	C20-C21-C22	2.89	131.33	127.28
25	C	490	BCR	C35-C13-C12	2.89	122.50	118.09
21	C	488	CLA	O2D-CGD-CBD	2.89	116.28	111.23
29	D	363	LMT	O1'-C1-C2	-2.89	99.57	109.37
25	B	527	BCR	C11-C10-C9	2.88	131.32	127.28
21	B	522	CLA	O2D-CGD-CBD	2.88	116.26	111.23
25	C	490	BCR	C30-C25-C24	2.88	123.46	115.65
27	C	494	LMG	C7-O1-C1	2.88	119.97	113.80
28	C	491	DGD	O3G-C3G-C2G	2.88	117.81	110.82
21	B	524	CLA	C3A-C2A-C1A	2.87	105.64	101.34
29	A	376	LMT	C7-C6-C5	-2.87	99.88	114.37
28	C	474	DGD	C4A-C3A-C2A	2.87	123.66	113.13
28	C	493	DGD	C1G-O1G-C1A	2.86	127.59	117.12
33	V	164	HEM	C3D-C4D-ND	2.86	113.31	110.17
28	C	492	DGD	CBA-CAA-C9A	-2.86	99.90	114.37
33	F	85	HEM	CAB-C3B-C4B	2.86	137.03	124.39
22	A	365	PHO	CMA-C3A-C4A	-2.86	108.46	114.61
25	B	529	BCR	C24-C23-C22	2.85	130.46	126.23
21	B	525	CLA	C1-C2-C3	2.85	130.87	126.20
21	B	517	CLA	CAA-C2A-C1A	-2.85	102.65	111.97
32	D	357	PL9	C10-C9-C11	-2.84	110.29	115.23
21	B	521	CLA	C2A-C1A-CHA	2.84	128.80	123.87
21	B	521	CLA	CED-O2D-CGD	2.84	122.36	115.92
28	C	493	DGD	C8B-C7B-C6B	-2.84	100.02	114.37
21	C	484	CLA	C3D-C4D-ND	2.84	114.60	109.99
30	D	361	SQD	O47-C7-C8	2.84	117.62	111.48
30	D	361	SQD	C31-C30-C29	2.84	132.52	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	364	CLA	C1-C2-C3	2.82	130.82	126.20
33	F	85	HEM	CAB-C3B-C2B	-2.82	119.26	128.43
21	B	521	CLA	C3D-C4D-ND	2.82	114.57	109.99
21	C	488	CLA	C2A-C3A-C4A	2.82	106.42	101.87
21	B	526	CLA	CED-O2D-CGD	2.82	122.31	115.92
28	D	362	DGD	O2G-C2G-C1G	2.81	118.44	108.34
21	A	363	CLA	C3D-C4D-ND	2.81	114.56	109.99
21	B	520	CLA	C2A-C1A-CHA	2.81	128.74	123.87
25	B	529	BCR	C11-C10-C9	2.81	131.21	127.28
25	A	369	BCR	C37-C22-C23	2.80	122.37	118.09
25	J	112	BCR	C32-C1-C2	-2.80	98.19	108.95
22	D	355	PHO	C4D-ND-C1D	-2.80	105.52	108.87
28	B	533	DGD	O1G-C1A-O1A	-2.79	116.65	123.63
21	B	514	CLA	C3A-C2A-C1A	2.78	105.50	101.34
33	V	164	HEM	CAB-C3B-C4B	2.78	136.67	124.39
21	B	513	CLA	CHB-C4A-NA	2.78	128.41	124.40
30	L	213	SQD	C3-C4-C5	-2.78	105.20	110.23
21	C	478	CLA	O1D-CGD-CBD	-2.78	119.04	124.52
28	A	375	DGD	O3G-C3G-C2G	-2.78	104.07	110.82
29	O	274	LMT	C4-C3-C2	-2.78	100.34	114.37
21	A	363	CLA	C4B-C3B-C2B	-2.77	103.85	107.30
25	C	490	BCR	C37-C22-C23	2.77	122.32	118.09
25	C	490	BCR	C40-C30-C29	-2.77	98.31	108.95
25	J	112	BCR	C35-C13-C12	2.77	122.32	118.09
28	C	493	DGD	C8A-C7A-C6A	-2.77	100.37	114.37
21	B	511	CLA	C1-C2-C3	2.77	130.73	126.20
25	C	489	BCR	C1-C6-C7	2.77	123.15	115.65
30	L	213	SQD	O9-S-C6	-2.77	102.63	106.76
33	V	164	HEM	CAA-C2A-C1A	-2.76	119.55	124.94
21	B	512	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
32	D	357	PL9	C2-C1-C6	2.76	122.27	119.00
25	D	358	BCR	C23-C22-C21	-2.75	114.68	119.01
29	I	274	LMT	C4-C3-C2	-2.75	100.44	114.37
21	C	478	CLA	C2A-C1A-CHA	2.75	128.65	123.87
21	A	366	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
25	J	115	BCR	C21-C20-C19	2.75	131.17	123.20
27	J	492	LMG	O7-C8-C9	2.75	118.21	108.34
21	B	517	CLA	O2A-CGA-CBA	2.75	120.22	111.83
21	B	511	CLA	C2A-C1A-CHA	2.75	128.64	123.87
21	C	488	CLA	CED-O2D-CGD	2.75	122.15	115.92
21	C	478	CLA	C3D-C4D-ND	2.75	114.45	109.99
25	J	112	BCR	C34-C9-C8	2.75	122.28	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	478	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
21	B	524	CLA	C3D-C4D-ND	2.74	114.45	109.99
21	C	478	CLA	CED-O2D-CGD	2.74	122.13	115.92
21	B	515	CLA	CED-O2D-CGD	2.74	122.12	115.92
21	B	521	CLA	C5-C3-C2	2.73	127.30	121.17
21	B	513	CLA	CAA-C2A-C3A	-2.73	105.61	113.00
27	D	359	LMG	C38-C37-C36	2.73	128.16	114.37
21	B	516	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
29	D	536	LMT	O1'-C1'-C2'	-2.72	104.14	108.27
21	C	479	CLA	C3A-C2A-C1A	2.72	105.41	101.34
29	I	274	LMT	C1-O1'-C1'	2.71	118.32	113.68
30	L	213	SQD	C15-C14-C13	2.71	128.09	114.37
25	B	527	BCR	C36-C18-C19	2.71	122.23	118.09
27	D	359	LMG	C17-C16-C15	-2.71	100.66	114.37
21	C	480	CLA	C3D-C4D-ND	2.71	114.39	109.99
21	A	364	CLA	CED-O2D-CGD	2.71	122.07	115.92
21	B	511	CLA	CED-O2D-CGD	2.71	122.06	115.92
28	C	492	DGD	O2G-C2G-C3G	2.70	118.04	108.34
22	D	355	PHO	O1D-CGD-CBD	-2.70	120.62	124.72
21	B	519	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
21	B	517	CLA	C3D-C4D-ND	2.69	114.36	109.99
21	B	523	CLA	CED-O2D-CGD	2.69	122.02	115.92
21	A	362	CLA	C2A-C1A-CHA	2.69	128.53	123.87
21	B	517	CLA	CBA-CAA-C2A	2.69	121.79	113.79
28	B	533	DGD	C6D-C5D-C4D	-2.69	106.42	112.07
21	B	514	CLA	C3D-C4D-ND	2.69	114.36	109.99
21	B	519	CLA	C3D-C4D-ND	2.69	114.36	109.99
29	A	376	LMT	C4-C3-C2	-2.69	100.79	114.37
22	D	355	PHO	CMA-C3A-C4A	-2.68	108.83	114.61
21	C	481	CLA	C3D-C4D-ND	2.68	114.35	109.99
25	D	358	BCR	C35-C13-C12	2.68	122.19	118.09
21	C	479	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
21	A	362	CLA	CED-O2D-CGD	2.67	121.97	115.92
29	O	274	LMT	O1'-C1'-C2'	-2.67	104.22	108.27
30	C	475	SQD	O8-S-O9	-2.67	104.72	111.40
21	C	483	CLA	CED-O2D-CGD	2.67	121.96	115.92
21	C	487	CLA	CHA-C1A-NA	-2.66	120.36	126.39
25	C	490	BCR	C23-C24-C25	2.66	134.09	127.00
29	I	274	LMT	C7-C6-C5	-2.66	100.94	114.37
28	C	493	DGD	O6E-C1E-C2E	2.65	115.83	110.37
21	C	477	CLA	CBA-CAA-C2A	2.65	121.68	113.79
21	D	356	CLA	CAA-C2A-C1A	-2.65	103.29	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	489	BCR	C40-C30-C25	2.65	114.40	110.24
21	C	485	CLA	C1-C2-C3	2.65	130.54	126.20
21	B	522	CLA	O1D-CGD-CBD	-2.65	119.29	124.52
21	C	479	CLA	C3D-C4D-ND	2.65	114.29	109.99
21	D	356	CLA	C4B-C3B-C2B	-2.64	104.01	107.30
21	B	522	CLA	C1-C2-C3	2.64	130.52	126.20
21	B	520	CLA	O1D-CGD-CBD	-2.64	119.31	124.52
27	B	531	LMG	C14-C13-C12	2.64	127.69	114.37
29	D	536	LMT	C7-C6-C5	-2.63	101.07	114.37
21	C	486	CLA	O2D-CGD-CBD	2.63	115.82	111.23
27	C	494	LMG	C9-C8-C7	2.61	117.88	111.78
25	B	529	BCR	C16-C17-C18	2.61	130.94	127.28
26	A	371	LHG	O7-C7-C8	2.61	117.12	111.48
27	I	220	LMG	C19-C18-C17	-2.60	101.21	114.37
21	D	354	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
21	A	362	CLA	C3D-C4D-ND	2.60	114.22	109.99
28	C	492	DGD	O6E-C1E-C2E	2.60	115.71	110.37
25	B	527	BCR	C24-C23-C22	2.60	130.08	126.23
27	J	492	LMG	C39-C38-C37	2.59	127.48	114.37
28	B	533	DGD	C4A-C3A-C2A	2.59	122.66	113.13
27	D	359	LMG	O7-C8-C9	-2.59	99.04	108.34
21	D	356	CLA	C1-C2-C3	2.59	130.44	126.20
21	C	481	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
21	B	513	CLA	CED-O2D-CGD	2.58	121.77	115.92
21	B	518	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
28	B	533	DGD	O2G-C1B-O1B	-2.58	117.68	123.70
27	D	360	LMG	O8-C28-C29	2.57	119.69	111.83
21	B	518	CLA	C2A-C1A-CHA	2.57	128.34	123.87
28	D	362	DGD	O6E-C1E-O5D	2.57	116.13	110.04
25	Z	116	BCR	C15-C14-C13	2.57	130.88	127.28
21	C	488	CLA	CAA-C2A-C1A	-2.57	103.55	111.97
21	A	362	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
27	A	373	LMG	O8-C28-C29	2.57	119.67	111.83
21	C	477	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
21	B	517	CLA	C4B-C3B-C2B	-2.56	104.11	107.30
25	B	529	BCR	C40-C30-C25	2.56	114.26	110.24
33	F	85	HEM	CAA-CBA-CGA	2.56	120.45	113.67
21	C	486	CLA	C2A-C1A-CHA	2.56	128.31	123.87
21	B	522	CLA	C3D-C4D-ND	2.56	114.14	109.99
29	A	376	LMT	C1B-O1B-C4'	-2.56	111.92	117.98
30	C	475	SQD	C15-C14-C13	2.56	127.29	114.37
21	B	521	CLA	C6-C5-C3	2.55	119.69	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	528	DGD	O1G-C1A-C2A	2.55	119.62	111.83
28	C	474	DGD	C4D-C3D-C2D	2.55	115.31	110.83
25	Z	116	BCR	C19-C18-C17	-2.55	115.00	119.01
21	C	482	CLA	CAA-C2A-C1A	-2.55	103.62	111.97
28	C	491	DGD	O2G-C2G-C3G	2.55	117.48	108.34
21	C	485	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
25	D	358	BCR	C16-C17-C18	2.54	130.84	127.28
29	D	363	LMT	O1'-C1'-C2'	-2.54	104.42	108.27
21	B	518	CLA	C5-C3-C2	2.53	126.86	121.17
25	A	369	BCR	C7-C8-C9	2.53	129.98	126.23
21	B	513	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
27	C	494	LMG	C6-C5-C4	-2.53	106.81	113.02
27	M	217	LMG	O7-C10-O9	-2.53	117.79	123.70
28	C	493	DGD	CBA-CAA-C9A	-2.53	101.60	114.37
25	A	369	BCR	C30-C25-C24	2.52	122.50	115.65
21	B	512	CLA	C3D-C4D-ND	2.52	114.09	109.99
27	J	492	LMG	C34-C33-C32	-2.52	101.63	114.37
25	B	530	BCR	C30-C25-C24	2.52	122.48	115.65
21	C	483	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
21	B	520	CLA	C3D-C4D-ND	2.52	114.08	109.99
28	C	491	DGD	O6D-C1D-O3G	2.51	115.99	110.04
21	B	523	CLA	C3D-C4D-ND	2.51	114.07	109.99
25	B	530	BCR	C35-C13-C12	2.51	121.92	118.09
30	C	475	SQD	C45-O47-C7	2.51	123.80	117.80
32	D	357	PL9	C25-C24-C23	-2.51	117.19	123.63
21	C	484	CLA	C4B-C3B-C2B	-2.51	104.19	107.30
33	F	85	HEM	C3D-C4D-ND	2.50	112.92	110.17
21	C	481	CLA	C1D-ND-C4D	-2.50	104.56	106.31
21	D	354	CLA	C3A-C2A-C1A	2.50	105.09	101.34
21	A	363	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
21	B	514	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
25	A	369	BCR	C2-C1-C6	2.49	114.06	110.44
25	J	112	BCR	C40-C30-C25	2.49	114.16	110.24
21	A	364	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
28	A	375	DGD	O1G-C1A-C2A	2.49	119.43	111.83
21	C	477	CLA	C3D-C4D-ND	2.49	114.03	109.99
33	V	164	HEM	C4B-C3B-C2B	-2.49	104.99	107.28
21	A	364	CLA	CAA-C2A-C1A	-2.49	103.83	111.97
32	D	357	PL9	C40-C39-C41	2.49	119.54	115.23
29	D	536	LMT	O1B-C1B-C2B	2.49	114.20	108.09
30	F	224	SQD	C32-C31-C30	2.48	130.13	113.36
21	D	354	CLA	CED-O2D-CGD	2.48	121.53	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	526	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
22	A	365	PHO	C2B-C1B-NB	2.47	111.22	109.43
27	J	492	LMG	C13-C12-C11	2.47	122.20	113.13
25	B	530	BCR	C37-C22-C23	2.47	121.86	118.09
21	C	485	CLA	C3D-C4D-ND	2.46	113.99	109.99
21	B	517	CLA	C11-C12-C13	2.46	124.15	115.97
21	C	480	CLA	C2A-C1A-CHA	2.46	128.14	123.87
25	A	369	BCR	C35-C13-C12	2.46	121.85	118.09
25	B	530	BCR	C34-C9-C8	2.46	121.85	118.09
27	M	217	LMG	C12-C11-C10	-2.46	104.68	113.69
21	D	356	CLA	C3D-C4D-ND	2.46	113.98	109.99
33	F	85	HEM	C3B-C4B-NB	-2.45	107.70	109.47
22	A	365	PHO	CED-O2D-CGD	2.45	121.48	115.92
21	B	516	CLA	C12-C11-C10	-2.45	102.30	113.28
21	B	511	CLA	C3A-C2A-C1A	2.45	105.00	101.34
28	A	375	DGD	C1D-O6D-C5D	-2.45	108.94	113.72
30	L	213	SQD	C45-O47-C7	2.44	123.65	117.80
25	X	107	BCR	C37-C22-C23	2.44	121.82	118.09
21	C	482	CLA	C3D-C4D-ND	2.43	113.94	109.99
29	A	376	LMT	O1'-C1'-C2'	-2.43	104.58	108.27
25	B	530	BCR	C3-C4-C5	2.43	118.39	114.06
27	C	494	LMG	O8-C9-C8	-2.43	101.40	108.40
21	K	483	CLA	CED-O2D-CGD	2.43	121.42	115.92
29	T	226	LMT	C1-O1'-C1'	-2.42	109.54	113.68
28	C	493	DGD	O6E-C5E-C4E	2.42	114.07	109.70
25	C	490	BCR	C32-C1-C6	2.42	114.04	110.24
30	F	224	SQD	C15-C14-C13	2.42	126.60	114.37
21	C	486	CLA	C2C-C1C-NC	-2.42	107.44	109.98
25	B	527	BCR	C32-C1-C6	2.42	114.03	110.24
32	D	357	PL9	C3-C2-C1	-2.41	118.52	122.59
25	Z	116	BCR	C35-C13-C12	2.41	121.78	118.09
21	B	514	CLA	C2A-C1A-CHA	2.41	128.06	123.87
21	D	354	CLA	C2A-C1A-CHA	2.41	128.06	123.87
21	K	483	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
25	J	115	BCR	C40-C30-C25	2.41	114.03	110.24
21	D	356	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
21	C	485	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
25	B	530	BCR	C16-C17-C18	2.40	130.64	127.28
21	B	512	CLA	C2A-C1A-CHA	2.40	128.03	123.87
28	C	474	DGD	O1B-C1B-C2B	-2.39	114.42	123.78
28	C	491	DGD	C3A-C2A-C1A	2.39	122.47	113.69
26	A	371	LHG	O8-C6-C5	2.39	115.29	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	V	164	HEM	C4C-NC-C1C	2.39	109.72	105.82
32	D	357	PL9	C26-C27-C28	2.39	123.82	112.02
30	L	213	SQD	C17-C16-C15	2.38	126.41	114.37
28	C	493	DGD	CFB-CEB-CDB	-2.38	102.33	114.37
25	J	112	BCR	C37-C22-C23	2.38	121.73	118.09
25	B	530	BCR	C40-C30-C25	2.38	113.98	110.24
21	C	478	CLA	C1-C2-C3	2.38	130.09	126.20
33	V	164	HEM	C4D-C3D-C2D	-2.37	103.44	106.89
21	A	364	CLA	C3D-C4D-ND	2.37	113.84	109.99
21	C	483	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
30	L	213	SQD	O47-C7-C8	2.37	116.60	111.48
28	B	533	DGD	O3G-C3G-C2G	-2.37	105.06	110.82
21	C	481	CLA	C2C-C1C-NC	-2.37	107.50	109.98
25	B	527	BCR	C15-C14-C13	2.36	130.59	127.28
21	B	516	CLA	CAA-C2A-C1A	-2.36	104.24	111.97
21	C	480	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
21	B	525	CLA	C4B-C3B-C2B	-2.36	104.37	107.30
25	Z	116	BCR	C36-C18-C19	2.36	121.69	118.09
25	J	112	BCR	C16-C17-C18	2.36	130.59	127.28
27	J	492	LMG	O7-C10-O9	-2.36	118.19	123.70
21	C	482	CLA	C2A-C1A-CHA	2.36	127.96	123.87
21	K	483	CLA	C3D-C4D-ND	2.36	113.82	109.99
28	D	362	DGD	CBA-CAA-C9A	-2.35	102.47	114.37
21	B	516	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
25	J	112	BCR	C12-C13-C14	-2.35	115.31	119.01
21	C	482	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
21	B	518	CLA	CED-O2D-CGD	2.35	121.24	115.92
28	A	375	DGD	C6E-C5E-C4E	-2.35	107.26	113.02
25	J	115	BCR	C31-C1-C2	2.34	117.95	108.95
27	C	494	LMG	C19-C18-C17	-2.34	102.52	114.37
22	D	355	PHO	CBC-CAC-C3C	-2.34	109.52	112.87
21	B	513	CLA	C3D-C4D-ND	2.34	113.79	109.99
33	V	164	HEM	C2A-C1A-NA	2.34	112.75	110.15
21	C	487	CLA	C3A-C2A-C1A	2.34	104.84	101.34
22	A	365	PHO	OBD-CAD-C3D	2.33	131.53	127.89
21	B	520	CLA	C4B-C3B-C2B	-2.33	104.40	107.30
22	D	355	PHO	OBD-CAD-CBD	-2.33	122.40	125.82
25	D	358	BCR	C40-C30-C25	2.33	113.90	110.24
25	B	527	BCR	C34-C9-C8	2.33	121.64	118.09
21	A	362	CLA	C7-C6-C5	-2.33	107.06	113.26
21	D	354	CLA	CHB-C1B-NB	2.32	127.53	124.05
28	A	375	DGD	C8B-C7B-C6B	-2.32	102.64	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	483	CLA	C3D-C4D-ND	2.32	113.75	109.99
25	B	529	BCR	C32-C1-C6	2.31	113.87	110.24
25	A	369	BCR	C32-C1-C6	2.31	113.87	110.24
21	B	525	CLA	CED-O2D-CGD	2.31	121.16	115.92
21	C	487	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
25	X	107	BCR	C19-C18-C17	-2.30	115.39	119.01
21	K	483	CLA	C12-C11-C10	-2.30	102.97	113.28
21	C	482	CLA	C5-C3-C2	2.30	126.33	121.17
21	D	356	CLA	CED-O2D-CGD	2.30	121.13	115.92
21	C	482	CLA	O1D-CGD-CBD	-2.30	119.99	124.52
25	X	107	BCR	C1-C6-C7	2.29	121.88	115.65
28	C	491	DGD	C4E-C3E-C2E	-2.29	106.81	110.83
25	Z	116	BCR	C1-C6-C5	-2.29	119.50	122.64
28	D	362	DGD	C8A-C7A-C6A	-2.29	102.80	114.37
27	B	531	LMG	O8-C28-C29	2.29	118.81	111.83
28	D	362	DGD	O2G-C2G-C3G	-2.28	100.15	108.34
30	C	475	SQD	C17-C16-C15	2.28	125.89	114.37
33	V	164	HEM	CAA-C2A-C3A	2.28	132.18	127.07
33	F	85	HEM	CHD-C4C-NC	2.28	126.93	124.45
27	J	492	LMG	O8-C28-C29	2.28	118.77	111.83
21	B	524	CLA	CAA-CBA-CGA	-2.27	106.75	113.21
25	B	530	BCR	C32-C1-C6	2.27	113.81	110.24
28	C	491	DGD	O6E-C5E-C4E	2.27	113.79	109.70
25	B	529	BCR	C16-C15-C14	2.27	128.17	123.52
25	Z	116	BCR	C1-C6-C7	2.27	121.81	115.65
21	B	526	CLA	C3D-C4D-ND	2.27	113.68	109.99
26	C	476	LHG	C6-C5-C4	2.27	117.08	111.78
28	C	492	DGD	C7A-C6A-C5A	2.27	125.83	114.37
25	D	358	BCR	C12-C13-C14	-2.27	115.44	119.01
21	B	515	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
21	B	512	CLA	CED-O2D-CGD	2.26	121.04	115.92
27	M	217	LMG	C14-C13-C12	-2.26	102.95	114.37
27	I	220	LMG	C14-C13-C12	2.25	125.76	114.37
21	B	511	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
25	A	369	BCR	C21-C20-C19	2.25	129.73	123.20
21	C	488	CLA	CBA-CAA-C2A	2.25	120.49	113.79
25	A	369	BCR	C40-C30-C25	2.25	113.77	110.24
25	B	530	BCR	C1-C6-C7	2.25	121.74	115.65
25	C	489	BCR	C7-C8-C9	2.24	129.55	126.23
21	C	488	CLA	C3D-C4D-ND	2.24	113.62	109.99
27	D	359	LMG	C6-C5-C4	-2.24	107.53	113.02
21	B	511	CLA	O1D-CGD-CBD	-2.24	120.11	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	515	CLA	C4B-C3B-C2B	-2.23	104.52	107.30
21	C	488	CLA	C2C-C1C-NC	-2.23	107.64	109.98
21	C	486	CLA	C3D-C4D-ND	2.23	113.62	109.99
28	B	533	DGD	C7A-C6A-C5A	-2.23	103.10	114.37
25	A	369	BCR	C23-C22-C21	-2.23	115.50	119.01
27	C	494	LMG	C17-C16-C15	-2.23	103.11	114.37
21	B	523	CLA	C4B-C3B-C2B	-2.23	104.53	107.30
32	D	357	PL9	C53-C6-C1	2.22	119.84	115.28
25	B	529	BCR	C7-C8-C9	2.22	129.52	126.23
25	X	107	BCR	C36-C18-C19	2.22	121.48	118.09
21	B	511	CLA	C3D-C4D-ND	2.22	113.60	109.99
25	Z	116	BCR	C40-C30-C25	2.22	113.73	110.24
28	C	474	DGD	O6E-C5E-C4E	2.22	113.70	109.70
28	C	493	DGD	C6A-C5A-C4A	-2.22	103.15	114.37
30	F	224	SQD	C17-C16-C15	2.22	125.58	114.37
25	A	369	BCR	C8-C7-C6	2.22	132.92	127.00
28	B	533	DGD	C3G-C2G-C1G	-2.21	106.62	111.78
21	B	516	CLA	C3D-C4D-ND	2.21	113.58	109.99
21	B	519	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
28	A	375	DGD	O6E-C5E-C6E	2.21	111.92	106.44
21	C	488	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
25	J	112	BCR	C36-C18-C19	2.21	121.46	118.09
28	B	533	DGD	C5B-C4B-C3B	-2.21	103.21	114.37
30	D	361	SQD	C15-C14-C13	2.20	125.51	114.37
21	B	517	CLA	C12-C11-C10	-2.20	103.41	113.28
28	C	493	DGD	CDB-CCB-CBB	-2.20	103.24	114.37
33	F	85	HEM	C4C-NC-C1C	2.20	109.41	105.82
27	C	494	LMG	O1-C1-C2	-2.20	104.93	108.27
21	B	524	CLA	C4B-C3B-C2B	-2.20	104.57	107.30
28	A	375	DGD	C1G-O1G-C1A	2.20	125.14	117.12
21	C	479	CLA	C2A-C1A-CHA	2.19	127.67	123.87
22	D	355	PHO	C1-C2-C3	2.19	129.78	126.20
21	A	364	CLA	CMD-C2D-C1D	2.19	128.58	124.73
25	J	112	BCR	C40-C30-C29	-2.18	100.56	108.95
21	B	524	CLA	C1D-ND-C4D	-2.18	104.78	106.31
21	B	521	CLA	CHD-C1D-ND	-2.18	121.73	124.80
21	C	484	CLA	C12-C11-C10	-2.18	103.50	113.28
21	C	481	CLA	CED-O2D-CGD	2.18	120.86	115.92
25	Z	116	BCR	C12-C13-C14	-2.18	115.58	119.01
21	A	366	CLA	C3D-C4D-ND	2.18	113.53	109.99
28	C	491	DGD	C5A-C4A-C3A	2.17	125.36	114.37
25	C	489	BCR	C23-C24-C25	2.17	132.80	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	363	LMT	C4-C3-C2	-2.17	103.39	114.37
21	D	354	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
21	C	486	CLA	C12-C11-C10	-2.17	103.57	113.28
27	D	360	LMG	C1-O6-C5	-2.16	109.49	113.72
25	B	530	BCR	C28-C27-C26	2.16	117.91	114.06
21	B	511	CLA	CHA-C1A-NA	-2.16	121.49	126.39
27	C	494	LMG	C12-C11-C10	2.16	121.62	113.69
21	B	517	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
27	A	373	LMG	C1-O6-C5	-2.16	109.50	113.72
30	F	224	SQD	O9-S-C6	-2.16	103.53	106.76
29	A	376	LMT	C9-C8-C7	-2.16	103.46	114.37
33	F	85	HEM	C2A-C1A-NA	2.16	112.55	110.15
21	C	487	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
28	B	533	DGD	CDA-CCA-CBA	-2.16	103.47	114.37
21	B	523	CLA	O1D-CGD-CBD	-2.15	120.27	124.52
28	B	528	DGD	C1D-O6D-C5D	-2.15	109.51	113.72
25	B	530	BCR	C12-C13-C14	-2.15	115.62	119.01
29	I	274	LMT	O1'-C1'-C2'	-2.15	105.01	108.27
21	B	516	CLA	O2D-CGD-CBD	2.15	114.99	111.23
21	B	521	CLA	C4-C3-C5	-2.15	111.50	115.23
28	B	528	DGD	C1E-O6E-C5E	-2.15	109.52	113.72
27	I	220	LMG	O6-C1-O1	2.15	115.12	110.04
21	A	363	CLA	CHD-C4C-NC	2.15	127.56	124.23
21	C	484	CLA	O1D-CGD-CBD	-2.15	120.29	124.52
30	C	475	SQD	O47-C7-C8	2.14	116.12	111.48
28	B	533	DGD	C3G-O3G-C1D	-2.14	109.20	113.80
27	D	359	LMG	O7-C10-C11	-2.14	106.85	111.48
25	C	490	BCR	C12-C13-C14	-2.14	115.64	119.01
21	C	477	CLA	C1-C2-C3	2.14	129.70	126.20
27	J	492	LMG	O9-C10-C11	-2.14	115.42	123.78
28	D	362	DGD	O3D-C3D-C2D	2.14	115.42	110.38
21	A	366	CLA	CED-O2D-CGD	2.13	120.75	115.92
21	D	354	CLA	C11-C10-C8	2.13	123.04	115.97
30	F	224	SQD	C31-C30-C29	2.13	133.91	115.25
30	L	213	SQD	O8-S-O7	2.13	116.72	111.40
28	C	493	DGD	C5B-C4B-C3B	2.13	125.11	114.37
25	A	369	BCR	C1-C6-C7	2.12	121.41	115.65
21	B	514	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
21	B	526	CLA	CBA-CAA-C2A	2.12	120.10	113.79
25	B	530	BCR	C36-C18-C19	2.12	121.32	118.09
28	C	491	DGD	O3G-C1D-C2D	-2.12	105.06	108.27
27	J	492	LMG	C9-O8-C28	2.11	124.81	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	369	BCR	C12-C13-C14	-2.11	115.70	119.01
30	F	224	SQD	O48-C23-O10	-2.10	118.36	123.63
25	A	369	BCR	C10-C11-C12	2.10	129.29	123.20
21	B	517	CLA	C9-C8-C7	-2.10	103.78	111.27
28	C	493	DGD	C4D-C3D-C2D	2.10	114.52	110.83
28	B	533	DGD	C4B-C3B-C2B	2.10	120.85	113.13
21	C	478	CLA	C1D-ND-C4D	-2.09	104.84	106.31
28	B	528	DGD	C1G-O1G-C1A	-2.09	109.47	117.12
25	X	107	BCR	C23-C22-C21	-2.09	115.72	119.01
27	J	492	LMG	C35-C34-C33	2.09	124.95	114.37
28	D	362	DGD	C4A-C3A-C2A	-2.09	105.44	113.13
21	B	525	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
21	C	481	CLA	OBD-CAD-C3D	2.09	133.30	128.42
27	M	217	LMG	O8-C9-C8	-2.08	102.39	108.40
21	C	477	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
27	D	360	LMG	C9-O8-C28	-2.08	109.50	117.12
27	C	494	LMG	C30-C29-C28	2.08	121.33	113.69
21	C	485	CLA	C4D-CHA-C1A	2.08	123.73	121.24
25	Z	116	BCR	C30-C25-C24	2.08	121.29	115.65
25	B	527	BCR	C37-C22-C23	2.08	121.26	118.09
27	I	220	LMG	C16-C15-C14	2.08	124.87	114.37
25	B	529	BCR	C28-C27-C26	2.08	117.76	114.06
27	A	373	LMG	C9-O8-C28	-2.08	109.53	117.12
21	B	514	CLA	CED-O2D-CGD	2.07	120.62	115.92
25	D	358	BCR	C11-C10-C9	2.07	130.18	127.28
21	B	513	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
21	B	518	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
28	B	533	DGD	O1B-C1B-C2B	-2.07	115.69	123.78
25	X	107	BCR	C11-C12-C13	2.07	132.03	126.36
25	C	490	BCR	C28-C27-C26	2.07	117.74	114.06
25	C	490	BCR	C1-C6-C7	2.06	121.25	115.65
30	F	224	SQD	O47-C7-C8	2.06	115.94	111.48
30	L	213	SQD	C13-C12-C11	2.06	124.80	114.37
27	D	359	LMG	C32-C31-C30	-2.06	103.95	114.37
25	D	358	BCR	C36-C18-C19	2.06	121.24	118.09
21	C	482	CLA	CMD-C2D-C1D	2.06	128.36	124.73
30	L	213	SQD	C19-C18-C17	2.06	124.78	114.37
29	O	274	LMT	O1B-C1B-C2B	2.06	113.15	108.09
28	D	362	DGD	C5A-C4A-C3A	2.06	124.77	114.37
28	C	493	DGD	O2G-C2G-C3G	2.06	115.72	108.34
21	C	477	CLA	CHC-C1C-NC	2.06	127.41	124.31
29	O	274	LMT	O5B-C5B-C6B	2.05	111.53	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	369	BCR	C1-C6-C5	-2.05	119.83	122.64
21	B	515	CLA	C1D-ND-C4D	-2.05	104.87	106.31
21	A	366	CLA	C1-C2-C3	2.05	129.56	126.20
21	B	525	CLA	CHA-C1A-NA	-2.05	121.74	126.39
33	F	85	HEM	C4D-C3D-C2D	-2.05	103.91	106.89
25	A	369	BCR	C36-C18-C19	2.05	121.22	118.09
21	A	364	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
25	C	489	BCR	C8-C7-C6	2.04	132.44	127.00
21	A	364	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
21	C	480	CLA	CHC-C1C-NC	2.03	127.38	124.31
21	K	483	CLA	C4B-C3B-C2B	-2.03	104.77	107.30
21	C	481	CLA	C12-C11-C10	-2.03	104.18	113.28
29	A	376	LMT	C1'-O5'-C5'	-2.03	109.76	113.72
21	B	521	CLA	CMD-C2D-C1D	2.03	128.30	124.73
25	A	369	BCR	C34-C9-C8	2.03	121.19	118.09
30	F	224	SQD	O8-S-O7	2.03	116.47	111.40
27	D	360	LMG	C7-O1-C1	-2.03	109.45	113.80
21	B	517	CLA	C9-C8-C10	-2.03	104.05	111.27
21	B	521	CLA	C1-C2-C3	2.02	129.51	126.20
25	C	490	BCR	C32-C1-C2	-2.02	101.18	108.95
25	D	358	BCR	C1-C6-C7	2.02	121.13	115.65
21	D	354	CLA	C3D-C4D-ND	2.02	113.27	109.99
21	B	524	CLA	C2A-C1A-CHA	2.02	127.37	123.87
21	B	512	CLA	CAA-CBA-CGA	-2.02	107.49	113.21
21	B	521	CLA	C11-C12-C13	2.02	122.66	115.97
28	B	528	DGD	C6D-O5D-C1E	-2.01	109.48	113.80
29	O	274	LMT	C7-C6-C5	-2.01	104.19	114.37
28	C	474	DGD	O2D-C2D-C1D	2.01	114.87	110.08
33	F	85	HEM	C2B-C1B-NB	2.01	112.15	109.84
25	C	489	BCR	C30-C25-C24	2.01	121.11	115.65
30	F	224	SQD	C13-C12-C11	2.01	124.54	114.37
21	B	515	CLA	C12-C11-C10	-2.01	104.27	113.28
27	M	217	LMG	C7-O1-C1	-2.01	109.49	113.80
27	D	359	LMG	C34-C33-C32	-2.01	104.22	114.37
28	B	528	DGD	C3G-O3G-C1D	-2.01	109.49	113.80
28	D	362	DGD	C3A-C2A-C1A	2.01	121.05	113.69
25	Z	116	BCR	C37-C22-C23	2.01	121.15	118.09
30	D	361	SQD	O8-S-O9	-2.00	106.39	111.40
21	B	517	CLA	OBD-CAD-C3D	2.00	133.10	128.42
21	B	516	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
28	C	491	DGD	C3G-C2G-C1G	2.00	116.45	111.78
25	C	490	BCR	C10-C11-C12	2.00	129.00	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	483	CLA	C12-C11-C10	-2.00	104.31	113.28
27	J	492	LMG	C32-C31-C30	-2.00	104.25	114.37
21	C	486	CLA	C4B-C3B-C2B	-2.00	104.81	107.30

All (74) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	362	CLA	ND
21	A	362	CLA	C8
21	A	363	CLA	ND
21	A	363	CLA	C8
21	A	366	CLA	ND
21	A	366	CLA	C8
21	A	364	CLA	ND
21	A	364	CLA	C8
21	B	511	CLA	ND
21	B	511	CLA	C8
21	B	512	CLA	ND
21	B	512	CLA	C8
21	B	513	CLA	ND
21	B	513	CLA	C8
21	B	514	CLA	ND
21	B	514	CLA	C8
21	B	515	CLA	ND
21	B	515	CLA	C8
21	B	516	CLA	ND
21	B	516	CLA	C8
21	B	517	CLA	ND
21	B	517	CLA	C8
21	B	518	CLA	ND
21	B	518	CLA	C8
21	B	519	CLA	ND
21	B	519	CLA	C8
21	B	520	CLA	ND
21	B	520	CLA	C8
21	B	521	CLA	ND
21	B	521	CLA	C8
21	B	522	CLA	ND
21	B	522	CLA	C8
21	B	523	CLA	ND
21	B	523	CLA	C8
21	B	524	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	524	CLA	C8
21	B	525	CLA	ND
21	B	525	CLA	C8
21	B	526	CLA	ND
21	B	526	CLA	C8
21	C	477	CLA	ND
21	C	477	CLA	C8
21	C	478	CLA	ND
21	C	478	CLA	C8
21	C	479	CLA	ND
21	C	479	CLA	C8
21	C	480	CLA	ND
21	C	480	CLA	C8
21	C	481	CLA	ND
21	C	481	CLA	C8
21	C	482	CLA	ND
21	C	482	CLA	C8
21	C	483	CLA	ND
21	C	483	CLA	C8
21	C	484	CLA	ND
21	C	484	CLA	C8
21	C	485	CLA	ND
21	C	485	CLA	C8
21	C	486	CLA	ND
21	C	486	CLA	C8
21	C	487	CLA	ND
21	C	487	CLA	C8
21	C	488	CLA	ND
21	C	488	CLA	C8
21	D	354	CLA	ND
21	D	354	CLA	C8
21	D	356	CLA	ND
21	D	356	CLA	C8
21	K	483	CLA	ND
21	K	483	CLA	C8
22	A	365	PHO	C8
22	D	355	PHO	C8
28	C	492	DGD	C1E
28	C	493	DGD	C1E

All (685) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	B	511	CLA	C11-C12-C13-C14
21	B	516	CLA	C4-C3-C5-C6
21	B	524	CLA	CAD-CBD-CGD-O2D
21	C	477	CLA	CAD-CBD-CGD-O1D
21	C	477	CLA	CAD-CBD-CGD-O2D
21	C	480	CLA	CHA-CBD-CGD-O1D
21	C	480	CLA	CHA-CBD-CGD-O2D
21	C	483	CLA	C4-C3-C5-C6
21	K	483	CLA	CHA-CBD-CGD-O1D
21	K	483	CLA	CHA-CBD-CGD-O2D
23	A	367	MES	C7-C8-S-O2S
23	A	367	MES	C7-C8-S-O3S
25	A	369	BCR	C6-C7-C8-C9
25	B	527	BCR	C1-C6-C7-C8
25	B	527	BCR	C5-C6-C7-C8
25	B	527	BCR	C6-C7-C8-C9
25	C	489	BCR	C6-C7-C8-C9
25	C	490	BCR	C6-C7-C8-C9
25	C	490	BCR	C23-C24-C25-C26
25	C	490	BCR	C23-C24-C25-C30
25	D	358	BCR	C1-C6-C7-C8
25	D	358	BCR	C5-C6-C7-C8
25	D	358	BCR	C6-C7-C8-C9
25	J	115	BCR	C6-C7-C8-C9
25	J	112	BCR	C6-C7-C8-C9
25	X	107	BCR	C1-C6-C7-C8
25	X	107	BCR	C5-C6-C7-C8
25	Z	116	BCR	C1-C6-C7-C8
25	Z	116	BCR	C5-C6-C7-C8
26	C	476	LHG	O1-C1-C2-C3
26	C	476	LHG	C8-C7-O7-C5
27	B	531	LMG	C7-C8-O7-C10
27	D	360	LMG	C11-C10-O7-C8
27	J	492	LMG	O7-C8-C9-O8
28	C	474	DGD	O6E-C1E-O5D-C6D
28	C	491	DGD	O6E-C1E-O5D-C6D
28	C	492	DGD	O6E-C1E-O5D-C6D
28	C	493	DGD	O2G-C2G-C3G-O3G
28	C	493	DGD	O6E-C1E-O5D-C6D
28	D	362	DGD	O1G-C1G-C2G-O2G
28	D	362	DGD	O6E-C1E-O5D-C6D
30	C	475	SQD	C8-C7-O47-C45
30	D	361	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
30	D	361	SQD	C8-C7-O47-C45
30	D	361	SQD	C5-C6-S-O7
30	D	361	SQD	C5-C6-S-O8
30	D	361	SQD	C5-C6-S-O9
30	F	224	SQD	O5-C1-O6-C44
30	F	224	SQD	O5-C5-C6-S
30	F	224	SQD	C5-C6-S-O8
30	L	213	SQD	C2-C1-O6-C44
30	L	213	SQD	O49-C7-O47-C45
30	L	213	SQD	C8-C7-O47-C45
32	D	357	PL9	C26-C27-C28-C29
32	D	357	PL9	C39-C41-C42-C43
32	D	357	PL9	C46-C47-C48-C49
33	F	85	HEM	C2B-C3B-CAB-CBB
33	F	85	HEM	C4B-C3B-CAB-CBB
33	F	85	HEM	C2C-C3C-CAC-CBC
33	F	85	HEM	C4C-C3C-CAC-CBC
33	V	164	HEM	C3A-C2A-CAA-CBA
33	V	164	HEM	C2B-C3B-CAB-CBB
33	V	164	HEM	C4B-C3B-CAB-CBB
29	I	274	LMT	C3'-C4'-O1B-C1B
22	D	355	PHO	CBD-CGD-O2D-CED
21	B	517	CLA	C13-C15-C16-C17
21	B	522	CLA	C10-C11-C12-C13
30	F	224	SQD	O10-C23-O48-C46
28	B	528	DGD	O6D-C5D-C6D-O5D
28	C	493	DGD	O6D-C5D-C6D-O5D
26	C	476	LHG	O9-C7-O7-C5
27	D	360	LMG	O9-C10-O7-C8
30	C	475	SQD	O49-C7-O47-C45
21	A	362	CLA	C3-C5-C6-C7
21	A	364	CLA	C3-C5-C6-C7
21	B	511	CLA	C3-C5-C6-C7
21	B	514	CLA	C3-C5-C6-C7
21	B	519	CLA	C3-C5-C6-C7
21	C	478	CLA	C3-C5-C6-C7
21	C	484	CLA	C3-C5-C6-C7
29	B	535	LMT	C5'-C4'-O1B-C1B
21	A	366	CLA	CBA-CGA-O2A-C1
30	F	224	SQD	C24-C23-O48-C46
28	B	528	DGD	C4E-C5E-C6E-O5E
29	A	376	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
21	B	515	CLA	C4-C3-C5-C6
21	B	517	CLA	C4-C3-C5-C6
21	B	525	CLA	C4-C3-C5-C6
21	C	484	CLA	C4-C3-C5-C6
21	B	515	CLA	C2-C3-C5-C6
21	B	516	CLA	C2-C3-C5-C6
21	B	517	CLA	C2-C3-C5-C6
21	B	525	CLA	C2-C3-C5-C6
21	C	483	CLA	C2-C3-C5-C6
21	C	484	CLA	C2-C3-C5-C6
21	B	520	CLA	C2A-CAA-CBA-CGA
21	B	522	CLA	C2A-CAA-CBA-CGA
21	B	517	CLA	C3-C5-C6-C7
21	C	479	CLA	C3-C5-C6-C7
21	C	481	CLA	C3-C5-C6-C7
21	C	485	CLA	C3-C5-C6-C7
21	A	363	CLA	CBA-CGA-O2A-C1
21	B	524	CLA	CBA-CGA-O2A-C1
21	C	483	CLA	CBA-CGA-O2A-C1
27	I	220	LMG	C18-C19-C20-C21
28	C	491	DGD	C7A-C8A-C9A-CAA
32	D	357	PL9	C7-C8-C9-C10
21	A	363	CLA	O1A-CGA-O2A-C1
21	A	366	CLA	O1A-CGA-O2A-C1
21	C	483	CLA	O1A-CGA-O2A-C1
21	D	354	CLA	O1A-CGA-O2A-C1
26	A	371	LHG	O10-C23-O8-C6
27	B	531	LMG	C36-C37-C38-C39
27	C	494	LMG	C18-C19-C20-C21
27	C	494	LMG	C36-C37-C38-C39
27	D	359	LMG	C36-C37-C38-C39
27	D	360	LMG	C36-C37-C38-C39
27	J	492	LMG	C36-C37-C38-C39
27	M	217	LMG	C18-C19-C20-C21
28	B	533	DGD	C7B-C8B-C9B-CAB
29	D	536	LMT	C3-C4-C5-C6
21	C	482	CLA	C3-C5-C6-C7
27	B	531	LMG	C18-C19-C20-C21
27	D	359	LMG	C18-C19-C20-C21
27	J	492	LMG	C18-C19-C20-C21
28	C	474	DGD	C7A-C8A-C9A-CAA
28	C	492	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
28	C	493	DGD	C7B-C8B-C9B-CAB
28	D	362	DGD	C7A-C8A-C9A-CAA
29	A	376	LMT	C3-C4-C5-C6
29	D	363	LMT	C3-C4-C5-C6
29	I	274	LMT	C3-C4-C5-C6
29	T	226	LMT	C3-C4-C5-C6
21	B	522	CLA	CBA-CGA-O2A-C1
27	A	373	LMG	C29-C28-O8-C9
21	B	524	CLA	O1A-CGA-O2A-C1
21	B	511	CLA	C2C-C3C-CAC-CBC
27	A	373	LMG	O10-C28-O8-C9
28	B	528	DGD	C7B-C8B-C9B-CAB
29	O	274	LMT	C3-C4-C5-C6
28	B	528	DGD	C4D-C5D-C6D-O5D
28	B	533	DGD	C7A-C8A-C9A-CAA
28	C	474	DGD	C7B-C8B-C9B-CAB
28	D	362	DGD	C7B-C8B-C9B-CAB
27	A	373	LMG	O6-C5-C6-O5
22	D	355	PHO	O1D-CGD-O2D-CED
21	A	362	CLA	CBA-CGA-O2A-C1
21	D	354	CLA	CBA-CGA-O2A-C1
26	A	371	LHG	C24-C23-O8-C6
21	C	479	CLA	C4-C3-C5-C6
21	C	479	CLA	C2-C3-C5-C6
32	D	357	PL9	C24-C26-C27-C28
28	A	375	DGD	C7B-C8B-C9B-CAB
28	C	492	DGD	C7A-C8A-C9A-CAA
28	C	493	DGD	C7A-C8A-C9A-CAA
33	V	164	HEM	C1A-C2A-CAA-CBA
28	B	528	DGD	O6E-C5E-C6E-O5E
21	C	481	CLA	C2A-CAA-CBA-CGA
21	A	362	CLA	O1A-CGA-O2A-C1
21	B	522	CLA	O1A-CGA-O2A-C1
28	B	533	DGD	O6E-C1E-O5D-C6D
29	B	535	LMT	C3-C4-C5-C6
21	C	485	CLA	CBA-CGA-O2A-C1
30	D	361	SQD	C24-C23-O48-C46
28	B	528	DGD	C7A-C8A-C9A-CAA
30	D	361	SQD	O10-C23-O48-C46
21	B	518	CLA	CBA-CGA-O2A-C1
21	C	478	CLA	CBA-CGA-O2A-C1
21	C	488	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	D	360	LMG	C29-C28-O8-C9
26	C	476	LHG	C23-C24-C25-C26
21	B	523	CLA	C4-C3-C5-C6
21	B	523	CLA	C2-C3-C5-C6
21	C	480	CLA	C3-C5-C6-C7
21	B	518	CLA	C11-C12-C13-C14
21	B	520	CLA	C14-C13-C15-C16
21	B	523	CLA	C11-C12-C13-C14
21	C	477	CLA	C6-C7-C8-C9
21	C	480	CLA	C11-C12-C13-C14
21	C	481	CLA	C6-C7-C8-C9
21	C	482	CLA	C6-C7-C8-C9
21	C	486	CLA	C11-C12-C13-C14
22	D	355	PHO	C11-C12-C13-C14
22	D	355	PHO	C14-C13-C15-C16
27	A	373	LMG	C4-C5-C6-O5
21	B	521	CLA	C2A-CAA-CBA-CGA
21	C	488	CLA	O1A-CGA-O2A-C1
27	D	360	LMG	O10-C28-O8-C9
29	O	274	LMT	C5'-C4'-O1B-C1B
28	C	474	DGD	O2G-C2G-C3G-O3G
22	A	365	PHO	C13-C15-C16-C17
21	A	363	CLA	C10-C11-C12-C13
22	A	365	PHO	C15-C16-C17-C18
21	B	516	CLA	C11-C12-C13-C15
21	B	518	CLA	C12-C13-C15-C16
21	C	488	CLA	C11-C12-C13-C15
21	B	514	CLA	CBA-CGA-O2A-C1
21	B	518	CLA	O1A-CGA-O2A-C1
21	C	478	CLA	O1A-CGA-O2A-C1
21	A	362	CLA	C13-C15-C16-C17
21	B	513	CLA	C10-C11-C12-C13
21	C	480	CLA	C13-C15-C16-C17
22	D	355	PHO	C13-C15-C16-C17
21	B	516	CLA	C2A-CAA-CBA-CGA
21	B	518	CLA	C2A-CAA-CBA-CGA
21	C	477	CLA	C2A-CAA-CBA-CGA
21	B	511	CLA	C4C-C3C-CAC-CBC
21	B	516	CLA	C13-C15-C16-C17
26	A	371	LHG	C23-C24-C25-C26
27	A	373	LMG	C10-C11-C12-C13
27	D	360	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	C	475	SQD	C23-C24-C25-C26
21	B	523	CLA	C3-C5-C6-C7
21	B	512	CLA	C10-C11-C12-C13
21	B	525	CLA	C13-C15-C16-C17
21	C	480	CLA	C10-C11-C12-C13
21	C	485	CLA	O1A-CGA-O2A-C1
21	A	366	CLA	C13-C15-C16-C17
21	C	479	CLA	C13-C15-C16-C17
28	D	362	DGD	CFB-CGB-CHB-CIB
21	B	511	CLA	C13-C15-C16-C17
28	B	533	DGD	CFB-CGB-CHB-CIB
28	C	492	DGD	CFB-CGB-CHB-CIB
28	C	493	DGD	CFB-CGB-CHB-CIB
21	B	513	CLA	O1A-CGA-O2A-C1
21	C	486	CLA	C13-C15-C16-C17
21	B	513	CLA	CBA-CGA-O2A-C1
21	C	487	CLA	CBA-CGA-O2A-C1
21	B	514	CLA	O1A-CGA-O2A-C1
28	B	528	DGD	C1B-C2B-C3B-C4B
21	C	488	CLA	C2A-CAA-CBA-CGA
21	B	511	CLA	CBA-CGA-O2A-C1
21	B	512	CLA	CBA-CGA-O2A-C1
21	C	479	CLA	CBA-CGA-O2A-C1
21	C	482	CLA	CBA-CGA-O2A-C1
21	A	362	CLA	C10-C11-C12-C13
21	C	482	CLA	C10-C11-C12-C13
21	B	511	CLA	O1A-CGA-O2A-C1
32	D	357	PL9	C35-C34-C36-C37
21	B	526	CLA	C3-C5-C6-C7
27	D	360	LMG	C2-C1-O1-C7
30	C	475	SQD	C2-C1-O6-C44
32	D	357	PL9	C34-C36-C37-C38
21	D	356	CLA	C13-C15-C16-C17
21	C	487	CLA	C2A-CAA-CBA-CGA
28	B	528	DGD	C1G-C2G-O2G-C1B
21	A	363	CLA	C3-C5-C6-C7
21	B	514	CLA	C10-C11-C12-C13
27	D	360	LMG	O6-C1-O1-C7
28	B	528	DGD	C2B-C1B-O2G-C2G
30	C	475	SQD	C24-C23-O48-C46
28	C	492	DGD	O6D-C5D-C6D-O5D
21	B	516	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	B	522	CLA	C2-C1-O2A-CGA
21	C	482	CLA	O1A-CGA-O2A-C1
21	C	487	CLA	O1A-CGA-O2A-C1
30	F	224	SQD	C10-C11-C12-C13
27	A	373	LMG	C28-C29-C30-C31
27	A	373	LMG	C30-C31-C32-C33
26	C	476	LHG	O1-C1-C2-O2
21	A	363	CLA	C2A-CAA-CBA-CGA
30	F	224	SQD	C11-C12-C13-C14
22	D	355	PHO	C5-C6-C7-C8
28	B	528	DGD	O1B-C1B-O2G-C2G
21	C	487	CLA	C10-C11-C12-C13
27	D	360	LMG	C13-C14-C15-C16
30	C	475	SQD	C17-C18-C19-C20
21	B	512	CLA	O1A-CGA-O2A-C1
21	C	479	CLA	O1A-CGA-O2A-C1
29	O	274	LMT	C3'-C4'-O1B-C1B
26	C	476	LHG	C13-C14-C15-C16
30	F	224	SQD	C12-C13-C14-C15
21	C	483	CLA	C13-C15-C16-C17
27	D	360	LMG	C11-C12-C13-C14
30	F	224	SQD	C25-C26-C27-C28
30	L	213	SQD	C27-C28-C29-C30
30	C	475	SQD	O10-C23-O48-C46
25	A	369	BCR	C1-C6-C7-C8
25	B	530	BCR	C1-C6-C7-C8
25	B	530	BCR	C5-C6-C7-C8
25	B	530	BCR	C23-C24-C25-C26
25	B	530	BCR	C23-C24-C25-C30
25	C	489	BCR	C1-C6-C7-C8
25	C	489	BCR	C5-C6-C7-C8
25	C	489	BCR	C23-C24-C25-C26
25	C	489	BCR	C23-C24-C25-C30
27	A	373	LMG	C36-C37-C38-C39
21	B	524	CLA	C13-C15-C16-C17
25	B	527	BCR	C22-C23-C24-C25
30	D	361	SQD	O5-C1-O6-C44
30	D	361	SQD	C2-C1-O6-C44
21	A	363	CLA	C13-C15-C16-C17
26	A	371	LHG	C11-C10-C9-C8
26	A	371	LHG	C28-C29-C30-C31
21	C	488	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	L	213	SQD	C25-C26-C27-C28
30	F	224	SQD	C27-C28-C29-C30
21	D	356	CLA	C2A-CAA-CBA-CGA
21	B	516	CLA	C10-C11-C12-C13
27	A	373	LMG	C15-C16-C17-C18
21	C	486	CLA	C10-C11-C12-C13
30	F	224	SQD	C11-C10-C9-C8
28	B	528	DGD	C1A-C2A-C3A-C4A
27	D	359	LMG	O1-C7-C8-O7
27	M	217	LMG	O1-C7-C8-O7
28	A	375	DGD	O1G-C1G-C2G-O2G
27	D	360	LMG	C12-C13-C14-C15
21	B	525	CLA	CBA-CGA-O2A-C1
21	D	356	CLA	C3-C5-C6-C7
21	B	518	CLA	C13-C15-C16-C17
26	A	371	LHG	C24-C25-C26-C27
26	A	371	LHG	C26-C27-C28-C29
27	A	373	LMG	C11-C12-C13-C14
21	B	522	CLA	C11-C12-C13-C15
21	B	525	CLA	C6-C7-C8-C10
21	B	525	CLA	C12-C13-C15-C16
21	C	477	CLA	C6-C7-C8-C10
21	C	477	CLA	C12-C13-C15-C16
21	C	480	CLA	C11-C12-C13-C15
21	C	480	CLA	C12-C13-C15-C16
21	C	485	CLA	C6-C7-C8-C10
21	D	354	CLA	C11-C12-C13-C15
30	F	224	SQD	C15-C16-C17-C18
26	C	476	LHG	C12-C13-C14-C15
26	C	476	LHG	C11-C12-C13-C14
21	D	354	CLA	C10-C11-C12-C13
21	A	362	CLA	C6-C7-C8-C9
21	A	363	CLA	C14-C13-C15-C16
21	A	364	CLA	C11-C12-C13-C14
21	B	523	CLA	C14-C13-C15-C16
21	B	524	CLA	C6-C7-C8-C9
21	D	354	CLA	C11-C12-C13-C14
21	B	525	CLA	O1A-CGA-O2A-C1
30	C	475	SQD	C25-C26-C27-C28
30	D	361	SQD	C10-C11-C12-C13
26	A	371	LHG	C4-C5-C6-O8
27	A	373	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	D	359	LMG	O1-C7-C8-C9
27	I	220	LMG	O1-C7-C8-C9
27	M	217	LMG	O1-C7-C8-C9
28	A	375	DGD	C1G-C2G-C3G-O3G
28	D	362	DGD	O1G-C1G-C2G-C3G
30	C	475	SQD	C10-C11-C12-C13
21	C	480	CLA	O1A-CGA-O2A-C1
28	D	362	DGD	O6D-C5D-C6D-O5D
21	C	477	CLA	O1A-CGA-O2A-C1
21	B	521	CLA	C13-C15-C16-C17
21	C	477	CLA	CBA-CGA-O2A-C1
22	A	365	PHO	O2A-C1-C2-C3
27	C	494	LMG	C7-C8-O7-C10
27	D	359	LMG	C7-C8-O7-C10
27	D	360	LMG	C7-C8-O7-C10
27	J	492	LMG	C9-C8-O7-C10
30	C	475	SQD	C24-C25-C26-C27
27	A	373	LMG	C37-C38-C39-C40
30	C	475	SQD	C29-C30-C31-C32
27	D	360	LMG	C16-C17-C18-C19
21	B	521	CLA	CBA-CGA-O2A-C1
21	C	480	CLA	CBA-CGA-O2A-C1
30	C	475	SQD	C11-C12-C13-C14
21	B	524	CLA	C4-C3-C5-C6
32	D	357	PL9	C12-C11-C9-C10
30	F	224	SQD	C29-C30-C31-C32
30	L	213	SQD	C19-C20-C21-C22
27	A	373	LMG	C16-C17-C18-C19
30	L	213	SQD	C10-C11-C12-C13
27	A	373	LMG	O7-C8-C9-O8
30	C	475	SQD	O6-C44-C45-O47
30	D	361	SQD	O6-C44-C45-O47
30	F	224	SQD	C24-C25-C26-C27
27	A	373	LMG	C14-C15-C16-C17
21	K	483	CLA	C4-C3-C5-C6
32	D	357	PL9	C45-C44-C46-C47
21	D	356	CLA	CBA-CGA-O2A-C1
21	A	362	CLA	C14-C13-C15-C16
21	B	514	CLA	C11-C12-C13-C14
21	B	520	CLA	C11-C12-C13-C14
21	B	522	CLA	C6-C7-C8-C9
21	B	522	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	525	CLA	C6-C7-C8-C9
21	B	525	CLA	C14-C13-C15-C16
21	C	477	CLA	C14-C13-C15-C16
21	C	480	CLA	C14-C13-C15-C16
21	C	483	CLA	C14-C13-C15-C16
22	D	355	PHO	C3-C5-C6-C7
21	A	362	CLA	C6-C7-C8-C10
21	A	362	CLA	C12-C13-C15-C16
21	A	363	CLA	C12-C13-C15-C16
21	A	366	CLA	C12-C13-C15-C16
21	B	511	CLA	C11-C12-C13-C15
21	B	514	CLA	C11-C12-C13-C15
21	B	518	CLA	C11-C12-C13-C15
21	B	520	CLA	C11-C12-C13-C15
21	B	523	CLA	C6-C7-C8-C10
21	B	523	CLA	C12-C13-C15-C16
21	B	524	CLA	C6-C7-C8-C10
21	C	479	CLA	C11-C12-C13-C15
22	D	355	PHO	C6-C7-C8-C10
22	D	355	PHO	C12-C13-C15-C16
26	A	371	LHG	C9-C10-C11-C12
27	A	373	LMG	C12-C13-C14-C15
21	B	521	CLA	O1A-CGA-O2A-C1
21	B	520	CLA	C4-C3-C5-C6
21	B	520	CLA	C2-C3-C5-C6
21	K	483	CLA	C2-C3-C5-C6
21	B	515	CLA	CBA-CGA-O2A-C1
21	B	524	CLA	C2C-C3C-CAC-CBC
27	A	373	LMG	C29-C30-C31-C32
28	A	375	DGD	O1G-C1G-C2G-C3G
28	B	533	DGD	O1G-C1G-C2G-C3G
28	B	528	DGD	C1G-C2G-C3G-O3G
28	C	491	DGD	C1G-C2G-C3G-O3G
28	C	492	DGD	C1G-C2G-C3G-O3G
30	D	361	SQD	O6-C44-C45-C46
30	L	213	SQD	C17-C18-C19-C20
29	A	376	LMT	C3'-C4'-O1B-C1B
25	A	369	BCR	C23-C24-C25-C30
21	C	485	CLA	C10-C11-C12-C13
28	B	528	DGD	C2B-C3B-C4B-C5B
21	B	517	CLA	C2A-CAA-CBA-CGA
26	C	476	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
27	B	531	LMG	O7-C8-C9-O8
27	D	360	LMG	O7-C8-C9-O8
28	B	533	DGD	O2G-C2G-C3G-O3G
28	C	491	DGD	O2G-C2G-C3G-O3G
32	D	357	PL9	C4-C3-C7-C8
21	C	482	CLA	C4-C3-C5-C6
21	A	364	CLA	CBA-CGA-O2A-C1
21	A	366	CLA	C14-C13-C15-C16
21	B	521	CLA	C6-C7-C8-C9
25	J	115	BCR	C22-C23-C24-C25
28	B	528	DGD	O6E-C1E-O5D-C6D
30	D	361	SQD	C12-C13-C14-C15
26	C	476	LHG	C9-C10-C11-C12
21	C	482	CLA	C2-C3-C5-C6
23	A	367	MES	C7-C8-S-O1S
21	B	511	CLA	C12-C13-C15-C16
21	C	478	CLA	C12-C13-C15-C16
21	C	481	CLA	C11-C12-C13-C15
21	C	486	CLA	C12-C13-C15-C16
27	D	360	LMG	C15-C16-C17-C18
21	A	364	CLA	O1A-CGA-O2A-C1
21	B	515	CLA	O1A-CGA-O2A-C1
21	B	517	CLA	C10-C11-C12-C13
21	C	479	CLA	C10-C11-C12-C13
21	B	511	CLA	C4-C3-C5-C6
32	D	357	PL9	C43-C44-C46-C47
33	V	164	HEM	C2C-C3C-CAC-CBC
22	A	365	PHO	C3-C5-C6-C7
27	I	220	LMG	C7-C8-O7-C10
28	A	375	DGD	C3G-C2G-O2G-C1B
28	C	491	DGD	C3G-C2G-O2G-C1B
28	C	492	DGD	C1G-C2G-O2G-C1B
28	C	493	DGD	C3G-C2G-O2G-C1B
21	D	356	CLA	O1A-CGA-O2A-C1
30	C	475	SQD	O5-C1-O6-C44
26	C	476	LHG	C4-C5-C6-O8
27	J	492	LMG	C7-C8-C9-O8
28	B	533	DGD	C1G-C2G-C3G-O3G
28	C	493	DGD	C1G-C2G-C3G-O3G
28	D	362	DGD	C1G-C2G-C3G-O3G
33	V	164	HEM	C4C-C3C-CAC-CBC
28	B	528	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
21	A	364	CLA	C6-C7-C8-C9
21	C	485	CLA	C6-C7-C8-C9
21	C	488	CLA	C11-C12-C13-C14
28	B	528	DGD	C4B-C5B-C6B-C7B
30	L	213	SQD	C16-C17-C18-C19
21	B	513	CLA	CAA-CBA-CGA-O2A
21	C	478	CLA	C10-C11-C12-C13
21	B	519	CLA	C13-C15-C16-C17
26	A	371	LHG	O2-C2-C3-O3
26	A	371	LHG	C25-C26-C27-C28
21	B	526	CLA	CBA-CGA-O2A-C1
21	B	519	CLA	C10-C11-C12-C13
21	B	526	CLA	O1A-CGA-O2A-C1
21	B	511	CLA	C2-C3-C5-C6
21	D	354	CLA	C2A-CAA-CBA-CGA
30	C	475	SQD	C5-C6-S-O9
21	B	514	CLA	C12-C13-C15-C16
22	A	365	PHO	C12-C13-C15-C16
26	C	476	LHG	C26-C27-C28-C29
28	B	528	DGD	C2A-C3A-C4A-C5A
22	D	355	PHO	C4-C3-C5-C6
21	B	511	CLA	C2A-CAA-CBA-CGA
21	B	513	CLA	C2A-CAA-CBA-CGA
21	B	523	CLA	C6-C7-C8-C9
21	C	478	CLA	C14-C13-C15-C16
21	C	481	CLA	C11-C12-C13-C14
30	L	213	SQD	C14-C15-C16-C17
27	I	220	LMG	O1-C7-C8-O7
28	A	375	DGD	O2G-C2G-C3G-O3G
28	B	533	DGD	O1G-C1G-C2G-O2G
28	C	474	DGD	O1G-C1G-C2G-O2G
28	D	362	DGD	O2G-C2G-C3G-O3G
30	L	213	SQD	O6-C44-C45-O47
27	D	360	LMG	C7-C8-C9-O8
21	B	522	CLA	CAD-CBD-CGD-O2D
21	C	485	CLA	CAD-CBD-CGD-O2D
21	C	487	CLA	CAD-CBD-CGD-O2D
30	C	475	SQD	C9-C10-C11-C12
30	C	475	SQD	C12-C13-C14-C15
21	B	522	CLA	CAD-CBD-CGD-O1D
21	B	524	CLA	CAD-CBD-CGD-O1D
21	C	484	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	C	484	CLA	CHA-CBD-CGD-O2D
21	C	485	CLA	CAD-CBD-CGD-O1D
21	C	487	CLA	CAD-CBD-CGD-O1D
26	C	476	LHG	C4-O6-P-O4
25	J	115	BCR	C5-C6-C7-C8
21	B	524	CLA	C2-C3-C5-C6
22	D	355	PHO	C2-C3-C5-C6
26	A	371	LHG	C2-C3-O3-P
21	B	524	CLA	C4C-C3C-CAC-CBC
21	C	481	CLA	CBA-CGA-O2A-C1
27	D	360	LMG	C30-C31-C32-C33
28	C	474	DGD	C1G-C2G-O2G-C1B
28	D	362	DGD	C1G-C2G-O2G-C1B
29	B	535	LMT	C3'-C4'-O1B-C1B
21	C	479	CLA	C11-C12-C13-C14
21	C	486	CLA	C14-C13-C15-C16
22	D	355	PHO	C6-C7-C8-C9
21	B	512	CLA	C6-C7-C8-C10
27	A	373	LMG	C35-C36-C37-C38
21	C	485	CLA	C4-C3-C5-C6
27	A	373	LMG	C18-C19-C20-C21
26	A	371	LHG	O7-C5-C6-O8
28	C	493	DGD	O1G-C1G-C2G-O2G
21	A	366	CLA	C3-C5-C6-C7
28	C	492	DGD	O1G-C1G-C2G-C3G
30	L	213	SQD	O6-C44-C45-C46
21	B	511	CLA	C14-C13-C15-C16
21	B	514	CLA	C14-C13-C15-C16
21	B	517	CLA	CBA-CGA-O2A-C1
27	D	360	LMG	C19-C20-C21-C22
21	B	522	CLA	C4-C3-C5-C6
21	C	485	CLA	C2-C3-C5-C6
21	B	517	CLA	O1A-CGA-O2A-C1
21	B	520	CLA	C12-C13-C15-C16
21	C	482	CLA	C6-C7-C8-C10
21	C	483	CLA	C11-C12-C13-C15
21	C	487	CLA	C6-C7-C8-C10
21	B	520	CLA	O1A-CGA-O2A-C1
30	L	213	SQD	C13-C14-C15-C16
27	D	360	LMG	C18-C19-C20-C21
21	B	526	CLA	C13-C15-C16-C17
21	C	482	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	B	520	CLA	C13-C15-C16-C17
21	B	519	CLA	C4-C3-C5-C6
21	B	512	CLA	C14-C13-C15-C16
21	B	513	CLA	C11-C12-C13-C14
21	B	513	CLA	C14-C13-C15-C16
21	B	515	CLA	C11-C12-C13-C14
21	B	520	CLA	C6-C7-C8-C9
21	B	526	CLA	C11-C12-C13-C14
21	C	483	CLA	C11-C12-C13-C14
26	C	476	LHG	C11-C10-C9-C8
26	C	476	LHG	C10-C11-C12-C13
21	A	364	CLA	C13-C15-C16-C17
28	B	533	DGD	C1G-C2G-O2G-C1B
21	B	522	CLA	C2-C3-C5-C6
21	B	516	CLA	C3-C5-C6-C7
21	C	488	CLA	C2C-C3C-CAC-CBC
25	A	369	BCR	C5-C6-C7-C8
25	A	369	BCR	C23-C24-C25-C26
33	F	85	HEM	CAA-CBA-CGA-O1A
21	C	481	CLA	C4-C3-C5-C6
32	D	357	PL9	C30-C29-C31-C32
21	B	526	CLA	C6-C7-C8-C10
21	C	484	CLA	C12-C13-C15-C16
26	A	371	LHG	C1-C2-C3-O3
21	B	526	CLA	C4-C3-C5-C6
32	D	357	PL9	C2-C3-C7-C8
33	F	85	HEM	CAD-CBD-CGD-O2D
21	A	364	CLA	C14-C13-C15-C16
21	B	519	CLA	C14-C13-C15-C16
21	C	484	CLA	C14-C13-C15-C16
30	D	361	SQD	C11-C10-C9-C8
21	A	364	CLA	C4-C3-C5-C6
21	B	519	CLA	C2-C3-C5-C6
21	B	520	CLA	CBA-CGA-O2A-C1
30	C	475	SQD	O6-C44-C45-C46
30	L	213	SQD	C44-C45-C46-O48
33	F	85	HEM	CAA-CBA-CGA-O2A
33	F	85	HEM	CAD-CBD-CGD-O1D
21	C	482	CLA	CAA-CBA-CGA-O2A
21	B	521	CLA	C10-C11-C12-C13
21	C	484	CLA	CAA-CBA-CGA-O2A
21	B	518	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	V	164	HEM	CAD-CBD-CGD-O1D
21	B	526	CLA	C2-C3-C5-C6
21	B	515	CLA	C11-C12-C13-C15
33	V	164	HEM	CAA-CBA-CGA-O2A
21	B	516	CLA	C11-C12-C13-C14
21	B	522	CLA	C14-C13-C15-C16
30	D	361	SQD	C45-C44-O6-C1
33	V	164	HEM	CAD-CBD-CGD-O2D
21	B	521	CLA	C2-C1-O2A-CGA
21	B	524	CLA	C2-C1-O2A-CGA
21	C	479	CLA	C2-C1-O2A-CGA
30	C	475	SQD	C11-C10-C9-C8
21	B	513	CLA	CAA-CBA-CGA-O1A
21	B	515	CLA	CAA-CBA-CGA-O2A
25	X	107	BCR	C6-C7-C8-C9
33	V	164	HEM	CAA-CBA-CGA-O1A
27	A	373	LMG	C32-C33-C34-C35
30	F	224	SQD	O6-C44-C45-C46
21	C	480	CLA	CAA-CBA-CGA-O2A
30	F	224	SQD	O47-C45-C46-O48
21	B	512	CLA	C6-C7-C8-C9
22	A	365	PHO	C14-C13-C15-C16
21	C	483	CLA	CAA-CBA-CGA-O2A
21	B	512	CLA	C12-C13-C15-C16
21	B	513	CLA	C12-C13-C15-C16
21	B	519	CLA	C12-C13-C15-C16
21	B	522	CLA	C12-C13-C15-C16
21	B	523	CLA	C11-C12-C13-C15
21	C	481	CLA	C6-C7-C8-C10
21	C	484	CLA	C11-C12-C13-C15
21	C	486	CLA	C11-C12-C13-C15
21	D	354	CLA	C6-C7-C8-C10
21	C	487	CLA	C2C-C3C-CAC-CBC
21	B	523	CLA	C2-C1-O2A-CGA
21	B	520	CLA	CAA-CBA-CGA-O2A
22	D	355	PHO	CAA-CBA-CGA-O2A
30	C	475	SQD	C15-C16-C17-C18
21	C	479	CLA	CAA-CBA-CGA-O2A
30	L	213	SQD	C4-C5-C6-S
26	C	476	LHG	C25-C26-C27-C28
21	D	356	CLA	C6-C7-C8-C9
28	C	474	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
21	A	363	CLA	C4B-C3B-CAB-CBB
21	A	364	CLA	C4B-C3B-CAB-CBB
21	B	511	CLA	C4B-C3B-CAB-CBB
21	B	513	CLA	C4B-C3B-CAB-CBB
21	B	515	CLA	C4B-C3B-CAB-CBB
21	B	516	CLA	C4B-C3B-CAB-CBB
21	B	523	CLA	C4B-C3B-CAB-CBB
21	C	477	CLA	C4B-C3B-CAB-CBB
21	C	479	CLA	C4B-C3B-CAB-CBB
21	C	480	CLA	C4B-C3B-CAB-CBB
21	C	481	CLA	C4B-C3B-CAB-CBB
21	C	484	CLA	C4B-C3B-CAB-CBB
21	D	354	CLA	C4B-C3B-CAB-CBB
28	B	528	DGD	O6D-C1D-O3G-C3G
21	B	511	CLA	CAA-CBA-CGA-O2A
30	C	475	SQD	O47-C7-C8-C9
22	D	355	PHO	C15-C16-C17-C18
30	D	361	SQD	C11-C12-C13-C14
21	B	521	CLA	CAA-CBA-CGA-O2A
21	K	483	CLA	CAA-CBA-CGA-O2A
21	B	520	CLA	C3-C5-C6-C7
21	C	484	CLA	C2-C1-O2A-CGA
21	D	356	CLA	C2-C1-O2A-CGA
22	D	355	PHO	C2-C1-O2A-CGA
21	A	364	CLA	C11-C12-C13-C15
21	C	481	CLA	C12-C13-C15-C16
21	D	356	CLA	C6-C7-C8-C10
21	D	354	CLA	CAA-CBA-CGA-O2A
21	A	364	CLA	C2C-C3C-CAC-CBC
32	D	357	PL9	C21-C22-C23-C24
21	C	480	CLA	CAA-CBA-CGA-O1A
32	D	357	PL9	C28-C29-C31-C32
21	B	514	CLA	C13-C15-C16-C17
21	C	483	CLA	CAA-CBA-CGA-O1A
30	C	475	SQD	O49-C7-C8-C9
30	F	224	SQD	C7-C8-C9-C10
21	B	526	CLA	C6-C7-C8-C9
21	K	483	CLA	C14-C13-C15-C16
22	D	355	PHO	CAA-CBA-CGA-O1A
27	D	360	LMG	C8-C7-O1-C1
21	C	481	CLA	O1A-CGA-O2A-C1
21	B	520	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	F	224	SQD	C44-C45-C46-O48
21	B	521	CLA	CAA-CBA-CGA-O1A
32	D	357	PL9	C11-C12-C13-C14
32	D	357	PL9	C41-C42-C43-C44
26	A	371	LHG	O7-C7-C8-C9
21	C	484	CLA	C13-C15-C16-C17
21	B	511	CLA	CAA-CBA-CGA-O1A
21	B	514	CLA	CAA-CBA-CGA-O2A
30	L	213	SQD	O47-C7-C8-C9
21	C	478	CLA	CAA-CBA-CGA-O2A
21	D	354	CLA	CAA-CBA-CGA-O1A
26	A	371	LHG	O9-C7-C8-C9

There are no ring outliers.

77 monomers are involved in 672 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	536	LMT	1	0
21	C	482	CLA	7	0
23	A	367	MES	13	0
25	D	358	BCR	8	0
25	B	529	BCR	5	0
28	C	492	DGD	14	0
25	B	530	BCR	2	0
29	O	274	LMT	1	0
27	M	217	LMG	3	0
21	A	362	CLA	19	0
33	V	164	HEM	5	0
21	B	516	CLA	7	0
21	C	479	CLA	19	0
30	C	475	SQD	5	0
28	A	375	DGD	1	0
29	T	226	LMT	1	0
21	C	486	CLA	21	0
21	B	525	CLA	6	0
25	B	527	BCR	1	0
32	D	357	PL9	30	0
27	D	360	LMG	30	0
21	A	364	CLA	7	0
21	C	480	CLA	14	0
21	C	488	CLA	6	0
22	D	355	PHO	15	0

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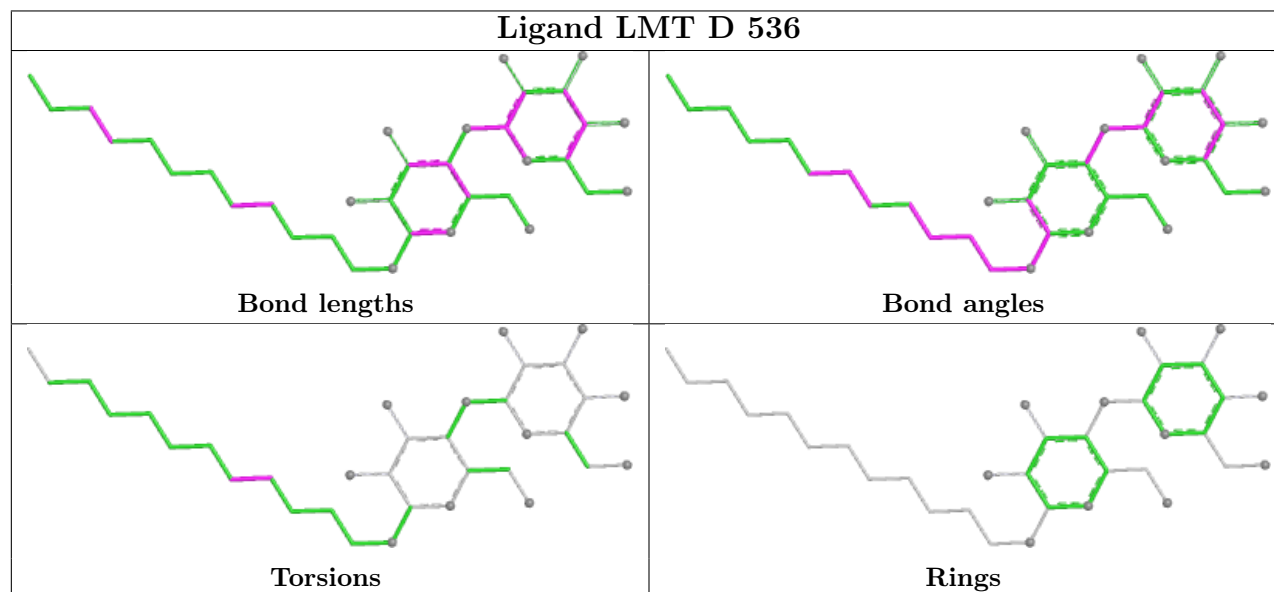
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21	B	511	CLA	3	0
21	B	512	CLA	9	0
27	C	494	LMG	6	0
29	D	363	LMT	2	0
30	D	361	SQD	9	0
21	B	517	CLA	19	0
21	C	487	CLA	15	0
27	A	373	LMG	40	0
27	J	492	LMG	4	0
21	B	524	CLA	5	0
25	J	115	BCR	7	0
21	B	521	CLA	13	0
21	B	522	CLA	10	0
25	C	490	BCR	7	0
21	A	363	CLA	14	0
21	B	513	CLA	23	0
29	I	274	LMT	2	0
21	B	519	CLA	6	0
28	B	528	DGD	23	0
21	C	484	CLA	13	0
26	A	371	LHG	7	0
21	C	483	CLA	11	0
21	B	523	CLA	5	0
21	C	477	CLA	9	0
25	Z	116	BCR	5	0
29	B	535	LMT	2	0
28	B	533	DGD	18	0
25	C	489	BCR	17	0
27	B	531	LMG	6	0
21	C	481	CLA	16	0
21	B	518	CLA	12	0
21	B	515	CLA	9	0
25	A	369	BCR	9	0
21	C	478	CLA	13	0
21	B	514	CLA	9	0
21	D	354	CLA	15	0
25	J	112	BCR	12	0
21	C	485	CLA	2	0
21	B	526	CLA	4	0
22	A	365	PHO	6	0
28	C	474	DGD	8	0

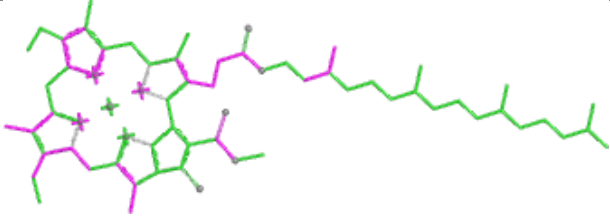
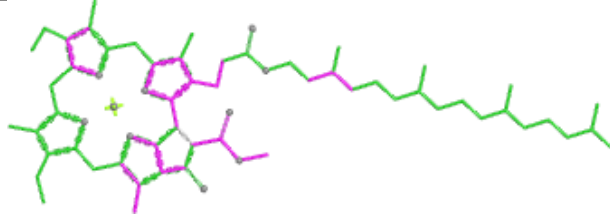
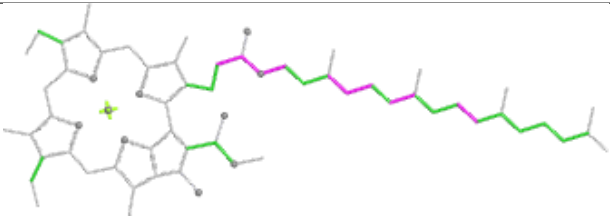
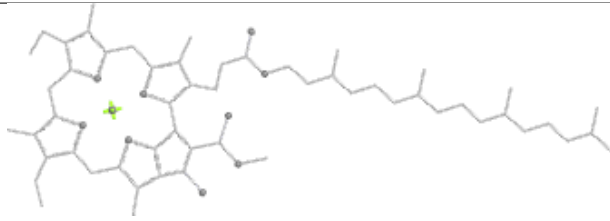
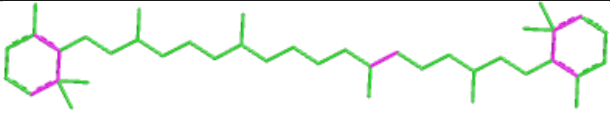
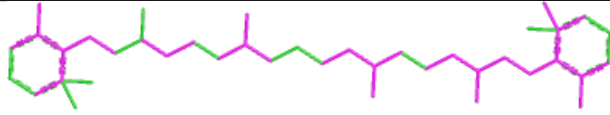
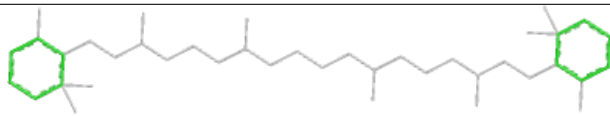
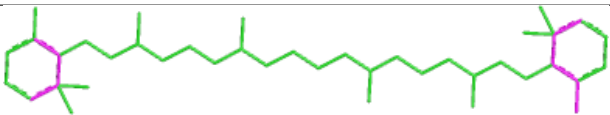
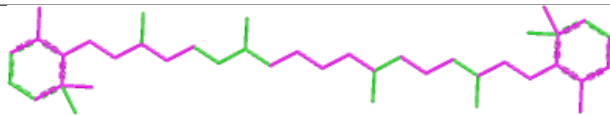
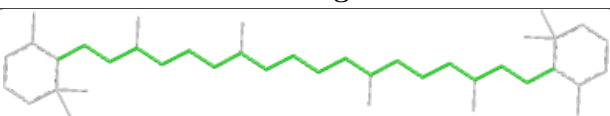
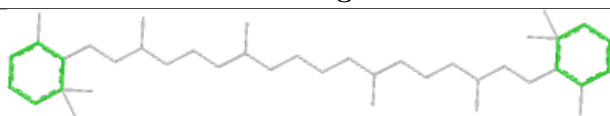
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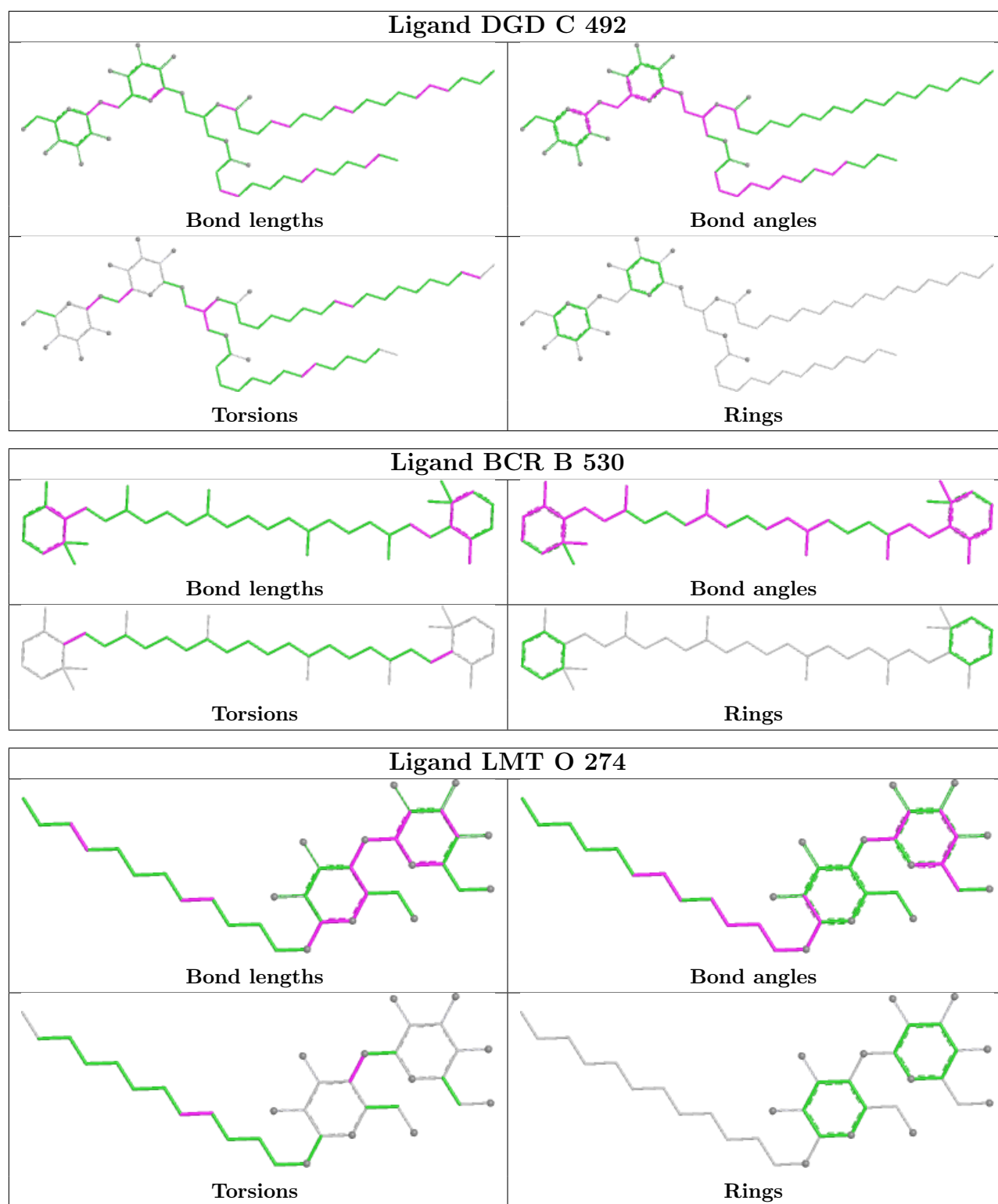
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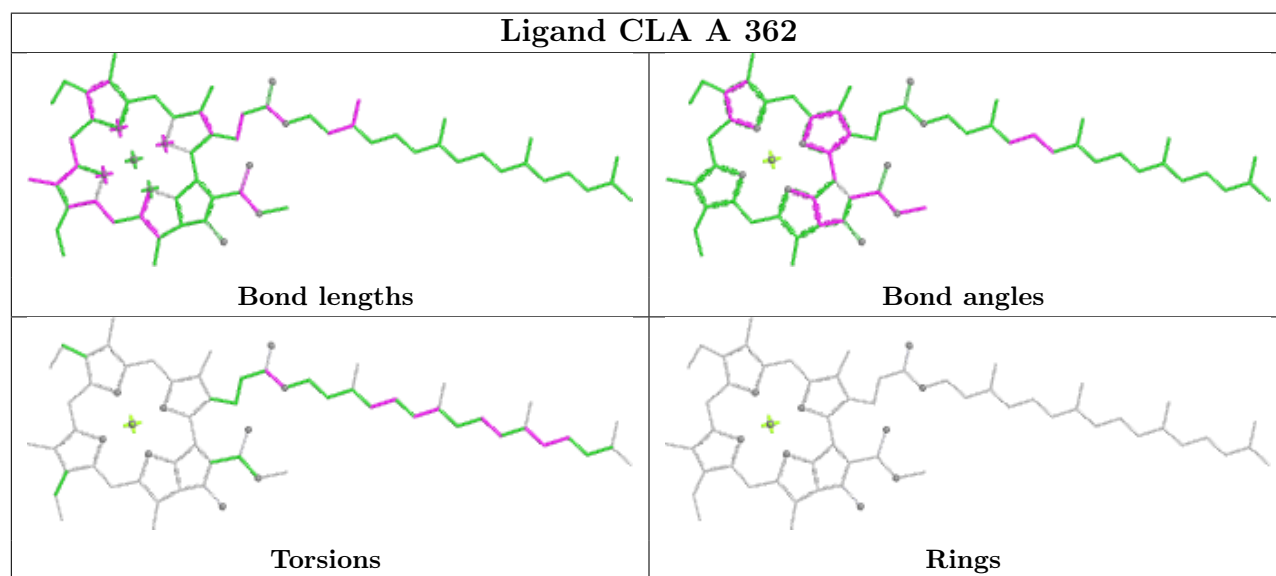
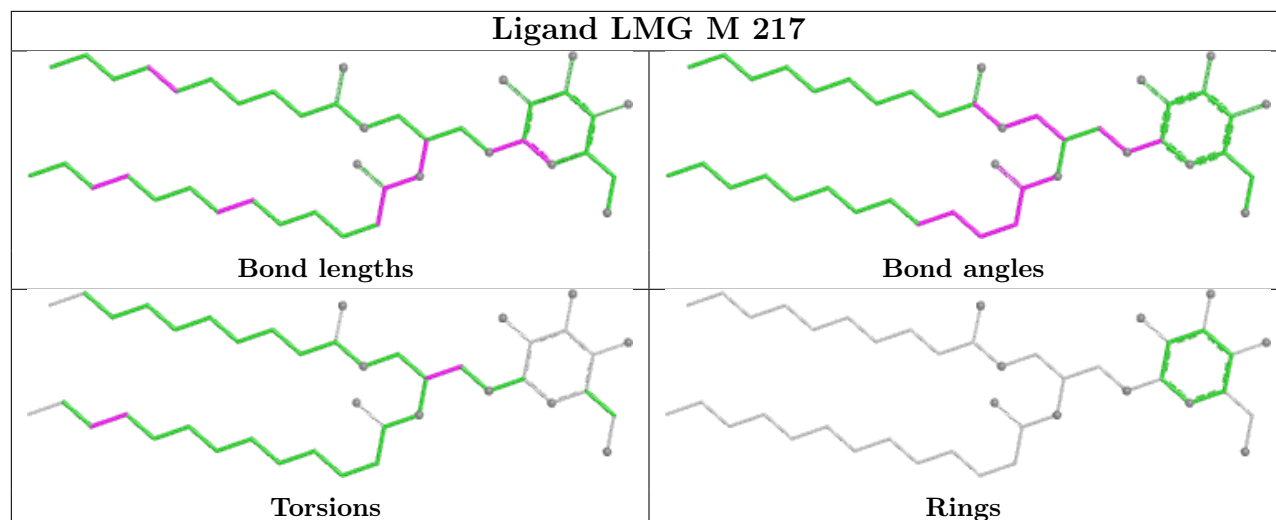
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	X	107	BCR	5	0
33	F	85	HEM	6	0
21	D	356	CLA	3	0
28	C	493	DGD	40	0
30	L	213	SQD	2	0
21	A	366	CLA	9	0
26	C	476	LHG	5	0
27	D	359	LMG	6	0
21	B	520	CLA	7	0
28	C	491	DGD	17	0

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

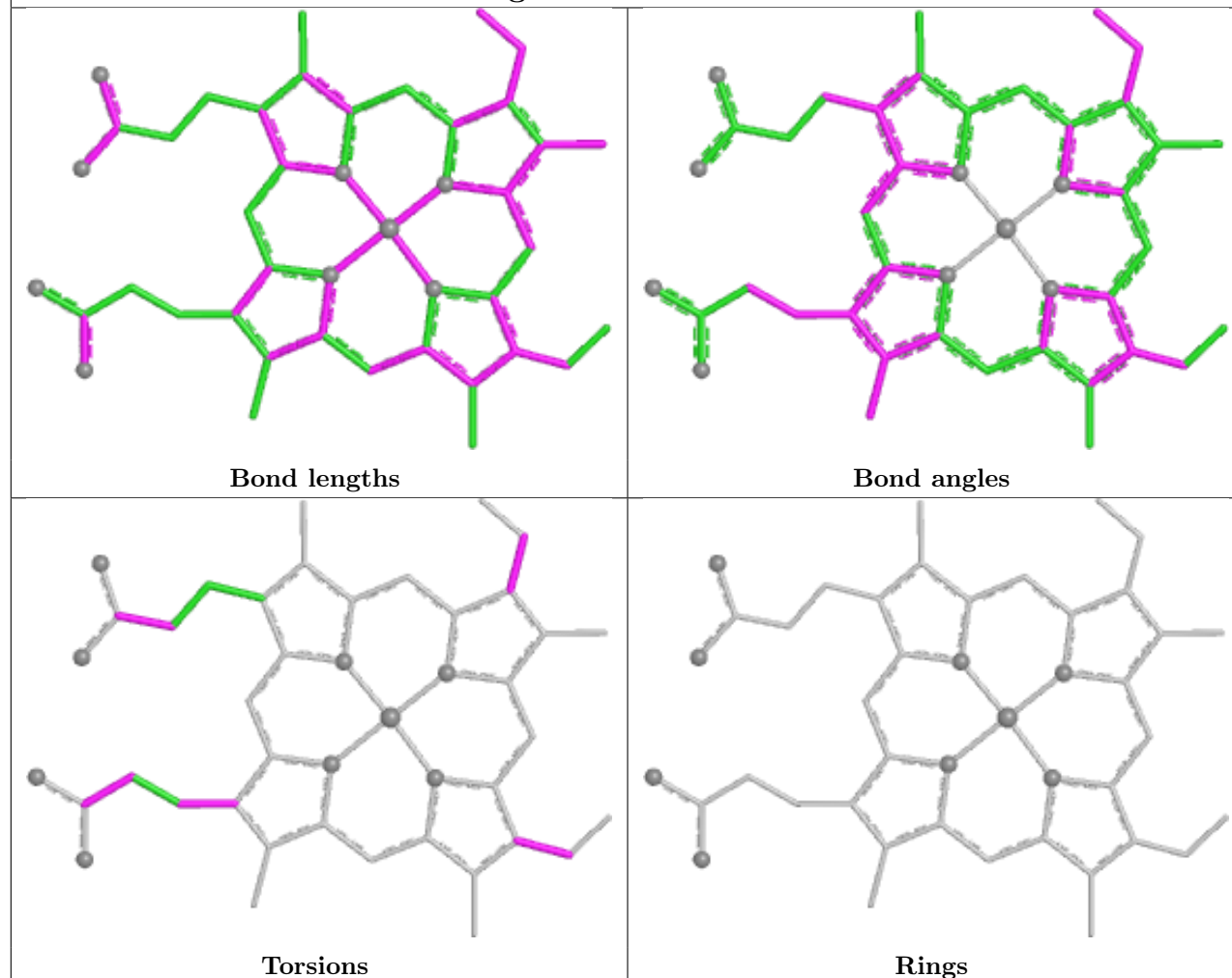


Ligand CLA C 482	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 358	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 529	
 Bond lengths	 Bond angles
 Torsions	 Rings

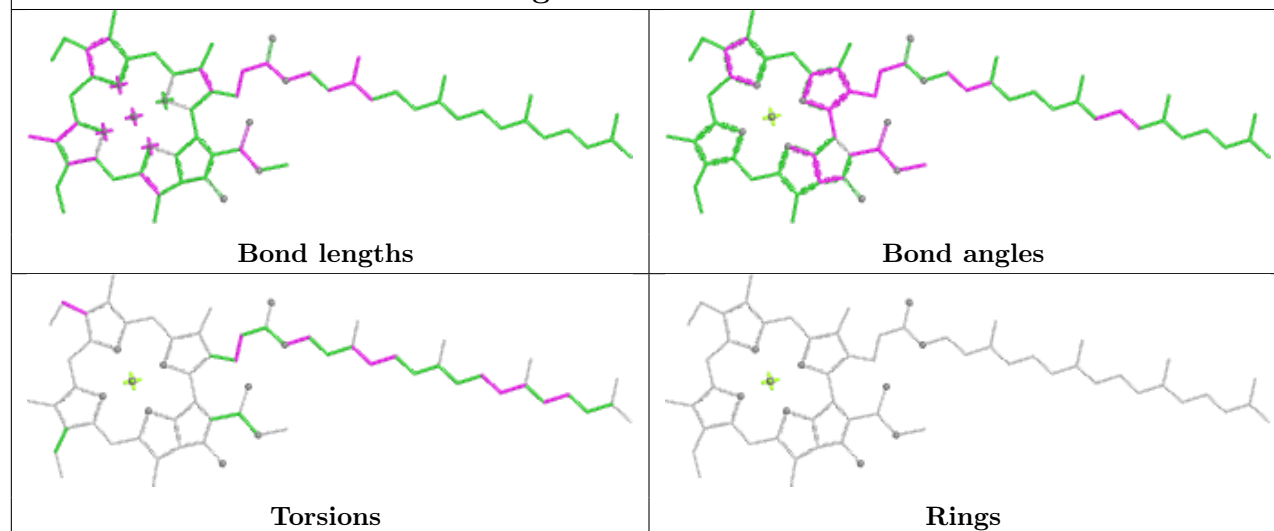


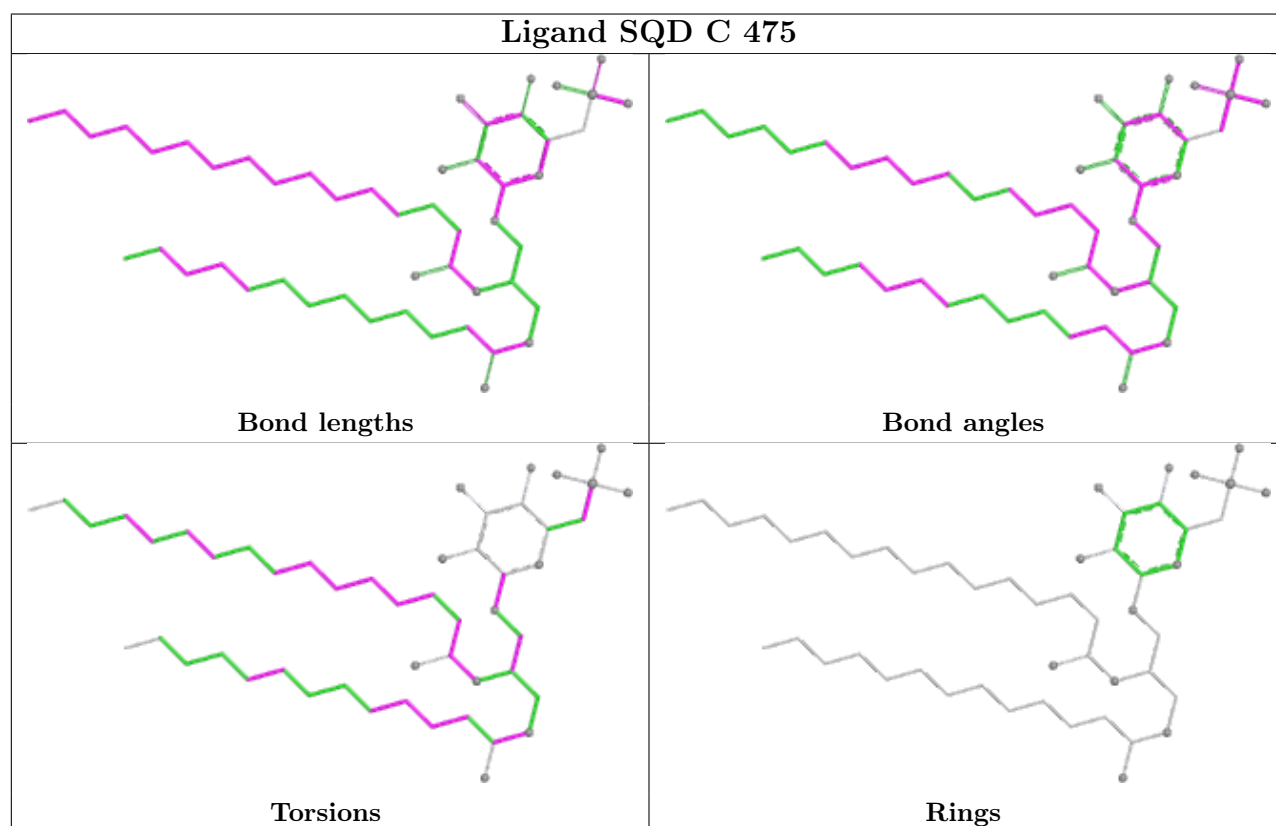
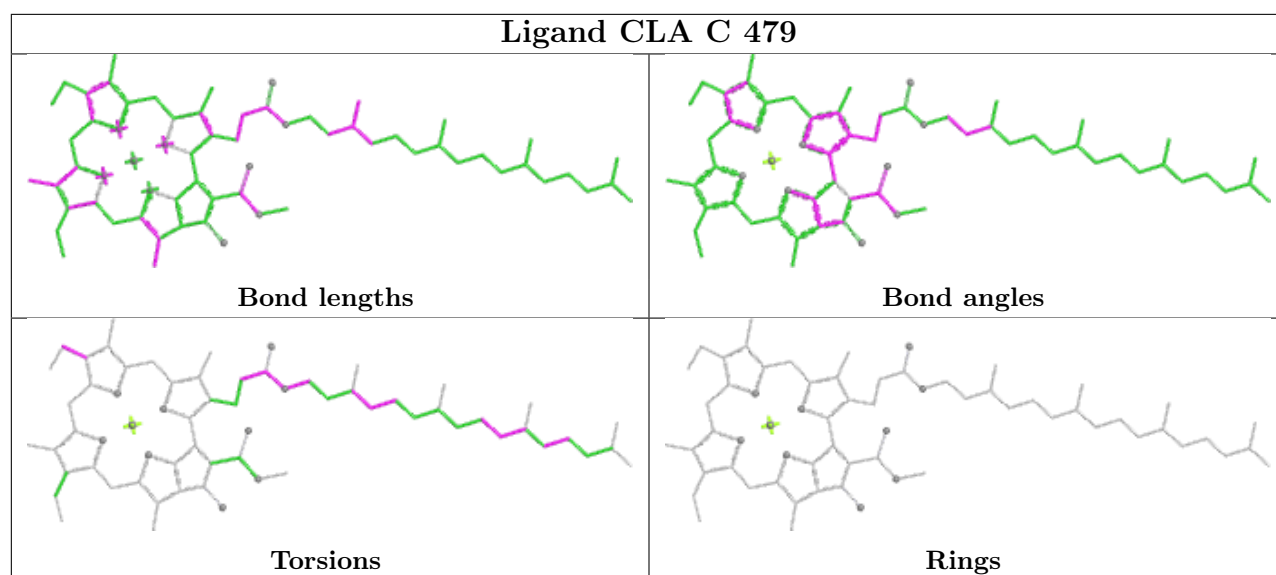


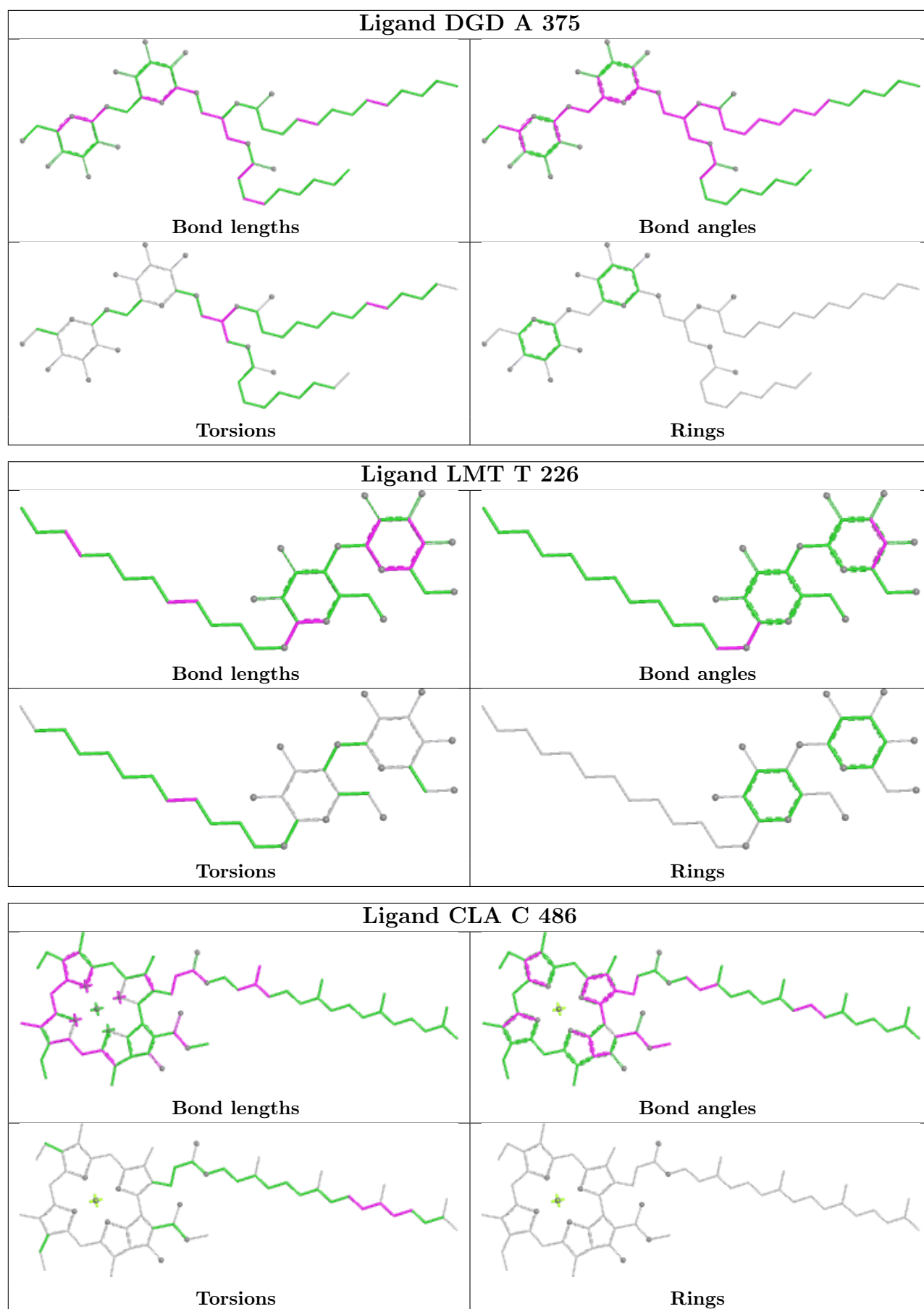
Ligand HEM V 164

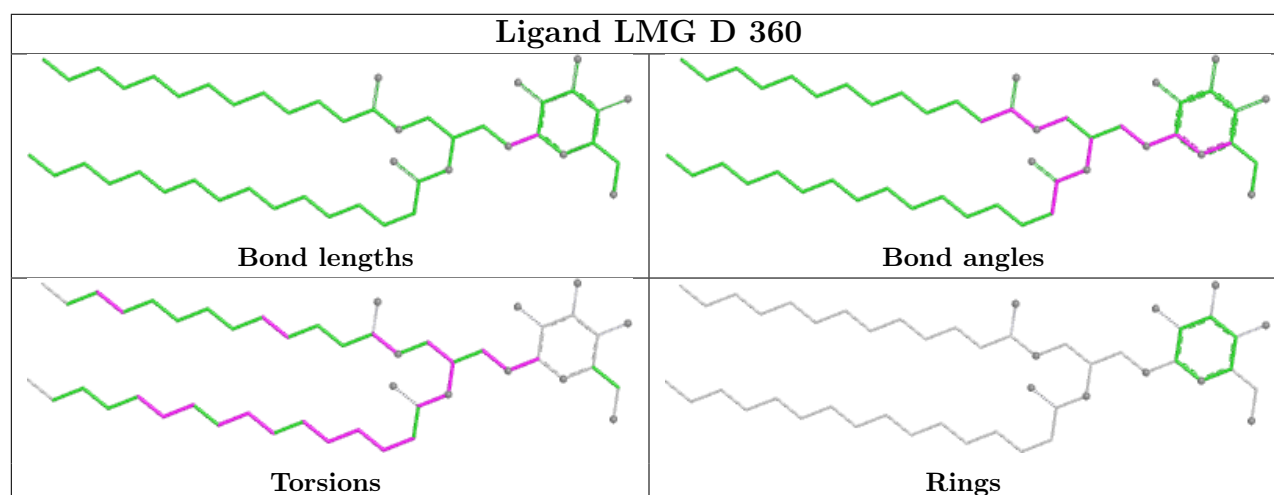
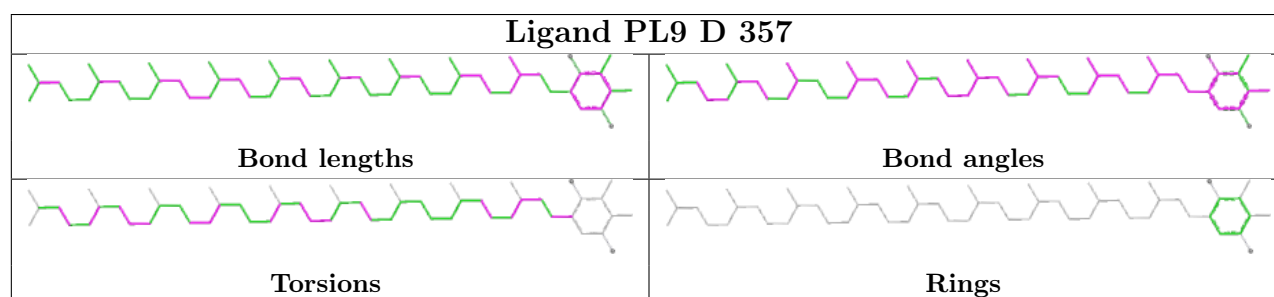
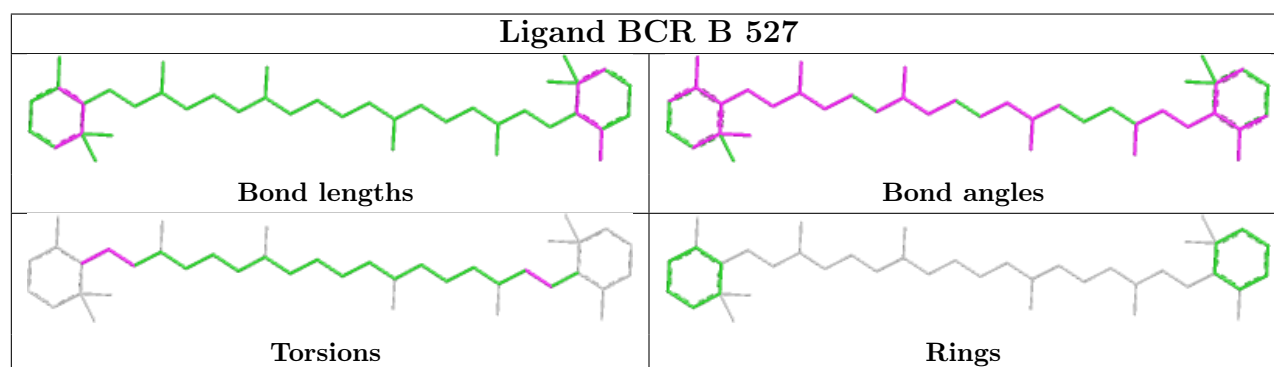
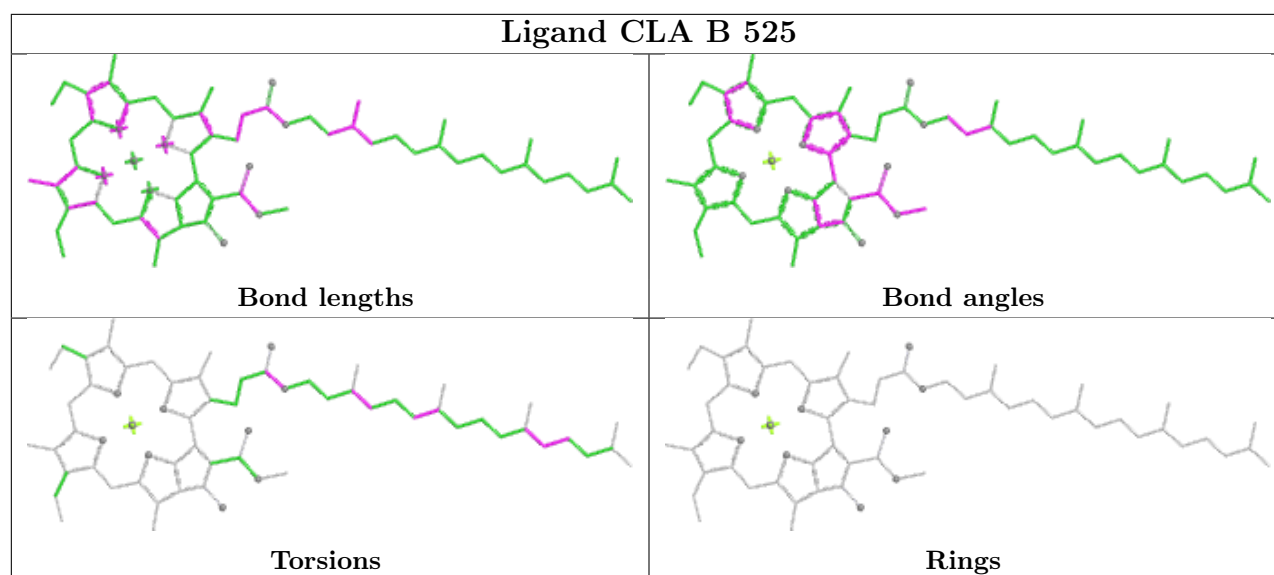


Ligand CLA B 516

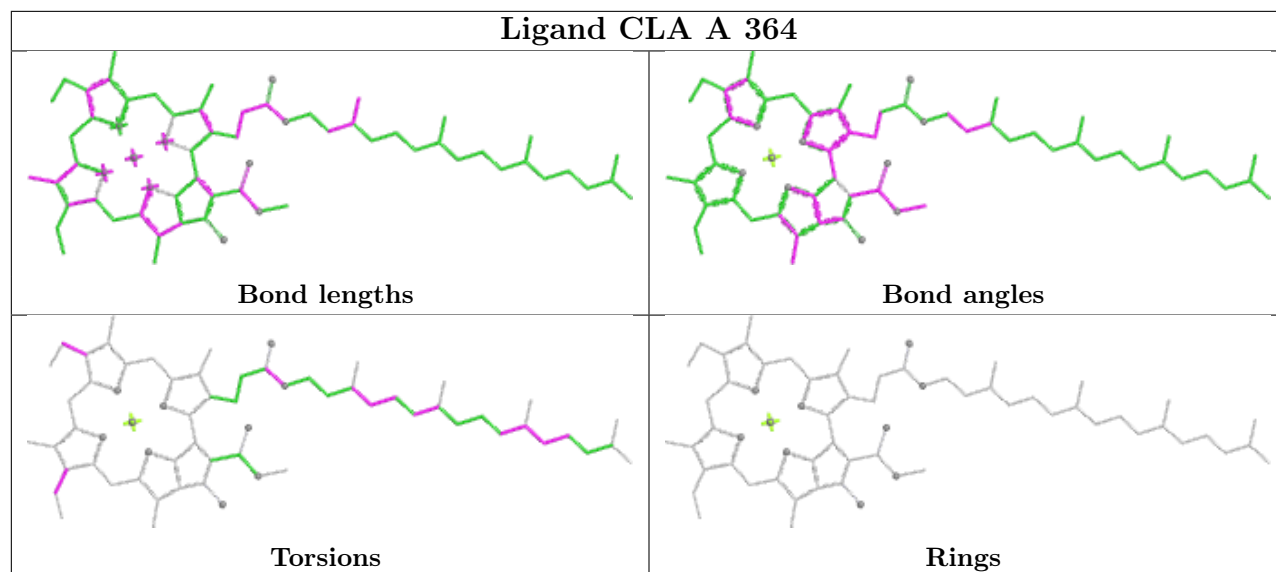




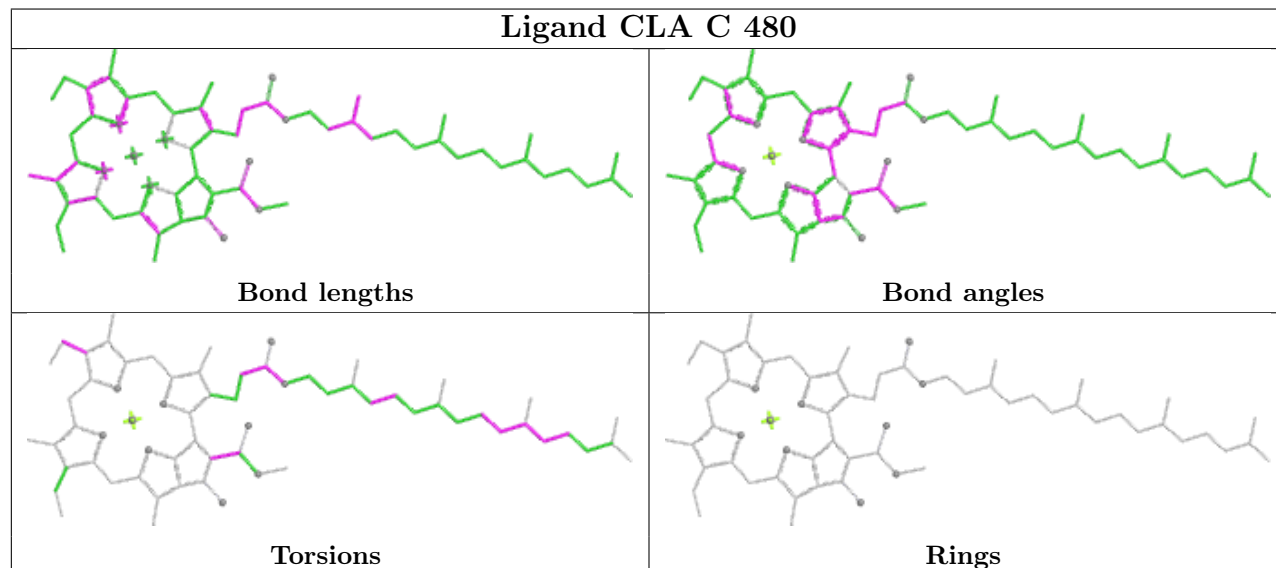




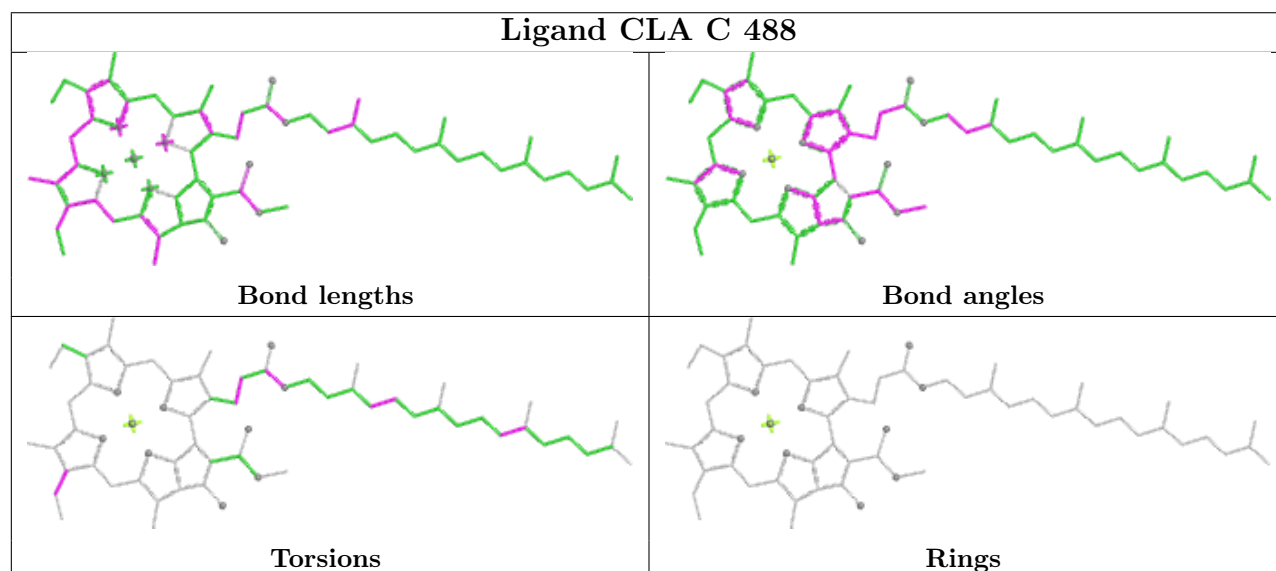
Ligand CLA A 364

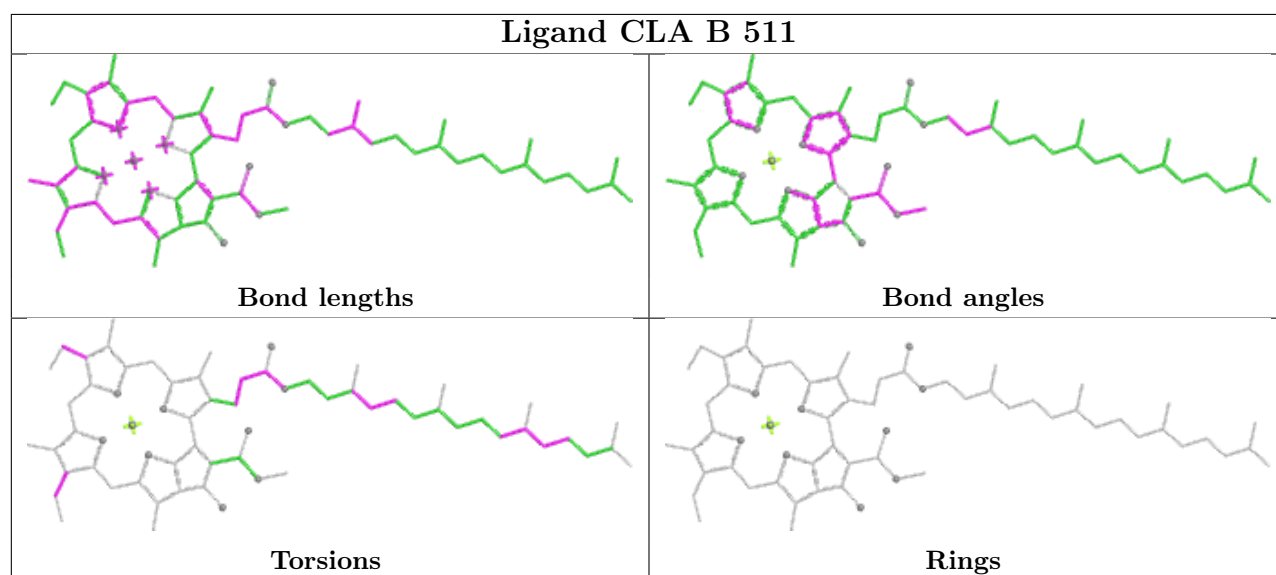
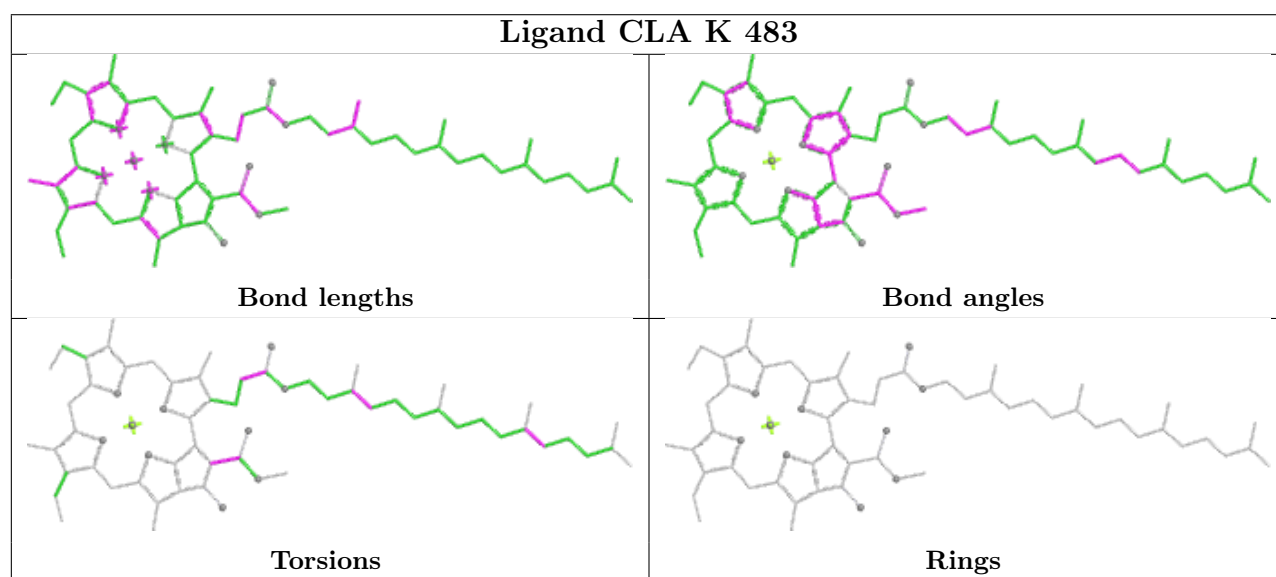
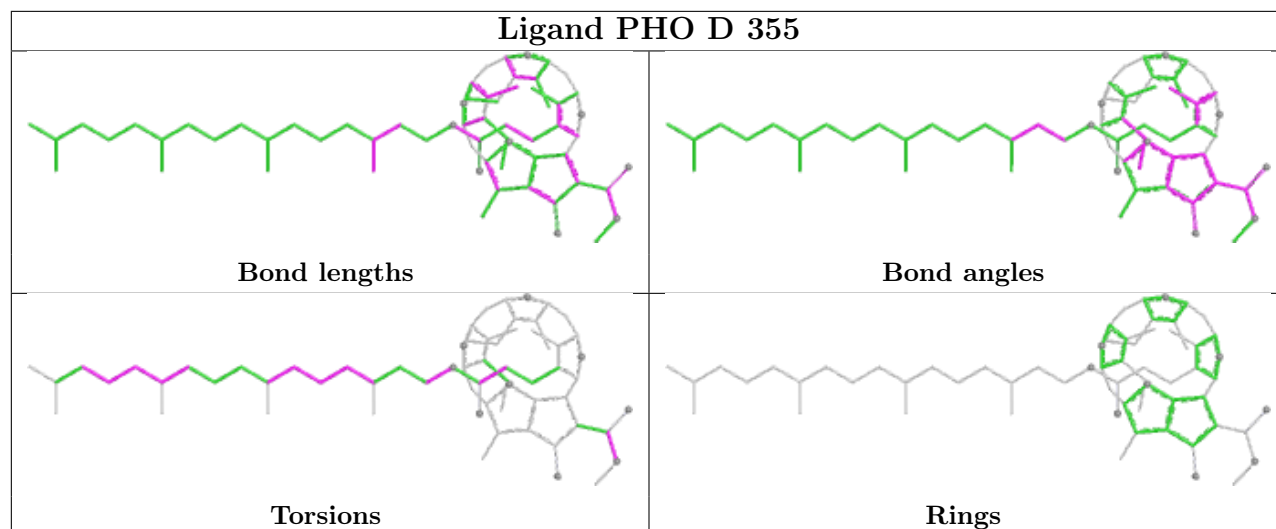


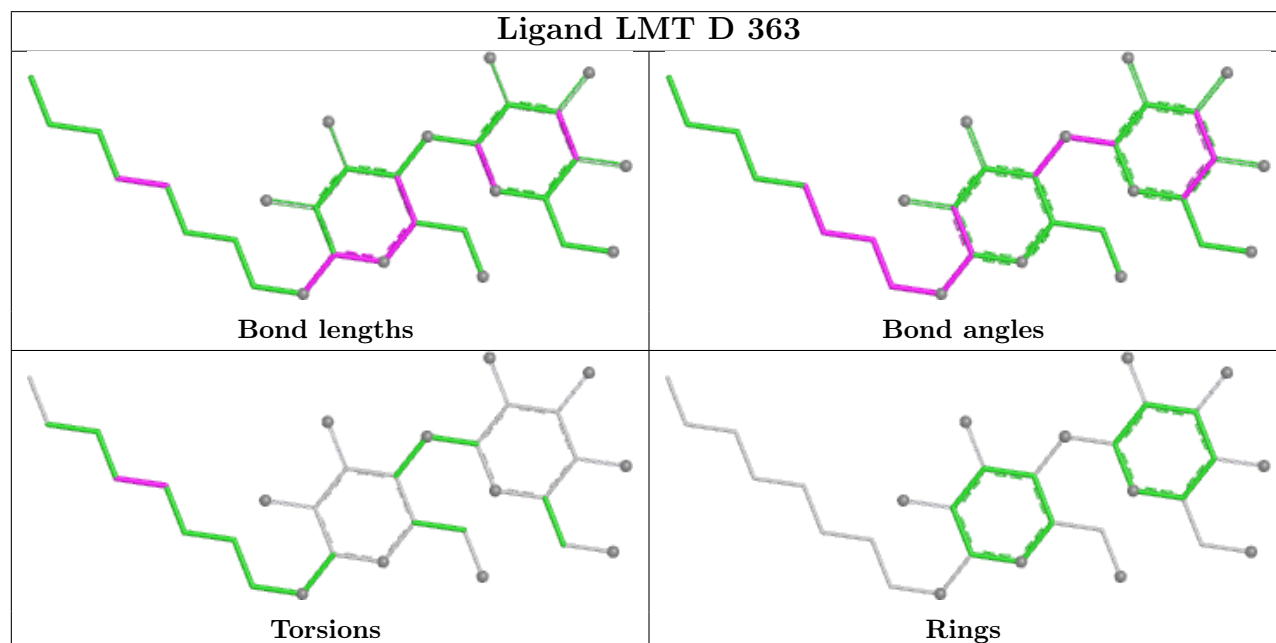
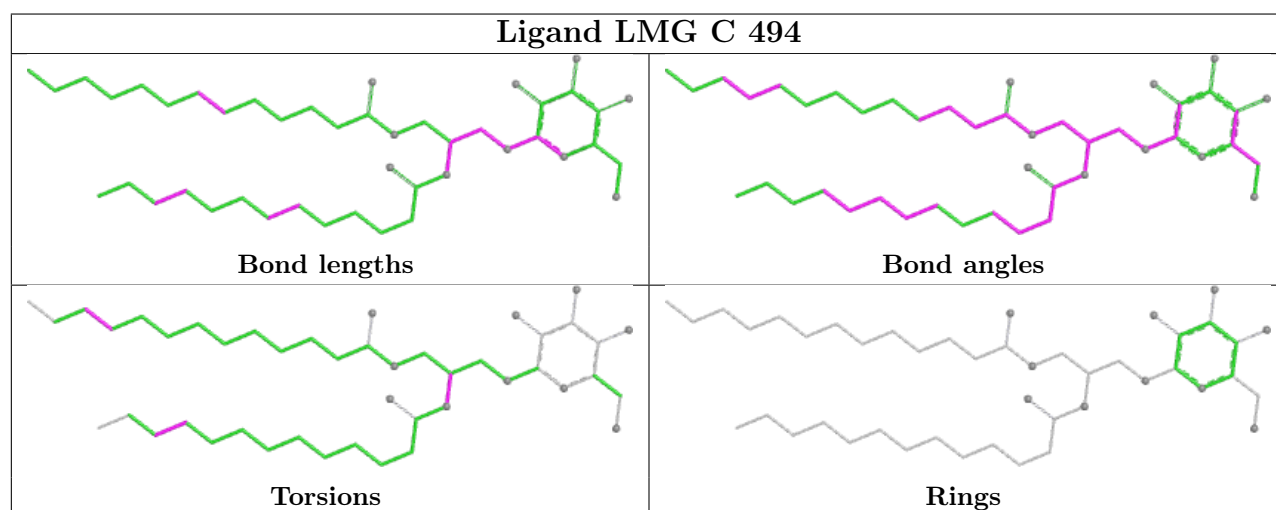
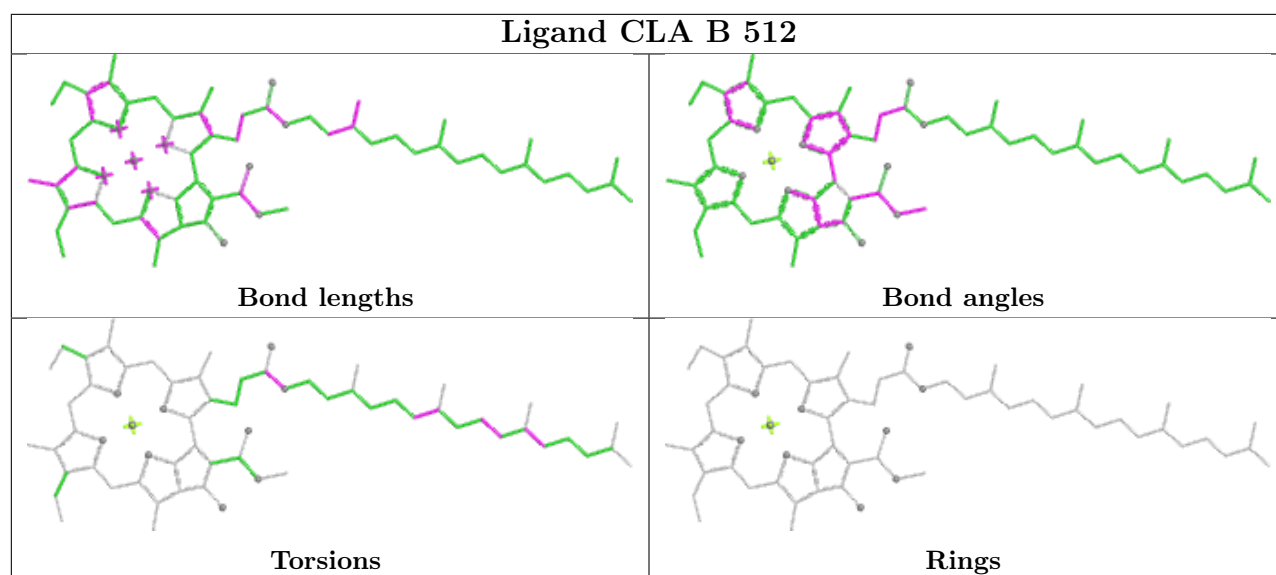
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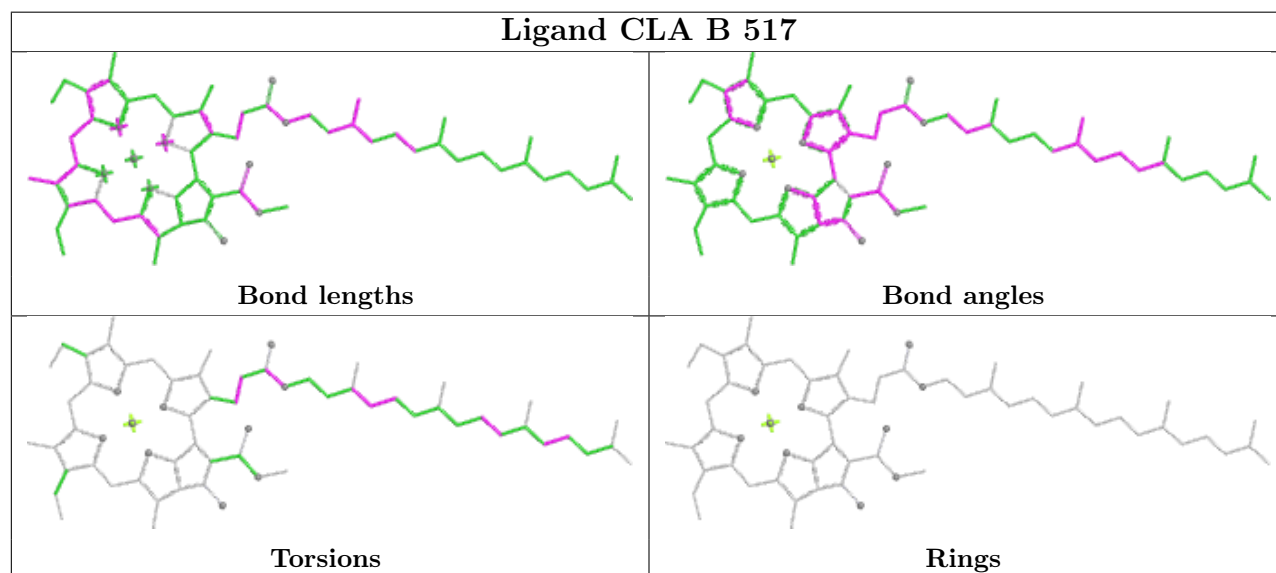
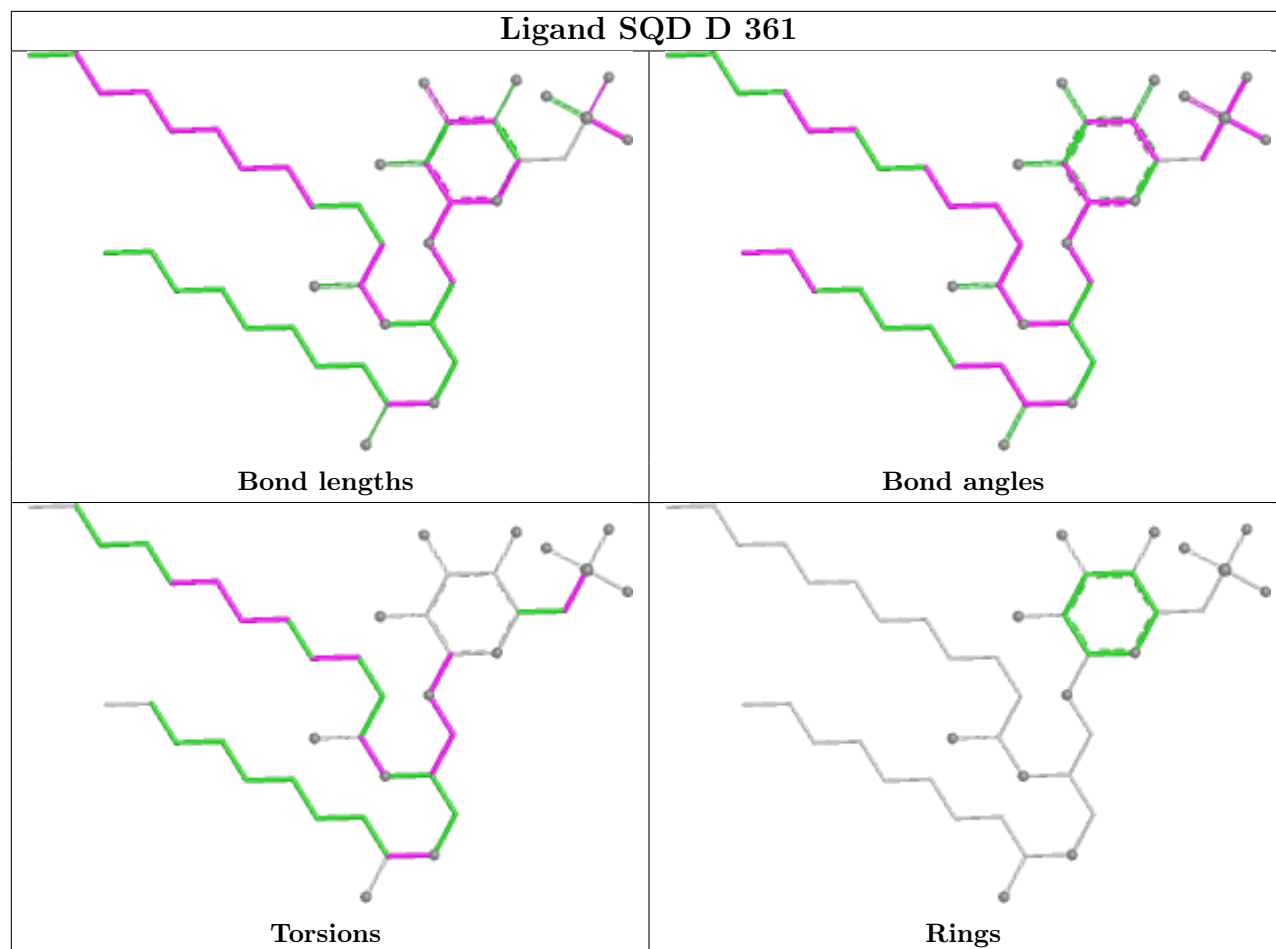


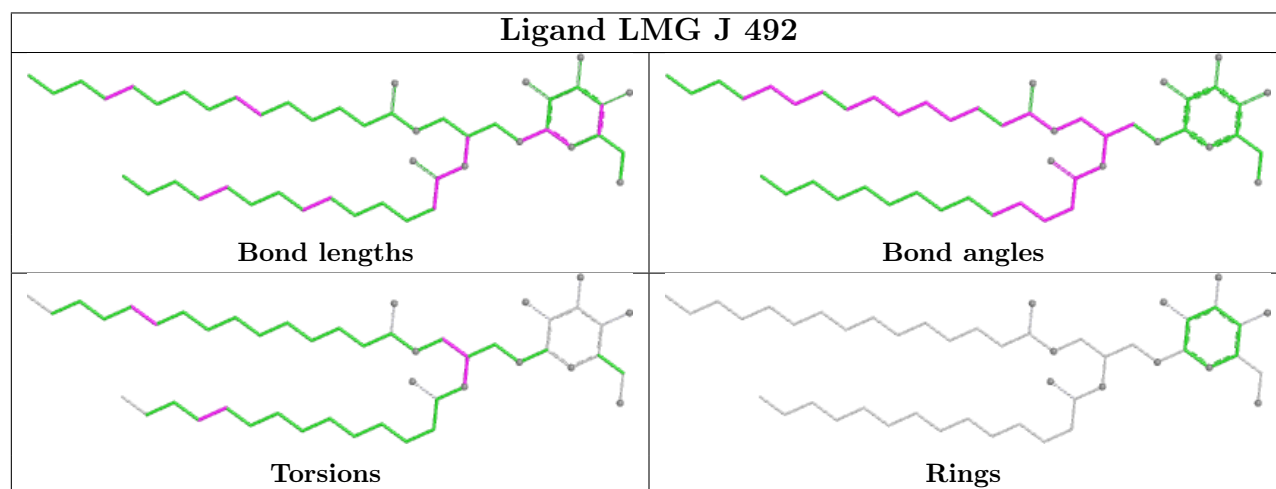
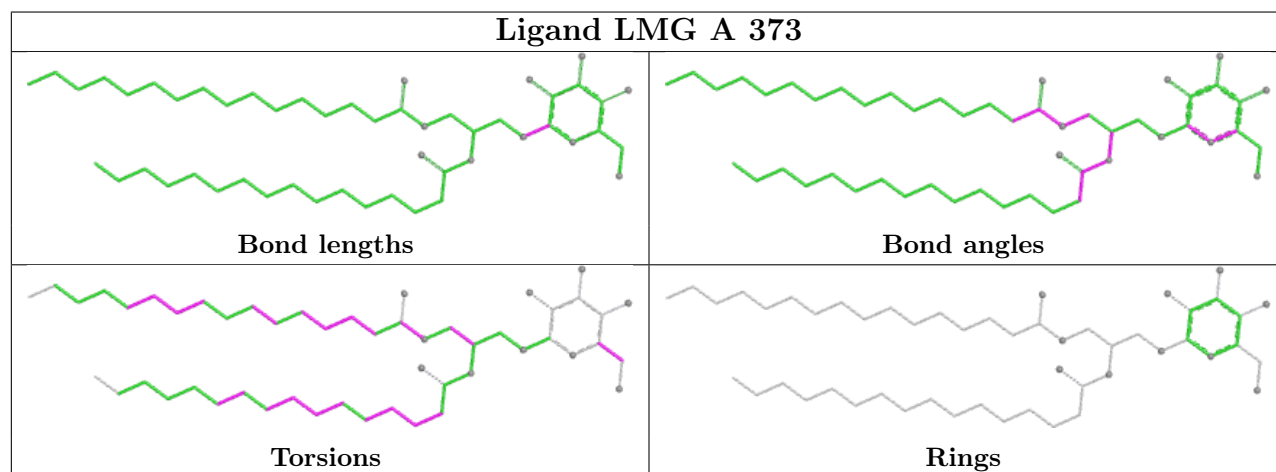
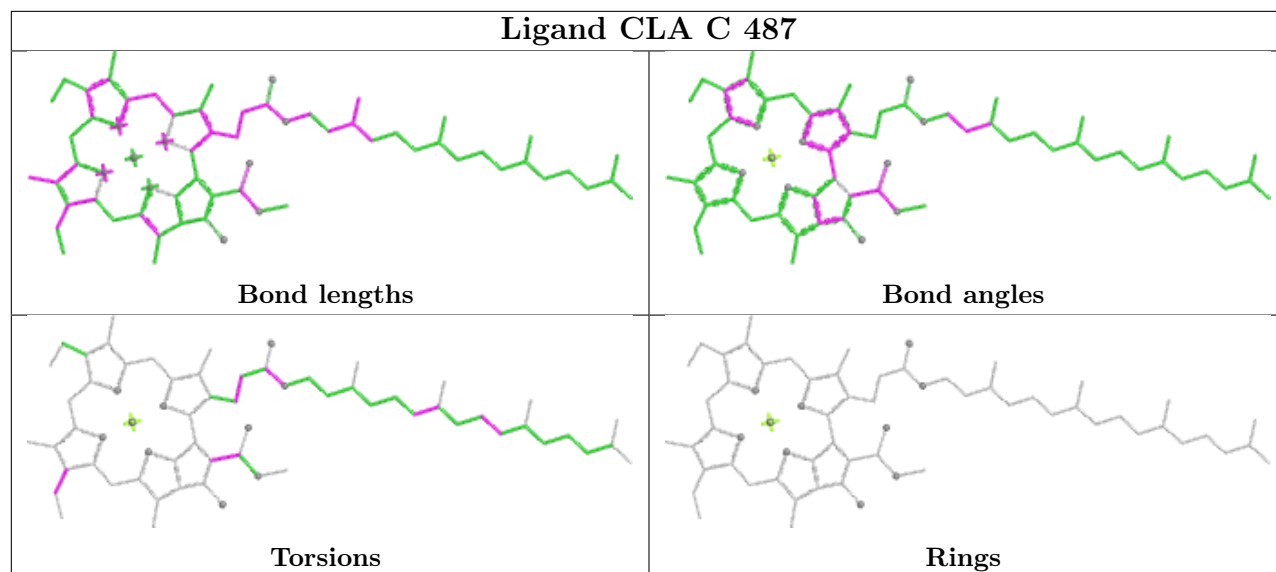
Ligand CLA C 488



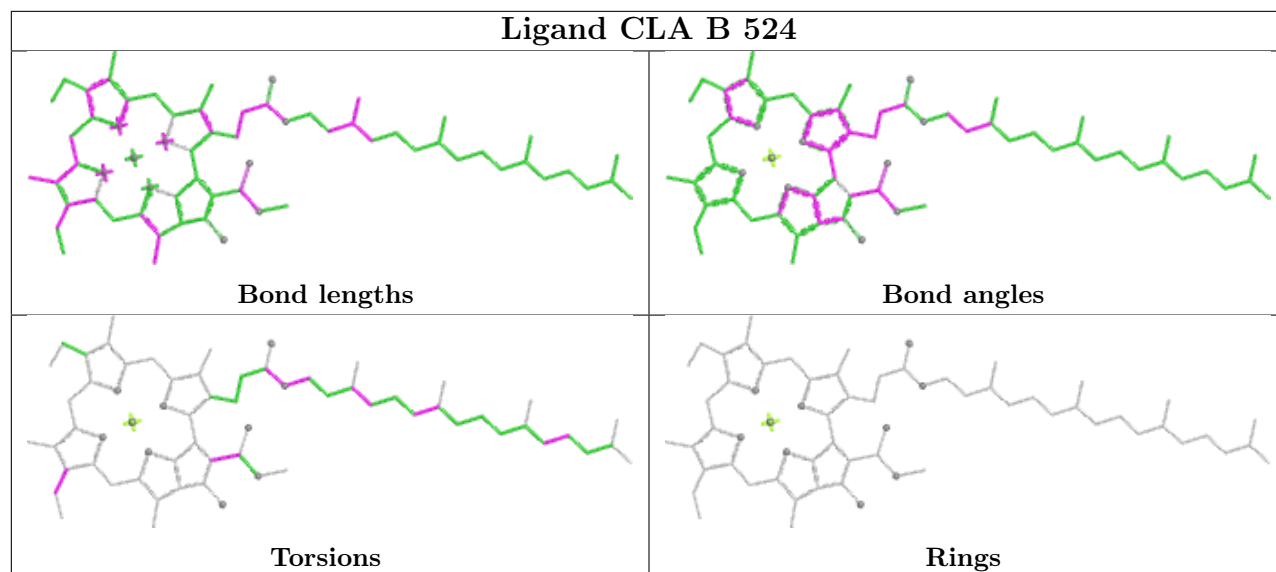




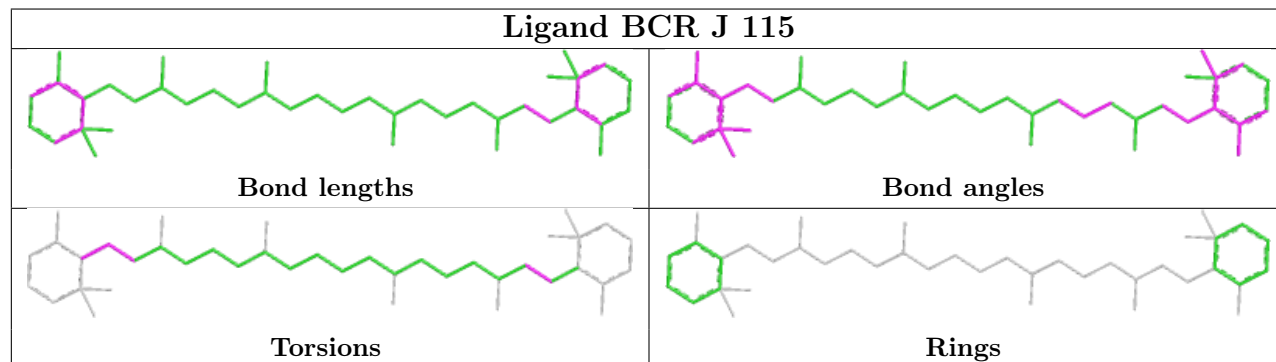




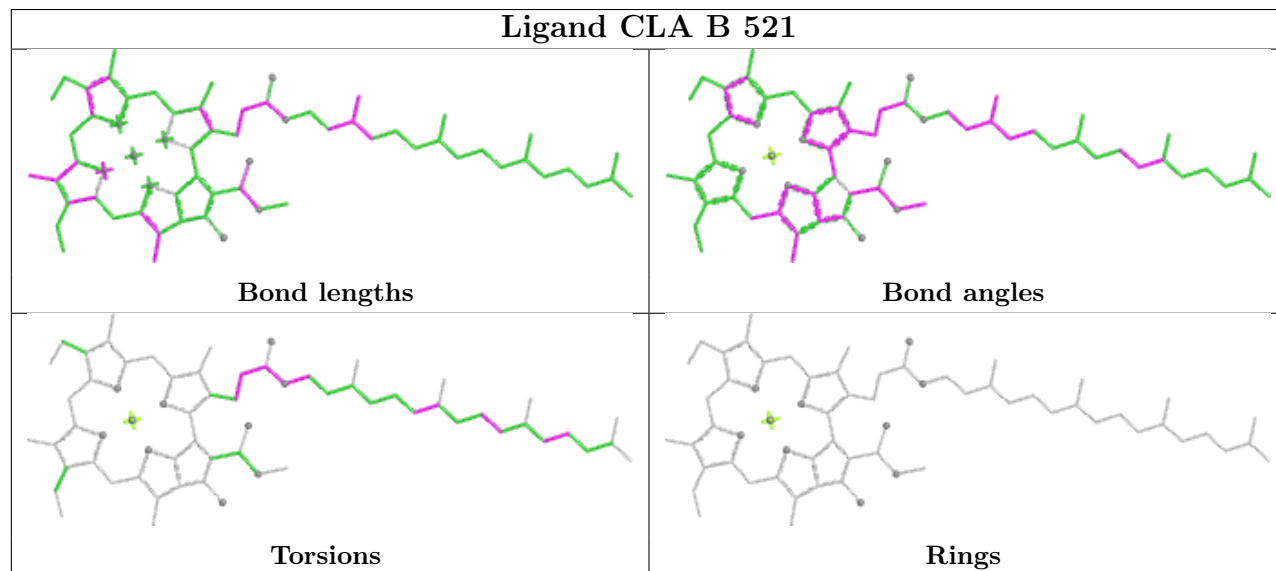
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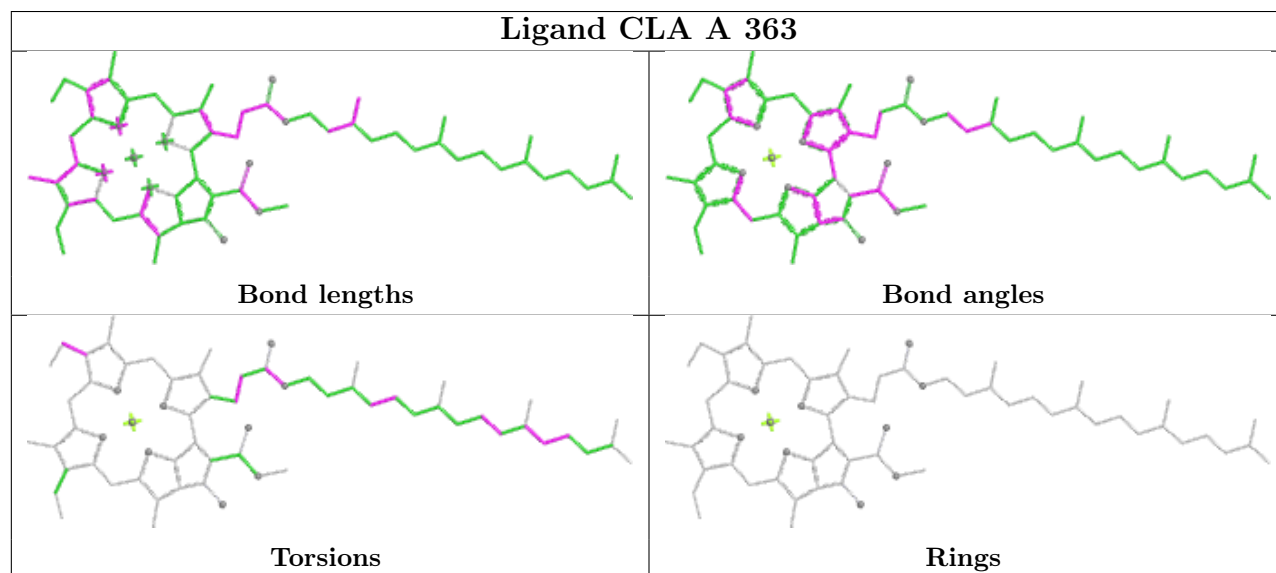
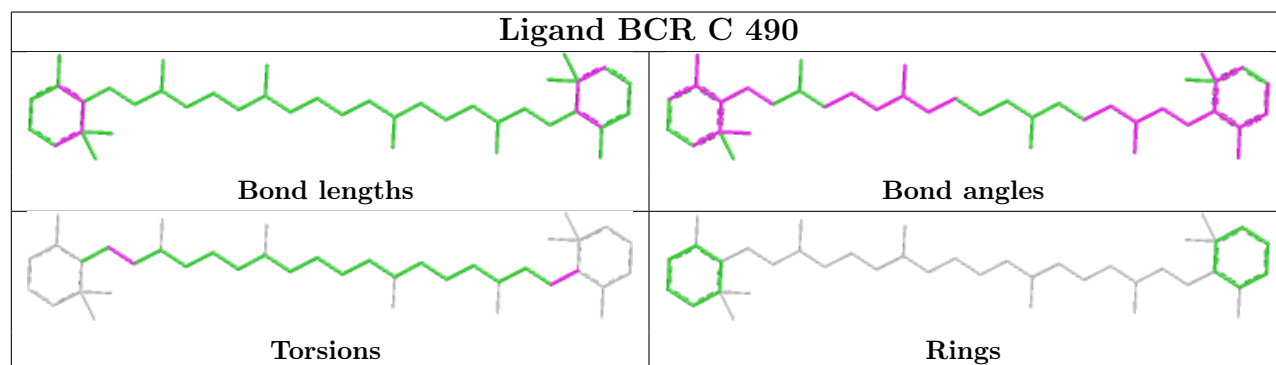
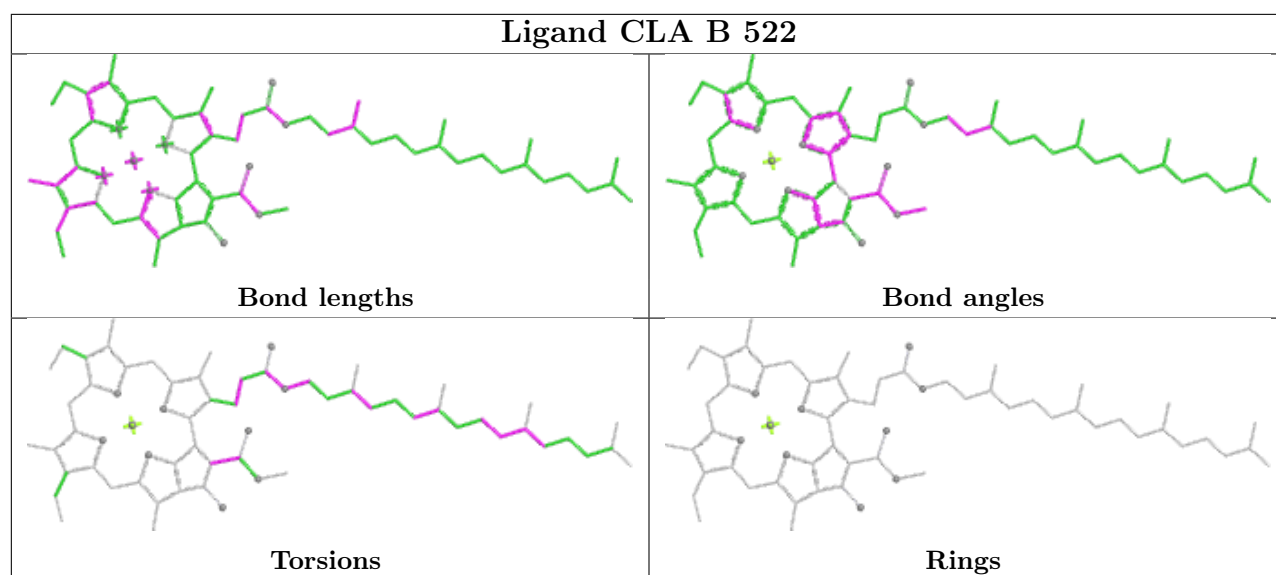


Ligand BCR J 115

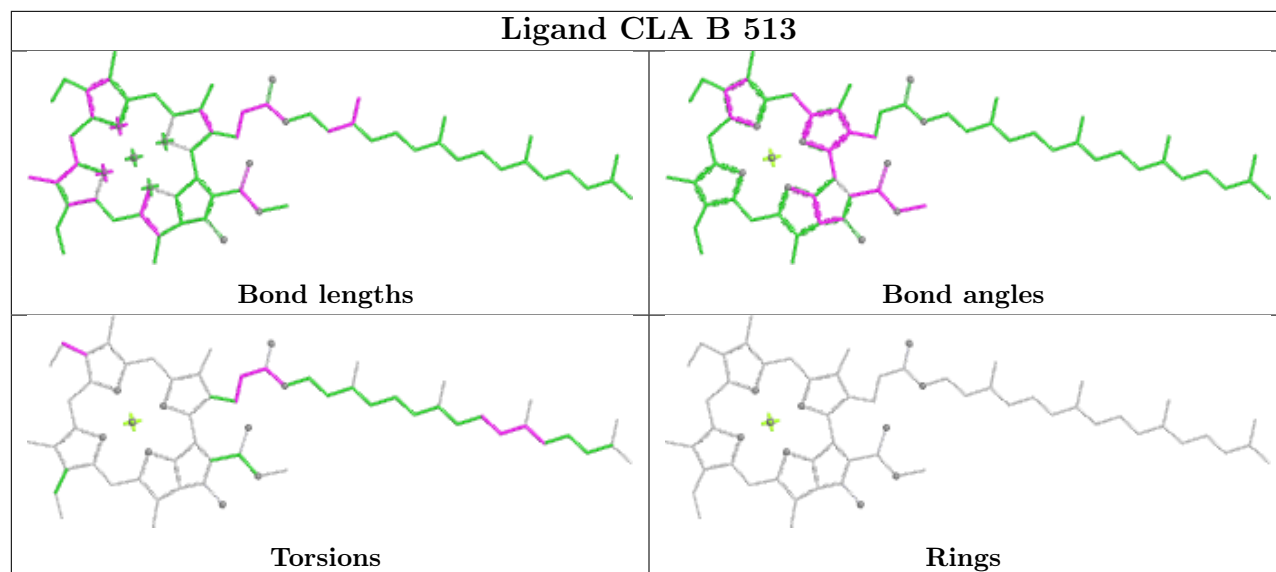


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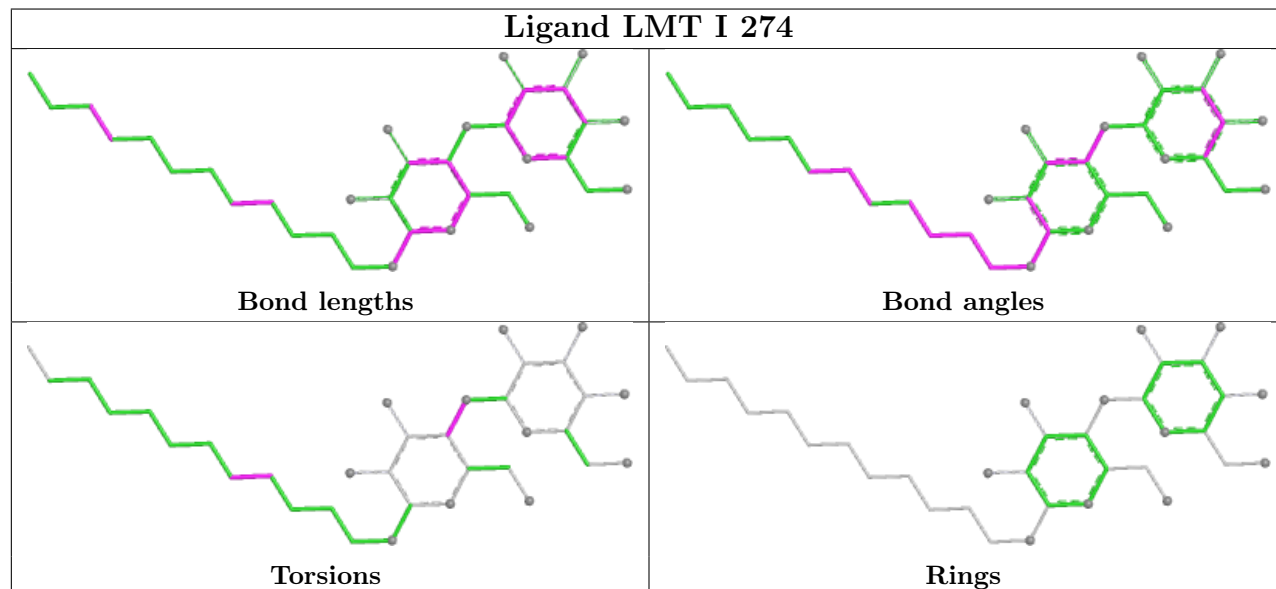




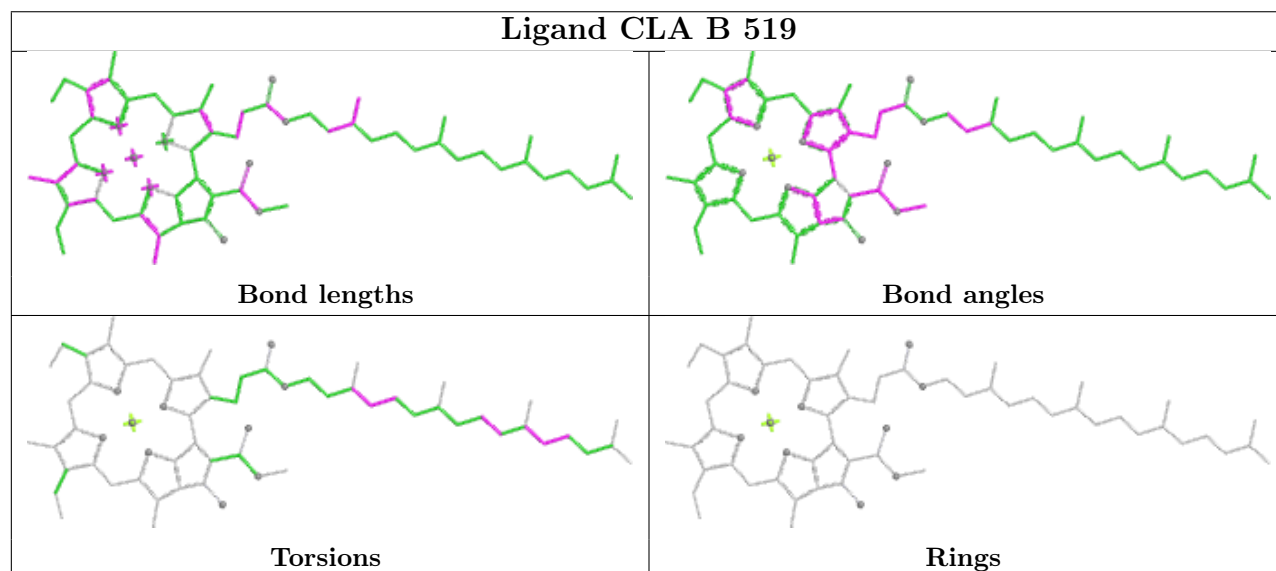
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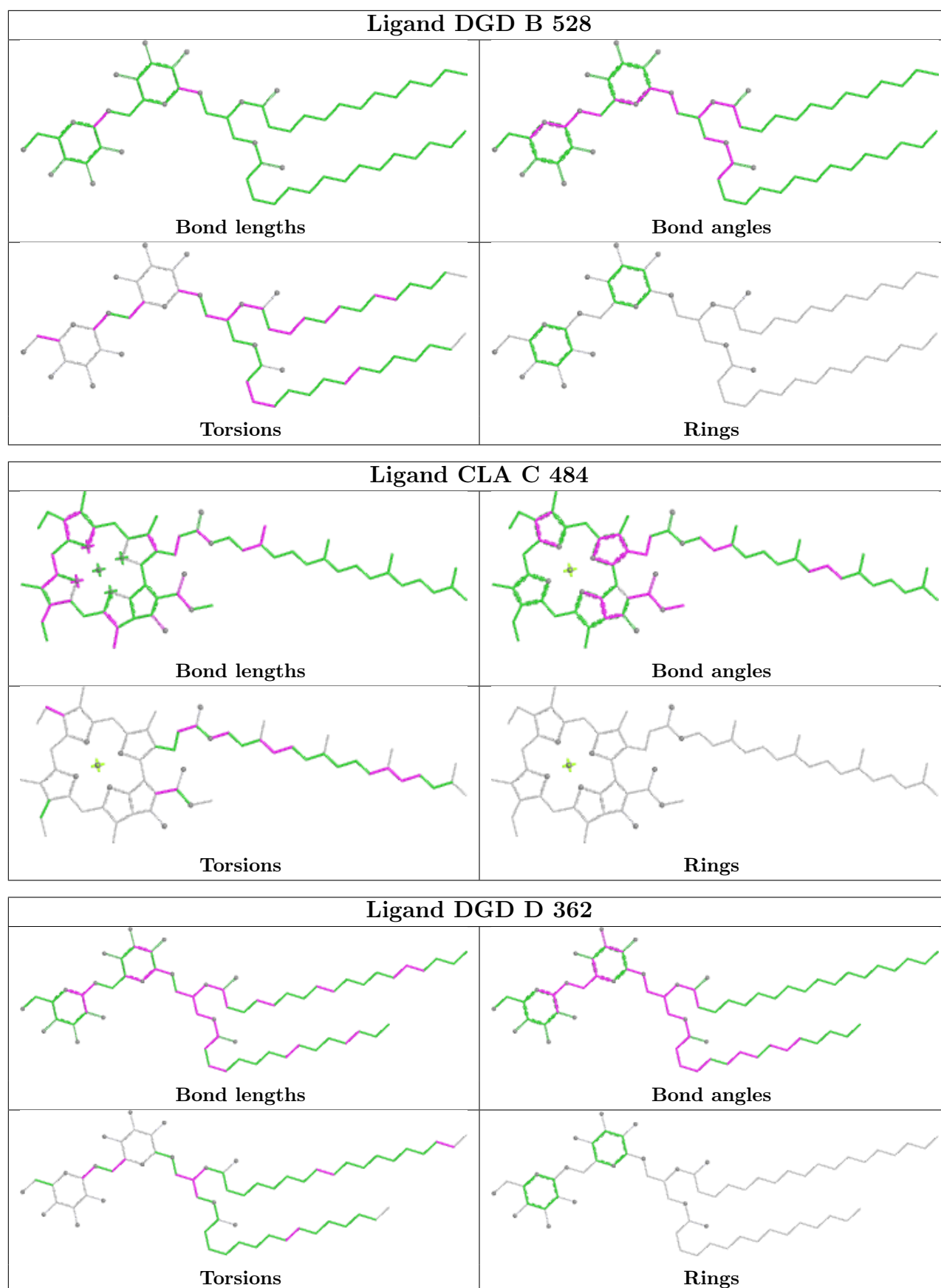


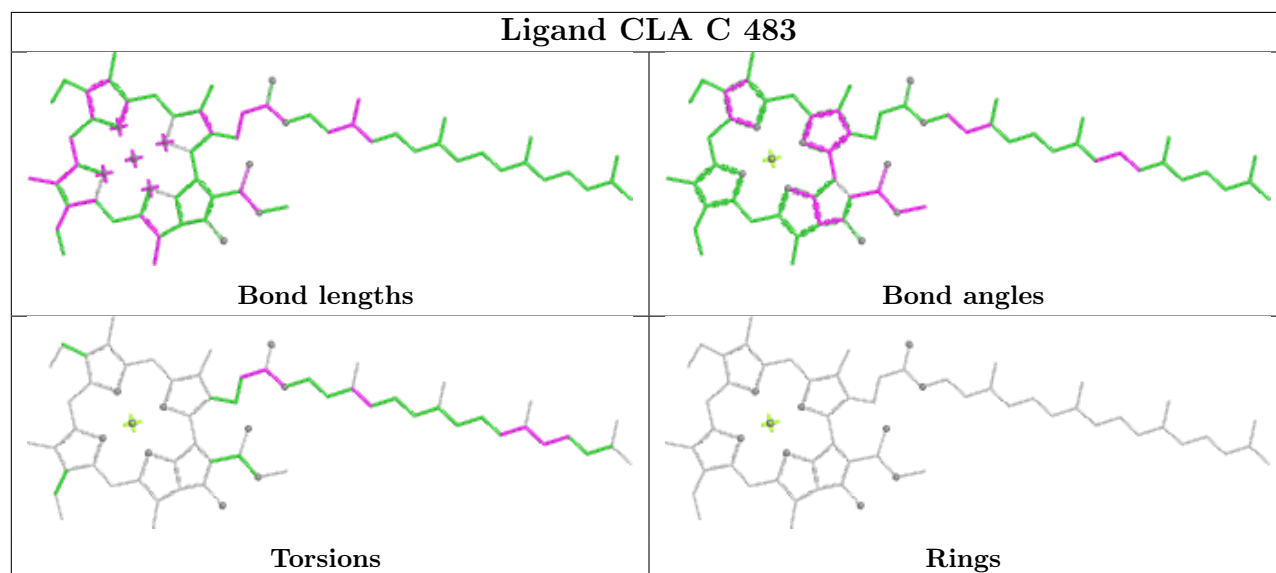
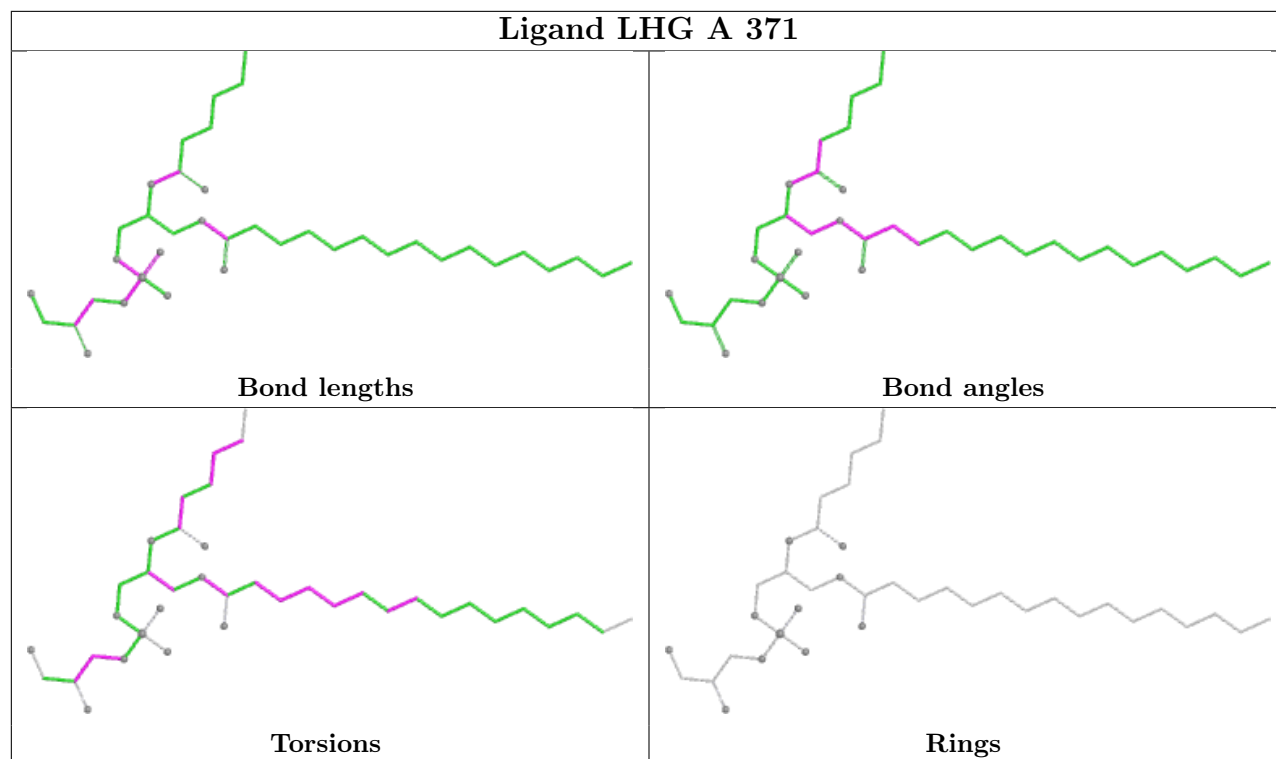
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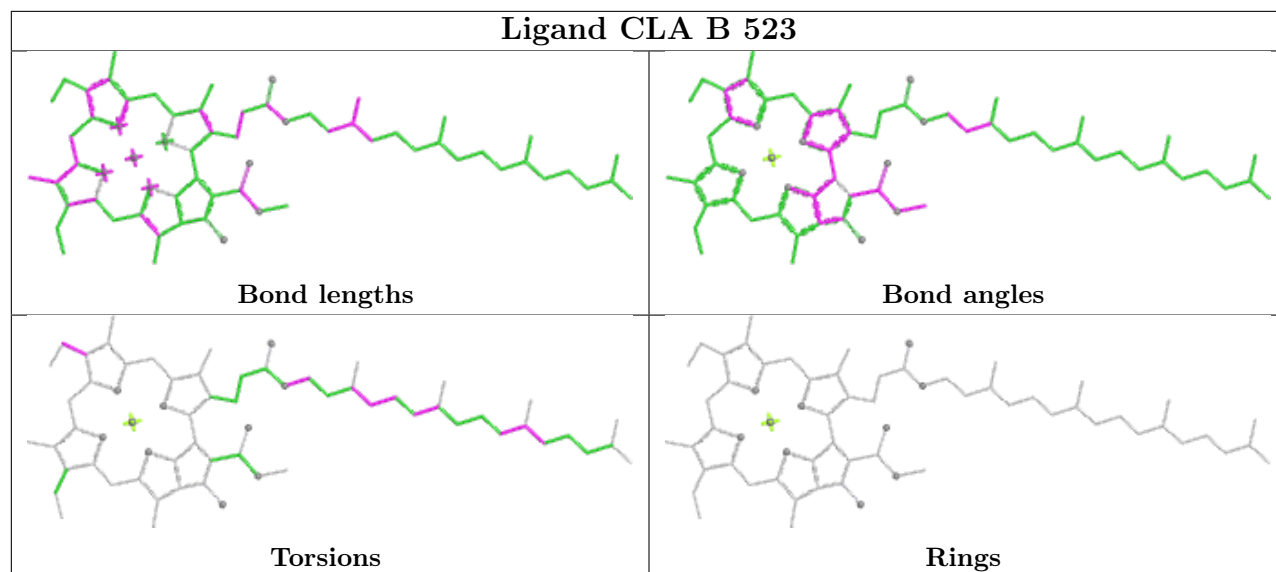
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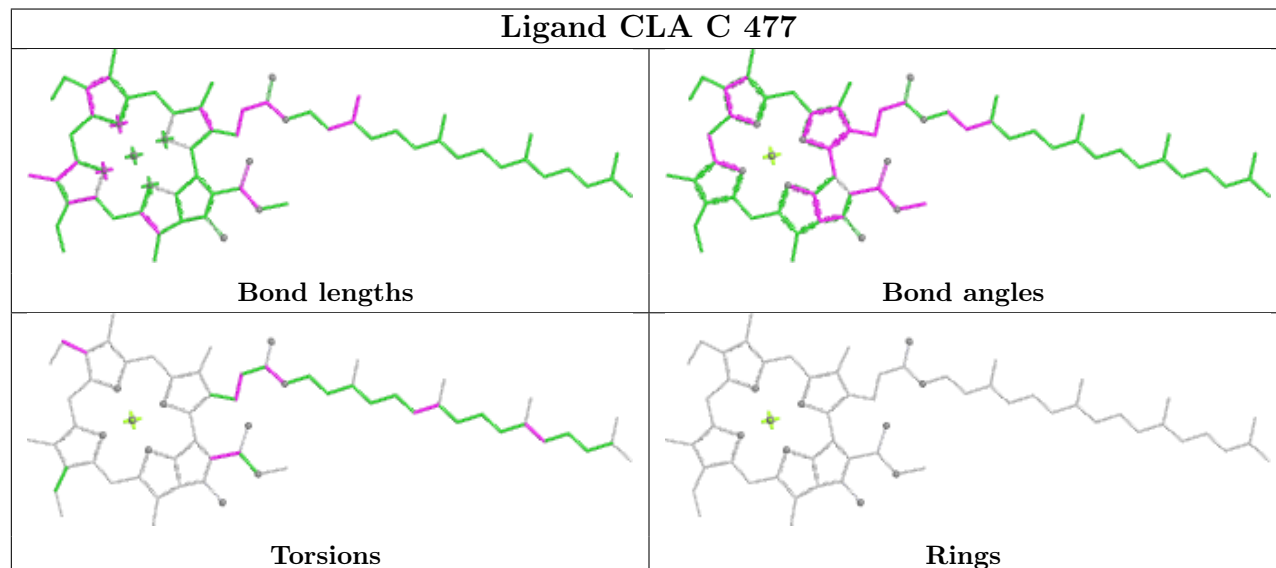




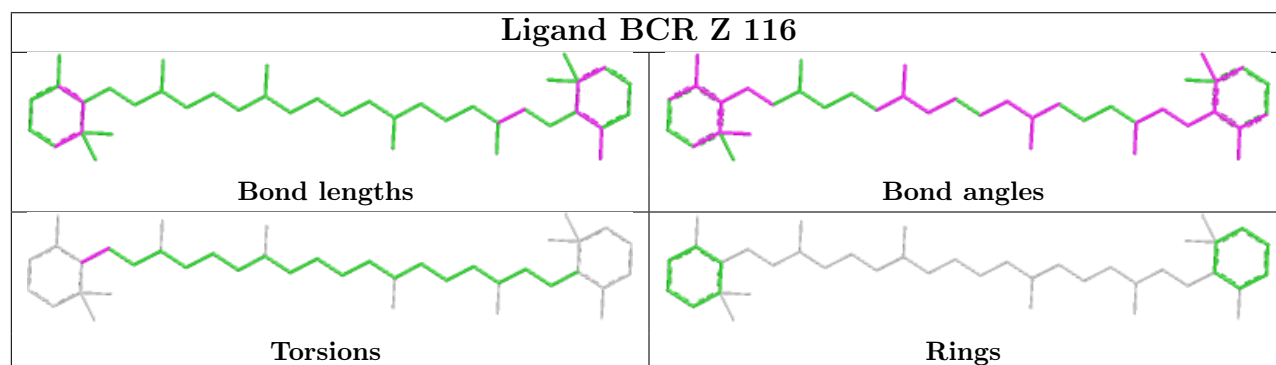
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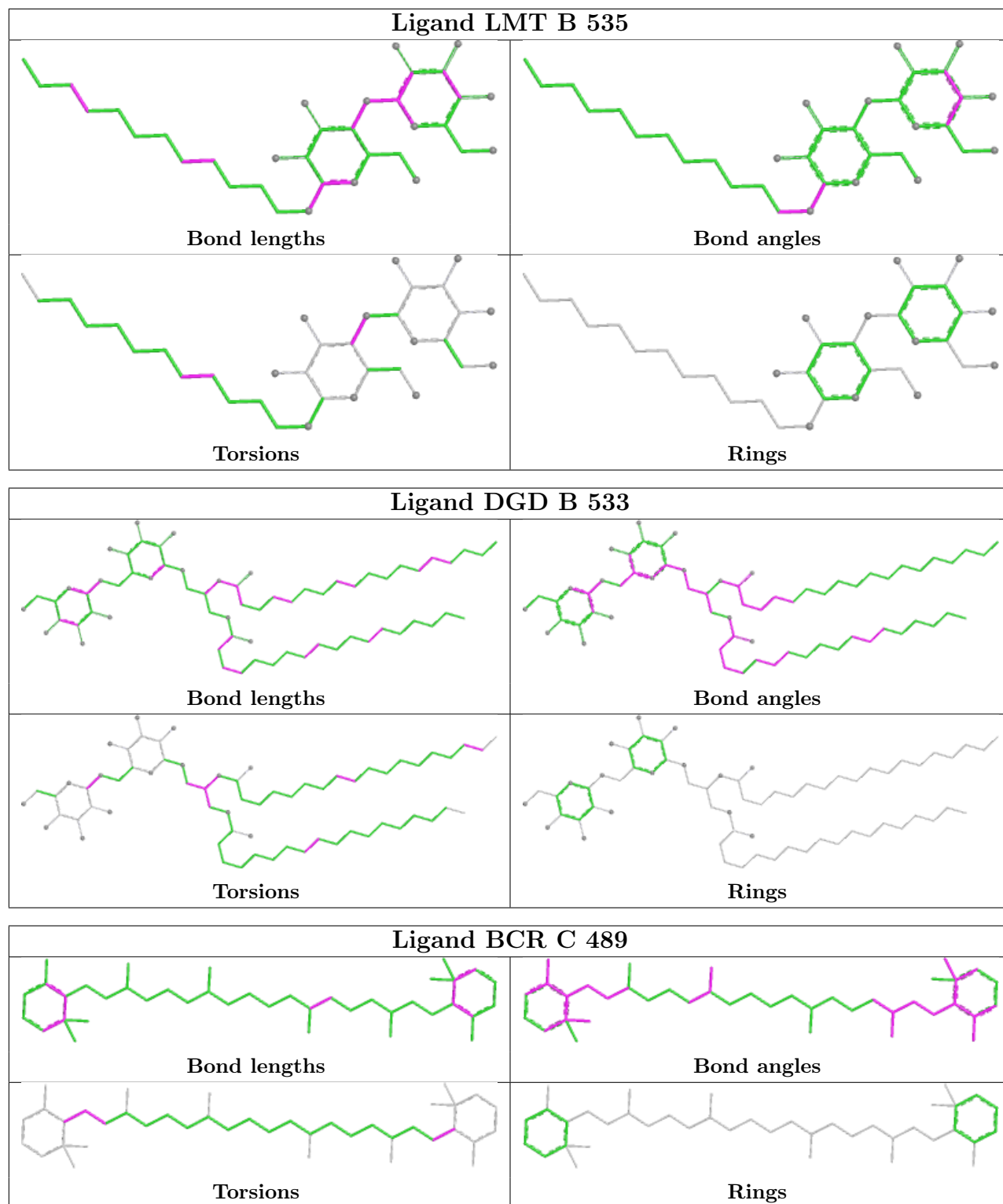


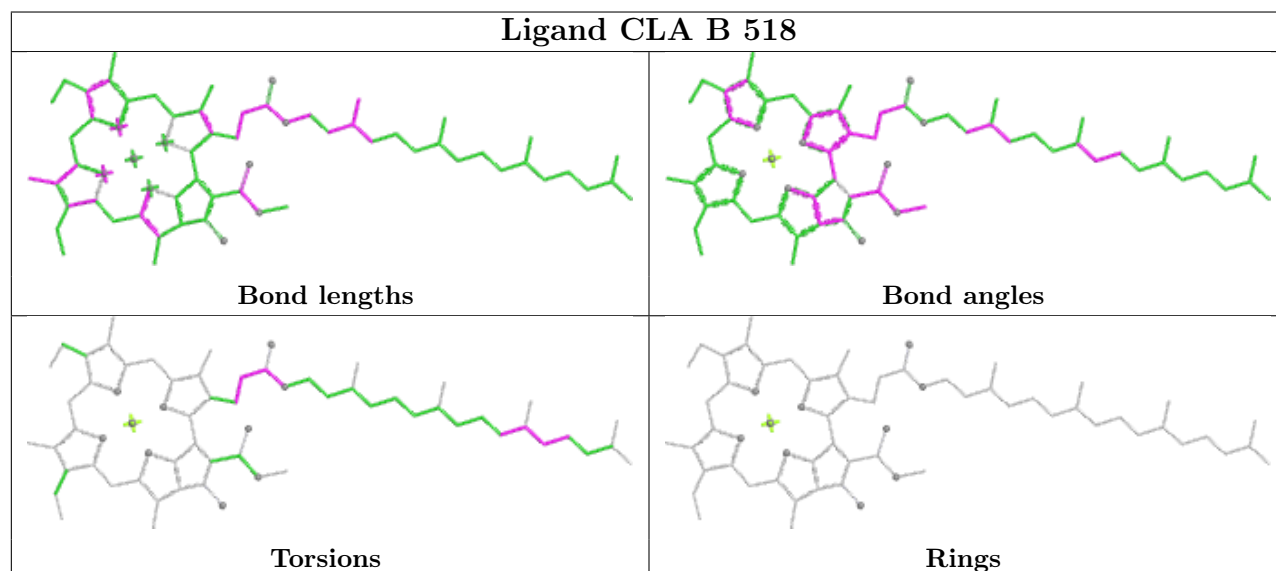
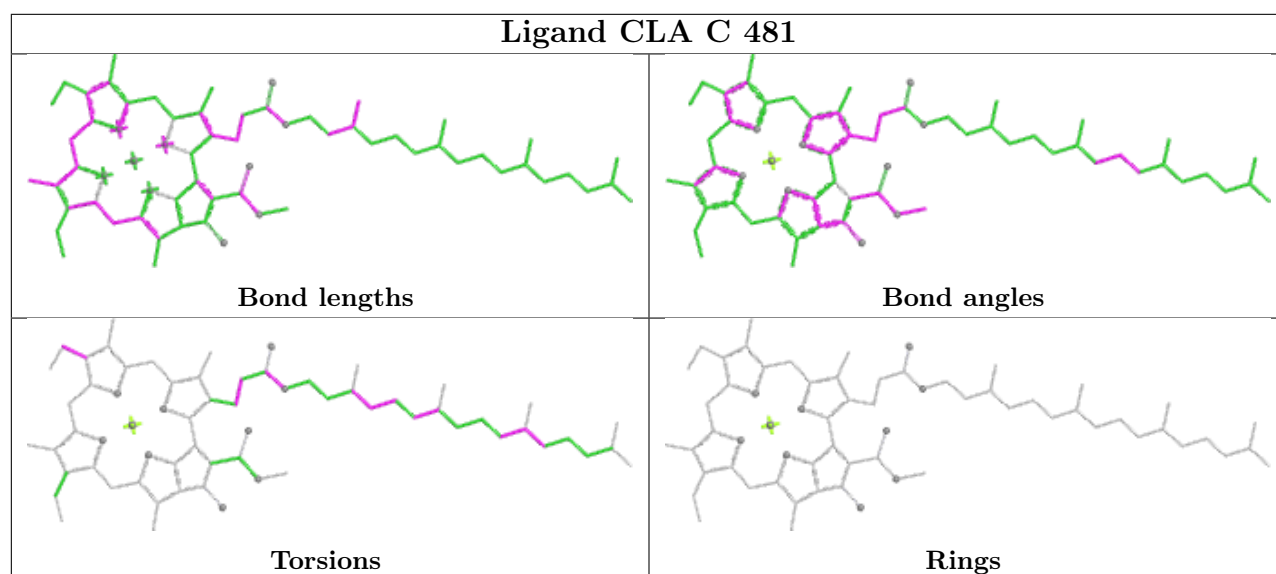
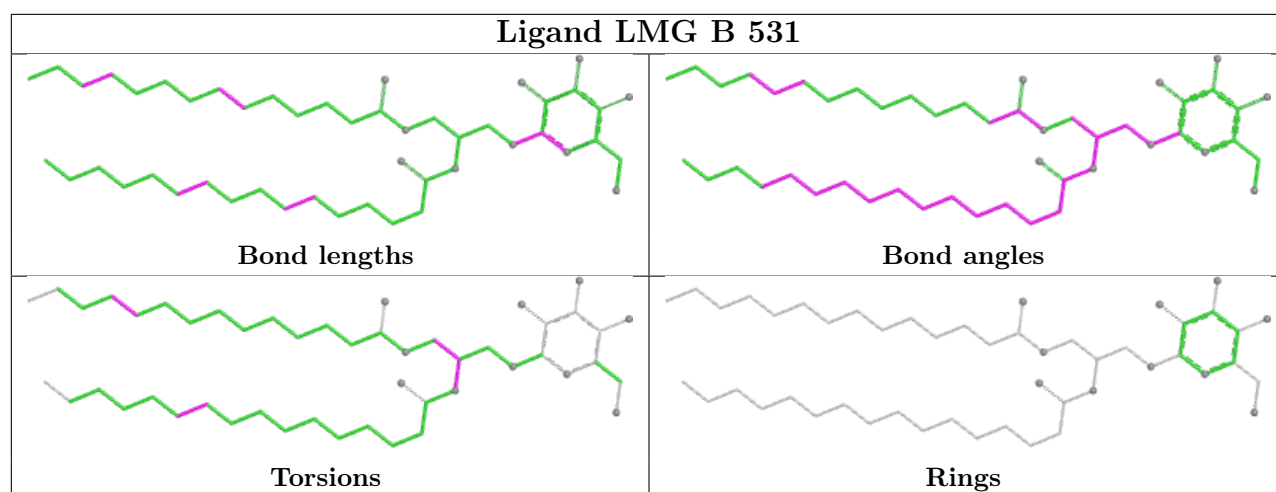
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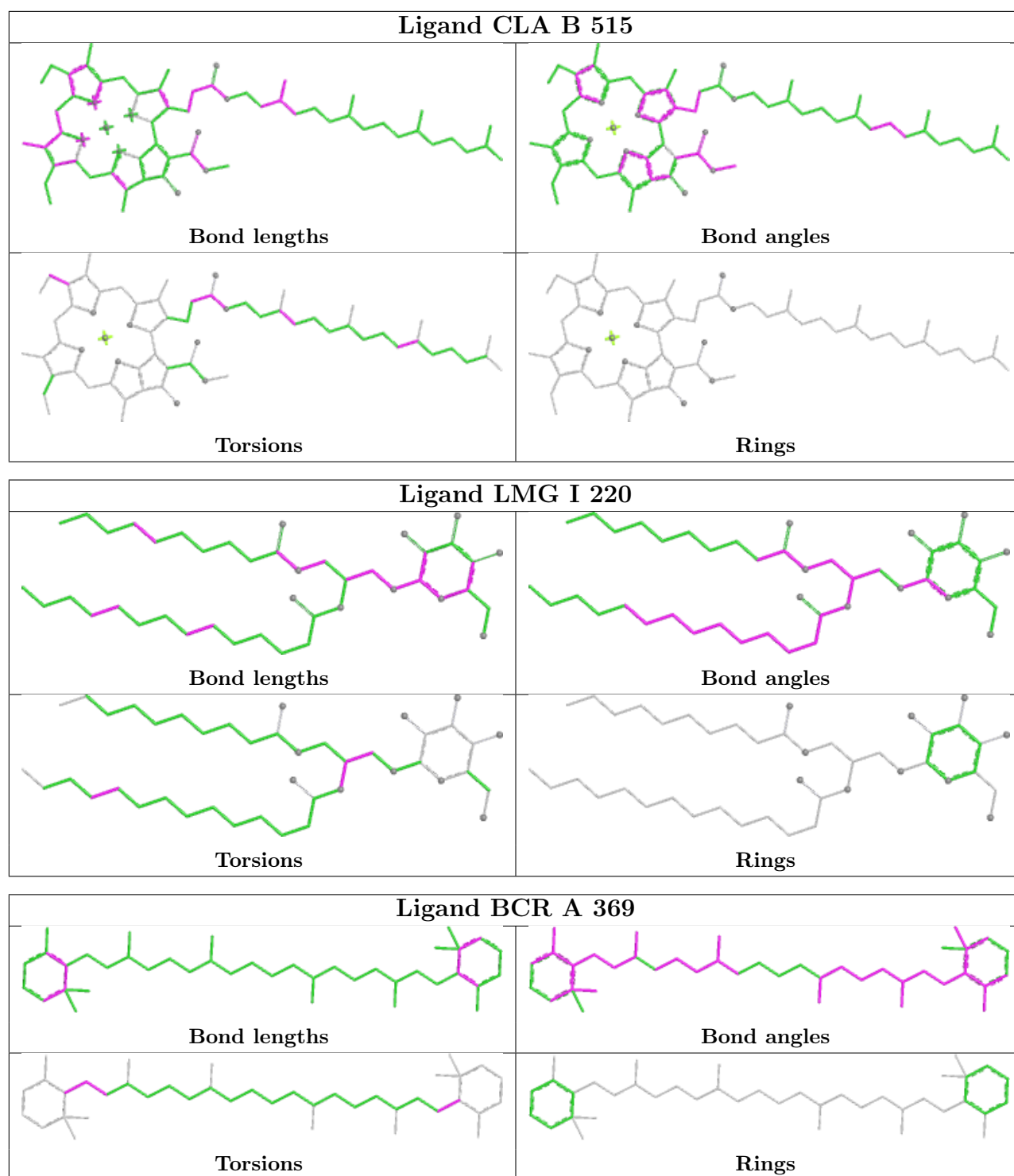


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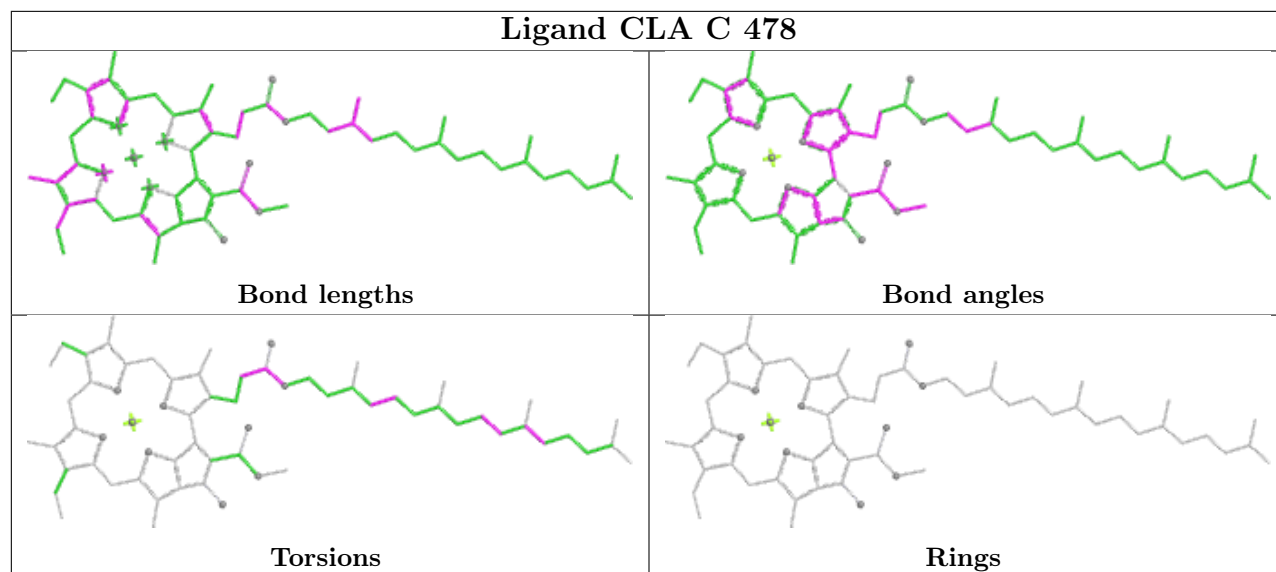




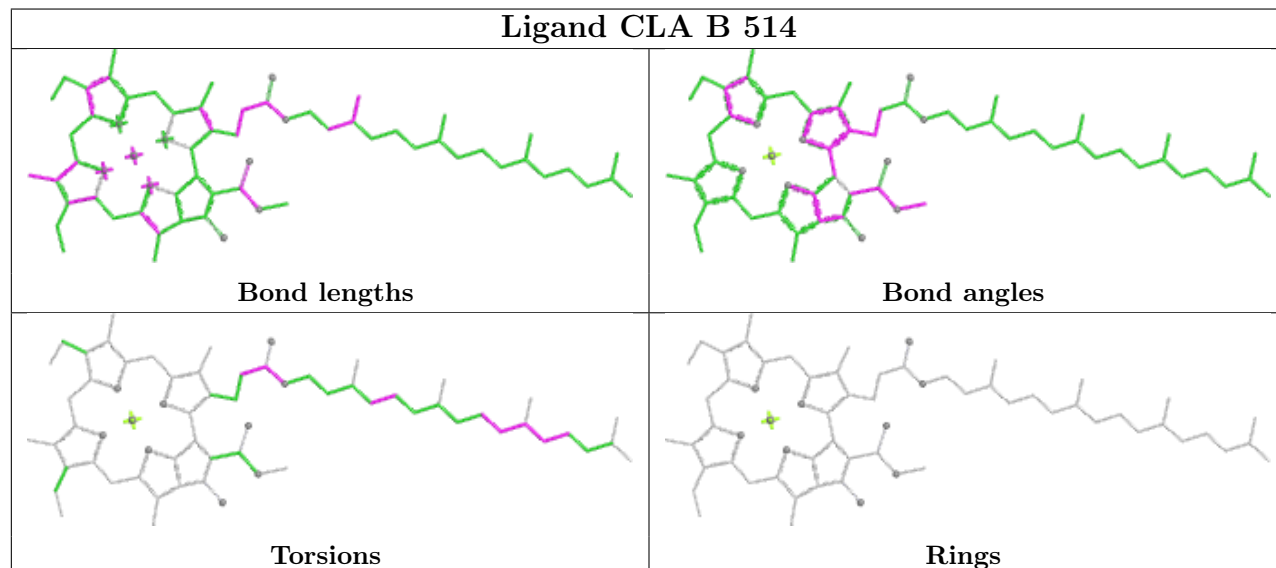




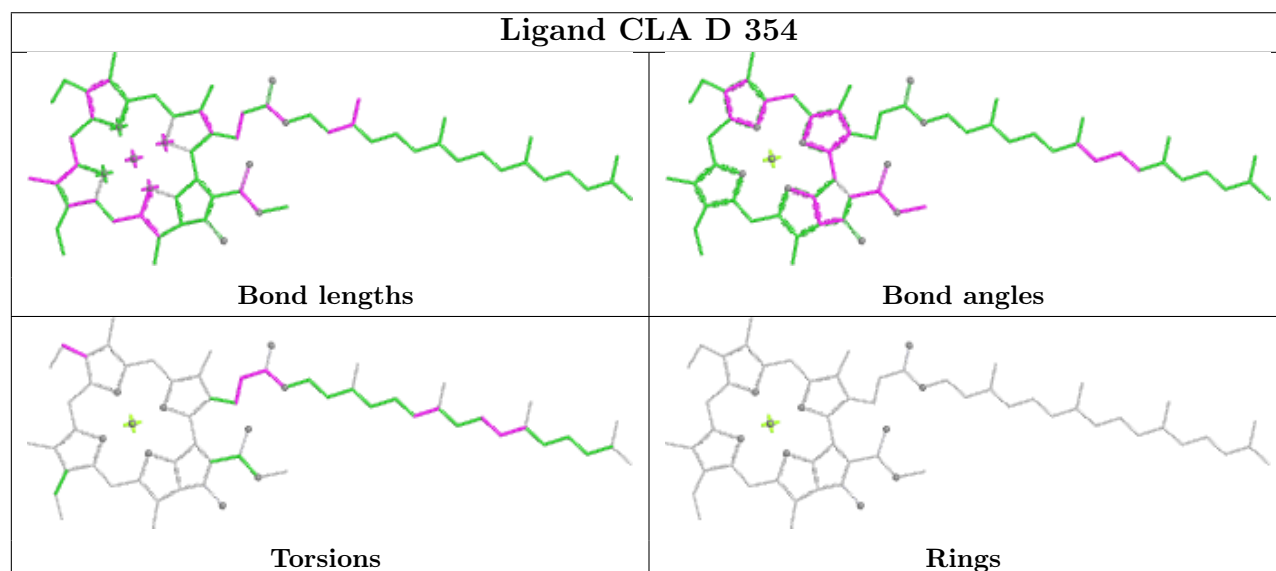
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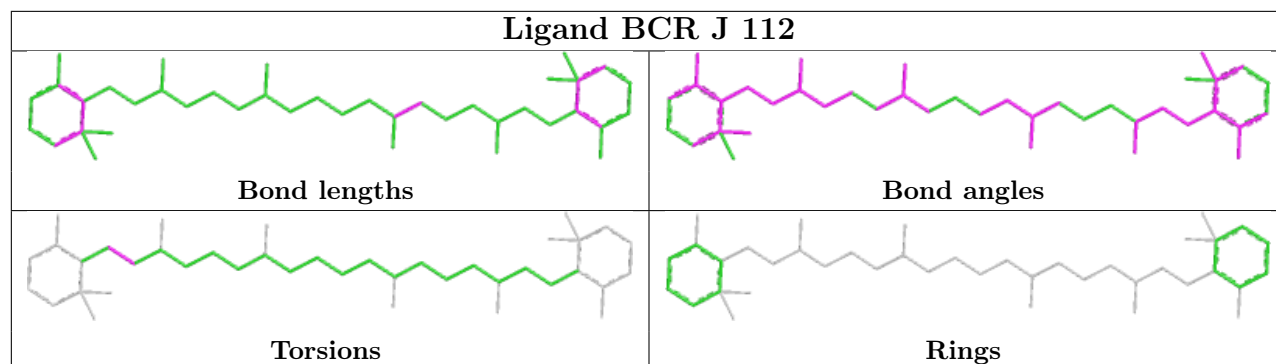
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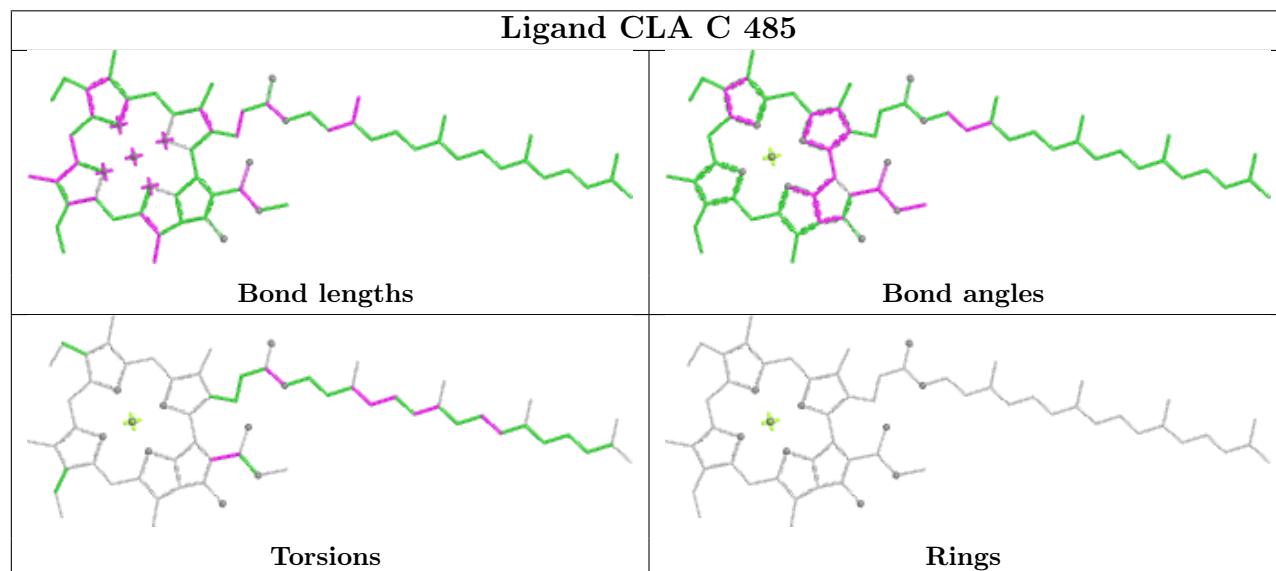
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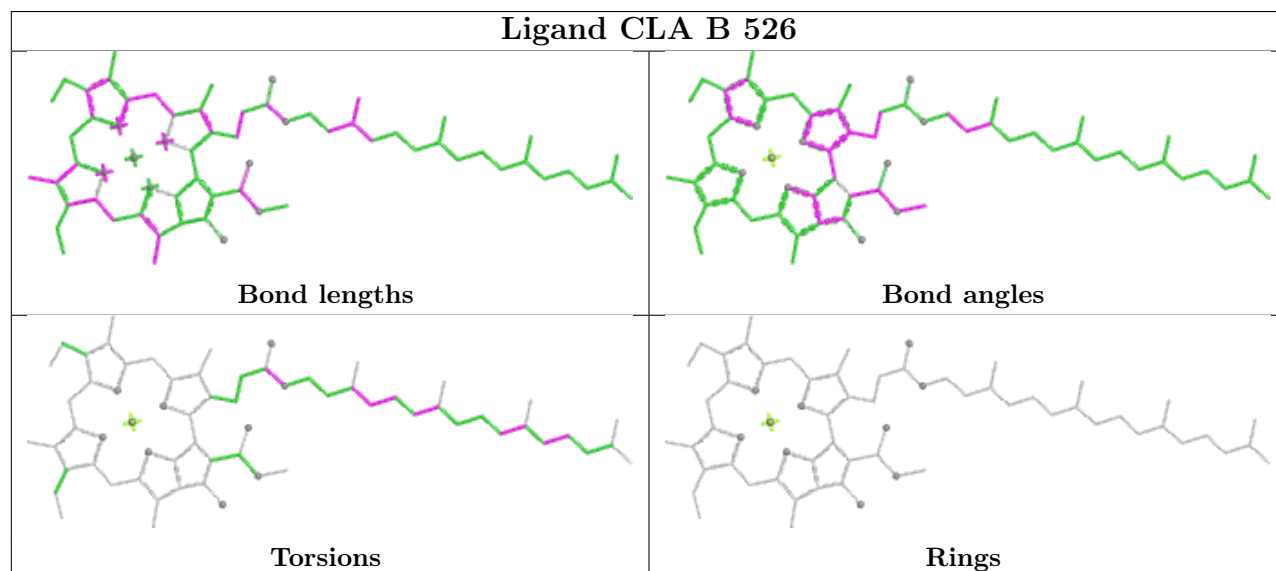
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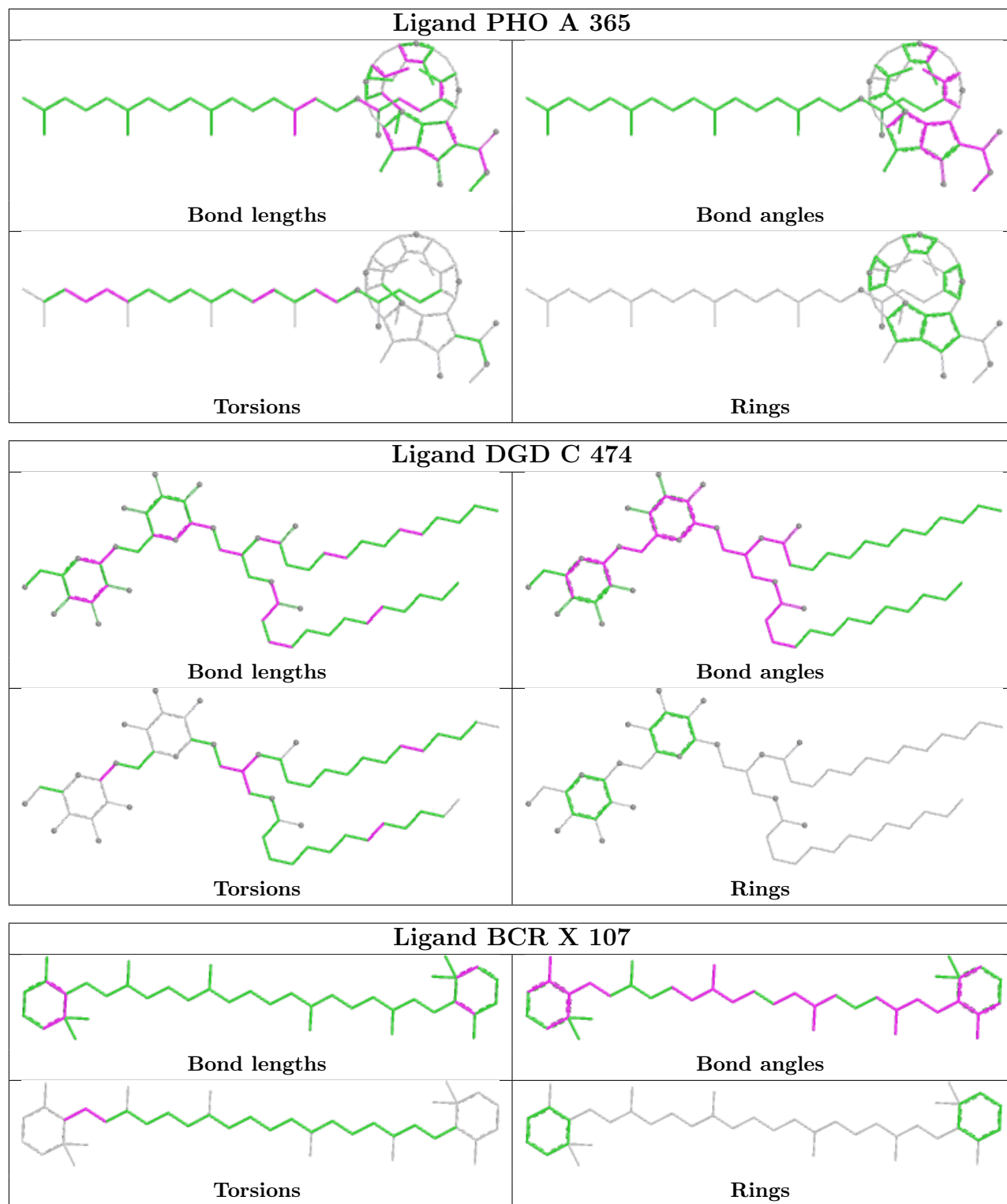


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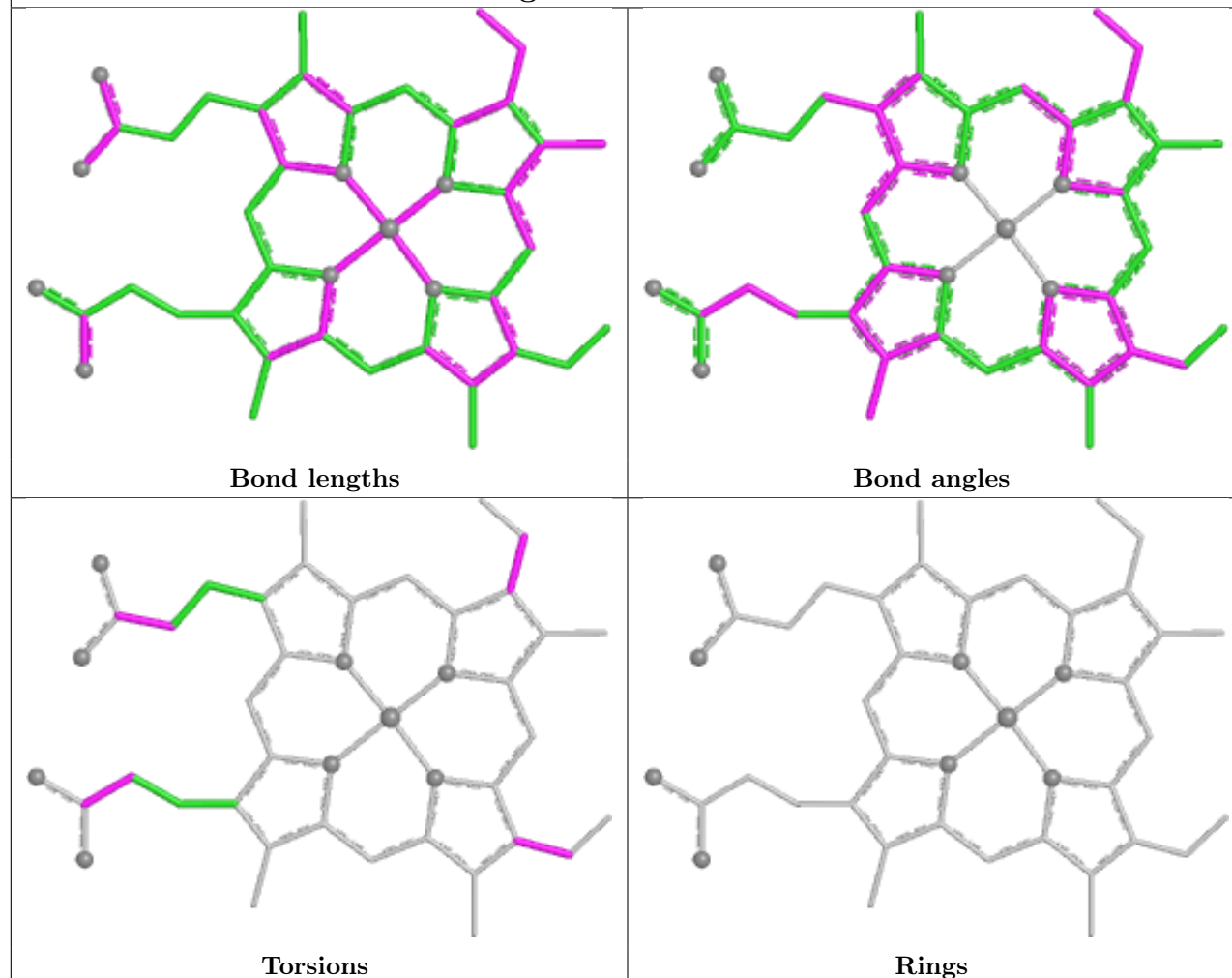


Ligand CLA B 526

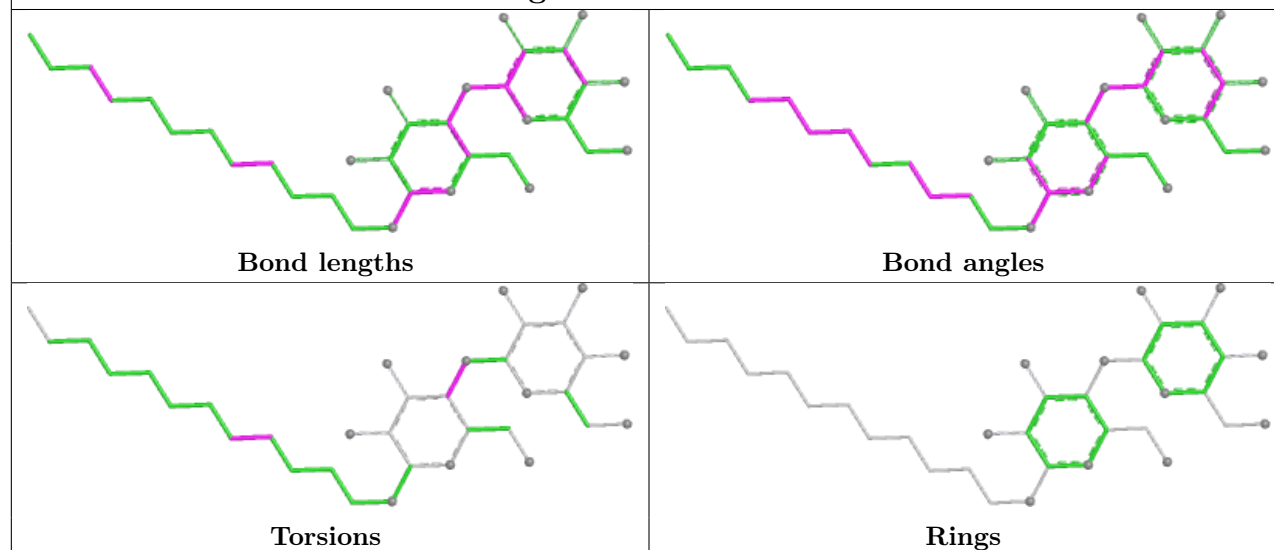


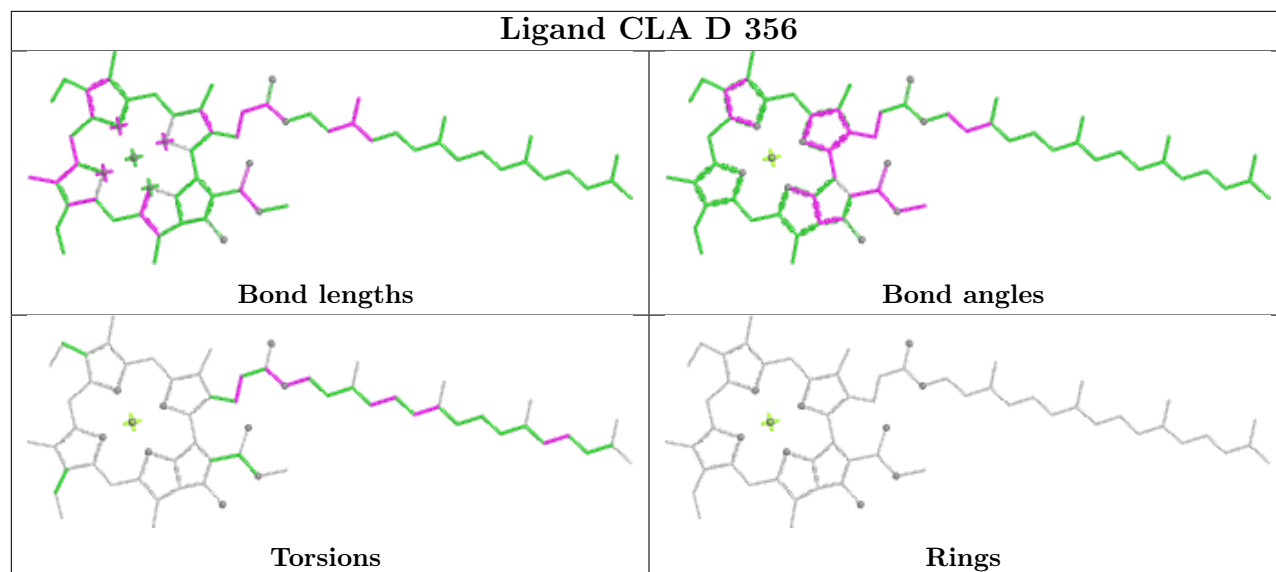
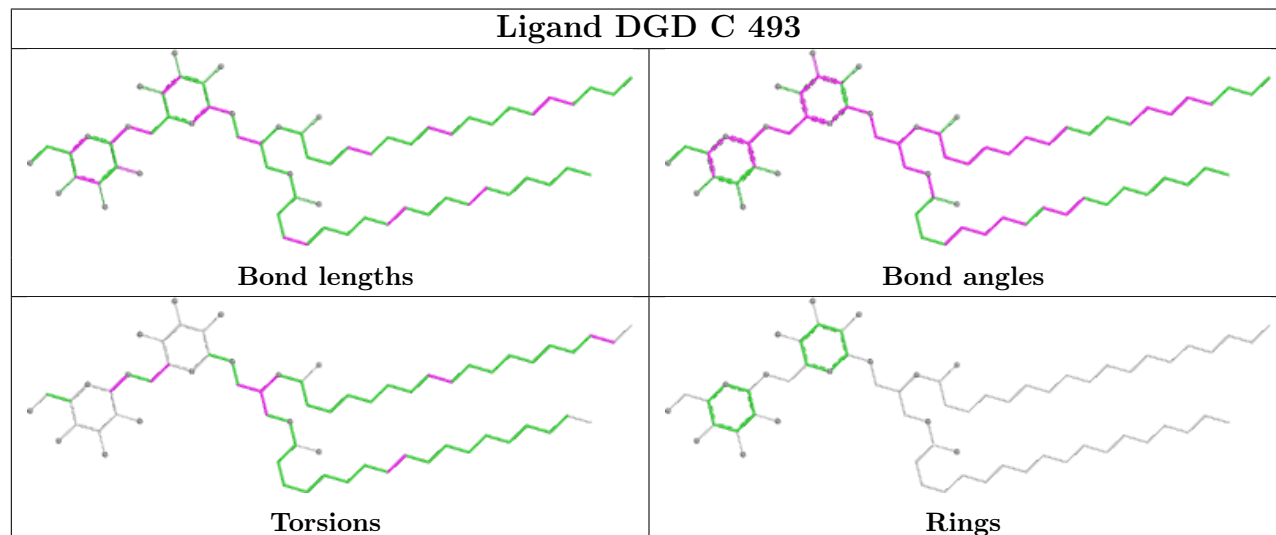


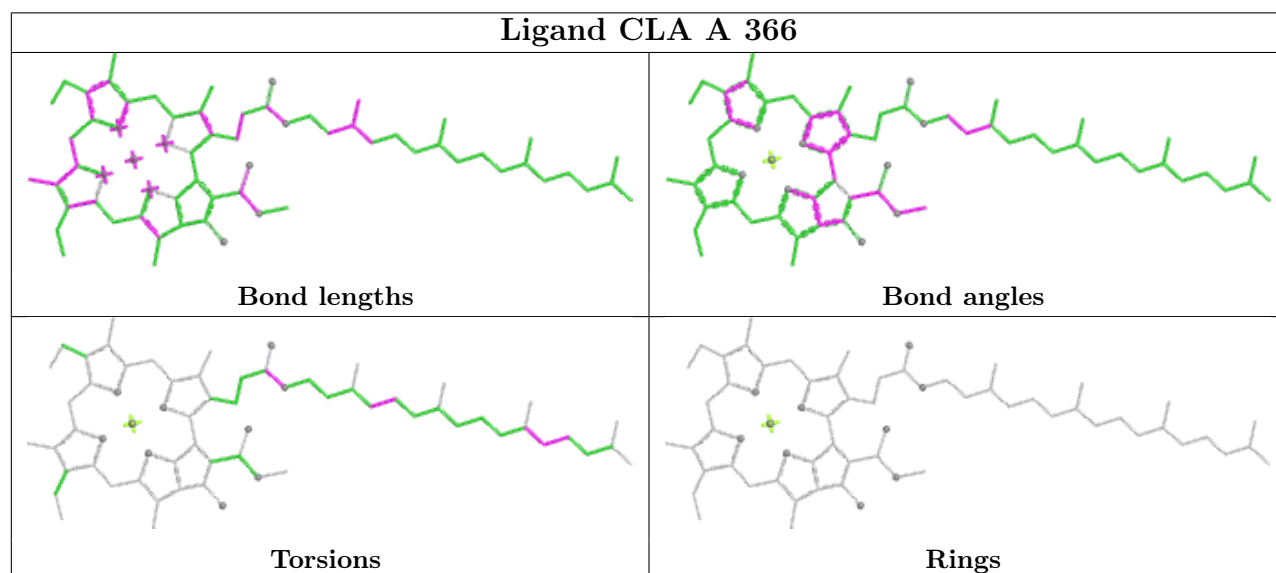
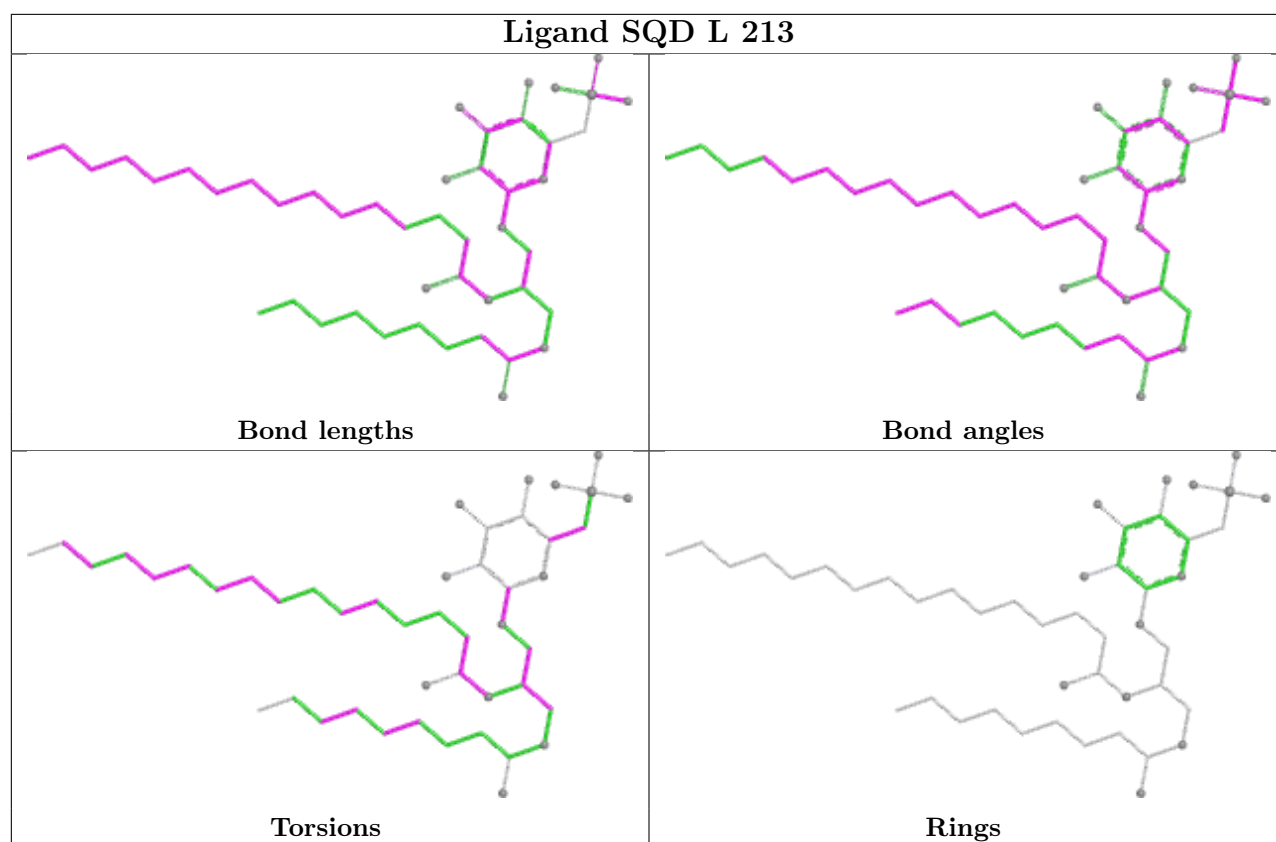
Ligand HEM F 85

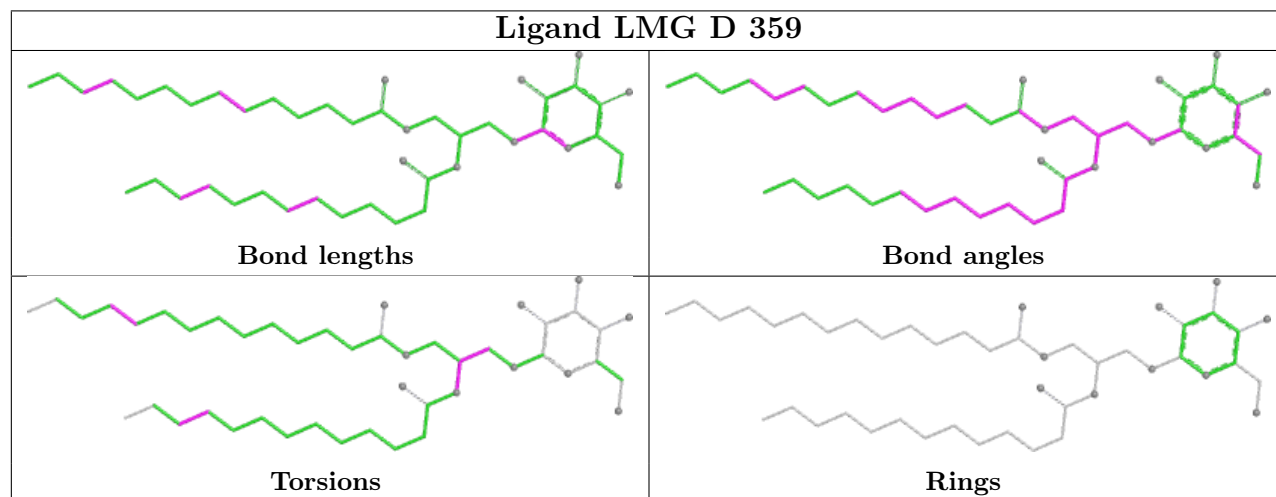
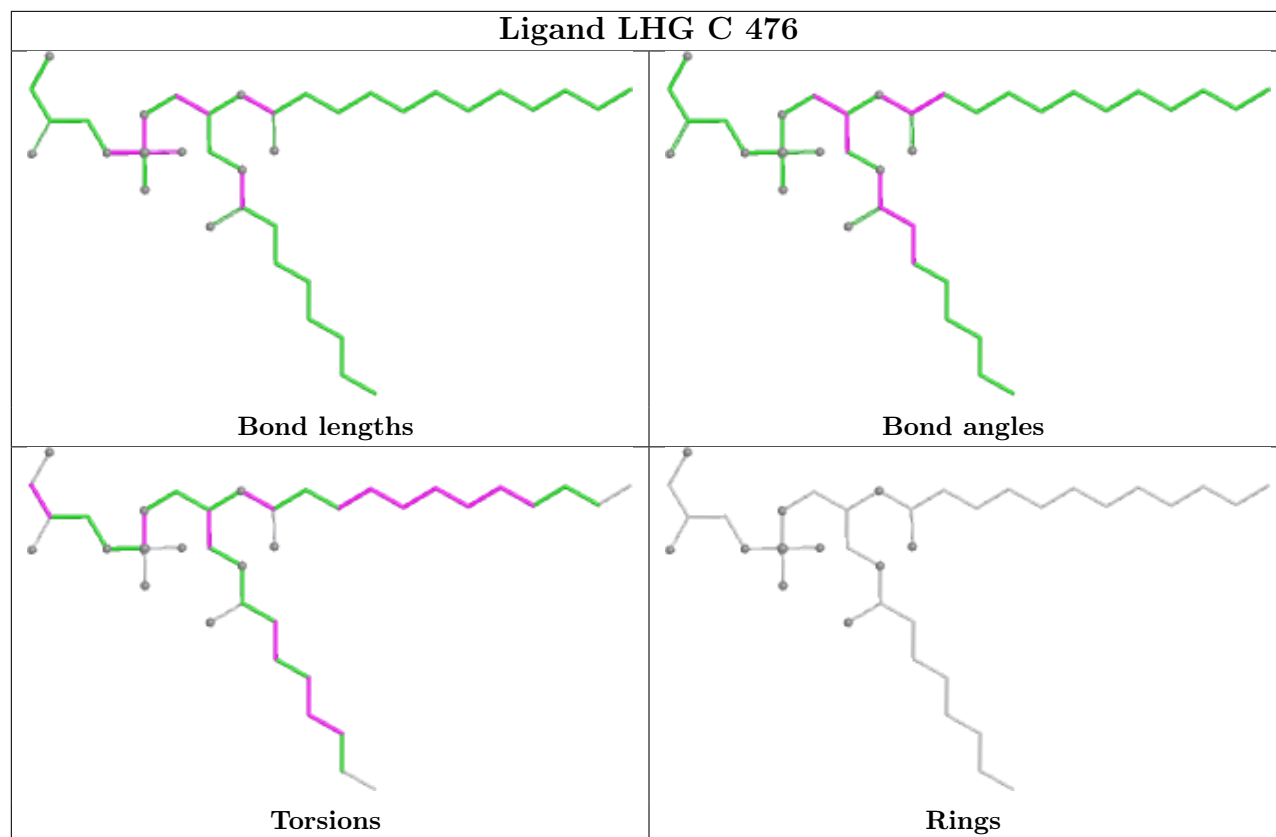


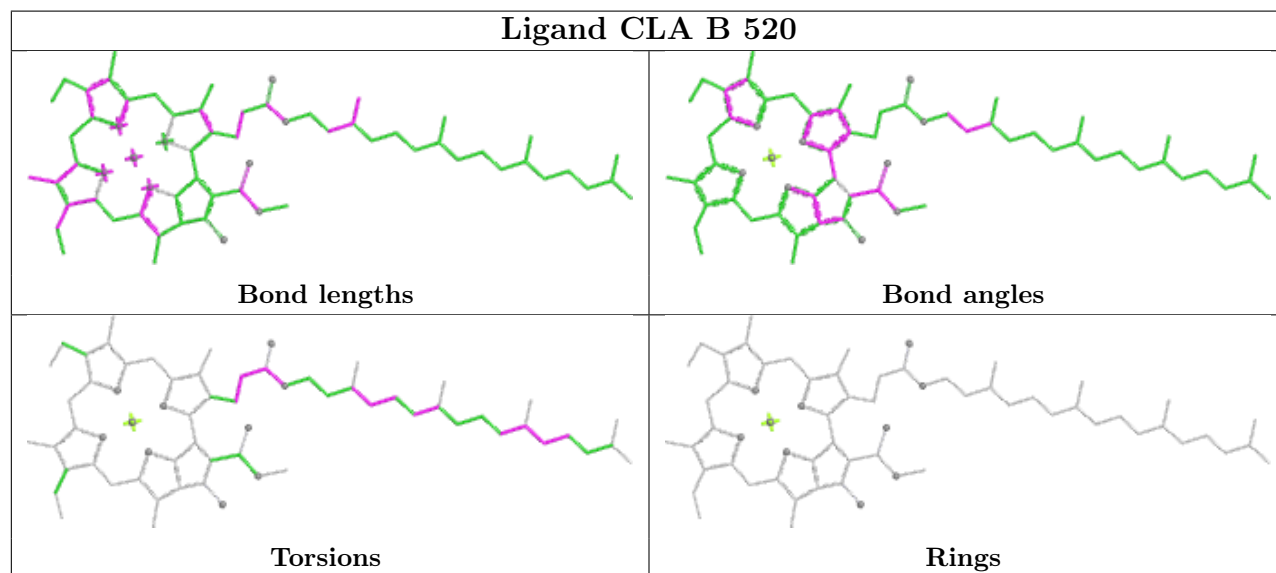
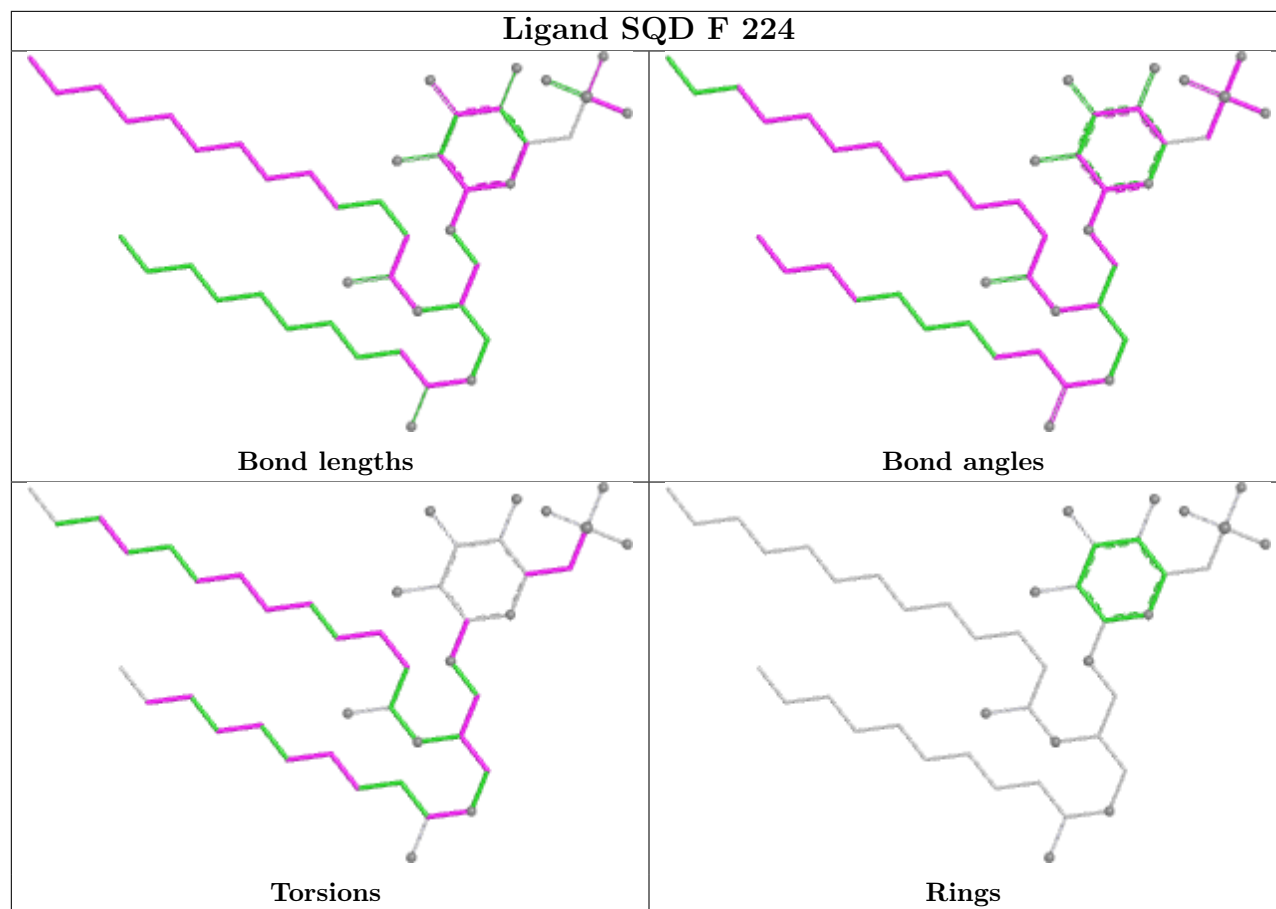
Ligand LMT A 376

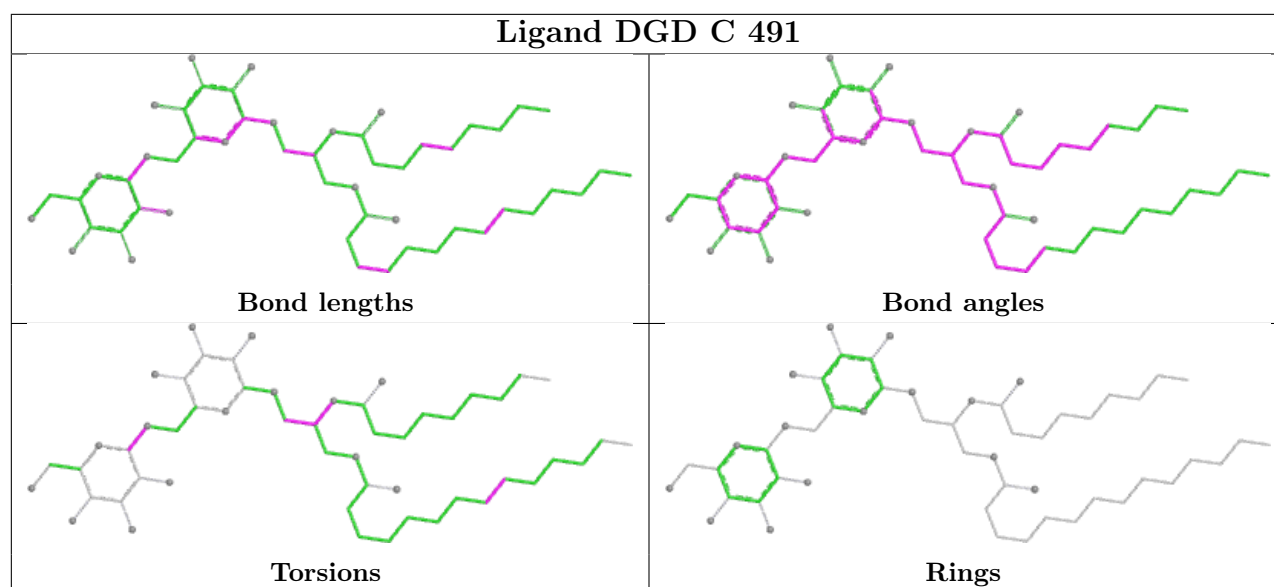


Ligand CLA D 356**Ligand DGD C 493**









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.00	7 (2%) 63 37	134, 163, 180, 180	0
2	B	485/510 (95%)	-0.03	8 (1%) 70 43	129, 158, 178, 180	0
3	C	448/461 (97%)	-0.03	4 (0%) 81 56	136, 168, 180, 180	0
4	D	340/352 (96%)	0.09	9 (2%) 57 33	126, 154, 179, 180	0
5	E	77/83 (92%)	-0.16	0 100 100	138, 157, 179, 180	0
6	F	38/44 (86%)	-0.29	0 100 100	138, 157, 169, 177	0
7	H	65/65 (100%)	0.06	3 (4%) 37 21	139, 164, 177, 180	0
8	I	35/38 (92%)	-0.34	0 100 100	163, 172, 180, 180	0
9	J	34/40 (85%)	-0.28	0 100 100	141, 155, 169, 171	0
10	K	37/37 (100%)	0.07	1 (2%) 56 32	156, 166, 179, 180	0
11	L	37/37 (100%)	-0.34	0 100 100	152, 168, 180, 180	0
12	M	34/36 (94%)	0.03	0 100 100	153, 165, 180, 180	0
13	O	243/246 (98%)	-0.06	2 (0%) 82 58	143, 174, 180, 180	0
14	T	30/32 (93%)	-0.27	0 100 100	152, 169, 180, 180	0
15	U	97/104 (93%)	-0.08	0 100 100	141, 160, 171, 179	0
16	V	137/137 (100%)	0.02	2 (1%) 72 44	136, 160, 171, 174	0
17	y	28/46 (60%)	-0.22	0 100 100	158, 175, 180, 180	0
18	X	35/40 (87%)	-0.15	1 (2%) 53 30	144, 156, 174, 178	0
19	Z	62/62 (100%)	-0.05	0 100 100	166, 178, 180, 180	0
All	All	2597/2714 (95%)	-0.03	37 (1%) 73 46	126, 164, 180, 180	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	341	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
7	H	56	ASP	3.8
4	D	130	PHE	3.7
1	A	30	VAL	3.5
4	D	35	ILE	3.4
1	A	188	ALA	3.2
2	B	198	VAL	3.0
1	A	336	ALA	3.0
2	B	21	ALA	3.0
16	V	103	LYS	2.9
1	A	61	ASP	2.7
1	A	18	CYS	2.7
3	C	204	LEU	2.7
7	H	2	ALA	2.7
4	D	140	PRO	2.6
4	D	264	LYS	2.4
2	B	187	PRO	2.4
16	V	62	ALA	2.4
4	D	314	PHE	2.4
18	X	21	ILE	2.3
13	O	166	THR	2.3
7	H	24	GLY	2.3
1	A	248	ILE	2.3
10	K	27	VAL	2.3
2	B	116	VAL	2.2
4	D	78	VAL	2.2
3	C	375	LEU	2.2
2	B	386	ALA	2.2
2	B	336	ILE	2.1
1	A	171	GLY	2.1
4	D	165	SER	2.1
2	B	473	THR	2.1
13	O	162	ILE	2.1
2	B	476	ARG	2.0
4	D	306	ALA	2.0
3	C	460	ASP	2.0
4	D	346	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	LHG	C	476	37/49	0.39	0.12	143,176,180,180	0
27	LMG	M	217	42/55	0.43	0.13	166,180,180,180	0
30	SQD	F	224	45/54	0.65	0.15	152,179,180,180	0
25	BCR	J	115	40/40	0.67	0.14	171,180,180,180	0
29	LMT	T	226	35/35	0.68	0.11	156,180,180,180	0
29	LMT	O	274	35/35	0.68	0.08	180,180,180,180	0
27	LMG	I	220	43/55	0.69	0.10	158,180,180,180	0
30	SQD	L	213	47/54	0.69	0.10	155,178,180,180	0
28	DGD	D	362	63/66	0.71	0.12	177,180,180,180	0
28	DGD	A	375	52/66	0.72	0.09	164,180,180,180	0
29	LMT	A	376	35/35	0.72	0.12	162,180,180,180	0
27	LMG	C	494	45/55	0.73	0.10	168,180,180,180	0
34	CA	K	56	1/1	0.73	0.08	180,180,180,180	0
29	LMT	B	535	35/35	0.74	0.11	163,180,180,180	0
29	LMT	D	536	35/35	0.75	0.17	168,173,180,180	0
27	LMG	D	360	48/55	0.76	0.17	140,169,176,177	0
30	SQD	C	475	51/54	0.77	0.10	156,172,180,180	0
29	LMT	D	363	31/35	0.77	0.13	170,180,180,180	0
34	CA	O	273	1/1	0.77	0.17	180,180,180,180	0
21	CLA	B	526	65/65	0.78	0.12	167,177,180,180	0
21	CLA	B	511	65/65	0.78	0.15	148,179,180,180	0
28	DGD	C	492	62/66	0.78	0.12	153,171,180,180	0
28	DGD	C	474	56/66	0.79	0.13	158,180,180,180	0
28	DGD	C	493	66/66	0.80	0.13	159,174,180,180	0
29	LMT	I	274	35/35	0.82	0.11	170,180,180,180	0
28	DGD	B	533	66/66	0.82	0.12	166,179,180,180	0
25	BCR	B	530	40/40	0.83	0.13	173,180,180,180	0
21	CLA	C	482	65/65	0.83	0.15	148,179,180,180	0
27	LMG	D	359	46/55	0.83	0.13	142,163,180,180	0
25	BCR	C	490	40/40	0.84	0.16	164,169,180,180	0
25	BCR	B	527	40/40	0.85	0.13	161,169,176,178	0
27	LMG	A	373	51/55	0.85	0.18	169,174,180,180	0

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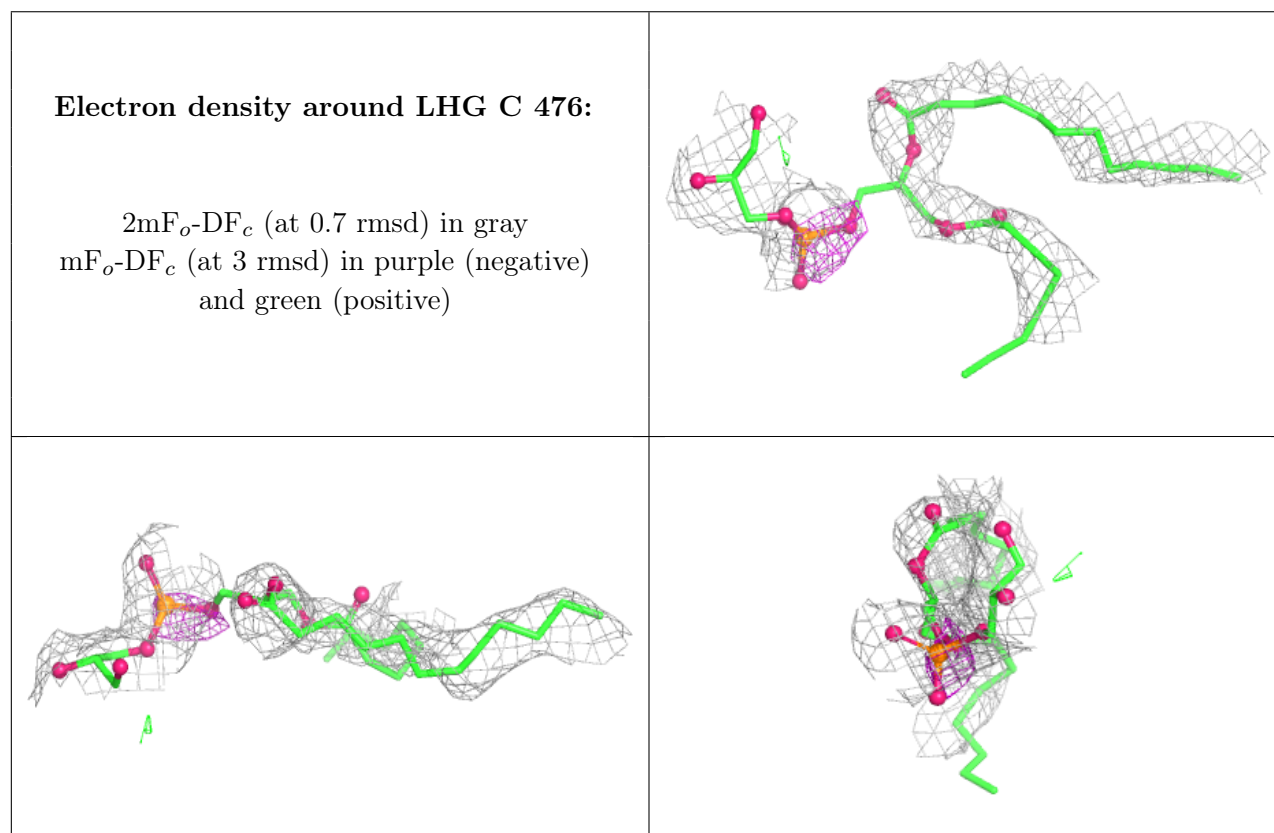
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	LMG	J	492	48/55	0.85	0.15	155,175,180,180	0
28	DGD	B	528	58/66	0.85	0.16	126,136,172,173	0
25	BCR	B	529	40/40	0.86	0.15	166,169,173,174	0
21	CLA	C	488	65/65	0.87	0.10	169,176,179,180	0
21	CLA	A	363	65/65	0.87	0.13	154,161,175,177	0
27	LMG	B	531	49/55	0.87	0.16	160,167,175,176	0
21	CLA	B	524	65/65	0.87	0.11	157,180,180,180	0
25	BCR	Z	116	40/40	0.88	0.16	163,165,170,171	0
30	SQD	D	361	43/54	0.88	0.11	160,173,180,180	0
21	CLA	C	486	65/65	0.88	0.15	143,180,180,180	0
25	BCR	J	112	40/40	0.89	0.18	157,160,172,173	0
21	CLA	A	364	65/65	0.90	0.12	126,141,175,177	0
21	CLA	C	477	65/65	0.90	0.14	163,169,179,180	0
21	CLA	C	481	65/65	0.90	0.12	152,180,180,180	0
21	CLA	B	525	65/65	0.91	0.12	148,167,180,180	0
21	CLA	C	487	65/65	0.91	0.13	176,180,180,180	0
21	CLA	C	479	65/65	0.91	0.13	162,180,180,180	0
24	OEC	A	368	5/9	0.91	0.11	118,138,151,154	0
21	CLA	C	484	65/65	0.91	0.12	168,177,180,180	0
25	BCR	X	107	40/40	0.91	0.14	154,158,161,163	0
21	CLA	D	356	65/65	0.92	0.13	149,154,162,164	0
28	DGD	C	491	53/66	0.92	0.14	155,160,166,168	0
23	MES	A	367	12/12	0.92	0.11	136,144,152,153	0
21	CLA	C	480	65/65	0.92	0.10	151,159,180,180	0
25	BCR	A	369	40/40	0.92	0.14	164,171,178,178	0
21	CLA	C	485	65/65	0.92	0.14	170,176,178,180	0
21	CLA	B	516	65/65	0.92	0.10	152,155,180,180	0
31	BCT	D	353	4/4	0.92	0.07	169,170,170,171	0
21	CLA	A	366	65/65	0.92	0.09	152,162,164,166	0
21	CLA	C	483	65/65	0.92	0.12	164,180,180,180	0
21	CLA	K	483	65/65	0.93	0.10	155,160,174,176	0
25	BCR	C	489	40/40	0.93	0.16	152,169,171,171	0
21	CLA	C	478	65/65	0.93	0.11	153,155,166,170	0
32	PL9	D	357	55/55	0.93	0.13	146,153,161,162	0
26	LHG	A	371	39/49	0.93	0.11	156,175,179,180	0
21	CLA	B	518	65/65	0.93	0.12	150,164,167,169	0
22	PHO	A	365	64/64	0.94	0.10	143,154,162,164	0
22	PHO	D	355	64/64	0.94	0.11	140,162,169,171	0
21	CLA	B	521	65/65	0.94	0.11	149,169,175,179	0
21	CLA	D	354	65/65	0.94	0.14	135,154,164,168	0
25	BCR	D	358	40/40	0.94	0.11	135,151,162,162	0
33	HEM	F	85	43/43	0.94	0.11	154,159,162,163	0

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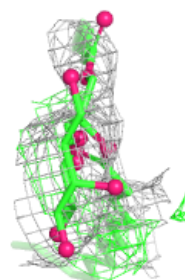
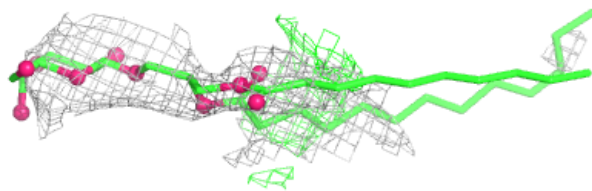
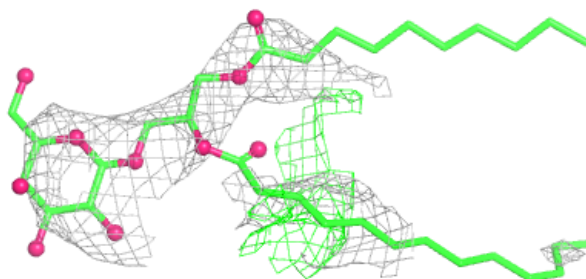
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	CLA	B	517	65/65	0.94	0.11	144,160,164,167	0
21	CLA	B	512	65/65	0.94	0.14	142,165,172,173	0
21	CLA	B	514	65/65	0.95	0.13	139,146,168,169	0
21	CLA	B	519	65/65	0.95	0.11	152,157,158,159	0
21	CLA	A	362	65/65	0.95	0.12	149,154,159,163	0
21	CLA	B	522	65/65	0.95	0.12	134,144,163,165	0
21	CLA	B	523	65/65	0.95	0.10	134,142,169,170	0
21	CLA	B	513	65/65	0.95	0.12	133,170,171,172	0
21	CLA	B	515	65/65	0.96	0.12	142,162,168,170	0
34	CA	F	225	1/1	0.97	0.07	142,142,142,142	0
21	CLA	B	520	65/65	0.97	0.14	150,162,165,167	0
33	HEM	V	164	43/43	0.97	0.11	89,102,122,129	0
20	FE2	A	361	1/1	0.99	0.03	160,160,160,160	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

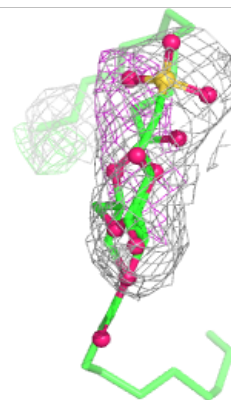
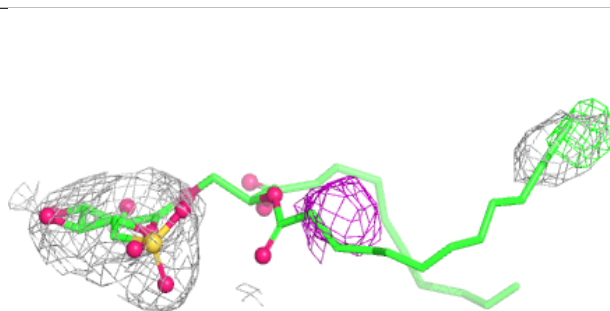
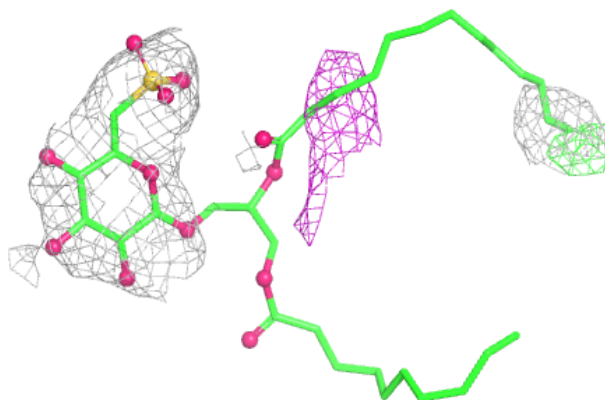


Electron density around LMG M 217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

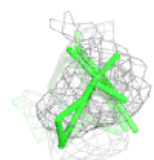
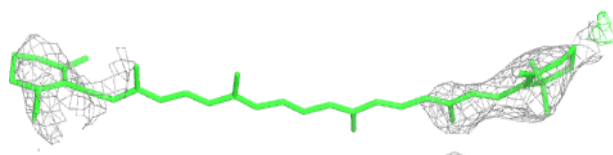
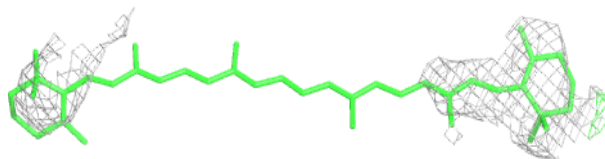
**Electron density around SQD F 224:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

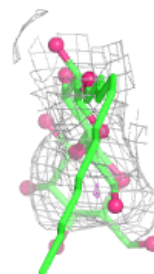
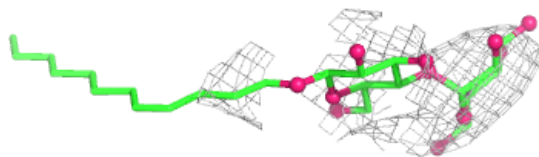
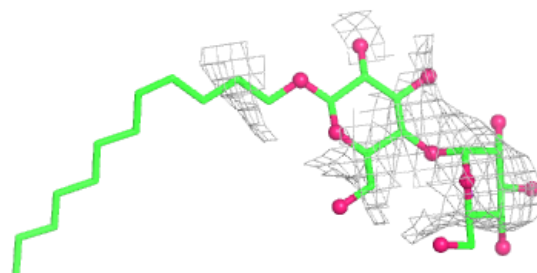


Electron density around BCR J 115:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

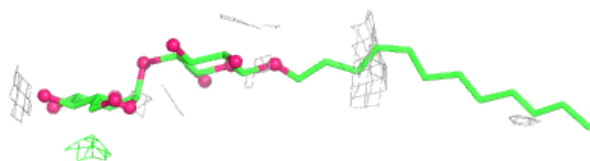
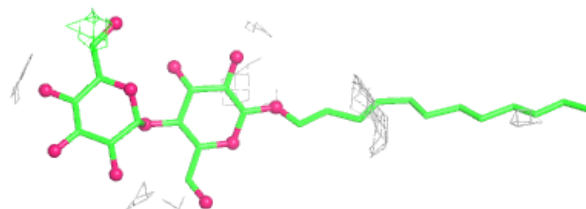
**Electron density around LMT T 226:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

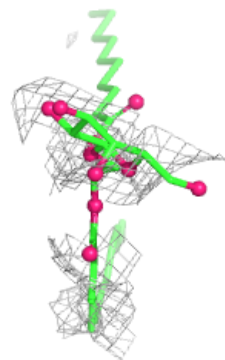
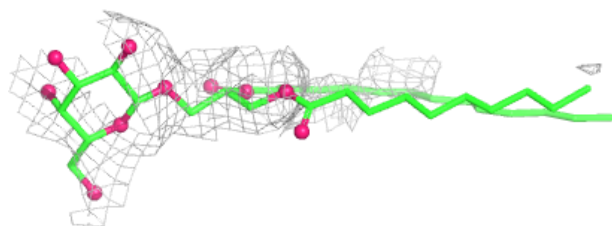


Electron density around LMT O 274:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

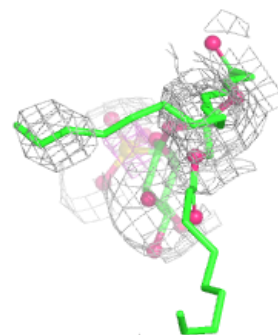
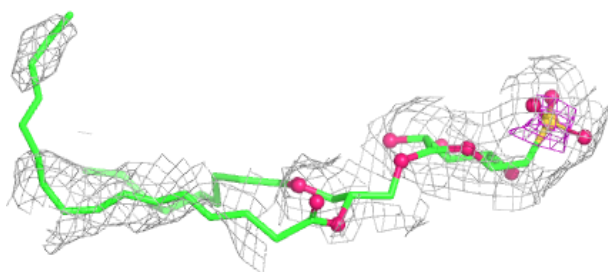
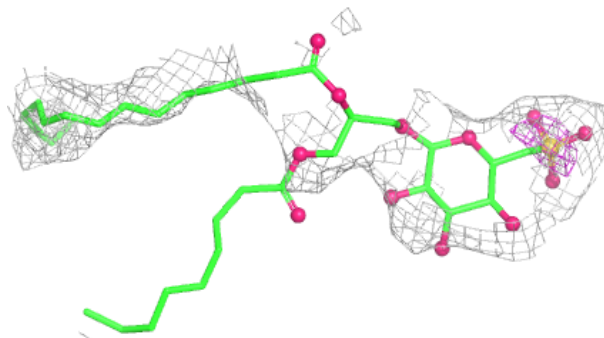
**Electron density around LMG I 220:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

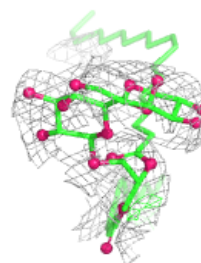
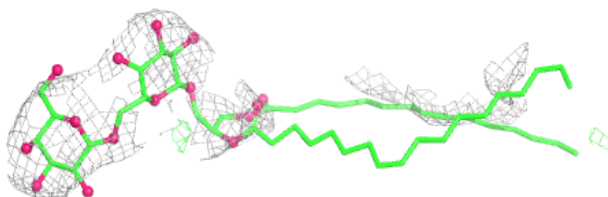
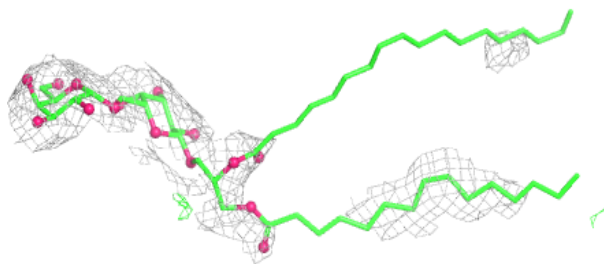


Electron density around SQD L 213:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

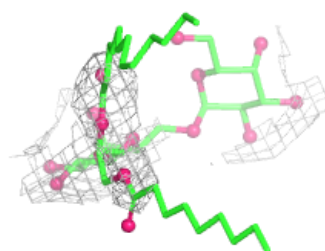
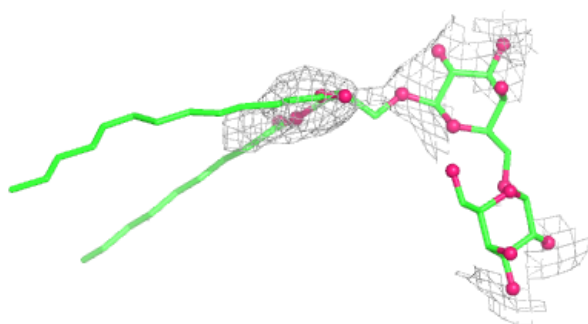
**Electron density around DGD D 362:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

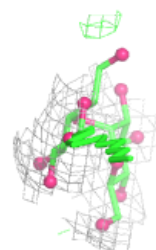
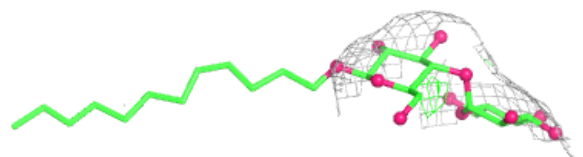
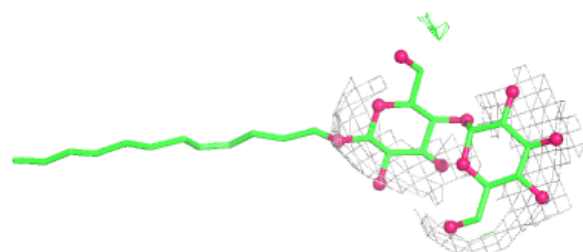


Electron density around DGD A 375:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

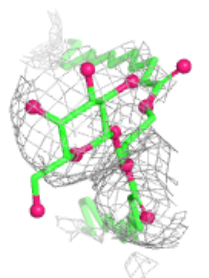
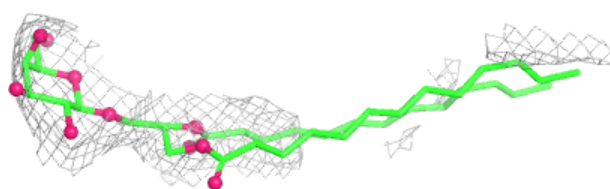
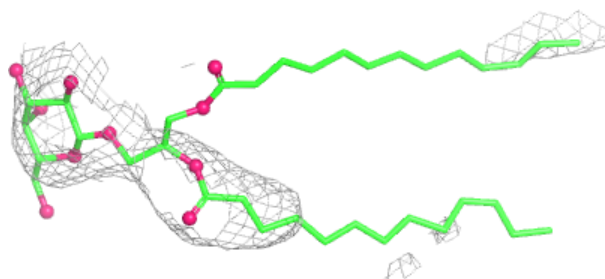
**Electron density around LMT A 376:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

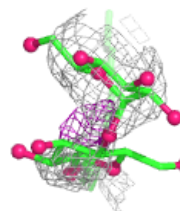
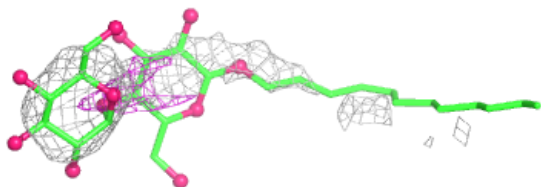
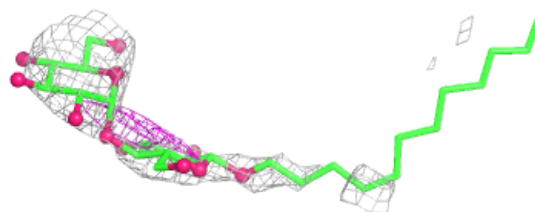


Electron density around LMG C 494:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

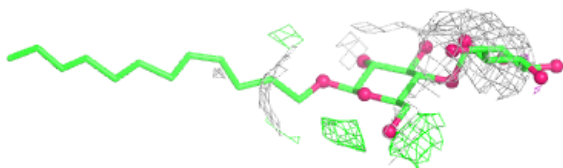
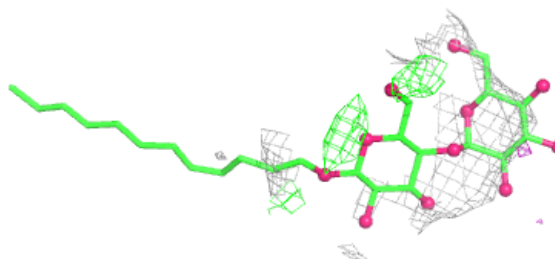
**Electron density around LMT B 535:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

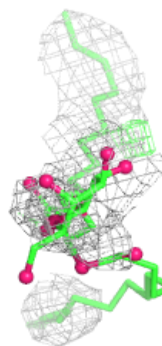
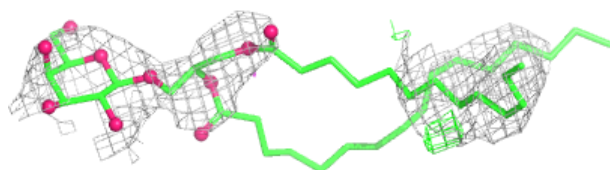
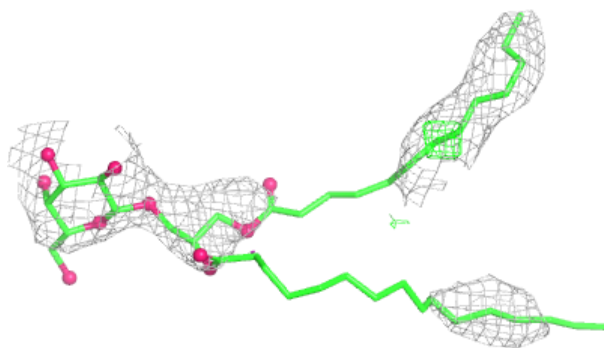


Electron density around LMT D 536:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

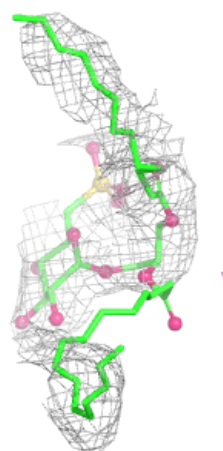
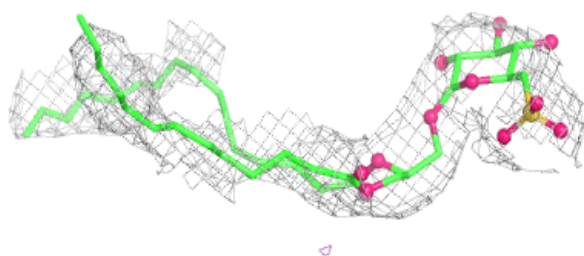
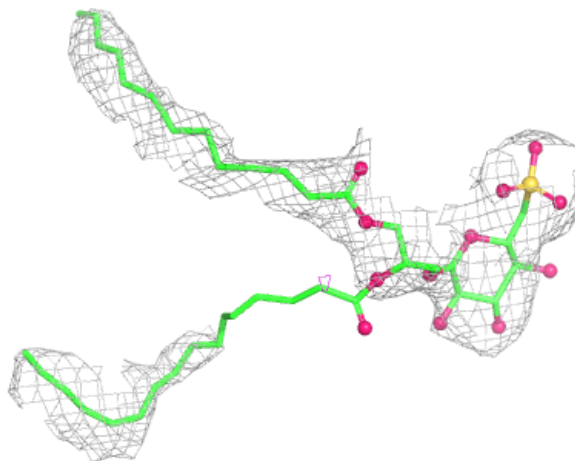
**Electron density around LMG D 360:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



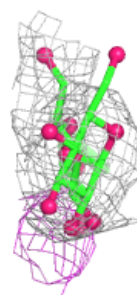
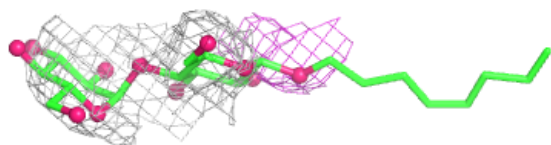
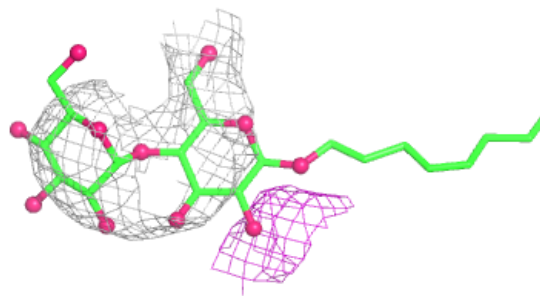
Electron density around SQD C 475:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



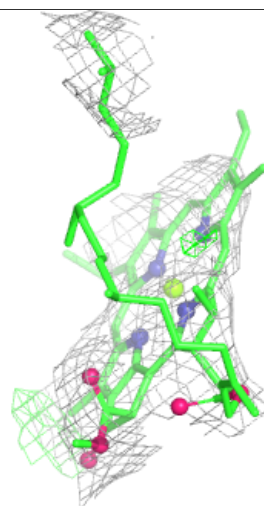
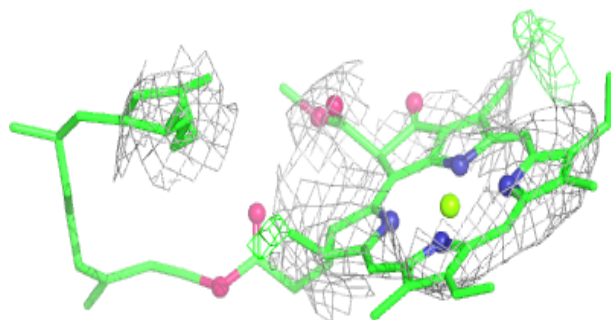
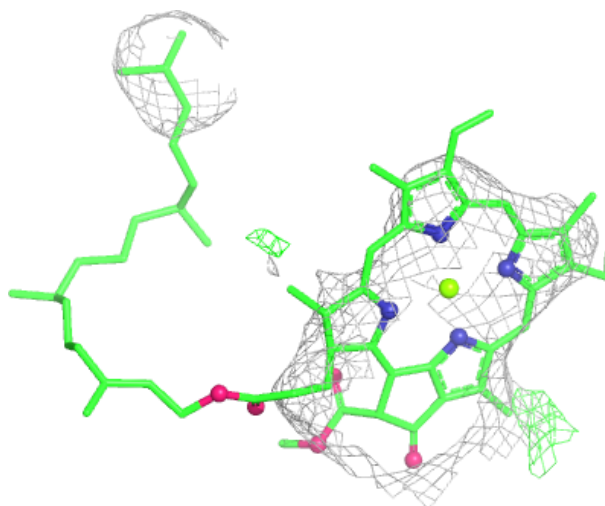
Electron density around LMT D 363:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



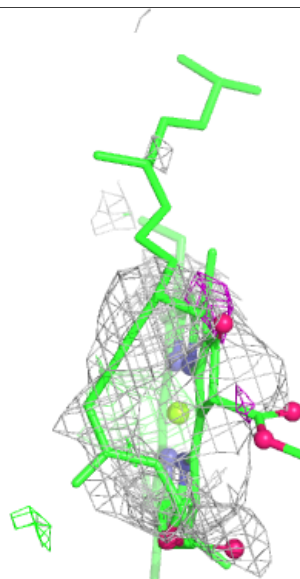
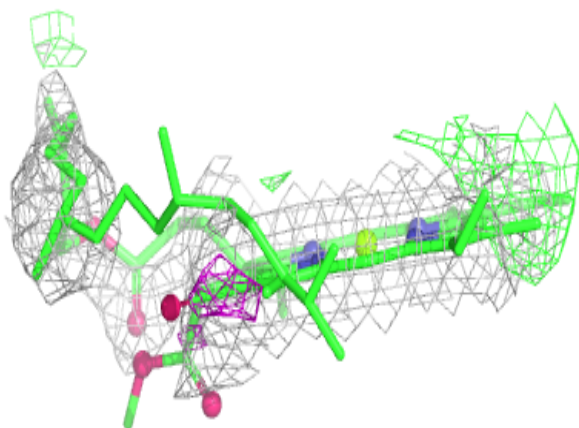
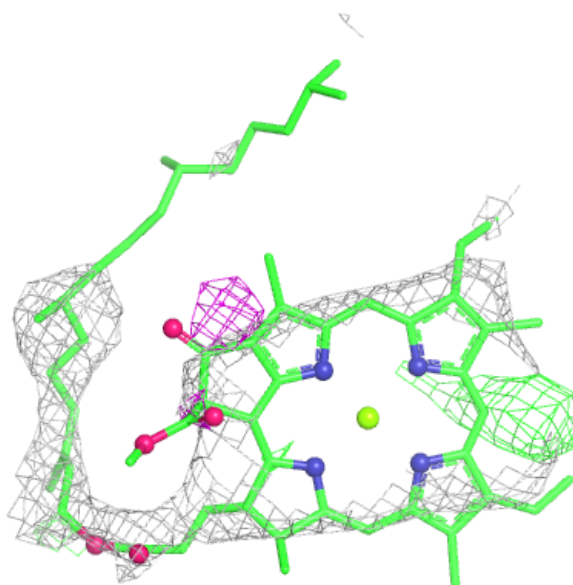
Electron density around CLA B 526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



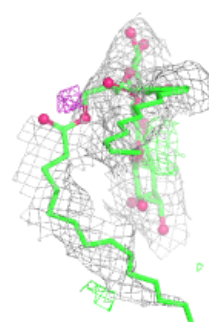
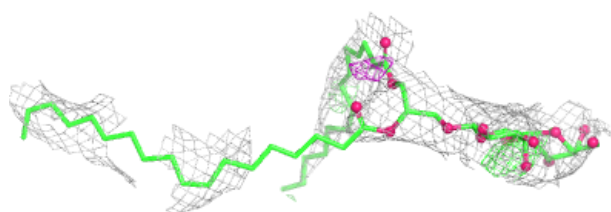
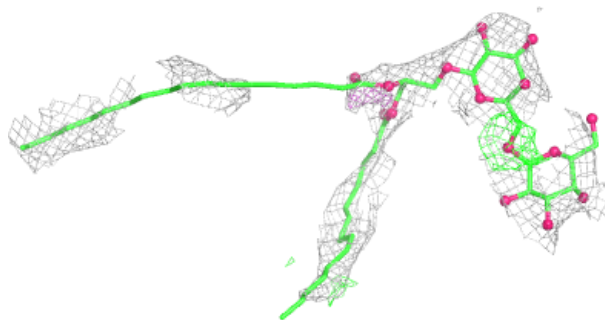
Electron density around CLA B 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

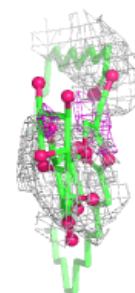
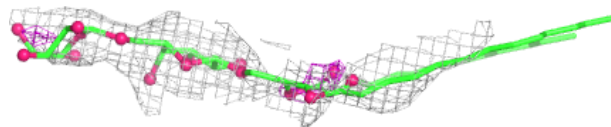


Electron density around DGD C 492:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

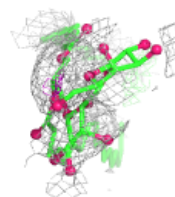
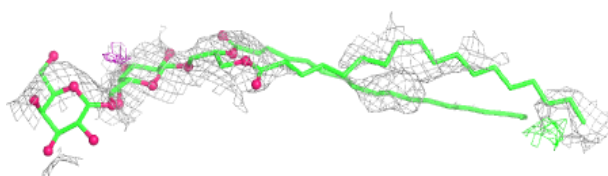
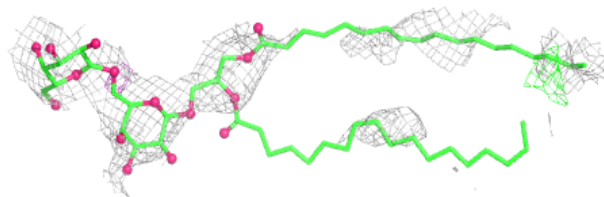
**Electron density around DGD C 474:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

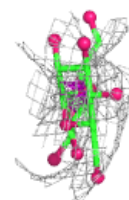
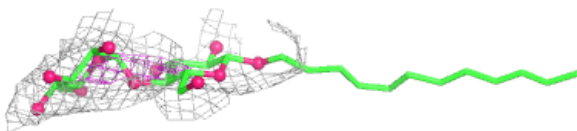
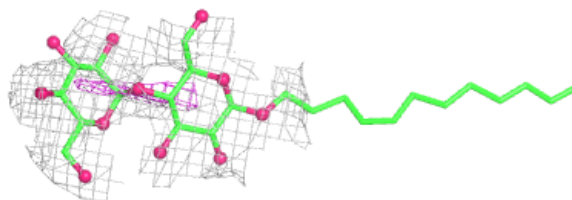


Electron density around DGD C 493:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

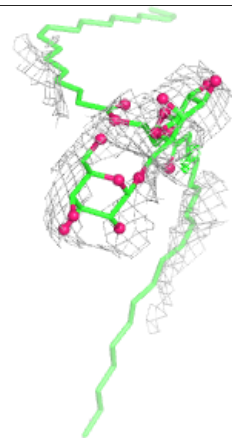
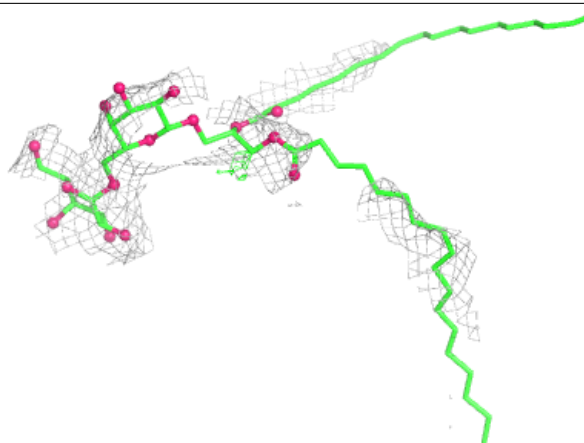
**Electron density around LMT I 274:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

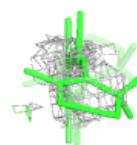
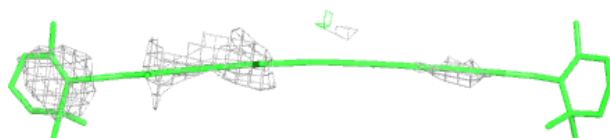
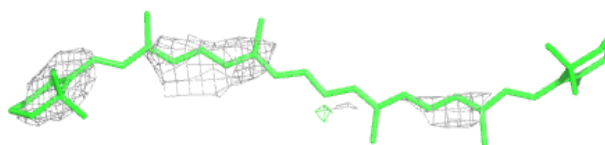


Electron density around DGD B 533:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

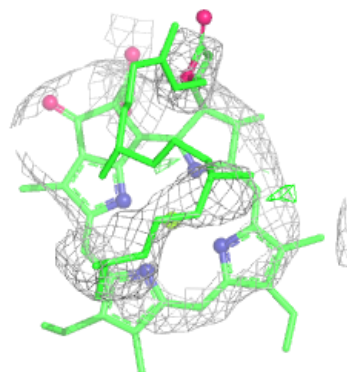
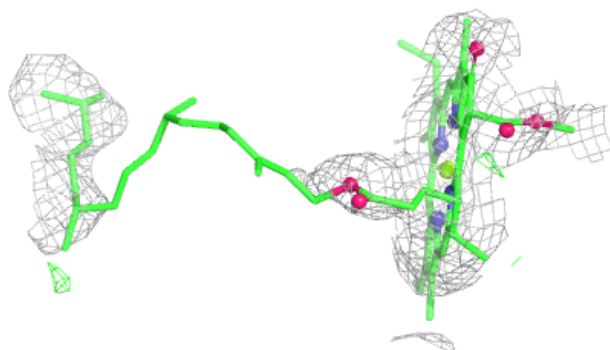
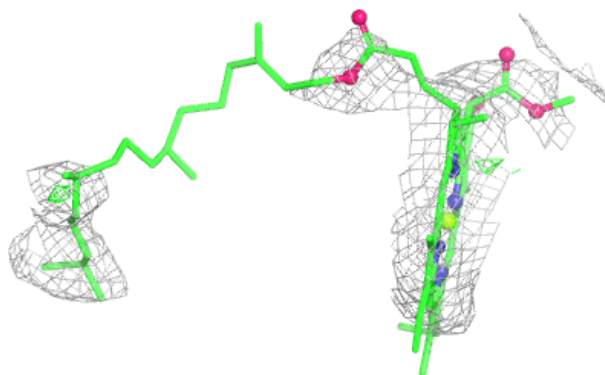
**Electron density around BCR B 530:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

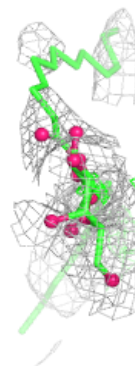
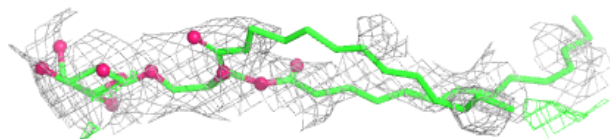
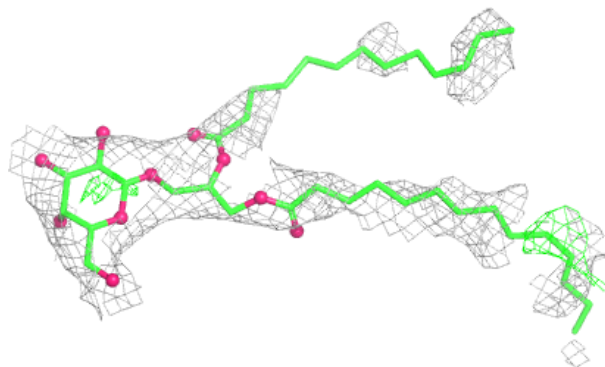


Electron density around CLA C 482:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

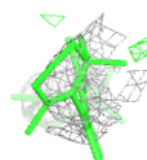
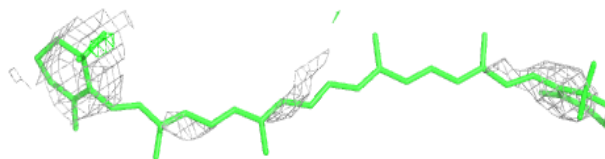
**Electron density around LMG D 359:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

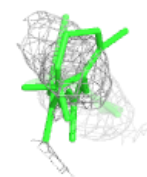
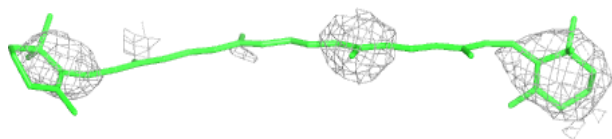
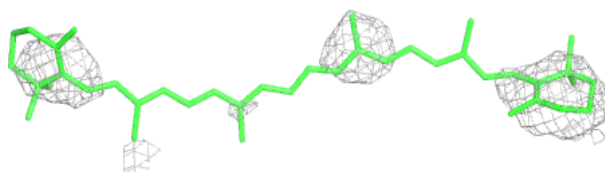


Electron density around BCR C 490:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

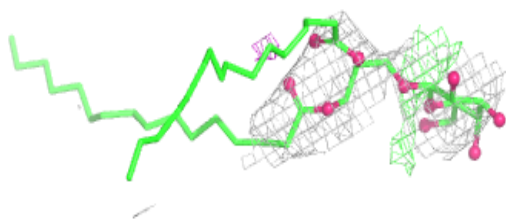
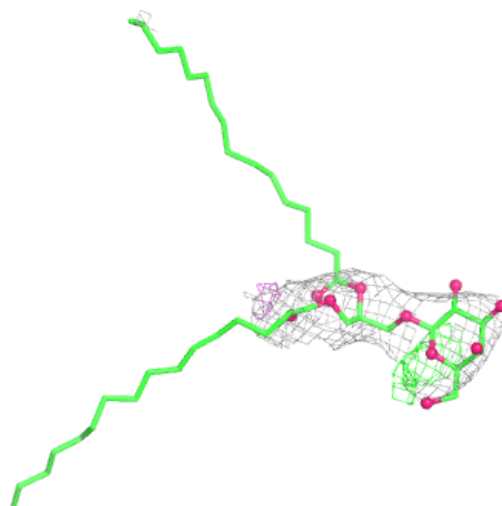
**Electron density around BCR B 527:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



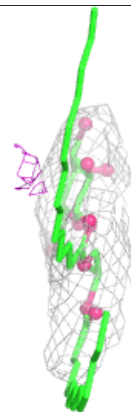
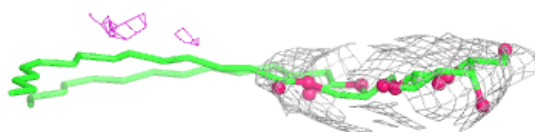
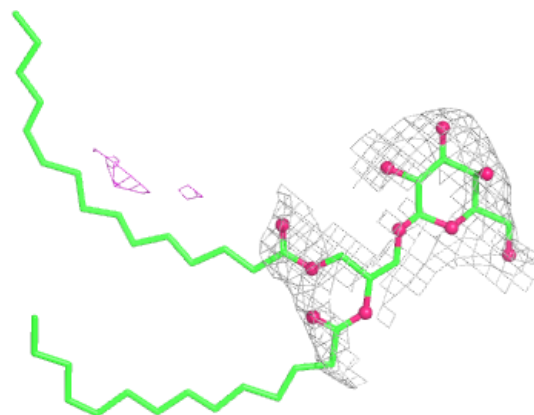
Electron density around LMG A 373:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

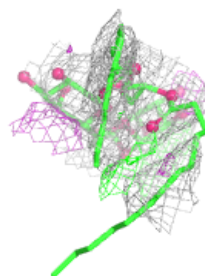
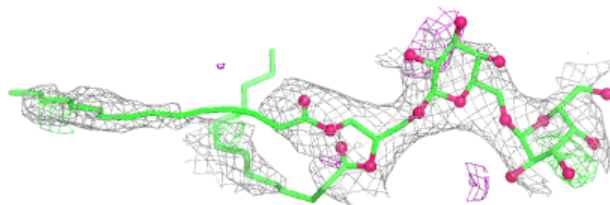
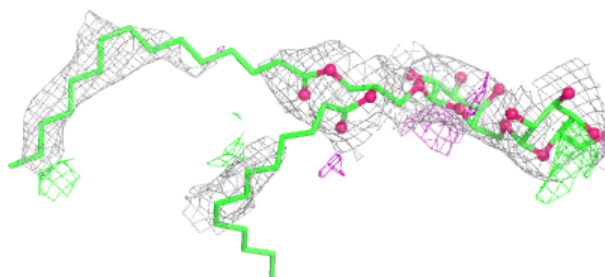


Electron density around LMG J 492:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

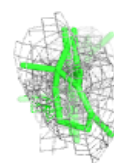
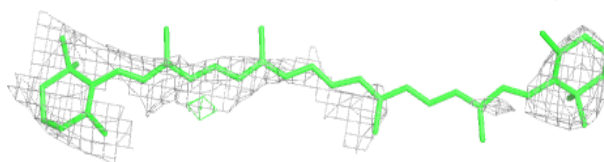
**Electron density around DGD B 528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

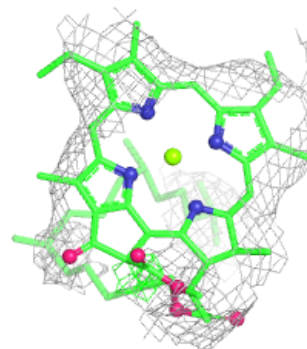
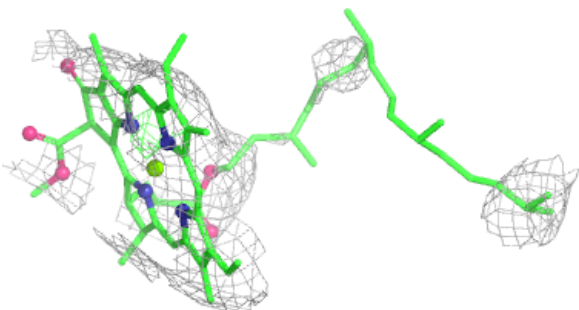
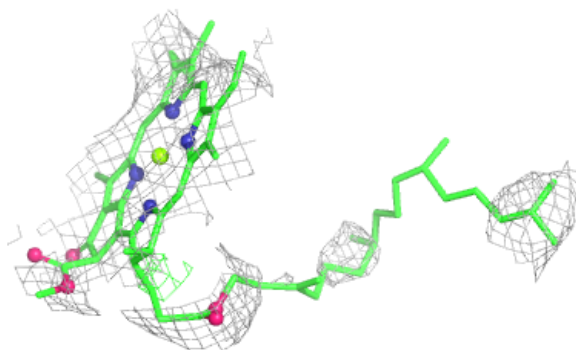


Electron density around BCR B 529:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

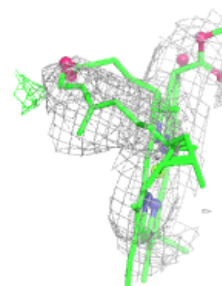
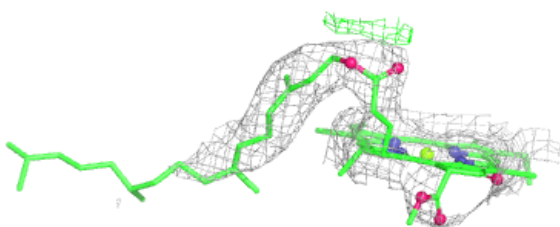
**Electron density around CLA C 488:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

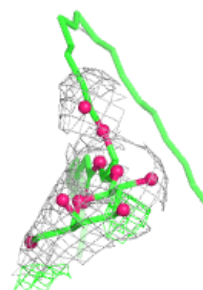
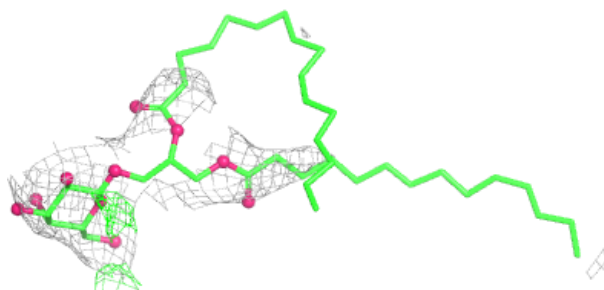


Electron density around CLA A 363:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

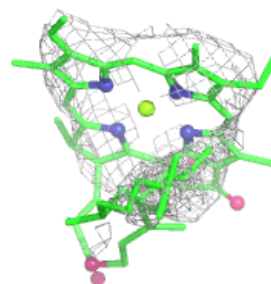
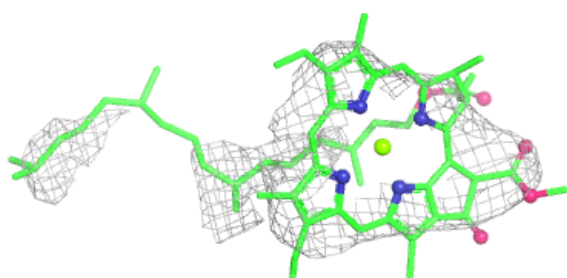
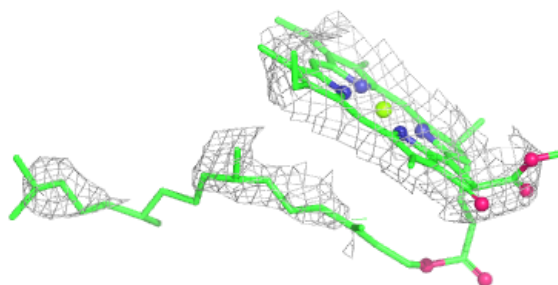
**Electron density around LMG B 531:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

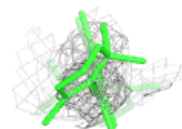
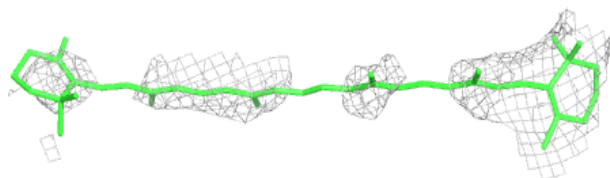
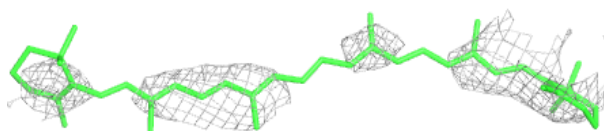


Electron density around CLA B 524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

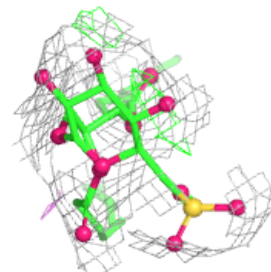
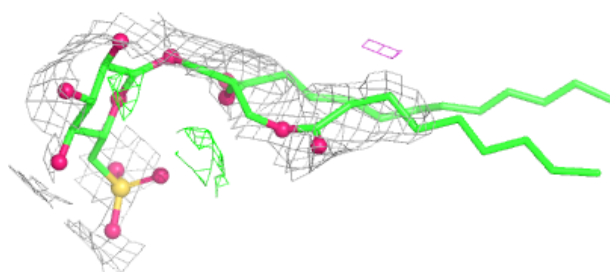
**Electron density around BCR Z 116:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

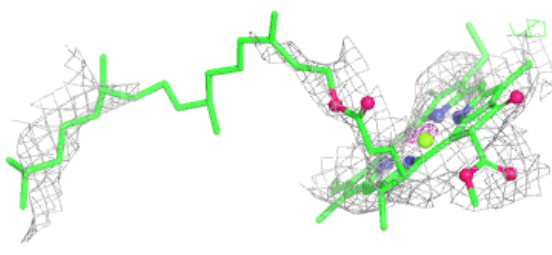
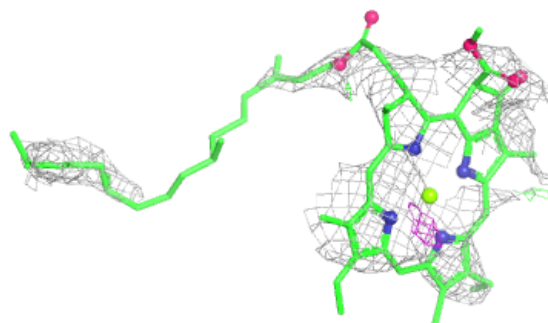


Electron density around SQD D 361:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

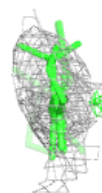
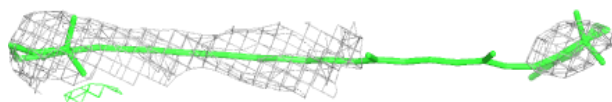
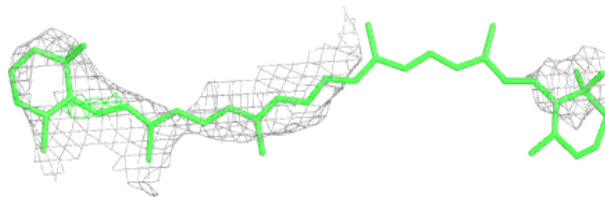
**Electron density around CLA C 486:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

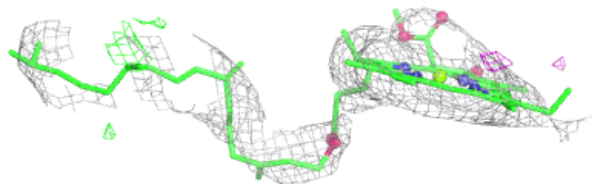
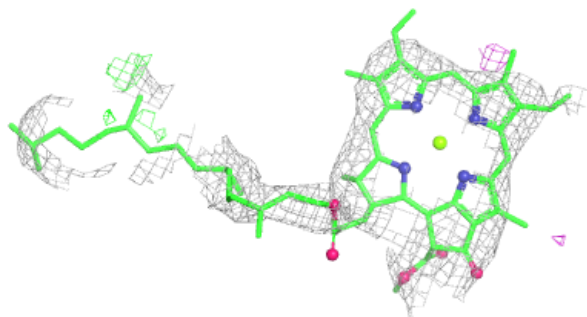


Electron density around BCR J 112:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

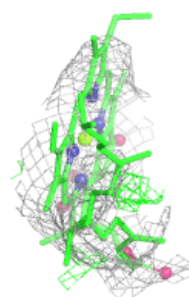
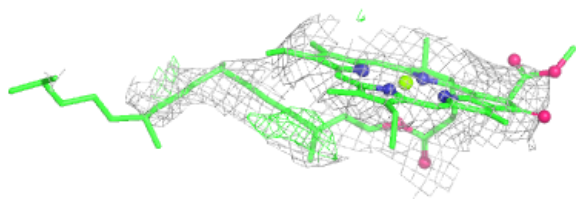
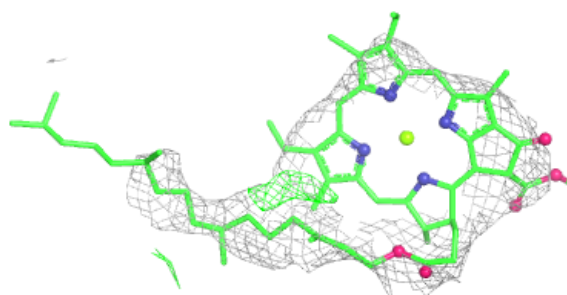
**Electron density around CLA A 364:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

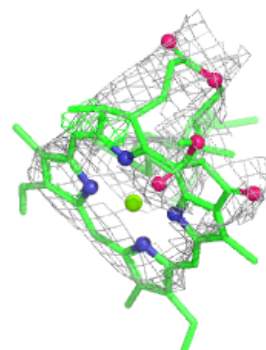
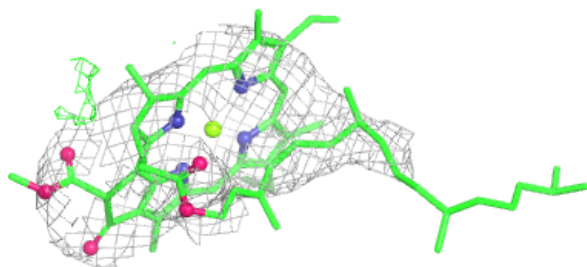


Electron density around CLA C 477:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

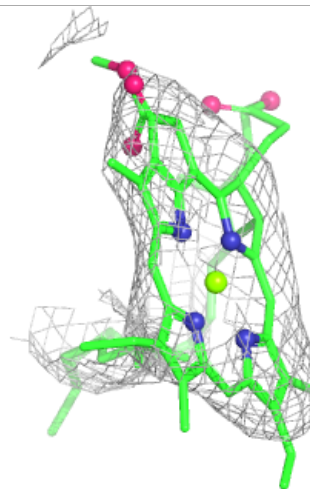
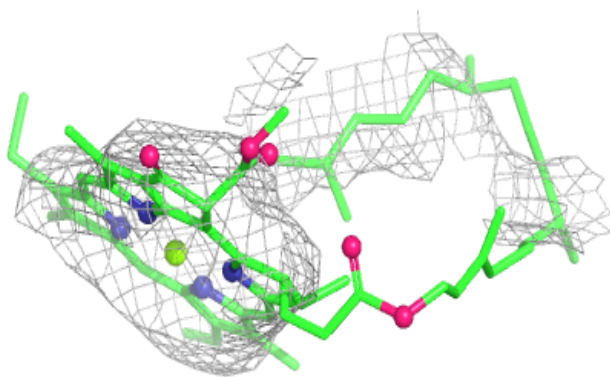
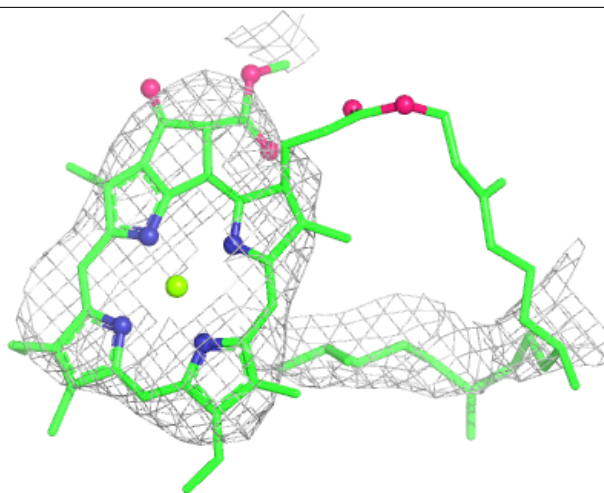
**Electron density around CLA C 481:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



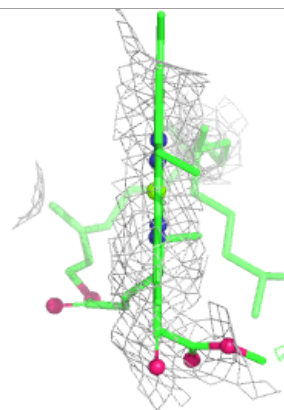
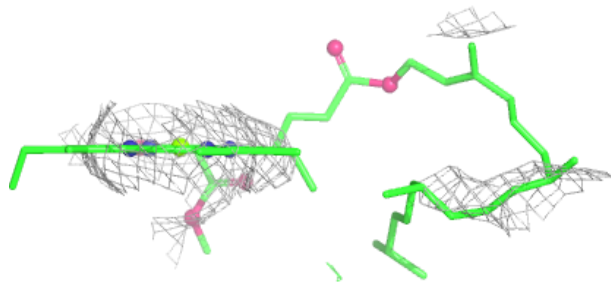
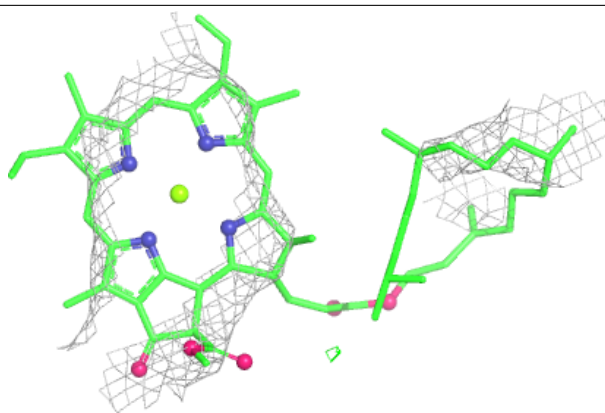
Electron density around CLA B 525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



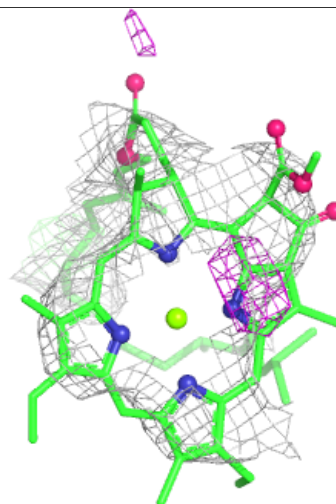
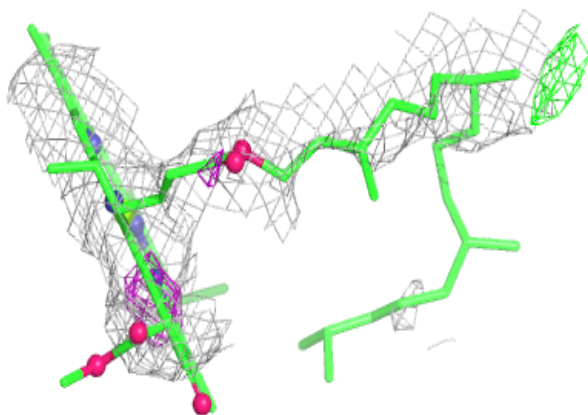
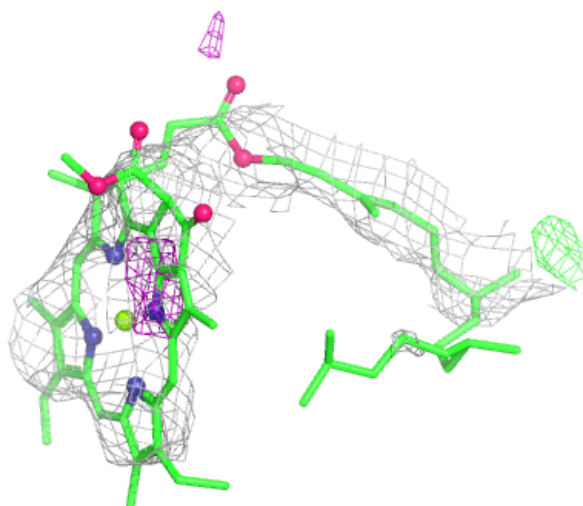
Electron density around CLA C 487:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



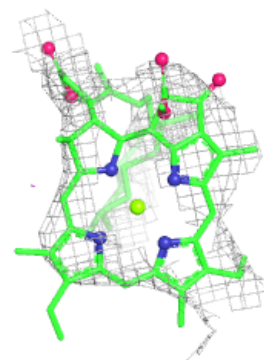
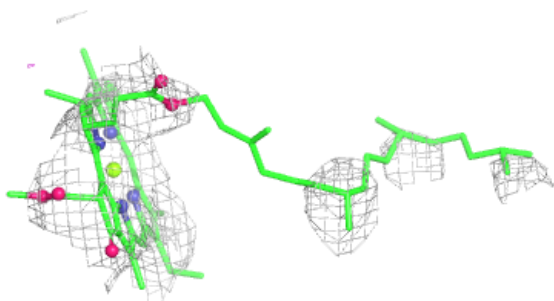
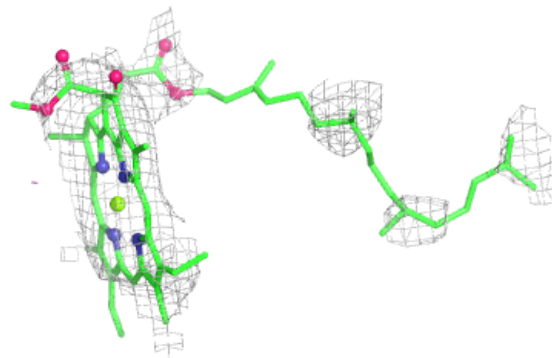
Electron density around CLA C 479:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

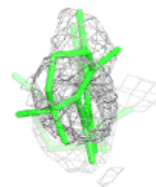
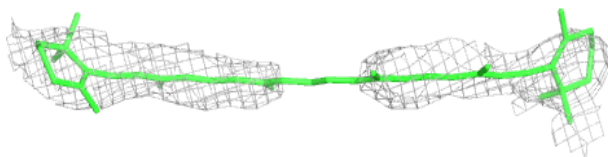
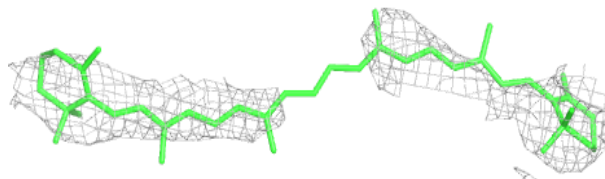


Electron density around CLA C 484:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

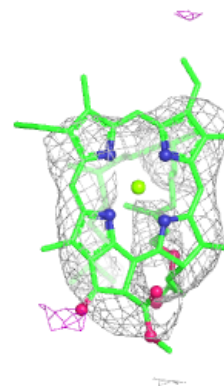
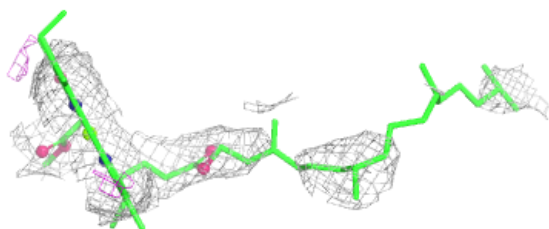
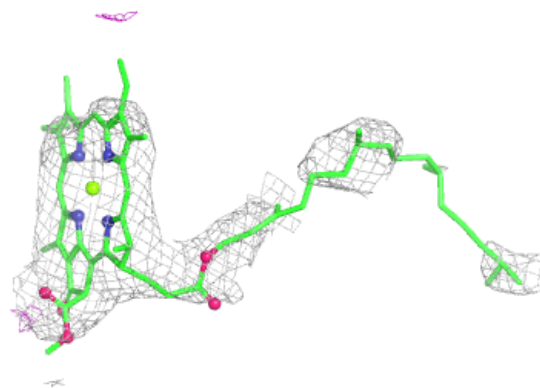
**Electron density around BCR X 107:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

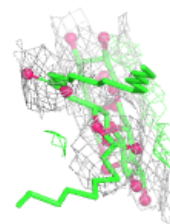
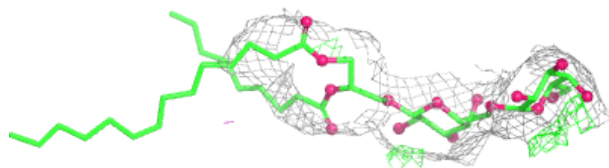
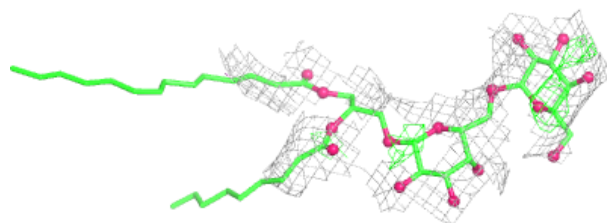


Electron density around CLA D 356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

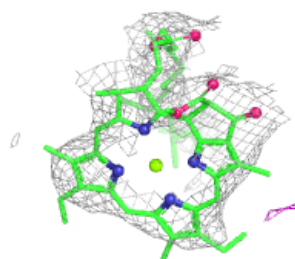
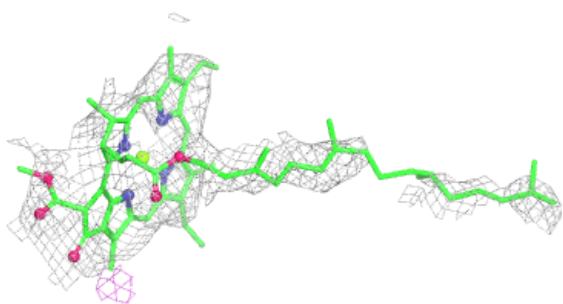
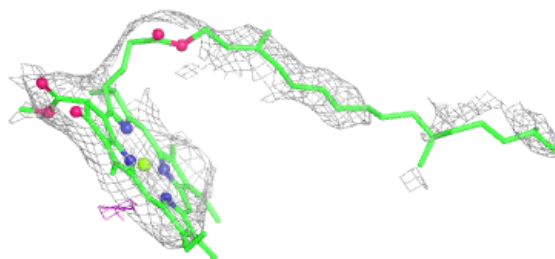
**Electron density around DGD C 491:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

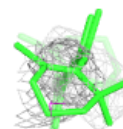
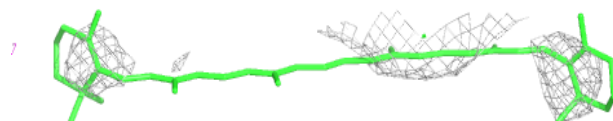
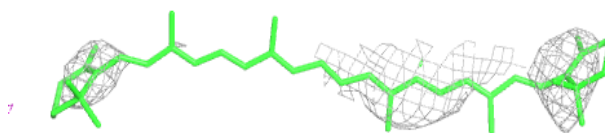


Electron density around CLA C 480:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

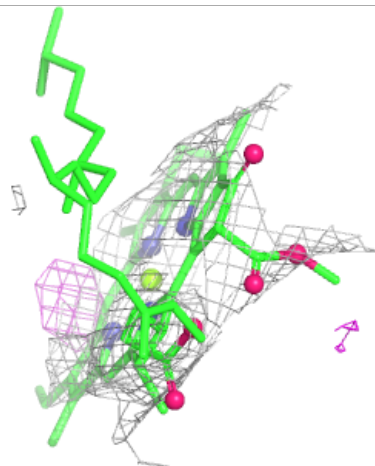
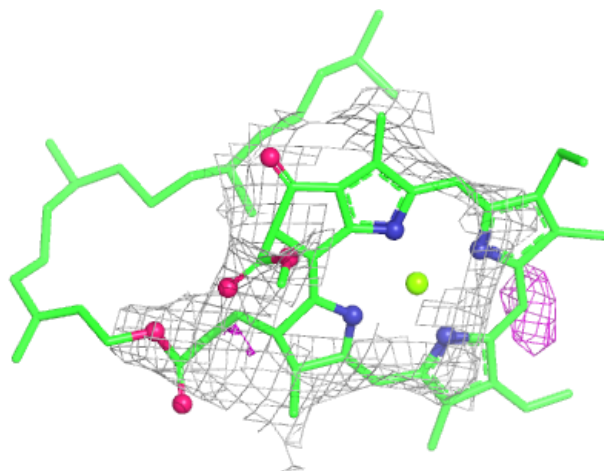
**Electron density around BCR A 369:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



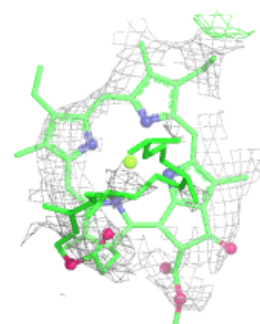
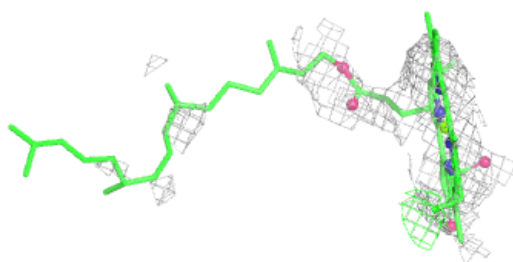
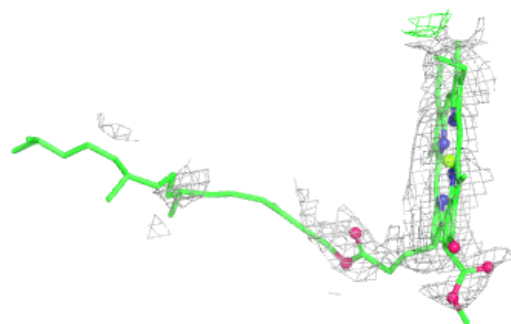
Electron density around CLA C 485:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

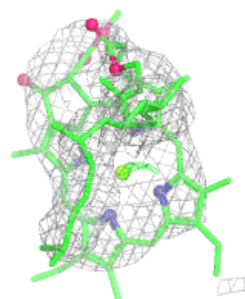
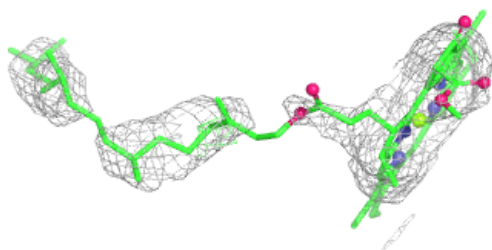
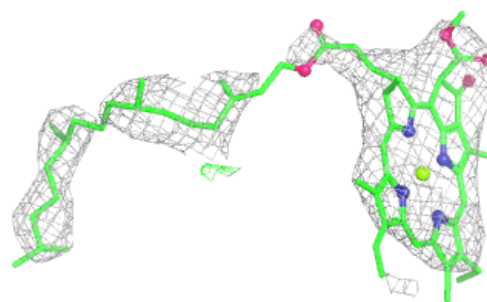


Electron density around CLA B 516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

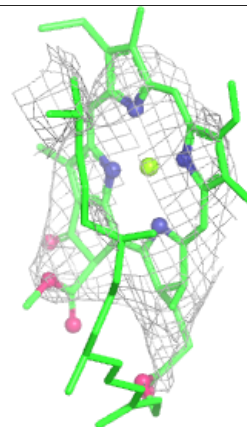
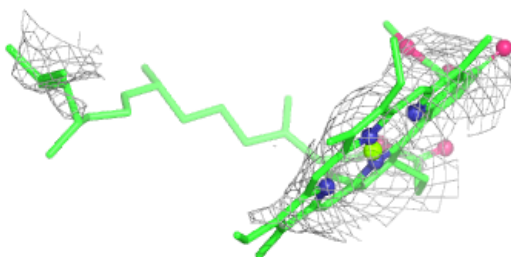
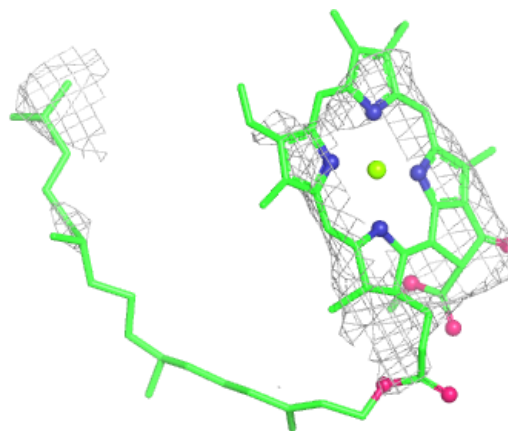
**Electron density around CLA A 366:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



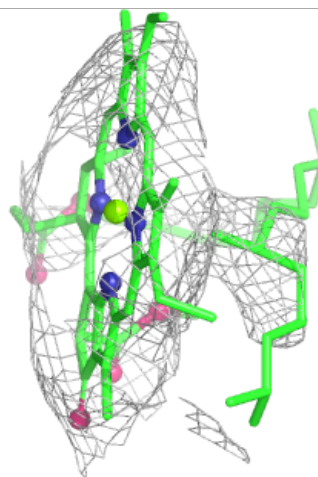
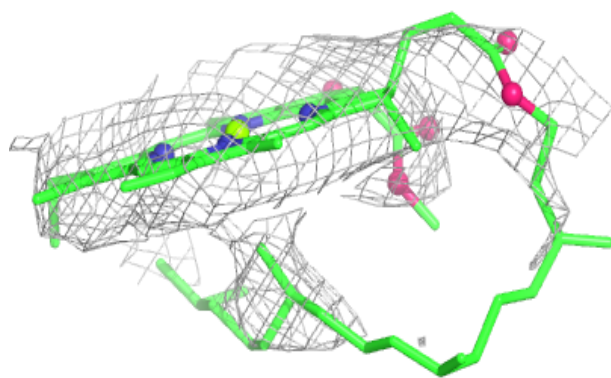
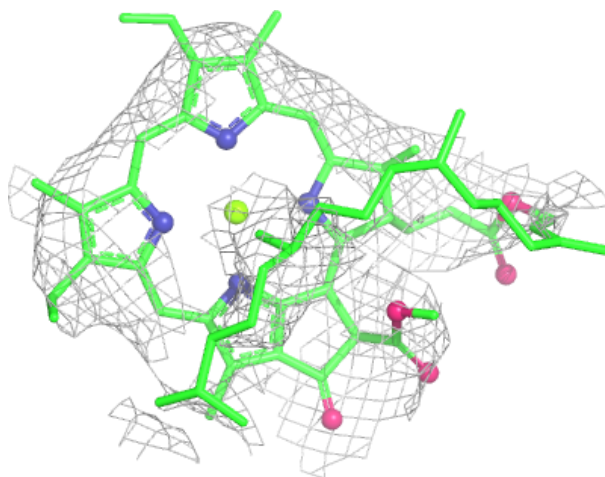
Electron density around CLA C 483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



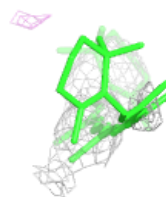
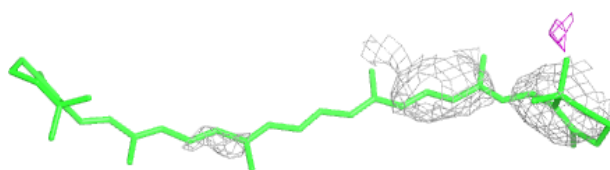
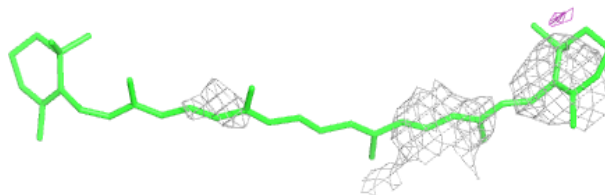
Electron density around CLA K 483:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

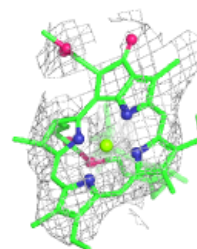
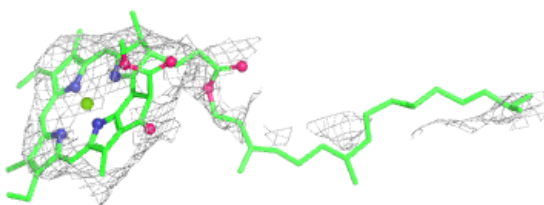


Electron density around BCR C 489:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

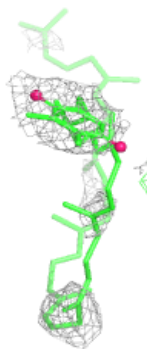
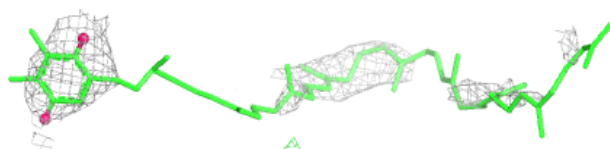
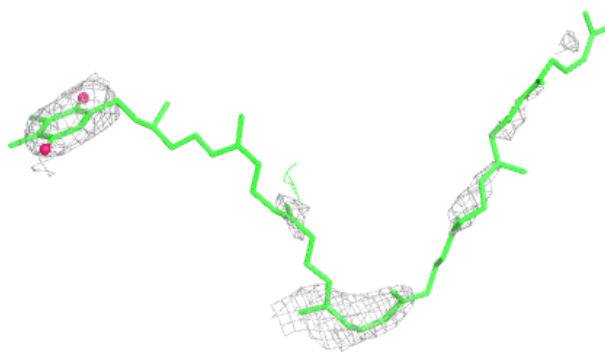
**Electron density around CLA C 478:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

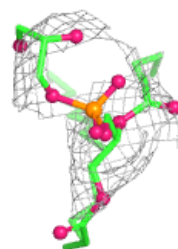
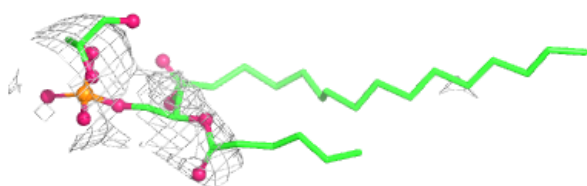
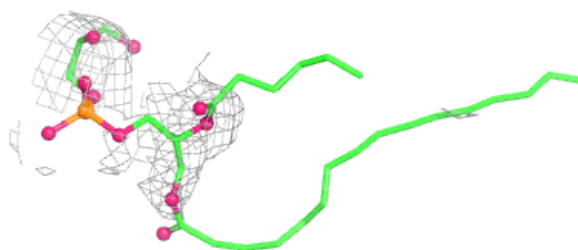


Electron density around PL9 D 357:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

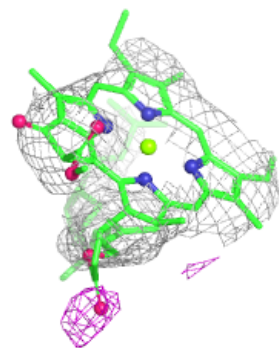
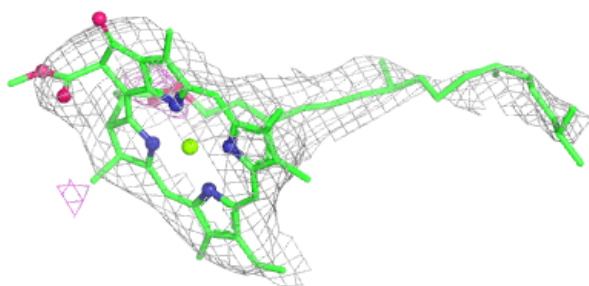
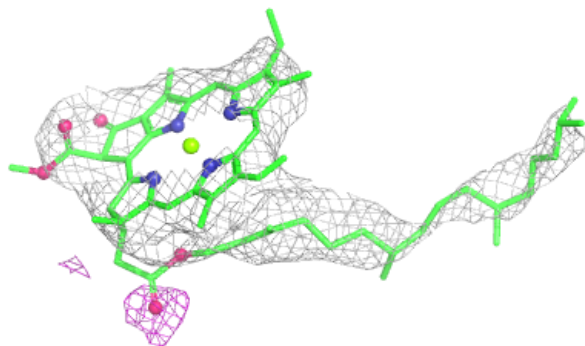
**Electron density around LHG A 371:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

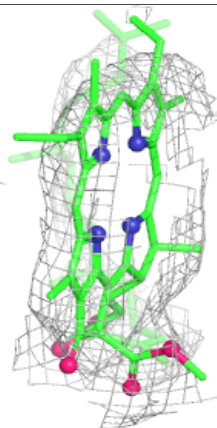
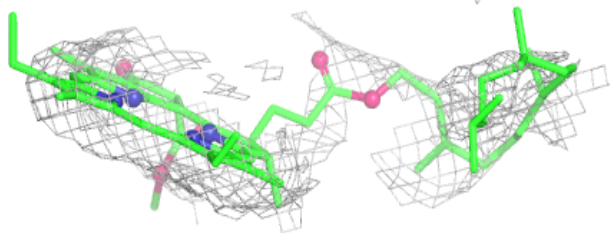
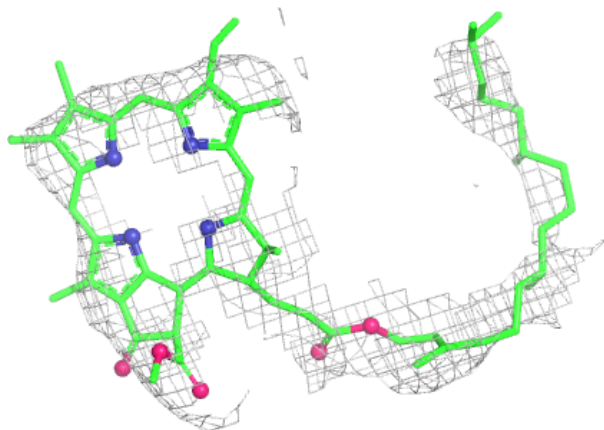


Electron density around CLA B 518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

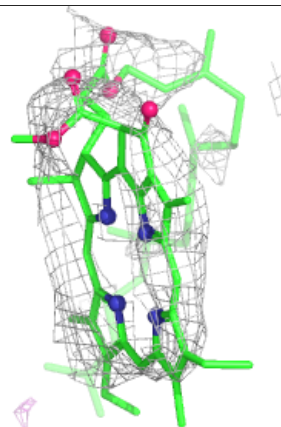
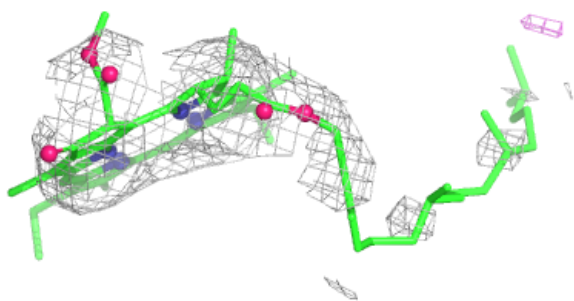
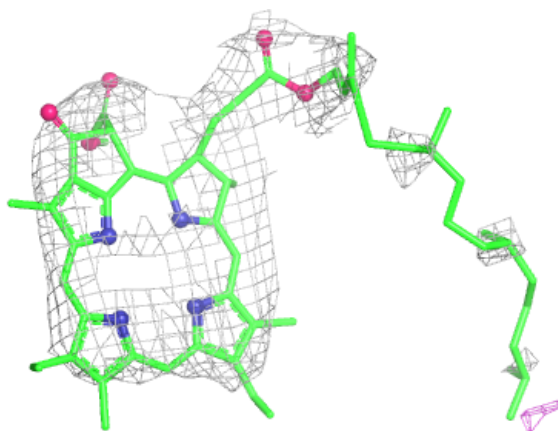
**Electron density around PHO A 365:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



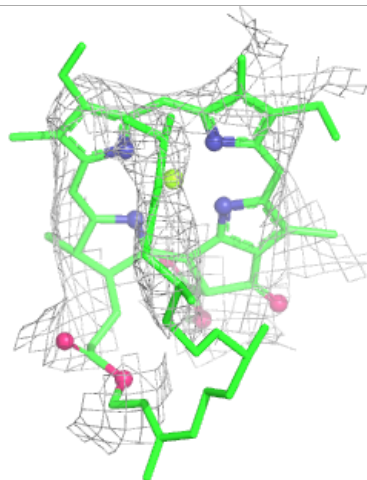
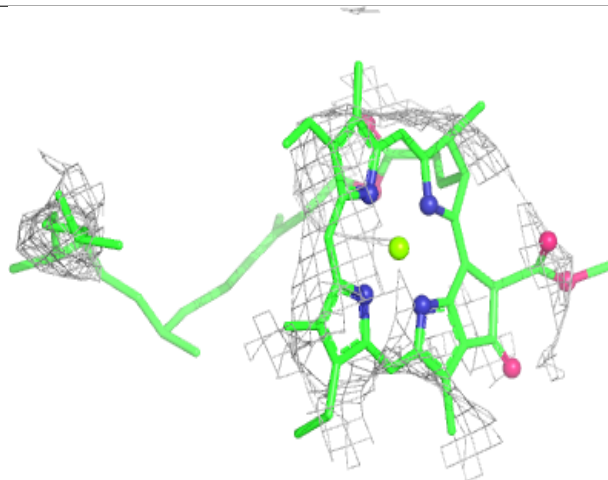
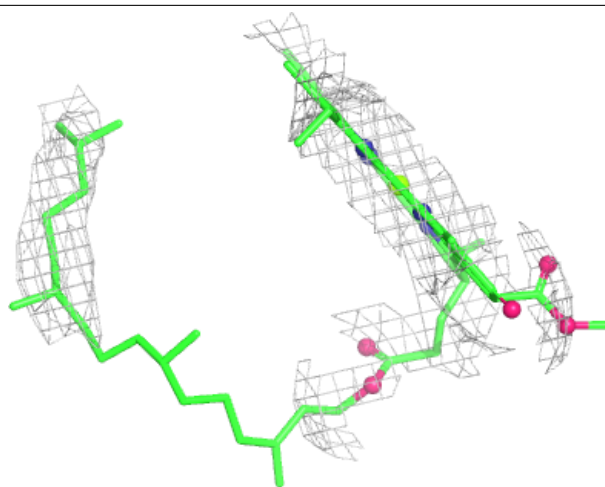
Electron density around PHO D 355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



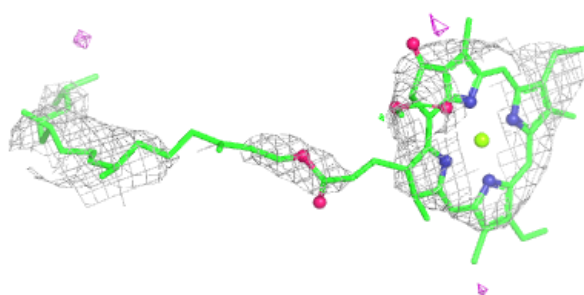
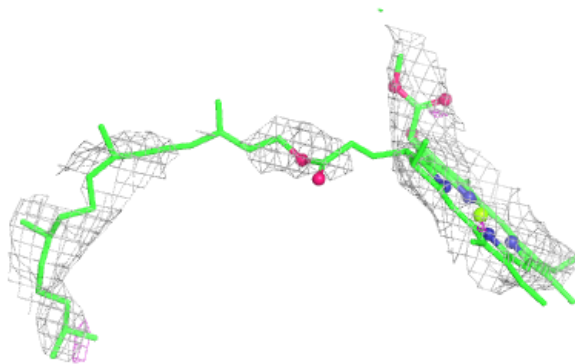
Electron density around CLA B 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

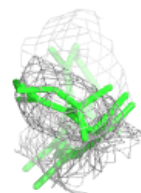
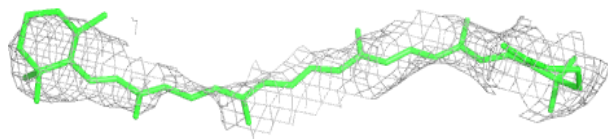
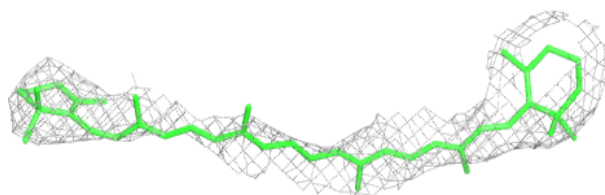


Electron density around CLA D 354:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

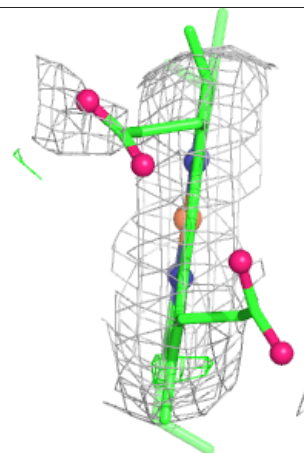
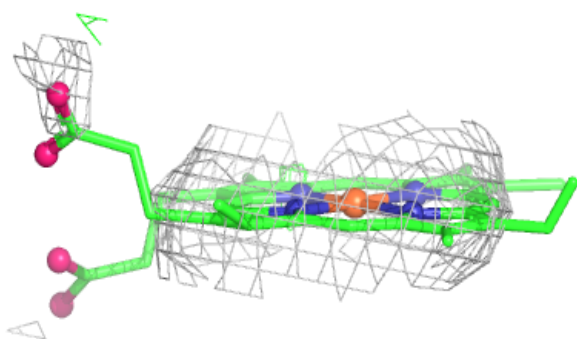
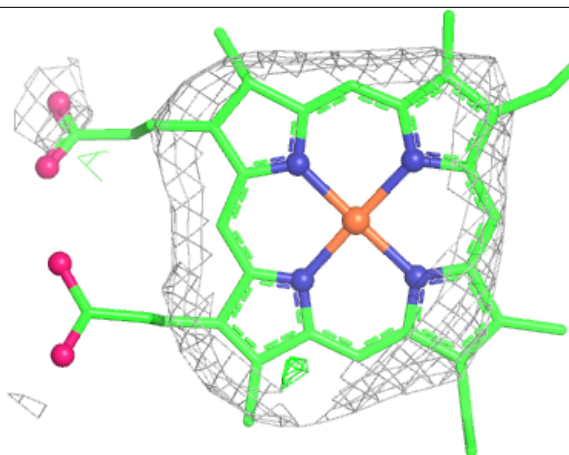
**Electron density around BCR D 358:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



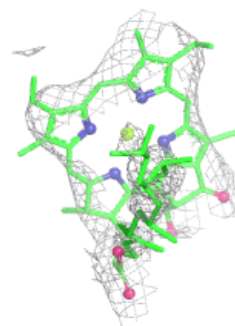
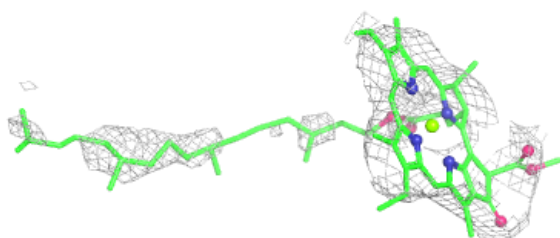
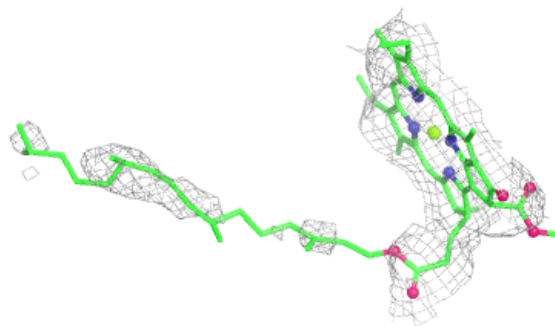
Electron density around HEM F 85:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

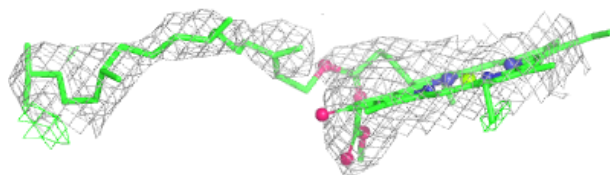
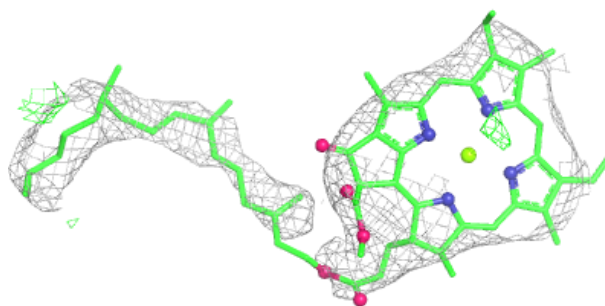


Electron density around CLA B 517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

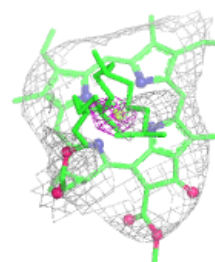
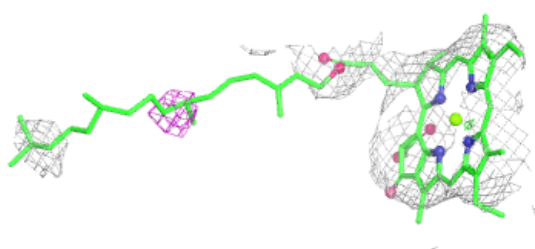
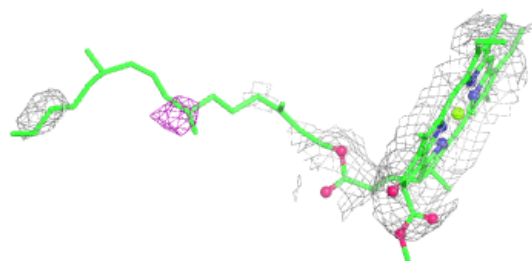
**Electron density around CLA B 512:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

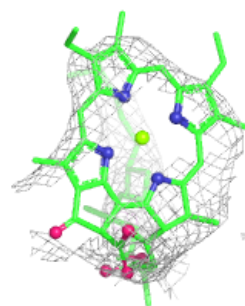
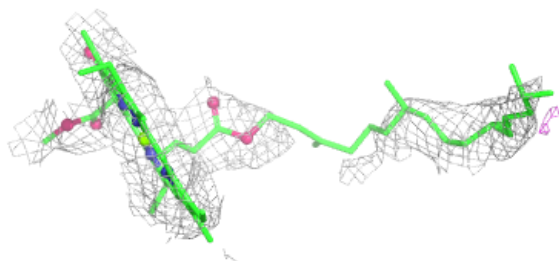
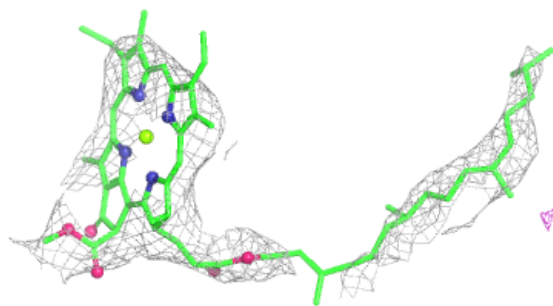


Electron density around CLA B 514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

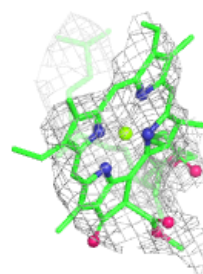
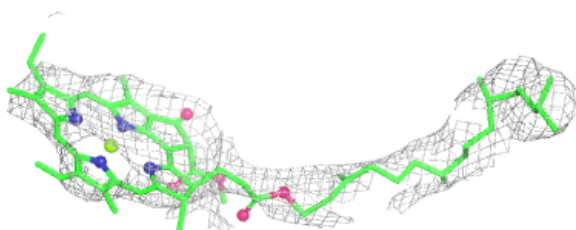
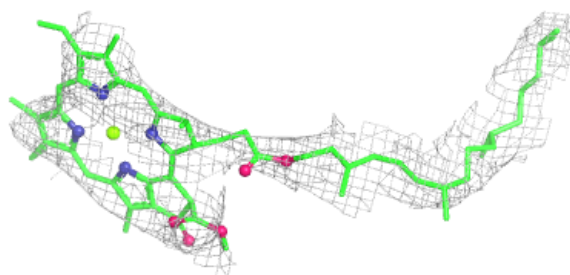
**Electron density around CLA B 519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

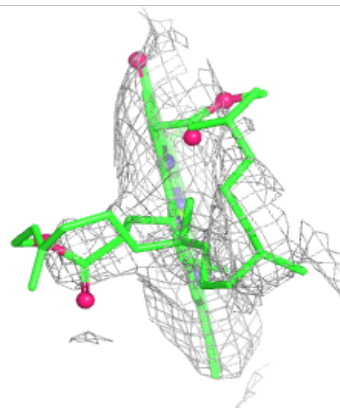
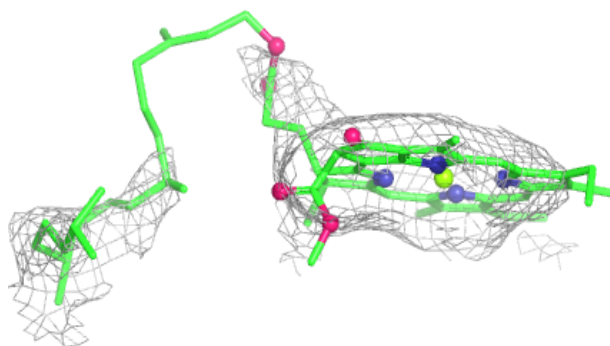
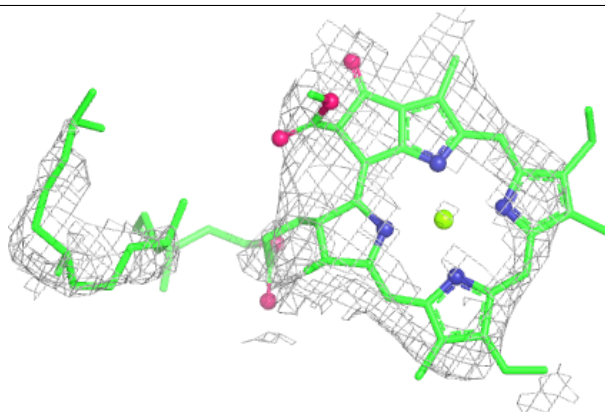


Electron density around CLA A 362:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

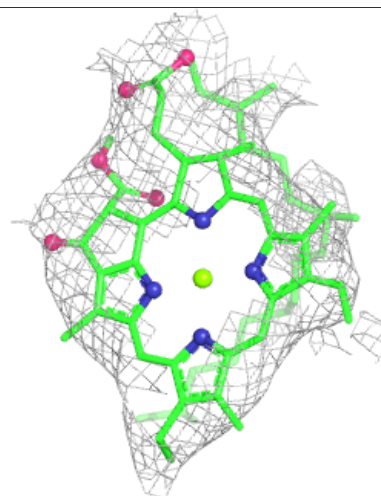
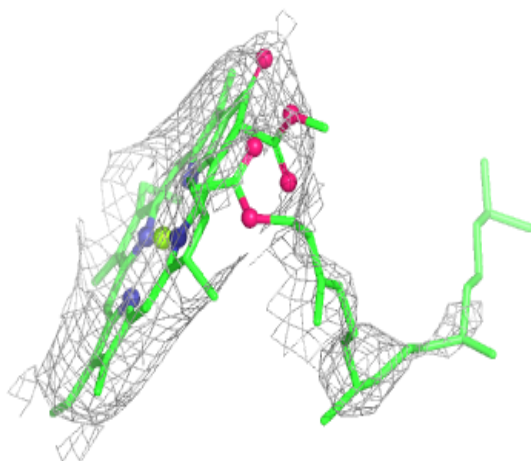
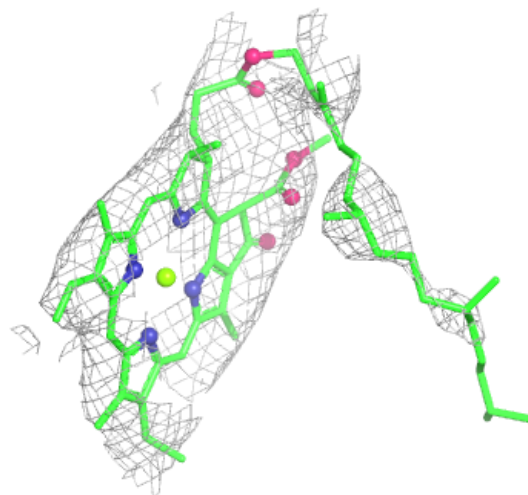
**Electron density around CLA B 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



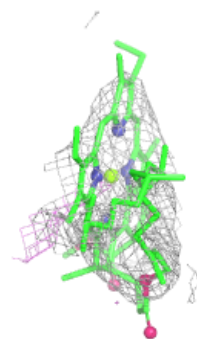
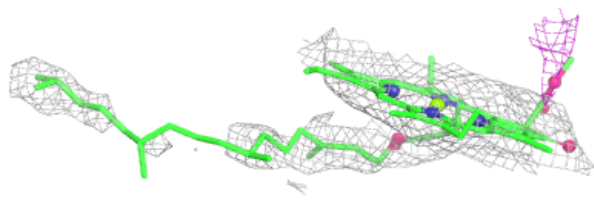
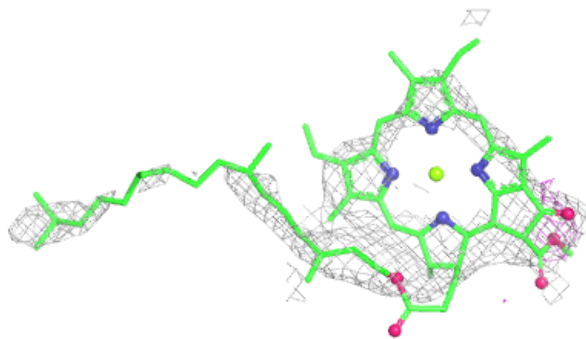
Electron density around CLA B 523:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

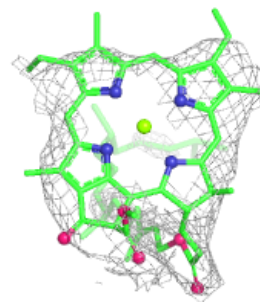
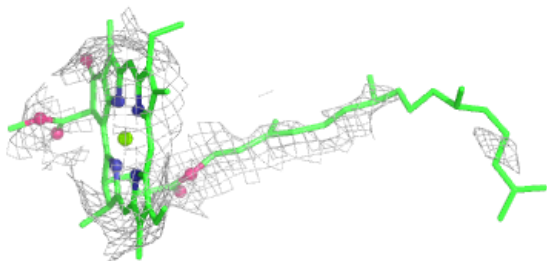
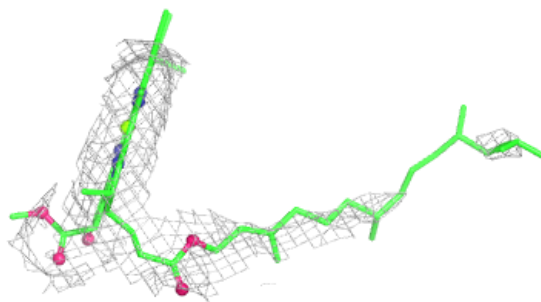


Electron density around CLA B 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

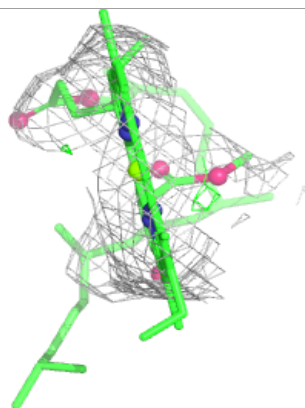
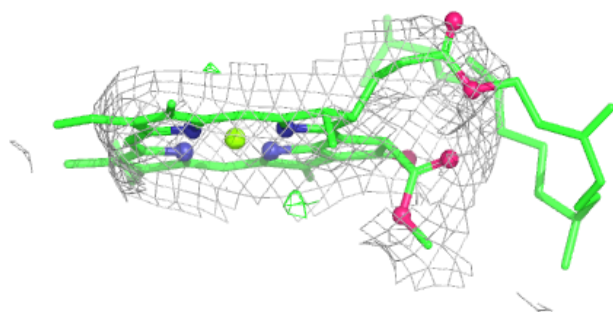
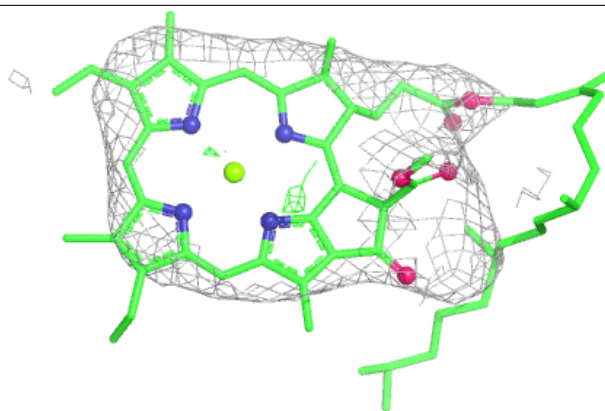
**Electron density around CLA B 515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

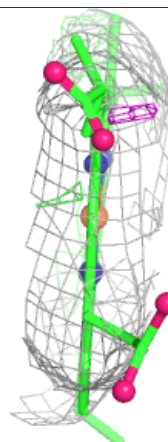
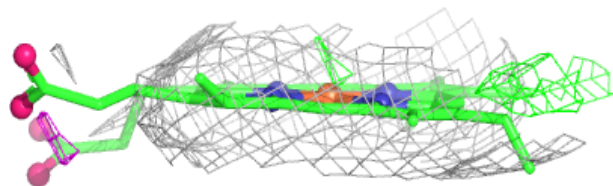
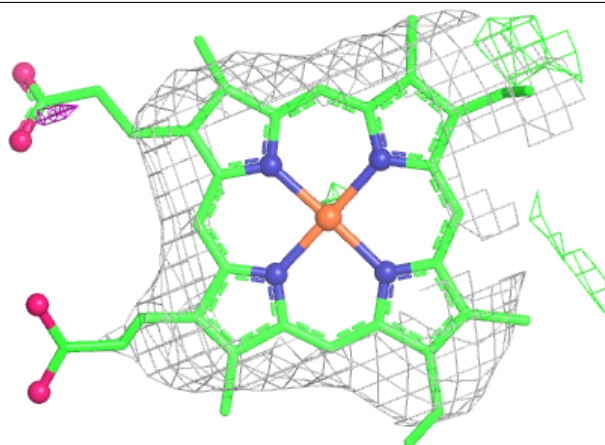


Electron density around CLA B 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HEM V 164:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.