Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:26 AM EDT

PDB ID	:	3PL9 / pdb_00003pl9
Title	:	Crystal structure of spinach minor light-harvesting complex CP29 at 2.80 angstrom resolution
Authors	:	Pan, X.W.; Li, M.; Wan, T.; Wang, L.F.; Jia, C.J.; Hou, Z.Q.; Zhao, X.L.; Zhang, J.P.; Chang, W.R.
Deposited on	:	2010-11-14
Resolution	:	2.80 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:

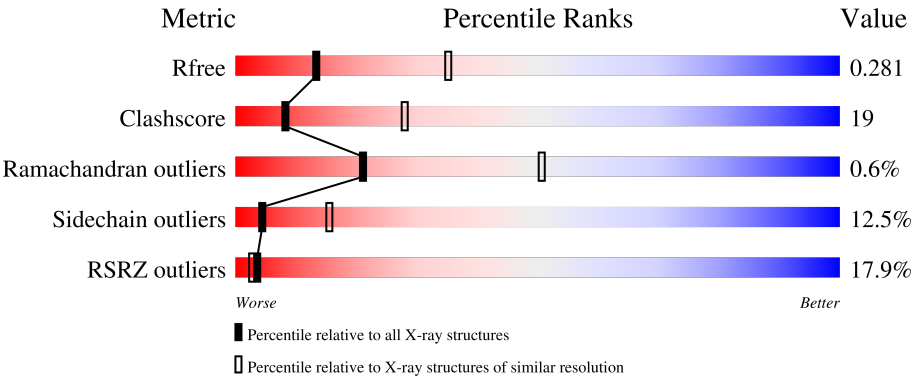
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	243	12% 32% 24% 8% 36%

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
2	CLA	A	602	X	-	-	-
2	CLA	A	604	X	-	-	-
2	CLA	A	609	X	-	-	-
2	CLA	A	610	X	-	-	-
2	CLA	A	611	X	-	-	-
2	CLA	A	612	X	-	-	-
2	CLA	A	613	X	-	-	-
2	CLA	A	615	X	-	-	-
3	CHL	A	606	X	-	-	-
3	CHL	A	607	X	-	-	-
3	CHL	A	608	X	-	-	-
3	CHL	A	614	X	-	-	-

2 Entry composition

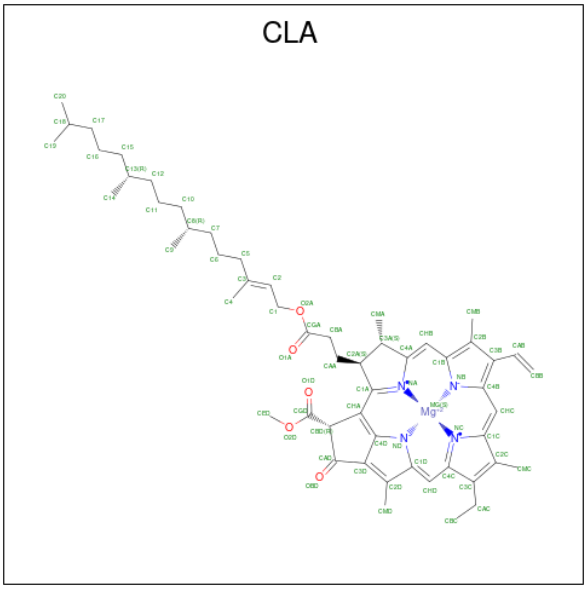
There are 9 unique types of molecules in this entry. The entry contains 2317 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll A-B binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1217	790	204	219	4			

- Molecule 2 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



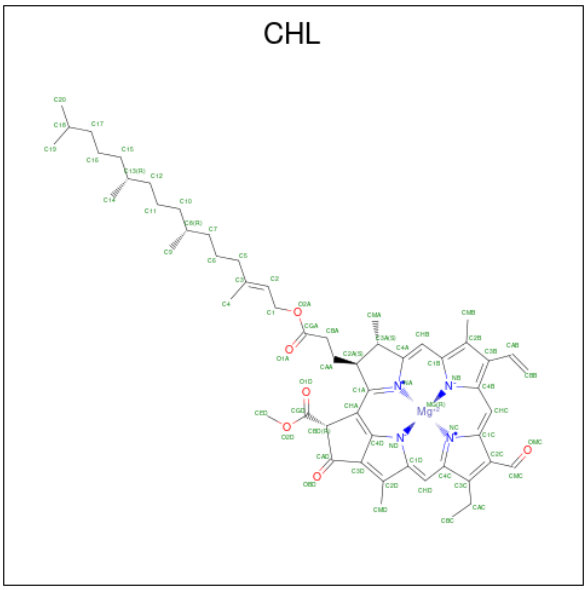
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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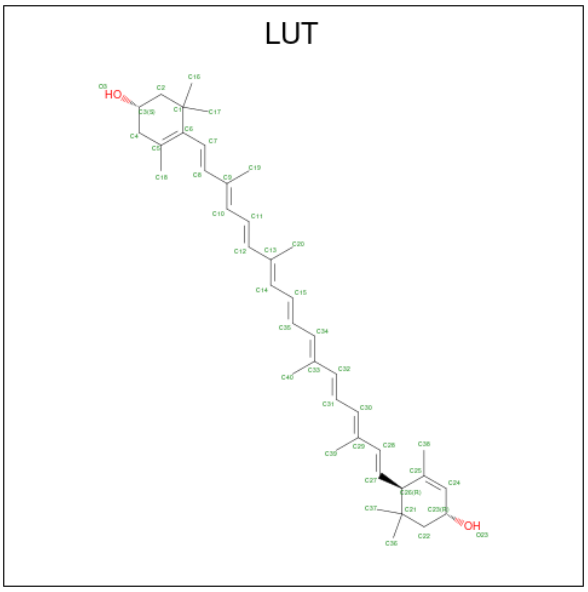
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
2	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 3 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



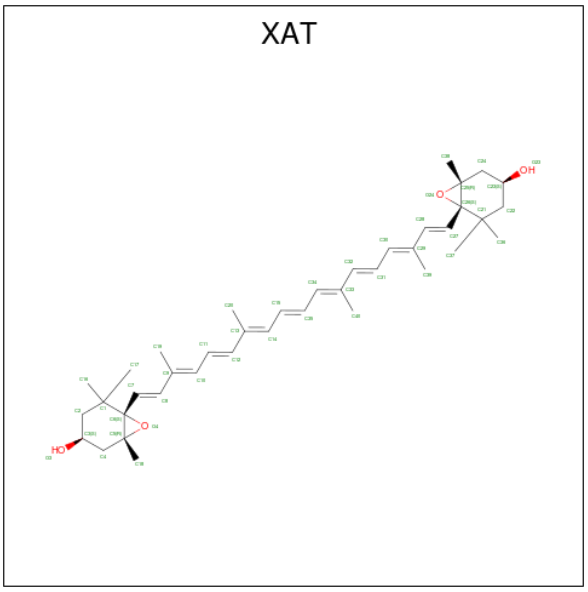
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
3	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			42	40	2		

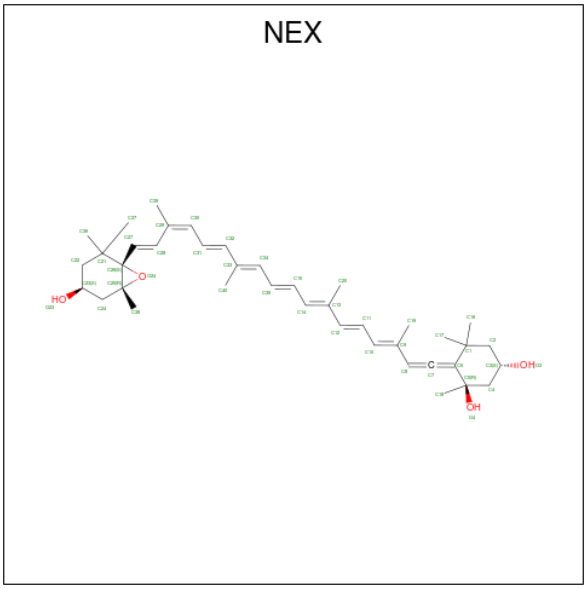
- Molecule 5 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			44	40	4		

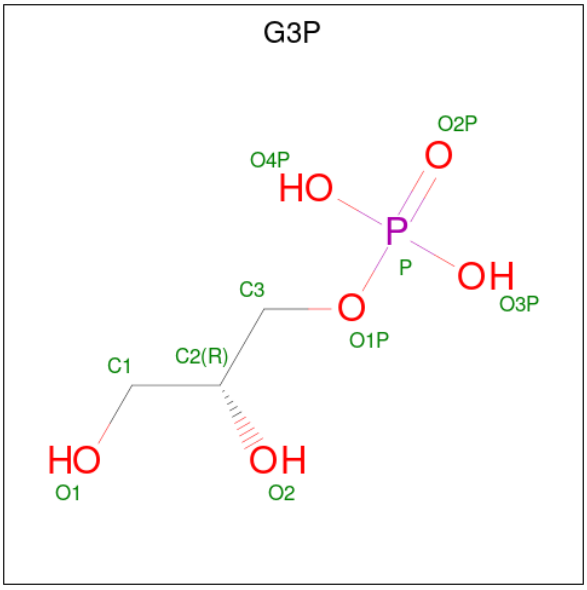
- Molecule 6 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2, 2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA

DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (CCD ID: NEX) (formula: $C_{40}H_{56}O_4$).



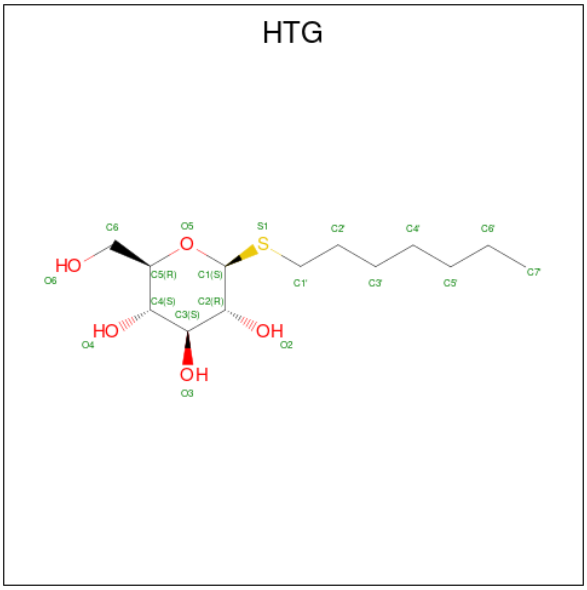
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 44 40 4	0	0

- Molecule 7 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 10 3 6 1	0	0

- Molecule 8 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O S 17 13 3 1	0	0
8	A	1	Total C O S 15 9 5 1	0	0

- Molecule 9 is water.

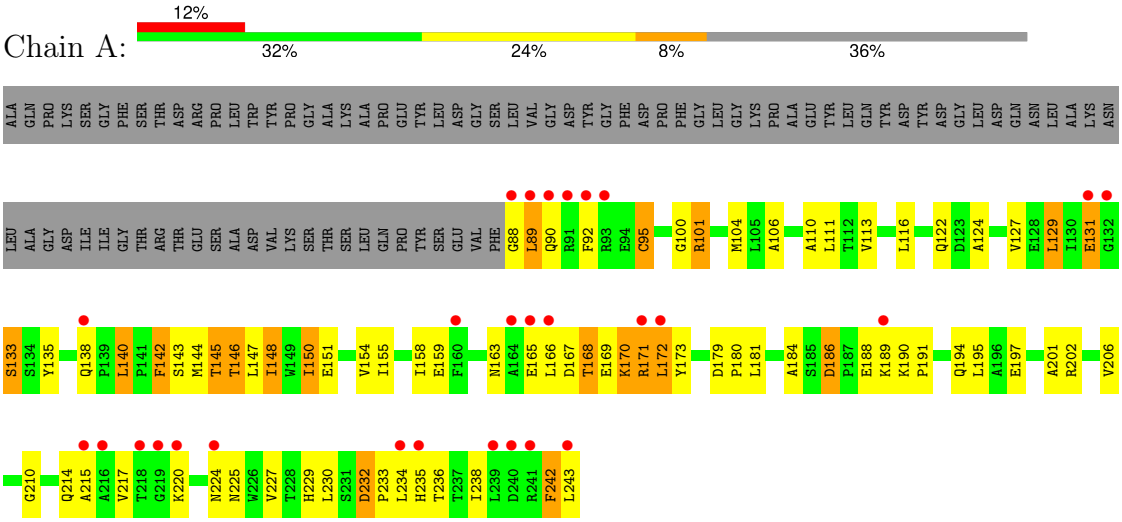
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	79	Total O 79 79	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	68.79Å 68.79Å 425.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.56 – 2.80 42.56 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.4 (42.56-2.80) 92.4 (42.56-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.41 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.282 , 0.293 0.276 , 0.281	Depositor DCC
R_{free} test set	738 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 73.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	2317	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NEX, CHL, HTG, XAT, G3P, LUT, CLA

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	0.51	0/1246	1.06	14/1694 (0.8%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	VAL	N-CA-C	6.87	117.65	110.72
1	A	133	SER	N-CA-C	-6.75	99.53	110.20
1	A	142	PHE	N-CA-C	6.19	119.02	110.35
1	A	217	VAL	N-CA-C	6.12	117.67	111.00
1	A	232	ASP	CA-C-N	6.06	126.22	119.32
1	A	232	ASP	C-N-CA	6.06	126.22	119.32
1	A	171	ARG	N-CA-C	-5.99	105.82	113.01
1	A	186	ASP	CA-C-N	5.80	125.48	119.56
1	A	186	ASP	C-N-CA	5.80	125.48	119.56
1	A	131	GLU	N-CA-C	-5.77	101.42	110.36
1	A	170	LYS	N-CA-C	-5.36	106.75	113.72
1	A	234	LEU	N-CA-C	5.07	116.89	111.36
1	A	140	LEU	CA-C-N	5.00	124.44	119.24
1	A	140	LEU	C-N-CA	5.00	124.44	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1217	0	1233	75	0
2	A	585	0	647	24	0
3	A	264	0	278	9	0
4	A	42	0	56	4	0
5	A	44	0	55	1	0
6	A	44	0	56	3	0
7	A	10	0	7	0	0
8	A	32	0	37	5	0
9	A	79	0	0	5	0
All	All	2317	0	2369	89	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 19.

All (89) 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)
8:A:632:HTG:O5	8:A:632:HTG:C1	1.64	1.43
1:A:146:THR:O	1:A:150:ILE:HD13	1.78	0.83
1:A:206:VAL:HG11	2:A:615:CLA:H41	1.60	0.82
1:A:151:GLU:HG3	1:A:155:ILE:HD13	1.64	0.80
1:A:220:LYS:HD3	1:A:224:ASN:ND2	1.96	0.79
1:A:242:PHE:HB3	9:A:313:HOH:O	1.84	0.76
1:A:143:SER:O	1:A:147:LEU:HB2	1.88	0.74
1:A:88:GLY:N	9:A:322:HOH:O	2.20	0.73
1:A:166:LEU:H	8:A:632:HTG:H2'1	1.55	0.70
1:A:155:ILE:HD11	3:A:606:CHL:HMA1	1.72	0.70
8:A:632:HTG:C1	8:A:632:HTG:C5	2.70	0.69
1:A:135:TYR:HD2	2:A:604:CLA:HBA1	1.59	0.68
1:A:124:ALA:CB	2:A:604:CLA:HED1	2.24	0.67
1:A:158:ILE:HG22	9:A:247:HOH:O	1.92	0.67
1:A:131:GLU:HB3	9:A:310:HOH:O	1.95	0.67
2:A:613:CLA:H193	4:A:620:LUT:H193	1.78	0.65
1:A:210:GLY:O	1:A:214:GLN:HG3	1.97	0.64
1:A:158:ILE:HD11	6:A:623:NEX:H34	1.78	0.64
1:A:89:LEU:O	1:A:92:PHE:N	2.31	0.63
1:A:230:LEU:HD21	3:A:614:CHL:HMC	1.81	0.63
1:A:104:MET:HE2	1:A:201:ALA:HB2	1.82	0.62
1:A:184:ALA:HB3	2:A:610:CLA:HED3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HG22	1:A:146:THR:N	2.14	0.61
1:A:142:PHE:HB2	1:A:147:LEU:HD13	1.83	0.60
1:A:173:TYR:CE1	1:A:194:GLN:HG2	2.37	0.60
1:A:229:HIS:HA	1:A:236:THR:OG1	2.02	0.59
1:A:232:ASP:OD2	1:A:235:HIS:HB2	2.02	0.59
1:A:124:ALA:HB1	2:A:604:CLA:HED1	1.85	0.58
1:A:129:LEU:HB2	1:A:144:MET:HE3	1.86	0.57
1:A:151:GLU:HG3	1:A:155:ILE:CD1	2.32	0.57
1:A:100:GLY:HA3	1:A:201:ALA:HB1	1.86	0.56
1:A:172:LEU:HB3	1:A:173:TYR:CD2	2.42	0.54
1:A:206:VAL:HG11	2:A:615:CLA:H51	1.90	0.54
1:A:147:LEU:HD12	3:A:606:CHL:HED3	1.91	0.52
1:A:238:ILE:HD13	2:A:613:CLA:OBD	2.10	0.52
1:A:101:ARG:NH1	1:A:197:GLU:OE1	2.41	0.52
1:A:202:ARG:O	1:A:206:VAL:HG23	2.10	0.52
1:A:167:ASP:O	1:A:169:GLU:N	2.42	0.51
1:A:151:GLU:CG	1:A:155:ILE:HD13	2.37	0.51
1:A:95:CYS:SG	2:A:603:CLA:HAA2	2.50	0.51
1:A:122:GLN:HE21	1:A:215:ALA:HB1	1.75	0.50
1:A:145:THR:CG2	1:A:146:THR:N	2.74	0.50
1:A:159:GLU:HG3	2:A:609:CLA:C4B	2.42	0.50
1:A:179:ASP:N	1:A:180:PRO:HD3	2.27	0.50
1:A:95:CYS:HB3	2:A:602:CLA:HMB2	1.94	0.49
1:A:155:ILE:CD1	3:A:606:CHL:HMA1	2.42	0.49
1:A:225:ASN:HB3	2:A:613:CLA:HED2	1.94	0.49
2:A:615:CLA:HHC	2:A:615:CLA:HBB1	1.95	0.49
1:A:155:ILE:N	1:A:155:ILE:HD12	2.28	0.49
1:A:165:GLU:OE1	3:A:608:CHL:HBC1	2.13	0.49
1:A:159:GLU:HG3	2:A:609:CLA:NB	2.28	0.48
1:A:144:MET:O	1:A:148:ILE:HG23	2.14	0.48
2:A:613:CLA:HBB1	2:A:613:CLA:HHC	1.96	0.47
3:A:606:CHL:HBA2	6:A:623:NEX:H403	1.96	0.47
1:A:166:LEU:N	8:A:632:HTG:H2'1	2.27	0.47
1:A:89:LEU:O	1:A:90:GLN:C	2.57	0.47
1:A:166:LEU:HA	1:A:171:ARG:HD2	1.95	0.47
1:A:238:ILE:HG13	1:A:238:ILE:O	2.16	0.46
1:A:163:ASN:ND2	1:A:171:ARG:HH12	2.13	0.46
3:A:607:CHL:H93	3:A:607:CHL:HBA2	1.98	0.45
1:A:225:ASN:N	1:A:225:ASN:HD22	2.14	0.45
1:A:89:LEU:C	1:A:89:LEU:CD1	2.90	0.44
3:A:606:CHL:H61	6:A:623:NEX:H402	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:603:CLA:HBB1	2:A:603:CLA:HHC	1.99	0.44
1:A:186:ASP:HB3	1:A:189:LYS:HD2	2.00	0.44
1:A:233:PRO:HD2	3:A:614:CHL:H151	1.99	0.44
1:A:186:ASP:C	1:A:186:ASP:OD2	2.60	0.43
1:A:195:LEU:HD11	2:A:615:CLA:HMD2	2.00	0.43
1:A:195:LEU:CD1	2:A:615:CLA:HMD2	2.49	0.43
1:A:143:SER:OG	1:A:146:THR:HG23	2.17	0.43
1:A:163:ASN:ND2	1:A:171:ARG:NH1	2.66	0.43
1:A:110:ALA:O	1:A:113:VAL:HG12	2.19	0.43
2:A:613:CLA:HMB2	4:A:620:LUT:H7	2.01	0.43
2:A:609:CLA:HBB1	2:A:609:CLA:HHC	2.01	0.43
2:A:604:CLA:HMA3	9:A:244:HOH:O	2.18	0.42
1:A:179:ASP:HA	4:A:620:LUT:H24	2.00	0.42
1:A:190:LYS:HB2	1:A:191:PRO:HD3	2.01	0.42
2:A:613:CLA:H91	2:A:613:CLA:H143	2.01	0.42
1:A:101:ARG:HD2	2:A:610:CLA:C4C	2.50	0.41
1:A:225:ASN:N	1:A:225:ASN:ND2	2.65	0.41
1:A:227:VAL:O	1:A:227:VAL:HG12	2.20	0.41
1:A:181:LEU:HD12	4:A:620:LUT:H222	2.03	0.41
1:A:106:ALA:HA	5:A:622:XAT:H181	2.03	0.41
1:A:133:SER:HB2	1:A:140:LEU:O	2.21	0.41
1:A:172:LEU:HB3	1:A:173:TYR:CE2	2.56	0.41
1:A:206:VAL:CG1	2:A:615:CLA:H41	2.41	0.41
1:A:170:LYS:HE2	1:A:170:LYS:HB3	1.86	0.41
1:A:168:THR:HA	1:A:171:ARG:HG3	2.02	0.40
8:A:632:HTG:O5	8:A:632:HTG:C2	2.60	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	154/243 (63%)	141 (92%)	12 (8%)	1 (1%)	21 51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	THR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	128/198 (65%)	112 (88%)	16 (12%)	4 15

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	95	CYS
1	A	101	ARG
1	A	111	LEU
1	A	116	LEU
1	A	127	VAL
1	A	129	LEU
1	A	138	GLN
1	A	145	THR
1	A	146	THR
1	A	148	ILE
1	A	150	ILE
1	A	172	LEU
1	A	188	GLU
1	A	242	PHE
1	A	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	163	ASN
1	A	224	ASN
1	A	225	ASN
1	A	235	HIS

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)

19 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	CLA	A	613	1	69,73,73	1.28	7 (10%)	82,113,113	1.99	11 (13%)
4	LUT	A	620	-	42,43,43	1.08	3 (7%)	51,60,60	1.40	6 (11%)
3	CHL	A	606	9	70,74,74	1.49	7 (10%)	79,114,114	1.94	17 (21%)
5	XAT	A	622	-	41,47,47	1.02	2 (4%)	54,74,74	1.51	5 (9%)
8	HTG	A	631	-	17,17,19	3.69	9 (52%)	19,20,24	2.89	5 (26%)
2	CLA	A	612	1	69,73,73	1.53	8 (11%)	82,113,113	1.86	16 (19%)
7	G3P	A	630	2	9,9,9	1.38	1 (11%)	10,12,12	1.27	1 (10%)
2	CLA	A	609	1	69,73,73	1.32	9 (13%)	82,113,113	1.79	15 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CLA	A	611	7	69,73,73	1.51	8 (11%)	82,113,113	1.79	13 (15%)
2	CLA	A	604	9	69,73,73	1.34	7 (10%)	82,113,113	2.07	16 (19%)
3	CHL	A	614	1	70,74,74	1.49	7 (10%)	79,114,114	2.06	17 (21%)
2	CLA	A	602	1	69,73,73	1.41	6 (8%)	82,113,113	1.90	16 (19%)
6	NEX	A	623	-	40,46,46	2.10	4 (10%)	50,70,70	1.45	7 (14%)
3	CHL	A	607	9	70,74,74	1.40	6 (8%)	79,114,114	2.02	17 (21%)
2	CLA	A	610	1	69,73,73	1.32	6 (8%)	82,113,113	1.94	18 (21%)
8	HTG	A	632	-	15,15,19	4.63	8 (53%)	19,20,24	2.71	3 (15%)
3	CHL	A	608	9	70,74,74	1.72	10 (14%)	79,114,114	2.17	17 (21%)
2	CLA	A	603	1	69,73,73	1.35	7 (10%)	82,113,113	1.74	11 (13%)
2	CLA	A	615	7	69,73,73	1.36	8 (11%)	82,113,113	1.59	14 (17%)

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
2	CLA	A	613	1	2/2/15/20	12/39/115/115	-
4	LUT	A	620	-	-	2/29/67/67	0/2/2/2
3	CHL	A	606	9	2/2/15/21	17/41/117/117	-
5	XAT	A	622	-	-	0/31/93/93	0/4/4/4
8	HTG	A	631	-	-	3/10/23/30	0/1/1/1
2	CLA	A	612	1	2/2/15/20	13/39/115/115	-
7	G3P	A	630	2	-	0/8/8/8	-
2	CLA	A	609	1	2/2/15/20	14/39/115/115	-
2	CLA	A	611	7	1/1/15/20	20/39/115/115	-
2	CLA	A	604	9	2/2/15/20	13/39/115/115	-
3	CHL	A	614	1	2/2/15/21	16/41/117/117	-
2	CLA	A	602	1	1/1/15/20	17/39/115/115	-
6	NEX	A	623	-	-	4/27/83/83	0/3/3/3
3	CHL	A	607	9	2/2/15/21	21/41/117/117	-
2	CLA	A	610	1	1/1/15/20	15/39/115/115	-
8	HTG	A	632	-	-	0/6/26/30	0/1/1/1
3	CHL	A	608	9	2/2/15/21	15/41/117/117	-
2	CLA	A	603	1	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CLA	A	615	7	1/1/15/20	11/39/115/115	-

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	632	HTG	O5-C1	14.04	1.64	1.42
6	A	623	NEX	C7-C6	10.54	1.42	1.30
8	A	631	HTG	O5-C1	8.32	1.55	1.42
3	A	608	CHL	O2A-CGA	8.08	1.56	1.33
2	A	612	CLA	O2D-CGD	6.67	1.49	1.33
3	A	614	CHL	MG-NA	6.43	2.21	2.06
8	A	631	HTG	O5-C5	6.42	1.54	1.44
3	A	608	CHL	MG-NA	6.27	2.21	2.06
2	A	611	CLA	MG-NA	6.26	2.21	2.06
2	A	602	CLA	O2D-CGD	6.15	1.48	1.33
3	A	606	CHL	O2A-CGA	5.91	1.50	1.33
8	A	632	HTG	C1-C2	5.50	1.62	1.53
3	A	607	CHL	O2A-CGA	5.48	1.49	1.33
6	A	623	NEX	C7-C8	5.48	1.40	1.31
3	A	614	CHL	O2A-CGA	5.43	1.49	1.33
3	A	607	CHL	O2D-CGD	5.38	1.46	1.33
2	A	612	CLA	MG-NA	5.04	2.18	2.06
2	A	610	CLA	O2A-CGA	5.01	1.48	1.33
2	A	603	CLA	O2D-CGD	4.99	1.45	1.33
8	A	631	HTG	C4-C5	4.99	1.64	1.51
2	A	602	CLA	MG-NA	4.95	2.18	2.06
3	A	606	CHL	MG-NA	4.71	2.17	2.06
8	A	631	HTG	C1-C2	4.69	1.60	1.53
2	A	604	CLA	O2A-CGA	4.69	1.47	1.33
8	A	631	HTG	O2-C2	4.69	1.53	1.43
2	A	603	CLA	MG-NA	4.65	2.17	2.06
2	A	609	CLA	O2D-CGD	4.60	1.44	1.33
2	A	603	CLA	O2A-CGA	4.60	1.46	1.33
2	A	615	CLA	O2A-CGA	4.60	1.46	1.33
3	A	607	CHL	MG-NA	4.59	2.17	2.06
2	A	613	CLA	O2A-CGA	4.58	1.46	1.33
3	A	606	CHL	MG-ND	-4.54	1.96	2.05
3	A	614	CHL	O2D-CGD	4.51	1.44	1.33
8	A	632	HTG	C4-C5	4.51	1.62	1.53
2	A	611	CLA	O2A-CGA	4.51	1.46	1.33
2	A	612	CLA	O2A-CGA	4.49	1.46	1.33
2	A	615	CLA	MG-NA	4.47	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	613	CLA	MG-NA	4.45	2.16	2.06
2	A	602	CLA	O2A-CGA	4.45	1.46	1.33
8	A	632	HTG	O5-C5	4.43	1.55	1.44
8	A	632	HTG	C4-C3	4.36	1.63	1.52
2	A	611	CLA	O2D-CGD	4.30	1.43	1.33
2	A	604	CLA	O2D-CGD	4.20	1.43	1.33
8	A	632	HTG	C3-C2	3.88	1.62	1.52
3	A	608	CHL	O2D-CGD	3.87	1.42	1.33
2	A	604	CLA	MG-NA	3.86	2.15	2.06
2	A	609	CLA	MG-NA	3.86	2.15	2.06
2	A	609	CLA	O2A-CGA	3.85	1.44	1.33
2	A	604	CLA	O2D-CED	-3.82	1.36	1.45
8	A	631	HTG	C1-S1	3.80	1.87	1.80
2	A	613	CLA	O2D-CGD	3.71	1.42	1.33
7	A	630	G3P	P-O2P	3.66	1.61	1.50
2	A	611	CLA	O2D-CED	-3.64	1.37	1.45
2	A	610	CLA	MG-NA	3.61	2.14	2.06
8	A	631	HTG	C4-C3	3.58	1.61	1.52
2	A	610	CLA	O2D-CED	-3.57	1.37	1.45
8	A	631	HTG	C6-C5	3.55	1.59	1.51
4	A	620	LUT	C1-C6	3.53	1.58	1.53
2	A	610	CLA	O2D-CGD	3.52	1.41	1.33
5	A	622	XAT	O23-C23	3.47	1.53	1.43
3	A	608	CHL	C2-C3	3.38	1.40	1.33
8	A	632	HTG	C6-C5	3.36	1.63	1.51
3	A	606	CHL	C2-C3	3.34	1.40	1.33
8	A	631	HTG	C3-C2	3.25	1.57	1.52
2	A	615	CLA	O2D-CGD	3.19	1.41	1.33
2	A	611	CLA	C5-C3	3.11	1.57	1.51
3	A	606	CHL	C5-C3	3.10	1.57	1.51
3	A	606	CHL	O2D-CGD	3.09	1.40	1.33
2	A	609	CLA	MG-ND	-3.08	1.99	2.05
2	A	604	CLA	MG-ND	-3.08	1.99	2.05
2	A	612	CLA	C2-C3	3.08	1.40	1.33
3	A	614	CHL	C2-C3	3.07	1.40	1.33
2	A	611	CLA	C2-C3	3.07	1.40	1.33
3	A	608	CHL	O2D-CED	-3.07	1.38	1.45
2	A	615	CLA	O2D-CED	-3.05	1.38	1.45
4	A	620	LUT	C23-C24	3.02	1.54	1.50
2	A	604	CLA	C2-C3	3.00	1.40	1.33
2	A	602	CLA	C2-C3	2.99	1.40	1.33
2	A	612	CLA	MG-ND	-2.96	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	603	CLA	C2-C3	2.96	1.39	1.33
2	A	610	CLA	C2-C3	2.94	1.39	1.33
2	A	609	CLA	C2-C3	2.93	1.39	1.33
3	A	607	CHL	C2-C3	2.90	1.39	1.33
3	A	608	CHL	C5-C3	2.86	1.57	1.51
2	A	611	CLA	MG-ND	-2.83	2.00	2.05
2	A	612	CLA	CMB-C2B	2.82	1.56	1.50
2	A	613	CLA	C2-C3	2.81	1.39	1.33
3	A	606	CHL	O2D-CED	-2.81	1.39	1.45
2	A	613	CLA	O2D-CED	-2.78	1.39	1.45
2	A	609	CLA	O2D-CED	-2.73	1.39	1.45
3	A	608	CHL	CMB-C2B	2.68	1.56	1.50
6	A	623	NEX	C28-C29	2.66	1.51	1.46
6	A	623	NEX	C1-C6	2.66	1.59	1.54
2	A	603	CLA	CMB-C2B	2.62	1.56	1.50
2	A	615	CLA	CMB-C2B	2.59	1.56	1.50
2	A	613	CLA	MG-ND	-2.56	2.00	2.05
2	A	609	CLA	CMB-C2B	2.53	1.56	1.50
2	A	602	CLA	CMB-C2B	2.50	1.55	1.50
2	A	615	CLA	C2-C3	2.48	1.38	1.33
3	A	608	CHL	C4-C3	2.46	1.56	1.50
3	A	607	CHL	CMB-C2B	2.45	1.55	1.50
2	A	613	CLA	CMC-C2C	2.44	1.55	1.50
4	A	620	LUT	C24-C25	2.44	1.36	1.33
2	A	610	CLA	CMB-C2B	2.42	1.55	1.50
2	A	612	CLA	C5-C3	2.40	1.56	1.51
3	A	614	CHL	C5-C3	2.38	1.56	1.51
3	A	608	CHL	CAA-C2A	2.33	1.58	1.54
2	A	609	CLA	C5-C3	2.33	1.56	1.51
2	A	603	CLA	MG-NB	-2.31	2.01	2.05
3	A	614	CHL	O2D-CED	-2.30	1.40	1.45
2	A	615	CLA	C5-C3	2.22	1.55	1.51
3	A	608	CHL	CBD-CGD	2.19	1.59	1.52
2	A	611	CLA	C4-C3	2.17	1.56	1.50
2	A	612	CLA	C4-C3	2.17	1.56	1.50
5	A	622	XAT	C8-C7	2.09	1.37	1.32
2	A	609	CLA	C4-C3	2.08	1.55	1.50
2	A	615	CLA	CMC-C2C	2.06	1.55	1.50
8	A	632	HTG	C1-S1	2.05	1.84	1.80
3	A	607	CHL	O2D-CED	-2.04	1.40	1.45
2	A	603	CLA	C5-C3	2.03	1.55	1.51
2	A	604	CLA	C5-C3	2.03	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	CLA	CBD-CGD	2.02	1.58	1.52
3	A	614	CHL	C4-C3	2.01	1.55	1.50

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	632	HTG	C1'-S1-C1	10.30	122.70	100.45
8	A	631	HTG	C1'-S1-C1	10.08	122.22	100.45
2	A	612	CLA	C4A-NA-C1A	8.16	110.40	106.68
2	A	613	CLA	C4A-NA-C1A	7.93	110.30	106.68
2	A	603	CLA	C4A-NA-C1A	7.92	110.29	106.68
2	A	613	CLA	C1-C2-C3	7.68	138.78	126.20
3	A	607	CHL	C4A-NA-C1A	7.65	110.17	106.68
3	A	614	CHL	C1-C2-C3	7.56	138.59	126.20
3	A	608	CHL	C1-C2-C3	7.55	138.57	126.20
2	A	602	CLA	C4A-NA-C1A	7.54	110.12	106.68
2	A	609	CLA	C4A-NA-C1A	7.50	110.10	106.68
2	A	610	CLA	C4A-NA-C1A	7.48	110.09	106.68
3	A	606	CHL	C4A-NA-C1A	7.31	110.01	106.68
3	A	608	CHL	C4A-NA-C1A	7.24	109.98	106.68
3	A	614	CHL	C4A-NA-C1A	7.18	109.95	106.68
2	A	611	CLA	C4A-NA-C1A	7.14	109.94	106.68
2	A	604	CLA	C4A-NA-C1A	7.08	109.91	106.68
2	A	615	CLA	C4A-NA-C1A	6.77	109.77	106.68
2	A	604	CLA	CBA-CAA-C2A	6.70	133.74	113.79
2	A	602	CLA	CED-O2D-CGD	6.52	130.71	115.92
3	A	607	CHL	C1-C2-C3	6.43	136.73	126.20
3	A	608	CHL	O2A-CGA-CBA	6.35	131.21	111.83
5	A	622	XAT	C24-C23-C22	6.22	122.42	110.79
2	A	609	CLA	C1-C2-C3	6.17	136.31	126.20
3	A	608	CHL	OMC-CMC-C2C	5.86	138.84	125.62
6	A	623	NEX	C4-C3-C2	-5.78	99.98	110.79
3	A	608	CHL	CBA-CAA-C2A	5.78	130.98	113.79
2	A	604	CLA	CMB-C2B-C1B	-5.60	116.89	125.42
2	A	609	CLA	CED-O2D-CGD	5.49	128.37	115.92
2	A	602	CLA	O2D-CGD-CBD	5.44	120.73	111.23
3	A	606	CHL	C1-C2-C3	5.39	135.02	126.20
2	A	604	CLA	O2D-CGD-CBD	5.21	120.33	111.23
2	A	612	CLA	CED-O2D-CGD	5.09	127.46	115.92
2	A	612	CLA	C1-C2-C3	5.07	134.50	126.20
2	A	613	CLA	C6-C5-C3	5.02	125.69	113.47
2	A	611	CLA	CED-O2D-CGD	5.00	127.25	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	614	CHL	O2A-CGA-CBA	4.99	127.06	111.83
3	A	607	CHL	OMC-CMC-C2C	4.97	136.83	125.62
2	A	613	CLA	CBA-CAA-C2A	4.95	128.51	113.79
3	A	606	CHL	C7-C6-C5	4.85	126.19	113.26
2	A	613	CLA	CAA-CBA-CGA	4.84	126.95	113.21
2	A	602	CLA	CBA-CAA-C2A	4.71	127.81	113.79
2	A	602	CLA	O1D-CGD-CBD	-4.71	115.23	124.52
3	A	607	CHL	CED-O2D-CGD	4.69	126.55	115.92
3	A	607	CHL	CBA-CAA-C2A	4.68	127.71	113.79
2	A	610	CLA	CED-O2D-CGD	4.58	126.31	115.92
2	A	610	CLA	CMB-C2B-C1B	-4.58	118.45	125.42
2	A	610	CLA	O2A-CGA-CBA	4.54	125.66	111.83
2	A	610	CLA	CBA-CAA-C2A	4.50	127.18	113.79
5	A	622	XAT	C7-C8-C9	4.48	132.48	125.53
2	A	603	CLA	CED-O2D-CGD	4.46	126.03	115.92
2	A	603	CLA	O2D-CGD-CBD	4.43	118.98	111.23
2	A	611	CLA	C1-C2-C3	4.36	133.34	126.20
2	A	603	CLA	C1-C2-C3	4.35	133.32	126.20
2	A	610	CLA	C7-C6-C5	4.33	124.80	113.26
3	A	614	CHL	CED-O2D-CGD	4.32	125.71	115.92
3	A	614	CHL	CAA-CBA-CGA	4.32	125.47	113.21
2	A	611	CLA	CAA-C2A-C3A	-4.30	101.38	113.00
2	A	604	CLA	O1D-CGD-CBD	-4.23	116.18	124.52
2	A	604	CLA	C6-C5-C3	4.22	123.75	113.47
3	A	614	CHL	C11-C10-C8	4.21	129.95	115.97
2	A	603	CLA	O1D-CGD-CBD	-4.19	116.25	124.52
2	A	610	CLA	C1-C2-C3	4.17	133.03	126.20
2	A	615	CLA	O2A-CGA-CBA	4.12	124.41	111.83
5	A	622	XAT	O23-C23-C22	4.12	118.17	109.75
4	A	620	LUT	C18-C5-C6	4.09	128.95	124.48
8	A	631	HTG	C4-C3-C2	-4.09	105.75	111.76
2	A	611	CLA	C6-C5-C3	4.01	123.23	113.47
3	A	606	CHL	C16-C15-C13	4.00	129.26	115.97
2	A	613	CLA	C6-C7-C8	4.00	129.25	115.97
2	A	603	CLA	O2A-CGA-CBA	3.98	123.96	111.83
2	A	611	CLA	O2A-CGA-CBA	3.97	123.94	111.83
3	A	606	CHL	CBA-CAA-C2A	3.95	125.54	113.79
4	A	620	LUT	C18-C5-C4	-3.94	107.17	114.42
2	A	604	CLA	CMB-C2B-C3B	3.94	135.82	126.55
2	A	612	CLA	O2A-CGA-CBA	3.94	123.85	111.83
2	A	602	CLA	O2A-CGA-CBA	3.92	123.77	111.83
3	A	606	CHL	O2A-CGA-CBA	3.91	123.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	609	CLA	CBA-CAA-C2A	3.88	125.35	113.79
3	A	614	CHL	C11-C12-C13	3.87	128.82	115.97
2	A	612	CLA	CBA-CAA-C2A	3.79	125.06	113.79
4	A	620	LUT	C38-C25-C24	-3.79	114.40	123.36
2	A	604	CLA	C1-C2-C3	3.78	132.38	126.20
3	A	606	CHL	C6-C5-C3	3.72	122.54	113.47
3	A	607	CHL	CBC-CAC-C3C	3.69	122.41	112.42
2	A	611	CLA	CAA-CBA-CGA	3.66	123.60	113.21
2	A	610	CLA	C16-C15-C13	3.64	128.06	115.97
2	A	609	CLA	O2A-CGA-CBA	3.63	122.91	111.83
3	A	607	CHL	O2A-CGA-CBA	3.62	122.86	111.83
2	A	615	CLA	C1-C2-C3	3.56	132.03	126.20
2	A	604	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
3	A	608	CHL	O2D-CGD-CBD	3.51	117.37	111.23
2	A	610	CLA	C11-C10-C8	3.48	127.54	115.97
2	A	615	CLA	C16-C15-C13	3.47	127.51	115.97
2	A	613	CLA	CED-O2D-CGD	3.46	123.77	115.92
3	A	614	CHL	CAA-C2A-C1A	3.44	123.24	111.97
8	A	632	HTG	O5-C1-C2	-3.41	105.61	110.32
3	A	614	CHL	C6-C5-C3	3.41	121.77	113.47
3	A	606	CHL	C4-C3-C5	-3.41	109.31	115.23
8	A	631	HTG	O5-C1-C2	-3.39	105.65	110.32
2	A	604	CLA	C11-C10-C8	3.36	127.12	115.97
2	A	610	CLA	CMB-C2B-C3B	3.35	134.42	126.55
3	A	607	CHL	CAA-C2A-C1A	3.32	122.87	111.97
3	A	614	CHL	C16-C15-C13	3.27	126.84	115.97
6	A	623	NEX	C24-C23-C22	3.27	116.90	110.79
3	A	608	CHL	O1A-CGA-CBA	-3.25	111.06	123.78
2	A	611	CLA	C11-C12-C13	3.22	126.68	115.97
4	A	620	LUT	C3-C4-C5	3.15	120.03	112.18
5	A	622	XAT	C38-C25-C24	-3.14	110.72	114.24
2	A	604	CLA	C9-C8-C10	3.13	122.43	111.27
2	A	611	CLA	CAA-C2A-C1A	3.12	122.20	111.97
6	A	623	NEX	C26-C27-C28	3.11	132.57	125.99
2	A	612	CLA	C16-C15-C13	3.07	126.17	115.97
3	A	608	CHL	CAA-CBA-CGA	3.04	121.83	113.21
3	A	608	CHL	C6-C7-C8	3.03	126.05	115.97
2	A	612	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
8	A	631	HTG	C2'-C1'-S1	-2.99	102.28	112.36
3	A	606	CHL	C11-C12-C13	2.98	125.88	115.97
3	A	606	CHL	O2D-CGD-CBD	2.95	116.39	111.23
2	A	615	CLA	C4-C3-C5	2.95	120.34	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	606	CHL	CAA-C2A-C3A	-2.94	105.05	113.00
3	A	606	CHL	C11-C10-C8	2.92	125.67	115.97
2	A	604	CLA	O2A-CGA-CBA	2.88	120.60	111.83
2	A	610	CLA	C16-C17-C18	2.84	128.62	115.94
2	A	602	CLA	C1-C2-C3	2.84	130.85	126.20
2	A	612	CLA	C2A-C1A-CHA	2.84	128.79	123.87
3	A	608	CHL	C3B-C4B-NB	-2.80	108.03	110.53
2	A	611	CLA	C3B-C4B-NB	-2.77	108.06	110.53
2	A	613	CLA	C5-C3-C2	-2.75	114.99	121.17
4	A	620	LUT	C1-C6-C5	-2.75	118.87	122.64
2	A	604	CLA	CAA-CBA-CGA	2.75	121.01	113.21
2	A	602	CLA	C3B-C4B-NB	-2.73	108.10	110.53
2	A	603	CLA	C16-C15-C13	2.72	125.02	115.97
2	A	602	CLA	C4-C3-C5	-2.71	110.52	115.23
2	A	615	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
2	A	604	CLA	CMA-C3A-C4A	-2.71	104.48	111.77
2	A	610	CLA	C11-C12-C13	2.71	124.97	115.97
8	A	631	HTG	O5-C5-C6	2.70	111.16	106.83
3	A	614	CHL	C1D-ND-C4D	-2.69	104.42	106.31
4	A	620	LUT	C1-C2-C3	2.69	119.49	113.59
2	A	615	CLA	C3B-C4B-NB	-2.69	108.13	110.53
2	A	604	CLA	C11-C12-C13	2.69	124.89	115.97
2	A	612	CLA	C3B-C4B-NB	-2.68	108.14	110.53
6	A	623	NEX	O24-C25-C24	2.64	115.96	113.49
7	A	630	G3P	O3P-P-O1P	2.62	113.49	106.67
2	A	615	CLA	C11-C12-C13	2.58	124.55	115.97
3	A	614	CHL	C4-C3-C5	-2.57	110.77	115.23
2	A	612	CLA	C6-C5-C3	2.54	119.65	113.47
2	A	615	CLA	C14-C13-C15	2.54	120.31	111.27
2	A	609	CLA	C6-C5-C3	2.53	119.63	113.47
3	A	608	CHL	C11-C10-C8	2.53	124.36	115.97
2	A	610	CLA	C9-C8-C7	2.52	120.26	111.27
3	A	608	CHL	C9-C8-C7	2.51	120.24	111.27
3	A	607	CHL	C3B-C4B-NB	-2.51	108.29	110.53
2	A	611	CLA	C7-C6-C5	2.51	119.94	113.26
5	A	622	XAT	O24-C25-C24	2.51	115.84	113.49
2	A	609	CLA	C16-C15-C13	2.50	124.26	115.97
3	A	608	CHL	C14-C13-C12	2.50	120.17	111.27
2	A	612	CLA	C14-C13-C15	2.49	120.15	111.27
2	A	612	CLA	CAA-CBA-CGA	2.49	120.28	113.21
3	A	608	CHL	O1D-CGD-CBD	-2.49	119.61	124.52
3	A	614	CHL	C3B-C4B-NB	-2.47	108.32	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	611	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
2	A	604	CLA	C2A-C1A-CHA	2.46	128.13	123.87
3	A	607	CHL	C16-C15-C13	2.44	124.07	115.97
2	A	613	CLA	C4D-CHA-C1A	2.44	124.15	121.24
2	A	613	CLA	O2A-CGA-CBA	2.41	119.19	111.83
2	A	615	CLA	C11-C10-C8	2.40	123.95	115.97
8	A	632	HTG	O5-C5-C6	2.39	112.37	106.44
2	A	609	CLA	C2A-C1A-CHA	2.39	128.01	123.87
3	A	608	CHL	O2A-CGA-O1A	-2.38	117.68	123.63
2	A	612	CLA	CAC-C3C-C4C	2.38	127.88	124.79
3	A	614	CHL	O2A-CGA-O1A	-2.37	117.71	123.63
2	A	609	CLA	C12-C11-C10	-2.35	102.73	113.28
2	A	613	CLA	C7-C6-C5	2.35	119.52	113.26
3	A	614	CHL	C9-C8-C10	2.34	119.63	111.27
2	A	615	CLA	CBC-CAC-C3C	2.34	118.78	112.42
2	A	610	CLA	C2A-C1A-CHA	2.34	127.93	123.87
3	A	607	CHL	C16-C17-C18	2.34	126.38	115.94
3	A	608	CHL	CED-O2D-CGD	2.33	121.20	115.92
3	A	607	CHL	C7-C6-C5	2.33	119.47	113.26
3	A	607	CHL	C17-C16-C15	2.32	123.70	113.28
2	A	602	CLA	CMC-C2C-C1C	2.32	128.66	125.03
2	A	609	CLA	C3B-C4B-NB	-2.32	108.46	110.53
2	A	615	CLA	CED-O2D-CGD	2.29	121.11	115.92
2	A	615	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
2	A	602	CLA	C2A-C1A-CHA	2.28	127.83	123.87
6	A	623	NEX	C1-C2-C3	2.27	118.57	113.59
3	A	607	CHL	C14-C13-C12	2.24	119.27	111.27
3	A	606	CHL	C5-C3-C2	2.24	126.19	121.17
3	A	606	CHL	C2A-C1A-CHA	2.22	127.72	123.87
2	A	609	CLA	C11-C12-C13	2.20	123.28	115.97
2	A	602	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
2	A	610	CLA	C1D-ND-C4D	-2.19	104.77	106.31
2	A	609	CLA	C17-C16-C15	2.19	123.11	113.28
2	A	612	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
3	A	614	CHL	O1A-CGA-CBA	-2.19	115.23	123.78
2	A	603	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
2	A	611	CLA	C2A-C1A-CHA	2.18	127.65	123.87
2	A	612	CLA	CAA-C2A-C1A	2.18	119.11	111.97
2	A	612	CLA	CHA-C1A-NA	-2.17	121.47	126.39
3	A	614	CHL	C4D-CHA-C1A	2.17	123.83	121.24
2	A	603	CLA	C3B-C4B-NB	-2.17	108.60	110.53
2	A	609	CLA	O2A-CGA-O1A	-2.16	118.22	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	610	CLA	C14-C13-C15	2.16	118.96	111.27
3	A	607	CHL	C11-C10-C8	2.15	123.13	115.97
3	A	606	CHL	O2A-CGA-O1A	-2.14	118.28	123.63
2	A	610	CLA	C19-C18-C17	2.14	124.20	111.55
2	A	603	CLA	CAA-C2A-C1A	2.14	118.97	111.97
2	A	603	CLA	C6-C7-C8	2.13	123.05	115.97
3	A	607	CHL	C2A-C1A-CHA	2.12	127.55	123.87
2	A	615	CLA	C6-C5-C3	2.12	118.62	113.47
2	A	602	CLA	C7-C6-C5	-2.12	107.62	113.26
3	A	606	CHL	C3B-C4B-NB	-2.11	108.65	110.53
3	A	607	CHL	O2A-CGA-O1A	-2.10	118.37	123.63
2	A	609	CLA	C2B-C1B-NB	-2.10	108.15	110.33
3	A	608	CHL	C1D-ND-C4D	-2.10	104.84	106.31
2	A	610	CLA	O1A-CGA-CBA	-2.10	115.59	123.78
2	A	602	CLA	C11-C10-C8	-2.08	109.04	115.97
6	A	623	NEX	C37-C21-C36	2.08	110.39	107.37
6	A	623	NEX	C38-C25-C24	-2.07	111.91	114.24
2	A	602	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
3	A	606	CHL	O1D-CGD-CBD	-2.04	120.49	124.52
2	A	602	CLA	C9-C8-C7	2.02	118.47	111.27
2	A	609	CLA	C4D-CHA-C1A	2.02	123.65	121.24

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	602	CLA	C8
2	A	604	CLA	C8
2	A	604	CLA	C13
2	A	609	CLA	C8
2	A	609	CLA	C13
2	A	610	CLA	C13
2	A	611	CLA	C13
2	A	612	CLA	C8
2	A	612	CLA	C13
2	A	613	CLA	C8
2	A	613	CLA	C13
2	A	615	CLA	C13
3	A	606	CHL	C8
3	A	606	CHL	C13
3	A	607	CHL	C8
3	A	607	CHL	C13
3	A	608	CHL	C8

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Mol	Chain	Res	Type	Atom
3	A	608	CHL	C13
3	A	614	CHL	C8
3	A	614	CHL	C13

All (211) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	CLA	C3A-C2A-CAA-CBA
2	A	603	CLA	CHA-CBD-CGD-O1D
2	A	603	CLA	CBD-CGD-O2D-CED
2	A	604	CLA	CHA-CBD-CGD-O1D
2	A	604	CLA	CHA-CBD-CGD-O2D
2	A	612	CLA	CBD-CGD-O2D-CED
2	A	613	CLA	CBD-CGD-O2D-CED
3	A	606	CHL	C2B-C3B-CAB-CBB
3	A	606	CHL	C4B-C3B-CAB-CBB
3	A	606	CHL	CHA-CBD-CGD-O1D
3	A	606	CHL	CHA-CBD-CGD-O2D
3	A	608	CHL	C1A-C2A-CAA-CBA
8	A	631	HTG	C4-C5-C6-O6
8	A	631	HTG	O5-C5-C6-O6
2	A	612	CLA	O1D-CGD-O2D-CED
3	A	606	CHL	CBD-CGD-O2D-CED
3	A	607	CHL	CBD-CGD-O2D-CED
2	A	603	CLA	O1D-CGD-O2D-CED
3	A	606	CHL	O1D-CGD-O2D-CED
2	A	615	CLA	O1A-CGA-O2A-C1
3	A	614	CHL	O1A-CGA-O2A-C1
2	A	613	CLA	O1D-CGD-O2D-CED
2	A	602	CLA	O1A-CGA-O2A-C1
2	A	609	CLA	C3-C5-C6-C7
3	A	608	CHL	C3-C5-C6-C7
2	A	615	CLA	CBA-CGA-O2A-C1
3	A	614	CHL	CBA-CGA-O2A-C1
2	A	610	CLA	CBD-CGD-O2D-CED
2	A	611	CLA	CBD-CGD-O2D-CED
3	A	608	CHL	CBD-CGD-O2D-CED
3	A	607	CHL	O1D-CGD-O2D-CED
2	A	602	CLA	C3-C5-C6-C7
2	A	610	CLA	C3-C5-C6-C7
2	A	602	CLA	CBA-CGA-O2A-C1
2	A	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
2	A	611	CLA	O1A-CGA-O2A-C1
2	A	612	CLA	O1A-CGA-O2A-C1
3	A	614	CHL	C3-C5-C6-C7
2	A	609	CLA	CBA-CGA-O2A-C1
2	A	612	CLA	CBA-CGA-O2A-C1
3	A	608	CHL	CBA-CGA-O2A-C1
2	A	603	CLA	O1A-CGA-O2A-C1
2	A	611	CLA	O1D-CGD-O2D-CED
2	A	611	CLA	CBA-CGA-O2A-C1
2	A	609	CLA	O1A-CGA-O2A-C1
3	A	608	CHL	O1A-CGA-O2A-C1
3	A	607	CHL	O1A-CGA-O2A-C1
3	A	607	CHL	CBA-CGA-O2A-C1
2	A	613	CLA	C5-C6-C7-C8
2	A	604	CLA	C11-C10-C8-C9
2	A	615	CLA	C14-C13-C15-C16
3	A	606	CHL	C14-C13-C15-C16
3	A	608	CHL	C6-C7-C8-C9
2	A	604	CLA	C2A-CAA-CBA-CGA
3	A	608	CHL	O1D-CGD-O2D-CED
2	A	602	CLA	C10-C11-C12-C13
2	A	613	CLA	C15-C16-C17-C18
2	A	610	CLA	C12-C13-C15-C16
2	A	609	CLA	C5-C6-C7-C8
2	A	611	CLA	C2A-CAA-CBA-CGA
3	A	607	CHL	C3-C5-C6-C7
2	A	609	CLA	C10-C11-C12-C13
2	A	613	CLA	C10-C11-C12-C13
2	A	610	CLA	O1D-CGD-O2D-CED
3	A	606	CHL	C13-C15-C16-C17
3	A	607	CHL	C2C-C3C-CAC-CBC
3	A	608	CHL	C15-C16-C17-C18
3	A	614	CHL	C5-C6-C7-C8
2	A	602	CLA	C5-C6-C7-C8
2	A	611	CLA	C8-C10-C11-C12
2	A	612	CLA	C13-C15-C16-C17
2	A	604	CLA	C5-C6-C7-C8
3	A	614	CHL	C13-C15-C16-C17
3	A	607	CHL	C13-C15-C16-C17
2	A	602	CLA	C16-C17-C18-C20
2	A	611	CLA	C16-C17-C18-C20
2	A	612	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
6	A	623	NEX	C11-C10-C9-C8
2	A	602	CLA	C16-C17-C18-C19
2	A	609	CLA	C16-C17-C18-C20
2	A	611	CLA	C16-C17-C18-C19
2	A	612	CLA	C16-C17-C18-C19
2	A	613	CLA	C13-C15-C16-C17
2	A	609	CLA	C16-C17-C18-C19
2	A	611	CLA	C3-C5-C6-C7
2	A	611	CLA	C3A-C2A-CAA-CBA
3	A	606	CHL	C3A-C2A-CAA-CBA
2	A	609	CLA	CBD-CGD-O2D-CED
3	A	607	CHL	C4C-C3C-CAC-CBC
2	A	613	CLA	C8-C10-C11-C12
2	A	603	CLA	C16-C17-C18-C20
2	A	602	CLA	CBD-CGD-O2D-CED
2	A	610	CLA	C13-C15-C16-C17
2	A	612	CLA	C8-C10-C11-C12
3	A	614	CHL	C2-C3-C5-C6
2	A	602	CLA	C1A-C2A-CAA-CBA
2	A	611	CLA	C1A-C2A-CAA-CBA
3	A	606	CHL	C1A-C2A-CAA-CBA
3	A	614	CHL	C1A-C2A-CAA-CBA
2	A	602	CLA	C11-C10-C8-C7
2	A	604	CLA	C6-C7-C8-C10
2	A	604	CLA	C11-C10-C8-C7
2	A	604	CLA	C12-C13-C15-C16
2	A	609	CLA	C6-C7-C8-C10
2	A	613	CLA	C11-C12-C13-C15
3	A	607	CHL	C8-C10-C11-C12
2	A	603	CLA	C14-C13-C15-C16
2	A	609	CLA	C6-C7-C8-C9
2	A	609	CLA	C11-C10-C8-C9
2	A	611	CLA	C14-C13-C15-C16
2	A	613	CLA	C11-C12-C13-C14
3	A	614	CHL	C14-C13-C15-C16
3	A	614	CHL	C4-C3-C5-C6
3	A	608	CHL	C5-C6-C7-C8
2	A	611	CLA	C4-C3-C5-C6
3	A	606	CHL	CBA-CGA-O2A-C1
2	A	613	CLA	C3-C5-C6-C7
8	A	631	HTG	C4'-C5'-C6'-C7'
2	A	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	A	603	CLA	C16-C17-C18-C19
2	A	604	CLA	C14-C13-C15-C16
3	A	607	CHL	C6-C7-C8-C9
2	A	610	CLA	C4B-C3B-CAB-CBB
2	A	603	CLA	C12-C13-C15-C16
2	A	609	CLA	C11-C10-C8-C7
2	A	610	CLA	C6-C7-C8-C10
2	A	610	CLA	C11-C10-C8-C7
2	A	613	CLA	C11-C10-C8-C7
3	A	606	CHL	C6-C7-C8-C10
3	A	614	CHL	C12-C13-C15-C16
3	A	606	CHL	C15-C16-C17-C18
2	A	611	CLA	C2-C3-C5-C6
2	A	610	CLA	C16-C17-C18-C19
3	A	606	CHL	C4-C3-C5-C6
3	A	606	CHL	O1A-CGA-O2A-C1
4	A	620	LUT	C1-C6-C7-C8
3	A	607	CHL	C15-C16-C17-C18
2	A	603	CLA	C11-C12-C13-C15
2	A	612	CLA	C6-C7-C8-C10
3	A	606	CHL	C2-C3-C5-C6
2	A	612	CLA	C3-C5-C6-C7
2	A	612	CLA	C6-C7-C8-C9
2	A	610	CLA	C16-C17-C18-C20
3	A	614	CHL	C16-C17-C18-C19
2	A	615	CLA	O1D-CGD-O2D-CED
3	A	607	CHL	C16-C17-C18-C20
2	A	611	CLA	C6-C7-C8-C10
2	A	602	CLA	C2A-CAA-CBA-CGA
2	A	602	CLA	C11-C10-C8-C9
2	A	604	CLA	C6-C7-C8-C9
2	A	613	CLA	C11-C10-C8-C9
6	A	623	NEX	C7-C8-C9-C10
2	A	603	CLA	CHA-CBD-CGD-O2D
2	A	615	CLA	C16-C17-C18-C20
3	A	614	CHL	C16-C17-C18-C20
2	A	609	CLA	C13-C15-C16-C17
2	A	602	CLA	C11-C12-C13-C14
2	A	603	CLA	C11-C12-C13-C14
3	A	606	CHL	C6-C7-C8-C9
3	A	607	CHL	C14-C13-C15-C16
2	A	615	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
3	A	607	CHL	C11-C12-C13-C15
2	A	611	CLA	C13-C15-C16-C17
3	A	608	CHL	C2C-C3C-CAC-CBC
2	A	615	CLA	C16-C17-C18-C19
2	A	610	CLA	C6-C7-C8-C9
2	A	611	CLA	C12-C13-C15-C16
2	A	604	CLA	C3A-C2A-CAA-CBA
6	A	623	NEX	C39-C29-C30-C31
2	A	602	CLA	C14-C13-C15-C16
2	A	611	CLA	C11-C10-C8-C9
2	A	612	CLA	C14-C13-C15-C16
2	A	615	CLA	C6-C7-C8-C9
6	A	623	NEX	C28-C29-C30-C31
2	A	603	CLA	C3-C5-C6-C7
4	A	620	LUT	C5-C6-C7-C8
3	A	608	CHL	C16-C17-C18-C20
2	A	603	CLA	C4-C3-C5-C6
2	A	604	CLA	C4-C3-C5-C6
2	A	603	CLA	C2-C3-C5-C6
2	A	612	CLA	C11-C12-C13-C15
3	A	607	CHL	C6-C7-C8-C10
3	A	607	CHL	C11-C10-C8-C7
3	A	608	CHL	C10-C11-C12-C13
3	A	608	CHL	C16-C17-C18-C19
3	A	607	CHL	C4-C3-C5-C6
3	A	614	CHL	C6-C7-C8-C9
3	A	607	CHL	C16-C17-C18-C19
3	A	608	CHL	C3A-C2A-CAA-CBA
2	A	610	CLA	C5-C6-C7-C8
3	A	607	CHL	C10-C11-C12-C13
2	A	611	CLA	C6-C7-C8-C9
3	A	608	CHL	C14-C13-C15-C16
2	A	609	CLA	O1D-CGD-O2D-CED
2	A	611	CLA	C11-C10-C8-C7
2	A	610	CLA	C2B-C3B-CAB-CBB
2	A	615	CLA	CAA-CBA-CGA-O2A
2	A	603	CLA	C1A-C2A-CAA-CBA
2	A	602	CLA	CAA-CBA-CGA-O2A
2	A	603	CLA	CAA-CBA-CGA-O2A
2	A	615	CLA	C6-C7-C8-C10
3	A	614	CHL	C3A-C2A-CAA-CBA
2	A	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	610	CLA	C14-C13-C15-C16
3	A	607	CHL	C11-C12-C13-C14
2	A	603	CLA	CAA-CBA-CGA-O1A
3	A	614	CHL	CAA-CBA-CGA-O2A
2	A	615	CLA	CAA-CBA-CGA-O1A
2	A	602	CLA	CAA-CBA-CGA-O1A
3	A	607	CHL	CAA-CBA-CGA-O2A
3	A	614	CHL	CAA-CBA-CGA-O1A

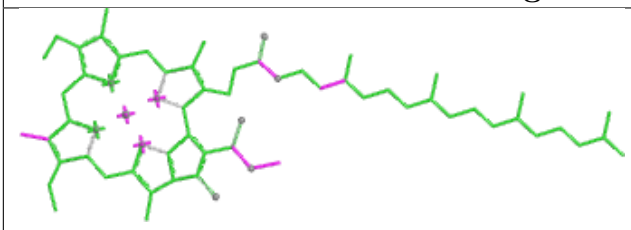
There are no ring outliers.

15 monomers are involved in 42 short contacts:

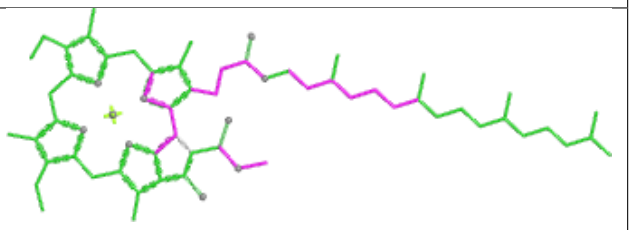
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	613	CLA	6	0
4	A	620	LUT	4	0
3	A	606	CHL	5	0
5	A	622	XAT	1	0
2	A	609	CLA	3	0
2	A	604	CLA	4	0
3	A	614	CHL	2	0
2	A	602	CLA	1	0
6	A	623	NEX	3	0
3	A	607	CHL	1	0
2	A	610	CLA	2	0
8	A	632	HTG	5	0
3	A	608	CHL	1	0
2	A	603	CLA	2	0
2	A	615	CLA	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

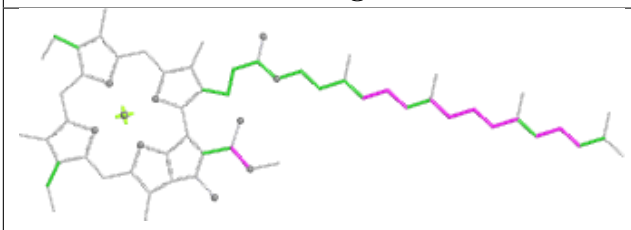
Ligand CLA A 613



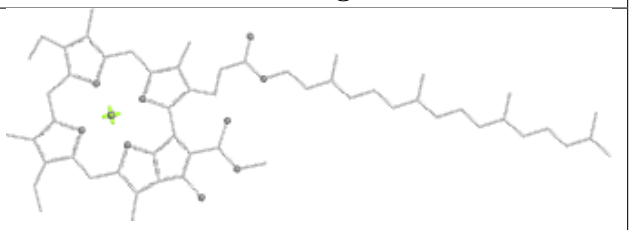
Bond lengths



Bond angles

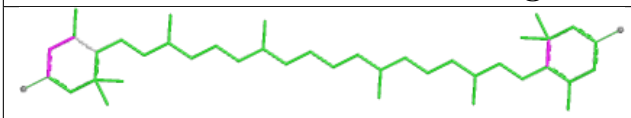


Torsions

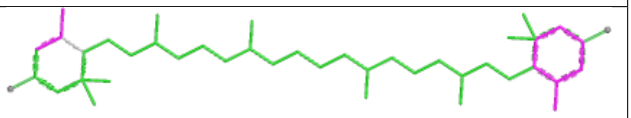


Rings

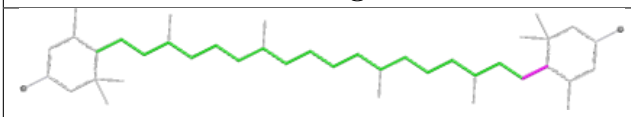
Ligand LUT A 620



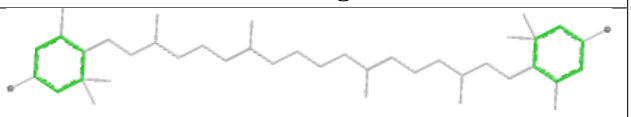
Bond lengths



Bond angles

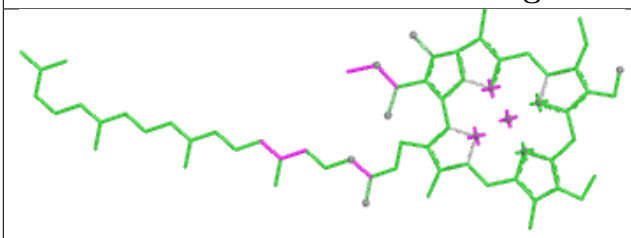


Torsions

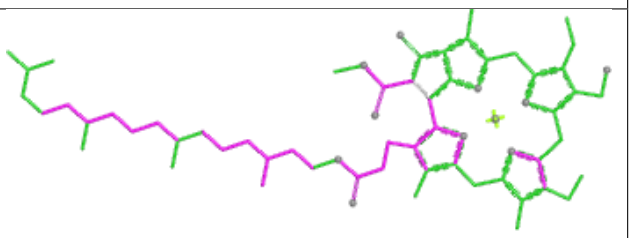


Rings

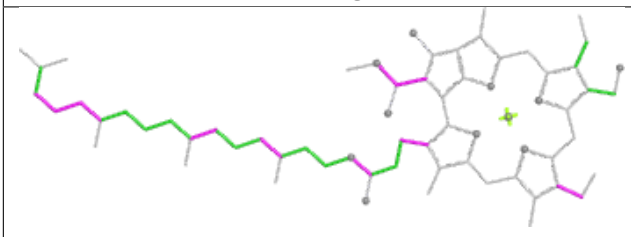
Ligand CHL A 606



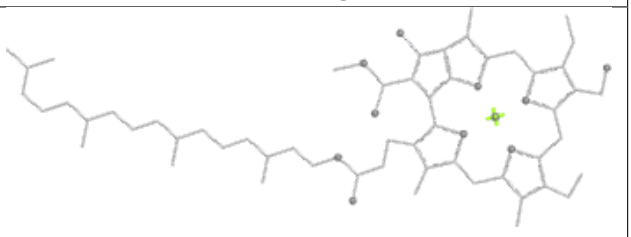
Bond lengths



Bond angles

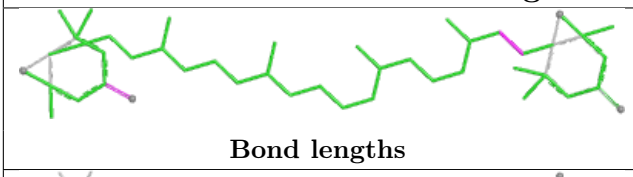


Torsions

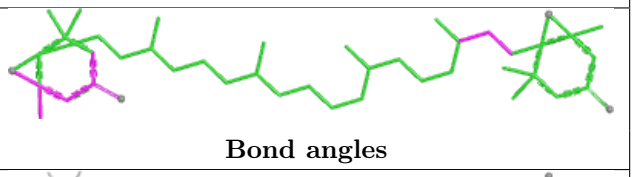


Rings

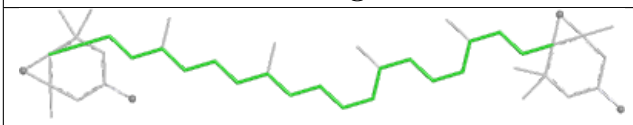
Ligand XAT A 622



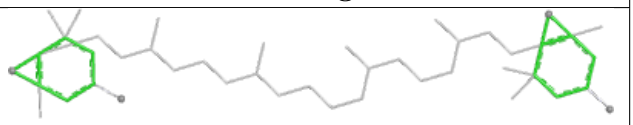
Bond lengths



Bond angles

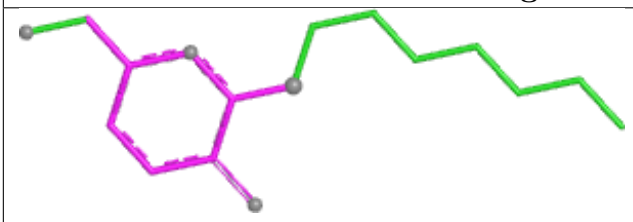


Torsions

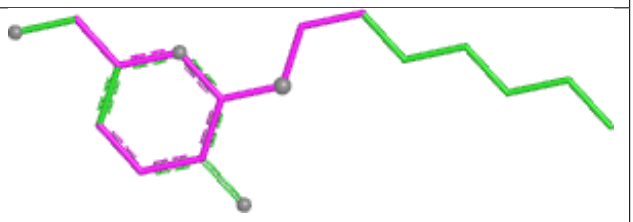


Rings

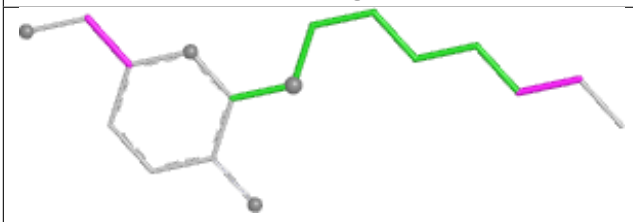
Ligand HTG A 631



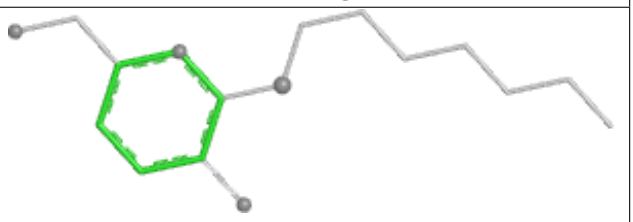
Bond lengths



Bond angles

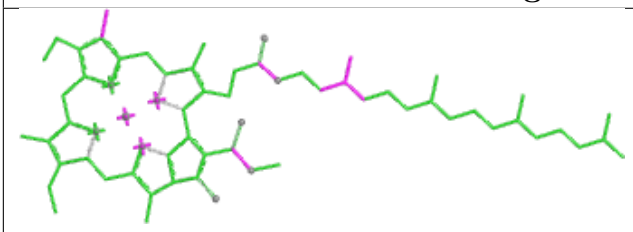


Torsions

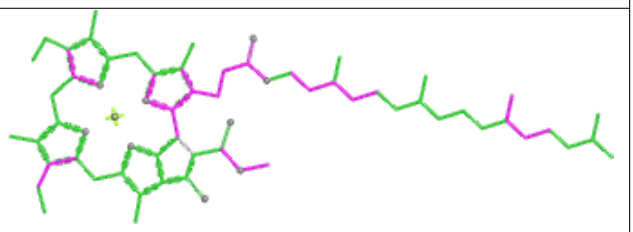


Rings

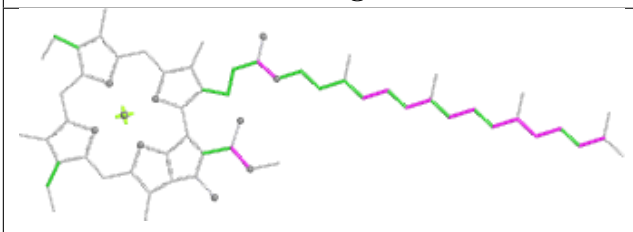
Ligand CLA A 612



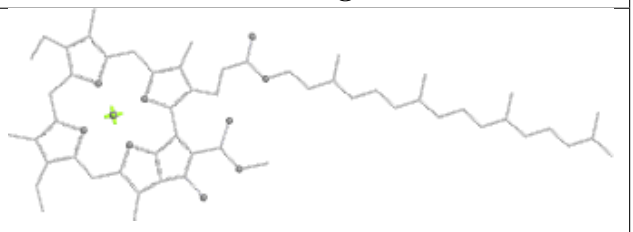
Bond lengths



Bond angles

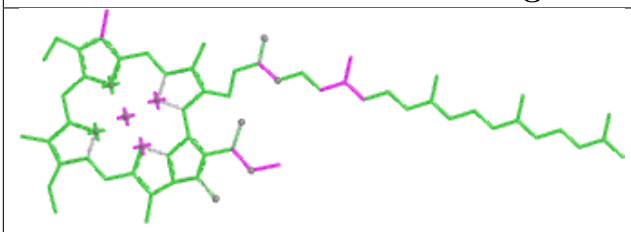


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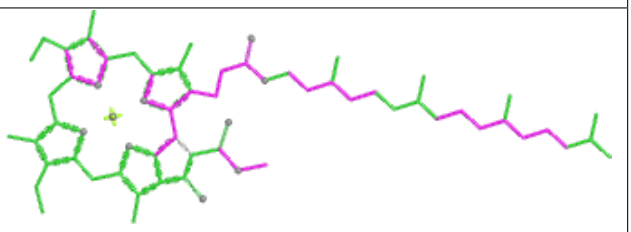


Rings

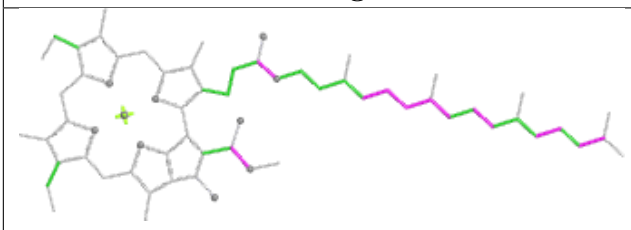
Ligand CLA A 609



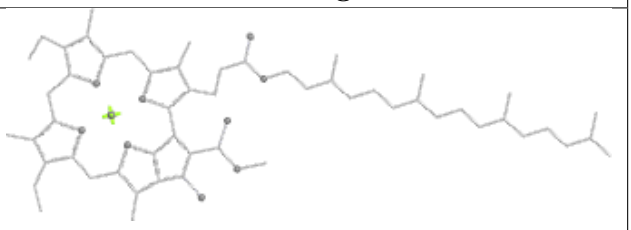
Bond lengths



Bond angles

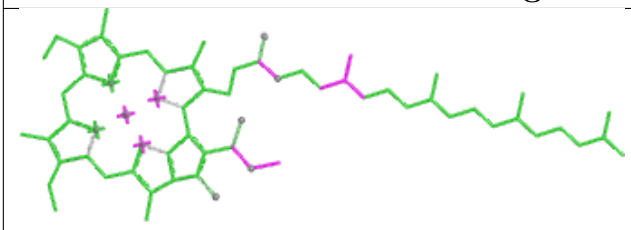


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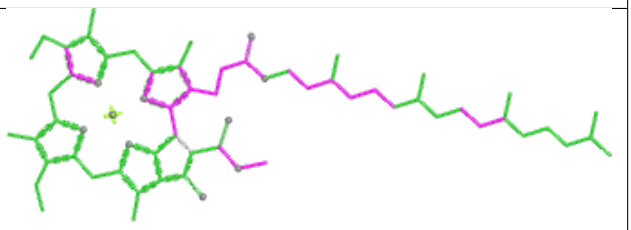


Rings

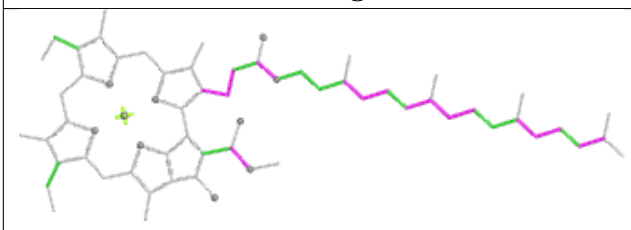
Ligand CLA A 611



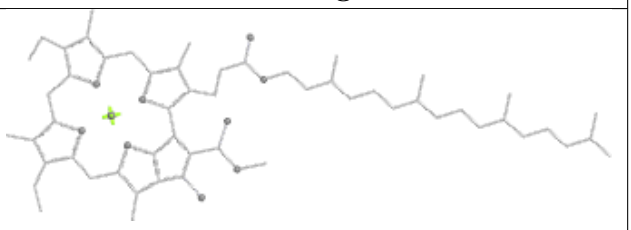
Bond lengths



Bond angles

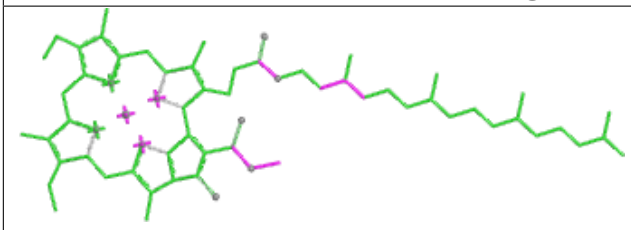


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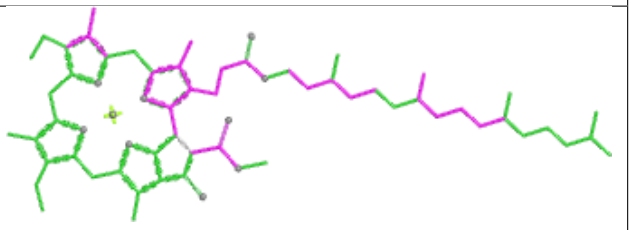


Rings

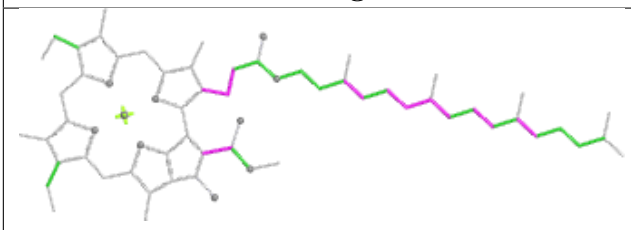
Ligand CLA A 604



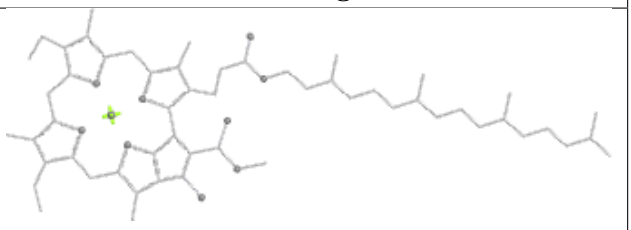
Bond lengths



Bond angles

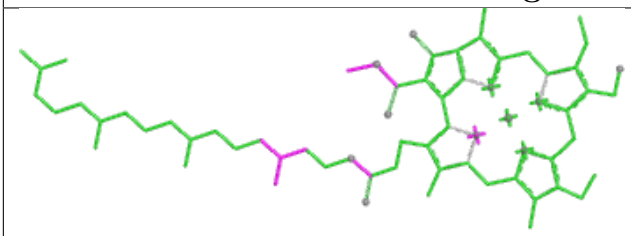


Torsions

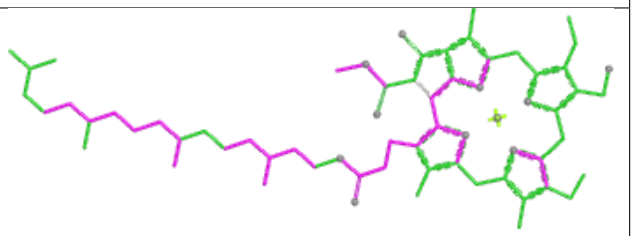


Rings

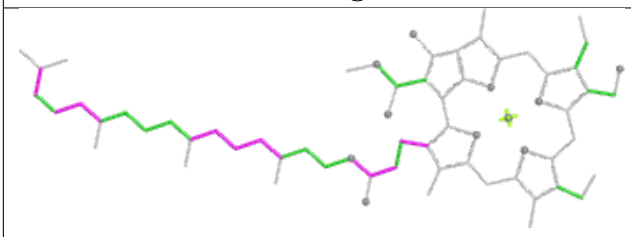
Ligand CHL A 614



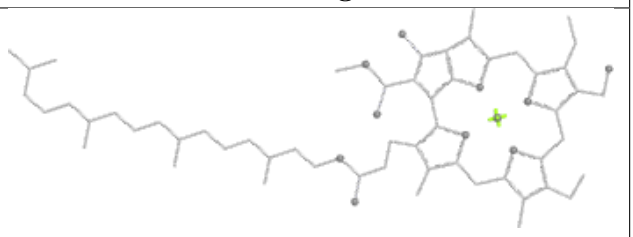
Bond lengths



Bond angles

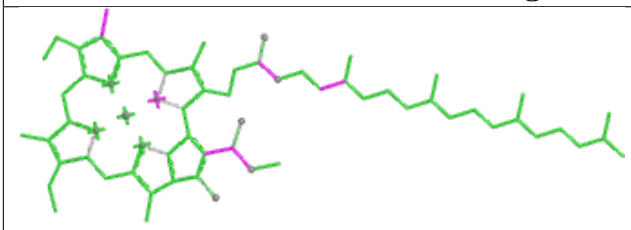


Torsions

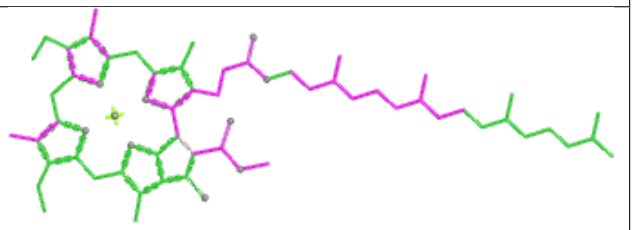


Rings

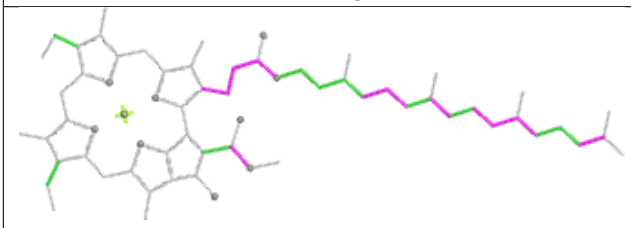
Ligand CLA A 602



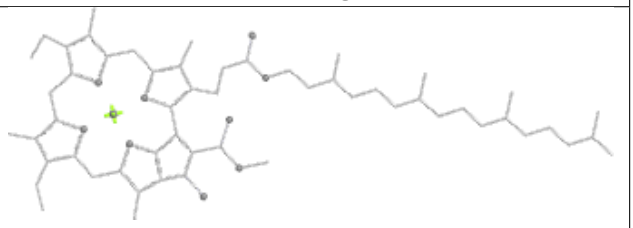
Bond lengths



Bond angles

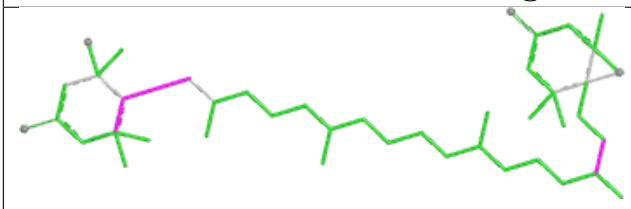


Torsions

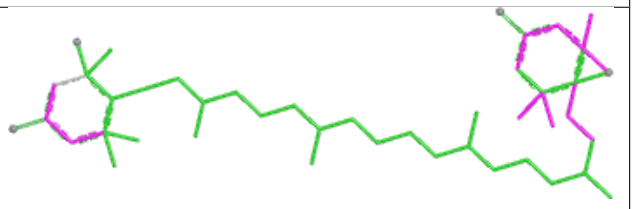


Rings

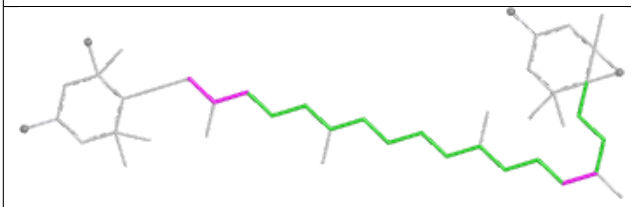
Ligand NEX A 623



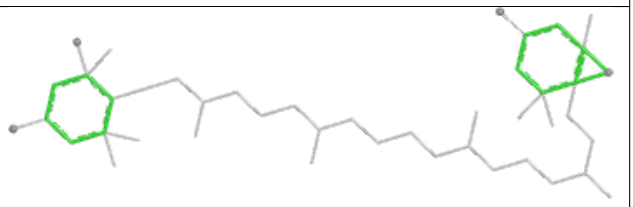
Bond lengths



Bond angles

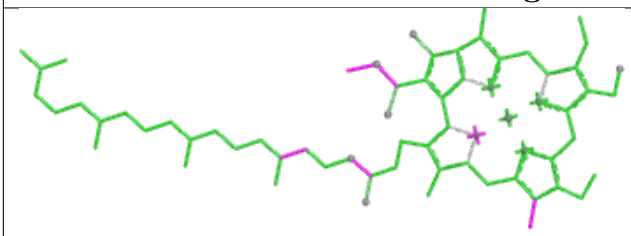


Torsions

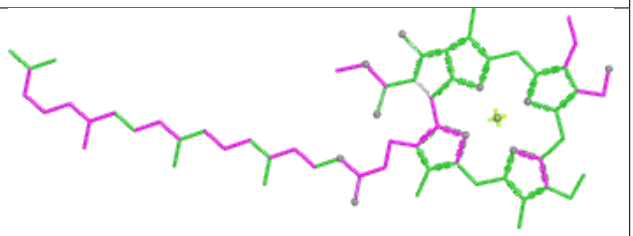


Rings

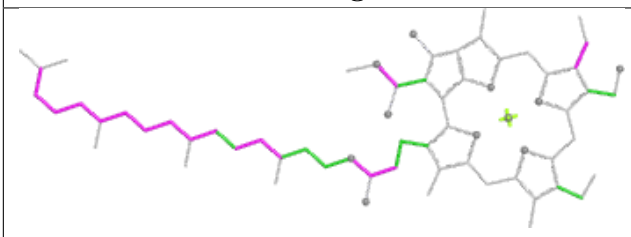
Ligand CHL A 607



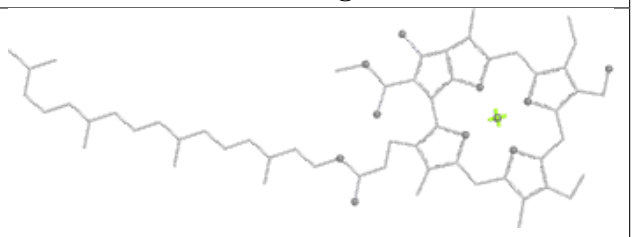
Bond lengths



Bond angles

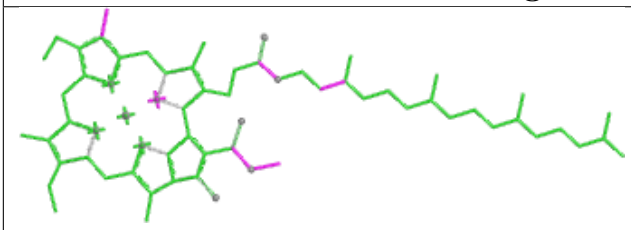


Torsions

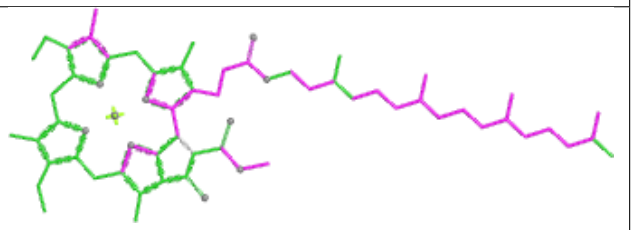


Rings

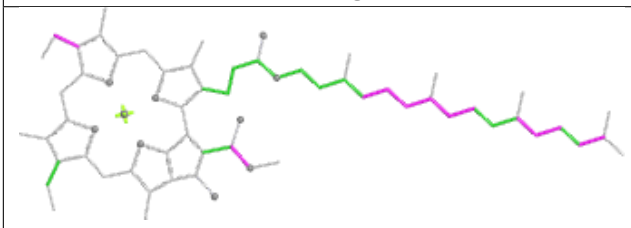
Ligand CLA A 610



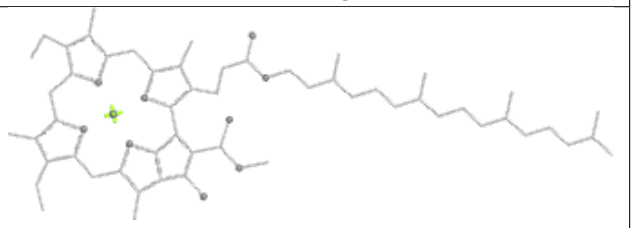
Bond lengths



Bond angles

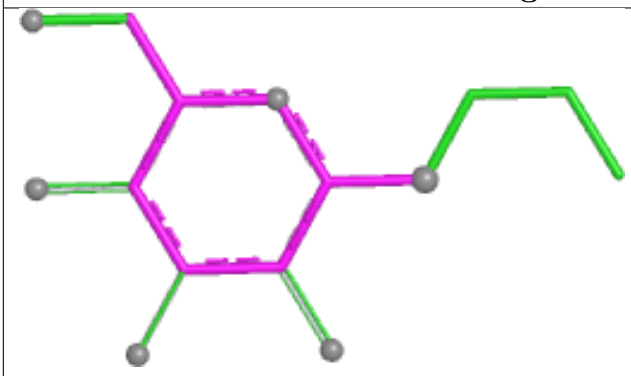


Torsions

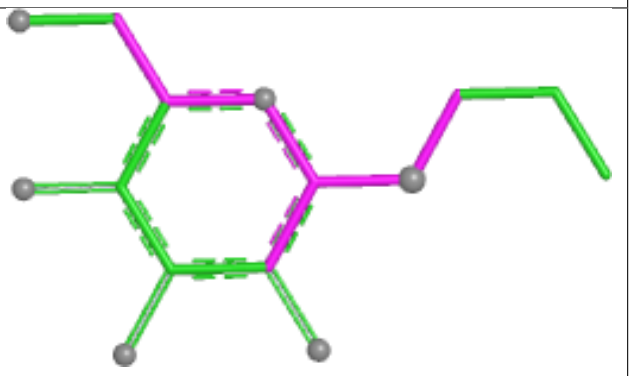


Rings

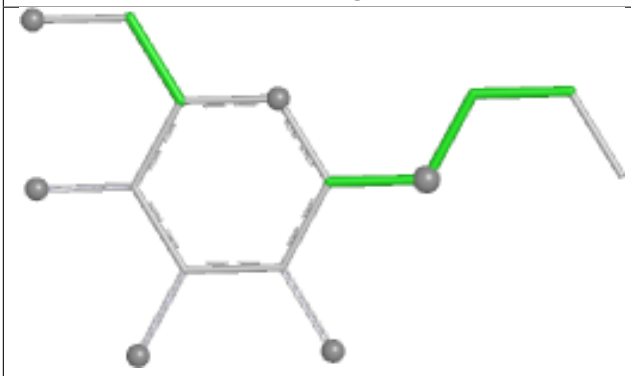
Ligand HTG A 632



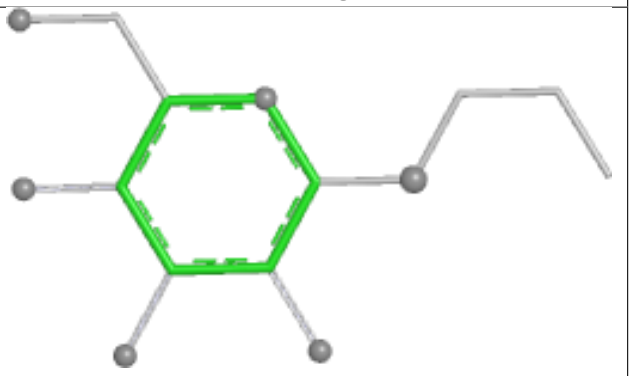
Bond lengths



Bond angles

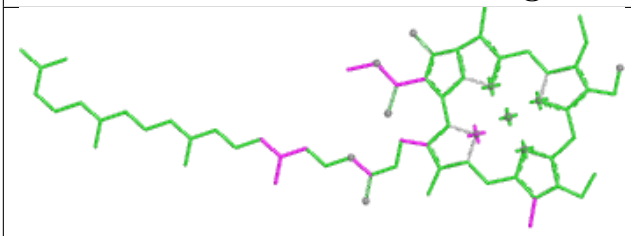


Torsions

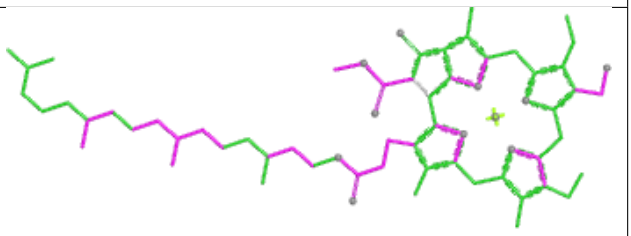


Rings

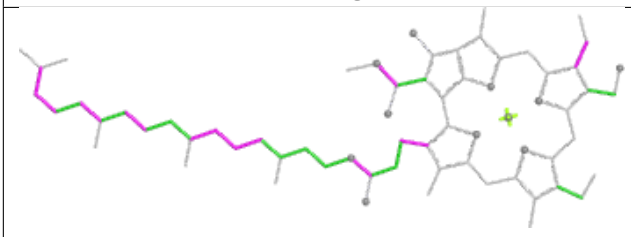
Ligand CHL A 608



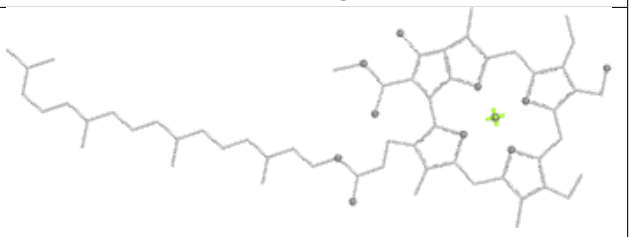
Bond lengths



Bond angles

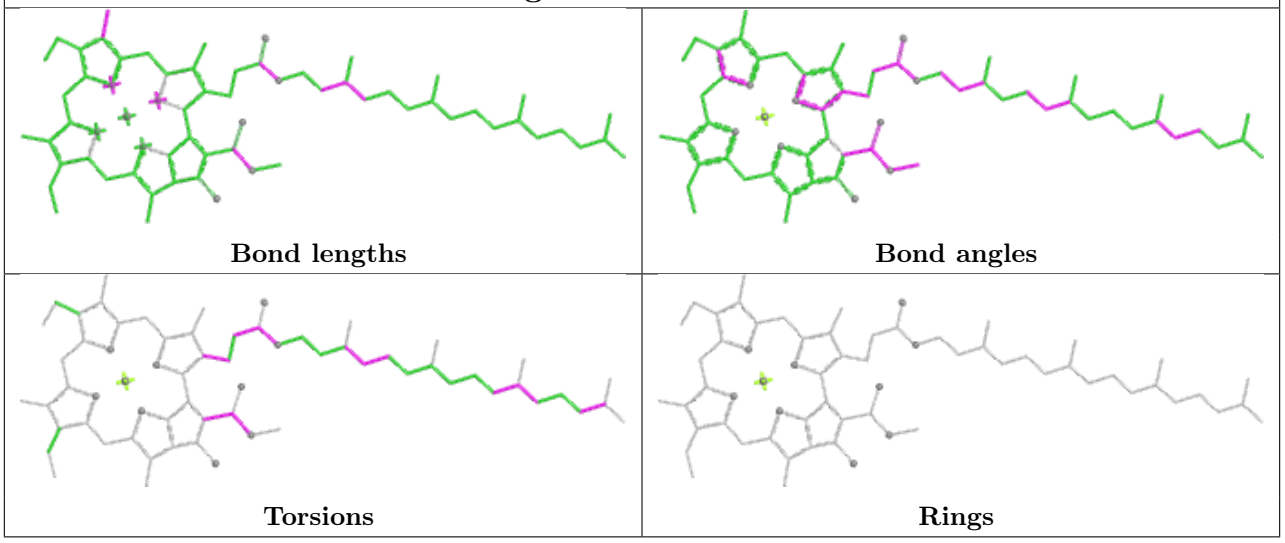


Torsions

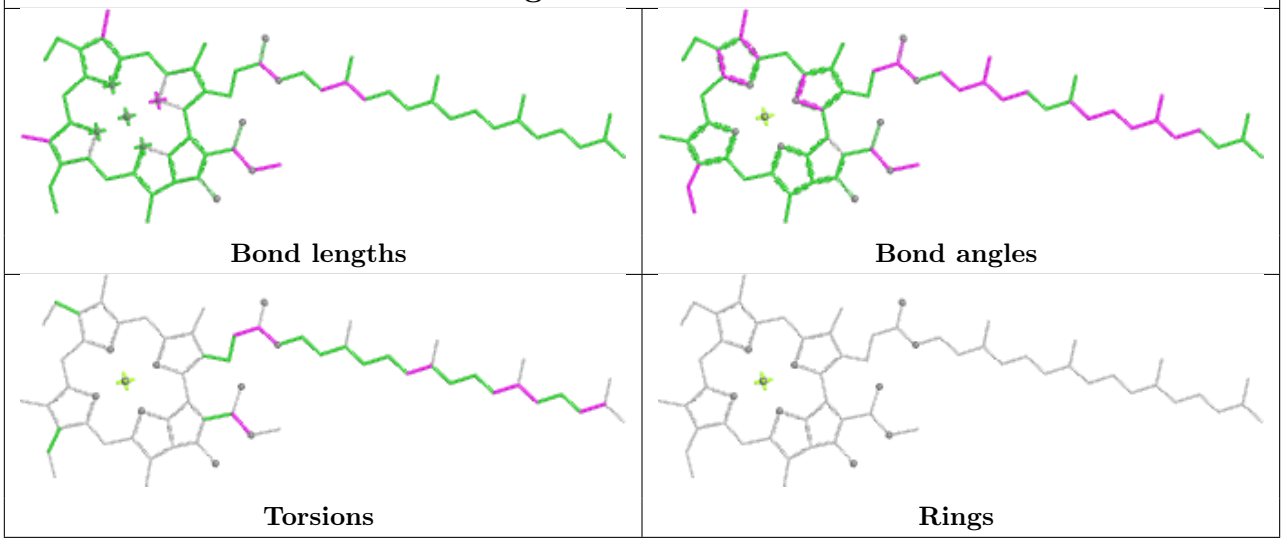


Rings

Ligand CLA A 603



Ligand CLA A 615



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, 95^{th} 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	156/243 (64%)	0.85	28 (17%)	3 3	18, 41, 96, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	234	LEU	5.0
1	A	88	GLY	4.5
1	A	166	LEU	4.4
1	A	243	LEU	3.9
1	A	90	GLN	3.7
1	A	89	LEU	3.7
1	A	164	ALA	3.4
1	A	220	LYS	3.1
1	A	91	ARG	3.0
1	A	171	ARG	2.9
1	A	219	GLY	2.8
1	A	160	PHE	2.8
1	A	131	GLU	2.6
1	A	92	PHE	2.6
1	A	93	ARG	2.6
1	A	216	ALA	2.5
1	A	215	ALA	2.4
1	A	172	LEU	2.4
1	A	189	LYS	2.3
1	A	218	THR	2.2
1	A	239	LEU	2.2
1	A	235	HIS	2.1
1	A	241	ARG	2.1
1	A	224	ASN	2.1
1	A	240	ASP	2.1
1	A	132	GLY	2.1
1	A	165	GLU	2.1

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
1	A	138	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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.

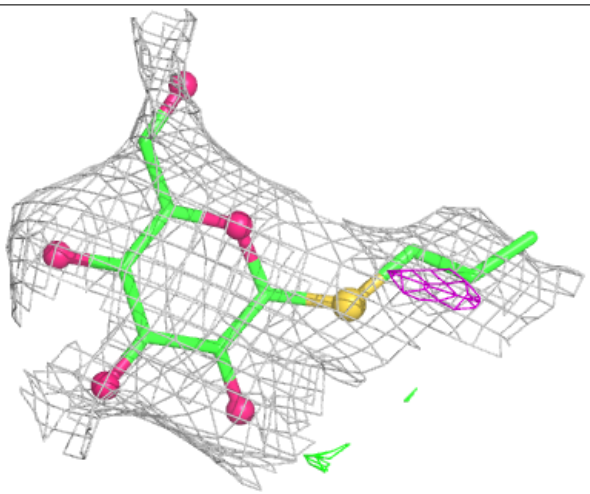
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	HTG	A	632	15/19	0.75	0.20	85,87,89,89	0
8	HTG	A	631	17/19	0.82	0.24	85,86,88,89	0
3	CHL	A	608	66/66	0.83	0.22	32,63,90,94	0
3	CHL	A	614	66/66	0.83	0.23	36,52,133,134	0
2	CLA	A	602	65/65	0.86	0.23	37,74,125,129	0
3	CHL	A	607	66/66	0.86	0.22	39,53,154,156	0
2	CLA	A	612	65/65	0.87	0.28	24,54,143,144	0
6	NEX	A	623	44/44	0.87	0.17	22,49,158,159	0
2	CLA	A	603	65/65	0.88	0.22	40,61,157,158	0
2	CLA	A	609	65/65	0.89	0.20	38,56,119,125	0
2	CLA	A	615	65/65	0.89	0.19	15,35,141,144	0
7	G3P	A	630	10/10	0.90	0.17	69,78,82,82	0
3	CHL	A	606	66/66	0.91	0.19	18,38,127,129	0
2	CLA	A	610	65/65	0.92	0.14	29,44,54,67	0
5	XAT	A	622	44/44	0.92	0.18	21,53,122,127	0
2	CLA	A	604	65/65	0.92	0.14	23,44,99,100	0
4	LUT	A	620	42/42	0.94	0.10	21,31,37,39	0
2	CLA	A	613	65/65	0.94	0.16	41,49,109,125	0
2	CLA	A	611	65/65	0.94	0.16	13,28,162,165	0

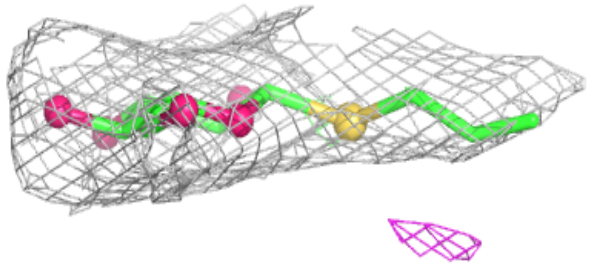
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

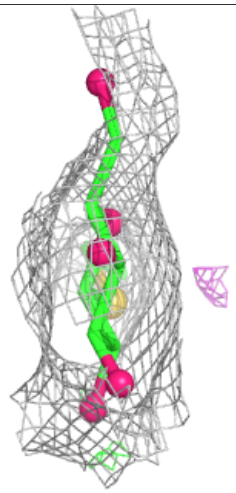
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HTG A 632:

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

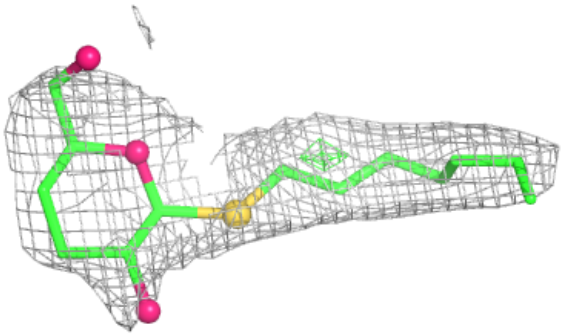


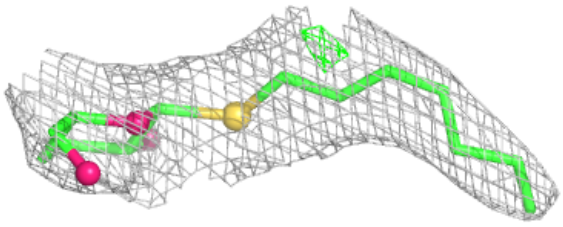


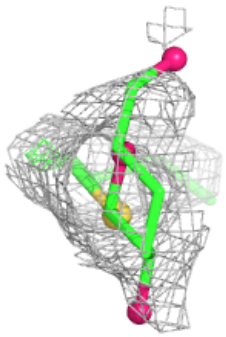


Electron density around HTG A 631:

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

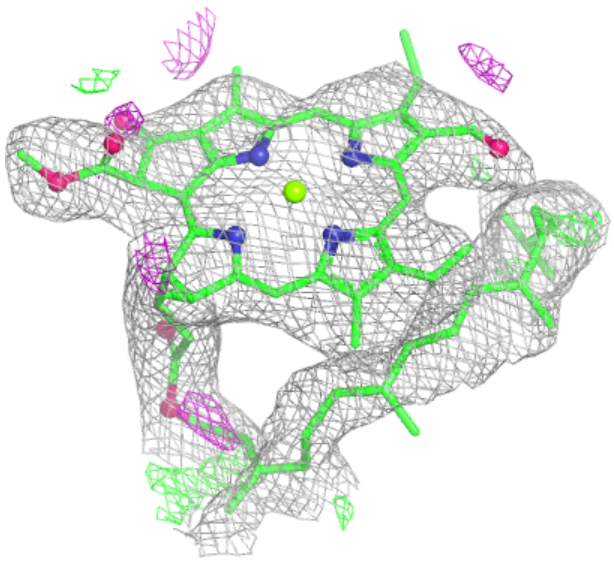


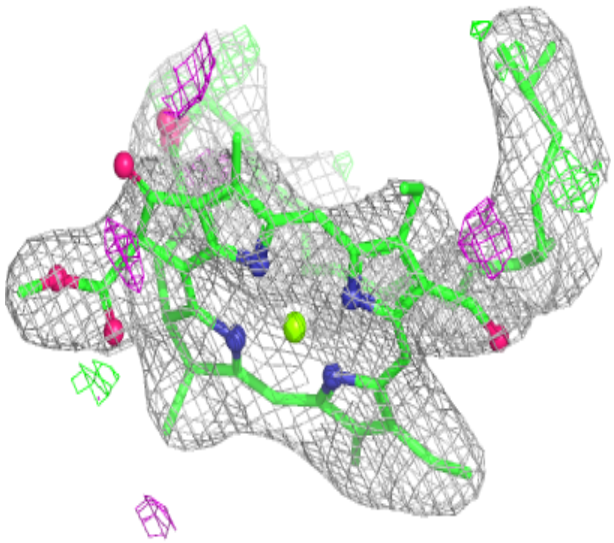


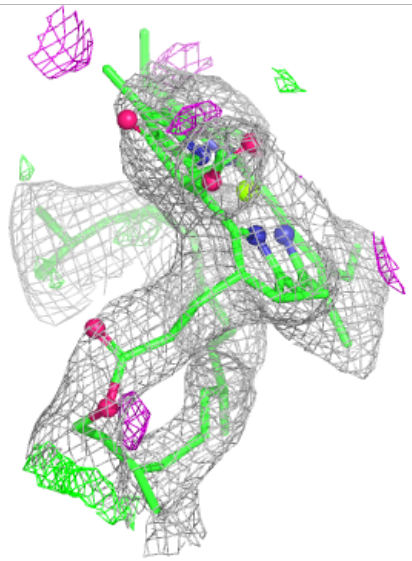


Electron density around CHL A 608:

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

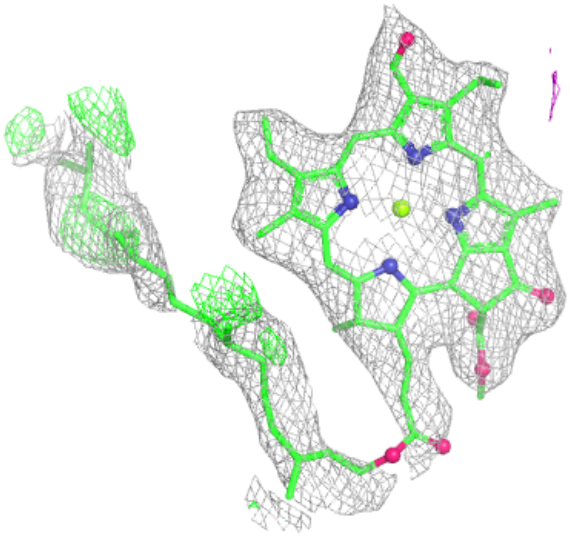


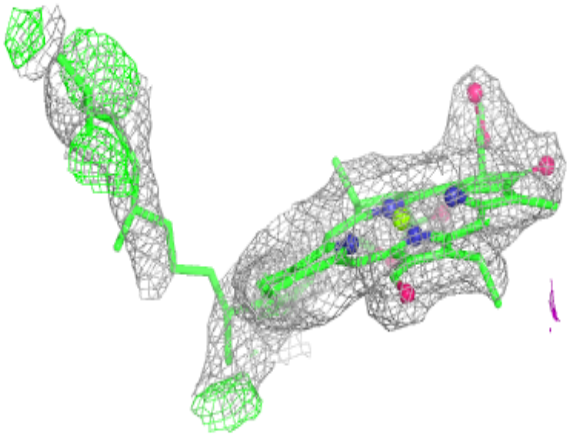


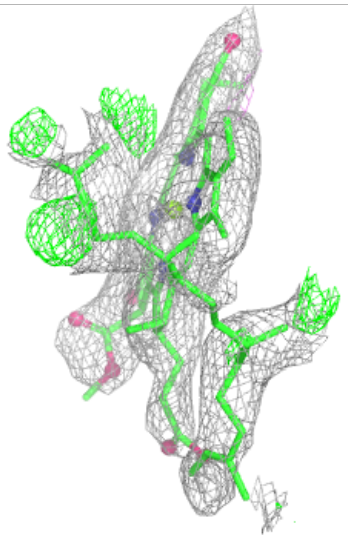


Electron density around CHL A 614:

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

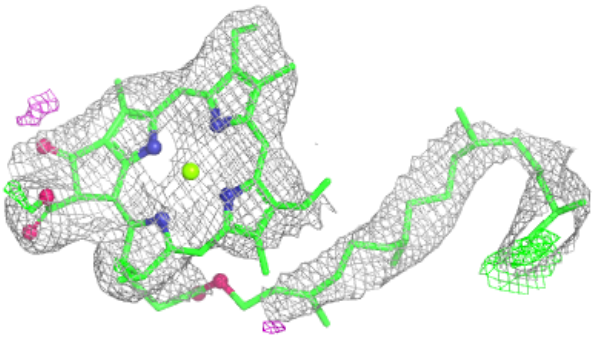


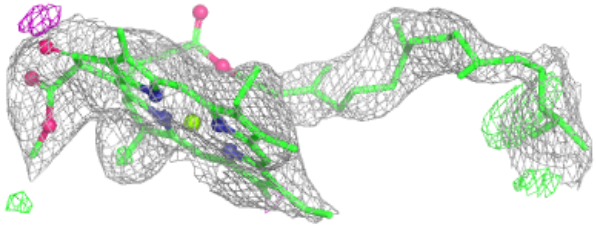




Electron density around CLA A 602:

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

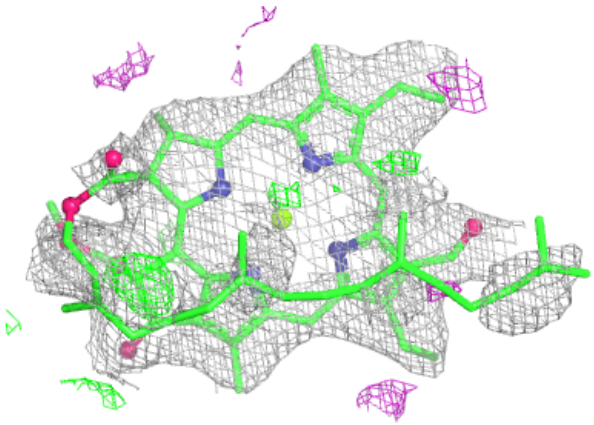


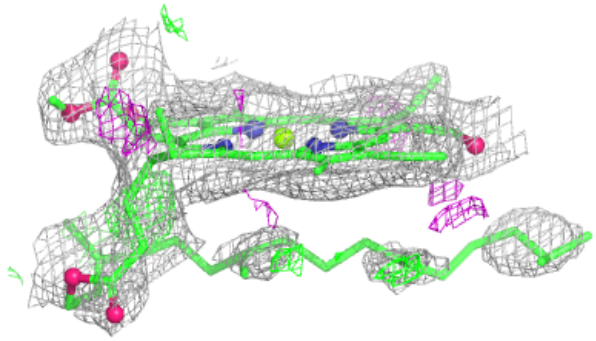




Electron density around CHL A 607:

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

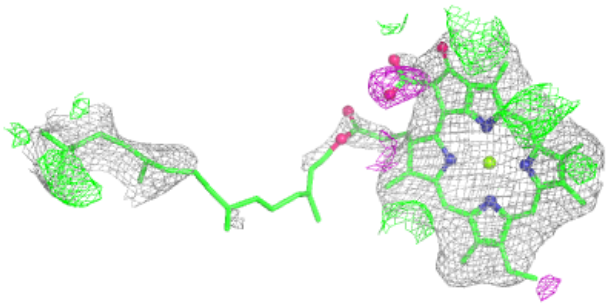


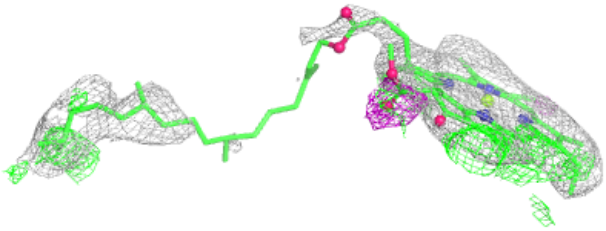


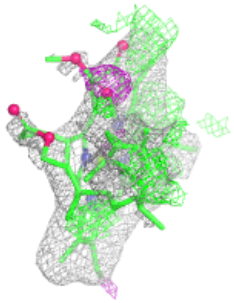


Electron density around CLA A 612:

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

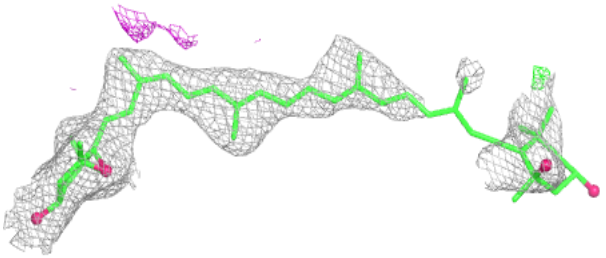


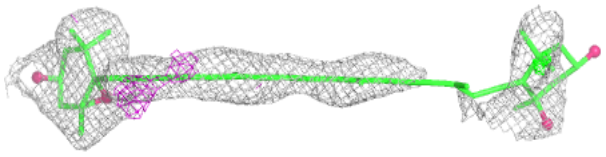


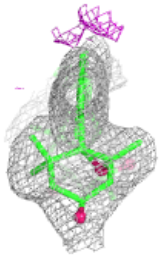


Electron density around NEX A 623:

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

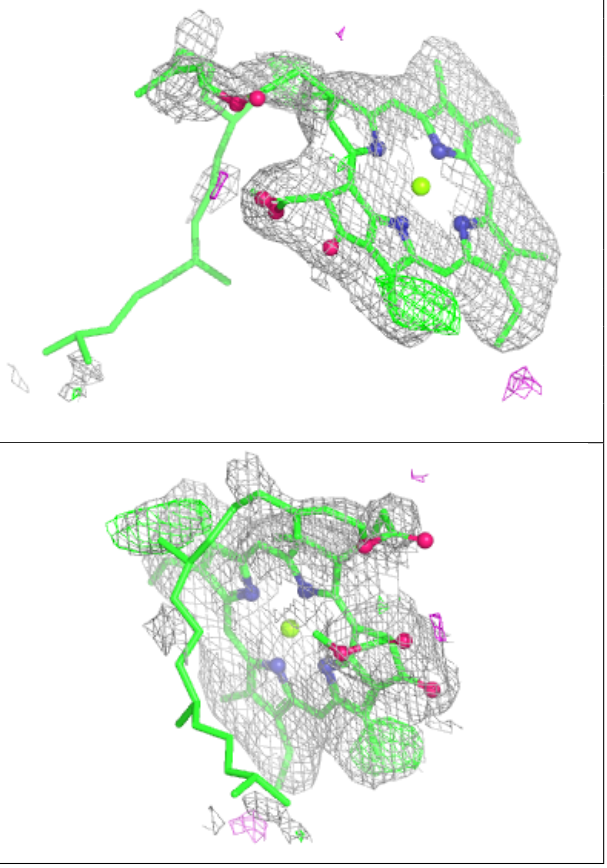


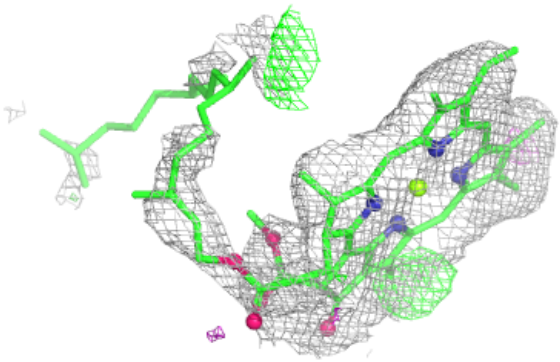




Electron density around CLA A 603:

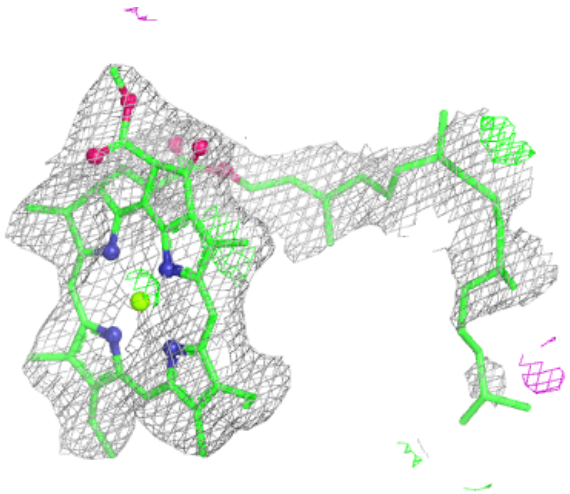
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

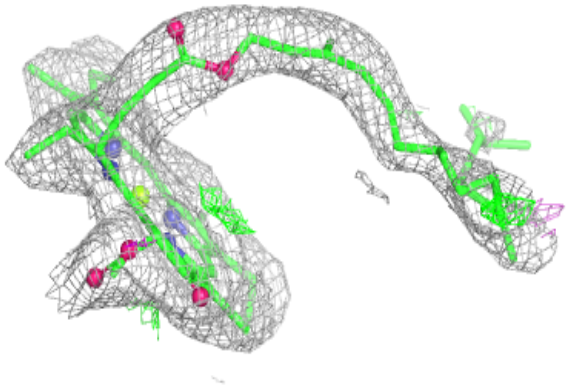


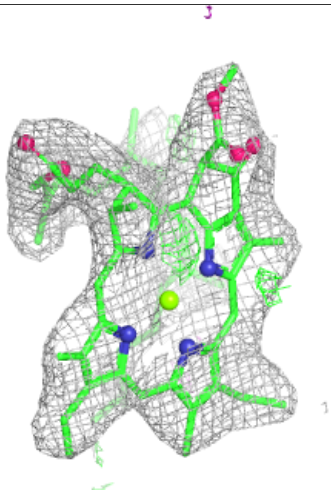


Electron density around CLA A 609:

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

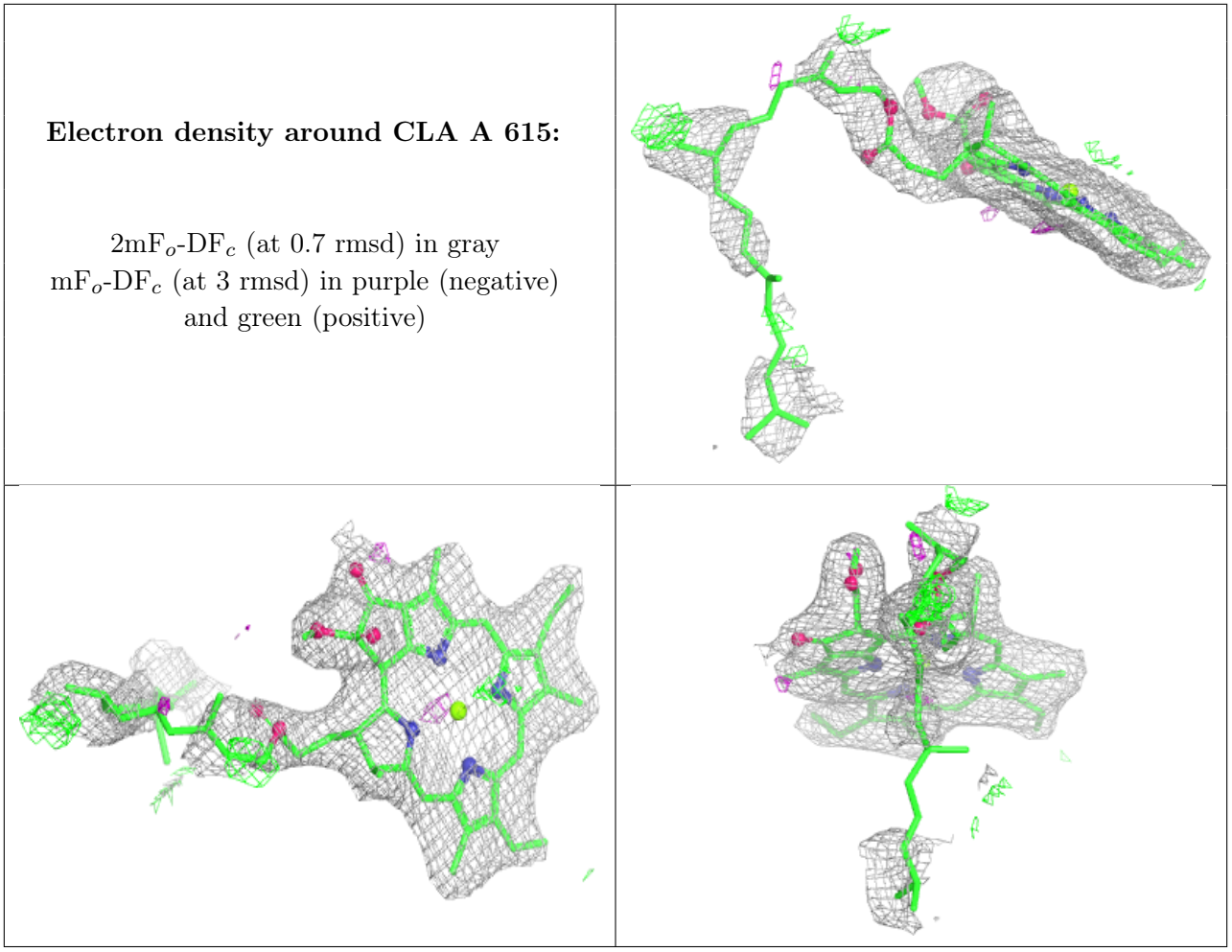






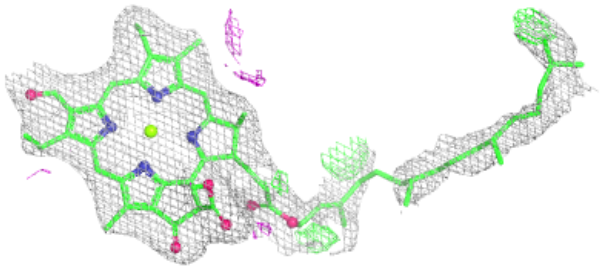
Electron density around CLA A 615:

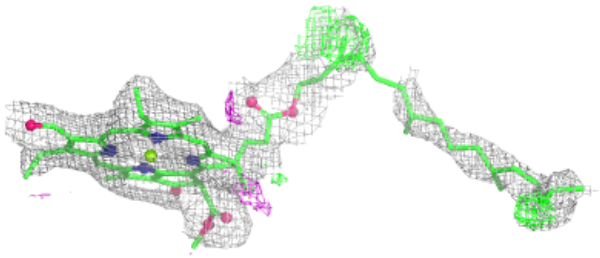
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

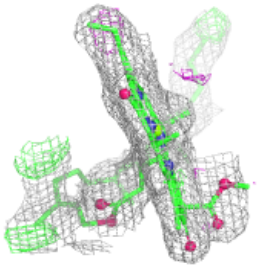


Electron density around CHL A 606:

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

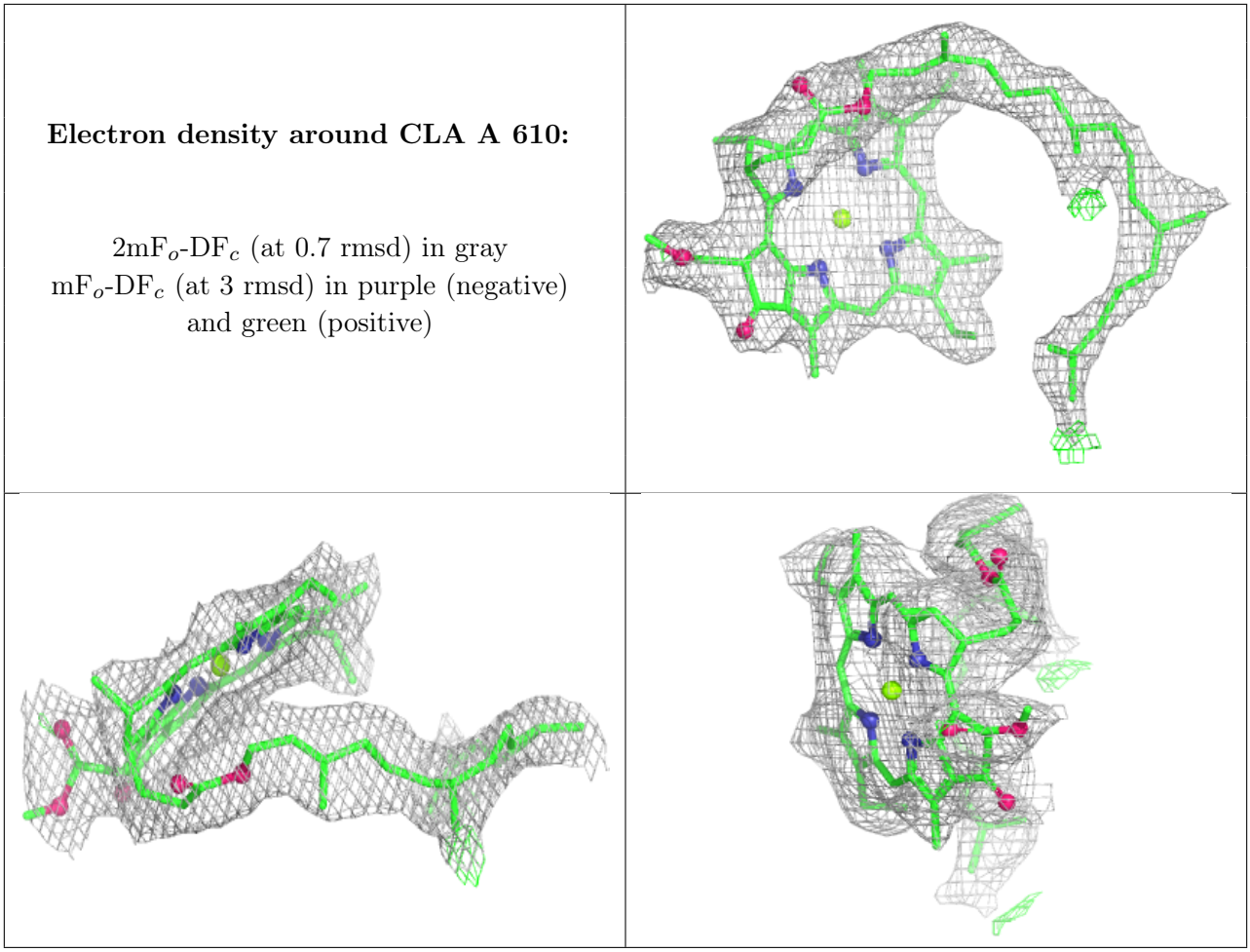






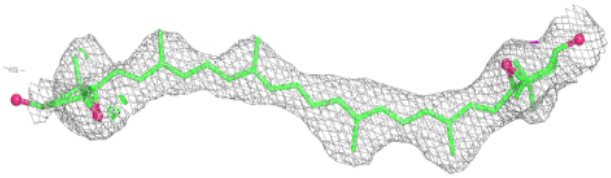
Electron density around CLA A 610:

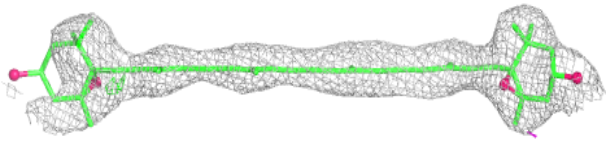
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

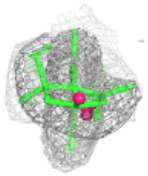


Electron density around XAT A 622:

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

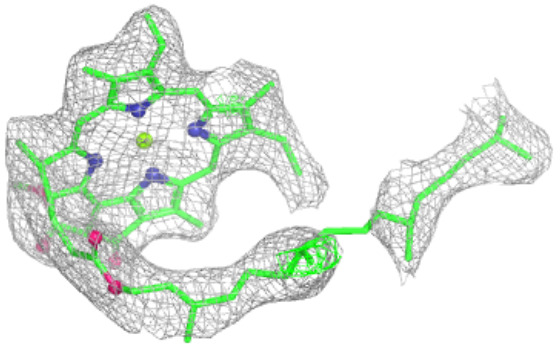


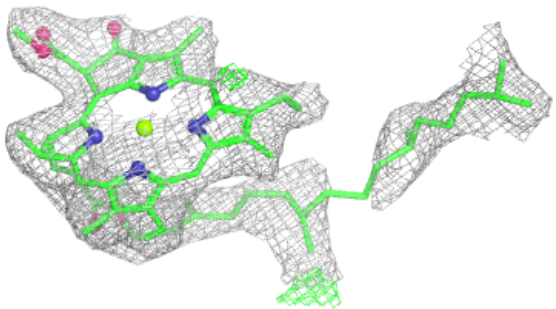




Electron density around CLA A 604:

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

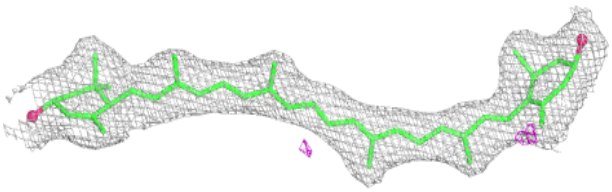


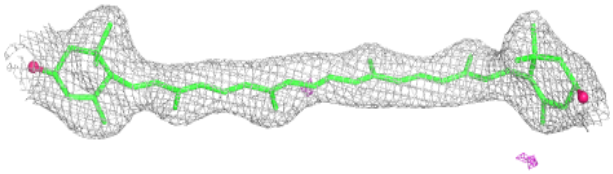


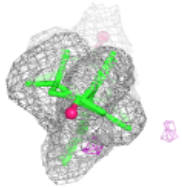


Electron density around LUT A 620:

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

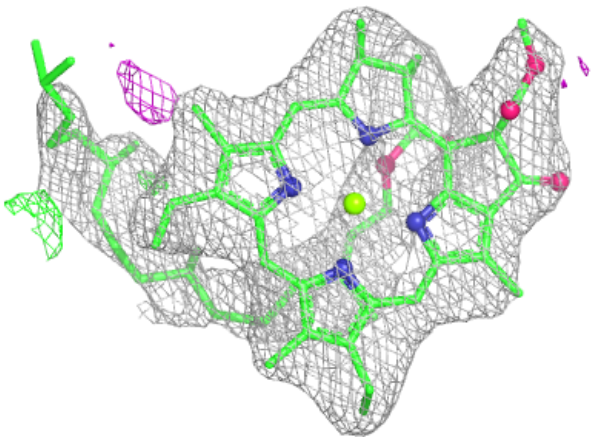


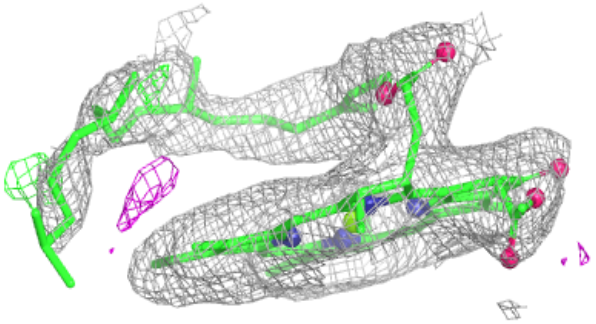


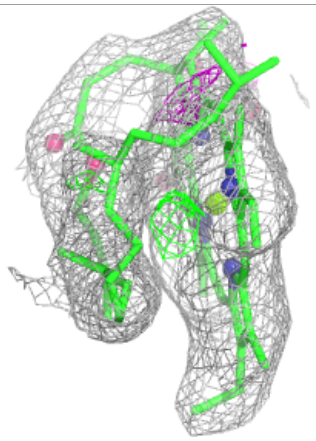


Electron density around CLA A 613:

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

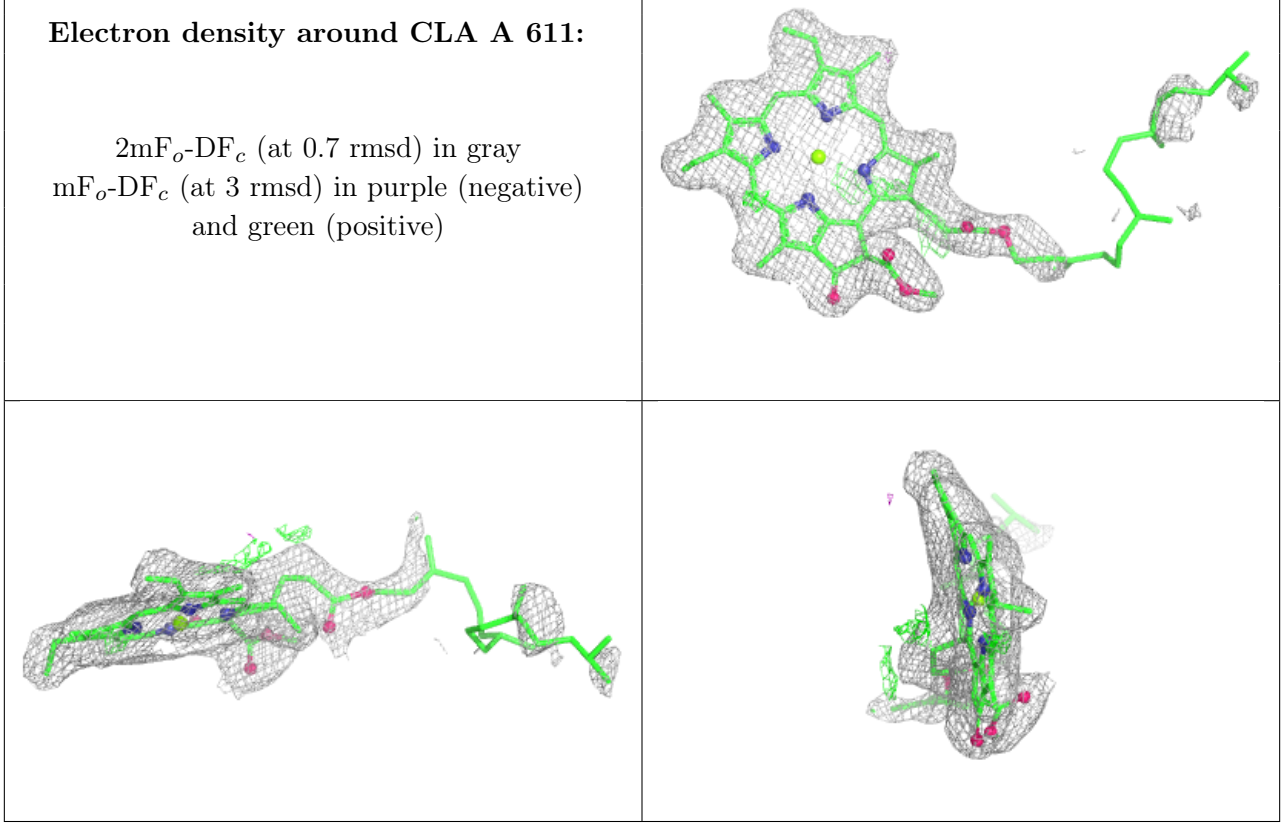






Electron density around CLA A 611:

$2mF_o$-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

There are no such residues in this entry.