

wwPDB X-ray Structure Validation Summary Report (i)

Mar 18, 2024 – 12:24 PM JST

PDB ID : 6A2W

Title : Crystal structure of fucoxanthin chlorophyll a/c complex from Phaeodactylum

tricornutum

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Deposited on : 2018-06-13

Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

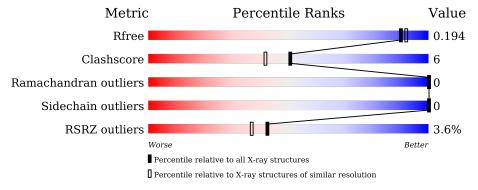
Validation Pipeline (wwPDB-VP) : 2.36

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 1.80 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.



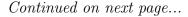
Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	
			4%	
1	A	167	94%	5% •

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
5	CLA	A	401	X	-	-	-
5	CLA	A	402	X	-	-	-





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	A	404	X	-	-	-
5	CLA	A	405	X	-	-	-
5	CLA	A	406	X	-	-	-
5	CLA	A	407	X	-	-	-
5	CLA	A	409	X	-	-	-
8	LMT	A	410	-	-	-	X



2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 2518 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.

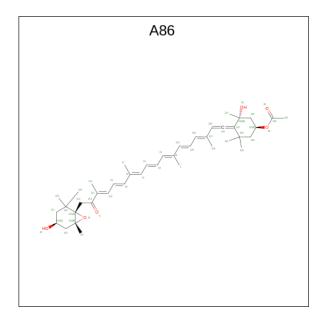
• Molecule 1 is a protein called Protein fucoxanthin chlorophyl a/c protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	166	Total 1308	C 847	N 216	O 241	S 4	0	3	0

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0

• Molecule 3 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7, 8-hexahydro-5,6-epoxy-beta,beta-caroten-3'- yl acetate (three-letter code: A86) (formula: $C_{42}H_{58}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total C C 48 42 6) ;	0	0

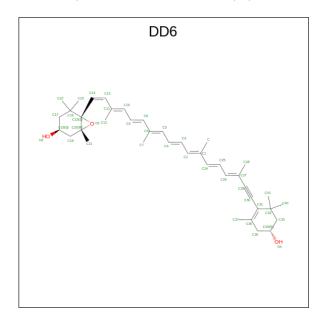
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 48 42 6	0	0
3	A	1	Total C O 48 42 6	0	0
3	A	1	Total C O 48 42 6	0	0
3	A	1	Total C O 48 42 6	0	0
3	A	1	Total C O 48 42 6	0	0
3	A	1	Total C O 48 42 6	0	0

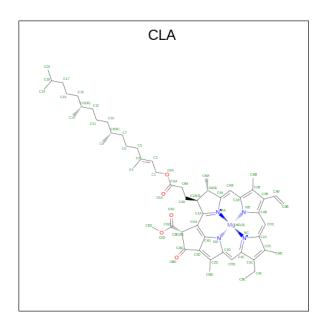
• Molecule 4 is (3S,3'R,5R,6S,7cis)-7',8'-didehydro-5,6-dihydro-5,6-epoxy-beta,beta-carotene-3,3'-diol (three-letter code: DD6) (formula: $C_{40}H_{54}O_3$).



Mol	Chain	Residues	Ato	oms		ZeroOcc	AltConf
4	A	1	Total 43	C 40	O 3	0	0

• Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).

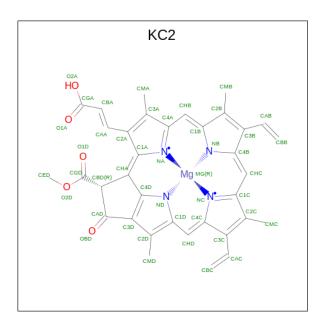




Mol	Chain	Residues		At	oms			ZeroOcc	AltConf
5	A	1	Total	С	Mg	N	О	0	0
9	Λ	1	61	51	1	4	5	U	U
5	A	1	Total	С	Mg	N	О	0	0
	Λ	1	65	55	1	4	5	U	0
5	A	1	Total	С	Mg	N	О	0	0
9	Λ	1	65	55	1	4	5	U	
5	A	1	Total	С	Mg	N	О	0	0
9	Λ	1	46	36	1	4	5	U	0
5	A	1	Total	С	Mg	N	О	0	0
9	Λ	1	65	55	1	4	5	U	
5	A	1	Total	С	Mg	N	О	0	0
	Α	1	65	55	1	4	5	U	U
5	۸	1	Total	С	Mg	N	О	0	0
3	Λ	1	41	33	1	4	3	U	

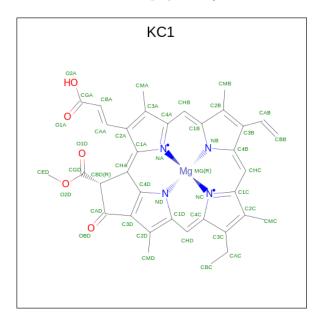
 \bullet Molecule 6 is Chlorophyll c2 (three-letter code: KC2) (formula: $\rm C_{35}H_{28}MgN_4O_5).$





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

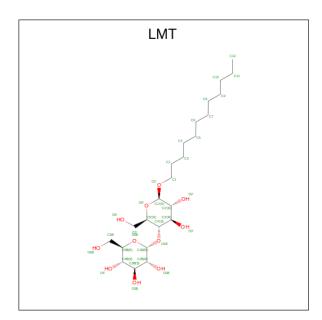
 \bullet Molecule 7 is Chlorophyll c1 (three-letter code: KC1) (formula: $\mathrm{C_{35}H_{30}MgN_4O_5}).$



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 45	C 35	Mg 1	N 4	O 5	0	0

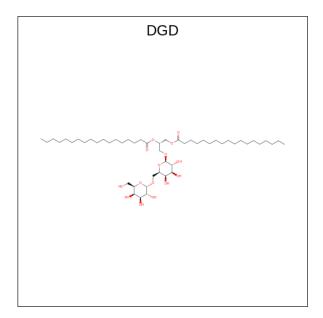
 \bullet Molecule 8 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 31	C 20	O 11	0	0

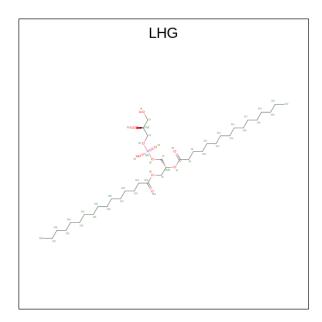
• Molecule 9 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 39	C 34	O 5	0	0

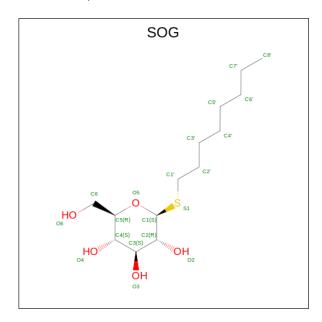
 \bullet Molecule 10 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $\rm C_{38}H_{75}O_{10}P).$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	٨	1	Total	С	О	Р	0	0
10	A	1	33	24	8	1	0	U

 \bullet Molecule 11 is octyl 1-thio-beta-D-glucopyranoside (three-letter code: SOG) (formula: $\rm C_{14}H_{28}O_5S).$



Mol	Chain	Residues	Ator	ns	ZeroOcc	AltConf
11	A	1	Total C 20 14		0	0
11	A	1	Total C		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 20			0	0
11	A	1	Total 15			0	0

• Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		Atoms		Atoms		ZeroOcc	AltConf
12	A	7	Total 73	C 73	0	0				

• Molecule 13 is water.

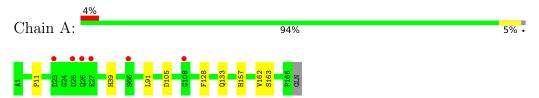
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	80	Total O 80 80	0	0



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: Protein fucoxanthin chlorophyl a/c protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	47.75Å 115.72Å 141.26Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 - 1.80	Depositor
Resolution (A)	19.98 - 1.80	EDS
% Data completeness	67.0 (19.98-1.80)	Depositor
(in resolution range)	67.0 (19.98-1.80)	EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.11 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
D D.	0.175 , 0.197	Depositor
R, R_{free}	0.173 , 0.194	DCC
R_{free} test set	1860 reflections (7.55%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.42, 89.4	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2518	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, SOG, LMT, DD6, A86, DGD, UNL, KC1, CA, CLA, KC2

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).

ſ	Mol	Chain	Bond	lengths	Bond angles		
			RMSZ	# Z > 5	RMSZ	# Z > 5	
ſ	1	A	0.43	0/1342	0.57	0/1811	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1308	0	1297	9	0
2	A	2	0	0	0	0
3	A	336	0	0	1	0
4	A	43	0	0	0	0
5	A	408	0	411	17	0
6	A	45	0	0	0	0
7	A	45	0	0	0	0
8	A	31	0	35	0	0
9	A	39	0	62	4	0
10	A	33	0	42	1	0
11	A	75	0	99	4	0
12	A	73	0	0	0	0
13	A	80	0	0	1	0
All	All	2518	0	1946	25	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 25 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:105:ASP:OD1	13:A:501:HOH:O	2.09	0.70
9:A:411:DGD:HBW2	9:A:411:DGD:HA92	1.76	0.68
5:A:401:CLA:HBB1	5:A:401:CLA:HMB1	1.85	0.57
1:A:91:LEU:HD23	5:A:405:CLA:HBC3	1.91	0.52
11:A:416:SOG:S1	11:A:416:SOG:O6	2.57	0.52

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	167/167 (100%)	165 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	134/132 (102%)	134 (100%)	0	100	100	



There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 2 are monoatomic and 7 are unknown - leaving 24 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	Trino	Chain	Res	Link	В	ond leng	$_{ m gths}$	Во	ond angl	es
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A86	A	302	-	44,50,50	1.13	2 (4%)	51,76,76	1.63	8 (15%)
5	CLA	A	407	1	65,73,73	1.28	6 (9%)	76,113,113	1.54	15 (19%)
3	A86	A	306	-	44,50,50	1.65	8 (18%)	51,76,76	2.29	17 (33%)
7	KC1	A	408	1	48,53,53	2.80	20 (41%)	55,89,89	4.48	32 (58%)
3	A86	A	307	-	44,50,50	1.10	2 (4%)	51,76,76	1.70	10 (19%)
4	DD6	A	308	-	39,45,45	2.24	4 (10%)	52,67,67	2.49	14 (26%)
5	CLA	A	406	1	65,73,73	1.49	6 (9%)	76,113,113	1.54	11 (14%)
8	LMT	A	410	-	32,32,36	1.05	4 (12%)	43,43,47	1.48	4 (9%)
10	LHG	A	412	-	32,32,48	0.86	2 (6%)	36,37,54	1.63	4 (11%)



Mol	Type	Chain	Res	Link	В	ond leng	gths	Во	ond angl	es
WIOI	Type	Chain	rtes	Lilik	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
11	SOG	A	414	_	20,20,20	1.13	1 (5%)	24,25,25	1.27	2 (8%)
9	DGD	A	411	-	38,38,67	0.68	1 (2%)	40,40,81	1.35	3 (7%)
3	A86	A	303	-	44,50,50	1.15	3 (6%)	51,76,76	1.72	7 (13%)
5	CLA	A	401	13	61,69,73	1.45	5 (8%)	71,108,113	1.41	7 (9%)
11	SOG	A	416	-	15,15,20	1.11	1 (6%)	18,20,25	1.34	2 (11%)
11	SOG	A	413	-	20,20,20	0.95	1 (5%)	24,25,25	1.03	1 (4%)
3	A86	A	301	-	44,50,50	1.18	2 (4%)	51,76,76	2.34	18 (35%)
6	KC2	A	403	-	48,53,53	3.13	21 (43%)	54,89,89	4.44	31 (57%)
5	CLA	A	405	1	46,54,73	1.68	7 (15%)	53,90,113	1.80	15 (28%)
11	SOG	A	415	-	20,20,20	0.91	1 (5%)	24,25,25	0.93	1 (4%)
3	A86	A	304	-	44,50,50	1.11	3 (6%)	51,76,76	1.69	10 (19%)
5	CLA	A	404	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	10 (13%)
5	CLA	A	409	-	41,49,73	1.81	6 (14%)	47,84,113	1.66	7 (14%)
3	A86	A	305	-	44,50,50	1.21	2 (4%)	51,76,76	2.23	8 (15%)
5	CLA	A	402	1	65,73,73	1.47	6 (9%)	76,113,113	1.56	12 (15%)

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
3	A86	A	302	-	-	4/34/90/90	0/3/3/3
5	CLA	A	407	1	1/1/15/20	12/37/115/115	-
3	A86	A	306	-	-	2/34/90/90	0/3/3/3
7	KC1	A	408	1	-	1/15/71/71	-
3	A86	A	307	-	-	3/34/90/90	0/3/3/3
4	DD6	A	308	-	-	9/26/80/80	0/3/3/3
5	CLA	A	406	1	1/1/15/20	5/37/115/115	-
8	LMT	A	410	-	-	9/17/57/61	0/2/2/2
10	LHG	A	412	-	-	16/34/34/53	-
11	SOG	A	414	-	-	5/11/31/31	0/1/1/1
9	DGD	A	411	-	-	25/40/40/95	-
3	A86	A	303	-	-	2/34/90/90	0/3/3/3
5	CLA	A	401	13	1/1/14/20	10/33/111/115	-
11	SOG	A	416	-	-	3/6/26/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	SOG	A	413	-	-	2/11/31/31	0/1/1/1
3	A86	A	301	-	-	3/34/90/90	0/3/3/3
6	KC2	A	403	-	-	4/15/71/71	-
5	CLA	A	405	1	1/1/11/20	5/15/93/115	-
11	SOG	A	415	-	-	3/11/31/31	0/1/1/1
3	A86	A	304	-	-	0/34/90/90	0/3/3/3
5	CLA	A	404	1	1/1/15/20	5/37/115/115	-
5	CLA	A	409	-	1/1/10/20	3/8/86/115	-
3	A86	A	305	-	-	3/34/90/90	0/3/3/3
5	CLA	A	402	1	1/1/15/20	12/37/115/115	-

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
4	A	308	DD6	C29-C27	-9.27	1.24	1.42
4	A	308	DD6	C30-C31	-7.95	1.25	1.42
6	A	403	KC2	C4C-NC	7.83	1.49	1.37
5	A	406	CLA	C4B-NB	7.60	1.42	1.35
6	A	403	KC2	C4D-ND	7.55	1.41	1.35

The worst 5 of 249 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
7	A	408	KC1	CHC-C4B-NB	11.65	135.16	124.45
6	A	403	KC2	C1A-NA-C4A	-10.63	101.92	106.71
6	A	403	KC2	CHC-C4B-NB	10.17	133.80	124.45
7	A	408	KC1	CHD-C4C-C3C	-10.05	106.46	125.33
3	A	306	A86	C17-C16-C15	10.05	119.41	109.16

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	401	CLA	ND
5	A	402	CLA	ND
5	A	404	CLA	ND
5	A	405	CLA	ND
5	A	406	CLA	ND

5 of 146 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
3	A	301	A86	O5-C38-O4-C34
3	A	302	A86	C-C1-C24-C25
4	A	308	DD6	C-C1-C24-C25
4	A	308	DD6	C2-C1-C24-C25
4	A	308	DD6	C10-C11-C13-C14

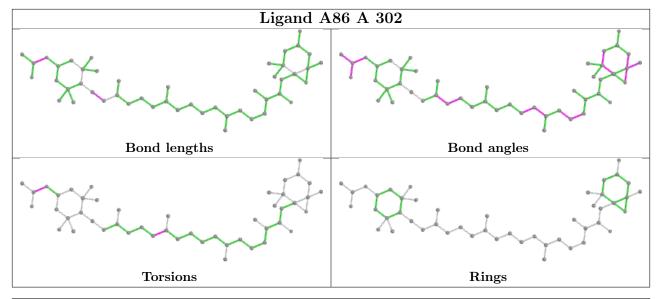
There are no ring outliers.

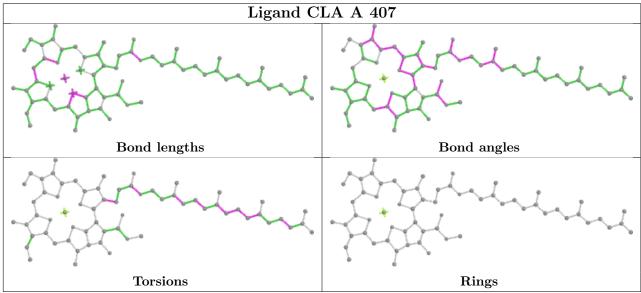
13 monomers are involved in 23 short contacts:

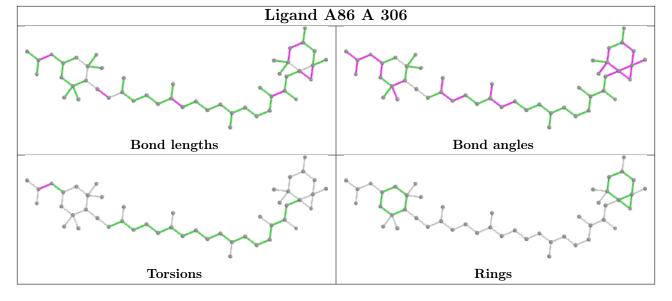
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	CLA	2	0
5	A	406	CLA	3	0
10	A	412	LHG	1	0
11	A	414	SOG	1	0
9	A	411	DGD	4	0
3	A	303	A86	1	0
5	A	401	CLA	2	0
11	A	416	SOG	1	0
11	A	413	SOG	2	0
5	A	405	CLA	2	0
5	A	404	CLA	1	0
5	A	409	CLA	4	0
5	A	402	CLA	3	0

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.

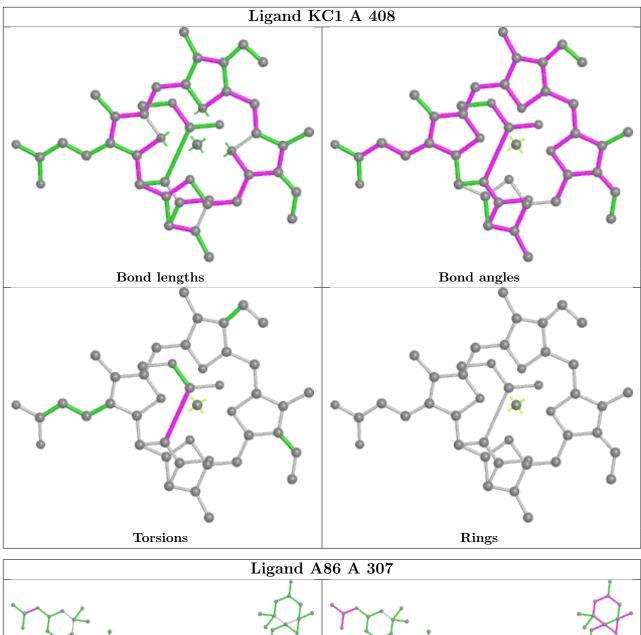


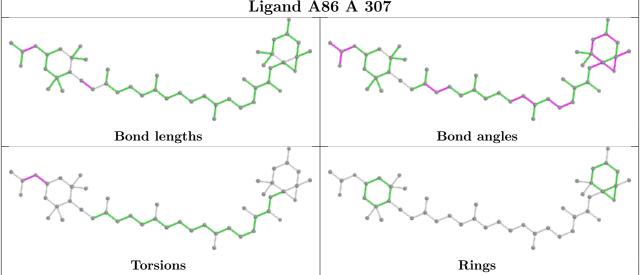




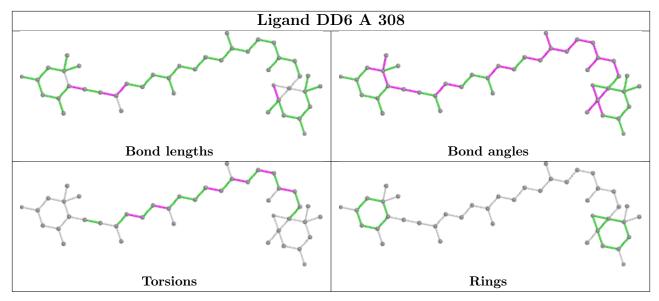


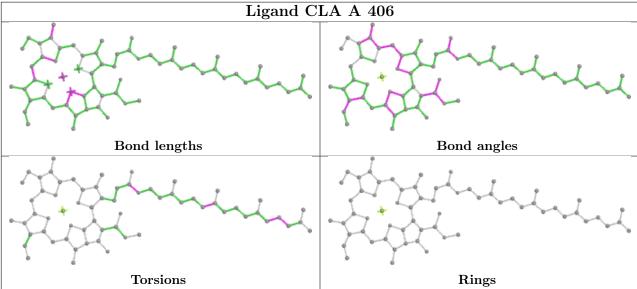




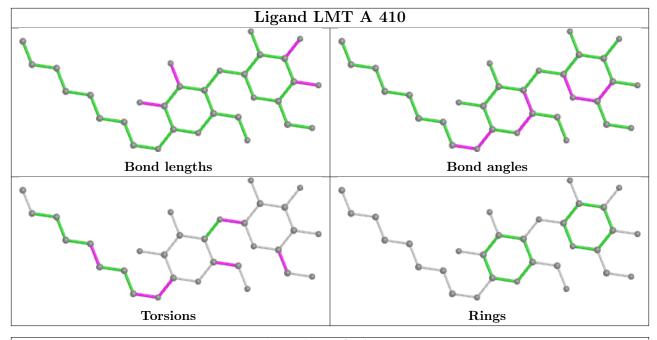


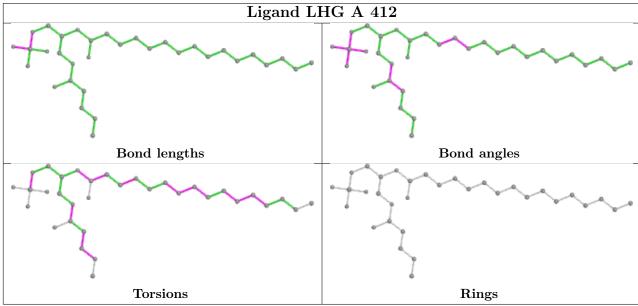




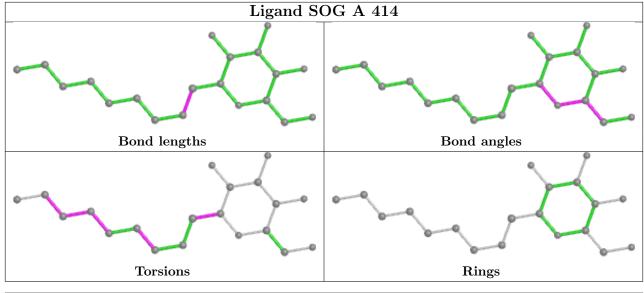


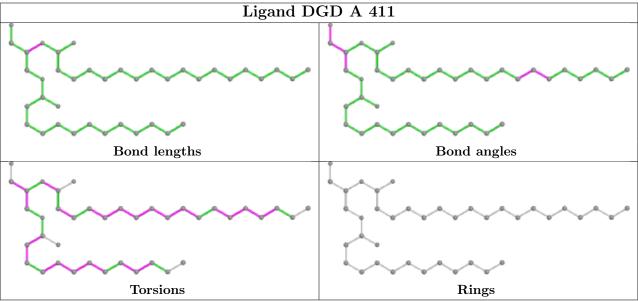


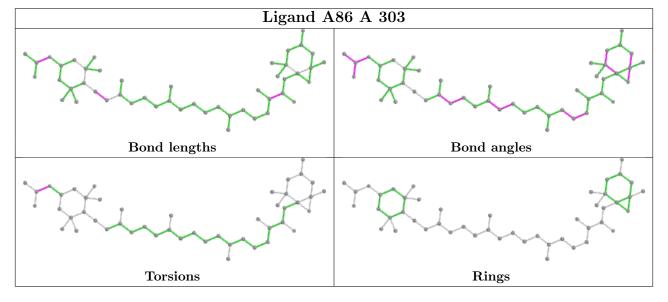




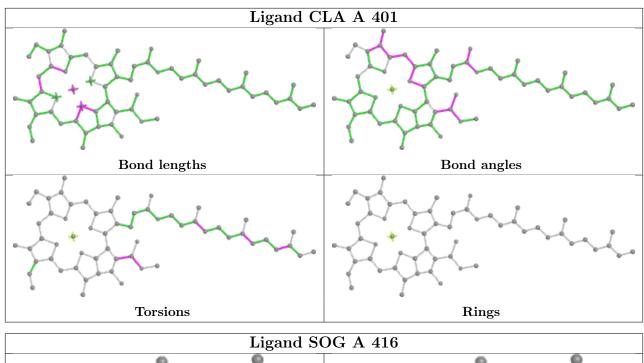


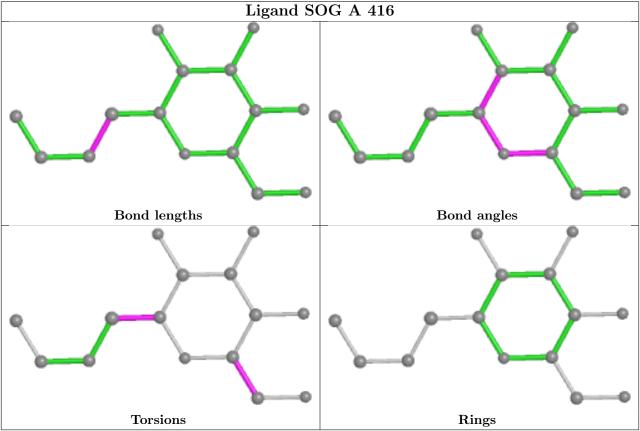




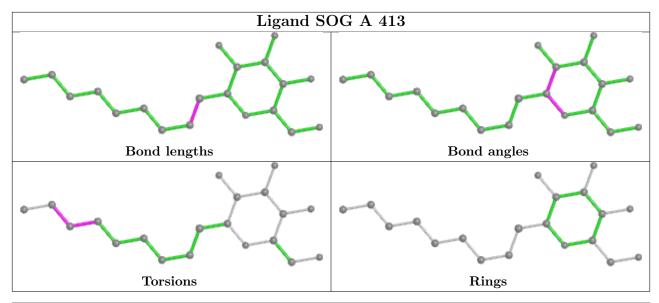


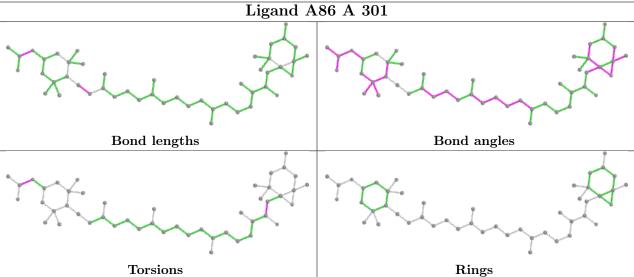




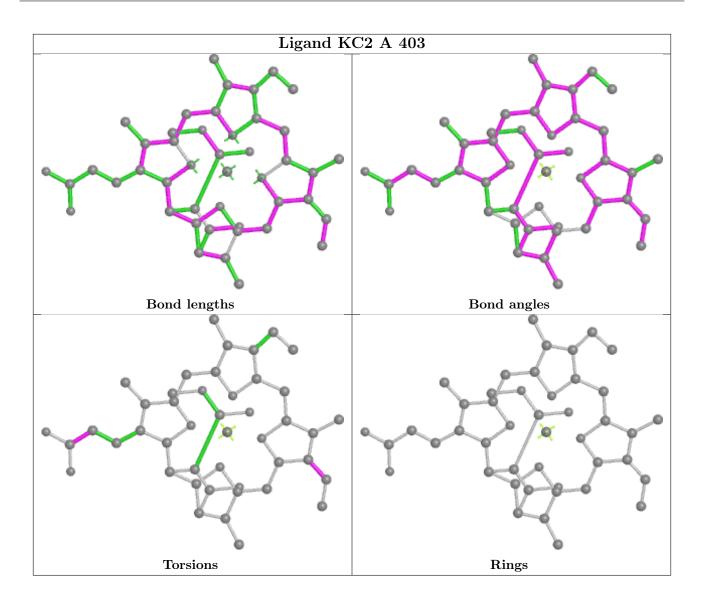




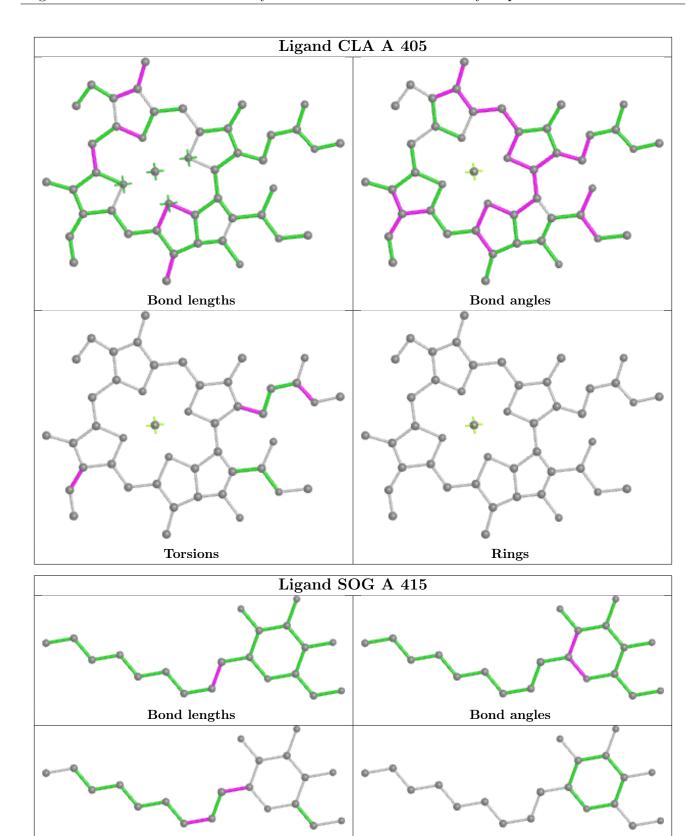








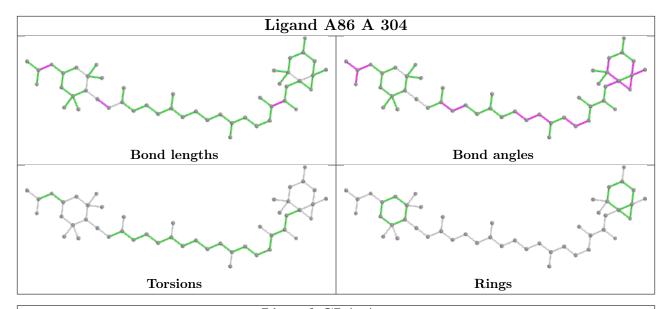


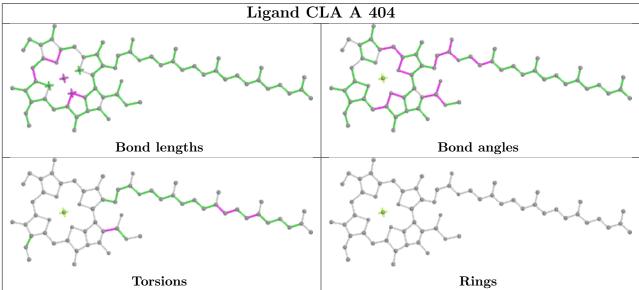




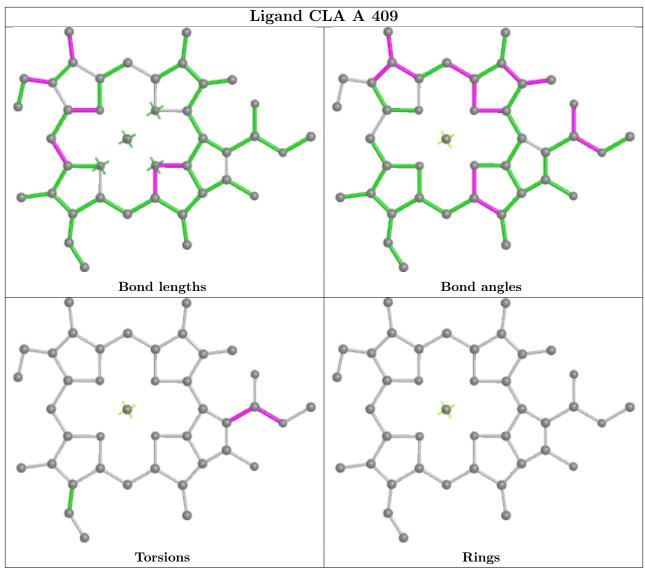
Rings

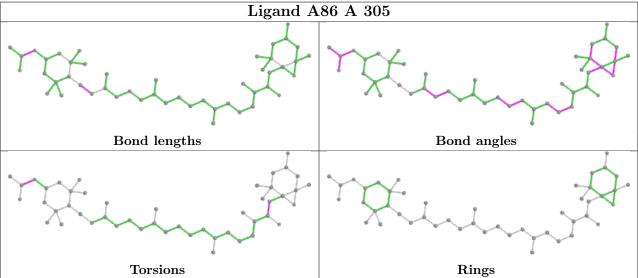
Torsions



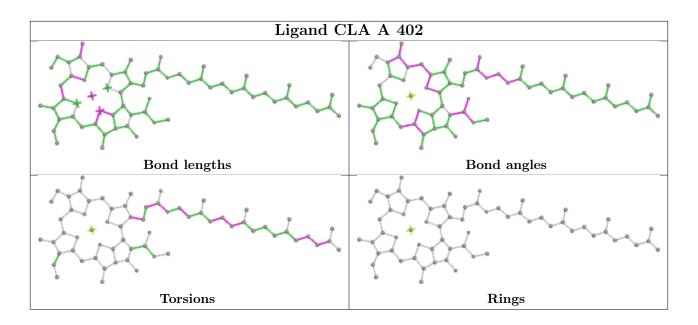












5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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 $>$	#R5	\mathbf{SRZ}	>2	$OWAB(A^2)$	Q<0.9
1	A	166/167 (99%)	-0.10	6 (3%)	42	37	18, 36, 63, 79	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	GLU	3.3
1	A	25	ASP	2.5
1	A	23	ASP	2.4
1	A	66	SER	2.3
1	A	26	GLN	2.3

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 monosaccharides 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
8	LMT	A	410	31/35	0.51	0.40	49,110,124,127	0
4	DD6	A	308	43/43	0.52	0.30	70,84,104,109	0

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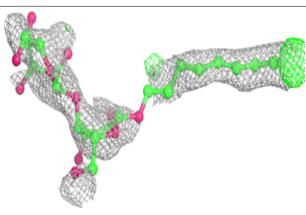
Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B\text{-}factors}({f \AA}^2)$	Q<0.9
9	DGD	A	411	39/66	0.59	0.33	68,86,99,105	0
10	LHG	A	412	33/49	0.62	0.20	45,66,123,127	0
11	SOG	A	414	20/20	0.65	0.24	43,93,104,109	0
11	SOG	A	415	20/20	0.66	0.20	55,100,105,110	0
12	UNL	A	423	10/-	0.68	0.16	62,64,65,65	0
12	UNL	A	420	12/-	0.69	0.21	56,60,64,64	0
11	SOG	A	416	15/20	0.70	0.30	90,96,104,105	0
12	UNL	A	422	7/-	0.71	0.15	43,54,60,61	0
11	SOG	A	413	20/20	0.73	0.30	48,105,119,120	0
12	UNL	A	418	12/-	0.79	0.12	58,61,68,69	0
12	UNL	A	421	12/-	0.79	0.30	52,55,67,69	0
3	A86	A	304	48/48	0.87	0.13	21,28,59,76	0
3	A86	A	306	48/48	0.89	0.12	35,49,72,85	0
12	UNL	A	419	8/-	0.89	0.11	49,54,56,59	0
12	UNL	A	417	12/-	0.89	0.11	47,52,59,60	0
3	A86	A	301	48/48	0.90	0.14	26,43,93,105	0
2	CA	A	202	1/1	0.90	0.08	76,76,76,76	0
5	CLA	A	405	46/65	0.93	0.10	31,43,60,75	0
5	CLA	A	407	65/65	0.93	0.14	15,25,75,83	0
3	A86	A	302	48/48	0.94	0.09	18,28,66,73	0
5	CLA	A	402	65/65	0.94	0.14	25,37,74,79	0
5	CLA	A	409	41/65	0.95	0.10	31,44,61,67	0
5	CLA	A	404	65/65	0.95	0.10	18,25,51,59	0
3	A86	A	303	48/48	0.95	0.09	20,27,51,58	0
5	CLA	A	406	65/65	0.95	0.10	19,28,70,78	0
3	A86	A	307	48/48	0.95	0.08	23,31,55,58	0
3	A86	A	305	48/48	0.96	0.09	17,28,50,63	0
5	CLA	A	401	61/65	0.96	0.09	21,35,66,71	0
6	KC2	A	403	45/45	0.97	0.07	24,30,43,57	0
7	KC1	A	408	45/45	0.97	0.09	19,24,31,56	0
2	CA	A	201	1/1	0.99	0.05	39,39,39,39	0

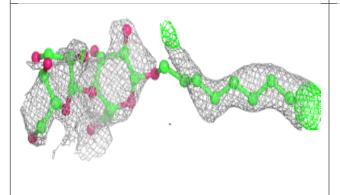
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

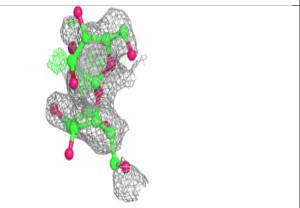


Electron density around LMT A 410:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

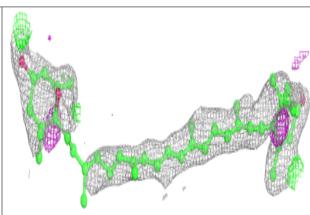


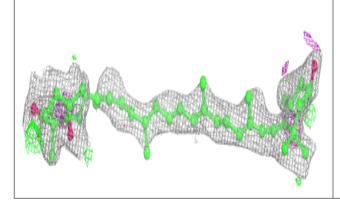


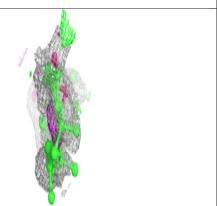


Electron density around DD6 A 308:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



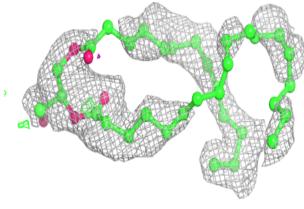


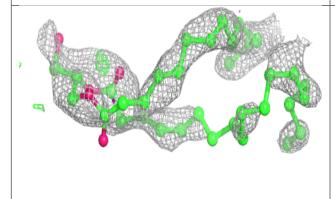


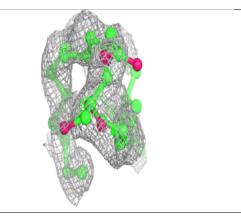


Electron density around DGD A 411:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

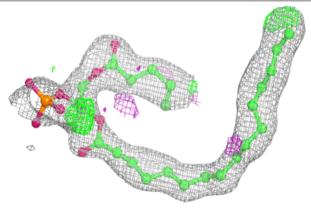


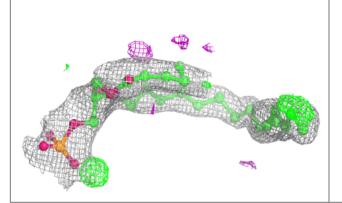


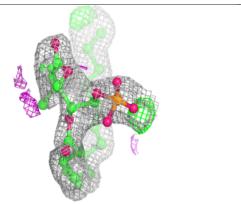


Electron density around LHG A 412:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



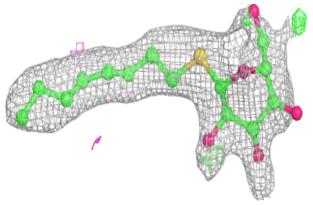


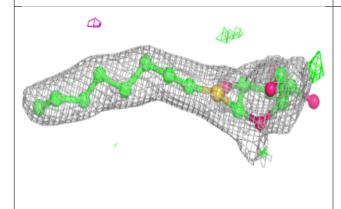


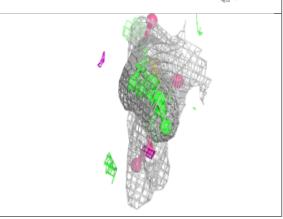


Electron density around SOG A 414:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

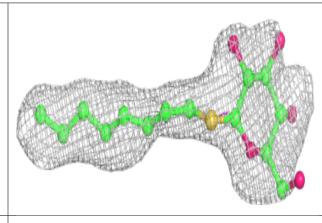


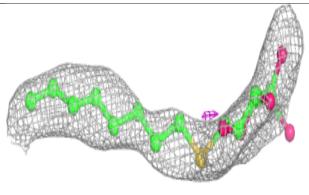


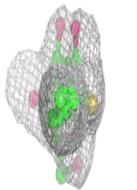


Electron density around SOG A 415:

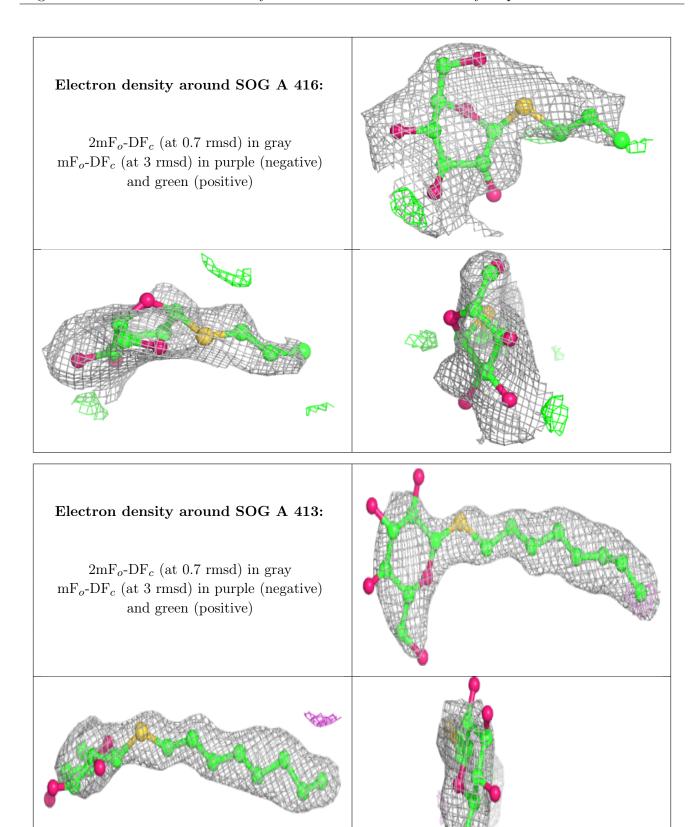
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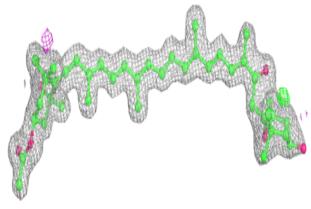


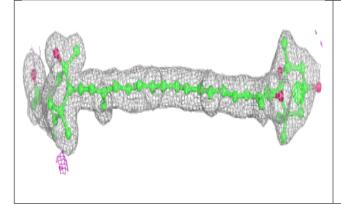


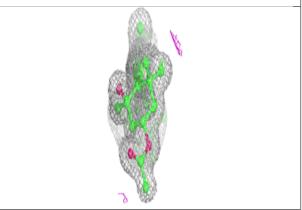


Electron density around A86 A 304:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

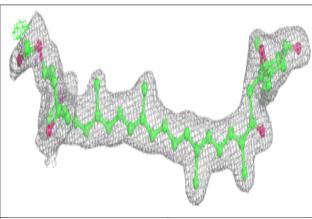


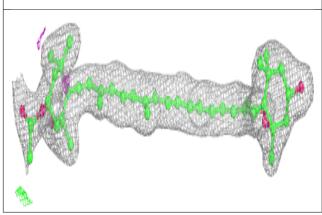


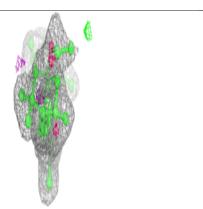


Electron density around A86 A 306:

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m -DF}_c$ (at 0.7 rmsd) in gray ${
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m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



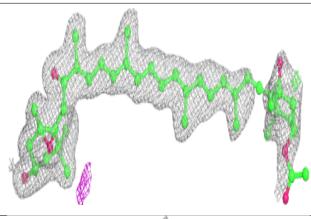


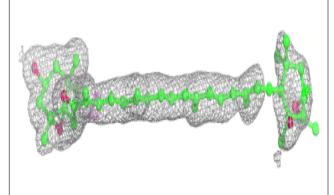


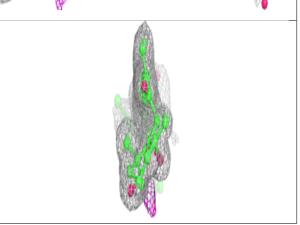


Electron density around A86 A 301:

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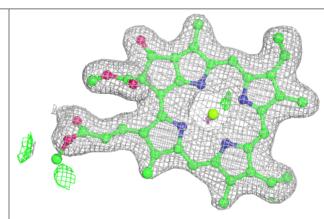


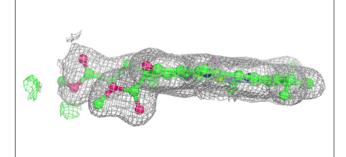


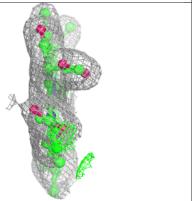


Electron density around CLA A 405:

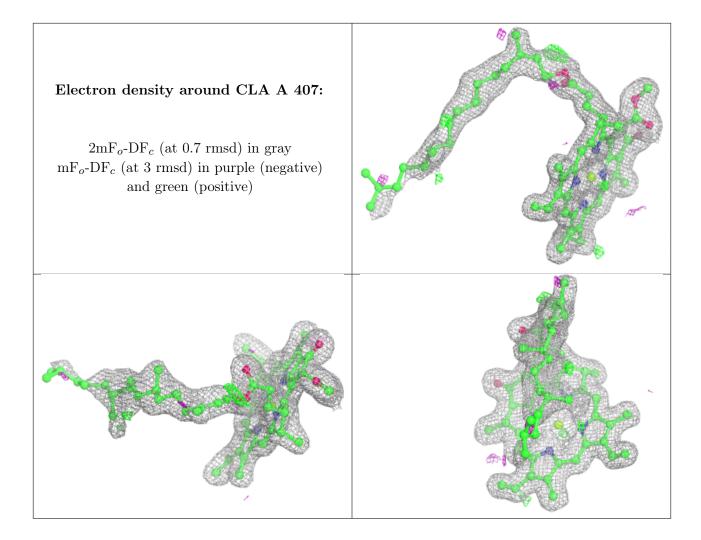
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







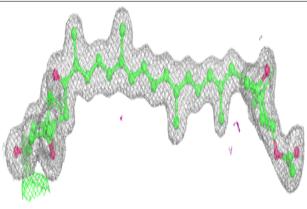


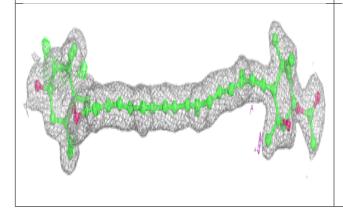


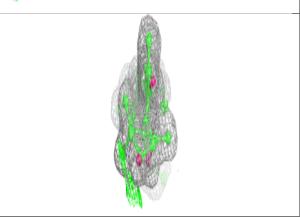


Electron density around A86 A 302:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

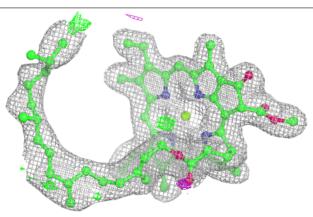


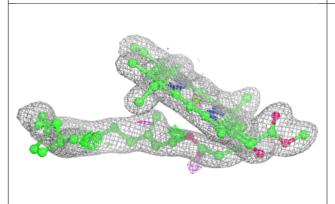


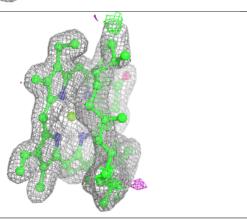


Electron density around CLA A 402:

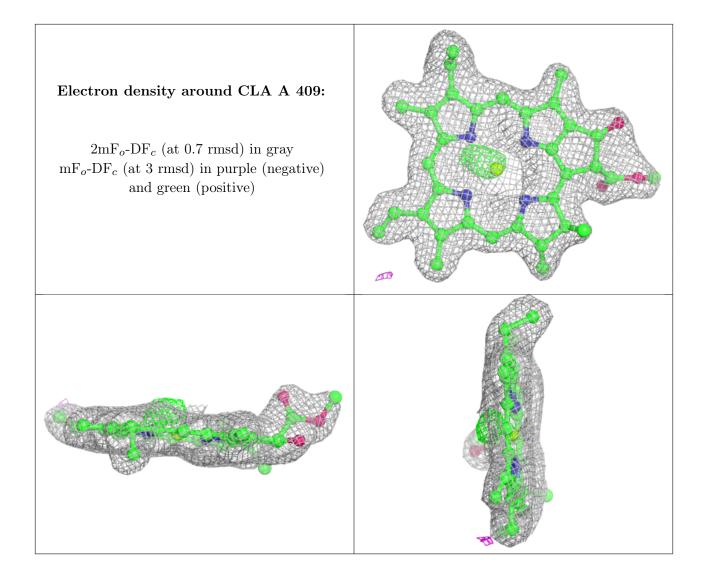
 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)







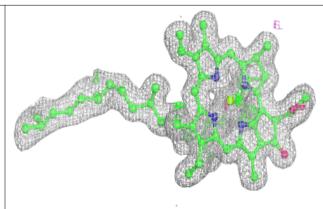


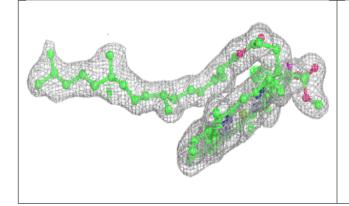


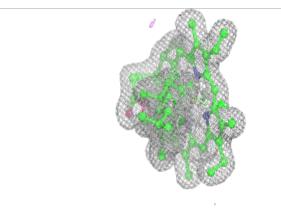


Electron density around CLA A 404:

 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

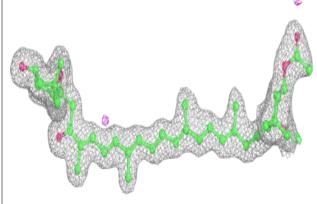


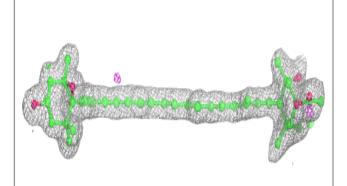


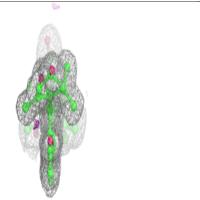


Electron density around A86 A 303:

 $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



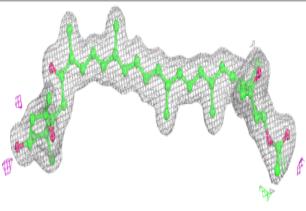


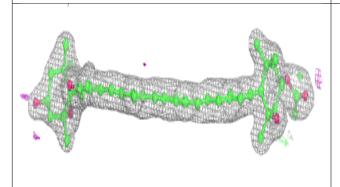


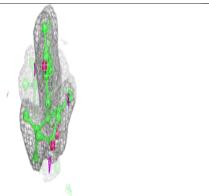


Electron density around A86 A 307:

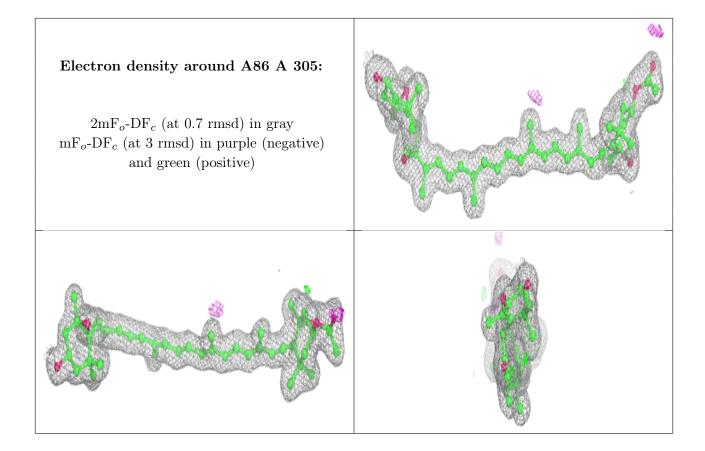
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



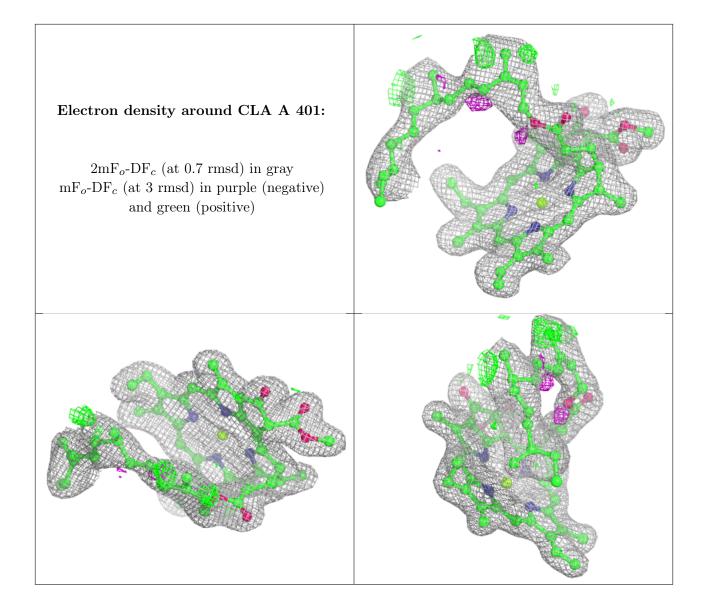




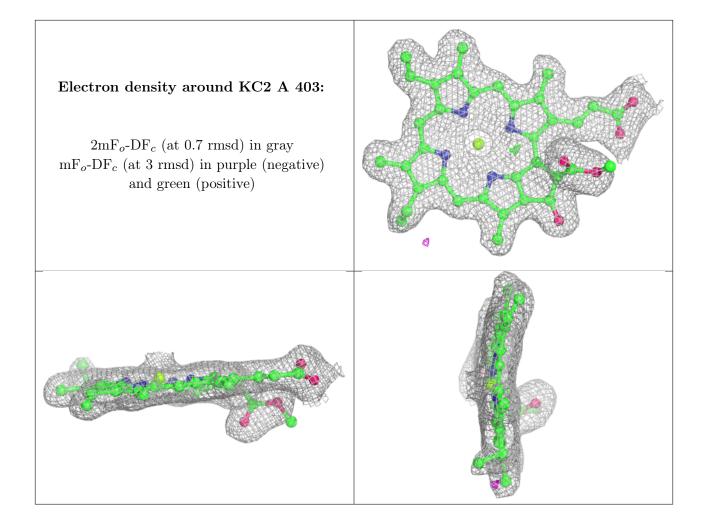




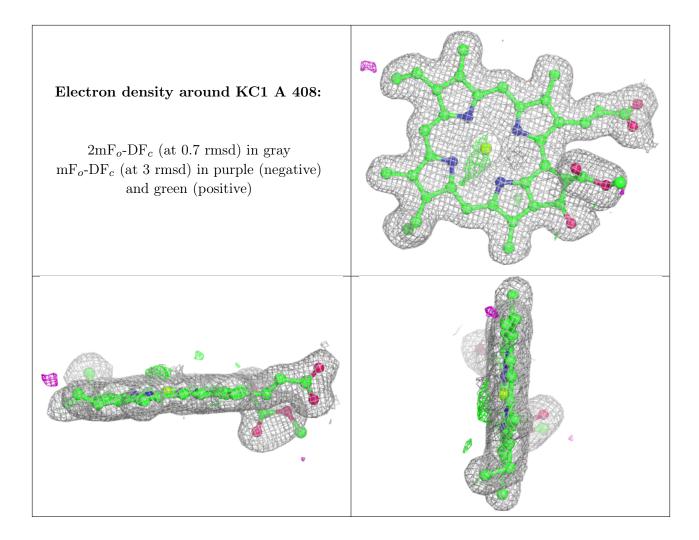












6.5 Other polymers (i)

There are no such residues in this entry.

