wwPDB X-ray Structure Validation Summary Report (i)

Aug 3, 2026 – 08:29 AM EDT

PDB ID	:	5WEH / pdb_00005weh
Title	:	Cytochrome c oxidase from Rhodobacter sphaeroides in the reduced state
Authors	:	Liu, J.; Ferguson-Miller, F.; Ling, Q.; Hiser, C.
Deposited on	:	2017-07-10
Resolution	:	3.45 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 (i)) were used in the production of this report:

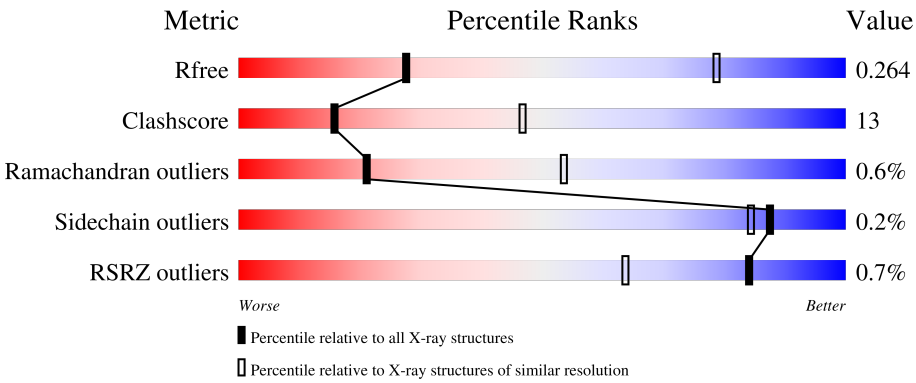
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

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	566	% 74% 22% • •
1	G	566	70% 27% •
2	B	262	% 80% 17% •
2	H	262	2% 66% 29% • •
3	C	266	2% 82% 17% •

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Mol	Chain	Length	Quality of chain
3	I	266	80% 19%
4	D	50	74% 6% 20%
4	J	50	80% 16%

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	HEA	A	601	-	X	-	-
5	HEA	A	602	-	-	X	-
5	HEA	G	602	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17909 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4254	2848	666	710	30	0	0	0
1	G	547	4292	2873	677	711	31	0	0	0

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	254	1956	1275	320	355	6	0	0	0
2	H	253	1927	1265	316	340	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	HIS	-	expression tag	UNP Q03736
B	283	HIS	-	expression tag	UNP Q03736
B	284	HIS	-	expression tag	UNP Q03736
B	285	HIS	-	expression tag	UNP Q03736
B	286	HIS	-	expression tag	UNP Q03736
B	287	HIS	-	expression tag	UNP Q03736
H	282	HIS	-	expression tag	UNP Q03736
H	283	HIS	-	expression tag	UNP Q03736
H	284	HIS	-	expression tag	UNP Q03736
H	285	HIS	-	expression tag	UNP Q03736
H	286	HIS	-	expression tag	UNP Q03736
H	287	HIS	-	expression tag	UNP Q03736

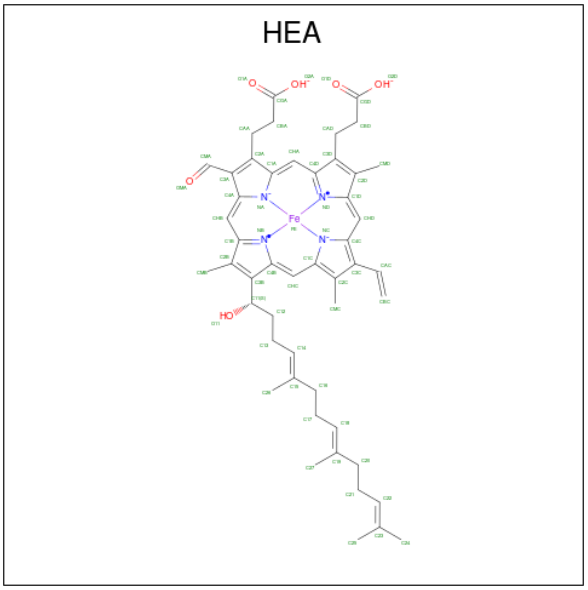
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	264	2064	1387	331	334	12	0	0	0
3	I	264	2095	1417	332	334	12	0	0	0

- Molecule 4 is a protein called Aa3-type cytochrome c oxidase subunit IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	40	276	183	43	49	1	0	0	0
4	J	42	299	195	49	53	2	0	0	0

- Molecule 5 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	60	49	1	4	6	0	0
5	A	1	60	49	1	4	6	0	0
5	G	1	60	49	1	4	6	0	0
5	G	1	60	49	1	4	6	0	0

- Molecule 6 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cu 1 1	0	0
6	G	1	Total Cu 1 1	0	0
6	B	2	Total Cu 2 2	0	0
6	H	2	Total Cu 2 2	0	0

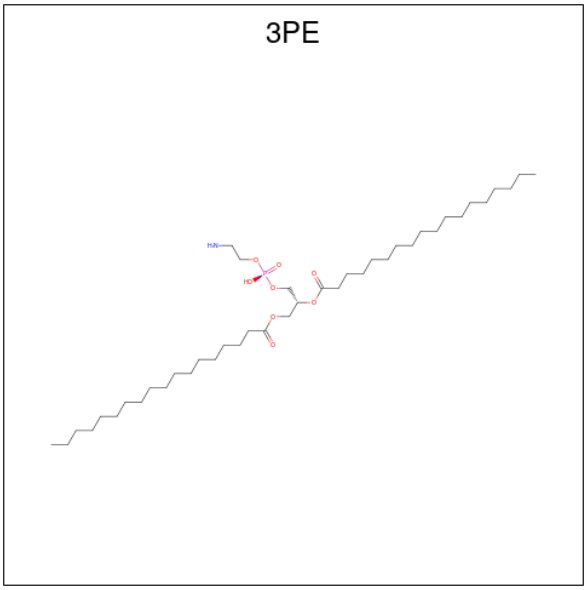
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	G	1	Total Mg 1 1	0	0

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

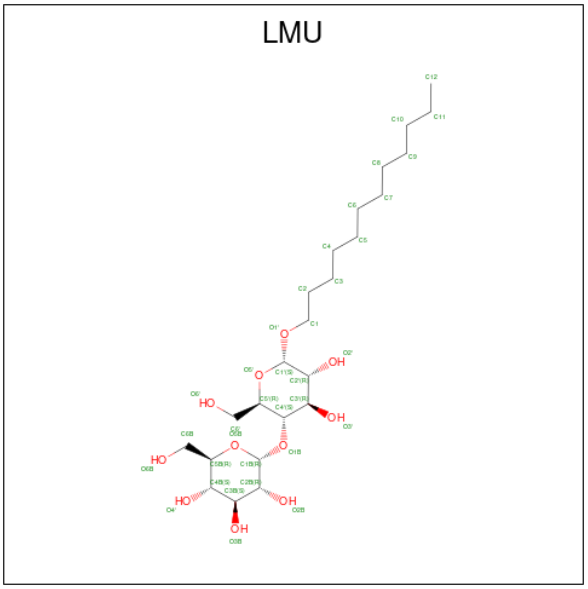
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	21	11	1	8	1	0	0
9	A	1	45	35	1	8	1	0	0
9	G	1	33	23	1	8	1	0	0
9	G	1	44	34	1	8	1	0	0
9	C	1	41	31	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	D	1	51	41	1	8	1	0	0
9	I	1	40	30	1	8	1	0	0
9	I	1	32	22	1	8	1	0	0
9	I	1	23	13	1	8	1	0	0
9	J	1	35	25	1	8	1	0	0

- Molecule 10 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	G	1	20	9	11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	G	1	24	13	11	0	0
			Total	C	O		
10	C	1	35	24	11	0	0

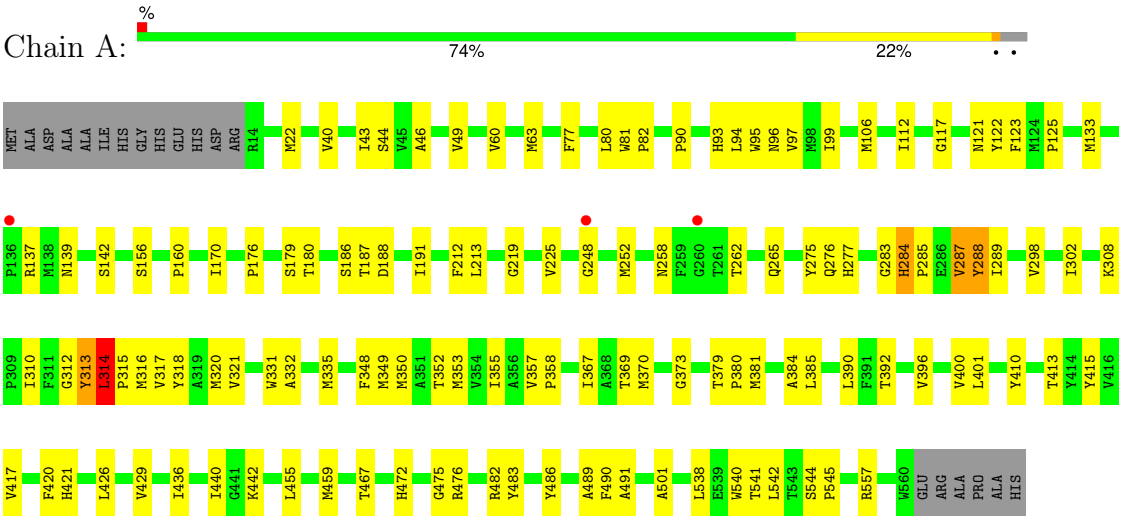
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	1	1	1	0	0

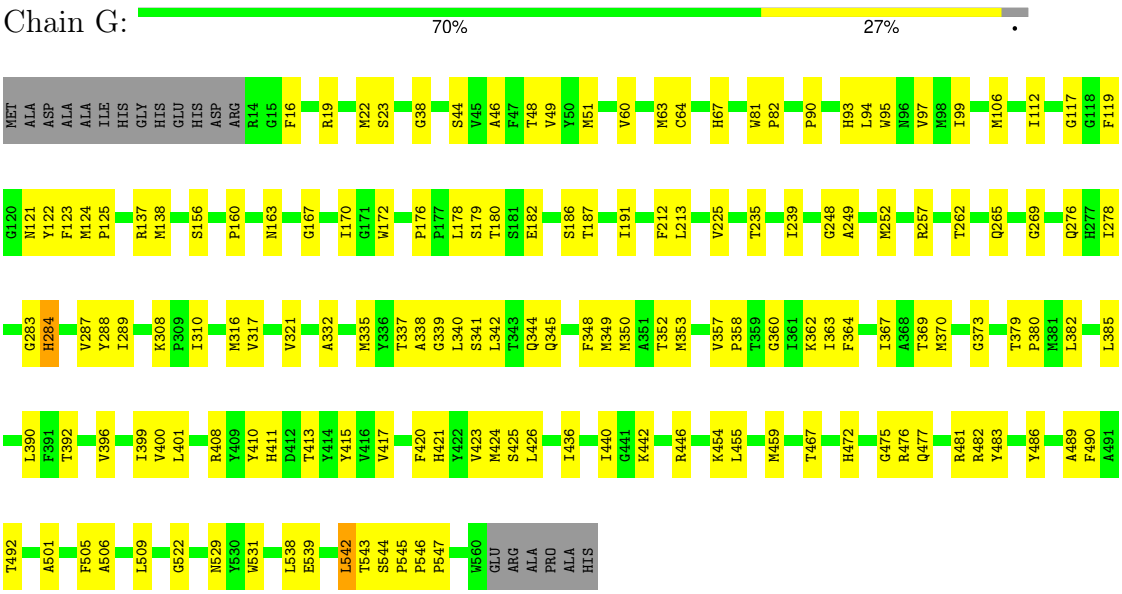
3 Residue-property plots (i)

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: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: %
80% 17% •

GLN GLN GLN SER L30 E31 I32 I33 G34 R35 P36 Q37 P38 G39 D58 I61 L62 I65 F83 P99 T105 P108 I109 P130 T139 G140 Y141 Q142 W143 Y147 S158 I161 G167 Q179 E182 Y185 L192 A193 T194 D195 T196 V199

V202 T211 H217 G233 W239 E245 G246 I247 Q251 L255 S259 H260 A261 K268 V269 H283 HIS HIS HIS HIS

• Molecule 2: Cytochrome c oxidase subunit 2

Chain H: 2%
66% 29% • •

GLN GLN GLN SER L30 E31 I32 I33 G34 R35 P36 Q37 P38 G39 Q44 P45 S48 P49 V50 A51 T52 Q53 D58 I61 L62 I65 I68 V72 F83 H84 E85 K86 P99 L100 E101 W104 T105 I106 V107 P108 I109 F124 Q127 P130 E131 A132

T135 V136 T139 G140 Y141 Q142 W143 Y144 W145 G146 Y147 P150 D151 E152 E153 F156 I161 Q178 I181 Y185 L192 A193 T194 D195 T196 A197 M198 V199 V200 P201 V202 T205 V206 D214 V215 I216 H217 S218 W219 K227 V231 R234 L235 W239 E245

G246 I247 F248 Q251 C252 S253 I258 S259 H260 A261 T266 V267 K268 V269 H282 HIS HIS HIS HIS HIS

• Molecule 3: Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3)

Chain C: 2%
82% 17% •

MET ALA H3 D8 Y9 H10 I11 L12 P13 P14 S15 I16 W17 A21 W35 G40 P41 T54 L67 T72 P73 V74 V75 R76 L77 G78 L79 R80 W81 I84 L85 M88 V91 H104 P108 S113 F120 P130 L133 P134 L135 I136 L155

R162 D163 V164 L168 Y184 F193 I197 G207 F211 V215 V222 C223 L224 R229 G230 H231 K236 G239 H248 V252 I263 Q266

• Molecule 3: Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3)

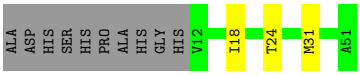
Chain I:
80% 19% •

MET ALA H3 D8 L12 I16 W17 A21 I46 V50 T54 W59 T64 E68 T72 P73 V74 V75 R76 L77 G78 L79 R80 W81 I84 L85 M88 W99 P108 S113 P114 I115 I116 F120 P121 P122 F128 D129 P130 H152

N160 R161 R162 D163 L168 A189 I197 F211 I214 V215 I218 L224 Q228 R229 G230 K236 I244 W245 H248 V252 I263 W264 G265 Q266

• Molecule 4: Aa3-type cytochrome c oxidase subunit IV

Chain D:
74% 6% 20%



• Molecule 4: Aa3-type cytochrome c oxidase subunit IV

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	339.22Å 339.22Å 89.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.45 – 3.45 28.45 – 3.45	Depositor EDS
% Data completeness (in resolution range)	92.1 (28.45-3.45) 92.1 (28.45-3.45)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.73 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.223 , 0.262 0.224 , 0.264	Depositor DCC
R_{free} test set	1442 reflections (2.79%)	wwPDB-VP
Wilson B-factor (Å^2)	105.8	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.000 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17909	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, LMU, CA, MG, HEA, 3PE

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	0.26	2/4413 (0.0%)	0.56	9/6035 (0.1%)
1	G	0.24	3/4452 (0.1%)	0.53	5/6079 (0.1%)
2	B	0.19	0/2015	0.50	0/2765
2	H	0.30	0/1985	0.58	0/2726
3	C	0.17	0/2149	0.43	0/2943
3	I	0.19	0/2184	0.43	0/2991
4	D	0.17	0/280	0.47	0/384
4	J	0.17	0/303	0.45	0/411
All	All	0.23	5/17781 (0.0%)	0.51	14/24334 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	283	GLY	C-N	-7.07	1.22	1.34
1	G	284	HIS	C-N	5.57	1.46	1.33
1	A	287	VAL	C-N	5.46	1.42	1.33
1	A	288	TYR	C-N	5.33	1.40	1.34
1	G	288	TYR	C-N	5.22	1.40	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	288	TYR	CA-C-N	9.18	134.97	120.47
1	G	288	TYR	C-N-CA	9.18	134.97	120.47
1	A	283	GLY	O-C-N	-8.37	114.16	122.19
1	A	284	HIS	CA-C-N	-8.31	109.45	119.84
1	A	284	HIS	C-N-CA	-8.31	109.45	119.84

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	4254	0	4102	105	0
1	G	4292	0	4174	133	0
2	B	1956	0	1868	32	0
2	H	1927	0	1867	82	0
3	C	2064	0	1935	39	0
3	I	2095	0	1989	43	0
4	D	276	0	270	3	0
4	J	299	0	299	3	0
5	A	120	0	108	44	0
5	G	120	0	108	44	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	G	1	0	0	0	0
6	H	2	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	1	0	0	0	0
8	G	1	0	0	0	0
9	A	66	0	83	6	0
9	C	92	0	141	10	0
9	D	51	0	82	1	0
9	G	77	0	105	3	0
9	I	95	0	112	3	0
9	J	35	0	47	1	0
10	C	35	0	46	2	0
10	G	44	0	28	15	0
11	A	1	0	0	0	0
All	All	17909	0	17364	469	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 469 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)
5:A:602:HEA:CHA	5:A:602:HEA:C1A	1.75	1.63
5:G:602:HEA:C4B	5:G:602:HEA:CHC	1.80	1.59
5:G:603:HEA:CHC	5:G:603:HEA:C4B	1.80	1.59
5:G:603:HEA:CHD	5:G:603:HEA:C1D	1.81	1.59
5:A:601:HEA:CHC	5:A:601:HEA:C4B	1.79	1.58

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	545/566 (96%)	502 (92%)	40 (7%)	3 (1%)	21	53
1	G	545/566 (96%)	504 (92%)	39 (7%)	2 (0%)	30	62
2	B	252/262 (96%)	227 (90%)	23 (9%)	2 (1%)	16	49
2	H	251/262 (96%)	220 (88%)	26 (10%)	5 (2%)	6	32
3	C	262/266 (98%)	247 (94%)	15 (6%)	0	100	100
3	I	262/266 (98%)	246 (94%)	15 (6%)	1 (0%)	30	62
4	D	38/50 (76%)	37 (97%)	1 (3%)	0	100	100
4	J	40/50 (80%)	39 (98%)	1 (2%)	0	100	100
All	All	2195/2288 (96%)	2022 (92%)	160 (7%)	13 (1%)	21	53

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	45	PRO
2	H	153	GLU
1	G	16	PHE
2	H	51	ALA
1	A	313	TYR

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	431/459 (94%)	430 (100%)	1 (0%)	87	84
1	G	439/459 (96%)	438 (100%)	1 (0%)	87	84
2	B	199/221 (90%)	199 (100%)	0	100	100
2	H	195/221 (88%)	194 (100%)	1 (0%)	81	81
3	C	200/216 (93%)	200 (100%)	0	100	100
3	I	207/216 (96%)	207 (100%)	0	100	100
4	D	24/36 (67%)	24 (100%)	0	100	100
4	J	27/36 (75%)	27 (100%)	0	100	100
All	All	1722/1864 (92%)	1719 (100%)	3 (0%)	87	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	LEU
1	G	542	LEU
2	H	151	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	251	GLN
3	I	182	GLN
3	I	157	HIS
2	B	237	GLN
2	H	53	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 10 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	LMU	C	303	-	36,36,36	1.23	3 (8%)	47,47,47	1.50	5 (10%)
10	LMU	G	609	-	25,25,36	1.26	2 (8%)	36,36,47	0.99	2 (5%)
9	3PE	A	607	-	44,44,50	0.93	4 (9%)	47,49,55	1.11	3 (6%)
9	3PE	I	302	-	31,31,50	1.10	4 (12%)	34,36,55	1.10	2 (5%)
9	3PE	J	101	-	34,34,50	1.00	3 (8%)	37,39,55	1.03	1 (2%)
10	LMU	G	601	-	13,13,36	0.65	0	10,10,47	0.59	0
9	3PE	C	302	-	50,50,50	0.89	4 (8%)	53,55,55	1.08	2 (3%)
5	HEA	G	603	1	67,67,67	7.25	32 (47%)	81,103,103	5.15	49 (60%)
5	HEA	G	602	1	67,67,67	7.17	32 (47%)	81,103,103	5.13	50 (61%)
9	3PE	G	608	-	43,43,50	0.95	4 (9%)	46,48,55	1.09	2 (4%)
5	HEA	A	601	1	67,67,67	7.01	32 (47%)	81,103,103	5.23	57 (70%)
9	3PE	G	607	-	32,32,50	1.08	4 (12%)	35,37,55	1.12	2 (5%)
9	3PE	I	303	-	22,22,50	1.29	4 (18%)	25,27,55	1.06	2 (8%)
9	3PE	D	101	-	50,50,50	0.91	3 (6%)	53,55,55	1.07	2 (3%)
9	3PE	C	301	-	40,40,50	1.02	3 (7%)	43,45,55	1.11	2 (4%)
9	3PE	A	606	-	20,20,50	1.34	4 (20%)	23,25,55	1.06	2 (8%)
9	3PE	I	301	-	39,39,50	1.02	4 (10%)	42,44,55	1.12	2 (4%)
5	HEA	A	602	1	67,67,67	7.21	32 (47%)	81,103,103	4.96	48 (59%)

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
10	LMU	C	303	-	-	12/21/61/61	0/2/2/2
10	LMU	G	609	-	-	5/10/50/61	0/2/2/2
9	3PE	A	607	-	-	26/48/48/54	-
9	3PE	I	302	-	-	15/35/35/54	-
9	3PE	J	101	-	-	19/37/37/54	-
10	LMU	G	601	-	-	4/8/8/61	-
9	3PE	C	302	-	-	29/54/54/54	-
5	HEA	G	603	1	-	12/36/76/76	-
5	HEA	G	602	1	-	11/36/76/76	-
9	3PE	G	608	-	-	25/47/47/54	-
5	HEA	A	601	1	-	17/36/76/76	-
9	3PE	G	607	-	-	9/36/36/54	-
9	3PE	I	303	-	-	17/26/26/54	-
9	3PE	D	101	-	-	31/54/54/54	-
9	3PE	C	301	-	-	16/44/44/54	-
9	3PE	A	606	-	-	11/24/24/54	-
9	3PE	I	301	-	-	22/43/43/54	-
5	HEA	A	602	1	-	17/36/76/76	-

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEA	CHC-C1C	22.92	1.90	1.39
5	G	602	HEA	CHD-C1D	22.87	1.84	1.38
5	A	601	HEA	CHD-C1D	22.52	1.83	1.38
5	G	603	HEA	CHC-C1C	21.95	1.88	1.39
5	G	602	HEA	CHD-C4C	21.53	1.87	1.39

The worst 5 of 233 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	601	HEA	CHB-C4A-C3A	-14.37	100.98	125.21
5	G	602	HEA	CHB-C4A-C3A	-13.71	102.09	125.21
5	G	603	HEA	CHA-C4D-C3D	-13.04	105.75	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	602	HEA	C3C-C4C-NC	13.02	120.76	109.80
5	G	603	HEA	C1D-ND-C4D	-12.75	90.11	105.21

There are no chirality outliers.

5 of 298 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEA	C2A-C3A-CMA-OMA
5	A	601	HEA	C4A-C3A-CMA-OMA
5	A	601	HEA	C2C-C3C-CAC-CBC
5	A	601	HEA	C4C-C3C-CAC-CBC
5	A	601	HEA	C11-C12-C13-C14

There are no ring outliers.

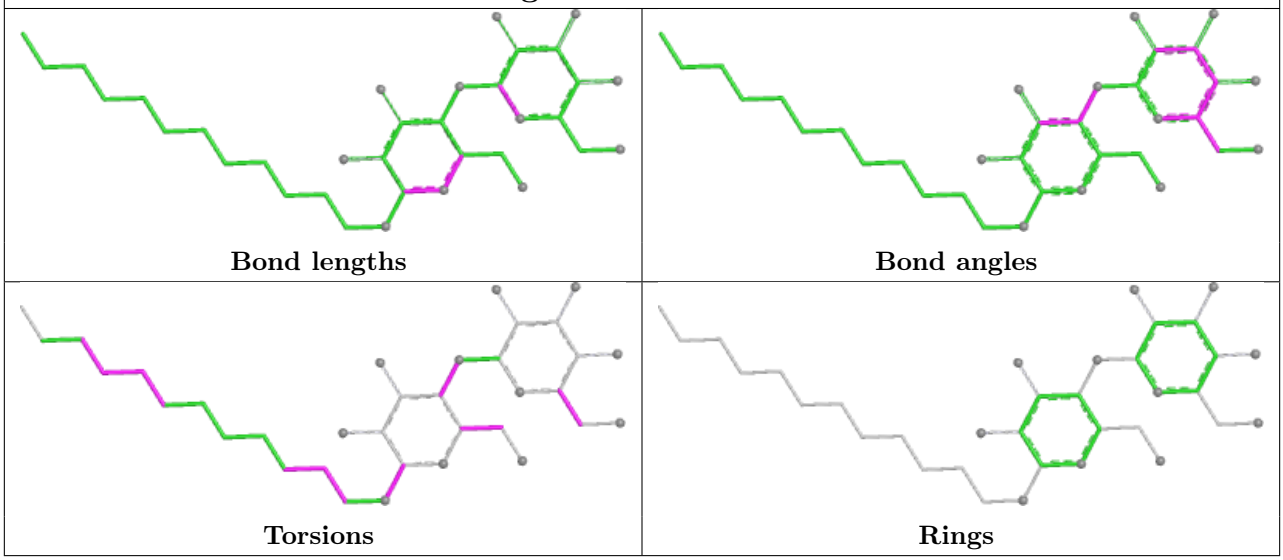
16 monomers are involved in 126 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	303	LMU	2	0
9	A	607	3PE	4	0
9	J	101	3PE	1	0
10	G	601	LMU	15	0
9	C	302	3PE	6	0
5	G	603	HEA	19	0
5	G	602	HEA	25	0
9	G	608	3PE	2	0
5	A	601	HEA	19	0
9	G	607	3PE	1	0
9	I	303	3PE	1	0
9	D	101	3PE	1	0
9	C	301	3PE	4	0
9	A	606	3PE	2	0
9	I	301	3PE	2	0
5	A	602	HEA	25	0

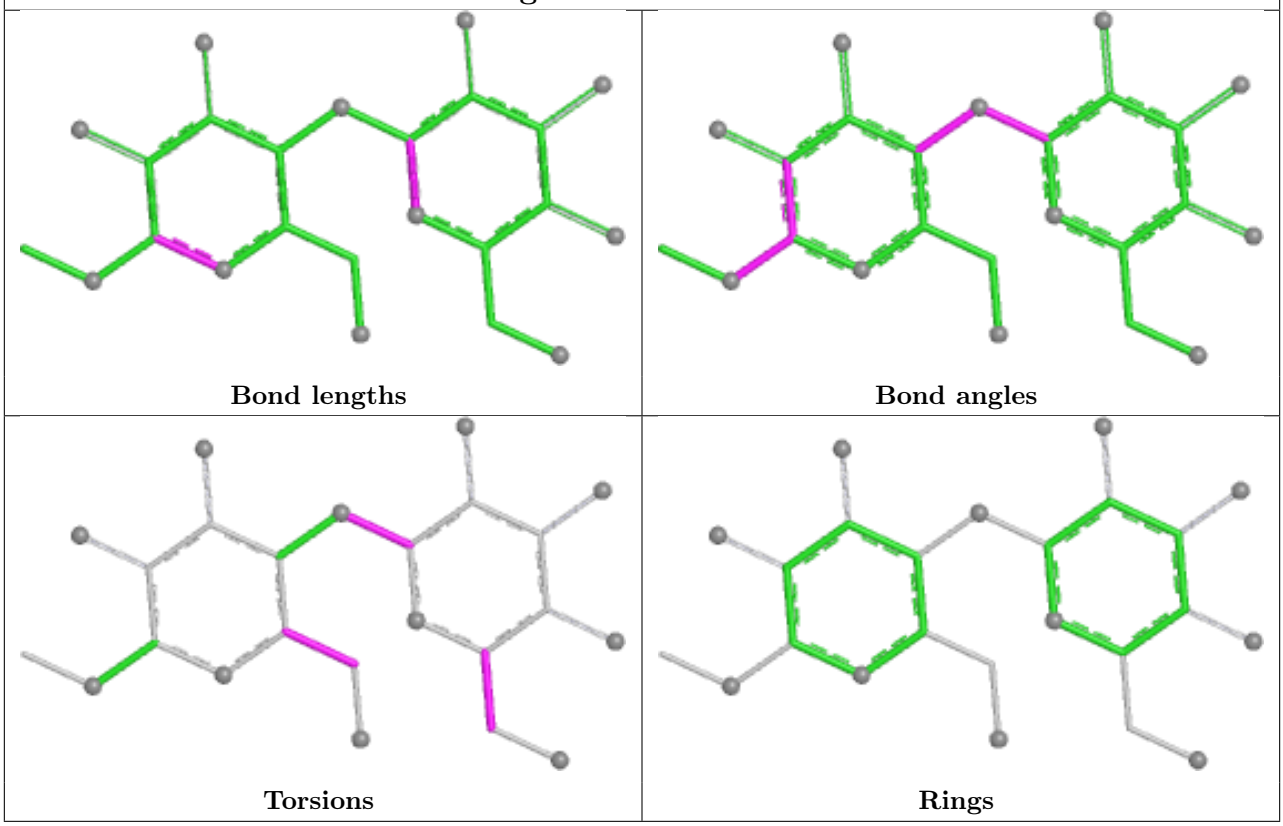
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

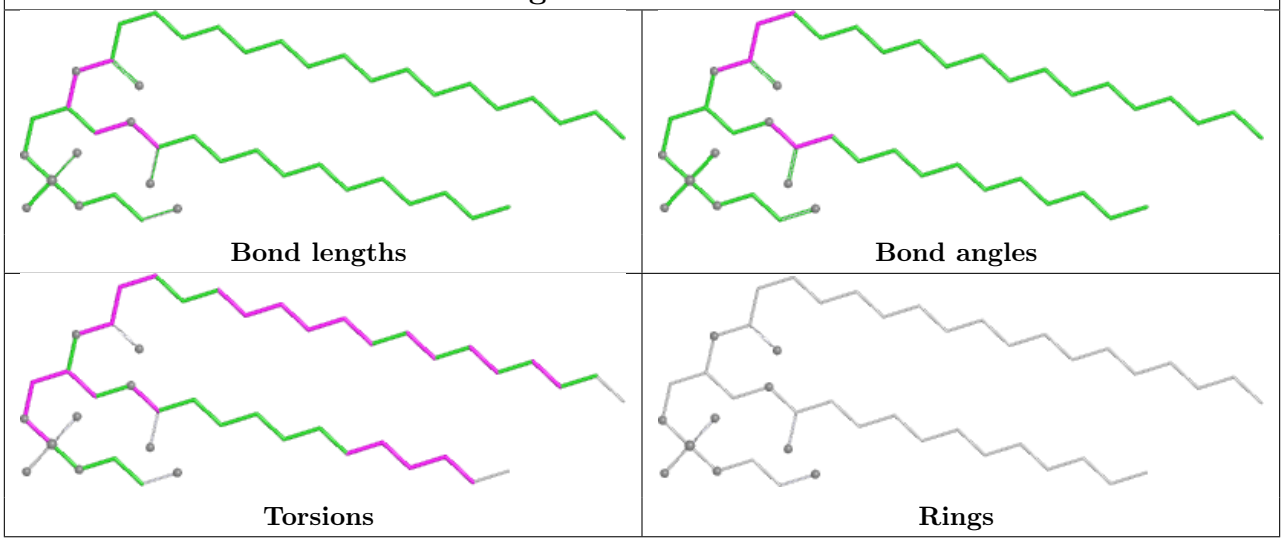
Ligand LMU C 303



Ligand LMU G 609



Ligand 3PE A 607



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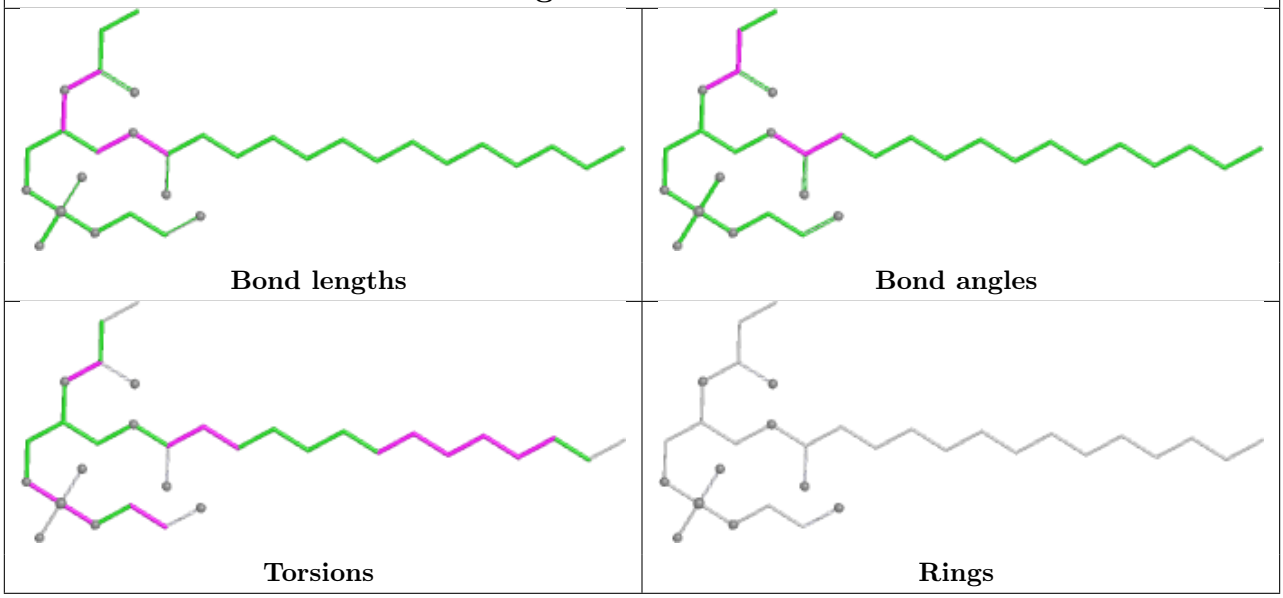

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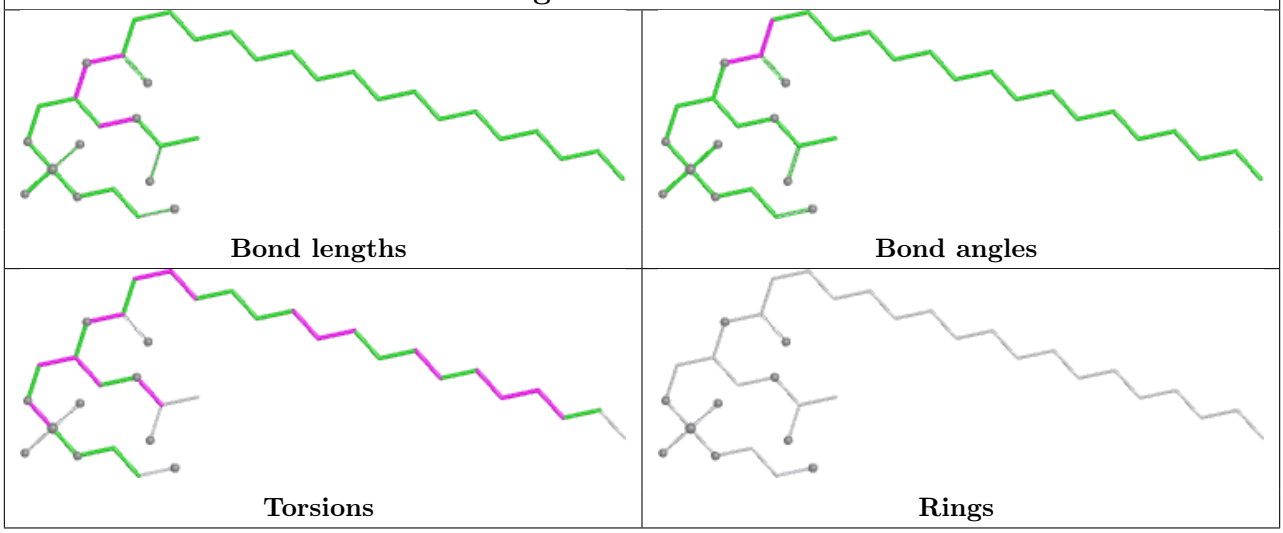

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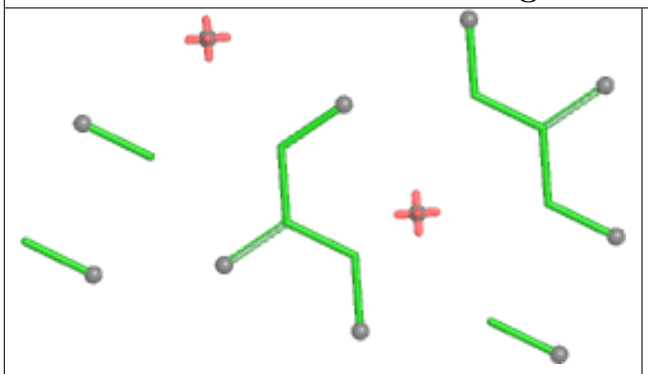
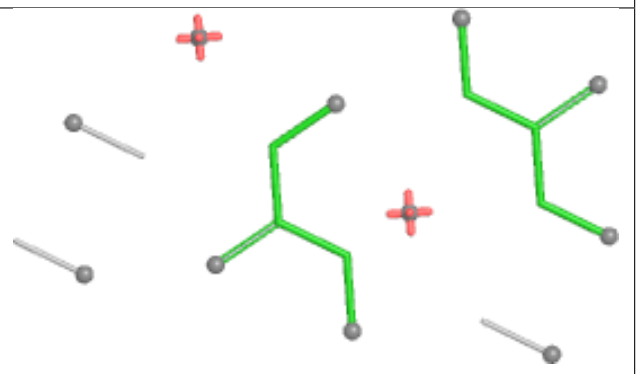
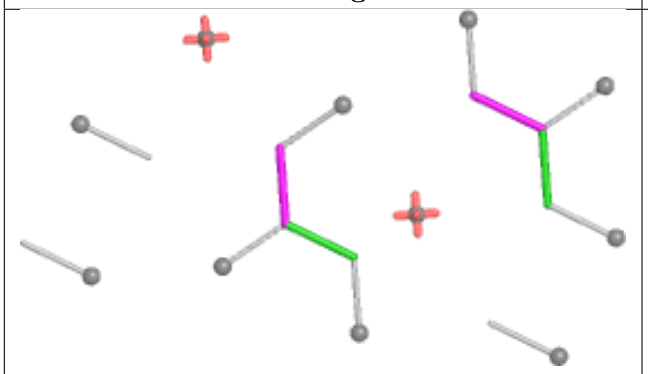


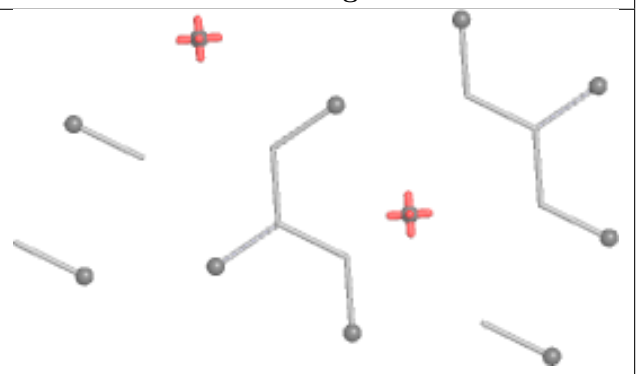
Bond lengths



Bond angles

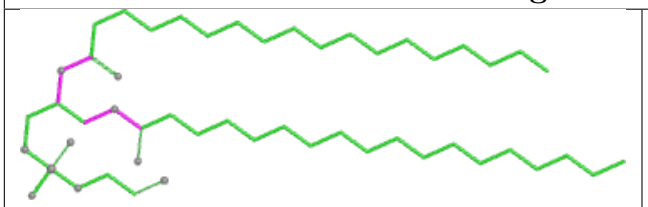


Torsions



Rings

Ligand 3PE C 302



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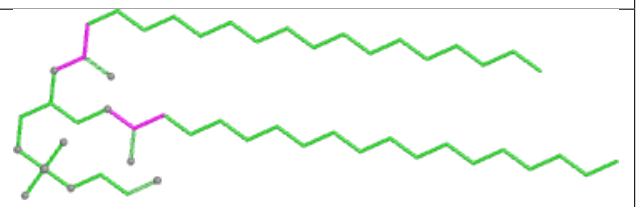

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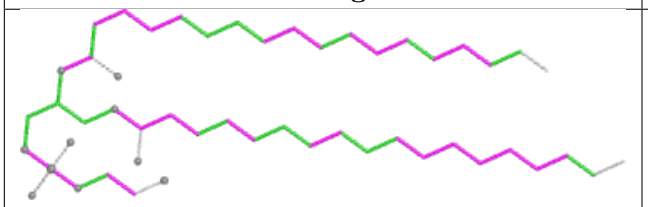

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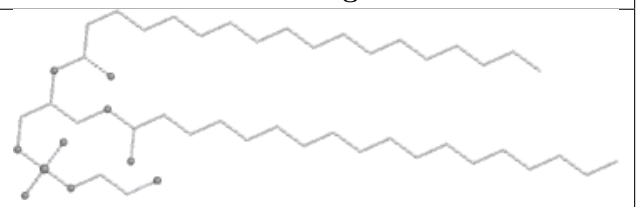
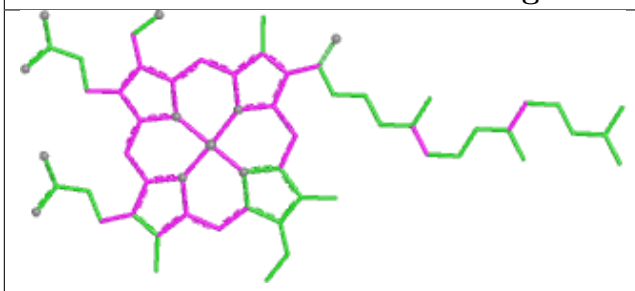
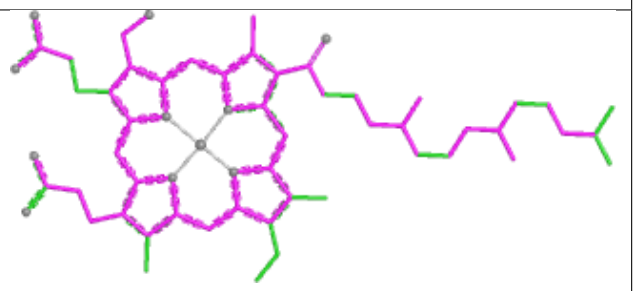
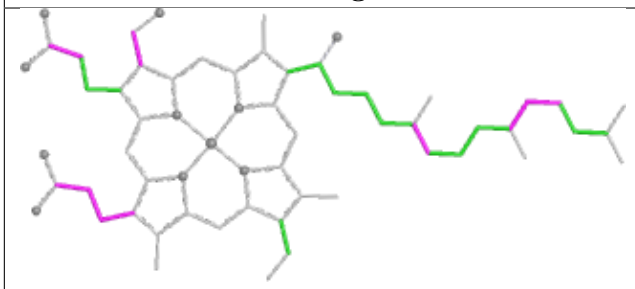
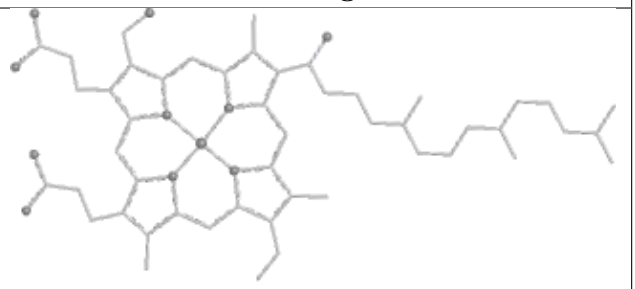
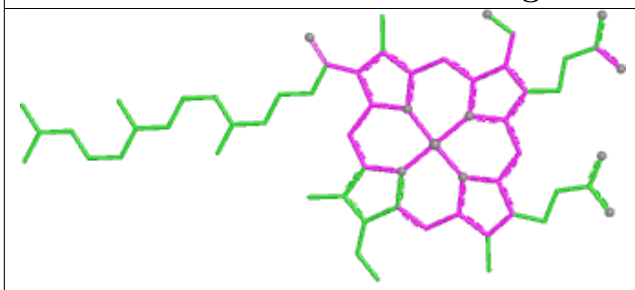
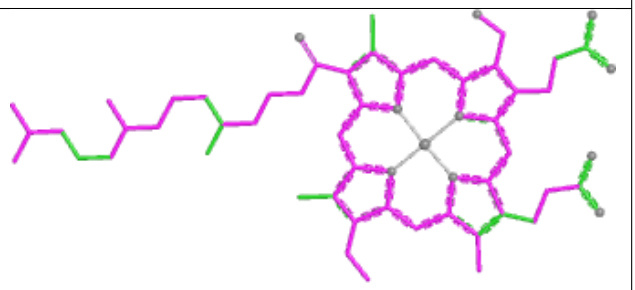
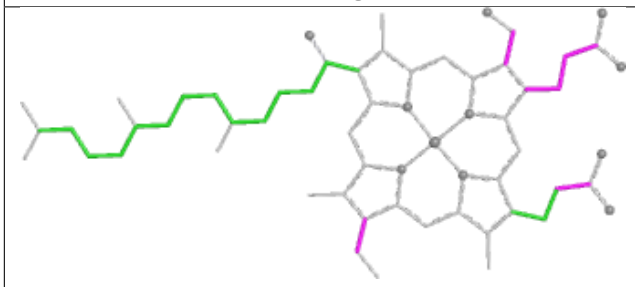
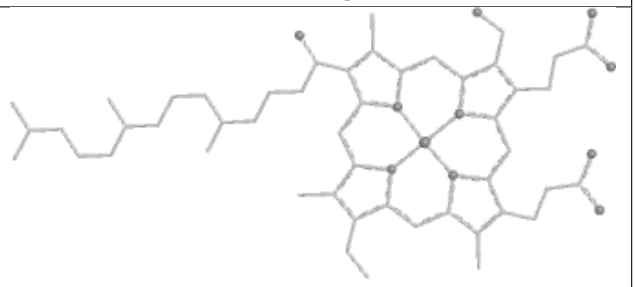
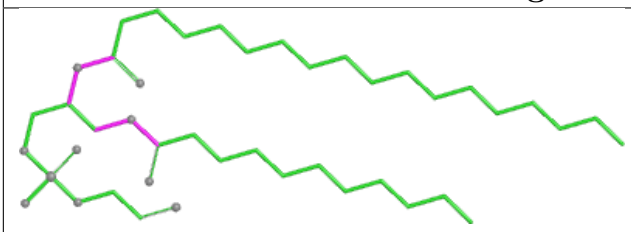


Rings

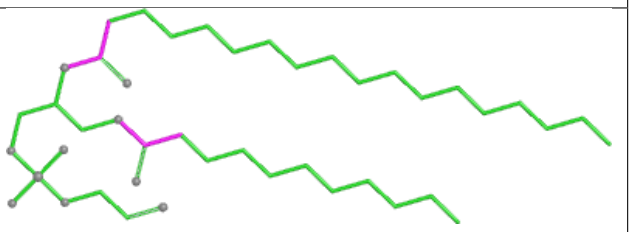
Ligand HEA G 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA G 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

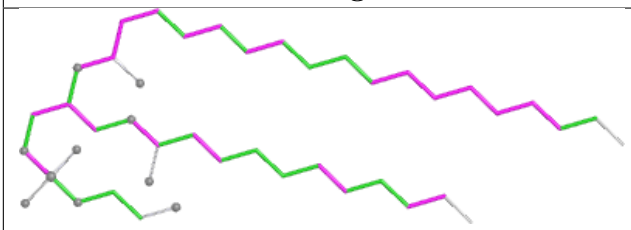
Ligand 3PE G 608



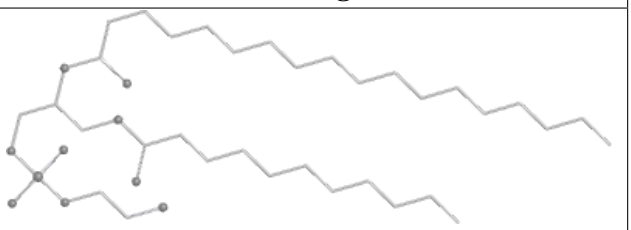
Bond lengths



Bond angles

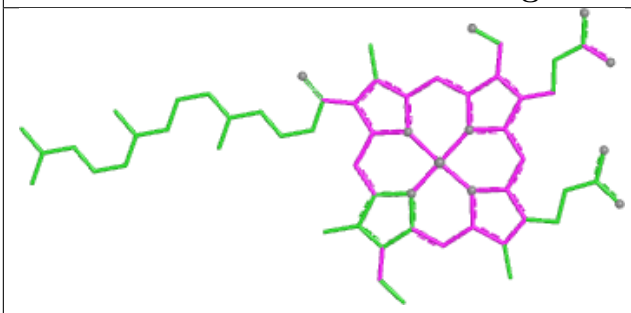


Torsions



Rings

Ligand HEA A 601



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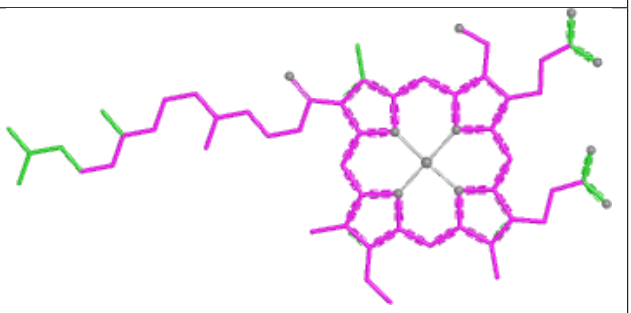
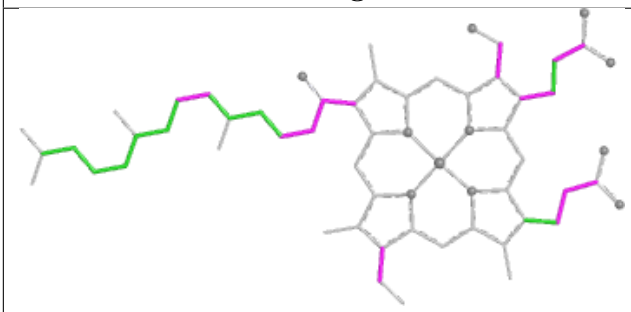


Bond angles



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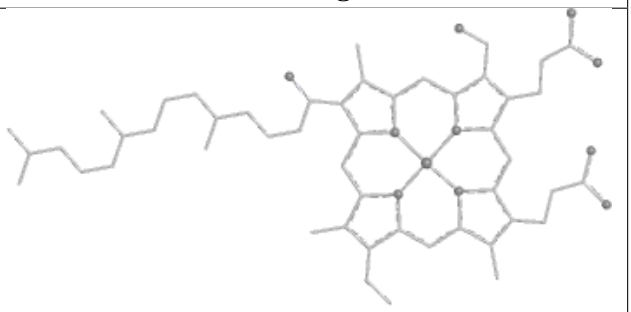

Rings

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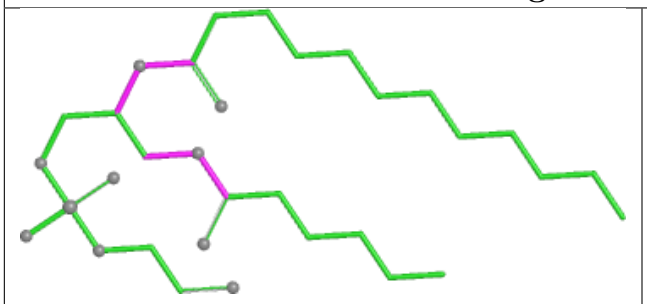

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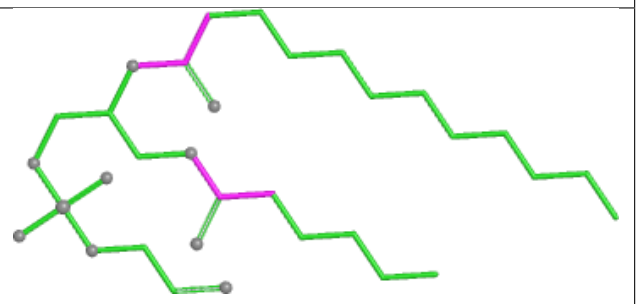
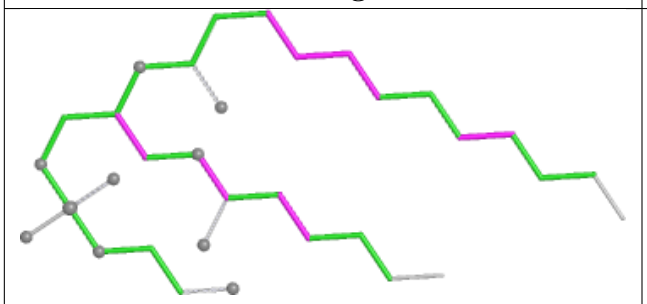


Bond angles



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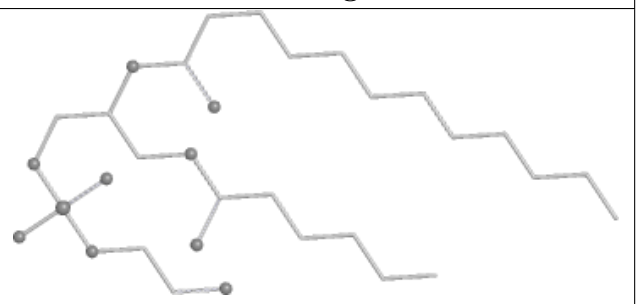
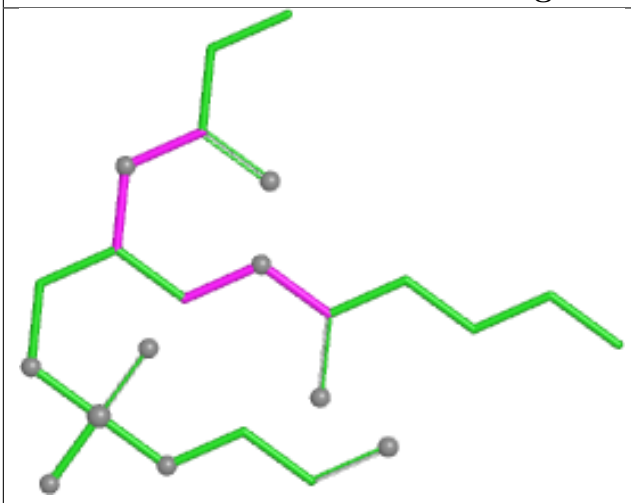


Rings

Ligand 3PE I 303



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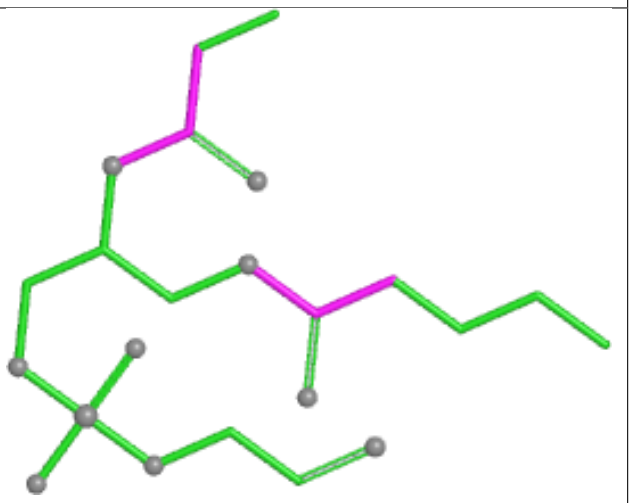
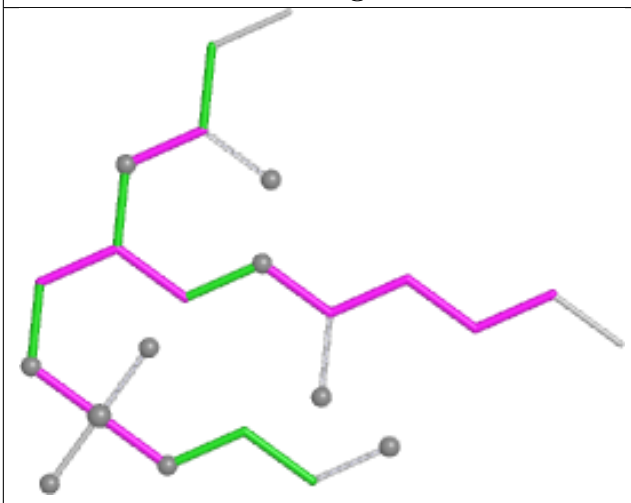
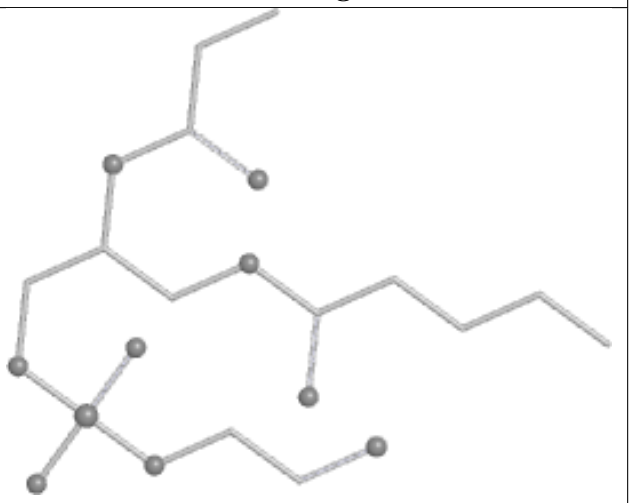


Bond angles

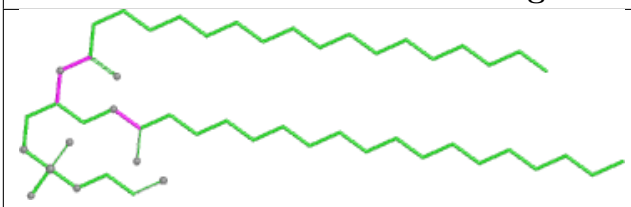


Torsions



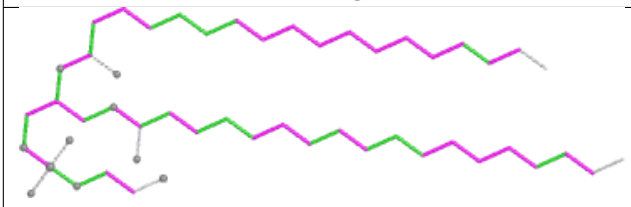
Rings

Ligand 3PE D 101



Bond lengths

Bond angles

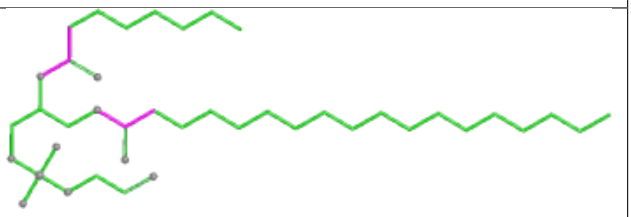


Torsions

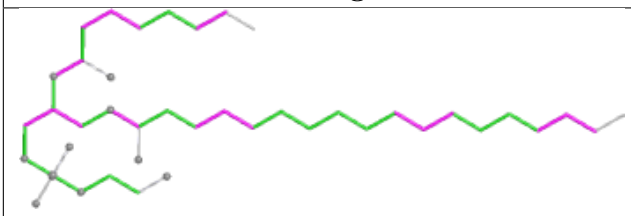
Rings

Ligand 3PE C 301

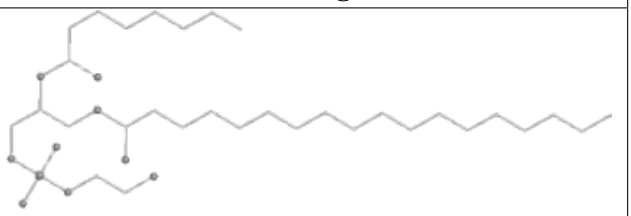
Bond lengths



Bond angles

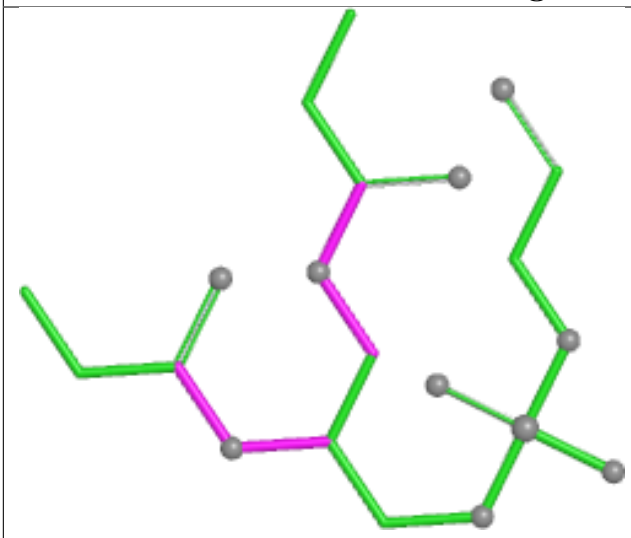


Torsions

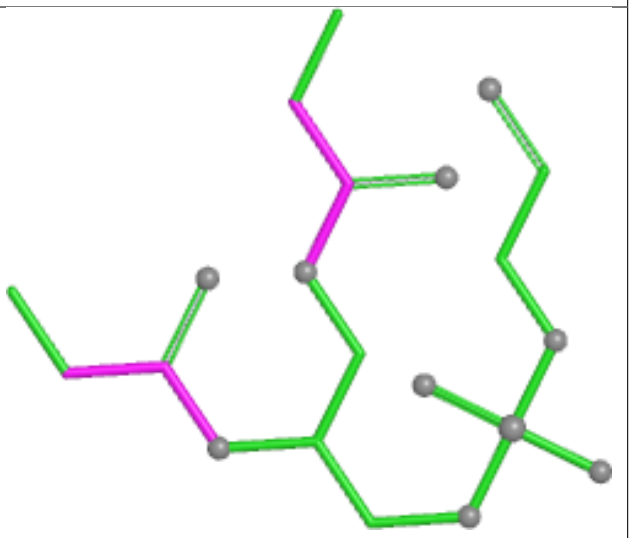


Rings

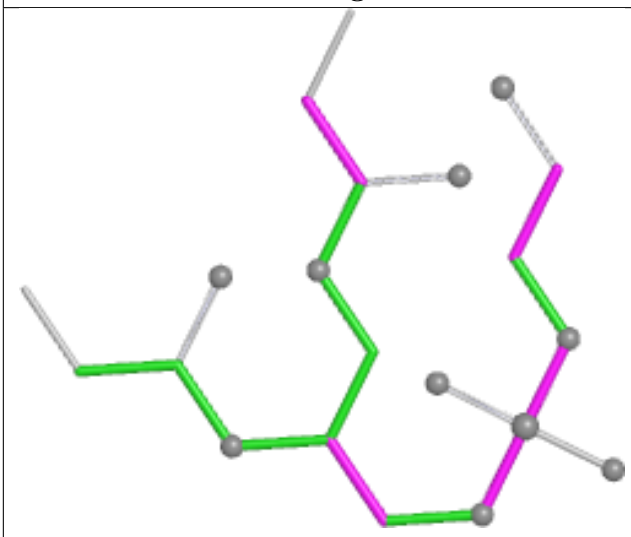
Ligand 3PE A 606



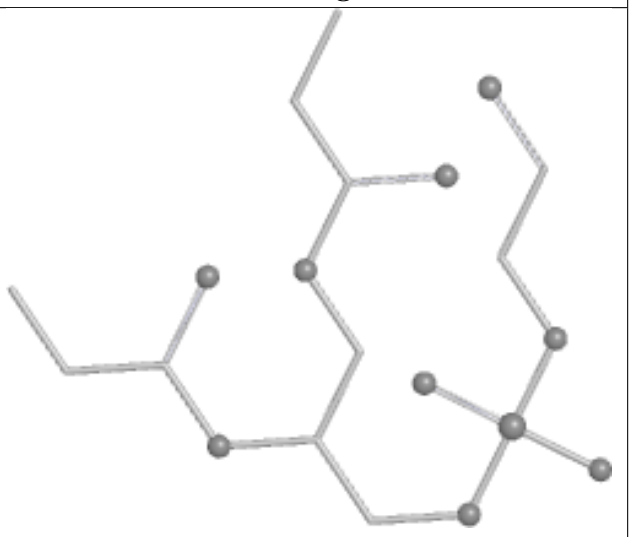
Bond lengths



Bond angles

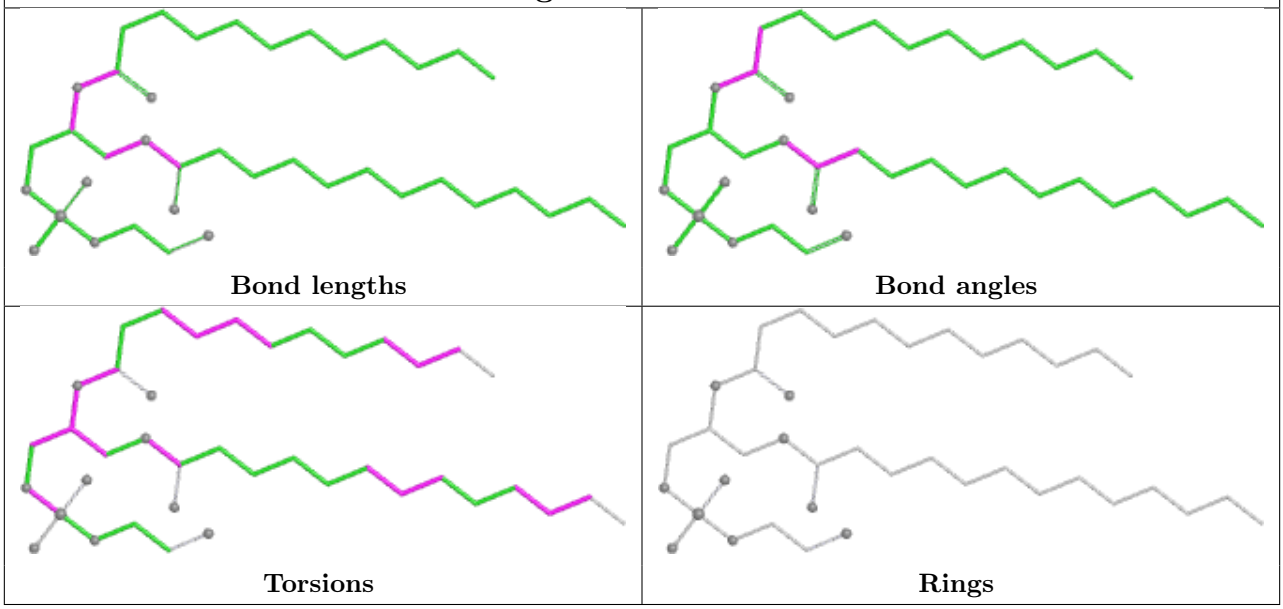


Torsions

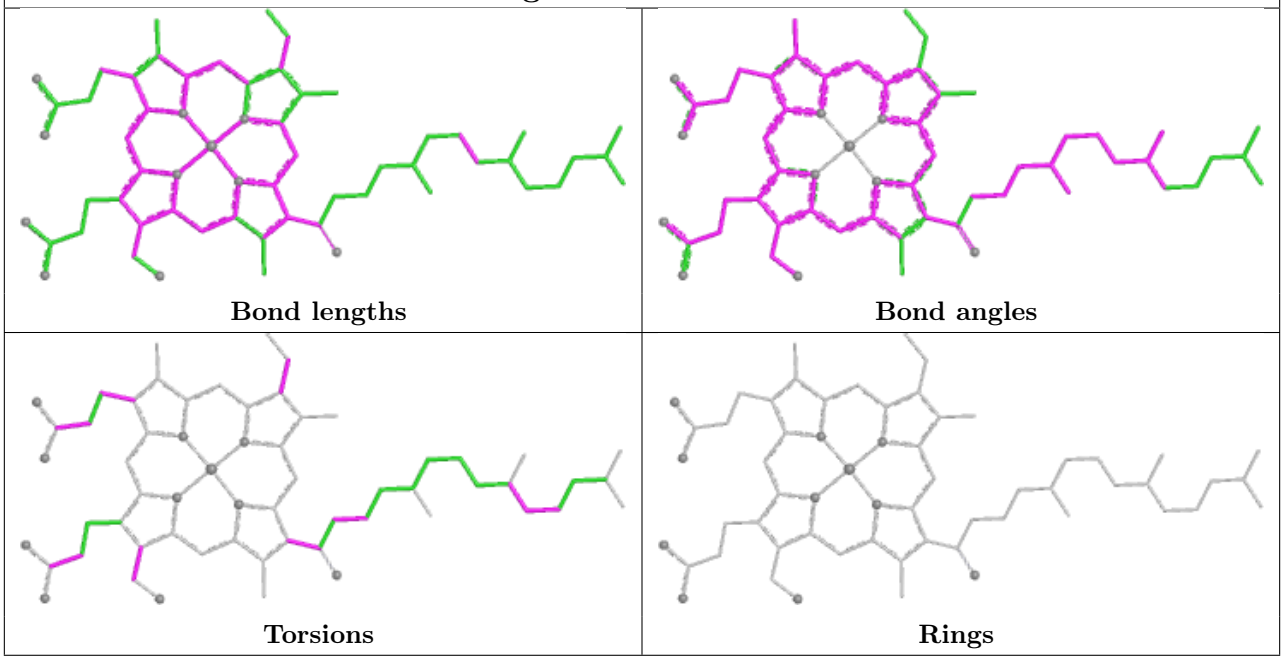


Rings

Ligand 3PE I 301



Ligand HEA A 602



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	547/566 (96%)	0.03	3 (0%)	87	70	76, 103, 142, 188	0
1	G	547/566 (96%)	-0.08	0	100	100	75, 103, 136, 180	0
2	B	254/262 (96%)	0.26	2 (0%)	82	61	83, 118, 152, 165	0
2	H	253/262 (96%)	0.20	4 (1%)	70	46	95, 135, 168, 178	0
3	C	264/266 (99%)	0.33	6 (2%)	61	38	92, 135, 168, 185	0
3	I	264/266 (99%)	-0.16	1 (0%)	88	73	79, 115, 151, 179	0
4	D	40/50 (80%)	-0.07	0	100	100	90, 120, 148, 160	0
4	J	42/50 (84%)	-0.02	0	100	100	88, 114, 143, 166	0
All	All	2211/2288 (96%)	0.06	16 (0%)	84	64	75, 113, 157, 188	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	113	SER	2.9
3	C	10	HIS	2.8
3	C	164	VAL	2.6
3	C	14	PRO	2.5
1	A	260	GLY	2.5

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)

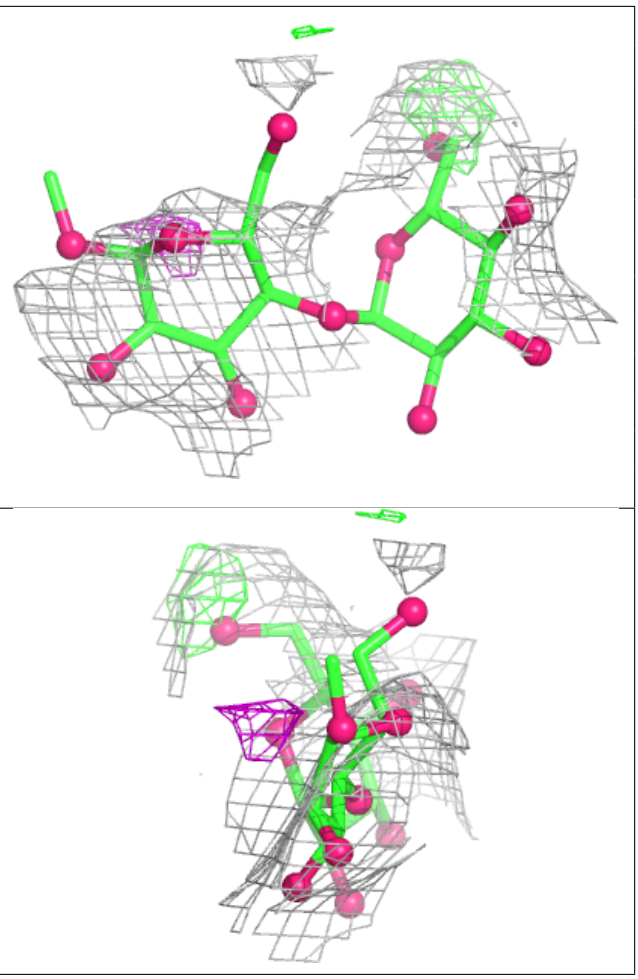
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	LMU	G	609	24/35	0.67	0.13	131,164,170,176	0
9	3PE	I	303	23/51	0.68	0.16	101,155,183,196	0
10	LMU	G	601	20/35	0.69	0.12	84,115,124,143	5
10	LMU	C	303	35/35	0.74	0.13	108,150,203,214	0
9	3PE	I	302	32/51	0.75	0.16	86,124,183,198	0
9	3PE	C	301	41/51	0.79	0.17	100,157,200,216	0
9	3PE	A	606	21/51	0.81	0.17	97,112,119,134	21
7	MG	A	604	1/1	0.84	0.13	95,95,95,95	0
9	3PE	J	101	35/51	0.88	0.13	97,123,164,172	0
9	3PE	G	608	44/51	0.89	0.15	78,110,175,179	0
9	3PE	A	607	45/51	0.89	0.16	65,93,109,138	45
9	3PE	C	302	51/51	0.89	0.15	92,111,150,185	0
7	MG	G	605	1/1	0.90	0.14	86,86,86,86	0
6	CU1	H	302	1/1	0.90	0.08	107,107,107,107	0
6	CU1	G	604	1/1	0.90	0.12	94,94,94,94	0
9	3PE	D	101	51/51	0.91	0.12	74,105,145,150	0
9	3PE	G	607	33/51	0.92	0.13	70,82,98,107	0
9	3PE	I	301	40/51	0.92	0.16	88,112,150,154	0
8	CA	A	605	1/1	0.93	0.09	102,102,102,102	0
8	CA	G	606	1/1	0.93	0.07	103,103,103,103	0
5	HEA	G	603	60/60	0.95	0.12	94,105,122,134	0
5	HEA	A	601	60/60	0.95	0.15	86,98,107,127	0
5	HEA	A	602	60/60	0.95	0.15	87,97,105,113	0
5	HEA	G	602	60/60	0.97	0.12	83,95,104,106	0
6	CU1	A	603	1/1	0.97	0.06	81,81,81,81	0
6	CU1	H	301	1/1	0.98	0.05	117,117,117,117	0
6	CU1	B	301	1/1	0.98	0.12	105,105,105,105	0
6	CU1	B	302	1/1	0.99	0.07	102,102,102,102	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.

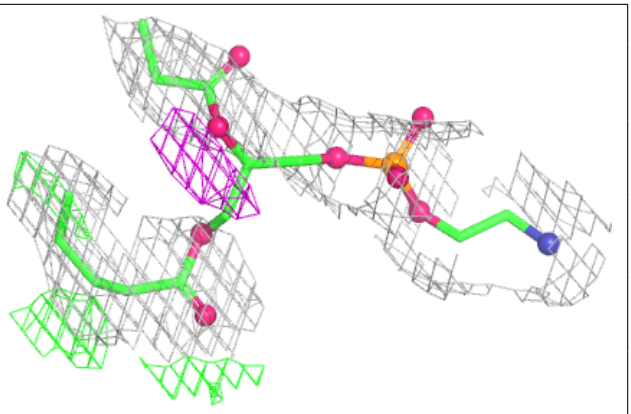
Electron density around LMU G 609:

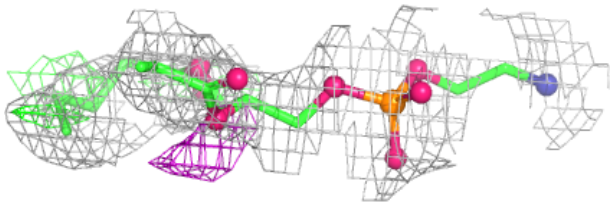
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

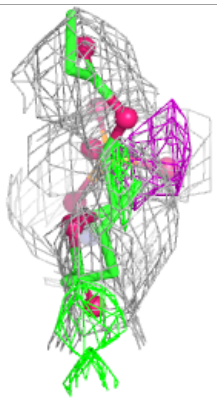


Electron density around 3PE I 303:

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

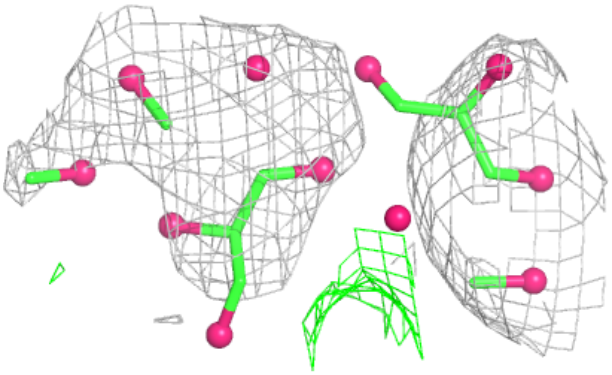


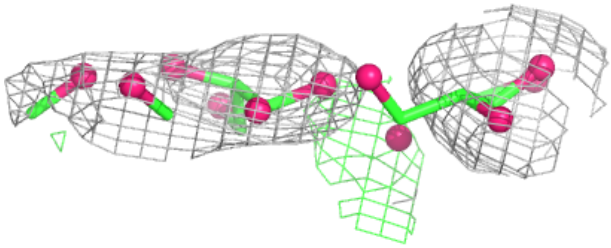


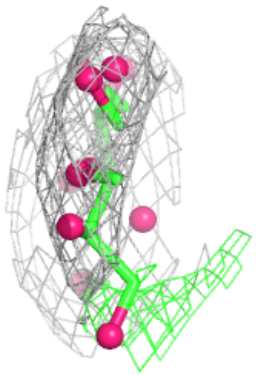


Electron density around LMU G 601:

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

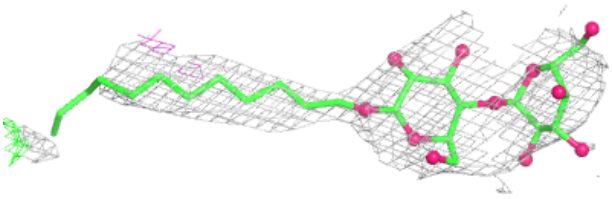


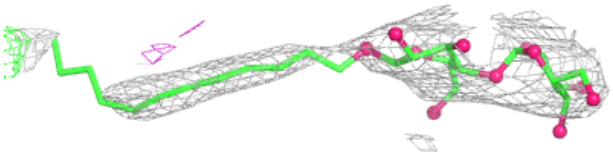


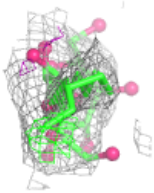


Electron density around LMU C 303:

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

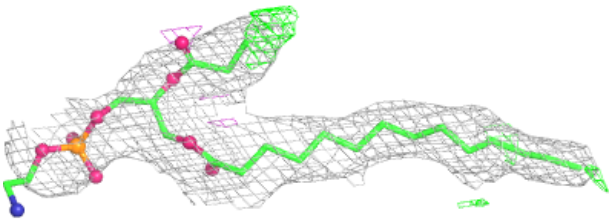


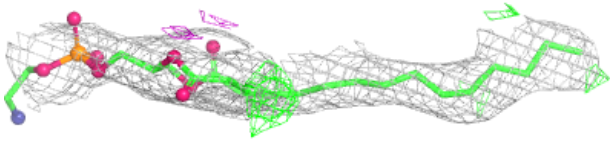




Electron density around 3PE I 302:

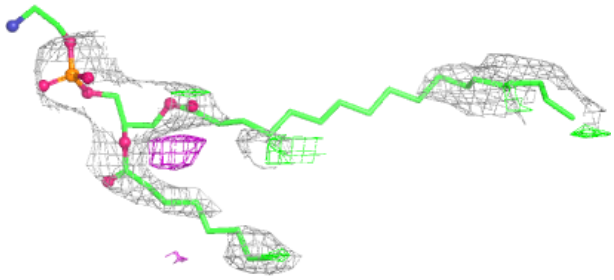
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

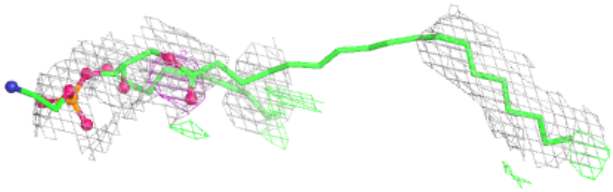




Electron density around 3PE C 301:

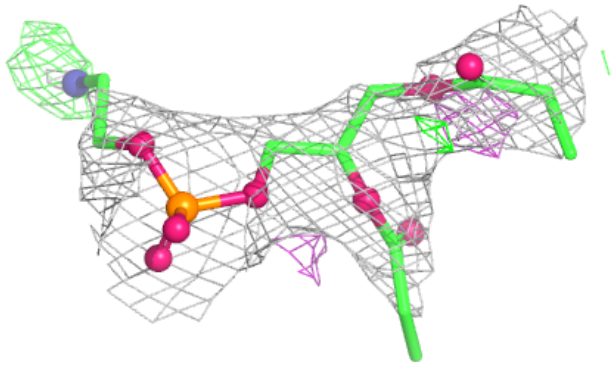
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

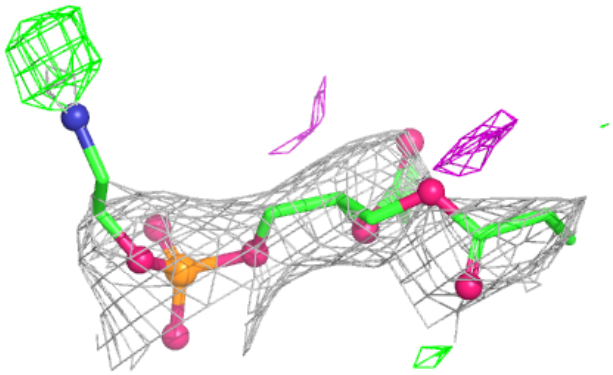


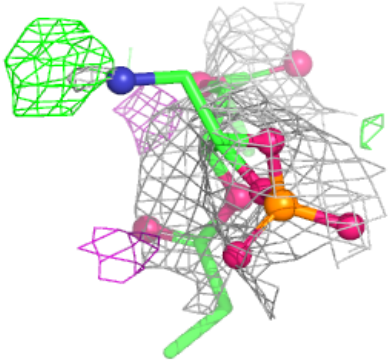


Electron density around 3PE A 606:

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

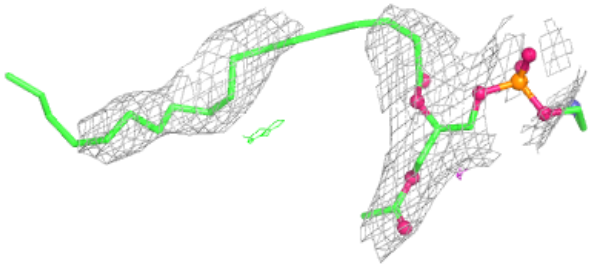


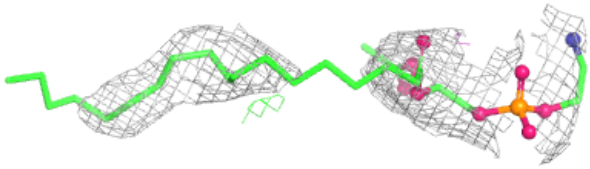


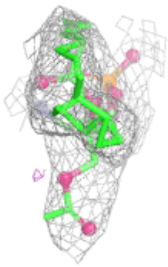


Electron density around 3PE J 101:

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

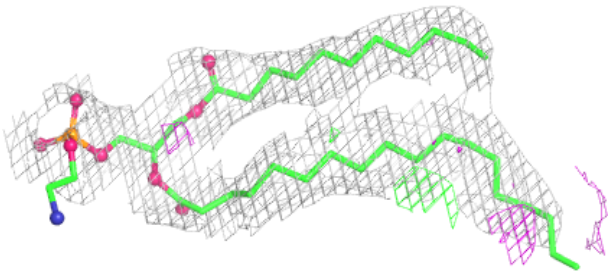


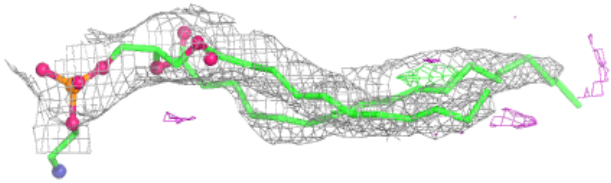


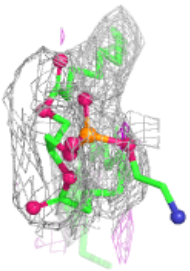


Electron density around 3PE G 608:

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

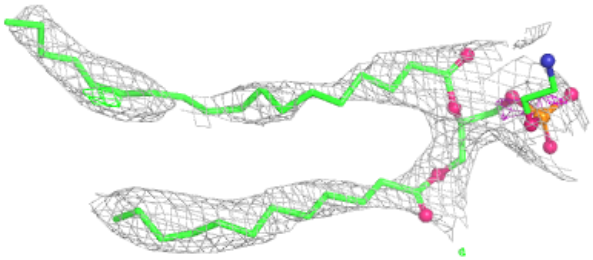


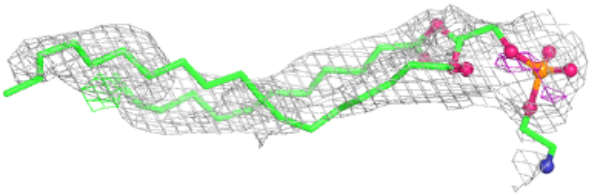




Electron density around 3PE A 607:

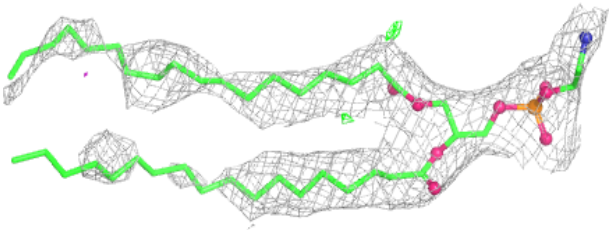
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

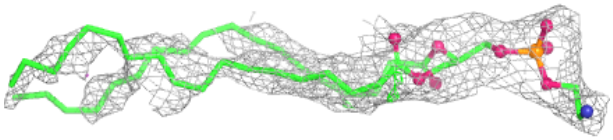


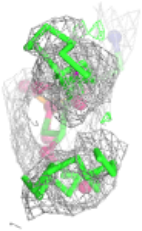


Electron density around 3PE C 302:

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

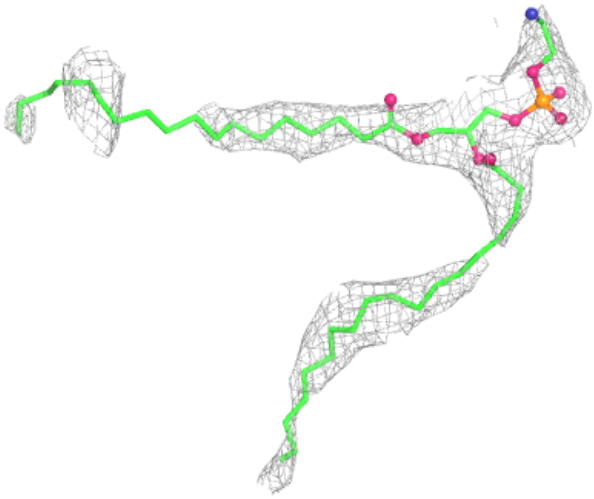


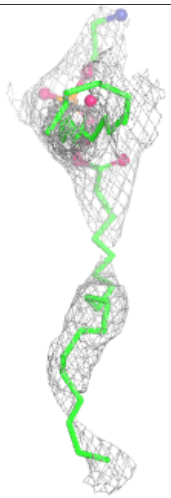




Electron density around 3PE D 101:

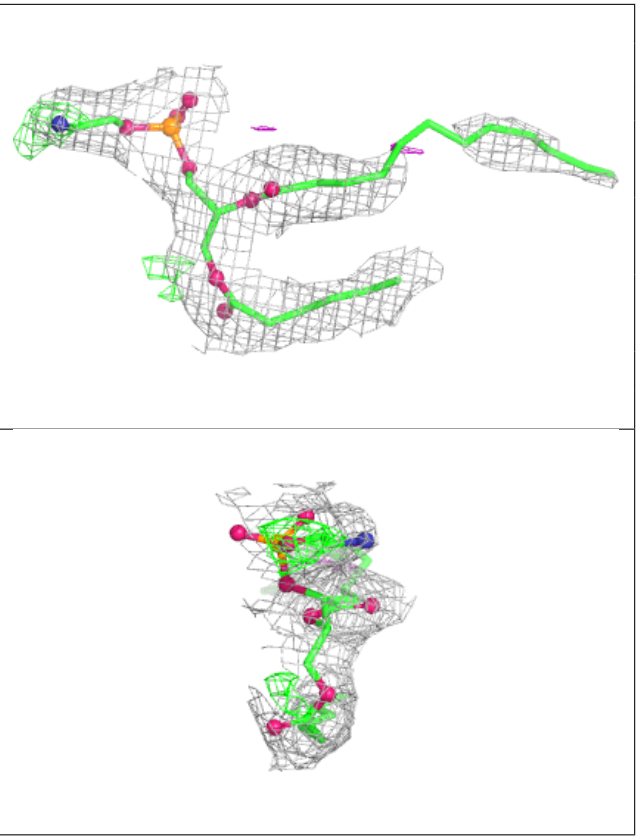
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





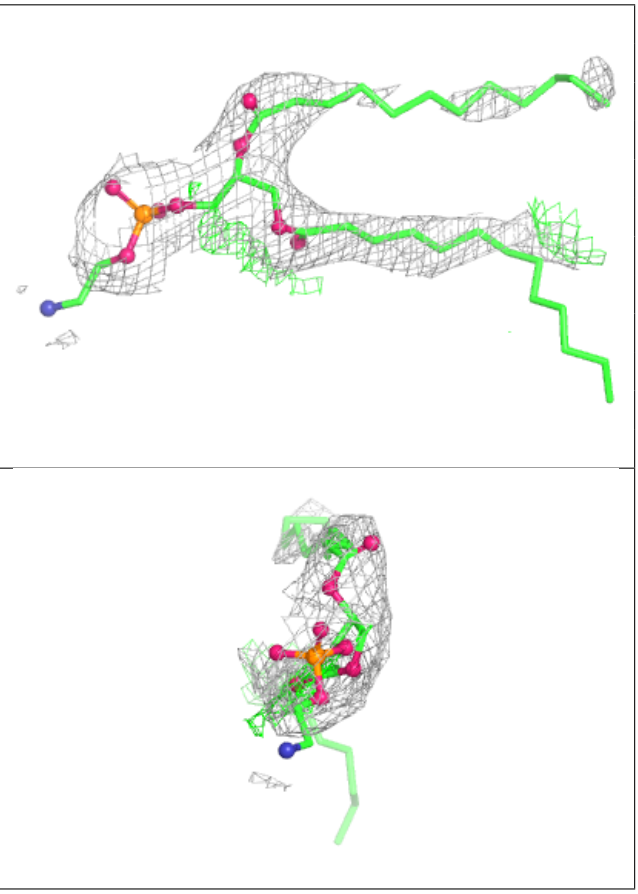
Electron density around 3PE G 607:

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



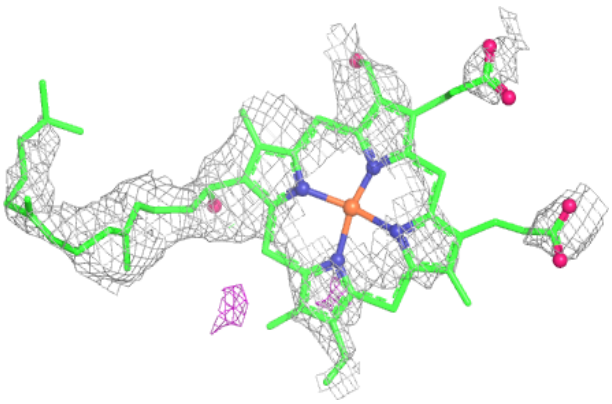
Electron density around 3PE I 301:

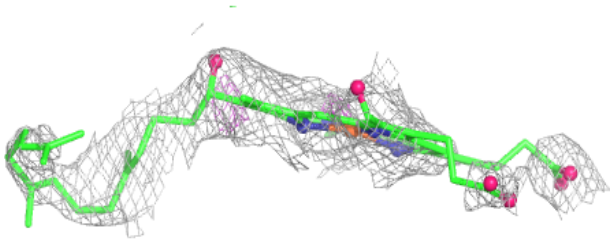
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

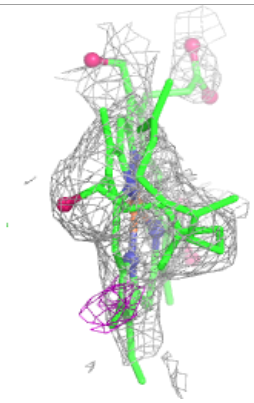


Electron density around HEA G 603:

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

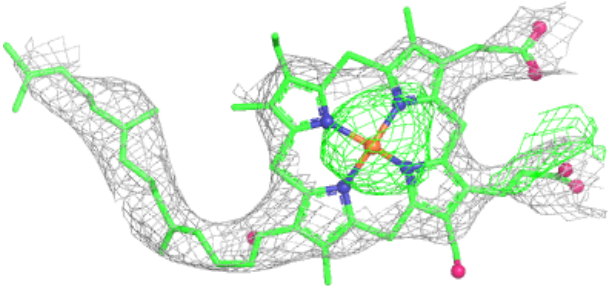


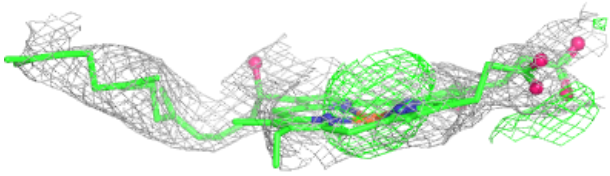


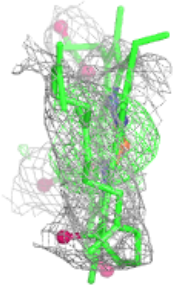


Electron density around HEA A 601:

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

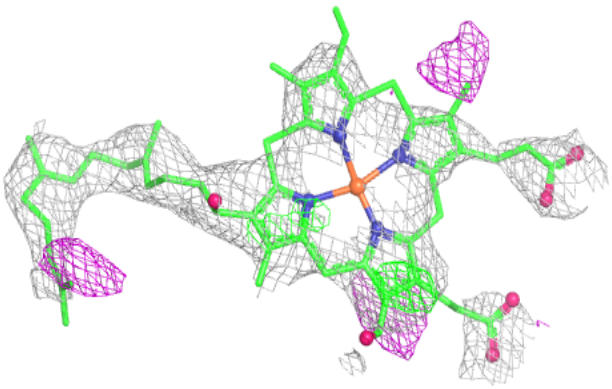


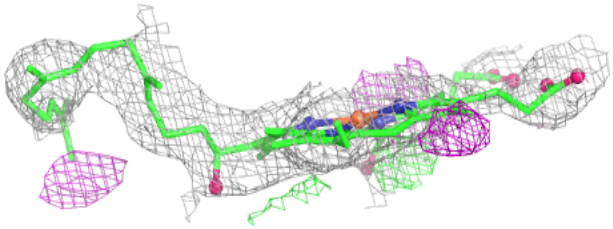




Electron density around HEA A 602:

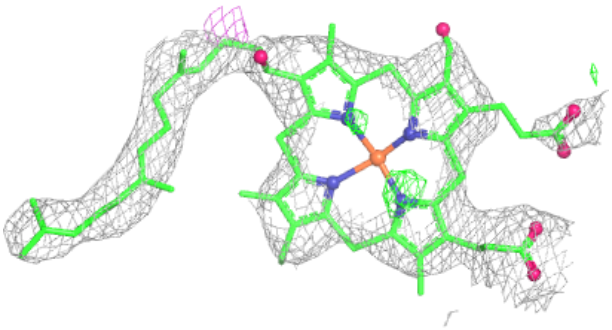
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

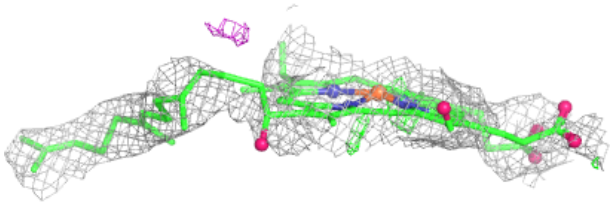




Electron density around HEA G 602:

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





6.5 Other polymers (i)

There are no such residues in this entry.