



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2021 – 12:35 PM EDT

PDB ID : 5WEH  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.22  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 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) : 2.22

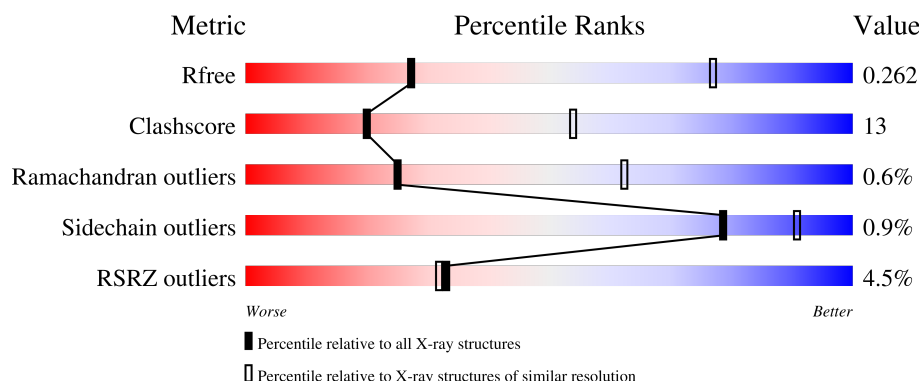
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div>3%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	G	566	<div> <div>%</div> <div>72%</div> <div>24%</div> <div>..</div> </div>
2	B	262	<div> <div>7%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	H	262	<div> <div>12%</div> <div>67%</div> <div>28%</div> <div>..</div> </div>
3	C	266	<div> <div>7%</div> <div>83%</div> <div>17%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	I	266	
4	D	50	
4	J	50	

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
10	LMU	G	609	-	-	-	X
5	HEA	A	602	X	-	X	-
5	HEA	G	602	-	-	X	-
5	HEA	G	603	X	-	-	-
7	MG	G	605	-	-	-	X
9	3PE	C	301	-	-	-	X
9	3PE	I	303	-	-	-	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
1	A	547	Total	C	N	O	S	0	0	0
			4254	2848	666	710	30			
1	G	547	Total	C	N	O	S	0	0	0
			4292	2873	677	711	31			

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

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

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

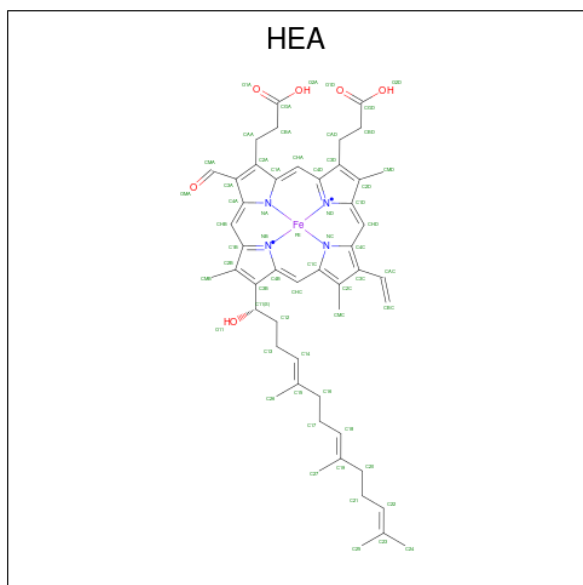
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3).

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

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

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

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



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

- Molecule 6 is COPPER (I) ION (three-letter code: 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

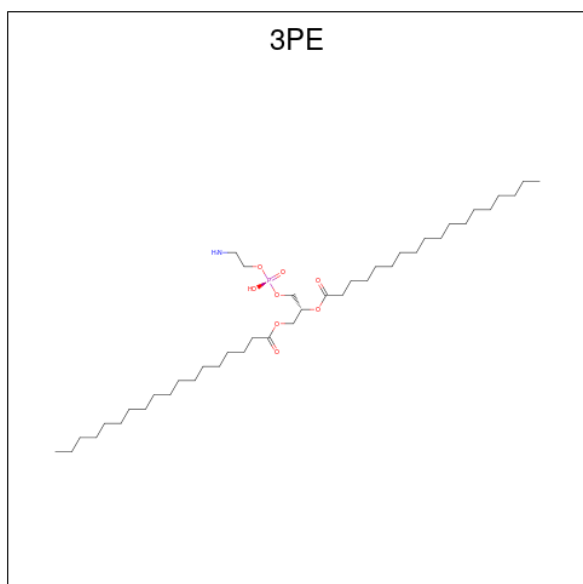
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: CA) (formula: Ca).

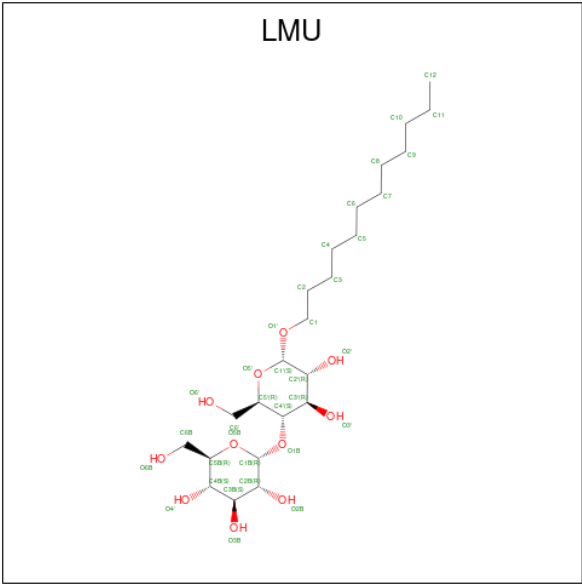
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Ca 1 1	0	0
8	G	1	Total Ca 1 1	0	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C<sub>41</sub>H<sub>82</sub>NO<sub>8</sub>P).



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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	G	1	Total	C	O	0	0
			20	9	11		
10	G	1	Total	C	O	0	0
			24	13	11		
10	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 11 is water.

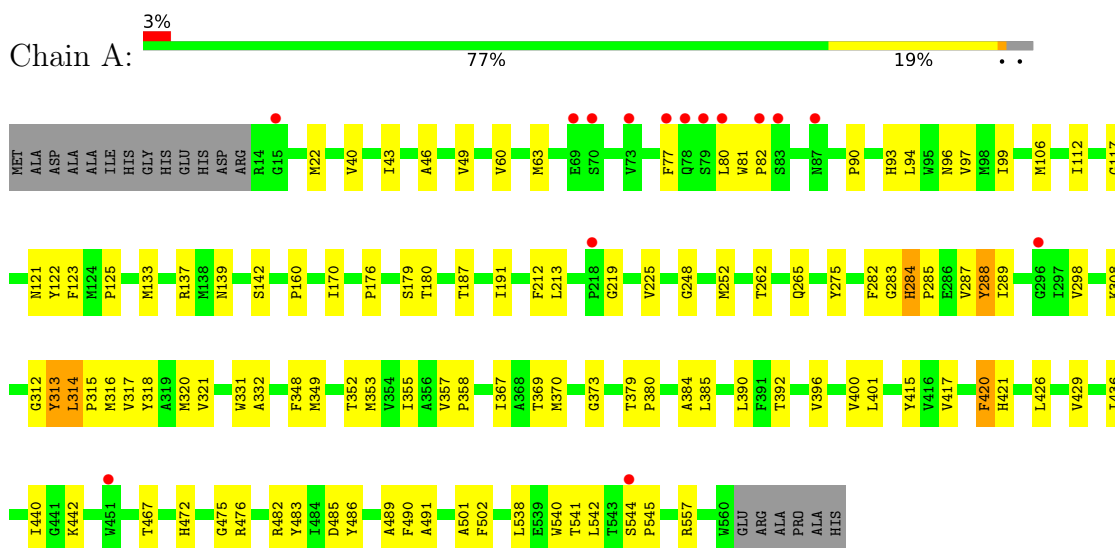
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			1	1		



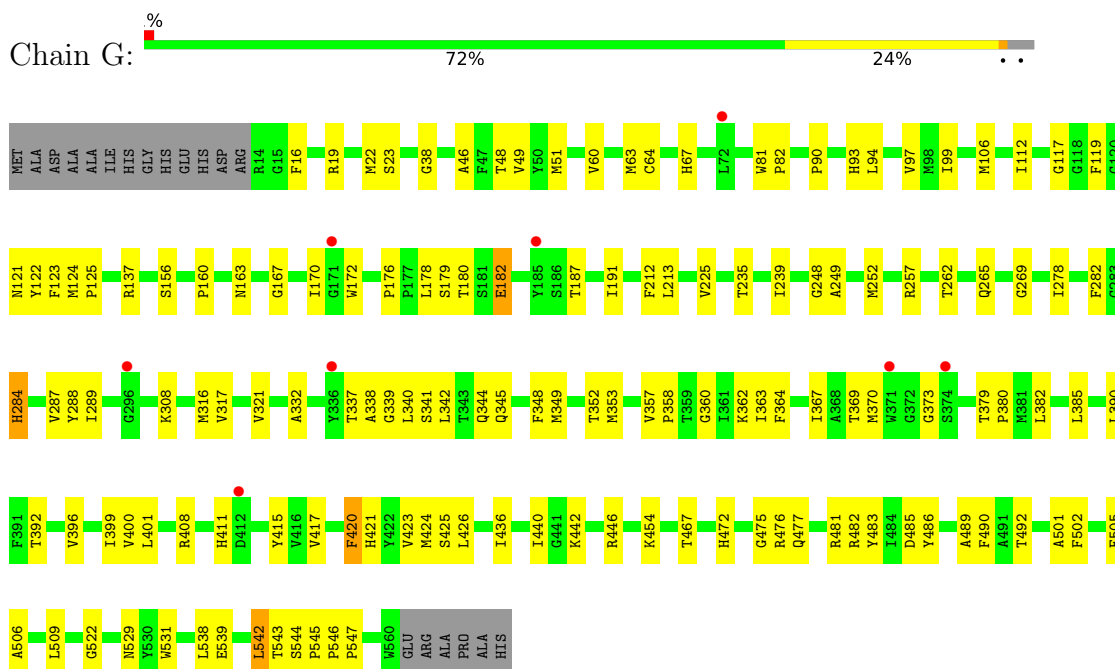
### 3 Residue-property plots [i](#)

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.

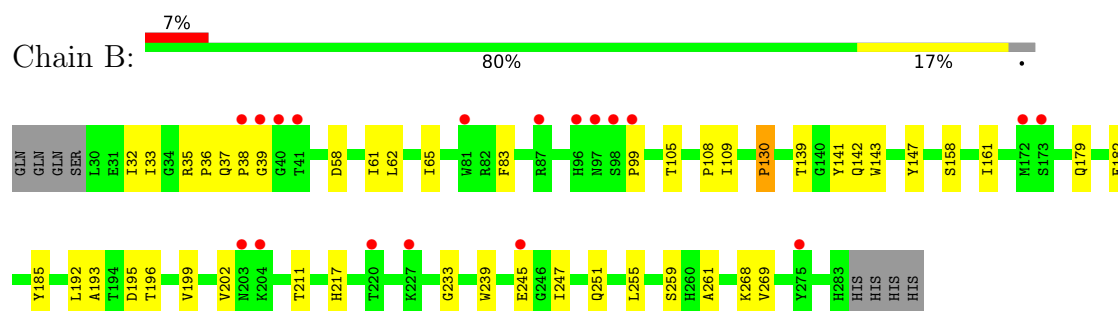
#### • Molecule 1: Cytochrome c oxidase subunit 1



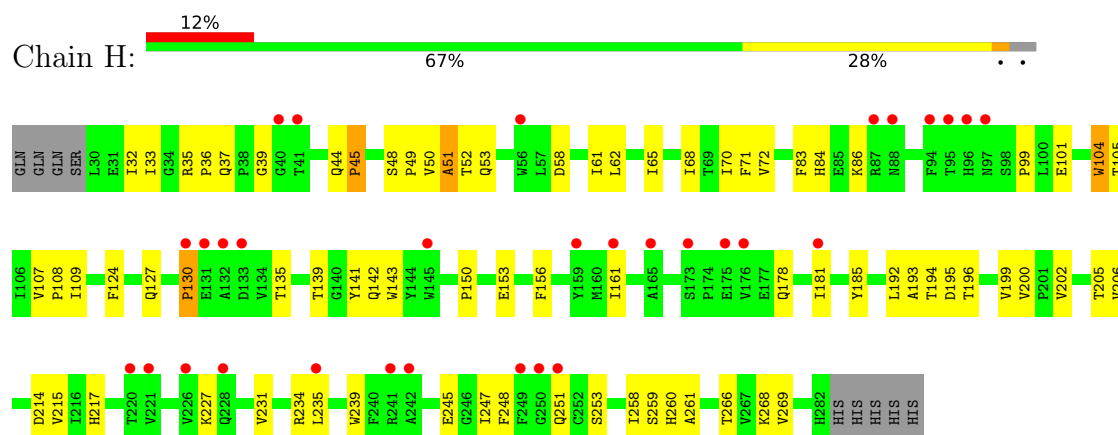
#### • Molecule 1: Cytochrome c oxidase subunit 1



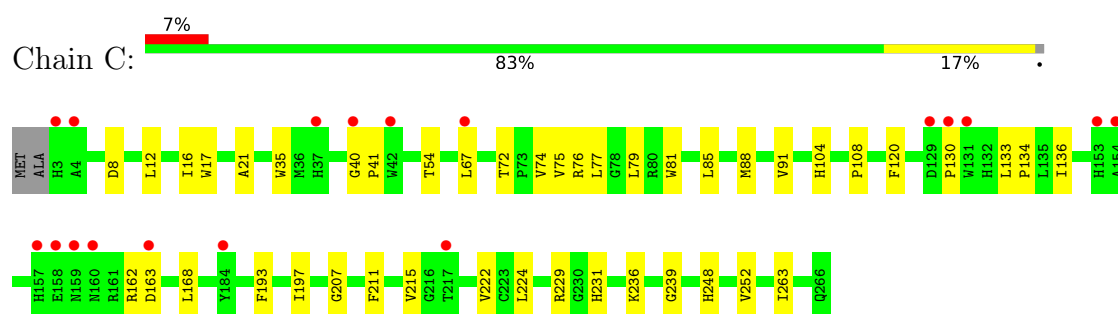
- Molecule 2: Cytochrome c oxidase subunit 2



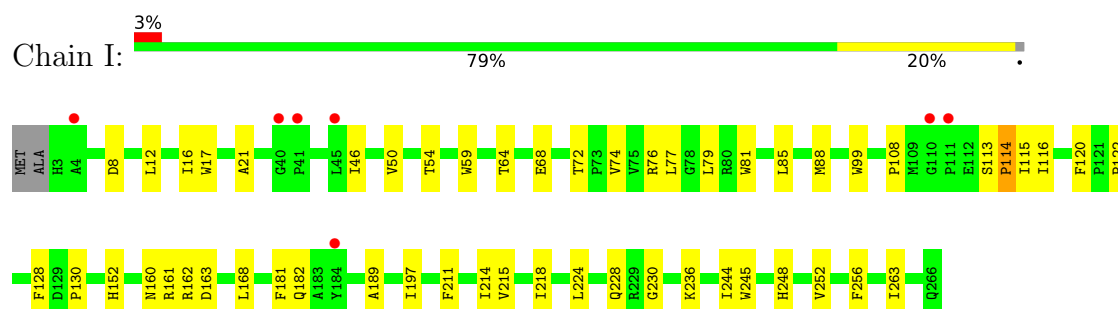
- Molecule 2: Cytochrome c oxidase subunit 2



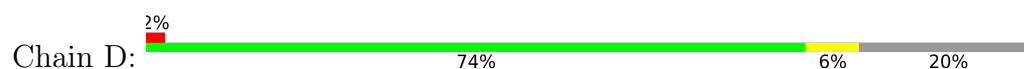
- Molecule 3: Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3)

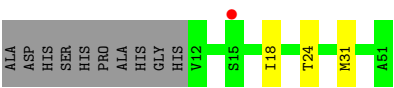


- Molecule 3: Cytochrome c oxidase polypeptide III (Cytochrome AA3 subunit 3)

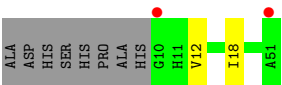
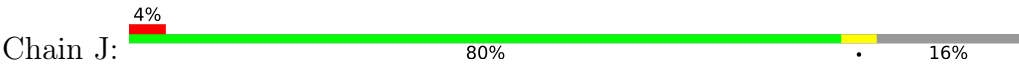


- Molecule 4: Aa3-type cytochrome c oxidase subunit IV





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



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	339.22Å 339.22Å 89.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.45 – 3.45 29.73 – 3.42	Depositor EDS
% Data completeness (in resolution range)	92.1 (28.45-3.45) 91.6 (29.73-3.42)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.73 (at 3.39Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.223 , 0.262 0.222 , 0.262	Depositor DCC
$R_{free}$ test set	1408 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	105.8	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 79.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.31	0/4413	0.49	3/6035 (0.0%)
1	G	0.31	1/4452 (0.0%)	0.49	2/6079 (0.0%)
2	B	0.27	0/2015	0.52	0/2765
2	H	0.32	0/1985	0.53	0/2726
3	C	0.27	0/2149	0.43	0/2943
3	I	0.29	0/2184	0.43	0/2991
4	D	0.25	0/280	0.39	0/384
4	J	0.26	0/303	0.41	0/411
All	All	0.30	1/17781 (0.0%)	0.48	5/24334 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	284	HIS	C-N	6.64	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	TYR	O-C-N	-5.83	113.36	122.70
1	G	288	TYR	O-C-N	-5.64	113.68	122.70
1	A	283	GLY	O-C-N	-5.34	114.16	122.70
1	G	288	TYR	C-N-CA	5.31	134.97	121.70
1	A	284	HIS	C-N-CD	5.12	139.16	128.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4254	0	4102	94	0
1	G	4292	0	4174	125	0
2	B	1956	0	1868	32	0
2	H	1927	0	1867	81	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	43	0
5	G	120	0	108	42	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	2	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	445	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.

All (445) 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
5:A:602:HEA:CHD	5:A:602:HEA:C1D	1.80	1.57
5:A:602:HEA:CHD	5:A:602:HEA:C4C	1.84	1.55
5:A:602:HEA:CHC	5:A:602:HEA:C4B	1.79	1.55
5:A:601:HEA:CHD	5:A:601:HEA:C1D	1.83	1.54
5:A:601:HEA:CHC	5:A:601:HEA:C1C	1.82	1.53
5:G:602:HEA:CHD	5:G:602:HEA:C1D	1.84	1.52
5:G:602:HEA:CHC	5:G:602:HEA:C1C	1.84	1.51
5:G:603:HEA:CHD	5:G:603:HEA:C4C	1.87	1.50
5:G:602:HEA:CHD	5:G:602:HEA:C4C	1.87	1.49
5:G:603:HEA:CHC	5:G:603:HEA:C1C	1.88	1.49
5:A:601:HEA:CHD	5:A:601:HEA:C4C	1.86	1.49
5:A:602:HEA:CHC	5:A:602:HEA:C1C	1.90	1.44
1:A:314:LEU:HG	1:A:315:PRO:CD	1.56	1.35
2:H:50:VAL:HG23	2:H:51:ALA:N	1.54	1.12
2:H:50:VAL:CG2	2:H:51:ALA:H	1.65	1.08
1:A:314:LEU:CG	1:A:315:PRO:HD3	1.88	1.01
1:A:314:LEU:HD23	1:A:314:LEU:H	1.26	0.98
2:H:50:VAL:CG2	2:H:51:ALA:N	2.14	0.98
3:C:8:ASP:HB3	3:C:72:THR:HG21	1.47	0.96
1:G:163:ASN:CB	2:H:258:ILE:HD11	1.96	0.96
1:A:314:LEU:CG	1:A:315:PRO:CD	2.42	0.95
2:H:48:SER:HB2	2:H:49:PRO:CD	1.99	0.93
1:A:314:LEU:HG	1:A:315:PRO:HD3	0.92	0.91
1:A:106:MET:HB3	5:A:601:HEA:HAC	1.53	0.90
10:G:601:LMU:C4B	10:G:601:LMU:C6B	2.50	0.90
10:G:601:LMU:C4'	10:G:601:LMU:C2'	2.48	0.90
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.53	0.88
2:H:142:GLN:N	2:H:214:ASP:OD2	2.06	0.88
1:G:542:LEU:H	1:G:542:LEU:HD12	1.38	0.87
1:G:81:TRP:HD1	1:G:82:PRO:HD2	1.38	0.87
2:H:48:SER:HB2	2:H:49:PRO:HD2	1.58	0.84
2:H:48:SER:OG	2:H:50:VAL:HG22	1.77	0.83
5:A:602:HEA:CHD	5:A:602:HEA:C3C	2.55	0.83
2:H:50:VAL:O	2:H:53:GLN:N	2.11	0.83
1:G:163:ASN:HB3	2:H:258:ILE:HD11	1.61	0.82
1:A:314:LEU:N	1:A:315:PRO:HD2	1.94	0.82
1:G:360:GLY:HA2	5:G:603:HEA:H18	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:602:HEA:CHC	5:G:602:HEA:C2C	2.60	0.80
2:B:32:ILE:HG22	2:B:35:ARG:HD2	1.65	0.79
2:H:50:VAL:HG22	2:H:51:ALA:H	1.47	0.78
5:A:601:HEA:CHC	5:A:601:HEA:C2C	2.60	0.77
1:A:314:LEU:HG	1:A:315:PRO:HD2	1.64	0.76
5:G:603:HEA:CHD	5:G:603:HEA:C3C	2.64	0.75
10:G:601:LMU:C2'	10:G:601:LMU:O1'	2.34	0.75
1:G:63:MET:HG2	1:G:94:LEU:HD23	1.68	0.75
1:A:63:MET:HG2	1:A:94:LEU:HD23	1.67	0.74
1:G:542:LEU:HD12	1:G:542:LEU:N	2.03	0.74
1:G:137:ARG:HH21	3:I:12:LEU:HD21	1.50	0.73
1:A:314:LEU:HD23	1:A:314:LEU:N	2.01	0.72
2:H:50:VAL:O	2:H:52:THR:N	2.22	0.72
1:G:442:LYS:NZ	1:G:542:LEU:O	2.21	0.71
5:A:601:HEA:CHD	5:A:601:HEA:C3C	2.67	0.71
10:G:601:LMU:O1B	10:G:601:LMU:C2B	2.39	0.71
1:A:313:TYR:O	1:A:316:MET:HB2	1.91	0.71
1:G:182:GLU:O	1:G:257:ARG:NH2	2.24	0.70
2:H:50:VAL:HG23	2:H:51:ALA:H	1.27	0.70
3:C:72:THR:HG22	3:C:75:VAL:HG23	1.74	0.70
10:G:601:LMU:C2'	10:G:601:LMU:O3'	2.39	0.70
1:A:314:LEU:H	1:A:314:LEU:CD2	2.01	0.70
1:A:312:GLY:O	1:A:315:PRO:HG2	1.92	0.70
1:A:321:VAL:HG13	9:A:607:3PE:H372	1.74	0.69
10:G:601:LMU:C4'	10:G:601:LMU:O3'	2.41	0.69
5:G:602:HEA:HBA1	5:G:602:HEA:HHA	1.73	0.69
5:A:602:HEA:CHC	5:A:602:HEA:C2C	2.69	0.68
1:G:344:GLN:NE2	9:J:101:3PE:O12	2.27	0.68
1:G:543:THR:HG22	1:G:547:PRO:HD3	1.73	0.68
1:G:99:ILE:HD12	5:G:602:HEA:HBA2	1.75	0.68
10:G:601:LMU:C6B	10:G:601:LMU:O5B	2.41	0.68
1:A:77:PHE:HA	1:A:80:LEU:HD13	1.76	0.67
1:G:38:GLY:HA2	5:G:602:HEA:H253	1.76	0.67
1:G:262:THR:HG23	3:I:197:ILE:HD13	1.75	0.67
5:G:602:HEA:CHC	5:G:602:HEA:C3B	2.72	0.67
1:A:287:VAL:HB	5:A:602:HEA:HHD	1.76	0.67
5:A:601:HEA:C4B	5:A:601:HEA:C1C	2.73	0.67
2:H:32:ILE:HG22	2:H:35:ARG:HD3	1.77	0.67
1:G:284:HIS:O	1:G:287:VAL:HG22	1.95	0.67
1:G:106:MET:HB3	5:G:602:HEA:HAC	1.76	0.66
1:A:314:LEU:CG	1:A:315:PRO:HD2	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:LEU:HD21	2:H:124:PHE:HD1	1.60	0.66
10:G:601:LMU:C4B	10:G:601:LMU:O5B	2.43	0.66
5:G:603:HEA:CHC	5:G:603:HEA:C2C	2.71	0.66
5:A:602:HEA:C1D	5:A:602:HEA:C4C	2.74	0.66
1:A:417:VAL:O	1:A:421:HIS:ND1	2.17	0.66
1:G:163:ASN:HB2	2:H:258:ILE:HD11	1.77	0.65
5:G:603:HEA:C1D	5:G:603:HEA:C4C	2.75	0.65
1:A:287:VAL:HG11	5:A:602:HEA:HMD2	1.79	0.65
5:A:601:HEA:CHC	5:A:601:HEA:C3B	2.73	0.64
5:A:602:HEA:CHD	5:A:602:HEA:CAC	2.76	0.64
1:G:341:SER:HB3	1:G:344:GLN:HG3	1.79	0.64
3:I:21:ALA:HB2	3:I:54:THR:HG21	1.78	0.64
1:A:482:ARG:HD3	2:B:255:LEU:HB2	1.80	0.64
3:C:91:VAL:HG13	9:C:302:3PE:H3E1	1.80	0.64
9:A:607:3PE:H2G2	9:C:302:3PE:H2G2	1.81	0.63
5:G:602:HEA:C4B	5:G:602:HEA:C1C	2.76	0.63
2:H:245:GLU:HA	2:H:269:VAL:HG13	1.81	0.62
2:B:202:VAL:HG11	2:B:245:GLU:HG3	1.80	0.62
2:H:44:GLN:O	2:H:45:PRO:O	2.16	0.62
1:A:106:MET:HB3	5:A:601:HEA:CAC	2.29	0.62
2:H:231:VAL:HG23	2:H:234:ARG:HB2	1.81	0.62
2:H:48:SER:CB	2:H:49:PRO:CD	2.70	0.62
3:I:17:TRP:HD1	3:I:54:THR:HG23	1.65	0.62
1:G:48:THR:HA	1:G:51:MET:HE2	1.80	0.62
3:C:21:ALA:HB2	3:C:54:THR:HG21	1.81	0.61
2:B:245:GLU:HA	2:B:269:VAL:HG13	1.83	0.61
2:B:199:VAL:HA	2:B:268:LYS:O	2.01	0.61
1:A:287:VAL:CG1	5:A:602:HEA:HMD2	2.31	0.61
1:G:64:CYS:HB2	1:G:67:HIS:CD2	2.35	0.60
2:H:50:VAL:O	2:H:51:ALA:C	2.39	0.60
1:A:284:HIS:O	1:A:287:VAL:HG22	2.01	0.60
3:C:17:TRP:HD1	3:C:54:THR:HG23	1.66	0.60
2:H:199:VAL:HA	2:H:268:LYS:O	2.01	0.60
2:B:33:ILE:O	2:B:35:ARG:HG2	2.02	0.59
2:B:147:TYR:HE1	2:B:158:SER:HB3	1.65	0.59
5:G:603:HEA:CHD	5:G:603:HEA:CAC	2.80	0.59
2:H:135:THR:O	2:H:150:PRO:HD2	2.02	0.59
3:I:8:ASP:CB	3:I:72:THR:HG21	2.30	0.59
1:A:317:VAL:HG12	1:A:318:TYR:N	2.18	0.59
1:A:390:LEU:HD13	1:A:426:LEU:HB3	1.85	0.58
1:A:212:PHE:CE2	1:A:225:VAL:HG11	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:602:HEA:C4B	5:A:602:HEA:C1C	2.81	0.58
5:G:602:HEA:CHD	5:G:602:HEA:C3C	2.75	0.57
5:A:602:HEA:HHC	5:A:602:HEA:H122	1.86	0.57
1:G:81:TRP:CD1	1:G:82:PRO:HD2	2.30	0.57
2:H:32:ILE:CG2	2:H:35:ARG:HD3	2.34	0.57
5:A:602:HEA:C1A	5:A:602:HEA:C4D	2.80	0.57
1:G:212:PHE:CE2	1:G:225:VAL:HG11	2.40	0.57
10:G:601:LMU:C2'	10:G:601:LMU:O5'	2.52	0.56
1:A:262:THR:HG22	1:A:265:GLN:HB2	1.87	0.56
9:A:607:3PE:H2H1	9:C:302:3PE:H2I3	1.87	0.56
2:H:105:THR:O	2:H:109:ILE:HG13	2.05	0.56
1:G:538:LEU:O	1:G:542:LEU:HD11	2.06	0.56
3:C:162:ARG:HG3	3:C:163:ASP:N	2.20	0.56
3:C:222:VAL:HG11	9:C:301:3PE:H351	1.86	0.56
1:G:269:GLY:C	3:I:197:ILE:HD11	2.26	0.56
1:G:390:LEU:HD13	1:G:426:LEU:HB3	1.87	0.56
3:C:104:HIS:ND1	3:C:197:ILE:HG12	2.21	0.56
5:G:603:HEA:CHD	5:G:603:HEA:C2D	2.78	0.56
3:I:85:LEU:HD23	3:I:88:MET:HE1	1.86	0.56
1:A:137:ARG:HB2	3:C:12:LEU:HD13	1.88	0.56
3:C:236:LYS:HE3	9:C:301:3PE:HN3	1.71	0.56
1:A:415:TYR:HB2	1:A:475:GLY:HA3	1.88	0.55
2:B:202:VAL:CG1	2:B:245:GLU:HG3	2.37	0.55
1:A:417:VAL:HG13	1:A:421:HIS:HE1	1.72	0.55
1:G:392:THR:HG23	5:G:603:HEA:H171	1.88	0.55
1:G:415:TYR:HB2	1:G:475:GLY:HA3	1.89	0.55
1:G:364:PHE:HB3	2:H:104:TRP:CZ3	2.42	0.55
9:G:608:3PE:H341	9:G:608:3PE:H272	1.88	0.55
2:B:233:GLY:HA2	4:J:12:VAL:HG11	1.87	0.55
1:G:538:LEU:O	1:G:542:LEU:CD1	2.54	0.54
1:G:539:GLU:HA	1:G:542:LEU:HD13	1.90	0.54
1:G:477:GLN:NE2	2:H:37:GLN:H	2.05	0.54
1:A:96:ASN:O	1:A:99:ILE:HG13	2.08	0.54
5:G:602:HEA:CHC	5:G:602:HEA:CMC	2.86	0.54
3:I:152:HIS:HB2	3:I:244:ILE:HD13	1.89	0.54
1:G:249:ALA:HA	1:G:252:MET:HE3	1.89	0.54
1:G:417:VAL:O	1:G:421:HIS:ND1	2.22	0.54
3:C:81:TRP:HH2	4:D:24:THR:HG22	1.73	0.54
10:G:601:LMU:C2B	10:G:601:LMU:O5B	2.56	0.53
3:I:224:LEU:O	3:I:228:GLN:HG2	2.08	0.53
1:A:482:ARG:NH2	5:A:601:HEA:O2D	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:37:GLN:O	2:H:39:GLY:N	2.40	0.53
2:H:65:ILE:HA	2:H:68:ILE:HG12	1.89	0.53
1:A:400:VAL:HG22	2:B:61:ILE:HG21	1.90	0.53
1:G:539:GLU:HA	1:G:542:LEU:CD1	2.38	0.53
1:G:112:ILE:HG12	1:G:289:ILE:HG22	1.91	0.53
2:H:194:THR:HG22	2:H:266:THR:OG1	2.09	0.53
1:G:106:MET:HB3	5:G:602:HEA:CAC	2.39	0.53
2:H:84:HIS:CE1	2:H:86:LYS:HG2	2.43	0.53
1:G:483:TYR:OH	2:H:251:GLN:HB3	2.08	0.53
3:I:17:TRP:CD1	3:I:54:THR:HG23	2.44	0.53
1:G:411:HIS:O	2:H:227:LYS:HE3	2.09	0.52
2:B:211:THR:HG21	4:J:12:VAL:HG13	1.91	0.52
2:H:178:GLN:HA	2:H:181:ILE:HD12	1.91	0.52
1:A:176:PRO:HB3	1:A:180:THR:HG23	1.92	0.52
1:G:379:THR:HB	1:G:380:PRO:HD3	1.92	0.52
2:H:200:VAL:HG11	2:H:206:VAL:HG21	1.90	0.52
3:I:161:ARG:NH2	3:I:230:GLY:HA2	2.25	0.52
1:G:396:VAL:HA	1:G:399:ILE:HD12	1.91	0.52
2:B:185:TYR:HE1	2:B:247:ILE:HD13	1.75	0.52
1:A:112:ILE:HG12	1:A:289:ILE:HG22	1.92	0.52
2:B:36:PRO:HD2	2:B:192:LEU:HD11	1.92	0.52
3:C:17:TRP:CD1	3:C:54:THR:HG23	2.44	0.52
3:C:85:LEU:HD23	3:C:88:MET:HE1	1.91	0.52
1:A:93:HIS:O	1:A:97:VAL:HG23	2.10	0.51
1:A:170:ILE:HG21	1:A:179:SER:HB3	1.90	0.51
3:C:207:GLY:HA3	10:C:303:LMU:H71	1.91	0.51
1:G:373:GLY:O	2:H:83:PHE:HB3	2.11	0.51
1:G:542:LEU:H	1:G:542:LEU:CD1	2.15	0.51
1:A:22:MET:HG2	3:C:16:ILE:HA	1.93	0.51
1:A:476:ARG:NH2	2:B:58:ASP:OD2	2.43	0.51
1:A:139:ASN:O	1:A:142:SER:OG	2.24	0.51
5:A:601:HEA:C1D	5:A:601:HEA:C4C	2.89	0.50
5:A:602:HEA:CHC	5:A:602:HEA:H122	2.40	0.50
1:A:417:VAL:HA	1:A:420:PHE:CE2	2.46	0.50
1:A:401:LEU:HD22	5:A:602:HEA:HBA2	1.91	0.50
3:I:130:PRO:HB2	3:I:263:ILE:HD13	1.92	0.50
1:A:442:LYS:NZ	1:A:542:LEU:O	2.43	0.50
2:H:143:TRP:CG	2:H:259:SER:HB2	2.46	0.50
1:G:117:GLY:O	1:G:121:ASN:HB2	2.11	0.50
2:H:62:LEU:HA	2:H:65:ILE:HG12	1.93	0.50
1:G:417:VAL:HG13	1:G:421:HIS:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:VAL:HG21	1:A:90:PRO:HB3	1.94	0.49
2:B:37:GLN:O	2:B:39:GLY:N	2.45	0.49
2:B:161:ILE:HD12	2:B:193:ALA:HB1	1.94	0.49
1:A:99:ILE:HD13	1:A:482:ARG:HG2	1.95	0.49
3:I:160:ASN:ND2	3:I:163:ASP:OD2	2.46	0.49
1:A:373:GLY:O	2:B:83:PHE:HB3	2.12	0.49
1:G:342:LEU:HD21	2:H:124:PHE:CD1	2.45	0.49
3:C:229:ARG:NH1	3:C:229:ARG:HB2	2.27	0.49
3:I:72:THR:HG22	3:I:74:VAL:H	1.77	0.49
3:I:128:PHE:HZ	3:I:189:ALA:HA	1.77	0.49
1:G:93:HIS:O	1:G:97:VAL:HG23	2.13	0.49
1:G:425:SER:HA	5:G:602:HEA:HBC1	1.94	0.49
1:A:213:LEU:HD13	3:C:81:TRP:CZ3	2.48	0.49
5:A:601:HEA:CHD	5:A:601:HEA:C2D	2.81	0.49
1:G:357:VAL:HB	1:G:358:PRO:HD3	1.95	0.49
2:H:50:VAL:C	2:H:52:THR:N	2.66	0.48
1:A:176:PRO:HD3	1:A:275:TYR:CD2	2.48	0.48
1:A:312:GLY:C	1:A:315:PRO:HG2	2.33	0.48
1:A:367:ILE:HA	1:A:370:MET:HE2	1.94	0.48
1:A:483:TYR:OH	2:B:251:GLN:HB3	2.13	0.48
1:G:170:ILE:HG21	1:G:179:SER:HB3	1.95	0.48
1:G:176:PRO:HB3	1:G:180:THR:HG23	1.96	0.48
1:G:317:VAL:O	1:G:321:VAL:HG23	2.13	0.48
1:G:370:MET:SD	1:G:385:LEU:HD21	2.54	0.48
3:C:77:LEU:HG	3:C:81:TRP:HE1	1.78	0.48
3:I:236:LYS:HD2	9:I:301:3PE:H112	1.94	0.48
1:A:332:ALA:HB3	1:A:348:PHE:CG	2.49	0.48
2:H:200:VAL:CG1	2:H:206:VAL:HG21	2.42	0.48
1:G:342:LEU:HD13	2:H:127:GLN:HB2	1.95	0.48
1:G:367:ILE:HA	1:G:370:MET:HE2	1.95	0.48
9:C:302:3PE:H331	9:D:101:3PE:H322	1.95	0.48
1:A:317:VAL:O	1:A:320:MET:N	2.47	0.48
2:B:143:TRP:CG	2:B:259:SER:HB2	2.49	0.48
1:A:314:LEU:CD2	1:A:315:PRO:HD2	2.44	0.48
1:G:213:LEU:HD13	3:I:81:TRP:CZ3	2.49	0.48
1:G:396:VAL:HB	2:H:65:ILE:HB	1.95	0.48
3:C:130:PRO:HB2	3:C:263:ILE:HD13	1.95	0.47
3:I:76:ARG:HD3	3:I:236:LYS:HG2	1.95	0.47
3:C:168:LEU:HB2	3:C:224:LEU:HD13	1.96	0.47
3:C:193:PHE:HB2	10:C:303:LMU:H11	1.96	0.47
2:H:161:ILE:HD12	2:H:193:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:SD	1:A:385:LEU:HD21	2.55	0.47
1:A:417:VAL:HG13	1:A:421:HIS:CE1	2.49	0.47
3:C:248:HIS:O	3:C:252:VAL:HG23	2.15	0.47
2:H:185:TYR:HE1	2:H:247:ILE:HD13	1.79	0.47
3:I:59:TRP:CZ3	9:I:301:3PE:H361	2.50	0.47
1:G:529:ASN:ND2	1:G:531:TRP:H	2.13	0.47
1:G:60:VAL:HG21	1:G:90:PRO:HB3	1.97	0.47
3:C:239:GLY:N	9:C:301:3PE:O12	2.40	0.47
2:H:202:VAL:HG22	2:H:269:VAL:HG22	1.96	0.47
1:A:288:TYR:OH	1:A:355:ILE:HG21	2.14	0.47
1:A:544:SER:HB3	1:A:545:PRO:HD3	1.96	0.47
2:H:234:ARG:HA	3:I:113:SER:OG	2.15	0.47
3:I:46:ILE:O	3:I:50:VAL:HG12	2.14	0.47
3:I:77:LEU:HG	3:I:81:TRP:HE1	1.80	0.47
1:G:411:HIS:ND1	5:G:603:HEA:O1A	2.47	0.47
1:G:467:THR:HG23	1:G:501:ALA:HB2	1.97	0.47
2:H:44:GLN:O	2:H:45:PRO:C	2.53	0.47
9:A:606:3PE:H111	3:C:12:LEU:HD11	1.96	0.47
1:G:332:ALA:HB3	1:G:348:PHE:CG	2.50	0.47
5:G:602:HEA:OMA	5:G:602:HEA:HBB	2.14	0.47
5:A:602:HEA:CHD	5:A:602:HEA:C2D	2.83	0.47
2:H:130:PRO:HG2	2:H:205:THR:HG21	1.97	0.47
3:I:74:VAL:HG12	4:J:18:ILE:HG23	1.96	0.47
3:I:245:TRP:CE2	9:I:303:3PE:H222	2.49	0.46
1:A:308:LYS:HD3	1:A:369:THR:O	2.15	0.46
1:A:392:THR:HG23	5:A:602:HEA:H171	1.97	0.46
1:G:278:ILE:HG12	3:I:99:TRP:CE3	2.50	0.46
1:G:308:LYS:HD3	1:G:369:THR:O	2.16	0.46
2:B:105:THR:O	2:B:109:ILE:HG13	2.16	0.46
2:H:195:ASP:OD1	2:H:196:THR:N	2.49	0.46
2:H:227:LYS:HE2	2:H:253:SER:CB	2.46	0.46
1:G:417:VAL:HA	1:G:420:PHE:CE2	2.51	0.46
5:G:602:HEA:HBA1	5:G:602:HEA:CHA	2.43	0.46
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.96	0.46
1:G:446:ARG:NH1	1:G:522:GLY:O	2.48	0.46
3:C:108:PRO:HG3	3:C:120:PHE:HB2	1.98	0.46
1:A:287:VAL:O	5:A:602:HEA:HAC	2.16	0.46
1:A:396:VAL:HB	2:B:65:ILE:HB	1.97	0.46
5:G:603:HEA:HHA	5:G:603:HEA:HAD2	1.81	0.46
2:H:234:ARG:HA	3:I:113:SER:HG	1.80	0.46
2:H:235:LEU:H	3:I:114:PRO:HD3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:VAL:HG21	5:A:601:HEA:H161	1.98	0.46
5:G:603:HEA:CHC	5:G:603:HEA:CMC	2.94	0.46
3:I:160:ASN:OD1	3:I:162:ARG:HG2	2.15	0.46
1:A:81:TRP:CD2	1:A:82:PRO:HD2	2.51	0.46
2:B:195:ASP:OD1	2:B:196:THR:N	2.49	0.46
1:G:337:THR:HG21	2:H:227:LYS:HZ2	1.81	0.46
2:H:48:SER:HG	2:H:50:VAL:HG22	1.80	0.46
3:I:77:LEU:O	3:I:81:TRP:HD1	1.99	0.46
1:G:137:ARG:HE	3:I:12:LEU:CD2	2.28	0.45
2:B:179:GLN:O	2:B:182:GLU:HB2	2.16	0.45
1:A:379:THR:HB	1:A:380:PRO:HD3	1.98	0.45
3:I:64:THR:O	3:I:68:GLU:HB2	2.16	0.45
1:G:38:GLY:CA	5:G:602:HEA:H253	2.43	0.45
1:G:187:THR:O	1:G:191:ILE:HG12	2.17	0.45
1:G:436:ILE:O	1:G:440:ILE:HB	2.16	0.45
3:C:67:LEU:HD11	3:C:231:HIS:CE1	2.51	0.45
2:H:48:SER:HB2	2:H:49:PRO:HD3	1.92	0.45
1:G:22:MET:HG2	3:I:16:ILE:HA	1.98	0.45
3:C:85:LEU:HA	3:C:88:MET:HE3	1.97	0.45
10:G:601:LMU:O1'	10:G:601:LMU:O5'	2.34	0.45
3:C:74:VAL:HG13	4:D:18:ILE:HG22	1.99	0.45
2:H:101:GLU:O	2:H:104:TRP:NE1	2.50	0.45
1:A:248:GLY:O	1:A:252:MET:HG3	2.16	0.45
1:A:483:TYR:CZ	2:B:261:ALA:HA	2.51	0.45
1:G:400:VAL:HG22	2:H:61:ILE:HG21	1.97	0.45
1:G:417:VAL:HG13	1:G:421:HIS:CE1	2.52	0.45
3:C:236:LYS:HB3	9:C:301:3PE:N	2.31	0.45
3:I:248:HIS:O	3:I:252:VAL:HG23	2.17	0.45
1:A:287:VAL:HB	5:A:602:HEA:CHD	2.45	0.45
1:G:338:ALA:O	1:G:339:GLY:C	2.56	0.45
1:G:249:ALA:HB2	1:G:278:ILE:HG22	2.00	0.45
1:G:360:GLY:O	1:G:363:ILE:HG22	2.16	0.45
10:G:601:LMU:O1B	10:G:601:LMU:O5B	2.35	0.45
2:H:101:GLU:HA	2:H:104:TRP:CE2	2.52	0.44
2:H:104:TRP:C	2:H:104:TRP:CD1	2.91	0.44
2:H:139:THR:HB	2:H:141:TYR:CE2	2.52	0.44
1:A:212:PHE:HE2	1:A:225:VAL:HG11	1.81	0.44
1:G:424:MET:SD	5:G:602:HEA:CBC	3.05	0.44
2:H:130:PRO:HD3	2:H:239:TRP:CD1	2.53	0.44
1:A:40:VAL:HA	1:A:43:ILE:HD12	1.98	0.44
9:A:607:3PE:H292	4:D:31:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:345:GLN:OE1	1:G:408:ARG:NH2	2.46	0.44
1:G:543:THR:HG23	1:G:545:PRO:O	2.17	0.44
2:H:104:TRP:HD1	2:H:105:THR:N	2.15	0.44
1:A:538:LEU:O	1:A:541:THR:OG1	2.34	0.44
5:A:602:HEA:CHC	5:A:602:HEA:CMC	2.96	0.44
9:A:606:3PE:H122	3:C:79:LEU:HD21	1.99	0.44
3:C:77:LEU:O	3:C:81:TRP:HD1	2.01	0.44
1:A:332:ALA:HB3	1:A:348:PHE:CD2	2.52	0.44
5:A:601:HEA:CHC	5:A:601:HEA:C11	2.96	0.44
1:G:352:THR:HG22	5:G:603:HEA:HMB2	1.99	0.44
3:I:108:PRO:HG3	3:I:120:PHE:HB2	1.98	0.44
1:A:46:ALA:O	1:A:49:VAL:HG12	2.18	0.44
1:A:331:TRP:HH2	9:C:302:3PE:H242	1.82	0.44
1:G:99:ILE:HG21	1:G:482:ARG:HG2	1.99	0.44
1:G:332:ALA:HB3	1:G:348:PHE:CD2	2.53	0.44
1:A:187:THR:O	1:A:191:ILE:HG12	2.17	0.43
1:G:156:SER:O	1:G:167:GLY:HA2	2.18	0.43
1:G:472:HIS:O	1:G:476:ARG:HG3	2.18	0.43
1:G:477:GLN:HA	1:G:477:GLN:OE1	2.18	0.43
5:G:603:HEA:CHD	5:G:603:HEA:HAC	2.48	0.43
1:G:420:PHE:HA	1:G:423:VAL:HG12	2.00	0.43
1:A:125:PRO:HG3	1:A:133:MET:SD	2.58	0.43
5:A:601:HEA:CHC	5:A:601:HEA:H11	2.49	0.43
1:G:178:LEU:HA	2:H:215:VAL:HG11	2.00	0.43
1:G:481:ARG:O	2:H:260:HIS:HE1	2.01	0.43
3:I:115:ILE:HG13	3:I:116:ILE:H	1.84	0.43
1:A:219:GLY:HA3	1:A:557:ARG:HE	1.84	0.43
1:A:298:VAL:HG13	1:A:384:ALA:HB1	2.01	0.43
1:A:467:THR:HG23	1:A:501:ALA:HB2	2.00	0.43
3:I:211:PHE:O	3:I:215:VAL:HG23	2.19	0.43
3:I:85:LEU:HA	3:I:88:MET:HE3	2.00	0.43
1:G:51:MET:SD	1:G:99:ILE:HD13	2.59	0.43
1:G:213:LEU:HD13	3:I:81:TRP:HZ3	1.83	0.43
3:C:91:VAL:HG11	9:C:302:3PE:H2H1	2.00	0.43
1:A:314:LEU:HD23	1:A:315:PRO:HD2	2.00	0.43
1:A:436:ILE:O	1:A:440:ILE:HB	2.19	0.43
10:G:601:LMU:C2'	10:G:601:LMU:C5'	2.97	0.43
1:G:477:GLN:HB3	1:G:490:PHE:HE1	1.84	0.42
1:G:424:MET:HA	5:G:603:HEA:CBC	2.48	0.42
5:A:601:HEA:H11	5:A:601:HEA:HHC	2.00	0.42
5:A:602:HEA:H242	2:B:108:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:TRP:CD1	5:G:602:HEA:HAD2	2.54	0.42
3:C:76:ARG:HA	3:C:79:LEU:HD12	2.01	0.42
1:A:349:MET:O	1:A:353:MET:HG3	2.19	0.42
1:G:321:VAL:HG13	9:G:608:3PE:H372	2.02	0.42
1:G:476:ARG:NH2	2:H:58:ASP:OD2	2.52	0.42
1:G:489:ALA:HB3	2:H:36:PRO:HG2	2.01	0.42
2:H:104:TRP:O	2:H:108:PRO:HD2	2.20	0.42
5:A:601:HEA:CHC	5:A:601:HEA:CMC	2.97	0.42
1:G:124:MET:HB3	1:G:125:PRO:HD3	2.01	0.42
1:G:248:GLY:O	1:G:252:MET:HG3	2.19	0.42
2:B:130:PRO:HD3	2:B:239:TRP:CD1	2.54	0.42
2:H:101:GLU:O	2:H:104:TRP:CD1	2.73	0.42
2:H:107:VAL:HB	2:H:108:PRO:HD3	2.01	0.42
1:A:314:LEU:O	1:A:317:VAL:HB	2.20	0.42
1:G:119:PHE:HZ	1:G:436:ILE:HG13	1.85	0.42
1:G:492:THR:OG1	2:H:39:GLY:HA2	2.19	0.42
2:B:62:LEU:HA	2:B:65:ILE:HG12	2.02	0.42
2:H:36:PRO:HD2	2:H:192:LEU:HD11	2.01	0.42
1:G:349:MET:O	1:G:353:MET:HG3	2.19	0.42
2:H:142:GLN:HA	2:H:217:HIS:HE1	1.85	0.42
1:G:46:ALA:O	1:G:49:VAL:HG12	2.19	0.42
3:C:133:LEU:O	3:C:136:ILE:HB	2.20	0.42
3:I:168:LEU:HB2	3:I:224:LEU:HD13	2.02	0.42
1:G:483:TYR:CZ	2:H:261:ALA:HA	2.55	0.42
1:G:545:PRO:HA	1:G:546:PRO:HD3	1.95	0.42
2:B:161:ILE:HD12	2:B:193:ALA:CB	2.50	0.42
2:B:202:VAL:HG13	2:B:269:VAL:HG22	2.02	0.42
1:G:506:ALA:HA	1:G:509:LEU:HD12	2.01	0.41
1:A:482:ARG:HA	5:A:601:HEA:O1A	2.20	0.41
1:G:424:MET:HE2	5:G:603:HEA:HMD3	2.01	0.41
3:I:214:ILE:O	3:I:218:ILE:HG12	2.20	0.41
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.55	0.41
10:G:601:LMU:C4B	10:G:601:LMU:O6B	2.69	0.41
1:A:472:HIS:O	1:A:476:ARG:HG3	2.21	0.41
1:G:235:THR:HG23	1:G:289:ILE:HA	2.01	0.41
1:G:122:TYR:HB3	1:G:123:PHE:CD1	2.55	0.41
1:G:262:THR:OG1	1:G:265:GLN:O	2.38	0.41
1:A:213:LEU:HD13	3:C:81:TRP:HZ3	1.86	0.41
1:G:316:MET:SD	1:G:362:LYS:HG2	2.60	0.41
1:G:340:LEU:HB2	1:G:345:GLN:HG3	2.03	0.41
1:G:187:THR:HB	1:G:257:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:TYR:O	2:H:143:TRP:N	2.54	0.41
2:H:161:ILE:HD12	2:H:193:ALA:CB	2.50	0.41
1:A:117:GLY:O	1:A:121:ASN:HB2	2.21	0.41
1:G:239:ILE:HG13	1:G:289:ILE:HG12	2.02	0.41
1:G:367:ILE:HD11	2:H:72:VAL:HG13	2.02	0.41
3:C:133:LEU:HB3	3:C:134:PRO:HD3	2.03	0.41
2:H:33:ILE:HB	2:H:248:PHE:CE1	2.55	0.41
1:A:284:HIS:O	1:A:285:PRO:C	2.56	0.41
2:H:70:ILE:HG13	2:H:71:PHE:N	2.36	0.41
1:A:489:ALA:HA	2:B:38:PRO:HA	2.03	0.40
5:G:602:HEA:C1D	5:G:602:HEA:C4C	2.97	0.40
3:C:211:PHE:O	3:C:215:VAL:HG23	2.21	0.40
3:I:76:ARG:HA	3:I:79:LEU:HD12	2.03	0.40
1:A:442:LYS:HD3	1:A:540:TRP:CE3	2.56	0.40
1:G:544:SER:OG	1:G:545:PRO:HD3	2.22	0.40
2:B:139:THR:HB	2:B:141:TYR:CE2	2.56	0.40
1:A:352:THR:HG22	5:A:602:HEA:HMB2	2.03	0.40
1:G:19:ARG:O	1:G:23:SER:HB2	2.21	0.40
1:G:212:PHE:HE2	1:G:225:VAL:HG11	1.85	0.40
1:G:382:LEU:HD11	1:G:454:LYS:HG2	2.02	0.40
1:G:401:LEU:C	5:G:603:HEA:HMA	2.41	0.40
1:G:477:GLN:HE21	2:H:37:GLN:H	1.68	0.40
1:G:486:TYR:CD2	1:G:490:PHE:HB2	2.56	0.40
5:G:602:HEA:CHC	5:G:602:HEA:H11	2.51	0.40
2:B:142:GLN:HA	2:B:217:HIS:HE1	1.87	0.40
3:I:128:PHE:CZ	3:I:189:ALA:HA	2.55	0.40
1:G:505:PHE:CE2	1:G:509:LEU:HD11	2.57	0.40
1:G:539:GLU:O	1:G:542:LEU:HD13	2.21	0.40
10:G:601:LMU:O1'	10:G:601:LMU:O2'	2.40	0.40
5:G:602:HEA:H11	5:G:602:HEA:HHC	2.04	0.40
3:C:35:TRP:CD1	3:C:41:PRO:HB3	2.56	0.40
3:C:40:GLY:HA2	3:C:41:PRO:HD2	1.93	0.40
1:A:122:TYR:HB3	1:A:123:PHE:CD1	2.57	0.40
2:H:156:PHE:CD1	2:H:156:PHE:N	2.89	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	25	62
1	G	545/566 (96%)	504 (92%)	39 (7%)	2 (0%)	34	70
2	B	252/262 (96%)	227 (90%)	23 (9%)	2 (1%)	19	57
2	H	251/262 (96%)	220 (88%)	26 (10%)	5 (2%)	7	37
3	C	262/266 (98%)	247 (94%)	15 (6%)	0	100	100
3	I	262/266 (98%)	246 (94%)	15 (6%)	1 (0%)	34	70
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%)	25	62

All (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
1	A	491	ALA
2	B	130	PRO
2	H	99	PRO
2	H	130	PRO
1	A	160	PRO
1	G	160	PRO
2	B	99	PRO
3	I	122	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/459 (94%)	426 (99%)	5 (1%)	71	87
1	G	439/459 (96%)	433 (99%)	6 (1%)	67	85
2	B	199/221 (90%)	199 (100%)	0	100	100
2	H	195/221 (88%)	194 (100%)	1 (0%)	88	95
3	C	200/216 (93%)	200 (100%)	0	100	100
3	I	207/216 (96%)	203 (98%)	4 (2%)	57	80
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%)	1706 (99%)	16 (1%)	78	91

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

Mol	Chain	Res	Type
1	A	282	PHE
1	A	314	LEU
1	A	420	PHE
1	A	485	ASP
1	A	502	PHE
1	G	182	GLU
1	G	282	PHE
1	G	420	PHE
1	G	485	ASP
1	G	502	PHE
1	G	542	LEU
2	H	104	TRP
3	I	114	PRO
3	I	181	PHE
3	I	182	GLN
3	I	256	PHE

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

Mol	Chain	Res	Type
1	A	334	HIS
2	B	217	HIS
2	H	217	HIS
2	H	260	HIS
3	I	157	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	G	609	-	25,25,36	1.28	2 (8%)	36,36,47	0.97	2 (5%)
9	3PE	C	301	-	40,40,50	1.01	3 (7%)	43,45,55	1.09	2 (4%)
9	3PE	A	606	-	20,20,50	1.32	4 (20%)	23,25,55	1.18	2 (8%)
9	3PE	J	101	-	34,34,50	0.98	3 (8%)	37,39,55	1.02	1 (2%)
9	3PE	G	608	-	43,43,50	0.93	3 (6%)	46,48,55	1.08	2 (4%)
9	3PE	I	301	-	39,39,50	1.00	4 (10%)	42,44,55	1.11	2 (4%)
9	3PE	A	607	-	44,44,50	0.92	4 (9%)	47,49,55	1.10	3 (6%)
9	3PE	D	101	-	50,50,50	0.90	3 (6%)	53,55,55	1.06	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEA	G	602	1	44,67,67	4.79	17 (38%)	37,103,103	3.32	22 (59%)
10	LMU	G	601	-	13,13,36	0.63	0	10,10,47	0.55	0
9	3PE	C	302	-	50,50,50	0.88	4 (8%)	53,55,55	1.07	2 (3%)
9	3PE	G	607	-	32,32,50	1.06	3 (9%)	35,37,55	1.10	2 (5%)
9	3PE	I	302	-	31,31,50	1.08	4 (12%)	34,36,55	1.16	2 (5%)
10	LMU	C	303	-	36,36,36	1.23	3 (8%)	47,47,47	1.48	5 (10%)
5	HEA	A	601	1	44,67,67	4.71	16 (36%)	37,103,103	3.15	18 (48%)
5	HEA	A	602	1	44,67,67	5.06	15 (34%)	37,103,103	3.07	14 (37%)
5	HEA	G	603	1	44,67,67	5.06	18 (40%)	37,103,103	2.75	17 (45%)
9	3PE	I	303	-	22,22,50	1.27	4 (18%)	25,27,55	1.13	2 (8%)

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	G	609	-	-	4/10/50/61	0/2/2/2
9	3PE	C	301	-	-	18/44/44/54	-
9	3PE	A	606	-	-	11/24/24/54	-
9	3PE	J	101	-	-	21/37/37/54	-
9	3PE	G	608	-	-	25/47/47/54	-
9	3PE	I	301	-	-	24/43/43/54	-
5	HEA	G	603	1	1/1/7/16	4/24/76/76	-
9	3PE	A	607	-	-	25/48/48/54	-
5	HEA	G	602	1	-	3/24/76/76	-
9	3PE	D	101	-	-	33/54/54/54	-
10	LMU	G	601	-	-	4/8/8/61	-
9	3PE	C	302	-	-	30/54/54/54	-
9	3PE	G	607	-	-	12/36/36/54	-
9	3PE	I	302	-	-	15/35/35/54	-
10	LMU	C	303	-	-	12/21/61/61	0/2/2/2
5	HEA	A	602	1	1/1/7/16	6/24/76/76	-
5	HEA	A	601	1	-	7/24/76/76	-
9	3PE	I	303	-	-	17/26/26/54	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	HEA	C1C-CHC	17.92	1.90	1.41
5	G	603	HEA	C1C-CHC	17.14	1.88	1.41
5	G	602	HEA	C4C-CHD	16.81	1.87	1.41
5	G	603	HEA	C4C-CHD	16.60	1.87	1.41
5	A	601	HEA	C4C-CHD	16.41	1.86	1.41
5	A	602	HEA	C4C-CHD	15.81	1.84	1.41
5	G	602	HEA	C1C-CHC	15.67	1.84	1.41
5	A	601	HEA	C1C-CHC	15.00	1.82	1.41
5	A	602	HEA	C1B-CHB	10.56	1.70	1.41
5	A	601	HEA	C1B-CHB	10.46	1.70	1.41
5	A	602	HEA	C4D-CHA	10.41	1.69	1.41
5	G	602	HEA	C4D-CHA	10.41	1.69	1.41
5	G	603	HEA	C4D-CHA	10.33	1.69	1.41
5	G	602	HEA	C1B-CHB	10.16	1.69	1.41
5	A	601	HEA	C4D-CHA	10.06	1.69	1.41
5	G	603	HEA	C1B-CHB	9.88	1.68	1.41
5	G	603	HEA	C3A-C2A	8.36	1.52	1.40
5	G	602	HEA	C1A-C2A	7.74	1.60	1.42
5	G	603	HEA	C4D-ND	7.59	1.51	1.36
5	A	601	HEA	C1B-NB	7.30	1.51	1.36
5	A	602	HEA	C1B-NB	7.17	1.50	1.36
5	A	602	HEA	C4D-ND	7.01	1.50	1.36
5	A	601	HEA	C1A-C2A	6.52	1.57	1.42
5	G	603	HEA	C1B-NB	6.30	1.49	1.36
5	A	602	HEA	C1A-C2A	6.18	1.56	1.42
5	G	602	HEA	C1B-NB	6.02	1.48	1.36
5	A	602	HEA	C3A-C2A	5.98	1.48	1.40
5	G	603	HEA	C1A-C2A	5.87	1.55	1.42
5	A	602	HEA	C4B-C3B	5.82	1.55	1.42
5	G	603	HEA	C4B-C3B	5.67	1.55	1.42
5	A	601	HEA	C4D-ND	5.40	1.47	1.36
5	A	601	HEA	C4B-C3B	5.38	1.54	1.42
5	A	602	HEA	C1D-C2D	5.22	1.54	1.42
5	G	602	HEA	C1D-C2D	5.03	1.53	1.42
5	G	603	HEA	C1D-C2D	4.85	1.53	1.42
5	G	602	HEA	C3A-C2A	4.76	1.47	1.40
5	A	601	HEA	C3A-C2A	4.73	1.46	1.40
5	G	602	HEA	C4B-C3B	4.57	1.52	1.42
5	A	602	HEA	C1C-NC	4.29	1.45	1.36
10	C	303	LMU	O5'-C1'	4.22	1.52	1.41
5	G	602	HEA	C4D-ND	4.05	1.44	1.36
5	G	602	HEA	C1C-NC	3.84	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	609	LMU	O5B-C1B	3.67	1.51	1.41
5	A	601	HEA	C1D-C2D	3.53	1.50	1.42
5	A	602	HEA	CAD-C3D	3.46	1.57	1.52
10	G	609	LMU	O5'-C1'	3.46	1.50	1.41
5	A	602	HEA	C3B-C11	3.45	1.55	1.52
10	C	303	LMU	O5B-C1B	3.40	1.50	1.41
5	A	601	HEA	C3A-CMA	3.38	1.54	1.46
5	A	601	HEA	C3B-C11	3.34	1.55	1.52
5	G	602	HEA	C4C-NC	3.24	1.42	1.36
5	G	603	HEA	C4C-NC	3.21	1.42	1.36
5	G	603	HEA	C1C-NC	3.19	1.42	1.36
5	G	603	HEA	CAD-C3D	3.08	1.56	1.52
5	G	602	HEA	C3C-C2C	-3.01	1.36	1.40
5	G	603	HEA	CAA-C2A	2.95	1.57	1.52
5	A	602	HEA	C4C-NC	2.89	1.42	1.36
5	G	603	HEA	C3B-C11	2.85	1.55	1.52
5	A	602	HEA	C3C-CAC	2.73	1.53	1.47
5	A	601	HEA	C3C-CAC	2.70	1.53	1.47
9	D	101	3PE	O31-C31	2.68	1.41	1.33
9	C	301	3PE	O31-C31	2.65	1.41	1.33
5	G	602	HEA	C3A-CMA	2.57	1.52	1.46
5	A	601	HEA	CAA-C2A	2.54	1.56	1.52
5	G	602	HEA	C3B-C11	2.52	1.54	1.52
5	G	603	HEA	C16-C15	2.51	1.56	1.51
9	G	608	3PE	O31-C31	2.51	1.40	1.33
9	I	303	3PE	O31-C31	2.51	1.40	1.33
9	A	606	3PE	O21-C2	-2.50	1.40	1.46
5	A	601	HEA	C3C-C2C	-2.48	1.36	1.40
9	I	301	3PE	O31-C31	2.46	1.40	1.33
9	G	607	3PE	O31-C31	2.44	1.40	1.33
5	G	603	HEA	C3A-CMA	2.43	1.52	1.46
9	A	607	3PE	O31-C31	2.42	1.40	1.33
9	A	606	3PE	O31-C31	2.42	1.40	1.33
9	I	301	3PE	O21-C21	2.40	1.41	1.34
9	I	302	3PE	O31-C31	2.40	1.40	1.33
9	I	302	3PE	O21-C21	2.37	1.41	1.34
9	C	301	3PE	O21-C21	2.36	1.41	1.34
9	J	101	3PE	O21-C2	-2.35	1.40	1.46
9	A	607	3PE	O21-C21	2.34	1.40	1.34
9	C	302	3PE	O31-C31	2.34	1.40	1.33
9	C	302	3PE	O21-C21	2.34	1.40	1.34
9	I	303	3PE	O21-C2	-2.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	607	3PE	O21-C21	2.32	1.40	1.34
9	D	101	3PE	O21-C21	2.32	1.40	1.34
9	G	607	3PE	O21-C2	-2.31	1.40	1.46
9	G	608	3PE	O21-C2	-2.30	1.40	1.46
9	A	607	3PE	O21-C2	-2.30	1.40	1.46
5	G	602	HEA	O11-C11	-2.29	1.37	1.42
5	G	603	HEA	C20-C19	2.28	1.56	1.51
9	I	301	3PE	O21-C2	-2.28	1.40	1.46
9	C	301	3PE	O21-C2	-2.26	1.40	1.46
9	C	302	3PE	O21-C2	-2.26	1.40	1.46
9	I	302	3PE	O21-C2	-2.24	1.41	1.46
9	I	303	3PE	O21-C21	2.24	1.40	1.34
9	G	608	3PE	O21-C21	2.21	1.40	1.34
9	D	101	3PE	O21-C2	-2.21	1.41	1.46
9	J	101	3PE	O21-C21	2.19	1.40	1.34
9	C	302	3PE	O31-C3	-2.16	1.40	1.45
9	A	606	3PE	O21-C21	2.15	1.40	1.34
9	A	606	3PE	O31-C3	-2.13	1.40	1.45
9	A	607	3PE	O31-C3	-2.11	1.40	1.45
10	C	303	LMU	O5'-C5'	2.10	1.49	1.44
9	I	302	3PE	O31-C3	-2.09	1.40	1.45
9	J	101	3PE	O31-C3	-2.07	1.40	1.45
9	I	301	3PE	O31-C3	-2.07	1.40	1.45
5	G	602	HEA	C3D-C2D	2.06	1.43	1.37
5	A	601	HEA	C3D-C2D	2.05	1.43	1.37
9	I	303	3PE	O31-C3	-2.03	1.40	1.45

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	602	HEA	CAD-CBD-CGD	-9.48	96.76	112.67
5	A	602	HEA	C3C-C4C-NC	8.94	120.76	109.21
5	A	601	HEA	CAD-CBD-CGD	-8.77	97.96	112.67
5	A	601	HEA	C3C-C4C-NC	7.83	119.34	109.21
5	G	602	HEA	C3C-C4C-NC	7.81	119.31	109.21
5	A	602	HEA	CAD-CBD-CGD	-7.49	100.11	112.67
5	A	602	HEA	CBD-CAD-C3D	7.36	126.06	112.49
5	G	603	HEA	C3C-C4C-NC	6.85	118.07	109.21
5	G	602	HEA	C3A-C4A-NA	6.68	123.56	110.94
5	A	602	HEA	CAA-CBA-CGA	-6.35	102.01	112.67
5	G	602	HEA	C13-C14-C15	-6.09	113.00	127.66
5	G	603	HEA	CAD-CBD-CGD	-5.88	102.81	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEA	C3A-C4A-NA	5.83	121.95	110.94
5	G	603	HEA	C1B-C2B-C3B	-5.38	103.25	107.00
5	A	601	HEA	CBA-CAA-C2A	4.89	121.49	112.48
10	C	303	LMU	O5B-C5B-C4B	4.59	118.02	109.69
5	G	603	HEA	OMA-CMA-C3A	-4.47	115.18	124.91
5	A	602	HEA	C13-C14-C15	-4.19	117.57	127.66
5	G	602	HEA	C16-C17-C18	-4.17	98.18	111.88
5	G	603	HEA	C13-C14-C15	-4.16	117.65	127.66
9	D	101	3PE	O21-C21-C22	4.15	120.45	111.50
9	C	302	3PE	O21-C21-C22	4.15	120.44	111.50
5	G	602	HEA	C1B-C2B-C3B	-4.14	104.12	107.00
9	I	301	3PE	O21-C21-C22	4.12	120.37	111.50
5	A	601	HEA	CAA-CBA-CGA	-4.11	105.77	112.67
10	C	303	LMU	C3B-C4B-C5B	4.10	117.55	110.24
5	G	603	HEA	O11-C11-C3B	-4.03	100.40	112.00
5	A	601	HEA	C1B-C2B-C3B	-4.01	104.20	107.00
5	G	603	HEA	C3A-C4A-NA	4.00	118.49	110.94
10	C	303	LMU	O1B-C4'-C3'	3.96	117.81	107.28
5	A	601	HEA	CMD-C2D-C3D	3.91	132.32	124.94
9	C	301	3PE	O21-C21-C22	3.88	119.86	111.50
9	G	608	3PE	O21-C21-C22	3.86	119.83	111.50
9	J	101	3PE	O21-C21-C22	3.85	119.80	111.50
5	A	602	HEA	C3A-C4A-NA	3.82	118.16	110.94
5	A	601	HEA	CAA-C2A-C3A	-3.75	117.61	126.86
9	G	607	3PE	O21-C21-C22	3.71	119.49	111.50
9	A	607	3PE	O21-C21-C22	3.65	119.36	111.50
5	G	602	HEA	CBA-CAA-C2A	3.63	119.17	112.48
9	I	302	3PE	O21-C21-C22	3.56	120.72	110.80
5	G	602	HEA	C12-C13-C14	3.55	121.61	112.23
5	A	601	HEA	C16-C15-C14	-3.53	113.96	121.12
5	A	601	HEA	C26-C15-C16	3.48	121.12	115.27
9	I	303	3PE	O21-C21-C22	3.44	120.40	110.80
5	G	602	HEA	C13-C12-C11	3.44	119.52	114.35
5	G	602	HEA	C27-C19-C20	3.34	120.89	115.27
5	G	603	HEA	C26-C15-C16	3.32	120.85	115.27
9	A	606	3PE	O31-C31-C32	3.26	119.93	111.38
5	G	603	HEA	CBD-CAD-C3D	3.25	118.48	112.49
5	G	603	HEA	C27-C19-C20	3.24	120.73	115.27
9	A	606	3PE	O21-C21-C22	3.22	119.79	110.80
5	G	602	HEA	C25-C23-C24	3.19	121.66	114.60
5	A	601	HEA	C21-C20-C19	-3.15	102.62	112.98
9	C	301	3PE	O31-C31-C32	3.14	121.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	603	HEA	CMC-C2C-C3C	3.12	130.52	124.68
5	G	602	HEA	CMC-C2C-C3C	3.09	130.46	124.68
5	A	602	HEA	C17-C18-C19	-3.07	120.27	127.66
5	G	603	HEA	C17-C18-C19	-3.05	120.31	127.66
5	A	602	HEA	OMA-CMA-C3A	-2.99	118.40	124.91
5	G	602	HEA	C17-C18-C19	-2.93	120.61	127.66
5	G	602	HEA	C20-C21-C22	-2.91	102.33	111.88
9	I	302	3PE	O31-C31-C32	2.88	120.94	111.91
5	G	603	HEA	CMC-C2C-C1C	-2.83	124.11	128.46
5	A	602	HEA	C26-C15-C16	2.83	120.03	115.27
9	D	101	3PE	O31-C31-C32	2.80	120.70	111.91
9	G	607	3PE	O31-C31-C32	2.79	120.67	111.91
5	A	601	HEA	O11-C11-C12	2.72	120.04	109.55
5	G	603	HEA	CBA-CAA-C2A	-2.69	107.53	112.48
9	I	301	3PE	O31-C31-C32	2.67	120.29	111.91
9	G	608	3PE	O31-C31-C32	2.64	120.19	111.91
9	I	303	3PE	O31-C31-C32	2.63	120.16	111.91
5	A	601	HEA	C16-C17-C18	-2.62	103.26	111.88
5	A	601	HEA	C13-C12-C11	2.62	118.28	114.35
5	A	602	HEA	O11-C11-C3B	-2.61	104.48	112.00
5	A	602	HEA	C12-C13-C14	-2.59	105.41	112.23
5	G	602	HEA	C12-C11-C3B	-2.58	105.79	112.56
10	G	609	LMU	C1B-O1B-C4'	-2.55	111.66	117.96
10	C	303	LMU	C4B-C3B-C2B	2.55	115.27	110.82
9	C	302	3PE	O31-C31-C32	2.54	119.89	111.91
5	G	603	HEA	C21-C22-C23	-2.50	119.21	127.75
5	G	602	HEA	C27-C19-C18	-2.46	117.37	123.68
5	A	602	HEA	C4B-C3B-C2B	-2.46	105.15	106.87
10	C	303	LMU	C6B-C5B-C4B	-2.44	107.28	113.00
10	G	609	LMU	O1'-C1'-C2'	2.42	110.99	108.15
9	A	607	3PE	O31-C31-C32	2.39	119.41	111.91
5	G	602	HEA	CAA-C2A-C3A	-2.28	121.25	126.86
5	A	602	HEA	C27-C19-C20	2.22	119.01	115.27
5	G	602	HEA	O11-C11-C12	2.22	118.11	109.55
5	A	601	HEA	C12-C13-C14	2.21	118.08	112.23
5	A	602	HEA	C17-C16-C15	-2.20	105.74	112.98
5	A	601	HEA	C13-C14-C15	-2.14	122.50	127.66
5	A	601	HEA	C17-C18-C19	-2.14	122.50	127.66
5	G	602	HEA	C24-C23-C22	-2.13	116.49	122.65
9	A	607	3PE	C23-C22-C21	-2.11	105.94	113.62
5	G	602	HEA	OMA-CMA-C3A	-2.08	120.37	124.91
5	G	603	HEA	CAA-C2A-C3A	2.08	131.99	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	603	HEA	C26-C15-C14	-2.08	118.34	123.68
5	G	602	HEA	C4B-C3B-C2B	-2.06	105.43	106.87
5	A	601	HEA	O11-C11-C3B	-2.06	106.06	112.00
5	G	602	HEA	C26-C15-C16	-2.03	111.85	115.27

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	602	HEA	NA
5	G	603	HEA	NA

All (271) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEA	C1A-C2A-CAA-CBA
5	A	601	HEA	C3A-C2A-CAA-CBA
5	A	601	HEA	C3B-C11-C12-C13
5	A	601	HEA	O11-C11-C12-C13
5	A	601	HEA	C11-C12-C13-C14
5	A	602	HEA	C2D-C3D-CAD-CBD
5	A	602	HEA	C4D-C3D-CAD-CBD
5	A	602	HEA	C11-C12-C13-C14
5	A	602	HEA	C19-C20-C21-C22
5	G	602	HEA	C1A-C2A-CAA-CBA
5	G	602	HEA	C3A-C2A-CAA-CBA
5	G	603	HEA	O11-C11-C12-C13
9	A	606	3PE	C11-O13-P-O14
9	A	606	3PE	O11-C1-C2-O21
9	A	607	3PE	C1-O11-P-O14
9	A	607	3PE	C22-C21-O21-C2
9	G	608	3PE	C1-O11-P-O12
9	G	608	3PE	C1-O11-P-O14
9	G	608	3PE	O11-C1-C2-O21
9	C	302	3PE	C1-O11-P-O12
9	C	302	3PE	C1-O11-P-O13
9	C	302	3PE	C1-O11-P-O14
9	C	302	3PE	O13-C11-C12-N
9	D	101	3PE	C1-O11-P-O12
9	D	101	3PE	C1-O11-P-O13
9	D	101	3PE	C1-O11-P-O14
9	D	101	3PE	O13-C11-C12-N
9	I	301	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
9	I	301	3PE	C1-O11-P-O14
9	I	302	3PE	C11-O13-P-O14
9	I	302	3PE	O13-C11-C12-N
9	I	302	3PE	C22-C21-O21-C2
9	I	303	3PE	C1-O11-P-O12
9	I	303	3PE	C1-O11-P-O13
9	I	303	3PE	C1-O11-P-O14
9	I	303	3PE	C11-O13-P-O11
9	I	303	3PE	C11-O13-P-O14
9	I	303	3PE	C22-C21-O21-C2
10	G	601	LMU	O2B-C2B-C3B-C4B
10	C	303	LMU	C2'-C1'-O1'-C1
10	C	303	LMU	O5'-C1'-O1'-C1
9	C	301	3PE	O32-C31-O31-C3
9	I	301	3PE	O32-C31-O31-C3
9	A	607	3PE	O22-C21-O21-C2
9	I	302	3PE	O22-C21-O21-C2
9	I	303	3PE	O22-C21-O21-C2
9	C	301	3PE	C32-C31-O31-C3
9	I	301	3PE	C32-C31-O31-C3
9	G	608	3PE	C32-C31-O31-C3
9	C	301	3PE	O22-C21-O21-C2
9	G	608	3PE	O32-C31-O31-C3
10	G	609	LMU	O5B-C5B-C6B-O6B
9	A	607	3PE	C32-C31-O31-C3
9	D	101	3PE	C32-C31-O31-C3
9	C	301	3PE	C22-C21-O21-C2
9	I	301	3PE	C22-C21-O21-C2
10	C	303	LMU	C3'-C4'-O1B-C1B
10	C	303	LMU	O5B-C5B-C6B-O6B
9	A	607	3PE	O32-C31-O31-C3
10	G	609	LMU	C4B-C5B-C6B-O6B
9	D	101	3PE	O32-C31-O31-C3
9	J	101	3PE	C32-C31-O31-C3
9	A	607	3PE	O11-C1-C2-O21
9	I	301	3PE	O22-C21-O21-C2
9	G	608	3PE	C22-C21-O21-C2
10	G	609	LMU	C4'-C5'-C6'-O6'
9	I	303	3PE	C32-C31-O31-C3
10	G	601	LMU	O1B-C4'-C5'-O5'
9	G	607	3PE	C31-C32-C33-C34
9	I	302	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	C	301	3PE	C21-C22-C23-C24
9	I	303	3PE	C31-C32-C33-C34
9	I	303	3PE	O32-C31-O31-C3
5	A	601	HEA	C15-C16-C17-C18
9	A	606	3PE	C1-O11-P-O13
9	A	606	3PE	C11-O13-P-O11
9	A	607	3PE	C1-O11-P-O13
9	G	608	3PE	C1-O11-P-O13
9	I	301	3PE	C1-O11-P-O13
9	I	302	3PE	C1-O11-P-O13
9	I	302	3PE	C11-O13-P-O11
9	J	101	3PE	C1-O11-P-O13
9	C	302	3PE	C32-C31-O31-C3
9	G	608	3PE	O22-C21-O21-C2
9	J	101	3PE	O32-C31-O31-C3
9	C	302	3PE	C36-C37-C38-C39
9	C	301	3PE	C32-C33-C34-C35
10	C	303	LMU	C11-C10-C9-C8
9	D	101	3PE	C2C-C2D-C2E-C2F
9	G	608	3PE	C2E-C2F-C2G-C2H
9	C	302	3PE	O32-C31-O31-C3
9	A	607	3PE	C28-C29-C2A-C2B
9	J	101	3PE	C2E-C2F-C2G-C2H
9	I	301	3PE	C22-C23-C24-C25
9	C	302	3PE	C28-C29-C2A-C2B
9	D	101	3PE	C3C-C3D-C3E-C3F
10	G	601	LMU	O1B-C4'-C5'-C6'
9	C	302	3PE	C22-C21-O21-C2
9	C	301	3PE	C22-C23-C24-C25
9	C	302	3PE	C31-C32-C33-C34
9	G	608	3PE	C23-C24-C25-C26
9	G	608	3PE	C2A-C2B-C2C-C2D
9	G	608	3PE	C2C-C2D-C2E-C2F
9	A	607	3PE	C38-C39-C3A-C3B
9	I	301	3PE	C35-C36-C37-C38
9	D	101	3PE	C2B-C2C-C2D-C2E
9	A	607	3PE	C25-C26-C27-C28
9	G	608	3PE	C2B-C2C-C2D-C2E
9	C	302	3PE	C3D-C3E-C3F-C3G
9	C	301	3PE	C3A-C3B-C3C-C3D
9	C	302	3PE	C3A-C3B-C3C-C3D
9	J	101	3PE	C2C-C2D-C2E-C2F

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Mol	Chain	Res	Type	Atoms
9	C	302	3PE	O22-C21-O21-C2
9	A	607	3PE	C27-C28-C29-C2A
9	D	101	3PE	C35-C36-C37-C38
9	D	101	3PE	C26-C27-C28-C29
5	A	602	HEA	C18-C19-C20-C21
9	A	607	3PE	C36-C37-C38-C39
9	G	607	3PE	C22-C23-C24-C25
9	C	302	3PE	C3C-C3D-C3E-C3F
9	G	607	3PE	C27-C28-C29-C2A
10	G	609	LMU	O5'-C5'-C6'-O6'
9	G	607	3PE	C32-C31-O31-C3
9	C	302	3PE	C2E-C2F-C2G-C2H
5	A	602	HEA	C27-C19-C20-C21
9	G	607	3PE	O32-C31-O31-C3
9	A	607	3PE	C21-C22-C23-C24
9	A	607	3PE	C2C-C2D-C2E-C2F
9	D	101	3PE	C37-C38-C39-C3A
9	J	101	3PE	C27-C28-C29-C2A
9	J	101	3PE	C22-C21-O21-C2
9	D	101	3PE	O11-C1-C2-O21
9	D	101	3PE	C3B-C3C-C3D-C3E
9	G	608	3PE	C2D-C2E-C2F-C2G
9	J	101	3PE	O22-C21-O21-C2
9	D	101	3PE	C22-C21-O21-C2
9	G	608	3PE	C31-C32-C33-C34
9	A	606	3PE	O11-C1-C2-C3
9	G	608	3PE	O11-C1-C2-C3
9	D	101	3PE	O11-C1-C2-C3
9	I	303	3PE	O11-C1-C2-C3
9	D	101	3PE	C3D-C3E-C3F-C3G
9	D	101	3PE	C27-C28-C29-C2A
9	J	101	3PE	C26-C27-C28-C29
9	C	302	3PE	C21-C22-C23-C24
9	I	301	3PE	C36-C37-C38-C39
9	J	101	3PE	C22-C23-C24-C25
9	I	301	3PE	C39-C3A-C3B-C3C
9	G	608	3PE	C1-C2-C3-O31
9	I	301	3PE	C1-C2-C3-O31
9	A	607	3PE	C24-C25-C26-C27
9	I	303	3PE	C32-C33-C34-C35
9	C	302	3PE	C3E-C3F-C3G-C3H
9	D	101	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	C	301	3PE	C3E-C3F-C3G-C3H
9	I	302	3PE	C38-C39-C3A-C3B
9	G	608	3PE	C38-C39-C3A-C3B
9	I	302	3PE	C36-C37-C38-C39
9	J	101	3PE	O21-C2-C3-O31
9	D	101	3PE	C2A-C2B-C2C-C2D
9	I	301	3PE	C29-C2A-C2B-C2C
10	C	303	LMU	C1-C2-C3-C4
9	C	302	3PE	C27-C28-C29-C2A
9	A	607	3PE	C2E-C2F-C2G-C2H
9	A	607	3PE	O11-C1-C2-C3
9	I	301	3PE	O11-C1-C2-C3
9	A	606	3PE	O13-C11-C12-N
9	J	101	3PE	C21-C22-C23-C24
9	D	101	3PE	O22-C21-O21-C2
9	A	607	3PE	C39-C3A-C3B-C3C
9	G	607	3PE	C1-C2-C3-O31
9	I	303	3PE	C1-C2-C3-O31
9	J	101	3PE	C1-C2-C3-O31
9	D	101	3PE	C22-C23-C24-C25
9	D	101	3PE	C21-C22-C23-C24
9	D	101	3PE	C34-C35-C36-C37
10	G	601	LMU	O2B-C2B-C3B-O3B
9	J	101	3PE	O11-C1-C2-O21
9	I	301	3PE	O21-C2-C3-O31
9	A	607	3PE	C2-C1-O11-P
9	D	101	3PE	C3F-C3G-C3H-C3I
9	C	301	3PE	O11-C1-C2-C3
9	C	301	3PE	C3F-C3G-C3H-C3I
10	C	303	LMU	C7-C8-C9-C10
9	A	607	3PE	C1-C2-C3-O31
9	C	301	3PE	C1-C2-C3-O31
9	C	302	3PE	C2B-C2C-C2D-C2E
9	C	302	3PE	C22-C23-C24-C25
9	A	607	3PE	O21-C2-C3-O31
9	C	301	3PE	O21-C2-C3-O31
10	C	303	LMU	C6-C7-C8-C9
9	I	301	3PE	C24-C25-C26-C27
10	C	303	LMU	C5'-C4'-O1B-C1B
9	D	101	3PE	C29-C2A-C2B-C2C
9	A	607	3PE	C37-C38-C39-C3A
9	A	606	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
9	A	606	3PE	C1-O11-P-O14
9	A	606	3PE	C11-O13-P-O12
9	A	607	3PE	C1-O11-P-O12
9	I	302	3PE	C1-O11-P-O12
9	J	101	3PE	C1-O11-P-O12
9	J	101	3PE	C1-O11-P-O14
9	G	608	3PE	C25-C26-C27-C28
9	D	101	3PE	C2F-C2G-C2H-C2I
9	I	301	3PE	C23-C24-C25-C26
9	I	301	3PE	O11-C1-C2-O21
9	I	303	3PE	O11-C1-C2-O21
9	J	101	3PE	C2A-C2B-C2C-C2D
9	G	607	3PE	O21-C2-C3-O31
9	I	303	3PE	O21-C2-C3-O31
10	C	303	LMU	O1'-C1-C2-C3
9	D	101	3PE	C28-C29-C2A-C2B
9	I	301	3PE	C28-C29-C2A-C2B
9	D	101	3PE	C2D-C2E-C2F-C2G
9	G	608	3PE	O21-C2-C3-O31
9	C	301	3PE	C11-O13-P-O11
9	C	302	3PE	C11-O13-P-O11
9	D	101	3PE	C11-O13-P-O11
9	I	301	3PE	C11-O13-P-O11
9	J	101	3PE	C11-O13-P-O11
9	D	101	3PE	C1-C2-C3-O31
9	C	302	3PE	C23-C24-C25-C26
9	A	606	3PE	O32-C31-C32-C33
9	D	101	3PE	C3A-C3B-C3C-C3D
9	J	101	3PE	O11-C1-C2-C3
9	G	608	3PE	C29-C2A-C2B-C2C
9	I	301	3PE	C3-C2-O21-C21
9	C	302	3PE	C39-C3A-C3B-C3C
9	I	301	3PE	C3A-C3B-C3C-C3D
9	A	606	3PE	O31-C31-C32-C33
9	A	607	3PE	C26-C27-C28-C29
9	G	607	3PE	C23-C24-C25-C26
9	J	101	3PE	C2D-C2E-C2F-C2G
9	G	607	3PE	C24-C25-C26-C27
10	C	303	LMU	C4'-C5'-C6'-O6'
9	A	607	3PE	C2A-C2B-C2C-C2D
9	I	302	3PE	C39-C3A-C3B-C3C
5	G	602	HEA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
5	G	603	HEA	C19-C20-C21-C22
9	J	101	3PE	O13-C11-C12-N
9	C	301	3PE	C33-C34-C35-C36
9	I	303	3PE	O31-C31-C32-C33
9	C	302	3PE	O31-C31-C32-C33
9	I	302	3PE	C3A-C3B-C3C-C3D
9	G	608	3PE	O21-C21-C22-C23
9	G	608	3PE	C21-C22-C23-C24
9	C	302	3PE	C33-C34-C35-C36
9	I	302	3PE	C37-C38-C39-C3A
5	G	603	HEA	C27-C19-C20-C21
9	G	608	3PE	C35-C36-C37-C38
9	C	302	3PE	O32-C31-C32-C33
10	C	303	LMU	C4B-C5B-C6B-O6B
9	C	302	3PE	C3B-C3C-C3D-C3E
9	C	302	3PE	C2D-C2E-C2F-C2G
9	I	302	3PE	O31-C31-C32-C33
9	G	607	3PE	C11-O13-P-O12
9	C	301	3PE	C1-O11-P-O14
9	C	302	3PE	C11-O13-P-O14
9	G	608	3PE	O22-C21-C22-C23
9	I	303	3PE	O32-C31-C32-C33
9	C	302	3PE	C2A-C2B-C2C-C2D
9	I	301	3PE	C1-C2-O21-C21
9	C	301	3PE	C39-C3A-C3B-C3C
5	G	603	HEA	C26-C15-C16-C17
9	C	301	3PE	C25-C26-C27-C28
9	I	302	3PE	O32-C31-C32-C33
5	A	601	HEA	C20-C21-C22-C23
9	G	607	3PE	O31-C31-C32-C33
9	D	101	3PE	O21-C21-C22-C23
9	I	301	3PE	O21-C21-C22-C23
9	G	607	3PE	O32-C31-C32-C33

There are no ring outliers.

15 monomers are involved in 122 short contacts:

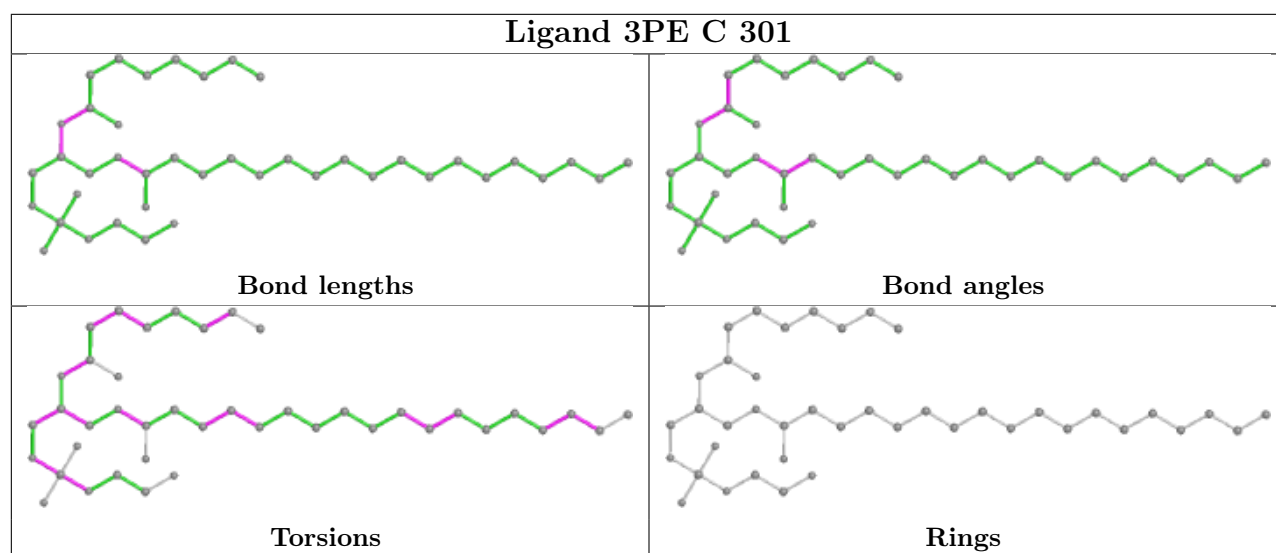
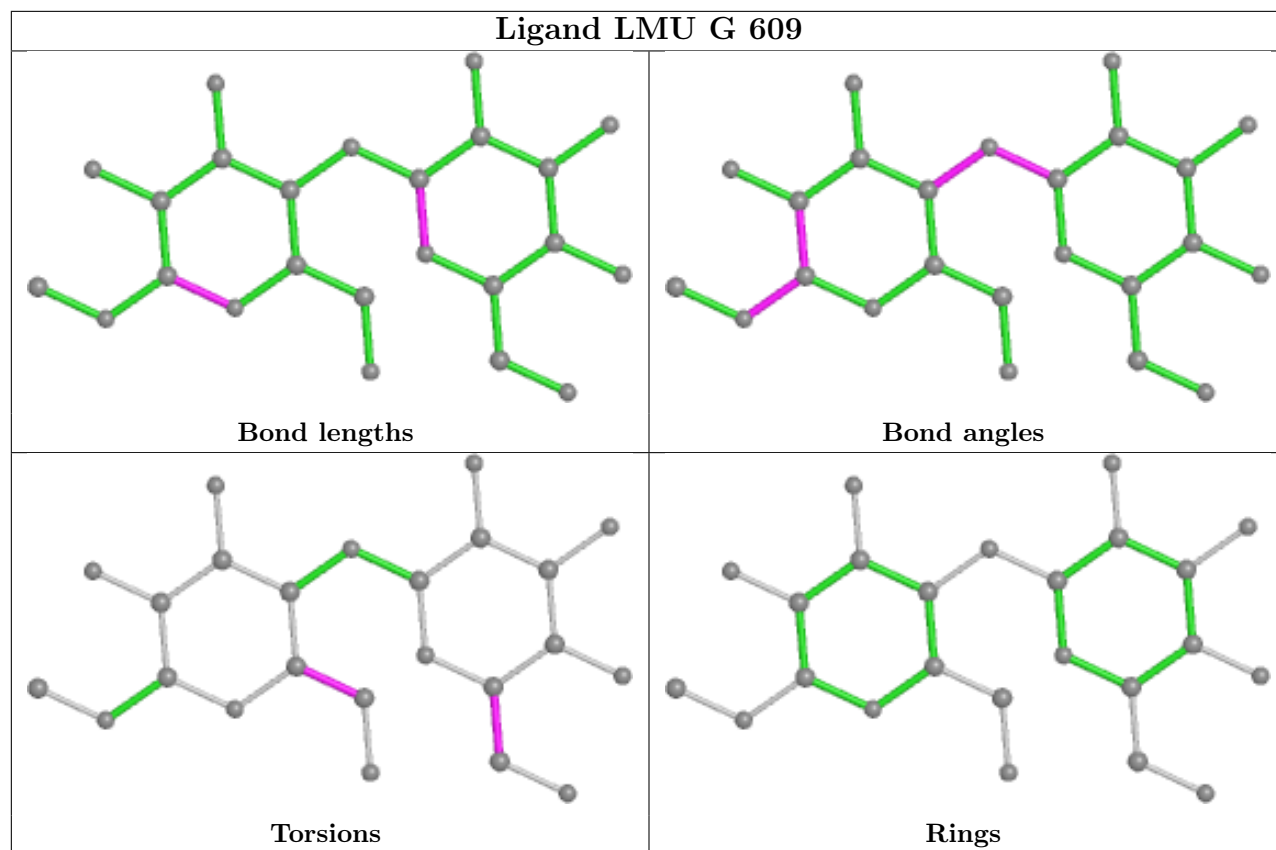
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	301	3PE	4	0
9	A	606	3PE	2	0
9	J	101	3PE	1	0
9	G	608	3PE	2	0

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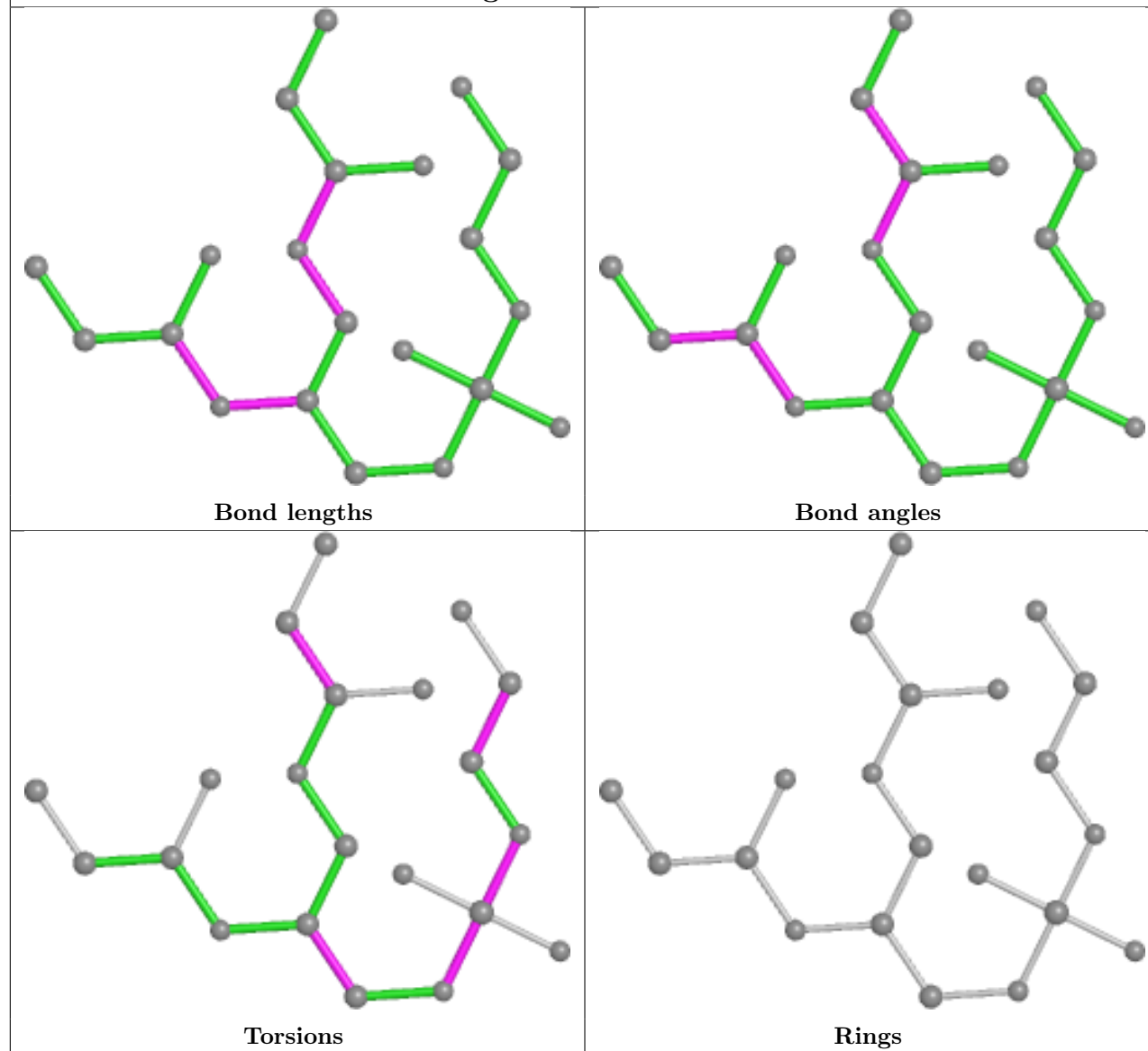
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	301	3PE	2	0
9	A	607	3PE	4	0
9	D	101	3PE	1	0
5	G	602	HEA	23	0
10	G	601	LMU	15	0
9	C	302	3PE	6	0
10	C	303	LMU	2	0
5	A	601	HEA	19	0
5	A	602	HEA	24	0
5	G	603	HEA	19	0
9	I	303	3PE	1	0

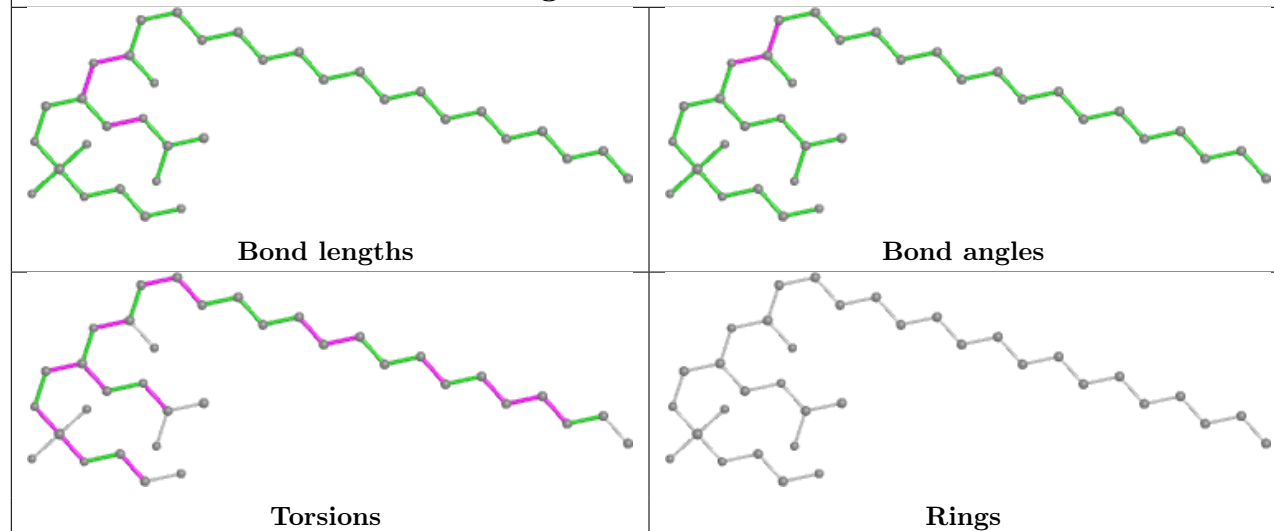
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

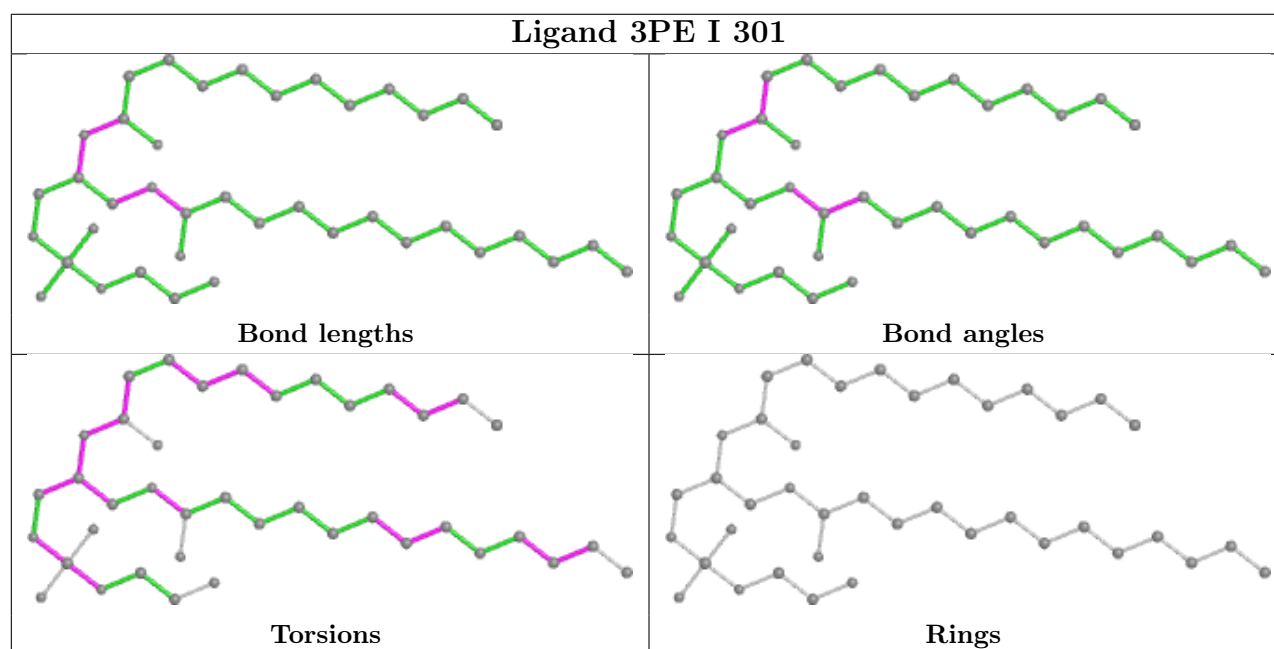
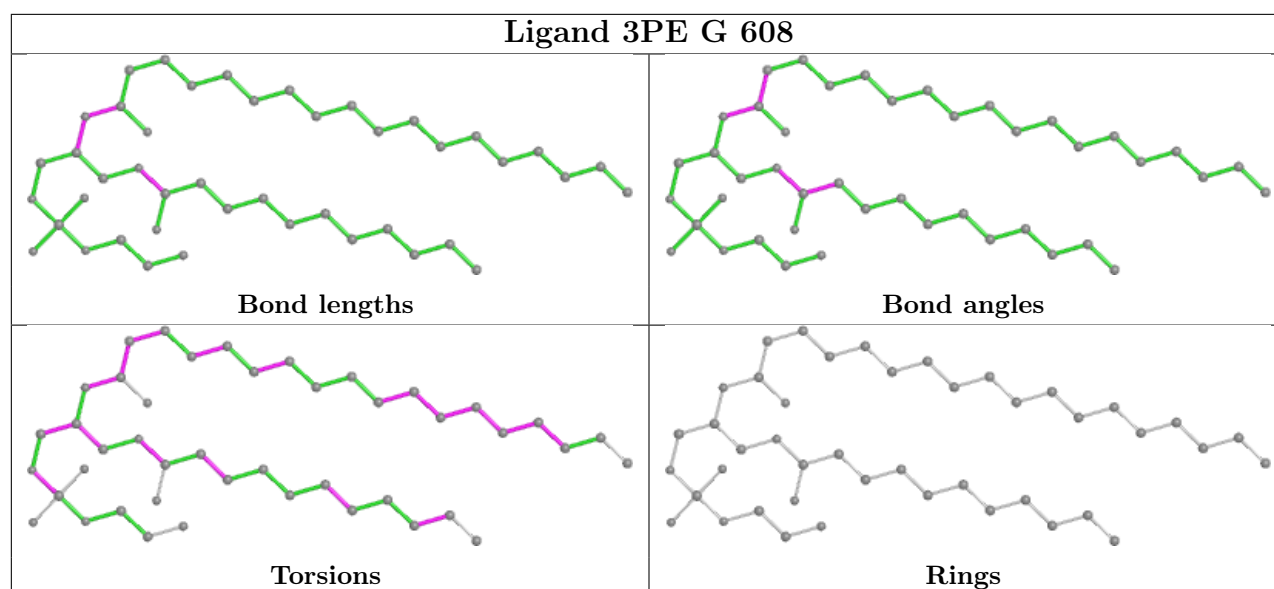


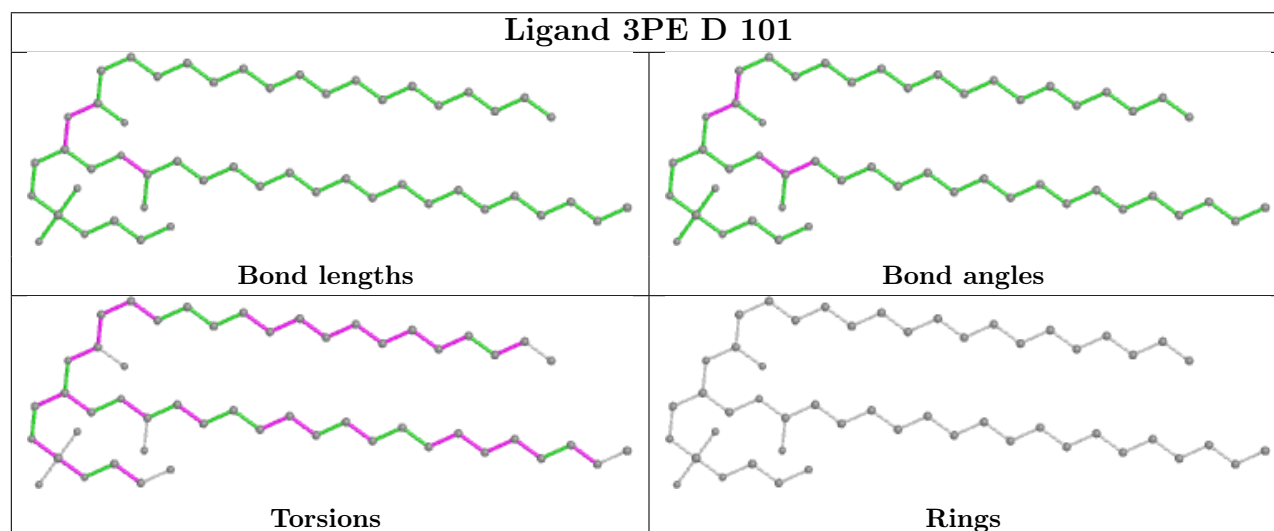
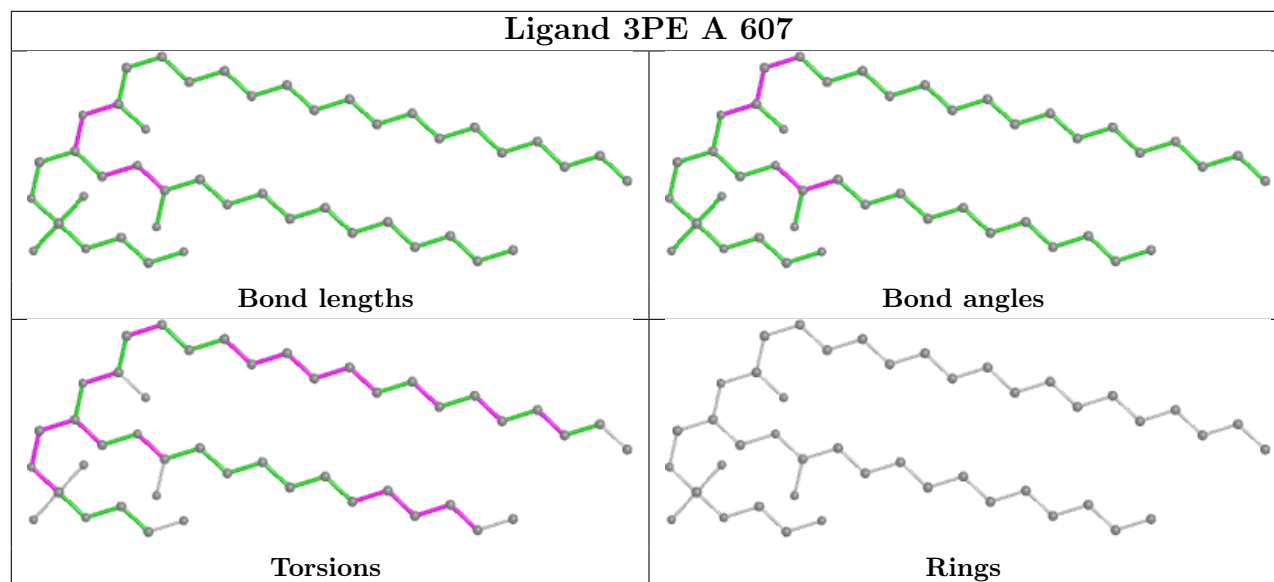
## Ligand 3PE A 606

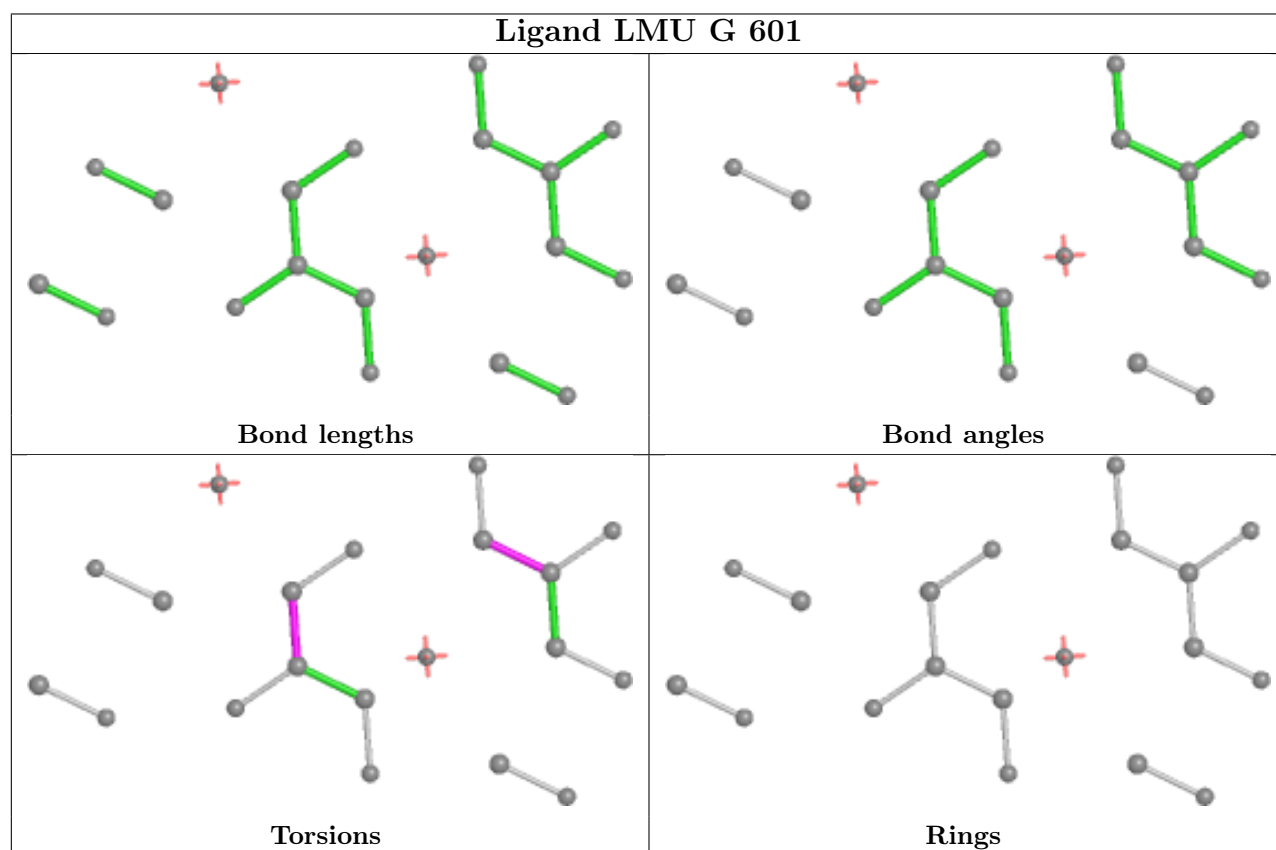
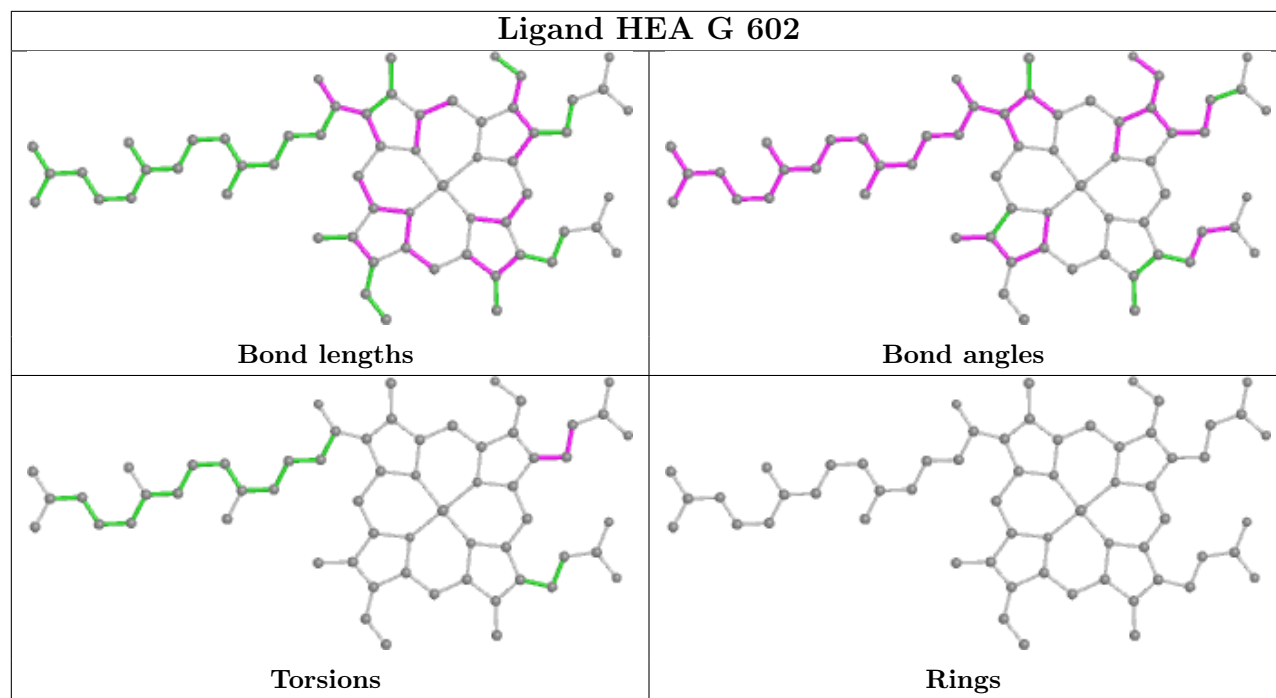


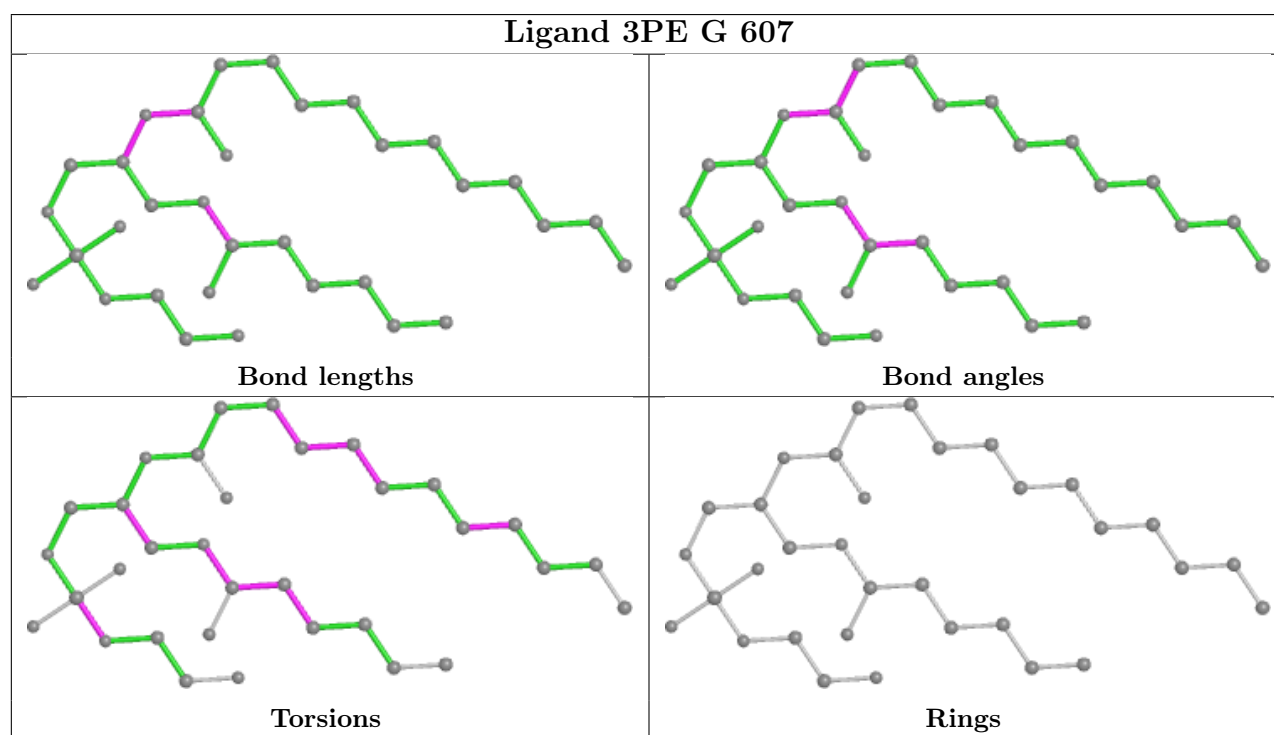
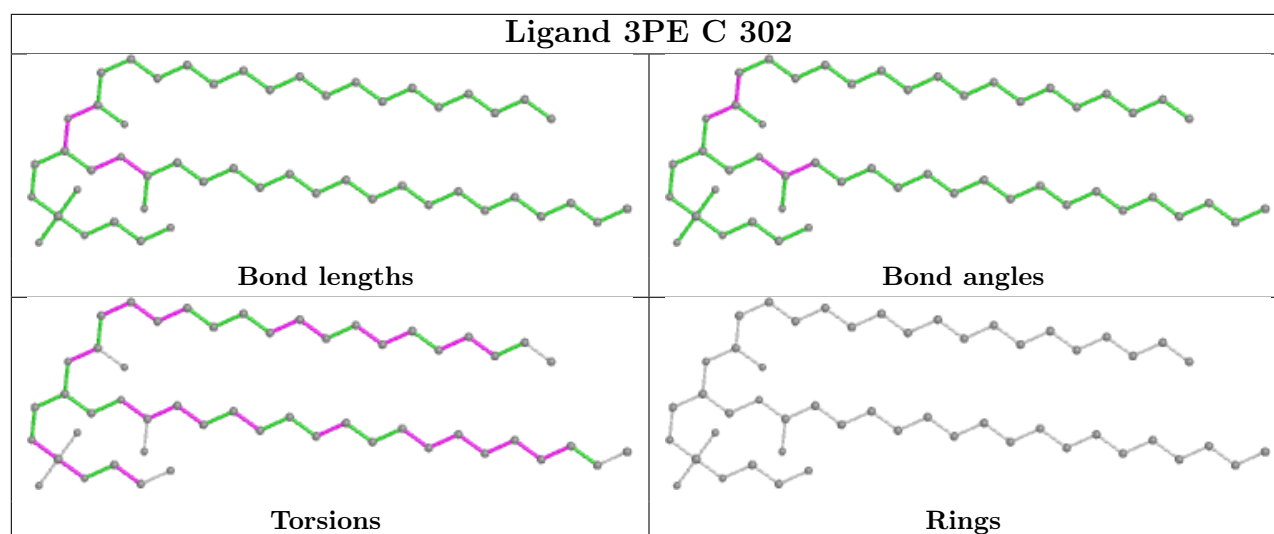
## Ligand 3PE J 101





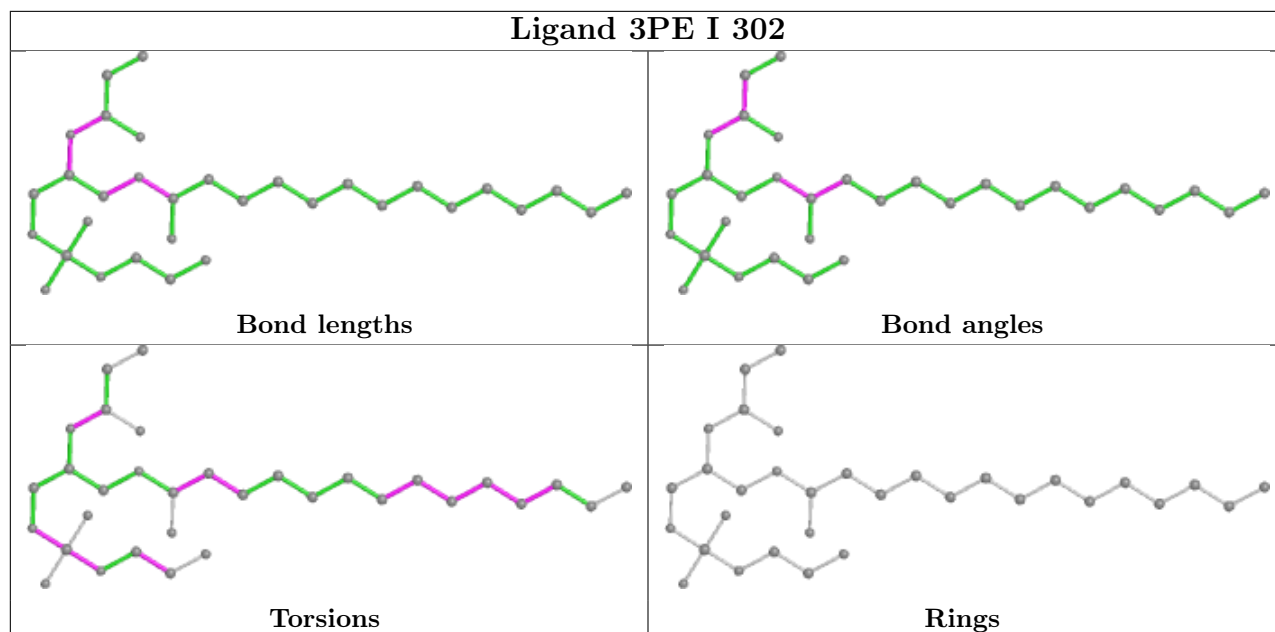




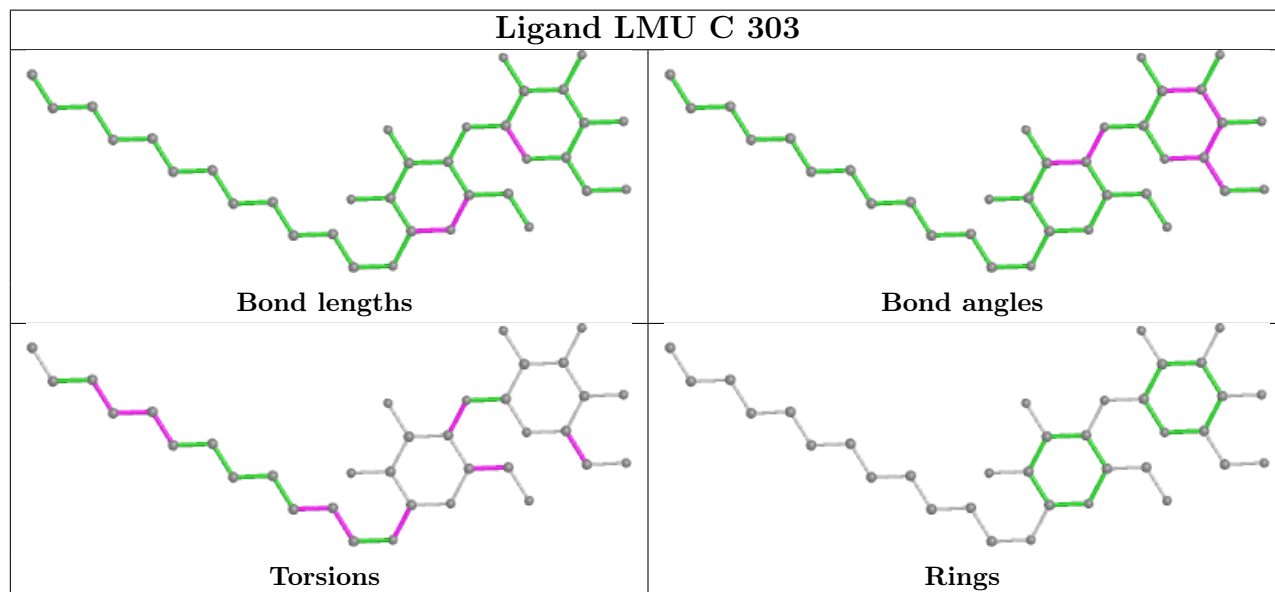


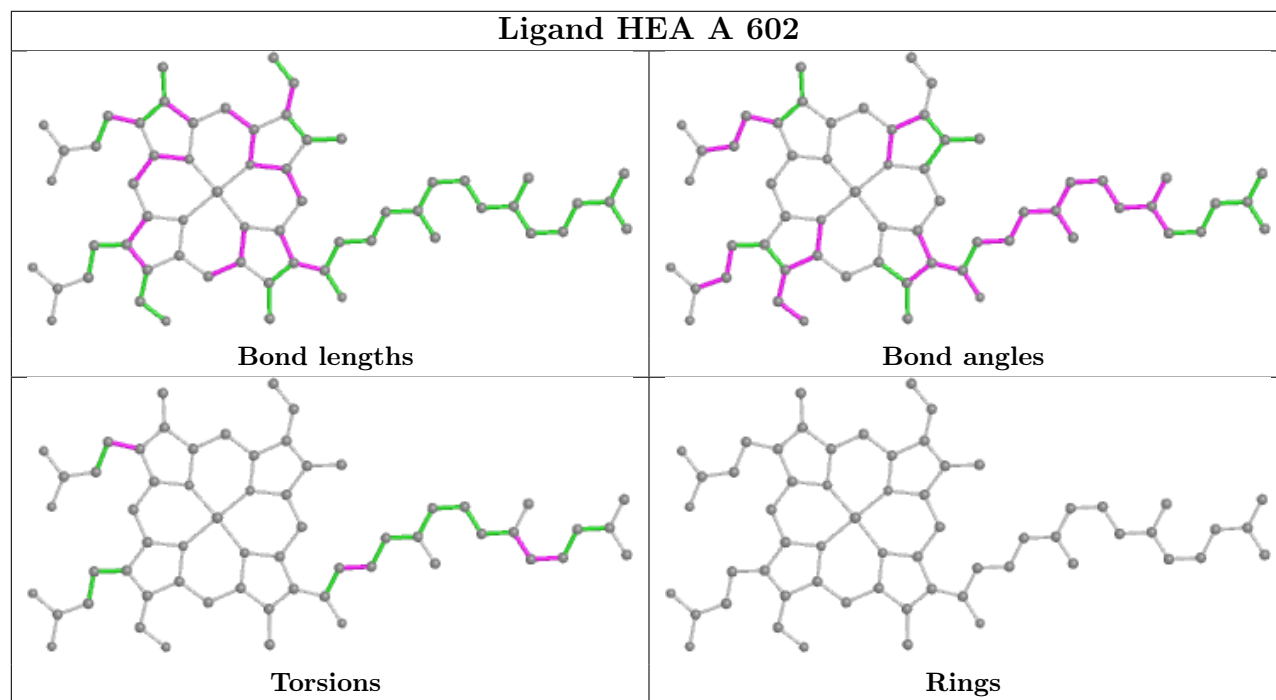
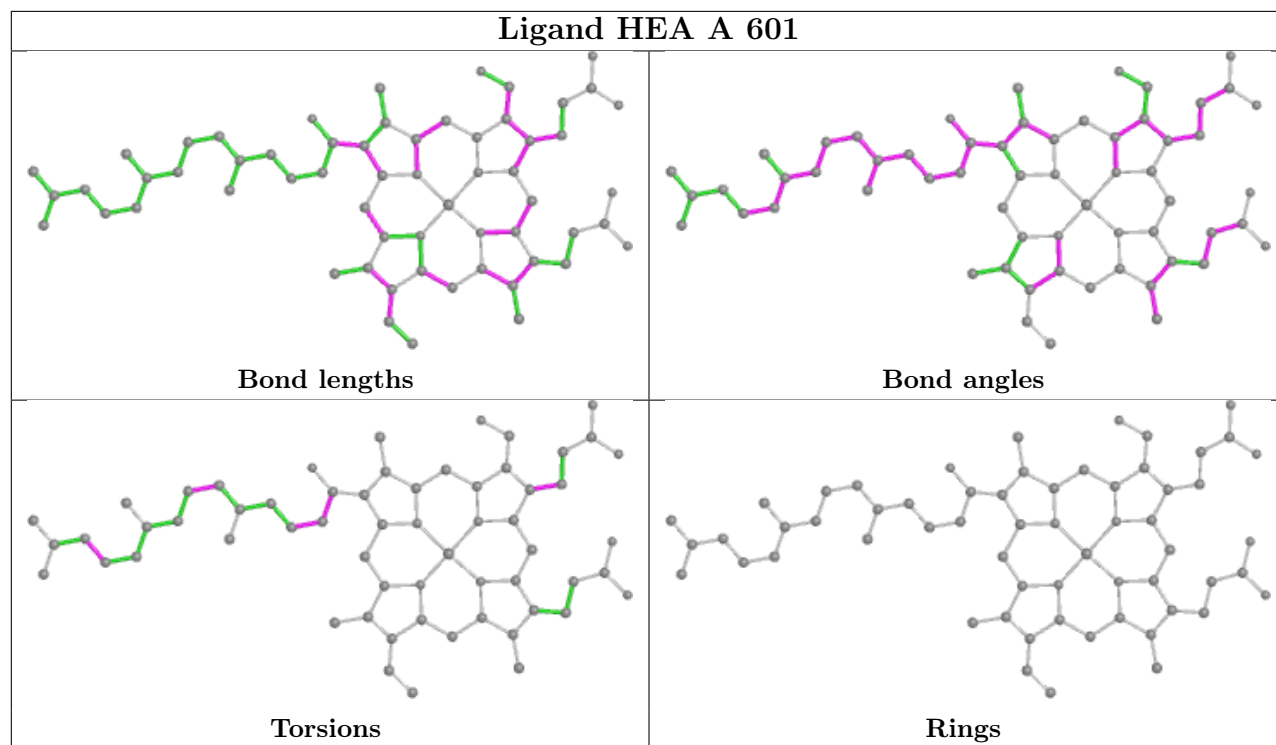


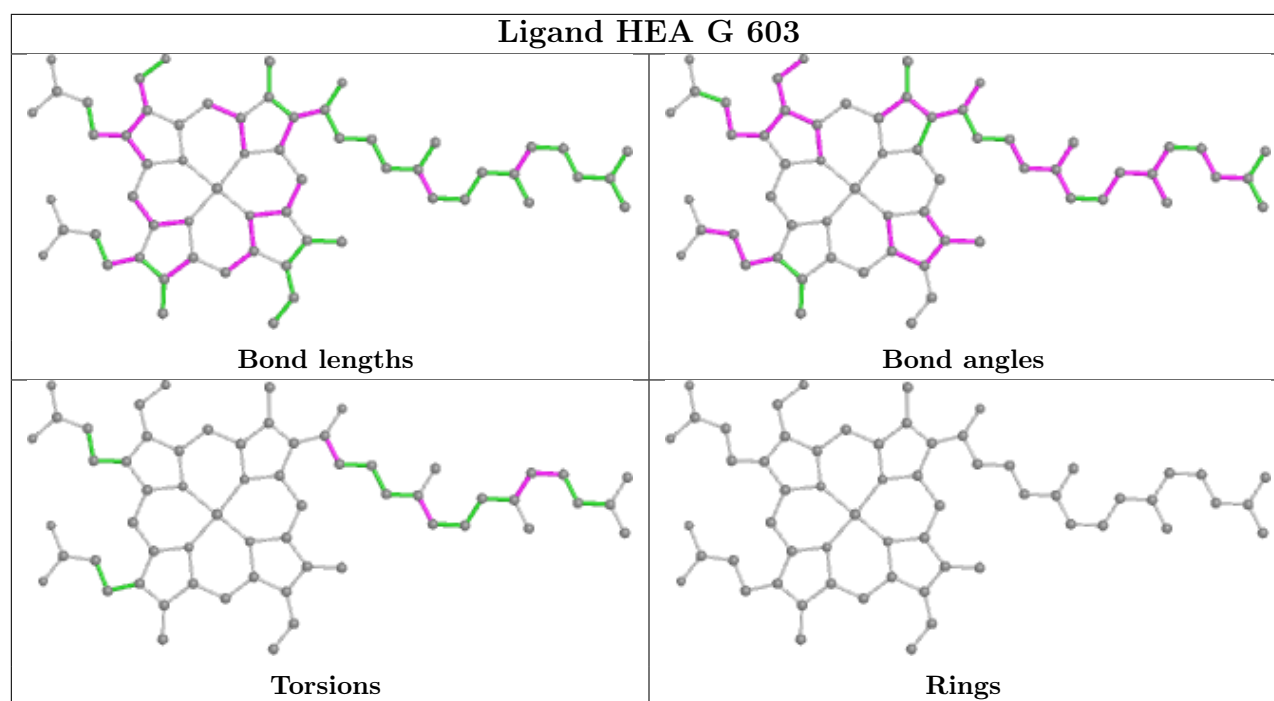
## Ligand 3PE I 302

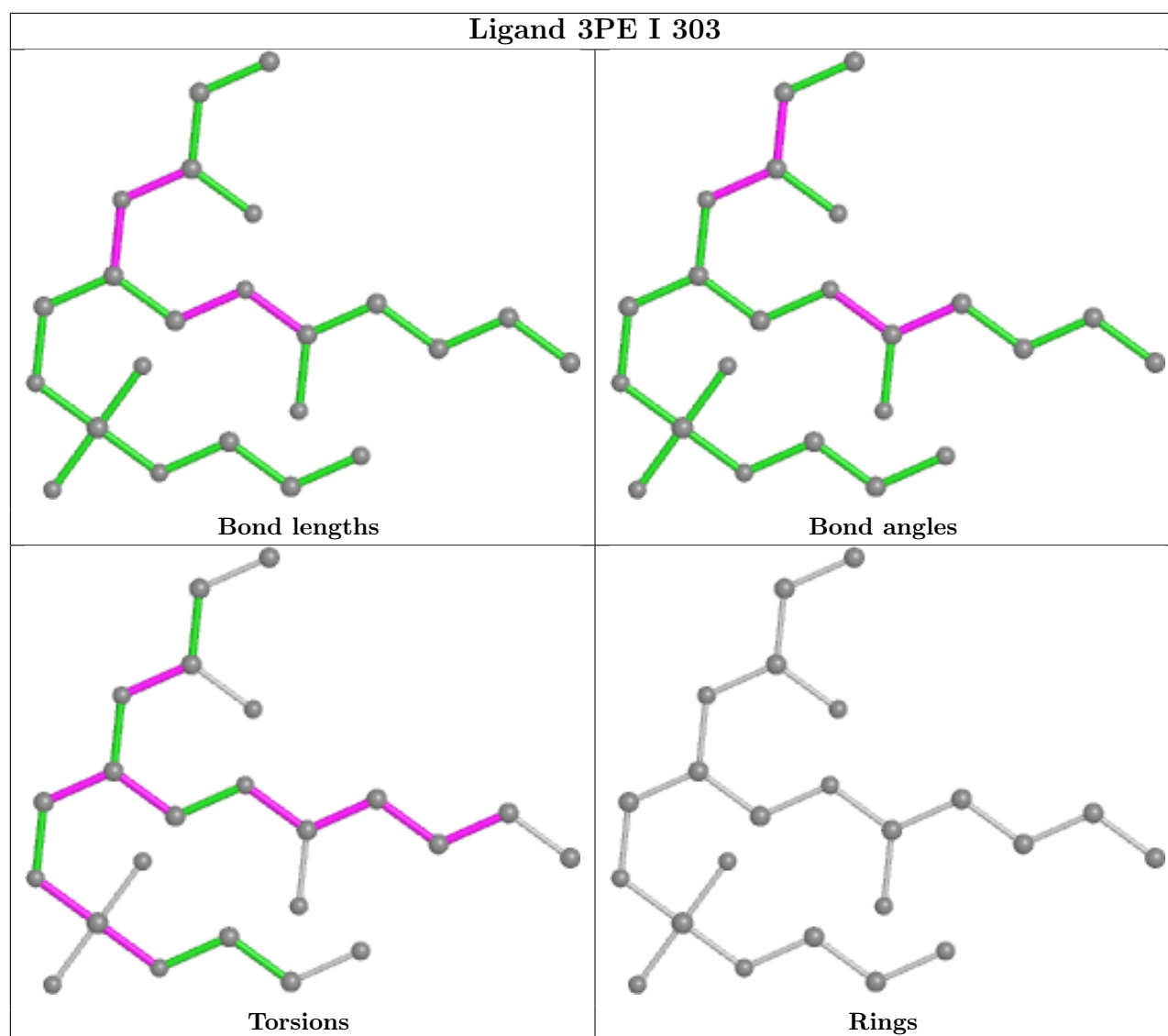


## Ligand LMU C 303









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	547/566 (96%)	0.05	15 (2%) 54 52	76, 103, 142, 188	0
1	G	547/566 (96%)	-0.02	8 (1%) 73 71	75, 103, 136, 180	0
2	B	254/262 (96%)	0.31	18 (7%) 16 18	83, 118, 152, 165	0
2	H	253/262 (96%)	0.59	31 (12%) 4 6	95, 135, 168, 178	0
3	C	264/266 (99%)	0.42	18 (6%) 17 19	92, 135, 168, 185	0
3	I	264/266 (99%)	-0.02	7 (2%) 54 52	79, 115, 151, 179	0
4	D	40/50 (80%)	0.14	1 (2%) 57 54	90, 120, 148, 160	0
4	J	42/50 (84%)	-0.17	2 (4%) 30 30	88, 114, 143, 166	0
All	All	2211/2288 (96%)	0.16	100 (4%) 33 32	75, 113, 157, 188	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	42	TRP	5.1
2	H	250	GLY	5.0
3	C	163	ASP	4.7
2	H	132	ALA	4.3
3	C	159	ASN	4.0
2	H	173	SER	3.9
3	C	3	HIS	3.8
2	H	94	PHE	3.7
1	A	69	GLU	3.7
2	H	41	THR	3.6
2	B	40	GLY	3.6
2	H	96	HIS	3.6
3	C	67	LEU	3.4
2	H	220	THR	3.3
3	C	160	ASN	3.3
4	J	51	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	130	PRO	3.1
3	I	41	PRO	3.1
2	H	176	VAL	3.1
2	B	204	LYS	3.1
1	A	15	GLY	3.0
3	C	184	TYR	3.0
1	G	374	SER	3.0
3	C	4	ALA	3.0
1	G	336	TYR	3.0
2	H	226	VAL	3.0
2	B	87	ARG	3.0
3	I	111	PRO	2.9
1	G	412	ASP	2.9
2	H	97	ASN	2.9
3	C	217	THR	2.8
2	H	133	ASP	2.8
1	G	296	GLY	2.8
2	B	41	THR	2.8
2	H	175	GLU	2.8
2	B	275	TYR	2.7
2	H	221	VAL	2.7
2	B	81	TRP	2.7
1	A	70	SER	2.7
3	C	154	ALA	2.7
1	A	218	PRO	2.6
1	A	296	GLY	2.6
2	H	131	GLU	2.6
3	I	110	GLY	2.6
2	H	165	ALA	2.6
3	C	40	GLY	2.5
2	H	87	ARG	2.5
2	H	161	ILE	2.5
1	A	73	VAL	2.5
2	H	145	TRP	2.5
3	C	158	GLU	2.5
2	B	173	SER	2.5
2	B	220	THR	2.5
2	H	95	THR	2.5
3	C	37	HIS	2.5
2	H	130	PRO	2.5
1	A	544	SER	2.5
3	C	131	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	241	ARG	2.4
2	B	98	SER	2.4
2	H	159	TYR	2.4
3	C	129	ASP	2.4
2	H	181	ILE	2.4
2	B	172	MET	2.4
1	A	87	ASN	2.4
1	A	80	LEU	2.4
2	H	249	PHE	2.4
2	H	56	TRP	2.3
2	H	242	ALA	2.3
1	A	79	SER	2.3
3	I	40	GLY	2.3
4	D	15	SER	2.3
2	B	97	ASN	2.3
3	I	4	ALA	2.3
3	C	157	HIS	2.3
2	H	88	ASN	2.3
2	B	99	PRO	2.3
2	B	38	PRO	2.2
2	B	227	LYS	2.2
2	B	39	GLY	2.2
2	H	228	GLN	2.2
1	A	451	TRP	2.2
1	G	72	LEU	2.2
4	J	10	GLY	2.2
3	I	184	TYR	2.2
1	G	185	TYR	2.2
2	H	40	GLY	2.1
1	A	83	SER	2.1
2	B	245	GLU	2.1
1	G	171	GLY	2.1
1	G	371	TRP	2.1
2	B	96	HIS	2.1
1	A	77	PHE	2.0
1	A	78	GLN	2.0
2	H	251	GLN	2.0
3	C	153	HIS	2.0
2	H	235	LEU	2.0
1	A	82	PRO	2.0
2	B	203	ASN	2.0
3	I	45	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	LMU	G	609	24/35	0.51	0.44	131,164,170,176	0
9	3PE	I	303	23/51	0.56	0.43	101,155,183,196	0
10	LMU	G	601	20/35	0.62	0.31	84,115,124,143	5
7	MG	G	605	1/1	0.66	0.58	86,86,86,86	0
9	3PE	C	301	41/51	0.74	0.48	100,157,200,216	0
9	3PE	I	302	32/51	0.78	0.34	86,124,183,198	0
10	LMU	C	303	35/35	0.79	0.38	108,150,203,214	0
8	CA	A	605	1/1	0.80	0.13	102,102,102,102	0
9	3PE	C	302	51/51	0.81	0.36	92,111,150,185	0
9	3PE	A	607	45/51	0.82	0.48	65,93,109,138	45
6	CU1	G	604	1/1	0.82	0.11	94,94,94,94	0
9	3PE	G	608	44/51	0.84	0.39	78,110,175,179	0
9	3PE	A	606	21/51	0.85	0.32	97,112,119,134	21
9	3PE	I	301	40/51	0.86	0.34	88,112,150,154	0
7	MG	A	604	1/1	0.86	0.58	95,95,95,95	0
9	3PE	J	101	35/51	0.89	0.38	97,123,164,172	0
9	3PE	D	101	51/51	0.89	0.31	74,105,145,150	0
9	3PE	G	607	33/51	0.90	0.33	70,82,98,107	0
6	CU1	H	302	1/1	0.90	0.22	107,107,107,107	0
8	CA	G	606	1/1	0.92	0.10	103,103,103,103	0
5	HEA	G	603	60/60	0.92	0.26	94,105,122,134	0
5	HEA	A	602	60/60	0.92	0.29	87,97,105,113	0
5	HEA	G	602	60/60	0.93	0.30	83,95,104,106	0
5	HEA	A	601	60/60	0.93	0.30	86,98,107,127	0
6	CU1	A	603	1/1	0.94	0.14	81,81,81,81	0
6	CU1	B	301	1/1	0.96	0.26	105,105,105,105	0
6	CU1	H	301	1/1	0.98	0.16	117,117,117,117	0

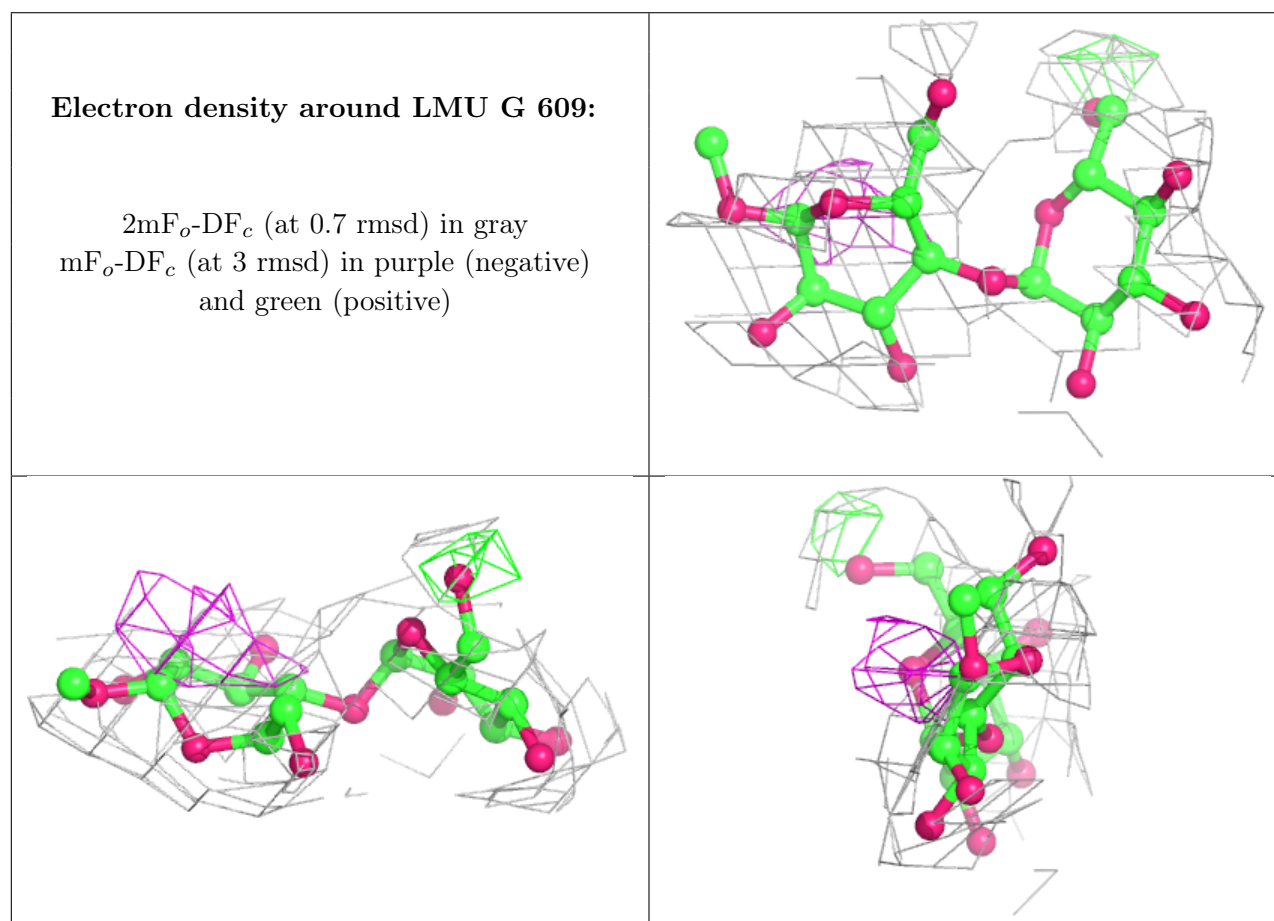
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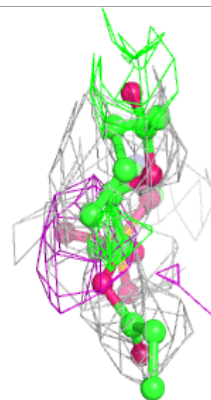
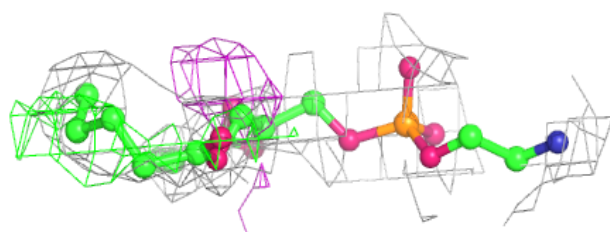
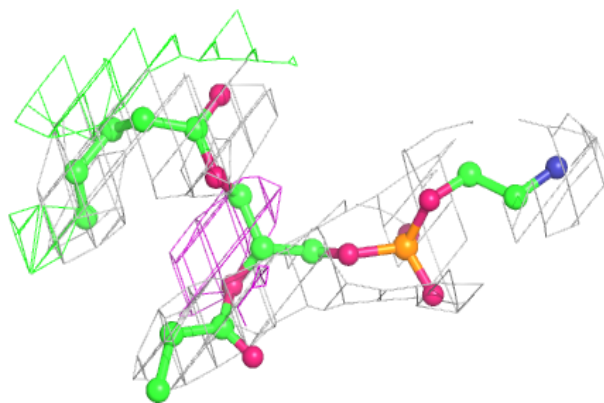
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CU1	B	302	1/1	0.98	0.17	102,102,102,102	0

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.

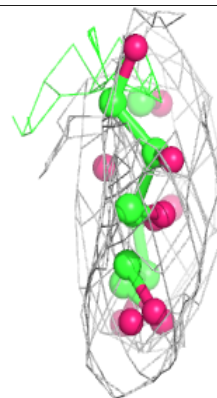
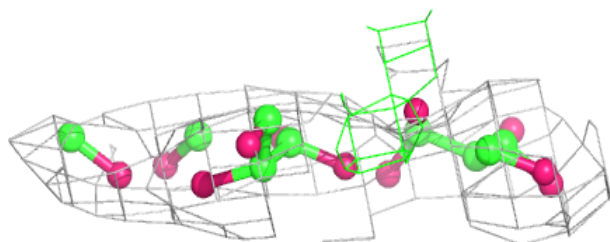
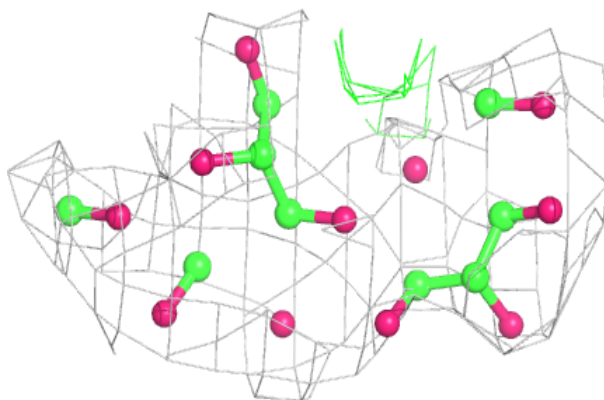


**Electron density around 3PE I 303:**

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

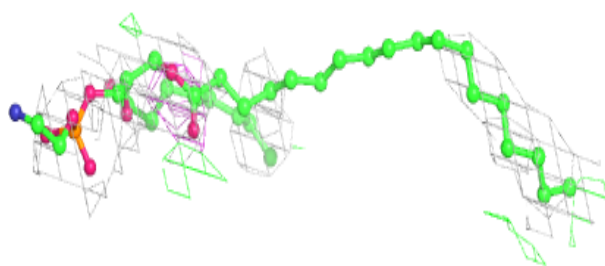
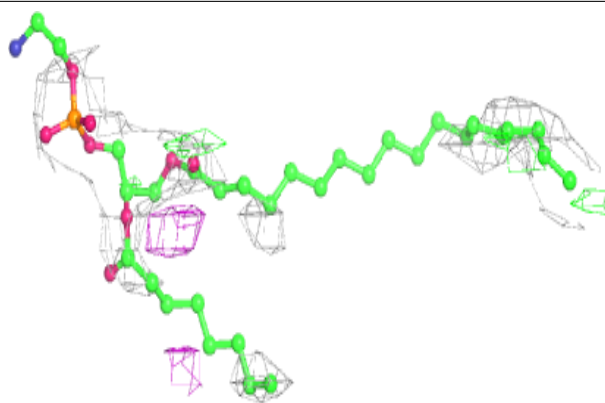
**Electron density around LMU G 601:**

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

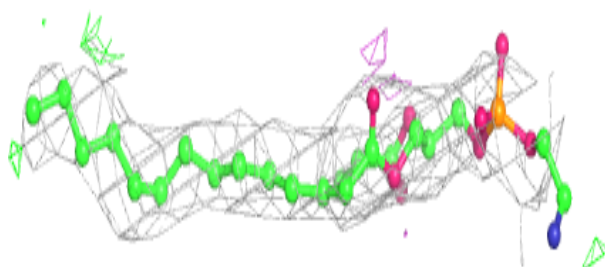
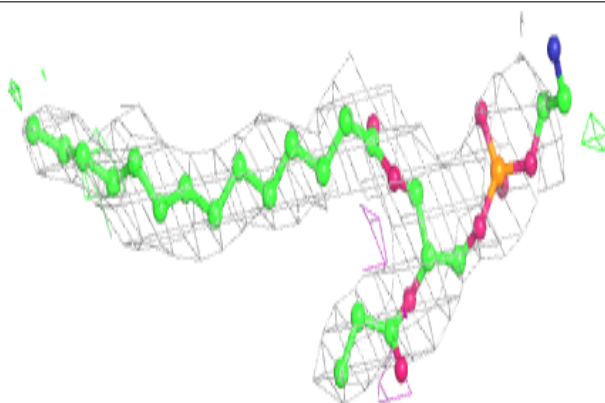


**Electron density around 3PE C 301:**

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

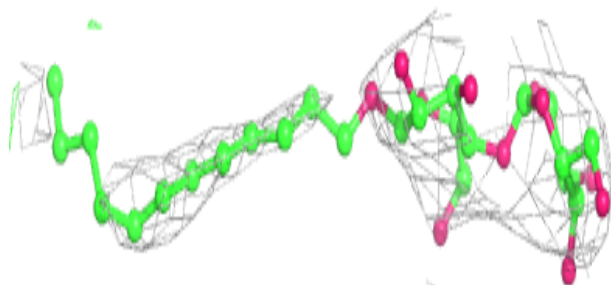
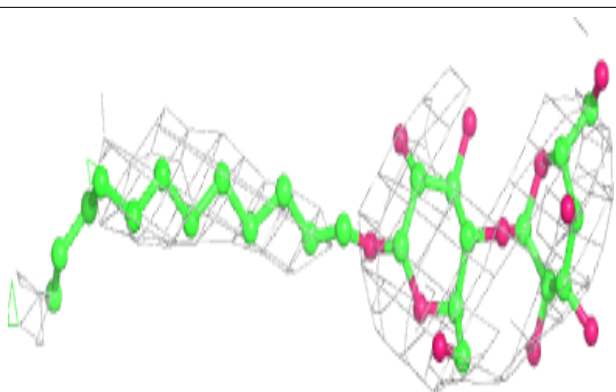
**Electron density around 3PE I 302:**

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

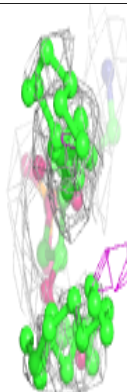
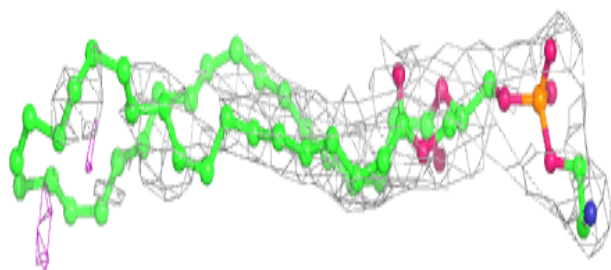
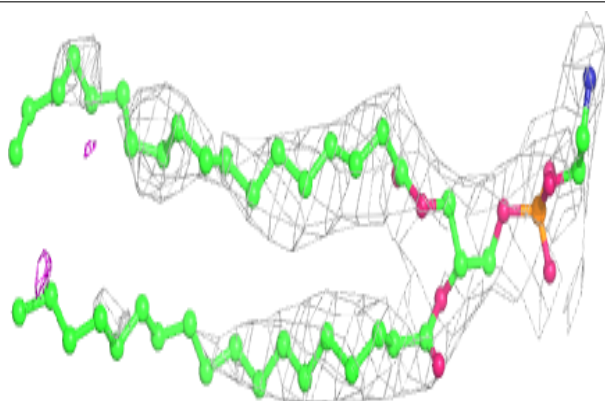


**Electron density around LMU C 303:**

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

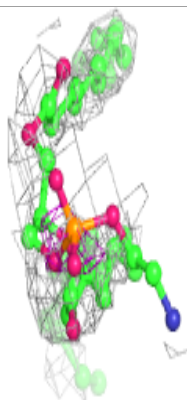
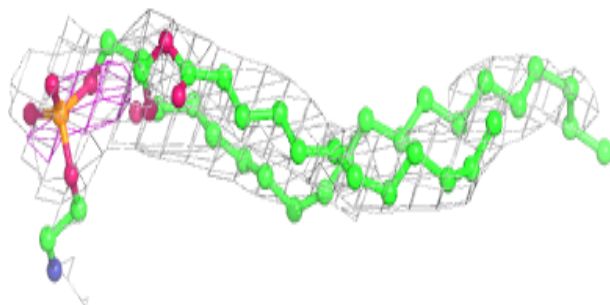
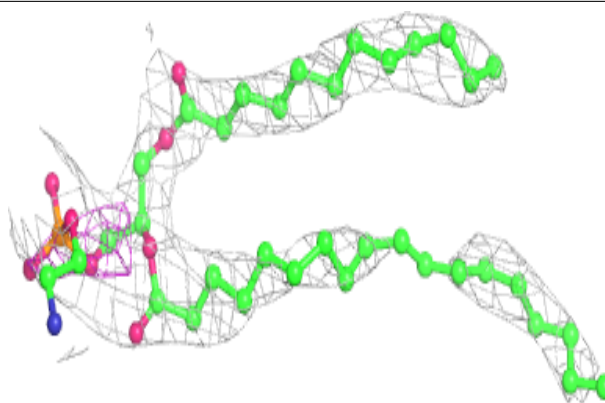
**Electron density around 3PE C 302:**

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

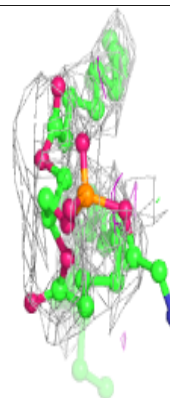
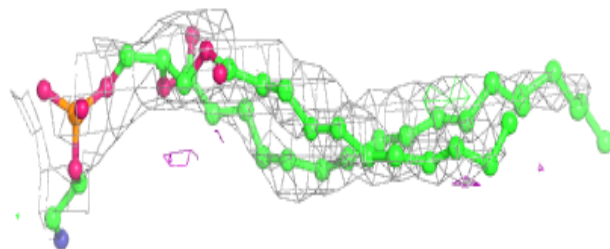
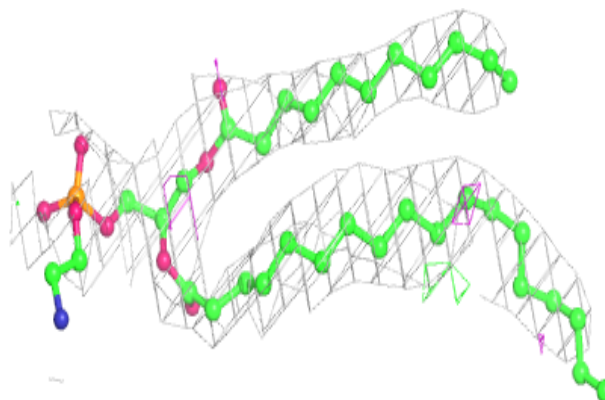


**Electron density around 3PE A 607:**

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

**Electron density around 3PE G 608:**

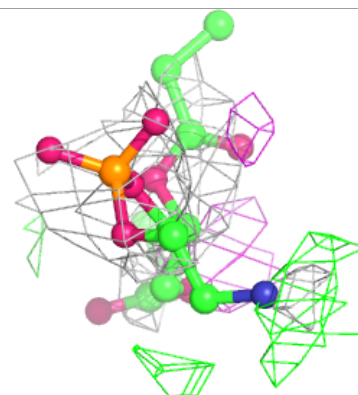
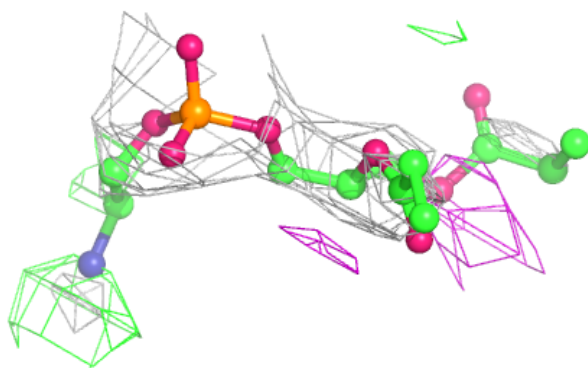
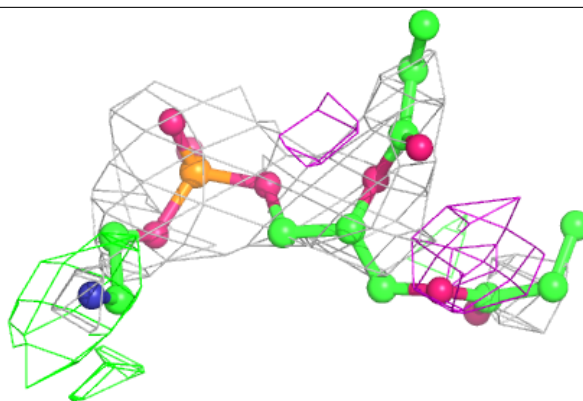
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



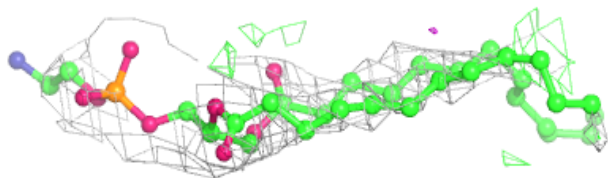
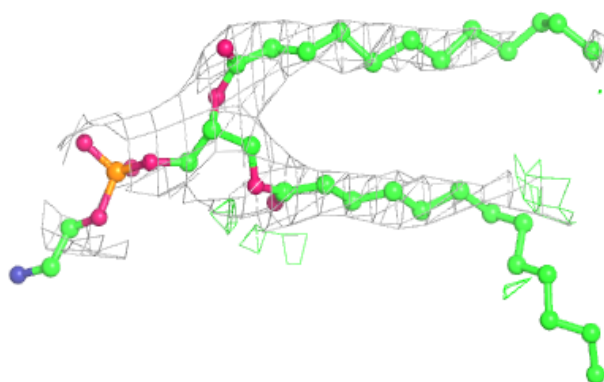


**Electron density around 3PE A 606:**

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

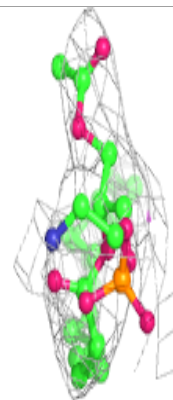
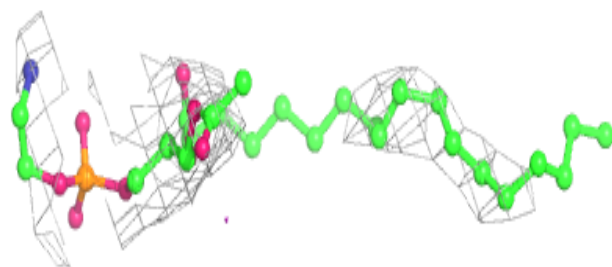
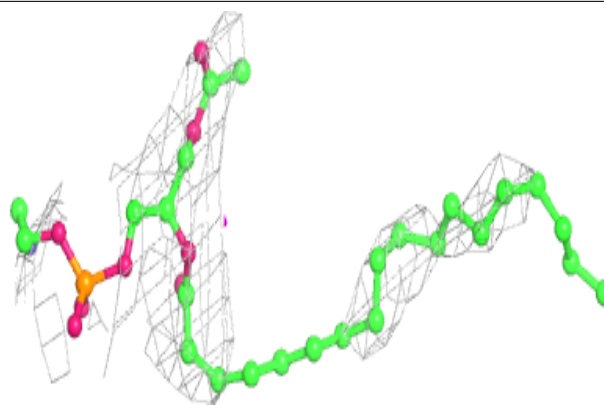
**Electron density around 3PE I 301:**

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



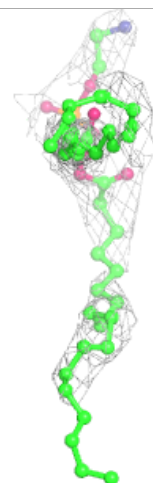
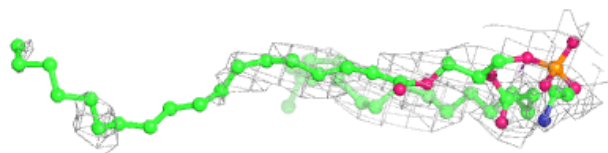
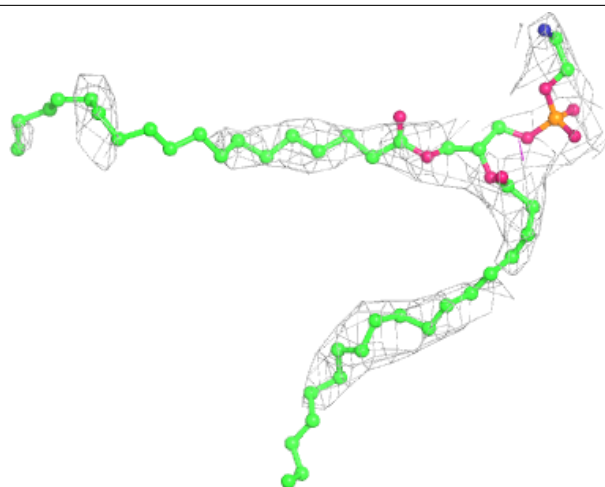
**Electron density around 3PE J 101:**

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



**Electron density around 3PE D 101:**

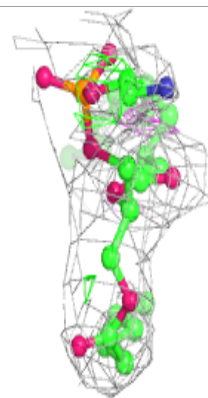
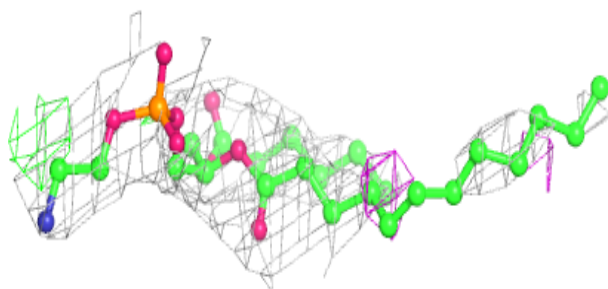
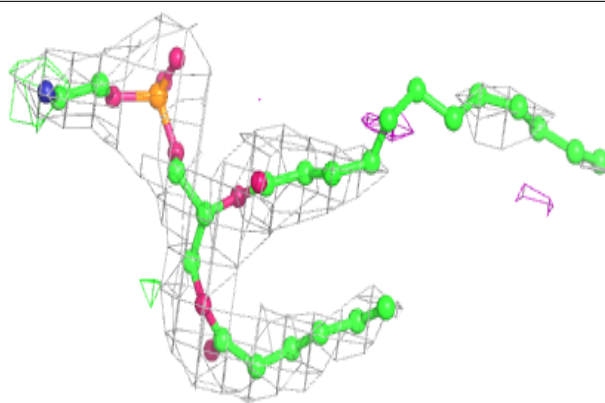
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



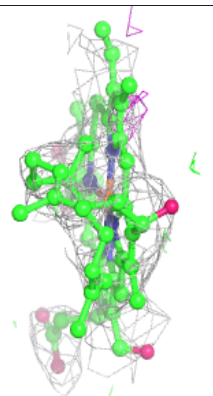
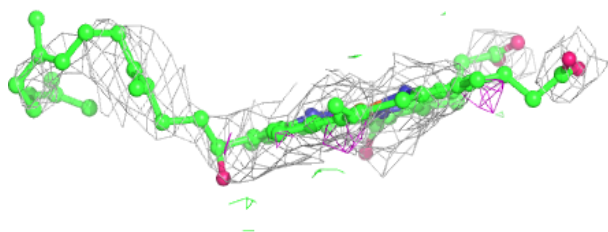
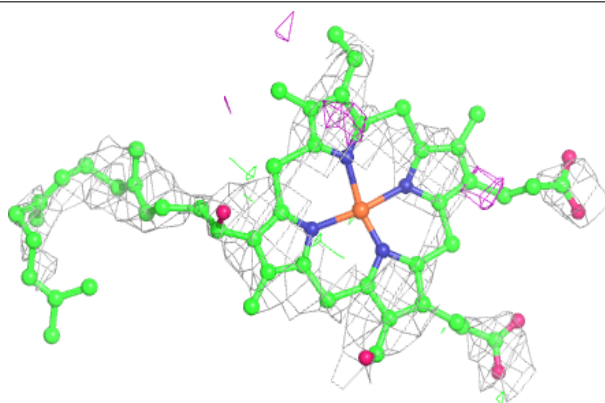


**Electron density around 3PE G 607:**

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

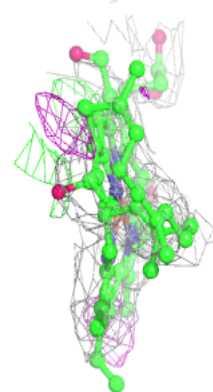
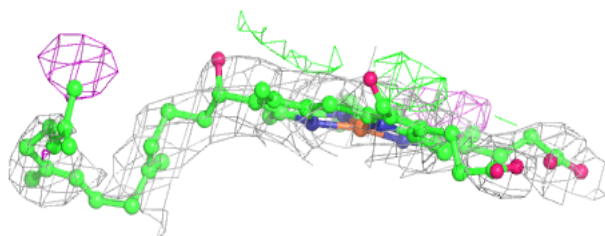
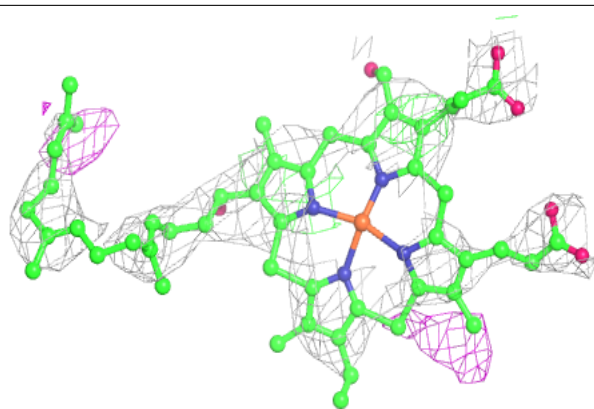
**Electron density around HEA G 603:**

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

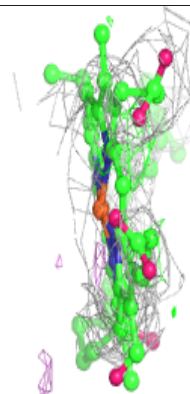
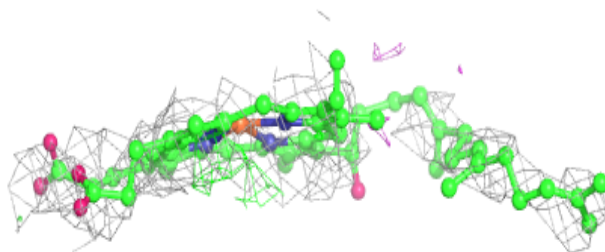
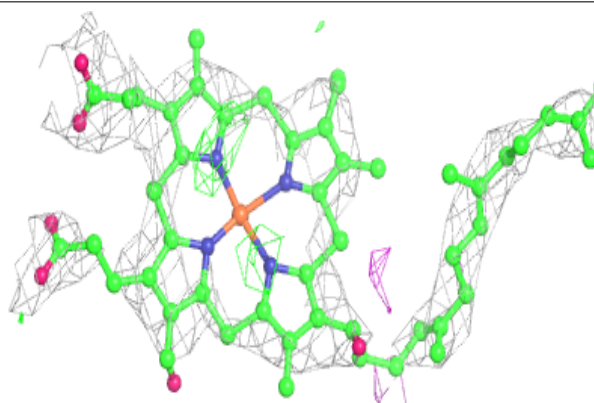


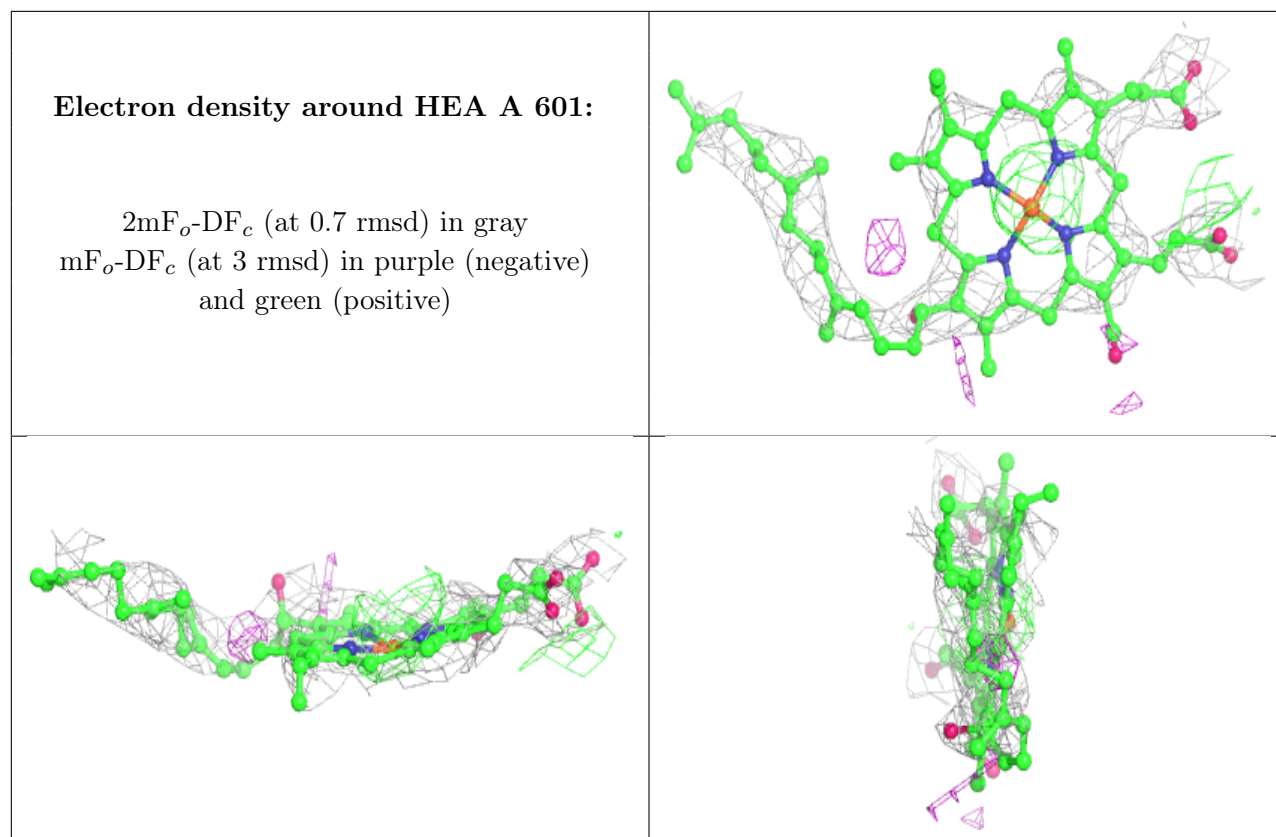
**Electron density around HEA A 602:**

$2mF_o-DF_c$  (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.