



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 06:17 PM BST

PDB ID : 4TNW
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and POPC in a lipid-modulated conformation
Authors : Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on : 2014-06-05
Resolution : 3.20 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 ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

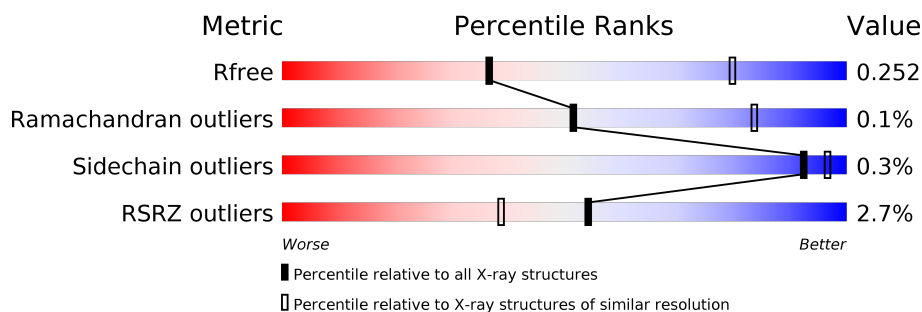
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



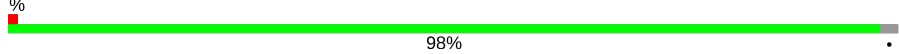
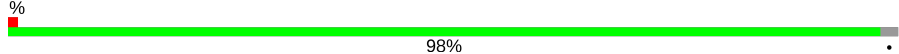
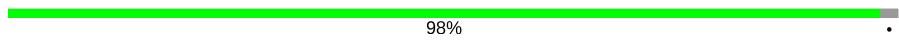
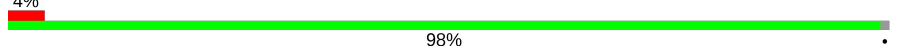
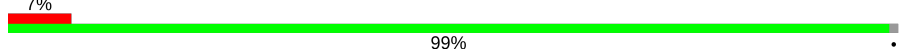
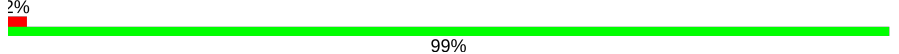
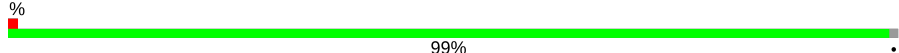
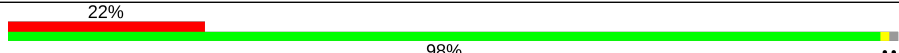
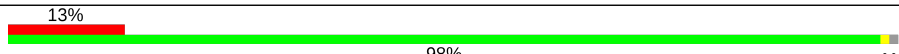
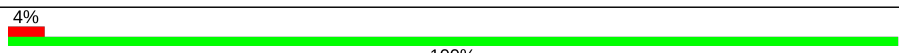
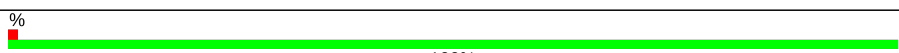
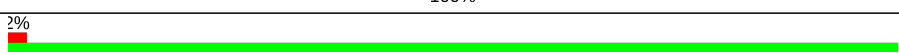
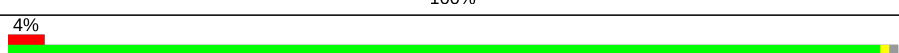
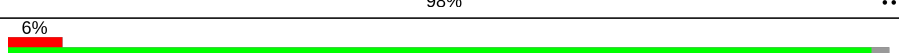
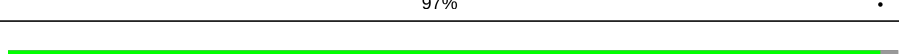
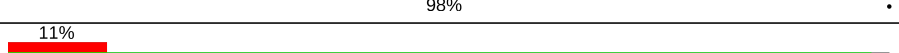
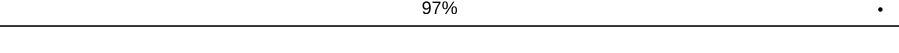
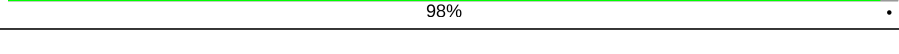
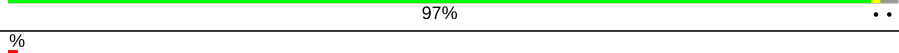
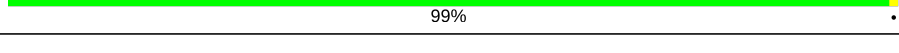
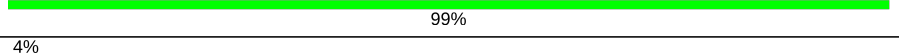
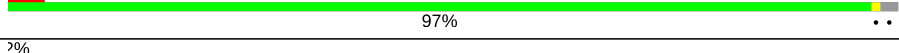
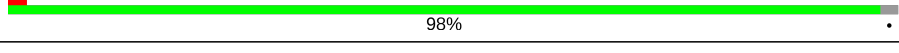
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	347	98% .
1	B	347	% 98% .
1	C	347	% 98% .
1	D	347	97% ..
1	E	347	% 98% .
1	P	347	98% .
1	Q	347	98% .

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Mol	Chain	Length	Quality of chain
1	R	347	%  98% .
1	S	347	%  98% .
1	T	347	 98% .
2	F	224	4%  98% .
2	G	224	7%  99% .
2	H	224	2%  99% .
2	I	224	%  99% .
2	J	224	22%  98% ..
2	U	224	13%  98% ..
2	V	224	4%  100% .
2	W	224	%  100% .
2	X	224	2%  100% .
2	Y	224	4%  98% ..
3	K	215	6%  97% .
3	L	215	 98% .
3	M	215	11%  97% .
3	N	215	 98% .
3	O	215	 97% ..
3	Z	215	%  99% .
3	f	215	 99% .
3	g	215	4%  97% ..
3	h	215	2%  98% .
3	i	215	 98% .

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	POV	A	402	-	-	-	X
5	POV	D	401	-	-	-	X
5	POV	P	403	-	-	-	X
5	POV	R	401	-	-	-	X
5	POV	T	401	-	-	-	X
6	CL	A	403	-	-	-	X
8	LMT	B	403	-	-	-	X
8	LMT	D	403	-	-	-	X
8	LMT	E	402	-	-	-	X
8	LMT	P	402	-	-	-	X
8	LMT	S	402	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 60818 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 Avermectin-sensitive glutamate-gated chloride channel GluCl alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2744	1786	449	494	15			
1	B	341	Total	C	N	O	S	0	0	0
			2734	1780	446	493	15			
1	C	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	D	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	P	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	Q	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	R	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	S	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			
1	T	340	Total	C	N	O	S	0	0	0
			2724	1774	443	492	15			

There are 110 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP G5EBR3
A	304	GLY	-	linker	UNP G5EBR3
A	305	THR	-	linker	UNP G5EBR3
A	340	HIS	-	expression tag	UNP G5EBR3
A	341	HIS	-	expression tag	UNP G5EBR3
A	342	HIS	-	expression tag	UNP G5EBR3
A	343	HIS	-	expression tag	UNP G5EBR3
A	344	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	345	HIS	-	expression tag	UNP G5EBR3
A	346	HIS	-	expression tag	UNP G5EBR3
A	347	HIS	-	expression tag	UNP G5EBR3
B	303	ALA	-	linker	UNP G5EBR3
B	304	GLY	-	linker	UNP G5EBR3
B	305	THR	-	linker	UNP G5EBR3
B	340	HIS	-	expression tag	UNP G5EBR3
B	341	HIS	-	expression tag	UNP G5EBR3
B	342	HIS	-	expression tag	UNP G5EBR3
B	343	HIS	-	expression tag	UNP G5EBR3
B	344	HIS	-	expression tag	UNP G5EBR3
B	345	HIS	-	expression tag	UNP G5EBR3
B	346	HIS	-	expression tag	UNP G5EBR3
B	347	HIS	-	expression tag	UNP G5EBR3
C	303	ALA	-	linker	UNP G5EBR3
C	304	GLY	-	linker	UNP G5EBR3
C	305	THR	-	linker	UNP G5EBR3
C	340	HIS	-	expression tag	UNP G5EBR3
C	341	HIS	-	expression tag	UNP G5EBR3
C	342	HIS	-	expression tag	UNP G5EBR3
C	343	HIS	-	expression tag	UNP G5EBR3
C	344	HIS	-	expression tag	UNP G5EBR3
C	345	HIS	-	expression tag	UNP G5EBR3
C	346	HIS	-	expression tag	UNP G5EBR3
C	347	HIS	-	expression tag	UNP G5EBR3
D	303	ALA	-	linker	UNP G5EBR3
D	304	GLY	-	linker	UNP G5EBR3
D	305	THR	-	linker	UNP G5EBR3
D	340	HIS	-	expression tag	UNP G5EBR3
D	341	HIS	-	expression tag	UNP G5EBR3
D	342	HIS	-	expression tag	UNP G5EBR3
D	343	HIS	-	expression tag	UNP G5EBR3
D	344	HIS	-	expression tag	UNP G5EBR3
D	345	HIS	-	expression tag	UNP G5EBR3
D	346	HIS	-	expression tag	UNP G5EBR3
D	347	HIS	-	expression tag	UNP G5EBR3
E	303	ALA	-	linker	UNP G5EBR3
E	304	GLY	-	linker	UNP G5EBR3
E	305	THR	-	linker	UNP G5EBR3
E	340	HIS	-	expression tag	UNP G5EBR3
E	341	HIS	-	expression tag	UNP G5EBR3
E	342	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	343	HIS	-	expression tag	UNP G5EBR3
E	344	HIS	-	expression tag	UNP G5EBR3
E	345	HIS	-	expression tag	UNP G5EBR3
E	346	HIS	-	expression tag	UNP G5EBR3
E	347	HIS	-	expression tag	UNP G5EBR3
P	303	ALA	-	linker	UNP G5EBR3
P	304	GLY	-	linker	UNP G5EBR3
P	305	THR	-	linker	UNP G5EBR3
P	340	HIS	-	expression tag	UNP G5EBR3
P	341	HIS	-	expression tag	UNP G5EBR3
P	342	HIS	-	expression tag	UNP G5EBR3
P	343	HIS	-	expression tag	UNP G5EBR3
P	344	HIS	-	expression tag	UNP G5EBR3
P	345	HIS	-	expression tag	UNP G5EBR3
P	346	HIS	-	expression tag	UNP G5EBR3
P	347	HIS	-	expression tag	UNP G5EBR3
Q	303	ALA	-	linker	UNP G5EBR3
Q	304	GLY	-	linker	UNP G5EBR3
Q	305	THR	-	linker	UNP G5EBR3
Q	340	HIS	-	expression tag	UNP G5EBR3
Q	341	HIS	-	expression tag	UNP G5EBR3
Q	342	HIS	-	expression tag	UNP G5EBR3
Q	343	HIS	-	expression tag	UNP G5EBR3
Q	344	HIS	-	expression tag	UNP G5EBR3
Q	345	HIS	-	expression tag	UNP G5EBR3
Q	346	HIS	-	expression tag	UNP G5EBR3
Q	347	HIS	-	expression tag	UNP G5EBR3
R	303	ALA	-	linker	UNP G5EBR3
R	304	GLY	-	linker	UNP G5EBR3
R	305	THR	-	linker	UNP G5EBR3
R	340	HIS	-	expression tag	UNP G5EBR3
R	341	HIS	-	expression tag	UNP G5EBR3
R	342	HIS	-	expression tag	UNP G5EBR3
R	343	HIS	-	expression tag	UNP G5EBR3
R	344	HIS	-	expression tag	UNP G5EBR3
R	345	HIS	-	expression tag	UNP G5EBR3
R	346	HIS	-	expression tag	UNP G5EBR3
R	347	HIS	-	expression tag	UNP G5EBR3
S	303	ALA	-	linker	UNP G5EBR3
S	304	GLY	-	linker	UNP G5EBR3
S	305	THR	-	linker	UNP G5EBR3
S	340	HIS	-	expression tag	UNP G5EBR3

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Chain	Residue	Modelled	Actual	Comment	Reference
S	341	HIS	-	expression tag	UNP G5EBR3
S	342	HIS	-	expression tag	UNP G5EBR3
S	343	HIS	-	expression tag	UNP G5EBR3
S	344	HIS	-	expression tag	UNP G5EBR3
S	345	HIS	-	expression tag	UNP G5EBR3
S	346	HIS	-	expression tag	UNP G5EBR3
S	347	HIS	-	expression tag	UNP G5EBR3
T	303	ALA	-	linker	UNP G5EBR3
T	304	GLY	-	linker	UNP G5EBR3
T	305	THR	-	linker	UNP G5EBR3
T	340	HIS	-	expression tag	UNP G5EBR3
T	341	HIS	-	expression tag	UNP G5EBR3
T	342	HIS	-	expression tag	UNP G5EBR3
T	343	HIS	-	expression tag	UNP G5EBR3
T	344	HIS	-	expression tag	UNP G5EBR3
T	345	HIS	-	expression tag	UNP G5EBR3
T	346	HIS	-	expression tag	UNP G5EBR3
T	347	HIS	-	expression tag	UNP G5EBR3

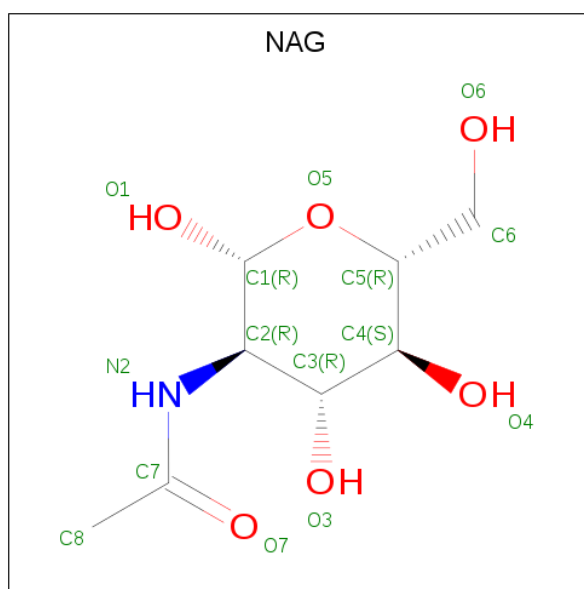
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	G	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	H	223	Total	C	N	O	S	0	0	0
			1701	1077	278	338	8			
2	I	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			
2	U	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	V	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	W	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	X	224	Total	C	N	O	S	0	0	0
			1707	1080	279	339	9			
2	Y	221	Total	C	N	O	S	0	0	0
			1682	1067	273	334	8			
2	J	222	Total	C	N	O	S	0	0	0
			1693	1073	277	335	8			

- Molecule 3 is a protein called Mouse monoclonal Fab fragment, light chain.

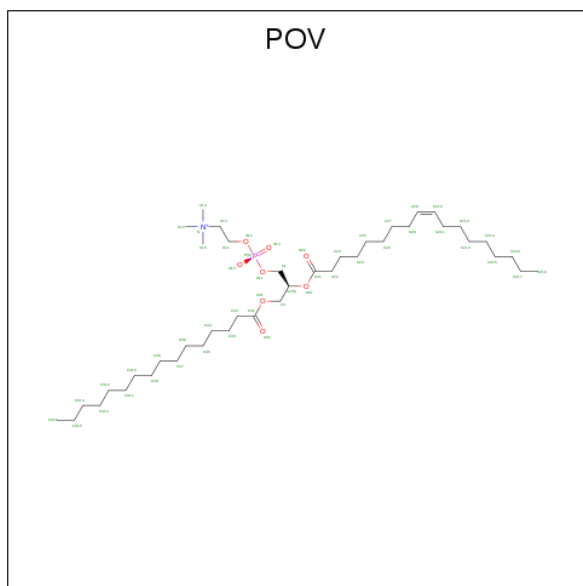
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	6			
3	L	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	N	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	O	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	Z	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	f	215	Total	C	N	O	S	0	0	0
			1626	1018	274	327	7			
3	g	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	h	211	Total	C	N	O	S	0	0	0
			1601	1005	270	320	6			
3	i	214	Total	C	N	O	S	0	0	0
			1620	1015	273	325	7			
3	M	210	Total	C	N	O	S	0	0	0
			1590	999	266	319	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	P	1	Total	C	N	O	0	0
			14	8	1	5		
4	Q	1	Total	C	N	O	0	0
			14	8	1	5		
4	S	1	Total	C	N	O	0	0
			14	8	1	5		
4	T	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	14	1	7	1		
5	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		

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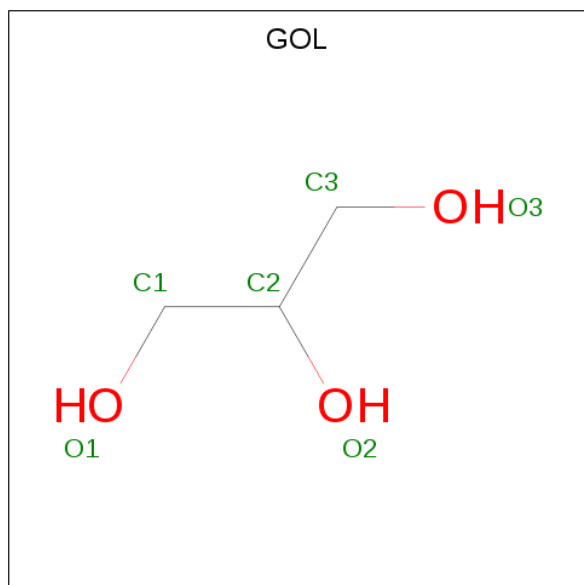
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	P	1	Total	C	N	O	P	0	0
			42	32	1	8	1		
5	Q	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
5	R	1	Total	C	N	O	P	0	0
			34	24	1	8	1		
5	R	1	Total	C	O	P		0	0
			35	26	8	1			
5	T	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

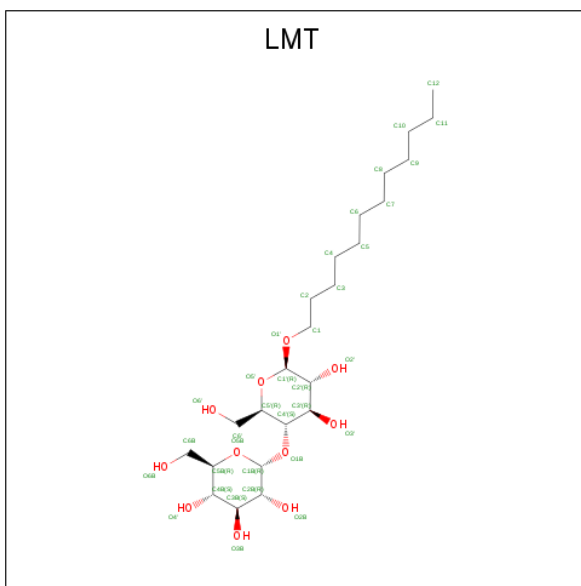
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

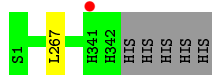
- Molecule 8 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:

$\text{C}_{24}\text{H}_{46}\text{O}_{11})$.

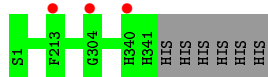
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 23	C 12	O 11	0	0
8	C	1	Total 23	C 12	O 11	0	0
8	D	1	Total 23	C 12	O 11	0	0
8	E	1	Total 23	C 12	O 11	0	0
8	P	1	Total 23	C 12	O 11	0	0
8	S	1	Total 23	C 12	O 11	0	0
8	T	1	Total 23	C 12	O 11	0	0

i

- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



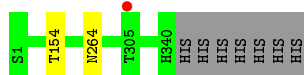
- Chain B:  98%



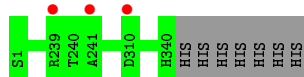
- Chain C:  98%



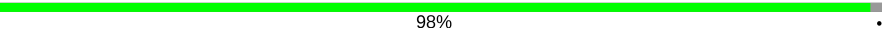
- Chain D:  97%



- Chain E:  98%



- 

Chain P:  98%



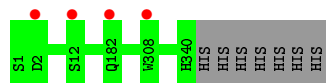
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain Q:  98%



- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain R:  98%



- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain S:  98%



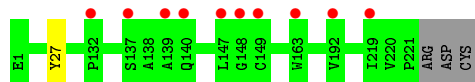
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain T:  98%



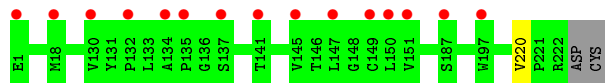
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:  98%

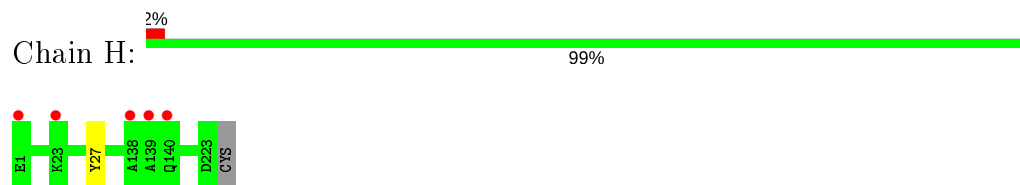


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

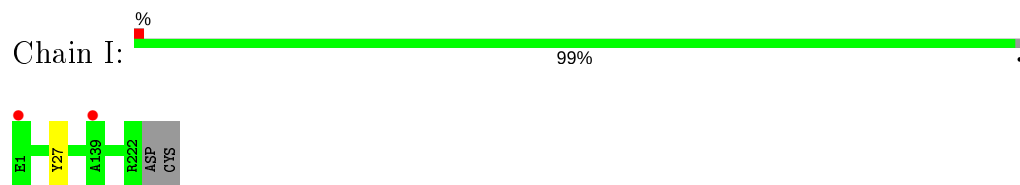
Chain G:  99%



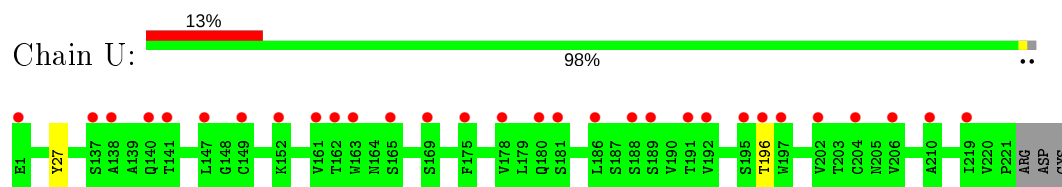
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



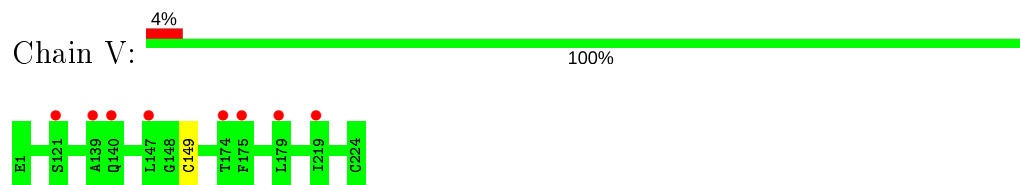
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



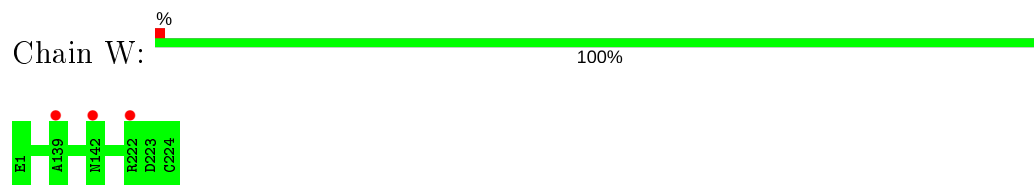
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



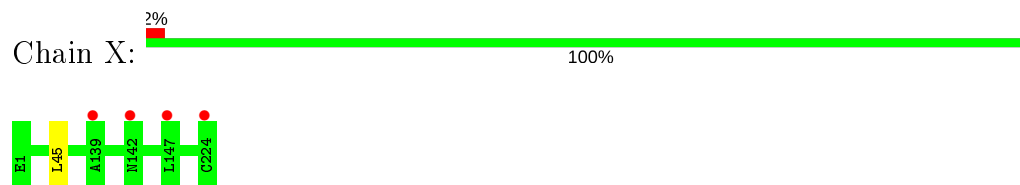
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

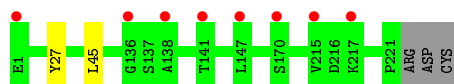


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

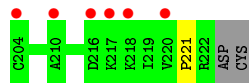
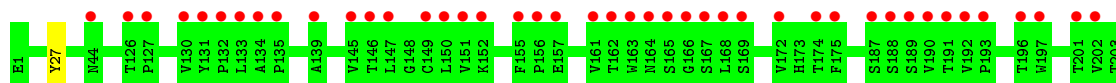


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

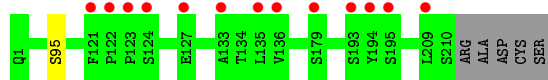




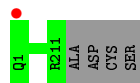
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



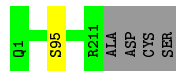
- Molecule 3: Mouse monoclonal Fab fragment, light chain



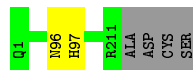
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



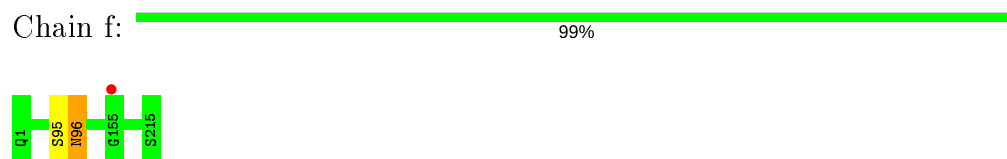
- Molecule 3: Mouse monoclonal Fab fragment, light chain



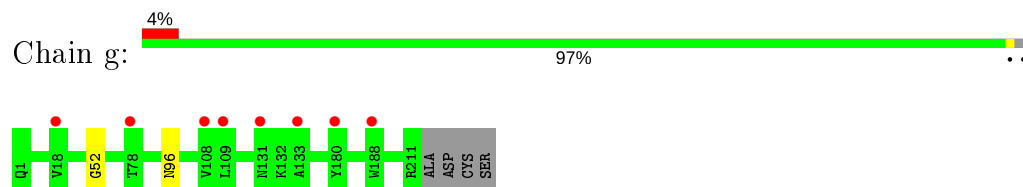
- Molecule 3: Mouse monoclonal Fab fragment, light chain



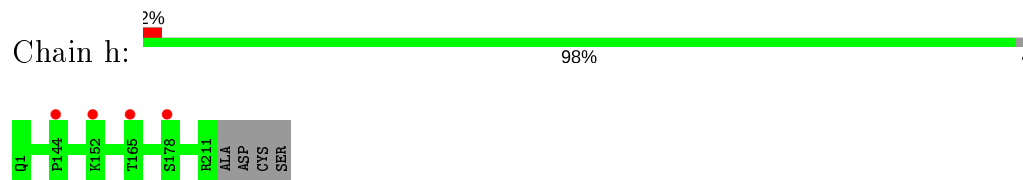
- Molecule 3: Mouse monoclonal Fab fragment, light chain



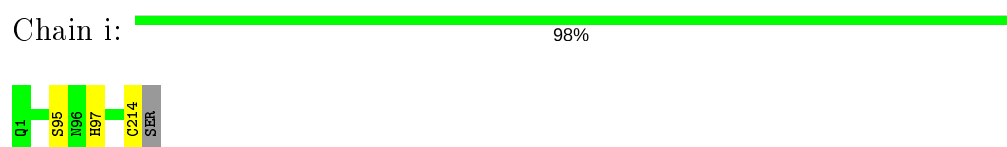
- Molecule 3: Mouse monoclonal Fab fragment, light chain



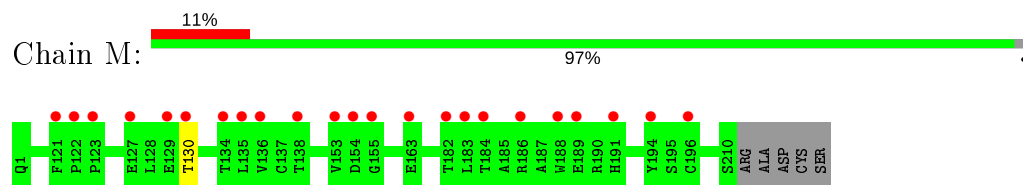
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	453.75Å 192.87Å 196.14Å 90.00° 92.27° 90.00°	Depositor
Resolution (Å)	58.70 – 3.20 59.51 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.6 (58.70-3.20) 88.8 (59.51-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.227 , 0.251 0.230 , 0.252	Depositor DCC
R_{free} test set	14870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	60818	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POV, GOL, LMT, NAG, CL

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	0.24	0/2819	0.44	0/3847
1	B	0.23	0/2808	0.43	0/3832
1	C	0.23	0/2797	0.43	0/3817
1	D	0.25	0/2797	0.48	0/3817
1	E	0.24	0/2797	0.44	0/3817
1	P	0.24	0/2797	0.45	0/3817
1	Q	0.24	0/2797	0.45	0/3817
1	R	0.24	0/2797	0.43	0/3817
1	S	0.23	0/2797	0.43	0/3817
1	T	0.24	0/2797	0.45	0/3817
2	F	0.21	0/1728	0.40	0/2360
2	G	0.22	0/1739	0.41	0/2374
2	H	0.22	0/1747	0.41	0/2385
2	I	0.21	0/1739	0.40	0/2374
2	J	0.23	0/1739	0.42	0/2374
2	U	0.21	0/1728	0.40	0/2360
2	V	0.21	0/1753	0.40	0/2393
2	W	0.21	0/1753	0.40	0/2393
2	X	0.22	0/1753	0.42	0/2393
2	Y	0.21	0/1728	0.41	0/2360
3	K	0.22	0/1628	0.42	0/2226
3	L	0.22	0/1639	0.43	0/2240
3	M	0.22	0/1628	0.43	0/2226
3	N	0.23	0/1639	0.43	0/2240
3	O	0.22	0/1639	0.42	0/2240
3	Z	0.23	0/1664	0.43	0/2274
3	f	0.22	0/1664	0.42	0/2274
3	g	0.22	0/1639	0.42	0/2240
3	h	0.22	0/1639	0.41	0/2240
3	i	0.22	0/1658	0.43	0/2266
All	All	0.23	0/61847	0.43	0/84447

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	340/347 (98%)	327 (96%)	13 (4%)	0	100	100
1	B	339/347 (98%)	325 (96%)	14 (4%)	0	100	100
1	C	338/347 (97%)	324 (96%)	14 (4%)	0	100	100
1	D	338/347 (97%)	328 (97%)	10 (3%)	0	100	100
1	E	338/347 (97%)	325 (96%)	13 (4%)	0	100	100
1	P	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	Q	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	R	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
1	S	338/347 (97%)	325 (96%)	12 (4%)	1 (0%)	41	74
1	T	338/347 (97%)	326 (96%)	12 (4%)	0	100	100
2	F	219/224 (98%)	206 (94%)	13 (6%)	0	100	100
2	G	220/224 (98%)	203 (92%)	17 (8%)	0	100	100
2	H	221/224 (99%)	206 (93%)	15 (7%)	0	100	100
2	I	220/224 (98%)	206 (94%)	14 (6%)	0	100	100
2	J	220/224 (98%)	203 (92%)	16 (7%)	1 (0%)	29	67
2	U	219/224 (98%)	205 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	222/224 (99%)	203 (91%)	19 (9%)	0	100	100
2	W	222/224 (99%)	209 (94%)	13 (6%)	0	100	100
2	X	222/224 (99%)	206 (93%)	16 (7%)	0	100	100
2	Y	219/224 (98%)	202 (92%)	17 (8%)	0	100	100
3	K	208/215 (97%)	193 (93%)	14 (7%)	1 (0%)	29	67
3	L	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
3	M	208/215 (97%)	193 (93%)	15 (7%)	0	100	100
3	N	209/215 (97%)	194 (93%)	14 (7%)	1 (0%)	29	67
3	O	209/215 (97%)	194 (93%)	15 (7%)	0	100	100
3	Z	213/215 (99%)	193 (91%)	19 (9%)	1 (0%)	29	67
3	f	213/215 (99%)	195 (92%)	16 (8%)	2 (1%)	17	56
3	g	209/215 (97%)	196 (94%)	11 (5%)	2 (1%)	15	54
3	h	209/215 (97%)	194 (93%)	15 (7%)	0	100	100
3	i	212/215 (99%)	199 (94%)	12 (6%)	1 (0%)	29	67
All	All	7686/7860 (98%)	7256 (94%)	420 (6%)	10 (0%)	51	83

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	95	SER
3	N	95	SER
3	i	95	SER
3	f	95	SER
1	S	309	ASN

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	311/316 (98%)	310 (100%)	1 (0%)	92	96
1	B	310/316 (98%)	310 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	309/316 (98%)	309 (100%)	0	100	100
1	D	309/316 (98%)	307 (99%)	2 (1%)	86	94
1	E	309/316 (98%)	309 (100%)	0	100	100
1	P	309/316 (98%)	308 (100%)	1 (0%)	92	96
1	Q	309/316 (98%)	308 (100%)	1 (0%)	92	96
1	R	309/316 (98%)	309 (100%)	0	100	100
1	S	309/316 (98%)	309 (100%)	0	100	100
1	T	309/316 (98%)	309 (100%)	0	100	100
2	F	190/193 (98%)	189 (100%)	1 (0%)	88	95
2	G	191/193 (99%)	190 (100%)	1 (0%)	88	95
2	H	192/193 (100%)	191 (100%)	1 (0%)	88	95
2	I	191/193 (99%)	190 (100%)	1 (0%)	88	95
2	J	191/193 (99%)	190 (100%)	1 (0%)	88	95
2	U	190/193 (98%)	188 (99%)	2 (1%)	73	88
2	V	193/193 (100%)	192 (100%)	1 (0%)	88	95
2	W	193/193 (100%)	193 (100%)	0	100	100
2	X	193/193 (100%)	192 (100%)	1 (0%)	88	95
2	Y	190/193 (98%)	188 (99%)	2 (1%)	73	88
3	K	178/182 (98%)	178 (100%)	0	100	100
3	L	179/182 (98%)	179 (100%)	0	100	100
3	M	178/182 (98%)	177 (99%)	1 (1%)	86	94
3	N	179/182 (98%)	179 (100%)	0	100	100
3	O	179/182 (98%)	177 (99%)	2 (1%)	73	88
3	Z	182/182 (100%)	181 (100%)	1 (0%)	88	95
3	f	182/182 (100%)	181 (100%)	1 (0%)	88	95
3	g	179/182 (98%)	179 (100%)	0	100	100
3	h	179/182 (98%)	179 (100%)	0	100	100
3	i	181/182 (100%)	179 (99%)	2 (1%)	73	88
All	All	6803/6910 (98%)	6780 (100%)	23 (0%)	92	96

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	264	ASN
2	U	196	THR
2	J	27	TYR
2	U	27	TYR
2	V	149	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	N	170	GLN
3	O	97	HIS
3	f	39	GLN
3	L	200	HIS
3	Z	97	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 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	401	1	14,14,15	0.29	0	17,19,21	1.06	1 (5%)
8	LMT	E	402	-	24,24,36	1.05	2 (8%)	35,35,47	1.13	2 (5%)
5	POV	R	402	-	34,34,51	1.14	2 (5%)	38,39,59	1.30	5 (13%)
8	LMT	P	402	-	24,24,36	1.05	2 (8%)	35,35,47	1.16	2 (5%)
5	POV	R	401	-	33,33,51	1.17	2 (6%)	39,41,59	1.12	3 (7%)
7	GOL	B	401	-	5,5,5	0.36	0	5,5,5	0.26	0
4	NAG	D	402	1	14,14,15	0.35	0	17,19,21	1.38	2 (11%)
4	NAG	B	402	1	14,14,15	0.26	0	17,19,21	0.80	0
4	NAG	Q	402	1	14,14,15	0.26	0	17,19,21	0.66	0
4	NAG	P	401	1	14,14,15	0.33	0	17,19,21	0.80	1 (5%)
4	NAG	S	401	1	14,14,15	0.34	0	17,19,21	1.34	1 (5%)
5	POV	T	401	-	42,42,51	1.04	2 (4%)	48,50,59	1.12	4 (8%)
8	LMT	D	403	-	24,24,36	1.09	2 (8%)	35,35,47	1.14	2 (5%)
4	NAG	T	402	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
8	LMT	S	402	-	24,24,36	1.06	2 (8%)	35,35,47	1.22	3 (8%)
5	POV	P	403	-	41,41,51	1.06	2 (4%)	47,49,59	1.10	4 (8%)
8	LMT	C	402	-	24,24,36	1.11	2 (8%)	35,35,47	1.11	4 (11%)
4	NAG	E	401	1	14,14,15	0.26	0	17,19,21	0.63	0
5	POV	Q	401	-	45,45,51	1.02	2 (4%)	51,53,59	1.04	3 (5%)
4	NAG	C	401	1	14,14,15	0.39	0	17,19,21	0.85	1 (5%)
5	POV	D	401	-	25,25,51	1.35	2 (8%)	31,33,59	1.30	3 (9%)
8	LMT	T	403	-	24,24,36	1.05	2 (8%)	35,35,47	1.23	5 (14%)
5	POV	A	402	-	22,22,51	1.10	1 (4%)	27,29,59	1.18	2 (7%)
8	LMT	B	403	-	24,24,36	1.03	1 (4%)	35,35,47	1.42	6 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
8	LMT	E	402	-	-	3/8/48/61	0/2/2/2
5	POV	R	402	-	-	12/36/36/55	-
8	LMT	P	402	-	-	1/8/48/61	0/2/2/2
5	POV	R	401	-	-	18/37/37/55	-
7	GOL	B	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	402	1	-	3/6/23/26	0/1/1/1
4	NAG	B	402	1	-	0/6/23/26	0/1/1/1
4	NAG	Q	402	1	-	0/6/23/26	0/1/1/1
4	NAG	P	401	1	-	4/6/23/26	0/1/1/1
4	NAG	S	401	1	-	0/6/23/26	0/1/1/1
5	POV	T	401	-	-	17/46/46/55	-
8	LMT	D	403	-	-	4/8/48/61	0/2/2/2
4	NAG	T	402	1	-	3/6/23/26	0/1/1/1
8	LMT	S	402	-	-	1/8/48/61	0/2/2/2
5	POV	P	403	-	-	15/45/45/55	-
8	LMT	C	402	-	-	6/8/48/61	0/2/2/2
4	NAG	E	401	1	-	2/6/23/26	0/1/1/1
5	POV	Q	401	-	-	16/49/49/55	-
4	NAG	C	401	1	-	6/6/23/26	0/1/1/1
5	POV	D	401	-	-	12/29/29/55	-
8	LMT	T	403	-	-	2/8/48/61	0/2/2/2
5	POV	A	402	-	-	5/25/25/55	-
8	LMT	B	403	-	-	4/8/48/61	0/2/2/2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	POV	O31-C31	4.47	1.46	1.33
5	P	403	POV	O31-C31	4.34	1.46	1.33
5	Q	401	POV	O31-C31	4.32	1.46	1.33
5	R	401	POV	O31-C31	4.25	1.45	1.33
5	T	401	POV	O31-C31	4.21	1.45	1.33

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	401	NAG	C1-O5-C5	4.52	118.32	112.19
4	D	402	NAG	C1-O5-C5	-4.36	106.29	112.19
5	R	402	POV	O21-C21-C22	4.31	120.79	111.50
5	T	401	POV	O21-C21-C22	4.19	120.53	111.50
5	A	402	POV	O21-C21-C22	4.07	120.28	111.50

There are no chirality outliers.

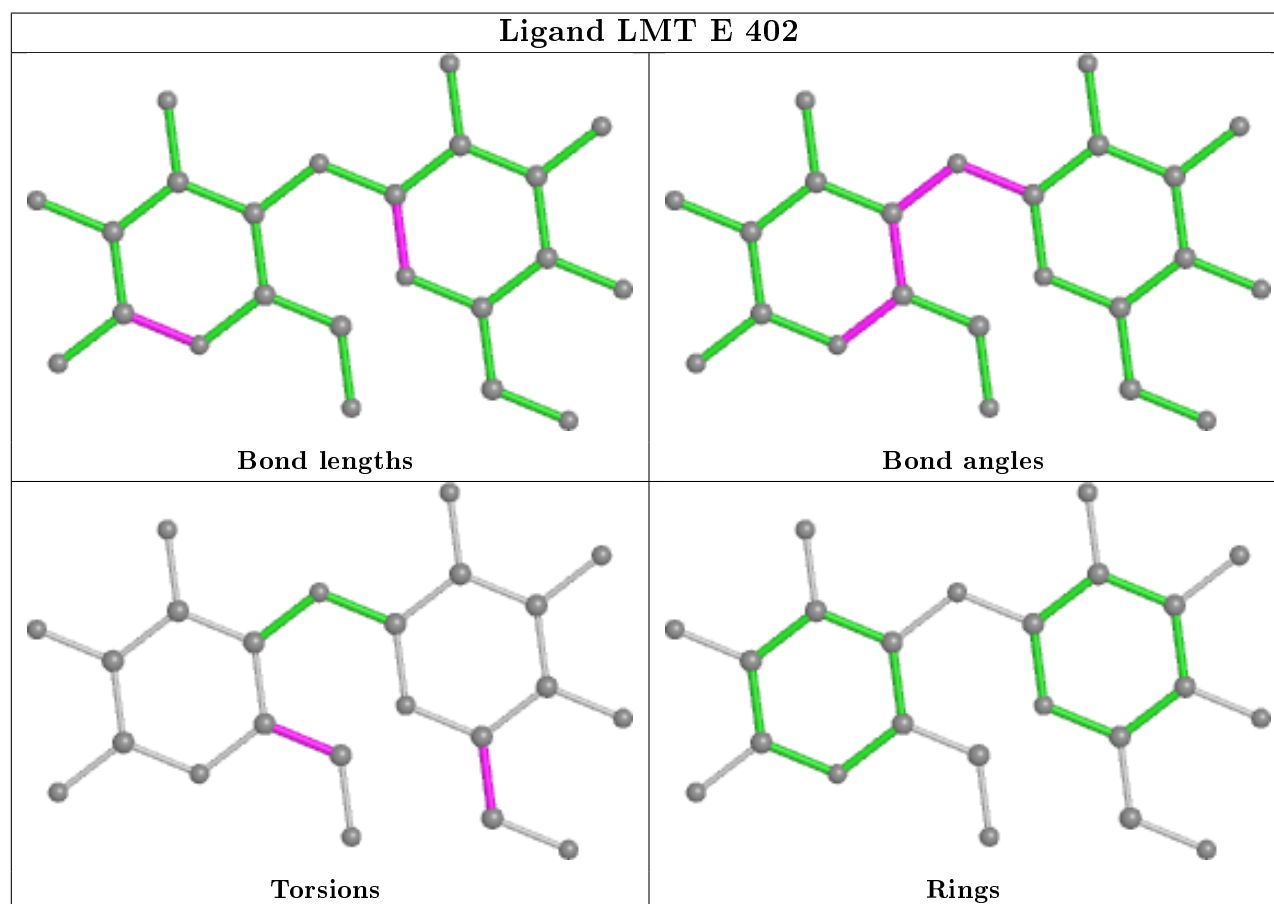
5 of 138 torsion outliers are listed below:

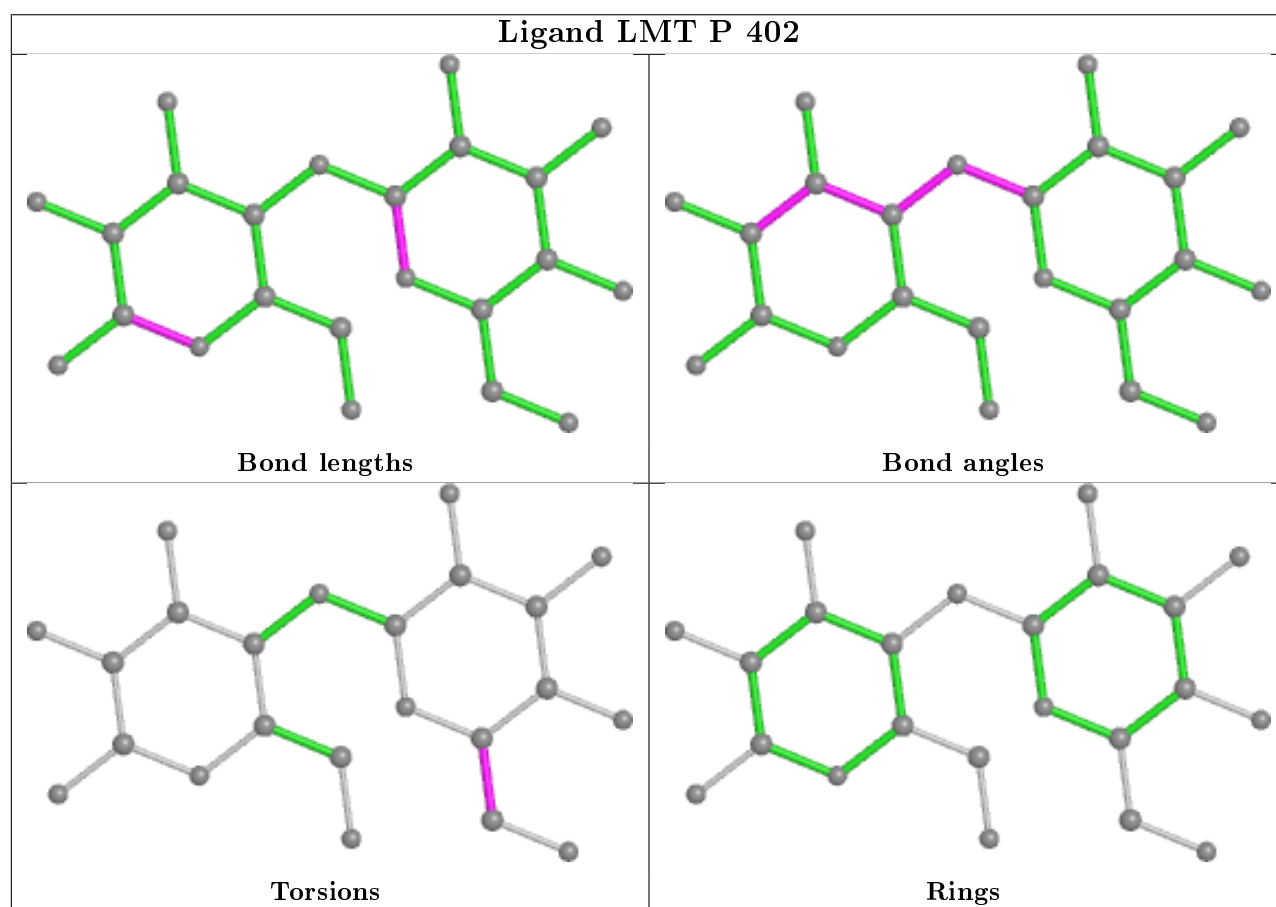
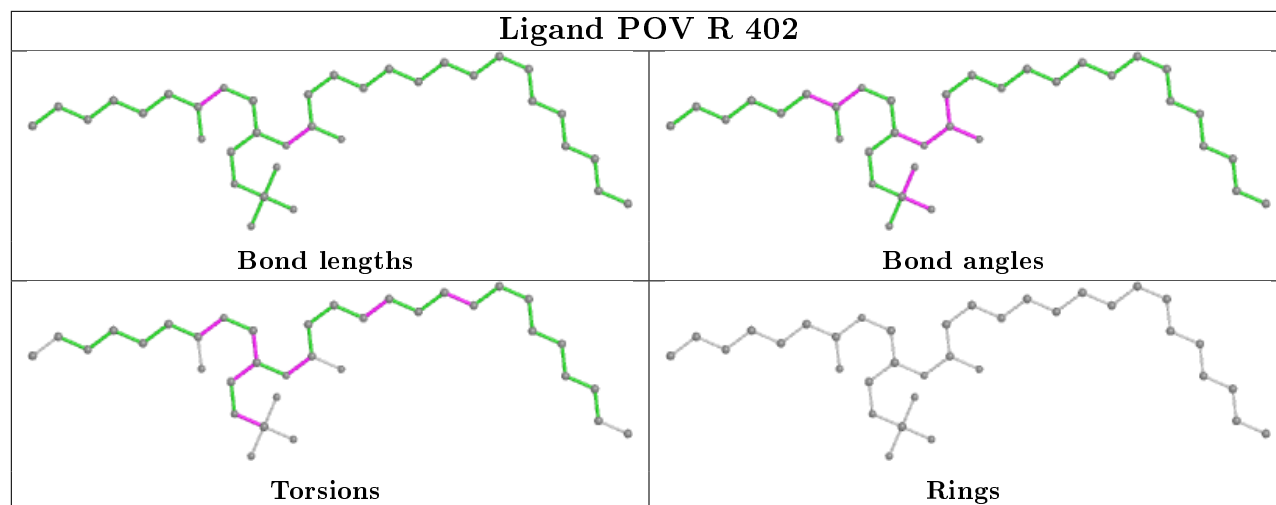
Mol	Chain	Res	Type	Atoms
5	R	402	POV	C1-O11-P-O12
5	R	401	POV	C1-O11-P-O14
5	R	401	POV	O22-C21-O21-C2
7	B	401	GOL	O1-C1-C2-C3
5	D	401	POV	C11-O12-P-O14

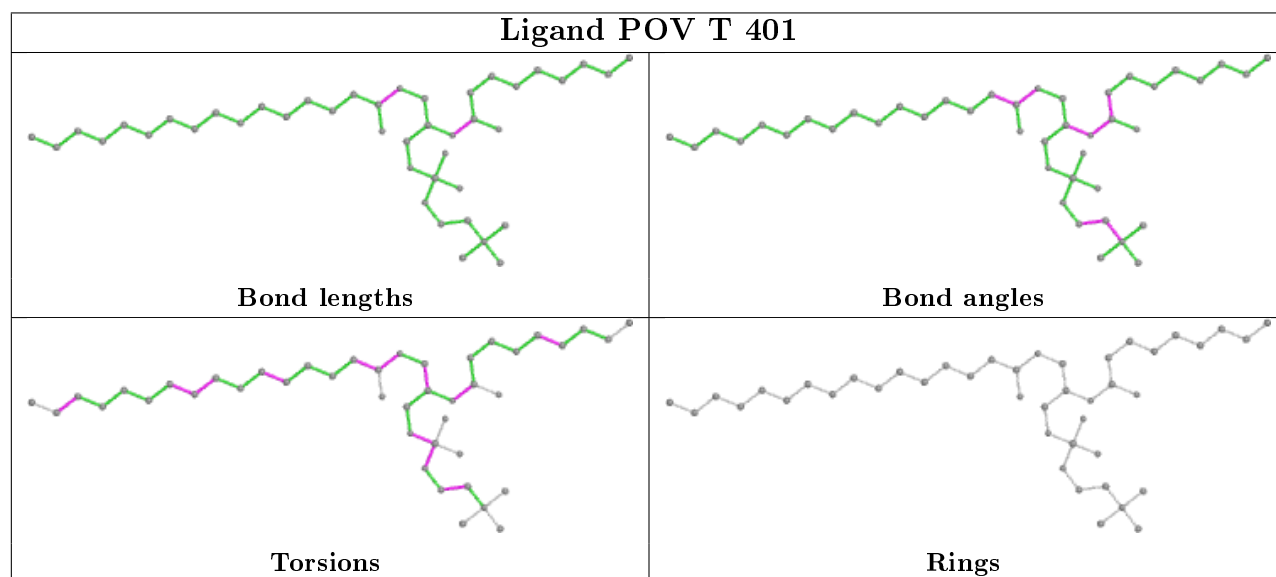
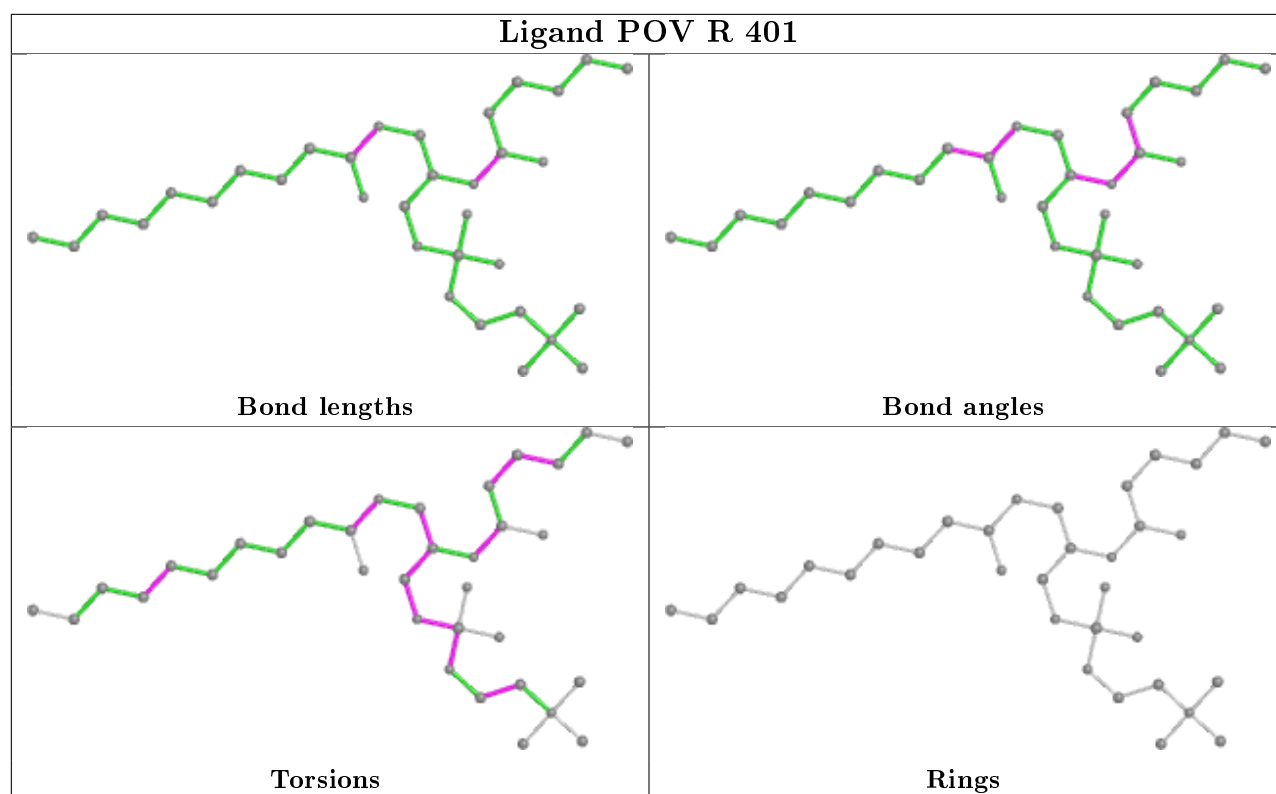
There are no ring outliers.

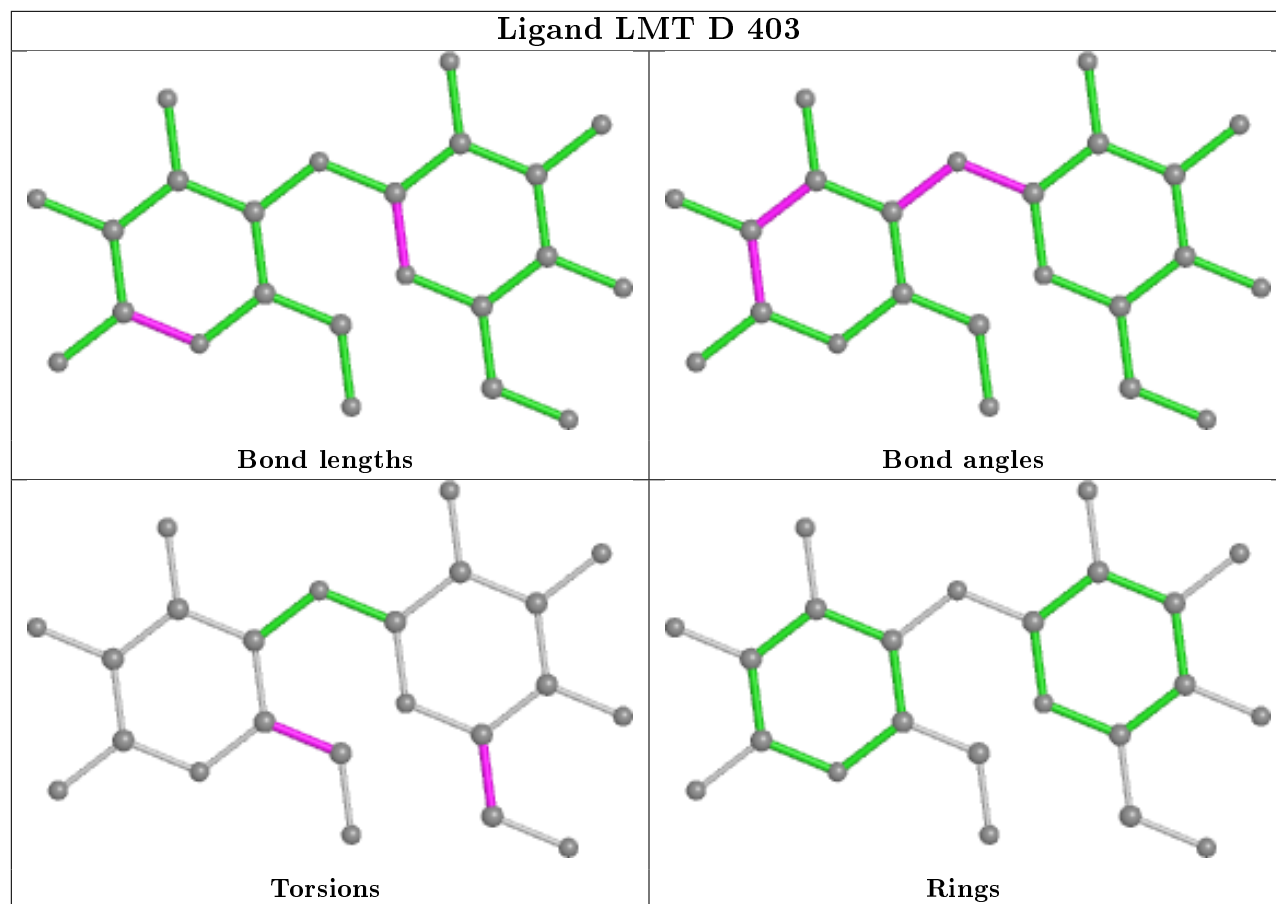
No monomer is involved in short contacts.

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.

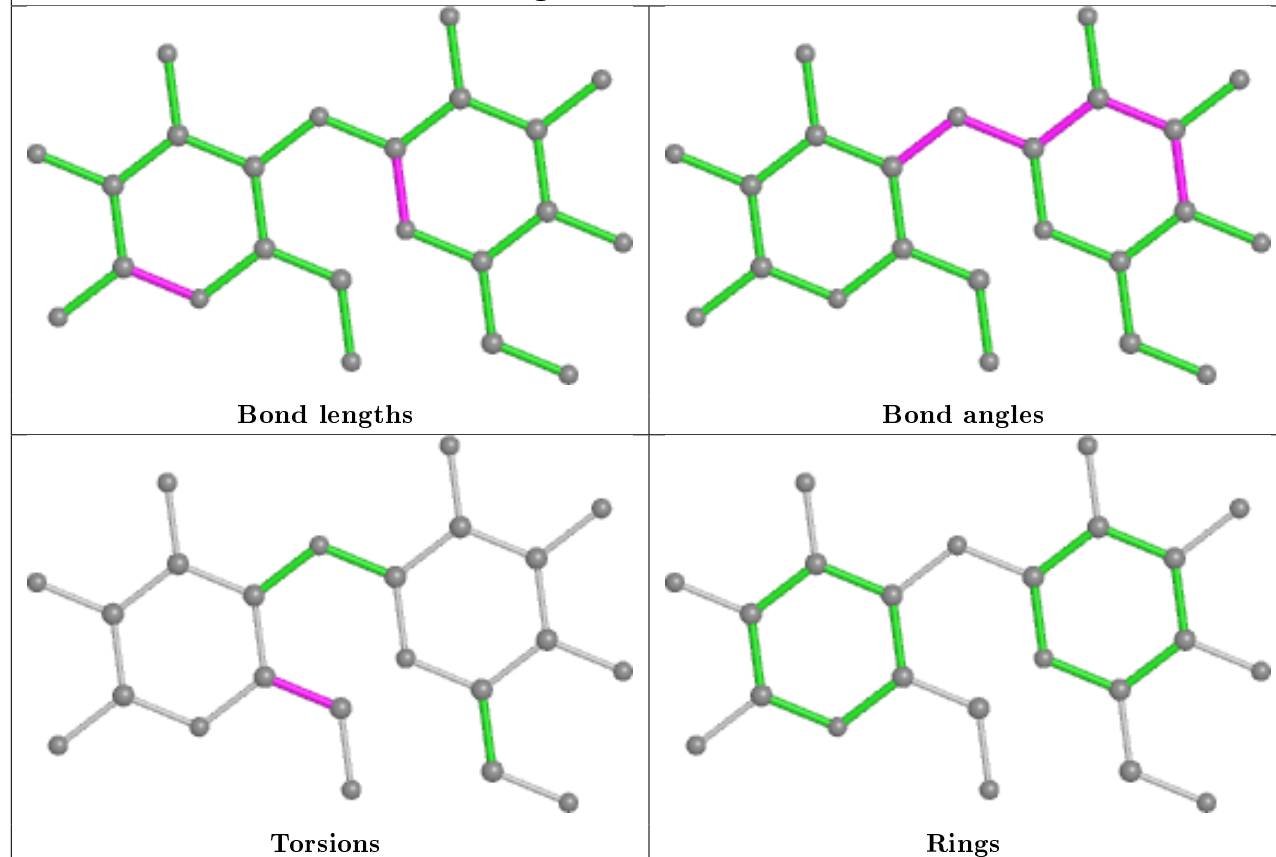




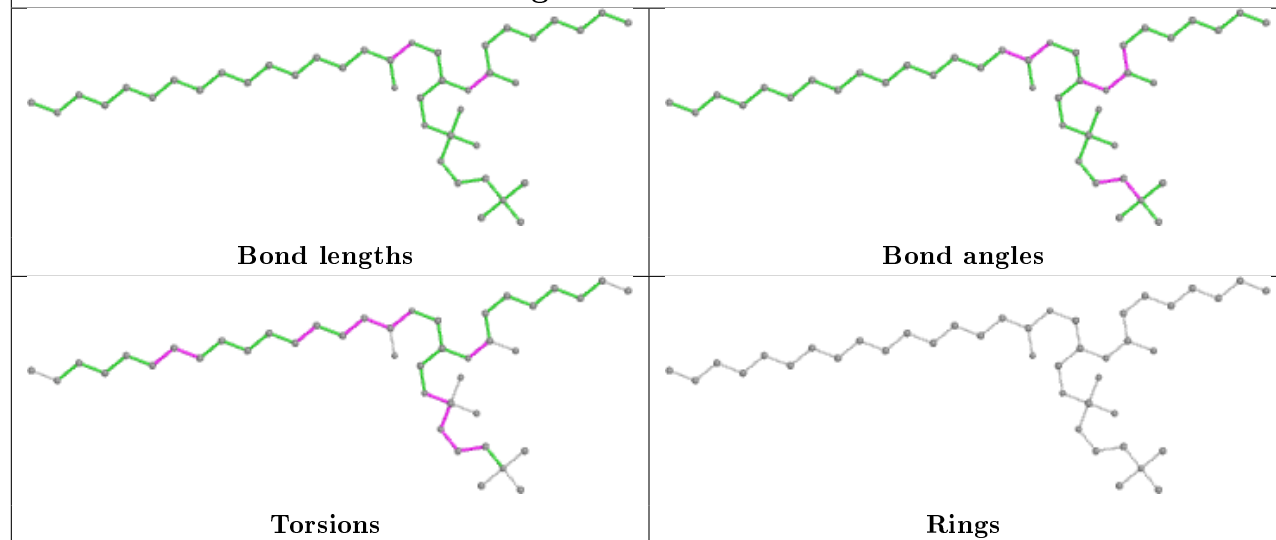


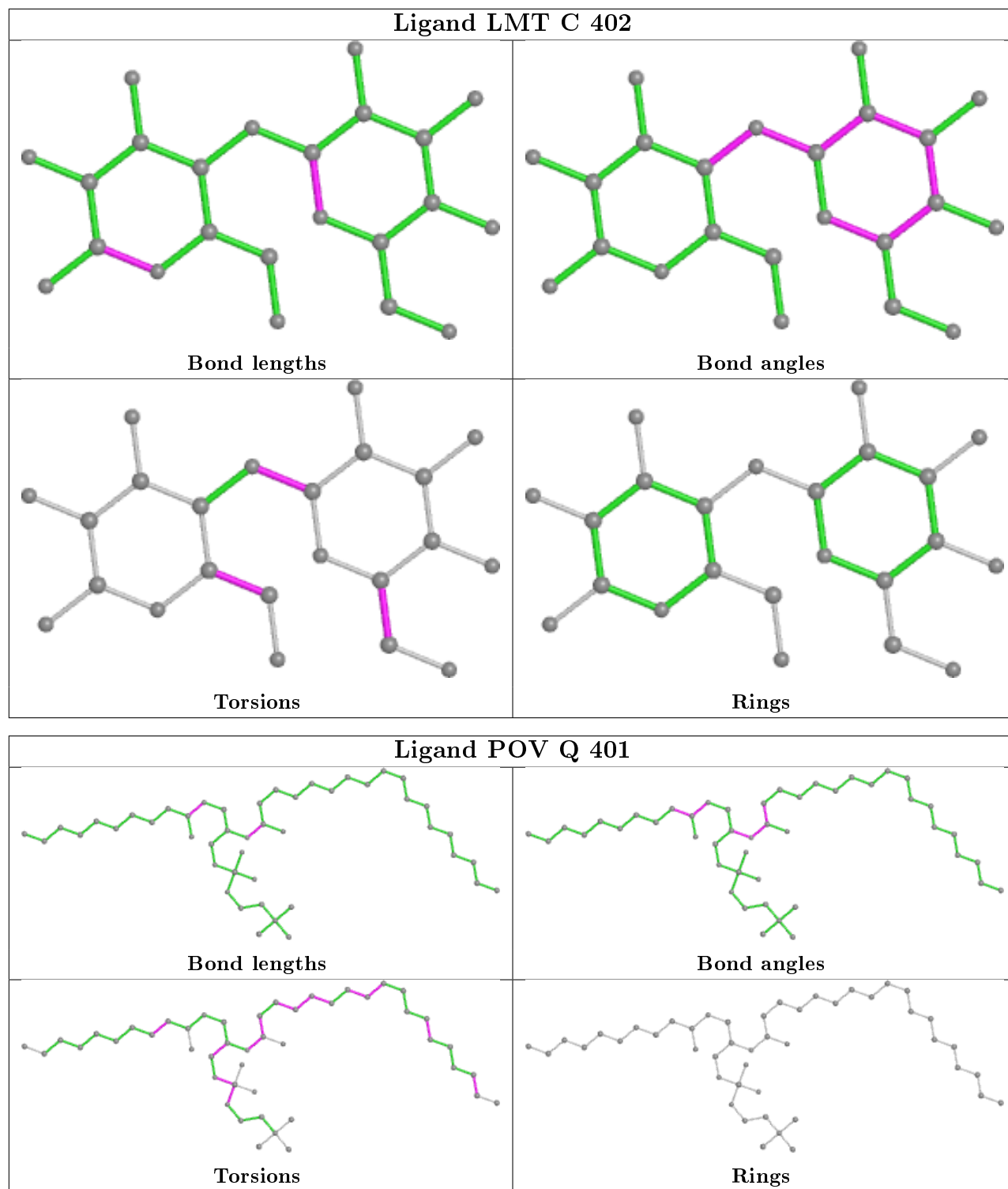


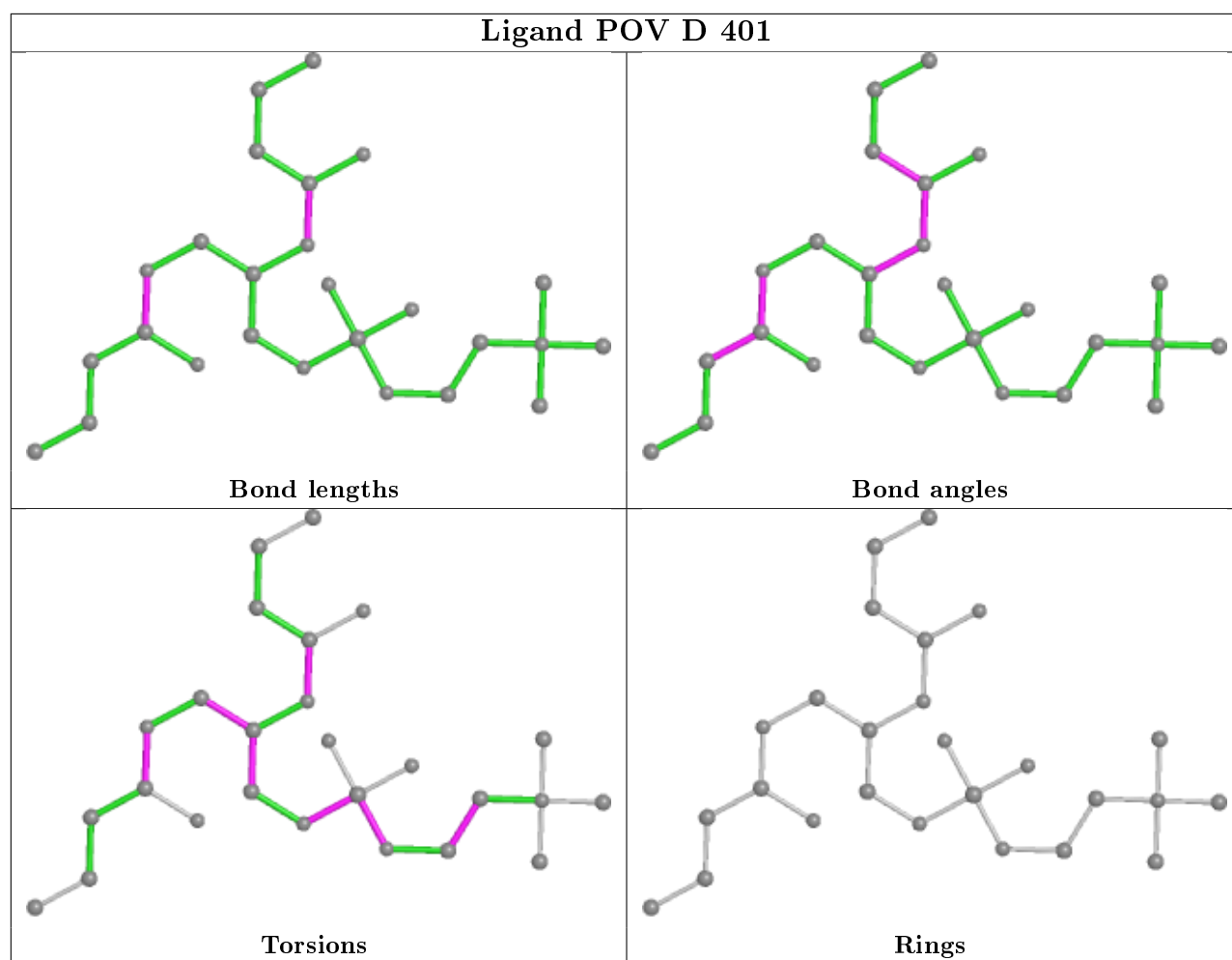
Ligand LMT S 402

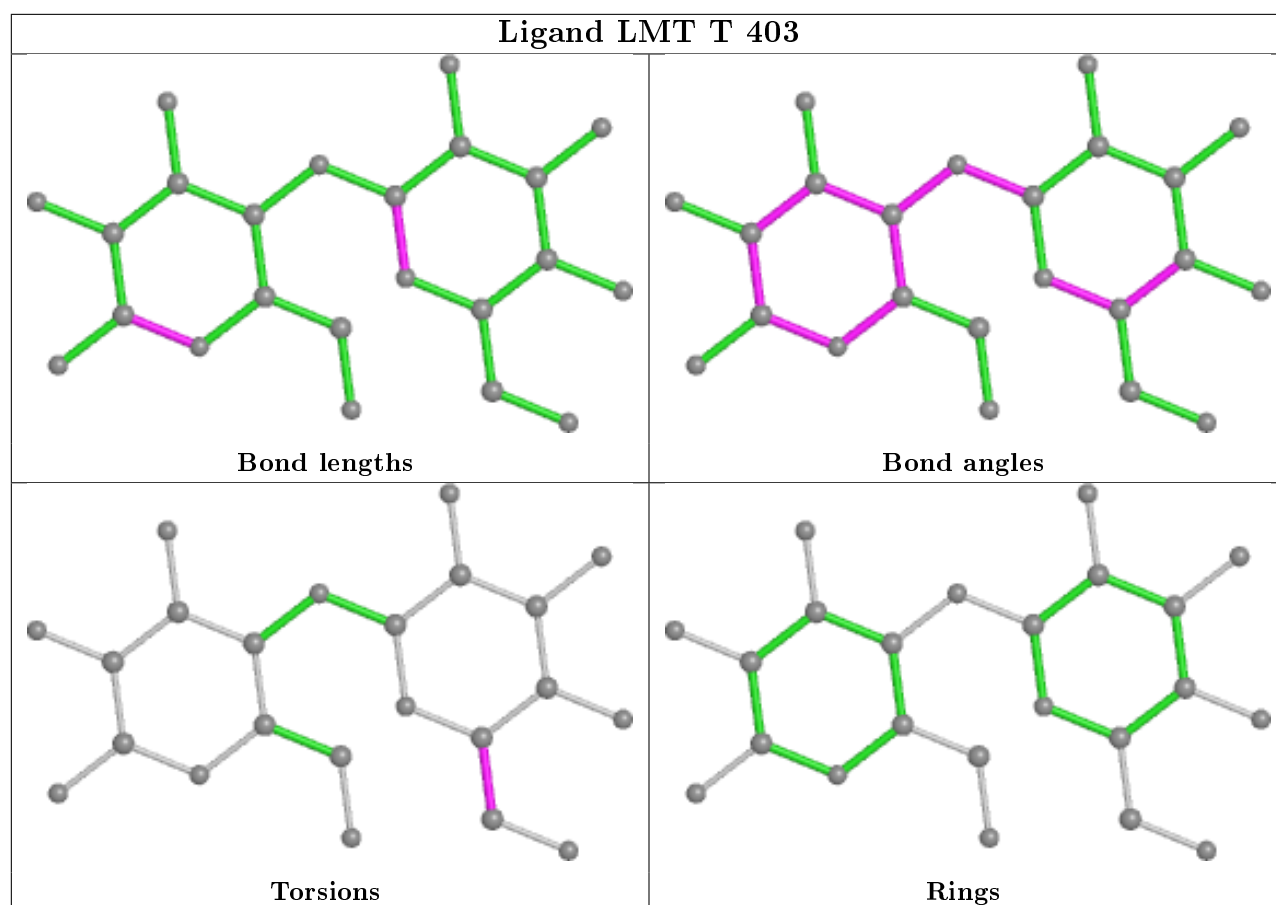


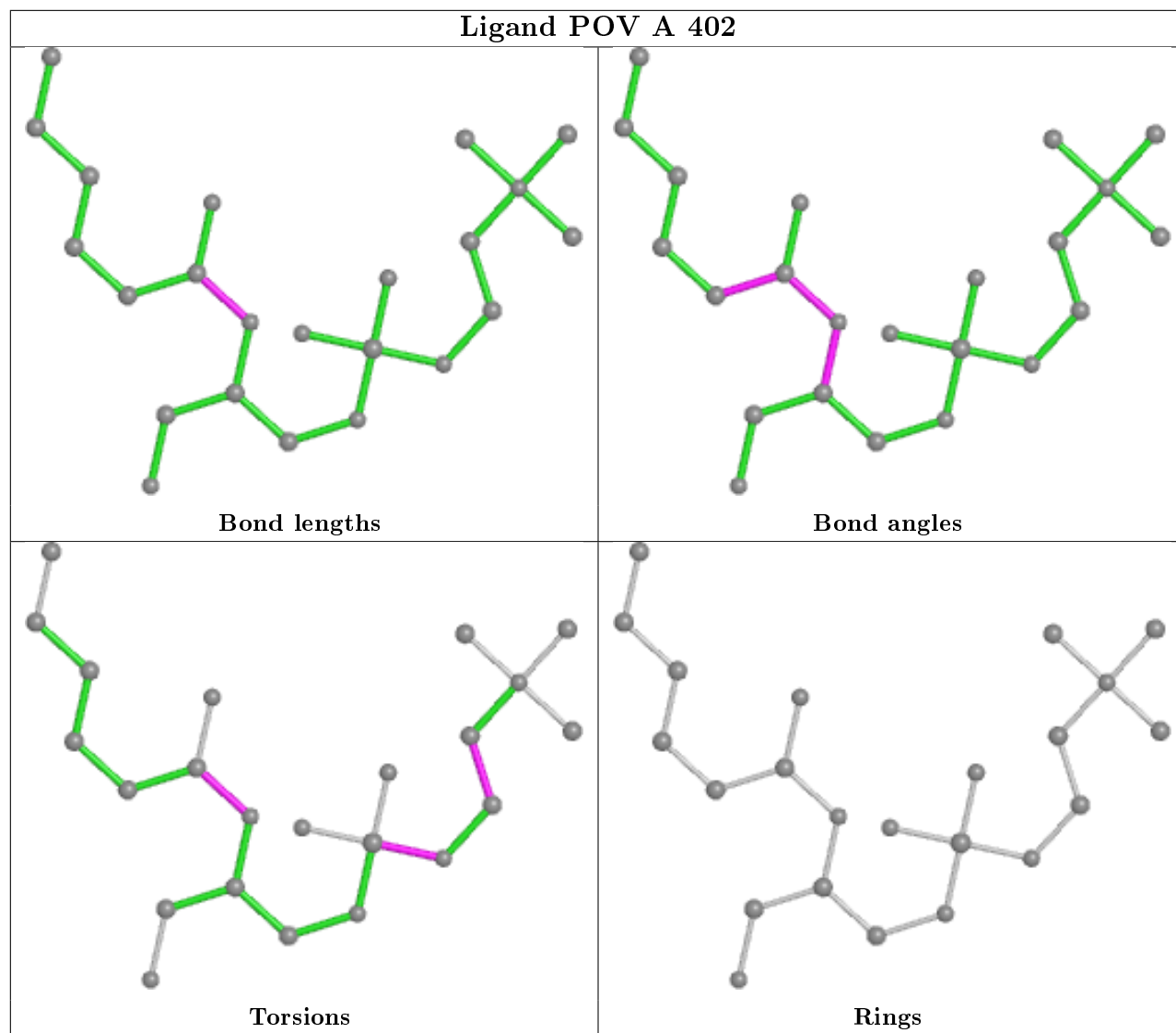
Ligand POV P 403

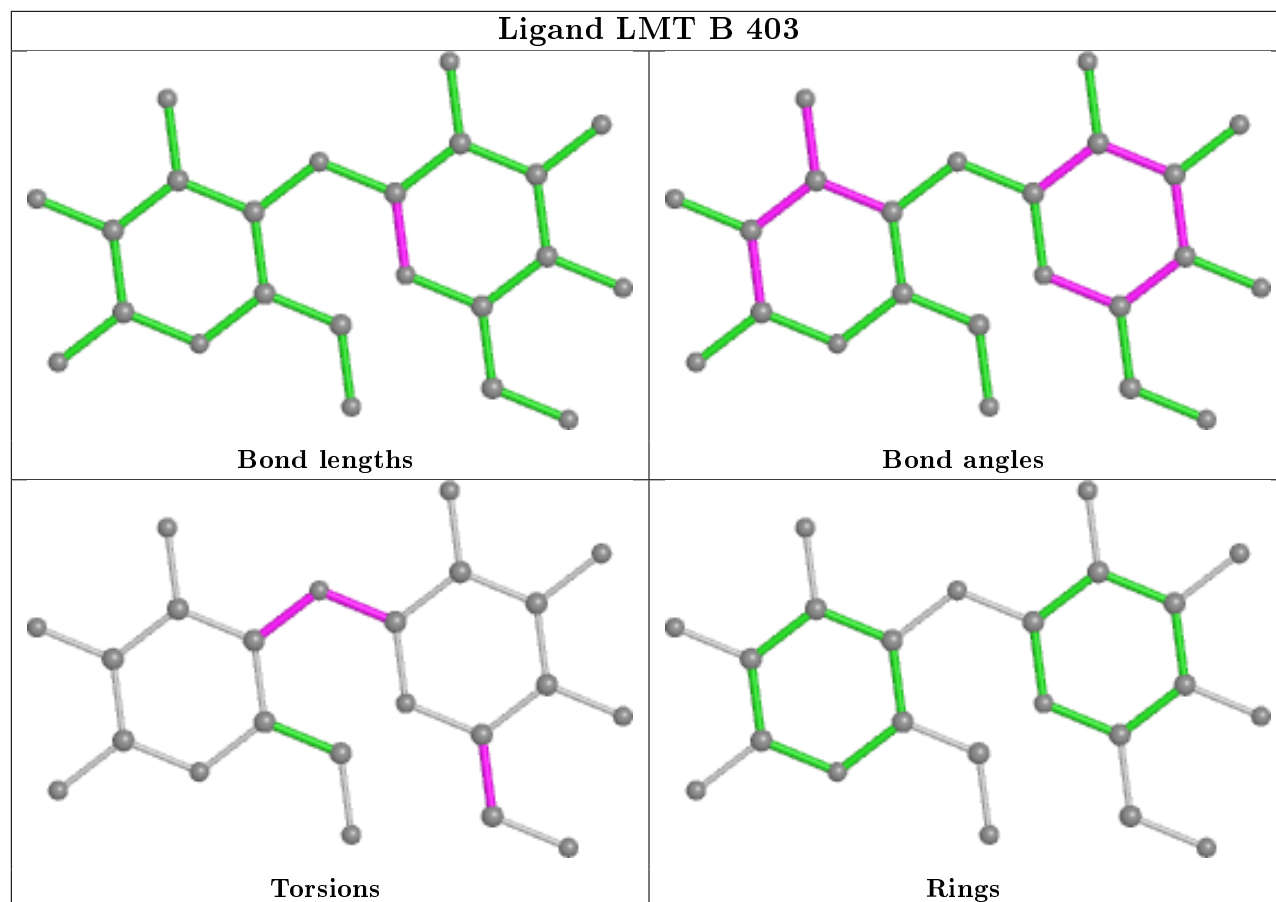












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	342/347 (98%)	0.05	1 (0%) 94 92	56, 102, 165, 226	0
1	B	341/347 (98%)	0.03	3 (0%) 84 75	58, 109, 175, 270	0
1	C	340/347 (97%)	0.02	2 (0%) 89 83	58, 106, 185, 251	0
1	D	340/347 (97%)	-0.02	1 (0%) 94 92	54, 106, 170, 263	0
1	E	340/347 (97%)	0.02	3 (0%) 84 75	57, 105, 170, 230	0
1	P	340/347 (97%)	-0.03	1 (0%) 94 92	51, 93, 156, 239	0
1	Q	340/347 (97%)	-0.05	1 (0%) 94 92	58, 99, 167, 242	0
1	R	340/347 (97%)	-0.07	4 (1%) 79 67	58, 97, 158, 274	0
1	S	340/347 (97%)	0.08	4 (1%) 79 67	53, 89, 144, 247	0
1	T	340/347 (97%)	-0.01	1 (0%) 94 92	49, 88, 151, 210	0
2	F	221/224 (98%)	0.12	10 (4%) 33 21	68, 113, 202, 265	0
2	G	222/224 (99%)	0.39	15 (6%) 17 10	75, 142, 230, 309	0
2	H	223/224 (99%)	-0.00	5 (2%) 62 48	52, 100, 158, 275	0
2	I	222/224 (99%)	-0.02	2 (0%) 84 75	63, 105, 192, 239	0
2	J	222/224 (99%)	0.81	49 (22%) 0 0	64, 146, 281, 313	0
2	U	221/224 (98%)	0.64	30 (13%) 3 2	75, 131, 220, 317	0
2	V	224/224 (100%)	0.12	8 (3%) 42 27	70, 117, 169, 269	0
2	W	224/224 (100%)	-0.06	3 (1%) 77 65	68, 102, 155, 257	0
2	X	224/224 (100%)	0.00	4 (1%) 68 55	57, 98, 169, 249	0
2	Y	221/224 (98%)	0.23	8 (3%) 42 27	64, 127, 195, 277	0
3	K	210/215 (97%)	0.15	13 (6%) 20 11	59, 114, 222, 295	0
3	L	211/215 (98%)	-0.09	1 (0%) 91 86	49, 91, 170, 224	0
3	M	210/215 (97%)	0.46	23 (10%) 5 3	69, 130, 248, 270	0
3	N	211/215 (98%)	-0.07	0 100 100	66, 116, 158, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	211/215 (98%)	-0.05	0 100 100	65, 108, 143, 157	0
3	Z	215/215 (100%)	0.19	2 (0%) 84 75	71, 120, 160, 199	0
3	f	215/215 (100%)	-0.12	1 (0%) 91 86	69, 104, 153, 231	0
3	g	211/215 (98%)	0.23	8 (3%) 40 26	71, 127, 173, 218	0
3	h	211/215 (98%)	0.25	4 (1%) 66 53	75, 137, 177, 249	0
3	i	214/215 (99%)	-0.06	0 100 100	60, 99, 135, 165	0
All	All	7746/7860 (98%)	0.09	207 (2%) 54 39	49, 107, 191, 317	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	165	SER	8.9
2	V	140	GLN	8.6
2	X	142	ASN	7.0
2	J	147	LEU	6.7
2	J	218	LYS	5.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CL	A	403	1/1	0.54	0.61	119,119,119,119	0
8	LMT	P	402	23/35	0.56	0.43	221,221,221,221	0
7	GOL	B	401	6/6	0.58	0.35	115,145,151,167	0
8	LMT	T	403	23/35	0.58	0.38	156,202,217,222	0

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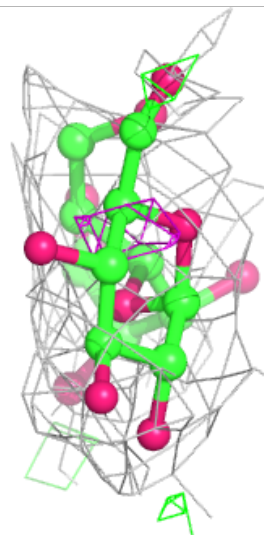
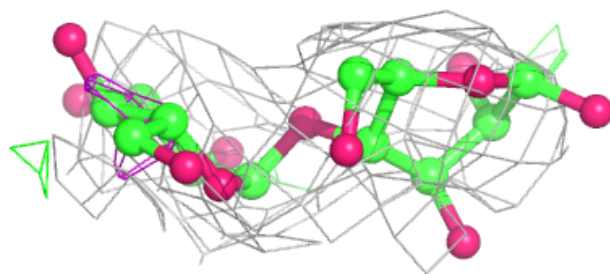
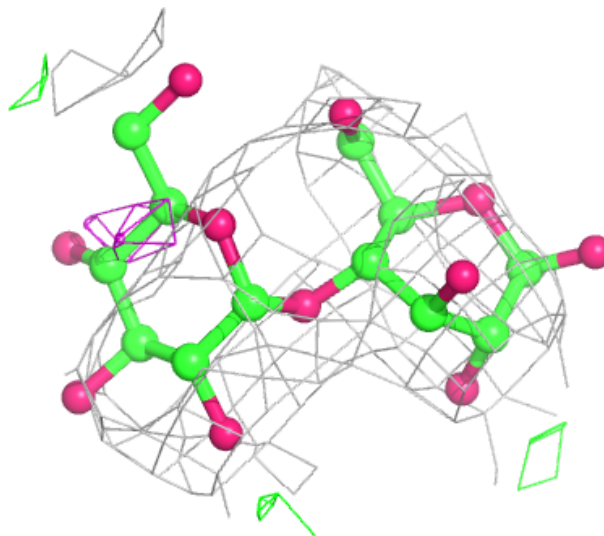
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	LMT	S	402	23/35	0.62	0.51	169,214,224,235	0
8	LMT	E	402	23/35	0.63	0.63	218,239,254,257	0
4	NAG	T	402	14/15	0.68	0.34	153,200,210,211	0
8	LMT	B	403	23/35	0.70	0.55	176,217,235,242	0
5	POV	A	402	23/52	0.73	0.62	137,177,208,241	0
5	POV	R	401	34/52	0.73	0.43	99,146,200,535	0
5	POV	D	401	26/52	0.76	0.63	125,176,201,334	0
5	POV	T	401	43/52	0.77	0.47	77,129,177,205	0
5	POV	P	403	42/52	0.78	0.43	82,125,179,206	0
8	LMT	C	402	23/35	0.79	0.32	179,179,179,179	0
8	LMT	D	403	23/35	0.79	0.58	196,218,239,247	0
4	NAG	D	402	14/15	0.80	0.19	153,197,214,221	0
4	NAG	S	401	14/15	0.81	0.22	153,184,189,195	0
5	POV	Q	401	46/52	0.81	0.67	108,149,198,237	0
5	POV	R	402	35/52	0.81	0.50	96,123,186,208	0
4	NAG	Q	402	14/15	0.82	0.23	146,184,202,207	0
4	NAG	C	401	14/15	0.84	0.27	191,210,218,223	0
4	NAG	P	401	14/15	0.85	0.24	133,182,192,201	0
4	NAG	A	401	14/15	0.86	0.23	137,181,192,196	0
4	NAG	B	402	14/15	0.87	0.25	139,168,176,177	0
6	CL	P	404	1/1	0.89	0.20	90,90,90,90	0
4	NAG	E	401	14/15	0.90	0.16	157,190,206,212	0

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

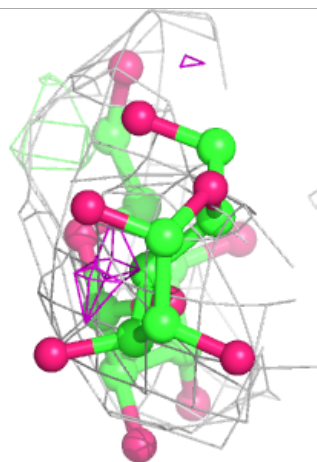
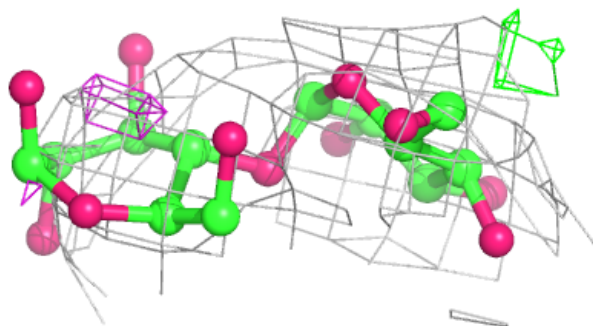
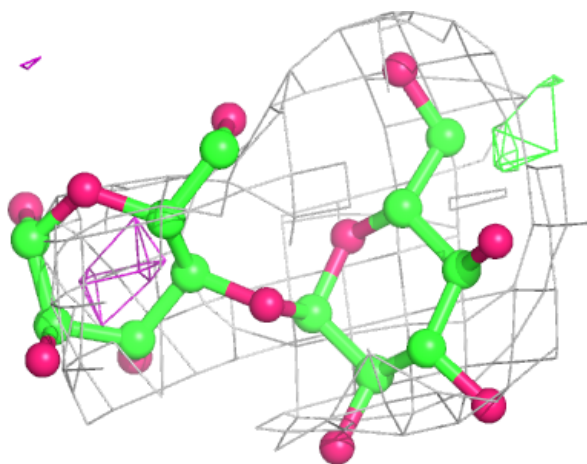
Electron density around LMT P 402:

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



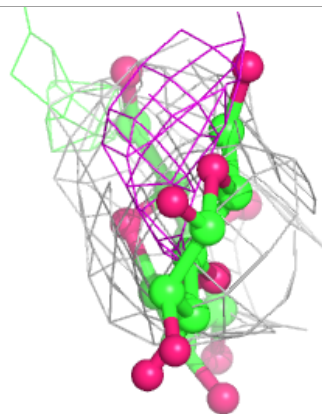
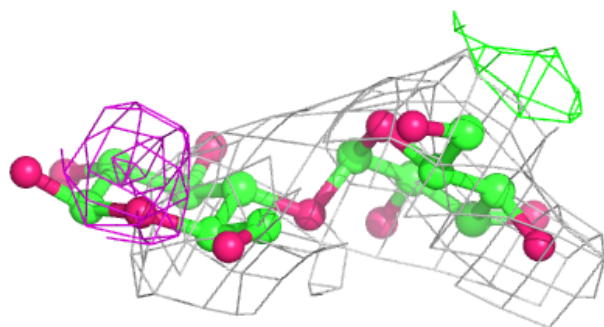
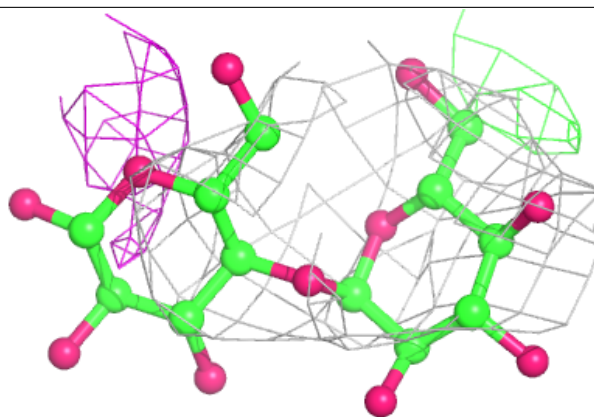
Electron density around LMT T 403:

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



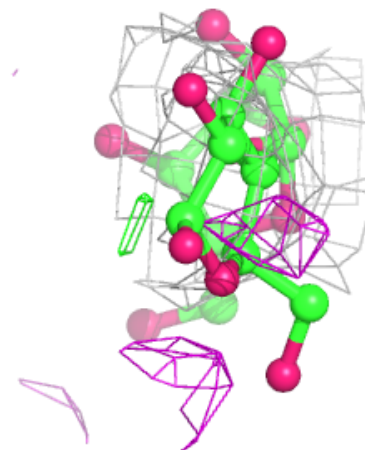
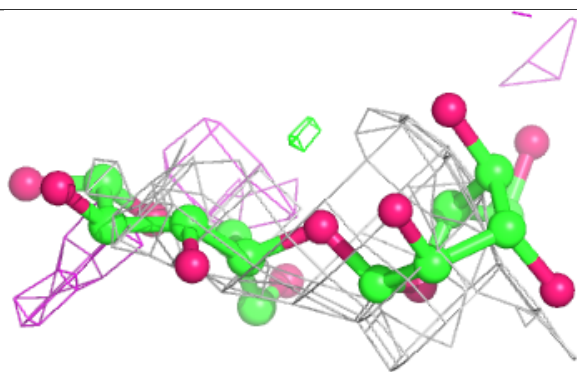
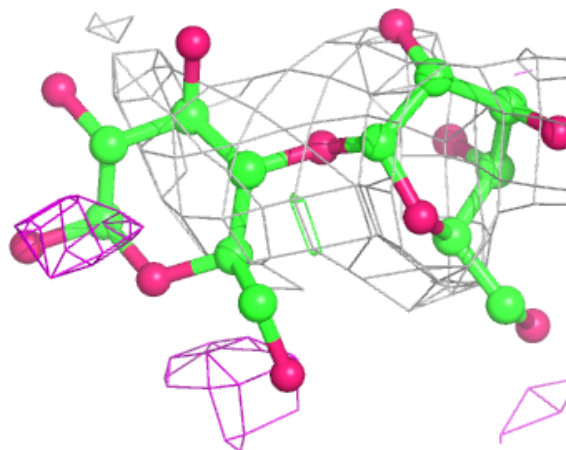
Electron density around LMT S 402:

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



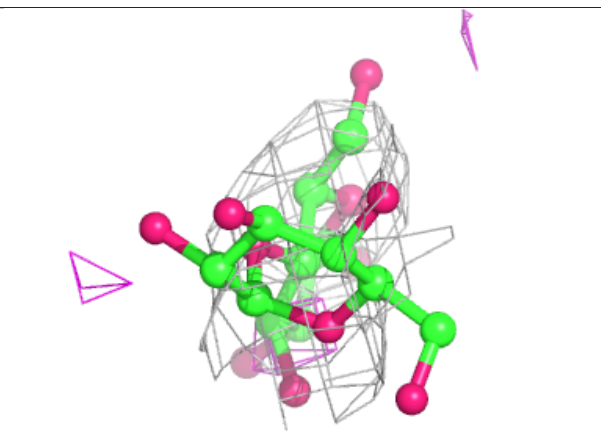
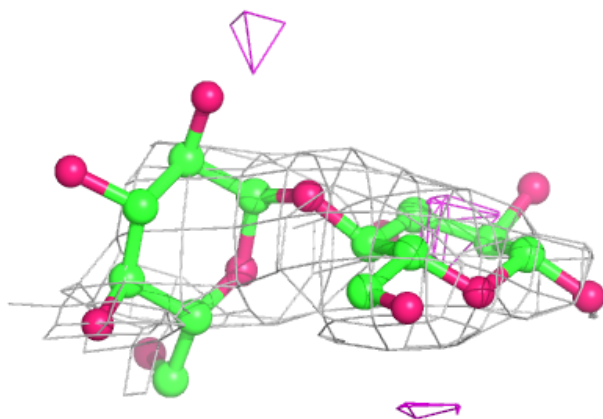
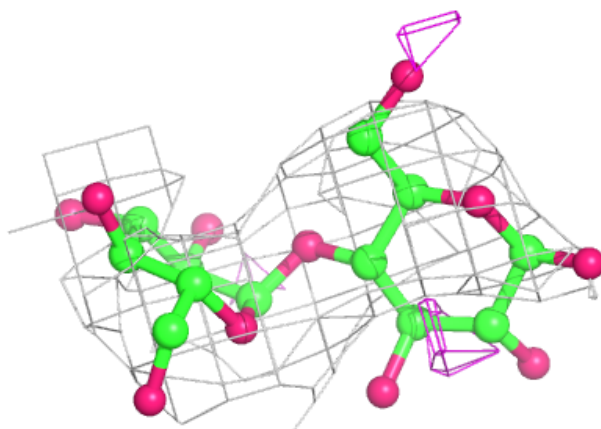
Electron density around LMT E 402:

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

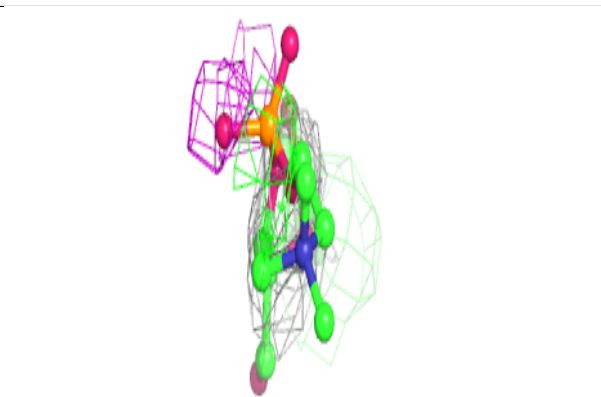
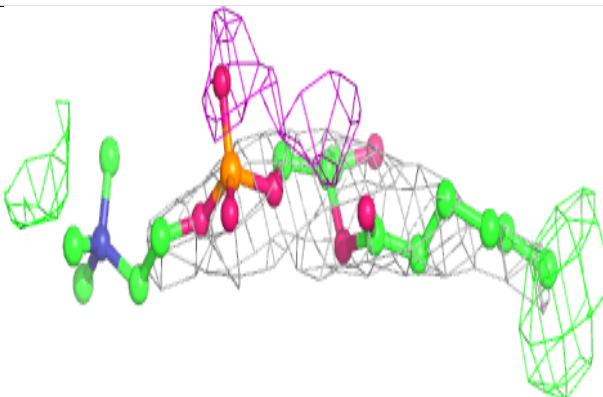
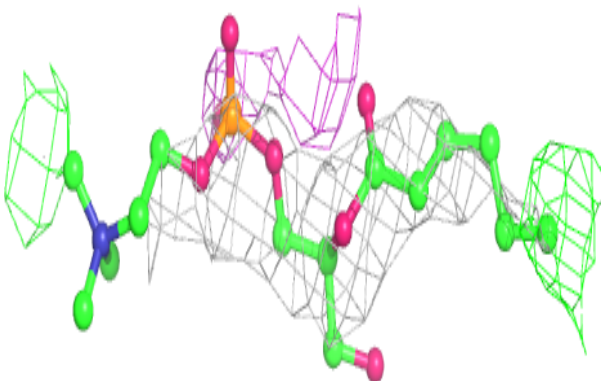


Electron density around LMT B 403:

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

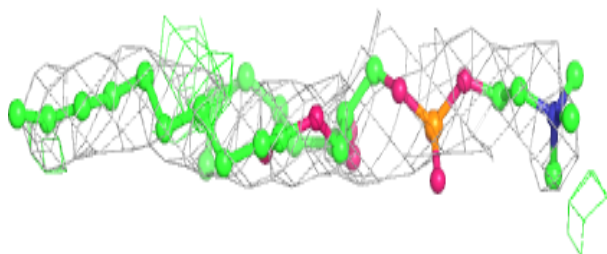
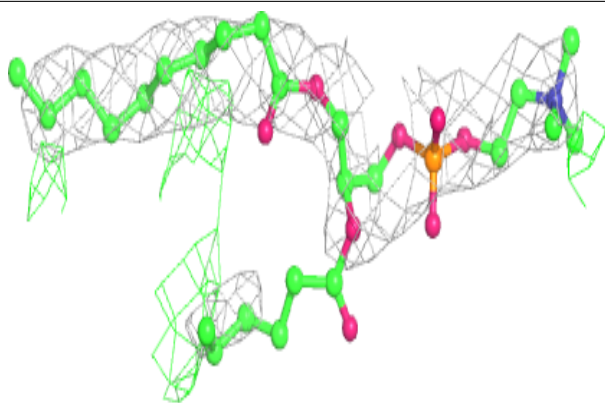
**Electron density around POV A 402:**

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and green (positive)

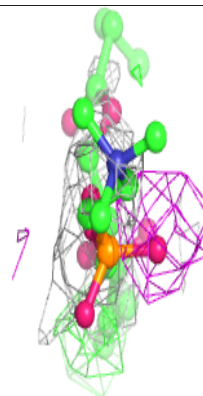
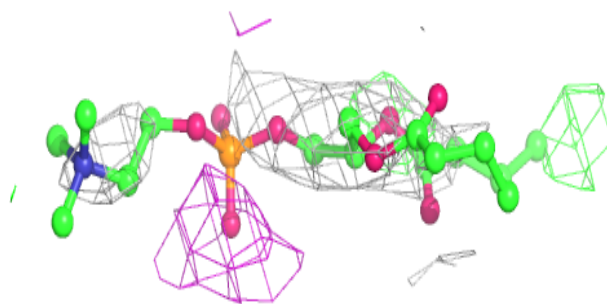
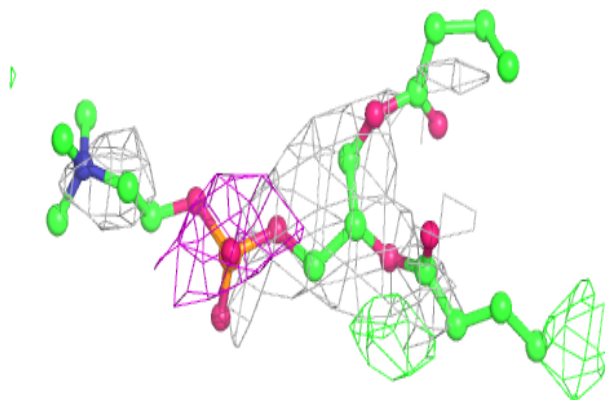


Electron density around POV R 401:

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and green (positive)

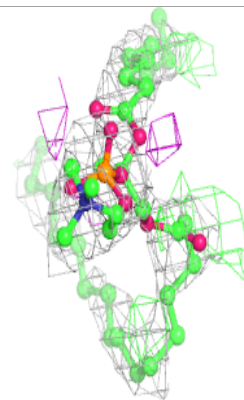
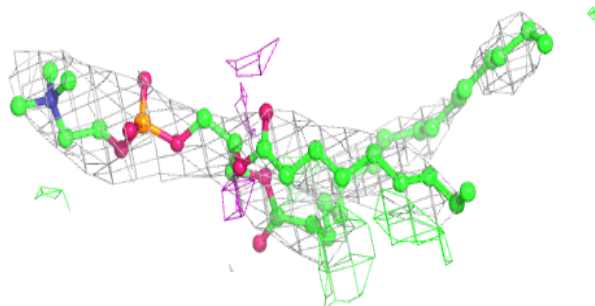
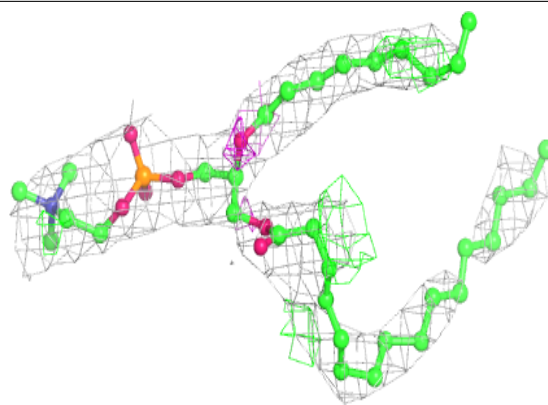
**Electron density around POV D 401:**

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

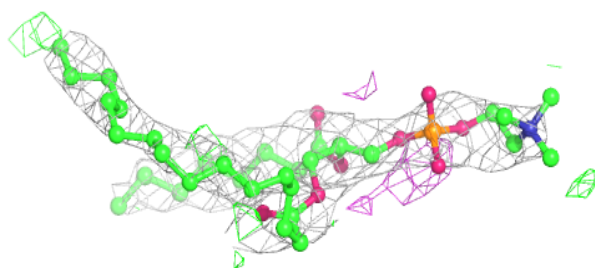
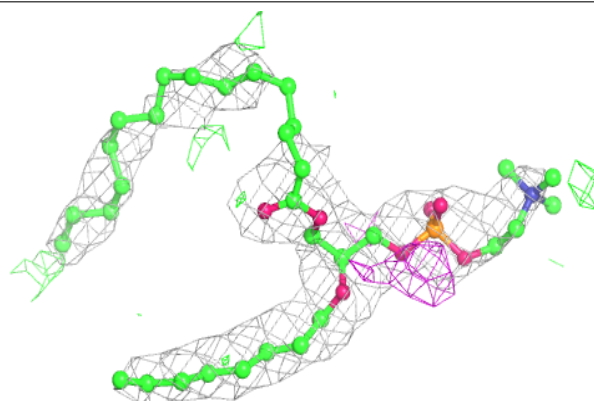


Electron density around POV T 401:

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

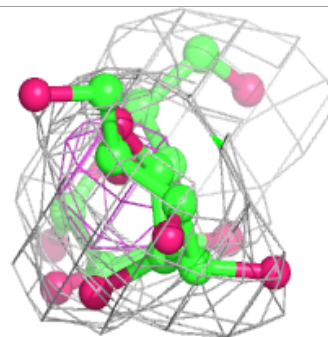
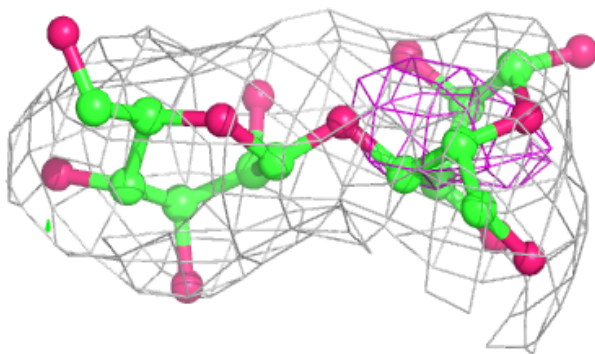
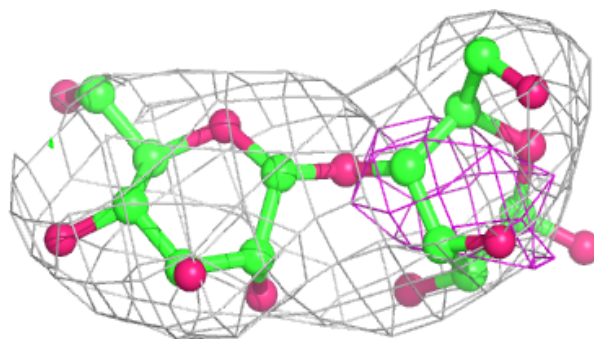
**Electron density around POV P 403:**

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



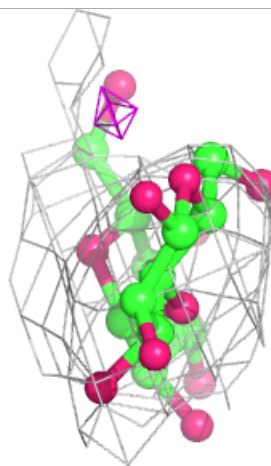
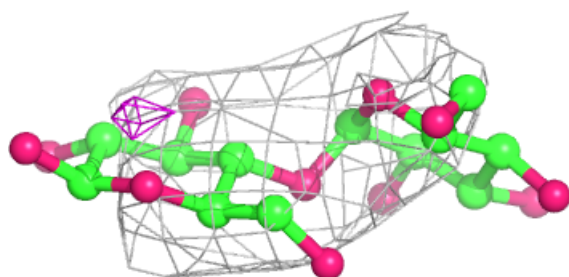
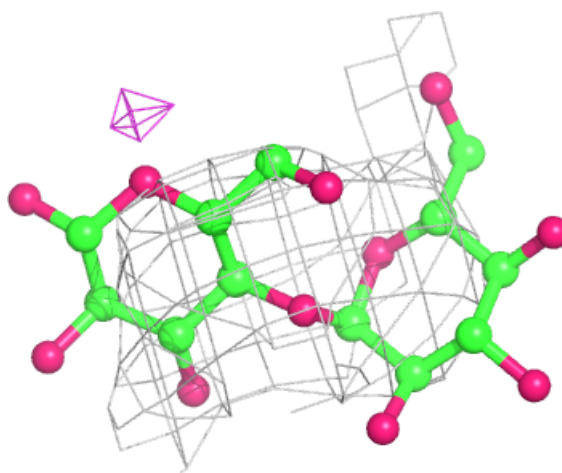
Electron density around LMT C 402:

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



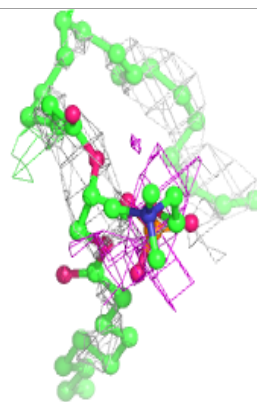
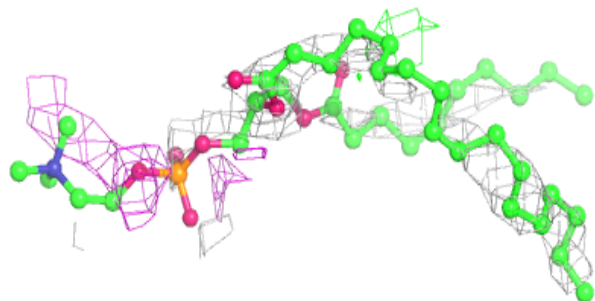
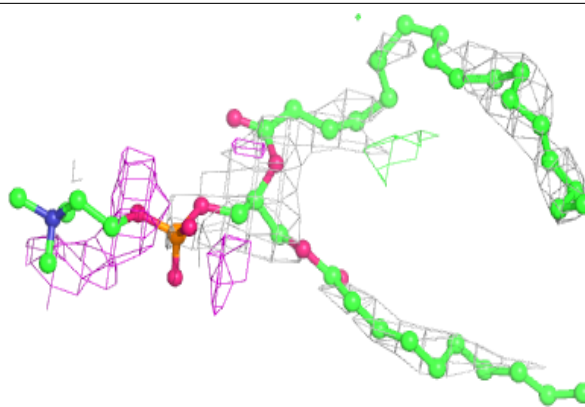
Electron density around LMT D 403:

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



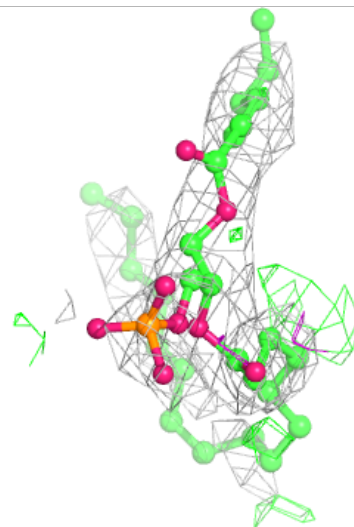
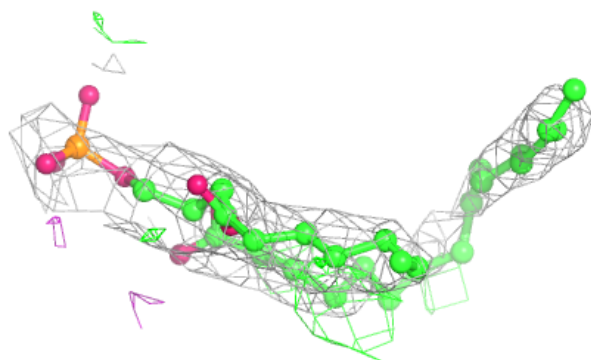
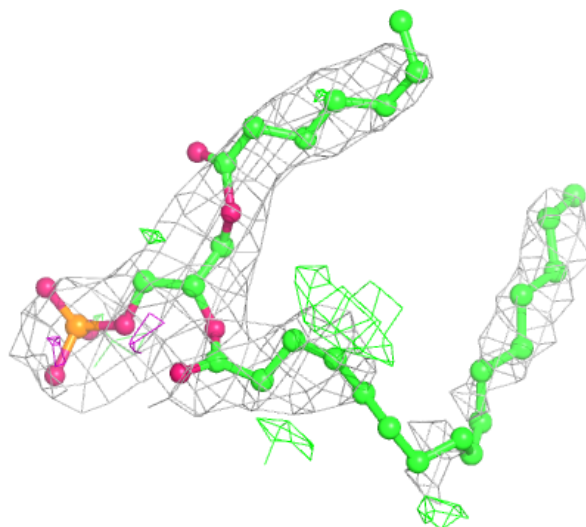
Electron density around POV Q 401:

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



Electron density around POV R 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.