Full wwPDB X-ray Structure Validation Report (i)

Sep 16, 2023 – 08:51 PM EDT

PDB ID	:	4TNV
Title	:	C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab in a non-conducting conformation
Authors	:	Althoff, T.; Hibbs, R.E.; Banerjee, S.; Gouaux, E.
Deposited on	:	2014-06-05
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

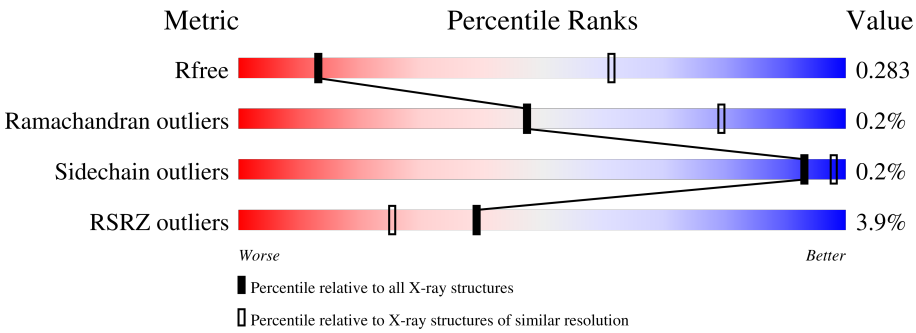
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	%, 97%, .
1	B	347	4%, 97%, .
1	C	347	%, 97%, .
1	D	347	3%, 97%, .
1	E	347	5%, 97%, .
1	P	347	2%, 97%, .

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Mol	Chain	Length	Quality of chain
1	Q	347	2% 97%
1	R	347	% 97%
1	S	347	2% 97%
1	T	347	% 97%
2	F	224	3% 99%
2	G	224	4% 100%
2	H	224	99%
2	I	224	2% 99%
2	J	224	13% 100%
2	U	224	12% 99%
2	V	224	5% 99%
2	W	224	3% 100%
2	X	224	% 99%
2	Y	224	15% 98%
3	K	215	3% 98%
3	L	215	% 97%
3	M	215	10% 98%
3	N	215	2% 98%
3	O	215	% 98%
3	Z	215	2% 100%
3	f	215	2% 99%
3	g	215	18% 98%
3	h	215	6% 98%
3	i	215	100%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CL	P	403	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 60408 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
			Total	C	N	O	S			
1	A	337	2695	1755	438	487	15	0	0	0
1	B	337	2695	1755	438	487	15	0	0	0
1	C	337	2695	1755	438	487	15	0	0	0
1	D	337	2695	1755	438	487	15	0	0	0
1	E	337	2695	1755	438	487	15	0	0	0
1	P	337	2695	1755	438	487	15	0	0	0
1	Q	337	2695	1755	438	487	15	0	0	0
1	R	337	2695	1755	438	487	15	0	0	0
1	S	337	2695	1755	438	487	15	0	0	0
1	T	337	2695	1755	438	487	15	0	0	0

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

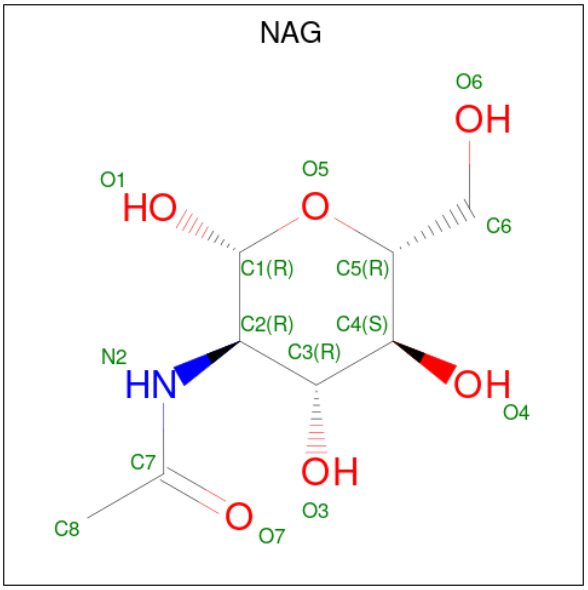
- Molecule 2 is a protein called Mouse monoclonal Fab fragment, heavy chain.

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

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

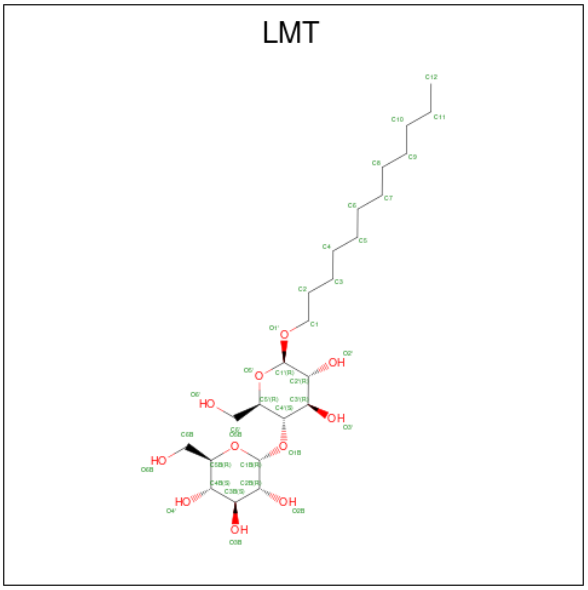
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	K	212	1606	1008	271	321	6	0	0	0
			Total	C	N	O	S			
3	L	211	1601	1005	270	320	6	0	0	0
			Total	C	N	O	S			
3	N	211	1601	1005	270	320	6	0	0	0
			Total	C	N	O	S			
3	O	211	1601	1005	270	320	6	0	0	0
			Total	C	N	O	S			
3	Z	215	1626	1018	274	327	7	0	0	0
			Total	C	N	O	S			
3	f	214	1620	1015	273	325	7	0	0	0
			Total	C	N	O	S			
3	g	211	1601	1005	270	320	6	0	0	0
			Total	C	N	O	S			
3	h	211	1601	1005	270	320	6	0	0	0
			Total	C	N	O	S			
3	i	214	1620	1015	273	325	7	0	0	0
			Total	C	N	O	S			
3	M	211	1601	1005	270	320	6	0	0	0

- 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
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0
4	C	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0
4	E	1	14	8	1	5	0	0
4	P	1	14	8	1	5	0	0
4	Q	1	14	8	1	5	0	0
4	R	1	14	8	1	5	0	0
4	S	1	14	8	1	5	0	0
4	T	1	14	8	1	5	0	0

- Molecule 5 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	23	12	11	0	0

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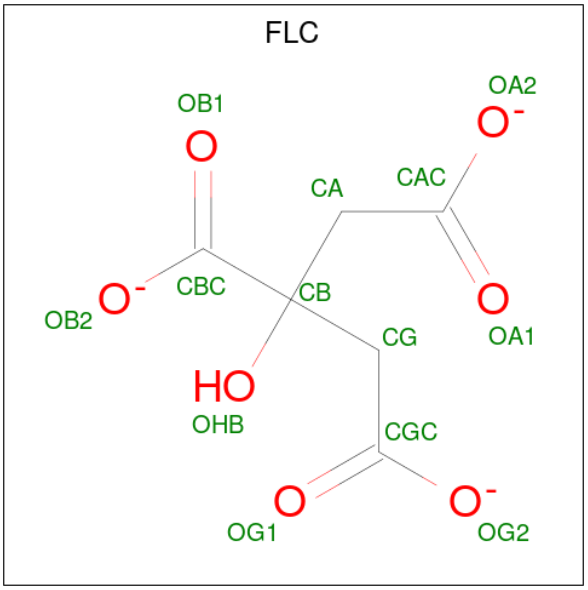
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	23	12	11	0	0
5	C	1	23	12	11	0	0
5	D	1	23	12	11	0	0
5	E	1	23	12	11	0	0
5	P	1	23	12	11	0	0
5	Q	1	23	12	11	0	0
5	R	1	23	12	11	0	0
5	S	1	23	12	11	0	0
5	T	1	25	14	11	0	0

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	13	6	7	0	0
6	T	1	13	6	7	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

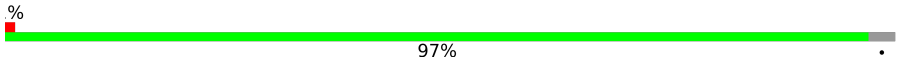
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	P	2	2	2	0	0

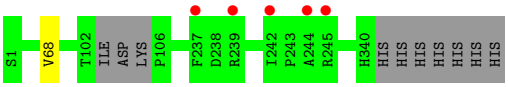
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

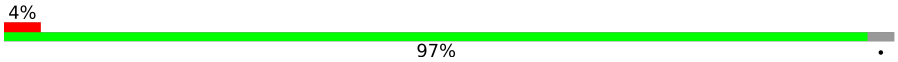
Chain A:

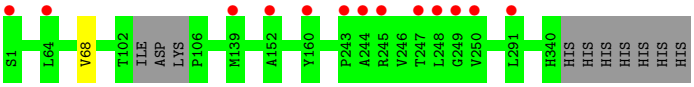




• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

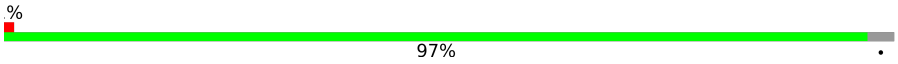
Chain B:

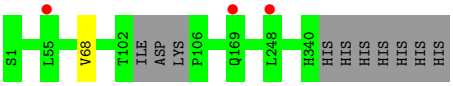




• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

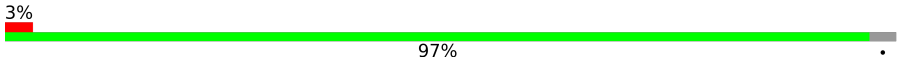
Chain C:

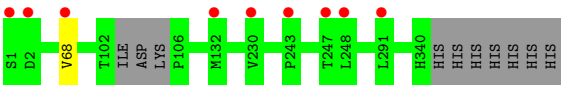




• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

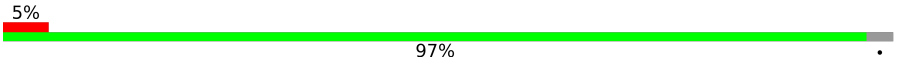
Chain D:

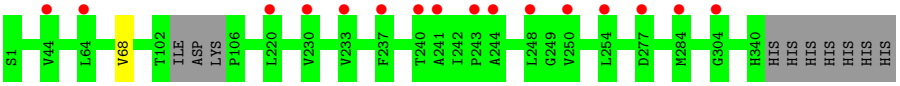




• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

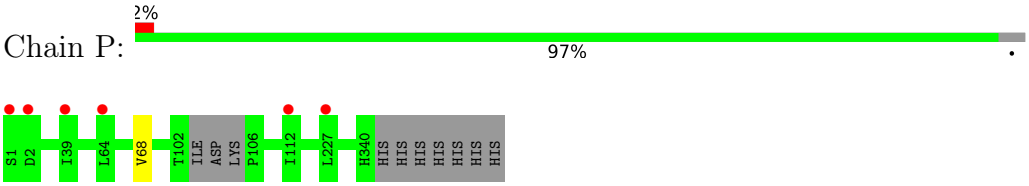
Chain E:





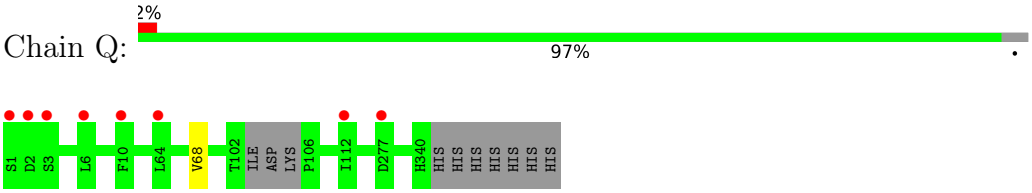
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain P:



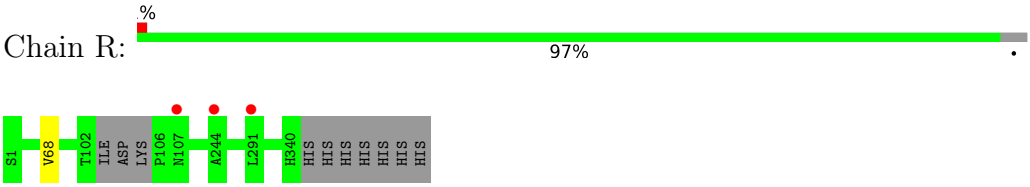
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain Q:



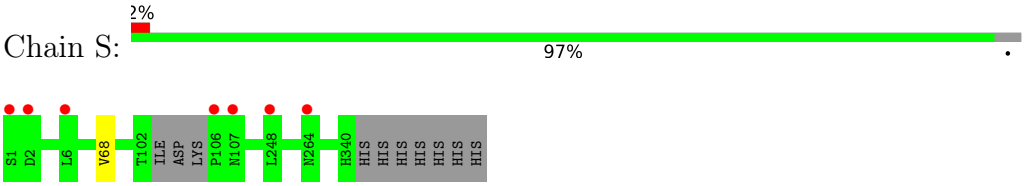
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain R:



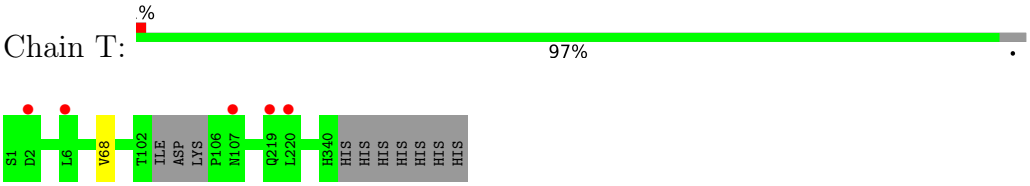
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain S:



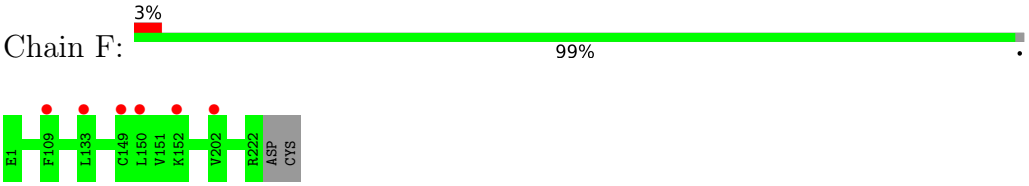
• Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain T:



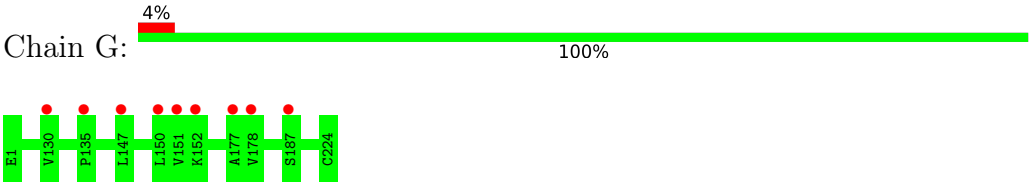
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:



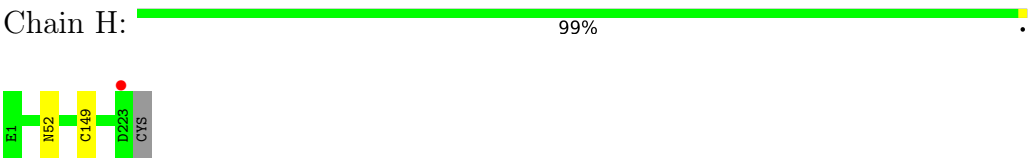
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G:



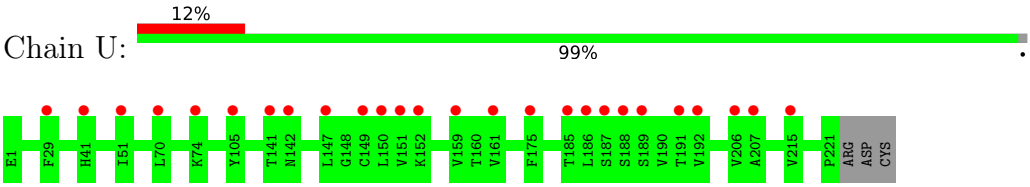
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H:



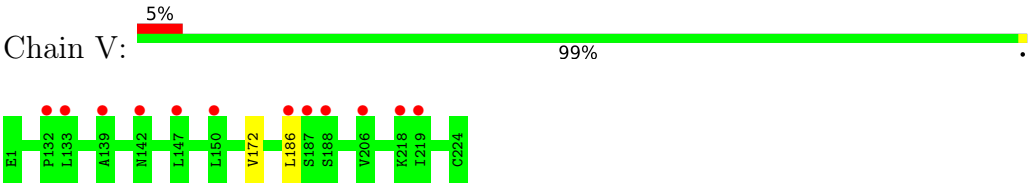
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain U:



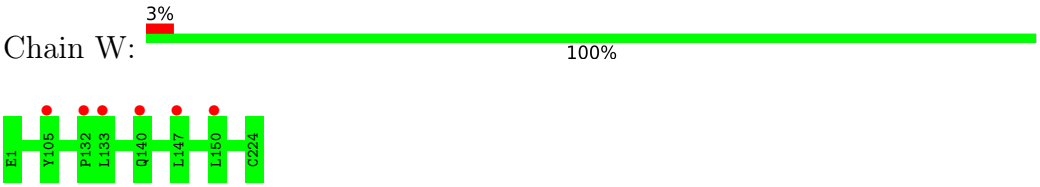
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain V:



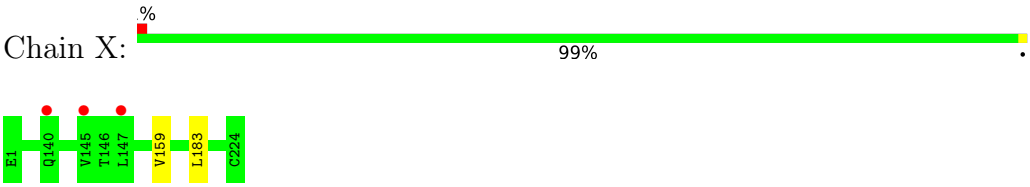
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain W:



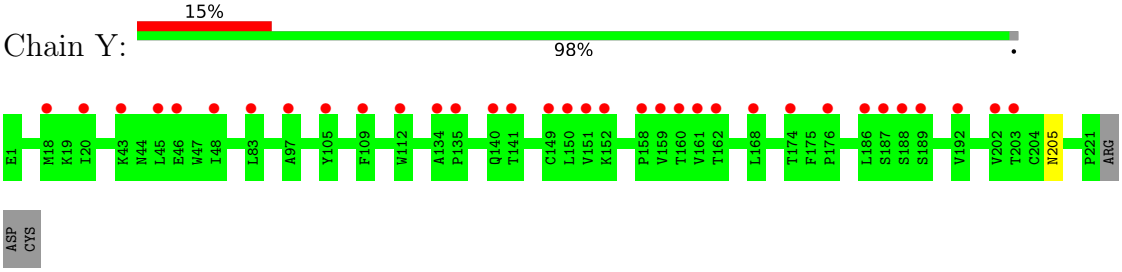
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain X:



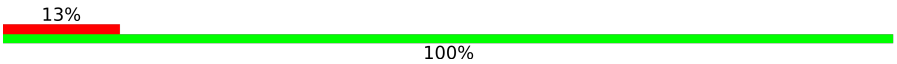
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

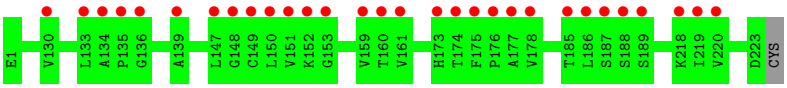
Chain Y:



• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

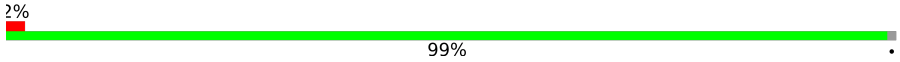
Chain J:





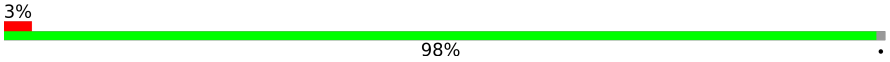
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

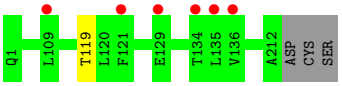
Chain I:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

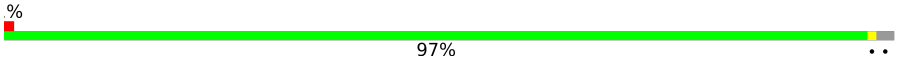
Chain K:

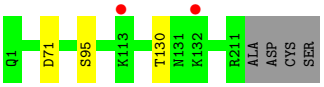




• Molecule 3: Mouse monoclonal Fab fragment, light chain

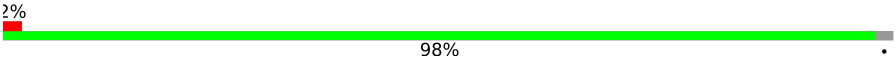
Chain L:

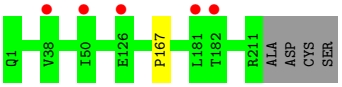




• Molecule 3: Mouse monoclonal Fab fragment, light chain

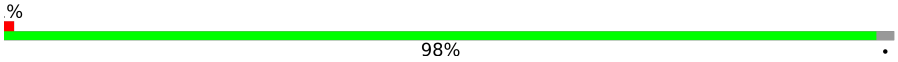
Chain N:

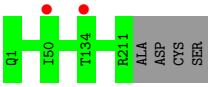




• Molecule 3: Mouse monoclonal Fab fragment, light chain

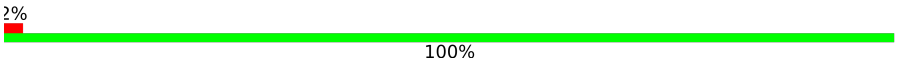
Chain O:





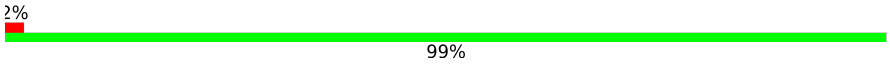
• Molecule 3: Mouse monoclonal Fab fragment, light chain

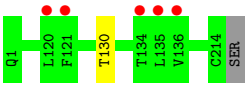
Chain Z:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

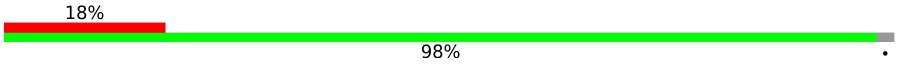
Chain f:

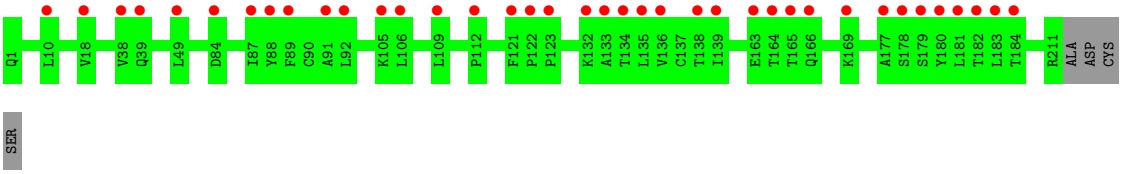




• Molecule 3: Mouse monoclonal Fab fragment, light chain

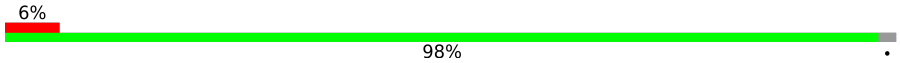
Chain g:

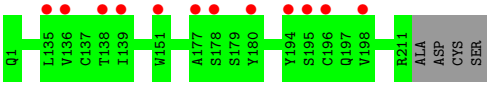




• Molecule 3: Mouse monoclonal Fab fragment, light chain

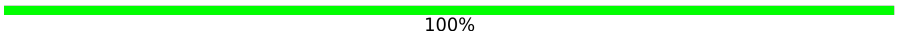
Chain h:





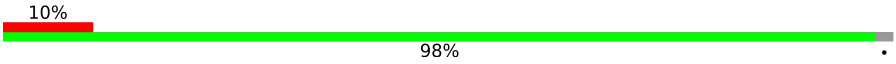
• Molecule 3: Mouse monoclonal Fab fragment, light chain

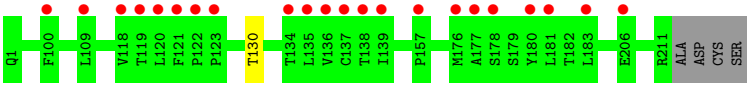
Chain i:



• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain M:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	455.81Å 195.68Å 196.18Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	58.44 – 3.60 58.44 – 3.60	Depositor EDS
% Data completeness (in resolution range)	88.3 (58.44-3.60) 88.4 (58.44-3.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.261 , 0.283 0.262 , 0.283	Depositor DCC
R_{free} test set	8783 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	121.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 89.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	60408	wwPDB-VP
Average B, all atoms (Å^2)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, NAG, FLC, 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	0.28	0/2767	0.45	0/3776
1	B	0.27	0/2767	0.45	0/3776
1	C	0.28	0/2767	0.46	0/3776
1	D	0.28	0/2767	0.45	0/3776
1	E	0.27	0/2767	0.44	0/3776
1	P	0.29	0/2767	0.46	0/3776
1	Q	0.30	0/2767	0.47	0/3776
1	R	0.30	0/2767	0.47	0/3776
1	S	0.31	0/2767	0.48	0/3776
1	T	0.30	0/2767	0.47	0/3776
2	F	0.25	0/1739	0.43	0/2374
2	G	0.25	0/1753	0.42	0/2393
2	H	0.28	0/1747	0.45	0/2385
2	I	0.25	0/1739	0.43	0/2374
2	J	0.27	0/1747	0.45	0/2385
2	U	0.24	0/1728	0.43	0/2360
2	V	0.25	0/1753	0.44	0/2393
2	W	0.27	0/1753	0.44	0/2393
2	X	0.26	0/1753	0.45	0/2393
2	Y	0.24	0/1728	0.44	0/2360
3	K	0.27	0/1644	0.45	0/2247
3	L	0.30	0/1639	0.48	0/2240
3	M	0.25	0/1639	0.46	0/2240
3	N	0.24	0/1639	0.43	0/2240
3	O	0.25	0/1639	0.44	0/2240
3	Z	0.25	0/1664	0.45	0/2274
3	f	0.28	0/1658	0.45	0/2266
3	g	0.24	0/1639	0.45	0/2240
3	h	0.25	0/1639	0.44	0/2240
3	i	0.28	0/1658	0.46	0/2266
All	All	0.27	0/61568	0.45	0/84063

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	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	41	75
1	B	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	41	75
1	C	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	41	75
1	D	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	41	75
1	E	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	41	75
1	P	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	41	75
1	Q	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	41	75
1	R	333/347 (96%)	322 (97%)	10 (3%)	1 (0%)	41	75
1	S	333/347 (96%)	320 (96%)	12 (4%)	1 (0%)	41	75
1	T	333/347 (96%)	321 (96%)	11 (3%)	1 (0%)	41	75
2	F	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	G	222/224 (99%)	197 (89%)	25 (11%)	0	100	100
2	H	221/224 (99%)	198 (90%)	23 (10%)	0	100	100
2	I	220/224 (98%)	204 (93%)	16 (7%)	0	100	100
2	J	221/224 (99%)	200 (90%)	21 (10%)	0	100	100
2	U	219/224 (98%)	195 (89%)	24 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	222/224 (99%)	196 (88%)	25 (11%)	1 (0%)	29	68
2	W	222/224 (99%)	199 (90%)	23 (10%)	0	100	100
2	X	222/224 (99%)	201 (90%)	21 (10%)	0	100	100
2	Y	219/224 (98%)	192 (88%)	27 (12%)	0	100	100
3	K	210/215 (98%)	190 (90%)	20 (10%)	0	100	100
3	L	209/215 (97%)	195 (93%)	13 (6%)	1 (0%)	29	68
3	M	209/215 (97%)	190 (91%)	19 (9%)	0	100	100
3	N	209/215 (97%)	193 (92%)	15 (7%)	1 (0%)	29	68
3	O	209/215 (97%)	198 (95%)	11 (5%)	0	100	100
3	Z	213/215 (99%)	192 (90%)	20 (9%)	1 (0%)	29	68
3	f	212/215 (99%)	198 (93%)	14 (7%)	0	100	100
3	g	209/215 (97%)	185 (88%)	24 (12%)	0	100	100
3	h	209/215 (97%)	191 (91%)	18 (9%)	0	100	100
3	i	212/215 (99%)	192 (91%)	20 (9%)	0	100	100
All	All	7639/7860 (97%)	7122 (93%)	503 (7%)	14 (0%)	47	79

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL
1	E	68	VAL
1	P	68	VAL
1	Q	68	VAL
1	R	68	VAL
1	S	68	VAL
1	T	68	VAL
2	V	172	VAL
3	Z	152	LYS
3	L	95	SER
3	N	167	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/316 (96%)	305 (100%)	0	100	100
1	B	305/316 (96%)	305 (100%)	0	100	100
1	C	305/316 (96%)	305 (100%)	0	100	100
1	D	305/316 (96%)	305 (100%)	0	100	100
1	E	305/316 (96%)	305 (100%)	0	100	100
1	P	305/316 (96%)	305 (100%)	0	100	100
1	Q	305/316 (96%)	305 (100%)	0	100	100
1	R	305/316 (96%)	305 (100%)	0	100	100
1	S	305/316 (96%)	305 (100%)	0	100	100
1	T	305/316 (96%)	305 (100%)	0	100	100
2	F	191/193 (99%)	191 (100%)	0	100	100
2	G	193/193 (100%)	193 (100%)	0	100	100
2	H	192/193 (100%)	190 (99%)	2 (1%)	76	88
2	I	191/193 (99%)	191 (100%)	0	100	100
2	J	192/193 (100%)	192 (100%)	0	100	100
2	U	190/193 (98%)	190 (100%)	0	100	100
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%)	191 (99%)	2 (1%)	76	88
2	Y	190/193 (98%)	189 (100%)	1 (0%)	88	95
3	K	179/182 (98%)	178 (99%)	1 (1%)	86	94
3	L	179/182 (98%)	177 (99%)	2 (1%)	73	88
3	M	179/182 (98%)	178 (99%)	1 (1%)	86	94
3	N	179/182 (98%)	179 (100%)	0	100	100
3	O	179/182 (98%)	179 (100%)	0	100	100
3	Z	182/182 (100%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	f	181/182 (100%)	180 (99%)	1 (1%)	86	94
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%)	181 (100%)	0	100	100
All	All	6765/6910 (98%)	6754 (100%)	11 (0%)	93	98

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	52	ASN
2	H	149	CYS
3	K	119	THR
3	L	71	ASP
3	L	130	THR
2	V	186	LEU
2	X	159	VAL
2	X	183	LEU
2	Y	205	ASN
3	f	130	THR
3	M	130	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	55	ASN
2	H	52	ASN
3	L	170	GLN
2	Y	55	ASN
2	Y	205	ASN
3	Z	96	ASN
3	f	96	ASN
3	g	172	ASN
3	g	197	GLN
3	h	96	ASN
3	i	96	ASN
2	J	55	ASN
3	M	96	ASN

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 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
5	LMT	Q	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.41	5 (14%)
5	LMT	B	402	-	24,24,36	1.16	2 (8%)	35,35,47	1.27	5 (14%)
6	FLC	A	403	-	12,12,12	0.99	0	17,17,17	1.16	2 (11%)
5	LMT	A	402	-	24,24,36	1.11	2 (8%)	35,35,47	1.24	3 (8%)
5	LMT	C	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.30	5 (14%)
4	NAG	P	401	1	14,14,15	0.52	0	17,19,21	1.56	2 (11%)
4	NAG	D	401	1	14,14,15	0.46	0	17,19,21	1.10	1 (5%)
6	FLC	T	403	-	12,12,12	1.05	0	17,17,17	1.30	2 (11%)
5	LMT	D	402	-	24,24,36	1.05	2 (8%)	35,35,47	1.09	2 (5%)
5	LMT	P	402	-	24,24,36	1.08	2 (8%)	35,35,47	1.11	3 (8%)
5	LMT	R	402	-	24,24,36	1.07	2 (8%)	35,35,47	1.00	1 (2%)
4	NAG	T	401	1	14,14,15	0.35	0	17,19,21	0.68	0
4	NAG	R	401	1	14,14,15	0.47	0	17,19,21	0.67	0
5	LMT	S	402	-	24,24,36	1.08	2 (8%)	35,35,47	1.19	3 (8%)
4	NAG	Q	401	1	14,14,15	0.68	0	17,19,21	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	401	1	14,14,15	0.69	0	17,19,21	1.07	1 (5%)
4	NAG	E	401	1	14,14,15	0.33	0	17,19,21	0.63	0
4	NAG	A	401	1	14,14,15	0.26	0	17,19,21	0.62	0
4	NAG	S	401	1	14,14,15	0.36	0	17,19,21	1.23	1 (5%)
5	LMT	E	402	-	24,24,36	1.11	2 (8%)	35,35,47	1.10	2 (5%)
4	NAG	C	401	1	14,14,15	0.57	0	17,19,21	1.93	6 (35%)
5	LMT	T	402	-	26,26,36	1.14	2 (7%)	37,37,47	0.96	1 (2%)

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
5	LMT	Q	402	-	-	4/8/48/61	0/2/2/2
5	LMT	B	402	-	-	3/8/48/61	0/2/2/2
6	FLC	A	403	-	-	0/16/16/16	-
5	LMT	A	402	-	-	5/8/48/61	0/2/2/2
5	LMT	C	402	-	-	3/8/48/61	0/2/2/2
4	NAG	P	401	1	-	4/6/23/26	0/1/1/1
4	NAG	D	401	1	-	4/6/23/26	0/1/1/1
6	FLC	T	403	-	-	3/16/16/16	-
5	LMT	D	402	-	-	4/8/48/61	0/2/2/2
5	LMT	P	402	-	-	2/8/48/61	0/2/2/2
5	LMT	R	402	-	-	4/8/48/61	0/2/2/2
4	NAG	T	401	1	-	4/6/23/26	0/1/1/1
4	NAG	R	401	1	-	4/6/23/26	0/1/1/1
5	LMT	S	402	-	-	5/8/48/61	0/2/2/2
4	NAG	Q	401	1	-	6/6/23/26	0/1/1/1
4	NAG	B	401	1	-	6/6/23/26	0/1/1/1
4	NAG	E	401	1	-	3/6/23/26	0/1/1/1
4	NAG	A	401	1	-	2/6/23/26	0/1/1/1
4	NAG	S	401	1	-	4/6/23/26	0/1/1/1
5	LMT	E	402	-	-	2/8/48/61	0/2/2/2
4	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	LMT	T	402	-	-	4/11/51/61	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	LMT	O5B-C1B	3.20	1.50	1.41
5	E	402	LMT	O5B-C1B	3.01	1.49	1.41
5	Q	402	LMT	O5B-C1B	3.01	1.49	1.41
5	C	402	LMT	O5B-C1B	2.97	1.49	1.41
5	A	402	LMT	O5B-C1B	2.95	1.49	1.41
5	T	402	LMT	O5B-C1B	2.91	1.49	1.41
5	S	402	LMT	O5B-C1B	2.86	1.49	1.41
5	P	402	LMT	O5B-C1B	2.79	1.49	1.41
5	D	402	LMT	O5B-C1B	2.77	1.48	1.41
5	R	402	LMT	O5B-C1B	2.76	1.48	1.41
5	T	402	LMT	O5'-C1'	2.68	1.48	1.41
5	P	402	LMT	O5'-C1'	2.39	1.48	1.42
5	E	402	LMT	O5'-C1'	2.26	1.48	1.42
5	S	402	LMT	O5'-C1'	2.21	1.48	1.42
5	A	402	LMT	O5'-C1'	2.19	1.48	1.42
5	R	402	LMT	O5'-C1'	2.18	1.48	1.42
5	B	402	LMT	O5'-C1'	2.17	1.48	1.42
5	D	402	LMT	O5'-C1'	2.17	1.48	1.42
5	Q	402	LMT	O5'-C1'	2.16	1.48	1.42
5	C	402	LMT	O5'-C1'	2.02	1.47	1.42

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	401	NAG	C1-O5-C5	5.10	119.10	112.19
4	C	401	NAG	C1-O5-C5	4.75	118.63	112.19
5	A	402	LMT	O5B-C5B-C4B	3.93	116.83	109.69
5	B	402	LMT	O5B-C5B-C4B	3.91	116.80	109.69
5	Q	402	LMT	C2'-C3'-C4'	3.84	118.45	109.68
5	C	402	LMT	O5'-C5'-C4'	3.71	117.58	109.75
4	S	401	NAG	C1-O5-C5	-3.65	107.25	112.19
4	C	401	NAG	C2-N2-C7	-3.60	117.78	122.90
6	A	403	FLC	OB2-CBC-CB	3.36	118.89	113.05
5	Q	402	LMT	C1B-O1B-C4'	-3.33	109.72	117.96
5	S	402	LMT	C2'-C3'-C4'	3.22	117.03	109.68
4	P	401	NAG	O5-C1-C2	3.20	116.35	111.29
6	T	403	FLC	OB2-CBC-CB	3.19	118.59	113.05
5	B	402	LMT	C1B-O5B-C5B	3.16	119.89	113.69
5	Q	402	LMT	C3'-C4'-C5'	3.06	117.94	110.93
4	D	401	NAG	C1-O5-C5	-3.05	108.06	112.19
5	S	402	LMT	O5B-C5B-C4B	2.96	115.07	109.69
5	P	402	LMT	O5'-C1'-C2'	2.95	115.55	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	402	LMT	C1B-O1B-C4'	-2.85	110.92	117.96
4	C	401	NAG	C4-C3-C2	-2.74	107.00	111.02
5	E	402	LMT	C1B-O1B-C4'	-2.74	111.19	117.96
5	C	402	LMT	C3'-C4'-C5'	2.71	117.13	110.93
5	C	402	LMT	C2'-C3'-C4'	2.68	115.79	109.68
5	P	402	LMT	C1B-O1B-C4'	-2.67	111.36	117.96
5	T	402	LMT	C1B-O1B-C4'	-2.65	111.42	117.96
4	B	401	NAG	O5-C1-C2	-2.58	107.21	111.29
6	T	403	FLC	OB1-CBC-CB	-2.57	118.62	122.25
5	P	402	LMT	C1'-C2'-C3'	2.57	115.64	110.31
5	Q	402	LMT	O5B-C1B-C2B	2.56	115.76	110.35
5	Q	402	LMT	C1'-C2'-C3'	2.54	115.59	110.31
5	D	402	LMT	C2'-C3'-C4'	2.47	115.33	109.68
5	D	402	LMT	C1B-O1B-C4'	-2.46	111.86	117.96
5	C	402	LMT	C1B-C2B-C3B	2.40	114.98	110.00
5	C	402	LMT	C1B-O1B-C4'	-2.38	112.07	117.96
5	B	402	LMT	C6B-C5B-C4B	-2.37	107.46	113.00
4	C	401	NAG	O5-C5-C6	2.33	110.85	107.20
4	C	401	NAG	O5-C1-C2	2.31	114.93	111.29
6	A	403	FLC	OB1-CBC-CB	-2.31	118.99	122.25
5	E	402	LMT	O5B-C1B-C2B	2.28	115.18	110.35
5	B	402	LMT	O5'-C5'-C4'	2.28	114.56	109.75
5	S	402	LMT	C1'-C2'-C3'	2.28	115.05	110.31
5	B	402	LMT	O5B-C1B-C2B	2.25	115.10	110.35
4	C	401	NAG	C6-C5-C4	-2.23	107.79	113.00
5	A	402	LMT	C1B-O5B-C5B	2.17	117.95	113.69
5	A	402	LMT	C3B-C4B-C5B	2.12	114.01	110.24

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O7-C7-N2-C2
4	C	401	NAG	C8-C7-N2-C2
4	C	401	NAG	O7-C7-N2-C2
4	D	401	NAG	C8-C7-N2-C2
4	D	401	NAG	O7-C7-N2-C2
4	P	401	NAG	C8-C7-N2-C2
4	P	401	NAG	O7-C7-N2-C2
4	Q	401	NAG	O7-C7-N2-C2
4	R	401	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	R	401	NAG	O7-C7-N2-C2
4	S	401	NAG	C3-C2-N2-C7
4	S	401	NAG	C8-C7-N2-C2
4	S	401	NAG	O7-C7-N2-C2
5	A	402	LMT	O5B-C1B-O1B-C4'
5	B	402	LMT	O5B-C1B-O1B-C4'
5	Q	402	LMT	C4B-C5B-C6B-O6B
4	Q	401	NAG	C8-C7-N2-C2
4	Q	401	NAG	O5-C5-C6-O6
5	P	402	LMT	O5'-C5'-C6'-O6'
5	R	402	LMT	O5'-C5'-C6'-O6'
4	B	401	NAG	C1-C2-N2-C7
4	D	401	NAG	C1-C2-N2-C7
5	Q	402	LMT	O5'-C5'-C6'-O6'
5	D	402	LMT	O5'-C5'-C6'-O6'
4	A	401	NAG	C8-C7-N2-C2
4	A	401	NAG	O7-C7-N2-C2
4	T	401	NAG	C8-C7-N2-C2
4	B	401	NAG	O5-C5-C6-O6
5	T	402	LMT	O5B-C5B-C6B-O6B
5	C	402	LMT	C4'-C5'-C6'-O6'
5	D	402	LMT	O5B-C5B-C6B-O6B
5	T	402	LMT	C4'-C5'-C6'-O6'
5	T	402	LMT	O5'-C5'-C6'-O6'
4	Q	401	NAG	C4-C5-C6-O6
5	Q	402	LMT	O5B-C5B-C6B-O6B
4	B	401	NAG	C4-C5-C6-O6
4	E	401	NAG	C8-C7-N2-C2
4	T	401	NAG	O7-C7-N2-C2
5	S	402	LMT	O5B-C5B-C6B-O6B
5	P	402	LMT	C4'-C5'-C6'-O6'
4	Q	401	NAG	C1-C2-N2-C7
4	R	401	NAG	C1-C2-N2-C7
4	T	401	NAG	C4-C5-C6-O6
5	Q	402	LMT	C4'-C5'-C6'-O6'
5	R	402	LMT	C4'-C5'-C6'-O6'
5	D	402	LMT	C4'-C5'-C6'-O6'
5	S	402	LMT	C4B-C5B-C6B-O6B
4	E	401	NAG	O7-C7-N2-C2
5	S	402	LMT	O5B-C1B-O1B-C4'
5	A	402	LMT	C4B-C5B-C6B-O6B
5	C	402	LMT	O5'-C5'-C6'-O6'

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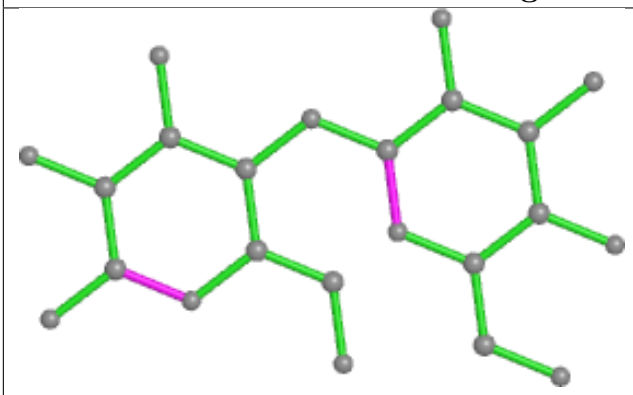
Mol	Chain	Res	Type	Atoms
5	R	402	LMT	C4B-C5B-C6B-O6B
4	P	401	NAG	O5-C5-C6-O6
4	T	401	NAG	O5-C5-C6-O6
5	S	402	LMT	C2B-C1B-O1B-C4'
5	T	402	LMT	C4B-C5B-C6B-O6B
5	A	402	LMT	C4'-C5'-C6'-O6'
5	B	402	LMT	C4'-C5'-C6'-O6'
5	S	402	LMT	O5'-C5'-C6'-O6'
5	E	402	LMT	O5B-C1B-O1B-C4'
5	D	402	LMT	C4B-C5B-C6B-O6B
5	A	402	LMT	O5'-C5'-C6'-O6'
5	R	402	LMT	O5B-C5B-C6B-O6B
6	T	403	FLC	CAC-CA-CB-CBC
5	B	402	LMT	O5'-C5'-C6'-O6'
6	T	403	FLC	CAC-CA-CB-OHB
5	A	402	LMT	O5B-C5B-C6B-O6B
4	P	401	NAG	C4-C5-C6-O6
4	B	401	NAG	C3-C2-N2-C7
4	D	401	NAG	C3-C2-N2-C7
4	Q	401	NAG	C3-C2-N2-C7
4	R	401	NAG	C3-C2-N2-C7
5	E	402	LMT	C2B-C1B-O1B-C4'
4	E	401	NAG	C4-C5-C6-O6
5	C	402	LMT	C4B-C5B-C6B-O6B
6	T	403	FLC	CAC-CA-CB-CG
4	S	401	NAG	C1-C2-N2-C7

There are no ring outliers.

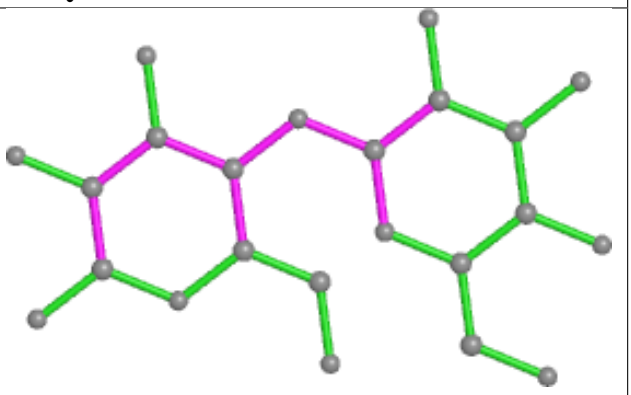
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

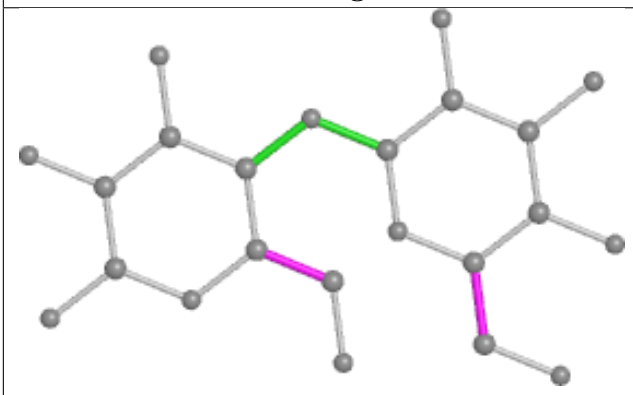
Ligand LMT Q 402



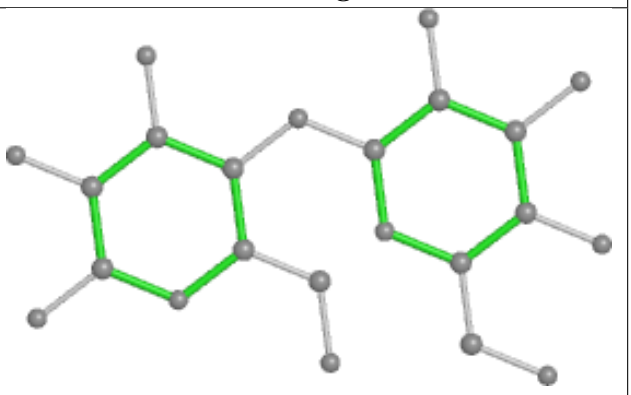
Bond lengths



Bond angles

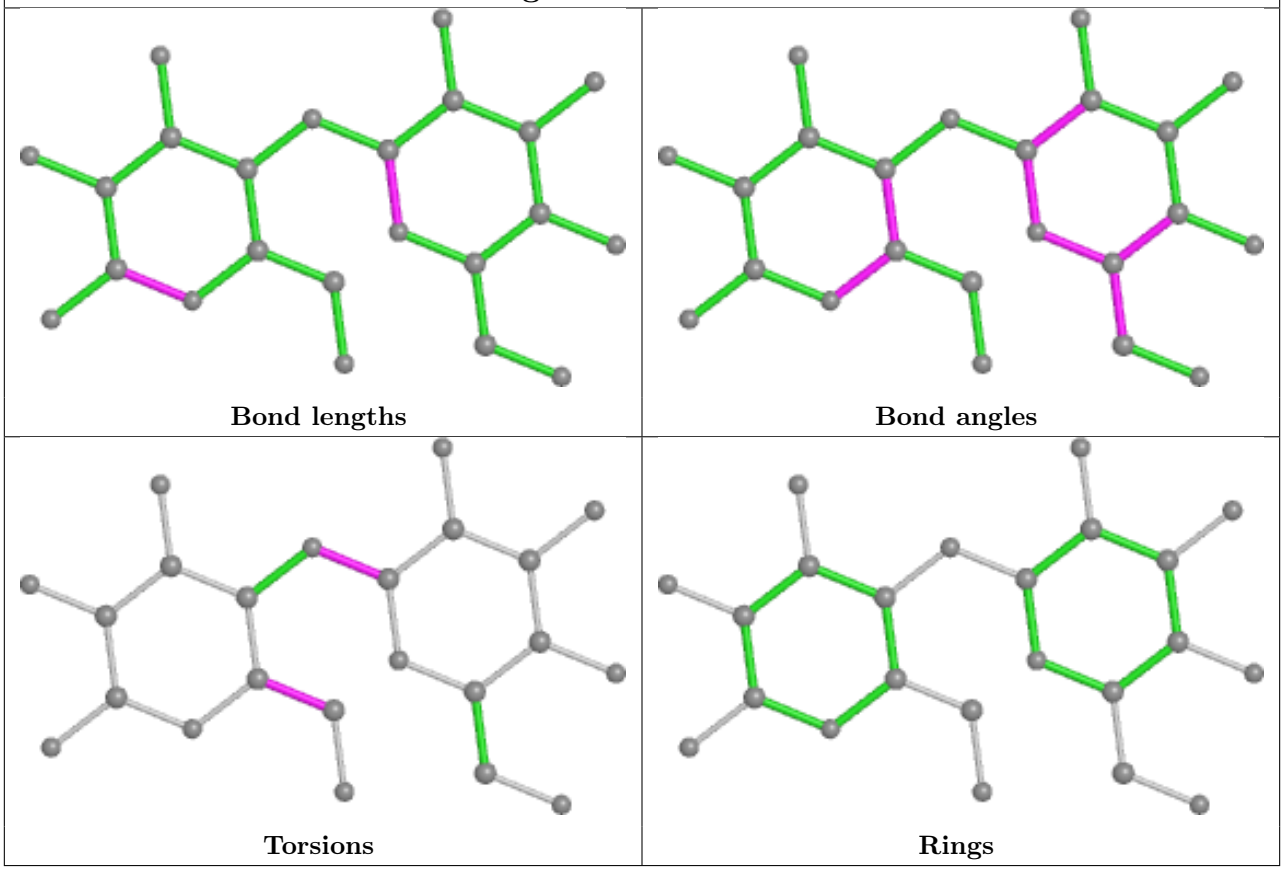


Torsions

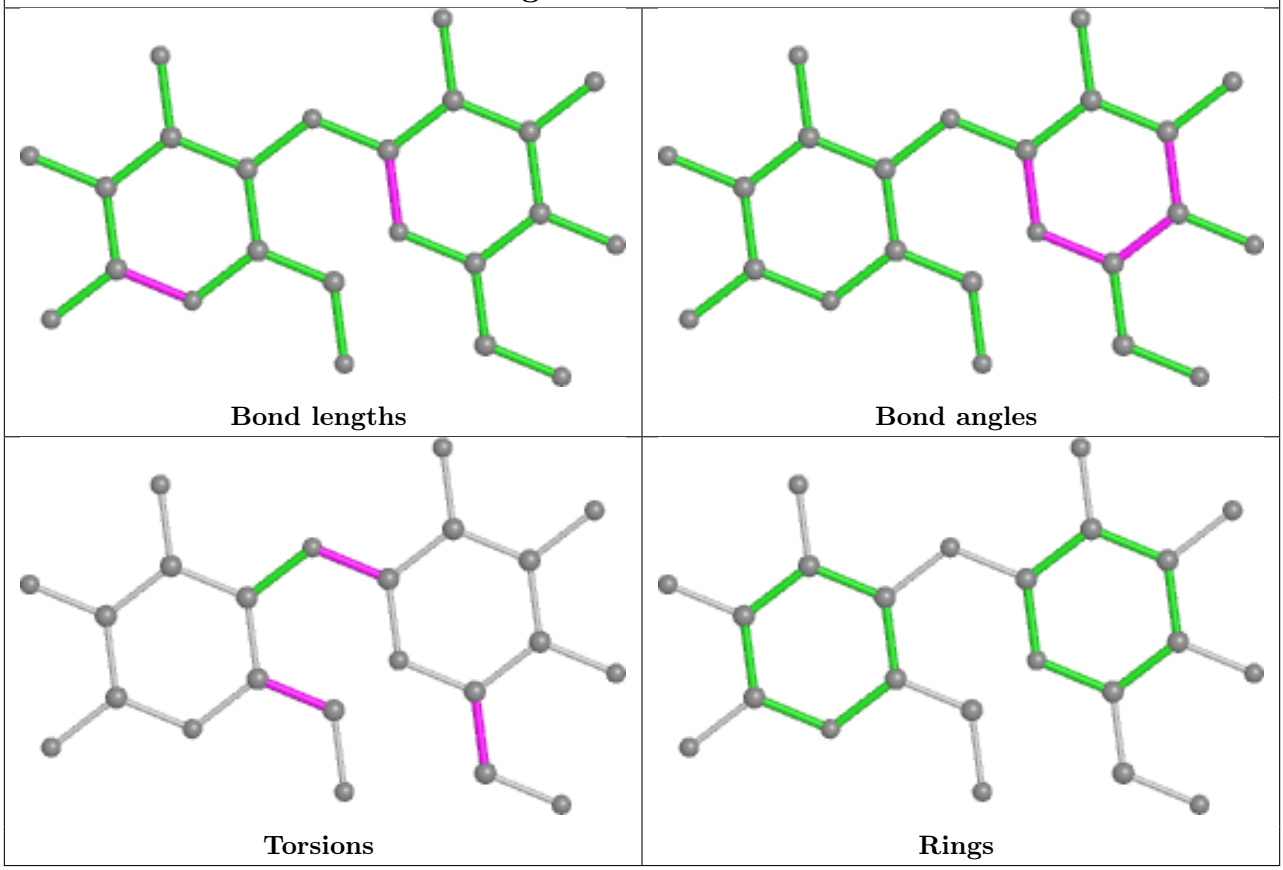


Rings

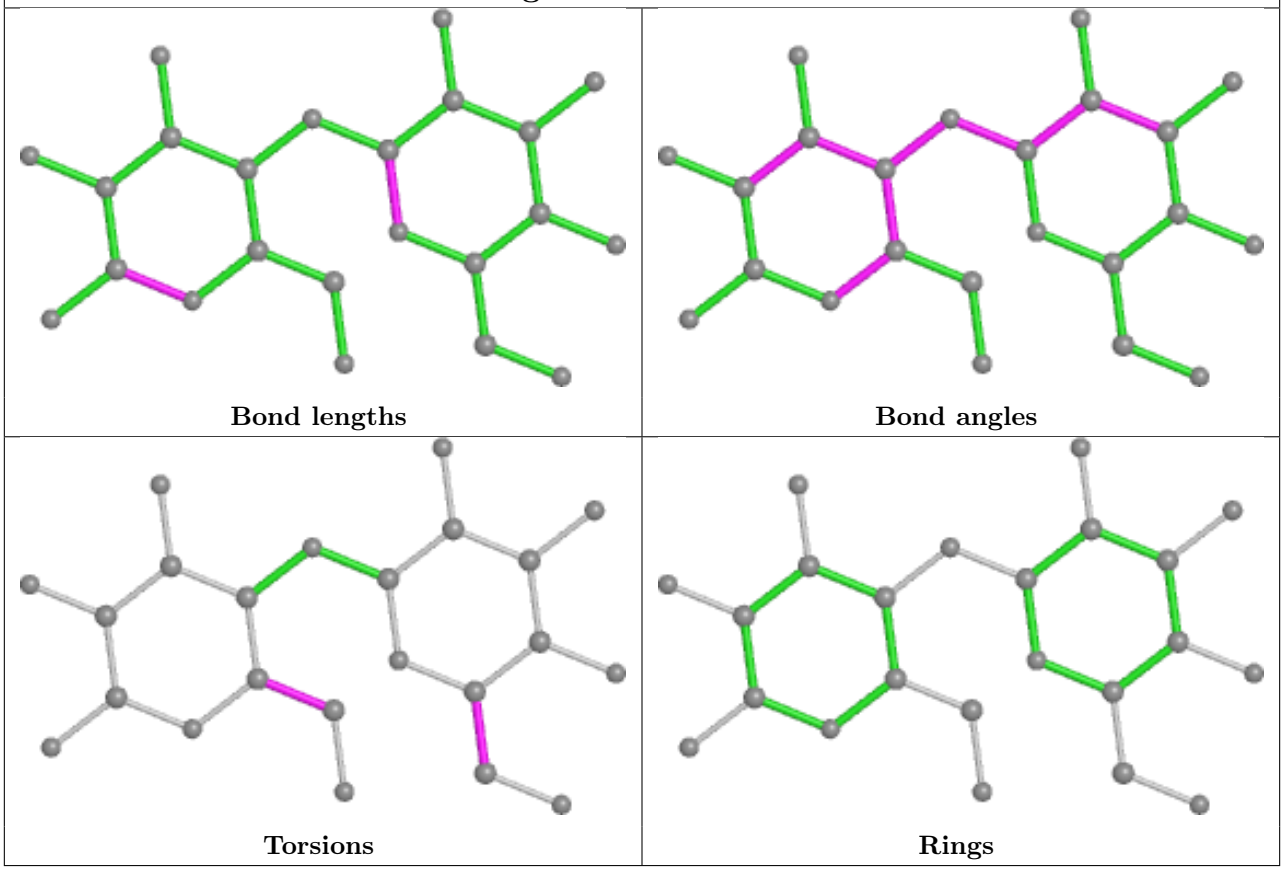
Ligand LMT B 402



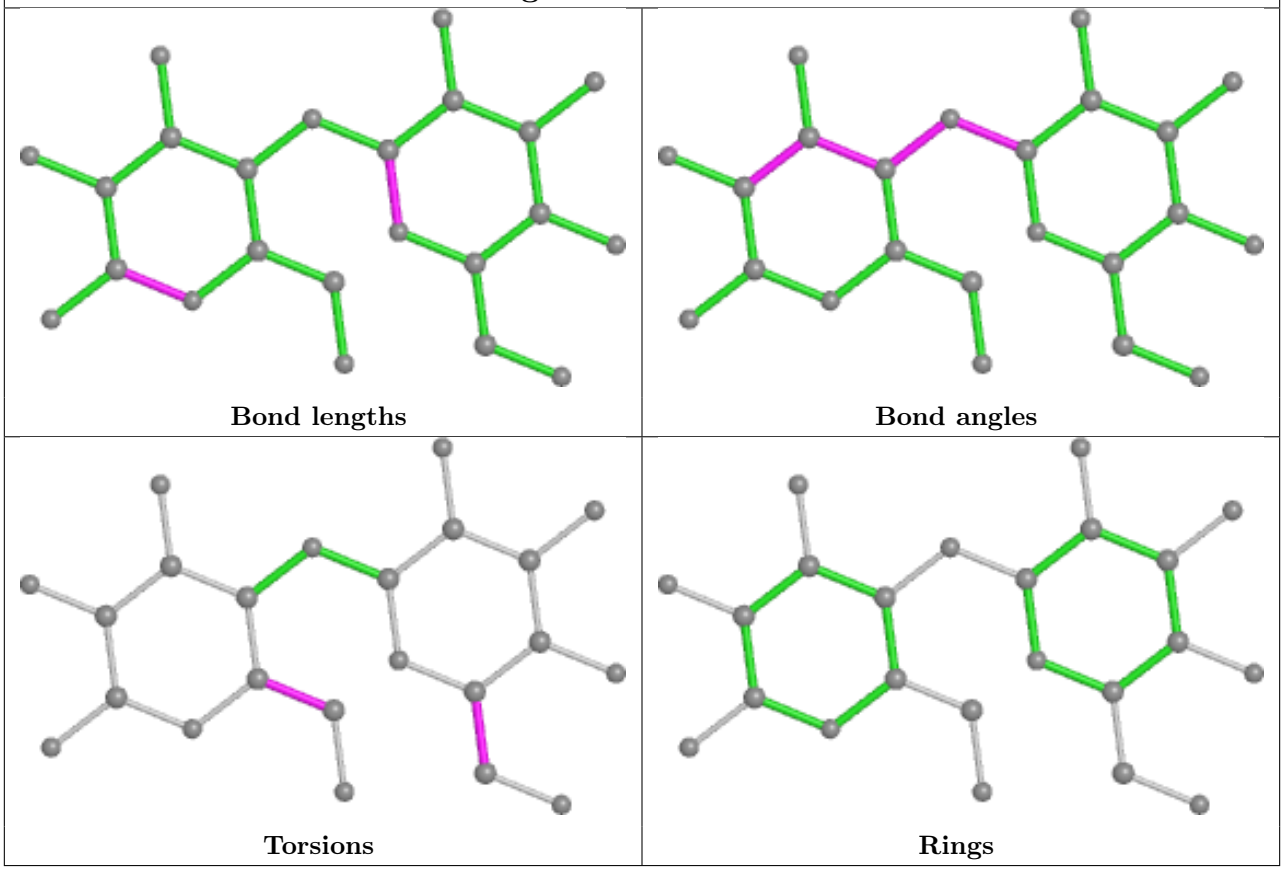
Ligand LMT A 402



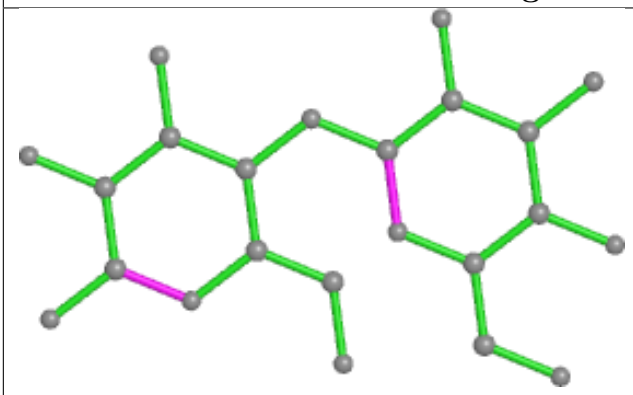
Ligand LMT C 402



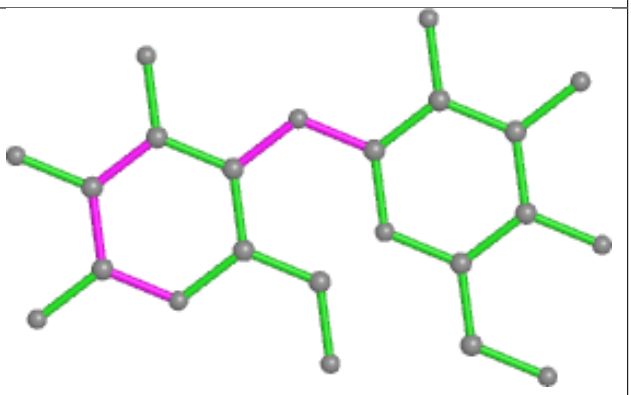
Ligand LMT D 402



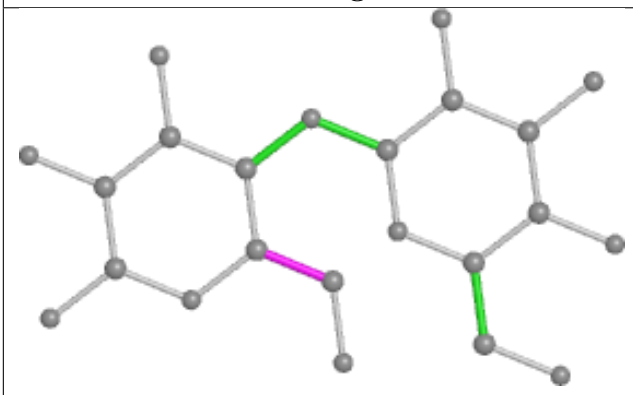
Ligand LMT P 402



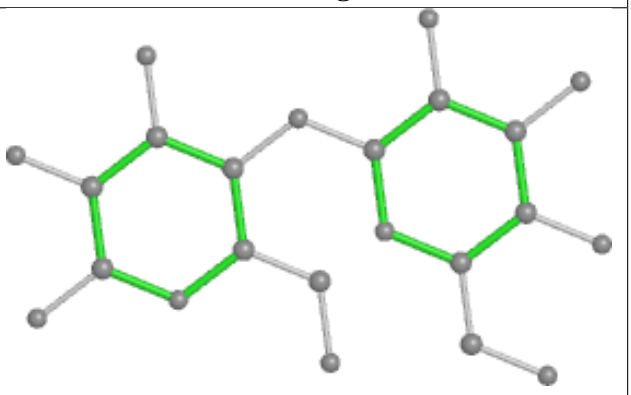
Bond lengths



Bond angles

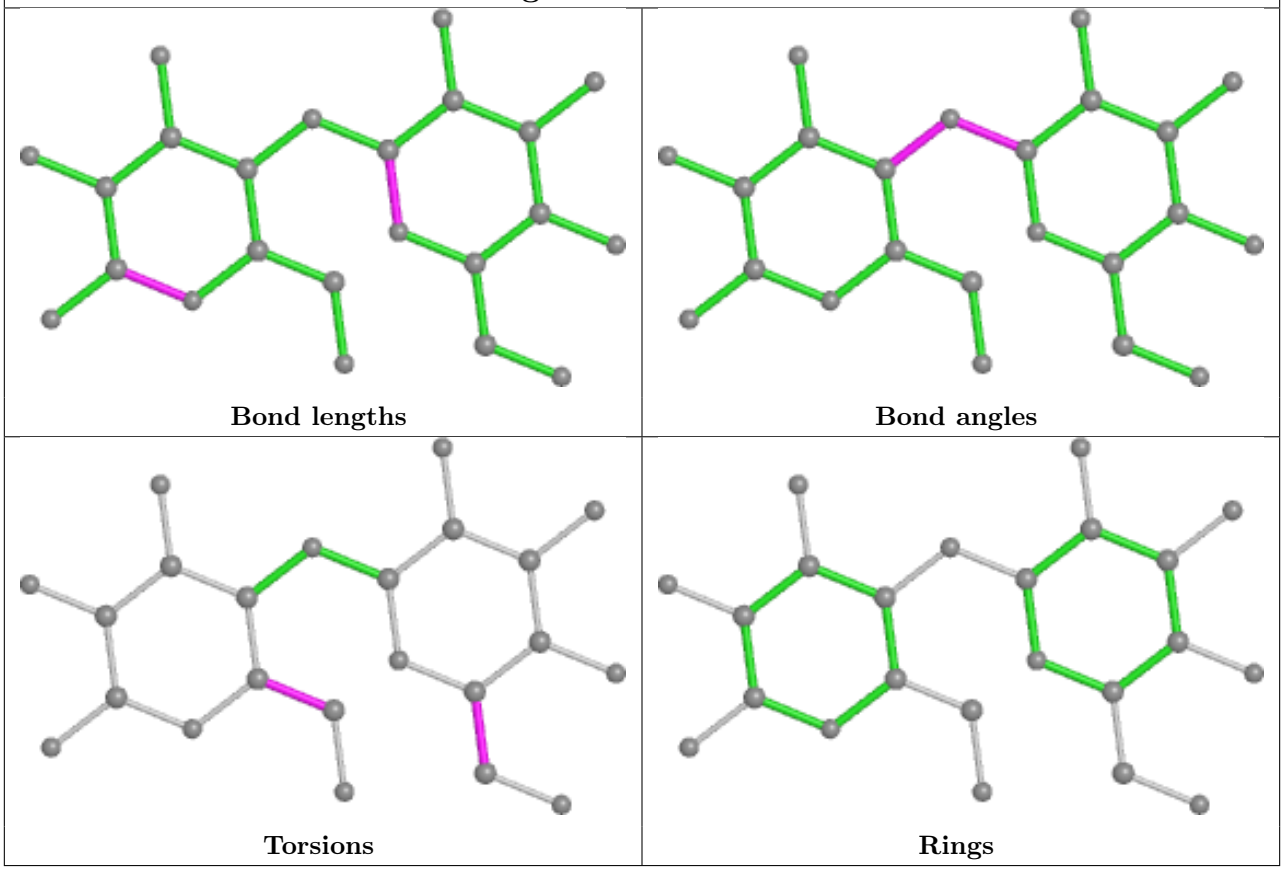


Torsions

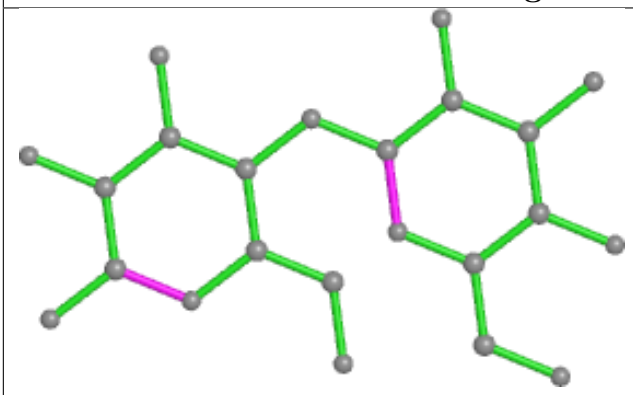


Rings

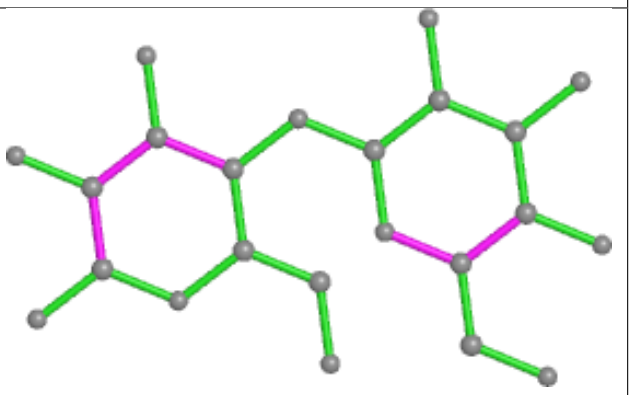
Ligand LMT R 402



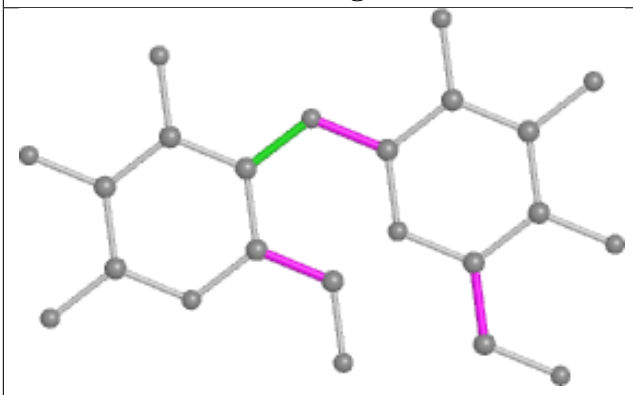
Ligand LMT S 402



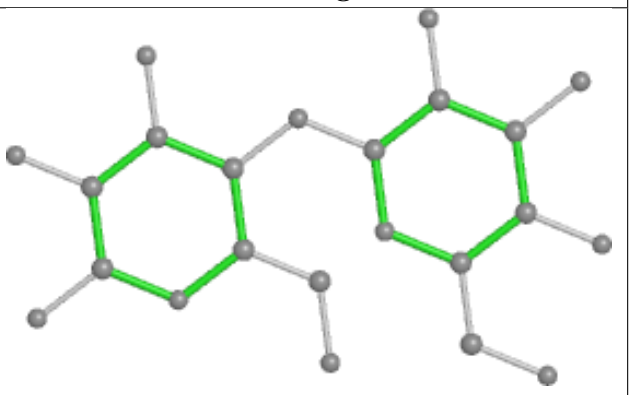
Bond lengths



Bond angles

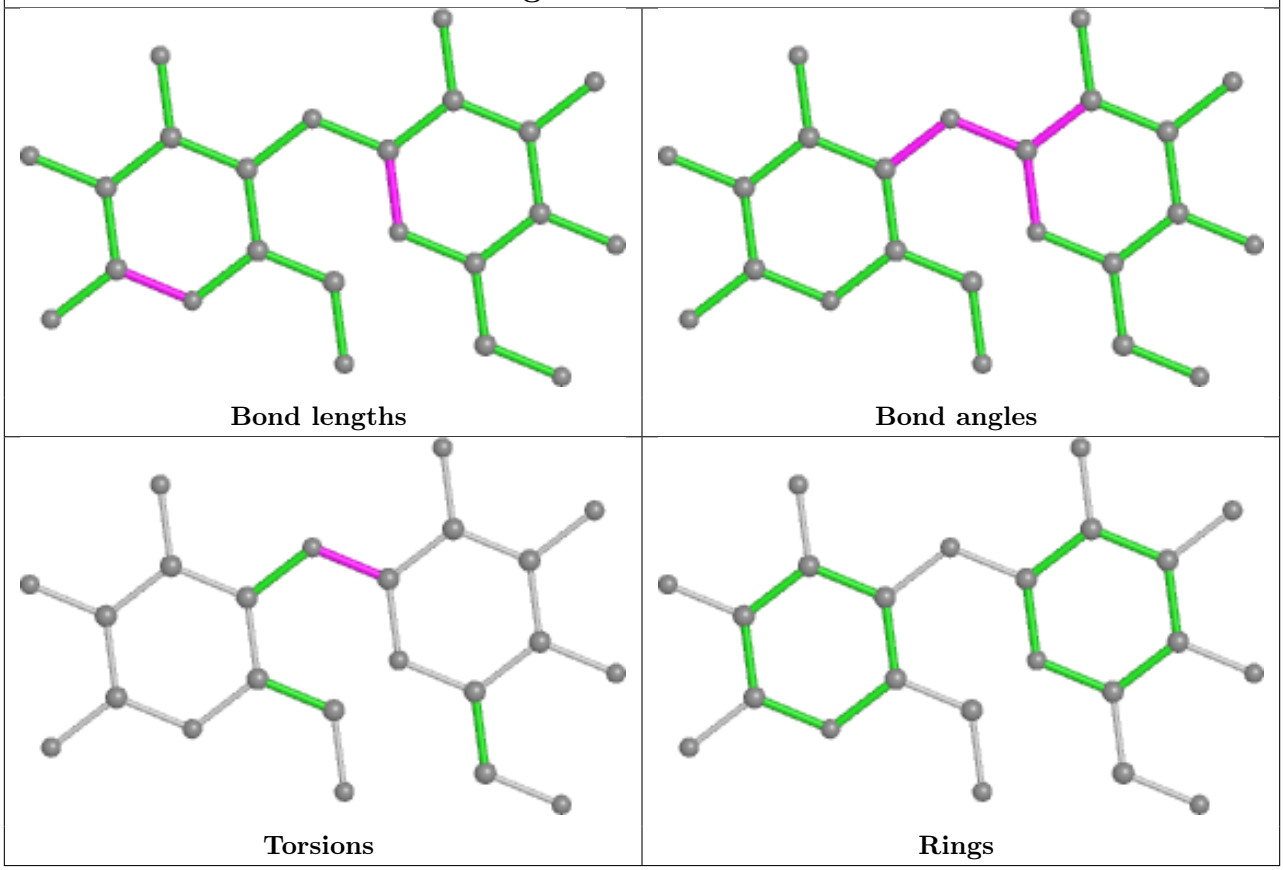


Torsions

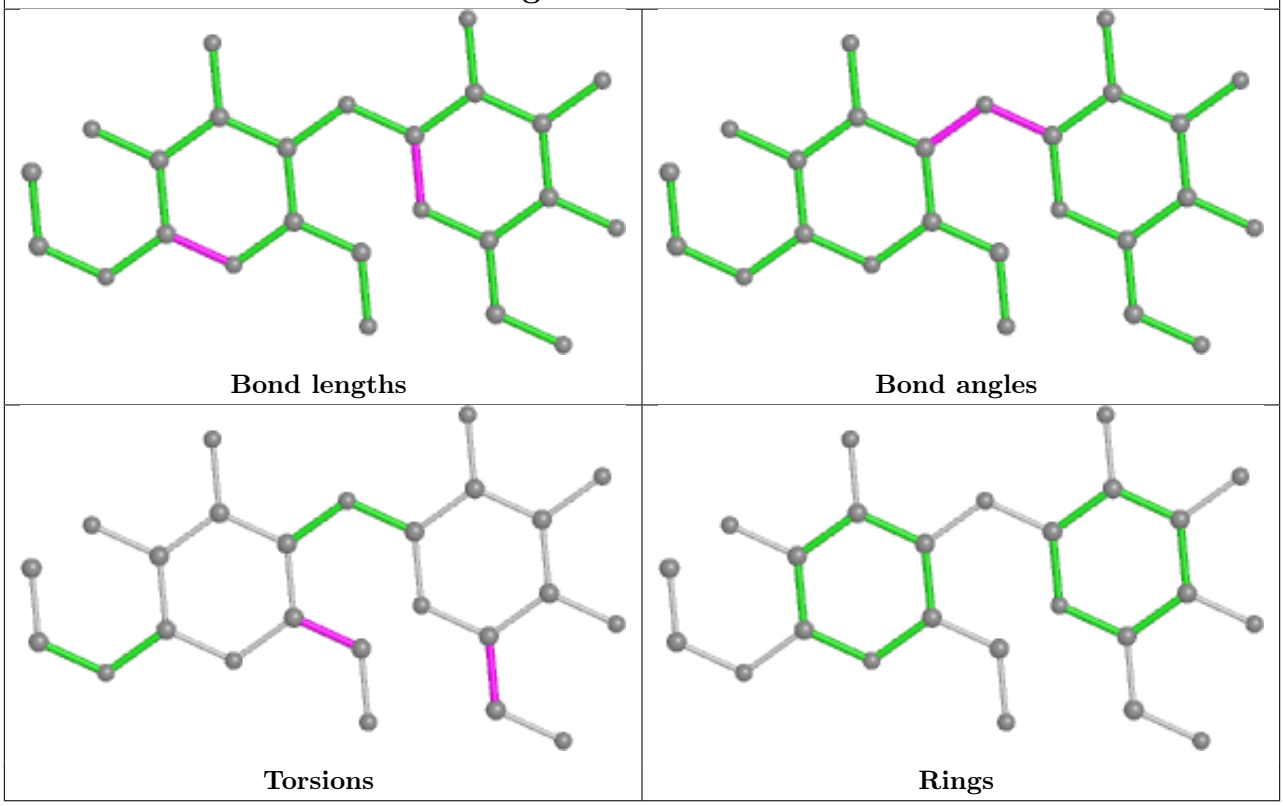


Rings

Ligand LMT E 402



Ligand LMT T 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	337/347 (97%)	0.19	5 (1%)	73	60	91, 137, 216, 241	0
1	B	337/347 (97%)	0.20	13 (3%)	39	25	100, 143, 229, 269	0
1	C	337/347 (97%)	0.18	3 (0%)	84	73	94, 140, 228, 260	0
1	D	337/347 (97%)	0.13	9 (2%)	54	38	103, 144, 219, 255	0
1	E	337/347 (97%)	0.22	16 (4%)	31	19	99, 146, 221, 259	0
1	P	337/347 (97%)	0.14	6 (1%)	68	53	92, 110, 180, 204	0
1	Q	337/347 (97%)	0.25	8 (2%)	59	42	88, 110, 175, 199	0
1	R	337/347 (97%)	0.14	3 (0%)	84	73	87, 105, 166, 183	0
1	S	337/347 (97%)	0.27	7 (2%)	63	48	83, 101, 171, 193	0
1	T	337/347 (97%)	0.15	5 (1%)	73	60	84, 109, 173, 203	0
2	F	222/224 (99%)	0.08	6 (2%)	54	38	112, 139, 215, 248	0
2	G	224/224 (100%)	0.09	9 (4%)	38	25	103, 168, 199, 209	0
2	H	223/224 (99%)	0.02	1 (0%)	92	86	84, 121, 151, 224	0
2	I	222/224 (99%)	-0.03	5 (2%)	60	44	105, 133, 203, 223	0
2	J	223/224 (99%)	0.51	30 (13%)	3	2	115, 162, 263, 278	0
2	U	221/224 (98%)	0.43	26 (11%)	4	3	121, 172, 241, 253	0
2	V	224/224 (100%)	0.04	12 (5%)	25	16	114, 154, 185, 261	0
2	W	224/224 (100%)	0.08	6 (2%)	54	38	102, 126, 145, 207	0
2	X	224/224 (100%)	0.04	3 (1%)	77	63	98, 118, 137, 187	0
2	Y	221/224 (98%)	0.68	34 (15%)	2	1	139, 197, 278, 297	0
3	K	212/215 (98%)	0.03	6 (2%)	53	37	104, 133, 187, 198	0
3	L	211/215 (98%)	0.04	2 (0%)	84	73	81, 109, 162, 172	0
3	M	211/215 (98%)	0.47	22 (10%)	6	3	118, 151, 247, 254	0
3	N	211/215 (98%)	-0.09	5 (2%)	59	42	111, 150, 173, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	O	211/215 (98%)	-0.11	2 (0%) 84 73	104, 134, 153, 160	0
3	Z	215/215 (100%)	0.06	5 (2%) 60 44	112, 161, 190, 244	0
3	f	214/215 (99%)	0.02	5 (2%) 60 44	101, 124, 138, 174	0
3	g	211/215 (98%)	0.81	38 (18%) 1 0	150, 223, 274, 281	0
3	h	211/215 (98%)	0.15	12 (5%) 23 14	119, 178, 207, 217	0
3	i	214/215 (99%)	0.02	0 100 100	99, 119, 138, 169	0
All	All	7719/7860 (98%)	0.17	304 (3%) 39 25	81, 134, 233, 297	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	g	164	THR	11.4
3	g	178	SER	10.5
3	M	123	PRO	9.6
2	Y	161	VAL	9.5
2	J	150	LEU	8.9
2	U	188	SER	8.8
2	J	161	VAL	8.8
3	g	135	LEU	8.7
3	g	165	THR	8.3
2	Y	188	SER	7.7
3	M	135	LEU	7.6
3	g	177	ALA	7.2
2	U	187	SER	7.1
2	J	176	PRO	6.9
2	J	175	PHE	6.7
2	U	161	VAL	6.6
2	Y	160	THR	6.6
3	g	133	ALA	6.5
3	M	122	PRO	6.5
1	A	244	ALA	6.4
2	J	187	SER	6.4
2	J	151	VAL	6.3
3	g	134	THR	6.3
2	J	147	LEU	6.2
3	M	206	GLU	6.2
3	g	136	VAL	6.2
2	Y	149	CYS	6.1
2	J	152	LYS	6.1
3	g	183	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
2	Y	189	SER	6.0
1	B	244	ALA	6.0
2	G	150	LEU	5.9
2	J	134	ALA	5.8
3	M	136	VAL	5.7
3	g	123	PRO	5.5
2	Y	187	SER	5.5
3	M	118	VAL	5.4
1	A	239	ARG	5.4
2	Y	150	LEU	5.3
3	M	177	ALA	5.2
3	g	163	GLU	5.2
1	S	107	ASN	5.2
2	J	133	LEU	5.2
1	B	248	LEU	5.2
2	J	149	CYS	5.2
3	g	166	GLN	5.1
2	J	148	GLY	5.0
2	J	130	VAL	5.0
2	U	159	VAL	4.9
2	Y	140	GLN	4.8
3	h	135	LEU	4.8
2	Y	162	THR	4.7
2	U	142	ASN	4.7
2	J	139	ALA	4.7
3	g	182	THR	4.7
3	g	88	TYR	4.6
3	g	122	PRO	4.6
2	U	186	LEU	4.6
2	J	186	LEU	4.5
2	I	130	VAL	4.5
2	U	189	SER	4.4
2	Y	135	PRO	4.4
1	Q	6	LEU	4.4
3	M	134	THR	4.3
1	S	2	ASP	4.3
2	G	151	VAL	4.3
3	g	84	ASP	4.3
2	Y	174	THR	4.3
3	M	180	TYR	4.2
3	M	121	PHE	4.2
2	U	192	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	Y	134	ALA	4.1
2	Y	141	THR	4.1
3	h	136	VAL	4.1
1	S	6	LEU	4.1
3	M	139	ILE	4.1
2	Y	159	VAL	4.0
2	I	150	LEU	4.0
3	h	139	ILE	4.0
1	E	244	ALA	4.0
1	D	247	THR	4.0
3	g	89	PHE	3.9
2	J	188	SER	3.9
2	J	189	SER	3.8
2	J	219	ILE	3.8
2	I	132	PRO	3.8
3	h	138	THR	3.8
2	G	130	VAL	3.8
1	A	242	ILE	3.7
2	X	140	GLN	3.7
2	Y	151	VAL	3.7
2	J	177	ALA	3.6
3	K	109	LEU	3.6
3	f	121	PHE	3.6
1	S	1	SER	3.6
2	J	174	THR	3.6
2	Y	152	LYS	3.6
1	T	6	LEU	3.5
1	D	68	VAL	3.5
2	U	74	LYS	3.5
2	I	161	VAL	3.5
3	g	18	VAL	3.4
1	B	291	LEU	3.4
2	U	152	LYS	3.4
1	D	291	LEU	3.4
2	J	185	THR	3.4
1	Q	1	SER	3.4
1	E	220	LEU	3.3
1	T	2	ASP	3.3
2	U	150	LEU	3.3
1	C	248	LEU	3.2
1	P	64	LEU	3.2
2	U	185	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	136	GLY	3.2
3	g	38	VAL	3.2
3	g	106	LEU	3.2
3	g	132	LYS	3.2
1	A	245	ARG	3.2
3	g	39	GLN	3.2
2	U	147	LEU	3.2
3	g	109	LEU	3.2
1	S	106	PRO	3.2
3	g	87	ILE	3.1
2	U	151	VAL	3.1
2	W	140	GLN	3.1
1	E	237	PHE	3.1
3	M	157	PRO	3.1
3	M	109	LEU	3.1
2	Y	158	PRO	3.1
2	V	150	LEU	3.1
2	Y	186	LEU	3.1
2	F	133	LEU	3.0
2	V	147	LEU	3.0
2	G	187	SER	3.0
2	J	159	VAL	3.0
3	g	139	ILE	3.0
2	F	150	LEU	3.0
1	Q	2	ASP	3.0
3	Z	64	PHE	3.0
3	M	178	SER	3.0
2	Y	202	VAL	3.0
3	K	136	VAL	2.9
2	V	188	SER	2.9
3	h	178	SER	2.9
1	P	2	ASP	2.9
2	W	150	LEU	2.9
1	Q	3	SER	2.9
1	A	237	PHE	2.9
1	Q	10	PHE	2.9
1	T	107	ASN	2.9
2	V	139	ALA	2.9
1	B	250	VAL	2.9
1	D	2	ASP	2.9
3	M	181	LEU	2.9
3	g	179	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	W	147	LEU	2.8
3	g	92	LEU	2.8
1	D	243	PRO	2.8
3	g	91	ALA	2.8
1	B	249	GLY	2.8
1	E	248	LEU	2.8
2	V	133	LEU	2.8
2	J	178	VAL	2.8
2	Y	48	ILE	2.8
2	H	223	ASP	2.7
1	R	107	ASN	2.7
3	N	50	ILE	2.7
3	N	182	THR	2.7
2	J	135	PRO	2.7
2	G	147	LEU	2.7
2	Y	18	MET	2.7
3	f	120	LEU	2.7
2	Y	109	PHE	2.7
3	K	134	THR	2.7
2	U	149	CYS	2.7
1	E	64	LEU	2.7
1	B	247	THR	2.7
2	J	160	THR	2.7
2	U	215	VAL	2.6
1	E	241	ALA	2.6
2	Y	168	LEU	2.6
3	h	151	TRP	2.6
2	G	178	VAL	2.6
2	U	206	VAL	2.6
3	K	135	LEU	2.6
1	B	64	LEU	2.6
2	Y	97	ALA	2.6
2	U	141	THR	2.6
2	V	142	ASN	2.6
2	V	218	LYS	2.6
1	D	132	MET	2.6
3	Z	120	LEU	2.6
1	C	55	LEU	2.5
2	U	175	PHE	2.5
2	U	191	THR	2.5
3	Z	49	LEU	2.5
3	M	138	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	W	105	TYR	2.5
3	g	138	THR	2.5
3	f	136	VAL	2.5
2	Y	43	LYS	2.5
3	O	134	THR	2.5
2	Y	83	LEU	2.5
2	Y	203	THR	2.5
1	D	248	LEU	2.5
3	M	100	PHE	2.5
2	U	51	ILE	2.5
2	J	153	GLY	2.5
2	G	177	ALA	2.4
1	C	169	GLN	2.4
3	g	112	PRO	2.4
3	h	177	ALA	2.4
2	U	105	TYR	2.4
1	B	245	ARG	2.4
2	F	109	PHE	2.4
3	g	184	THR	2.4
3	g	181	LEU	2.4
1	B	160	TYR	2.4
1	Q	64	LEU	2.4
2	F	152	LYS	2.4
3	h	195	SER	2.4
3	h	198	VAL	2.4
1	B	243	PRO	2.4
1	Q	112	ILE	2.4
1	E	230	VAL	2.3
3	O	50	ILE	2.3
1	P	39	ILE	2.3
3	g	180	TYR	2.3
3	h	194	TYR	2.3
1	B	1	SER	2.3
1	E	243	PRO	2.3
2	Y	112	TRP	2.3
2	Y	176	PRO	2.3
3	f	134	THR	2.3
2	Y	192	VAL	2.3
3	N	126	GLU	2.3
2	F	149	CYS	2.3
2	Y	45	LEU	2.3
3	Z	77	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	g	121	PHE	2.3
3	M	176	MET	2.3
1	E	254	LEU	2.2
1	D	230	VAL	2.2
1	E	233	VAL	2.2
1	T	220	LEU	2.2
1	E	250	VAL	2.2
2	J	218	LYS	2.2
2	V	132	PRO	2.2
2	Y	46	GLU	2.2
2	J	220	VAL	2.2
3	f	135	LEU	2.2
1	T	219	GLN	2.2
2	F	202	VAL	2.2
2	G	152	LYS	2.2
1	P	227	LEU	2.2
1	S	264	ASN	2.2
1	E	304	GLY	2.2
1	Q	277	ASP	2.2
2	Y	105	TYR	2.2
3	g	105	LYS	2.2
2	V	186	LEU	2.1
3	g	49	LEU	2.1
3	h	180	TYR	2.1
1	E	44	VAL	2.1
3	g	10	LEU	2.1
2	U	70	LEU	2.1
3	N	181	LEU	2.1
1	E	240	THR	2.1
1	D	1	SER	2.1
2	V	206	VAL	2.1
2	I	147	LEU	2.1
2	G	135	PRO	2.1
2	V	187	SER	2.1
3	h	196	CYS	2.1
1	R	244	ALA	2.1
2	X	147	LEU	2.1
2	Y	20	ILE	2.1
2	J	173	HIS	2.1
3	N	38	VAL	2.1
3	L	132	LYS	2.1
2	W	132	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	129	GLU	2.1
3	M	120	LEU	2.1
1	E	277	ASP	2.1
1	P	112	ILE	2.1
2	V	219	ILE	2.1
3	K	121	PHE	2.1
2	U	41	HIS	2.0
3	M	119	THR	2.0
3	M	137	CYS	2.0
3	M	183	LEU	2.0
1	E	284	MET	2.0
2	U	29	PHE	2.0
2	U	207	ALA	2.0
1	P	1	SER	2.0
3	g	169	LYS	2.0
2	X	145	VAL	2.0
3	Z	84	ASP	2.0
1	B	139	MET	2.0
1	B	152	ALA	2.0
1	R	291	LEU	2.0
1	S	248	LEU	2.0
2	W	133	LEU	2.0
3	L	113	LYS	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, 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.

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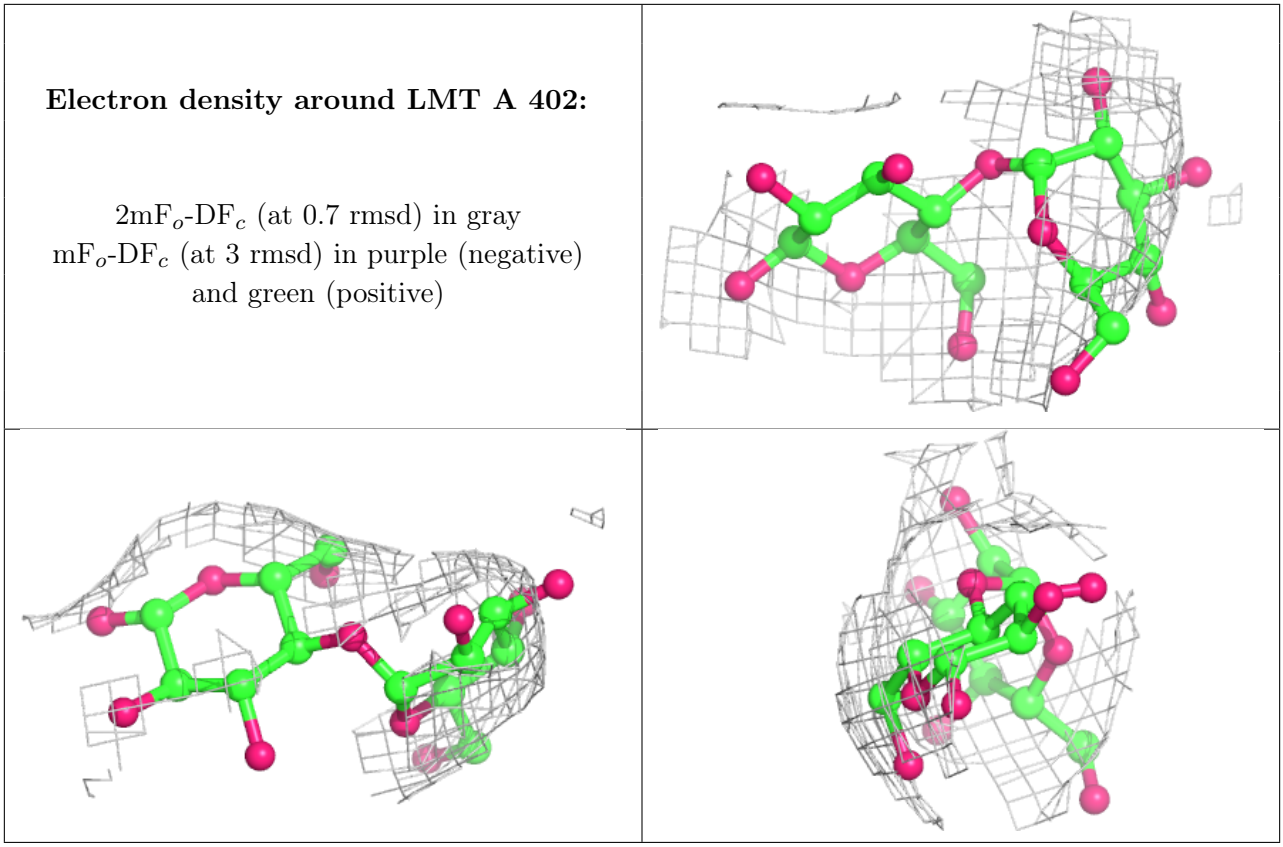
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LMT	A	402	23/35	0.65	0.24	211,211,211,211	0
5	LMT	C	402	23/35	0.67	0.33	173,173,173,173	0
5	LMT	R	402	23/35	0.68	0.37	149,149,149,149	0
5	LMT	B	402	23/35	0.70	0.36	181,181,181,181	0
5	LMT	E	402	23/35	0.75	0.25	177,177,177,177	0
5	LMT	Q	402	23/35	0.76	0.18	143,143,143,143	0
5	LMT	D	402	23/35	0.77	0.32	189,189,189,189	0
7	CL	P	403	1/1	0.77	1.87	115,115,115,115	0
5	LMT	P	402	23/35	0.79	0.28	149,149,149,149	0
4	NAG	Q	401	14/15	0.79	0.27	176,176,176,176	0
5	LMT	T	402	25/35	0.80	0.34	145,145,145,145	0
6	FLC	T	403	13/13	0.81	0.38	187,187,187,187	0
4	NAG	P	401	14/15	0.81	0.53	232,232,232,232	0
5	LMT	S	402	23/35	0.83	0.23	130,130,130,130	0
4	NAG	T	401	14/15	0.83	0.19	182,182,182,182	0
4	NAG	D	401	14/15	0.84	0.20	204,204,204,204	0
4	NAG	C	401	14/15	0.84	0.20	158,158,158,158	0
4	NAG	S	401	14/15	0.85	0.38	218,218,218,218	0
6	FLC	A	403	13/13	0.88	0.35	168,168,168,168	0
4	NAG	B	401	14/15	0.89	0.15	172,172,172,172	0
4	NAG	E	401	14/15	0.90	0.14	170,170,170,170	0
4	NAG	R	401	14/15	0.91	0.16	191,191,191,191	0
4	NAG	A	401	14/15	0.91	0.16	165,165,165,165	0
7	CL	P	404	1/1	0.91	2.53	115,115,115,115	0

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

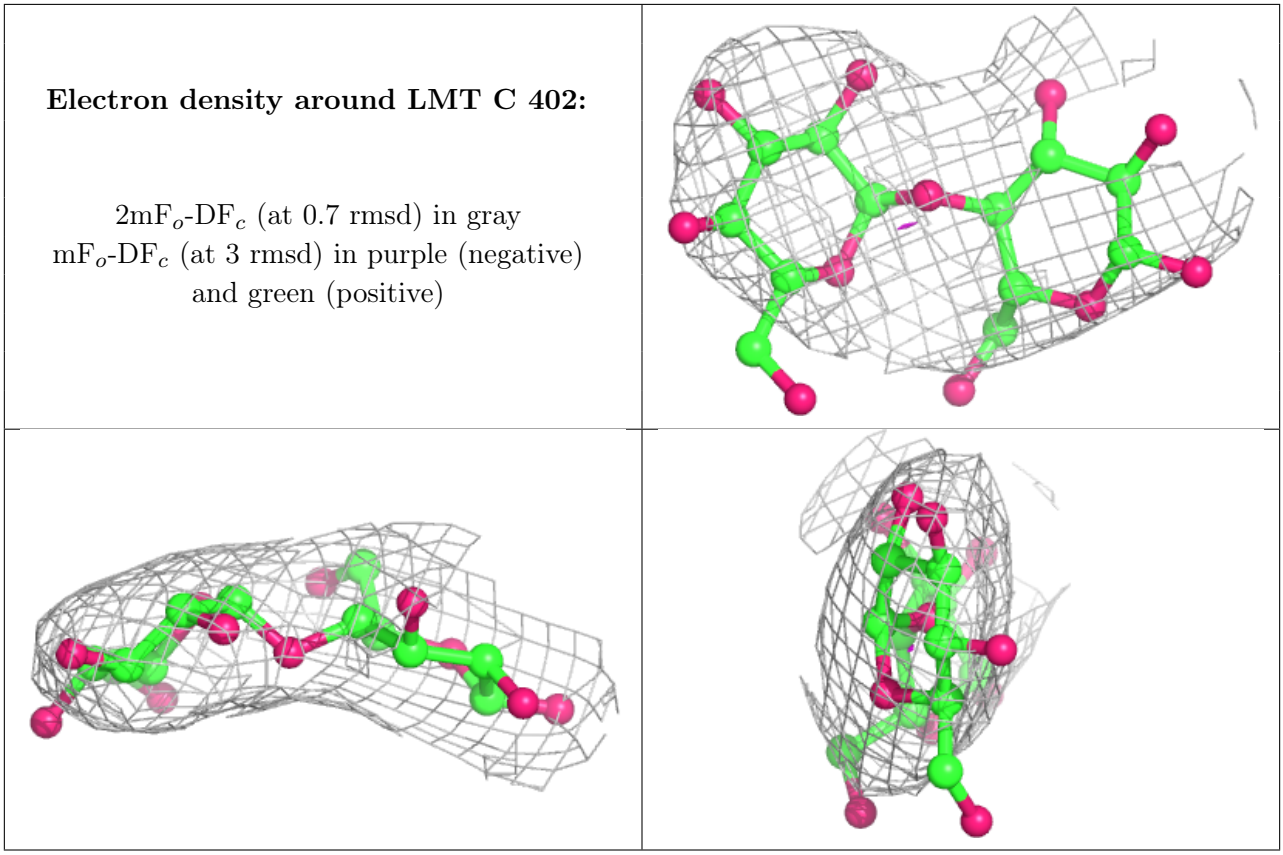
Electron density around LMT A 402:

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



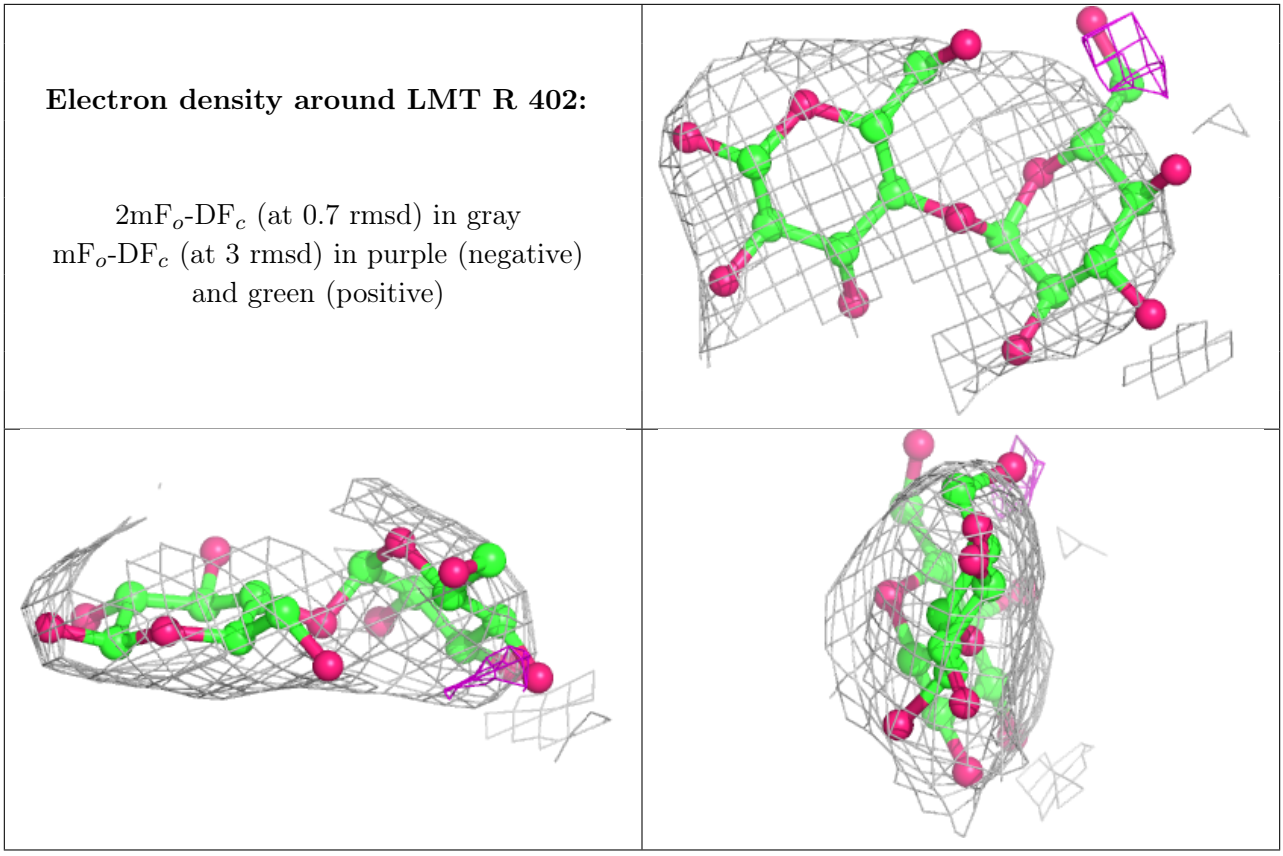
Electron density around LMT C 402:

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



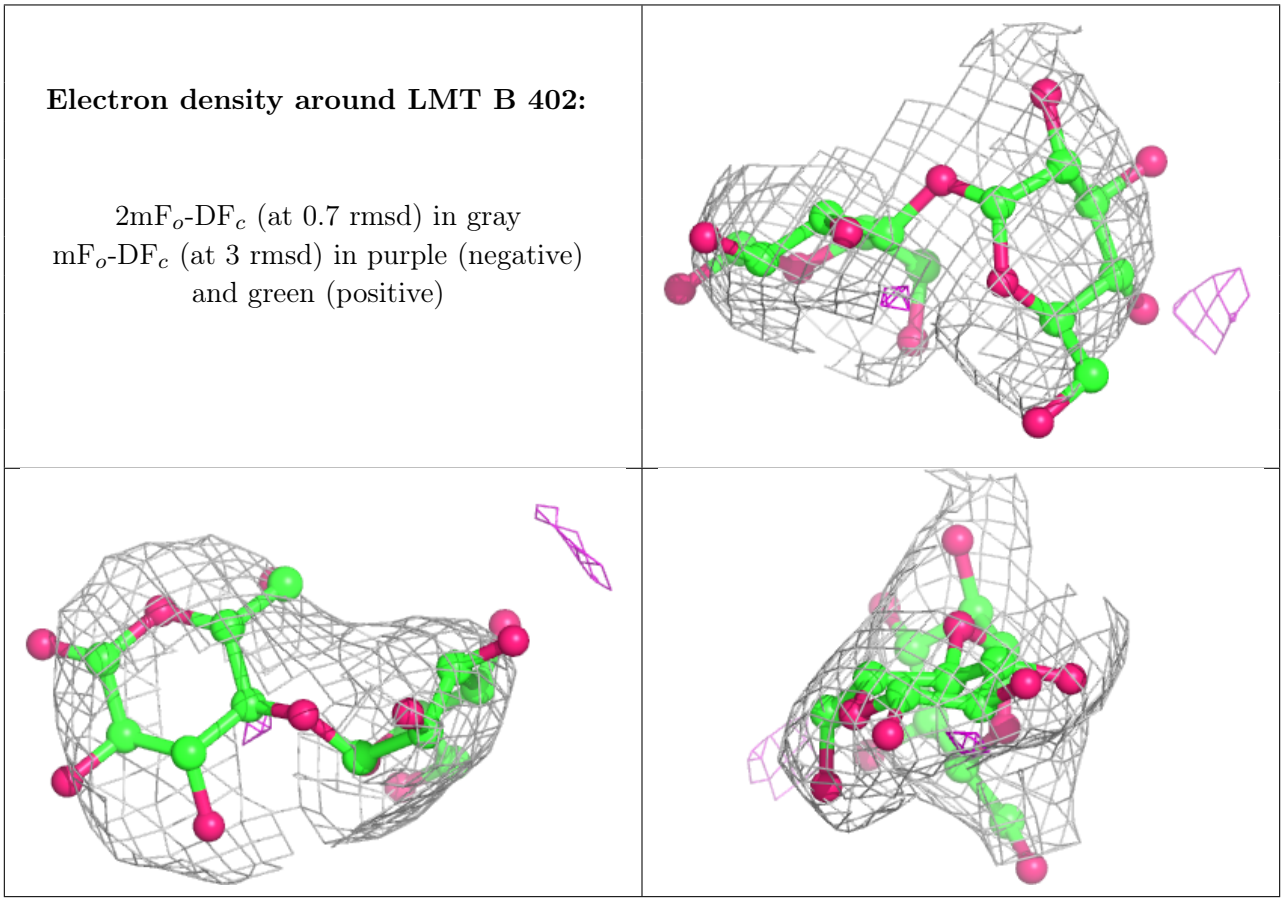
Electron density around LMT R 402:

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



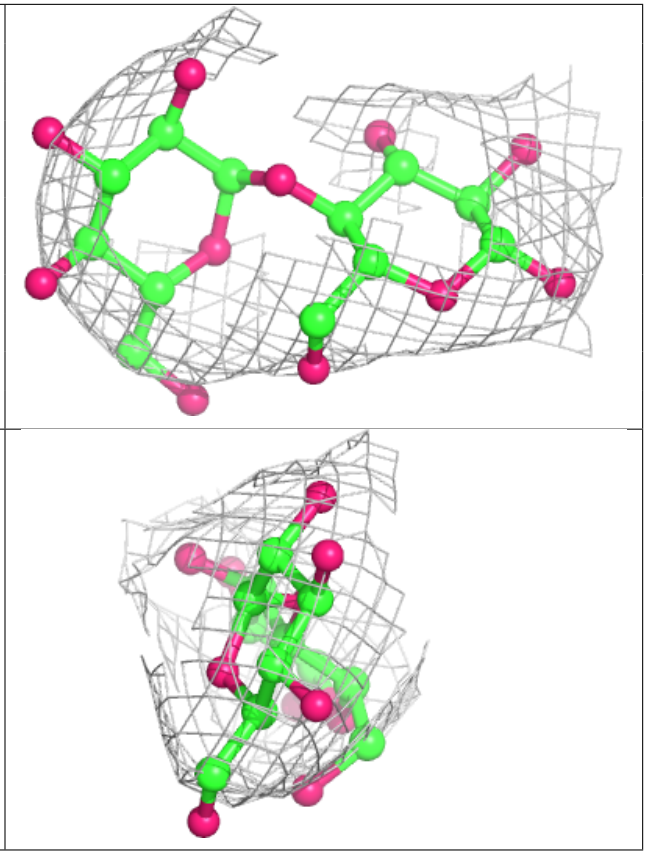
Electron density around LMT B 402:

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



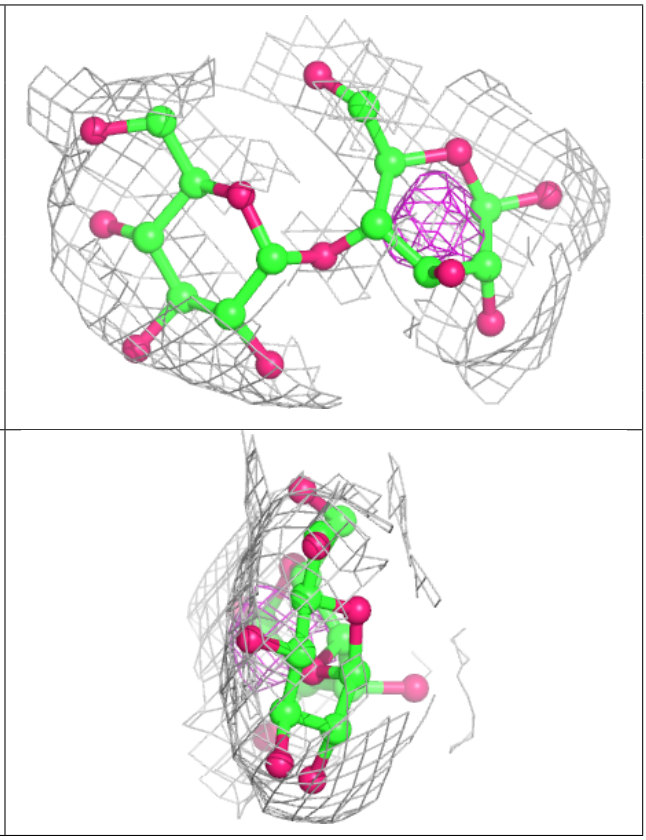
Electron density around LMT E 402:

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



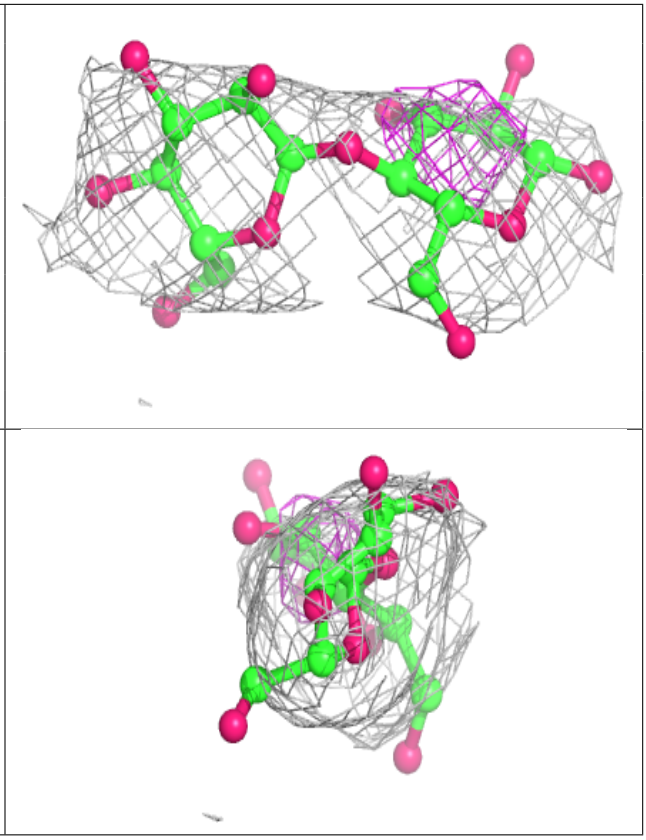
Electron density around LMT Q 402:

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



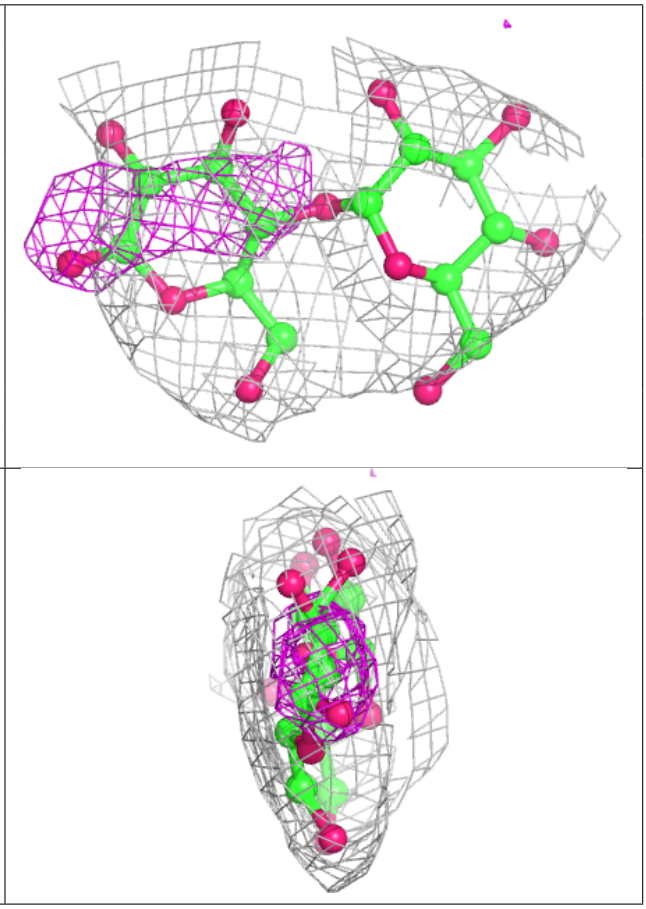
Electron density around LMT D 402:

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



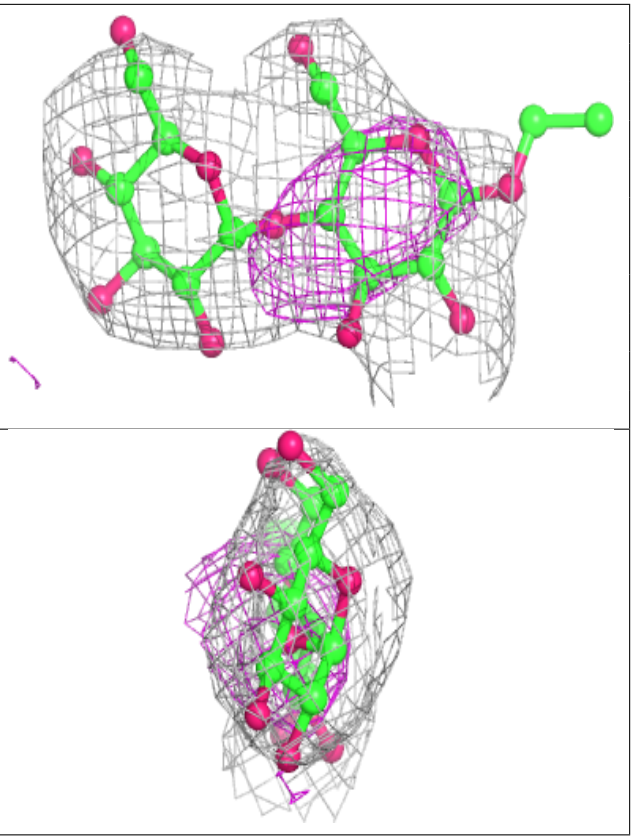
Electron density around LMT P 402:

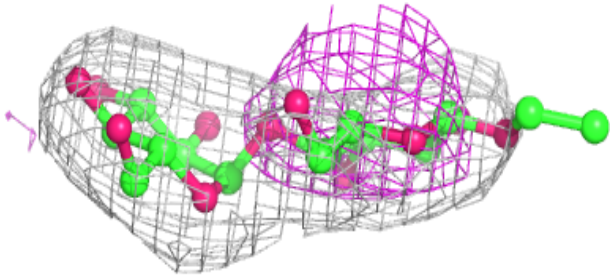
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LMT T 402:

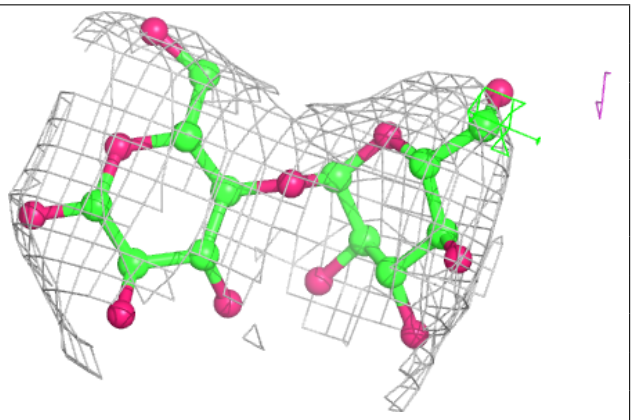
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

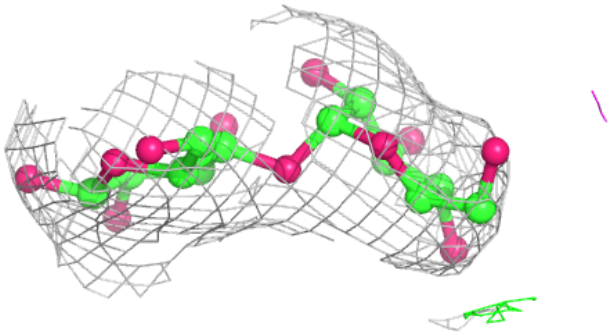


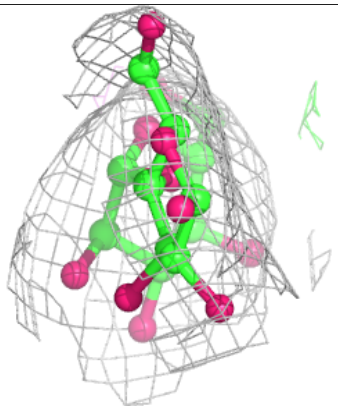


Electron density around LMT S 402:

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







6.5 Other polymers (i)

There are no such residues in this entry.