



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:50 AM BST

PDB ID : 3RI5
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and picrotoxin
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-12
Resolution : 3.40 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

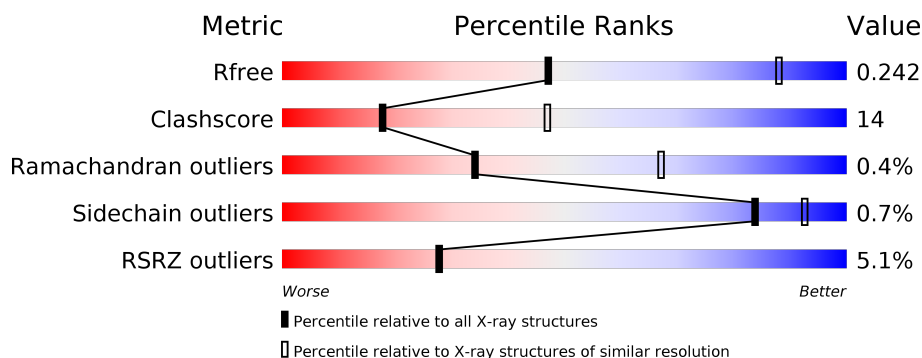
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	<div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	B	347	<div> <div>3%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	C	347	<div> <div>3%</div> <div>69%</div> <div>28%</div> <div>..</div> </div>
1	D	347	<div> <div>3%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
1	E	347	<div> <div>3%</div> <div>68%</div> <div>29%</div> <div>..</div> </div>
2	F	221	<div> <div>13%</div> <div>63%</div> <div>22%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	221	
2	H	221	
2	I	221	
2	J	221	
3	K	210	
3	L	210	
3	M	210	
3	N	210	
3	O	210	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	RI5	E	351	-	-	X	-
5	LMT	A	351	-	-	-	X
5	LMT	B	350	-	-	-	X
7	OCT	D	350	-	-	-	X
7	OCT	E	350	-	-	-	X
8	UND	B	352	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29167 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	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	B	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	C	339	Total	C	N	O	S	0	0	0
			2706	1762	438	491	15			
1	D	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2716	1768	441	492	15			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	ALA	-	linker	UNP O17793
A	304	GLY	-	linker	UNP O17793
A	305	THR	-	linker	UNP O17793
A	340	HIS	-	expression tag	UNP O17793
A	341	HIS	-	expression tag	UNP O17793
A	342	HIS	-	expression tag	UNP O17793
A	343	HIS	-	expression tag	UNP O17793
A	344	HIS	-	expression tag	UNP O17793
A	345	HIS	-	expression tag	UNP O17793
A	346	HIS	-	expression tag	UNP O17793
A	347	HIS	-	expression tag	UNP O17793
B	303	ALA	-	linker	UNP O17793
B	304	GLY	-	linker	UNP O17793
B	305	THR	-	linker	UNP O17793
B	340	HIS	-	expression tag	UNP O17793
B	341	HIS	-	expression tag	UNP O17793
B	342	HIS	-	expression tag	UNP O17793
B	343	HIS	-	expression tag	UNP O17793

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Chain	Residue	Modelled	Actual	Comment	Reference
B	344	HIS	-	expression tag	UNP O17793
B	345	HIS	-	expression tag	UNP O17793
B	346	HIS	-	expression tag	UNP O17793
B	347	HIS	-	expression tag	UNP O17793
C	303	ALA	-	linker	UNP O17793
C	304	GLY	-	linker	UNP O17793
C	305	THR	-	linker	UNP O17793
C	340	HIS	-	expression tag	UNP O17793
C	341	HIS	-	expression tag	UNP O17793
C	342	HIS	-	expression tag	UNP O17793
C	343	HIS	-	expression tag	UNP O17793
C	344	HIS	-	expression tag	UNP O17793
C	345	HIS	-	expression tag	UNP O17793
C	346	HIS	-	expression tag	UNP O17793
C	347	HIS	-	expression tag	UNP O17793
D	303	ALA	-	linker	UNP O17793
D	304	GLY	-	linker	UNP O17793
D	305	THR	-	linker	UNP O17793
D	340	HIS	-	expression tag	UNP O17793
D	341	HIS	-	expression tag	UNP O17793
D	342	HIS	-	expression tag	UNP O17793
D	343	HIS	-	expression tag	UNP O17793
D	344	HIS	-	expression tag	UNP O17793
D	345	HIS	-	expression tag	UNP O17793
D	346	HIS	-	expression tag	UNP O17793
D	347	HIS	-	expression tag	UNP O17793
E	303	ALA	-	linker	UNP O17793
E	304	GLY	-	linker	UNP O17793
E	305	THR	-	linker	UNP O17793
E	340	HIS	-	expression tag	UNP O17793
E	341	HIS	-	expression tag	UNP O17793
E	342	HIS	-	expression tag	UNP O17793
E	343	HIS	-	expression tag	UNP O17793
E	344	HIS	-	expression tag	UNP O17793
E	345	HIS	-	expression tag	UNP O17793
E	346	HIS	-	expression tag	UNP O17793
E	347	HIS	-	expression tag	UNP O17793

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	188	Total	C	N	O	S	0	0	0
			1441	915	234	285	7			

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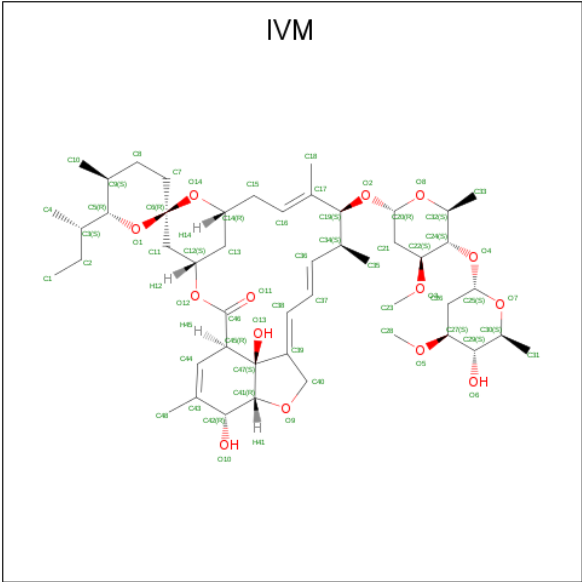
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	200	Total	C	N	O	S	0	0	0
			1529	973	248	301	7			
2	H	221	Total	C	N	O	S	0	0	0
			1683	1067	273	335	8			
2	I	199	Total	C	N	O	S	0	0	0
			1525	969	247	301	8			
2	J	215	Total	C	N	O	S	0	0	0
			1639	1043	265	324	7			

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

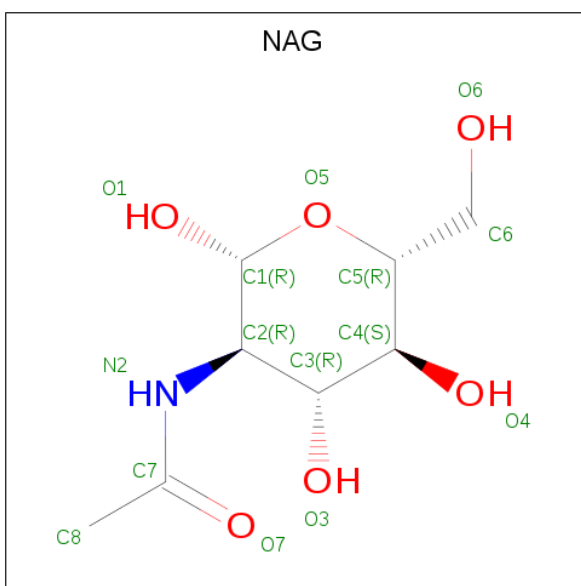
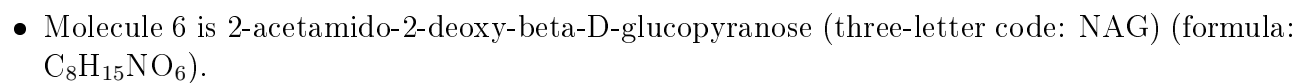
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	199	Total	C	N	O	S	0	0	0
			1496	941	246	303	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1579	993	261	319	6			
3	N	158	Total	C	N	O	S	0	0	0
			1156	728	192	233	3			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is (2aE,4E,5'S,6S,6'R,7S,8E,11R,13R,15S,17aR,20R,20aR,20bS)-6'-[(2S)-butan-2-yl]-20,20b-dihydroxy-5',6,8,19-tetramethyl-17-oxo-3',4',5',6,6',10,11,14,15,17,17a,20,20a,20b-tetradecahydro-2H,7H-spiro[11,15-methanofuro[4,3,2-pq][2,6]benzodioxacy clooctadecine-13,2'-pyran]-7-yl 2,6-dideoxy-4-O-(2,6-dideoxy-3-O-methyl-alpha-L-arabino-hexopyranosyl)-3-O-methyl-alpha-L-arabino-hexopyranoside (three-letter code: IVM) (formula: C₄₈H₇₄O₁₄).



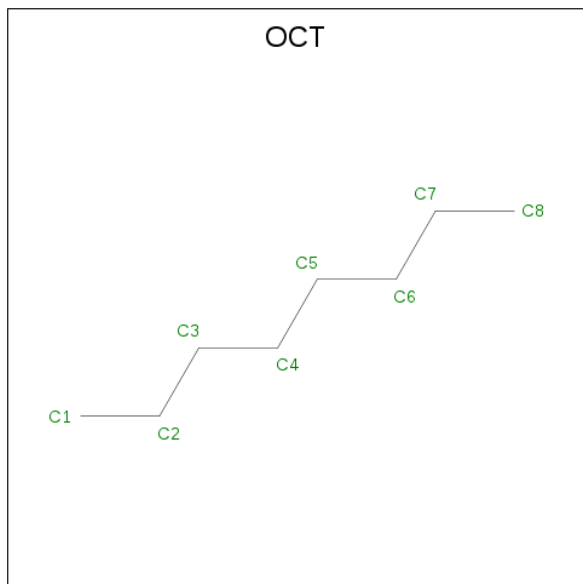
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			62	48	14		
4	B	1	Total	C	O	0	0
			62	48	14		
4	C	1	Total	C	O	0	0
			62	48	14		
4	D	1	Total	C	O	0	0
			62	48	14		
4	E	1	Total	C	O	0	0
			62	48	14		

- Molecule 5 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



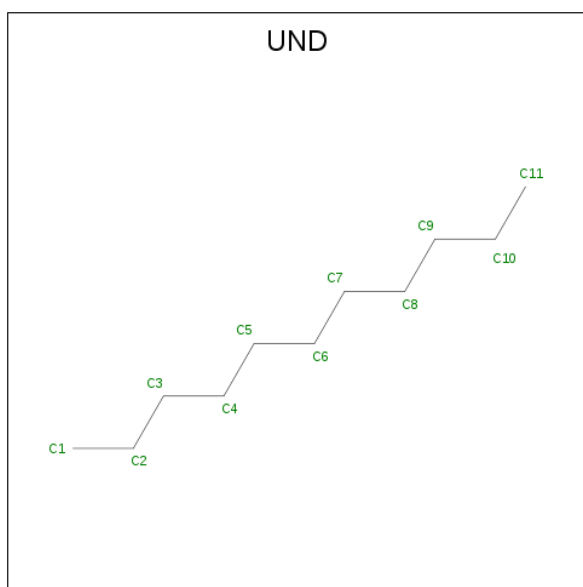
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is N-OCTANE (three-letter code: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C	0	0
			8	8		
7	D	1	Total	C	0	0
			8	8		
7	E	1	Total	C	0	0
			8	8		

- Molecule 8 is UNDECANE (three-letter code: UND) (formula: C₁₁H₂₄).

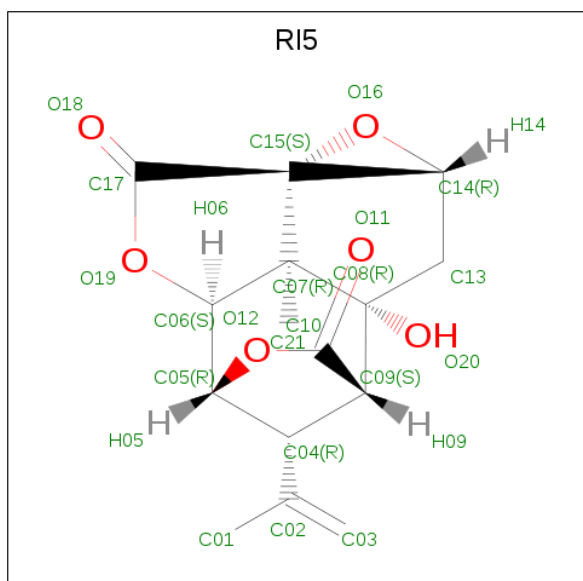


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 11 11	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total Cl 1 1	0	0

- Molecule 10 is (1aR,2aR,3S,6R,6aS,8aS,8bR,9R)-2a-hydroxy-8b-methyl-9-(prop-1-en-2-yl)hexahydro-3,6-methano-1,5,7-trioxacyclopenta[ij]c yclopropa[a]azulene-4,8(3H)-dione (three-letter code: RI5) (formula: C₁₅H₁₆O₆).

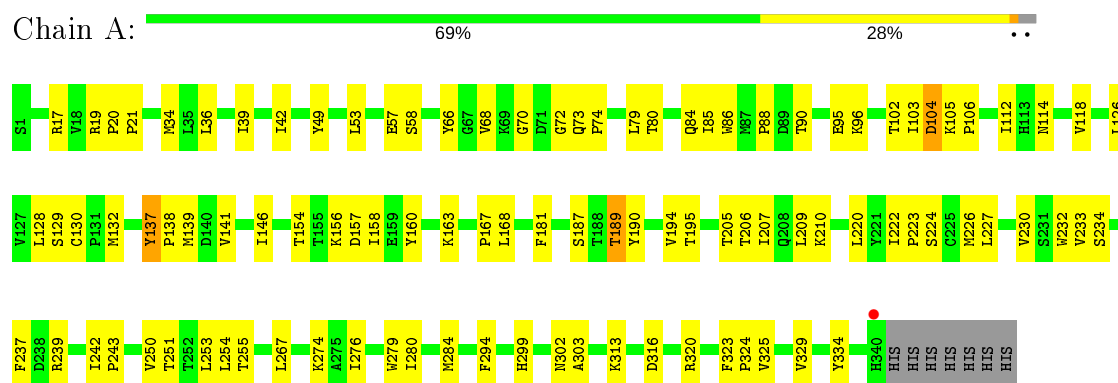


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			21	15	6		

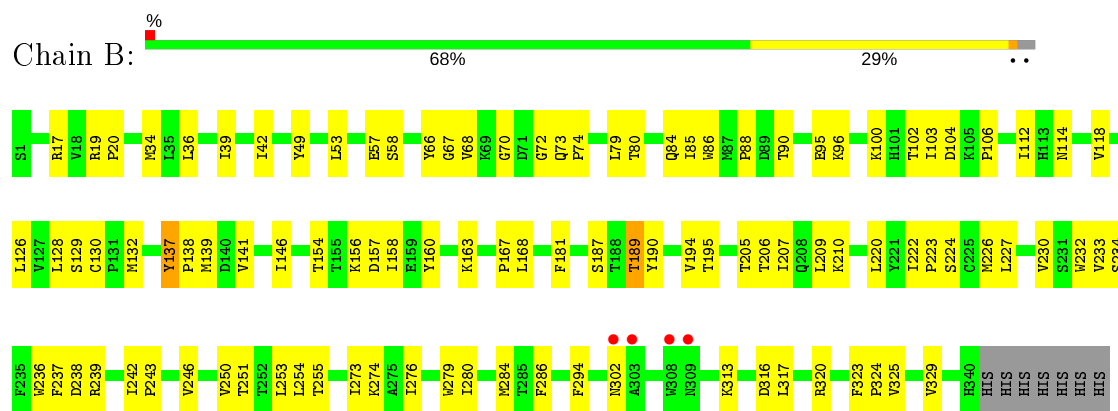
3 Residue-property plots

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.

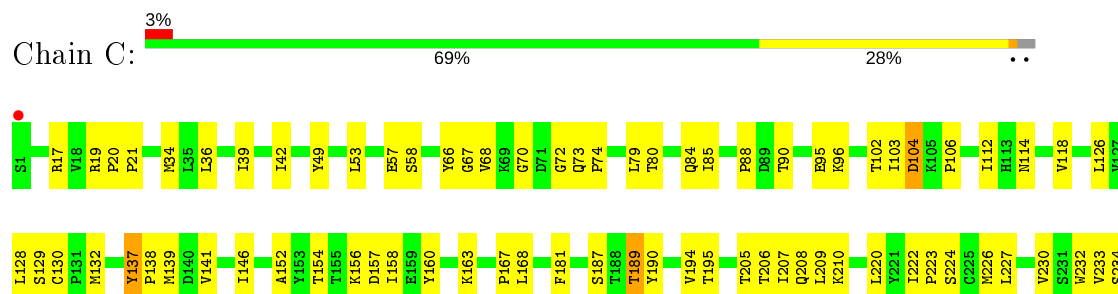
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

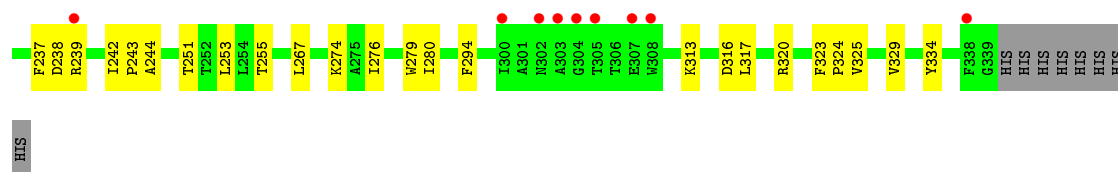


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



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

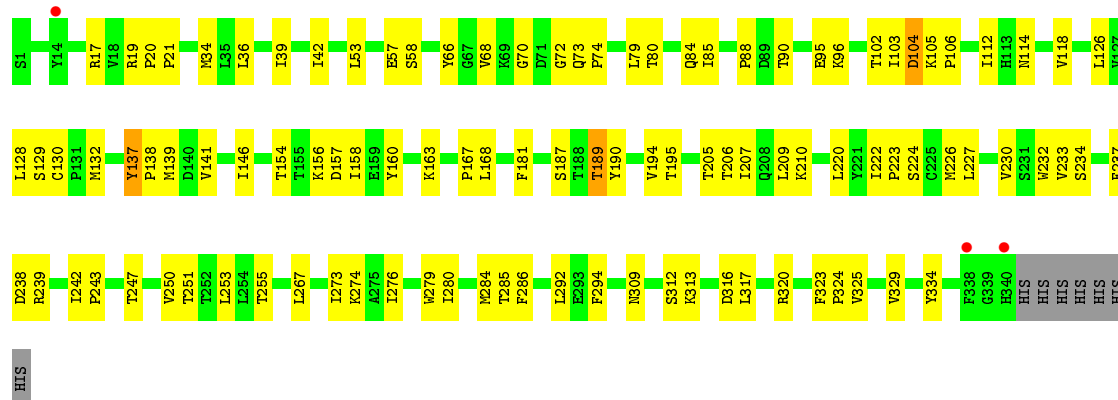




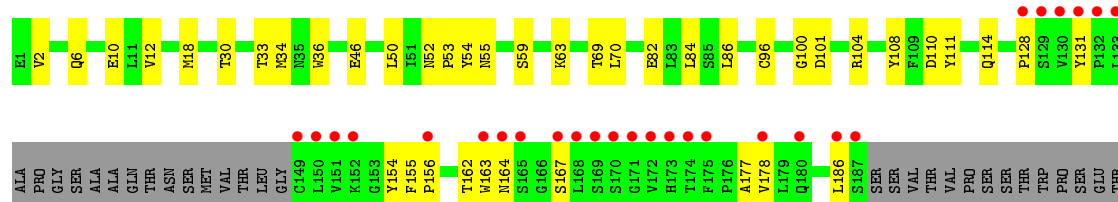
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

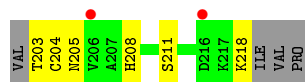


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

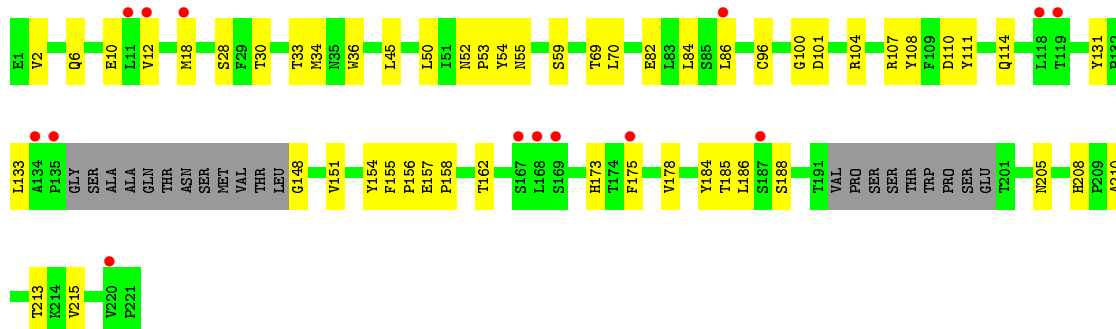


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

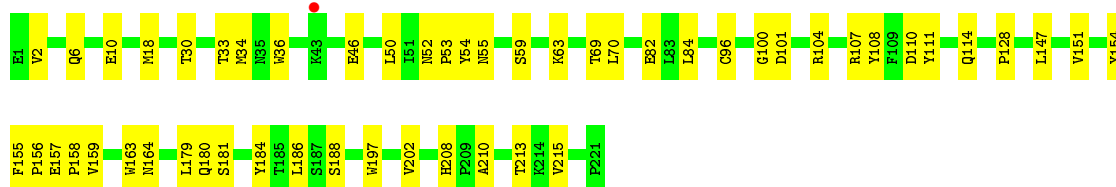




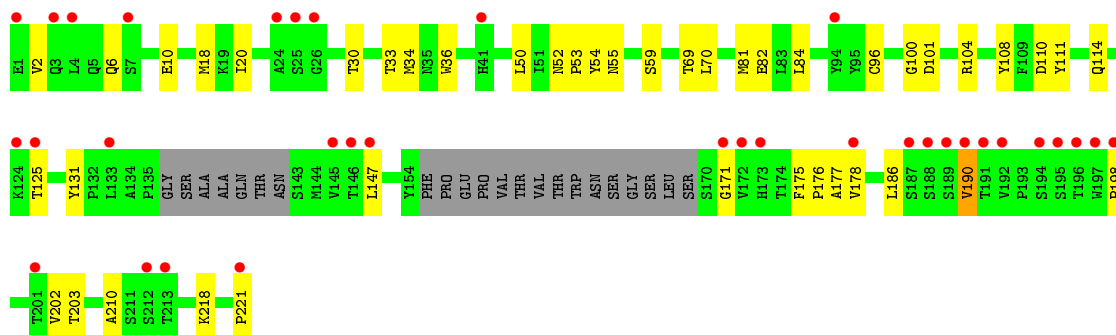
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



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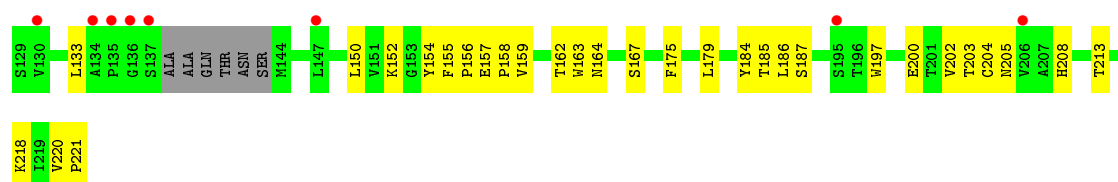


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

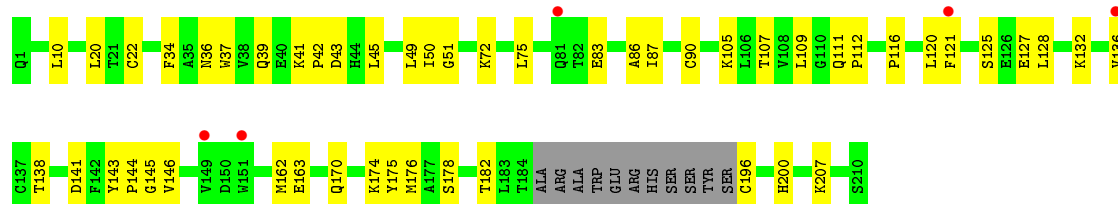


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

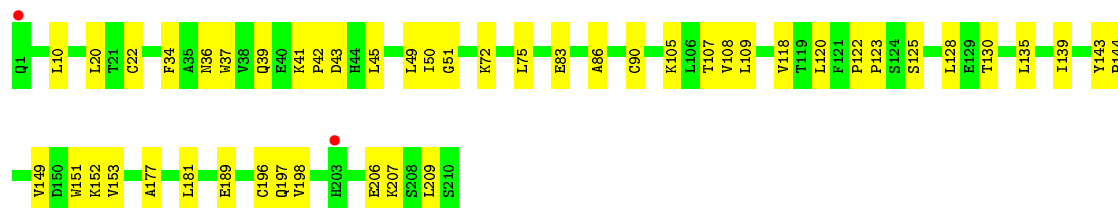
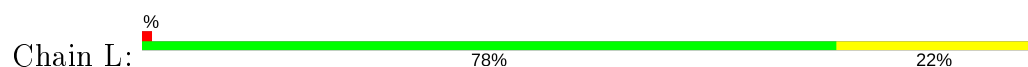




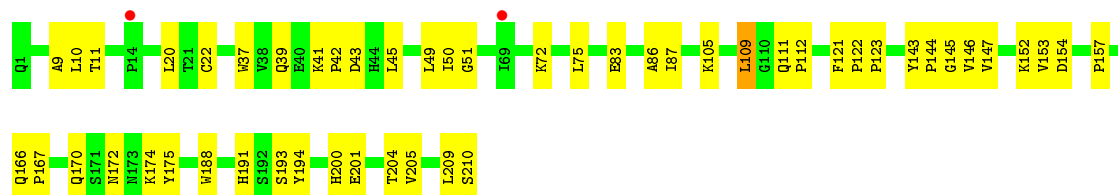
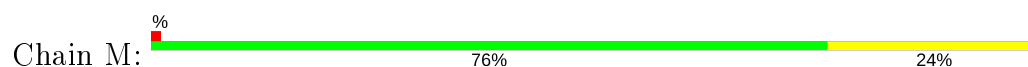
- Molecule 3: Mouse monoclonal Fab fragment, light chain



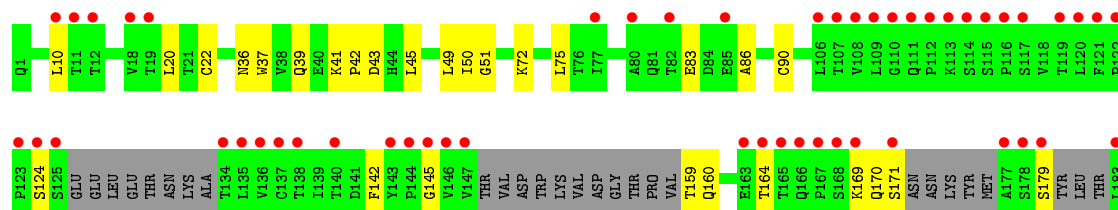
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain

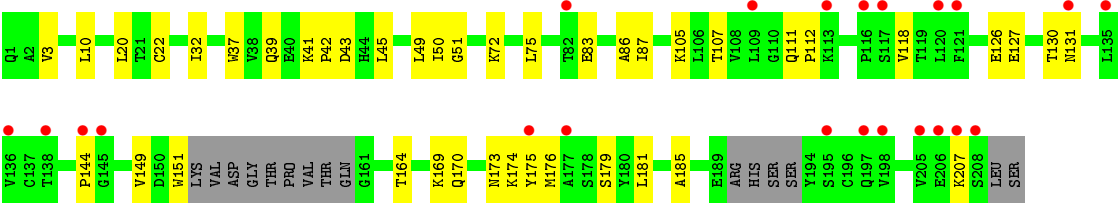


- Molecule 3: Mouse monoclonal Fab fragment, light chain



T184
A185
ARG
ALA
TRP
GLU
ARG
HIS
SER
SER
TYR
SER
CYS
GLN
VAL
THR
HIS
GLU
GLY
HIS
THR
VAL
GLU
LYS
SER
LEU
SER

- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.84Å 154.84Å 573.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 3.40 49.83 – 3.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.83-3.40) 98.8 (49.83-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.232 , 0.248 0.226 , 0.242	Depositor DCC
R_{free} test set	4809 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.8	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	29167	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: NAG, CL, IVM, RI5, LMT, UND, OCT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2789	0.41	0/3809
1	B	0.25	0/2789	0.40	0/3809
1	C	0.24	0/2778	0.40	0/3794
1	D	0.24	0/2789	0.40	0/3809
1	E	0.24	0/2789	0.40	0/3809
2	F	0.23	0/1479	0.40	0/2014
2	G	0.25	0/1569	0.44	0/2138
2	H	0.24	0/1729	0.42	0/2360
2	I	0.22	0/1564	0.41	0/2128
2	J	0.23	0/1684	0.42	0/2299
3	K	0.22	0/1529	0.42	0/2089
3	L	0.24	0/1629	0.42	0/2226
3	M	0.22	0/1616	0.42	0/2211
3	N	0.22	0/1178	0.42	0/1609
3	O	0.22	0/1504	0.43	0/2056
All	All	0.24	0/29415	0.41	0/40160

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2709	101	0
1	B	2716	0	2708	98	0
1	C	2706	0	2701	93	0
1	D	2716	0	2709	93	0
1	E	2716	0	2708	103	0
2	F	1441	0	1365	35	0
2	G	1529	0	1478	43	0
2	H	1683	0	1632	43	0
2	I	1525	0	1485	35	0
2	J	1639	0	1588	48	0
3	K	1496	0	1458	35	0
3	L	1591	0	1542	32	0
3	M	1579	0	1526	37	0
3	N	1156	0	1128	20	0
3	O	1470	0	1412	35	0
4	A	62	0	74	5	0
4	B	62	0	74	2	0
4	C	62	0	74	5	0
4	D	62	0	74	3	0
4	E	62	0	74	7	0
5	A	53	0	52	14	0
5	B	26	0	25	5	0
6	B	14	0	13	1	0
6	C	14	0	13	1	0
6	E	14	0	13	0	0
7	B	8	0	18	1	0
7	D	8	0	18	1	0
7	E	8	0	18	3	0
8	B	11	0	24	0	0
9	C	1	0	0	0	0
10	E	21	0	16	15	0
All	All	29167	0	28729	786	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 786 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:HIS:CD2	5:A:350:LMT:H12	1.79	1.17
1:A:299:HIS:HD2	5:A:350:LMT:H12	0.96	1.08
1:A:299:HIS:CD2	5:A:350:LMT:C1	2.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:THR:OG1	10:E:351:RI5:H13	1.57	1.01
1:A:299:HIS:HD2	5:A:350:LMT:C1	1.73	0.99

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	318 (94%)	18 (5%)	2 (1%)	25	57
1	B	338/347 (97%)	316 (94%)	20 (6%)	2 (1%)	25	57
1	C	337/347 (97%)	316 (94%)	19 (6%)	2 (1%)	25	57
1	D	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	57
1	E	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	25	57
2	F	182/221 (82%)	169 (93%)	12 (7%)	1 (0%)	29	61
2	G	194/221 (88%)	179 (92%)	14 (7%)	1 (0%)	29	61
2	H	219/221 (99%)	204 (93%)	15 (7%)	0	100	100
2	I	193/221 (87%)	181 (94%)	10 (5%)	2 (1%)	15	46
2	J	211/221 (96%)	197 (93%)	14 (7%)	0	100	100
3	K	195/210 (93%)	176 (90%)	18 (9%)	1 (0%)	29	61
3	L	208/210 (99%)	191 (92%)	16 (8%)	1 (0%)	29	61
3	M	208/210 (99%)	192 (92%)	16 (8%)	0	100	100
3	N	148/210 (70%)	133 (90%)	15 (10%)	0	100	100
3	O	189/210 (90%)	166 (88%)	23 (12%)	0	100	100
All	All	3636/3890 (94%)	3372 (93%)	248 (7%)	16 (0%)	34	67

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	190	VAL
1	A	68	VAL
1	B	68	VAL
1	C	68	VAL
1	D	68	VAL

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	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	B	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	C	306/316 (97%)	303 (99%)	3 (1%)	76	88
1	D	307/316 (97%)	304 (99%)	3 (1%)	76	88
1	E	307/316 (97%)	303 (99%)	4 (1%)	69	84
2	F	158/190 (83%)	158 (100%)	0	100	100
2	G	171/190 (90%)	170 (99%)	1 (1%)	86	94
2	H	190/190 (100%)	190 (100%)	0	100	100
2	I	172/190 (90%)	172 (100%)	0	100	100
2	J	185/190 (97%)	185 (100%)	0	100	100
3	K	169/178 (95%)	168 (99%)	1 (1%)	86	94
3	L	178/178 (100%)	175 (98%)	3 (2%)	60	80
3	M	176/178 (99%)	175 (99%)	1 (1%)	86	94
3	N	128/178 (72%)	128 (100%)	0	100	100
3	O	162/178 (91%)	161 (99%)	1 (1%)	86	94
All	All	3223/3420 (94%)	3200 (99%)	23 (1%)	84	92

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

Mol	Chain	Res	Type
1	D	104	ASP
1	E	95	GLU

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Mol	Chain	Res	Type
3	M	109	LEU
1	D	189	THR
1	E	104	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	180	GLN
2	H	5	GLN
3	N	166	GLN
2	G	5	GLN
2	H	62	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	IVM	A	349	-	65,68,68	0.79	1 (1%)	82,102,102	1.62	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	400	1	14,14,15	0.52	0	17,19,21	0.97	2 (11%)
7	OCT	E	350	-	7,7,7	0.28	0	6,6,6	0.42	0
4	IVM	E	349	-	65,68,68	0.81	1 (1%)	82,102,102	1.64	18 (21%)
4	IVM	C	350	-	65,68,68	0.82	1 (1%)	82,102,102	1.61	17 (20%)
5	LMT	A	351	-	28,28,36	1.47	4 (14%)	39,39,47	1.37	5 (12%)
8	UND	B	352	-	10,10,10	0.31	0	9,9,9	0.37	0
4	IVM	B	349	-	65,68,68	0.79	1 (1%)	82,102,102	1.62	17 (20%)
7	OCT	D	350	-	7,7,7	0.28	0	6,6,6	0.38	0
4	IVM	D	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.63	16 (19%)
5	LMT	B	350	-	27,27,36	1.54	4 (14%)	37,38,47	1.41	5 (13%)
6	NAG	C	400	1	14,14,15	0.37	0	17,19,21	1.92	2 (11%)
10	RI5	E	351	-	23,25,25	2.40	6 (26%)	26,46,46	2.20	10 (38%)
6	NAG	E	400	1	14,14,15	0.49	0	17,19,21	1.42	4 (23%)
5	LMT	A	350	-	27,27,36	1.50	4 (14%)	37,38,47	1.81	9 (24%)
7	OCT	B	351	-	7,7,7	0.25	0	6,6,6	0.41	0

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	IVM	A	349	-	-	6/45/141/141	0/6/7/7
6	NAG	B	400	1	-	0/6/23/26	0/1/1/1
7	OCT	E	350	-	-	0/5/5/5	-
4	IVM	E	349	-	-	6/45/141/141	0/6/7/7
4	IVM	C	350	-	-	6/45/141/141	0/6/7/7
5	LMT	A	351	-	-	6/13/53/61	0/2/2/2
8	UND	B	352	-	-	0/8/8/8	-
4	IVM	B	349	-	-	6/45/141/141	0/6/7/7
7	OCT	D	350	-	-	0/5/5/5	-
4	IVM	D	349	-	-	6/45/141/141	0/6/7/7
5	LMT	B	350	-	-	7/12/52/61	0/2/2/2
6	NAG	C	400	1	-	0/6/23/26	0/1/1/1
10	RI5	E	351	-	-	3/4/77/77	0/6/5/5
6	NAG	E	400	1	-	4/6/23/26	0/1/1/1
5	LMT	A	350	-	-	7/12/52/61	0/2/2/2
7	OCT	B	351	-	-	0/5/5/5	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	351	RI5	O12-C10	6.85	1.45	1.35
10	E	351	RI5	O19-C17	6.56	1.45	1.35
4	C	350	IVM	O12-C46	4.95	1.45	1.34
4	E	349	IVM	O12-C46	4.85	1.45	1.34
4	B	349	IVM	O12-C46	4.83	1.45	1.34

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	349	IVM	O12-C46-C45	6.72	120.69	110.97
4	A	349	IVM	O12-C46-C45	6.71	120.69	110.97
4	D	349	IVM	O12-C46-C45	6.63	120.56	110.97
4	C	350	IVM	O12-C46-C45	6.54	120.43	110.97
4	B	349	IVM	O12-C46-C45	6.44	120.30	110.97

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	349	IVM	O7-C25-O4-C24
4	A	349	IVM	C26-C25-O4-C24
4	E	349	IVM	O7-C25-O4-C24
4	E	349	IVM	C26-C25-O4-C24
4	C	350	IVM	O7-C25-O4-C24

There are no ring outliers.

14 monomers are involved in 63 short contacts:

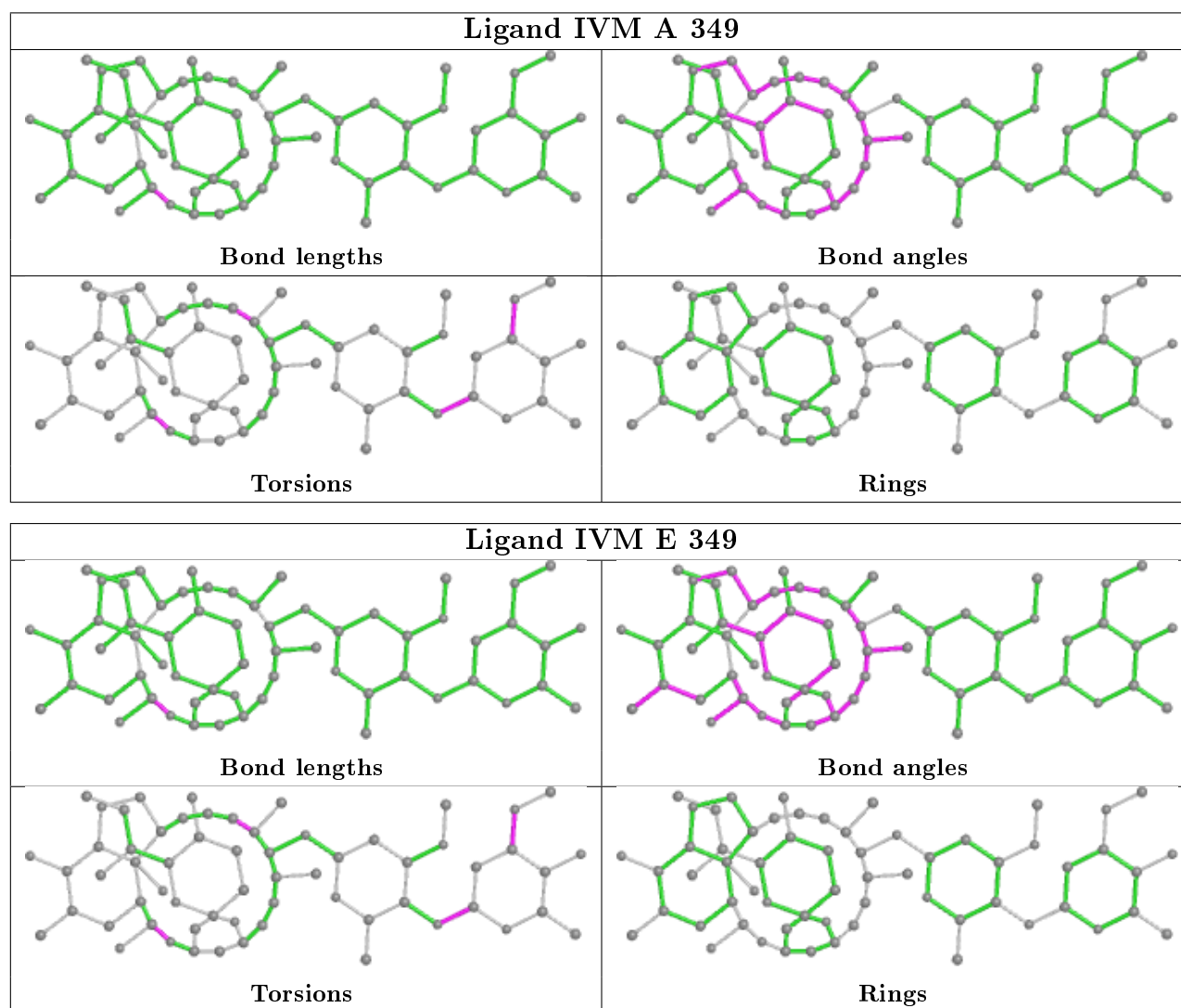
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	349	IVM	5	0
6	B	400	NAG	1	0
7	E	350	OCT	3	0
4	E	349	IVM	7	0
4	C	350	IVM	5	0
5	A	351	LMT	3	0
4	B	349	IVM	2	0
7	D	350	OCT	1	0
4	D	349	IVM	3	0
5	B	350	LMT	5	0
6	C	400	NAG	1	0

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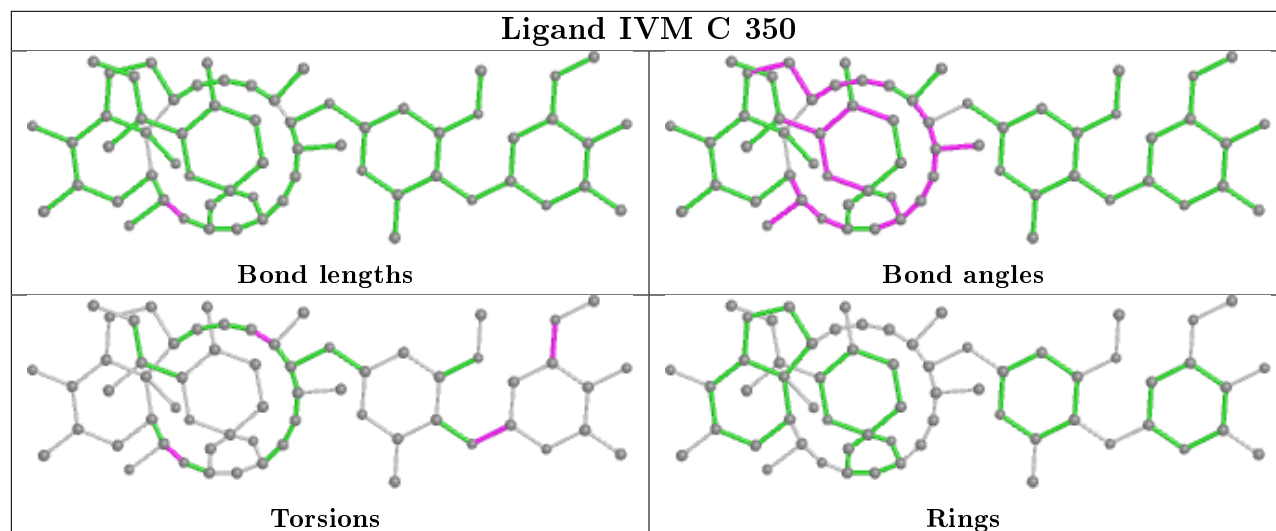
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	351	RI5	15	0
5	A	350	LMT	11	0
7	B	351	OCT	1	0

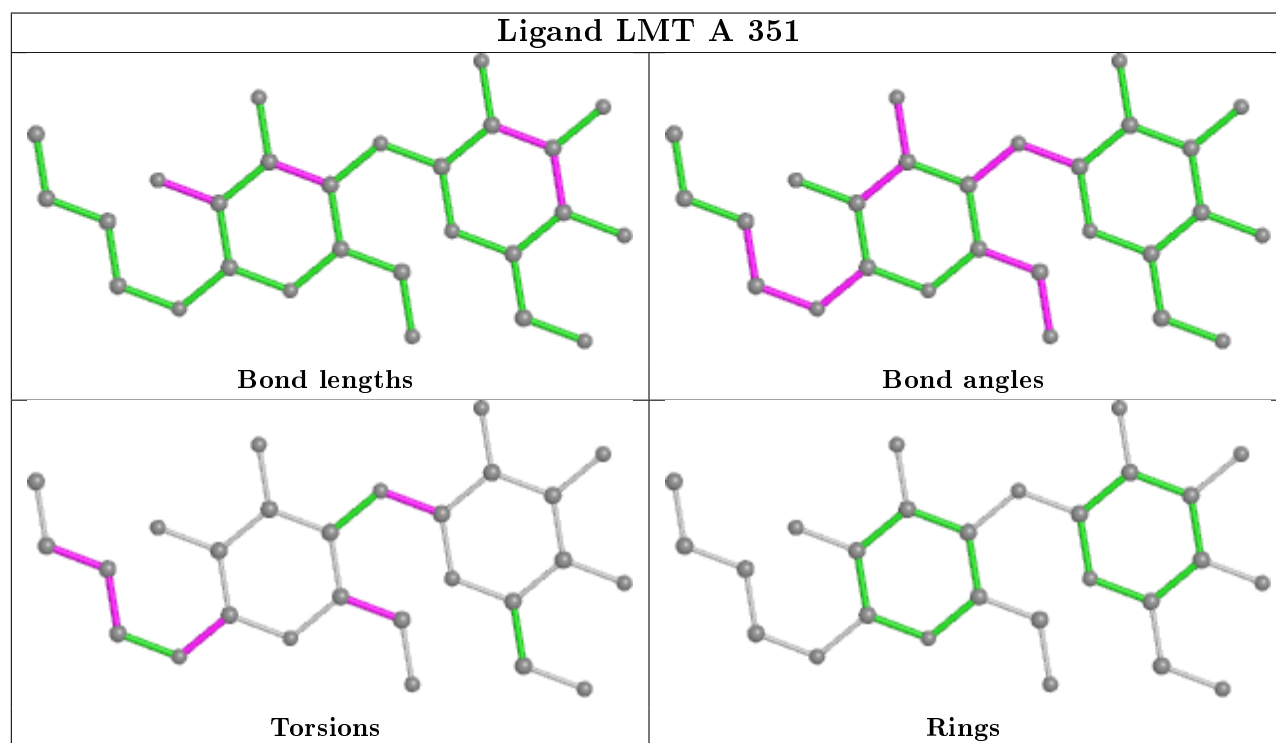
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

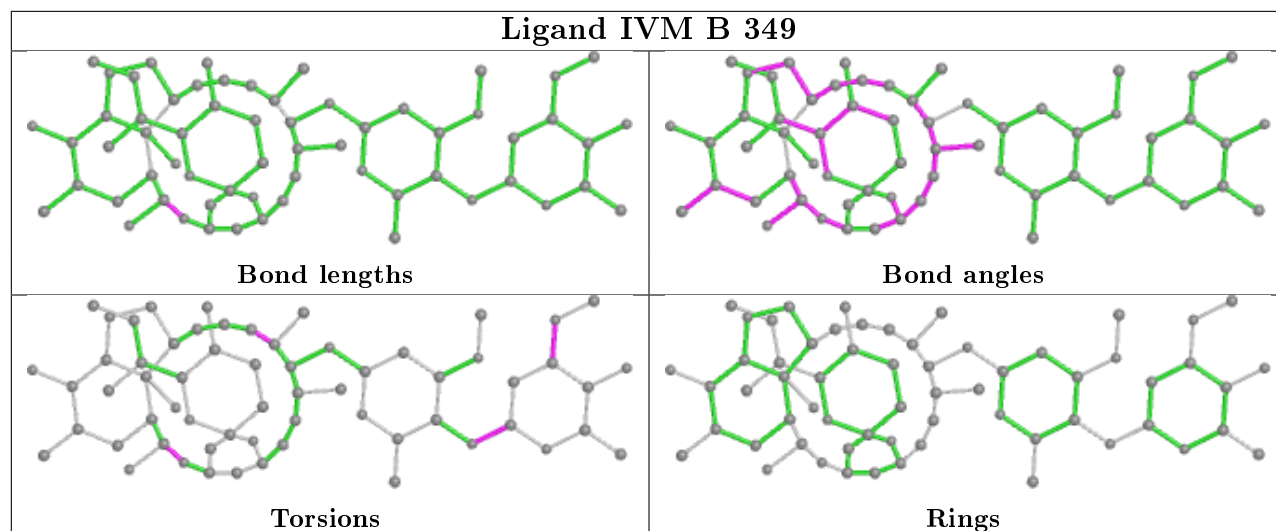
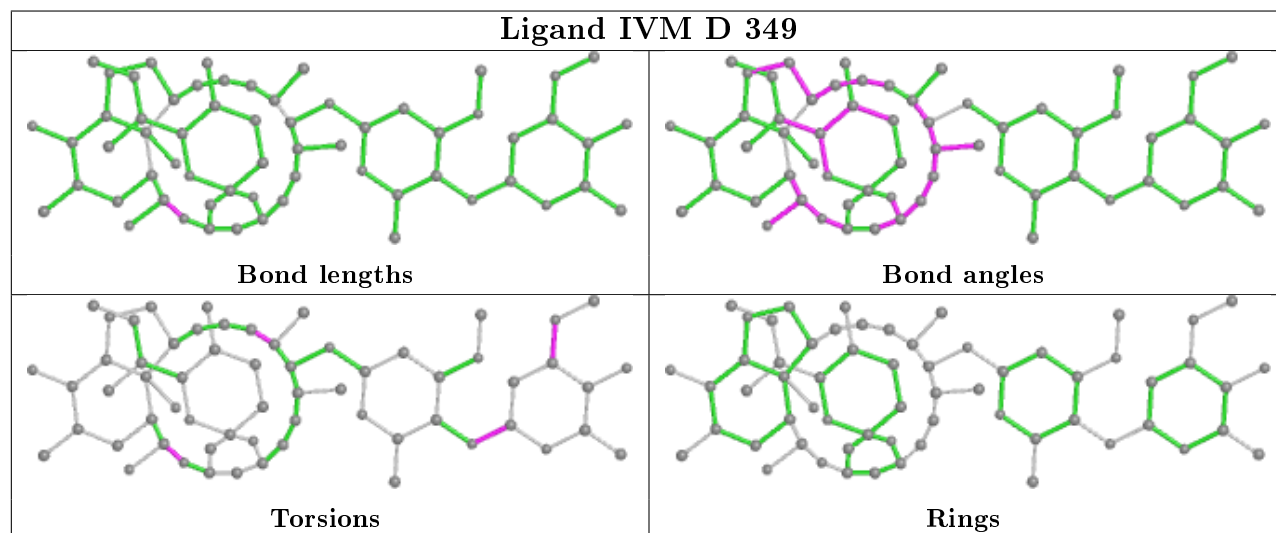


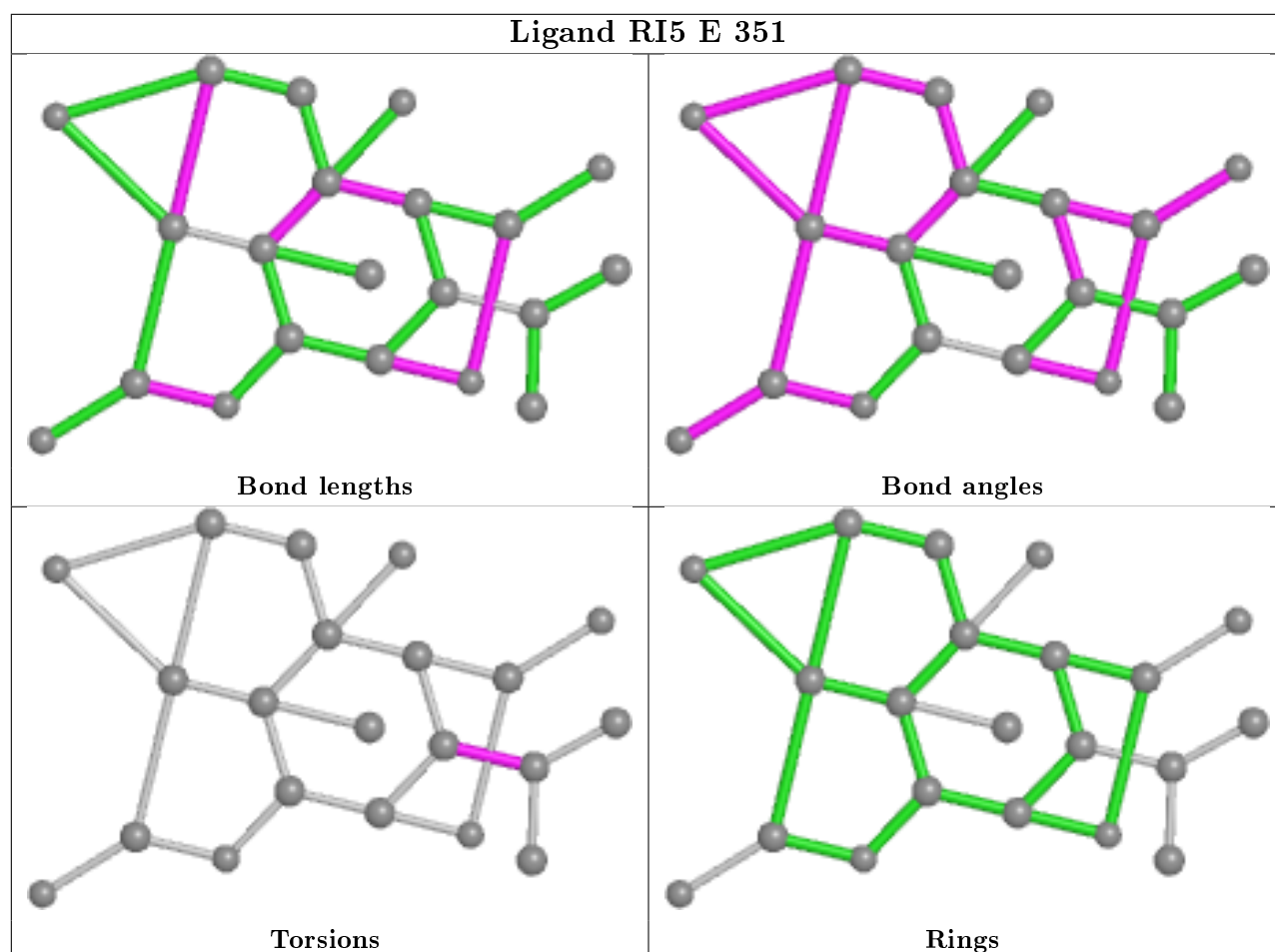
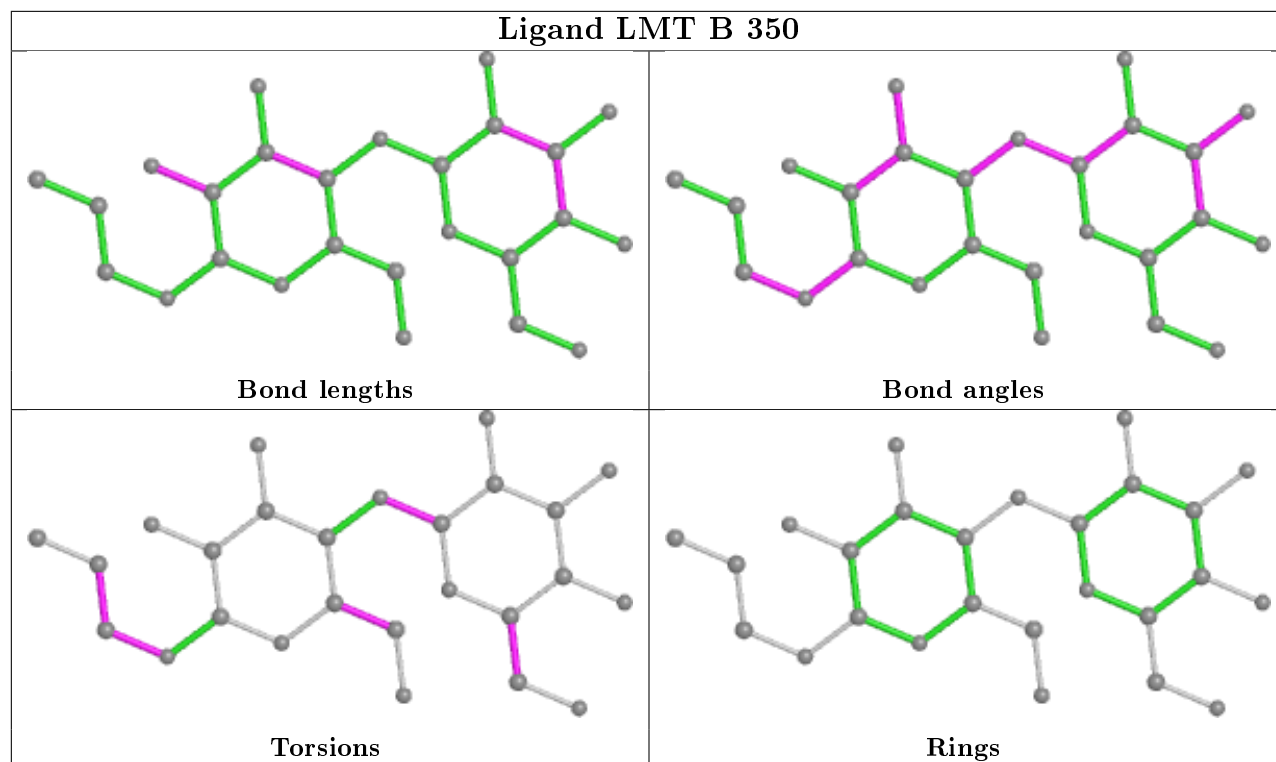
Ligand IVM C 350

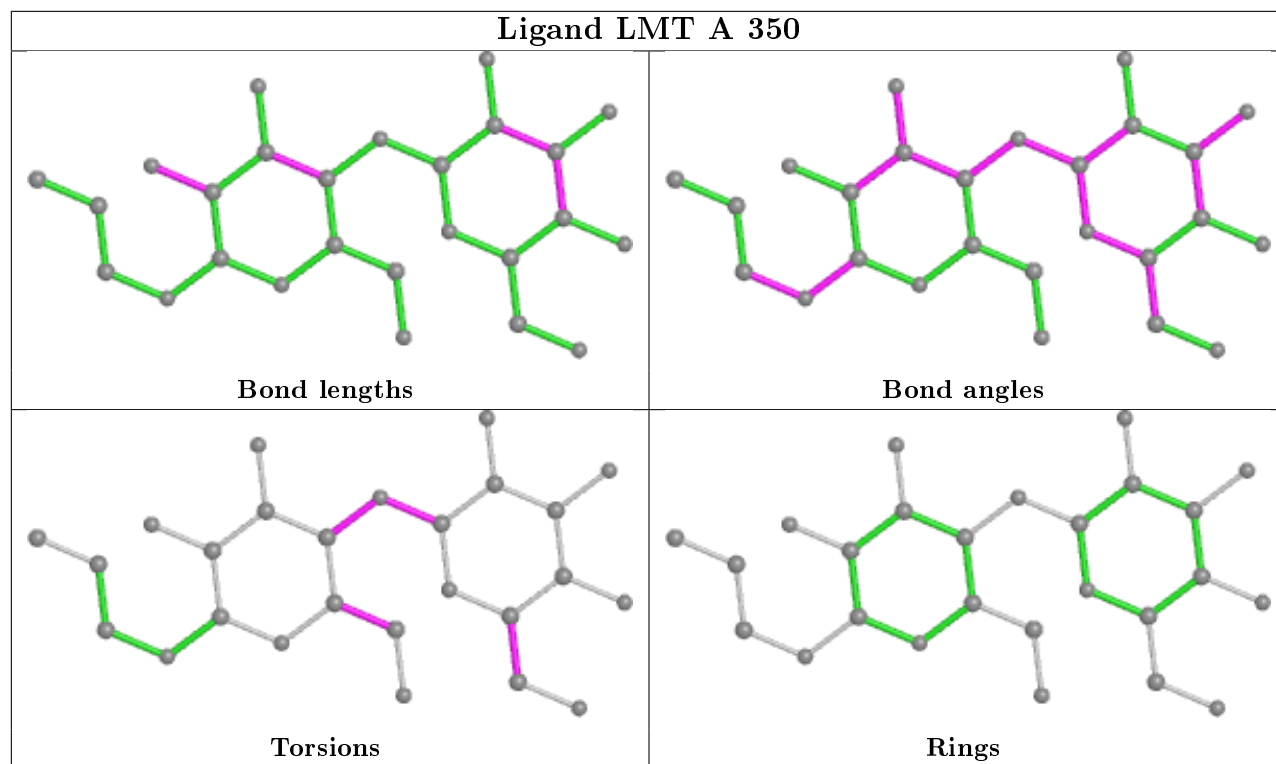


Ligand LMT A 351



Ligand IVM B 349**Ligand IVM D 349**





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	340/347 (97%)	-0.03	1 (0%) 94 93	42, 72, 125, 179	0
1	B	340/347 (97%)	-0.05	4 (1%) 79 77	47, 74, 129, 206	0
1	C	339/347 (97%)	0.06	10 (2%) 51 50	42, 76, 143, 234	0
1	D	340/347 (97%)	-0.07	4 (1%) 79 77	44, 80, 144, 252	0
1	E	340/347 (97%)	-0.04	3 (0%) 84 83	41, 76, 150, 230	0
2	F	188/221 (85%)	0.78	29 (15%) 2 2	59, 112, 184, 237	0
2	G	200/221 (90%)	0.44	14 (7%) 16 18	60, 99, 145, 177	0
2	H	221/221 (100%)	0.01	1 (0%) 91 90	47, 82, 139, 257	0
2	I	199/221 (90%)	0.79	34 (17%) 1 2	63, 112, 174, 207	0
2	J	215/221 (97%)	0.22	8 (3%) 41 40	55, 89, 149, 212	0
3	K	199/210 (94%)	0.13	5 (2%) 57 55	67, 107, 151, 198	0
3	L	210/210 (100%)	0.08	2 (0%) 82 81	44, 81, 129, 171	0
3	M	210/210 (100%)	0.07	2 (0%) 82 81	55, 92, 133, 197	0
3	N	158/210 (75%)	1.27	51 (32%) 0 0	65, 121, 197, 232	0
3	O	195/210 (92%)	0.72	22 (11%) 5 6	69, 117, 170, 218	0
All	All	3694/3890 (94%)	0.22	190 (5%) 28 28	41, 87, 159, 257	0

The worst 5 of 190 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	208	SER	7.5
2	J	137	SER	7.3
3	N	109	LEU	6.7
1	B	302	ASN	5.9
2	I	189	SER	5.6

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 ⓘ

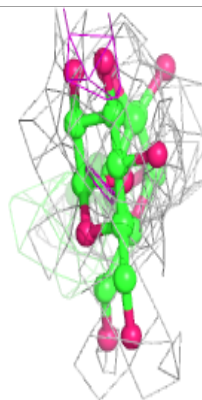
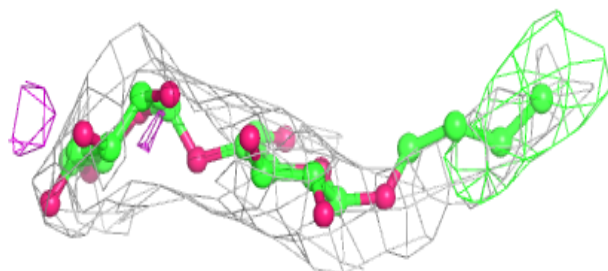
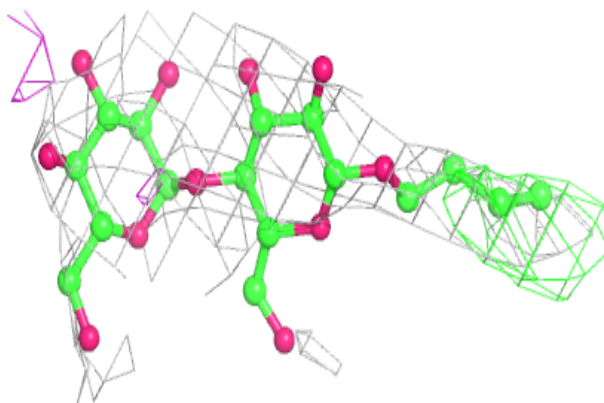
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	LMT	A	351	27/35	0.56	0.49	152,152,152,152	0
5	LMT	B	350	26/35	0.71	0.46	176,176,176,176	0
6	NAG	E	400	14/15	0.74	0.32	163,171,176,176	0
7	OCT	D	350	8/8	0.75	0.57	79,79,79,79	0
7	OCT	E	350	8/8	0.75	0.56	76,76,76,76	0
8	UND	B	352	11/11	0.77	0.42	74,74,74,74	0
6	NAG	C	400	14/15	0.84	0.19	128,130,131,132	0
6	NAG	B	400	14/15	0.85	0.48	123,124,129,130	0
5	LMT	A	350	26/35	0.86	0.29	111,111,111,111	0
7	OCT	B	351	8/8	0.87	0.40	68,68,68,68	0
10	RI5	E	351	21/21	0.88	0.27	213,213,213,213	0
4	IVM	D	349	62/62	0.89	0.28	69,77,96,97	0
4	IVM	C	350	62/62	0.90	0.32	60,73,95,98	0
4	IVM	E	349	62/62	0.91	0.32	73,81,101,103	0
4	IVM	B	349	62/62	0.91	0.23	54,62,79,80	0
4	IVM	A	349	62/62	0.92	0.26	68,76,101,105	0
9	CL	C	349	1/1	0.96	1.04	76,76,76,76	0

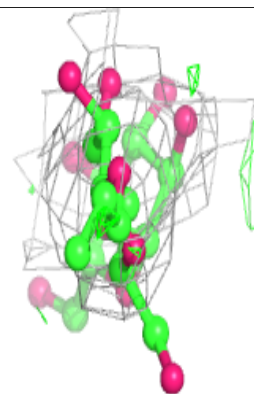
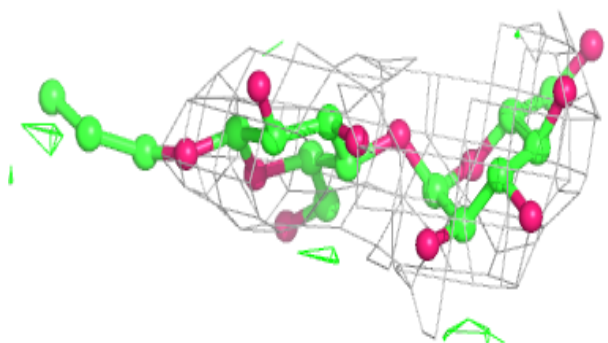
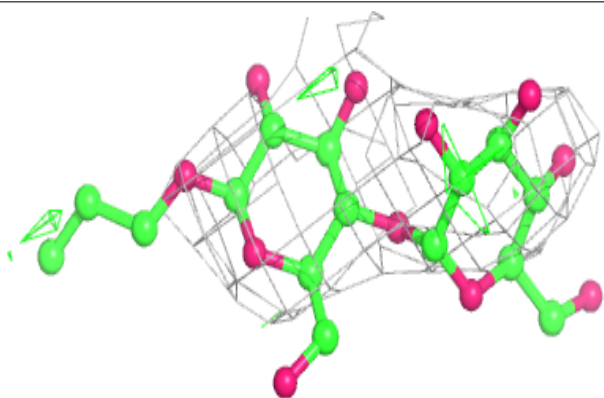
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 351:

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

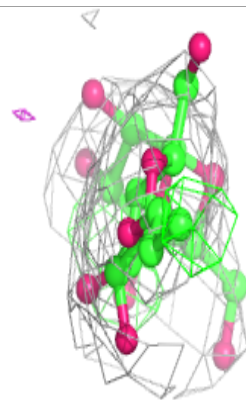
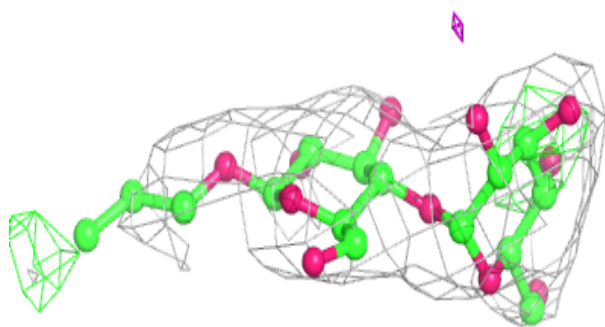
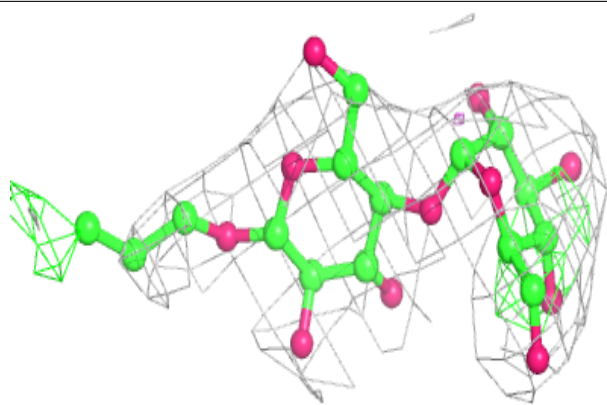
**Electron density around LMT B 350:**

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



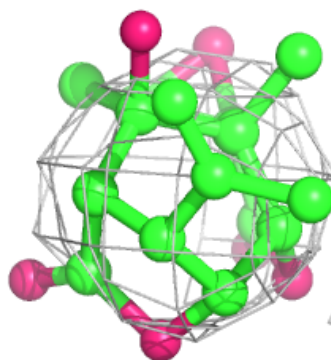
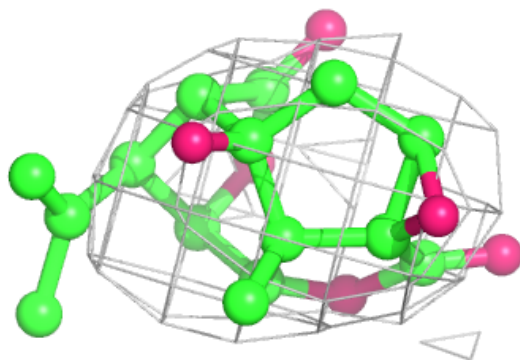
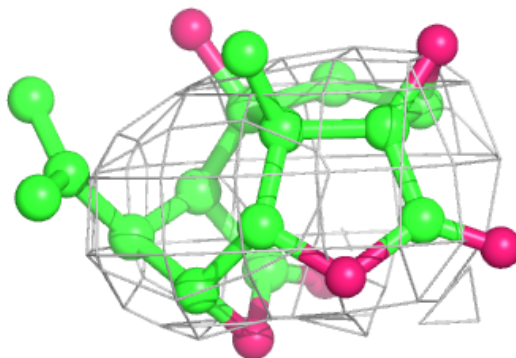
Electron density around LMT A 350:

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



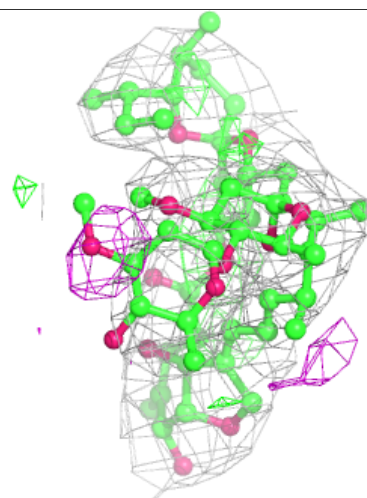
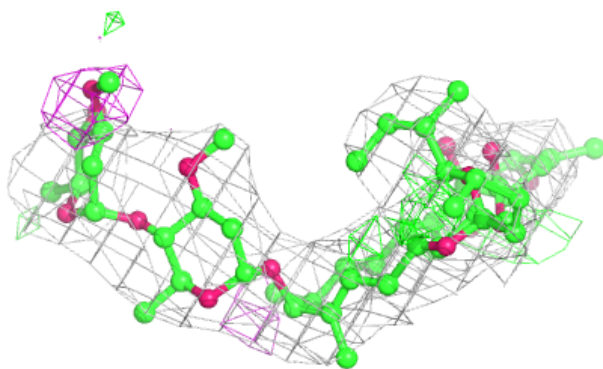
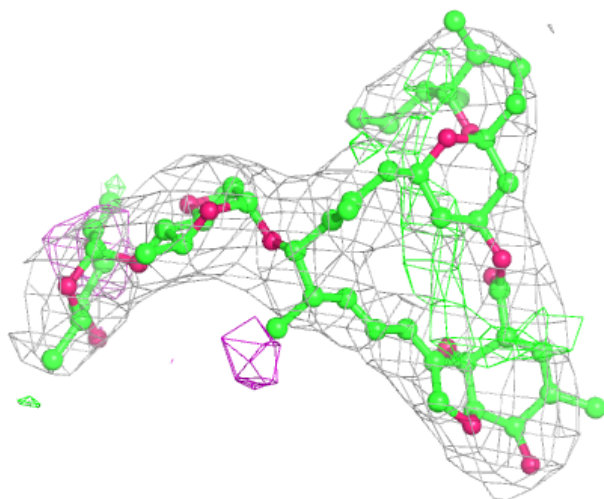
Electron density around RI5 E 351:

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



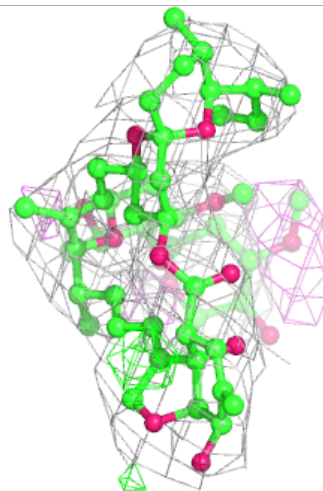
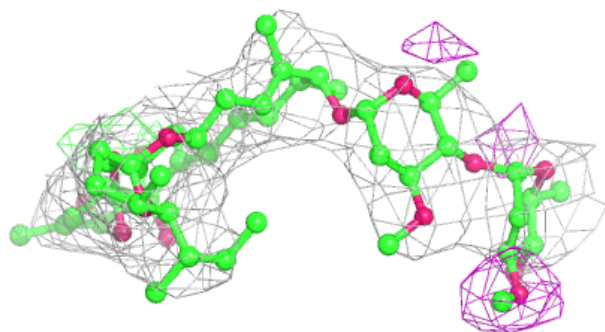
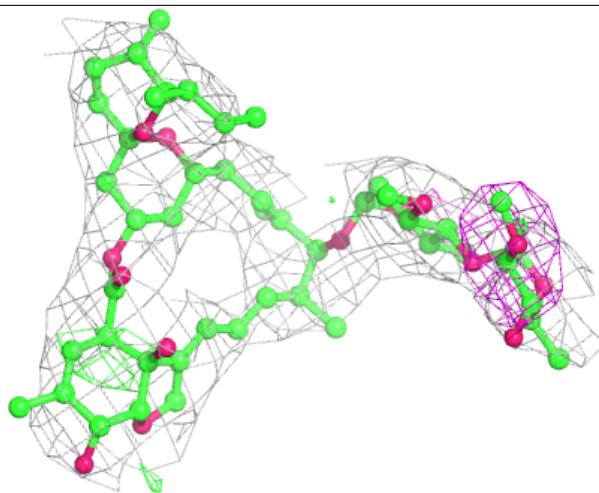
Electron density around IVM D 349:

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



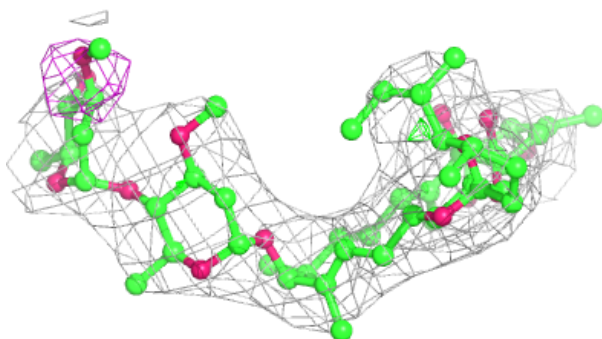
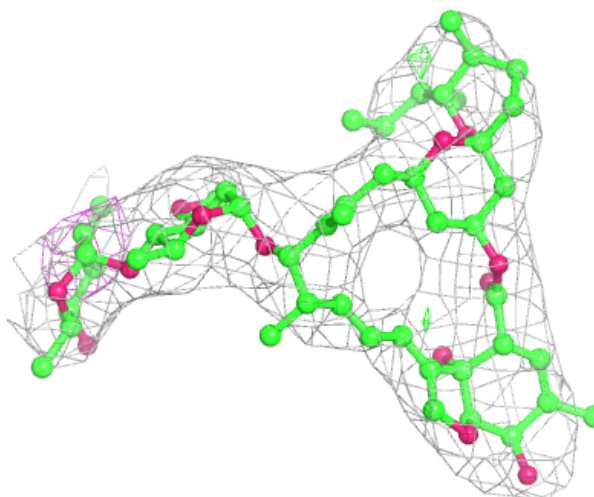
Electron density around IVM C 350:

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



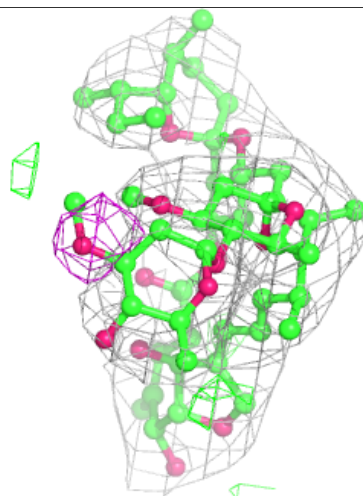
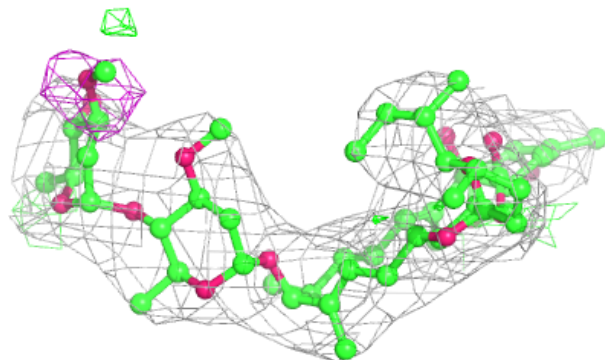
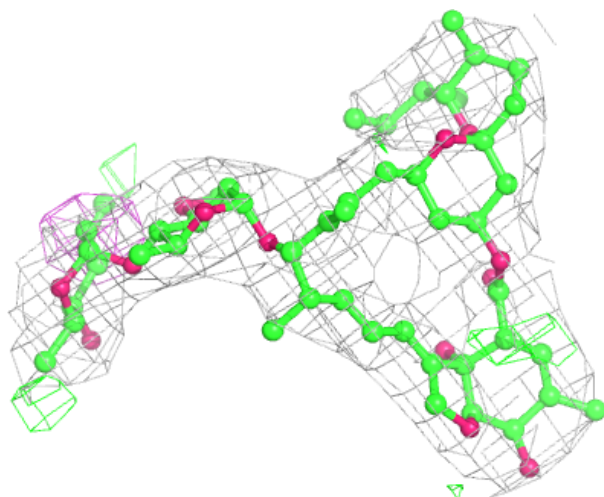
Electron density around IVM E 349:

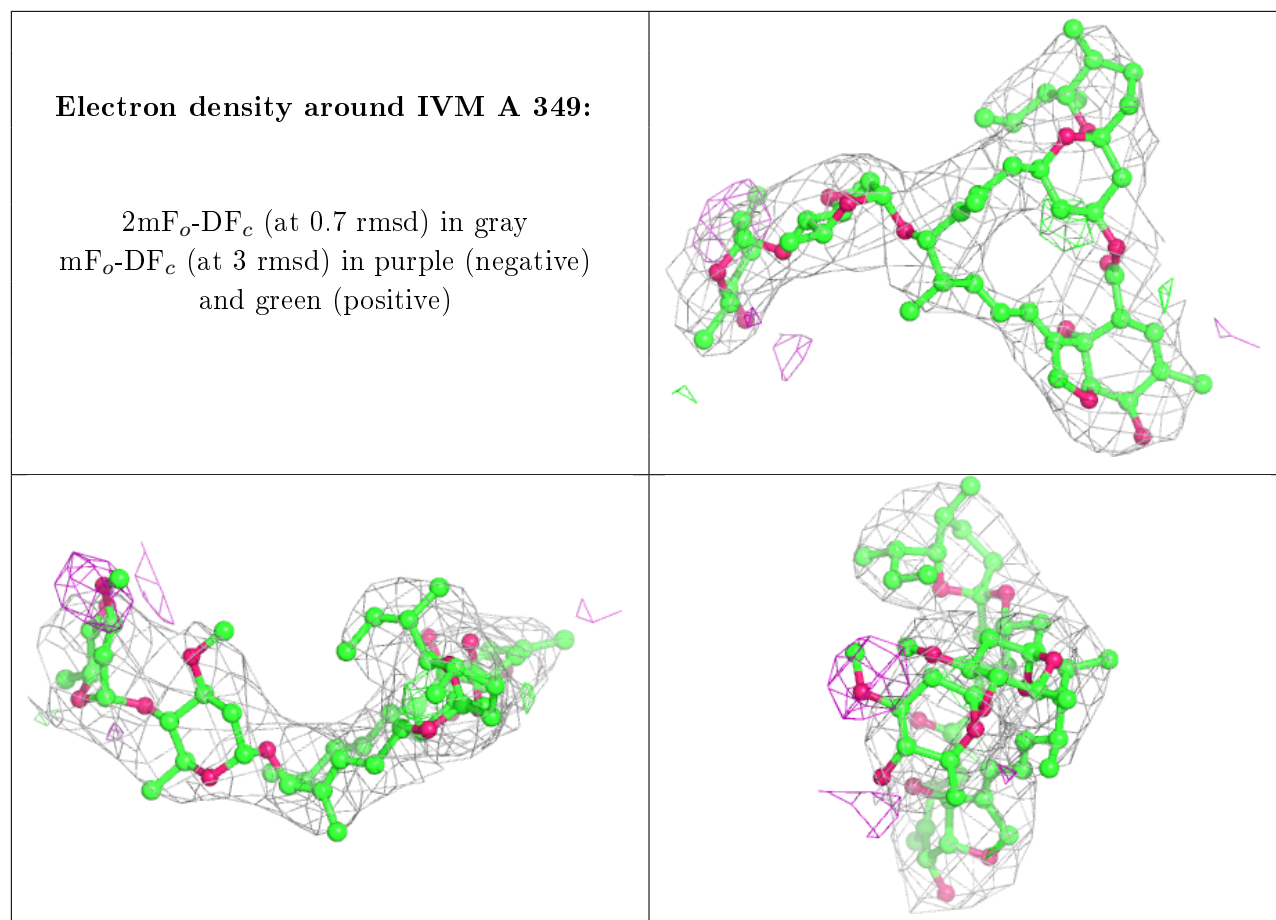
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IVM B 349:

$2mF_o-DF_c$ (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.