



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:12 AM UTC

PDB ID : 3RIA / pdb_00003ria
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and iodide.
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-13
Resolution : 3.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

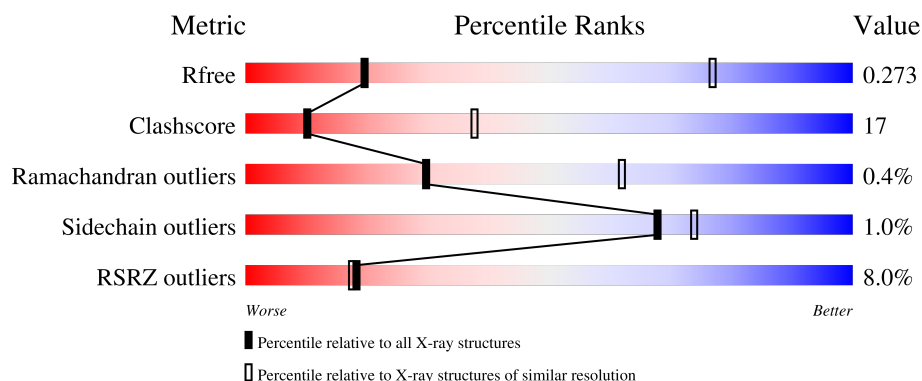
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. 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	4% 63% 35% .
1	B	347	5% 60% 37% ..
1	C	347	6% 61% 37% .
1	D	347	5% 62% 35% ..
1	E	347	4% 61% 36% ..

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Mol	Chain	Length	Quality of chain
2	F	221	
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
6	IOD	A	351	-	-	X	-
6	IOD	B	351	-	-	X	-
6	IOD	D	349	-	-	X	-
6	IOD	E	351	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 29159 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	191	Total	C	N	O	S	0	0	0
			1478	942	240	289	7			

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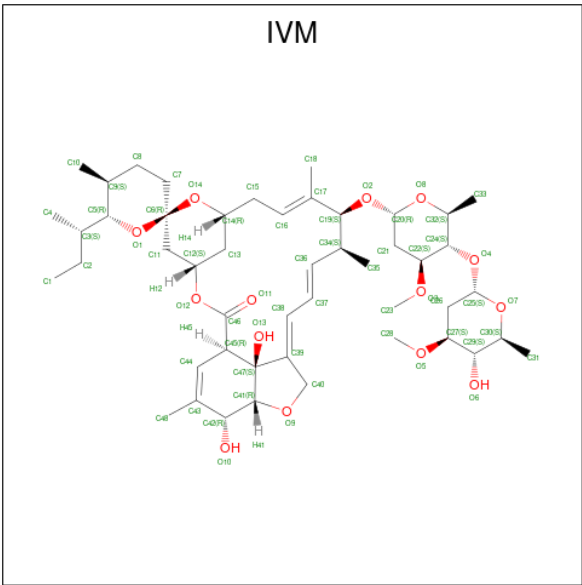
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	200	Total	C	N	O	S	0	0	0
			1529	973	248	301	7			
2	H	221	Total	C	N	O	S	0	0	0
			1683	1067	273	335	8			
2	I	199	Total	C	N	O	S	0	0	0
			1525	969	247	301	8			
2	J	215	Total	C	N	O	S	0	0	0
			1639	1043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

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

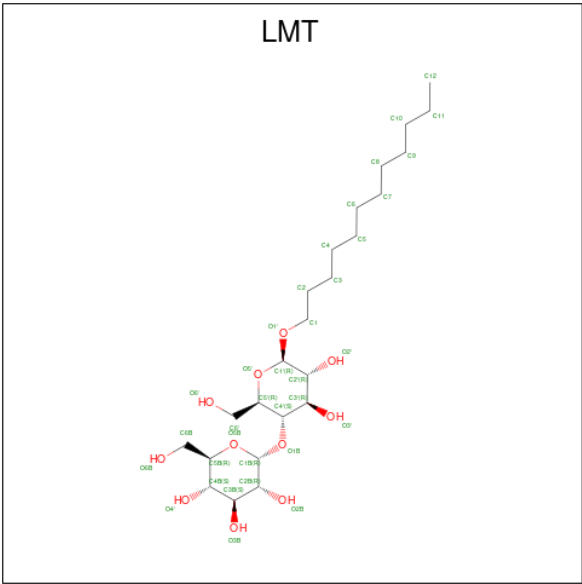
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	199	Total	C	N	O	S	0	0	0
			1496	941	246	303	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1584	996	263	319	6			
3	N	158	Total	C	N	O	S	0	0	0
			1165	736	192	233	4			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	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 (CCD ID: IVM) (formula: C₄₈H₇₄O₁₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			62	48	14		
4	C	1	Total	C	O	0	0
			62	48	14		
4	C	1	Total	C	O	0	0
			62	48	14		
4	E	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-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

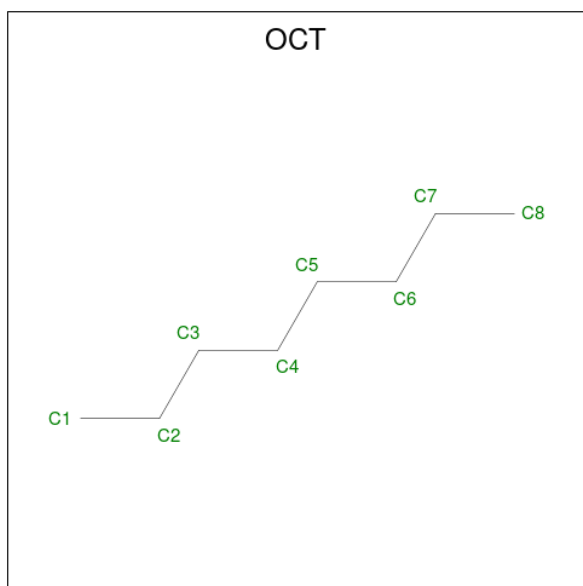


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			26	15	11		
5	A	1	Total	C	O	0	0
			27	16	11		
5	B	1	Total	C	O	0	0
			26	15	11		

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

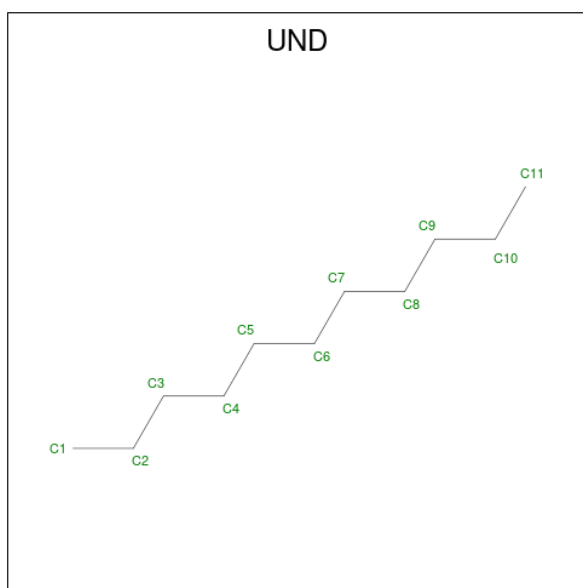
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	I	0	0
			1	1		
6	B	1	Total	I	0	0
			1	1		
6	D	1	Total	I	0	0
			1	1		
6	E	1	Total	I	0	0
			1	1		

- Molecule 7 is N-OCTANE (CCD ID: 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 (CCD ID: UND) (formula: $C_{11}H_{24}$).



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

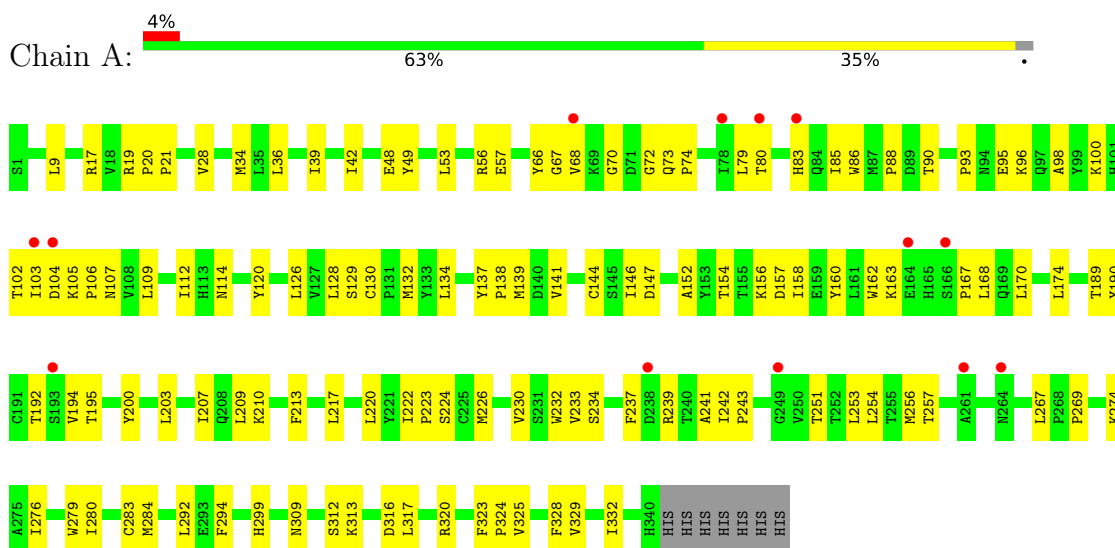
- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

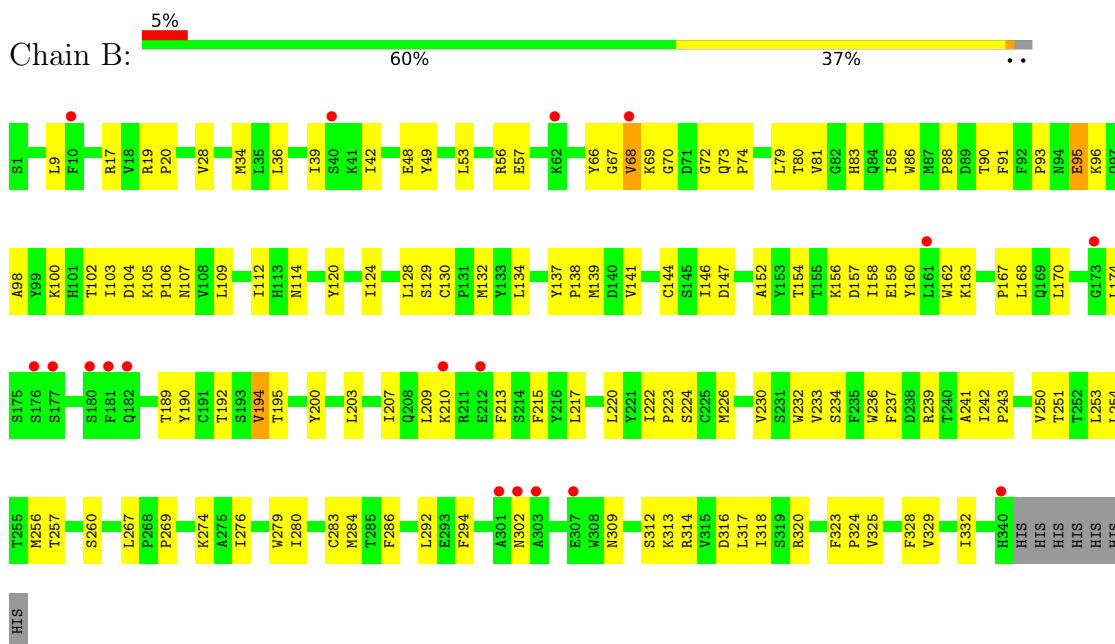
3 Residue-property plots [i](#)

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

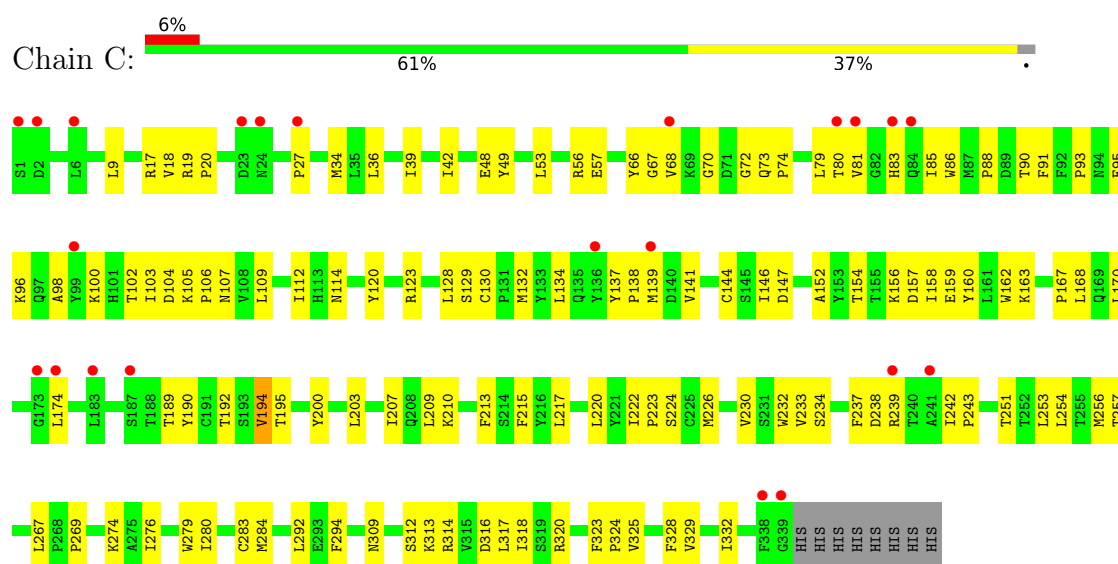
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



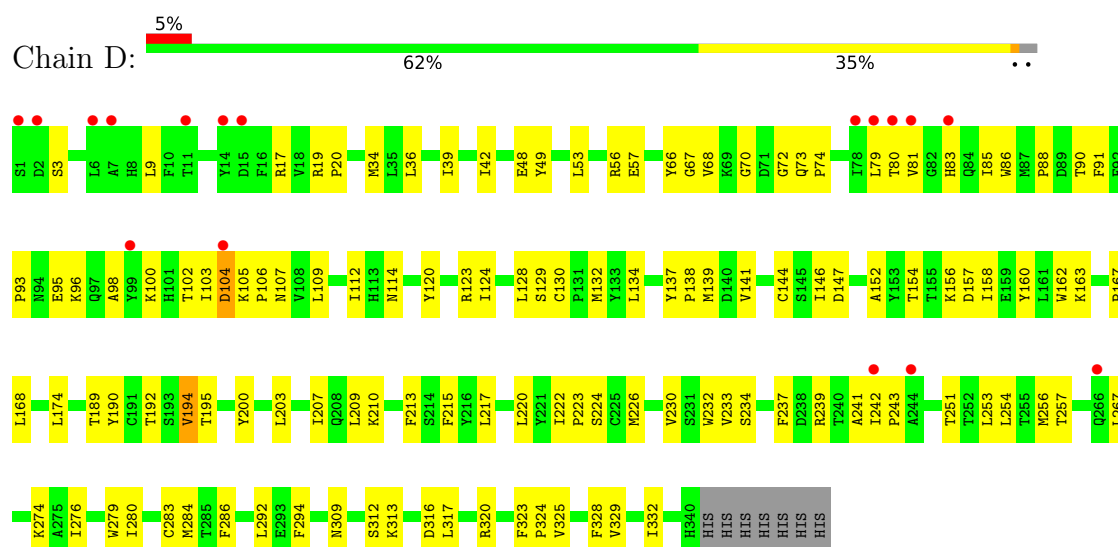
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



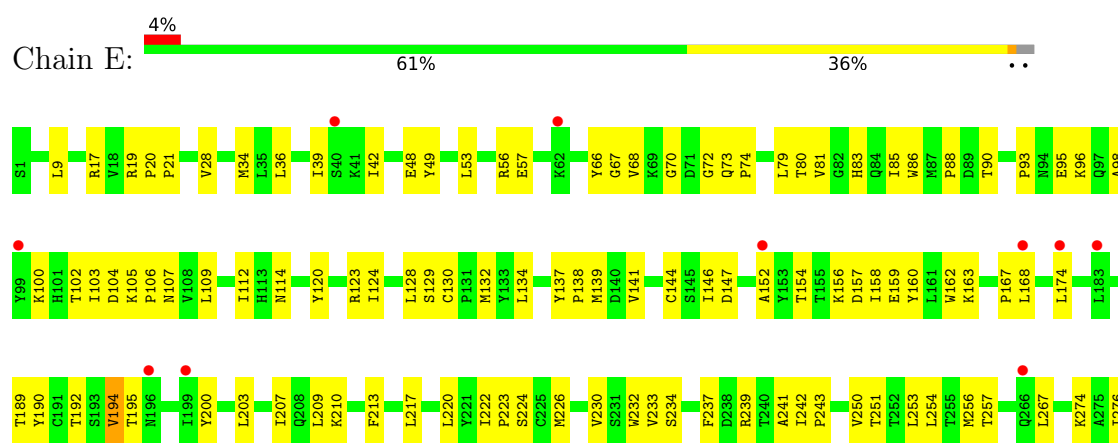
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

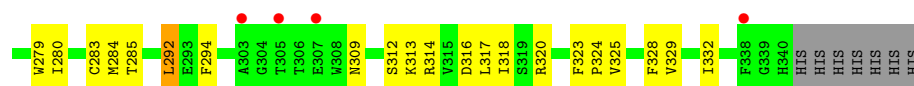


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

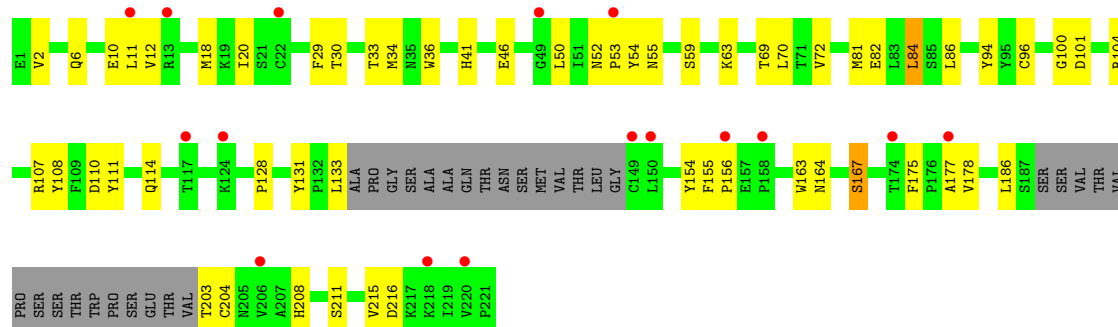


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

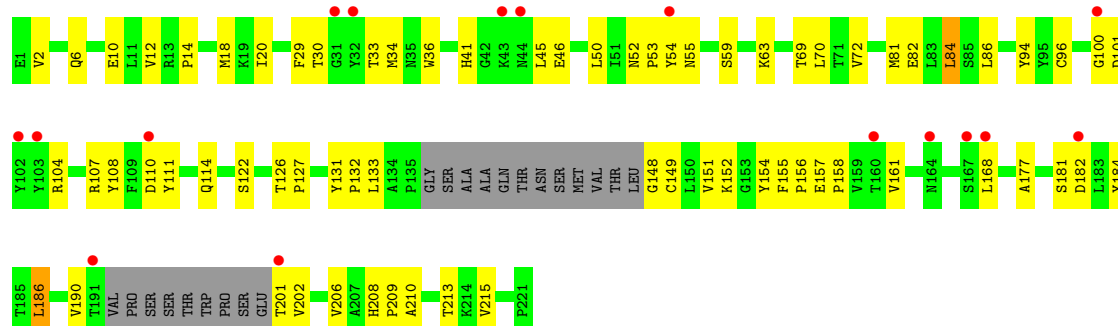




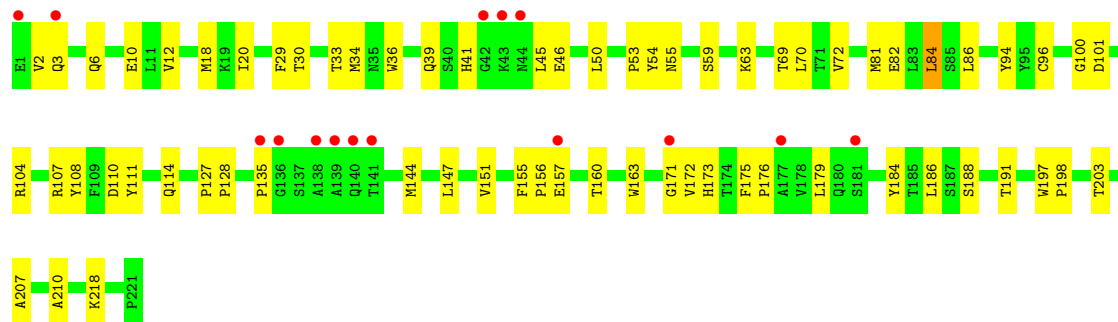
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

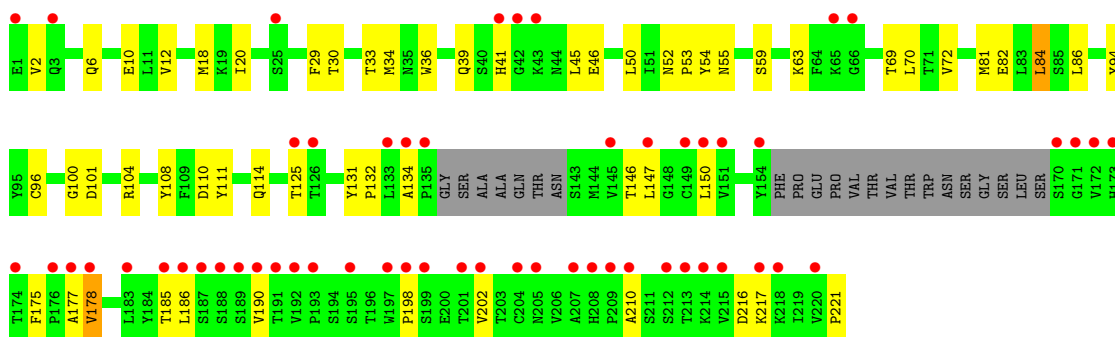


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

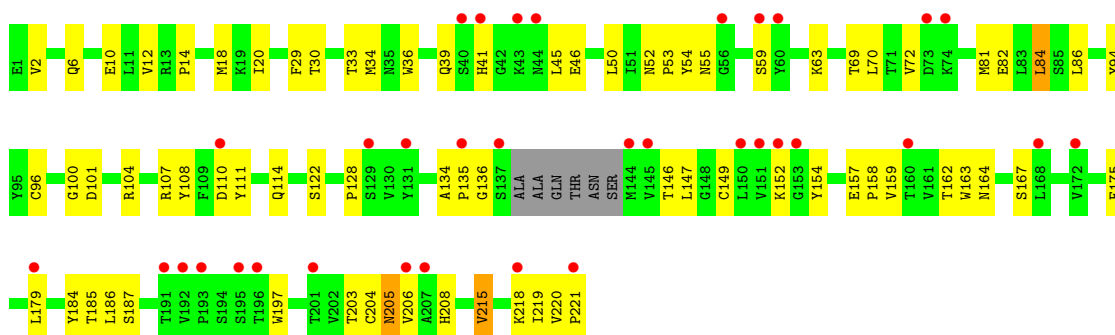


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

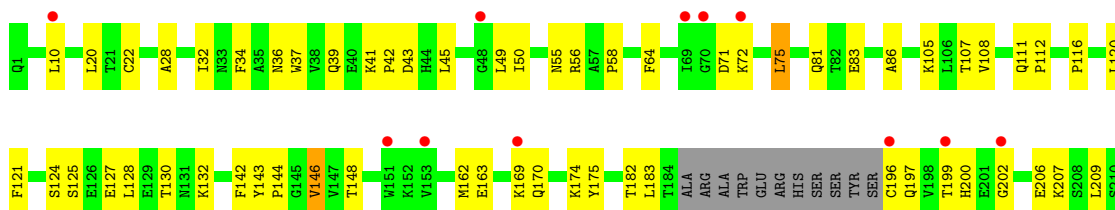




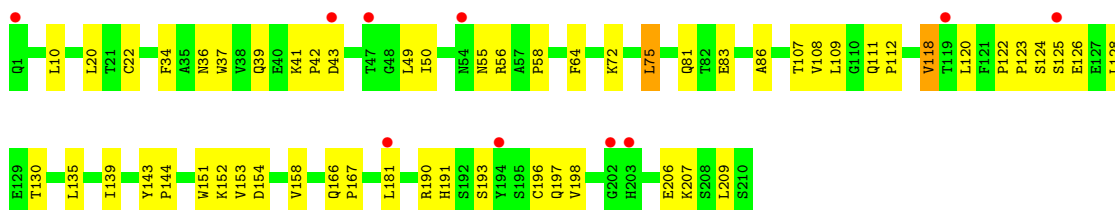
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



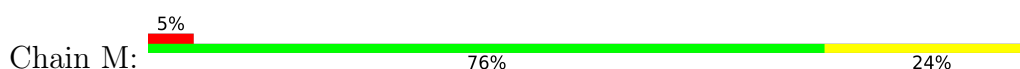
- Molecule 3: Mouse monoclonal Fab fragment, light chain



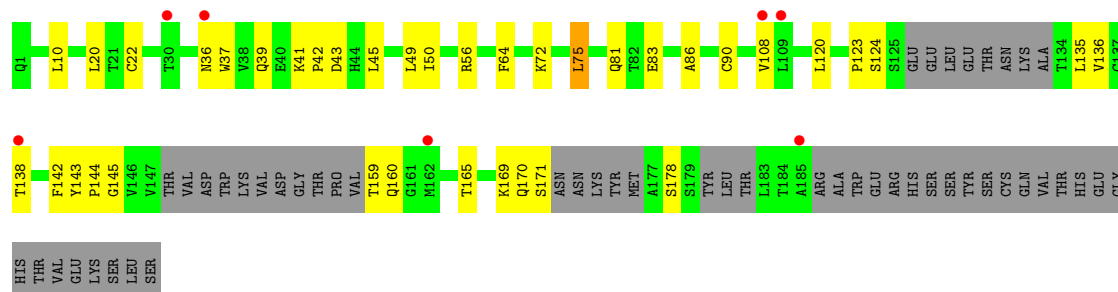
- Molecule 3: Mouse monoclonal Fab fragment, light chain



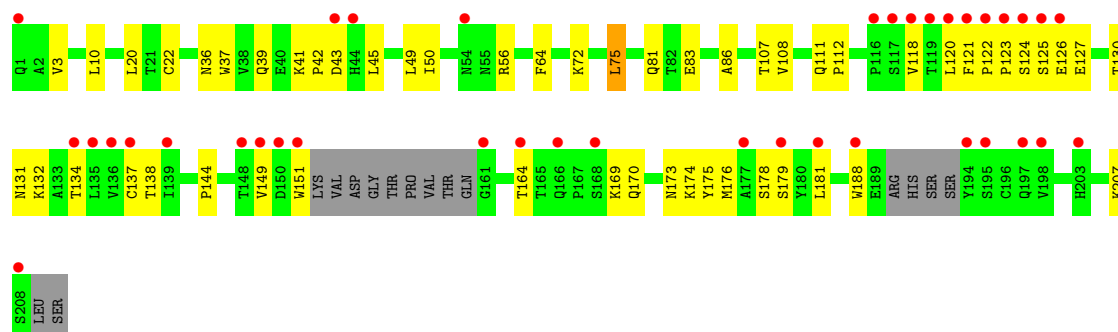
- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



- Molecule 3: Mouse monoclonal Fab fragment, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.10Å 155.10Å 578.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.77 – 3.80 38.77 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (38.77-3.80) 97.8 (38.77-3.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 3.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.266 , 0.280 0.254 , 0.273	Depositor DCC
R_{free} test set	3515 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	92.9	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	29159	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCT, IOD, CL, UND, LMT, IVM

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	0.32	0/2789	0.69	0/3809
1	B	0.31	0/2789	0.69	0/3809
1	C	0.31	0/2778	0.69	0/3794
1	D	0.30	0/2789	0.69	0/3809
1	E	0.31	0/2789	0.69	0/3809
2	F	0.28	0/1517	0.71	0/2062
2	G	0.28	0/1569	0.71	0/2138
2	H	0.29	0/1729	0.71	0/2360
2	I	0.29	0/1564	0.69	0/2128
2	J	0.29	0/1684	0.72	0/2299
3	K	0.27	0/1529	0.67	0/2089
3	L	0.30	0/1629	0.73	0/2226
3	M	0.29	0/1622	0.72	0/2219
3	N	0.27	0/1188	0.67	0/1621
3	O	0.34	0/1504	0.72	1/2056 (0.0%)
All	All	0.30	0/29469	0.70	1/40228 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	3	VAL	N-CA-C	5.32	116.33	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2716	0	2709	125	0
1	B	2716	0	2709	140	0
1	C	2706	0	2702	132	0
1	D	2716	0	2709	122	0
1	E	2716	0	2709	122	0
2	F	1478	0	1432	50	0
2	G	1529	0	1478	57	0
2	H	1683	0	1632	53	1
2	I	1525	0	1485	49	0
2	J	1639	0	1588	62	0
3	K	1496	0	1458	45	0
3	L	1591	0	1542	41	0
3	M	1584	0	1531	39	0
3	N	1165	0	1142	28	0
3	O	1470	0	1412	47	1
4	A	62	0	74	1	0
4	C	124	0	148	7	0
4	E	124	0	148	6	0
5	A	53	0	52	15	0
5	B	26	0	25	11	0
6	A	1	0	0	6	0
6	B	1	0	0	8	0
6	D	1	0	0	6	0
6	E	1	0	0	5	0
7	B	8	0	18	2	0
7	D	8	0	18	4	0
7	E	8	0	18	2	0
8	B	11	0	24	0	0
9	C	1	0	0	0	0
All	All	29159	0	28763	995	1

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 17.

The worst 5 of 995 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:241:ALA:HB1	6:A:351:IOD:I	1.62	1.68
1:D:241:ALA:HB1	6:D:349:IOD:I	1.65	1.65
1:D:241:ALA:CB	6:D:349:IOD:I	2.42	1.36
1:A:241:ALA:CB	6:A:351:IOD:I	2.44	1.33
1:E:241:ALA:HB1	6:E:351:IOD:I	2.03	1.27

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLN:NE2	3:O:125:SER:CB[3_554]	1.84	0.36

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	320 (95%)	17 (5%)	1 (0%)	36	67
1	B	338/347 (97%)	320 (95%)	17 (5%)	1 (0%)	36	67
1	C	337/347 (97%)	320 (95%)	16 (5%)	1 (0%)	36	67
1	D	338/347 (97%)	321 (95%)	16 (5%)	1 (0%)	36	67
1	E	338/347 (97%)	321 (95%)	16 (5%)	1 (0%)	36	67
2	F	185/221 (84%)	171 (92%)	12 (6%)	2 (1%)	11	41
2	G	194/221 (88%)	175 (90%)	19 (10%)	0	100	100
2	H	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
2	I	193/221 (87%)	181 (94%)	10 (5%)	2 (1%)	12	43
2	J	211/221 (96%)	200 (95%)	11 (5%)	0	100	100
3	K	195/210 (93%)	174 (89%)	20 (10%)	1 (0%)	24	57
3	L	208/210 (99%)	186 (89%)	20 (10%)	2 (1%)	12	43
3	M	208/210 (99%)	188 (90%)	20 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	N	148/210 (70%)	132 (89%)	15 (10%)	1 (1%)	18	51
3	O	189/210 (90%)	166 (88%)	23 (12%)	0	100	100
All	All	3639/3890 (94%)	3377 (93%)	249 (7%)	13 (0%)	30	62

5 of 13 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%)	305 (99%)	2 (1%)	76	77
1	B	307/316 (97%)	304 (99%)	3 (1%)	68	74
1	C	306/316 (97%)	304 (99%)	2 (1%)	76	77
1	D	307/316 (97%)	304 (99%)	3 (1%)	68	74
1	E	307/316 (97%)	305 (99%)	2 (1%)	76	77
2	F	165/190 (87%)	163 (99%)	2 (1%)	63	72
2	G	171/190 (90%)	167 (98%)	4 (2%)	44	63
2	H	190/190 (100%)	188 (99%)	2 (1%)	65	73
2	I	172/190 (90%)	170 (99%)	2 (1%)	63	72
2	J	185/190 (97%)	181 (98%)	4 (2%)	45	63
3	K	169/178 (95%)	168 (99%)	1 (1%)	78	79
3	L	178/178 (100%)	176 (99%)	2 (1%)	65	73
3	M	177/178 (99%)	176 (99%)	1 (1%)	78	79
3	N	130/178 (73%)	129 (99%)	1 (1%)	73	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	162/178 (91%)	161 (99%)	1 (1%)	78	79
All	All	3233/3420 (94%)	3201 (99%)	32 (1%)	68	74

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	118	VAL
3	M	75	LEU
2	F	41	HIS
1	E	292	LEU
3	N	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	180	GLN
3	K	96	ASN
2	I	5	GLN
2	J	5	GLN
3	K	197	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 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	348	-	67,68,68	0.91	2 (2%)	87,102,102	1.73	16 (18%)
5	LMT	B	348	-	27,27,36	1.50	4 (14%)	38,38,47	1.49	7 (18%)
5	LMT	A	350	-	28,28,36	1.48	4 (14%)	39,39,47	1.34	4 (10%)
4	IVM	C	349	-	67,68,68	0.93	2 (2%)	87,102,102	1.76	16 (18%)
5	LMT	A	349	-	27,27,36	1.54	6 (22%)	38,38,47	2.07	13 (34%)
7	OCT	E	350	-	7,7,7	0.13	0	6,6,6	0.49	0
4	IVM	E	348	-	67,68,68	0.91	2 (2%)	87,102,102	1.75	17 (19%)
8	UND	B	350	-	10,10,10	0.44	0	9,9,9	0.42	0
4	IVM	E	349	-	67,68,68	0.92	2 (2%)	87,102,102	1.74	15 (17%)
7	OCT	D	348	-	7,7,7	0.16	0	6,6,6	0.36	0
7	OCT	B	349	-	7,7,7	0.12	0	6,6,6	0.45	0
4	IVM	C	350	-	67,68,68	0.93	2 (2%)	87,102,102	1.76	16 (18%)

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	348	-	-	3/45/141/141	0/7/7/7
5	LMT	B	348	-	-	6/12/52/61	0/2/2/2
5	LMT	A	350	-	-	6/13/53/61	0/2/2/2
4	IVM	C	349	-	-	3/45/141/141	0/7/7/7
5	LMT	A	349	-	-	6/12/52/61	0/2/2/2
7	OCT	E	350	-	-	0/5/5/5	-
4	IVM	E	348	-	-	3/45/141/141	0/7/7/7
8	UND	B	350	-	-	0/8/8/8	-
4	IVM	E	349	-	-	3/45/141/141	0/7/7/7
7	OCT	D	348	-	-	0/5/5/5	-
7	OCT	B	349	-	-	0/5/5/5	-
4	IVM	C	350	-	-	3/45/141/141	0/7/7/7

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	349	IVM	O12-C46	5.03	1.45	1.34
4	E	348	IVM	O12-C46	5.00	1.45	1.34
4	A	348	IVM	O12-C46	4.93	1.45	1.34
4	E	349	IVM	O12-C46	4.92	1.45	1.34
4	C	350	IVM	O12-C46	4.84	1.45	1.34

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	348	IVM	O12-C46-C45	6.65	121.00	110.91
4	E	349	IVM	O12-C46-C45	6.57	120.89	110.91
4	C	350	IVM	O12-C46-C45	6.55	120.86	110.91
4	C	349	IVM	O12-C46-C45	6.53	120.82	110.91
4	A	348	IVM	O12-C46-C45	6.39	120.61	110.91

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	349	LMT	O5'-C1'-O1'-C1
5	A	350	LMT	C2'-C1'-O1'-C1
5	A	350	LMT	O5'-C1'-O1'-C1
5	A	349	LMT	C5'-C4'-O1B-C1B
5	B	348	LMT	C2B-C1B-O1B-C4'

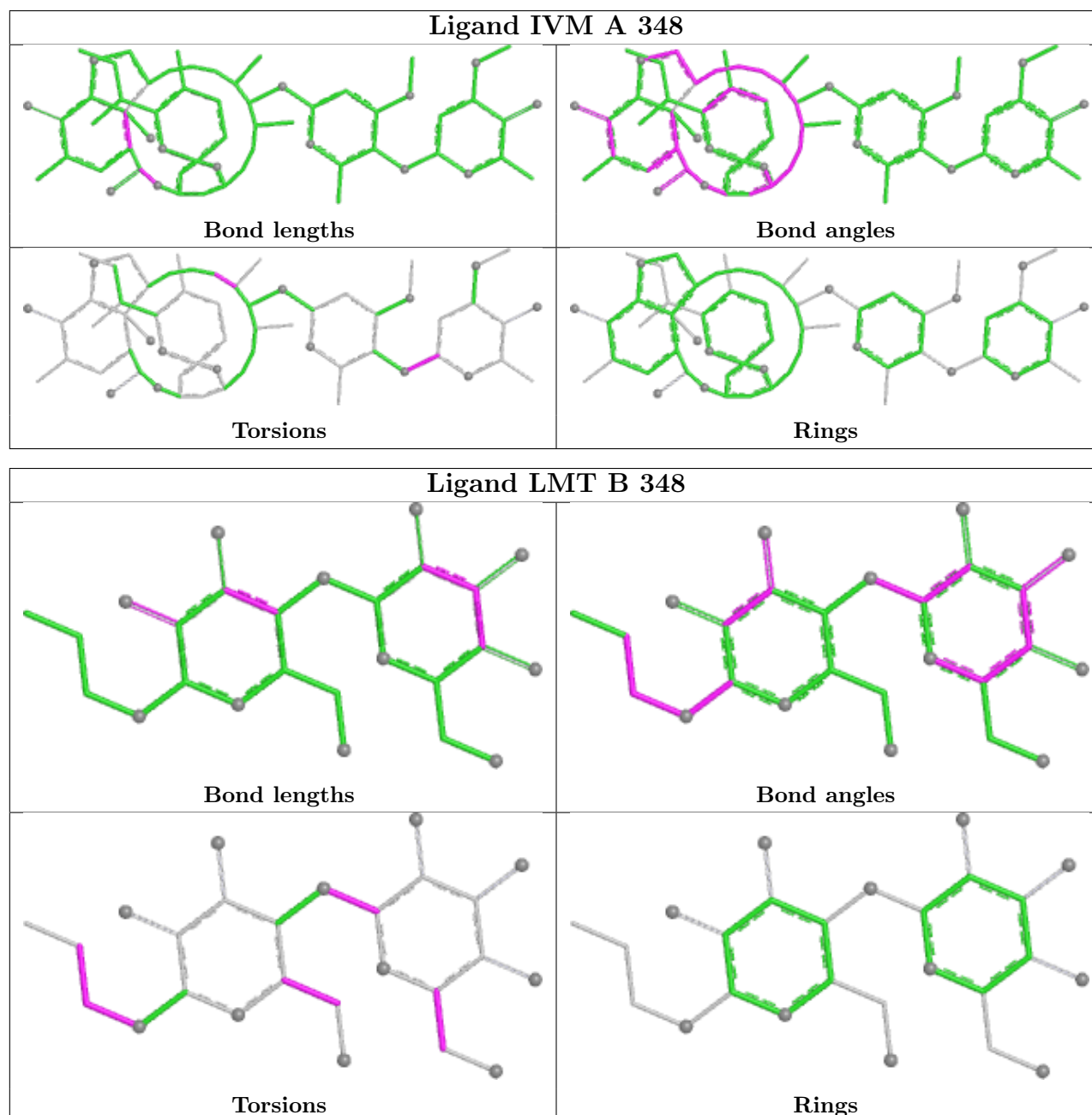
There are no ring outliers.

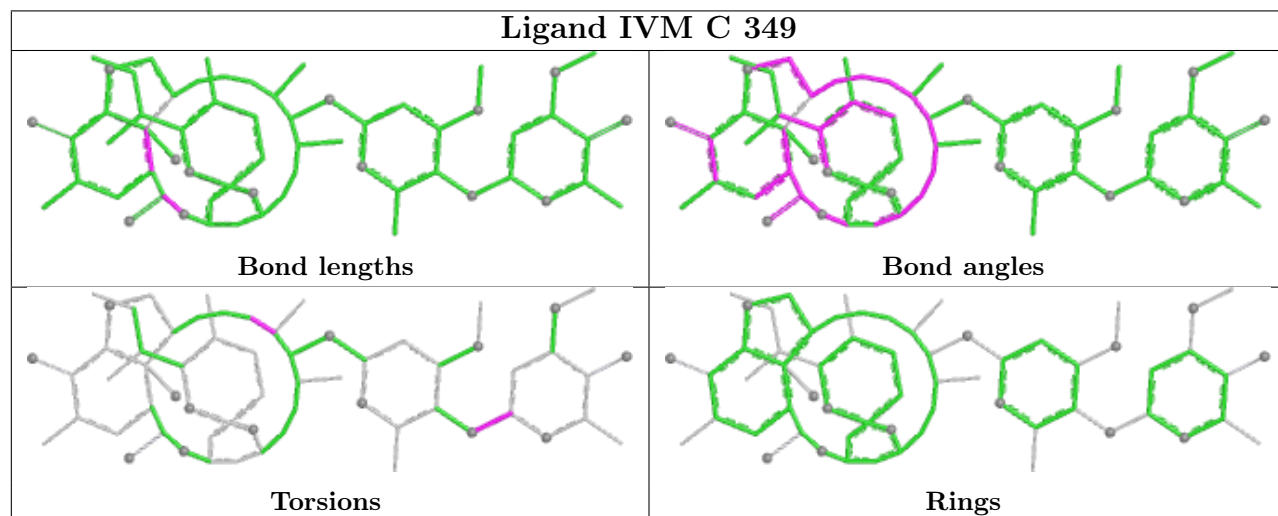
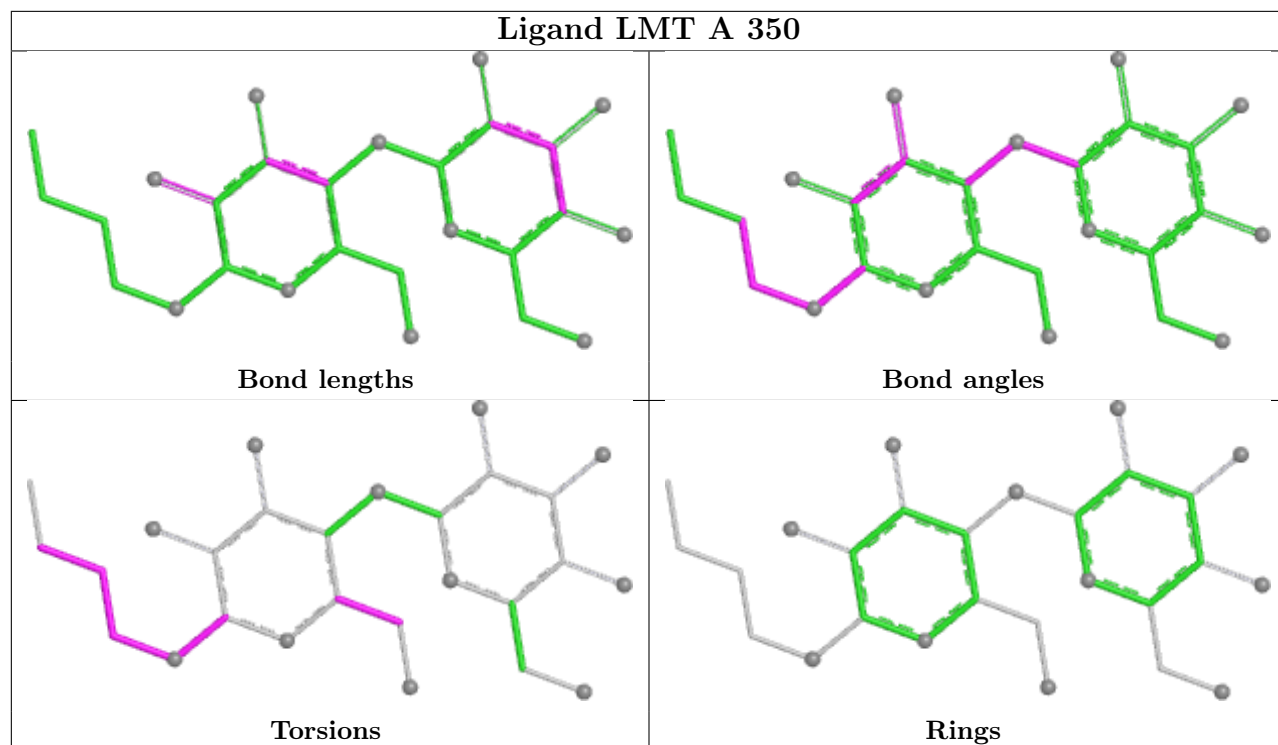
11 monomers are involved in 45 short contacts:

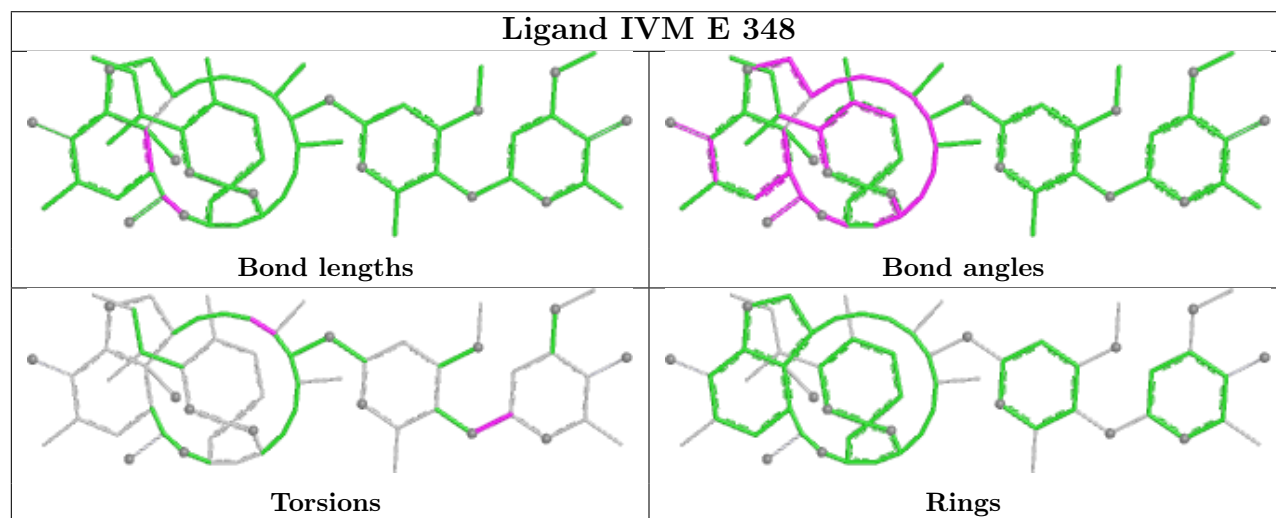
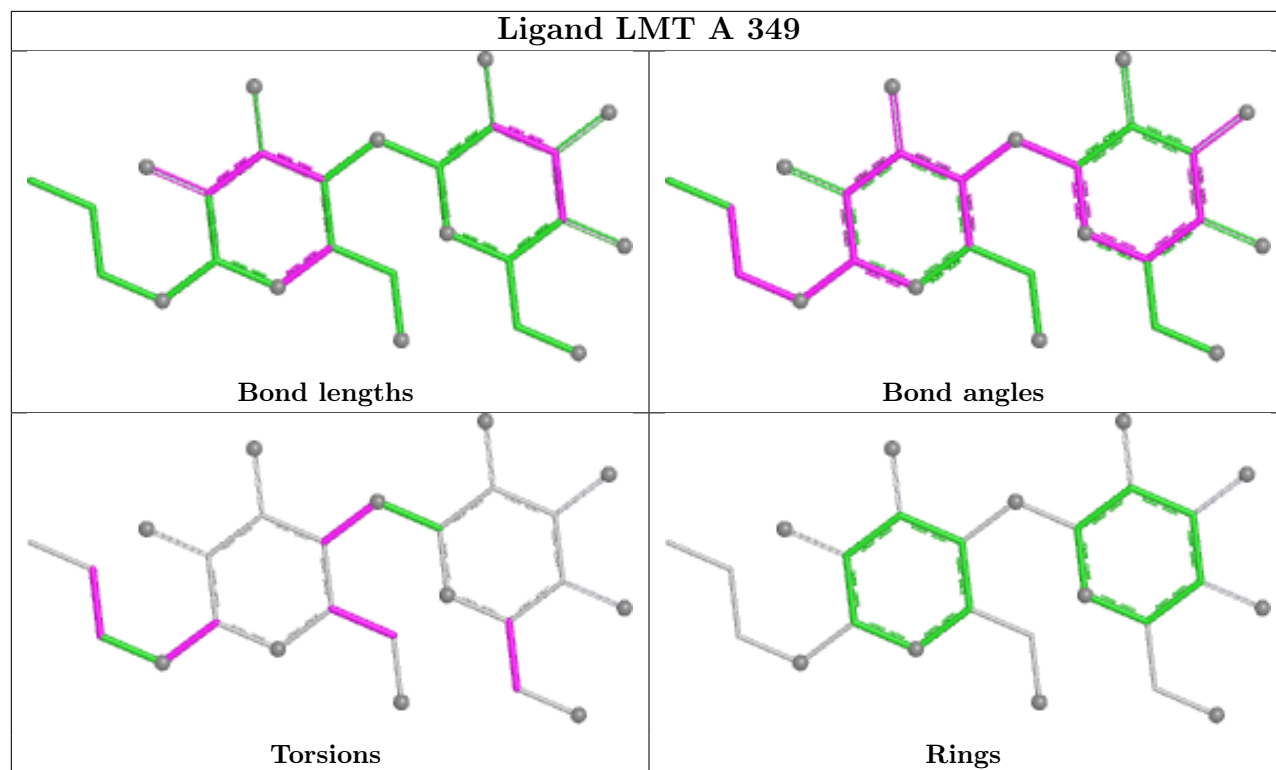
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	348	IVM	1	0
5	B	348	LMT	11	0
5	A	350	LMT	3	0
4	C	349	IVM	5	0
5	A	349	LMT	12	0
7	E	350	OCT	2	0
4	E	348	IVM	3	0
4	E	349	IVM	3	0
7	D	348	OCT	4	0
7	B	349	OCT	2	0
4	C	350	IVM	2	0

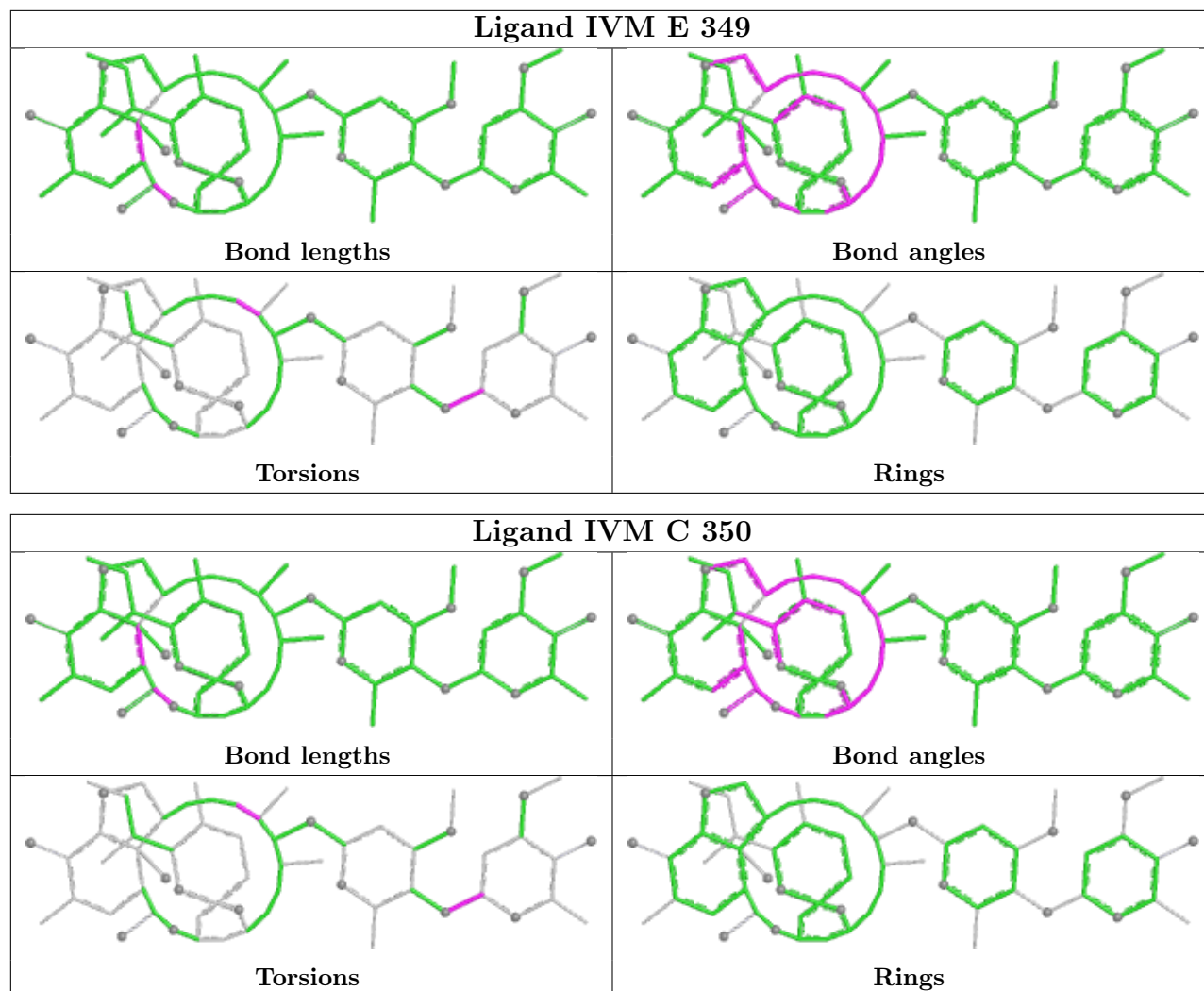
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.









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%)	0.42	13 (3%)	44	31	39, 71, 132, 192	0
1	B	340/347 (97%)	0.51	18 (5%)	32	24	34, 76, 138, 187	0
1	C	339/347 (97%)	0.57	22 (6%)	25	21	35, 77, 161, 223	0
1	D	340/347 (97%)	0.39	17 (5%)	34	25	41, 80, 164, 222	0
1	E	340/347 (97%)	0.40	14 (4%)	41	30	41, 78, 150, 239	0
2	F	191/221 (86%)	0.75	16 (8%)	17	17	63, 134, 212, 231	0
2	G	200/221 (90%)	0.46	16 (8%)	18	17	49, 89, 133, 163	0
2	H	221/221 (100%)	0.43	15 (6%)	23	20	37, 81, 140, 201	0
2	I	199/221 (90%)	1.35	56 (28%)	1	2	69, 132, 300, 344	0
2	J	215/221 (97%)	0.89	34 (15%)	5	8	49, 116, 197, 224	0
3	K	199/210 (94%)	0.60	11 (5%)	30	23	41, 93, 139, 170	0
3	L	210/210 (100%)	0.26	10 (4%)	35	26	28, 77, 126, 199	0
3	M	210/210 (100%)	0.64	10 (4%)	35	26	54, 117, 178, 210	0
3	N	158/210 (75%)	0.63	7 (4%)	39	28	73, 138, 202, 235	0
3	O	195/210 (92%)	1.10	38 (19%)	3	5	67, 141, 282, 346	0
All	All	3697/3890 (95%)	0.59	297 (8%)	18	17	28, 90, 202, 346	0

The worst 5 of 297 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	O	121	PHE	8.6
3	O	135	LEU	6.9
2	I	207	ALA	6.5
2	I	134	ALA	6.4
2	I	192	VAL	6.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

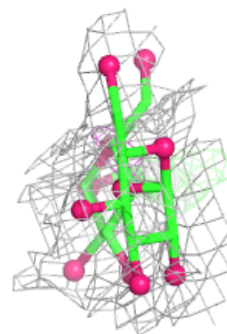
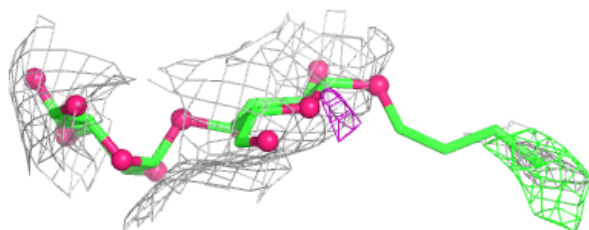
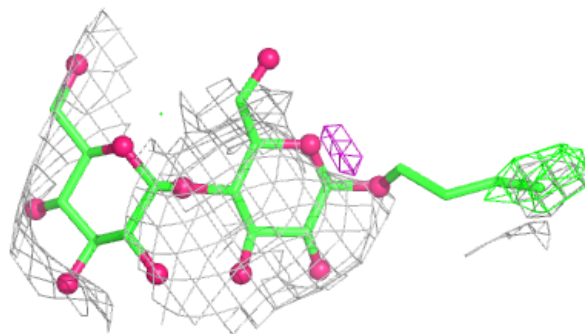
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	IOD	D	349	1/1	0.63	0.27	244,244,244,244	0
8	UND	B	350	11/11	0.67	0.28	80,80,80,80	0
7	OCT	B	349	8/8	0.70	0.28	70,70,70,70	0
5	LMT	A	350	27/35	0.71	0.20	145,145,145,145	0
5	LMT	B	348	26/35	0.73	0.19	153,153,153,153	0
7	OCT	E	350	8/8	0.77	0.34	83,83,83,83	0
5	LMT	A	349	26/35	0.85	0.14	116,116,116,116	0
7	OCT	D	348	8/8	0.85	0.24	66,66,66,66	0
9	CL	C	348	1/1	0.85	0.09	63,63,63,63	0
4	IVM	C	349	62/62	0.88	0.17	69,73,85,86	0
4	IVM	C	350	62/62	0.89	0.18	76,79,84,86	0
4	IVM	E	349	62/62	0.90	0.17	67,73,79,80	0
6	IOD	B	351	1/1	0.91	0.15	177,177,177,177	0
6	IOD	E	351	1/1	0.92	0.09	169,169,169,169	0
4	IVM	A	348	62/62	0.93	0.16	67,75,95,96	0
4	IVM	E	348	62/62	0.94	0.15	91,95,101,102	0
6	IOD	A	351	1/1	0.94	0.09	173,173,173,173	0

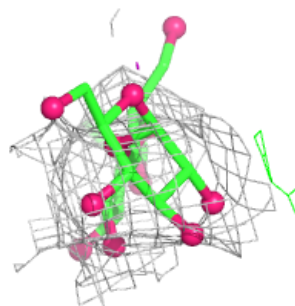
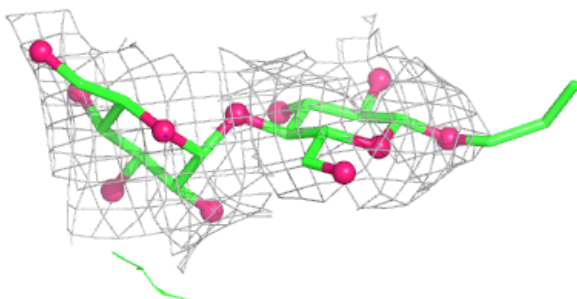
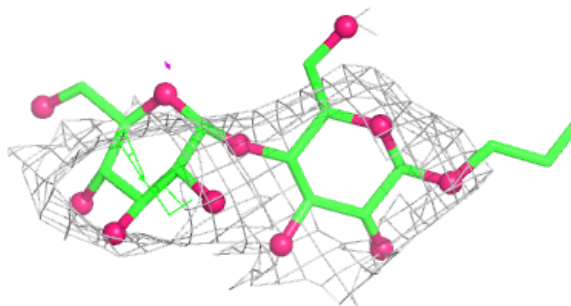
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 350:

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

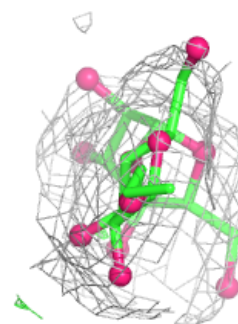
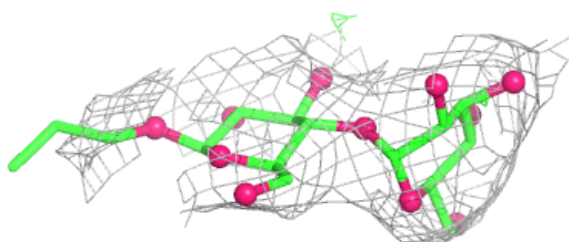
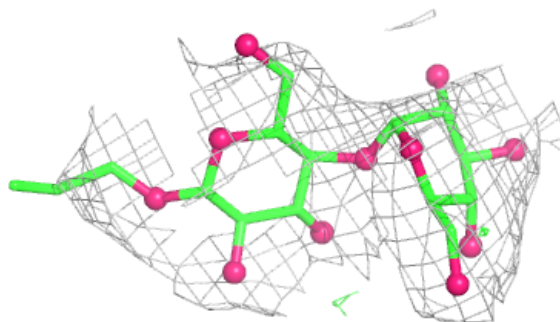
**Electron density around LMT B 348:**

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



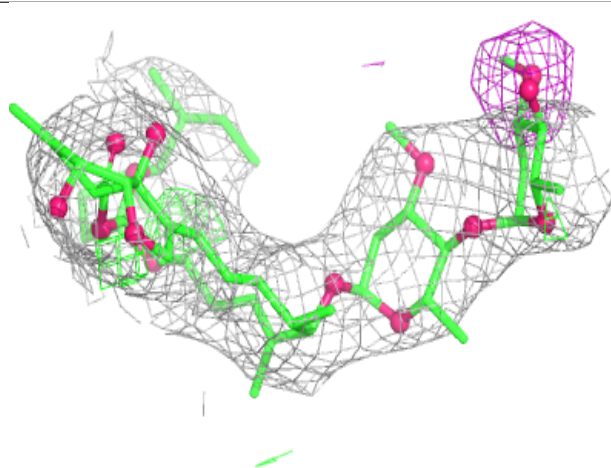
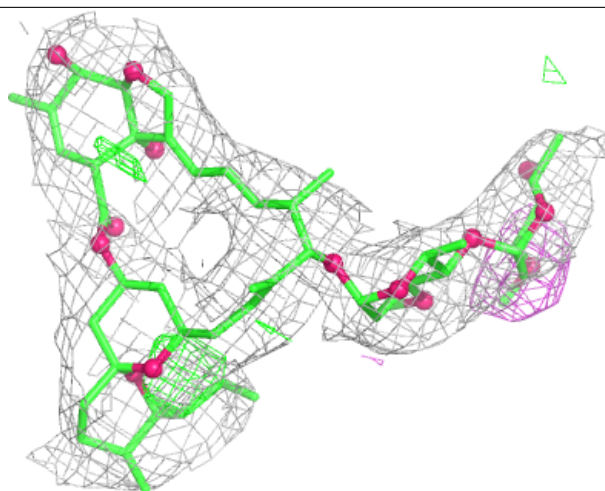
Electron density around LMT A 349:

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



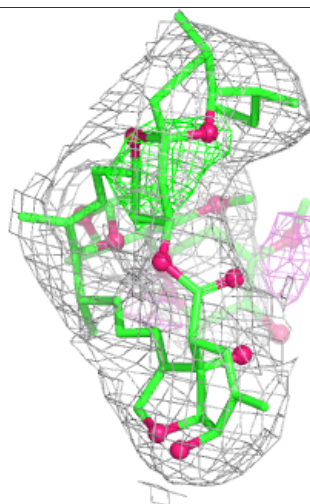
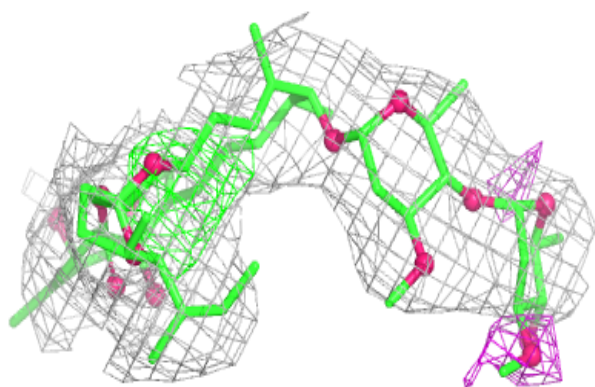
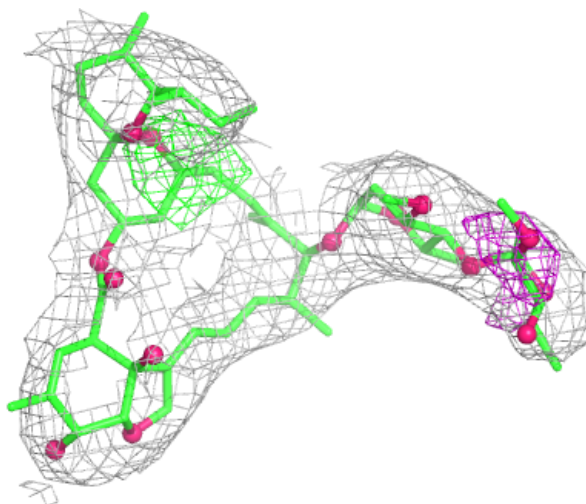
Electron density around IVM C 349:

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



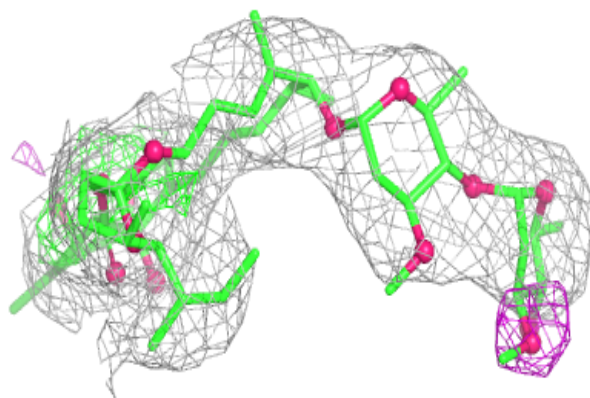
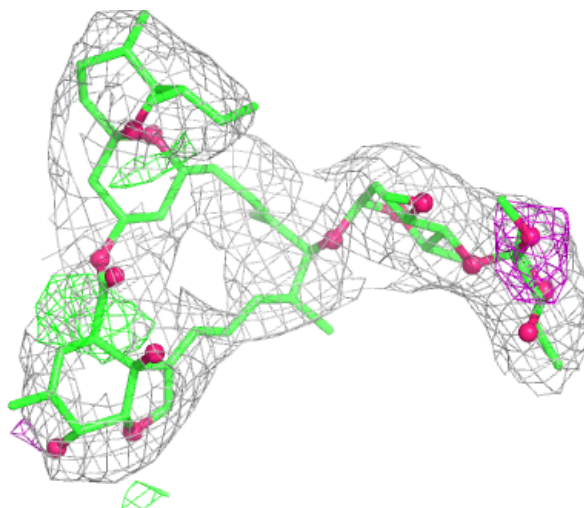
Electron density around IVM C 350:

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



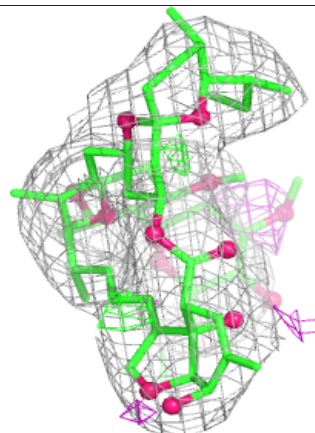
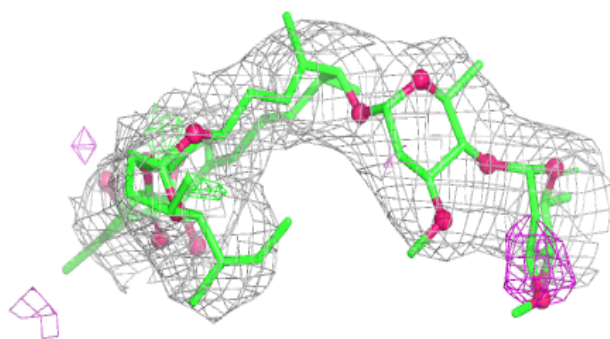
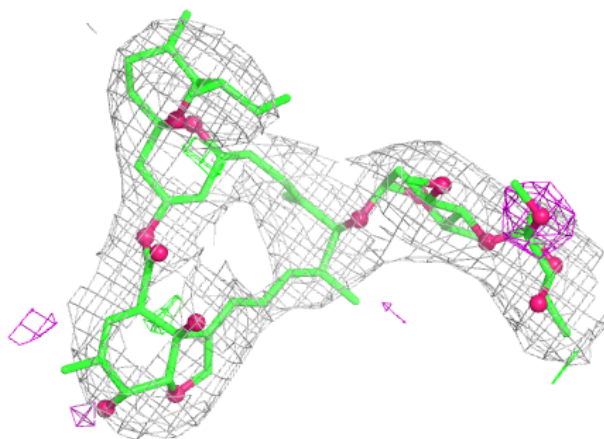
Electron density around IVM E 349:

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



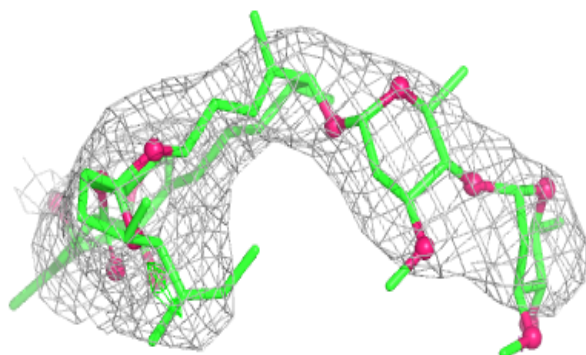
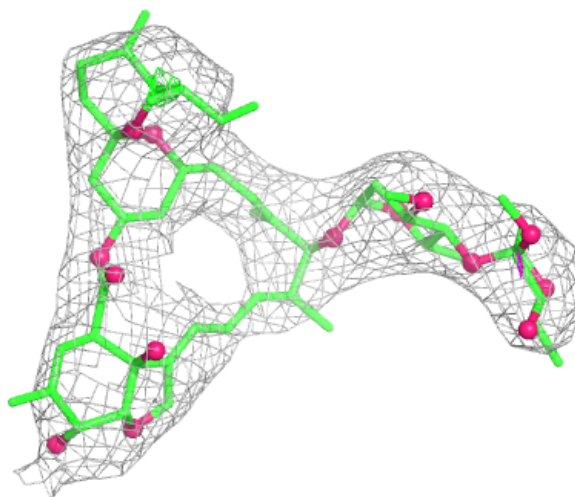
Electron density around IVM A 348:

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



Electron density around IVM E 348:

$2mF_o-DF_c$ (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.