



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:28 AM UTC

PDB ID : 3RIF / pdb_00003rif
Title : C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab, ivermectin and glutamate.
Authors : Hibbs, R.E.; Gouaux, E.
Deposited on : 2011-04-13
Resolution : 3.35 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

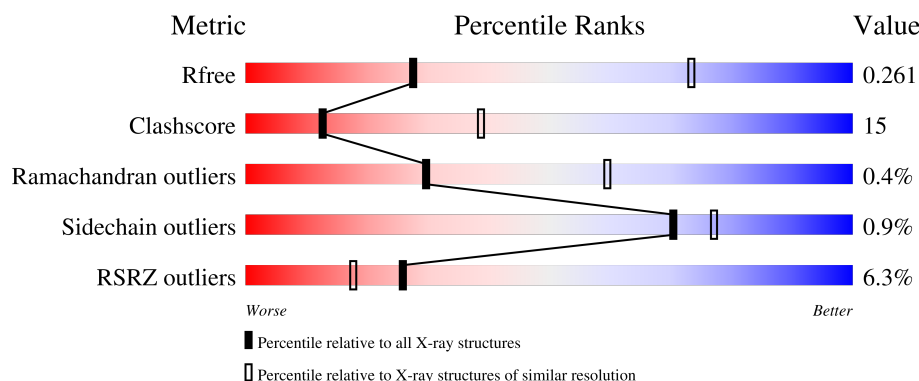
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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 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	6% 67% 31% .
1	B	347	6% 65% 32% ..
1	C	347	5% 65% 33% .
1	D	347	6% 65% 32% ..
1	E	347	4% 66% 32% .

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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	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 29020 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
			2720	1771	442	492	15			
1	B	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	C	339	Total	C	N	O	S	0	0	0
			2710	1765	439	491	15			
1	D	340	Total	C	N	O	S	0	0	0
			2720	1771	442	492	15			
1	E	340	Total	C	N	O	S	0	0	0
			2720	1771	442	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	171	Total	C	N	O	S	0	0	0
			1324	846	213	259	6			

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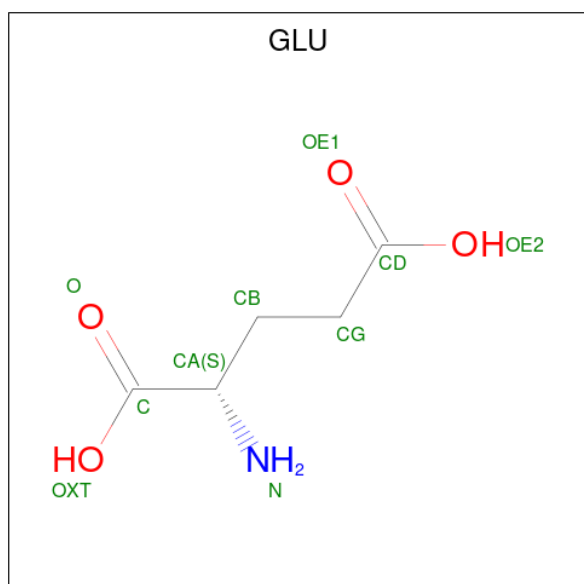
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	214	Total	C	N	O	S	0	0	0
			1631	1038	263	323	7			
2	H	221	Total	C	N	O	S	0	0	0
			1675	1061	271	335	8			
2	I	192	Total	C	N	O	S	0	0	0
			1466	932	238	288	8			
2	J	200	Total	C	N	O	S	0	0	0
			1526	971	247	301	7			

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

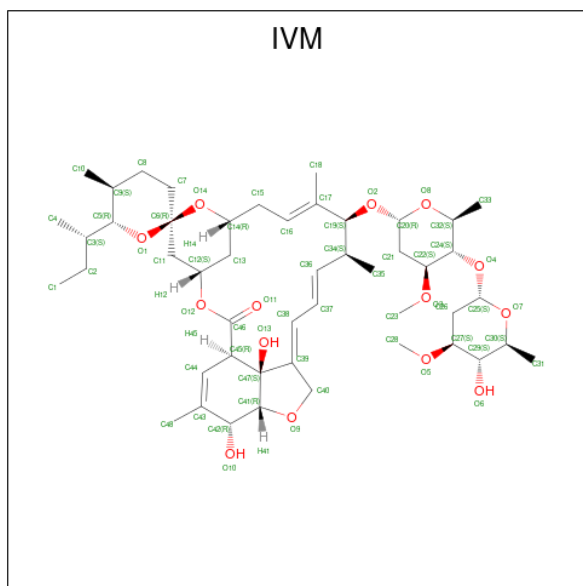
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	210	Total	C	N	O	S	0	0	0
			1579	993	260	320	6			
3	L	210	Total	C	N	O	S	0	0	0
			1591	999	266	320	6			
3	M	210	Total	C	N	O	S	0	0	0
			1576	991	262	317	6			
3	N	148	Total	C	N	O	S	0	0	0
			1075	678	180	214	3			
3	O	195	Total	C	N	O	S	0	0	0
			1470	927	243	294	6			

- Molecule 4 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



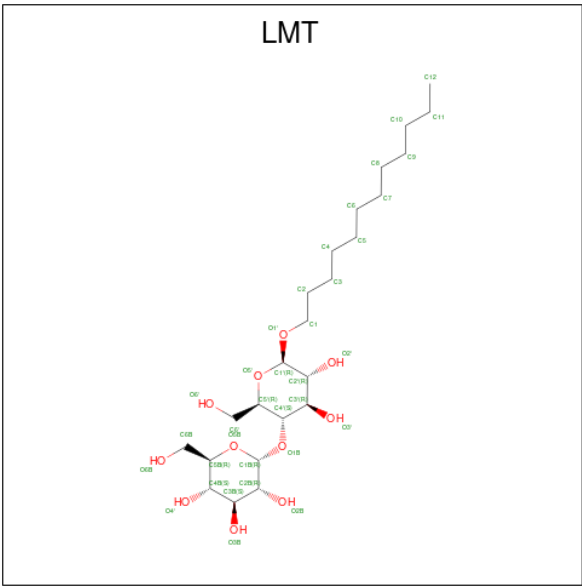
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	5	1	4		
4	B	1	Total	C	N	O	0	0
			10	5	1	4		
4	C	1	Total	C	N	O	0	0
			10	5	1	4		
4	D	1	Total	C	N	O	0	0
			10	5	1	4		
4	E	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 5 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
5	A	1	Total	C	O	0	0
			62	48	14		
5	A	1	Total	C	O	0	0
			62	48	14		
5	B	1	Total	C	O	0	0
			62	48	14		
5	D	1	Total	C	O	0	0
			62	48	14		
5	E	1	Total	C	O	0	0
			62	48	14		

- Molecule 6 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).

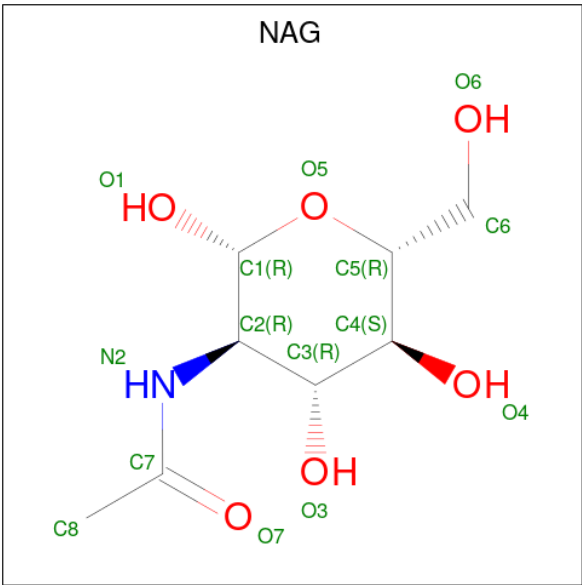


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			26	15	11		
6	A	1	Total	C	O	0	0
			27	16	11		
6	B	1	Total	C	O	0	0
			26	15	11		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

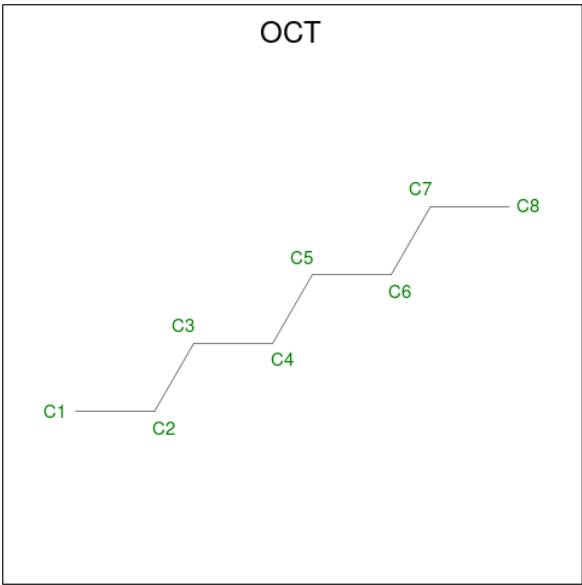
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 9 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



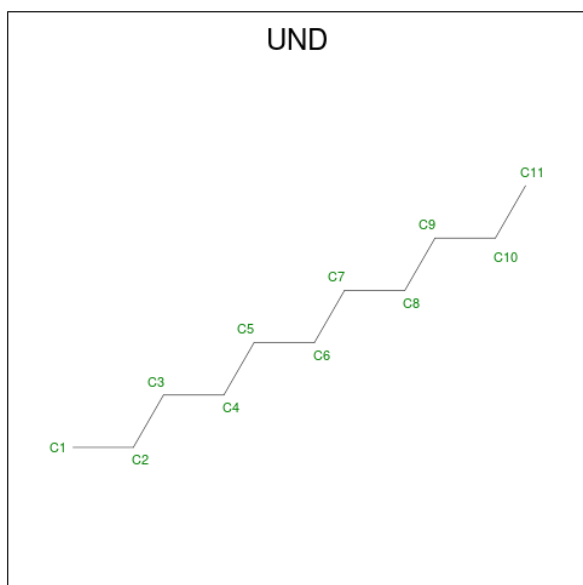
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			8	8		

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

- Molecule 10 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄).

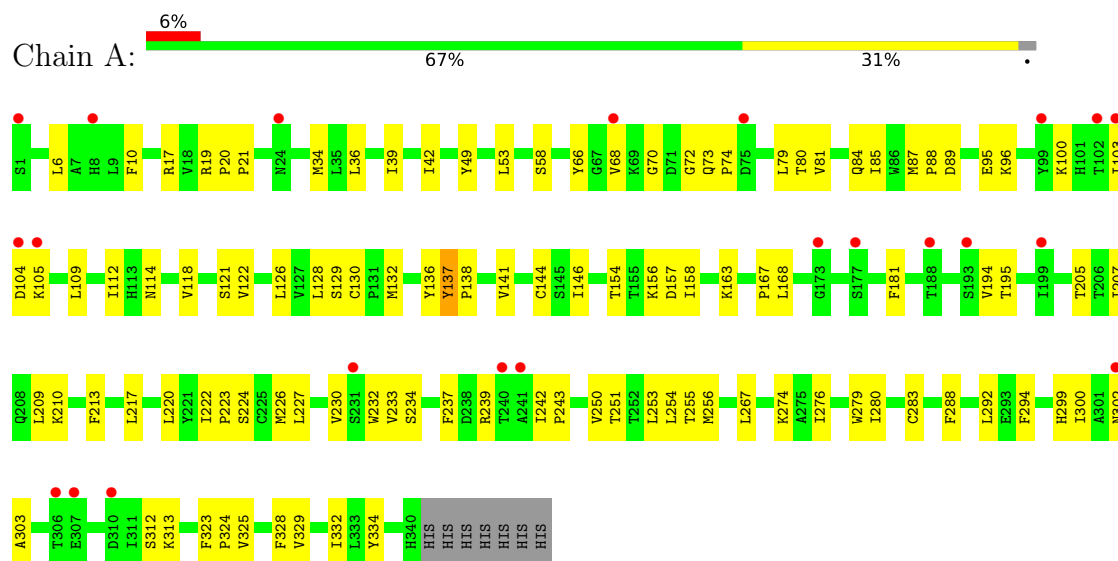


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C 11 11	0	0

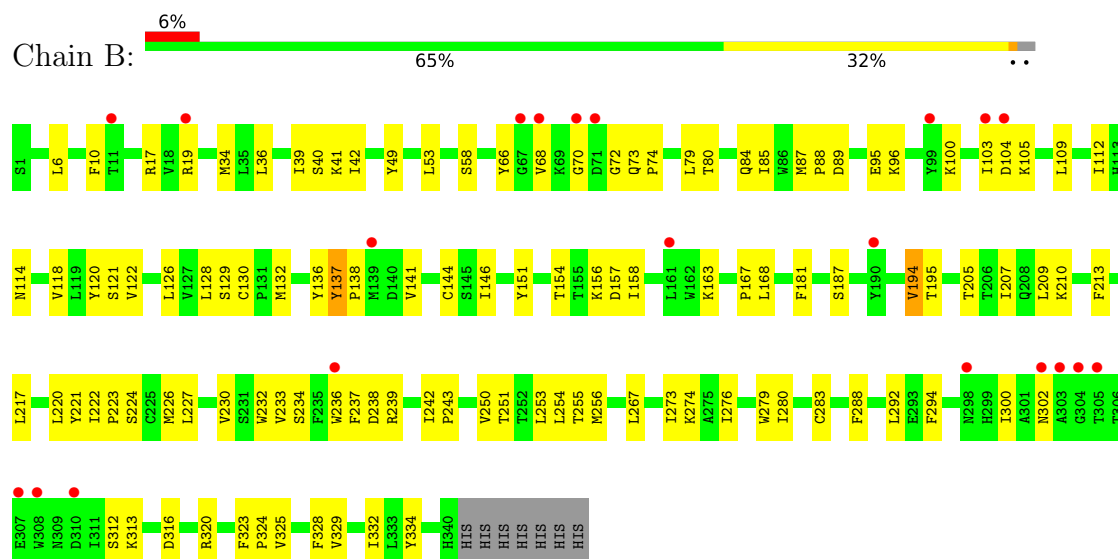
3 Residue-property plots

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.

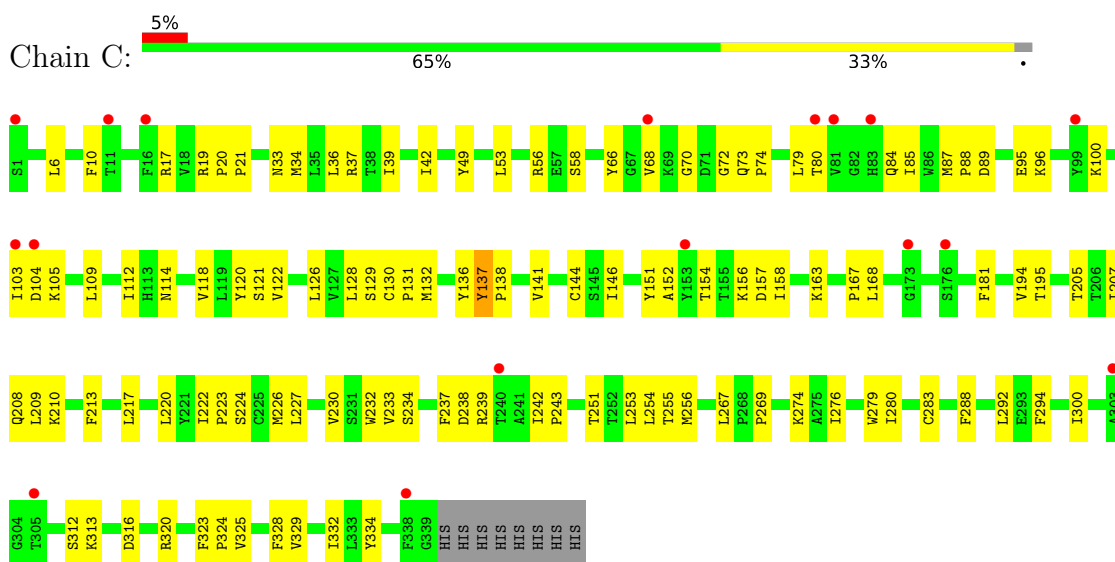
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



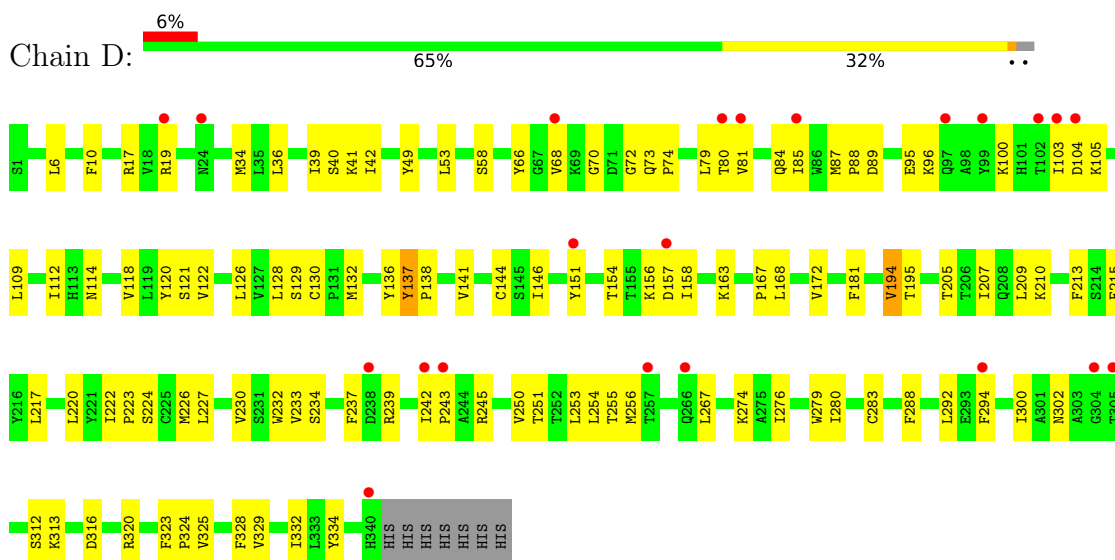
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



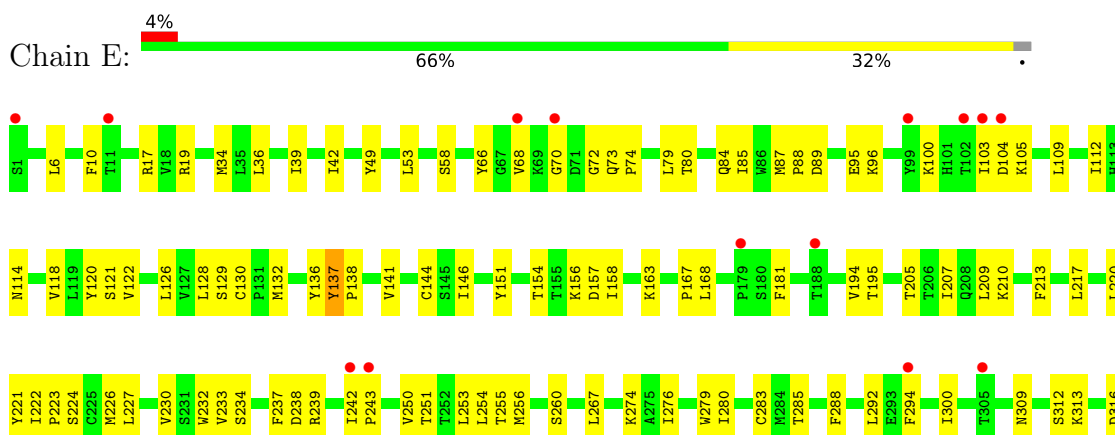
- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha



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

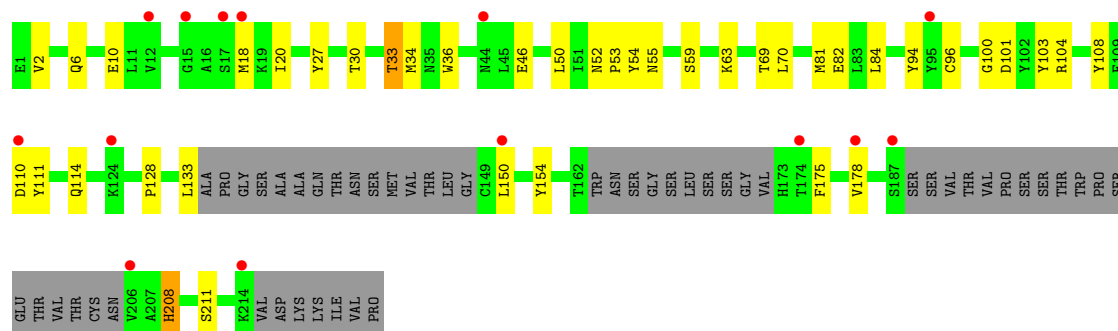


- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

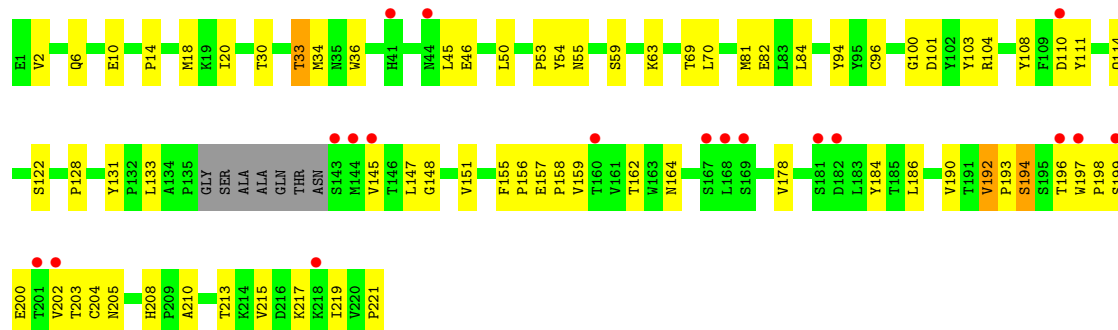




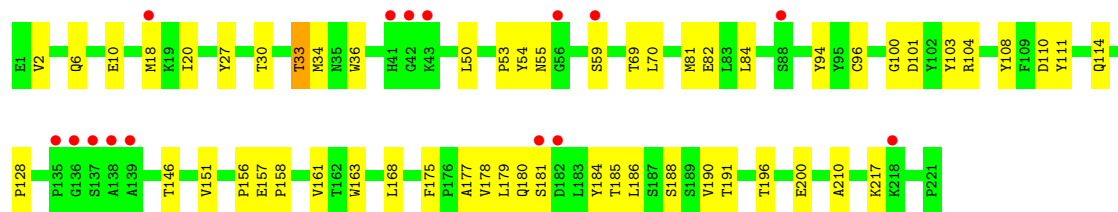
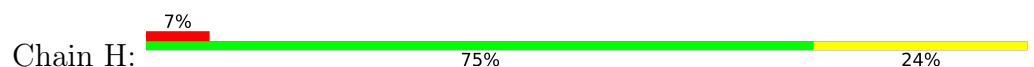
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain



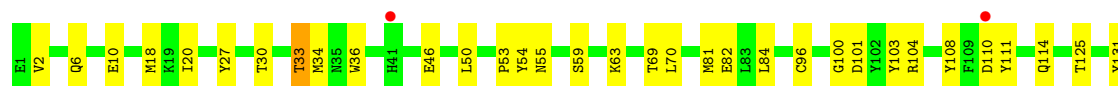
- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

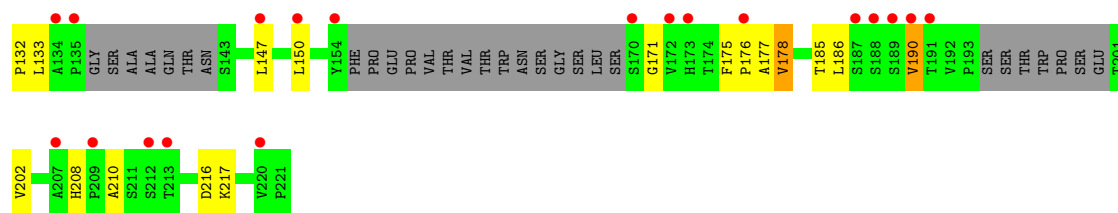


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

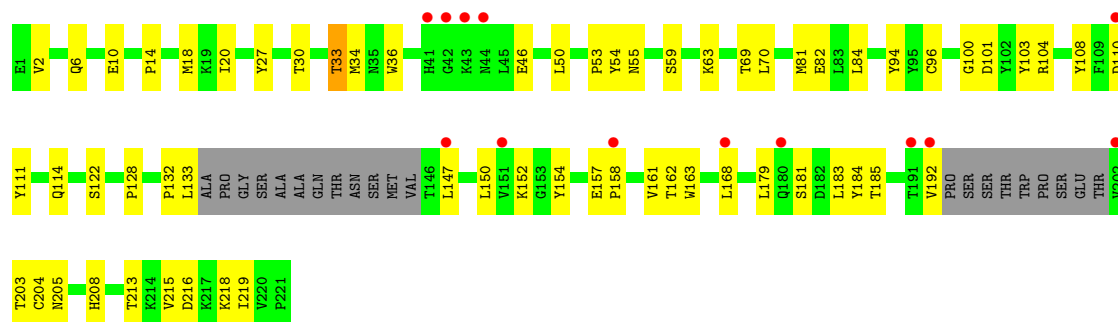


- Molecule 2: Mouse monoclonal Fab fragment, heavy chain

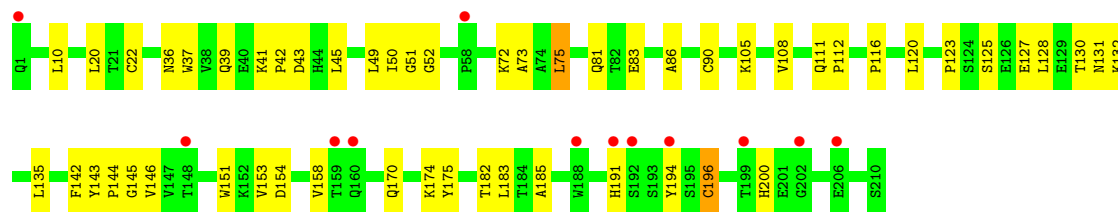
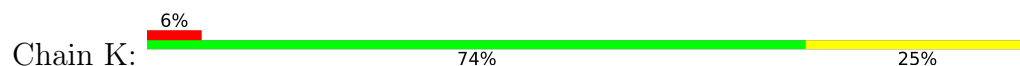




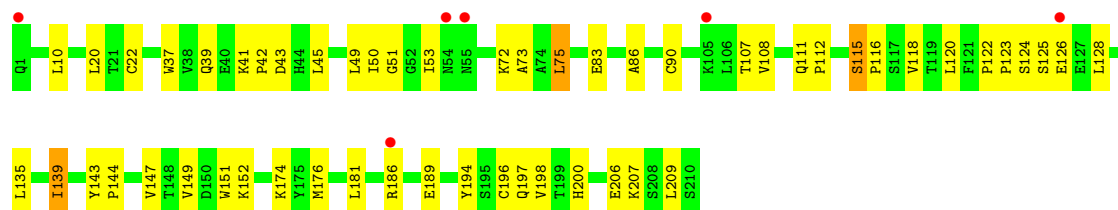
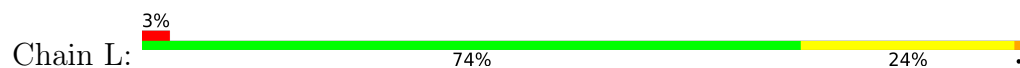
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain



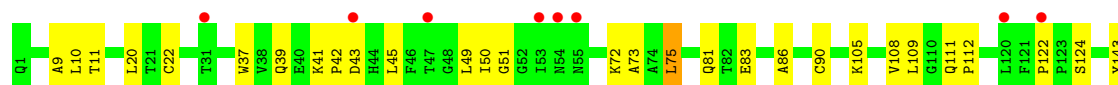
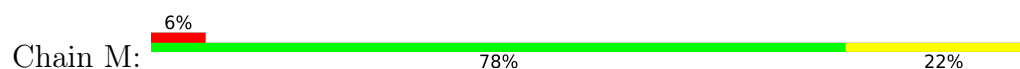
• Molecule 3: Mouse monoclonal Fab fragment, light chain

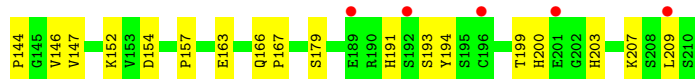


• Molecule 3: Mouse monoclonal Fab fragment, light chain



• Molecule 3: Mouse monoclonal Fab fragment, light chain

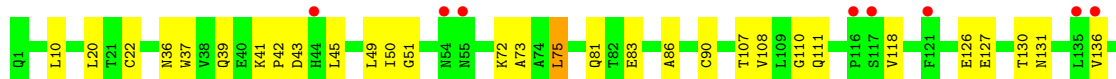




- Molecule 3: Mouse monoclonal Fab fragment, light chain



- 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	155.44Å 155.44Å 575.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.35 39.73 – 3.35	Depositor EDS
% Data completeness (in resolution range)	93.0 (39.73-3.35) 99.3 (39.73-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.248 , 0.271 0.242 , 0.261	Depositor DCC
R_{free} test set	5138 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.6	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	0.88	EDS
Total number of atoms	29020	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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: UND, LMT, CL, IVM, OCT, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/2793	0.67	0/3813
1	B	0.31	0/2793	0.66	0/3813
1	C	0.31	0/2782	0.67	0/3798
1	D	0.31	0/2793	0.67	0/3813
1	E	0.31	0/2793	0.67	0/3813
2	F	0.30	0/1359	0.70	2/1849 (0.1%)
2	G	0.32	0/1676	0.72	0/2290
2	H	0.30	0/1721	0.70	0/2352
2	I	0.31	0/1501	0.70	2/2040 (0.1%)
2	J	0.28	0/1565	0.70	0/2133
3	K	0.30	0/1617	0.69	0/2212
3	L	0.30	0/1629	0.70	2/2226 (0.1%)
3	M	0.31	0/1614	0.69	0/2210
3	N	0.32	0/1098	0.65	0/1503
3	O	0.31	0/1504	0.66	0/2056
All	All	0.31	0/29238	0.68	6/39921 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	115	SER	CA-C-N	5.09	125.00	119.76
3	L	115	SER	C-N-CA	5.09	125.00	119.76
2	I	208	HIS	CA-C-N	5.03	124.47	119.24
2	I	208	HIS	C-N-CA	5.03	124.47	119.24
2	F	208	HIS	CA-C-N	5.01	124.45	119.24

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	2720	0	2720	110	0
1	B	2720	0	2719	116	0
1	C	2710	0	2712	114	0
1	D	2720	0	2720	109	0
1	E	2720	0	2719	109	0
2	F	1324	0	1265	33	0
2	G	1631	0	1574	62	0
2	H	1675	0	1610	45	0
2	I	1466	0	1428	38	0
2	J	1526	0	1468	44	0
3	K	1579	0	1520	41	0
3	L	1591	0	1542	39	0
3	M	1576	0	1518	34	0
3	N	1075	0	1026	25	0
3	O	1470	0	1412	36	0
4	A	10	0	5	0	0
4	B	10	0	5	2	0
4	C	10	0	5	1	0
4	D	10	0	5	1	0
4	E	10	0	5	1	0
5	A	124	0	148	11	0
5	B	62	0	74	5	0
5	D	62	0	74	3	0
5	E	62	0	74	3	0
6	A	53	0	52	13	0
6	B	26	0	25	7	0
7	B	1	0	0	0	0
8	B	14	0	13	1	0
8	C	14	0	13	1	0
8	E	14	0	13	0	0
9	B	8	0	18	0	0
9	D	8	0	18	0	0
9	E	8	0	18	3	0
10	B	11	0	24	0	0
All	All	29020	0	28542	872	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 15.

The worst 5 of 872 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	6:A:404:LMT:H12	1.75	1.21
1:A:299:HIS:HD2	6:A:404:LMT:H12	1.25	0.97
1:B:100:LYS:HE2	1:C:104:ASP:H	1.27	0.96
1:D:89:ASP:HA	1:E:105:LYS:HG3	1.49	0.95
1:C:100:LYS:HE2	1:D:104:ASP:H	1.31	0.93

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%)	317 (94%)	19 (6%)	2 (1%)	21	51
1	B	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	21	51
1	C	337/347 (97%)	316 (94%)	19 (6%)	2 (1%)	21	51
1	D	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	21	51
1	E	338/347 (97%)	317 (94%)	19 (6%)	2 (1%)	21	51
2	F	163/221 (74%)	150 (92%)	12 (7%)	1 (1%)	21	51
2	G	210/221 (95%)	196 (93%)	13 (6%)	1 (0%)	24	55
2	H	219/221 (99%)	206 (94%)	13 (6%)	0	100	100
2	I	184/221 (83%)	172 (94%)	10 (5%)	2 (1%)	11	40
2	J	194/221 (88%)	180 (93%)	14 (7%)	0	100	100
3	K	208/210 (99%)	189 (91%)	19 (9%)	0	100	100
3	L	208/210 (99%)	195 (94%)	13 (6%)	0	100	100
3	M	208/210 (99%)	194 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	N	140/210 (67%)	128 (91%)	11 (8%)	1 (1%)	18 49
3	O	189/210 (90%)	168 (89%)	20 (11%)	1 (0%)	24 55
All	All	3612/3890 (93%)	3362 (93%)	234 (6%)	16 (0%)	30 59

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	B	137	TYR
1	C	137	TYR
1	D	137	TYR
1	E	137	TYR

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	308/316 (98%)	306 (99%)	2 (1%)	78 81
1	B	308/316 (98%)	306 (99%)	2 (1%)	78 81
1	C	307/316 (97%)	305 (99%)	2 (1%)	76 79
1	D	308/316 (98%)	306 (99%)	2 (1%)	78 81
1	E	308/316 (98%)	306 (99%)	2 (1%)	78 81
2	F	145/190 (76%)	144 (99%)	1 (1%)	76 79
2	G	184/190 (97%)	180 (98%)	4 (2%)	45 65
2	H	188/190 (99%)	186 (99%)	2 (1%)	65 75
2	I	164/190 (86%)	163 (99%)	1 (1%)	78 81
2	J	170/190 (90%)	168 (99%)	2 (1%)	63 74
3	K	176/178 (99%)	174 (99%)	2 (1%)	65 75
3	L	178/178 (100%)	173 (97%)	5 (3%)	38 62
3	M	175/178 (98%)	174 (99%)	1 (1%)	78 81
3	N	115/178 (65%)	114 (99%)	1 (1%)	70 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	162/178 (91%)	161 (99%)	1 (1%)	78	81
All	All	3196/3420 (94%)	3166 (99%)	30 (1%)	70	77

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	194	SER
3	M	75	LEU
2	I	33	THR
3	O	75	LEU
3	L	139	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	5	GLN
2	H	5	GLN
3	O	111	GLN
2	F	62	GLN
2	G	5	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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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
8	NAG	B	400	1	14,14,15	0.60	0	17,19,21	0.86	1 (5%)
5	IVM	A	402	-	67,68,68	0.88	2 (2%)	87,102,102	1.71	16 (18%)
5	IVM	A	403	-	67,68,68	0.88	2 (2%)	87,102,102	1.69	15 (17%)
4	GLU	B	401	-	8,9,9	1.12	1 (12%)	8,11,11	1.28	1 (12%)
9	OCT	B	405	-	7,7,7	0.25	0	6,6,6	0.43	0
10	UND	B	406	-	10,10,10	0.26	0	9,9,9	0.47	0
5	IVM	E	402	-	67,68,68	0.90	2 (2%)	87,102,102	1.70	15 (17%)
6	LMT	A	404	-	27,27,36	1.44	4 (14%)	38,38,47	1.81	11 (28%)
6	LMT	A	405	-	28,28,36	1.40	4 (14%)	39,39,47	1.41	5 (12%)
4	GLU	C	401	-	8,9,9	1.11	1 (12%)	8,11,11	1.22	1 (12%)
4	GLU	E	401	-	8,9,9	1.10	1 (12%)	8,11,11	1.24	1 (12%)
6	LMT	B	404	-	27,27,36	1.42	3 (11%)	38,38,47	1.51	8 (21%)
5	IVM	B	403	-	67,68,68	0.89	2 (2%)	87,102,102	1.68	15 (17%)
8	NAG	E	400	1	14,14,15	0.46	0	17,19,21	1.24	3 (17%)
8	NAG	C	400	1	14,14,15	0.49	0	17,19,21	1.69	2 (11%)
9	OCT	D	403	-	7,7,7	0.25	0	6,6,6	0.43	0
4	GLU	A	401	-	8,9,9	1.06	1 (12%)	8,11,11	1.28	1 (12%)
4	GLU	D	401	-	8,9,9	1.08	1 (12%)	8,11,11	1.26	1 (12%)
5	IVM	D	402	-	67,68,68	0.88	2 (2%)	87,102,102	1.69	15 (17%)
9	OCT	E	403	-	7,7,7	0.25	0	6,6,6	0.48	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
8	NAG	B	400	1	-	0/6/23/26	0/1/1/1
5	IVM	A	402	-	-	7/45/141/141	0/7/7/7
5	IVM	A	403	-	-	7/45/141/141	0/7/7/7
4	GLU	B	401	-	-	2/9/9/9	-
9	OCT	B	405	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	UND	B	406	-	-	0/8/8/8	-
5	IVM	E	402	-	-	7/45/141/141	0/7/7/7
6	LMT	A	404	-	-	9/12/52/61	0/2/2/2
6	LMT	A	405	-	-	4/13/53/61	0/2/2/2
4	GLU	C	401	-	-	5/9/9/9	-
4	GLU	E	401	-	-	3/9/9/9	-
6	LMT	B	404	-	-	5/12/52/61	0/2/2/2
5	IVM	B	403	-	-	7/45/141/141	0/7/7/7
8	NAG	E	400	1	-	4/6/23/26	0/1/1/1
8	NAG	C	400	1	-	0/6/23/26	0/1/1/1
9	OCT	D	403	-	-	0/5/5/5	-
4	GLU	A	401	-	-	3/9/9/9	-
4	GLU	D	401	-	-	2/9/9/9	-
5	IVM	D	402	-	-	7/45/141/141	0/7/7/7
9	OCT	E	403	-	-	0/5/5/5	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	402	IVM	O12-C46	4.94	1.45	1.34
5	B	403	IVM	O12-C46	4.93	1.45	1.34
5	A	402	IVM	O12-C46	4.92	1.45	1.34
5	A	403	IVM	O12-C46	4.91	1.45	1.34
5	D	402	IVM	O12-C46	4.87	1.45	1.34

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	403	IVM	O12-C46-C45	6.52	120.81	110.91
5	E	402	IVM	O12-C46-C45	6.48	120.75	110.91
5	A	402	IVM	O12-C46-C45	6.41	120.64	110.91
5	B	403	IVM	O12-C46-C45	6.36	120.56	110.91
5	D	402	IVM	O12-C46-C45	6.35	120.56	110.91

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	401	GLU	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
6	A	405	LMT	O5'-C1'-O1'-C1
8	E	400	NAG	C1-C2-N2-C7
8	E	400	NAG	C8-C7-N2-C2
8	E	400	NAG	O7-C7-N2-C2

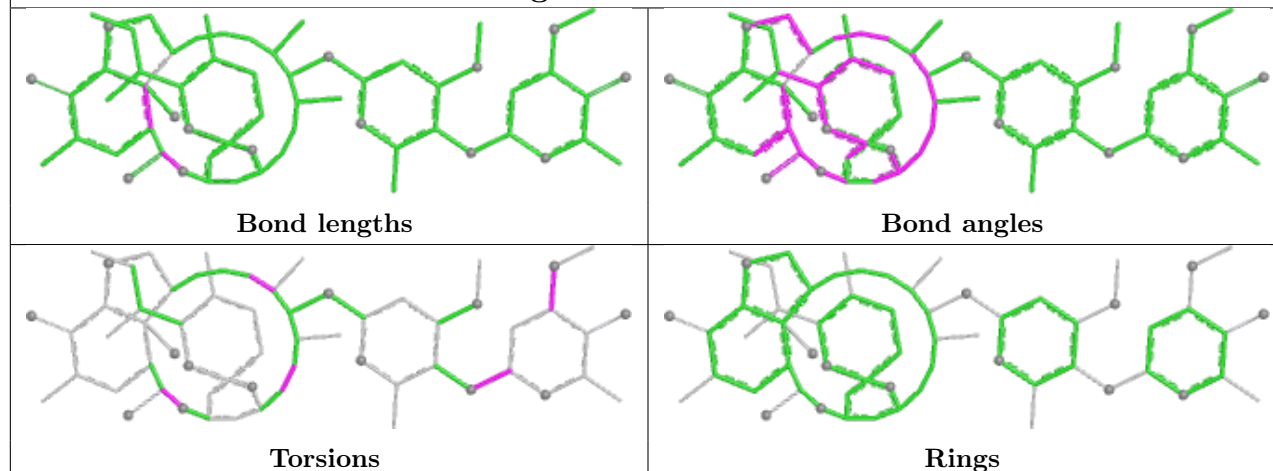
There are no ring outliers.

15 monomers are involved in 46 short contacts:

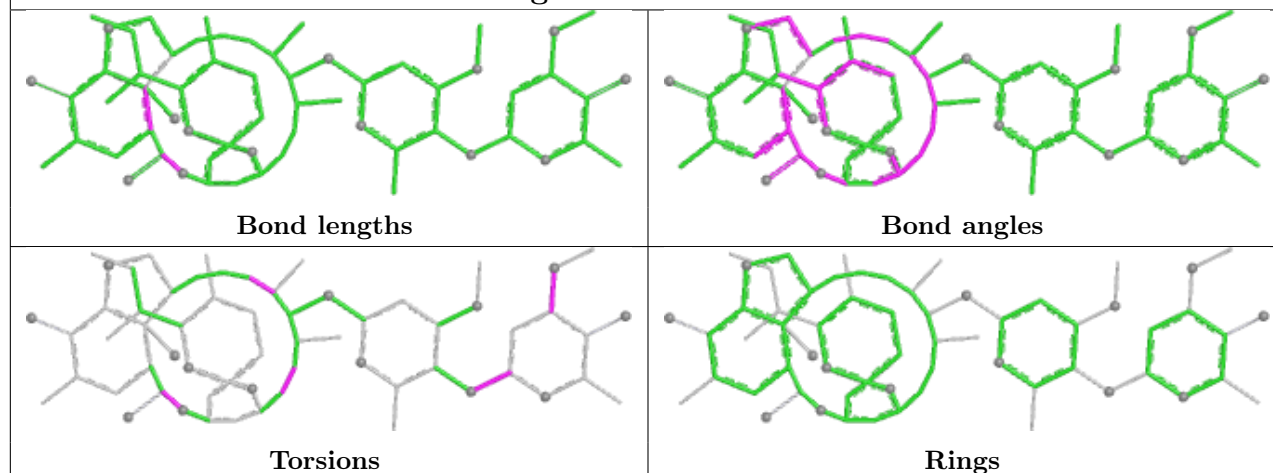
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	400	NAG	1	0
5	A	402	IVM	4	0
5	A	403	IVM	7	0
4	B	401	GLU	2	0
5	E	402	IVM	3	0
6	A	404	LMT	10	0
6	A	405	LMT	3	0
4	C	401	GLU	1	0
4	E	401	GLU	1	0
6	B	404	LMT	7	0
5	B	403	IVM	5	0
8	C	400	NAG	1	0
4	D	401	GLU	1	0
5	D	402	IVM	3	0
9	E	403	OCT	3	0

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.

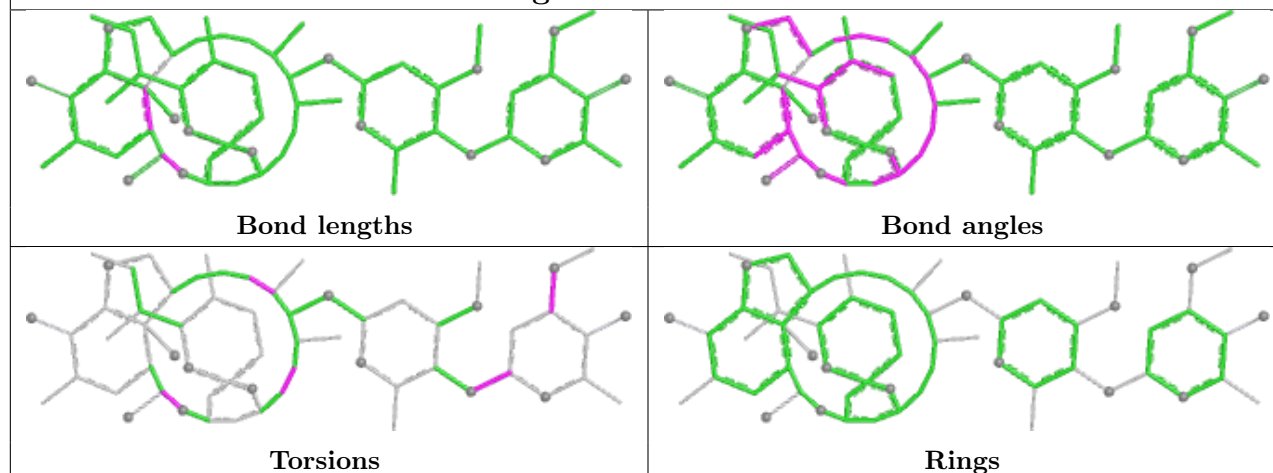
Ligand IVM A 402

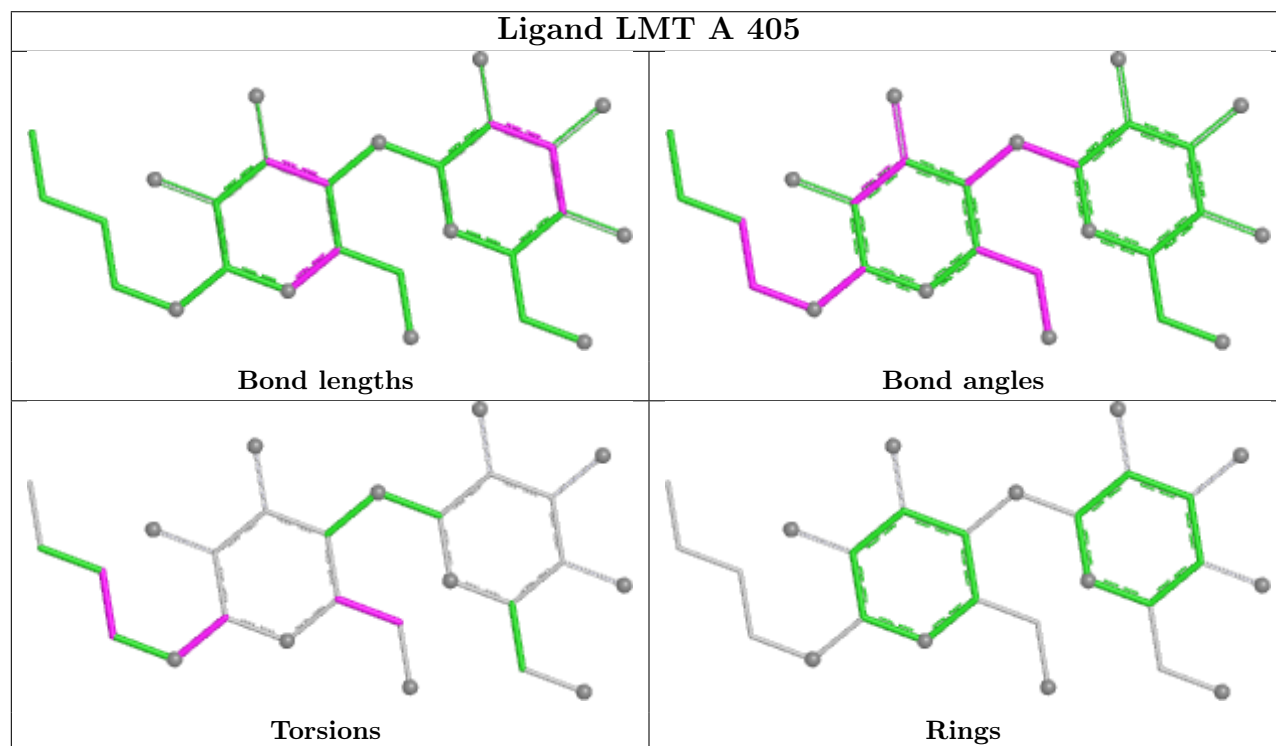
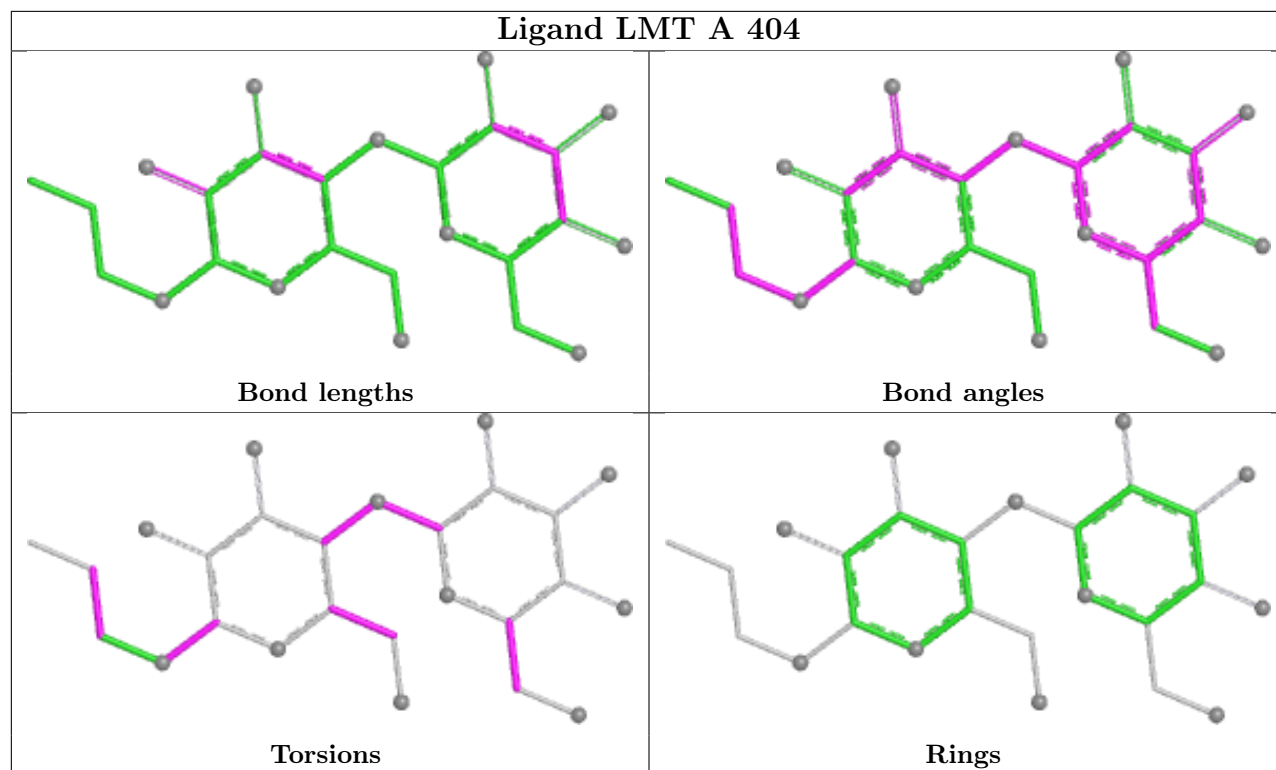


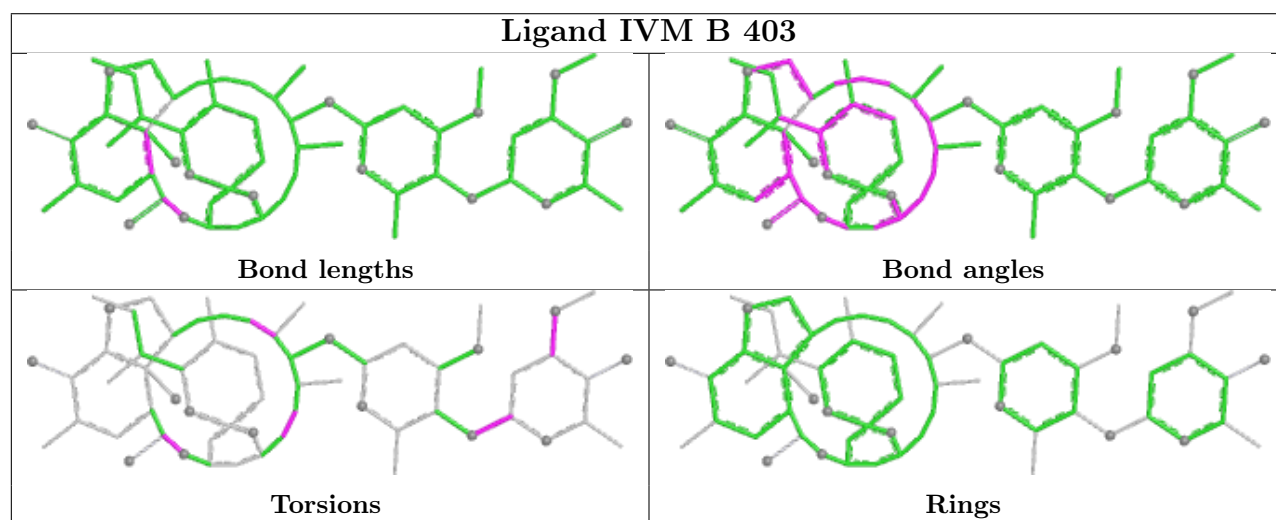
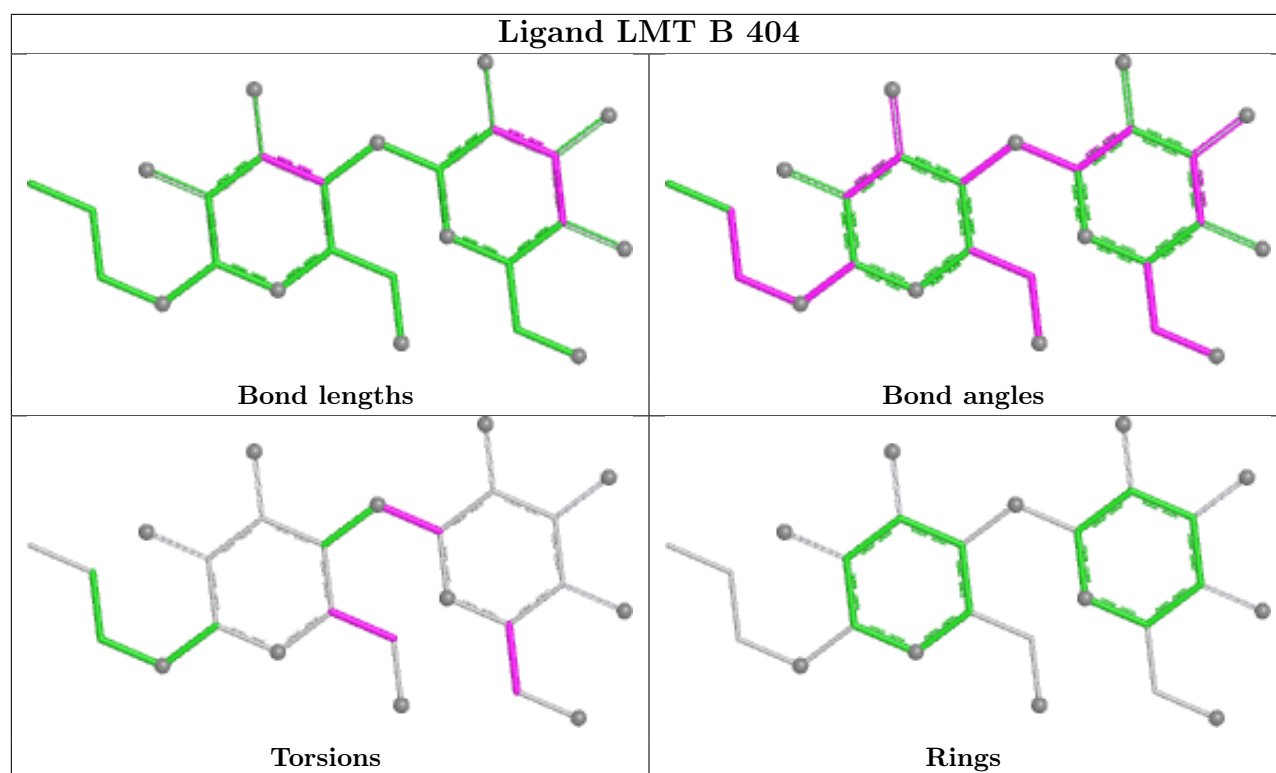
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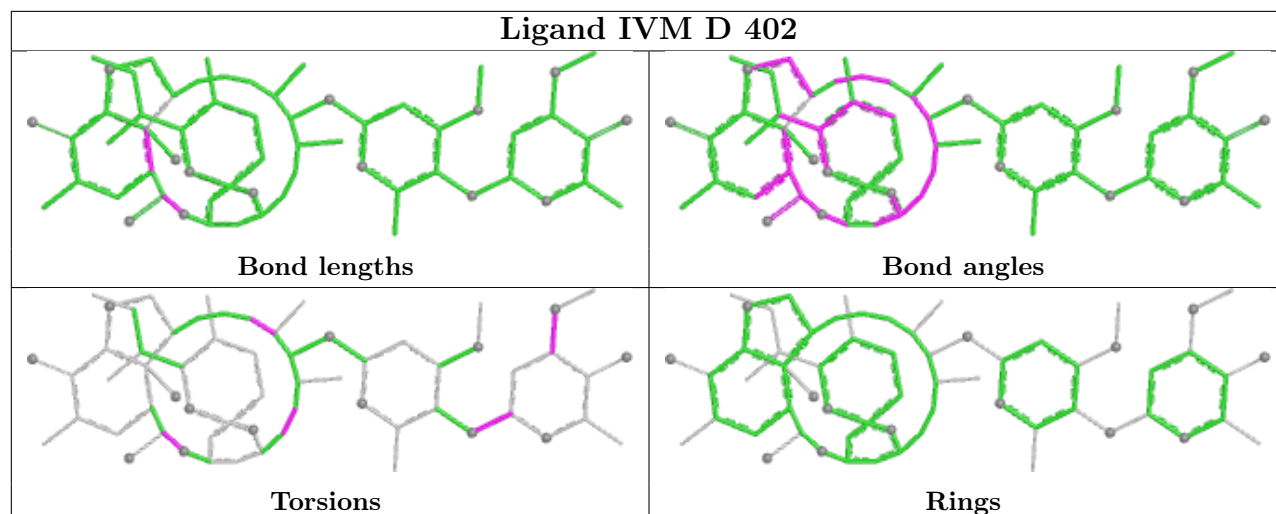


Ligand IVM E 402









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 ⓘ

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%)	0.38	22 (6%)	25	17	32, 66, 123, 196	0
1	B	340/347 (97%)	0.43	21 (6%)	26	18	38, 68, 125, 199	0
1	C	339/347 (97%)	0.33	17 (5%)	34	23	41, 71, 153, 279	0
1	D	340/347 (97%)	0.41	22 (6%)	25	17	39, 72, 159, 243	0
1	E	340/347 (97%)	0.34	15 (4%)	39	26	36, 69, 142, 210	0
2	F	171/221 (77%)	0.66	14 (8%)	17	14	58, 106, 163, 192	0
2	G	214/221 (96%)	0.44	18 (8%)	17	13	40, 89, 142, 182	0
2	H	221/221 (100%)	0.47	15 (6%)	23	16	42, 76, 131, 201	0
2	I	192/221 (86%)	0.81	21 (10%)	10	10	57, 110, 171, 201	0
2	J	200/221 (90%)	0.51	13 (6%)	25	17	49, 90, 158, 182	0
3	K	210/210 (100%)	0.49	12 (5%)	29	20	50, 95, 139, 209	0
3	L	210/210 (100%)	0.20	6 (2%)	53	36	38, 73, 114, 159	0
3	M	210/210 (100%)	0.42	13 (6%)	26	18	49, 93, 143, 165	0
3	N	148/210 (70%)	0.69	7 (4%)	36	25	58, 119, 178, 202	0
3	O	195/210 (92%)	0.73	17 (8%)	16	13	63, 113, 167, 190	0
All	All	3670/3890 (94%)	0.46	233 (6%)	26	18	32, 82, 155, 279	0

The worst 5 of 233 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	242	ILE	7.1
2	I	188	SER	5.5
1	B	68	VAL	5.0
3	O	208	SER	5.0
3	O	195	SER	5.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

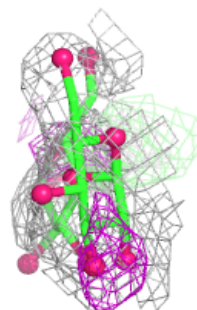
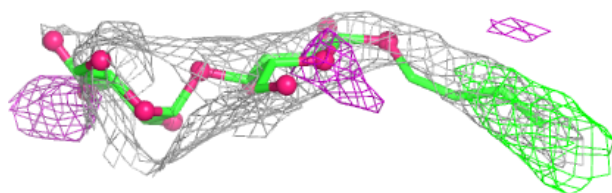
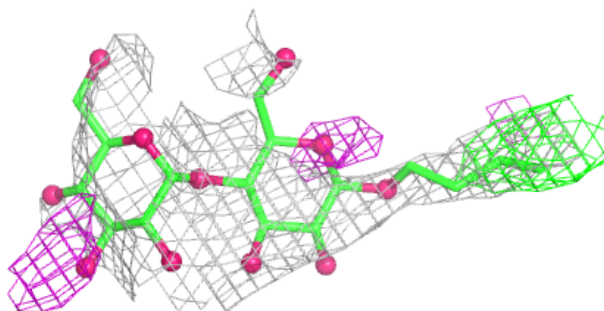
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
10	UND	B	406	11/11	0.60	0.25	60,60,60,60	0
6	LMT	A	405	27/35	0.63	0.22	143,143,143,143	0
9	OCT	E	403	8/8	0.65	0.36	79,79,79,79	0
8	NAG	E	400	14/15	0.66	0.20	172,176,179,180	0
6	LMT	B	404	26/35	0.69	0.21	145,145,145,145	0
8	NAG	C	400	14/15	0.72	0.15	128,132,137,137	0
8	NAG	B	400	14/15	0.77	0.13	138,141,143,145	0
9	OCT	D	403	8/8	0.77	0.26	59,59,59,59	0
7	CL	B	402	1/1	0.82	0.16	72,72,72,72	0
6	LMT	A	404	26/35	0.82	0.15	106,106,106,106	0
9	OCT	B	405	8/8	0.82	0.26	60,60,60,60	0
5	IVM	B	403	62/62	0.88	0.15	60,68,83,84	0
4	GLU	B	401	10/10	0.88	0.18	67,68,71,71	0
5	IVM	D	402	62/62	0.89	0.16	61,70,84,85	0
5	IVM	A	402	62/62	0.89	0.14	55,58,69,70	0
4	GLU	A	401	10/10	0.90	0.26	73,74,77,78	0
5	IVM	A	403	62/62	0.90	0.15	70,73,80,81	0
4	GLU	D	401	10/10	0.90	0.25	66,67,69,69	0
5	IVM	E	402	62/62	0.91	0.13	65,69,73,75	0
4	GLU	C	401	10/10	0.92	0.12	74,76,79,80	0
4	GLU	E	401	10/10	0.95	0.11	66,67,69,70	0

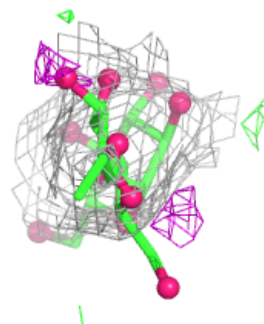
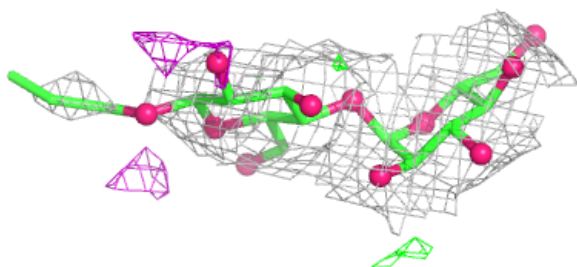
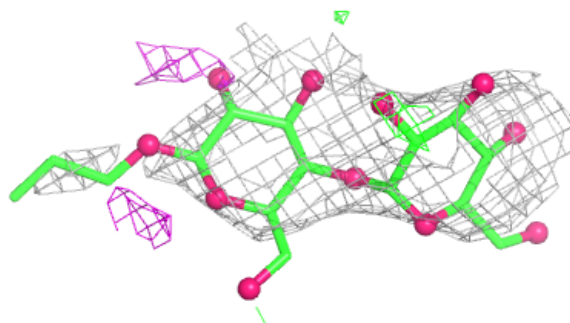
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 405:

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

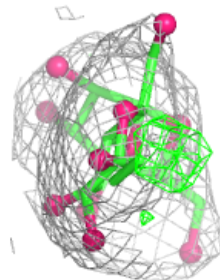
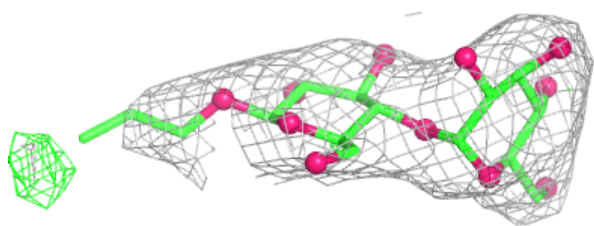
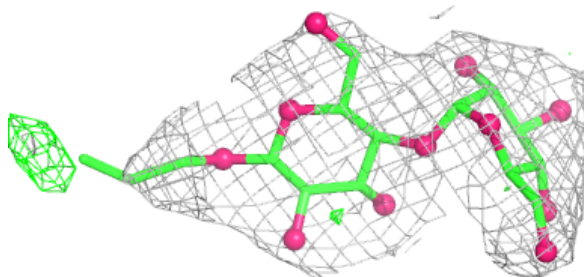
**Electron density around LMT B 404:**

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



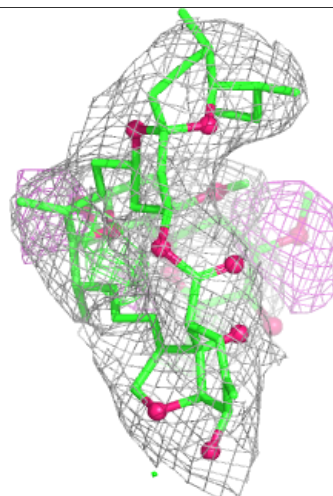
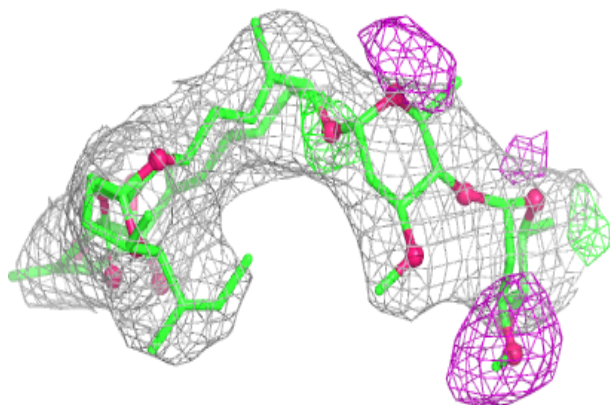
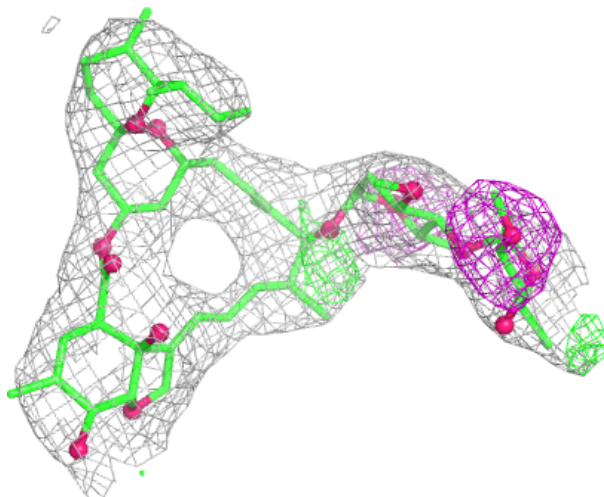
Electron density around LMT A 404:

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



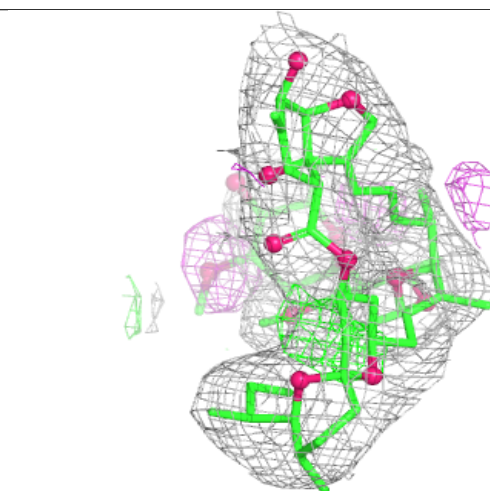
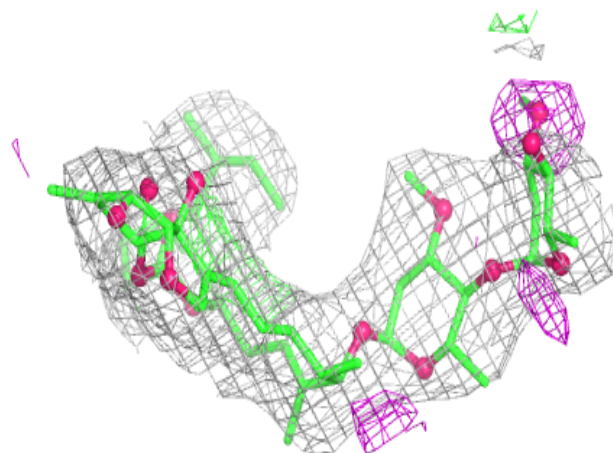
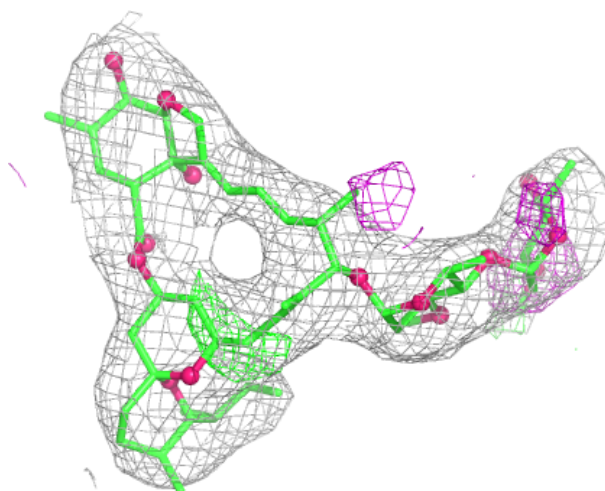
Electron density around IVM B 403:

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



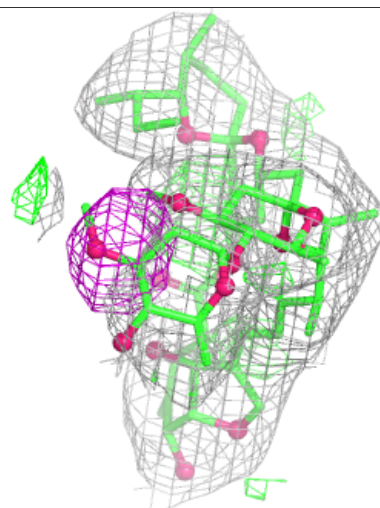
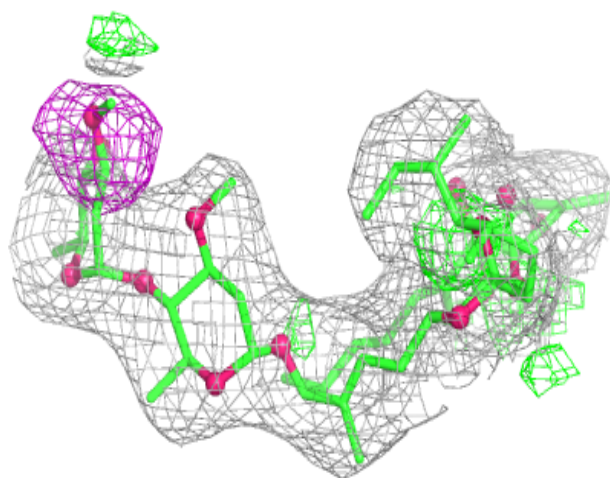
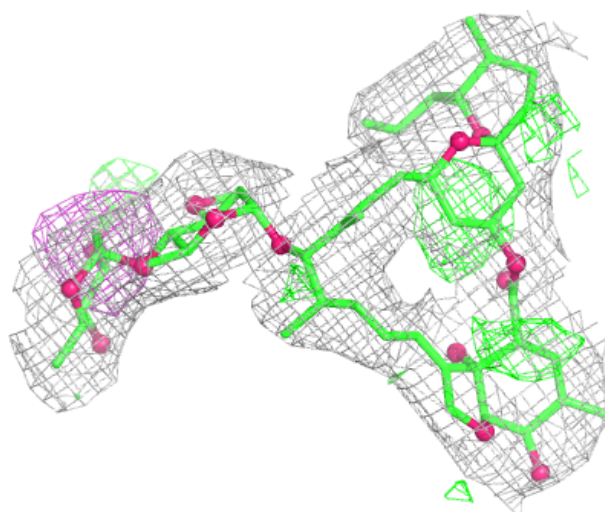
Electron density around IVM D 402:

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



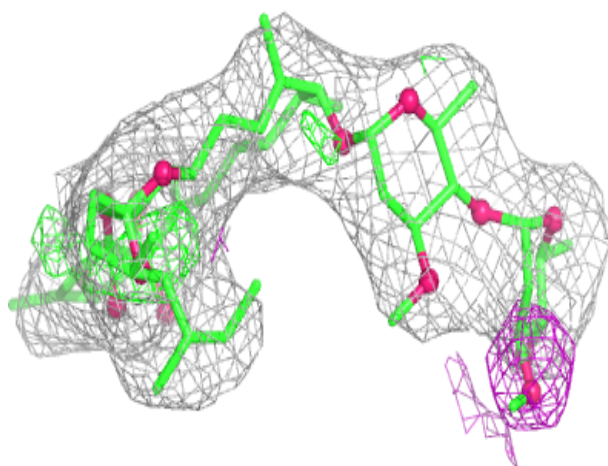
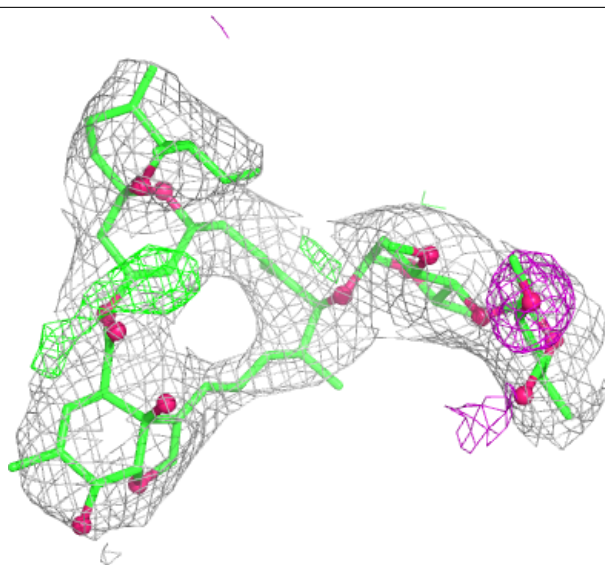
Electron density around IVM A 402:

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



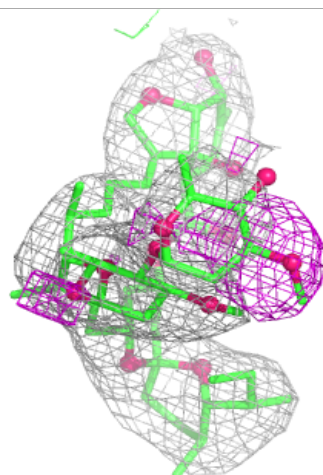
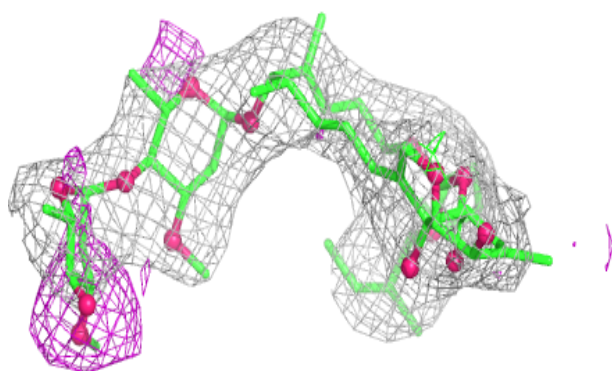
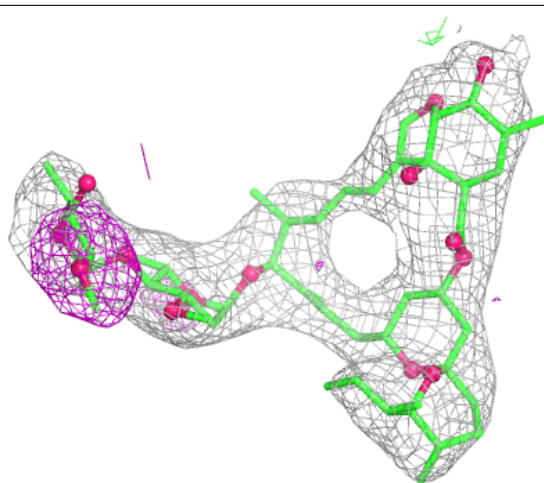
Electron density around IVM A 403:

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



Electron density around IVM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.