W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 3, 2023 – 01:27 AM EDT

PDB ID	:	3RHW
Title	:	C. elegans glutamate-gated chloride channel (GluCl) in complex with Fab and ivermectin
Authors	:	Hibbs, R.E.; Gouaux, E.
Deposited on	:	2011-04-12
Resolution	:	3.26 Å(reported)

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

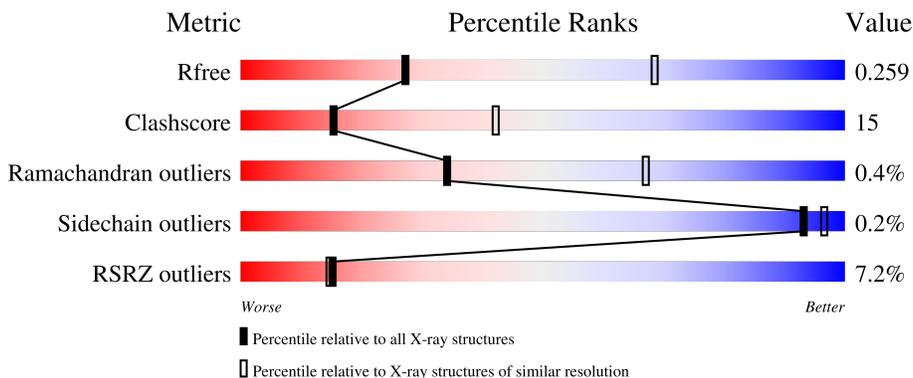|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.26 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.
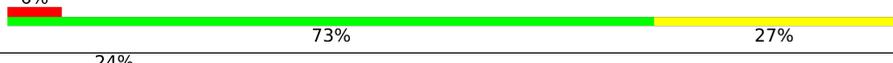
Metric	Percentile Ranks	Value
Rfree		0.259
Clashscore		15
Ramachandran outliers		0.4%
Sidechain outliers		0.2%
RSRZ outliers		7.2%

Worse *Better*

▐ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	347	2% / 64% / 33%
1	B	347	5% / 64% / 34%
1	C	347	5% / 64% / 33%
1	D	347	3% / 64% / 34%
1	E	347	3% / 64% / 34%

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Mol	Chain	Length	Quality of chain
2	F	221	14% ... 64% ... 22% ... 14%
2	G	221	5% ... 61% ... 30% ... 10%
2	H	221	6% ... 73% ... 27%
2	I	221	24% ... 67% ... 23% ... 10%
2	J	221	2% ... 67% ... 30% ... •
3	K	210	2% ... 72% ... 22% ... 5%
3	L	210	3% ... 74% ... 26%
3	M	210	3% ... 77% ... 23%
3	N	210	9% ... 60% ... 15% ... 25%
3	O	210	27% ... 70% ... 23% ... 7%

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	NAG	C	400	-	-	-	X
6	NAG	E	400	-	-	-	X

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 29197 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 2716	C 1768	N 441	O 492	S 15	0	0	0
1	B	340	Total 2716	C 1768	N 441	O 492	S 15	0	0	0
1	C	339	Total 2706	C 1762	N 438	O 491	S 15	0	0	0
1	D	340	Total 2716	C 1768	N 441	O 492	S 15	0	0	0
1	E	340	Total 2716	C 1768	N 441	O 492	S 15	0	0	0

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
			Total	C	N	O	S			
2	F	191	1478	942	240	289	7	0	0	0

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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 (three-letter code: IVM) (formula: $C_{48}H_{74}O_{14}$).

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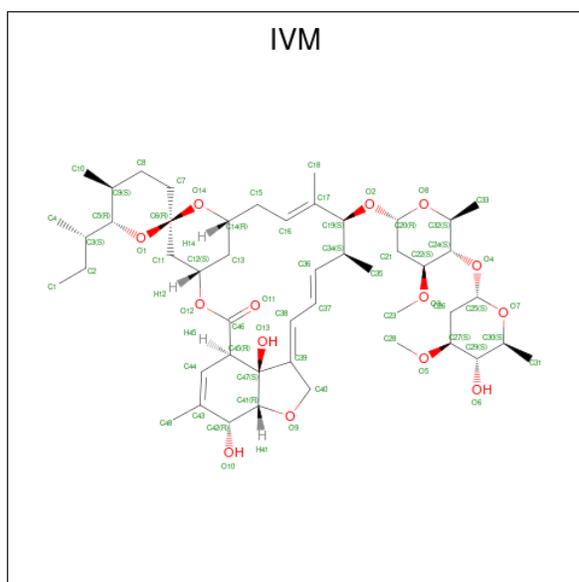
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 62	C 48	O 14	0	0
4	B	1	Total 62	C 48	O 14	0	0
4	B	1	Total 62	C 48	O 14	0	0
4	D	1	Total 62	C 48	O 14	0	0
4	D	1	Total 62	C 48	O 14	0	0

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

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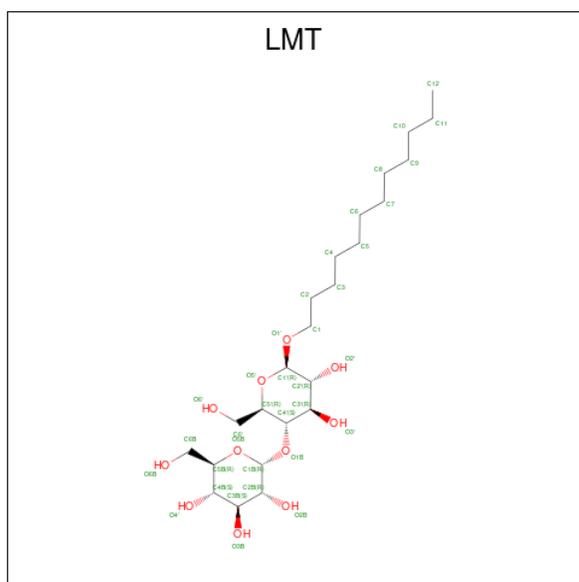
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 26	C 15	O 11	0	0
5	A	1	Total 27	C 16	O 11	0	0
5	B	1	Total 26	C 15	O 11	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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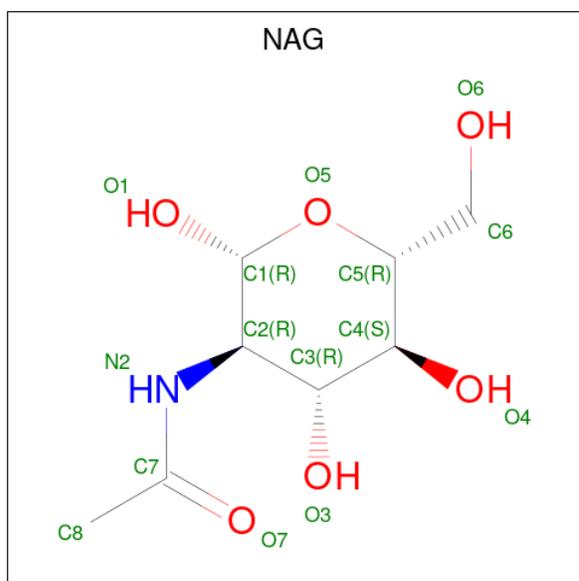
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total 14	C 8	N 1	O 5	0	0
6	C	1	Total 14	C 8	N 1	O 5	0	0
6	E	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).
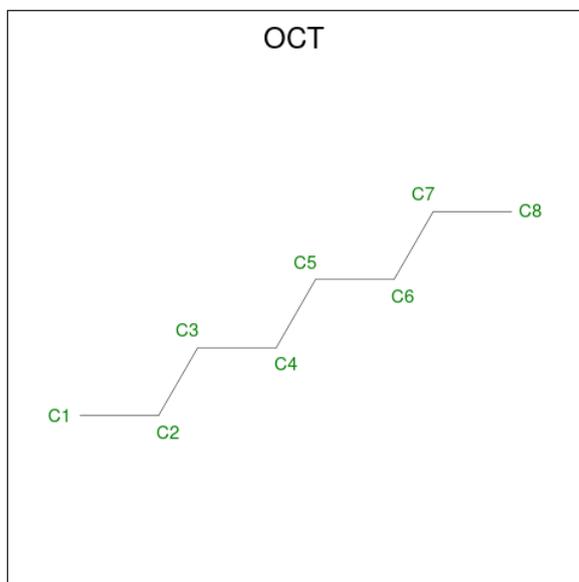
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 8	C 8	0	0
7	D	1	Total 8	C 8	0	0
7	E	1	Total 8	C 8	0	0

- Molecule 8 is UNDECANE (three-letter code: UND) (formula: $C_{11}H_{24}$).

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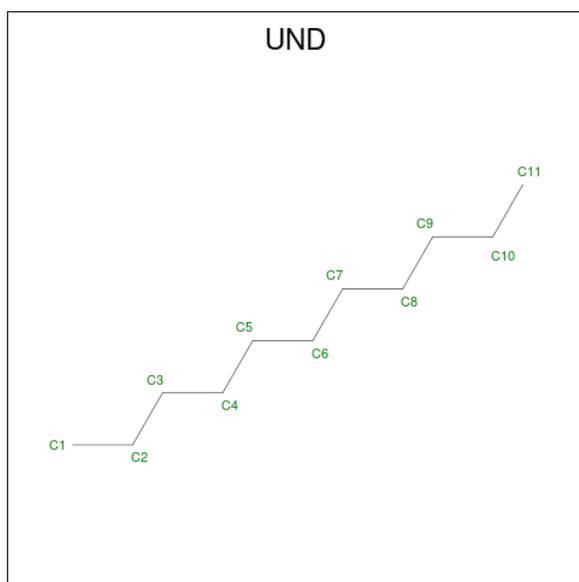
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 11	C 11	0	0

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

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Cl 1	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.

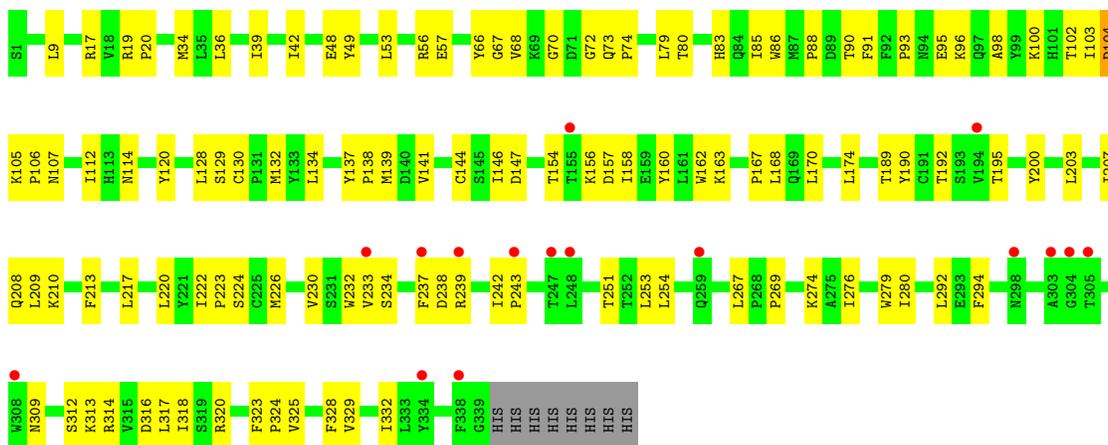- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha
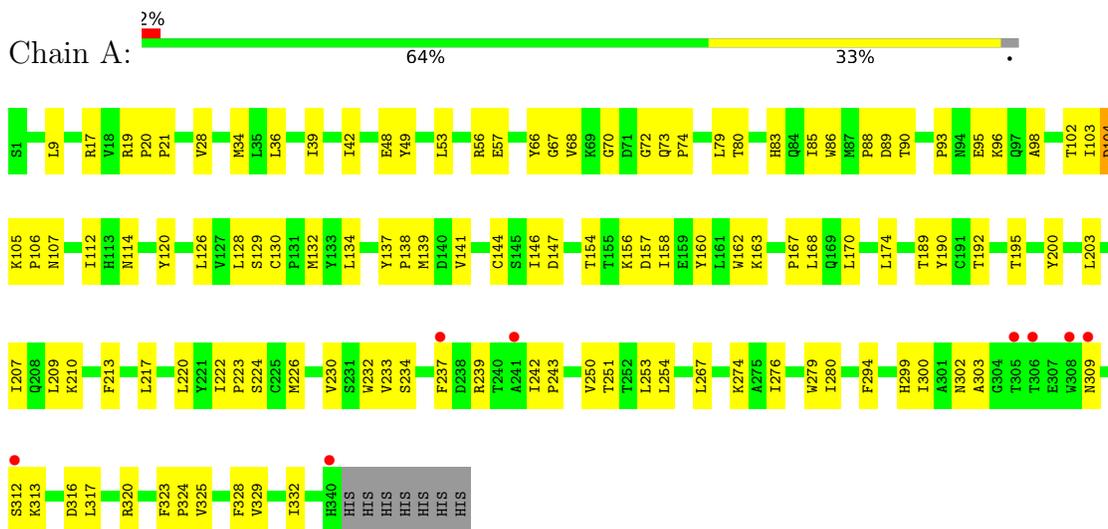
Chain A:

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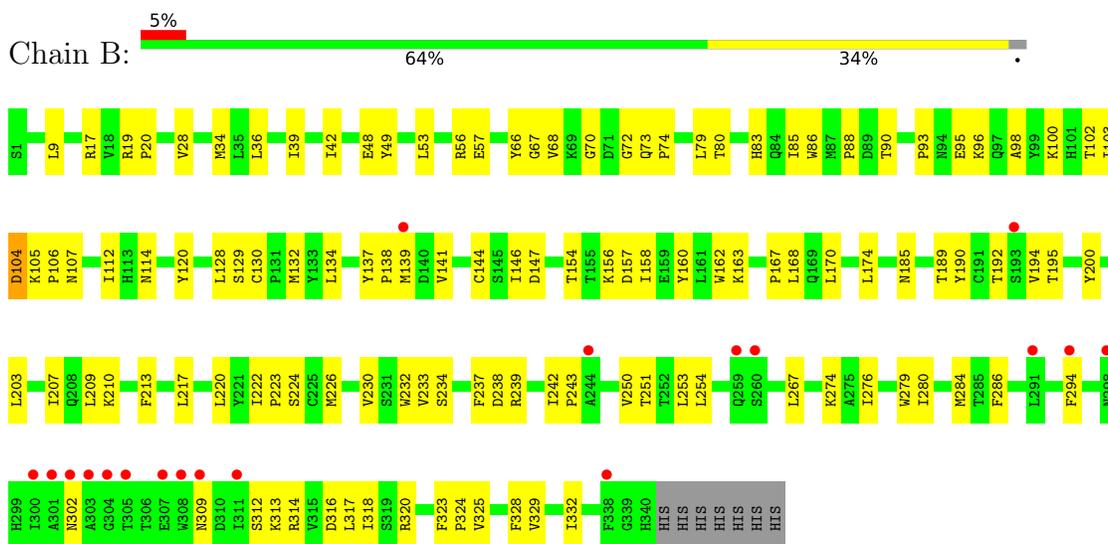
Chain B:

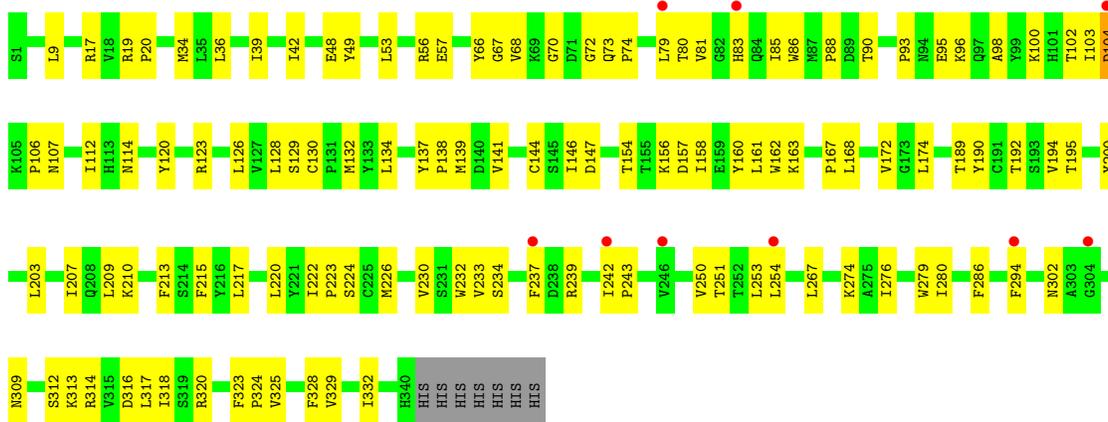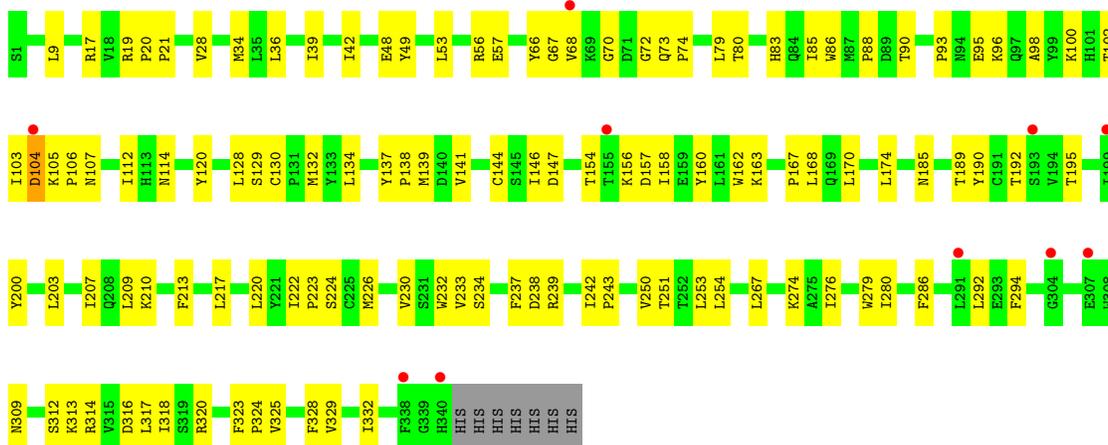- Molecule 1: Avermectin-sensitive glutamate-gated chloride channel GluCl alpha

Chain C:

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

Chain D:

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

Chain E:

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain F:

14%

64% 22% 14%

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain G:

5%

61% 30% 10%

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

Chain H:

6%

73% 27%

• Molecule 2: Mouse monoclonal Fab fragment, heavy chain
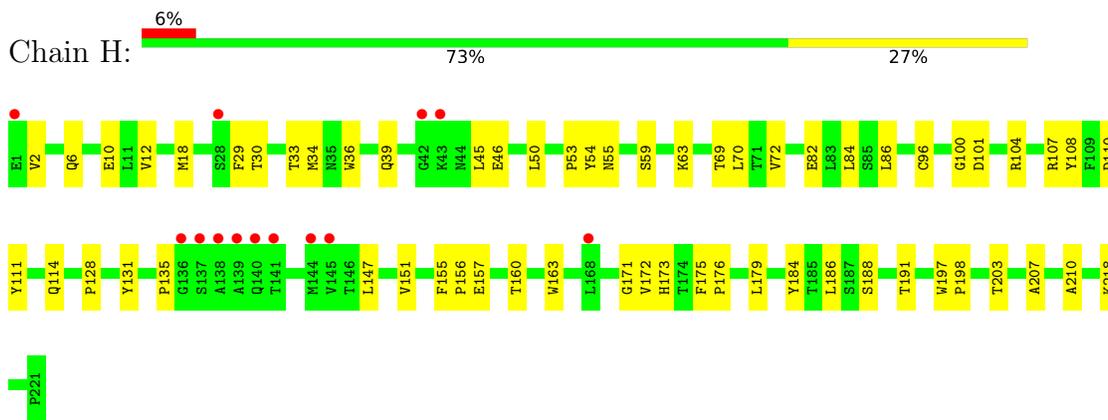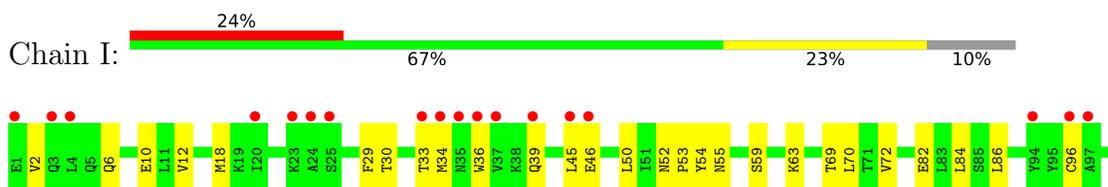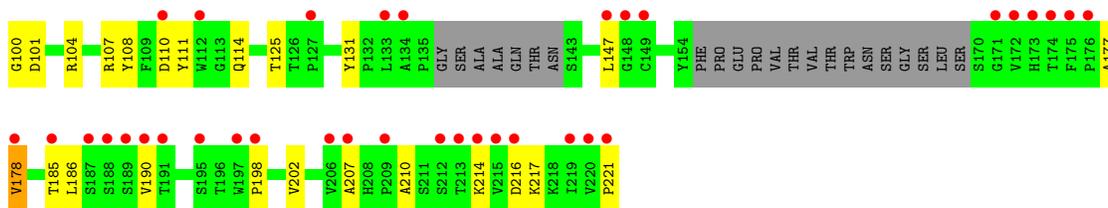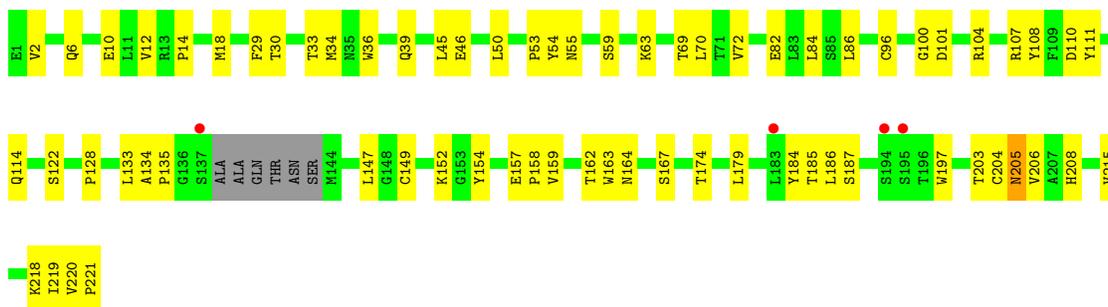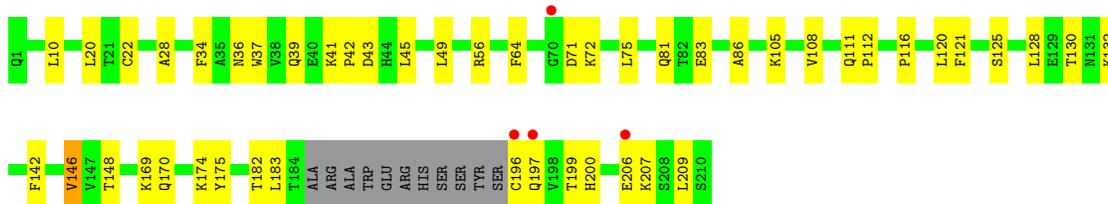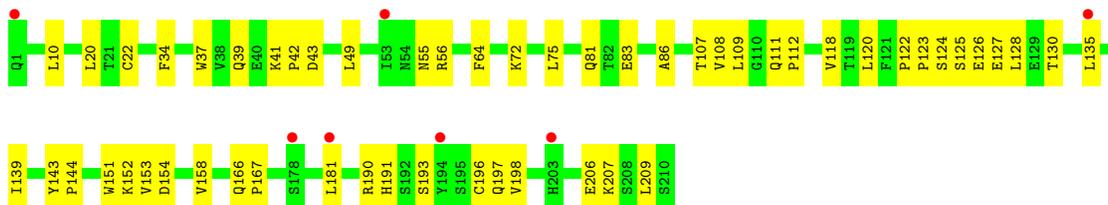
Chain I:

24%

67% 23% 10%
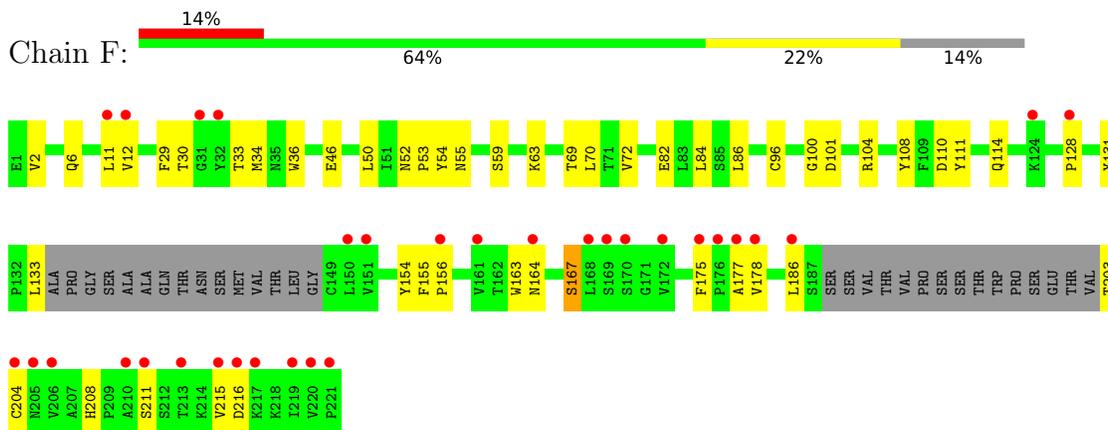
• Molecule 2: Mouse monoclonal Fab fragment, heavy chain

• Molecule 3: Mouse monoclonal Fab fragment, light chain

• Molecule 3: Mouse monoclonal Fab fragment, light chain

• Molecule 3: Mouse monoclonal Fab fragment, light chain

V153 D154 P157 Q166 P167 N172 N173 K174 Y175 M176 W188 S193 Y194 H200 E201 G202 H203 L209 S210

• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain N:

Q1 L10 L20 T21 C22 W37 V38 Q39 E40 K41 P42 D43 H44 L45 L49 R56 A57 P58 F64 K72 L75 Q81 T82 E83 A86 L106 T107 V108 L109 L120 P123 S124 S125 GLU GLU LEU GLU THR ASN LYS ALA T134 L135 V136 F142 Y143

P144 G145 V146 V147 THR VAL ASP TRP LYS VAL ASP GLY THR PRO VAL T159 Q160 G161 M162 E163 T164 T165 Q166 P167 S168 K169 Q170 S171 ASN ASN LYS TYR MET A177 S178 S179 TYR LEU THR L183 L184 A185 ARG ALA TRP GLU ARG HIS SER SER TYR SER CYS GLN VAL THR HIS GLU GLY GLY HIS

THR VAL GLU LYS SER LEU SER

• Molecule 3: Mouse monoclonal Fab fragment, light chain

Chain O:

Q1 A2 V3 L10 V18 T19 L20 T21 C22 I32 N33 F34 A35 N36 W37 V38 Q39 E40 K41 P42 D43 H44 L45 F46 L49 I50 R56 F64 K72 L75 Q81 T82 E83 A86 I87 Y88 F89 L92 V99 F100 G101 T104 K105 L106 T107 V108 L109

G110 Q111 P112 K113 P116 S117 V118 T119 L120 F121 P122 P123 E126 E127 T130 N131 K132 A133 T134 L135 V136 C137 T138 I139 T140 D141 F142 Y143 P144 V149 D150 W151 LYS VAL ASP GLY THR PRO VAL THR GLN G161 T164 P167 S168 K169 Q170 S171 N172 N173 K174 Y175 M176 A177

S178 S179 Y180 L181 T182 L183 W188 E189 ARG HIS SER SER Y194 S195 C196 Q197 V198 G202 H203 T204 V205 E206 K207 S208 LEU SER

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.85Å 154.85Å 574.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.50 – 3.26 109.50 – 3.26	Depositor EDS
% Data completeness (in resolution range)	93.7 (109.50-3.26) 99.7 (109.50-3.26)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.239 , 0.270 0.229 , 0.259	Depositor DCC
R_{free} test set	5474 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	86.7	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.5	EDS
L-test for twinning[2]	$<|L|>\ =0.47,\ <L^2>\ =0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	29197	wwPDB-VP
Average B, all atoms (Å^2)	87.0	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.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/3809
1	B	0.26	0/2789	0.42	0/3809
1	C	0.25	0/2778	0.42	0/3794
1	D	0.25	0/2789	0.42	0/3809
1	E	0.26	0/2789	0.42	0/3809
2	F	0.23	0/1517	0.41	0/2062
2	G	0.24	0/1569	0.44	0/2138
2	H	0.25	0/1729	0.43	0/2360
2	I	0.24	0/1564	0.42	0/2128
2	J	0.24	0/1684	0.43	0/2299
3	K	0.24	0/1529	0.43	0/2089
3	L	0.25	0/1629	0.45	0/2226
3	M	0.24	0/1622	0.43	0/2219
3	N	0.24	0/1188	0.44	0/1621
3	O	0.32	1/1504 (0.1%)	0.47	1/2056 (0.0%)
All	All	0.25	1/29469 (0.0%)	0.43	1/40228 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3	VAL	CB-CG2	8.11	1.69	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	3	VAL	CG1-CB-CG2	7.33	122.63	110.90

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	109	0
1	B	2716	0	2708	109	0
1	C	2706	0	2701	109	0
1	D	2716	0	2709	109	0
1	E	2716	0	2708	105	0
2	F	1478	0	1432	39	0
2	G	1529	0	1478	49	0
2	H	1683	0	1632	46	0
2	I	1525	0	1485	42	0
2	J	1639	0	1588	48	0
3	K	1496	0	1458	34	0
3	L	1591	0	1542	38	0
3	M	1584	0	1531	33	0
3	N	1165	0	1142	22	0
3	O	1470	0	1412	41	0
4	A	62	0	74	1	0
4	B	124	0	148	3	0
4	D	124	0	148	5	0
5	A	53	0	52	12	0
5	B	26	0	25	4	0
6	B	14	0	13	1	0
6	C	14	0	13	1	0
6	E	14	0	13	1	0
7	B	8	0	18	2	0
7	D	8	0	18	2	0
7	E	8	0	18	2	0
8	B	11	0	24	0	0
9	C	1	0	0	0	0
All	All	29197	0	28799	861	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 861 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:90:THR:HG22	1:A:160:TYR:OH	1.62	1.00
1:D:90:THR:HG22	1:D:160:TYR:OH	1.63	0.99
2:F:208:HIS:HD2	2:F:211:SER:H	1.10	0.98
1:B:90:THR:HG22	1:B:160:TYR:OH	1.63	0.98
1:E:90:THR:HG22	1:E:160:TYR:OH	1.65	0.96

There are no symmetry-related clashes.

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%)	321 (95%)	16 (5%)	1 (0%)	41	72
1	B	338/347 (97%)	320 (95%)	17 (5%)	1 (0%)	41	72
1	C	337/347 (97%)	320 (95%)	16 (5%)	1 (0%)	41	72
1	D	338/347 (97%)	321 (95%)	16 (5%)	1 (0%)	41	72
1	E	338/347 (97%)	322 (95%)	15 (4%)	1 (0%)	41	72
2	F	185/221 (84%)	171 (92%)	12 (6%)	2 (1%)	14	46
2	G	194/221 (88%)	176 (91%)	18 (9%)	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%)	15	47
2	J	211/221 (96%)	199 (94%)	12 (6%)	0	100	100
3	K	195/210 (93%)	173 (89%)	21 (11%)	1 (0%)	29	62
3	L	208/210 (99%)	186 (89%)	20 (10%)	2 (1%)	15	47
3	M	208/210 (99%)	189 (91%)	19 (9%)	0	100	100
3	N	148/210 (70%)	131 (88%)	16 (11%)	1 (1%)	22	56
3	O	189/210 (90%)	166 (88%)	23 (12%)	0	100	100
All	All	3639/3890 (94%)	3378 (93%)	248 (7%)	13 (0%)	34	67

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%)	306 (100%)	1 (0%)	92	96
1	B	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	C	306/316 (97%)	305 (100%)	1 (0%)	92	96
1	D	307/316 (97%)	306 (100%)	1 (0%)	92	96
1	E	307/316 (97%)	306 (100%)	1 (0%)	92	96
2	F	165/190 (87%)	165 (100%)	0	100	100
2	G	171/190 (90%)	170 (99%)	1 (1%)	86	91
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%)	184 (100%)	1 (0%)	88	93
3	K	169/178 (95%)	169 (100%)	0	100	100
3	L	178/178 (100%)	178 (100%)	0	100	100
3	M	177/178 (99%)	177 (100%)	0	100	100
3	N	130/178 (73%)	130 (100%)	0	100	100
3	O	162/178 (91%)	161 (99%)	1 (1%)	86	91
All	All	3233/3420 (94%)	3225 (100%)	8 (0%)	93	96

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	3	VAL
2	J	205	ASN
1	E	104	ASP
1	D	104	ASP
2	G	45	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	208	HIS
3	M	160	GLN
2	G	180	GLN
3	N	170	GLN
2	J	55	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	15 (18%)
5	LMT	B	350	-	27,27,36	1.54	4 (14%)	37,38,47	1.44	7 (18%)
7	OCT	D	350	-	7,7,7	0.17	0	6,6,6	0.36	0
4	IVM	B	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
4	IVM	D	349	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
4	IVM	B	348	-	65,68,68	0.80	1 (1%)	82,102,102	1.63	17 (20%)
5	LMT	A	349	-	27,27,36	1.59	6 (22%)	37,38,47	2.05	12 (32%)
4	IVM	D	348	-	65,68,68	0.80	1 (1%)	82,102,102	1.64	16 (19%)
6	NAG	B	400	1	14,14,15	0.57	0	17,19,21	1.70	3 (17%)
5	LMT	A	350	-	28,28,36	1.52	4 (14%)	39,39,47	1.32	4 (10%)
7	OCT	E	348	-	7,7,7	0.13	0	6,6,6	0.48	0
6	NAG	E	400	1	14,14,15	1.39	2 (14%)	17,19,21	1.90	5 (29%)
6	NAG	C	400	1	14,14,15	0.60	0	17,19,21	2.60	3 (17%)
7	OCT	B	351	-	7,7,7	0.13	0	6,6,6	0.44	0
8	UND	B	352	-	10,10,10	0.42	0	9,9,9	0.43	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	348	-	-	3/45/141/141	0/6/7/7
5	LMT	B	350	-	-	6/12/52/61	0/2/2/2
7	OCT	D	350	-	-	0/5/5/5	-
4	IVM	B	349	-	-	3/45/141/141	0/6/7/7
4	IVM	D	349	-	-	3/45/141/141	0/6/7/7
4	IVM	B	348	-	-	3/45/141/141	0/6/7/7
5	LMT	A	349	-	-	6/12/52/61	0/2/2/2
4	IVM	D	348	-	-	3/45/141/141	0/6/7/7
6	NAG	B	400	1	-	2/6/23/26	0/1/1/1
5	LMT	A	350	-	-	6/13/53/61	0/2/2/2
7	OCT	E	348	-	-	0/5/5/5	-
6	NAG	E	400	1	-	2/6/23/26	0/1/1/1
6	NAG	C	400	1	-	2/6/23/26	0/1/1/1
7	OCT	B	351	-	-	0/5/5/5	-
8	UND	B	352	-	-	0/8/8/8	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	349	IVM	O12-C46	4.93	1.45	1.34
4	D	349	IVM	O12-C46	4.87	1.45	1.34
4	A	348	IVM	O12-C46	4.85	1.45	1.34
4	B	348	IVM	O12-C46	4.84	1.45	1.34
4	D	348	IVM	O12-C46	4.78	1.45	1.34

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	400	NAG	O5-C1-C2	8.34	124.45	111.29
4	D	349	IVM	O12-C46-C45	6.93	121.00	110.97
4	A	348	IVM	O12-C46-C45	6.79	120.79	110.97
4	D	348	IVM	O12-C46-C45	6.72	120.69	110.97
4	B	349	IVM	O12-C46-C45	6.70	120.67	110.97

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	348	IVM	O7-C25-O4-C24
4	A	348	IVM	C26-C25-O4-C24
4	B	348	IVM	O7-C25-O4-C24
4	B	348	IVM	C26-C25-O4-C24
4	B	349	IVM	O7-C25-O4-C24

There are no ring outliers.

13 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	348	IVM	1	0
5	B	350	LMT	4	0
7	D	350	OCT	2	0
4	B	349	IVM	2	0
4	D	349	IVM	3	0
4	B	348	IVM	1	0
5	A	349	LMT	12	0
4	D	348	IVM	2	0
6	B	400	NAG	1	0
7	E	348	OCT	2	0
6	E	400	NAG	1	0

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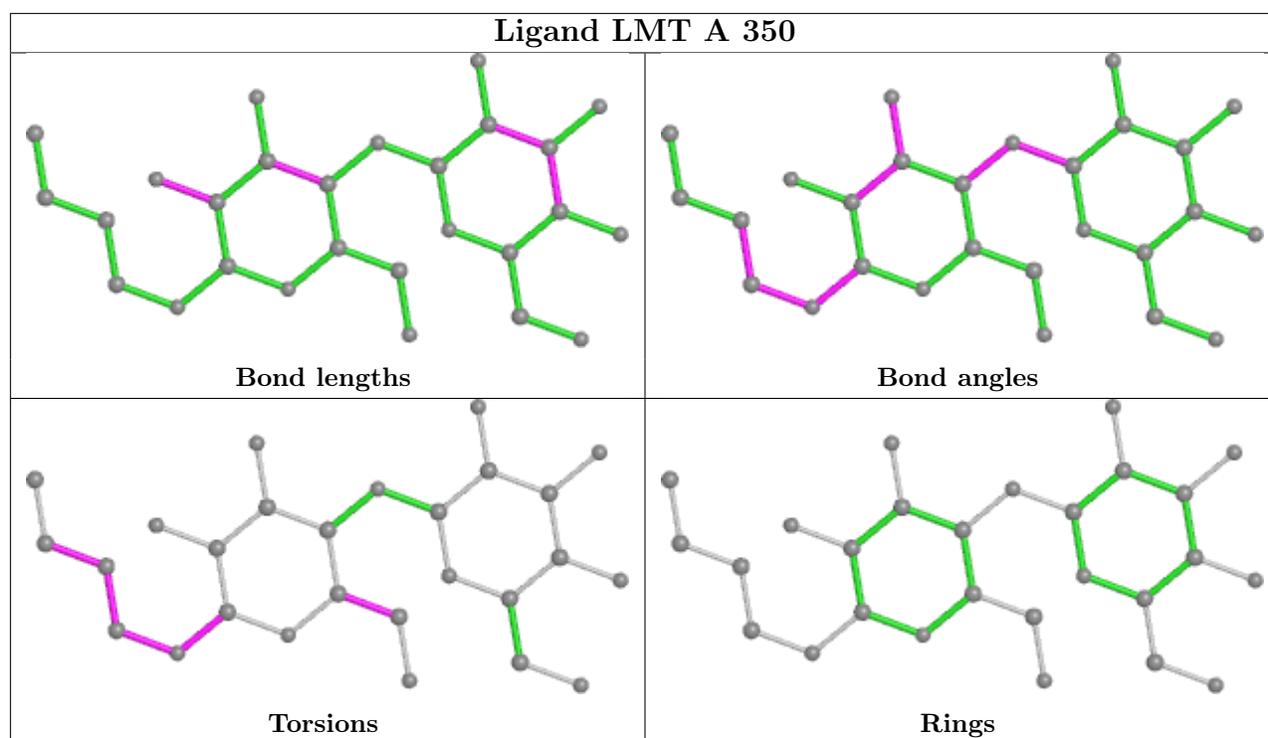| Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	400	NAG	1	0
7	B	351	OCT	2	0

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

Ligand IVM A 348

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT B 350

Bond lengths

Bond angles

Torsions

Rings

Ligand IVM B 349

Bond lengths

Bond angles

Torsions

Rings

Ligand IVM D 349

Bond lengths

Bond angles

Torsions

Rings

Ligand IVM B 348

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 349

Bond lengths

Bond angles

Torsions

Rings

Ligand IVM D 348

Bond lengths

Bond angles

Torsions

Rings

Ligand LMT A 350

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	340/347 (97%)	0.38	8 (2%)	59	55	35, 64, 128, 174	0
1	B	340/347 (97%)	0.45	19 (5%)	24	22	39, 66, 119, 196	0
1	C	339/347 (97%)	0.48	16 (4%)	31	28	44, 72, 144, 238	0
1	D	340/347 (97%)	0.42	9 (2%)	56	52	42, 73, 142, 215	0
1	E	340/347 (97%)	0.38	10 (2%)	51	50	38, 70, 138, 207	0
2	F	191/221 (86%)	1.06	32 (16%)	1	1	49, 102, 161, 181	0
2	G	200/221 (90%)	0.56	11 (5%)	25	23	52, 94, 146, 181	0
2	H	221/221 (100%)	0.52	13 (5%)	22	21	40, 77, 131, 280	0
2	I	199/221 (90%)	1.29	53 (26%)	0	0	56, 106, 170, 206	0
2	J	215/221 (97%)	0.36	4 (1%)	66	64	47, 80, 150, 240	0
3	K	199/210 (94%)	0.32	4 (2%)	65	63	61, 102, 149, 201	0
3	L	210/210 (100%)	0.42	7 (3%)	46	43	43, 74, 119, 157	0
3	M	210/210 (100%)	0.41	6 (2%)	51	50	46, 82, 126, 150	0
3	N	158/210 (75%)	0.82	19 (12%)	4	4	60, 106, 170, 198	0
3	O	195/210 (92%)	1.44	56 (28%)	0	0	61, 109, 160, 189	0
All	All	3697/3890 (95%)	0.58	267 (7%)	15	15	35, 80, 150, 280	0

The worst 5 of 267 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	188	SER	9.1
1	B	302	ASN	8.7
2	H	136	GLY	8.1
2	I	189	SER	7.3
3	O	208	SER	7.3

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	LMT	A	350	27/35	0.56	0.33	149,149,149,149	0
6	NAG	E	400	14/15	0.70	0.41	162,166,169,171	0
6	NAG	C	400	14/15	0.72	0.44	119,123,126,128	0
8	UND	B	352	11/11	0.72	0.25	63,63,63,63	0
5	LMT	B	350	26/35	0.73	0.35	166,166,166,166	0
6	NAG	B	400	14/15	0.79	0.38	132,137,140,142	0
7	OCT	E	348	8/8	0.82	0.44	74,74,74,74	0
7	OCT	D	350	8/8	0.82	0.39	61,61,61,61	0
5	LMT	A	349	26/35	0.85	0.31	110,110,110,110	0
7	OCT	B	351	8/8	0.86	0.56	68,68,68,68	0
4	IVM	D	348	62/62	0.93	0.35	57,75,99,115	0
4	IVM	D	349	62/62	0.93	0.33	52,68,94,111	0
4	IVM	A	348	62/62	0.94	0.32	56,70,97,114	0
4	IVM	B	348	62/62	0.94	0.34	47,63,89,106	0
4	IVM	B	349	62/62	0.94	0.36	55,70,97,114	0
9	CL	C	348	1/1	0.95	0.20	83,83,83,83	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)
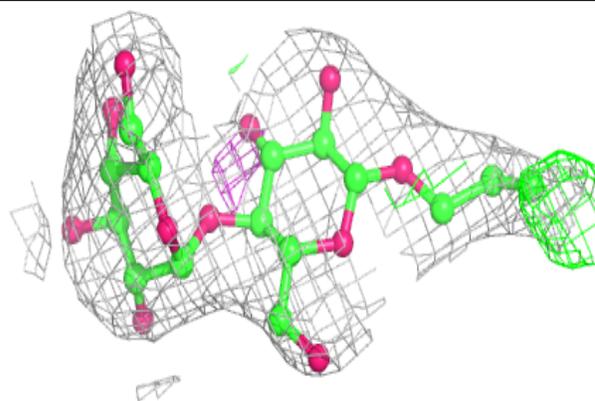and green (positive)
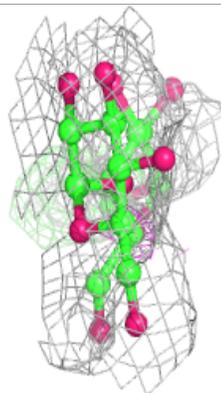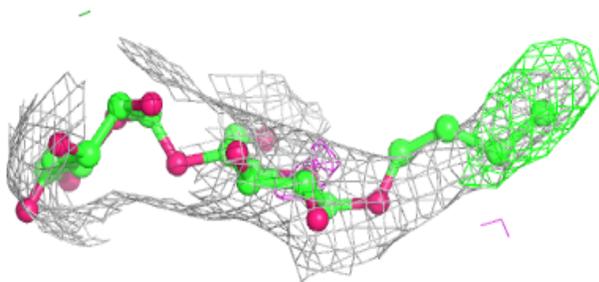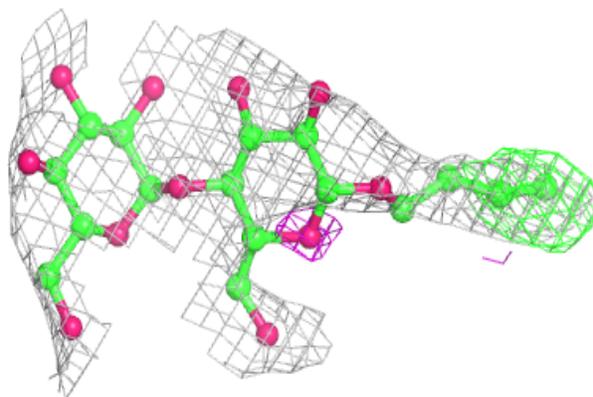
Electron density around LMT B 350:

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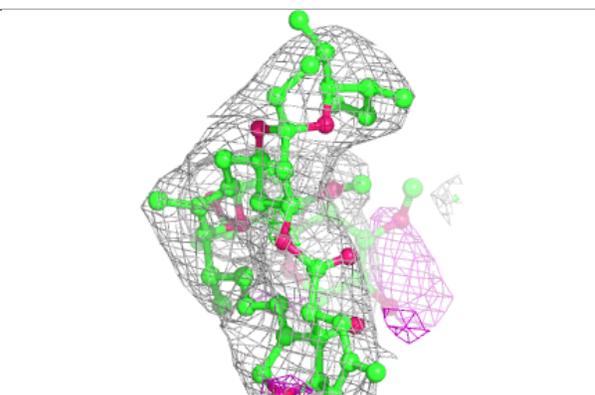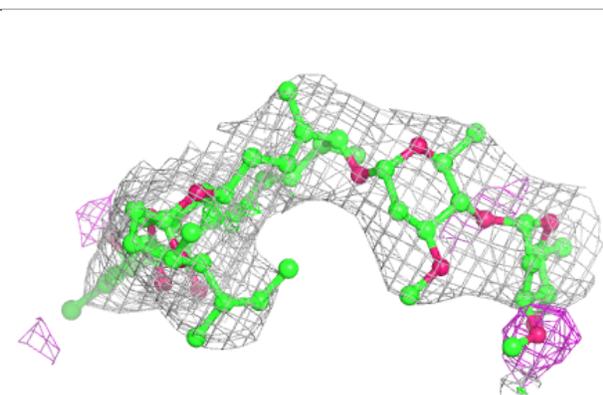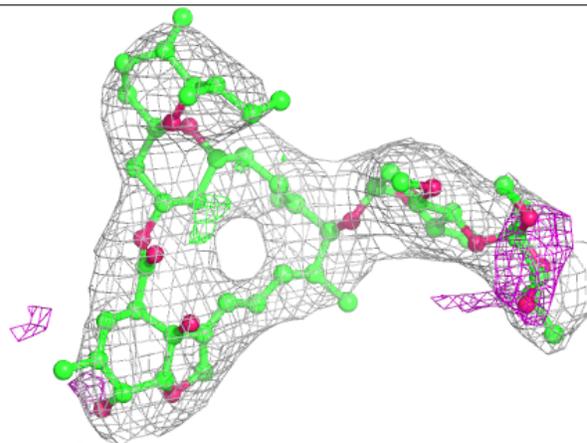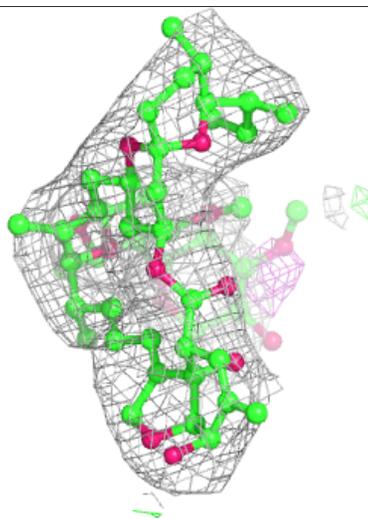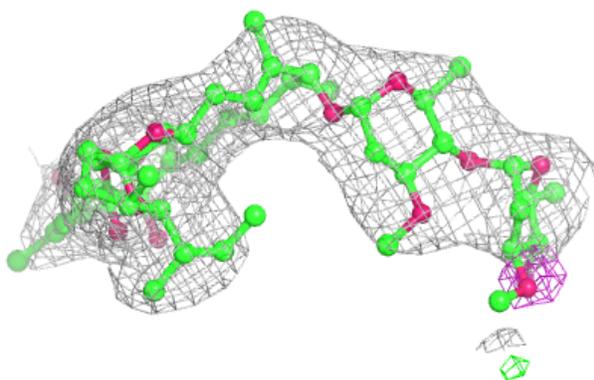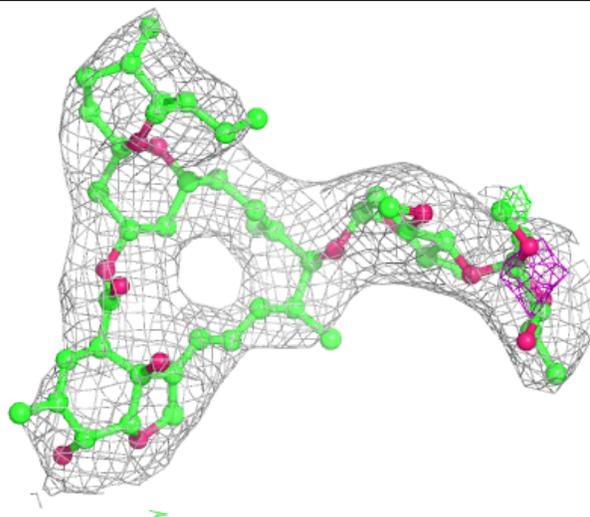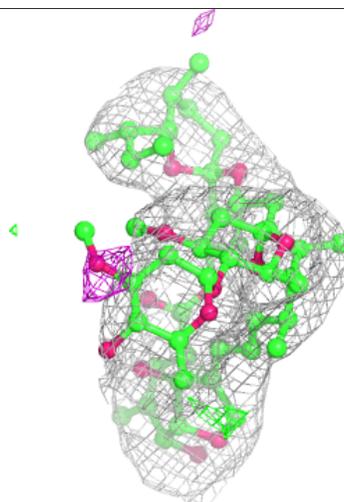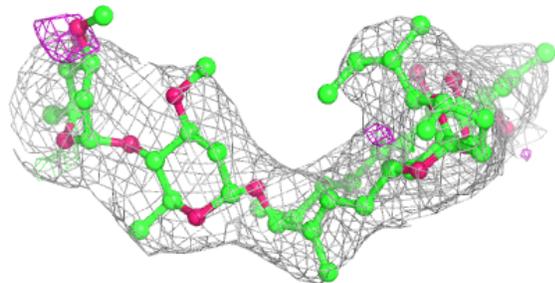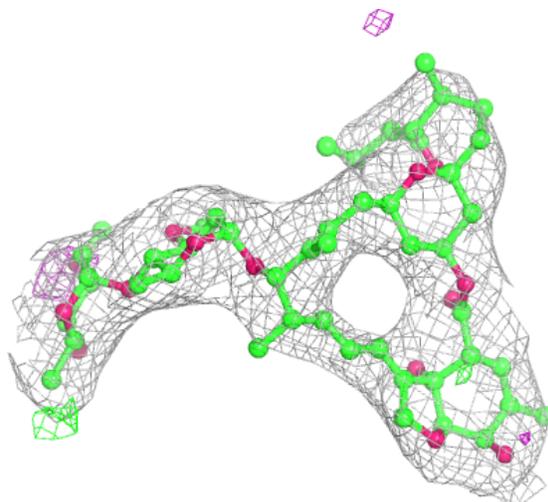mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
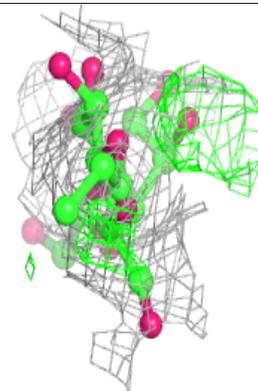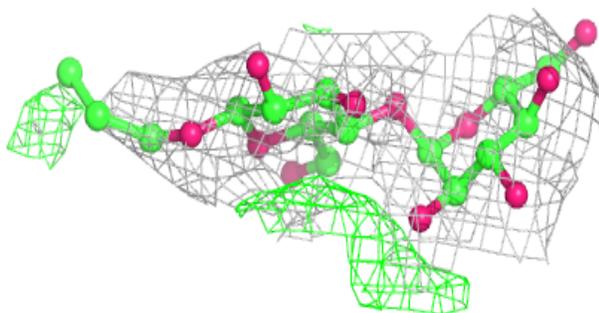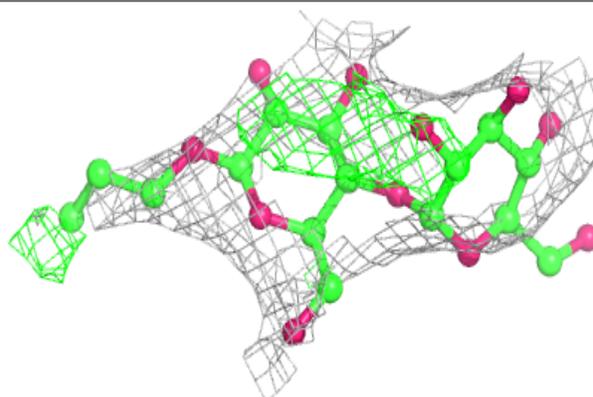
Electron density around LMT A 349:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
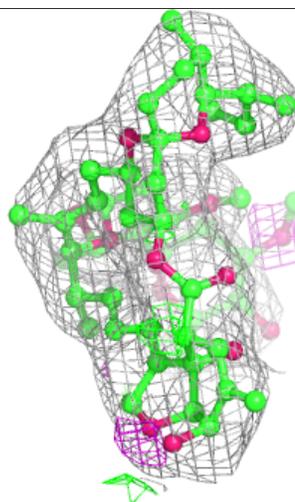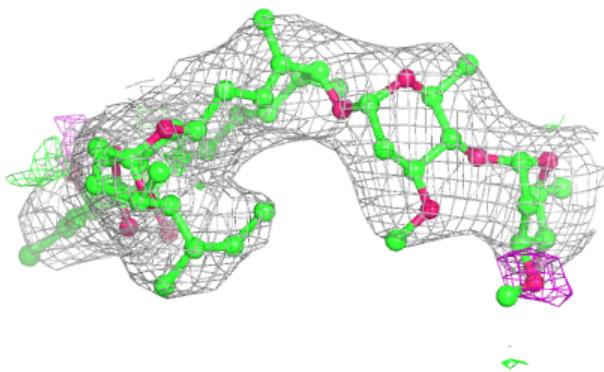and green (positive)
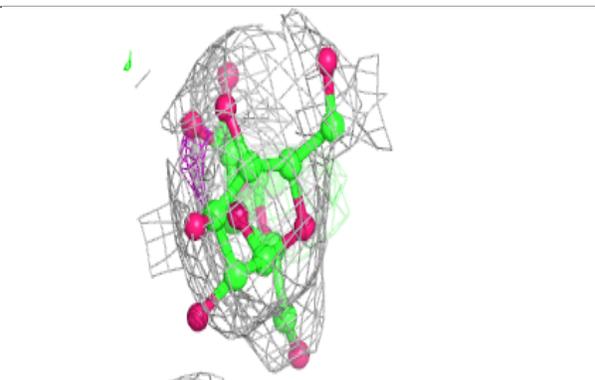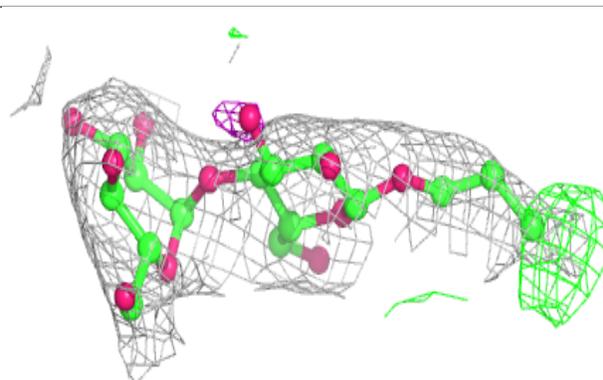
Electron density around IVM D 348:

$2mF_o$-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 D 349:

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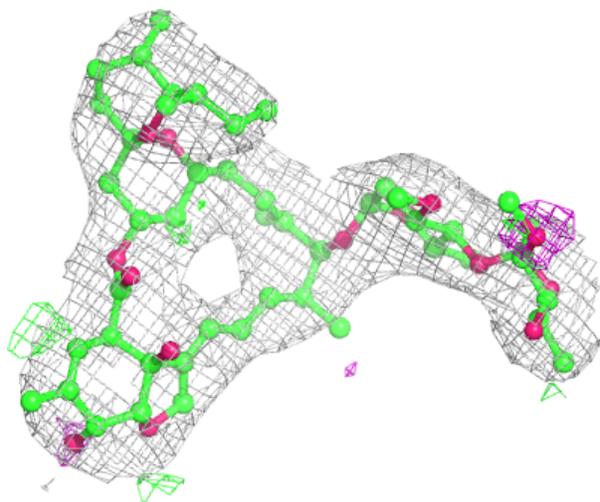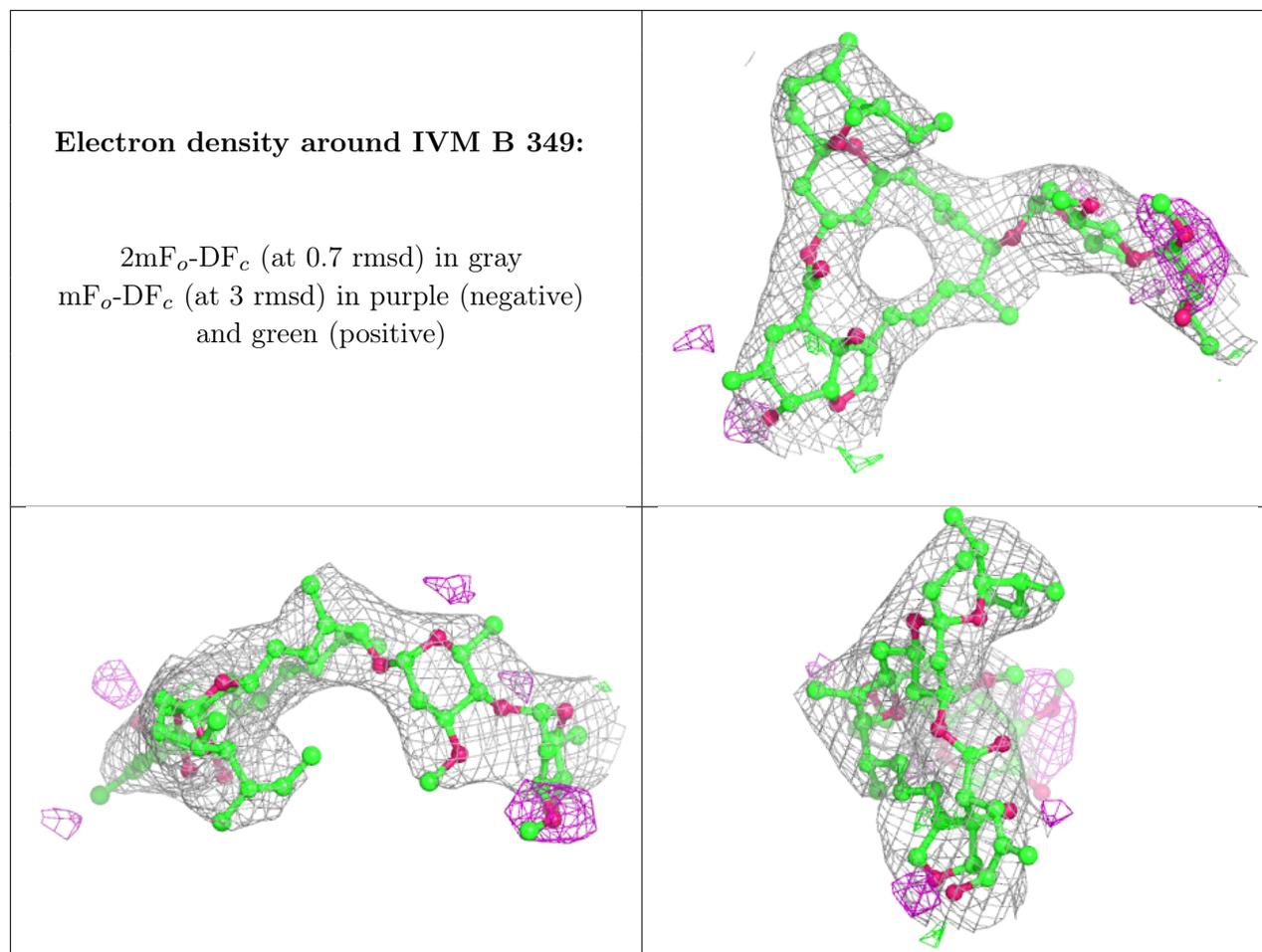and green (positive)

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 B 348:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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.