



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2024 – 03:42 pm BST

PDB ID : 3ZKR  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with bromoform  
Authors : Spurny, R.; Billen, B.; Howard, R.J.; Brams, M.; Debaveye, S.; Price, K.L.; Weston, D.A.; Strelkov, S.V.; Tytgat, J.; Bertrand, S.; Bertrand, D.; Lummis, S.C.R.; Ulens, C.  
Deposited on : 2013-01-24  
Resolution : 3.65 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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

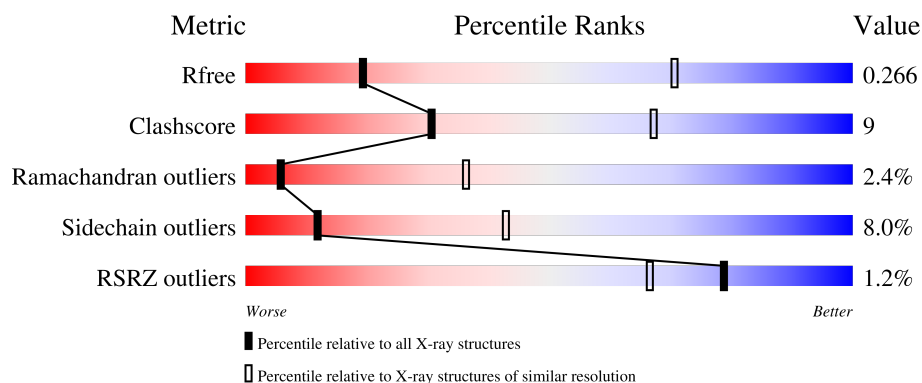
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	307	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>26%</div> <div>.</div> </div> </div>
1	B	307	<div> <div>71%</div> <div>27%</div> <div>.</div> </div>
1	C	307	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	D	307	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	E	307	
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

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
2	MBR	A	401	-	-	-	X
2	MBR	A	402	-	-	X	-
2	MBR	B	402	-	-	X	-
2	MBR	C	402	-	-	X	-
2	MBR	D	401	-	-	-	X
2	MBR	D	402	-	-	X	-
2	MBR	E	401	-	-	X	-
2	MBR	E	402	-	-	X	X
2	MBR	F	401	-	-	X	X
2	MBR	F	402	-	-	X	-
2	MBR	G	402	-	-	X	X
2	MBR	H	402	-	-	X	-
2	MBR	I	401	-	-	-	X
2	MBR	I	402	-	-	X	X
2	MBR	J	402	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25042 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

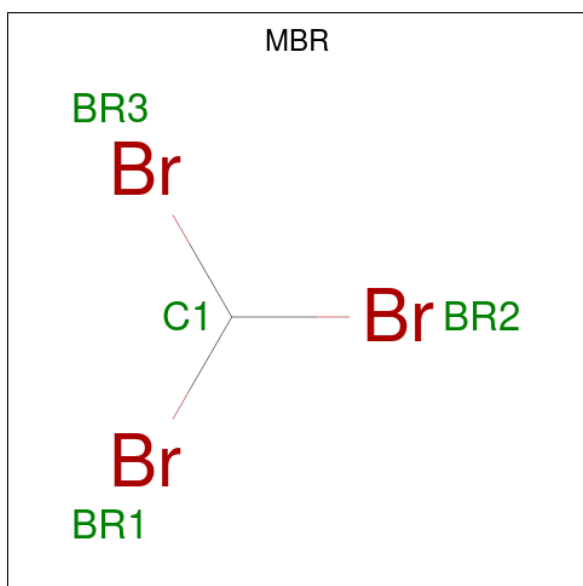
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	289	ASN	MET	conflict	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	289	ASN	MET	conflict	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	289	ASN	MET	conflict	UNP P0C7B7
D	164	GLY	-	insertion	UNP P0C7B7
D	289	ASN	MET	conflict	UNP P0C7B7
E	164	GLY	-	insertion	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	conflict	UNP P0C7B7
F	164	GLY	-	insertion	UNP P0C7B7
F	289	ASN	MET	conflict	UNP P0C7B7
G	164	GLY	-	insertion	UNP P0C7B7
G	289	ASN	MET	conflict	UNP P0C7B7
H	164	GLY	-	insertion	UNP P0C7B7
H	289	ASN	MET	conflict	UNP P0C7B7
I	164	GLY	-	insertion	UNP P0C7B7
I	289	ASN	MET	conflict	UNP P0C7B7
J	164	GLY	-	insertion	UNP P0C7B7
J	289	ASN	MET	conflict	UNP P0C7B7

- Molecule 2 is TRIBROMOMETHANE (three-letter code: MBR) (formula:  $\text{CHBr}_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Br 1 1	0	0
2	A	1	Total Br 1 1	0	0
2	A	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	B	1	Total Br 1 1	0	0
2	C	1	Total Br 1 1	0	0

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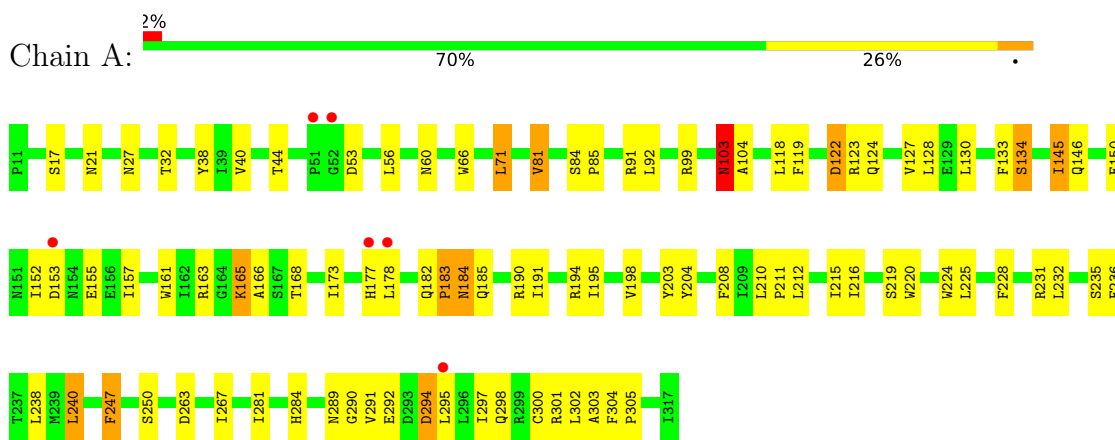
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Br 1	0	0
2	D	1	Total 1	Br 1	0	0
2	D	1	Total 1	Br 1	0	0
2	E	1	Total 1	Br 1	0	0
2	E	1	Total 1	Br 1	0	0
2	F	1	Total 1	Br 1	0	0
2	F	1	Total 1	Br 1	0	0
2	F	1	Total 1	Br 1	0	0
2	G	1	Total 1	Br 1	0	0
2	G	1	Total 1	Br 1	0	0
2	H	1	Total 1	Br 1	0	0
2	H	1	Total 1	Br 1	0	0
2	I	1	Total 1	Br 1	0	0
2	I	1	Total 1	Br 1	0	0
2	J	1	Total 1	Br 1	0	0
2	J	1	Total 1	Br 1	0	0

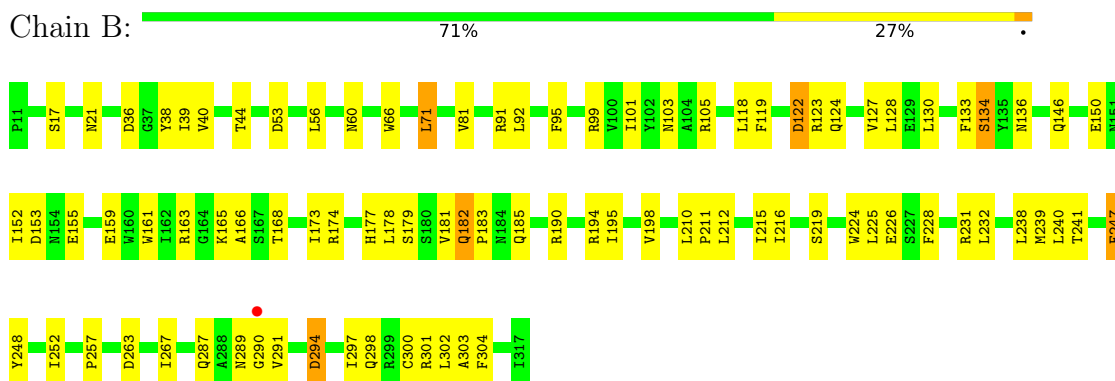
### 3 Residue-property plots [i](#)

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.

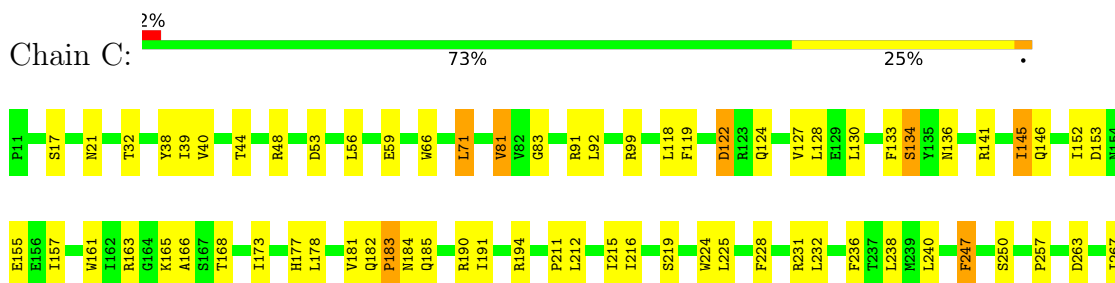
#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

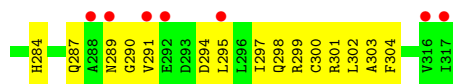


#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

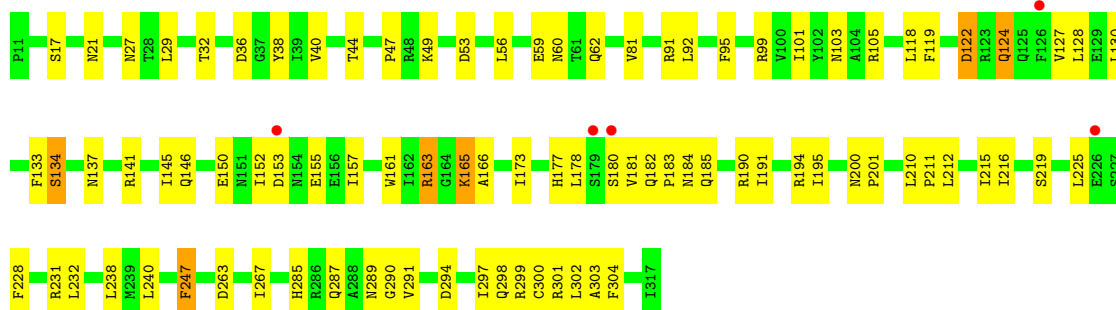


#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

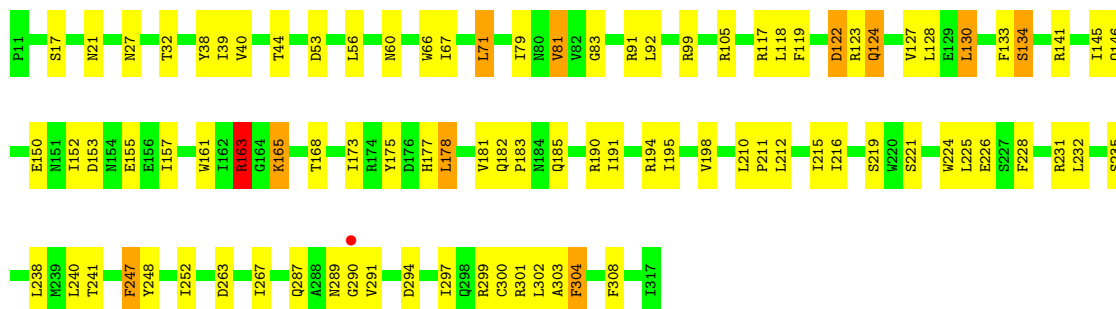




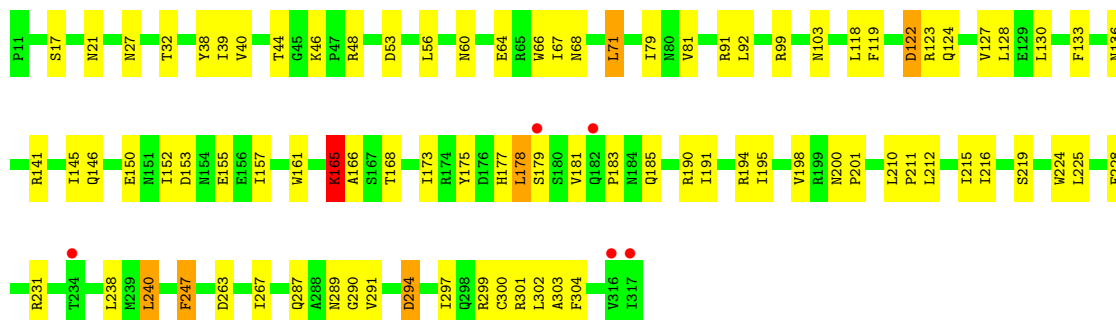
● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



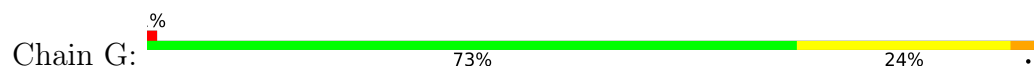
● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



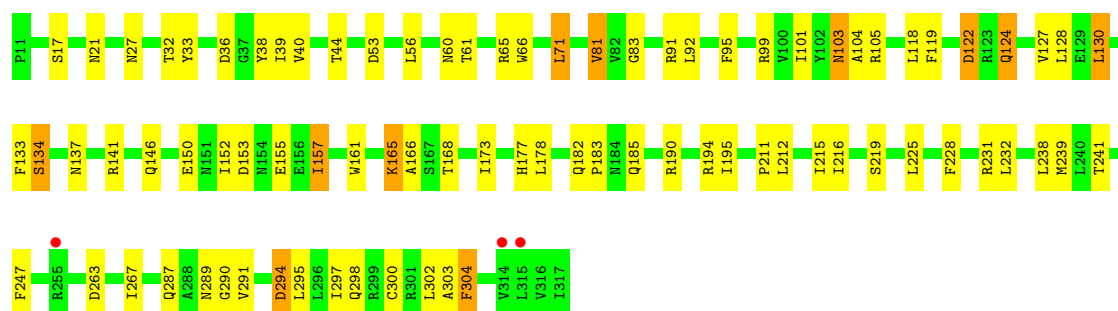
● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



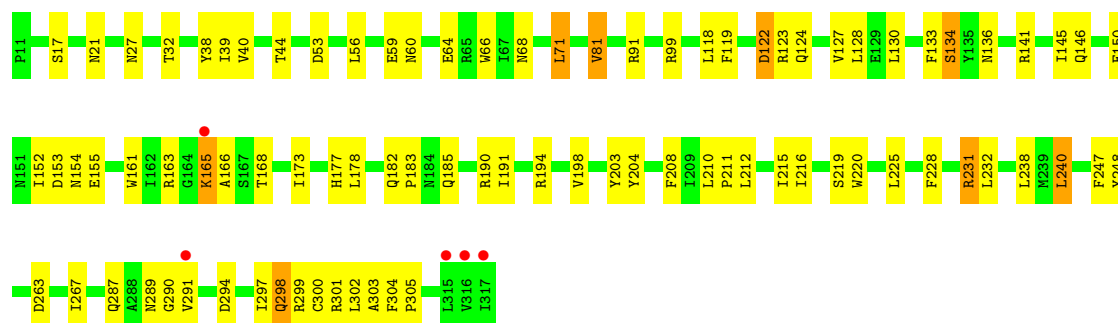
● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



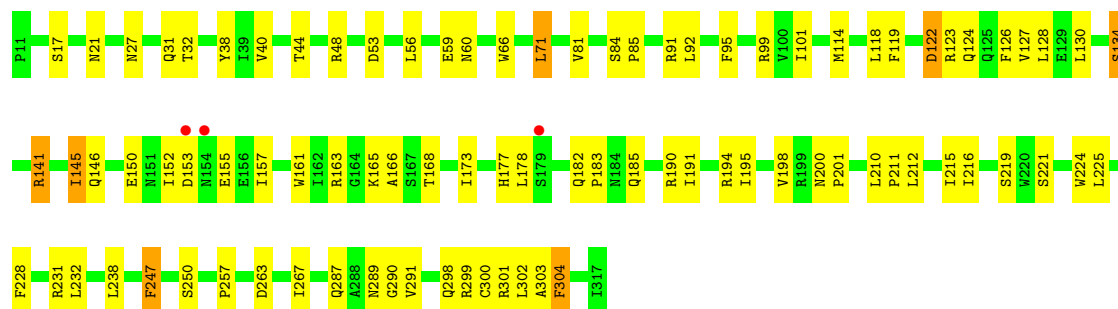




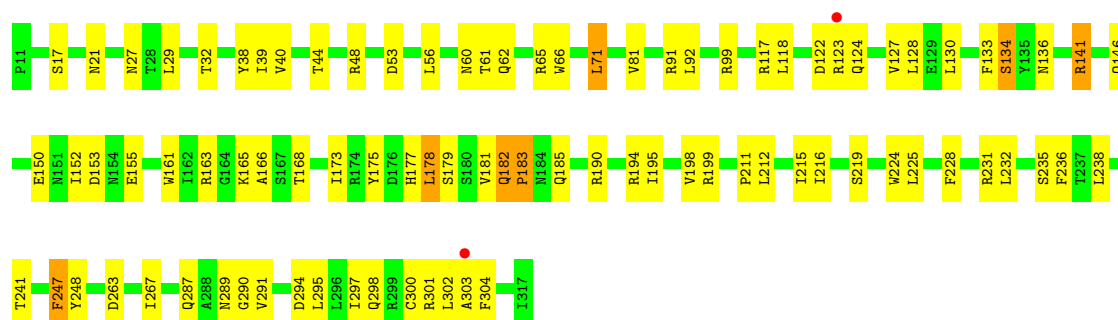
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.11Å 266.25Å 110.75Å 90.00° 109.78° 90.00°	Depositor
Resolution (Å)	44.08 – 3.65 44.08 – 3.65	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.08-3.65) 98.8 (44.08-3.65)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 3.66Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.229 , 0.264 0.232 , 0.266	Depositor DCC
$R_{free}$ test set	3184 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.2	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 45.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	25042	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MBR

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	0.41	2/2570 (0.1%)	0.66	0/3503
1	B	0.41	4/2570 (0.2%)	0.65	0/3503
1	C	0.38	0/2570	0.65	0/3503
1	D	0.46	4/2570 (0.2%)	0.75	5/3503 (0.1%)
1	E	0.42	2/2570 (0.1%)	0.80	6/3503 (0.2%)
1	F	0.41	2/2570 (0.1%)	0.93	8/3503 (0.2%)
1	G	0.45	3/2570 (0.1%)	0.68	0/3503
1	H	0.40	2/2570 (0.1%)	0.67	1/3503 (0.0%)
1	I	0.44	2/2570 (0.1%)	0.66	0/3503
1	J	0.37	0/2570	0.65	2/3503 (0.1%)
All	All	0.42	21/25700 (0.1%)	0.72	22/35030 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	ASN	CG-ND2	-7.94	1.13	1.32
1	D	124	GLN	CD-NE2	-7.72	1.13	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	103	ASN	CG-OD1	-7.47	1.07	1.24
1	G	124	GLN	CD-NE2	-7.36	1.14	1.32
1	E	124	GLN	CD-NE2	-6.89	1.15	1.32

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	LYS	O-C-N	-27.07	79.38	122.70
1	F	165	LYS	CA-C-O	-19.47	79.22	120.10
1	E	163	ARG	NE-CZ-NH1	18.98	129.79	120.30
1	F	165	LYS	CA-C-N	18.34	157.54	117.20
1	E	163	ARG	NE-CZ-NH2	-14.78	112.91	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Mainchain
1	D	165	LYS	Mainchain
1	D	47	PRO	Mainchain
1	E	165	LYS	Mainchain
1	F	165	LYS	Mainchain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2502	0	2469	60	1
1	B	2502	0	2469	49	0
1	C	2502	0	2469	53	0
1	D	2502	0	2469	50	1
1	E	2502	0	2469	67	0
1	F	2502	0	2469	53	0
1	G	2502	0	2469	50	0
1	H	2502	0	2469	49	0
1	I	2502	0	2469	54	0
1	J	2502	0	2469	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	4	0
2	B	2	0	0	3	0
2	C	2	0	0	3	0
2	D	2	0	0	3	0
2	E	2	0	0	8	0
2	F	3	0	0	6	0
2	G	2	0	0	5	0
2	H	2	0	0	4	0
2	I	2	0	0	5	0
2	J	2	0	0	4	0
All	All	25042	0	24690	456	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 9.

The worst 5 of 456 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:J:195:ILE:HD12	2:J:402:MBR:BR1	1.28	1.84
1:E:221:SER:HB3	2:E:401:MBR:BR1	1.37	1.76
1:I:195:ILE:HD12	2:I:402:MBR:BR1	1.57	1.56
1:C:128:LEU:HD13	2:C:402:MBR:BR1	1.61	1.52
1:J:195:ILE:CD1	2:J:402:MBR:BR1	2.19	1.44

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)
1:A:292:GLU:OE1	1:D:49:LYS:NZ[1_556]	2.01	0.19

## 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	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	4	32
1	B	305/307 (99%)	275 (90%)	21 (7%)	9 (3%)	4	32
1	C	305/307 (99%)	276 (90%)	23 (8%)	6 (2%)	7	40
1	D	305/307 (99%)	275 (90%)	22 (7%)	8 (3%)	5	34
1	E	305/307 (99%)	273 (90%)	26 (8%)	6 (2%)	7	40
1	F	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	6	37
1	G	305/307 (99%)	276 (90%)	21 (7%)	8 (3%)	5	34
1	H	305/307 (99%)	273 (90%)	25 (8%)	7 (2%)	6	37
1	I	305/307 (99%)	274 (90%)	24 (8%)	7 (2%)	6	37
1	J	305/307 (99%)	275 (90%)	23 (8%)	7 (2%)	6	37
All	All	3050/3070 (99%)	2748 (90%)	228 (8%)	74 (2%)	6	36

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	B	53	ASP
1	B	60	ASN
1	B	166	ALA
1	C	166	ALA

### 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	274/275 (100%)	253 (92%)	21 (8%)	13	44
1	B	274/275 (100%)	251 (92%)	23 (8%)	11	41
1	C	274/275 (100%)	250 (91%)	24 (9%)	10	40
1	D	274/275 (100%)	254 (93%)	20 (7%)	14	46
1	E	274/275 (100%)	251 (92%)	23 (8%)	11	41
1	F	274/275 (100%)	254 (93%)	20 (7%)	14	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	274/275 (100%)	251 (92%)	23 (8%)	11	41
1	H	274/275 (100%)	250 (91%)	24 (9%)	10	40
1	I	274/275 (100%)	254 (93%)	20 (7%)	14	46
1	J	274/275 (100%)	252 (92%)	22 (8%)	12	43
All	All	2740/2750 (100%)	2520 (92%)	220 (8%)	12	43

5 of 220 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	118	LEU
1	G	165	LYS
1	J	304	PHE
1	J	39	ILE
1	F	136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	177	HIS
1	G	103	ASN
1	F	103	ASN
1	E	298	GLN
1	F	298	GLN

### 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 [i](#)

Of 22 ligands modelled in this entry, 22 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/307 (100%)	-0.25	6 (1%) 65 50	73, 122, 214, 290	0
1	B	307/307 (100%)	-0.34	1 (0%) 94 89	73, 118, 212, 284	0
1	C	307/307 (100%)	-0.30	7 (2%) 60 44	74, 117, 214, 284	0
1	D	307/307 (100%)	-0.25	5 (1%) 72 58	77, 118, 215, 285	0
1	E	307/307 (100%)	-0.37	1 (0%) 94 89	77, 122, 213, 287	0
1	F	307/307 (100%)	-0.36	5 (1%) 72 58	80, 122, 214, 285	0
1	G	307/307 (100%)	-0.32	3 (0%) 82 71	77, 116, 214, 288	0
1	H	307/307 (100%)	-0.33	5 (1%) 72 58	78, 118, 210, 285	0
1	I	307/307 (100%)	-0.22	3 (0%) 82 71	73, 118, 214, 304	0
1	J	307/307 (100%)	-0.36	2 (0%) 87 79	86, 123, 217, 313	0
All	All	3070/3070 (100%)	-0.31	38 (1%) 79 66	73, 119, 215, 313	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	317	ILE	7.9
1	C	289	ASN	6.9
1	C	317	ILE	6.4
1	I	153	ASP	6.2
1	H	291	VAL	5.3

### 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 ⓘ

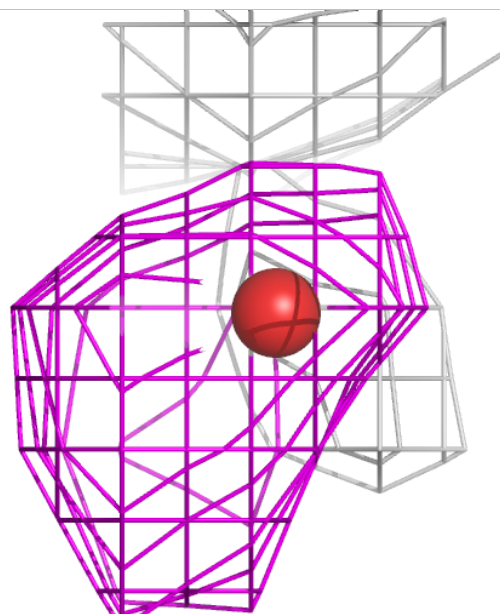
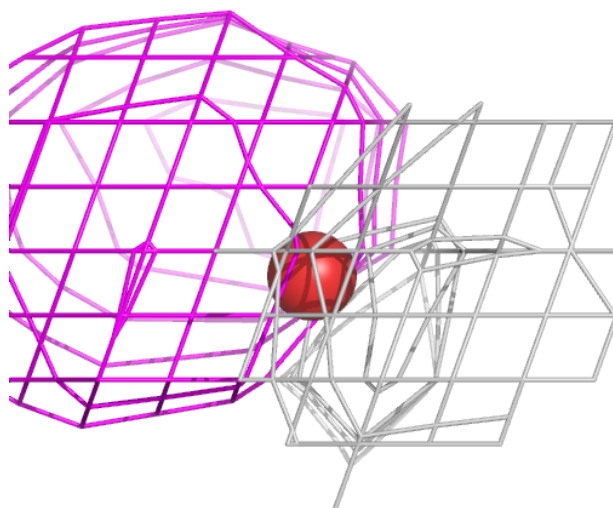
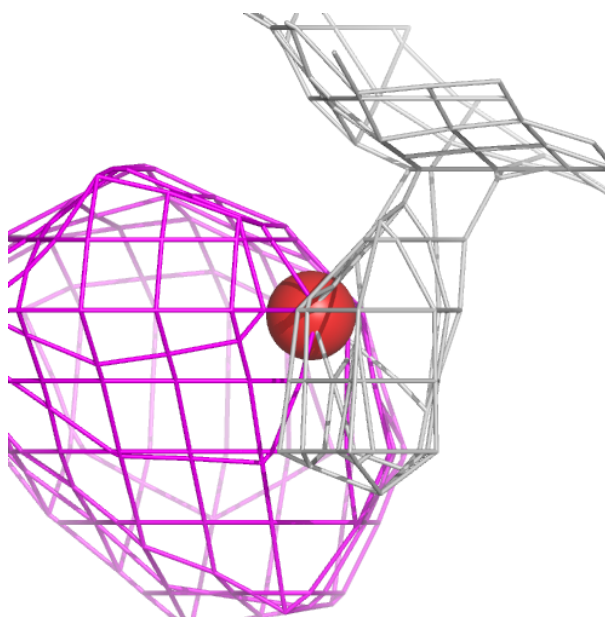
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MBR	J	401	1/4	0.19	0.38	212,212,212,212	0
2	MBR	F	401	1/4	0.37	0.77	201,201,201,201	0
2	MBR	C	401	1/4	0.39	0.32	193,193,193,193	0
2	MBR	A	401	1/4	0.51	1.12	210,210,210,210	0
2	MBR	D	401	1/4	0.59	0.52	186,186,186,186	0
2	MBR	H	401	1/4	0.64	0.13	195,195,195,195	0
2	MBR	E	402	1/4	0.65	1.38	211,211,211,211	0
2	MBR	I	401	1/4	0.68	0.57	186,186,186,186	0
2	MBR	B	401	1/4	0.69	0.11	200,200,200,200	0
2	MBR	A	403	1/4	0.71	0.21	154,154,154,154	0
2	MBR	G	401	1/4	0.74	0.12	190,190,190,190	0
2	MBR	I	402	1/4	0.78	2.39	212,212,212,212	0
2	MBR	F	403	1/4	0.78	0.14	166,166,166,166	0
2	MBR	G	402	1/4	0.79	2.77	186,186,186,186	0
2	MBR	H	402	1/4	0.83	0.78	198,198,198,198	0
2	MBR	E	401	1/4	0.89	0.31	190,190,190,190	0
2	MBR	F	402	1/4	0.90	0.93	196,196,196,196	0
2	MBR	J	402	1/4	0.90	3.30	202,202,202,202	0
2	MBR	B	402	1/4	0.93	1.74	195,195,195,195	0
2	MBR	C	402	1/4	0.93	0.84	195,195,195,195	0
2	MBR	A	402	1/4	0.95	1.67	201,201,201,201	0
2	MBR	D	402	1/4	0.96	3.41	185,185,185,185	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.

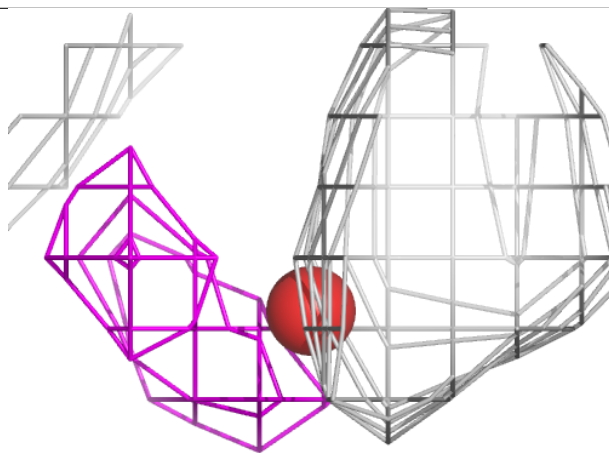
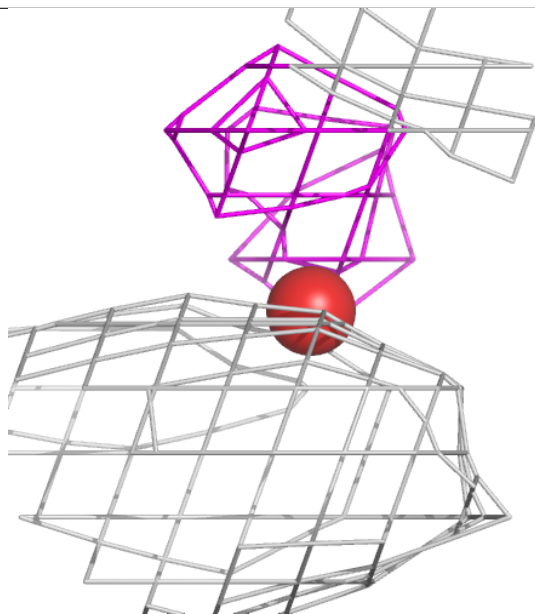
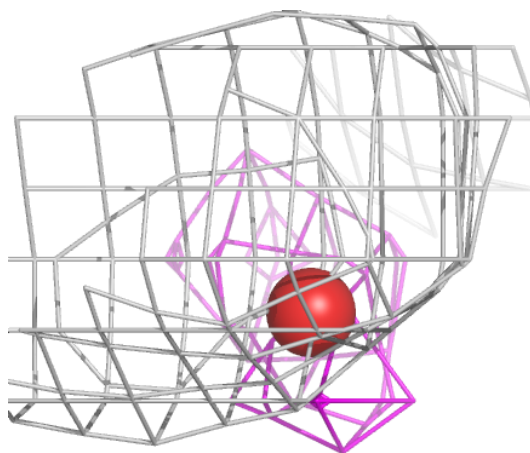
**Electron density around MBR F 401:**

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



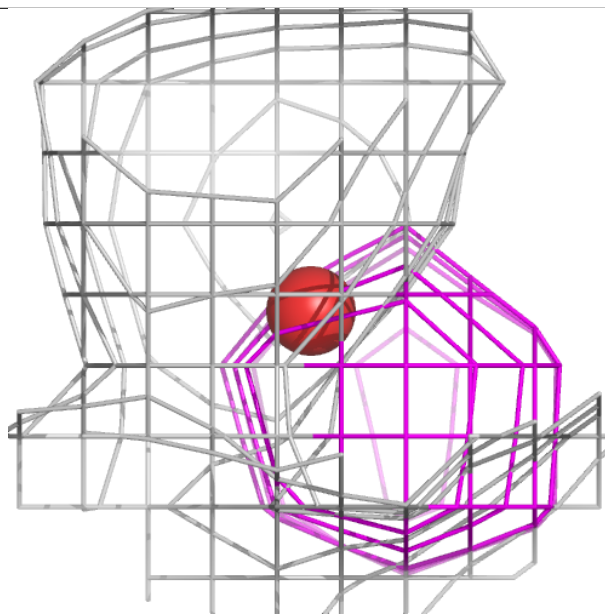
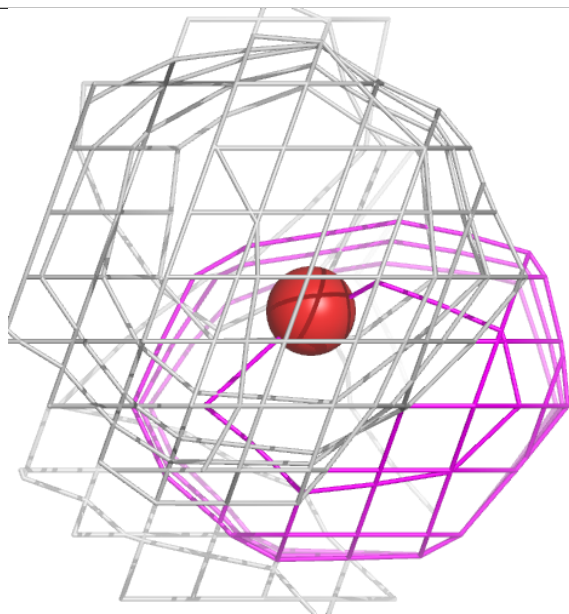
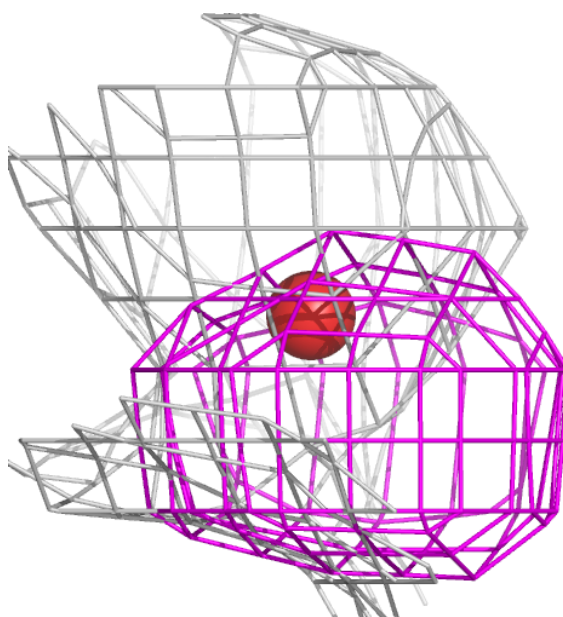
**Electron density around MBR A 401:**

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



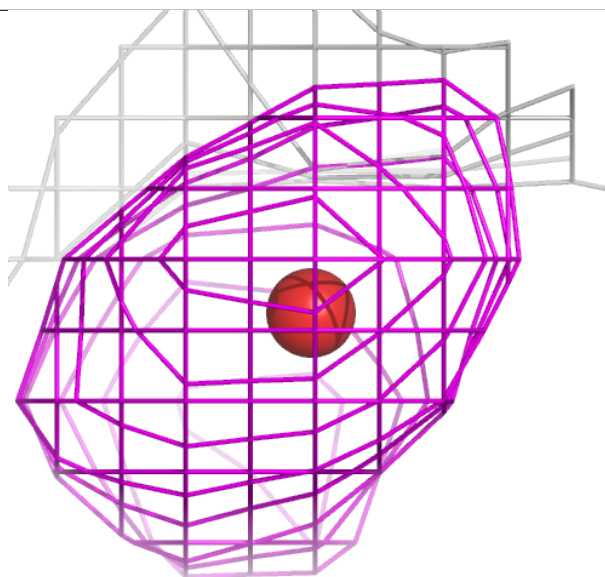
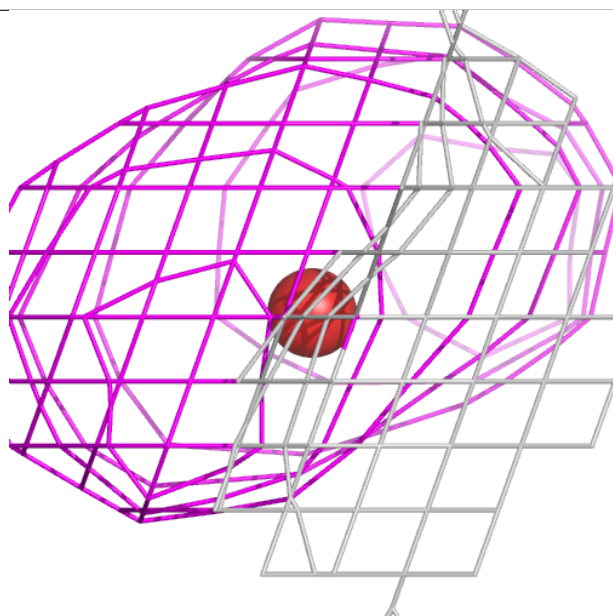
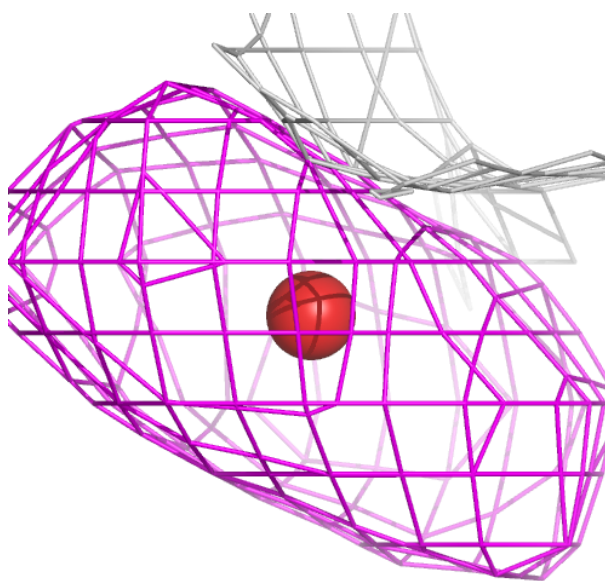
**Electron density around MBR D 401:**

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



**Electron density around MBR E 402:**

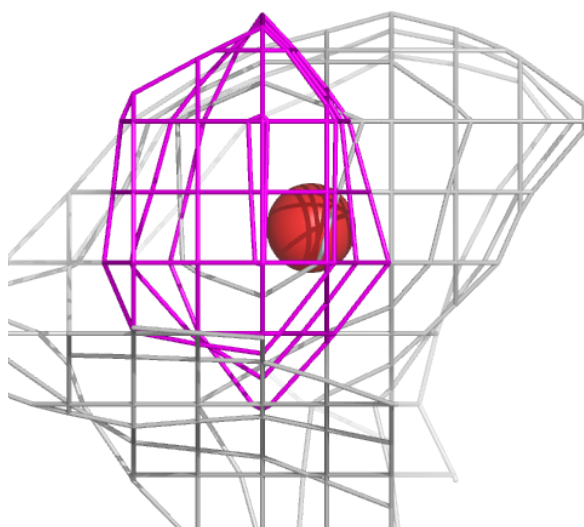
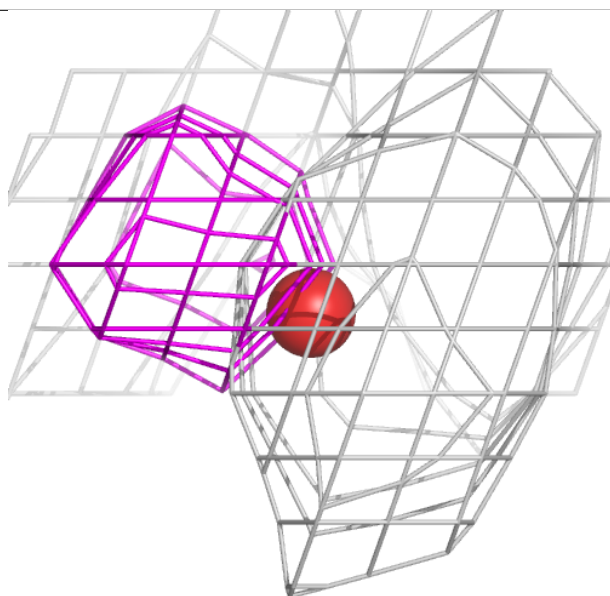
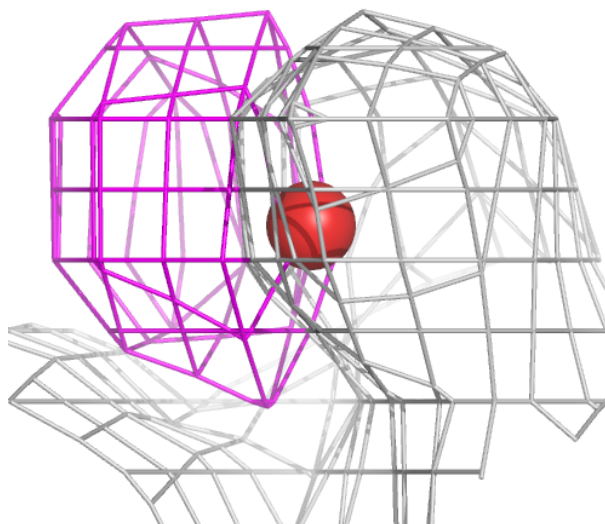
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





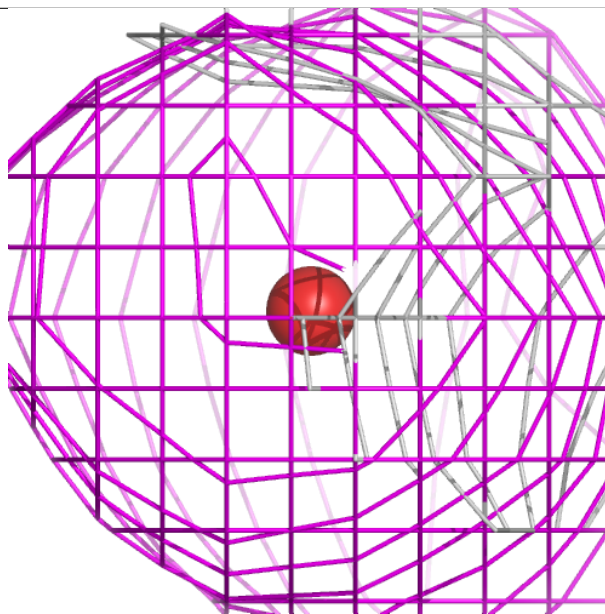
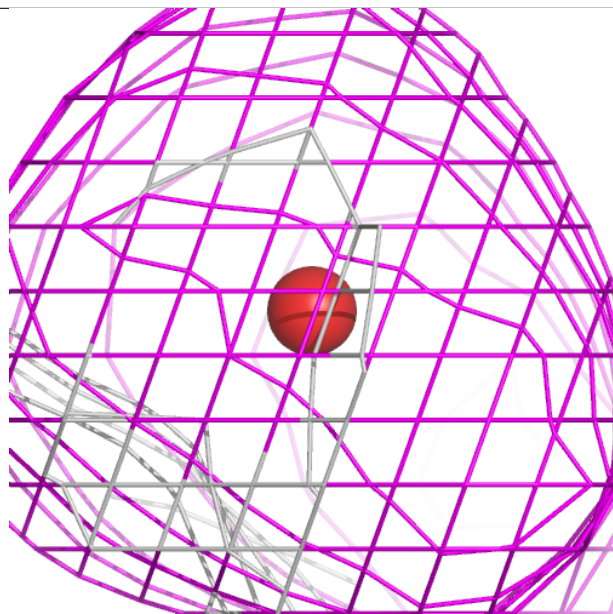
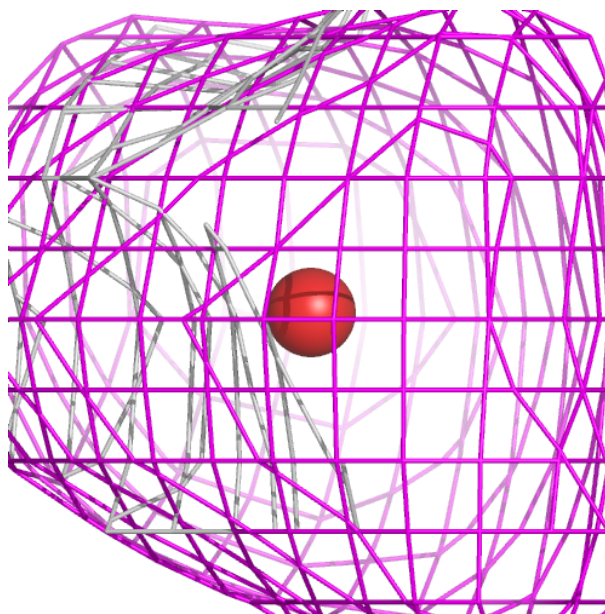
**Electron density around MBR I 401:**

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



**Electron density around MBR I 402:**

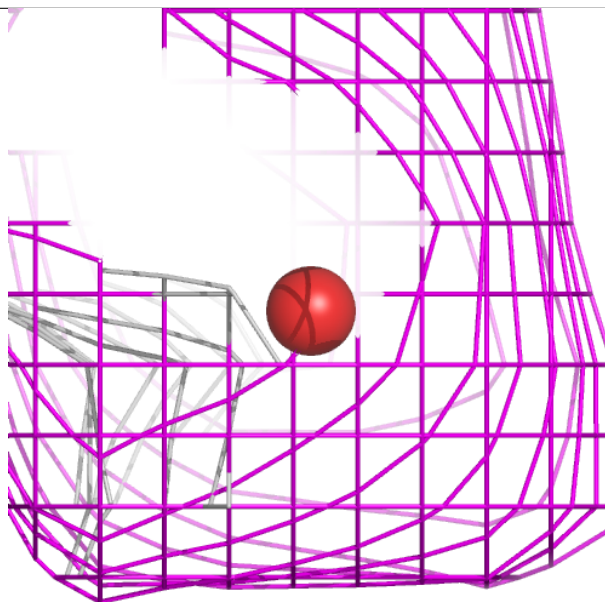
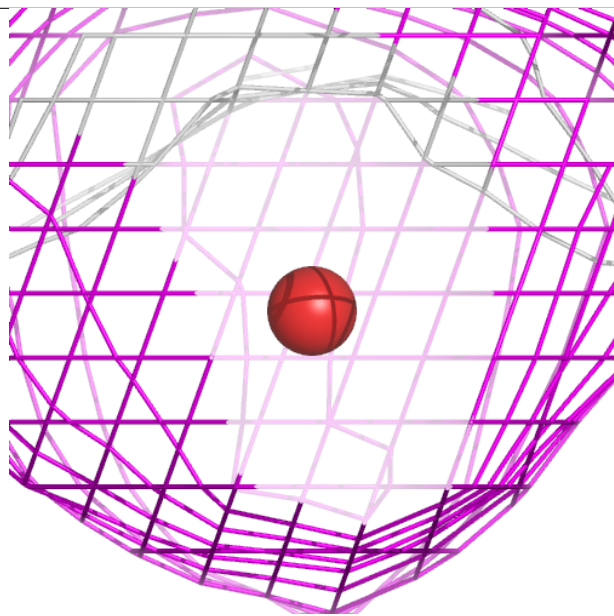
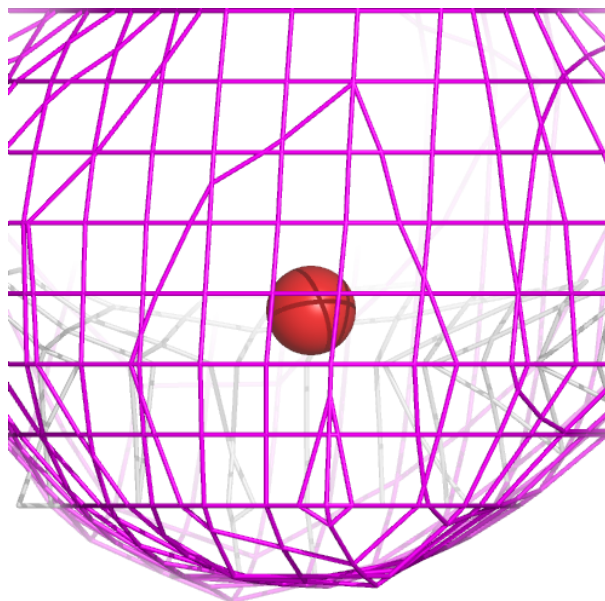
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MBR G 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 ⓘ

There are no such residues in this entry.