



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:25 am BST

PDB ID : 3RQW  
Title : Crystal structure of acetylcholine bound to a prokaryotic pentameric ligand-gated ion channel, ELIC  
Authors : Pan, J.J.; Chen, Q.; Yoshida, K.; Cohen, A.; Kong, X.P.; Xu, Y.; Tang, P.  
Deposited on : 2011-04-28  
Resolution : 2.91 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.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

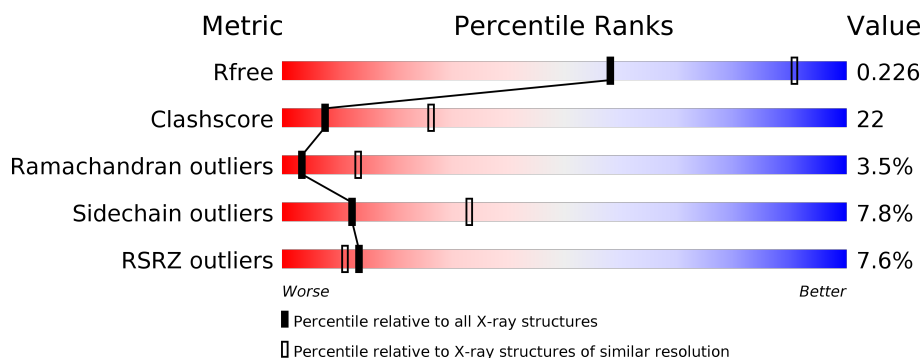
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	322	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	322	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	322	<div> <div>5%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>5%</div> <div>5%</div> </div> </div>
1	D	322	<div> <div>7%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>6%</div> <div>5%</div> </div> </div>
1	E	322	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>5%</div> <div>5%</div> </div> </div>
1	F	322	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>5%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	322	
1	H	322	
1	I	322	
1	J	322	

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
4	GOL	A	325	-	-	-	X
4	GOL	A	326	-	-	X	-
4	GOL	B	326	-	-	X	-
4	GOL	B	327	-	-	X	-
4	GOL	C	325	-	-	X	-
4	GOL	F	328	-	-	X	-
4	GOL	G	328	-	-	X	-
4	GOL	H	325	-	-	X	-
4	GOL	I	327	-	-	X	-
4	GOL	I	329	-	-	X	-
4	GOL	J	325	-	-	X	-

## 2 Entry composition

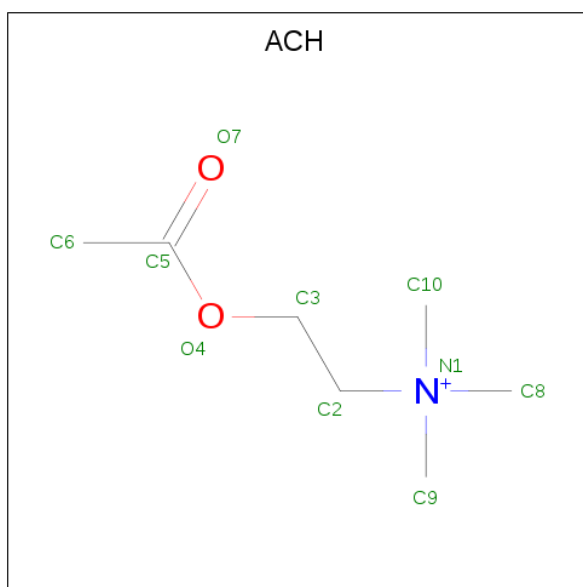
There are 5 unique types of molecules in this entry. The entry contains 25508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2505	1633	416	450	6			

- Molecule 2 is ACETYLCHOLINE (three-letter code: ACH) (formula: C<sub>7</sub>H<sub>16</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		
2	C	1	Total	C	N	O	0	0
			10	7	1	2		
2	D	1	Total	C	N	O	0	0
			10	7	1	2		
2	E	1	Total	C	N	O	0	0
			10	7	1	2		
2	F	1	Total	C	N	O	0	0
			10	7	1	2		
2	G	1	Total	C	N	O	0	0
			10	7	1	2		
2	H	1	Total	C	N	O	0	0
			10	7	1	2		
2	I	1	Total	C	N	O	0	0
			10	7	1	2		
2	J	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	G	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	I	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	J	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	G	1	Total C O 4 2 2	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	8	Total O 8 8	0	0
5	C	10	Total O 10 10	0	0
5	D	15	Total O 15 15	0	0
5	E	11	Total O 11 11	0	0
5	F	4	Total O 4 4	0	0

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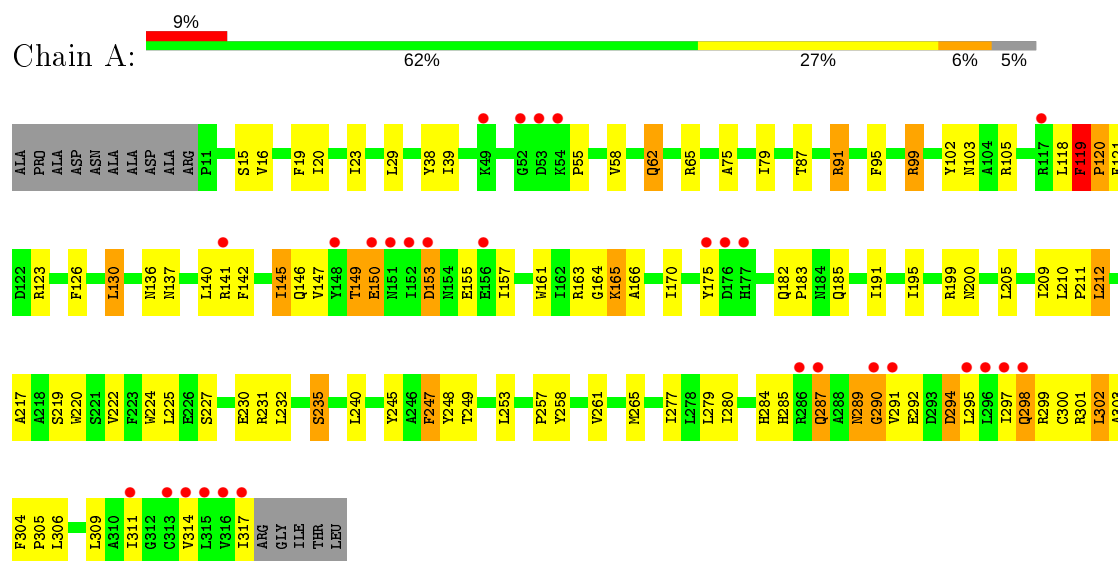
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	12	Total 12	O 12	0	0
5	H	7	Total 7	O 7	0	0
5	I	6	Total 6	O 6	0	0
5	J	7	Total 7	O 7	0	0

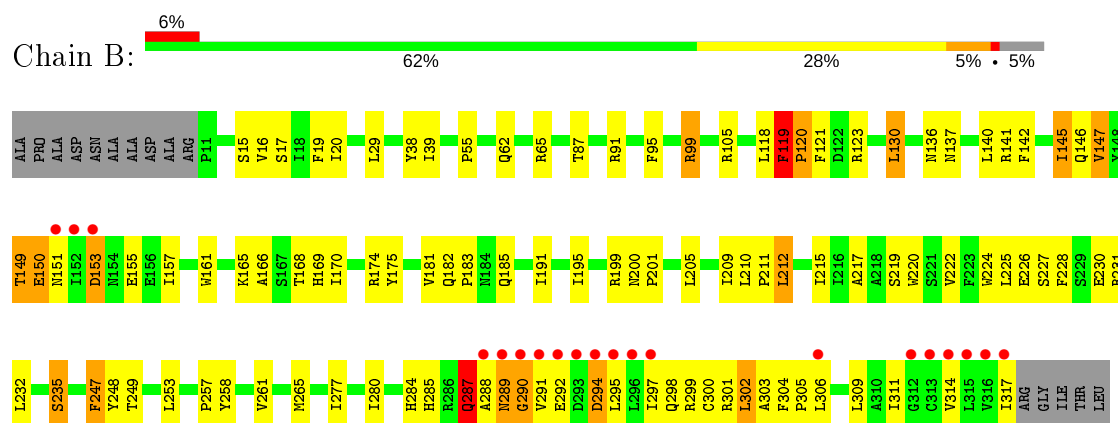
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

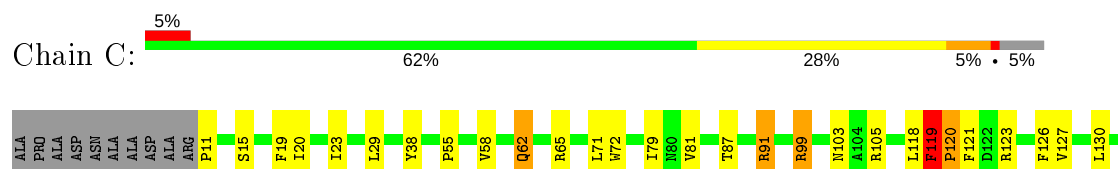
#### • Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

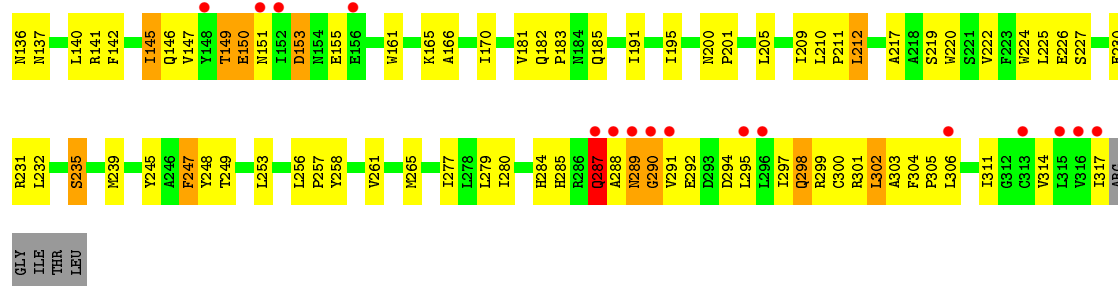


#### • Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



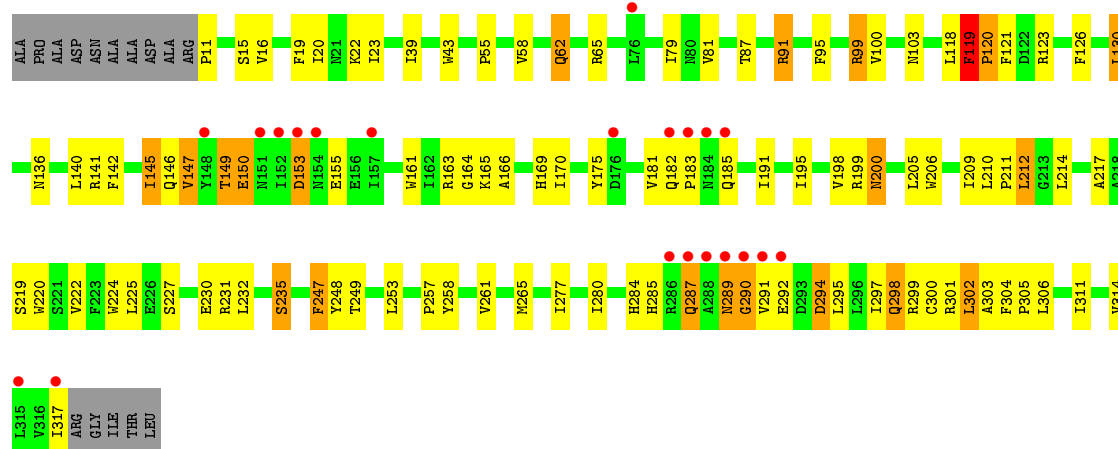
#### • Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*





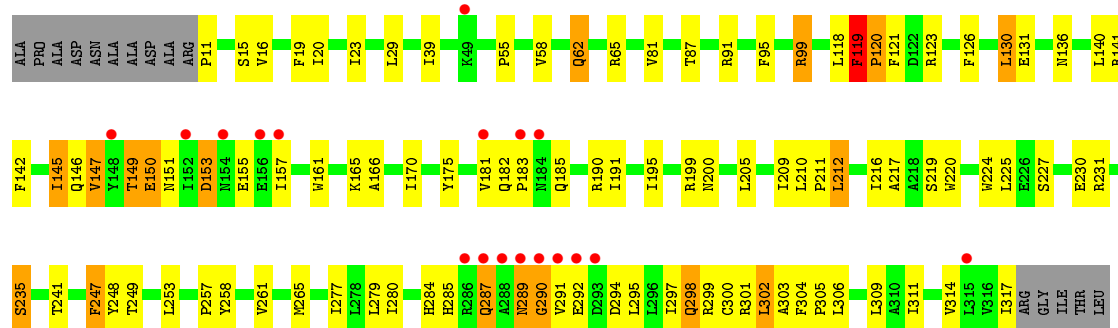
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

Chain D: 7% 62% 26% 6% 5%



• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

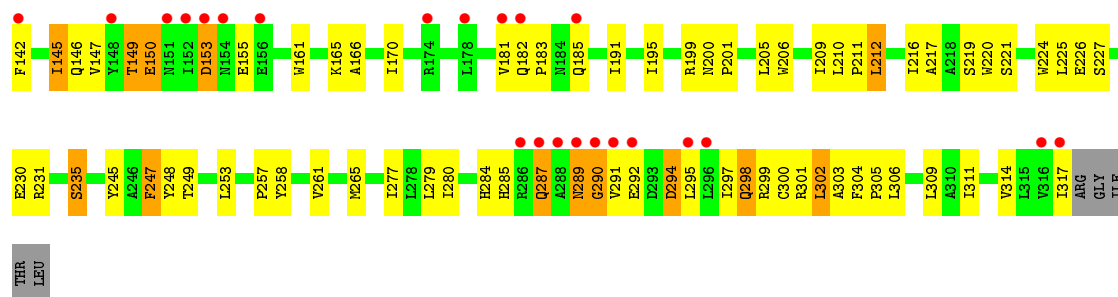
Chain E: 6% 64% 26% 5% 5%



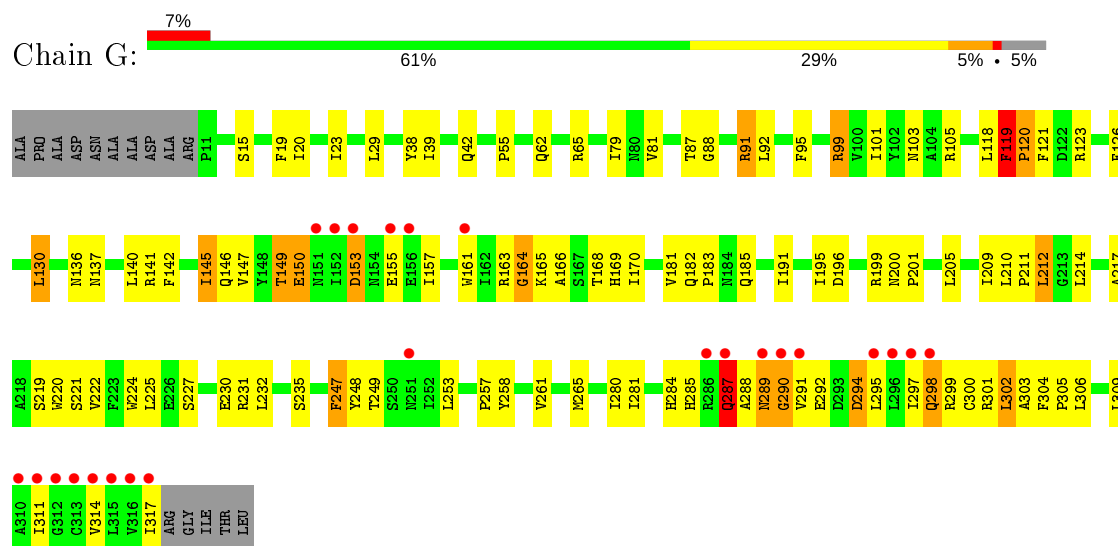
• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

Chain F: 7% 64% 27% 5% 5%

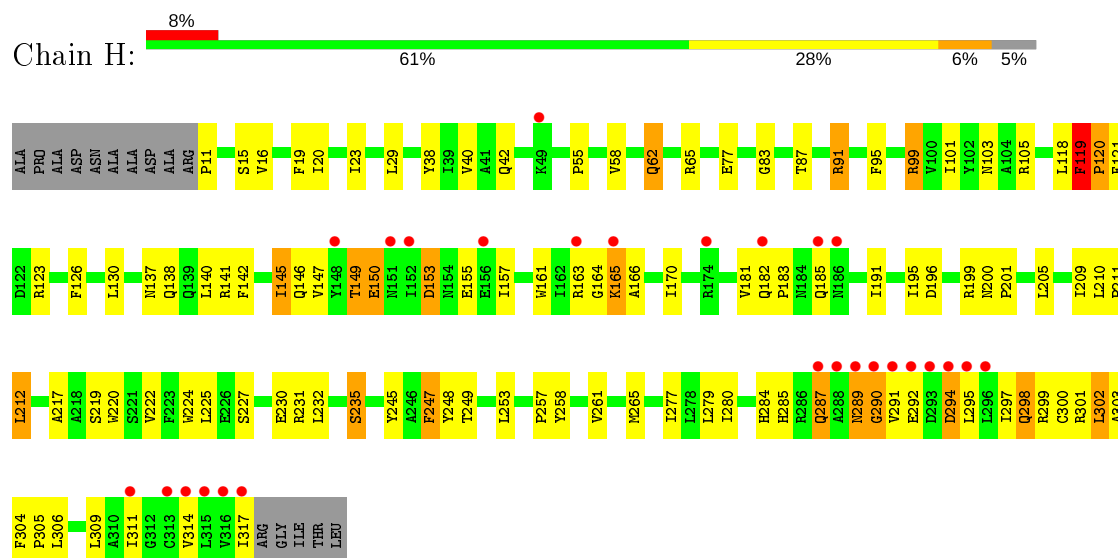




- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

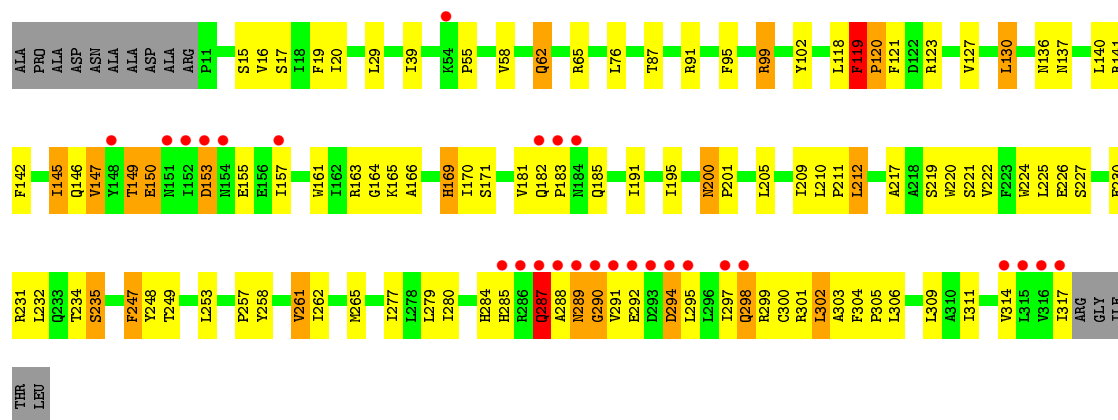


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*

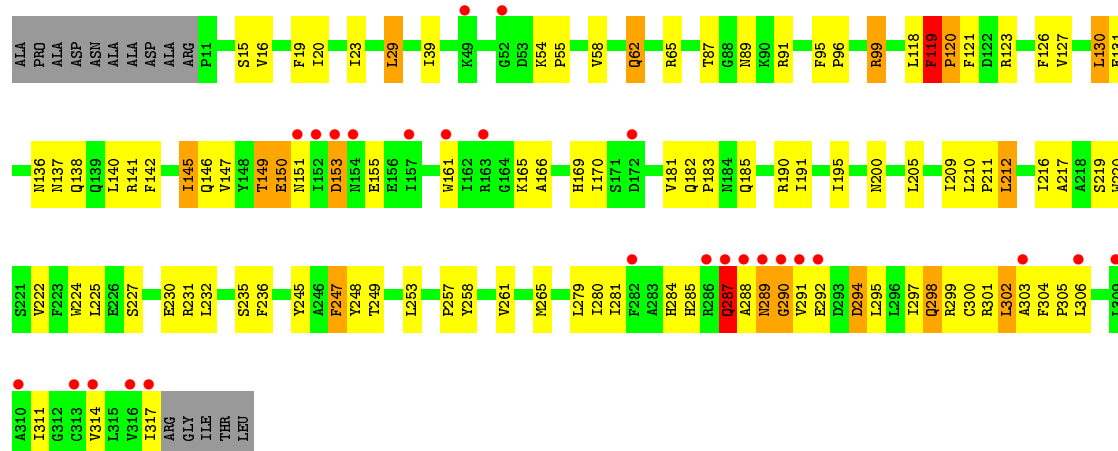


- Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*





• Molecule 1: ELIC Pentameric Ligand Gated Ion Channel from *Erwinia Chrysanthemi*



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.76Å 266.07Å 111.16Å 90.00° 107.82° 90.00°	Depositor
Resolution (Å)	24.98 – 2.91 29.80 – 2.91	Depositor EDS
% Data completeness (in resolution range)	92.5 (24.98-2.91) 98.0 (29.80-2.91)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.206 , 0.231 0.202 , 0.226	Depositor DCC
$R_{free}$ test set	6262 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	25508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: GOL, ACH, MES

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	0.38	0/2573	0.54	1/3507 (0.0%)
1	B	0.44	0/2573	0.57	1/3507 (0.0%)
1	C	0.43	0/2573	0.57	1/3507 (0.0%)
1	D	0.46	0/2573	0.58	1/3507 (0.0%)
1	E	0.42	0/2573	0.56	1/3507 (0.0%)
1	F	0.41	0/2573	0.55	1/3507 (0.0%)
1	G	0.43	0/2573	0.60	2/3507 (0.1%)
1	H	0.42	0/2573	0.57	1/3507 (0.0%)
1	I	0.43	0/2573	0.58	1/3507 (0.0%)
1	J	0.41	0/2573	0.56	1/3507 (0.0%)
All	All	0.42	0/25730	0.57	11/35070 (0.0%)

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	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
1	I	0	1
1	J	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	119	PHE	C-N-CD	-7.40	104.31	120.60
1	J	119	PHE	C-N-CD	-7.25	104.66	120.60
1	G	302	LEU	CA-CB-CG	7.10	131.62	115.30
1	E	119	PHE	C-N-CD	-7.04	105.12	120.60
1	G	119	PHE	C-N-CD	-7.01	105.17	120.60

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	PHE	Peptide
1	A	164	GLY	Peptide
1	B	119	PHE	Peptide
1	C	119	PHE	Peptide
1	D	119	PHE	Peptide

## 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	2505	0	2478	118	0
1	B	2505	0	2478	121	0
1	C	2505	0	2478	109	0
1	D	2505	0	2478	111	0
1	E	2505	0	2478	105	0
1	F	2505	0	2478	115	0
1	G	2505	0	2478	130	0
1	H	2505	0	2478	117	0
1	I	2505	0	2478	121	0
1	J	2505	0	2478	119	0
2	A	10	0	16	2	0
2	B	10	0	16	2	0
2	C	10	0	16	3	0
2	D	10	0	16	2	0
2	E	10	0	16	4	0
2	F	10	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	10	0	16	1	0
2	H	10	0	16	1	0
2	I	10	0	16	3	0
2	J	10	0	16	3	0
3	A	12	0	12	1	0
3	B	12	0	12	0	0
3	D	24	0	24	1	0
3	E	12	0	12	0	0
3	F	12	0	12	2	0
3	G	12	0	12	0	0
3	I	12	0	12	0	0
3	J	12	0	12	0	0
4	A	12	0	16	6	0
4	B	18	0	24	12	0
4	C	12	0	16	4	0
4	D	12	0	16	1	0
4	E	12	0	16	2	0
4	F	24	0	32	5	0
4	G	22	0	28	9	0
4	H	12	0	16	9	0
4	I	30	0	40	10	0
4	J	6	0	8	7	0
5	A	10	0	0	2	0
5	B	8	0	0	2	0
5	C	10	0	0	4	0
5	D	15	0	0	9	0
5	E	11	0	0	5	0
5	F	4	0	0	5	0
5	G	12	0	0	3	0
5	H	7	0	0	5	0
5	I	6	0	0	4	0
5	J	7	0	0	6	0
All	All	25508	0	25260	1114	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 22.

The worst 5 of 1114 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:C:136:ASN:O	4:C:325:GOL:H2	1.36	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:140:LEU:HD21	5:I:334:HOH:O	1.48	1.11
1:B:140:LEU:HD11	5:B:332:HOH:O	1.51	1.11
1:D:140:LEU:HD11	5:D:341:HOH:O	1.52	1.09
1:H:140:LEU:HD11	5:H:331:HOH:O	1.52	1.07

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	305/322 (95%)	270 (88%)	25 (8%)	10 (3%)	4	14
1	B	305/322 (95%)	271 (89%)	24 (8%)	10 (3%)	4	14
1	C	305/322 (95%)	267 (88%)	29 (10%)	9 (3%)	4	16
1	D	305/322 (95%)	269 (88%)	24 (8%)	12 (4%)	3	11
1	E	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	3	13
1	F	305/322 (95%)	268 (88%)	28 (9%)	9 (3%)	4	16
1	G	305/322 (95%)	265 (87%)	29 (10%)	11 (4%)	3	13
1	H	305/322 (95%)	268 (88%)	27 (9%)	10 (3%)	4	14
1	I	305/322 (95%)	271 (89%)	22 (7%)	12 (4%)	3	11
1	J	305/322 (95%)	267 (88%)	26 (8%)	12 (4%)	3	11
All	All	3050/3220 (95%)	2681 (88%)	263 (9%)	106 (4%)	3	13

5 of 106 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	120	PRO
1	A	149	THR

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Mol	Chain	Res	Type
1	A	165	LYS
1	B	119	PHE

### 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	275/284 (97%)	255 (93%)	20 (7%)	14	37
1	B	275/284 (97%)	253 (92%)	22 (8%)	12	32
1	C	275/284 (97%)	254 (92%)	21 (8%)	13	35
1	D	275/284 (97%)	251 (91%)	24 (9%)	10	29
1	E	275/284 (97%)	253 (92%)	22 (8%)	12	32
1	F	275/284 (97%)	255 (93%)	20 (7%)	14	37
1	G	275/284 (97%)	254 (92%)	21 (8%)	13	35
1	H	275/284 (97%)	256 (93%)	19 (7%)	15	40
1	I	275/284 (97%)	252 (92%)	23 (8%)	11	30
1	J	275/284 (97%)	253 (92%)	22 (8%)	12	32
All	All	2750/2840 (97%)	2536 (92%)	214 (8%)	12	33

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	130	LEU
1	F	212	LEU
1	J	91	ARG
1	E	212	LEU
1	E	317	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	151	ASN

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Mol	Chain	Res	Type
1	F	69	ASN
1	J	69	ASN
1	E	284	HIS
1	F	200	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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

46 ligands are modelled in this entry.

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	GOL	F	328	-	5,5,5	0.77	0	5,5,5	0.59	0
4	GOL	B	326	-	5,5,5	0.75	0	5,5,5	0.58	0
4	GOL	G	328	-	5,5,5	0.59	0	5,5,5	0.98	0
4	GOL	J	325	-	5,5,5	0.70	0	5,5,5	0.62	0
2	ACH	H	323	-	9,9,9	1.00	1 (11%)	12,12,12	0.89	1 (8%)
4	GOL	F	325	-	5,5,5	0.70	0	5,5,5	0.42	0
4	GOL	G	327	-	3,3,5	0.49	0	2,2,5	0.31	0
2	ACH	G	323	-	9,9,9	1.10	1 (11%)	12,12,12	0.62	0
4	GOL	C	324	-	5,5,5	0.60	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	D	325	-	12,12,12	2.24	1 (8%)	14,16,16	2.71	5 (35%)
2	ACH	C	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.78	0
4	GOL	H	324	-	5,5,5	0.45	0	5,5,5	0.77	0
4	GOL	F	327	-	5,5,5	0.83	0	5,5,5	0.29	0
4	GOL	D	327	-	5,5,5	0.69	0	5,5,5	0.55	0
3	MES	A	324	-	12,12,12	2.14	1 (8%)	14,16,16	2.53	7 (50%)
4	GOL	A	326	-	5,5,5	0.77	0	5,5,5	0.30	0
2	ACH	I	323	-	9,9,9	1.01	1 (11%)	12,12,12	0.75	0
3	MES	I	324	-	12,12,12	2.08	1 (8%)	14,16,16	2.44	8 (57%)
3	MES	D	324	-	12,12,12	2.14	1 (8%)	14,16,16	2.44	6 (42%)
2	ACH	J	323	-	9,9,9	1.04	1 (11%)	12,12,12	0.78	0
4	GOL	I	326	-	5,5,5	0.72	0	5,5,5	0.81	0
2	ACH	D	323	-	9,9,9	1.14	1 (11%)	12,12,12	0.86	0
2	ACH	F	323	-	9,9,9	1.05	1 (11%)	12,12,12	0.85	0
4	GOL	I	327	-	5,5,5	0.75	0	5,5,5	0.32	0
3	MES	F	324	-	12,12,12	2.18	1 (8%)	14,16,16	2.47	7 (50%)
2	ACH	E	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.72	0
3	MES	G	324	-	12,12,12	2.28	1 (8%)	14,16,16	2.49	8 (57%)
4	GOL	G	325	-	5,5,5	0.71	0	5,5,5	0.50	0
4	GOL	E	326	-	5,5,5	0.83	0	5,5,5	0.54	0
4	GOL	D	326	-	5,5,5	0.75	0	5,5,5	0.54	0
2	ACH	A	323	-	9,9,9	1.08	1 (11%)	12,12,12	0.67	0
4	GOL	H	325	-	5,5,5	0.94	0	5,5,5	0.42	0
3	MES	J	324	-	12,12,12	2.25	1 (8%)	14,16,16	2.51	7 (50%)
2	ACH	B	323	-	9,9,9	1.02	1 (11%)	12,12,12	0.74	0
4	GOL	B	327	-	5,5,5	0.81	0	5,5,5	0.67	0
4	GOL	E	325	-	5,5,5	0.78	0	5,5,5	0.31	0
3	MES	E	324	-	12,12,12	2.20	1 (8%)	14,16,16	2.41	7 (50%)
4	GOL	C	325	-	5,5,5	0.73	0	5,5,5	0.70	0
4	GOL	G	326	-	5,5,5	0.64	0	5,5,5	0.42	0
4	GOL	F	326	-	5,5,5	0.65	0	5,5,5	0.55	0
3	MES	B	324	-	12,12,12	2.15	1 (8%)	14,16,16	2.51	7 (50%)
4	GOL	A	325	-	5,5,5	0.73	0	5,5,5	0.59	0
4	GOL	I	325	-	5,5,5	0.76	0	5,5,5	0.40	0
4	GOL	B	325	-	5,5,5	0.68	0	5,5,5	0.64	0
4	GOL	I	328	-	5,5,5	0.69	0	5,5,5	0.46	0
4	GOL	I	329	-	5,5,5	0.83	0	5,5,5	0.57	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	GOL	F	328	-	-	4/4/4/4	-
4	GOL	B	326	-	-	2/4/4/4	-
4	GOL	G	328	-	-	1/4/4/4	-
4	GOL	J	325	-	-	0/4/4/4	-
2	ACH	H	323	-	-	0/7/7/7	-
4	GOL	F	325	-	-	2/4/4/4	-
4	GOL	G	327	-	-	1/1/1/4	-
2	ACH	G	323	-	-	1/7/7/7	-
4	GOL	C	324	-	-	4/4/4/4	-
3	MES	D	325	-	-	5/6/14/14	0/1/1/1
2	ACH	C	323	-	-	0/7/7/7	-
4	GOL	H	324	-	-	2/4/4/4	-
4	GOL	F	327	-	-	0/4/4/4	-
4	GOL	D	327	-	-	2/4/4/4	-
3	MES	A	324	-	-	5/6/14/14	0/1/1/1
4	GOL	A	326	-	-	0/4/4/4	-
2	ACH	I	323	-	-	1/7/7/7	-
3	MES	I	324	-	-	5/6/14/14	0/1/1/1
3	MES	D	324	-	-	4/6/14/14	0/1/1/1
2	ACH	J	323	-	-	0/7/7/7	-
4	GOL	I	326	-	-	1/4/4/4	-
2	ACH	D	323	-	-	0/7/7/7	-
2	ACH	F	323	-	-	0/7/7/7	-
4	GOL	I	327	-	-	0/4/4/4	-
3	MES	F	324	-	-	5/6/14/14	0/1/1/1
2	ACH	E	323	-	-	0/7/7/7	-
3	MES	G	324	-	-	4/6/14/14	0/1/1/1
4	GOL	G	325	-	-	3/4/4/4	-
4	GOL	E	326	-	-	0/4/4/4	-
4	GOL	D	326	-	-	0/4/4/4	-
2	ACH	A	323	-	-	0/7/7/7	-
4	GOL	H	325	-	-	2/4/4/4	-
3	MES	J	324	-	-	1/6/14/14	0/1/1/1
2	ACH	B	323	-	-	1/7/7/7	-
4	GOL	B	327	-	-	3/4/4/4	-
4	GOL	E	325	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	E	324	-	-	2/6/14/14	0/1/1/1
4	GOL	C	325	-	-	0/4/4/4	-
4	GOL	G	326	-	-	2/4/4/4	-
4	GOL	F	326	-	-	1/4/4/4	-
3	MES	B	324	-	-	4/6/14/14	0/1/1/1
4	GOL	A	325	-	-	0/4/4/4	-
4	GOL	I	325	-	-	0/4/4/4	-
4	GOL	B	325	-	-	3/4/4/4	-
4	GOL	I	328	-	-	4/4/4/4	-
4	GOL	I	329	-	-	2/4/4/4	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	324	MES	C8-S	-7.55	1.66	1.77
3	J	324	MES	C8-S	-7.49	1.66	1.77
3	D	325	MES	C8-S	-7.44	1.66	1.77
3	E	324	MES	C8-S	-7.28	1.67	1.77
3	F	324	MES	C8-S	-7.14	1.67	1.77

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	325	MES	O3S-S-C8	6.99	117.07	105.77
3	G	324	MES	O1S-S-C8	5.10	113.06	106.92
3	F	324	MES	C5-N4-C3	5.01	120.11	108.83
3	A	324	MES	C5-N4-C3	4.80	119.62	108.83
3	E	324	MES	C5-N4-C3	4.78	119.59	108.83

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	325	MES	C8-C7-N4-C3
3	D	325	MES	N4-C7-C8-S
4	B	325	GOL	C1-C2-C3-O3
4	D	327	GOL	O1-C1-C2-C3
3	A	324	MES	C7-C8-S-O1S

There are no ring outliers.

28 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	328	GOL	4	0
4	B	326	GOL	5	0
4	G	328	GOL	9	0
4	J	325	GOL	7	0
2	H	323	ACH	1	0
4	F	325	GOL	1	0
2	G	323	ACH	1	0
3	D	325	MES	1	0
2	C	323	ACH	3	0
4	H	324	GOL	3	0
4	D	327	GOL	1	0
3	A	324	MES	1	0
4	A	326	GOL	4	0
2	I	323	ACH	3	0
2	J	323	ACH	3	0
2	D	323	ACH	2	0
2	F	323	ACH	2	0
4	I	327	GOL	4	0
3	F	324	MES	2	0
2	E	323	ACH	4	0
4	E	326	GOL	2	0
2	A	323	ACH	2	0
4	H	325	GOL	6	0
2	B	323	ACH	2	0
4	B	327	GOL	7	0
4	C	325	GOL	4	0
4	A	325	GOL	2	0
4	I	329	GOL	6	0

## 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	307/322 (95%)	0.18	29 (9%) 8 6	57, 90, 172, 210	0
1	B	307/322 (95%)	0.02	20 (6%) 18 15	52, 87, 172, 213	0
1	C	307/322 (95%)	0.06	16 (5%) 27 24	51, 87, 173, 210	0
1	D	307/322 (95%)	0.02	21 (6%) 17 14	51, 84, 170, 210	0
1	E	307/322 (95%)	0.04	18 (5%) 22 19	54, 88, 170, 208	0
1	F	307/322 (95%)	0.08	24 (7%) 13 10	53, 94, 173, 208	0
1	G	307/322 (95%)	0.10	24 (7%) 13 10	51, 87, 168, 209	0
1	H	307/322 (95%)	0.26	27 (8%) 10 7	55, 89, 174, 208	0
1	I	307/322 (95%)	0.07	27 (8%) 10 7	57, 90, 172, 211	0
1	J	307/322 (95%)	0.05	26 (8%) 10 8	59, 94, 175, 208	0
All	All	3070/3220 (95%)	0.09	232 (7%) 13 11	51, 89, 174, 213	0

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	23.2
1	A	152	ILE	18.3
1	G	152	ILE	17.0
1	E	291	VAL	12.9
1	H	152	ILE	12.5

### 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 carbohydrates 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
4	GOL	B	326	6/6	0.68	0.21	83,110,138,150	0
4	GOL	A	325	6/6	0.73	0.49	69,109,127,135	0
4	GOL	E	325	6/6	0.73	0.22	85,99,110,130	0
4	GOL	I	327	6/6	0.78	0.38	88,92,119,126	0
4	GOL	H	324	6/6	0.79	0.20	56,69,111,111	0
4	GOL	F	325	6/6	0.80	0.38	84,100,114,125	0
4	GOL	C	324	6/6	0.81	0.41	79,89,98,113	0
4	GOL	J	325	6/6	0.82	0.15	64,92,106,114	0
4	GOL	H	325	6/6	0.83	0.57	80,85,104,115	0
4	GOL	B	325	6/6	0.83	0.35	77,88,103,117	0
3	MES	A	324	12/12	0.84	0.14	91,140,168,188	0
4	GOL	F	328	6/6	0.84	0.13	73,86,114,121	0
4	GOL	F	327	6/6	0.84	0.34	77,98,110,119	0
4	GOL	I	329	6/6	0.84	0.19	61,71,110,133	0
4	GOL	A	326	6/6	0.85	0.18	79,90,125,127	0
4	GOL	G	325	6/6	0.85	0.28	79,94,101,112	0
3	MES	F	324	12/12	0.86	0.19	106,147,159,185	0
3	MES	D	324	12/12	0.86	0.17	107,132,160,169	0
4	GOL	F	326	6/6	0.86	0.35	83,98,121,143	0
3	MES	D	325	12/12	0.86	0.15	85,140,157,157	0
4	GOL	G	328	6/6	0.87	0.18	50,79,101,104	0
4	GOL	G	326	6/6	0.87	0.29	91,96,115,116	0
3	MES	I	324	12/12	0.87	0.17	109,142,169,177	0
3	MES	J	324	12/12	0.87	0.13	139,157,169,184	0
4	GOL	I	325	6/6	0.88	0.10	88,93,105,121	0
4	GOL	I	328	6/6	0.88	0.77	87,95,119,124	0
4	GOL	B	327	6/6	0.88	0.14	55,62,83,90	0
3	MES	G	324	12/12	0.89	0.14	99,122,143,150	0
3	MES	E	324	12/12	0.90	0.09	123,143,171,178	0
4	GOL	G	327	4/6	0.90	0.34	86,96,104,106	0
4	GOL	I	326	6/6	0.91	0.26	73,91,114,119	0
4	GOL	D	327	6/6	0.91	0.25	51,79,98,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	C	325	6/6	0.91	0.13	60,66,78,92	0
4	GOL	D	326	6/6	0.91	0.39	96,100,101,106	0
4	GOL	E	326	6/6	0.92	0.16	67,89,129,133	0
2	ACH	J	323	10/10	0.93	0.20	56,74,82,89	0
3	MES	B	324	12/12	0.94	0.09	120,136,164,175	0
2	ACH	C	323	10/10	0.95	0.23	54,69,74,75	0
2	ACH	E	323	10/10	0.96	0.18	57,76,82,85	0
2	ACH	H	323	10/10	0.97	0.30	57,74,81,83	0
2	ACH	A	323	10/10	0.97	0.23	56,66,76,77	0
2	ACH	G	323	10/10	0.97	0.19	48,68,76,77	0
2	ACH	I	323	10/10	0.97	0.19	54,67,76,80	0
2	ACH	B	323	10/10	0.97	0.18	53,65,78,80	0
2	ACH	D	323	10/10	0.98	0.17	53,62,70,73	0
2	ACH	F	323	10/10	0.99	0.17	48,67,74,76	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.