WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 8, 2024 – 03:14 am GMT

PDB ID	:	6FIZ
Title	:	Crystal Structure of CNG mimicking NaK-EAPP mutant (T67A) cocrystallized with K+
Authors	:	Napolitano, L.M.R.; De March, M.; Steiner, R.A.; Onesti, S.
Deposited on	:	2018-01-19
Resolution	:	2.63 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

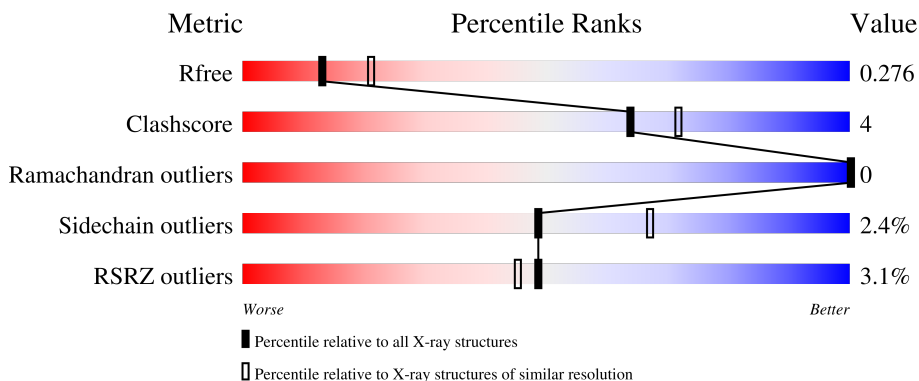|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.63 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		0.276
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		2.4%
RSRZ outliers		3.1%

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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	94	3% 87% 10% ·
1	B	94	9% 84% 11% · ·
1	C	94	9% 86% 11% ·
1	D	94	5% 85% 12% ·
1	E	94	5% 84% 12% · ·

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Mol	Chain	Length	Quality of chain
1	F	94	5% ... 83% ... 13% ··
1	G	94	2% ... 86% ... 11% ·
1	H	94	9% ... 88% ... 6% ··
1	I	94	90% ... 10%
1	J	94	% ... 84% ... 13% ·
1	K	94	85% ... 12% ·
1	L	94	90% ... 6% ·
1	M	94	90% ... 10%
1	N	94	89% ... 7% ·
1	O	94	93% ... ···
1	P	94	88% ... 9% ·

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	GLY	B	201	-	X	-	-
2	GLY	D	201	-	X	-	-
2	GLY	D	204	-	X	-	-
2	GLY	E	201	-	X	-	-
2	GLY	G	202	-	X	-	-
2	GLY	H	201	-	X	-	-
2	GLY	H	203	-	X	-	-
2	GLY	I	202	-	X	-	-
2	GLY	J	204	-	X	-	-
2	GLY	J	205	-	X	-	-
2	GLY	J	208	-	X	-	-
2	GLY	K	202	-	X	-	-
2	GLY	K	203	-	X	-	-
2	GLY	M	201	-	X	-	-
2	GLY	M	202	-	X	-	-
2	GLY	M	206	-	X	-	-
2	GLY	N	205	-	X	-	-
2	GLY	N	207	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLY	O	204	-	X	-	-
2	GLY	P	201	-	X	-	-
2	GLY	P	202	-	X	-	-
2	GLY	P	203	-	X	-	-
4	MPD	F	203	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11844 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 Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	91	Total 708	C 481	N 104	O 123	0	0	0
1	B	91	Total 708	C 481	N 104	O 123	0	0	0
1	C	91	Total 708	C 481	N 104	O 123	0	0	0
1	D	91	Total 708	C 481	N 104	O 123	0	0	0
1	E	91	Total 708	C 481	N 104	O 123	0	0	0
1	F	91	Total 708	C 481	N 104	O 123	0	0	0
1	G	91	Total 708	C 481	N 104	O 123	0	0	0
1	H	91	Total 708	C 481	N 104	O 123	0	0	0
1	I	94	Total 730	C 494	N 108	O 128	0	0	0
1	J	91	Total 717	C 487	N 106	O 124	0	1	0
1	K	91	Total 708	C 481	N 104	O 123	0	0	0
1	L	91	Total 708	C 481	N 104	O 123	0	0	0
1	M	94	Total 730	C 494	N 108	O 128	0	0	0
1	N	91	Total 708	C 481	N 104	O 123	0	0	0
1	O	91	Total 708	C 481	N 104	O 123	0	0	0
1	P	91	Total 708	C 481	N 104	O 123	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP Q81HW2
A	67	ALA	THR	engineered mutation	UNP Q16280
A	110	VAL	-	expression tag	UNP Q81HW2
A	111	VAL	-	expression tag	UNP Q81HW2
A	112	PRO	-	expression tag	UNP Q81HW2
B	19	ALA	-	expression tag	UNP Q81HW2
B	67	ALA	THR	engineered mutation	UNP Q16280
B	110	VAL	-	expression tag	UNP Q81HW2
B	111	VAL	-	expression tag	UNP Q81HW2
B	112	PRO	-	expression tag	UNP Q81HW2
C	19	ALA	-	expression tag	UNP Q81HW2
C	67	ALA	THR	engineered mutation	UNP Q16280
C	110	VAL	-	expression tag	UNP Q81HW2
C	111	VAL	-	expression tag	UNP Q81HW2
C	112	PRO	-	expression tag	UNP Q81HW2
D	19	ALA	-	expression tag	UNP Q81HW2
D	67	ALA	THR	engineered mutation	UNP Q16280
D	110	VAL	-	expression tag	UNP Q81HW2
D	111	VAL	-	expression tag	UNP Q81HW2
D	112	PRO	-	expression tag	UNP Q81HW2
E	19	ALA	-	expression tag	UNP Q81HW2
E	67	ALA	THR	engineered mutation	UNP Q16280
E	110	VAL	-	expression tag	UNP Q81HW2
E	111	VAL	-	expression tag	UNP Q81HW2
E	112	PRO	-	expression tag	UNP Q81HW2
F	19	ALA	-	expression tag	UNP Q81HW2
F	67	ALA	THR	engineered mutation	UNP Q16280
F	110	VAL	-	expression tag	UNP Q81HW2
F	111	VAL	-	expression tag	UNP Q81HW2
F	112	PRO	-	expression tag	UNP Q81HW2
G	19	ALA	-	expression tag	UNP Q81HW2
G	67	ALA	THR	engineered mutation	UNP Q16280
G	110	VAL	-	expression tag	UNP Q81HW2
G	111	VAL	-	expression tag	UNP Q81HW2
G	112	PRO	-	expression tag	UNP Q81HW2
H	19	ALA	-	expression tag	UNP Q81HW2
H	67	ALA	THR	engineered mutation	UNP Q16280
H	110	VAL	-	expression tag	UNP Q81HW2
H	111	VAL	-	expression tag	UNP Q81HW2
H	112	PRO	-	expression tag	UNP Q81HW2
I	19	ALA	-	expression tag	UNP Q81HW2
I	67	ALA	THR	engineered mutation	UNP Q16280

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Chain	Residue	Modelled	Actual	Comment	Reference
I	110	VAL	-	expression tag	UNP Q81HW2
I	111	VAL	-	expression tag	UNP Q81HW2
I	112	PRO	-	expression tag	UNP Q81HW2
J	19	ALA	-	expression tag	UNP Q81HW2
J	67	ALA	THR	engineered mutation	UNP Q16280
J	110	VAL	-	expression tag	UNP Q81HW2
J	111	VAL	-	expression tag	UNP Q81HW2
J	112	PRO	-	expression tag	UNP Q81HW2
K	19	ALA	-	expression tag	UNP Q81HW2
K	67	ALA	THR	engineered mutation	UNP Q16280
K	110	VAL	-	expression tag	UNP Q81HW2
K	111	VAL	-	expression tag	UNP Q81HW2
K	112	PRO	-	expression tag	UNP Q81HW2
L	19	ALA	-	expression tag	UNP Q81HW2
L	67	ALA	THR	engineered mutation	UNP Q16280
L	110	VAL	-	expression tag	UNP Q81HW2
L	111	VAL	-	expression tag	UNP Q81HW2
L	112	PRO	-	expression tag	UNP Q81HW2
M	19	ALA	-	expression tag	UNP Q81HW2
M	67	ALA	THR	engineered mutation	UNP Q16280
M	110	VAL	-	expression tag	UNP Q81HW2
M	111	VAL	-	expression tag	UNP Q81HW2
M	112	PRO	-	expression tag	UNP Q81HW2
N	19	ALA	-	expression tag	UNP Q81HW2
N	67	ALA	THR	engineered mutation	UNP Q16280
N	110	VAL	-	expression tag	UNP Q81HW2
N	111	VAL	-	expression tag	UNP Q81HW2
N	112	PRO	-	expression tag	UNP Q81HW2
O	19	ALA	-	expression tag	UNP Q81HW2
O	67	ALA	THR	engineered mutation	UNP Q16280
O	110	VAL	-	expression tag	UNP Q81HW2
O	111	VAL	-	expression tag	UNP Q81HW2
O	112	PRO	-	expression tag	UNP Q81HW2
P	19	ALA	-	expression tag	UNP Q81HW2
P	67	ALA	THR	engineered mutation	UNP Q16280
P	110	VAL	-	expression tag	UNP Q81HW2
P	111	VAL	-	expression tag	UNP Q81HW2
P	112	PRO	-	expression tag	UNP Q81HW2

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: $C_2H_5NO_2$).
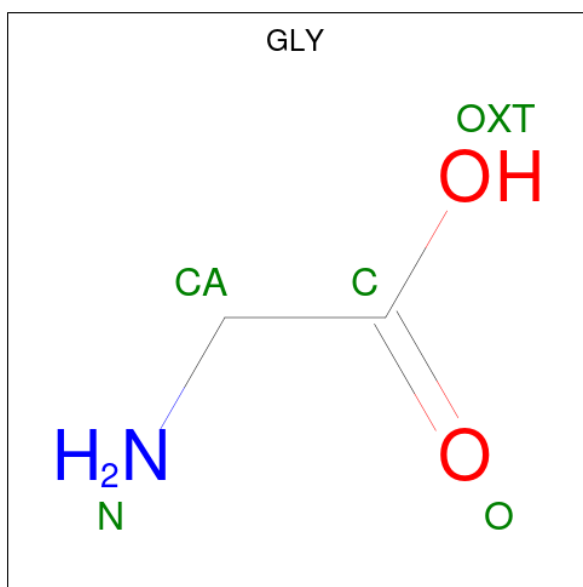
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 5	C 2	N 1	O 2	0	0
2	A	1	Total 5	C 2	N 1	O 2	0	0
2	B	1	Total 5	C 2	N 1	O 2	0	0
2	B	1	Total 5	C 2	N 1	O 2	0	0
2	B	1	Total 5	C 2	N 1	O 2	0	0
2	C	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	C 2	N 1	O 2	0	0
2	D	1	Total 5	C 2	N 1	O 2	0	0
2	E	1	Total 5	C 2	N 1	O 2	0	0
2	E	1	Total 5	C 2	N 1	O 2	0	0
2	E	1	Total 5	C 2	N 1	O 2	0	0
2	E	1	Total 5	C 2	N 1	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	N	O	0	0
			5	2	1	2		
2	F	1	Total	C	N	O	0	0
			5	2	1	2		
2	G	1	Total	C	N	O	0	0
			5	2	1	2		
2	G	1	Total	C	N	O	0	0
			5	2	1	2		
2	H	1	Total	C	N	O	0	0
			5	2	1	2		
2	H	1	Total	C	N	O	0	0
			5	2	1	2		
2	H	1	Total	C	N	O	0	0
			5	2	1	2		
2	H	1	Total	C	N	O	0	0
			5	2	1	2		
2	I	1	Total	C	N	O	0	0
			5	2	1	2		
2	I	1	Total	C	N	O	0	0
			5	2	1	2		
2	I	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	J	1	Total	C	N	O	0	0
			5	2	1	2		
2	K	1	Total	C	N	O	0	0
			5	2	1	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total 5	C 2	N 1	O 2	0	0
2	K	1	Total 5	C 2	N 1	O 2	0	0
2	L	1	Total 5	C 2	N 1	O 2	0	0
2	L	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	M	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	N	1	Total 5	C 2	N 1	O 2	0	0
2	O	1	Total 5	C 2	N 1	O 2	0	0
2	O	1	Total 5	C 2	N 1	O 2	0	0
2	O	1	Total 5	C 2	N 1	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total 5	C 2	N 1	O 2	0	0
2	P	1	Total 5	C 2	N 1	O 2	0	0
2	P	1	Total 5	C 2	N 1	O 2	0	0
2	P	1	Total 5	C 2	N 1	O 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	K 3	0	0
3	E	3	Total 3	K 3	0	0
3	I	3	Total 3	K 3	0	0
3	M	3	Total 3	K 3	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
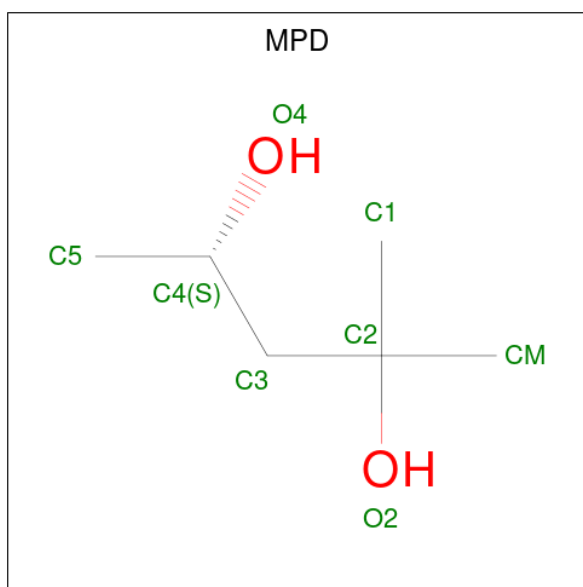
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 8	C 6	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 8	C 6	O 2	0	0
4	G	1	Total 8	C 6	O 2	0	0
4	J	1	Total 8	C 6	O 2	0	0
4	J	1	Total 8	C 6	O 2	0	0
4	M	1	Total 8	C 6	O 2	0	0
4	N	1	Total 8	C 6	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total 8	O 8	0	0
5	B	1	Total 1	O 1	0	0
5	C	4	Total 4	O 4	0	0
5	D	6	Total 6	O 6	0	0
5	E	3	Total 3	O 3	0	0
5	F	8	Total 8	O 8	0	0
5	G	4	Total 4	O 4	0	0
5	H	3	Total 3	O 3	0	0
5	I	6	Total 6	O 6	0	0
5	J	5	Total 5	O 5	0	0
5	K	6	Total 6	O 6	0	0
5	L	12	Total 12	O 12	0	0
5	M	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	11	Total 11	O 11	0	0
5	O	6	Total 6	O 6	0	0
5	P	7	Total 7	O 7	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.
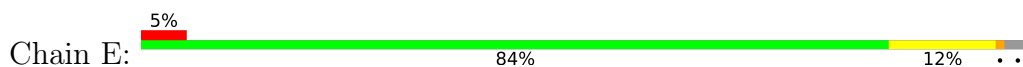
- Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

- Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
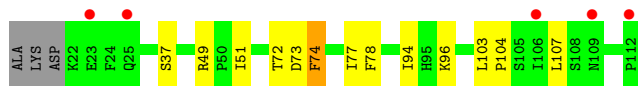

- Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

- Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
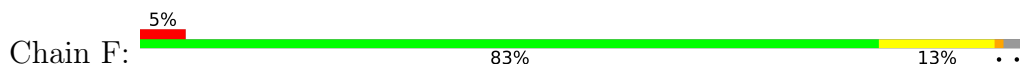

- Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

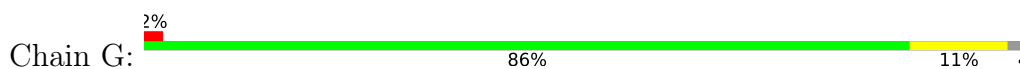• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
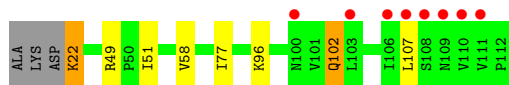

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
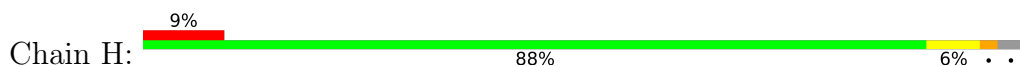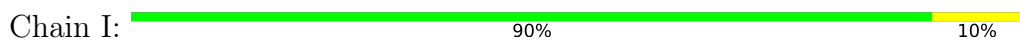

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
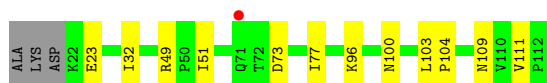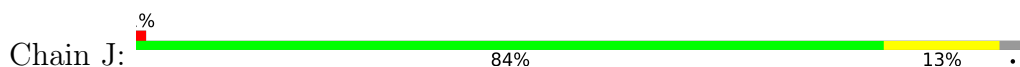
ALA LYS ASP K22 L30 L33 V64 D73 I77 K96 Q102 L103 P104 L107 P112

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

Chain L:

90% 6%

ALA LYS ASP K22 G65 I85 K96 L103 P104 L107 P112

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

Chain M:

90% 10%

A19 K20 D21 L33 I51 I87 L103 P104 L107 V111 P112

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

Chain N:

89% 7%

ALA LYS ASP K22 F74 I77 K96 L103 P104 N109 V110 V111 P112

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein
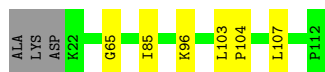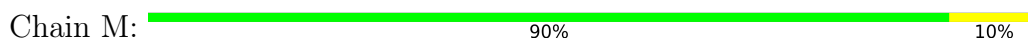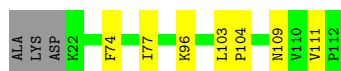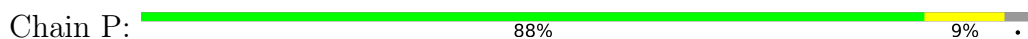
Chain O:

93%

ALA LYS ASP K22 K96 L103 P104 P112

• Molecule 1: Potassium channel protein,Cyclic nucleotide-gated olfactory channel,Potassium channel protein

Chain P:

88% 9%

ALA LYS ASP K22 E66 I94 H95 K96 L103 P104 L107 V111 P112

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.22Å 135.25Å 67.43Å 90.00° 91.95° 90.00°	Depositor
Resolution (Å)	67.62 – 2.63 67.62 – 2.63	Depositor EDS
% Data completeness (in resolution range)	84.5 (67.62-2.63) 92.7 (67.62-2.63)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.235 , 0.269 0.241 , 0.276	Depositor DCC
R_{free} test set	2291 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.108 for -h,-k,l	Xtriage
Reported twinning fraction	0.914 for H, K, L 0.086 for h,-k,-l	Depositor
Outliers	5 of 44750 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11844	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 78.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8231e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: K, MPD

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	0.70	0/726	0.66	0/994
1	B	0.68	0/726	0.69	0/994
1	C	0.68	0/726	0.69	0/994
1	D	0.66	0/726	0.66	0/994
1	E	0.68	0/726	0.70	0/994
1	F	0.67	0/726	0.67	0/994
1	G	0.70	0/726	0.68	0/994
1	H	0.69	0/726	0.68	0/994
1	I	0.68	0/748	0.67	0/1023
1	J	0.68	0/735	0.69	0/1005
1	K	0.69	0/726	0.68	0/994
1	L	0.69	0/726	0.67	0/994
1	M	0.70	0/748	0.70	0/1023
1	N	0.70	0/726	0.68	0/994
1	O	0.69	0/726	0.69	0/994
1	P	0.72	1/726 (0.1%)	0.68	0/994
All	All	0.69	1/11669 (0.0%)	0.68	0/15973

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	66	GLU	CD-OE2	-5.17	1.20	1.25

There are no bond angle outliers.

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	708	0	745	9	0
1	B	708	0	745	13	0
1	C	708	0	745	8	0
1	D	708	0	745	8	0
1	E	708	0	745	13	0
1	F	708	0	745	14	0
1	G	708	0	745	9	0
1	H	708	0	745	7	0
1	I	730	0	767	6	0
1	J	717	0	757	15	0
1	K	708	0	745	12	0
1	L	708	0	745	4	0
1	M	730	0	767	4	0
1	N	708	0	745	6	0
1	O	708	0	745	3	0
1	P	708	0	745	4	0
2	A	10	0	4	0	0
2	B	15	0	6	0	0
2	C	5	0	2	1	0
2	D	20	0	8	1	0
2	E	20	0	8	3	0
2	F	10	0	4	0	0
2	G	10	0	4	3	0
2	H	20	0	8	0	0
2	I	15	0	6	0	0
2	J	45	0	18	1	0
2	K	15	0	6	0	0
2	L	10	0	4	0	0
2	M	30	0	12	1	0
2	N	40	0	16	0	0
2	O	20	0	8	0	0
2	P	15	0	6	0	0
3	A	3	0	0	0	0
3	E	3	0	0	0	0
3	I	3	0	0	0	0
3	M	3	0	0	0	0
4	D	8	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	8	0	14	8	0
4	G	8	0	14	0	0
4	J	16	0	28	2	0
4	M	8	0	14	0	0
4	N	8	0	14	0	0
5	A	8	0	0	1	0
5	B	1	0	0	0	0
5	C	4	0	0	0	0
5	D	6	0	0	0	0
5	E	3	0	0	0	0
5	F	8	0	0	0	0
5	G	4	0	0	0	0
5	H	3	0	0	0	0
5	I	6	0	0	1	0
5	J	5	0	0	1	0
5	K	6	0	0	0	0
5	L	12	0	0	0	0
5	M	5	0	0	0	0
5	N	11	0	0	1	0
5	O	6	0	0	0	0
5	P	7	0	0	1	0
All	All	11844	0	12194	101	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 4.

The worst 5 of 101 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:E:83:ILE:HG23	1:E:87:ILE:HD12	1.38	1.06
1:E:83:ILE:HG23	1:E:87:ILE:CD1	1.99	0.90
1:J:96[B]:LYS:HE2	1:J:100:ASN:OD1	1.70	0.90
1:I:110:VAL:HG13	5:I:301:HOH:O	1.78	0.82
4:F:203:MPD:H52	4:F:203:MPD:H11	1.69	0.73

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	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	B	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	C	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	D	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	E	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	F	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	G	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	H	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	I	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	J	90/94 (96%)	89 (99%)	1 (1%)	0	100	100
1	K	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	L	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	M	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
1	N	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	O	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
1	P	89/94 (95%)	88 (99%)	1 (1%)	0	100	100
All	All	1431/1504 (95%)	1415 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	B	81/83 (98%)	77 (95%)	4 (5%)	25	39
1	C	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	D	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	E	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	F	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	G	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	H	81/83 (98%)	78 (96%)	3 (4%)	34	51
1	I	83/83 (100%)	81 (98%)	2 (2%)	49	67
1	J	82/83 (99%)	82 (100%)	0	100	100
1	K	81/83 (98%)	79 (98%)	2 (2%)	47	66
1	L	81/83 (98%)	80 (99%)	1 (1%)	71	83
1	M	83/83 (100%)	79 (95%)	4 (5%)	25	39
1	N	81/83 (98%)	81 (100%)	0	100	100
1	O	81/83 (98%)	80 (99%)	1 (1%)	71	83
1	P	81/83 (98%)	79 (98%)	2 (2%)	47	66
All	All	1301/1328 (98%)	1270 (98%)	31 (2%)	49	67

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	22	LYS
1	M	111	VAL
1	H	102	GLN
1	P	107	LEU
1	M	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 79 ligands modelled in this entry, 12 are monoatomic - leaving 67 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
2	GLY	D	201	-	4,4,4	1.02	0	3,4,4	2.39	2 (66%)
2	GLY	P	201	-	4,4,4	0.98	0	3,4,4	2.06	2 (66%)
2	GLY	M	201	-	4,4,4	0.81	0	3,4,4	1.92	2 (66%)
2	GLY	K	202	-	4,4,4	0.99	0	3,4,4	1.67	2 (66%)
2	GLY	J	207	-	4,4,4	1.05	0	3,4,4	1.36	0
2	GLY	M	203	-	4,4,4	0.98	0	3,4,4	1.59	1 (33%)
2	GLY	B	201	-	4,4,4	1.18	1 (25%)	3,4,4	1.90	1 (33%)
4	MPD	J	210	-	7,7,7	0.25	0	9,10,10	0.63	0
2	GLY	N	203	-	4,4,4	1.09	0	3,4,4	1.17	0
2	GLY	I	201	-	4,4,4	1.09	0	3,4,4	1.16	0
2	GLY	J	202	-	4,4,4	0.93	0	3,4,4	1.55	1 (33%)
2	GLY	C	201	-	4,4,4	0.92	0	3,4,4	1.34	0
2	GLY	H	202	-	4,4,4	1.15	1 (25%)	3,4,4	1.55	1 (33%)
2	GLY	H	201	-	4,4,4	1.14	0	3,4,4	1.83	2 (66%)
2	GLY	A	202	-	4,4,4	0.90	0	3,4,4	2.52	2 (66%)
2	GLY	N	204	-	4,4,4	1.18	1 (25%)	3,4,4	1.59	0
2	GLY	E	202	-	4,4,4	1.04	0	3,4,4	1.64	1 (33%)
2	GLY	J	206	-	4,4,4	1.12	1 (25%)	3,4,4	1.06	0
2	GLY	E	204	-	4,4,4	1.03	0	3,4,4	3.03	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GLY	D	204	-	4,4,4	1.16	1 (25%)	3,4,4	2.15	2 (66%)
4	MPD	M	210	-	7,7,7	0.16	0	9,10,10	0.72	0
2	GLY	J	201	-	4,4,4	0.98	0	3,4,4	1.49	0
2	GLY	E	201	-	4,4,4	1.36	1 (25%)	3,4,4	1.56	1 (33%)
2	GLY	E	203	-	4,4,4	1.20	1 (25%)	3,4,4	1.51	0
2	GLY	F	202	-	4,4,4	1.17	1 (25%)	3,4,4	1.44	0
2	GLY	H	203	-	4,4,4	1.08	1 (25%)	3,4,4	1.88	2 (66%)
2	GLY	N	207	-	4,4,4	1.05	1 (25%)	3,4,4	1.69	1 (33%)
2	GLY	N	208	-	4,4,4	1.15	1 (25%)	3,4,4	1.94	1 (33%)
2	GLY	N	202	-	4,4,4	1.09	1 (25%)	3,4,4	1.57	0
2	GLY	I	203	-	4,4,4	0.96	0	3,4,4	1.20	0
2	GLY	H	204	-	4,4,4	1.31	1 (25%)	3,4,4	0.82	0
2	GLY	L	202	-	4,4,4	1.15	1 (25%)	3,4,4	2.26	2 (66%)
2	GLY	D	203	-	4,4,4	0.56	0	3,4,4	1.83	1 (33%)
2	GLY	N	206	-	4,4,4	1.14	1 (25%)	3,4,4	1.33	0
2	GLY	B	203	-	4,4,4	1.10	1 (25%)	3,4,4	1.50	1 (33%)
2	GLY	J	204	-	4,4,4	0.91	0	3,4,4	1.82	2 (66%)
2	GLY	K	201	-	4,4,4	0.81	0	3,4,4	1.61	1 (33%)
2	GLY	J	208	-	4,4,4	1.16	1 (25%)	3,4,4	2.34	2 (66%)
4	MPD	G	203	-	7,7,7	0.24	0	9,10,10	0.47	0
2	GLY	L	201	-	4,4,4	1.18	1 (25%)	3,4,4	2.13	2 (66%)
2	GLY	J	203	-	4,4,4	1.15	1 (25%)	3,4,4	1.79	1 (33%)
2	GLY	N	205	-	4,4,4	0.69	0	3,4,4	2.18	2 (66%)
2	GLY	P	202	-	4,4,4	1.18	1 (25%)	3,4,4	2.00	1 (33%)
2	GLY	K	203	-	4,4,4	1.02	0	3,4,4	1.93	2 (66%)
2	GLY	I	202	-	4,4,4	1.07	1 (25%)	3,4,4	2.38	2 (66%)
2	GLY	O	202	-	4,4,4	0.99	0	3,4,4	2.23	2 (66%)
2	GLY	F	201	-	4,4,4	1.26	1 (25%)	3,4,4	1.05	0
2	GLY	M	205	-	4,4,4	1.01	0	3,4,4	1.75	1 (33%)
2	GLY	M	204	-	4,4,4	0.84	0	3,4,4	2.22	1 (33%)
2	GLY	O	204	-	4,4,4	1.27	1 (25%)	3,4,4	1.68	1 (33%)
4	MPD	F	203	-	7,7,7	0.29	0	9,10,10	0.53	0
2	GLY	D	202	-	4,4,4	1.38	1 (25%)	3,4,4	1.62	1 (33%)
2	GLY	O	203	-	4,4,4	1.23	1 (25%)	3,4,4	1.03	0
2	GLY	M	202	-	4,4,4	1.10	1 (25%)	3,4,4	2.25	2 (66%)
4	MPD	D	205	-	7,7,7	0.31	0	9,10,10	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	GLY	G	202	-	4,4,4	1.10	1 (25%)	3,4,4	2.13	2 (66%)
2	GLY	B	202	-	4,4,4	1.00	0	3,4,4	1.76	1 (33%)
2	GLY	J	209	-	4,4,4	1.17	1 (25%)	3,4,4	1.45	0
2	GLY	P	203	-	4,4,4	1.07	1 (25%)	3,4,4	2.35	2 (66%)
2	GLY	G	201	-	4,4,4	1.27	1 (25%)	3,4,4	1.23	0
4	MPD	J	211	-	7,7,7	0.35	0	9,10,10	0.55	0
2	GLY	A	201	-	4,4,4	1.02	0	3,4,4	1.54	1 (33%)
4	MPD	N	209	-	7,7,7	0.25	0	9,10,10	0.94	0
2	GLY	M	206	-	4,4,4	1.28	1 (25%)	3,4,4	1.93	1 (33%)
2	GLY	J	205	-	4,4,4	1.31	1 (25%)	3,4,4	1.84	1 (33%)
2	GLY	N	201	-	4,4,4	1.17	1 (25%)	3,4,4	1.31	0
2	GLY	O	201	-	4,4,4	0.95	0	3,4,4	0.80	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
2	GLY	D	201	-	-	2/2/2/2	-
2	GLY	P	201	-	-	2/2/2/2	-
2	GLY	M	201	-	-	2/2/2/2	-
2	GLY	K	202	-	-	2/2/2/2	-
2	GLY	J	207	-	-	0/2/2/2	-
2	GLY	M	203	-	-	2/2/2/2	-
2	GLY	B	201	-	-	2/2/2/2	-
4	MPD	J	210	-	-	3/5/5/5	-
2	GLY	N	203	-	-	0/2/2/2	-
2	GLY	I	201	-	-	2/2/2/2	-
2	GLY	J	202	-	-	2/2/2/2	-
2	GLY	C	201	-	-	2/2/2/2	-
2	GLY	H	202	-	-	0/2/2/2	-
2	GLY	H	201	-	-	2/2/2/2	-
2	GLY	A	202	-	-	0/2/2/2	-
2	GLY	N	204	-	-	0/2/2/2	-
2	GLY	E	202	-	-	2/2/2/2	-
2	GLY	J	206	-	-	0/2/2/2	-
2	GLY	E	204	-	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLY	D	204	-	-	2/2/2/2	-
4	MPD	M	210	-	-	2/5/5/5	-
2	GLY	J	201	-	-	2/2/2/2	-
2	GLY	E	201	-	-	2/2/2/2	-
2	GLY	E	203	-	-	2/2/2/2	-
2	GLY	F	202	-	-	2/2/2/2	-
2	GLY	H	203	-	-	2/2/2/2	-
2	GLY	N	207	-	-	2/2/2/2	-
2	GLY	N	208	-	-	0/2/2/2	-
2	GLY	N	202	-	-	2/2/2/2	-
2	GLY	I	203	-	-	2/2/2/2	-
2	GLY	H	204	-	-	2/2/2/2	-
2	GLY	L	202	-	-	0/2/2/2	-
2	GLY	D	203	-	-	2/2/2/2	-
2	GLY	N	206	-	-	2/2/2/2	-
2	GLY	B	203	-	-	1/2/2/2	-
2	GLY	J	204	-	-	2/2/2/2	-
2	GLY	K	201	-	-	2/2/2/2	-
2	GLY	J	208	-	-	2/2/2/2	-
4	MPD	G	203	-	-	0/5/5/5	-
2	GLY	L	201	-	-	0/2/2/2	-
2	GLY	J	203	-	-	0/2/2/2	-
2	GLY	N	205	-	-	2/2/2/2	-
2	GLY	P	202	-	-	2/2/2/2	-
2	GLY	K	203	-	-	2/2/2/2	-
2	GLY	I	202	-	-	2/2/2/2	-
2	GLY	O	202	-	-	0/2/2/2	-
2	GLY	F	201	-	-	0/2/2/2	-
2	GLY	M	205	-	-	2/2/2/2	-
2	GLY	M	204	-	-	0/2/2/2	-
2	GLY	O	204	-	-	2/2/2/2	-
4	MPD	F	203	-	-	3/5/5/5	-
2	GLY	D	202	-	-	0/2/2/2	-
2	GLY	O	203	-	-	0/2/2/2	-
2	GLY	M	202	-	-	2/2/2/2	-
4	MPD	D	205	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLY	G	202	-	-	2/2/2/2	-
2	GLY	B	202	-	-	2/2/2/2	-
2	GLY	J	209	-	-	0/2/2/2	-
2	GLY	P	203	-	-	2/2/2/2	-
2	GLY	G	201	-	-	1/2/2/2	-
4	MPD	J	211	-	-	2/5/5/5	-
2	GLY	A	201	-	-	2/2/2/2	-
4	MPD	N	209	-	-	2/5/5/5	-
2	GLY	M	206	-	-	2/2/2/2	-
2	GLY	J	205	-	-	2/2/2/2	-
2	GLY	N	201	-	-	2/2/2/2	-
2	GLY	O	201	-	-	2/2/2/2	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	202	GLY	OXT-C	-2.56	1.22	1.30
2	J	205	GLY	OXT-C	-2.55	1.22	1.30
2	M	206	GLY	OXT-C	-2.48	1.22	1.30
2	O	204	GLY	OXT-C	-2.46	1.22	1.30
2	H	204	GLY	OXT-C	-2.44	1.22	1.30

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	204	GLY	OXT-C-O	-3.82	113.79	123.30
2	E	204	GLY	OXT-C-CA	3.50	127.39	113.45
2	I	202	GLY	OXT-C-O	-3.48	114.62	123.30
2	J	208	GLY	OXT-C-O	-3.35	114.95	123.30
2	A	202	GLY	OXT-C-O	-3.31	115.04	123.30

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GLY	O-C-CA-N
2	B	201	GLY	OXT-C-CA-N
2	C	201	GLY	O-C-CA-N
2	D	201	GLY	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
2	D	204	GLY	OXT-C-CA-N

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	207	GLY	1	0
4	J	210	MPD	1	0
2	C	201	GLY	1	0
2	E	202	GLY	3	0
2	D	204	GLY	1	0
2	M	204	GLY	1	0
4	F	203	MPD	8	0
4	D	205	MPD	1	0
2	G	201	GLY	3	0
4	J	211	MPD	1	0

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	91/94 (96%)	-0.27	3 (3%)	46	43	24, 46, 92, 114	0
1	B	91/94 (96%)	0.22	8 (8%)	10	7	28, 47, 127, 183	0
1	C	91/94 (96%)	0.05	8 (8%)	10	7	25, 47, 125, 144	0
1	D	91/94 (96%)	-0.05	5 (5%)	25	22	27, 44, 107, 135	0
1	E	91/94 (96%)	-0.07	5 (5%)	25	22	25, 41, 116, 168	0
1	F	91/94 (96%)	0.04	5 (5%)	25	22	25, 42, 110, 131	0
1	G	91/94 (96%)	-0.27	2 (2%)	62	58	23, 42, 83, 119	0
1	H	91/94 (96%)	0.16	8 (8%)	10	7	25, 39, 127, 197	0
1	I	94/94 (100%)	-0.50	0	100	100	24, 41, 59, 80	0
1	J	91/94 (96%)	-0.48	1 (1%)	80	78	30, 42, 66, 72	0
1	K	91/94 (96%)	-0.46	0	100	100	30, 43, 58, 78	0
1	L	91/94 (96%)	-0.43	0	100	100	30, 42, 62, 79	0
1	M	94/94 (100%)	-0.57	0	100	100	25, 38, 54, 76	0
1	N	91/94 (96%)	-0.60	0	100	100	26, 39, 52, 56	0
1	O	91/94 (96%)	-0.48	0	100	100	28, 41, 58, 61	0
1	P	91/94 (96%)	-0.55	0	100	100	25, 37, 50, 60	0
All	All	1462/1504 (97%)	-0.27	45 (3%)	49	45	23, 41, 96, 197	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	ASN	12.6
1	H	109	ASN	10.8
1	E	25	GLN	8.5
1	G	112	PRO	7.9
1	C	112	PRO	7.5

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLY	I	201	5/5	0.65	0.25	66,69,75,79	0
2	GLY	J	207	5/5	0.72	0.26	55,63,69,70	0
2	GLY	N	207	5/5	0.73	0.21	55,58,65,77	0
4	MPD	D	205	8/8	0.73	0.39	50,58,60,62	0
2	GLY	M	202	5/5	0.74	0.28	62,63,64,71	0
2	GLY	O	202	5/5	0.76	0.26	47,48,54,56	0
2	GLY	H	203	5/5	0.76	0.27	57,61,68,69	0
2	GLY	H	204	5/5	0.77	0.23	72,79,83,84	0
2	GLY	J	208	5/5	0.78	0.21	54,55,57,61	0
2	GLY	G	202	5/5	0.78	0.23	55,62,63,71	0
2	GLY	M	206	5/5	0.78	0.26	70,70,72,74	0
2	GLY	L	202	5/5	0.79	0.24	49,52,55,55	0
2	GLY	J	203	5/5	0.79	0.20	58,64,66,72	0
2	GLY	P	201	5/5	0.80	0.28	65,67,72,78	0
2	GLY	J	209	5/5	0.82	0.22	63,64,73,81	0
2	GLY	P	202	5/5	0.82	0.18	42,47,49,54	0
2	GLY	I	202	5/5	0.82	0.21	51,53,58,58	0
2	GLY	D	203	5/5	0.83	0.24	47,47,50,52	0
2	GLY	J	201	5/5	0.84	0.17	49,53,55,60	0
2	GLY	B	201	5/5	0.86	0.23	51,57,61,61	0
2	GLY	M	201	5/5	0.86	0.14	59,61,69,71	0
2	GLY	F	202	5/5	0.86	0.24	58,62,70,71	0
2	GLY	M	204	5/5	0.86	0.16	35,37,42,47	0
2	GLY	D	201	5/5	0.86	0.17	60,62,65,66	0
4	MPD	G	203	8/8	0.86	0.22	62,70,73,76	0
2	GLY	A	201	5/5	0.87	0.22	61,68,71,71	0
2	GLY	J	204	5/5	0.88	0.20	48,52,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLY	O	201	5/5	0.88	0.19	51,59,62,65	0
2	GLY	K	203	5/5	0.88	0.16	64,68,70,72	0
2	GLY	O	204	5/5	0.88	0.18	53,53,56,61	0
2	GLY	L	201	5/5	0.88	0.18	55,60,64,66	0
2	GLY	J	205	5/5	0.88	0.12	65,66,71,72	0
2	GLY	N	203	5/5	0.88	0.15	42,48,52,55	0
2	GLY	N	206	5/5	0.88	0.15	49,50,64,69	0
2	GLY	E	204	5/5	0.89	0.16	28,30,33,34	0
2	GLY	N	202	5/5	0.89	0.17	58,58,60,64	0
2	GLY	D	204	5/5	0.89	0.14	47,49,51,55	0
2	GLY	M	205	5/5	0.90	0.14	49,52,57,59	0
2	GLY	B	203	5/5	0.90	0.17	68,72,74,76	0
2	GLY	O	203	5/5	0.90	0.23	67,67,71,72	0
2	GLY	N	208	5/5	0.90	0.26	58,63,65,66	0
2	GLY	J	206	5/5	0.91	0.16	52,62,68,69	0
2	GLY	J	202	5/5	0.91	0.12	48,59,64,66	0
2	GLY	D	202	5/5	0.91	0.13	48,49,55,61	0
2	GLY	F	201	5/5	0.91	0.20	44,53,58,61	0
2	GLY	E	203	5/5	0.91	0.18	54,54,58,58	0
4	MPD	M	210	8/8	0.91	0.20	42,51,61,76	0
2	GLY	N	201	5/5	0.92	0.17	57,58,59,60	0
2	GLY	I	203	5/5	0.92	0.14	53,56,59,61	0
3	K	A	205	1/1	0.92	0.10	21,21,21,21	0
2	GLY	H	201	5/5	0.93	0.12	47,54,60,65	0
3	K	I	206	1/1	0.93	0.16	24,24,24,24	0
2	GLY	G	201	5/5	0.93	0.12	48,49,55,60	0
4	MPD	F	203	8/8	0.93	0.18	61,65,66,69	0
2	GLY	A	202	5/5	0.93	0.14	48,53,61,70	0
2	GLY	K	201	5/5	0.93	0.17	44,50,55,56	0
4	MPD	N	209	8/8	0.93	0.18	50,57,65,67	0
2	GLY	K	202	5/5	0.94	0.20	61,62,65,67	0
2	GLY	B	202	5/5	0.94	0.14	46,48,53,55	0
2	GLY	N	204	5/5	0.94	0.18	52,52,61,67	0
2	GLY	N	205	5/5	0.94	0.15	37,41,46,48	0
2	GLY	E	201	5/5	0.95	0.12	37,39,44,45	0
2	GLY	P	203	5/5	0.95	0.12	52,56,59,60	0
2	GLY	M	203	5/5	0.95	0.13	60,63,67,69	0
4	MPD	J	210	8/8	0.95	0.18	41,49,52,55	0
2	GLY	C	201	5/5	0.95	0.14	28,38,43,48	0
3	K	M	209	1/1	0.95	0.15	15,15,15,15	0
2	GLY	E	202	5/5	0.96	0.16	49,54,57,67	0
4	MPD	J	211	8/8	0.96	0.12	43,50,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLY	H	202	5/5	0.97	0.13	40,43,45,57	0
3	K	E	206	1/1	0.98	0.08	22,22,22,22	0
3	K	E	207	1/1	0.98	0.09	20,20,20,20	0
3	K	I	204	1/1	0.98	0.08	30,30,30,30	0
3	K	A	204	1/1	0.98	0.05	23,23,23,23	0
3	K	A	203	1/1	0.98	0.11	34,34,34,34	0
3	K	E	205	1/1	0.98	0.09	24,24,24,24	0
3	K	I	205	1/1	0.99	0.13	27,27,27,27	0
3	K	M	207	1/1	0.99	0.06	21,21,21,21	0
3	K	M	208	1/1	1.00	0.13	21,21,21,21	0

6.5 Other polymers ⓘ

There are no such residues in this entry.