

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 15, 2023 – 11:13 AM JST

PDB ID	:	6IZ4
Title	:	Crystal Structure Analysis of TRIC counter-ion channels in calcium release
Authors	:	Wang, X.H.; Zeng, Y.; Gao, F.; Su, M.; Hendrickson, W.A.; Chen, Y.H.
Deposited on	:	2018-12-18
Resolution	:	3.10  Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	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 (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 3.10 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	А	314	2% <b>58%</b>	13%	29%		
1	В	314	2% 59%	13%	29%		
1	С	314	% • 60%	11%	29%		
1	D	314	% • 63%	8%	29%		
1	Е	314	2% 59%	12%	29%		
1	F	314	% 58%	13%	29%		



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Mol	Chain	Length		Quality of chain					
1	G	314	58%	13%	29%				
1	Н	314	2%	12%	29%				
1	Ι	314	-% <b>6</b> 0%	12%	29%				
1	J	314	% • 57%	14%	29%				
1	K	314	.% • 57%	14%	29%				
1	L	314	60%	11%	29%				

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# 2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21192 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	224	Total	С	Ν	0	S	0	0	0
1	A	224	1766	1166	285	299	16	0	0	0
1	Р	224	Total	С	Ν	0	S	0	0	0
1	D	224	1766	1166	285	299	16	0	0	0
1	C	224	Total	С	Ν	0	S	0	0	0
1		224	1766	1166	285	299	16	0	0	0
1	П	224	Total	С	Ν	0	S	0	0	0
1		224	1766	1166	285	299	16	0	0	0
1	F	224	Total	С	Ν	0	S	0	0	0
1	Ľ	224	1766	1166	285	299	16	0	0	0
1	Б	224	Total	С	Ν	0	S	0	0	0
1	Г		1766	1166	285	299	16	0	0	U
1	C	004	Total	С	Ν	0	S	0	0	0
1	G	224	1766	1166	285	299	16	0	0	0
1	и	224	Total	С	Ν	0	S	0	0	0
1	п	224	1766	1166	285	299	16	0	0	U
1	т	224	Total	С	Ν	0	S	0	0	0
1	1	224	1766	1166	285	299	16	0	0	0
1	т	224	Total	С	Ν	0	S	0	0	0
1	J	224	1766	1166	285	299	16	0	0	0
1	V	224	Total	С	Ν	0	S	0	0	0
1	n n	224	1766	1166	285	299	16	0		U
1	т	224	Total	С	Ν	Ο	S	0	0	0
1	L	<i>ZZ</i> 4	1766	1166	285	299	16	U	U	

• Molecule 1 is a protein called Trimeric intracellular cation channel type B-B.

There are 360 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	285	ALA	-	expression tag	UNP Q6GN30
А	286	ALA	-	expression tag	UNP Q6GN30
А	287	ALA	-	expression tag	UNP Q6GN30
А	288	GLU	-	expression tag	UNP Q6GN30
А	289	ASN	-	expression tag	UNP Q6GN30



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Chain	Residue	Modelled	Actual	Comment	Reference
А	290	LEU	-	expression tag	UNP Q6GN30
А	291	TYR	-	expression tag	UNP Q6GN30
A	292	PHE	-	expression tag	UNP Q6GN30
А	293	GLN	-	expression tag	UNP Q6GN30
А	294	GLY	-	expression tag	UNP Q6GN30
А	295	LEU	-	expression tag	UNP Q6GN30
А	296	GLU	-	expression tag	UNP Q6GN30
А	297	ASP	-	expression tag	UNP Q6GN30
А	298	TYR	-	expression tag	UNP Q6GN30
А	299	LYS	-	expression tag	UNP Q6GN30
А	300	ASP	-	expression tag	UNP Q6GN30
А	301	ASP	-	expression tag	UNP Q6GN30
А	302	ASP	-	expression tag	UNP Q6GN30
А	303	ASP	-	expression tag	UNP Q6GN30
А	304	LYS	-	expression tag	UNP Q6GN30
А	305	HIS	-	expression tag	UNP Q6GN30
А	306	HIS	-	expression tag	UNP Q6GN30
А	307	HIS	-	expression tag	UNP Q6GN30
А	308	HIS	-	expression tag	UNP Q6GN30
А	309	HIS	-	expression tag	UNP Q6GN30
А	310	HIS	-	expression tag	UNP Q6GN30
А	311	HIS	-	expression tag	UNP Q6GN30
А	312	HIS	-	expression tag	UNP Q6GN30
А	313	HIS	-	expression tag	UNP Q6GN30
А	314	HIS	-	expression tag	UNP Q6GN30
В	285	ALA	-	expression tag	UNP Q6GN30
В	286	ALA	-	expression tag	UNP Q6GN30
В	287	ALA	-	expression tag	UNP Q6GN30
В	288	GLU	-	expression tag	UNP Q6GN30
В	289	ASN	-	expression tag	UNP Q6GN30
В	290	LEU	-	expression tag	UNP Q6GN30
В	291	TYR	-	expression tag	UNP Q6GN30
В	292	PHE	-	expression tag	UNP Q6GN30
В	293	GLN	-	expression tag	UNP Q6GN30
В	294	GLY	-	expression tag	UNP Q6GN30
В	295	LEU	-	expression tag	UNP Q6GN30
В	296	GLU	-	expression tag	UNP Q6GN30
В	297	ASP	-	expression tag	UNP Q6GN30
В	298	TYR	-	expression tag	UNP Q6GN30
В	299	LYS	-	expression tag	UNP Q6GN30
В	300	ASP	-	expression tag	UNP Q6GN30
В	301	ASP	-	expression tag	UNP Q6GN30



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Chain	Residue	Modelled	Actual	Comment	Reference
В	302	ASP	-	expression tag	UNP Q6GN30
В	303	ASP	-	expression tag	UNP Q6GN30
В	304	LYS	-	expression tag	UNP Q6GN30
В	305	HIS	-	expression tag	UNP Q6GN30
В	306	HIS	-	expression tag	UNP Q6GN30
В	307	HIS	-	expression tag	UNP Q6GN30
В	308	HIS	-	expression tag	UNP Q6GN30
В	309	HIS	-	expression tag	UNP Q6GN30
В	310	HIS	_	expression tag	UNP Q6GN30
В	311	HIS	_	expression tag	UNP Q6GN30
В	312	HIS	-	expression tag	UNP Q6GN30
В	313	HIS	-	expression tag	UNP Q6GN30
В	314	HIS	-	expression tag	UNP Q6GN30
С	285	ALA	-	expression tag	UNP Q6GN30
С	286	ALA	-	expression tag	UNP Q6GN30
С	287	ALA	-	expression tag	UNP Q6GN30
С	288	GLU	-	expression tag	UNP Q6GN30
С	289	ASN	-	expression tag	UNP Q6GN30
С	290	LEU	_	expression tag	UNP Q6GN30
С	291	TYR	-	expression tag	UNP Q6GN30
С	292	PHE	-	expression tag	UNP Q6GN30
С	293	GLN	-	expression tag	UNP Q6GN30
С	294	GLY	-	expression tag	UNP Q6GN30
С	295	LEU	-	expression tag	UNP Q6GN30
С	296	GLU	-	expression tag	UNP Q6GN30
С	297	ASP	_	expression tag	UNP Q6GN30
С	298	TYR	_	expression tag	UNP Q6GN30
С	299	LYS	_	expression tag	UNP Q6GN30
С	300	ASP	-	expression tag	UNP Q6GN30
С	301	ASP	-	expression tag	UNP Q6GN30
С	302	ASP	_	expression tag	UNP Q6GN30
С	303	ASP	_	expression tag	UNP Q6GN30
С	304	LYS	_	expression tag	UNP Q6GN30
С	305	HIS	_	expression tag	UNP Q6GN30
С	306	HIS	-	expression tag	UNP Q6GN30
С	307	HIS	_	expression tag	UNP Q6GN30
С	308	HIS	_	expression tag	UNP Q6GN30
С	309	HIS	_	expression tag	UNP Q6GN30
С	310	HIS	_	expression tag	UNP Q6GN30
C	311	HIS	-	expression tag	UNP Q6GN30
C	312	HIS	-	expression tag	UNP Q6GN30
C	313	HIS	-	expression tag	UNP Q6GN30
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Chain	Residue	Modelled	Actual	Comment	Reference
С	314	HIS	-	expression tag	UNP Q6GN30
D	285	ALA	-	expression tag	UNP Q6GN30
D	286	ALA	-	expression tag	UNP Q6GN30
D	287	ALA	-	expression tag	UNP Q6GN30
D	288	GLU	-	expression tag	UNP Q6GN30
D	289	ASN	-	expression tag	UNP Q6GN30
D	290	LEU	-	expression tag	UNP Q6GN30
D	291	TYR	-	expression tag	UNP Q6GN30
D	292	PHE	-	expression tag	UNP Q6GN30
D	293	GLN	-	expression tag	UNP Q6GN30
D	294	GLY	-	expression tag	UNP Q6GN30
D	295	LEU	-	expression tag	UNP Q6GN30
D	296	GLU	-	expression tag	UNP Q6GN30
D	297	ASP	-	expression tag	UNP Q6GN30
D	298	TYR	-	expression tag	UNP Q6GN30
D	299	LYS	-	expression tag	UNP Q6GN30
D	300	ASP	-	expression tag	UNP Q6GN30
D	301	ASP	-	expression tag	UNP Q6GN30
D	302	ASP	-	expression tag	UNP Q6GN30
D	303	ASP	-	expression tag	UNP Q6GN30
D	304	LYS	-	expression tag	UNP Q6GN30
D	305	HIS	-	expression tag	UNP Q6GN30
D	306	HIS	-	expression tag	UNP Q6GN30
D	307	HIS	-	expression tag	UNP Q6GN30
D	308	HIS	-	expression tag	UNP Q6GN30
D	309	HIS	-	expression tag	UNP Q6GN30
D	310	HIS	-	expression tag	UNP Q6GN30
D	311	HIS	-	expression tag	UNP Q6GN30
D	312	HIS	-	expression tag	UNP Q6GN30
D	313	HIS	-	expression tag	UNP Q6GN30
D	314	HIS	-	expression tag	UNP Q6GN30
Е	285	ALA	-	expression tag	UNP Q6GN30
Е	286	ALA	-	expression tag	UNP Q6GN30
Е	287	ALA	-	expression tag	UNP Q6GN30
Е	288	GLU	-	expression tag	UNP Q6GN30
Е	289	ASN	-	expression tag	UNP Q6GN30
Е	290	LEU	-	expression tag	UNP Q6GN30
Е	291	TYR	-	expression tag	UNP Q6GN30
Е	292	PHE	-	expression tag	UNP Q6GN30
Е	293	GLN	-	expression tag	UNP Q6GN30
Е	294	GLY	-	expression tag	UNP Q6GN30
Е	295	LEU	-	expression tag	UNP Q6GN30



Chain	Residue	Modelled	Actual	Comment	Reference
E	296	GLU	-	expression tag	UNP Q6GN30
E	297	ASP	_	expression tag	UNP Q6GN30
E	298	TYR	_	expression tag	UNP Q6GN30
E	299	LYS	_	expression tag	UNP Q6GN30
E	300	ASP	-	expression tag	UNP Q6GN30
E	301	ASP	-	expression tag	UNP Q6GN30
E	302	ASP	-	expression tag	UNP Q6GN30
Е	303	ASP	-	expression tag	UNP Q6GN30
E	304	LYS	-	expression tag	UNP Q6GN30
Е	305	HIS	-	expression tag	UNP Q6GN30
Е	306	HIS	-	expression tag	UNP Q6GN30
Е	307	HIS	-	expression tag	UNP Q6GN30
Е	308	HIS	-	expression tag	UNP Q6GN30
Е	309	HIS	-	expression tag	UNP Q6GN30
Е	310	HIS	_	expression tag	UNP Q6GN30
Е	311	HIS	_	expression tag	UNP Q6GN30
Е	312	HIS	-	expression tag	UNP Q6GN30
Е	313	HIS	-	expression tag	UNP Q6GN30
Е	314	HIS	-	expression tag	UNP Q6GN30
F	285	ALA	-	expression tag	UNP Q6GN30
F	286	ALA	-	expression tag	UNP Q6GN30
F	287	ALA	-	expression tag	UNP Q6GN30
F	288	GLU	-	expression tag	UNP Q6GN30
F	289	ASN	-	expression tag	UNP Q6GN30
F	290	LEU	-	expression tag	UNP Q6GN30
F	291	TYR	-	expression tag	UNP Q6GN30
F	292	PHE	-	expression tag	UNP Q6GN30
F	293	GLN	-	expression tag	UNP Q6GN30
F	294	GLY	-	expression tag	UNP Q6GN30
F	295	LEU	-	expression tag	UNP Q6GN30
F	296	GLU	-	expression tag	UNP Q6GN30
F	297	ASP	-	expression tag	UNP Q6GN30
F	298	TYR	-	expression tag	UNP Q6GN30
F	299	LYS	-	expression tag	UNP Q6GN30
F	300	ASP	-	expression tag	UNP Q6GN30
F	301	ASP	-	expression tag	UNP Q6GN30
F	302	ASP	-	expression tag	UNP Q6GN30
F	303	ASP	-	expression tag	UNP Q6GN30
F	304	LYS	-	expression tag	UNP Q6GN30
F	305	HIS	-	expression tag	UNP $Q6\overline{GN30}$
F	306	HIS	-	expression tag	UNP Q6GN30
F	307	HIS	-	expression tag	UNP Q6GN30



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Chain	Residue	Modelled	Actual	Comment	Reference
F	308	HIS	-	expression tag	UNP Q6GN30
F	309	HIS	-	expression tag	UNP Q6GN30
F	310	HIS	-	expression tag	UNP Q6GN30
F	311	HIS	-	expression tag	UNP Q6GN30
F	312	HIS	-	expression tag	UNP Q6GN30
F	313	HIS	-	expression tag	UNP Q6GN30
F	314	HIS	-	expression tag	UNP Q6GN30
G	285	ALA	-	expression tag	UNP Q6GN30
G	286	ALA	-	expression tag	UNP Q6GN30
G	287	ALA	-	expression tag	UNP Q6GN30
G	288	GLU	-	expression tag	UNP Q6GN30
G	289	ASN	-	expression tag	UNP Q6GN30
G	290	LEU	-	expression tag	UNP Q6GN30
G	291	TYR	-	expression tag	UNP Q6GN30
G	292	PHE	-	expression tag	UNP Q6GN30
G	293	GLN	-	expression tag	UNP Q6GN30
G	294	GLY	-	expression tag	UNP Q6GN30
G	295	LEU	-	expression tag	UNP Q6GN30
G	296	GLU	-	expression tag	UNP Q6GN30
G	297	ASP	-	expression tag	UNP Q6GN30
G	298	TYR	-	expression tag	UNP Q6GN30
G	299	LYS	-	expression tag	UNP Q6GN30
G	300	ASP	-	expression tag	UNP Q6GN30
G	301	ASP	-	expression tag	UNP Q6GN30
G	302	ASP	-	expression tag	UNP Q6GN30
G	303	ASP	-	expression tag	UNP Q6GN30
G	304	LYS	-	expression tag	UNP Q6GN30
G	305	HIS	-	expression tag	UNP Q6GN30
G	306	HIS	-	expression tag	UNP Q6GN30
G	307	HIS	-	expression tag	UNP Q6GN30
G	308	HIS	-	expression tag	UNP Q6GN30
G	309	HIS	-	expression tag	UNP Q6GN30
G	310	HIS	-	expression tag	UNP Q6GN30
G	311	HIS	-	expression tag	UNP Q6GN30
G	312	HIS	-	expression tag	UNP Q6GN30
G	313	HIS	-	expression tag	UNP Q6GN30
G	314	HIS	-	expression tag	UNP Q6GN30
H	285	ALA	-	expression tag	UNP $Q6\overline{GN30}$
H	286	ALA	-	expression tag	UNP Q6GN30
Н	287	ALA	-	expression tag	UNP Q6GN30
Н	288	GLU	-	expression tag	UNP Q6GN30
Н	289	ASN	-	expression tag	UNP Q6GN30



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Chain	Residue	Modelled	Actual	Comment	Reference
Н	290	LEU	-	expression tag	UNP Q6GN30
Н	291	TYR	-	expression tag	UNP Q6GN30
Н	292	PHE	-	expression tag	UNP Q6GN30
Н	293	GLN	-	expression tag	UNP Q6GN30
Н	294	GLY	-	expression tag	UNP Q6GN30
Н	295	LEU	-	expression tag	UNP Q6GN30
Н	296	GLU	-	expression tag	UNP Q6GN30
Н	297	ASP	-	expression tag	UNP Q6GN30
Н	298	TYR	-	expression tag	UNP Q6GN30
Н	299	LYS	-	expression tag	UNP Q6GN30
Н	300	ASP	-	expression tag	UNP Q6GN30
Н	301	ASP	-	expression tag	UNP Q6GN30
Н	302	ASP	-	expression tag	UNP Q6GN30
Н	303	ASP	-	expression tag	UNP Q6GN30
Н	304	LYS	-	expression tag	UNP Q6GN30
Н	305	HIS	-	expression tag	UNP Q6GN30
Н	306	HIS	-	expression tag	UNP Q6GN30
Н	307	HIS	-	expression tag	UNP Q6GN30
Н	308	HIS	-	expression tag	UNP Q6GN30
Н	309	HIS	-	expression tag	UNP Q6GN30
Н	310	HIS	-	expression tag	UNP Q6GN30
Н	311	HIS	-	expression tag	UNP Q6GN30
Н	312	HIS	-	expression tag	UNP Q6GN30
Н	313	HIS	-	expression tag	UNP Q6GN30
Н	314	HIS	-	expression tag	UNP Q6GN30
Ι	285	ALA	-	expression tag	UNP Q6GN30
Ι	286	ALA	-	expression tag	UNP Q6GN30
Ι	287	ALA	-	expression tag	UNP Q6GN30
Ι	288	GLU	-	expression tag	UNP Q6GN30
Ι	289	ASN	-	expression tag	UNP Q6GN30
Ι	290	LEU	-	expression tag	UNP Q6GN30
Ι	291	TYR	-	expression tag	UNP Q6GN30
Ι	292	PHE	-	expression tag	UNP Q6GN30
Ι	293	GLN	-	expression tag	UNP Q6GN30
Ι	294	GLY	-	expression tag	UNP Q6GN30
Ι	295	LEU	-	expression tag	UNP Q6GN30
Ι	296	GLU	-	expression tag	UNP Q6GN30
Ι	297	ASP	-	expression tag	UNP Q6GN30
Ι	298	TYR	-	expression tag	UNP Q6GN30
Ι	299	LYS	-	expression tag	UNP Q6GN30
Ι	300	ASP	-	expression tag	UNP Q6GN30
Ι	301	ASP	-	expression tag	UNP Q6GN30



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Chain	Residue	Modelled	Actual	Comment	Reference
Ι	302	ASP	-	expression tag	UNP Q6GN30
Ι	303	ASP	-	expression tag	UNP Q6GN30
Ι	304	LYS	-	expression tag	UNP Q6GN30
Ι	305	HIS	-	expression tag	UNP Q6GN30
Ι	306	HIS	-	expression tag	UNP Q6GN30
Ι	307	HIS	-	expression tag	UNP Q6GN30
Ι	308	HIS	-	expression tag	UNP Q6GN30
Ι	309	HIS	-	expression tag	UNP Q6GN30
Ι	310	HIS	-	expression tag	UNP Q6GN30
Ι	311	HIS	-	expression tag	UNP Q6GN30
Ι	312	HIS	-	expression tag	UNP Q6GN30
Ι	313	HIS	-	expression tag	UNP Q6GN30
Ι	314	HIS	-	expression tag	UNP Q6GN30
J	285	ALA	-	expression tag	UNP Q6GN30
J	286	ALA	-	expression tag	UNP Q6GN30
J	287	ALA	-	expression tag	UNP Q6GN30
J	288	GLU	-	expression tag	UNP Q6GN30
J	289	ASN	-	expression tag	UNP Q6GN30
J	290	LEU	-	expression tag	UNP Q6GN30
J	291	TYR	-	expression tag	UNP Q6GN30
J	292	PHE	-	expression tag	UNP Q6GN30
J	293	GLN	-	expression tag	UNP Q6GN30
J	294	GLY	-	expression tag	UNP Q6GN30
J	295	LEU	-	expression tag	UNP Q6GN30
J	296	GLU	-	expression tag	UNP Q6GN30
J	297	ASP	-	expression tag	UNP Q6GN30
J	298	TYR	-	expression tag	UNP Q6GN30
J	299	LYS	-	expression tag	UNP Q6GN30
J	300	ASP	-	expression tag	UNP Q6GN30
J	301	ASP	-	expression tag	UNP Q6GN30
J	302	ASP	-	expression tag	UNP Q6GN30
J	303	ASP	-	expression tag	UNP Q6GN30
J	304	LYS	-	expression tag	UNP Q6GN30
J	305	HIS	-	expression tag	UNP Q6GN30
J	306	HIS	-	expression tag	UNP Q6GN30
J	307	HIS	-	expression tag	UNP Q6GN30
J	308	HIS	-	expression tag	UNP Q6GN30
J	309	HIS	-	expression tag	UNP Q6GN30
J	310	HIS	-	expression tag	UNP Q6GN30
J	311	HIS	-	expression tag	UNP Q6GN30
J	312	HIS	-	expression tag	UNP Q6GN30
J	313	HIS	-	expression tag	UNP Q6GN30



Chain	Residue	Modelled	Actual	Comment	Reference
J	314	HIS	-	expression tag	UNP Q6GN30
K	285	ALA	-	expression tag	UNP Q6GN30
K	286	ALA	-	expression tag	UNP Q6GN30
K	287	ALA	-	expression tag	UNP Q6GN30
K	288	GLU	-	expression tag	UNP Q6GN30
K	289	ASN	-	expression tag	UNP Q6GN30
K	290	LEU	-	expression tag	UNP Q6GN30
K	291	TYR	-	expression tag	UNP Q6GN30
K	292	PHE	-	expression tag	UNP Q6GN30
K	293	GLN	-	expression tag	UNP Q6GN30
K	294	GLY	-	expression tag	UNP Q6GN30
K	295	LEU	-	expression tag	UNP Q6GN30
K	296	GLU	-	expression tag	UNP Q6GN30
K	297	ASP	-	expression tag	UNP Q6GN30
K	298	TYR	-	expression tag	UNP Q6GN30
K	299	LYS	-	expression tag	UNP Q6GN30
K	300	ASP	-	expression tag	UNP Q6GN30
K	301	ASP	-	expression tag	UNP Q6GN30
K	302	ASP	-	expression tag	UNP Q6GN30
K	303	ASP	-	expression tag	UNP Q6GN30
K	304	LYS	-	expression tag	UNP Q6GN30
K	305	HIS	-	expression tag	UNP Q6GN30
K	306	HIS	-	expression tag	UNP Q6GN30
K	307	HIS	-	expression tag	UNP Q6GN30
K	308	HIS	-	expression tag	UNP Q6GN30
K	309	HIS	-	expression tag	UNP Q6GN30
K	310	HIS	-	expression tag	UNP Q6GN30
K	311	HIS	-	expression tag	UNP Q6GN30
K	312	HIS	-	expression tag	UNP Q6GN30
K	313	HIS	-	expression tag	UNP Q6GN30
K	314	HIS	-	expression tag	UNP Q6GN30
L	285	ALA	-	expression tag	UNP Q6GN30
L	286	ALA	-	expression tag	UNP Q6GN30
L	287	ALA	-	expression tag	UNP Q6GN30
L	288	GLU	-	expression tag	UNP Q6GN30
L	289	ASN	-	expression tag	UNP Q6GN30
L	290	LEU	-	expression tag	UNP Q6GN30
L	291	TYR	-	expression tag	UNP Q6GN30
L	292	PHE	-	expression tag	UNP Q6GN30
L	293	GLN	-	expression tag	UNP Q6GN30
L	294	GLY	-	expression tag	UNP $Q6\overline{GN30}$
L	295	LEU	-	expression tag	UNP Q6GN30

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Chain	Residue	Modelled	Actual	Comment	Reference
L	296	GLU	-	expression tag	UNP Q6GN30
L	297	ASP	-	expression tag	UNP Q6GN30
L	298	TYR	-	expression tag	UNP Q6GN30
L	299	LYS	-	expression tag	UNP Q6GN30
L	300	ASP	-	expression tag	UNP Q6GN30
L	301	ASP	-	expression tag	UNP Q6GN30
L	302	ASP	-	expression tag	UNP Q6GN30
L	303	ASP	-	expression tag	UNP Q6GN30
L	304	LYS	-	expression tag	UNP Q6GN30
L	305	HIS	-	expression tag	UNP Q6GN30
L	306	HIS	-	expression tag	UNP Q6GN30
L	307	HIS	-	expression tag	UNP Q6GN30
L	308	HIS	-	expression tag	UNP Q6GN30
L	309	HIS	-	expression tag	UNP Q6GN30
L	310	HIS	-	expression tag	UNP Q6GN30
L	311	HIS	-	expression tag	UNP Q6GN30
L	312	HIS	-	expression tag	UNP Q6GN30
L	313	HIS	-	expression tag	UNP Q6GN30
L	314	HIS	-	expression tag	UNP Q6GN30

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# 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: Trimeric intracellular cation channel type B-B







# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	290.25Å 290.25Å 195.80Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	49.93 - 3.10	Depositor
Resolution (A)	49.93 - 3.10	EDS
% Data completeness	90.9 (49.93-3.10)	Depositor
(in resolution range)	90.9 (49.93-3.10)	EDS
R <sub>merge</sub>	0.39	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.52 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.14rc2_3191	Depositor
P. P.	0.283 , $0.300$	Depositor
$n, n_{free}$	0.284 , $0.301$	DCC
$R_{free}$ test set	6778 reflections $(4.94%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	81.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , $60.2$	EDS
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	21192	wwPDB-VP
Average B, all atoms $(Å^2)$	75.0	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 36.05 % 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 5.3039e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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	
	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.25	0/1820	0.38	0/2470
1	В	0.25	0/1820	0.38	0/2470
1	С	0.26	0/1820	0.37	0/2470
1	D	0.25	0/1820	0.37	0/2470
1	Ε	0.25	0/1820	0.37	0/2470
1	F	0.27	0/1820	0.37	0/2470
1	G	0.25	0/1820	0.37	0/2470
1	Н	0.25	0/1820	0.37	0/2470
1	Ι	0.25	0/1820	0.37	0/2470
1	J	0.26	0/1820	0.38	0/2470
1	Κ	0.25	0/1820	0.37	0/2470
1	L	0.25	0/1820	0.38	0/2470
All	All	0.25	0/21840	0.38	0/29640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	А	1766	0	1763	29	0
1	В	1766	0	1763	27	0
1	С	1766	0	1763	24	0
1	D	1766	0	1763	17	0



0 0	contracta from proto as pagon						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes	
1	Е	1766	0	1763	25	0	
1	F	1766	0	1763	26	0	
1	G	1766	0	1763	22	0	
1	Н	1766	0	1763	20	0	
1	Ι	1766	0	1763	26	0	
1	J	1766	0	1763	33	0	
1	Κ	1766	0	1763	34	0	
1	L	1766	0	1763	25	0	
All	All	21192	0	21156	288	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 7.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:J:33:ARG:HB2	1:J:93:TYR:CZ	1.92	1.04
1:J:33:ARG:HB2	1:J:93:TYR:CE2	1.92	1.03
1:L:33:ARG:HB2	1:L:93:TYR:CZ	1.97	0.99
1:K:33:ARG:HB2	1:K:93:TYR:CZ	1.98	0.98
1:I:33:ARG:HB2	1:I:93:TYR:CZ	2.00	0.96
1:C:33:ARG:HB2	1:C:93:TYR:CE2	2.01	0.95
1:C:33:ARG:HB2	1:C:93:TYR:CZ	2.01	0.95
1:I:33:ARG:HB2	1:I:93:TYR:CE2	2.06	0.90
1:K:33:ARG:HB2	1:K:93:TYR:CE2	2.06	0.89
1:D:33:ARG:HB2	1:D:93:TYR:CE2	2.11	0.85
1:L:33:ARG:HB2	1:L:93:TYR:CE2	2.11	0.85
1:B:33:ARG:HB2	1:B:93:TYR:CZ	2.13	0.83
1:F:33:ARG:HB2	1:F:93:TYR:CZ	2.14	0.82
1:B:33:ARG:HB2	1:B:93:TYR:CE2	2.17	0.80
1:D:33:ARG:HB2	1:D:93:TYR:CZ	2.18	0.78
1:A:33:ARG:HB2	1:A:93:TYR:CZ	2.19	0.78
1:F:33:ARG:HB2	1:F:93:TYR:CE2	2.19	0.77
1:E:9:VAL:HG11	1:K:6:GLU:HA	1.66	0.76
1:J:33:ARG:HB2	1:J:93:TYR:OH	1.88	0.74
1:E:33:ARG:HB2	1:E:93:TYR:CZ	2.22	0.73
1:E:33:ARG:HB2	1:E:93:TYR:CE2	2.24	0.72
1:L:33:ARG:HB2	1:L:93:TYR:OH	1.88	0.72
1:J:33:ARG:CB	1:J:93:TYR:CE2	2.71	0.71
1:K:33:ARG:HB2	1:K:93:TYR:OH	1.90	0.71
1:A:33:ARG:HB2	1:A:93:TYR:CE2	2.25	0.70



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:I:33:ARG:HB2	1:I:93:TYR:OH	1.92	0.69
1:B:63:LEU:HB2	1:B:157:ILE:HD11	1.77	0.67
1:L:63:LEU:HB2	1:L:157:ILE:HD11	1.77	0.67
1:K:33:ARG:CA	1:K:93:TYR:OH	2.44	0.66
1:K:33:ARG:CB	1:K:93:TYR:CE2	2.79	0.65
1:L:184:VAL:HG11	1:L:215:LEU:HD13	1.78	0.65
1:J:195:GLN:NE2	1:J:202:ILE:O	2.24	0.64
1:C:184:VAL:HG11	1:C:215:LEU:HD13	1.79	0.64
1:K:184:VAL:HG11	1:K:215:LEU:HD13	1.80	0.64
1:D:184:VAL:HG11	1:D:215:LEU:HD13	1.80	0.64
1:H:184:VAL:HG11	1:H:215:LEU:HD13	1.79	0.63
1:C:33:ARG:HB2	1:C:93:TYR:OH	1.99	0.63
1:E:195:GLN:NE2	1:E:202:ILE:O	2.30	0.63
1:G:184:VAL:HG11	1:G:215:LEU:HD13	1.81	0.63
1:B:195:GLN:NE2	1:B:202:ILE:O	2.27	0.62
1:C:33:ARG:CB	1:C:93:TYR:CE2	2.80	0.62
1:E:184:VAL:HG11	1:E:215:LEU:HD13	1.81	0.62
1:B:184:VAL:HG11	1:B:215:LEU:HD13	1.83	0.61
1:F:184:VAL:HG11	1:F:215:LEU:HD13	1.82	0.61
1:A:184:VAL:HG11	1:A:215:LEU:HD13	1.82	0.61
1:J:33:ARG:CA	1:J:93:TYR:OH	2.49	0.60
1:K:195:GLN:NE2	1:K:202:ILE:O	2.28	0.60
1:B:33:ARG:HB2	1:B:93:TYR:OH	2.01	0.60
1:I:184:VAL:HG11	1:I:215:LEU:HD13	1.83	0.60
1:J:184:VAL:HG11	1:J:215:LEU:HD13	1.84	0.60
1:B:121:ARG:HD2	1:B:215:LEU:HD21	1.85	0.59
1:L:33:ARG:CA	1:L:93:TYR:OH	2.51	0.58
1:I:33:ARG:CB	1:I:93:TYR:CE2	2.84	0.58
1:D:63:LEU:HB2	1:D:157:ILE:HD11	1.85	0.58
1:F:33:ARG:HB2	1:F:93:TYR:OH	2.03	0.58
1:L:33:ARG:CB	1:L:93:TYR:CE2	2.86	0.58
1:H:195:GLN:NE2	1:H:202:ILE:O	2.29	0.58
1:E:29:VAL:HG22	1:E:53:ALA:HB1	1.86	0.58
1:G:195:GLN:NE2	1:G:202:ILE:O	2.25	0.57
1:D:195:GLN:NE2	1:D:202:ILE:O	2.29	0.57
1:K:33:ARG:CB	1:K:93:TYR:OH	2.53	0.57
1:K:173:ASN:ND2	1:L:164:VAL:O	2.37	0.57
1:B:205:HIS:CE1	1:H:9:VAL:HG12	2.40	0.57
1:I:121:ARG:HD2	1:I:215:LEU:HD21	1.86	0.56
1:I:33:ARG:CA	1:I:93:TYR:OH	2.54	0.56
1:J:33:ARG:CB	1:J:93:TYR:OH	2.52	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:121:ARG:HD2	1:A:215:LEU:HD21	1.87	0.56
1:G:63:LEU:HB2	1:G:157:ILE:HD11	1.88	0.55
1:A:195:GLN:NE2	1:A:202:ILE:O	2.28	0.55
1:L:33:ARG:CB	1:L:93:TYR:OH	2.54	0.55
1:C:33:ARG:CA	1:C:93:TYR:OH	2.55	0.55
1:H:35:GLN:OE1	1:H:165:ARG:NH1	2.39	0.55
1:K:28:SER:HB3	1:K:56:HIS:HB3	1.88	0.55
1:E:63:LEU:HB2	1:E:157:ILE:HD11	1.89	0.55
1:J:28:SER:HB3	1:J:56:HIS:HB3	1.89	0.55
1:F:9:VAL:HB	1:J:205:HIS:NE2	2.20	0.55
1:K:16:MET:HE2	1:K:123:TRP:CD1	2.42	0.55
1:D:121:ARG:HD2	1:D:215:LEU:HD21	1.89	0.54
1:L:121:ARG:HD2	1:L:215:LEU:HD21	1.90	0.54
1:J:173:ASN:ND2	1:K:164:VAL:O	2.41	0.54
1:F:16:MET:HE2	1:F:123:TRP:CD1	2.42	0.54
1:K:203:SER:OG	1:K:206:ASN:OD1	2.26	0.54
1:C:121:ARG:HD2	1:C:215:LEU:HD21	1.88	0.54
1:J:121:ARG:HD2	1:J:215:LEU:HD21	1.89	0.54
1:G:28:SER:HB3	1:G:56:HIS:HB3	1.89	0.54
1:J:203:SER:OG	1:J:206:ASN:OD1	2.26	0.53
1:K:121:ARG:HD2	1:K:215:LEU:HD21	1.90	0.53
1:F:28:SER:HB3	1:F:56:HIS:HB3	1.90	0.53
1:K:33:ARG:HA	1:K:93:TYR:OH	2.08	0.53
1:A:16:MET:HE2	1:A:123:TRP:CD1	2.43	0.53
1:A:161:GLU:OE2	1:A:165:ARG:NH1	2.41	0.53
1:B:203:SER:OG	1:B:206:ASN:OD1	2.25	0.53
1:E:121:ARG:HD2	1:E:215:LEU:HD21	1.89	0.53
1:H:121:ARG:HD2	1:H:215:LEU:HD21	1.91	0.53
1:D:35:GLN:OE1	1:D:165:ARG:NH1	2.42	0.53
1:E:203:SER:OG	1:E:206:ASN:OD1	2.26	0.53
1:G:16:MET:HE2	1:G:123:TRP:CD1	2.44	0.53
1:I:195:GLN:NE2	1:I:202:ILE:O	2.30	0.53
1:G:203:SER:OG	1:G:206:ASN:OD1	2.26	0.52
1:C:203:SER:OG	1:C:206:ASN:OD1	2.27	0.52
1:E:173:ASN:ND2	1:F:164:VAL:O	2.42	0.52
1:G:70:GLU:OE2	1:G:131:HIS:NE2	2.42	0.52
1:E:28:SER:HB3	1:E:56:HIS:HB3	1.93	0.51
1:L:203:SER:OG	1:L:206:ASN:OD1	2.28	0.51
1:F:70:GLU:OE2	1:F:131:HIS:NE2	2.41	0.51
1:F:121:ARG:HD2	1:F:215:LEU:HD21	1.91	0.51
1:K:63:LEU:HB2	1:K:157:ILE:HD11	1.91	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:76:LEU:HD12	1:B:82:ILE:HG13	1.93	0.51
1:D:33:ARG:CB	1:D:93:TYR:CE2	2.91	0.51
1:G:121:ARG:HD2	1:G:215:LEU:HD21	1.92	0.51
1:A:164:VAL:O	1:C:173:ASN:ND2	2.45	0.50
1:J:76:LEU:HD12	1:J:82:ILE:HG13	1.93	0.50
1:D:33:ARG:HB2	1:D:93:TYR:OH	2.10	0.50
1:E:35:GLN:OE1	1:E:165:ARG:NH1	2.44	0.50
1:J:70:GLU:OE2	1:J:131:HIS:NE2	2.39	0.50
1:C:63:LEU:HB2	1:C:157:ILE:HD11	1.92	0.50
1:L:52:SER:OG	1:L:161:GLU:OE2	2.28	0.50
1:H:16:MET:HE2	1:H:123:TRP:CD1	2.47	0.50
1:B:161:GLU:OE2	1:B:165:ARG:NH1	2.45	0.50
1:K:29:VAL:HG11	1:K:89:TRP:HA	1.93	0.50
1:A:63:LEU:HB2	1:A:157:ILE:HD11	1.93	0.50
1:I:33:ARG:CB	1:I:93:TYR:OH	2.58	0.50
1:C:28:SER:HB3	1:C:56:HIS:HB3	1.93	0.49
1:F:153:GLY:O	1:F:157:ILE:HG13	2.12	0.49
1:G:60:GLY:HA2	1:G:153:GLY:HA3	1.94	0.49
1:H:203:SER:OG	1:H:206:ASN:OD1	2.29	0.49
1:B:28:SER:HB3	1:B:56:HIS:HB3	1.95	0.49
1:C:16:MET:HE2	1:C:123:TRP:CD1	2.48	0.49
1:G:106:PHE:CD2	1:G:108:PRO:HD2	2.48	0.49
1:F:16:MET:HE2	1:F:123:TRP:HD1	1.78	0.48
1:I:153:GLY:O	1:I:157:ILE:HG13	2.13	0.48
1:A:33:ARG:NH2	1:A:92:VAL:O	2.45	0.48
1:C:33:ARG:CB	1:C:93:TYR:OH	2.62	0.48
1:A:203:SER:OG	1:A:206:ASN:OD1	2.31	0.48
1:I:70:GLU:OE2	1:I:131:HIS:NE2	2.33	0.48
1:I:203:SER:OG	1:I:206:ASN:OD1	2.31	0.48
1:A:33:ARG:HB2	1:A:93:TYR:OH	2.13	0.48
1:A:33:ARG:HA	1:A:93:TYR:OH	2.14	0.48
1:L:16:MET:HE2	1:L:123:TRP:CD1	2.49	0.48
1:A:33:ARG:CA	1:A:93:TYR:OH	2.62	0.47
1:A:136:TYR:OH	1:H:137:LYS:HE3	2.15	0.47
1:J:153:GLY:O	1:J:157:ILE:HG13	2.14	0.47
1:A:173:ASN:ND2	1:B:164:VAL:O	2.48	0.47
1:I:16:MET:HE2	1:I:123:TRP:CD1	2.50	0.47
1:J:16:MET:HE2	1:J:123:TRP:CD1	2.50	0.47
1:E:161:GLU:OE2	1:E:165:ARG:NH1	2.47	0.47
1:F:91:MET:O	1:F:95:PHE:HB2	2.15	0.47
1:F:203:SER:OG	1:F:206:ASN:OD1	2.33	0.47



	lo de page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:44:HIS:O	1:C:45:SER:OG	2.27	0.47	
1:L:76:LEU:HD12	1:L:82:ILE:HG13	1.97	0.47	
1:D:73:VAL:HG11	1:F:68:LEU:HD23	1.97	0.47	
1:L:153:GLY:O	1:L:157:ILE:HG13	2.14	0.47	
1:A:16:MET:HE2	1:A:123:TRP:HD1	1.80	0.46	
1:J:132:ALA:HB1	1:J:142:VAL:HG12	1.97	0.46	
1:F:60:GLY:HA2	1:F:153:GLY:HA3	1.97	0.46	
1:I:33:ARG:NH2	1:I:92:VAL:O	2.48	0.46	
1:A:153:GLY:O	1:A:157:ILE:HG13	2.16	0.46	
1:C:153:GLY:O	1:C:157:ILE:HG13	2.15	0.46	
1:E:106:PHE:CD2	1:E:108:PRO:HD2	2.51	0.46	
1:C:114:ALA:O	1:C:118:GLU:HG2	2.16	0.46	
1:K:60:GLY:HA2	1:K:153:GLY:HA3	1.97	0.46	
1:B:16:MET:HE2	1:B:123:TRP:CD1	2.51	0.46	
1:G:73:VAL:HG11	1:I:68:LEU:HD23	1.97	0.46	
1:H:153:GLY:O	1:H:157:ILE:HG13	2.15	0.46	
1:H:28:SER:HB3	1:H:56:HIS:HB3	1.98	0.46	
1:I:28:SER:HB3	1:I:56:HIS:HB3	1.98	0.46	
1:F:106:PHE:CD2	1:F:108:PRO:HD2	2.51	0.45	
1:A:44:HIS:O	1:A:45:SER:OG	2.30	0.45	
1:B:68:LEU:HD23	1:C:73:VAL:HG11	1.99	0.45	
1:I:44:HIS:O	1:I:45:SER:OG	2.31	0.45	
1:G:58:PHE:HB3	1:G:75:ILE:HG21	1.99	0.45	
1:I:118:GLU:HB3	1:I:215:LEU:HG	1.99	0.45	
1:A:118:GLU:OE2	1:A:121:ARG:NH1	2.49	0.45	
1:A:118:GLU:HB3	1:A:215:LEU:HG	1.99	0.45	
1:B:33:ARG:CB	1:B:93:TYR:CE2	2.95	0.45	
1:C:91:MET:O	1:C:95:PHE:HB2	2.17	0.45	
1:I:60:GLY:HA2	1:I:153:GLY:HA3	1.98	0.45	
1:E:205:HIS:NE2	1:K:9:VAL:HB	2.32	0.45	
1:J:164:VAL:O	1:L:173:ASN:ND2	2.49	0.45	
1:E:168:TRP:NE1	1:E:170:PRO:HG3	2.32	0.45	
1:H:52:SER:OG	1:H:161:GLU:OE2	2.30	0.45	
1:B:33:ARG:CA	1:B:93:TYR:OH	2.65	0.45	
1:K:33:ARG:CG	1:K:93:TYR:CE2	3.00	0.45	
1:L:195:GLN:NE2	1:L:202:ILE:O	2.32	0.45	
1:L:204:ARG:O	1:L:208:MET:HB2	2.16	0.45	
1:E:16:MET:HE2	1:E:123:TRP:CD1	2.52	0.44	
1:I:52:SER:OG	1:I:161:GLU:OE2	2.30	0.44	
1:F:111:LEU:HD11	1:F:224:LEU:HD21	1.97	0.44	
1:J:35:GLN:OE1	1:J:165:ARG:NH1	2.49	0.44	



	lo de page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:168:TRP:NE1	1:A:170:PRO:HG3	2.32	0.44	
1:J:33:ARG:CG	1:J:93:TYR:CE2	3.00	0.44	
1:F:29:VAL:HG22	1:F:53:ALA:HB1	2.00	0.44	
1:A:176:LEU:HA	1:B:45:SER:HB3	2.00	0.44	
1:K:106:PHE:CD2	1:K:108:PRO:HD2	2.53	0.44	
1:A:60:GLY:HA2	1:A:153:GLY:HA3	1.99	0.44	
1:G:168:TRP:NE1	1:G:170:PRO:HG3	2.33	0.44	
1:I:91:MET:O	1:I:95:PHE:HB2	2.18	0.44	
1:J:29:VAL:HG11	1:J:89:TRP:HA	2.00	0.44	
1:C:52:SER:OG	1:C:161:GLU:OE2	2.35	0.43	
1:E:44:HIS:O	1:E:45:SER:OG	2.34	0.43	
1:E:204:ARG:O	1:E:208:MET:HB2	2.17	0.43	
1:H:63:LEU:HB2	1:H:157:ILE:HD11	1.98	0.43	
1:J:144:ILE:HD13	1:J:190:VAL:HG22	2.00	0.43	
1:E:33:ARG:HB2	1:E:93:TYR:OH	2.18	0.43	
1:L:44:HIS:O	1:L:45:SER:OG	2.33	0.43	
1:D:164:VAL:O	1:F:173:ASN:ND2	2.51	0.43	
1:A:204:ARG:O	1:A:208:MET:HB2	2.18	0.43	
1:K:33:ARG:HG3	1:K:93:TYR:HE2	1.83	0.43	
1:K:95:PHE:CG	1:K:96:PRO:HD2	2.53	0.43	
1:D:60:GLY:HA2	1:D:153:GLY:HA3	2.00	0.43	
1:K:35:GLN:OE1	1:K:165:ARG:NH1	2.51	0.43	
1:B:114:ALA:O	1:B:118:GLU:HG2	2.19	0.43	
1:G:29:VAL:HG22	1:G:53:ALA:HB1	2.00	0.43	
1:I:63:LEU:HB2	1:I:157:ILE:HD11	2.01	0.43	
1:K:126:LEU:HD23	1:K:126:LEU:HA	1.90	0.43	
1:L:178:MET:HE2	1:L:178:MET:HB3	1.95	0.43	
1:A:41:ILE:O	1:A:45:SER:N	2.52	0.43	
1:H:60:GLY:HA2	1:H:153:GLY:HA3	2.00	0.43	
1:H:204:ARG:O	1:H:208:MET:HB2	2.18	0.43	
1:B:168:TRP:NE1	1:B:170:PRO:HG3	2.34	0.43	
1:B:60:GLY:HA2	1:B:153:GLY:HA3	2.00	0.42	
1:B:156:LEU:HD23	1:B:174:GLU:HG2	2.01	0.42	
1:C:60:GLY:HA2	1:C:153:GLY:HA3	2.00	0.42	
1:D:153:GLY:O	1:D:157:ILE:HG13	2.18	0.42	
1:D:176:LEU:HA	1:E:45:SER:HB3	2.02	0.42	
1:G:45:SER:HB3	1:I:176:LEU:HA	2.01	0.42	
1:G:95:PHE:CG	1:G:96:PRO:HD2	2.54	0.42	
1:K:114:ALA:O	1:K:118:GLU:HG2	2.19	0.42	
1:E:33:ARG:CA	1:E:93:TYR:OH	2.67	0.42	
1:H:106:PHE:CD2	1:H:108:PRO:HD2	2.54	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:K:77:ALA:O	1:K:79:THR:N	2.53	0.42	
1:A:35:GLN:OE1	1:A:165:ARG:NH1	2.53	0.42	
1:A:91:MET:O	1:A:95:PHE:HB2	2.18	0.42	
1:G:33:ARG:NH2	1:G:92:VAL:O	2.53	0.42	
1:G:153:GLY:O	1:G:157:ILE:HG13	2.20	0.42	
1:B:35:GLN:OE1	1:B:165:ARG:NH1	2.52	0.42	
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.88	0.42	
1:H:62:ILE:O	1:H:66:ILE:HG13	2.19	0.42	
1:J:33:ARG:CB	1:J:93:TYR:HE2	2.28	0.42	
1:K:204:ARG:O	1:K:208:MET:HB2	2.20	0.42	
1:C:168:TRP:NE1	1:C:170:PRO:HG3	2.35	0.42	
1:F:168:TRP:NE1	1:F:170:PRO:HG3	2.34	0.42	
1:G:114:ALA:O	1:G:118:GLU:HG2	2.20	0.42	
1:L:106:PHE:CD2	1:L:108:PRO:HD2	2.55	0.42	
1:L:114:ALA:O	1:L:118:GLU:HG2	2.19	0.42	
1:F:52:SER:OG	1:F:161:GLU:OE2	2.34	0.42	
1:E:114:ALA:O	1:E:118:GLU:HG2	2.20	0.41	
1:H:114:ALA:O	1:H:118:GLU:HG2	2.19	0.41	
1:L:33:ARG:NH2	1:L:92:VAL:O	2.53	0.41	
1:I:168:TRP:NE1	1:I:170:PRO:HG3	2.35	0.41	
1:H:97:TYR:HB2	1:H:99:LEU:HG	2.02	0.41	
1:J:63:LEU:HB2	1:J:157:ILE:HD11	2.01	0.41	
1:E:144:ILE:HD13	1:E:190:VAL:HG22	2.02	0.41	
1:K:29:VAL:HG22	1:K:53:ALA:HB1	2.02	0.41	
1:K:153:GLY:O	1:K:157:ILE:HG13	2.19	0.41	
1:C:33:ARG:NH2	1:C:92:VAL:O	2.53	0.41	
1:F:204:ARG:O	1:F:208:MET:HB2	2.20	0.41	
1:G:35:GLN:OE1	1:G:165:ARG:NH1	2.53	0.41	
1:G:91:MET:O	1:G:95:PHE:HB2	2.21	0.41	
1:J:33:ARG:N	1:J:93:TYR:OH	2.53	0.41	
1:J:60:GLY:HA2	1:J:153:GLY:HA3	2.03	0.41	
1:A:70:GLU:OE2	1:A:131:HIS:NE2	2.43	0.41	
1:B:95:PHE:CG	1:B:96:PRO:HD2	2.56	0.41	
1:C:35:GLN:OE1	1:C:165:ARG:NH1	2.54	0.41	
1:D:168:TRP:NE1	1:D:170:PRO:HG3	2.36	0.41	
1:E:33:ARG:NH2	1:E:92:VAL:O	2.54	0.41	
1:G:126:LEU:HD23	1:G:126:LEU:HA	1.87	0.41	
1:I:16:MET:HE2	1:I:123:TRP:HD1	1.86	0.41	
1:J:168:TRP:NE1	1:J:170:PRO:HG3	2.36	0.41	
1:B:207:LEU:HA	1:B:210:ILE:HG22	2.03	0.41	
1:D:118:GLU:OE2	1:D:121:ARG:NH1	2.52	0.41	



Atom_1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:I:106:PHE:CD2	1:I:108:PRO:HD2	2.56	0.41	
1:J:29:VAL:HG22	1:J:53:ALA:HB1	2.03	0.41	
1:J:114:ALA:O	1:J:118:GLU:HG2	2.21	0.41	
1:D:203:SER:OG	1:D:206:ASN:OD1	2.38	0.40	
1:F:33:ARG:CA	1:F:93:TYR:OH	2.69	0.40	
1:J:68:LEU:HD23	1:K:73:VAL:HG11	2.03	0.40	
1:K:76:LEU:HD12	1:K:76:LEU:HA	1.93	0.40	
1:H:126:LEU:HD23	1:H:126:LEU:HA	1.89	0.40	
1:J:45:SER:HB3	1:L:176:LEU:HA	2.03	0.40	
1:J:111:LEU:HD11	1:J:224:LEU:HD21	2.02	0.40	
1:B:153:GLY:O	1:B:157:ILE:HG13	2.21	0.40	
1:F:62:ILE:O	1:F:66:ILE:HG13	2.22	0.40	
1:H:95:PHE:CG	1:H:96:PRO:HD2	2.57	0.40	
1:L:33:ARG:HA	1:L:93:TYR:OH	2.21	0.40	
1:C:106:PHE:CD2	1:C:108:PRO:HD2	2.55	0.40	
1:F:182:VAL:O	1:F:185:THR:OG1	2.37	0.40	
1:K:91:MET:O	1:K:95:PHE:HB2	2.22	0.40	

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	Perce	entiles
1	А	222/314~(71%)	215~(97%)	4 (2%)	3(1%)	11	40
1	В	222/314~(71%)	213 (96%)	7 (3%)	2(1%)	17	52
1	С	222/314~(71%)	213 (96%)	7 (3%)	2(1%)	17	52
1	D	222/314~(71%)	215~(97%)	5 (2%)	2(1%)	17	52
1	Ε	222/314~(71%)	215 (97%)	5 (2%)	2(1%)	17	52
1	F	222/314~(71%)	215~(97%)	5 (2%)	2(1%)	17	52
1	G	222/314~(71%)	216 (97%)	4 (2%)	2 (1%)	17	52



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Н	222/314~(71%)	215~(97%)	4(2%)	3~(1%)	11 40
1	Ι	222/314~(71%)	214 (96%)	6 (3%)	2(1%)	17 52
1	J	222/314~(71%)	216~(97%)	4(2%)	2(1%)	17 52
1	Κ	222/314~(71%)	215~(97%)	4 (2%)	3~(1%)	11 40
1	L	222/314~(71%)	214 (96%)	6 (3%)	2(1%)	17 52
All	All	2664/3768~(71%)	2576 (97%)	61 (2%)	27 (1%)	15 49

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All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	137	LYS
1	Е	18	PRO
1	Н	18	PRO
1	L	18	PRO
1	А	18	PRO
1	А	137	LYS
1	В	18	PRO
1	С	18	PRO
1	D	18	PRO
1	F	18	PRO
1	F	137	LYS
1	G	18	PRO
1	G	137	LYS
1	Ι	18	PRO
1	Ι	137	LYS
1	J	18	PRO
1	J	137	LYS
1	Κ	18	PRO
1	Κ	137	LYS
1	L	137	LYS
1	В	137	LYS
1	D	137	LYS
1	К	78	ASN
1	Е	137	LYS
1	А	78	ASN
1	Н	137	LYS
1	Н	78	ASN



#### 6IZ4

#### 5.3.2 Protein sidechains (i)

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percent	iles
1	А	189/268~(70%)	186~(98%)	3~(2%)	62 8	34
1	В	189/268~(70%)	188 (100%)	1 (0%)	88 9	)4
1	С	189/268~(70%)	186~(98%)	3~(2%)	62 8	34
1	D	189/268~(70%)	186~(98%)	3~(2%)	62 8	34
1	Ε	189/268~(70%)	188 (100%)	1 (0%)	88 9	)4
1	F	189/268~(70%)	186~(98%)	3~(2%)	62 8	34
1	G	189/268~(70%)	187~(99%)	2(1%)	73 8	39
1	Н	189/268~(70%)	187~(99%)	2(1%)	73 8	39
1	Ι	189/268~(70%)	187~(99%)	2(1%)	73 8	39
1	J	189/268~(70%)	187~(99%)	2(1%)	73 8	39
1	Κ	189/268~(70%)	186~(98%)	3~(2%)	62 8	34
1	L	189/268~(70%)	187 (99%)	2 (1%)	73 8	39
All	All	2268/3216 (70%)	2241 (99%)	27(1%)	71 8	38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	26	LEU
1	А	43	SER
1	А	159	ASN
1	В	159	ASN
1	С	9	VAL
1	С	137	LYS
1	С	159	ASN
1	D	13	GLN
1	D	159	ASN
1	D	208	MET
1	Е	159	ASN
1	F	9	VAL
1	F	26	LEU
1	F	159	ASN



Mol	Chain	Res	Type
1	G	9	VAL
1	G	159	ASN
1	Н	6	GLU
1	Н	159	ASN
1	Ι	159	ASN
1	Ι	208	MET
1	J	159	ASN
1	J	208	MET
1	К	9	VAL
1	K	26	LEU
1	К	159	ASN
1	L	43	SER
1	L	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	135	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

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,  $95^{th}$  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 $>$	#RS	SRZ:	>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	224/314~(71%)	-0.14	5(2%)	62	41	42, 67, 106, 135	0
1	В	224/314~(71%)	-0.26	5 (2%)	62	41	38, 66, 106, 150	0
1	С	224/314~(71%)	-0.24	4 (1%)	68	47	40, 67, 110, 144	0
1	D	224/314~(71%)	-0.23	3(1%)	77	59	42, 67, 105, 143	0
1	Ε	224/314~(71%)	-0.15	5(2%)	62	41	46, 72, 116, 149	0
1	F	224/314~(71%)	-0.25	3(1%)	77	59	50, 73, 111, 149	0
1	G	224/314~(71%)	-0.23	3~(1%)	77	59	47, 74, 111, 160	0
1	Н	224/314~(71%)	-0.16	5(2%)	62	41	50, 71, 113, 149	0
1	Ι	224/314~(71%)	-0.19	4 (1%)	68	47	47, 74, 114, 139	0
1	J	224/314~(71%)	-0.25	3(1%)	77	59	46, 70, 112, 157	0
1	Κ	224/314~(71%)	-0.20	2~(0%)	84	69	45, 70, 109, 157	0
1	L	$22\overline{4/314}$ (71%)	-0.17	0 100	) 1	00	43, 68, 106, 134	0
All	All	$268\overline{8}/3768~(71\%)$	-0.21	42 (1%)	72	51	38, 70, 111, 160	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Н	5	SER	5.1
1	Κ	5	SER	4.6
1	J	13	GLN	4.6
1	Е	13	GLN	4.0
1	F	6	GLU	4.0
1	F	227	SER	4.0
1	Н	6	GLU	3.8
1	Е	138	ASP	3.5
1	А	5	SER	3.5
1	F	5	SER	3.3
1	D	6	GLU	3.1



Mol	Chain	Res	Type	RSRZ
1	Е	4	LEU	3.1
1	D	5	SER	3.0
1	D	4	LEU	3.0
1	А	200	LEU	3.0
1	С	199	TYR	3.0
1	Ι	227	SER	2.9
1	С	5	SER	2.9
1	С	6	GLU	2.8
1	K	6	GLU	2.7
1	G	5	SER	2.7
1	G	6	GLU	2.6
1	Ι	4	LEU	2.6
1	В	5	SER	2.5
1	А	4	LEU	2.3
1	В	13	GLN	2.3
1	С	200	LEU	2.3
1	Ι	172	SER	2.3
1	J	6	GLU	2.2
1	В	227	SER	2.2
1	А	227	SER	2.2
1	G	19	PHE	2.1
1	Н	199	TYR	2.1
1	J	19	PHE	2.1
1	Н	214	PHE	2.1
1	В	6	GLU	2.1
1	Ι	196	HIS	2.1
1	А	199	TYR	2.0
1	Е	173	ASN	2.0
1	Е	172	SER	2.0
1	Н	200	LEU	2.0
1	В	4	LEU	2.0

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## 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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

