



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:29 am BST

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](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  
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

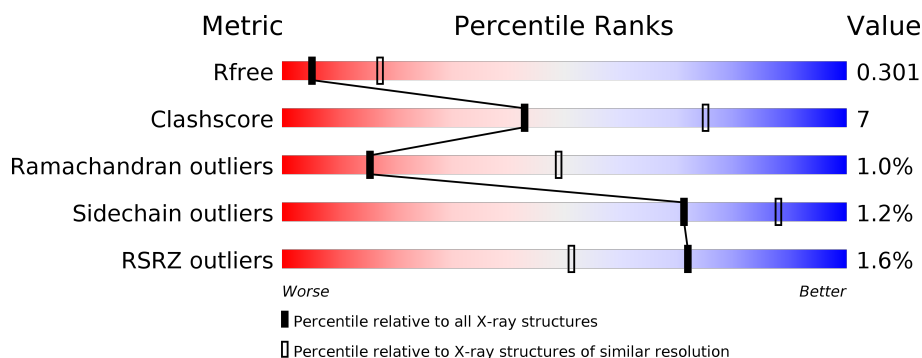
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 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	314	<div> <div>2%</div> <div>58%13%29%</div> </div>
1	B	314	<div> <div>2%</div> <div>59%13%29%</div> </div>
1	C	314	<div> <div>%</div> <div>60%11%29%</div> </div>
1	D	314	<div> <div>%</div> <div>63%8%29%</div> </div>
1	E	314	<div> <div>2%</div> <div>59%12%29%</div> </div>
1	F	314	<div> <div>%</div> <div>58%13%29%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	314	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>13%</div> <div>29%</div> </div> </div>
1	H	314	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>12%</div> <div>29%</div> </div> </div>
1	I	314	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>12%</div> <div>29%</div> </div> </div>
1	J	314	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>14%</div> <div>29%</div> </div> </div>
1	K	314	<div> <div>%</div> <div> <div></div> <div>57%</div> <div>14%</div> <div>29%</div> </div> </div>
1	L	314	<div> <div>%</div> <div> <div></div> <div>60%</div> <div>11%</div> <div>29%</div> </div> </div>

## 2 Entry composition

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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	B	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	C	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	D	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	E	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	F	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	G	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	H	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	I	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	J	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	K	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			
1	L	224	Total	C	N	O	S	0	0	0
			1766	1166	285	299	16			

There are 360 discrepancies between the modelled and reference sequences:

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

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

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

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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
E	303	ASP	-	expression tag	UNP Q6GN30
E	304	LYS	-	expression tag	UNP Q6GN30
E	305	HIS	-	expression tag	UNP Q6GN30
E	306	HIS	-	expression tag	UNP Q6GN30
E	307	HIS	-	expression tag	UNP Q6GN30
E	308	HIS	-	expression tag	UNP Q6GN30
E	309	HIS	-	expression tag	UNP Q6GN30
E	310	HIS	-	expression tag	UNP Q6GN30
E	311	HIS	-	expression tag	UNP Q6GN30
E	312	HIS	-	expression tag	UNP Q6GN30
E	313	HIS	-	expression tag	UNP Q6GN30
E	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 Q6GN30
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 Q6GN30
H	286	ALA	-	expression tag	UNP Q6GN30
H	287	ALA	-	expression tag	UNP Q6GN30
H	288	GLU	-	expression tag	UNP Q6GN30
H	289	ASN	-	expression tag	UNP Q6GN30

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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	302	ASP	-	expression tag	UNP Q6GN30
I	303	ASP	-	expression tag	UNP Q6GN30
I	304	LYS	-	expression tag	UNP Q6GN30
I	305	HIS	-	expression tag	UNP Q6GN30
I	306	HIS	-	expression tag	UNP Q6GN30
I	307	HIS	-	expression tag	UNP Q6GN30
I	308	HIS	-	expression tag	UNP Q6GN30
I	309	HIS	-	expression tag	UNP Q6GN30
I	310	HIS	-	expression tag	UNP Q6GN30
I	311	HIS	-	expression tag	UNP Q6GN30
I	312	HIS	-	expression tag	UNP Q6GN30
I	313	HIS	-	expression tag	UNP Q6GN30
I	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

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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 Q6GN30
L	295	LEU	-	expression tag	UNP Q6GN30

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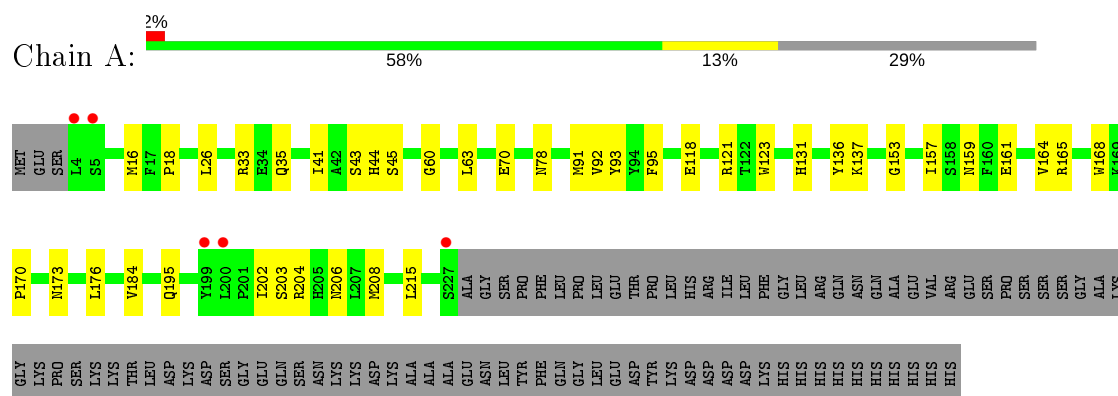
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Chain	Residue	Modelled	Actual	Comment	Reference
L	296	GLU	-	expression tag	UNP Q6GN30
L	297	ASP	-	expression tag	UNP Q6GN30
L	298	TYR	-	expression tag	UNP Q6GN30
L	299	LYS	-	expression tag	UNP Q6GN30
L	300	ASP	-	expression tag	UNP Q6GN30
L	301	ASP	-	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

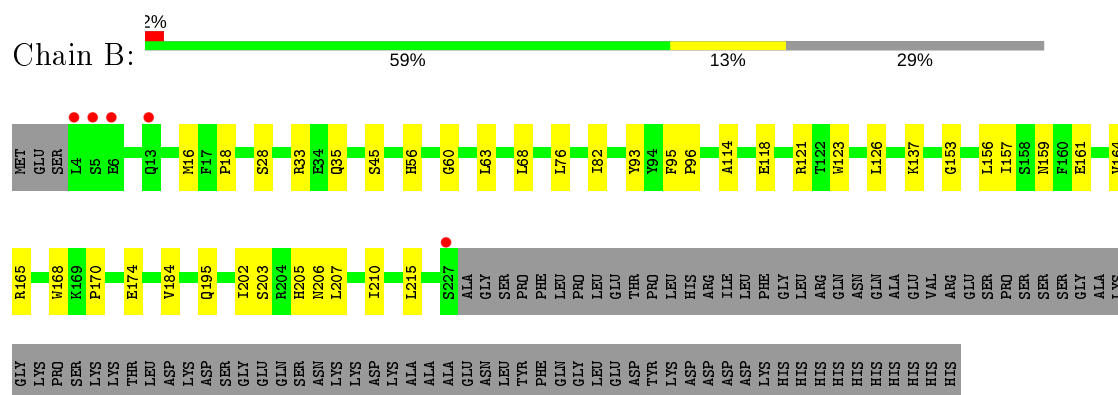
### 3 Residue-property plots [i](#)

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.

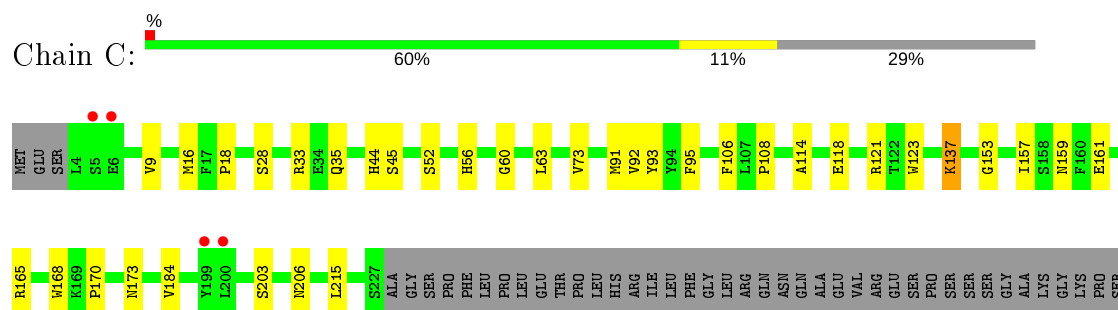
#### • Molecule 1: Trimeric intracellular cation channel type B-B



#### • Molecule 1: Trimeric intracellular cation channel type B-B



#### • Molecule 1: Trimeric intracellular cation channel type B-B



LYS  
LYS  
THR  
LEU  
ASP  
LYS  
ASP  
SER  
GLY  
GLN  
SER  
ASN  
LYS  
LYS  
ASP  
LYS  
ALA  
ALA  
GLU  
ASN  
LEU  
TYR  
PHE  
GLN  
GLY  
LEU  
GLU  
ASP  
TYR  
LYS  
ASP  
ASP  
ASP  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

• Molecule 1: Trimeric intracellular cation channel type B-B



MET GLU SER L4 S5 E6 Q13 P18 R33 R34 Q85 G60 L63 V73 Y93 E118 R121 K137 K153 G157 S168 N159 V164 R165 W168 R169 P170 L176 V184 Q195 I202 S203 N206 L207 M208 L215 S227 GLY

SER PRO PHE LEU PRO LEU GLU THR PRO HIS ARG ASP ILE LEU PHE GLY LEU ARG GLN ASN GLN Y93 VAL ARG GLU SER PRO SER SER GLY ALA LYS GLY LYS THR ASP LYS ASP SER GLY GLN SER ASN L202 N206 L207 M208 L215 S227 GLY

LEU TYR PHE GLN GLY LEU GLU ASP TYR TYR LYS ASP ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: Trimeric intracellular cation channel type B-B



MET GLU SER L4 V9 Q13 M16 P18 S28 V29 R33 R34 Q35 H44 S45 A53 H56 L63 V92 Y93 F106 L107 P108 A114 E118 R121 W123 K137 D138 I144 I157 S158 N159 F160 E161 R165 W168 K169 P170

E171 S172 M173 V184 V190 Q195 I202 S203 R204 H205 N206 M208 L215 S227 ALA GLY SER PRO PHE LEU LEU LEU THR PRO HIS L107 ARG ILE LEU PHE GLY LEU ARG GLN ASN ALA GLU VAL ARG GLU SER PRO SER SER SER GLY ALA LYS GLY LYS PRO

SER LYS THR LEU ASP LYS SER SER GLY GLN SER ASN LYS ASP LYS ALA ALA ALA GLU ASN LEU TYR PHE GLN GLY LEU LEU ASP TYR LYS ASP ASP ASP LYS HIS HIS HIS HIS HIS HIS HIS HIS

• Molecule 1: Trimeric intracellular cation channel type B-B



MET GLU SER L4 E6 V9 M16 F17 P18 L26 A27 V29 R33 S52 A53 H56 G60 G61 I62 I66 L67 L68 A69 E70 M91 V92 Y93 F95 F106 L107 P108 L111 R121 T122 W123 H131 K137 G153 I157 S158 N159

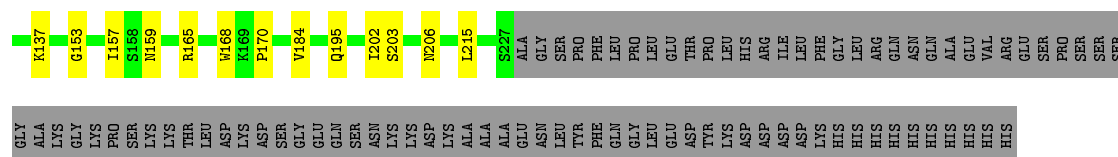
F160 E161 V164 W168 K169 P170 M173 V182 F183 V184 T185 S203 R204 H205 M206 L207 M208 L215 L224 S227 ALA GLY SER PRO PHE LEU LEU LEU THR PRO LEU LEU ARG ILE LEU PHE GLY LEU ARG GLN ASN GLN GLU VAL ARG GLU SER PRO SER

SER GLY ALA LYS LYS PRO SER LYS LYS THR ASP LYS ASP SER GLY GLN GLN ASN LYS HIS HIS HIS HIS HIS HIS HIS HIS

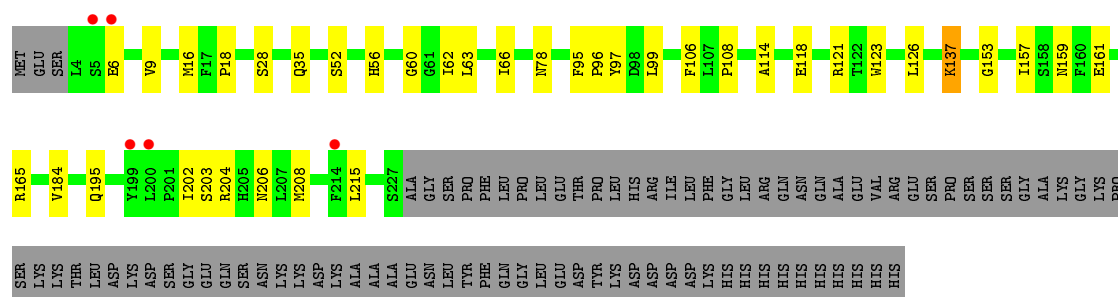
• Molecule 1: Trimeric intracellular cation channel type B-B



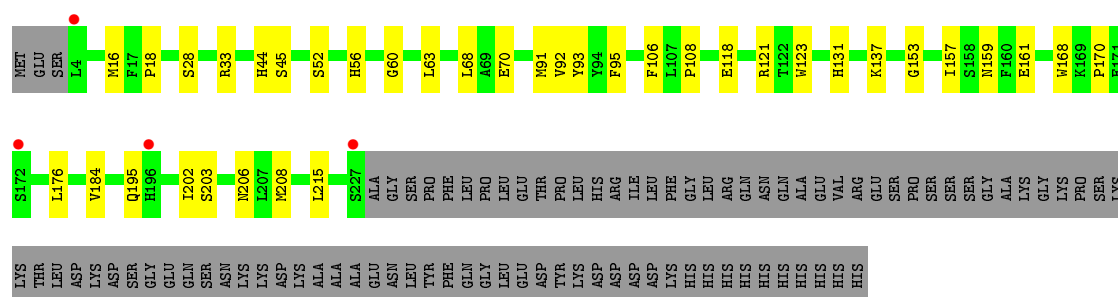
MET GLU SER L4 S5 E6 V9 M16 F17 P18 F19 S28 V29 R33 F34 Q35 S45 A53 H56 G57 F58 G59 G60 L63 E70 V73 G74 I75 M91 V92 F95 P96 F106 L107 P108 A114 E118 R121 T122 W123 L126 I157 S158 H131



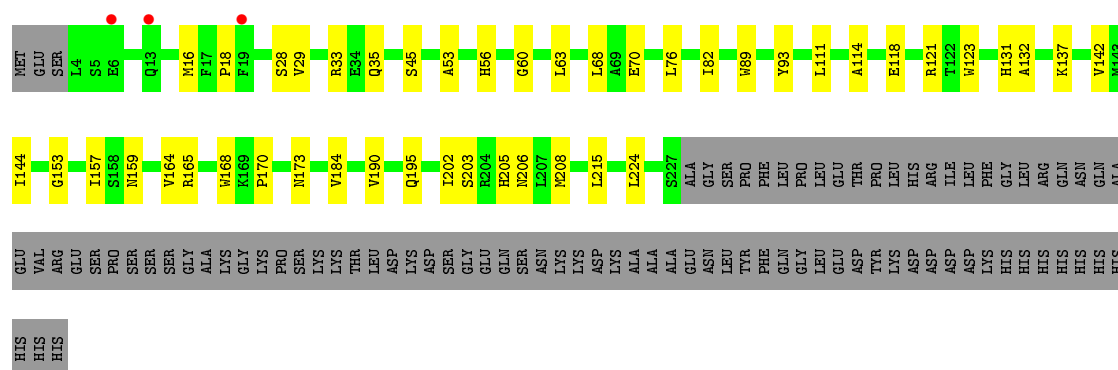
• Molecule 1: Trimeric intracellular cation channel type B-B



• Molecule 1: Trimeric intracellular cation channel type B-B



• Molecule 1: Trimeric intracellular cation channel type B-B



• Molecule 1: Trimeric intracellular cation channel type B-B





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 <sub>2</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	290.25Å 290.25Å 195.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.10 49.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.9 (49.93-3.10) 90.9 (49.93-3.10)	Depositor EDS
$R_{merge}$	0.39	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.14rc2_3191	Depositor
R, $R_{free}$	0.283 , 0.300 0.284 , 0.301	Depositor DCC
$R_{free}$ test set	6778 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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>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 [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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/1820	0.38	0/2470
1	B	0.25	0/1820	0.38	0/2470
1	C	0.26	0/1820	0.37	0/2470
1	D	0.25	0/1820	0.37	0/2470
1	E	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	H	0.25	0/1820	0.37	0/2470
1	I	0.25	0/1820	0.37	0/2470
1	J	0.26	0/1820	0.38	0/2470
1	K	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	A	1766	0	1763	29	0
1	B	1766	0	1763	27	0
1	C	1766	0	1763	24	0
1	D	1766	0	1763	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1766	0	1763	25	0
1	F	1766	0	1763	26	0
1	G	1766	0	1763	22	0
1	H	1766	0	1763	20	0
1	I	1766	0	1763	26	0
1	J	1766	0	1763	33	0
1	K	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 distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:161:GLU:OE2	1:A:165:ARG:NH1	2.41	0.53
1:A:16:MET:HE2	1:A:123:TRP:CD1	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:203:SER:OG	1:I:206:ASN:OD1	2.31	0.48
1:I:70:GLU:OE2	1:I:131:HIS:NE2	2.33	0.48
1:A:33:ARG:HA	1:A:93:TYR:OH	2.14	0.48
1:A:33:ARG:HB2	1:A:93:TYR:OH	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:H:153:GLY:O	1:H:157:ILE:HG13	2.15	0.46
1:G:73:VAL:HG11	1:I:68:LEU:HD23	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:204:ARG:O	1:E:208:MET:HB2	2.17	0.43
1:E:44:HIS:O	1:E:45:SER:OG	2.34	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:HA	1:K:126:LEU:HD23	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:204:ARG:O	1:H:208:MET:HB2	2.18	0.43
1:H:60:GLY:HA2	1:H:153:GLY:HA3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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:153:GLY:O	1:G:157:ILE:HG13	2.20	0.42
1:G:33:ARG:NH2	1:G:92:VAL:O	2.53	0.42
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.88	0.42
1:B:35:GLN:OE1	1:B:165:ARG:NH1	2.52	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:60:GLY:HA2	1:J:153:GLY:HA3	2.03	0.41
1:J:33:ARG:N	1:J:93:TYR:OH	2.53	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: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: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:C:35:GLN:OE1	1:C:165:ARG:NH1	2.54	0.41
1:G:126:LEU:HA	1:G:126:LEU:HD23	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:PHE:CD2	1:I:108:PRO:HD2	2.56	0.41
1:J:114:ALA:O	1:J:118:GLU:HG2	2.21	0.41
1:J:29:VAL:HG22	1:J:53:ALA:HB1	2.03	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:HA	1:K:76:LEU:HD12	1.93	0.40
1:H:126:LEU:HA	1:H:126:LEU:HD23	1.89	0.40
1:J:111:LEU:HD11	1:J:224:LEU:HD21	2.02	0.40
1:J:45:SER:HB3	1:L:176:LEU:HA	2.03	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 ⓘ

### 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	222/314 (71%)	215 (97%)	4 (2%)	3 (1%)	11	40
1	B	222/314 (71%)	213 (96%)	7 (3%)	2 (1%)	17	52
1	C	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	E	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	222/314 (71%)	215 (97%)	4 (2%)	3 (1%)	11	40
1	I	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	K	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

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	LYS
1	E	18	PRO
1	H	18	PRO
1	L	18	PRO
1	A	18	PRO
1	A	137	LYS
1	B	18	PRO
1	C	18	PRO
1	D	18	PRO
1	F	18	PRO
1	F	137	LYS
1	G	18	PRO
1	G	137	LYS
1	I	18	PRO
1	I	137	LYS
1	J	18	PRO
1	J	137	LYS
1	K	18	PRO
1	K	137	LYS
1	L	137	LYS
1	B	137	LYS
1	D	137	LYS
1	K	78	ASN
1	E	137	LYS
1	A	78	ASN
1	H	137	LYS
1	H	78	ASN

### 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	189/268 (70%)	186 (98%)	3 (2%)	62	84
1	B	189/268 (70%)	188 (100%)	1 (0%)	88	94
1	C	189/268 (70%)	186 (98%)	3 (2%)	62	84
1	D	189/268 (70%)	186 (98%)	3 (2%)	62	84
1	E	189/268 (70%)	188 (100%)	1 (0%)	88	94
1	F	189/268 (70%)	186 (98%)	3 (2%)	62	84
1	G	189/268 (70%)	187 (99%)	2 (1%)	73	89
1	H	189/268 (70%)	187 (99%)	2 (1%)	73	89
1	I	189/268 (70%)	187 (99%)	2 (1%)	73	89
1	J	189/268 (70%)	187 (99%)	2 (1%)	73	89
1	K	189/268 (70%)	186 (98%)	3 (2%)	62	84
1	L	189/268 (70%)	187 (99%)	2 (1%)	73	89
All	All	2268/3216 (70%)	2241 (99%)	27 (1%)	71	88

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

Mol	Chain	Res	Type
1	A	26	LEU
1	A	43	SER
1	A	159	ASN
1	B	159	ASN
1	C	9	VAL
1	C	137	LYS
1	C	159	ASN
1	D	13	GLN
1	D	159	ASN
1	D	208	MET
1	E	159	ASN
1	F	9	VAL
1	F	26	LEU
1	F	159	ASN

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

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

Mol	Chain	Res	Type
1	E	135	HIS

### 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 ⓘ

There are no ligands in this entry.

## 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, 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	224/314 (71%)	-0.14	5 (2%) 62 41	42, 67, 106, 135	0
1	B	224/314 (71%)	-0.26	5 (2%) 62 41	38, 66, 106, 150	0
1	C	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	E	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	H	224/314 (71%)	-0.16	5 (2%) 62 41	50, 71, 113, 149	0
1	I	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	K	224/314 (71%)	-0.20	2 (0%) 84 69	45, 70, 109, 157	0
1	L	224/314 (71%)	-0.17	0 100 100	43, 68, 106, 134	0
All	All	2688/3768 (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	H	5	SER	5.1
1	K	5	SER	4.6
1	J	13	GLN	4.6
1	E	13	GLN	4.0
1	F	6	GLU	4.0
1	F	227	SER	4.0
1	H	6	GLU	3.8
1	E	138	ASP	3.5
1	A	5	SER	3.5
1	F	5	SER	3.3
1	D	6	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	4	LEU	3.1
1	D	5	SER	3.0
1	D	4	LEU	3.0
1	A	200	LEU	3.0
1	C	199	TYR	3.0
1	I	227	SER	2.9
1	C	5	SER	2.9
1	C	6	GLU	2.8
1	K	6	GLU	2.7
1	G	5	SER	2.7
1	G	6	GLU	2.6
1	I	4	LEU	2.6
1	B	5	SER	2.5
1	A	4	LEU	2.3
1	B	13	GLN	2.3
1	C	200	LEU	2.3
1	I	172	SER	2.3
1	J	6	GLU	2.2
1	B	227	SER	2.2
1	A	227	SER	2.2
1	G	19	PHE	2.1
1	H	199	TYR	2.1
1	J	19	PHE	2.1
1	H	214	PHE	2.1
1	B	6	GLU	2.1
1	I	196	HIS	2.1
1	A	199	TYR	2.0
1	E	173	ASN	2.0
1	E	172	SER	2.0
1	H	200	LEU	2.0
1	B	4	LEU	2.0

## 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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.