



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 05:43 PM EDT

PDB ID : 6BBG  
Title : The CRAC channel Orai in an unlatched-closed conformation  
Authors : Long, S.B.; Hou, X.; Burstein, S.  
Deposited on : 2017-10-18  
Resolution : 6.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

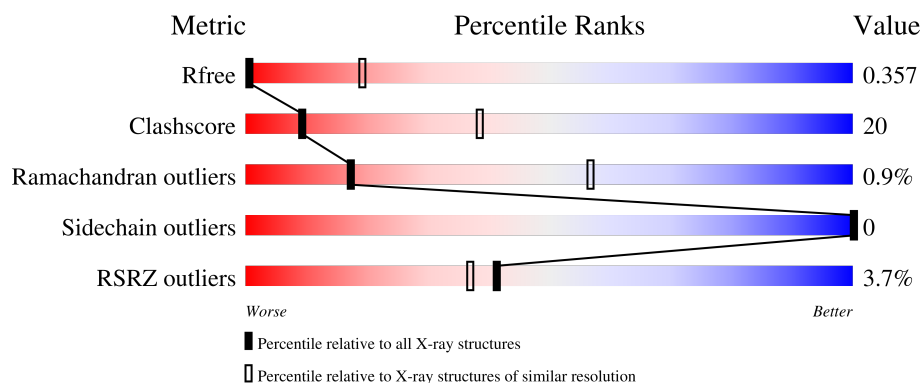
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

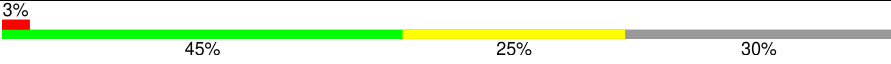
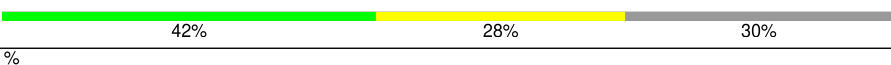
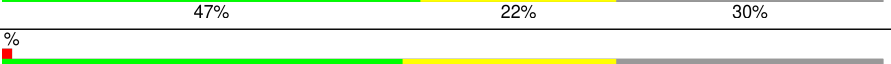
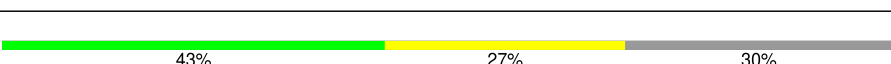

The reported resolution of this entry is 6.90 Å.

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.



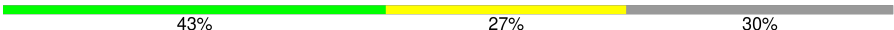

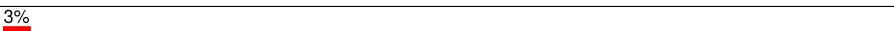
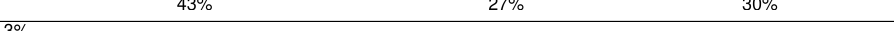

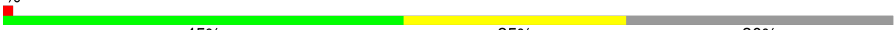

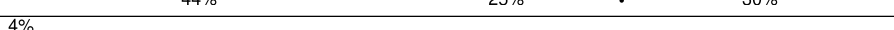

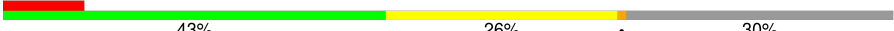



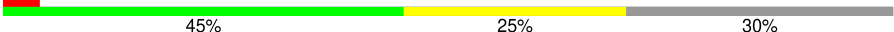

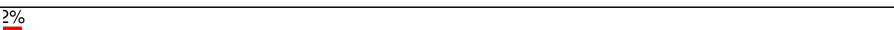


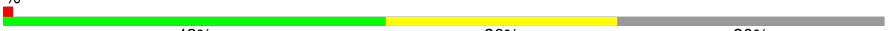
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1003 (9.70-3.90)
Clashscore	141614	1067 (9.70-3.90)
Ramachandran outliers	138981	1001 (9.70-3.90)
Sidechain outliers	138945	1001 (9.70-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	214	
1	B	214	
1	C	214	
1	D	214	
1	E	214	

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Mol	Chain	Length	Quality of chain
1	F	214	
1	G	214	
1	H	214	
1	I	214	
1	J	214	
1	K	214	
1	L	214	
1	M	214	
1	N	214	
1	O	214	
1	P	214	
1	Q	214	
1	R	214	
1	S	214	
1	T	214	
1	U	214	
1	V	214	
1	W	214	
1	X	214	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 27240 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 Calcium release-activated calcium channel protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	B	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	C	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	D	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	E	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	F	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	G	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	H	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	I	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	J	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	K	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	L	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	M	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	N	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	O	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	P	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	R	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	S	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	T	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	U	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	V	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	W	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			
1	X	150	Total	C	N	O	S	0	0	0
			1135	756	178	190	11			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	SER	CYS	engineered mutation	UNP Q9U6B8
A	283	THR	CYS	engineered mutation	UNP Q9U6B8
A	342	GLU	-	expression tag	UNP Q9U6B8
A	343	GLY	-	expression tag	UNP Q9U6B8
A	344	GLU	-	expression tag	UNP Q9U6B8
A	345	GLU	-	expression tag	UNP Q9U6B8
A	346	PHE	-	expression tag	UNP Q9U6B8
B	224	SER	CYS	engineered mutation	UNP Q9U6B8
B	283	THR	CYS	engineered mutation	UNP Q9U6B8
B	342	GLU	-	expression tag	UNP Q9U6B8
B	343	GLY	-	expression tag	UNP Q9U6B8
B	344	GLU	-	expression tag	UNP Q9U6B8
B	345	GLU	-	expression tag	UNP Q9U6B8
B	346	PHE	-	expression tag	UNP Q9U6B8
C	224	SER	CYS	engineered mutation	UNP Q9U6B8
C	283	THR	CYS	engineered mutation	UNP Q9U6B8
C	342	GLU	-	expression tag	UNP Q9U6B8
C	343	GLY	-	expression tag	UNP Q9U6B8
C	344	GLU	-	expression tag	UNP Q9U6B8
C	345	GLU	-	expression tag	UNP Q9U6B8
C	346	PHE	-	expression tag	UNP Q9U6B8
D	224	SER	CYS	engineered mutation	UNP Q9U6B8
D	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	342	GLU	-	expression tag	UNP Q9U6B8
D	343	GLY	-	expression tag	UNP Q9U6B8
D	344	GLU	-	expression tag	UNP Q9U6B8
D	345	GLU	-	expression tag	UNP Q9U6B8
D	346	PHE	-	expression tag	UNP Q9U6B8
E	224	SER	CYS	engineered mutation	UNP Q9U6B8
E	283	THR	CYS	engineered mutation	UNP Q9U6B8
E	342	GLU	-	expression tag	UNP Q9U6B8
E	343	GLY	-	expression tag	UNP Q9U6B8
E	344	GLU	-	expression tag	UNP Q9U6B8
E	345	GLU	-	expression tag	UNP Q9U6B8
E	346	PHE	-	expression tag	UNP Q9U6B8
F	224	SER	CYS	engineered mutation	UNP Q9U6B8
F	283	THR	CYS	engineered mutation	UNP Q9U6B8
F	342	GLU	-	expression tag	UNP Q9U6B8
F	343	GLY	-	expression tag	UNP Q9U6B8
F	344	GLU	-	expression tag	UNP Q9U6B8
F	345	GLU	-	expression tag	UNP Q9U6B8
F	346	PHE	-	expression tag	UNP Q9U6B8
G	224	SER	CYS	engineered mutation	UNP Q9U6B8
G	283	THR	CYS	engineered mutation	UNP Q9U6B8
G	342	GLU	-	expression tag	UNP Q9U6B8
G	343	GLY	-	expression tag	UNP Q9U6B8
G	344	GLU	-	expression tag	UNP Q9U6B8
G	345	GLU	-	expression tag	UNP Q9U6B8
G	346	PHE	-	expression tag	UNP Q9U6B8
H	224	SER	CYS	engineered mutation	UNP Q9U6B8
H	283	THR	CYS	engineered mutation	UNP Q9U6B8
H	342	GLU	-	expression tag	UNP Q9U6B8
H	343	GLY	-	expression tag	UNP Q9U6B8
H	344	GLU	-	expression tag	UNP Q9U6B8
H	345	GLU	-	expression tag	UNP Q9U6B8
H	346	PHE	-	expression tag	UNP Q9U6B8
I	224	SER	CYS	engineered mutation	UNP Q9U6B8
I	283	THR	CYS	engineered mutation	UNP Q9U6B8
I	342	GLU	-	expression tag	UNP Q9U6B8
I	343	GLY	-	expression tag	UNP Q9U6B8
I	344	GLU	-	expression tag	UNP Q9U6B8
I	345	GLU	-	expression tag	UNP Q9U6B8
I	346	PHE	-	expression tag	UNP Q9U6B8
J	224	SER	CYS	engineered mutation	UNP Q9U6B8
J	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	342	GLU	-	expression tag	UNP Q9U6B8
J	343	GLY	-	expression tag	UNP Q9U6B8
J	344	GLU	-	expression tag	UNP Q9U6B8
J	345	GLU	-	expression tag	UNP Q9U6B8
J	346	PHE	-	expression tag	UNP Q9U6B8
K	224	SER	CYS	engineered mutation	UNP Q9U6B8
K	283	THR	CYS	engineered mutation	UNP Q9U6B8
K	342	GLU	-	expression tag	UNP Q9U6B8
K	343	GLY	-	expression tag	UNP Q9U6B8
K	344	GLU	-	expression tag	UNP Q9U6B8
K	345	GLU	-	expression tag	UNP Q9U6B8
K	346	PHE	-	expression tag	UNP Q9U6B8
L	224	SER	CYS	engineered mutation	UNP Q9U6B8
L	283	THR	CYS	engineered mutation	UNP Q9U6B8
L	342	GLU	-	expression tag	UNP Q9U6B8
L	343	GLY	-	expression tag	UNP Q9U6B8
L	344	GLU	-	expression tag	UNP Q9U6B8
L	345	GLU	-	expression tag	UNP Q9U6B8
L	346	PHE	-	expression tag	UNP Q9U6B8
M	224	SER	CYS	engineered mutation	UNP Q9U6B8
M	283	THR	CYS	engineered mutation	UNP Q9U6B8
M	342	GLU	-	expression tag	UNP Q9U6B8
M	343	GLY	-	expression tag	UNP Q9U6B8
M	344	GLU	-	expression tag	UNP Q9U6B8
M	345	GLU	-	expression tag	UNP Q9U6B8
M	346	PHE	-	expression tag	UNP Q9U6B8
N	224	SER	CYS	engineered mutation	UNP Q9U6B8
N	283	THR	CYS	engineered mutation	UNP Q9U6B8
N	342	GLU	-	expression tag	UNP Q9U6B8
N	343	GLY	-	expression tag	UNP Q9U6B8
N	344	GLU	-	expression tag	UNP Q9U6B8
N	345	GLU	-	expression tag	UNP Q9U6B8
N	346	PHE	-	expression tag	UNP Q9U6B8
O	224	SER	CYS	engineered mutation	UNP Q9U6B8
O	283	THR	CYS	engineered mutation	UNP Q9U6B8
O	342	GLU	-	expression tag	UNP Q9U6B8
O	343	GLY	-	expression tag	UNP Q9U6B8
O	344	GLU	-	expression tag	UNP Q9U6B8
O	345	GLU	-	expression tag	UNP Q9U6B8
O	346	PHE	-	expression tag	UNP Q9U6B8
P	224	SER	CYS	engineered mutation	UNP Q9U6B8
P	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	342	GLU	-	expression tag	UNP Q9U6B8
P	343	GLY	-	expression tag	UNP Q9U6B8
P	344	GLU	-	expression tag	UNP Q9U6B8
P	345	GLU	-	expression tag	UNP Q9U6B8
P	346	PHE	-	expression tag	UNP Q9U6B8
Q	224	SER	CYS	engineered mutation	UNP Q9U6B8
Q	283	THR	CYS	engineered mutation	UNP Q9U6B8
Q	342	GLU	-	expression tag	UNP Q9U6B8
Q	343	GLY	-	expression tag	UNP Q9U6B8
Q	344	GLU	-	expression tag	UNP Q9U6B8
Q	345	GLU	-	expression tag	UNP Q9U6B8
Q	346	PHE	-	expression tag	UNP Q9U6B8
R	224	SER	CYS	engineered mutation	UNP Q9U6B8
R	283	THR	CYS	engineered mutation	UNP Q9U6B8
R	342	GLU	-	expression tag	UNP Q9U6B8
R	343	GLY	-	expression tag	UNP Q9U6B8
R	344	GLU	-	expression tag	UNP Q9U6B8
R	345	GLU	-	expression tag	UNP Q9U6B8
R	346	PHE	-	expression tag	UNP Q9U6B8
S	224	SER	CYS	engineered mutation	UNP Q9U6B8
S	283	THR	CYS	engineered mutation	UNP Q9U6B8
S	342	GLU	-	expression tag	UNP Q9U6B8
S	343	GLY	-	expression tag	UNP Q9U6B8
S	344	GLU	-	expression tag	UNP Q9U6B8
S	345	GLU	-	expression tag	UNP Q9U6B8
S	346	PHE	-	expression tag	UNP Q9U6B8
T	224	SER	CYS	engineered mutation	UNP Q9U6B8
T	283	THR	CYS	engineered mutation	UNP Q9U6B8
T	342	GLU	-	expression tag	UNP Q9U6B8
T	343	GLY	-	expression tag	UNP Q9U6B8
T	344	GLU	-	expression tag	UNP Q9U6B8
T	345	GLU	-	expression tag	UNP Q9U6B8
T	346	PHE	-	expression tag	UNP Q9U6B8
U	224	SER	CYS	engineered mutation	UNP Q9U6B8
U	283	THR	CYS	engineered mutation	UNP Q9U6B8
U	342	GLU	-	expression tag	UNP Q9U6B8
U	343	GLY	-	expression tag	UNP Q9U6B8
U	344	GLU	-	expression tag	UNP Q9U6B8
U	345	GLU	-	expression tag	UNP Q9U6B8
U	346	PHE	-	expression tag	UNP Q9U6B8
V	224	SER	CYS	engineered mutation	UNP Q9U6B8
V	283	THR	CYS	engineered mutation	UNP Q9U6B8

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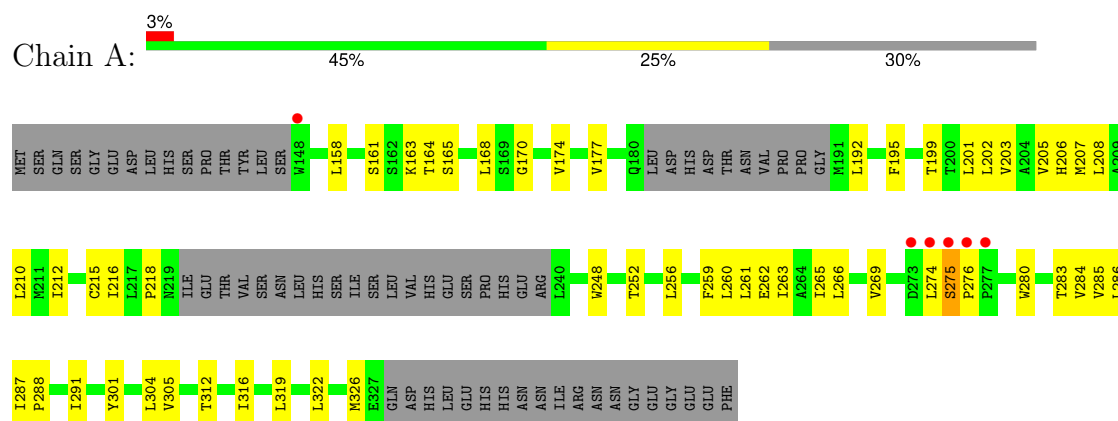
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Chain	Residue	Modelled	Actual	Comment	Reference
V	342	GLU	-	expression tag	UNP Q9U6B8
V	343	GLY	-	expression tag	UNP Q9U6B8
V	344	GLU	-	expression tag	UNP Q9U6B8
V	345	GLU	-	expression tag	UNP Q9U6B8
V	346	PHE	-	expression tag	UNP Q9U6B8
W	224	SER	CYS	engineered mutation	UNP Q9U6B8
W	283	THR	CYS	engineered mutation	UNP Q9U6B8
W	342	GLU	-	expression tag	UNP Q9U6B8
W	343	GLY	-	expression tag	UNP Q9U6B8
W	344	GLU	-	expression tag	UNP Q9U6B8
W	345	GLU	-	expression tag	UNP Q9U6B8
W	346	PHE	-	expression tag	UNP Q9U6B8
X	224	SER	CYS	engineered mutation	UNP Q9U6B8
X	283	THR	CYS	engineered mutation	UNP Q9U6B8
X	342	GLU	-	expression tag	UNP Q9U6B8
X	343	GLY	-	expression tag	UNP Q9U6B8
X	344	GLU	-	expression tag	UNP Q9U6B8
X	345	GLU	-	expression tag	UNP Q9U6B8
X	346	PHE	-	expression tag	UNP Q9U6B8

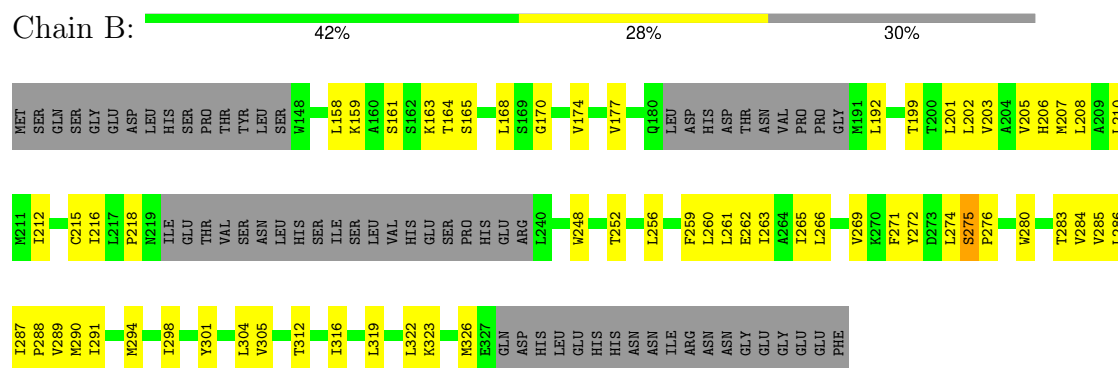
### 3 Residue-property plots [i](#)

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.

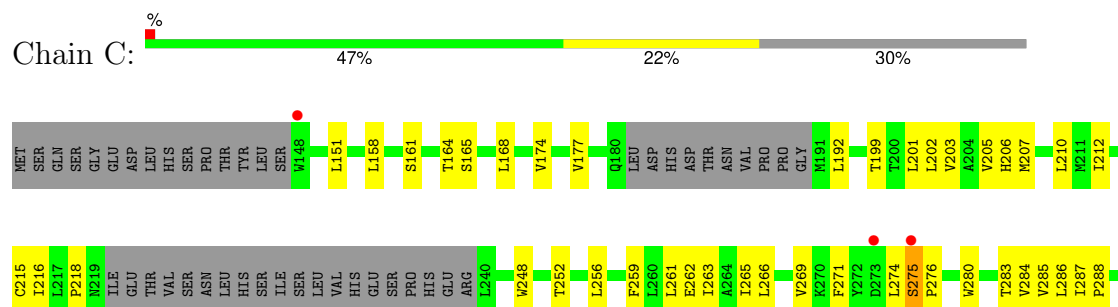
- Molecule 1: Calcium release-activated calcium channel protein 1

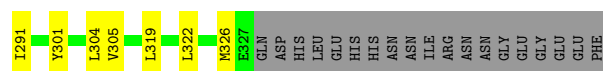


- Molecule 1: Calcium release-activated calcium channel protein 1

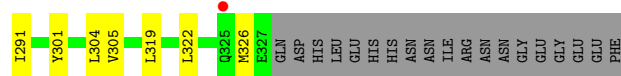
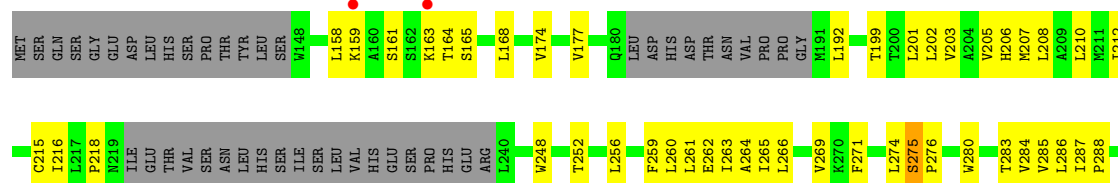


- Molecule 1: Calcium release-activated calcium channel protein 1

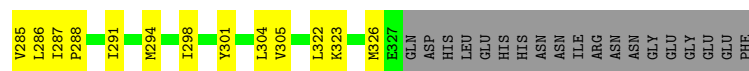
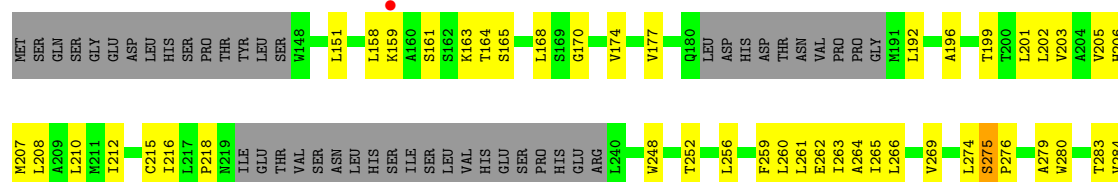




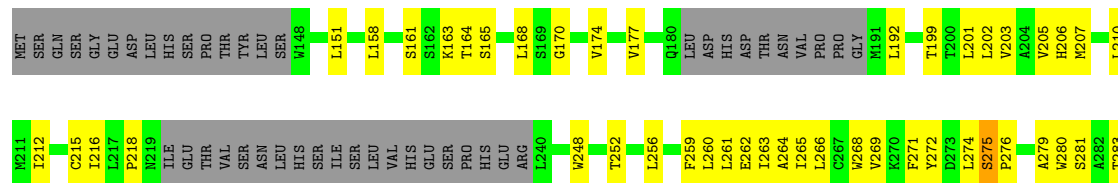
- Molecule 1: Calcium release-activated calcium channel protein 1



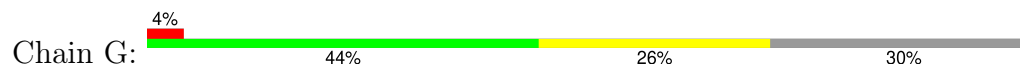
- Molecule 1: Calcium release-activated calcium channel protein 1

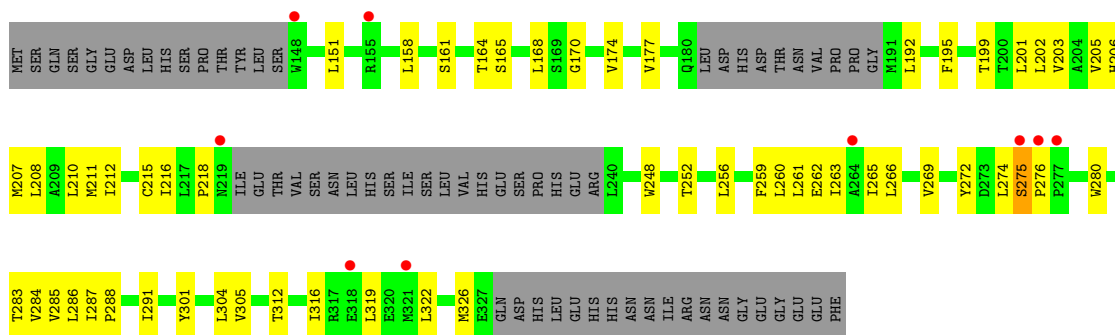


- Molecule 1: Calcium release-activated calcium channel protein 1

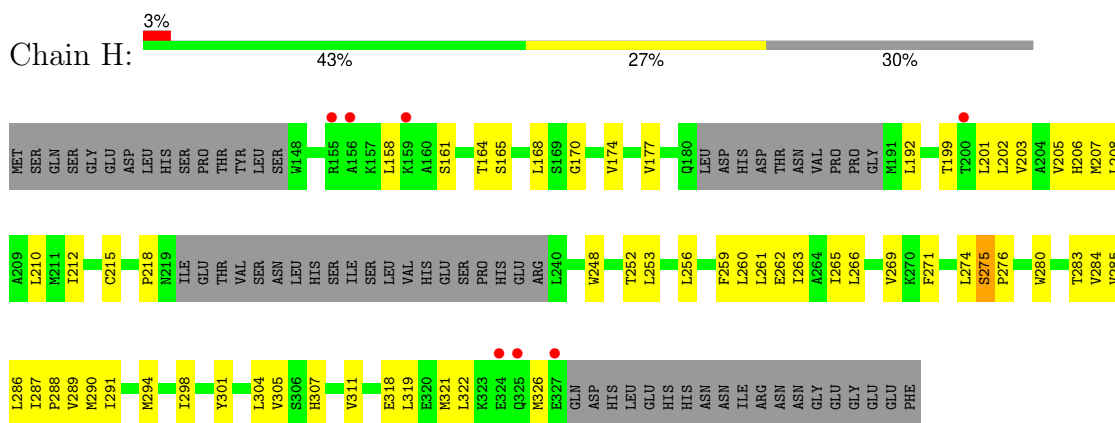


- Molecule 1: Calcium release-activated calcium channel protein 1

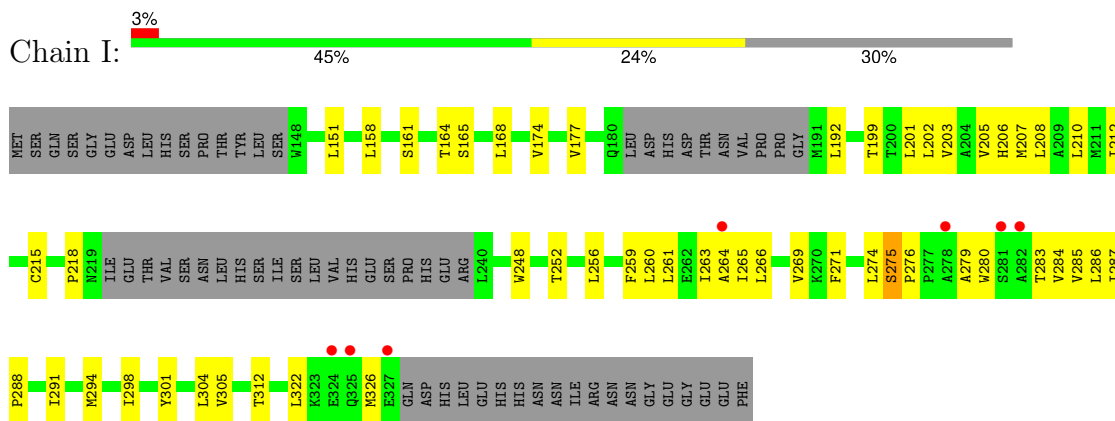




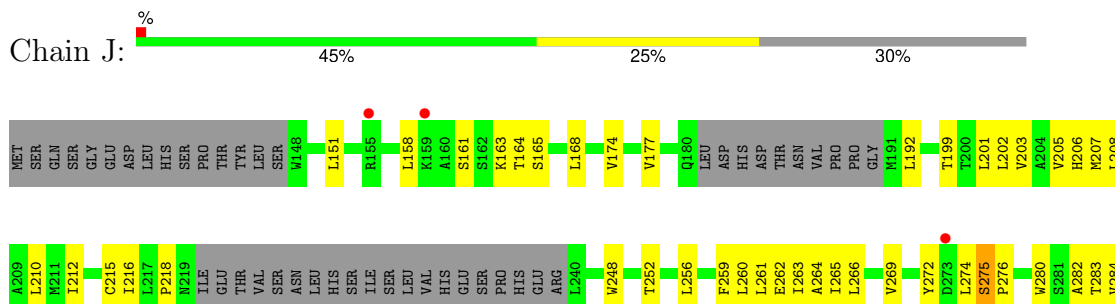
- Molecule 1: Calcium release-activated calcium channel protein 1



- Molecule 1: Calcium release-activated calcium channel protein 1

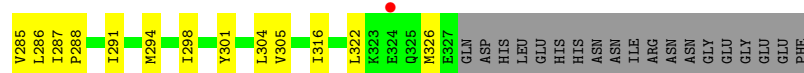
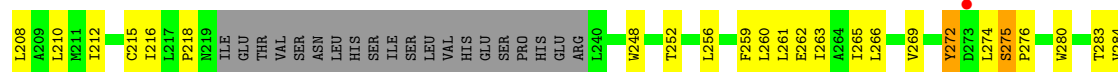
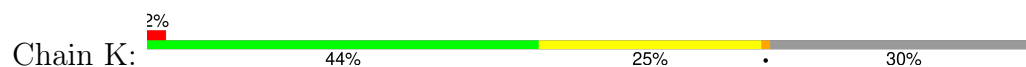


- Molecule 1: Calcium release-activated calcium channel protein 1

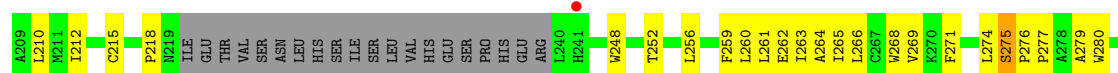
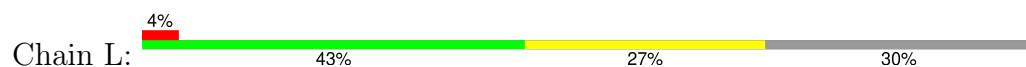




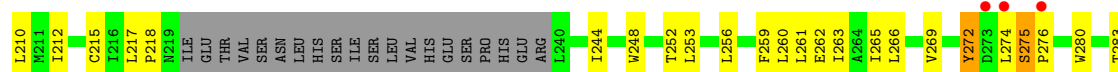
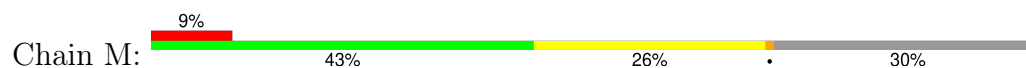
• Molecule 1: Calcium release-activated calcium channel protein 1



• Molecule 1: Calcium release-activated calcium channel protein 1

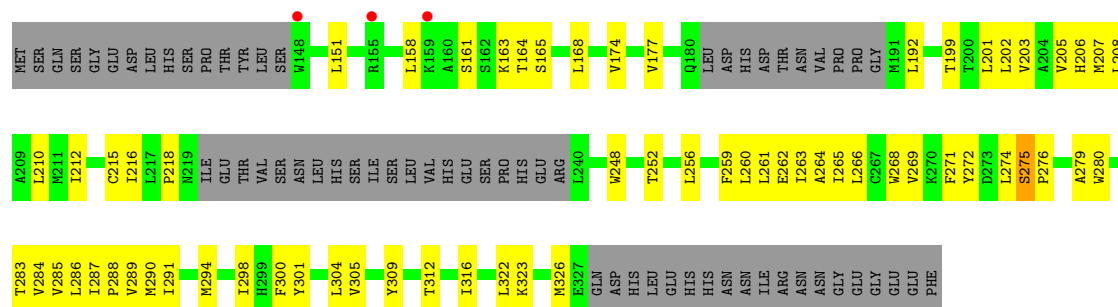


• Molecule 1: Calcium release-activated calcium channel protein 1

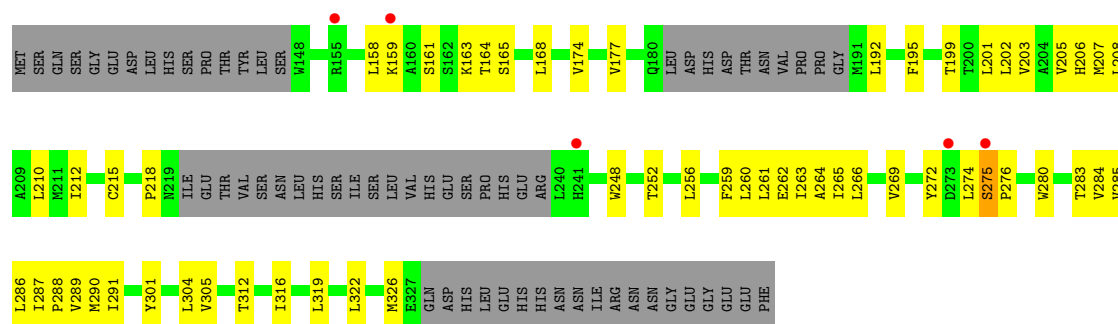


• Molecule 1: Calcium release-activated calcium channel protein 1

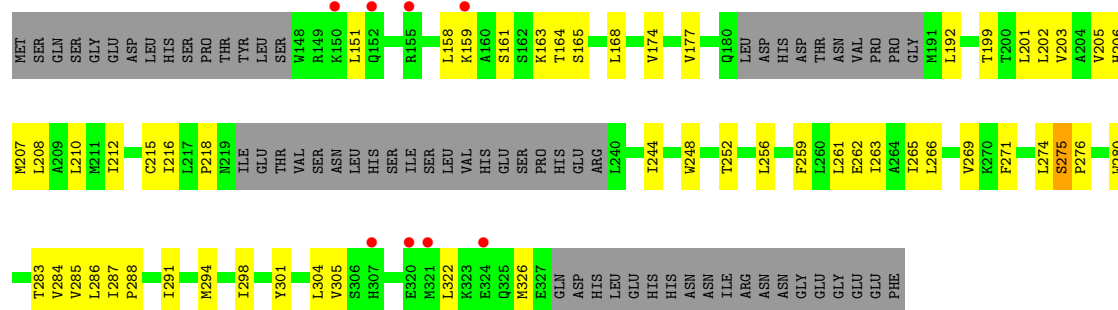




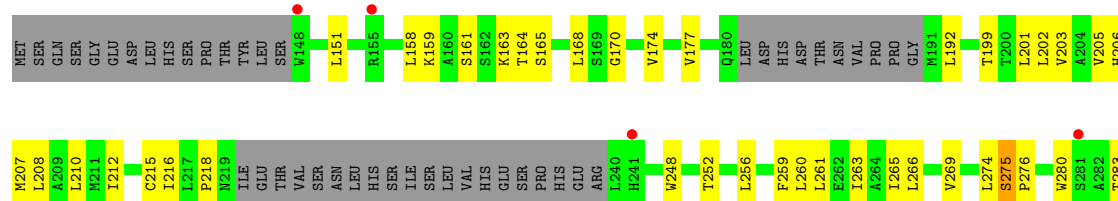
• Molecule 1: Calcium release-activated calcium channel protein 1



• Molecule 1: Calcium release-activated calcium channel protein 1

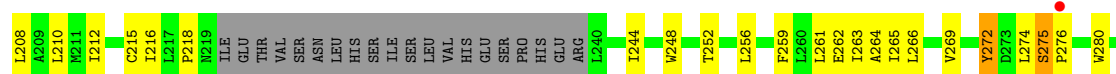
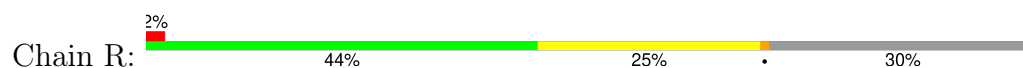


• Molecule 1: Calcium release-activated calcium channel protein 1

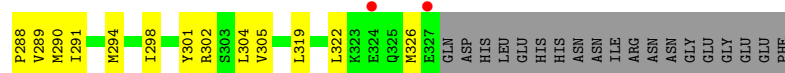




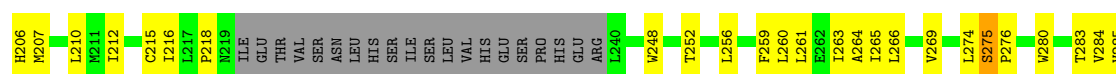
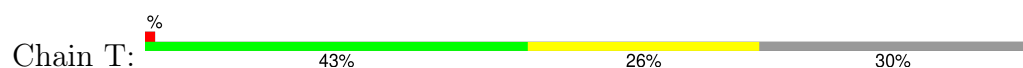
• Molecule 1: Calcium release-activated calcium channel protein 1



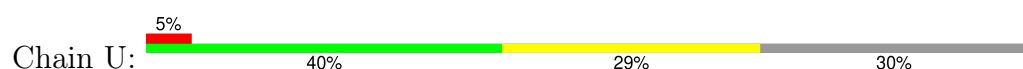
• Molecule 1: Calcium release-activated calcium channel protein 1

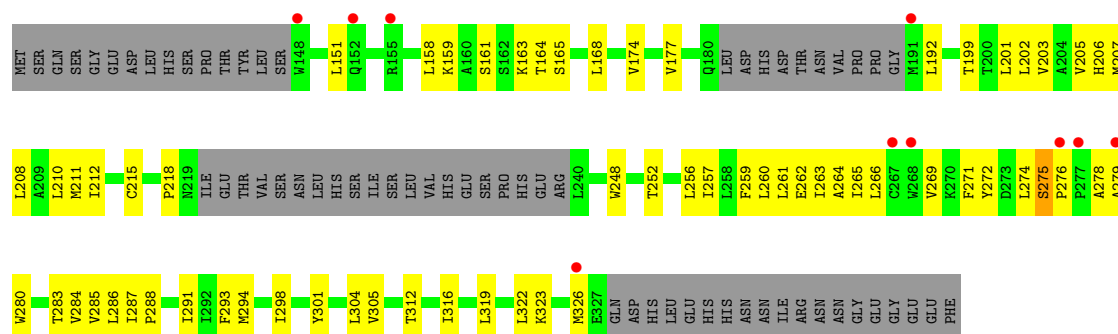


• Molecule 1: Calcium release-activated calcium channel protein 1

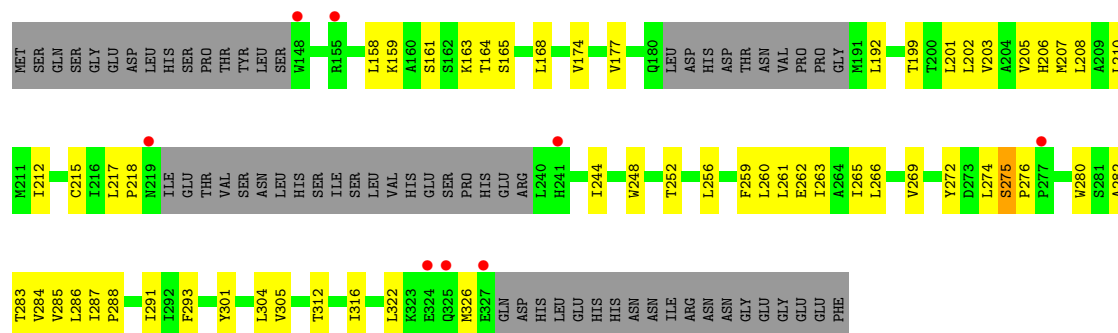
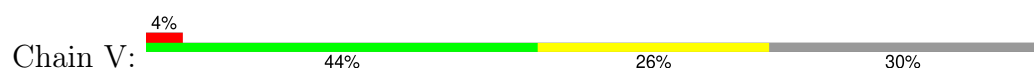


• Molecule 1: Calcium release-activated calcium channel protein 1

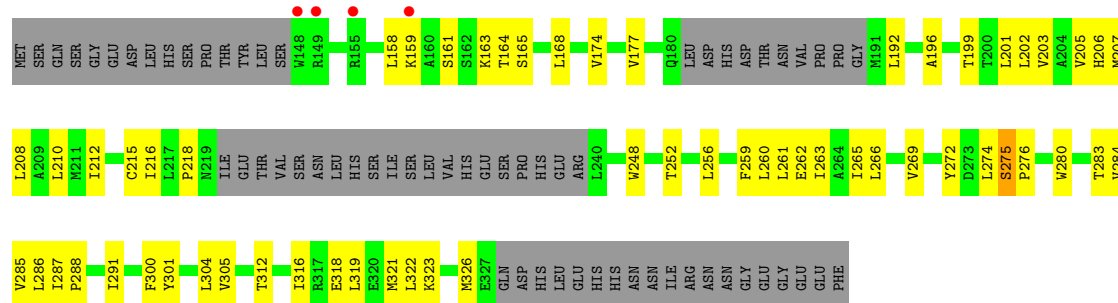
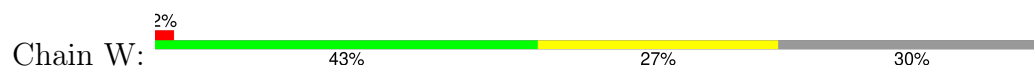




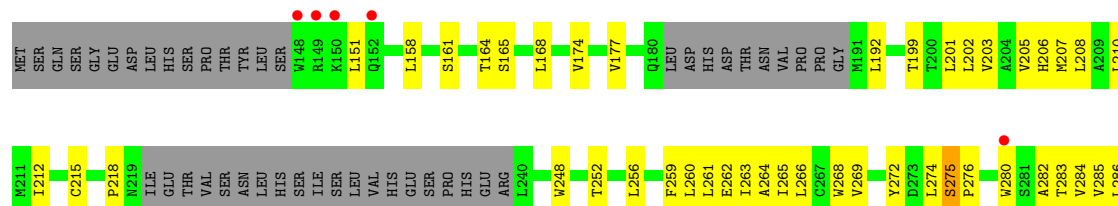
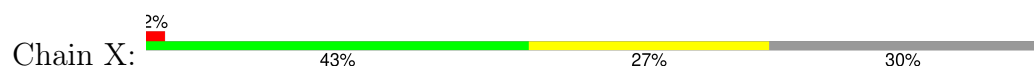
• Molecule 1: Calcium release-activated calcium channel protein 1



• Molecule 1: Calcium release-activated calcium channel protein 1



• Molecule 1: Calcium release-activated calcium channel protein 1





I287	P288	I291	Y301	L304	V305	E310	V311	T312	V313	I316	R317	E318	L319	L322	K323	M326	E327	GLN	ASP	HIS	LEU	GLU	HIS	HIS	ASN	ASN	ILE	ARG	ASN	ASN	GLY	GLU	GLY	GLU	PHE
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	250.38Å 250.38Å 210.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 6.90 19.98 – 6.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.98-6.90) 100.0 (19.98-6.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 6.98Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.334 , 0.354 0.340 , 0.357	Depositor DCC
$R_{free}$ test set	1071 reflections (10.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	657.4	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 509.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	27240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	599.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [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	0.26	0/1161	0.44	0/1579
1	B	0.26	0/1161	0.43	0/1579
1	C	0.26	0/1161	0.43	0/1579
1	D	0.26	0/1161	0.43	0/1579
1	E	0.26	0/1161	0.43	0/1579
1	F	0.26	0/1161	0.44	0/1579
1	G	0.26	0/1161	0.43	0/1579
1	H	0.26	0/1161	0.43	0/1579
1	I	0.26	0/1161	0.43	0/1579
1	J	0.26	0/1161	0.43	0/1579
1	K	0.26	0/1161	0.43	0/1579
1	L	0.26	0/1161	0.44	0/1579
1	M	0.26	0/1161	0.44	0/1579
1	N	0.26	0/1161	0.44	0/1579
1	O	0.26	0/1161	0.43	0/1579
1	P	0.26	0/1161	0.43	0/1579
1	Q	0.26	0/1161	0.44	0/1579
1	R	0.26	0/1161	0.43	0/1579
1	S	0.26	0/1161	0.43	0/1579
1	T	0.26	0/1161	0.43	0/1579
1	U	0.26	0/1161	0.44	0/1579
1	V	0.26	0/1161	0.43	0/1579
1	W	0.26	0/1161	0.44	0/1579
1	X	0.26	0/1161	0.44	0/1579
All	All	0.26	0/27864	0.44	0/37896

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 ⓘ

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	1135	0	1143	54	0
1	B	1135	0	1143	53	0
1	C	1135	0	1143	41	0
1	D	1135	0	1143	40	0
1	E	1135	0	1143	45	0
1	F	1135	0	1143	56	0
1	G	1135	0	1143	47	0
1	H	1135	0	1143	44	0
1	I	1135	0	1143	41	0
1	J	1135	0	1143	42	0
1	K	1135	0	1143	44	0
1	L	1135	0	1143	60	0
1	M	1135	0	1143	46	0
1	N	1135	0	1143	63	0
1	O	1135	0	1143	53	0
1	P	1135	0	1143	41	0
1	Q	1135	0	1143	54	0
1	R	1135	0	1143	43	0
1	S	1135	0	1143	48	0
1	T	1135	0	1143	45	0
1	U	1135	0	1143	58	0
1	V	1135	0	1143	45	0
1	W	1135	0	1143	57	0
1	X	1135	0	1143	61	0
All	All	27240	0	27432	1080	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 20.

The worst 5 of 1080 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:L:280:TRP:CE3	1:X:317:ARG:NH2	2.47	0.83
1:O:319:LEU:HD22	1:W:312:THR:HA	1.60	0.83
1:Q:308:LYS:HE3	1:U:322:LEU:HD21	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:268:TRP:HA	1:L:279:ALA:HB1	1.62	0.81
1:B:319:LEU:HD22	1:L:312:THR:HA	1.62	0.80

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	B	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11 46
1	C	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	D	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	E	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	F	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	G	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11 46
1	H	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	I	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	J	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	K	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11 46
1	L	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	M	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11 46
1	N	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22 63
1	O	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	22 63
1	P	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	Q	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22 63
1	R	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11	46
1	T	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22	63
1	U	144/214 (67%)	138 (96%)	4 (3%)	2 (1%)	11	46
1	V	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22	63
1	W	144/214 (67%)	139 (96%)	4 (3%)	1 (1%)	22	63
1	X	144/214 (67%)	139 (96%)	3 (2%)	2 (1%)	11	46
All	All	3456/5136 (67%)	3337 (97%)	87 (2%)	32 (1%)	17	57

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	272	TYR
1	S	272	TYR
1	X	272	TYR
1	B	272	TYR
1	B	275	SER

### 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	116/190 (61%)	116 (100%)	0	100	100
1	B	116/190 (61%)	116 (100%)	0	100	100
1	C	116/190 (61%)	116 (100%)	0	100	100
1	D	116/190 (61%)	116 (100%)	0	100	100
1	E	116/190 (61%)	116 (100%)	0	100	100
1	F	116/190 (61%)	116 (100%)	0	100	100
1	G	116/190 (61%)	116 (100%)	0	100	100
1	H	116/190 (61%)	116 (100%)	0	100	100
1	I	116/190 (61%)	116 (100%)	0	100	100
1	J	116/190 (61%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	116/190 (61%)	116 (100%)	0	100	100
1	L	116/190 (61%)	116 (100%)	0	100	100
1	M	116/190 (61%)	116 (100%)	0	100	100
1	N	116/190 (61%)	116 (100%)	0	100	100
1	O	116/190 (61%)	116 (100%)	0	100	100
1	P	116/190 (61%)	116 (100%)	0	100	100
1	Q	116/190 (61%)	116 (100%)	0	100	100
1	R	116/190 (61%)	116 (100%)	0	100	100
1	S	116/190 (61%)	116 (100%)	0	100	100
1	T	116/190 (61%)	116 (100%)	0	100	100
1	U	116/190 (61%)	116 (100%)	0	100	100
1	V	116/190 (61%)	116 (100%)	0	100	100
1	W	116/190 (61%)	116 (100%)	0	100	100
1	X	116/190 (61%)	116 (100%)	0	100	100
All	All	2784/4560 (61%)	2784 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 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	150/214 (70%)	-0.04	6 (4%) 38 34	554, 570, 607, 617	0
1	B	150/214 (70%)	-0.12	0 100 100	551, 565, 583, 588	0
1	C	150/214 (70%)	0.08	3 (2%) 65 58	551, 568, 583, 589	0
1	D	150/214 (70%)	-0.08	3 (2%) 65 58	557, 578, 606, 619	0
1	E	150/214 (70%)	-0.11	1 (0%) 87 82	562, 584, 628, 645	0
1	F	150/214 (70%)	0.03	1 (0%) 87 82	558, 579, 628, 644	0
1	G	150/214 (70%)	0.15	9 (6%) 21 21	586, 599, 609, 612	0
1	H	150/214 (70%)	0.21	7 (4%) 31 30	591, 616, 627, 631	0
1	I	150/214 (70%)	0.34	7 (4%) 31 30	590, 617, 634, 637	0
1	J	150/214 (70%)	0.09	3 (2%) 65 58	582, 600, 619, 622	0
1	K	150/214 (70%)	0.01	5 (3%) 46 41	578, 586, 595, 597	0
1	L	150/214 (70%)	0.25	8 (5%) 26 26	576, 585, 592, 595	0
1	M	150/214 (70%)	0.43	19 (12%) 3 7	591, 614, 659, 673	0
1	N	150/214 (70%)	0.04	3 (2%) 65 58	585, 607, 645, 657	0
1	O	150/214 (70%)	0.09	5 (3%) 46 41	594, 617, 646, 656	0
1	P	150/214 (70%)	0.18	8 (5%) 26 26	597, 631, 666, 674	0
1	Q	150/214 (70%)	0.18	5 (3%) 46 41	595, 629, 675, 686	0
1	R	150/214 (70%)	0.10	5 (3%) 46 41	582, 620, 668, 683	0
1	S	150/214 (70%)	0.11	4 (2%) 54 48	581, 591, 611, 617	0
1	T	150/214 (70%)	-0.03	3 (2%) 65 58	579, 585, 602, 610	0
1	U	150/214 (70%)	0.35	10 (6%) 17 18	580, 591, 606, 623	0
1	V	150/214 (70%)	0.34	8 (5%) 26 26	588, 604, 626, 645	0
1	W	150/214 (70%)	-0.05	4 (2%) 54 48	585, 604, 623, 630	0
1	X	150/214 (70%)	0.15	5 (3%) 46 41	583, 591, 617, 625	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
All	All	3600/5136 (70%)	0.11	132 (3%)	41	37	551, 596, 644, 686	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	273	ASP	5.0
1	H	155	ARG	4.9
1	M	310	GLU	4.4
1	M	311	VAL	4.2
1	O	159	LYS	4.0

## 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.