



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:29 AM UTC

PDB ID : 6BBH / pdb_00006bbh
Title : The CRAC channel Orai in an unlatched-closed conformation; K163W loss-of-function mutation
Authors : Long, S.B.; Hou, X.; Burstein, S.
Deposited on : 2017-10-18
Resolution : 6.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

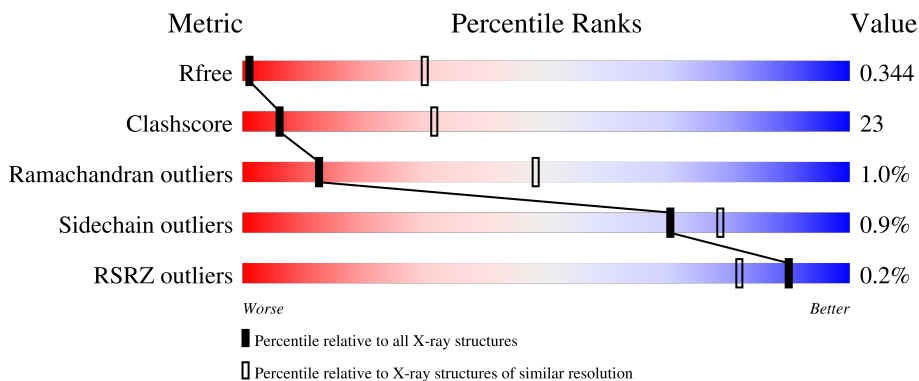
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.10 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.






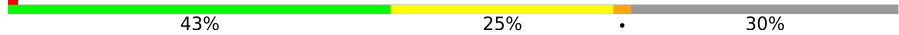
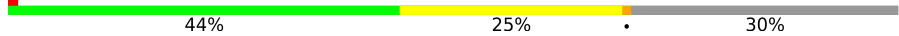
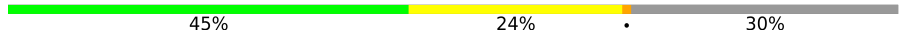
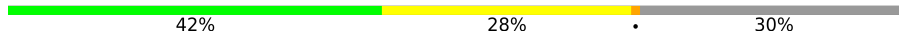
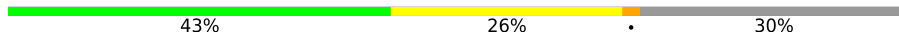
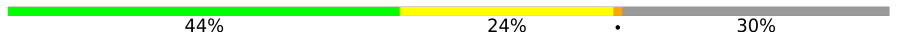
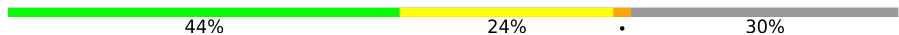
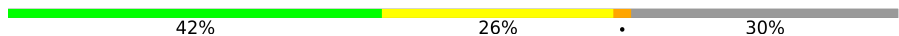
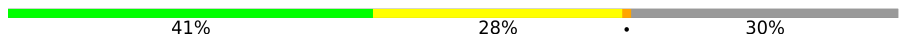
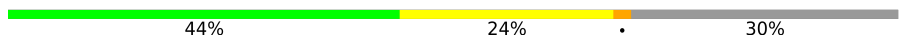
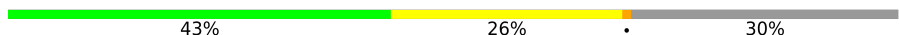





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1146 (8.20-4.00)
Clashscore	190562	1006 (8.08-4.02)
Ramachandran outliers	187476	1035 (8.20-4.00)
Sidechain outliers	187428	1001 (8.20-4.00)
RSRZ outliers	180081	1139 (8.20-4.00)

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 $\leq 5\%$. 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	 43% 26% 30%
1	G	214	 43% 26% 30%
1	H	214	 44% 23% 30%
1	I	214	 43% 25% 30%
1	J	214	 44% 25% 30%
1	K	214	 45% 24% 30%
1	L	214	 42% 28% 30%
1	M	214	 43% 26% 30%
1	N	214	 44% 24% 30%
1	O	214	 44% 24% 30%
1	P	214	 42% 26% 30%
1	Q	214	 41% 28% 30%
1	R	214	 44% 24% 30%
1	S	214	 43% 26% 30%
1	T	214	 44% 24% 30%
1	U	214	 42% 27% 30%
1	V	214	 43% 26% 30%
1	W	214	 43% 26% 30%
1	X	214	 40% 28% 30%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 27360 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
			Total	C	N	O	S			
1	A	150	1140	761	178	190	11	0	0	0
1	B	150	1140	761	178	190	11	0	0	0
1	C	150	1140	761	178	190	11	0	0	0
1	D	150	1140	761	178	190	11	0	0	0
1	E	150	1140	761	178	190	11	0	0	0
1	F	150	1140	761	178	190	11	0	0	0
1	G	150	1140	761	178	190	11	0	0	0
1	H	150	1140	761	178	190	11	0	0	0
1	I	150	1140	761	178	190	11	0	0	0
1	J	150	1140	761	178	190	11	0	0	0
1	K	150	1140	761	178	190	11	0	0	0
1	L	150	1140	761	178	190	11	0	0	0
1	M	150	1140	761	178	190	11	0	0	0
1	N	150	1140	761	178	190	11	0	0	0
1	O	150	1140	761	178	190	11	0	0	0
1	P	150	1140	761	178	190	11	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	R	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	S	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	T	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	U	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	V	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	W	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			
1	X	150	Total	C	N	O	S	0	0	0
			1140	761	178	190	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	163	TRP	LYS	engineered mutation	UNP Q9U6B8
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	346	PHE	-	expression tag	UNP Q9U6B8
D	163	TRP	LYS	engineered mutation	UNP Q9U6B8
D	224	SER	CYS	engineered mutation	UNP Q9U6B8
D	283	THR	CYS	engineered mutation	UNP Q9U6B8
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
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	163	TRP	LYS	engineered mutation	UNP Q9U6B8
J	224	SER	CYS	engineered mutation	UNP Q9U6B8
J	283	THR	CYS	engineered mutation	UNP Q9U6B8
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	UNP Q9U6B8
N	224	SER	CYS	engineered mutation	UNP Q9U6B8
N	283	THR	CYS	engineered mutation	UNP Q9U6B8

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Chain	Residue	Modelled	Actual	Comment	Reference
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	UNP Q9U6B8
P	224	SER	CYS	engineered mutation	UNP Q9U6B8
P	283	THR	CYS	engineered mutation	UNP Q9U6B8
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
S	344	GLU	-	expression tag	UNP Q9U6B8
S	345	GLU	-	expression tag	UNP Q9U6B8
S	346	PHE	-	expression tag	UNP Q9U6B8
T	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	UNP Q9U6B8
V	224	SER	CYS	engineered mutation	UNP Q9U6B8
V	283	THR	CYS	engineered mutation	UNP Q9U6B8
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	163	TRP	LYS	engineered mutation	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	163	TRP	LYS	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
X	346	PHE	-	expression tag	UNP Q9U6B8

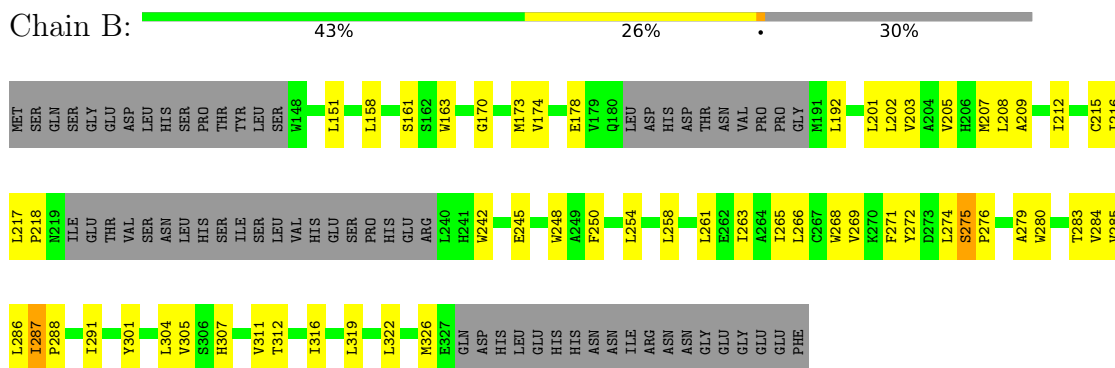
3 Residue-property plots [i](#)

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.

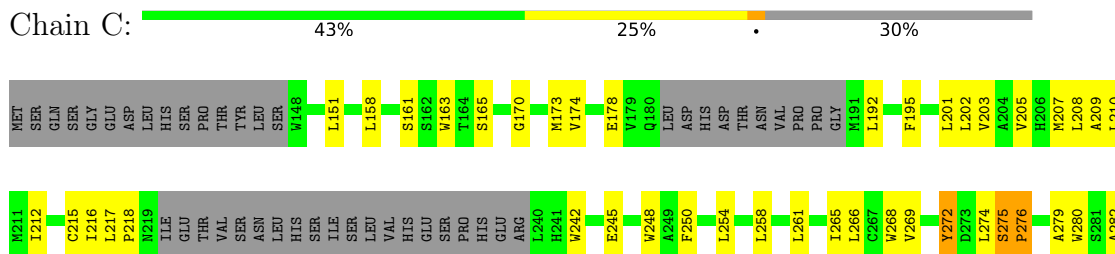
- Molecule 1: Calcium release-activated calcium channel protein 1



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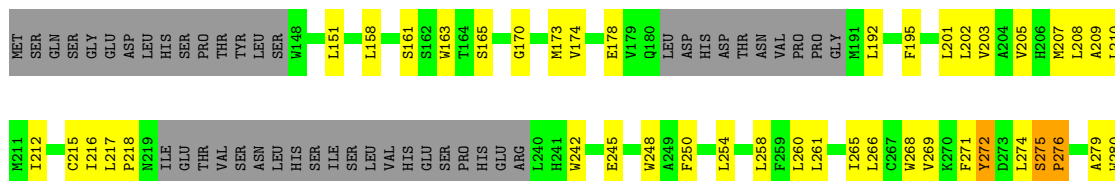


- Molecule 1: Calcium release-activated calcium channel protein 1

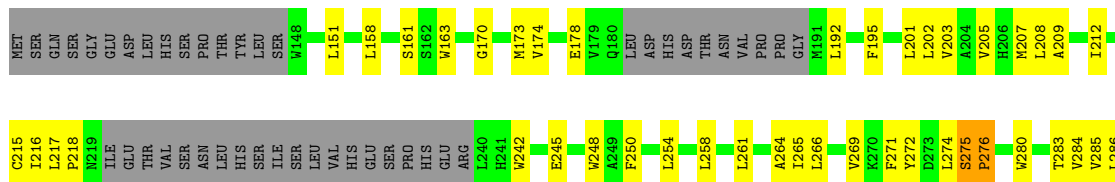




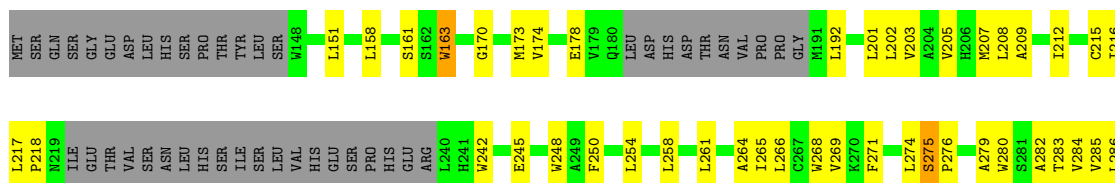
- Molecule 1: Calcium release-activated calcium channel protein 1



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

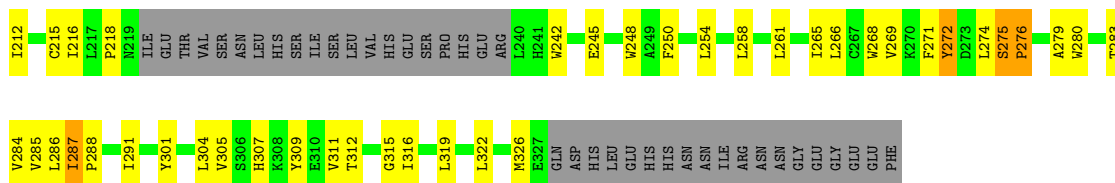


- Molecule 1: Calcium release-activated calcium channel protein 1

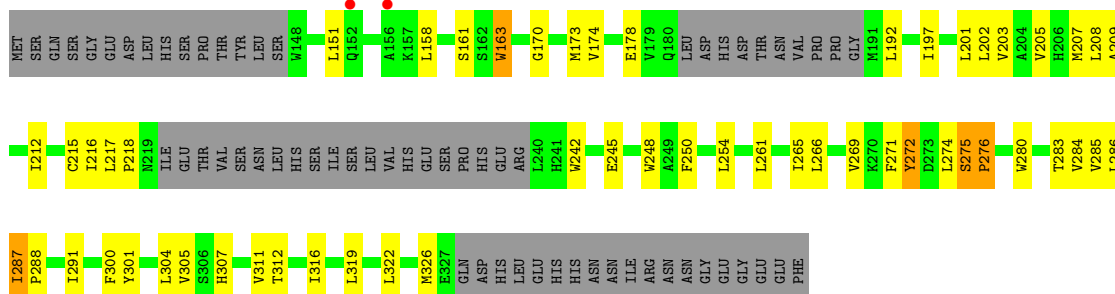
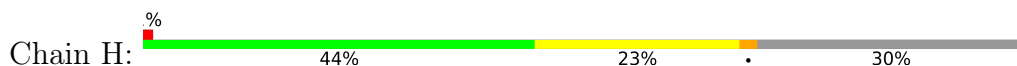


- Molecule 1: Calcium release-activated calcium channel protein 1

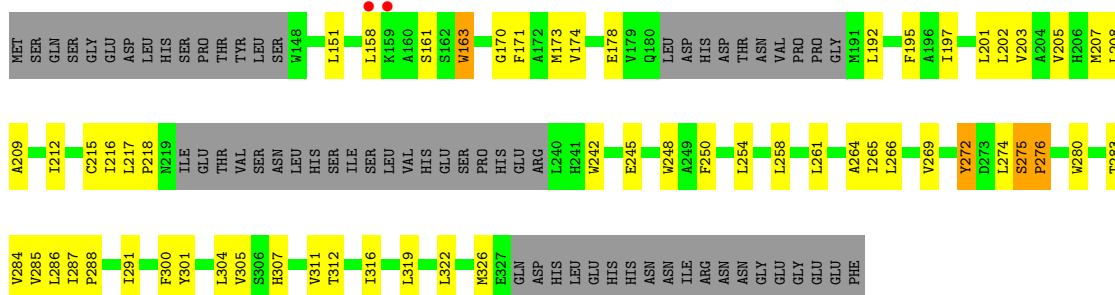




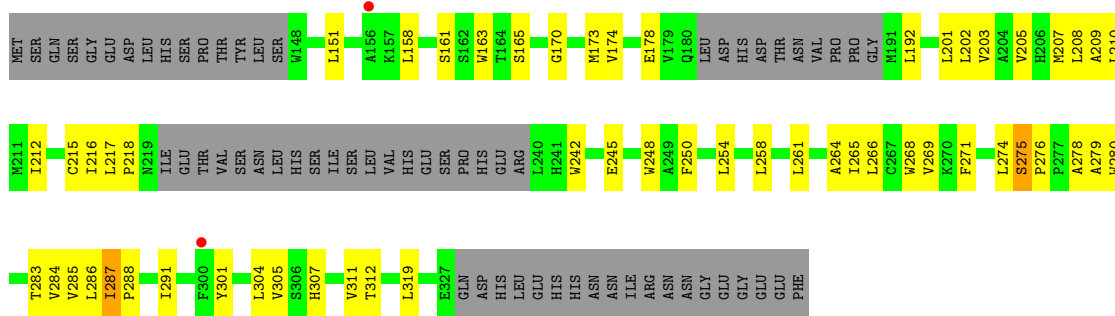
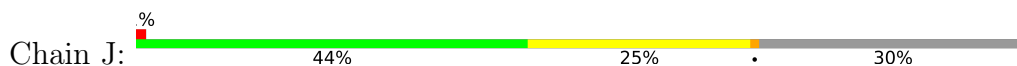
• Molecule 1: Calcium release-activated calcium channel protein 1



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

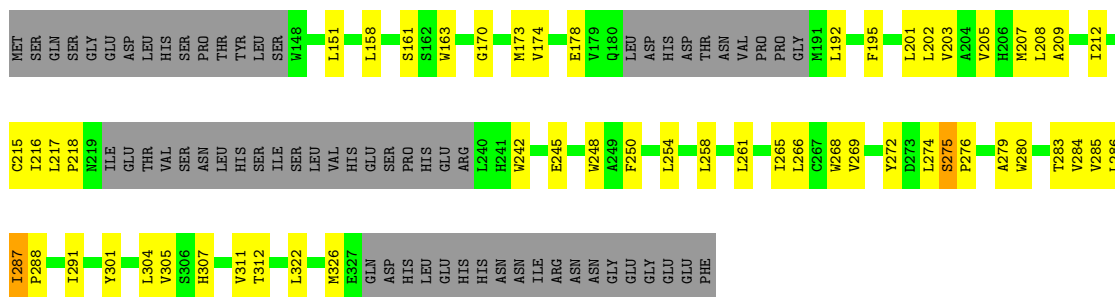


• Molecule 1: Calcium release-activated calcium channel protein 1



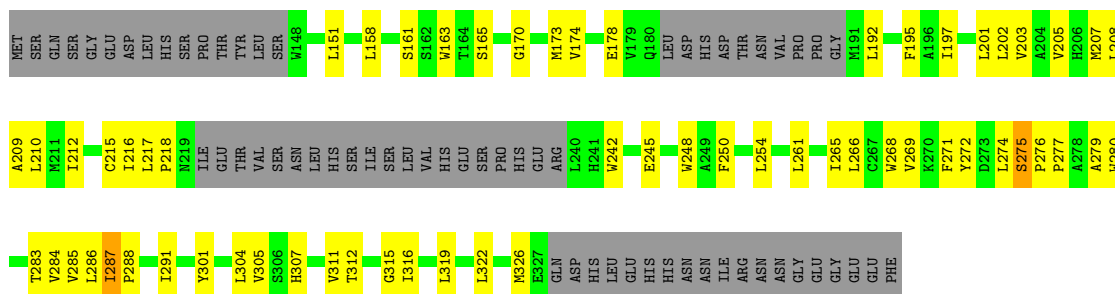
• Molecule 1: Calcium release-activated calcium channel protein 1

Chain K:  45% 24% 30%



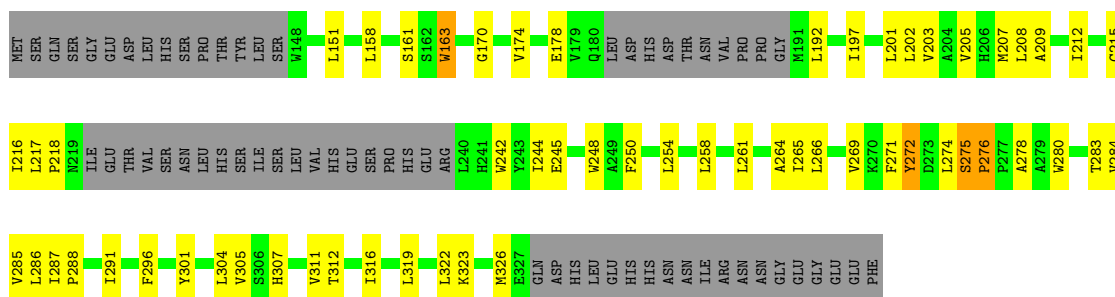
- Molecule 1: Calcium release-activated calcium channel protein 1

Chain L:  42% 28% 30%



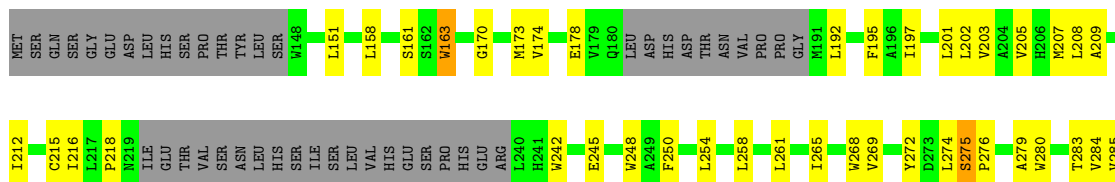
- Molecule 1: Calcium release-activated calcium channel protein 1

Chain M:  43% 26% 30%



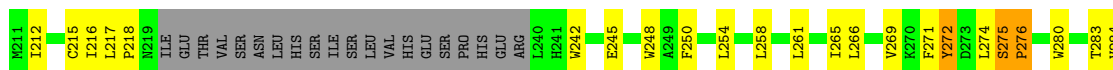
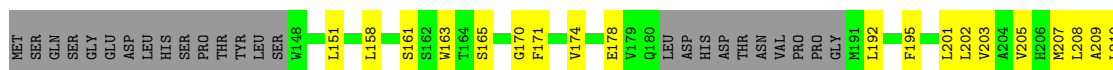
- Molecule 1: Calcium release-activated calcium channel protein 1

Chain N:  44% 24% 30%

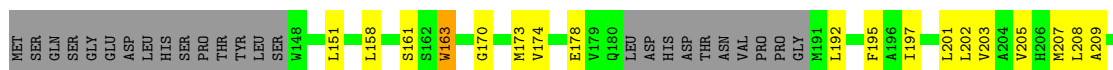




- Molecule 1: Calcium release-activated calcium channel protein 1



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

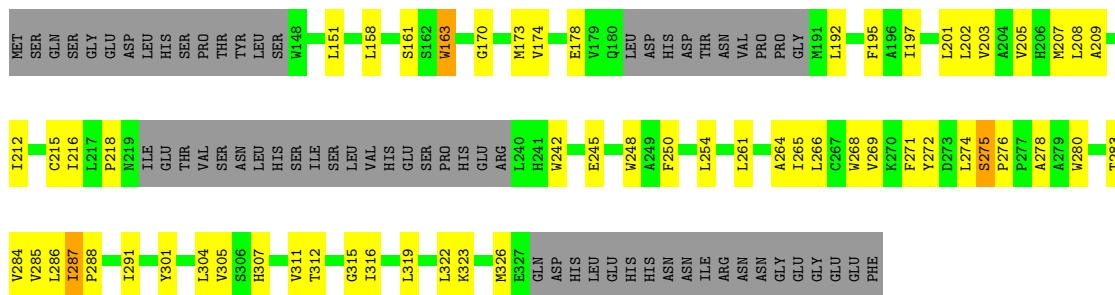


- Molecule 1: Calcium release-activated calcium channel protein 1

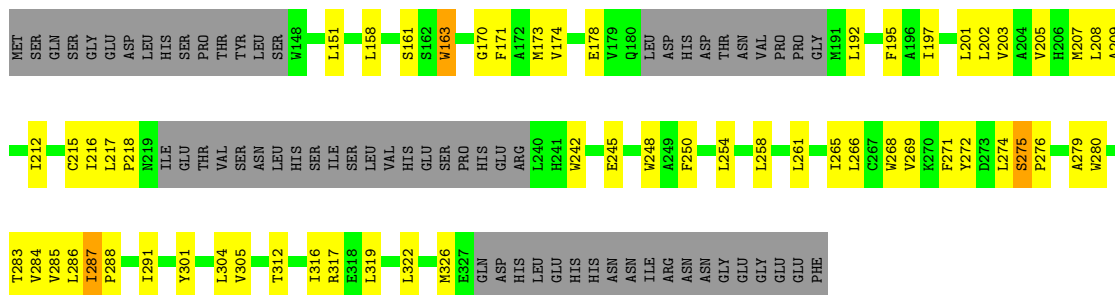


- Molecule 1: Calcium release-activated calcium channel protein 1

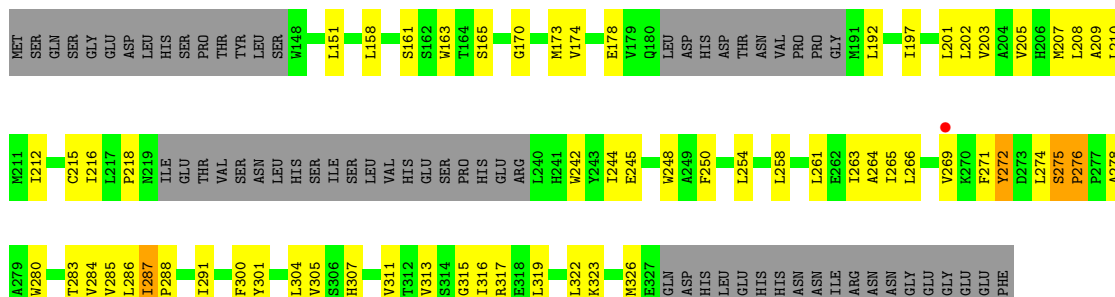




• Molecule 1: Calcium release-activated calcium channel protein 1



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



4 Data and refinement statistics i

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	247.46Å 247.46Å 210.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 6.10 19.99 – 6.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-6.10) 97.0 (19.99-6.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 5.92Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.314 , 0.341 0.316 , 0.344	Depositor DCC
R_{free} test set	1530 reflections (10.39%)	wwPDB-VP
Wilson B-factor (Å ²)	523.4	Xtrriage
Anisotropy	0.135	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 505.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.033 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27360	wwPDB-VP
Average B, all atoms (Å ²)	564.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.31	0/1168	0.76	1/1591 (0.1%)
1	B	0.31	0/1168	0.76	1/1591 (0.1%)
1	C	0.32	0/1168	0.76	2/1591 (0.1%)
1	D	0.31	0/1168	0.76	2/1591 (0.1%)
1	E	0.31	0/1168	0.76	2/1591 (0.1%)
1	F	0.31	0/1168	0.76	1/1591 (0.1%)
1	G	0.31	0/1168	0.76	2/1591 (0.1%)
1	H	0.31	0/1168	0.76	2/1591 (0.1%)
1	I	0.31	0/1168	0.76	1/1591 (0.1%)
1	J	0.31	0/1168	0.76	1/1591 (0.1%)
1	K	0.31	0/1168	0.76	1/1591 (0.1%)
1	L	0.31	0/1168	0.77	1/1591 (0.1%)
1	M	0.32	0/1168	0.76	1/1591 (0.1%)
1	N	0.31	0/1168	0.76	1/1591 (0.1%)
1	O	0.31	0/1168	0.76	2/1591 (0.1%)
1	P	0.32	0/1168	0.76	2/1591 (0.1%)
1	Q	0.31	0/1168	0.76	1/1591 (0.1%)
1	R	0.31	0/1168	0.76	1/1591 (0.1%)
1	S	0.31	0/1168	0.77	1/1591 (0.1%)
1	T	0.31	0/1168	0.76	1/1591 (0.1%)
1	U	0.32	0/1168	0.76	2/1591 (0.1%)
1	V	0.32	0/1168	0.76	1/1591 (0.1%)
1	W	0.31	0/1168	0.76	1/1591 (0.1%)
1	X	0.31	0/1168	0.76	2/1591 (0.1%)
All	All	0.31	0/28032	0.76	33/38184 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	276	PRO	N-CA-C	5.14	116.97	110.70
1	P	276	PRO	N-CA-C	5.11	116.93	110.70
1	W	287	ILE	CB-CA-C	-5.09	108.86	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	276	PRO	N-CA-C	5.08	116.90	110.70
1	D	287	ILE	CB-CA-C	-5.07	108.88	113.70

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	1140	0	1140	74	0
1	B	1140	0	1140	51	0
1	C	1140	0	1140	48	0
1	D	1140	0	1140	51	0
1	E	1140	0	1140	56	0
1	F	1140	0	1140	56	0
1	G	1140	0	1140	71	0
1	H	1140	0	1140	54	0
1	I	1140	0	1140	59	0
1	J	1140	0	1140	51	0
1	K	1140	0	1140	45	0
1	L	1140	0	1140	62	0
1	M	1140	0	1140	68	0
1	N	1140	0	1140	55	0
1	O	1140	0	1140	53	0
1	P	1140	0	1140	71	0
1	Q	1140	0	1140	81	0
1	R	1140	0	1140	57	0
1	S	1140	0	1140	65	0
1	T	1140	0	1140	64	0
1	U	1140	0	1140	84	0
1	V	1140	0	1140	72	0
1	W	1140	0	1140	59	0
1	X	1140	0	1140	65	0
All	All	27360	0	27360	1236	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 23.

The worst 5 of 1236 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:A:319:LEU:HB3	1:G:312:THR:HG23	1.16	1.12
1:Q:312:THR:HG23	1:U:319:LEU:HB3	1.15	1.09
1:Q:312:THR:HA	1:U:319:LEU:HD22	1.27	1.08
1:F:312:THR:HG23	1:H:319:LEU:HB3	1.34	1.08
1:E:319:LEU:HB3	1:I:312:THR:HG23	1.35	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	B	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	C	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	D	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	E	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	F	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	G	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	H	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	I	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	J	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	K	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	L	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	M	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	O	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	P	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	Q	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	R	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	S	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	T	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	U	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
1	V	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	W	144/214 (67%)	140 (97%)	3 (2%)	1 (1%)	18	56
1	X	144/214 (67%)	140 (97%)	2 (1%)	2 (1%)	9	40
All	All	3456/5136 (67%)	3360 (97%)	61 (2%)	35 (1%)	12	48

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	272	TYR
1	M	272	TYR
1	P	272	TYR
1	R	272	TYR
1	U	272	TYR

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	B	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	C	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	D	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	E	116/190 (61%)	115 (99%)	1 (1%)	70	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	G	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	H	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	I	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	J	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	K	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	L	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	M	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	N	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	O	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	P	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	Q	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	R	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	S	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	T	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	U	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	V	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	W	116/190 (61%)	115 (99%)	1 (1%)	70	79
1	X	116/190 (61%)	115 (99%)	1 (1%)	70	79
All	All	2784/4560 (61%)	2760 (99%)	24 (1%)	70	79

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	163	TRP
1	R	163	TRP
1	Q	163	TRP
1	S	163	TRP
1	G	163	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	206	HIS

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Mol	Chain	Res	Type
1	L	206	HIS
1	W	206	HIS
1	N	206	HIS
1	I	206	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 oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	150/214 (70%)	-0.63	0 100 100	476, 510, 583, 638	0
1	B	150/214 (70%)	-0.51	0 100 100	482, 530, 638, 721	0
1	C	150/214 (70%)	-0.49	1 (0%) 84 73	484, 541, 726, 777	0
1	D	150/214 (70%)	-0.56	0 100 100	477, 516, 709, 732	0
1	E	150/214 (70%)	-0.56	0 100 100	472, 496, 612, 670	0
1	F	150/214 (70%)	-0.64	0 100 100	472, 501, 589, 649	0
1	G	150/214 (70%)	-0.44	0 100 100	470, 520, 654, 754	0
1	H	150/214 (70%)	-0.43	2 (1%) 75 63	470, 518, 679, 724	0
1	I	150/214 (70%)	-0.49	2 (1%) 75 63	467, 505, 644, 674	0
1	J	150/214 (70%)	-0.54	2 (1%) 75 63	466, 506, 643, 724	0
1	K	150/214 (70%)	-0.72	0 100 100	467, 509, 650, 735	0
1	L	150/214 (70%)	-0.57	0 100 100	468, 511, 628, 700	0
1	M	150/214 (70%)	-0.75	0 100 100	542, 595, 765, 794	0
1	N	150/214 (70%)	-0.58	0 100 100	542, 594, 748, 791	0
1	O	150/214 (70%)	-0.46	0 100 100	539, 576, 659, 693	0
1	P	150/214 (70%)	-0.59	0 100 100	538, 589, 714, 741	0
1	Q	150/214 (70%)	-0.43	0 100 100	536, 575, 726, 746	0
1	R	150/214 (70%)	-0.53	0 100 100	537, 567, 725, 768	0
1	S	150/214 (70%)	-0.64	0 100 100	505, 571, 737, 786	0
1	T	150/214 (70%)	-0.54	0 100 100	499, 547, 764, 818	0
1	U	150/214 (70%)	-0.48	1 (0%) 84 73	499, 549, 804, 853	0
1	V	150/214 (70%)	-0.65	0 100 100	502, 562, 811, 833	0
1	W	150/214 (70%)	-0.51	0 100 100	506, 565, 755, 791	0
1	X	150/214 (70%)	-0.49	1 (0%) 84 73	509, 579, 754, 802	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3600/5136 (70%)	-0.55	9 (0%) 90 82	466, 547, 716, 853	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	269	VAL	3.8
1	I	158	LEU	3.1
1	H	156	ALA	2.7
1	J	156	ALA	2.6
1	U	156	ALA	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.