



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:12 pm GMT

PDB ID : 5TAZ  
EMDB ID: : EMD-8390  
Title : Structure of rabbit RyR1 (ryanodine dataset, class 3)  
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;  
Frank, J.  
Deposited on : 2016-09-10  
Resolution : 4.30 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

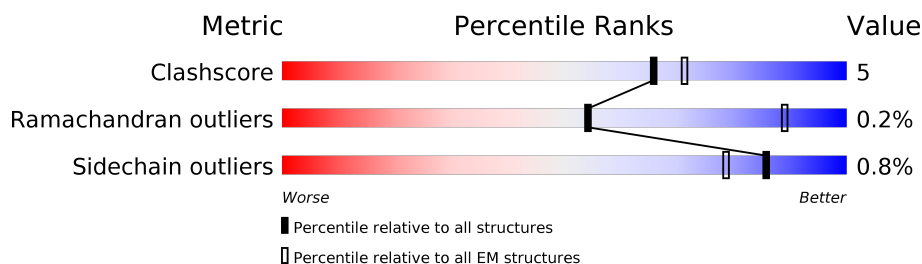
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.30 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	108	87% 12% .
1	F	108	89% 10% .
1	H	108	88% 11% .
1	J	108	89% 10% .
2	B	4416	84% 10% 5%
2	E	4416	84% 10% 5%
2	G	4416	84% 10% 5%
2	I	4416	85% 10% 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

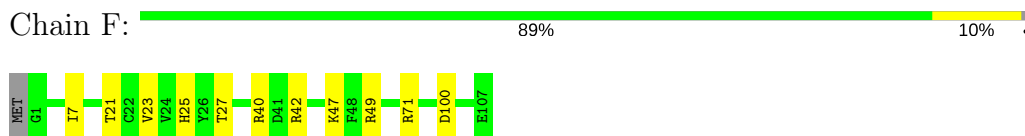
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

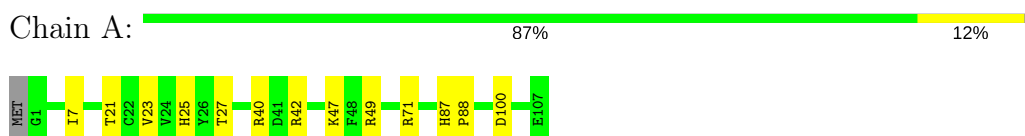
### 3 Residue-property plots

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. 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. 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.

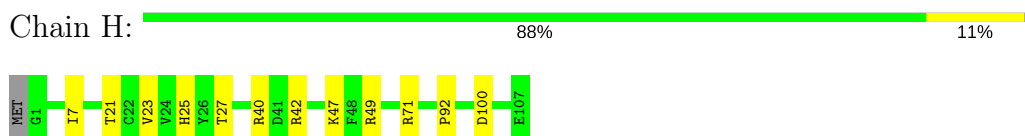
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



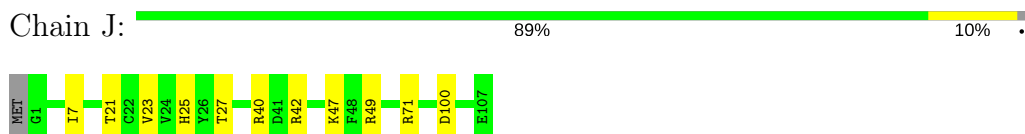
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



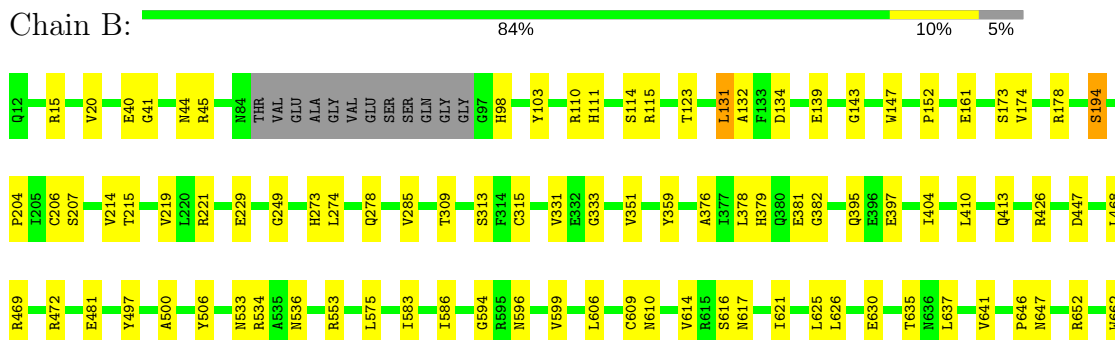
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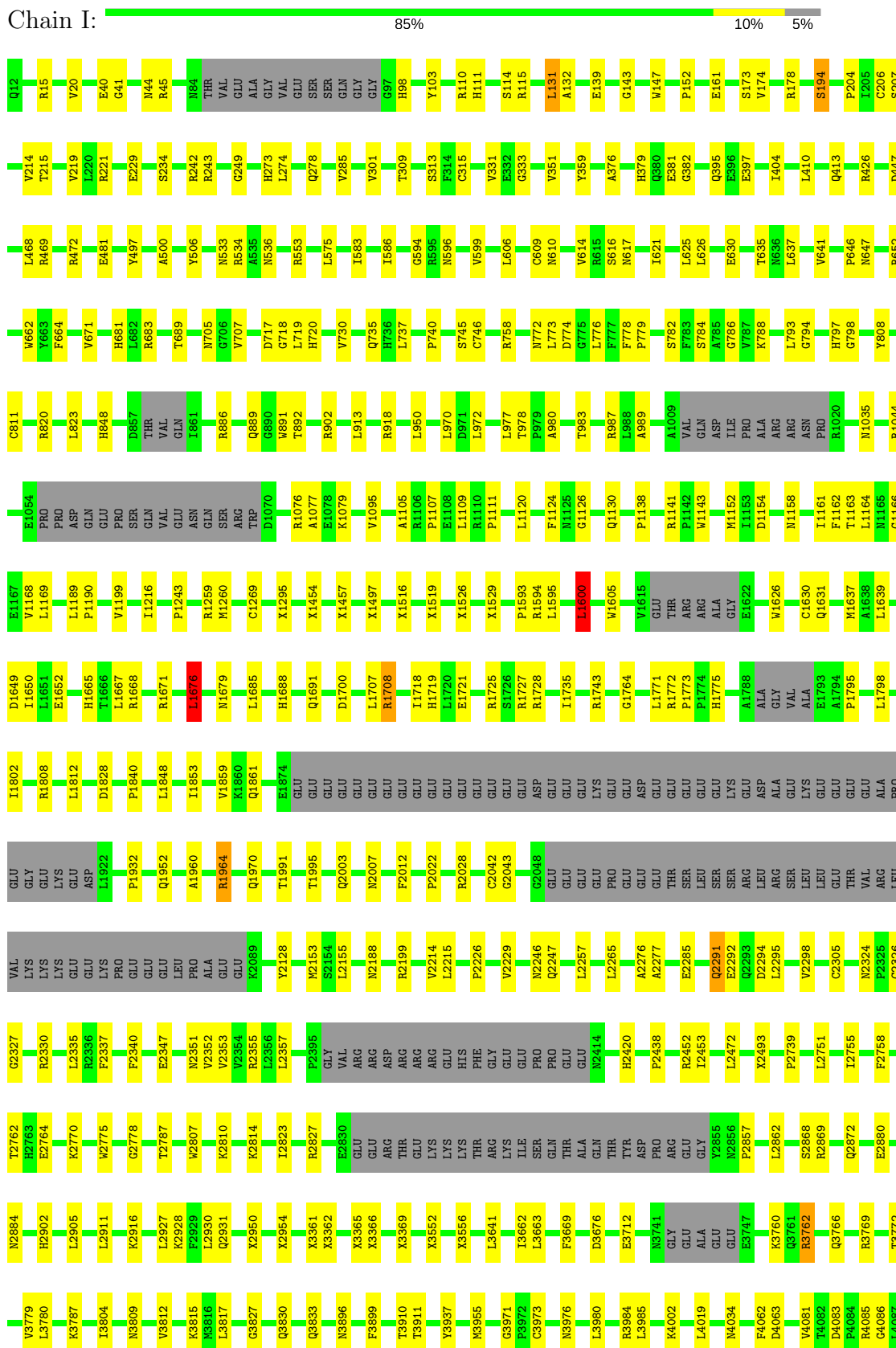
- Molecule 2: Ryanodine receptor 1





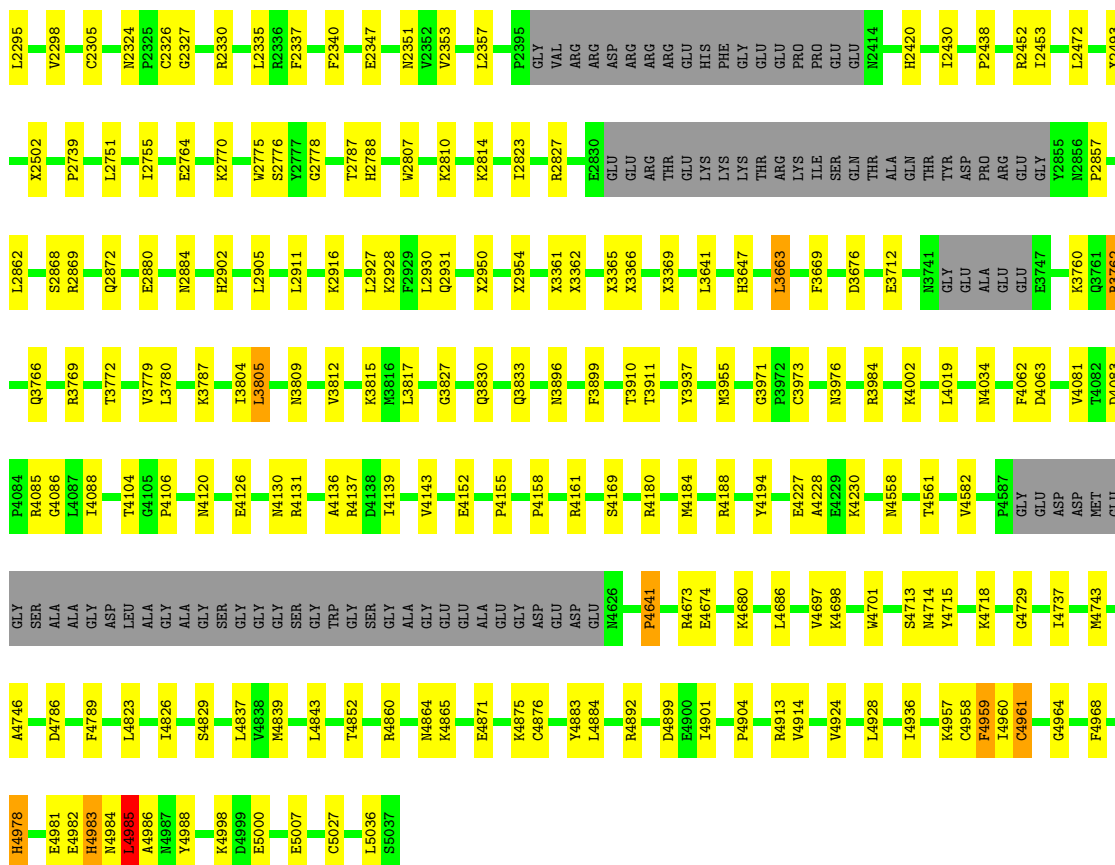

- Molecule 2: Ryanodine receptor 1

Chain I:

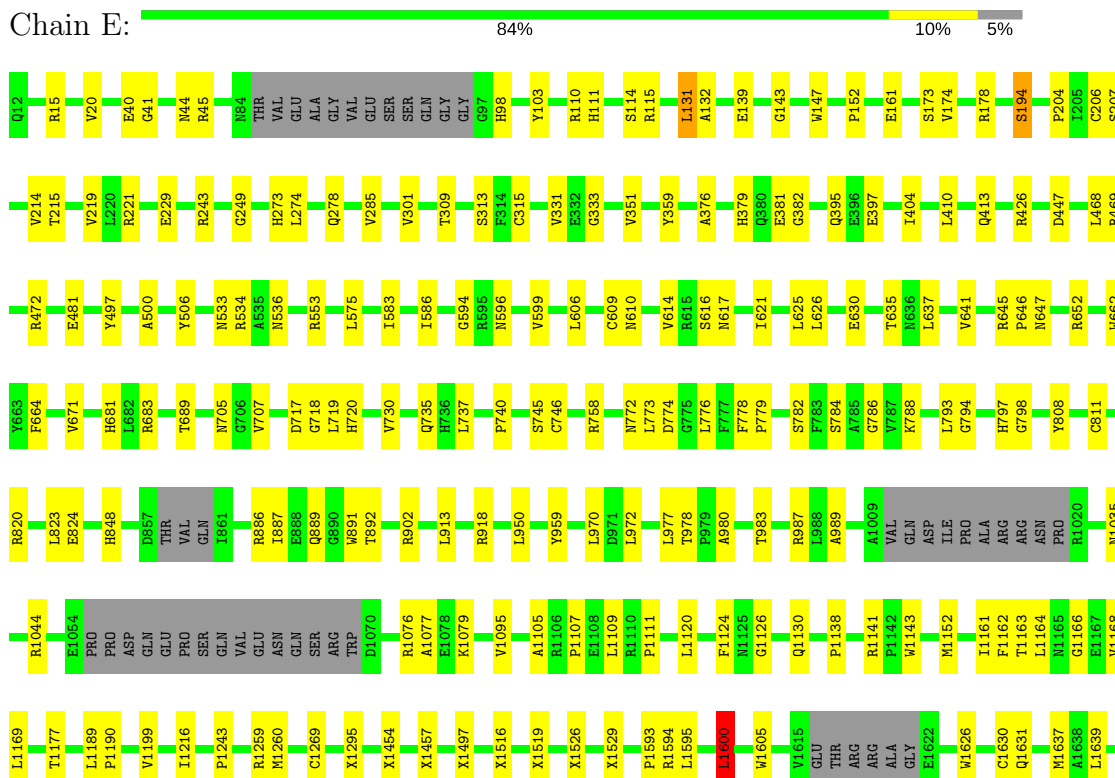








- Molecule 2: Ryanodine receptor 1



E4981	A4746	MET	T4982	R3762	S2868	L2751	C2305	LEV	LYS	R1908	D1649
E4982	D4786	GLU	D4083	Q3766	R2869	L2755	N2324	VAL	GLU	R1850	I1650
H4983	F4789	SER	R4085	R3769	Q2872	I2755	P2325	LYS	ASP	L1812	E1652
L4985		ALA	L4087	E2880	E2880	F2758	C2326	GLU	P1932	D1828	H1665
A4986	T4822	GLY	L4088	T3772	N2884	T2762	Q2327	GLU	LYS	P1840	T1668
A4987	L4923	ASP	T4104	R3773	H2902	E2763	R2330	PRO	GLU	I1853	R1668
Y4988	R4824	ALA	G4105	V3779	L2905	E2764	L2335	GLU	A1960		
K4998	T4925	GLY	P4106	L3780	L2905	K2770	R2336	GLU	GLU		
D4999	L4837	ALA	M4120	K3787	L2911	W2775	F2337	GLU	R1964	V1859	
E5000	F4838	GLY	M4120	K3787	L2911	W2775	F2340	LEV	Q1970	K1860	L1676
E5007	M4839	SER	E4126	T3804	K2916	G2778	E2347	ALA	GLU	Q1861	N1679
C5027	L4843	GLY	L3805	L3805	K2916	G2778	E2347	GLU	Q1973	E1874	L1685
L5036	T4852	GLY	M4130	N3809	L2927	T2787	N2351	K2089	GLU	GLU	
S5037	R4860	TRP	R4131	F3812	K2928	W2807	T2352	GLU	Y1977	GLU	H1688
		GLY	A4136	V3812	F2929	W2807	V2353		T1991	GLU	Q1691
	N4864	SER	R4137	K3815	L2930	K2810	L2357		T1995	GLU	D1700
	K4865	GLY	D4138	K3816	Q2931	K2810	L2357			GLU	
		ALA	L4139	L3817	X2950	K2814	F2395		Q2003	GLU	
	E4871	GLY	V4143	G3827	X2954	T2823	GLY	M2153	GLU	GLU	L1707
	K4875	GLU	E4152	F3827	X2954	T2823	VAL	S2154	N2007	GLU	R1708
	C4876	ALA	E4152	Q3830	X3361	R2827	ARG	L2155	F2012	GLU	I1718
		GLU	P4155	X3362	X3362	R2827	ASP	N2188		GLU	H1719
	Y4883	GLY	P4155	Q3833		E2830	ARG	N2196	P2022	GLU	L1720
	L4884	ASP	P4158	Q3833	X3365	GLU	ARG			GLU	E1721
		GLU	P4158	N3896	X3366	GLU	ARG	R2199	R2028	GLU	
	R4892	ASP	R4161	N3896	X3366	ARG	GLU		C2042	ASP	R1725
	D4899	GLU	S4169	F3999	X3369	THR	HIS	V2214	G2043	GLU	L1726
	F4900	GLU	S4169	F3999	X3369	GLY	PHE	L2215		GLU	R1727
	L4901		R4180	T3910	L3641	LYS	GLY	P2226	G2048	LYS	R1728
	P4904		R4180	T3911	H3647	LYS	GLU		GLU	GLU	
		E4674	M4184	Y3937	H3647	THR	PRO	V2229	GLU	GLU	I1735
	R4913		R4188	M3955	L3663	ARG	GLU	N2246	GLU	ASP	R1743
	V4914		Y4194	M3955	F3669	ILE	GLU	Q2247	PRO	GLU	G1764
	V4924	L4686	Y4194	G3971	F3669	SER	K2414	L2257	GLU	GLU	L1771
	L4928	V4697	E4227	P3972	D3676	GLN	H2420	L2265	GLU	GLU	R1772
		W4701	A4228	C3973	K3694	ALA	H2420	L2265	THR	LYS	H1775
	L4936		F4929	N3976	P3695	GLN	I2430	A2276	SER	ASP	
		S4713	K4230	R3984	E3712	TYR	P2438	A2277	LEV	ALA	A1788
	K4957	M4714	M4568	K4002	N3741	ASP	R2452	E2285	SER	GLU	ALA
	C4958	Y4715	T4561	L4019	GLY	ARG	E2285	E2285	ARG	LYS	GLY
	F4959	K4718	T4561	L4019	GLY	ARG	E2285	E2285	LEV	GLU	VAL
	L4960		V4582	N4034	ALA	GLY	Q2291	Q2291	ARG	GLU	ALA
	C4961		V4582	N4034	ALA	GLY	E2292	E2292	SER	GLU	E1793
		G4729	P4587	N4034	GLY	GLY	Q2293	Q2293	LEV	GLU	A1794
	G4964		GLY	D4063	GLU	GLU	D2294	D2294	LEV	ALA	P1795
	F4968		GLU	F4062	E3747	P2857	L2295	L2295	GLU	PRO	
			ASP	D4063	K3760	L2862	X2502	X2502	THR	GLU	L1798
			ASP	F4063	K3760	L2862		V2298	VAL	GLY	
			ASP	F4063	K3760	L2862		V2298	VAL	GLY	L1803

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.30	0/834	0.54	0/1123
1	F	0.30	0/834	0.54	0/1123
1	H	0.30	0/834	0.54	0/1123
1	J	0.30	0/834	0.54	0/1123
2	B	0.29	0/25428	0.53	6/34534 (0.0%)
2	E	0.29	0/25428	0.53	6/34534 (0.0%)
2	G	0.29	0/25428	0.53	6/34534 (0.0%)
2	I	0.29	0/25428	0.53	6/34534 (0.0%)
All	All	0.29	0/105048	0.53	24/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.91	133.50	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30
2	B	131	LEU	CA-CB-CG	7.90	133.47	115.30
2	E	131	LEU	CA-CB-CG	7.89	133.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1600	LEU	CA-CB-CG	6.81	130.95	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	194	SER	Peptide
2	B	808	TYR	Peptide

## 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	818	0	824	7	0
1	F	818	0	824	6	0
1	H	818	0	824	7	0
1	J	818	0	824	6	0
2	B	29499	0	24749	265	0
2	E	29499	0	24749	262	0
2	G	29499	0	24749	265	0
2	I	29499	0	24748	262	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102291	1047	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 5.

The worst 5 of 1047 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)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.18	1.32
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.18	1.32
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.18	1.30
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.18	1.30
2:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.67	1.02

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 PDB entries followed by that with respect to all EM entries.

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	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	51	85
2	E	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	51	85
2	G	3235/4416 (73%)	2900 (90%)	329 (10%)	6 (0%)	51	85
2	I	3235/4416 (73%)	2899 (90%)	330 (10%)	6 (0%)	51	85
All	All	13360/18096 (74%)	11973 (90%)	1363 (10%)	24 (0%)	54	85

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	4985	LEU
2	I	4985	LEU
2	G	4985	LEU
2	E	4985	LEU

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Mol	Chain	Res	Type
2	B	1708	ARG

### 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 PDB entries followed by that with respect to all EM entries.

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	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
2	E	2493/3022 (82%)	2471 (99%)	22 (1%)	82	91
2	G	2493/3022 (82%)	2471 (99%)	22 (1%)	82	91
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	85	92
All	All	10324/12444 (83%)	10238 (99%)	86 (1%)	86	92

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4959	PHE
2	G	1676	LEU
2	E	4120	ASN
2	I	4978	HIS
2	G	534	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 138 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3781	GLN
2	G	273	HIS
2	E	3809	ASN
2	I	3830	GLN

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Mol	Chain	Res	Type
2	I	4120	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14

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Mol	Chain	Number of breaks
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.83
1	I	4345:UNK	C	4540:PHE	N	73.83
1	G	4345:UNK	C	4540:PHE	N	73.83
1	E	4345:UNK	C	4540:PHE	N	73.83
1	B	3613:UNK	C	3639:THR	N	45.16