



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 01:11 pm GMT

PDB ID : 5TB1
EMDB ID: : EMD-8392
Title : Structure of rabbit RyR1 (EGTA-only dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 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
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

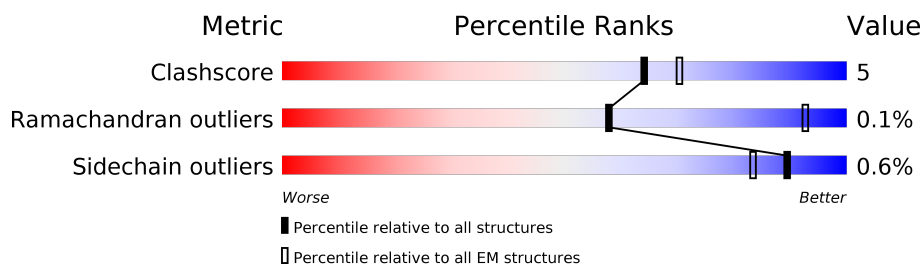
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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 ≥ 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	74% 25% .
1	F	108	73% 26% .
1	H	108	76% 23% .
1	J	108	77% 22% .
2	B	4416	84% 11% 5%
2	E	4416	84% 11% 5%
2	G	4416	84% 11% 5%
2	I	4416	84% 11% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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	E	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		

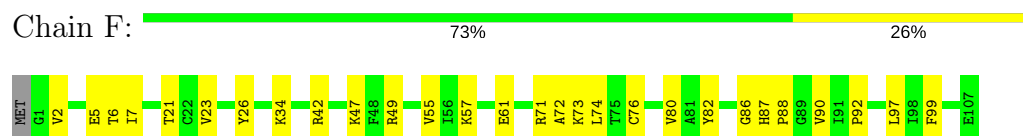
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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	

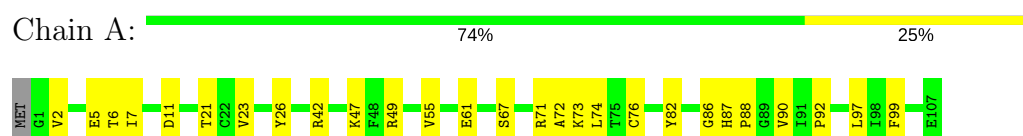
3 Residue-property plots

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.

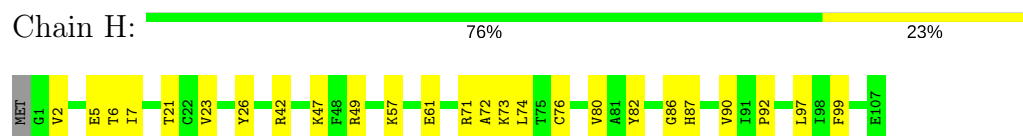
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



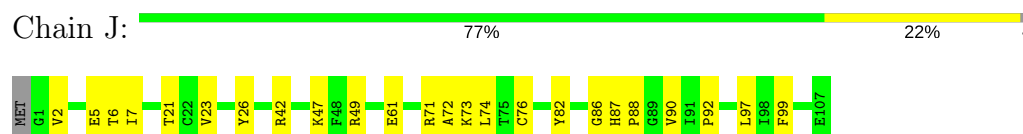
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



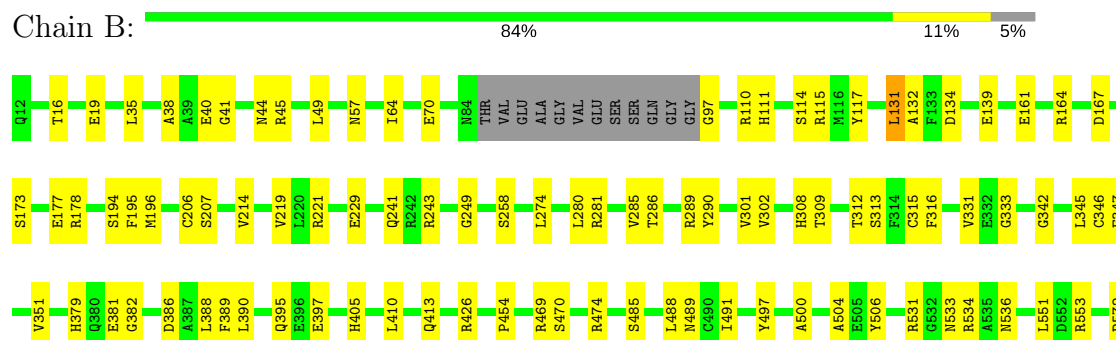
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



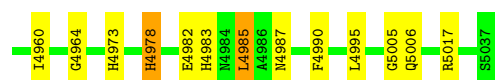
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1

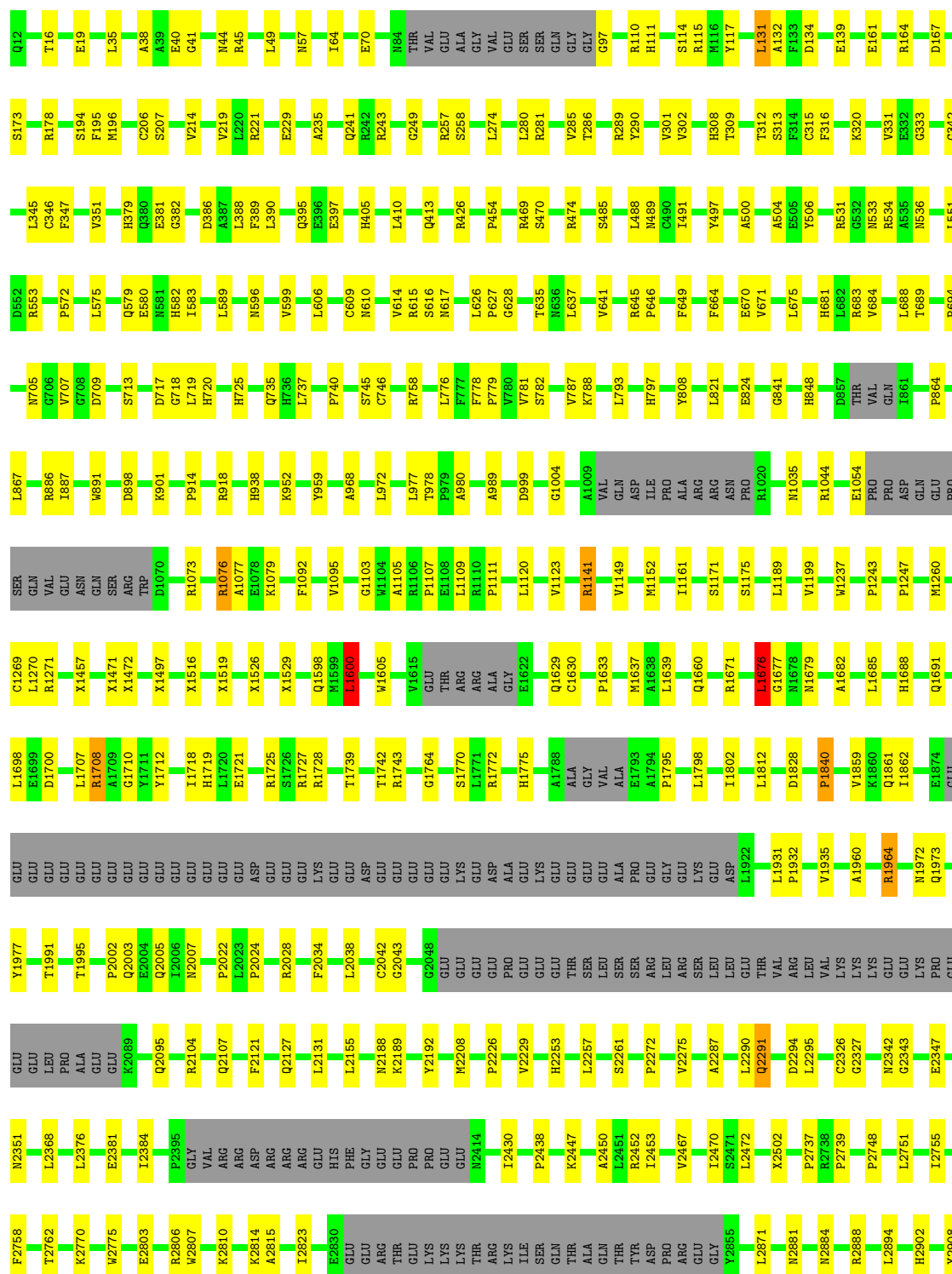


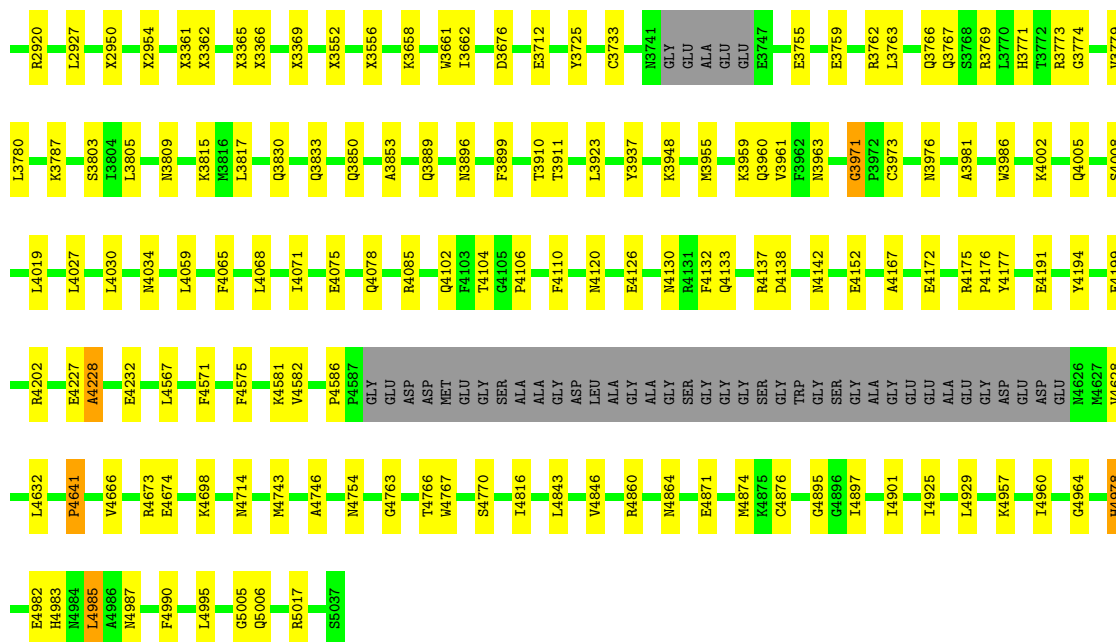


• Molecule 2: Ryanodine receptor 1

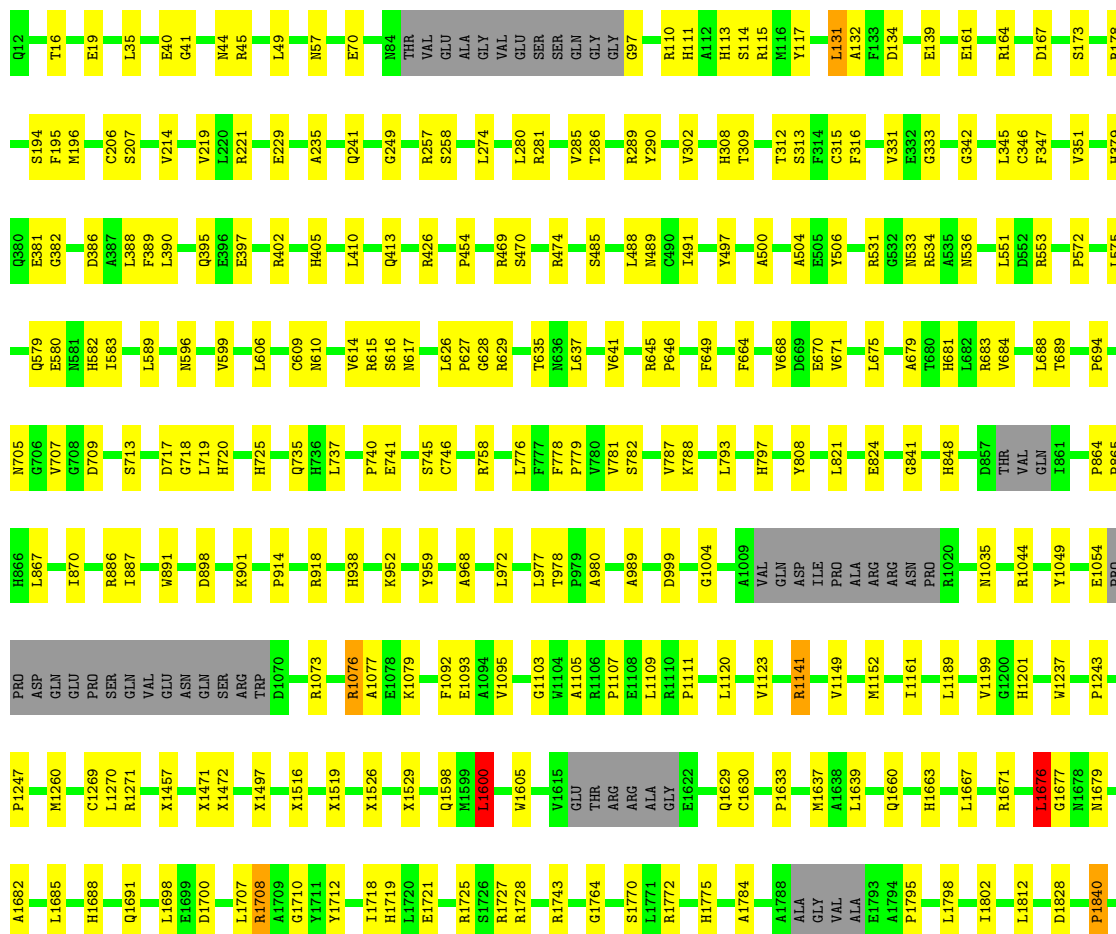
Chain I: 84% 11% 5%





• Molecule 2: Ryanodine receptor 1

Chain E: 84% 11% 5%



R4987	R4673	F4551	L4059	Q3830	X3365	K2810	R2104	Q2003	GLU	L1707	X1457	TRP	D891	D709
F4990	E4674	L4567	F4065	Q3833	X3366	K2814	Q2107	E2004	GLU	R1708	X1471	D1070	S713	
L4995	R4698	F4571	F4068	Q3850	X3369	A2815	F2121	Q2006	GLU	A1709	X1472	R1073	D898	
G5005	R4714	F4575	L4068	Q3853	X3552	T2823	Q2127	N2007	GLU	Y1711	X1497	R1076	K901	D717
Q5006	R4743	K4581	T4071	A3853	X3556	E2830	Q2022	P2022	GLU	A1077	X1516	A1077	H938	G718
R5017	R4746	V4582	E4075	Q3889	K3658	GLU	L2131	P2024	ASP	K1078	X1519	K1078	H725	L719
S5037	R4754	P4586	Q4078	N3896	K3661	GLU	L2155	R2028	GLU	F1092	X1526	F1092	K952	H720
		P4587	R4085	F3899	I3662	THR	K2188	C2042	LYS	E1093	X1529	A1094	Y959	Q735
	G4763	GLY	Q4102	T3910	D3676	GLU	K2189	G2043	GLU	V1095		V1095	A968	L737
	A4767	ASP	Q4103	T3911	E3712	LYS	Y2192	G2048	GLU	G1103	Q1598	G1103	L972	P740
	R4770	ASP	F4104	L3923	E3712	THR	N2208	GLU	GLU	A1104	N1599	A1104	L977	E741
		GLY	G4105	Y3937	Y3725	LYS	P2226	GLU	GLU	A1105	L1600	A1105	L977	S745
	I4816	SER	F4106	Y3937	K3741	GLY	Y2229	GLU	GLU	R1076	W1605	R1076	P979	C746
	L4843	ALA	F4110	K3948	GLY	GLY	H2253	GLU	GLU	E1108	V1615	E1108	A980	
	R4860	GLY	N4120	K3955	ALA	THR	H2257	THR	ALA	R1110	THR	R1110	A989	R758
		ASP	E4126	K3959	GLN	GLN	L2257	SER	GLU	P1111	ARG	P1111	D989	L776
	N4864	ALA	N4130	Q3960	THR	THR	S2261	LEU	LYS	L1120	ARG	L1120	G1004	F778
	E4871	ALA	R4131	F3962	ASP	GLN	S2261	SER	GLY	V1123	E1622	V1123	P779	W780
	F4132	GLY	F4132	N3963	PRO	THR	P2272	ARG	GLU	R1141		R1141	A1009	W781
	D4138	SER	D4138	E3759	GLU	GLU	Y2275	LEU	ALA	V1149	Q1629	V1149	VAL	S782
	C4875	GLY	N4142	R3762	GLY	GLY	A2287	SER	PRO	M152	C1630	M152	ASP	V787
	C4876	GLY	E4152	L3763	Y2885	Y2885	L2290	LEU	GLY	M161		M161	ILE	K789
	R4892	SER	E4152	Q3766	L2871	L2871	L2290	LEU	GLY	M1637		M1637	ALA	L793
	L4897	TRP	A4167	Q3767	N2881	N2881	Q2281	THR	LYS	A1638		A1638	ARG	H797
	T4901	SER	E4172	R3769	R2881	R2881	D2294	VAL	ASP	S1171	Q1660	S1171	ASN	Y808
	L4925	ALA	R4175	L3770	N2884	N2884	L2295	VAL	GLU	S1175		S1175	PRO	
	L4928	GLY	P4176	T3772	R2888	R2888	C2326	LYS	LYS	L1189	R1671	L1189	N1035	L821
	L4929	GLU	Y4177	R3773	L2894	L2894	Q2327	LYS	LYS	P1190		P1190	E824	
	R4957	ALA	E4191	G3774			N2342	GLU	GLU	V1199	L1676	V1199	R1044	G841
	L4960	GLY	Y4194	V3779	H2902	H2902	G2343	GLU	GLU	G1200	G1677	G1200	E1054	
	G4964	ASP	E4199	L3780	Y2908	Y2908	E2347	PRO	GLU	H1201	N1679	H1201	PRO	H848
	H4973	GLY	R4202	K3787	R2920	R2920	N2351	GLU	GLU	V1237	A1682	V1237	ASP	D857
	R4978	GLY	E4227	S3803	L2927	L2927	L2368	GLU	GLU	P1243	L1685	P1243	GLN	THR
		ALA	A4228	L3804	X2950	X2950	L2376	LEU	PRO	P1247		P1247	GLU	VAL
	E4982	GLY	E4232	L3805	X2954	X2954	L2381	ALA	ALA	M1260	H1688	M1260	SER	GLN
	H4983	GLY	E4232	N3809	Y2954	Y2954	E2381	GLU	GLU	Q1691	Q1691	Q1691	VAL	P864
	L4985	ALA	Q4547	K3815	X3361	X3361	L2384	GLU	GLU	C1269	L1698	C1269	ASN	L867
	A4986	GLY		L3816	X3362	X3362	L2384	GLU	GLU	L1270	E1699	L1270	GLN	R886
		GLY		L3817			P2395	GLU	GLU	D1700		D1700	SER	L887
		GLY						Q2095	P2002				ARG	

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

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	0.52	0/1123
1	F	0.30	0/834	0.52	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.29	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	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	16
2	E	0	16
2	G	0	16
2	I	0	16
All	All	0	64

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	G	131	LEU	CA-CB-CG	8.01	133.72	115.30
2	B	131	LEU	CA-CB-CG	8.00	133.69	115.30
2	E	131	LEU	CA-CB-CG	7.99	133.68	115.30
2	I	131	LEU	CA-CB-CG	7.99	133.66	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4985	LEU	CA-CB-CG	7.25	131.97	115.30

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	312	THR	Peptide
2	B	694	PRO	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	16	0
1	F	818	0	824	18	0
1	H	818	0	824	15	0
1	J	818	0	824	14	0
2	B	29499	0	24746	268	0
2	E	29499	0	24746	273	0
2	G	29499	0	24746	261	0
2	I	29499	0	24746	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
All	All	121272	0	102280	1100	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 1100 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:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.67
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.66
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.61	0.65

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 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%)	92 (88%)	13 (12%)	0	100	100
1	F	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	H	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
1	J	105/108 (97%)	92 (88%)	13 (12%)	0	100	100
2	B	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
2	E	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
2	G	3235/4416 (73%)	2887 (89%)	344 (11%)	4 (0%)	55	89
2	I	3235/4416 (73%)	2888 (89%)	343 (11%)	4 (0%)	55	89
All	All	13360/18096 (74%)	11919 (89%)	1425 (11%)	16 (0%)	58	89

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	B	1932	PRO

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%)	2477 (99%)	16 (1%)	89	94
2	E	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
2	G	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
2	I	2493/3022 (82%)	2477 (99%)	16 (1%)	89	94
All	All	10324/12444 (83%)	10260 (99%)	64 (1%)	89	94

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	4120	ASN
2	E	1076	ARG
2	G	4085	ARG
2	I	4978	HIS
2	E	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3950	ASN
2	E	413	GLN
2	G	3946	GLN
2	I	3963	ASN
2	I	4142	ASN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 4 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
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	73.36
1	I	4345:UNK	C	4540:PHE	N	73.36
1	E	4345:UNK	C	4540:PHE	N	73.36
1	G	4345:UNK	C	4540:PHE	N	73.36

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	46.46