



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2022 – 02:30 AM EDT

PDB ID : 5T9R
EMDB ID : EMD-8374
Title : Structure of rabbit RyR1 (Ca²⁺-only dataset, class 3)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-09
Resolution : 5.80 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

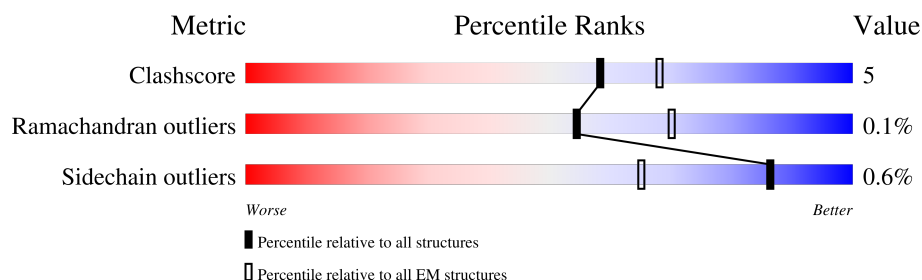
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	108	80% 19% .
1	F	108	80% 19% .
1	H	108	81% 18% .
1	J	108	81% 18% .
2	B	4676	79% 10% 11%
2	E	4676	79% 10% 11%
2	G	4676	79% 10% 11%
2	I	4676	78% 10% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 120756 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	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

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

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


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

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

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. 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.

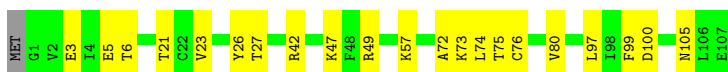
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




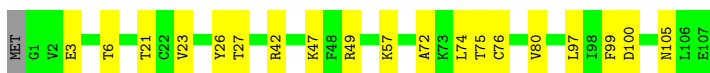
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 




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

Chain H: 




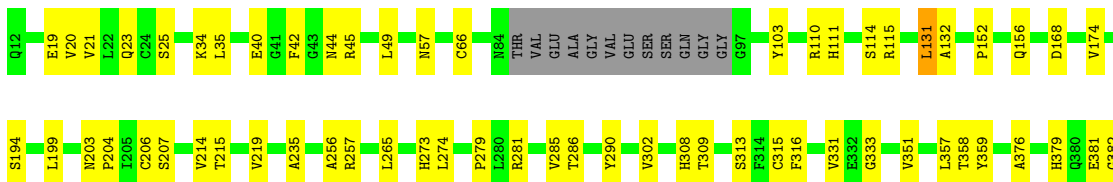
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

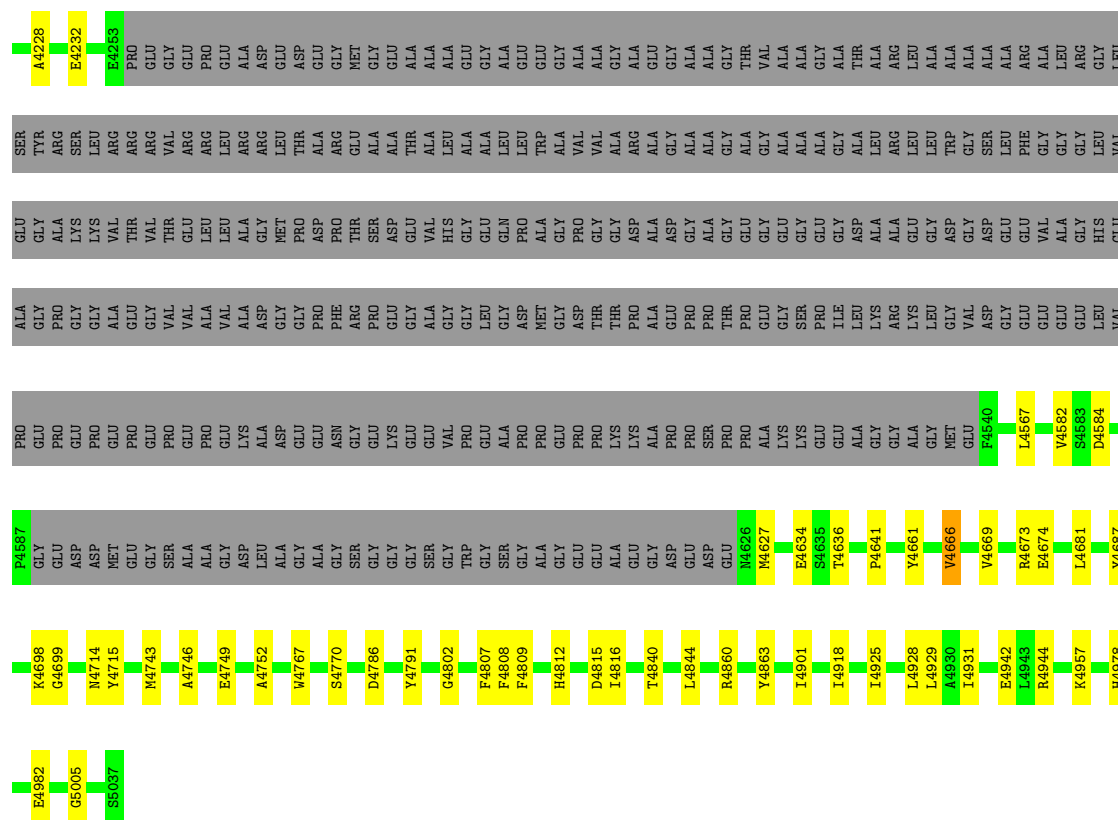


- Molecule 2: Ryanodine receptor 1

Chain B: 

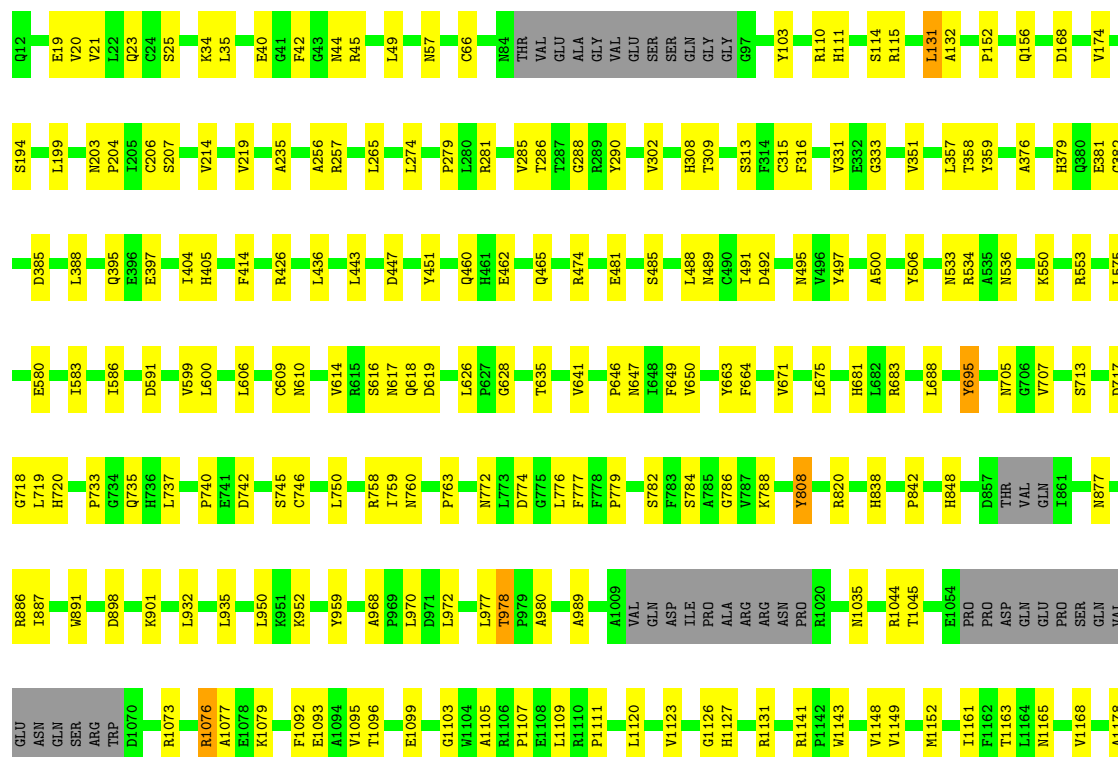


C3973	C3974	G3975	N3976	Q3977	Q3978	H3971	T3772	L3780	Q3781	H3988	S3784	K3787	L4002	L4003	L4013	L4019	N4034	V4049	K4067	I4071	E4075	Q4078	R4085	A4096	S4099	Q4102	F4103	G4105	P4106	N4120	E4126	N4130	R4131	E4152	R4159	M4184	I4190	E4191	R4192	Y4193			
GLU	GLU	E3747	N3976	T3772	T3772	H3771	T3772	L3780	Q3781	H3988	S3784	K3787	L4002	L4003	L4013	L4019	N4034	V4049	K4067	I4071	E4075	Q4078	R4085	A4096	S4099	Q4102	F4103	G4105	P4106	N4120	E4126	N4130	R4131	E4152	R4159	M4184	I4190	E4191	R4192	Y4193			
SER	GLN	THR	ALA	GLN	THR	THR	THR	TYR	ASP	ARG	GLU	GLY	Y2855	H2856	P2857	S2868	R2869	Q2872	N2884	R2888	L2927	L2930	X2945	X3362	X3366	X3552	X3556	K3658	V3661	I3662	I3674	D3696	L3710	T3711	E3712	Y3725	I3728	H3741	GLY	ALA			
L2472	X2517	X2521	X2674	X2675	X2676	P2737	R2738	P2739	P2748	L2751	T2755	F2758	T2762	H2763	E2764	K2770	W2775	G2778	T2787	P2789	M2790	E2803	R2806	W2807	K2810	I2823	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	THR	ARG	LYS			
Q2247	L2265	T2271	T2272	L2273	D2274	V2275	A2276	A2277	I2281	E2285	L2290	Q2291	V2299	A2303	C2326	C2327	R2330	F2337	V2341	N2342	G2343	E2347	N2351	P2395	GLY	ARG	ARG	ASP	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	R2452			
PRO	GLU	GLU	THR	SER	LEU	SER	ARG	LEU	ARG	LEU	GLU	VAL	ARG	LEU	VAL	LYS	LYS	PRG	ALA	GLU	GLU	PRG	E2089	R2104	Q2107	F2121	L2131	T2152	L2155	L2159	R2163	L2167	L2201	GLU	GLU	L2236							
GLU	GLU	GLU	LYS	ASP	ALA	GLU	GLU	GLU	GLU	ALA	PRO	GLY	GLY	LYS	ASP	L1922	L1926	L1931	P1932	V1935	A1960	R1964	Y1965	N1972	Q1973	Y1977	P2002	Q2003	E2004	Q2005	N2007	P2024	I2027	C2042	G2043	G2048	GLU	GLU	GLU	GLU			
ALA	GLY	VAL	E1793	E1794	P1795	A1796	R1797	L1798	I1802	L1807	R1808	L1812	D1828	P1840	L1848	I1853	F1854	V1859	K1860	Q1861	I1862	M1865	E1874	GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	LYS	GLU	GLU	GLU	GLU				
A1627	C1630	D1632	P1633	L1639	D1649	E1652	L1653	Q1660	H1665	L1667	R1668	R1671	L1676	G1677	N1678	M1679	W1688	V1689	D1690	L1698	E1699	D1700	R1708	A1709	G1710	Y1711	Y1712	I1718	H1719	L1720	E1721	R1725	R1728	S1729	R1743	A1788							
P1142	W1143	V1148	V1149	M1152	T1154	T1161	F1162	T1163	L1164	M1165	V1168	A1178	H1189	L1199	G1200	H1201	A1227	M1230	W1237	F1238	P1243	P1247	X1516	X1519	X1526	X1529	R1594	Q1598	M1599	L1600	V1605	S1606	V1615	THR	ARG	ALA	E1622						
N1035	Q1041	R1044	T1045	E1054	PRO	ASP	GLN	GLU	PRO	SER	VAL	ASN	GLN	SER	ARG	D1070	R1073	R1076	A1077	E1078	K1079	F1092	E1093	V1095	T1096	E1099	G1103	W1104	E1105	P1107	E1108	L1109	R1110	PRO	ALA	ARG	ASN	R1020	H1126	H1127	R1131	K1032	R1141
N877	R886	I887	W891	D898	K901	P914	R918	L932	L935	L950	K951	K952	Y959	A968	P969	L970	D971	L972	L977	T978	P979	A980	T983	R987	L988	A989	A1009	VAL	GLN	ASP	ILE	PRO	ALA	ARG	ASN	THR	VAL	GLN	I861	P864	P865		
G718	L719	H720	P733	G734	Q735	H736	L737	P740	E741	D742	S745	C746	N750	R758	I759	N760	P763	L626	F627	G628	T635	V641	P646	N647	I648	F649	V650	Y663	F664	V671	Y808	R820	H838	P842	H848	D857	THR	VAL	GLN	I861	P864	P865	
L575	E580	I583	I586	D591	V599	L600	L606	C609	N610	V614	R615	S616	N617	Q618	L626	E627	G628	T635	V641	P646	N647	I648	F649	V650	Y663	F664	V671	L675	H681	L682	R683	L688	Y695	N705	G706	V707	S713	D717					



● Molecule 2: Ryanodine receptor 1

Chain E: 79% 10% 11%

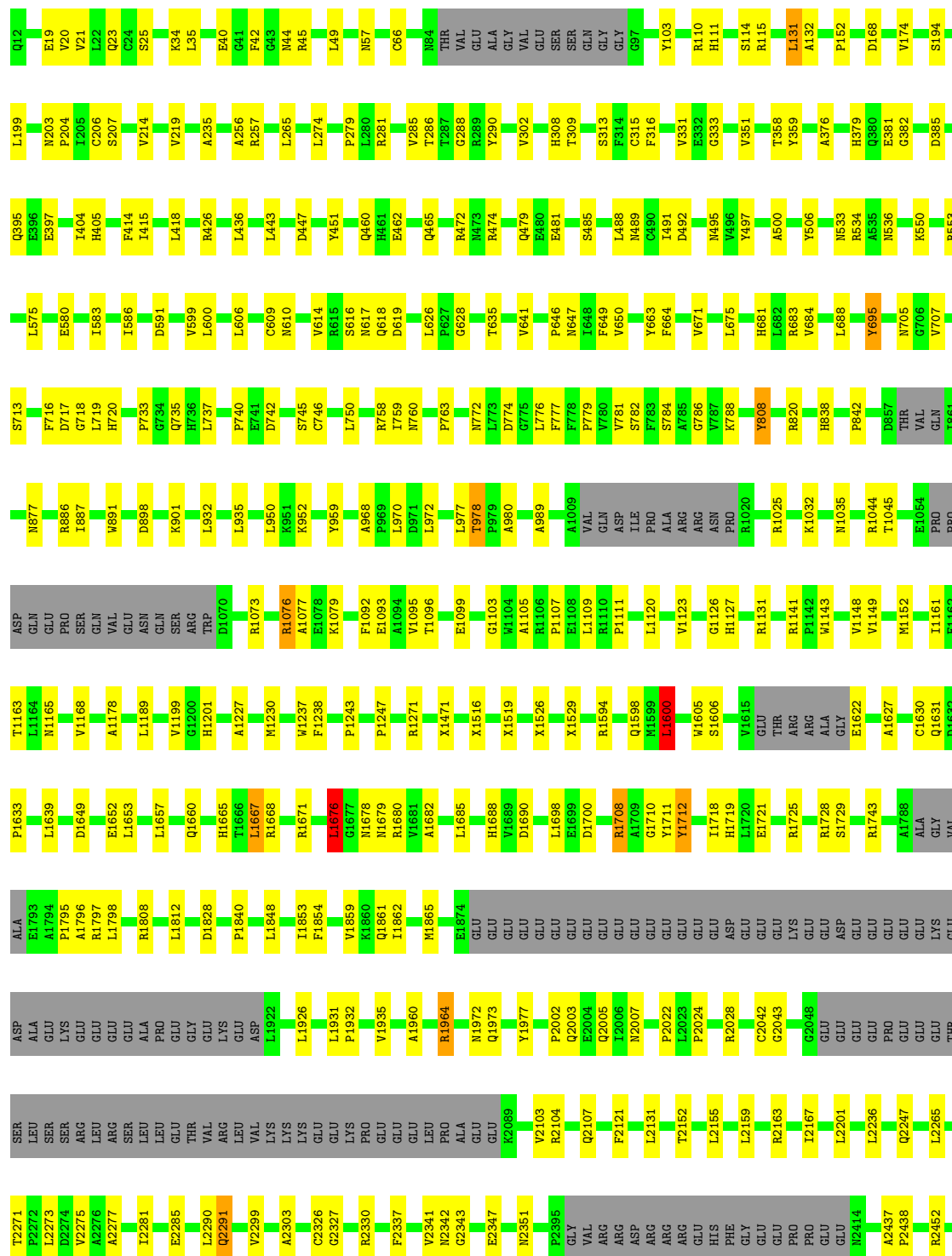






• Molecule 2: Ryanodine receptor 1

Chain I: 78% 10% 11%



PRO	H3994	T3772	ASP	X2521	T2271	THR	GLU	L1853	H1201	TRP	D998	L719	E530
GLU	H3998	L3780	PRO	P2737	P2272	SER	GLU	Q1560	A1227	D1070	X901	H720	E583
ALA	L4002	Q3781	ARG	R2738	L2273	LEU	ALA	H1665	M1230	R1073	L932	P733	I586
ASP	L4003	P2739	GLY	A2276	A2275	SER	PRO	T1666	W1237	R1076	L935	Q735	I566
GLU	L4013	A2277	Y2855	A2277	L1812	LEU	GLY	L1667	F1238	E1077	L950	H736	D891
MET	L4019	L2281	N2856	L2751	D1828	ARG	GLY	R1668	P1243	E1078	K951	L737	
GLY	L4034	E2285	P2857	L2755	P1840	SER	LYS	R1671	P1247	K1079	K952	P740	V599
ALA	L4049	F2758	Q2872	E2285	P1848	LEU	ASP	L1677		F1092	E741	L742	L600
ALA	Q3827	L2290	THR	L2290	L1848	GLU	L1922	G1678		A1094	Y959	S745	L606
GLU	Q3830	Q2291	VAL	Q2291	T1853	VAL	L1926	N1678	R1271	V1095	C746	C746	C609
GLY	Q3833	C2326	ARG	H2763	F1854	ARG	L1926	N1679	X1471	T1096	P969	C746	N610
GLU	Q3842	G2327	VAL	E2764	L1931	VAL	L1931	R1680		E1099	L970	L750	V614
GLU	L3842	G2343	LYS	K2770	P1932	LYS	P1932	V1681	X1497	G1103	D971	R758	R615
GLY	Q3850		LYS	W2775	V1935	LYS	V1935	L1682	X1516	W1104	L972	R759	S616
ALA	A3853		GLU	G2778	A1960	GLU	A1960	H1688	X1519	A1105	L977	N760	N617
ALA	F3880		PRO	T2787	R1964	PRO	R1964	V1689	X1526	R1106	P978	Q618	D619
GLY	A4096		GLU	H2788	N1972	GLU	N1972	D1690	X1529	E1108	A980	P763	
ALA	S4099		GLU	P2789	Q1973	GLU	Q1973	L1698	X1535	R1110	A989	N772	L626
THR	Q3889		LEU	M2790	Y1977	LEU	Y1977	D1700	R1594	P1111	A1009	L773	F627
VAL	N3896		ALA	N2351	P2395	ALA	P2395	R1708	L1595	L1120	VAL	G775	G628
ALA	N3897		GLY	E2347	GLY	GLY	GLY	A1709	Q1598	V1123	GLN	G776	T635
GLY	D3898		ARG	E2347	VAL	GLU	VAL	G1710	R1600	ASP	ASP	F777	V641
ALA	F3899		ASP	N2351	ARG	GLU	ARG	Y1712	L1600	PRD	PRD	P779	P646
THR	Q3900		ASP	E2803	ASP	GLU	N2007	I1718	V1605	G1126	ASN	F782	F649
ALA	N3901		ARG	A2815	ASP	GLU	Q2107	H1719	S1606	H1127	PRD	S784	V650
ARG	T3910		ARG	T2823	ARG	GLU	C2021	L1720		W1143	PRD	G786	Y663
LEU	T3911		ARG	E2830	ARG	GLU	P2022	E1721	V1615	V1148	R1020	V767	F664
ALA	S3929		HIS	G2830	ARG	GLU	L2023	I1725	GLY	V1149	N1035	K788	V671
ALA	Y3937		PHE	G2830	GLY	ASP	P2024	R1728	THR	M152	R1044	Y808	L675
ARG	M3955		GLY	GLY	GLU	GLU	R2028	S1729	ARG	M152	T1045	H838	
LEU	Q3960		GLU	GLU	GLU	GLU	F2034		ALA		E1054	P842	H831
LEU	T3974		PRO	THR	GLU	LYS	L2038	R1743	GLY	I1161	PRO	D857	L683
LEU	R4192		LYS	ARG	GLY	ASP	C2042	A1788	E1622	T1162	ASP	THR	L688
SER	A4228		THR	ARG	N2414	GLU	G2043	ALA	GLY	I1164	GLN	GLN	Y695
TYR	G3971		ARG	ARG	R2437	GLU	G2048	GLY	GLY	V1168	PRD	1861	N705
ARG	P3972		GLY	ILE	P2438	GLU	GLU	E1793	Q1631	T1163	ASP	THR	G706
SER	E4232		GLU	SER	R2452	GLU	GLU	A1794	P1633	I1164	GLN	GLN	V707
LEU	T3974		ALA	GLN	R2452	LYS	LYS	P1795	L1639	A1178	VAL	VAL	R886
ARG	G3975		GLU	ALA	L2472	GLU	PRO	A1796		L1189	GLU	GLU	S713
ARG	N3976		GLU	GLN	X2517	ASP	GLU	R1797	D1649	V1199	ASN	ASN	D717
VAL	Q3977		THR	THR		ALA	GLU	L1798	E1652	G1200	GLN	SER	G718
ARG	Q3978		TYR	TYR		LYS	GLU	I1802			ARG		

E4749	ALA	PRO	ALA	LEU	ARG
A4752	GLY	GLU	VAL	LEU	ARG
A4767	ASP	LYS	ALA	ASP	ARG
A4770	LEU	ALA	GLY	MET	LEU
D4786	ALA	ASP	GLY	PRO	THR
A4791	GLY	GLU	PRO	ASP	ALA
A4802	GLY	GLY	GLY	GLY	ALA
F4807	GLY	GLY	GLY	GLY	THR
F4808	SER	GLY	GLY	GLY	LEU
F4809	GLY	GLY	GLY	GLY	LEU
H4812	GLY	GLY	GLY	GLY	LEU
D4815	SER	PRO	ASP	PRO	TRP
I4816	ALA	PRO	MET	ALA	VAL
T4840	GLY	GLU	GLY	GLY	VAL
L4844	GLY	GLY	GLY	GLY	ALA
Y4863	GLY	GLY	GLY	GLY	ALA
Y4888	GLY	GLY	GLY	GLY	ARG
I4901	GLY	GLY	GLY	GLY	GLY
I4925	GLY	GLY	GLY	GLY	GLY
L4928	GLY	GLY	GLY	GLY	ALA
L4929	GLY	GLY	GLY	GLY	LEU
I4931	GLY	GLY	GLY	GLY	LEU
R4944	GLY	GLY	GLY	GLY	TRP
K4957	GLY	GLY	GLY	GLY	GLY
C4961	GLY	GLY	GLY	GLY	SER
T4977	GLY	GLY	GLY	GLY	GLY
H4978	GLY	GLY	GLY	GLY	GLY
E4981	GLY	GLY	GLY	GLY	GLY
H4983	GLY	GLY	GLY	GLY	GLY
G5005	GLY	GLY	GLY	GLY	GLY
S5037	GLY	GLY	GLY	GLY	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	E	0.29	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	G	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
2	I	0.30	1/25428 (0.0%)	0.54	8/34534 (0.0%)
All	All	0.29	4/105048 (0.0%)	0.54	32/142628 (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	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	695	TYR	C-N	13.13	1.59	1.34
2	I	695	TYR	C-N	13.12	1.59	1.34
2	B	695	TYR	C-N	13.12	1.59	1.34
2	E	695	TYR	C-N	13.12	1.59	1.34

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	131	LEU	CA-CB-CG	8.21	134.19	115.30
2	I	131	LEU	CA-CB-CG	8.21	134.18	115.30
2	G	131	LEU	CA-CB-CG	8.21	134.17	115.30
2	E	131	LEU	CA-CB-CG	8.20	134.16	115.30
2	E	1600	LEU	CA-CB-CG	7.39	132.30	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	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	11	0
1	F	818	0	824	12	0
1	H	818	0	824	10	0
1	J	818	0	824	10	0
2	B	29369	0	24721	266	0
2	E	29369	0	24720	263	0
2	G	29369	0	24720	262	0
2	I	29369	0	24720	265	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	120756	0	102177	1083	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 1083 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:G:788:LYS:HG2	2:G:1630:CYS:H	1.52	0.74
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.53	0.72
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.53	0.72
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.53	0.72
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.68

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%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2923 (90%)	308 (10%)	4 (0%)	51	85
2	E	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	51	85
2	G	3235/4676 (69%)	2922 (90%)	309 (10%)	4 (0%)	51	85
2	I	3235/4676 (69%)	2924 (90%)	307 (10%)	4 (0%)	51	85
All	All	13360/19136 (70%)	12064 (90%)	1280 (10%)	16 (0%)	54	85

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG

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Mol	Chain	Res	Type
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1840	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	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
2	E	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
2	G	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
2	I	2493/3202 (78%)	2477 (99%)	16 (1%)	86	92
All	All	10324/13164 (78%)	10260 (99%)	64 (1%)	86	92

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

Mol	Chain	Res	Type
2	G	3787	LYS
2	G	4034	ASN
2	E	1964	ARG
2	E	1676	LEU
2	G	4085	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	3950	ASN

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Mol	Chain	Res	Type
2	G	877	ASN
2	I	4034	ASN
2	G	113	HIS
2	G	2005	GLN

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 monosaccharides 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	B	12
2	G	12
2	E	12
2	I	12

The worst 5 of 48 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3613:UNK	C	3639:THR	N	43.37
1	G	3613:UNK	C	3639:THR	N	43.37
1	E	3613:UNK	C	3639:THR	N	43.34
1	I	3613:UNK	C	3639:THR	N	43.32
1	B	3163:UNK	C	3170:UNK	N	16.45

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8374. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.