



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 30, 2017 – 09:17 PM EST

PDB ID : 5GOA
EMDB ID: : EMD-9529
Title : Cryo-EM structure of RyR2 in open state
Authors : Peng, W.; Wu, J.P.; Yan, N.
Deposited on : 2016-07-26
Resolution : 4.20 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
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

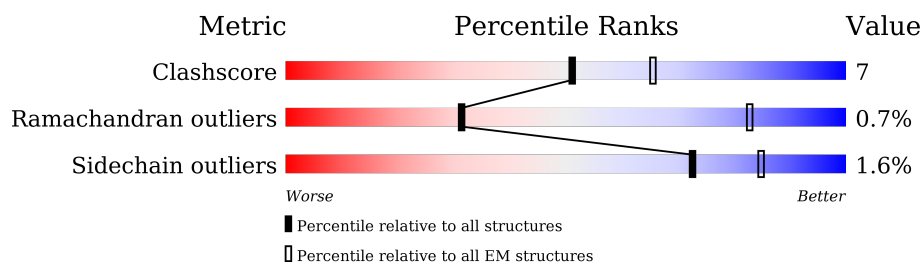
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	4968	<div> <div>54%</div> <div>14%</div> <div>•</div> <div>31%</div> </div>
1	B	4968	<div> <div>54%</div> <div>14%</div> <div>•</div> <div>31%</div> </div>
1	C	4968	<div> <div>54%</div> <div>14%</div> <div>•</div> <div>31%</div> </div>
1	D	4968	<div> <div>53%</div> <div>14%</div> <div>•</div> <div>31%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105072 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26267	16741	4498	4874	154		

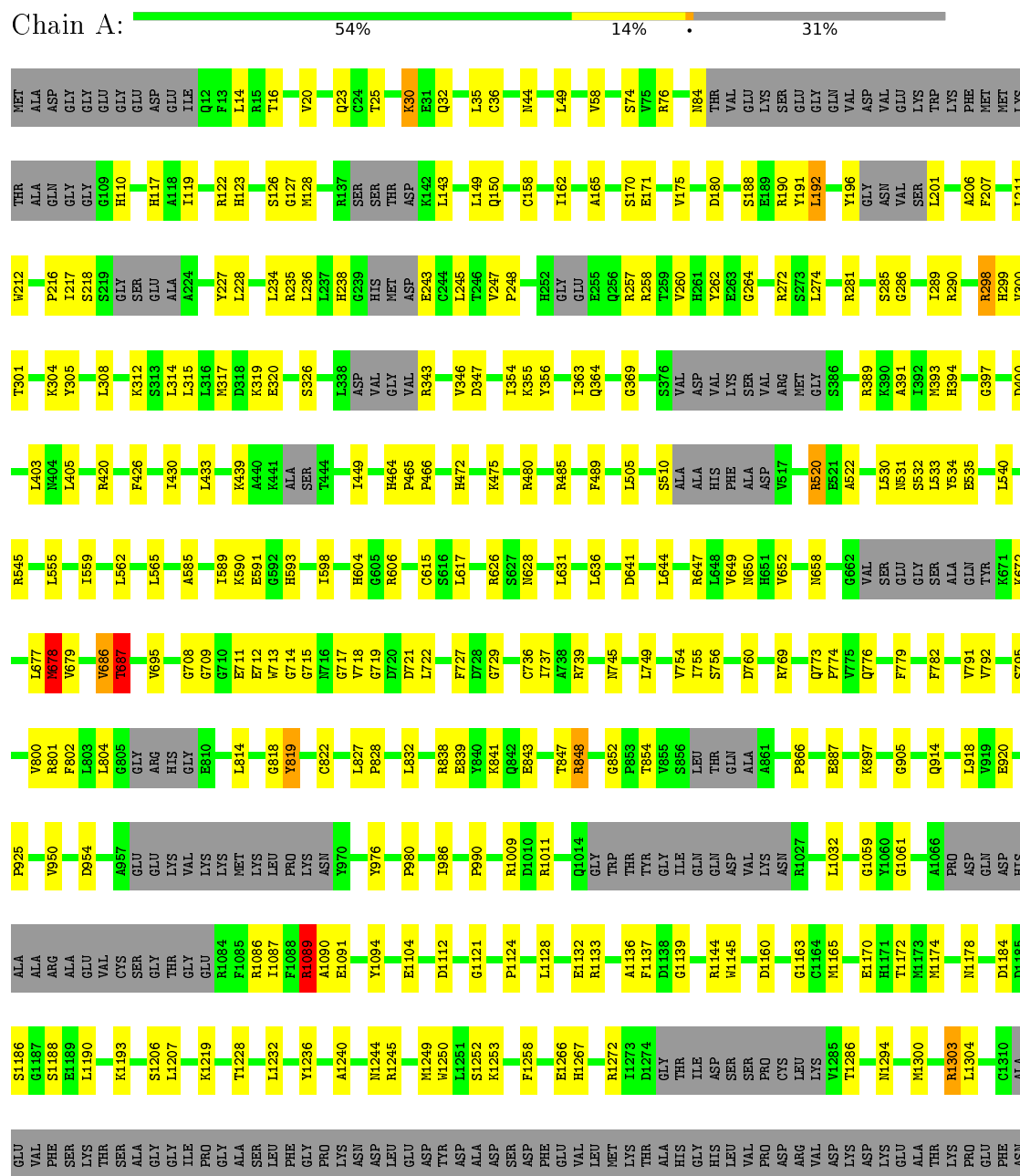
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	C	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 errors 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: RyR2

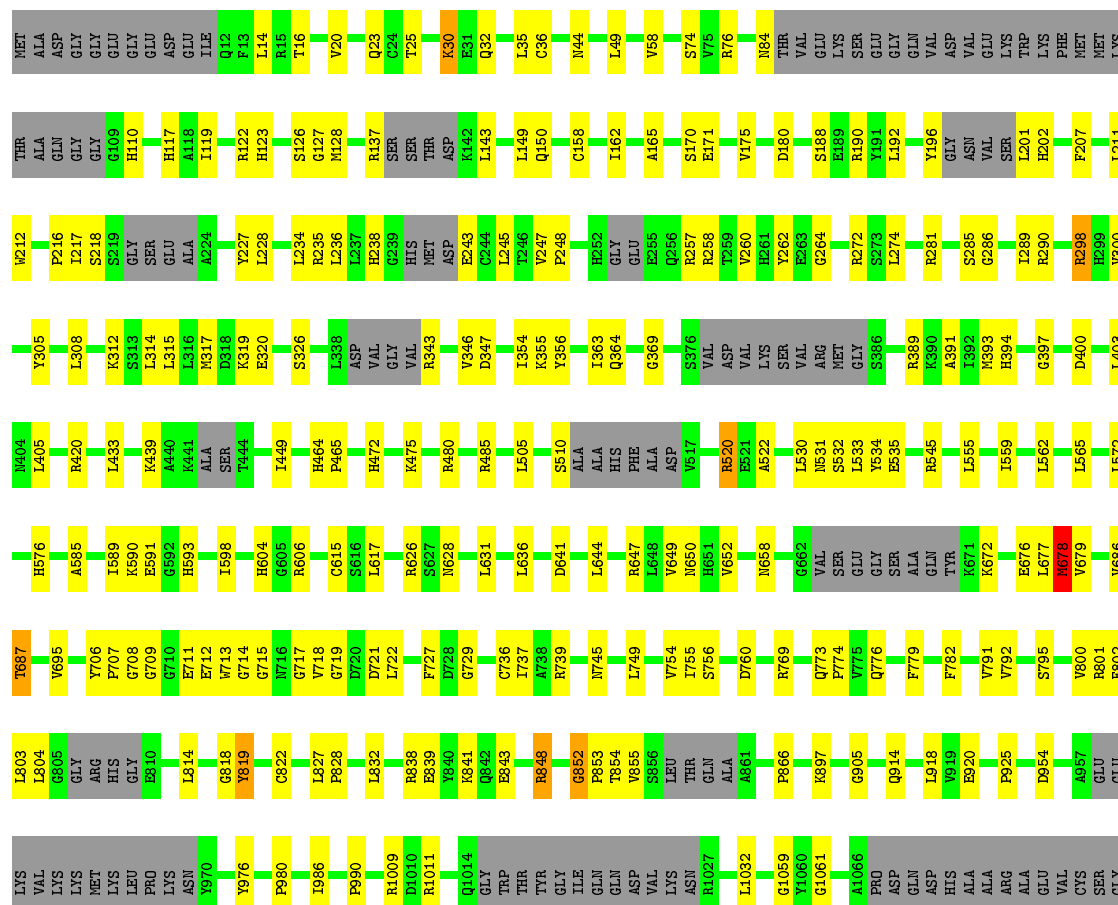





[illegible]



Category	Percentage
Very good	54%
Good	14%
Not good	31%
Very bad	1%



D2568	S2576	I2576	C2576	GLY	F2461	P2463	R2582	P2583	Q2587	M2469	R2475	P2476	Y2477	GLY	I2489	GLU	VAL	G2492	P2495	TRP	L2503	ASN	GLY	PHE	ALA	GLY	L2511	R2519	L2520	L2521	L2528	TRP	P2678	P2679	ASP	N178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A1090	E1091	Y1094	E1104	M1113	G1121	P1124	L1128	E1132	R1133	A1136	F1137	R1272	I1273	D1274	GLY	THR	I1E	ASP	D1160	G1163	C1164	M1165	E1170	H1171	T1172	M1173	M1174	N1178	D1184	D1185	S1186	S1187	S1188	L1189	E1189	K1193	P1202	THR	GLU	S1206	L1207	P1084	F1085	R1086	I1087	F1088	R1089	A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WORLDWIDE PDB
 PROTEIN DATA BANK

EMDataBank
 Unified Data Resource for 3DEM

L4866	Y4780	S4668	SER	LEU	LEU	VAL	ALA
F4871	G4672	G4672	GLU	ARG	ASP	GLY	PHE
R4875	Y4782	MET	ASN	GLN	ASP	ARG	THR
K4888	T4783	ASP	ALA	HIS	LEU	GLY	SER
	V4784	LYS	PHE	THR	SER	ASP	TTR
	F4789	ALA	GLY	HIS	SER	GLU	TRP
I4891	F4790	ALA	SER	ARG	PRO	GLY	SER
C4892	R4791	LEU	SER	TTR	ALA	GLU	VAL
	Y4794	ASP	ASP	GLY	PRO	ARG	PHE
	Y4795	PHE	SER	GLU	ILE	LYS	MET
Y4898	G4796	SER	SER	PRO	PRO	VAL	THR
H4904	S4797	ALA	PRO	VAL	VAL	GLU	LEU
	G4800	ARG	ARG	PRO	GLN	GLY	HIS
E4807		GLY	ILE	GLU	THR	THR	PHE
T4808	D4804	LYS	ALA	SER	LYS	LEU	ALA
H4809	M4805	PRO	PHE	ALA	PHE	PRO	ALA
K4806	K4806	LYS	THR	GLN	GLN	SER	SER
C4807	C4807	LYS	LYS	GLN	ASP	GLU	VAL
	M4810	ASP	H4880	LYS	LYS	LEU	ARG
	M4810	SER	Y4891	ILE	ALA	THR	GLY
H4817	H4817	SER	Y4891	ILE	LYS	ASP	PHE
M4818	M4818	LEU	K4895	THR	GLU	LEU	SER
	S4696	G4696	R4603	L4493	LYS	LYS	ARG
G4821	D4703	D4703	R4603	F4496	LYS	LEU	ILE
V4822	V4822	V4822	A4608	L4497	GLU	THR	GLY
R4823	R4823	Y4709	K4608	R4498	GLU	GLU	GLY
D4830	A4824	K4610	R4609	M4499	LYS	LEU	LEU
E4831	E4825	L4721	L4611	M4502	GLU	ASP	LEU
G4826	G4826	E4612	E4612	Y4508	ASN	LEU	GLY
G4827	G4827	Y4726	G4615	L4508	LYS	LEU	GLY
I4828	I4828	M4727	G4615	A4511	SER	SER	SER
I4832	I4832	L4732	L4616	A4511	GLU	ASP	LEU
P4835	P4835	F4733	Y4617	T4514	PRO	ILE	VAL
		H4734	E4620	M4515	GLU	PHE	GLU
		Y4735	E4620	M4515	LYS	GLY	GLY
E4839	E4839	F4739	T4627	L4518	ALA	LEU	ALA
Y4840	Y4840	F4740	K4628	L4519	GLU	ASP	LYS
E4841	E4841	F4740	G4629	L4519	GLY	LEU	LYS
		R4844	Q4630	S4524	ASP	ARG	LYS
		Y4747	Q4630	T4631	GLU	GLU	VAL
I4849	I4849	K4782	S4640	SER	GLY	GLY	ALA
T4850	T4850	T4783	F4641	SER	LYS	GLY	GLU
F4851	F4851	L4754	P4642	VAL	GLU	GLN	LEU
F4852	F4852	R4755	N4643	VAL	GLY	TTR	LEU
F4853	F4853	T4756	GLY	GLY	LYS	LYS	ALA
F4854	F4854	T4757	M4646	LYS	ALA	LEU	ASN
V4855	V4855	L4758	D4647	LYS	ILE	ILE	MET
			K4648	GLU	PRO	PRO	PRO
			F4649	ASP	HIS	ASP	ASP
		Q4767	V4650	LEU	LYS	ASN	PRO
A4861	A4861			THR	GLY	PRO	THR
I4862	I4862			ARG	LYS	ASN	GLN
I4863	I4863	L4770	D4665	SER	GLN	ALA	GLY
C4865	C4865	L4774	SER	SER	LYS	THR	GLY

- Molecule 1: RyR2

Chain C: 54% 14% 31%

[illegible]

[illegible]

I4153	I4014	I3899	F3790	R3674	PRO	LEU	TYR	VAL	HIS	ASN	VAL	P3104	LYS	G2907	I02723	Q2587
R4158	I4015	Q3904	F3791	L3677	ARG	ASP	SER	GLU	LEU	ILE	ASP	F3118	VAL	PHE	D2736	R2591
F4017	R3905	R3905	R3905	L3677	GLN	PRO	GLN	VAL	LYS	LYS	ALA	GLY	LEU	LYS	K2737	P2598
F4018	N3906	N3906	L3794	L3688	LYS	ILE	SER	PHE	VAL	ILE	SER	ASP	LEU	LEU	L2738	
F4019	F3907	F3907	L3797	F3689	ALA	TRP	LEU	TYR	TRP	ASN	GLY	LEU	ILE	LEU	V2742	
F4020	A3910	A3910	S3800	F3690	VAL	TRP	ILE	SER	GLY	ASN	ILE	ASP	ASP	LEU		
F4021	I3911	I3911	C3801	M3696	TRP	GLN	ILE	VAL	ASP	ASN	ARG	ASP	GLN	LEU	E2770	R2601
F4022	C3801	C3801	HIS	M3696	LYS	VAL	ALA	SER	LYS	GLY	THR	THR	PHE	THR	R2773	HIS
S4030	S3802	S3802	L3804	S3699	LEU	LEU	LEU	ALA	HIS	ILE	GLN	LYS	LYS	SER	I2776	K2605
F4031	D3805	D3805	C3700	C3700	TYR	TYR	ARG	PHE	ASN	ALA	ASP	ILE	ASN	ILE		K2606
F4032	HIS	HIS			LYS	LYS	ARG	GLU	GLU	GLU	PRO	MET	PRO	GLU	P2607	
S4045	ASP	ASP	ASP	ASP	LYS	ASP	LEU	LYS	LEU	GLY	HIS	VAL	ARG	ARG	P2625	
R4046	R3811	R3811	R3812	R3812	GLU	LEU	PRO	GLU	ILE	TRP	VAL	VAL	LEU	PHE	G2796	G2626
F4052	Q3813	Q3813	N3813	N3813	ASP	ASP	ASN	GLU	GLU	LEU	MET	GLU	MET	ALA	G2797	G2627
F4053	K3814	K3814	ALA	ASP	ARG	ARG	GLY	GLN	ASP	LYS	VAL	PHE	THR	ALA	TRP	GLY
F4056	GLU	GLU	GLU	GLY	VAL	PHE	LEU	ASN	GLU	ARG	VAL	PRO	ASN	ALA	ASN	GLY
T4060	I3925	I3925	GLY	GLU	VAL	GLU	ILE	VAL	PHE	LEU	VAL	VAL	LEU	PHE	ALA	THR
F4063	Q3926	Q3926	LEU	GLU	ALA	VAL	THR	VAL	THR	ALA	PRO	ASP	THR	GLN	TYR	PHE
F4067	N3932	N3932	GLY	GLU	CYS	GLN	LEU	GLN	LEU	PHE	LEU	ILE	ASN	GLN	ASN	ALA
F4071	Q3933	Q3933	MET	VAL	PHE	ASP	PRO	ASN	ALA	SER	CYS	ILE	F3009	LEU	ARG	A2634
F4072	VAL	VAL	VAL	LYS	ARG	PRO	GLY	GLU	ARG	GLN	SER	THR	THR	ILE	THR	
F4073	L3726	L3726	THR	L3714	MET	GLU	ASP	ILE	ASP	PRO	THR	ASN	T3028	ARG	ARG	L2653
D4074	GLU	GLU	GLU	R3732	ALA	LYS	GLN	ASN	LEU	ILE	MET	THR	SER	THR	ARG	SER
T4078	LYS	LYS	VAL	H3733	ILE	ASP	LEU	ILE	LEU	PRO	GLN	ALA	ILE	VAL	ILE	GLN
F4085	LEU	LEU	GLN	D3734	ALA	ILE	ASN	ASP	ASP	ILE	GLU	ALA	CYS	ALA	THR	LYS
F4086	D3833	D3833	ASN	G3735	ASN	THR	ARG	LYS	PHE	ARG	LEU	LEU	ALA	LEU	SER	P2668
R4087	G3736	G3736	VAL	G3737	PHE	VAL	SER	LYS	VAL	VAL	ASN	ASN	LEU	GLU	ASP	P2678
PHE	A3737	A3737	LEU	A3737	LEU	SER	LEU	LYS	ASP	ASP	PRO	THR	ARG	ASP	THR	P2679
HIS	M3740	M3740	HIS	M3741	LYS	LYS	LYS	MET	TYR	ASN	GLY	ASN	GLY	GLY	GLY	MET
F4090	G3850	G3850	LEU	L3742	THR	THR	THR	LYS	ARG	PRO	ALA	VAL	T3082	SER	TYR	ASN
L4102	D3854	D3854	GLU	L3742	GLU	GLU	GLU	ALA	ALA	LEU	GLU	GLU	HIS	ARG	VAL	TYR
T4114	L3975	L3975	LYS	S3748	VAL	VAL	GLU	ALA	LYS	MET	GLU	ASP	THR	SER	VAL	VAL
R4115	F3858	F3858	PRO	E3751	PRO	SER	LYS	VAL	TRP	GLU	CYS	VAL	ARG	LYS	SER	SER
L4116	T3875	T3875	THR	E3751	ARG	VAL	LEU	SER	LYS	LYS	CYS	GLY	ASN	GLY	MET	MET
Q4117	M3755	M3755	GLU	M3755	ASP	THR	ASP	ASP	LYS	LYS	ALA	PRO	GLN	GLU	MET	MET
L4122	F3878	F3878	GLU	M3755	GLU	GLU	ILE	GLU	PRO	LYS	ALA	ILE	LYS	PHE	LYS	GLN
F4130	E3888	E3888	ASP	L3767	ASP	ARG	ILE	ARG	ASN	LYS	ASN	PRO	GLY	PRO	THR	GLN
F4139	G3989	G3989	GLU	R3768	GLU	ARG	ARG	LYS	TRP	ALA	CYS	VAL	VAL	SER	THR	SER
L4134	N3990	N3990	GLY	G3769	GLY	GLY	SER	LYS	GLU	ALA	THR	GLU	THR	GLU	GLU	GLU
F4138	V3991	V3991	THR	G3770	THR	THR	ASN	MET	ALA	MET	HIS	LEU	GLN	MET	MET	MET
F4139	F3891	F3891	LYS	G3770	LYS	ILE	ILE	LYS	GLU	VAL	LYS	LYS	ILE	GLU	GLU	ASP
F4150	D4002	D4002	GLY	L3779	GLY	SER	THR	ARG	ASP	VAL	ASN	THR	ILE	ILE	ILE	SER
F4150	F4003	F4003	LEU	E3780	LEU	LEU	LEU	LYS	LEU	SER	THR	MET	ASN	LYS	GLU	GLY
F4150	L4004	L4004	VAL	L3781	VAL	GLN	GLN	GLY	PHE	THR	LEU	GLU	THR	PHE	PHE	GLY
F4150	K3896	K3896	GLU	L3782	ASP	ASP	ARG	ASP	MET	ASP	GLY	GLU	THR	PHE	PHE	ALA
F4150	K3783	K3783	LYS	K3783	ARG	ARG	MET	ASP	GLY	GLY	ILE	ILE	THR	ALA	ALA	

T4908	D4804	ARG	GLU	ILE	ARG	ILE	GLU	ILE	GLU	PRO	VAL	LYS	MET	ARG
H4909	K4805	GLU	GLU	ILE	GLU	ILE	GLU	GLU	GLU	THR	VAL	LEU	THR	MET
T4910	C4807	LYS	LYS	ALA	LYS	ALA	VAL	VAL	GLN	GLY	GLY	THR	PHE	PHE
H4914	M4810	PRO	PRO	H4859	PRO	H4859	GLU	GLU	GLU	THR	THR	THR	PHE	SER
M4915		LYS	LYS		LYS		SER	SER	LYS	LEU	PRO	ALA	ALA	LEU
T4916	H4817	LYS	LYS	H4880	LYS	H4880	ALA	PHE	GLN	PHE	PRO	ALA	ALA	LEU
M4918	M4818	ASP	ASP		ASP		ALA	PHE	GLN	GLN	GLU	GLU	VAL	THR
Y4919		SER	SER	Y4591	SER	Y4591	THR	THR	LYS	GLY	GLU	ASP	VAL	ARG
	G4821	SER	SER		SER		LYS	LYS	GLN	GLN	ASP	LEU	SER	ARG
Y4925	F4822	LEU	LEU	K4595	LEU	K4595	LYS	LYS	GLN	GLN	LEU	THR	ARG	SER
	R4823	S4696	S4696		ILE		ILE	I4486	LYS	LYS	THR	ALA	GLY	ALA
K4929	R4823			R4603		R4603	I4486	I4486	GLU	GLU	ASP	ASP	PHE	LEU
D4930	A4824			W4709		W4709	R4498	R4498	LYS	LYS	LEU	LEU	SER	LEU
E4931	G4825						M4499	M4499	GLU	GLU	LYS	ARG	ALA	ALA
G4937	G4826			L4721		L4721	R4609	R4609	GLU	GLU	ASP	GLY	ILE	ARG
E4938	G4827						K4610	K4610	LYS	LYS	LEU	ILE	ILE	ARG
Y4940	I4828			Y4726		Y4726	L4611	L4611	THR	THR	THR	GLY	GLY	TYR
Y4941				M4727		M4727	M4502	M4502	GLU	GLU	GLU	GLY	GLY	ASN
M4942							L4508	L4508	LYS	LYS	GLU	LEU	LEU	VAL
	P4835			L4732		L4732	G4615	G4615	GLU	GLU	SER	LEU	LEU	LEU
E4939				G4733		G4733	L4616	L4616	GLU	GLU	ASP	LEU	GLY	LEU
Y4940	E4839			H4734		H4734	Y4617	Y4617	ASN	ASN	ASP	LEU	GLY	LEU
Y4941	Y4840			Y4735		Y4735			LYS	LYS	LEU	LEU	GLY	LEU
M4945	E4841						E4620	E4620	SER	SER	ILE	LEU	VAL	MET
				F4739		F4739	L4518	L4518	GLU	GLU	ILE	LEU	VAL	MET
R4948				F4740		F4740	L4519	L4519	THR	THR	PHE	GLY	GLY	LEU
M4950	I4849						S4524	S4524	ALA	ALA	LEU	GLY	GLY	LEU
E4951	T4850			I4747		I4747	Q4629	Q4629	GLU	GLU	ASP	LYS	LYS	LYS
F4952	F4851			T4753		T4753	W4631	W4631	THR	THR	ARG	LYS	LYS	LYS
	F4852			L4754		L4754			SER	SER	VAL	LYS	LYS	LYS
F4853	F4853						S4640	S4640	SER	SER	ARG	LYS	LYS	LYS
F4854	F4854			I4757		I4757	F4641	F4641	VAL	VAL	GLY	GLY	VAL	MET
V4855	V4855			L4758		L4758	P4642	P4642	VAL	VAL	GLY	GLY	VAL	MET
							M4643	M4643	GLU	GLU	GLY	GLY	ASN	LYS
									THR	THR	THR	ILE	ASN	LYS
	A4861			Q4767		Q4767	W4646	W4646	LYS	LYS	TYR	LEU	ASN	LYS
	I4862						D4647	D4647	GLU	GLU	GLN	LEU	ASN	LYS
	I4863			L4770		L4770	K4648	K4648	LEU	LEU	LYS	ALA	ALA	LYS
G4865	G4865			L4774		L4774	F4649	F4649	PRO	PRO	LYS	LEU	ASN	LYS
L4866	L4866						Y4650	Y4650	THR	THR	ILE	ILE	MET	THR
									ARG	ARG	PRO	PRO	VAL	VAL
	F4871			Y4780		Y4780	D4665	D4665	SER	SER	HIS	HIS	ASP	ARG
	R4875			Y4782		Y4782	SER	SER	SER	SER	ASN	ASN	THR	THR
				T4783		T4783	S4668	S4668	SER	SER	GLY	GLY	GLN	ASP
				Y4784		Y4784			GLU	GLU	LYS	LYS	ASP	MET
	K4888						G4672	G4672	ASN	ASN	GLN	ALA	VAL	VAL
							MET	MET	ALA	ALA	GLY	GLY	GLU	THR
	I4891			F4789		F4789	ASP	ASP	ASN	ASN	LEU	LEU	VAL	ALA
	C4892			R4791		R4791	LYS	LYS	PHE	PHE	ARG	ARG	GLY	PHE
							ALA	ALA	GLY	GLY	GLN	ASP	GLY	PHE
	G4895			Y4794		Y4794	ALA	ALA	SER	SER	LEU	LEU	ASP	THR
				R4795		R4795	LEU	LEU	LEU	LEU	MET	MET	GLY	THR
	Y4898			K4796		K4796	ASP	ASP	ASP	THR	THR	THR	ASP	TYR
				S4797		S4797	SER	SER	SER	HIS	SER	SER	GLY	TRP
	H4904						SER	SER	SER	ARG	PRO	PRO	GLY	SER
				G4800		G4800	ASP	ASP	SER	TYR	ALA	ALA	GLU	VAL
	E4907						ILE	ILE	PRO	PRO	THR	THR	ARG	PHE

- Molecule 1: RyR2

Chain D:  53% 14% 31%

V686	H576	L433	I314	I217	ALA	MET
V687	A585	K439	L316	S218	GLN	ALA
V695	I589	A440	M317	GLY	GLY	ASP
G708	E590	K441	D818	GLY	G109	GLY
G709	E591	ALA	K319	GLU	H110	GLU
E711	E592	SER	E320	ALA	I119	GLU
E712	H593	I449	L338	Y227	R122	ASP
E713	I598	P465	VAL	L228	H123	GLU
G715	H604	P466	GLY	L234	S126	ILE
G716	G605	H472	R343	L236	G127	F13
G717	R606	E473	V446	L237	L236	L14
G718	D474	D475	D847	H238	M128	L15
G719	C615	K475	V356	G239	R137	T16
D720	S616	Q476	I364	HIS	SER	V20
D721	L617	M477	K355	NET	SER	Q23
D722	N628	N478	Y356	ASP	TTR	C24
F727	R626	R480	I363	E243	K142	T25
D728	S627	R485	Q364	C244	L143	K30
G729	N632	L488	G369	L245	L149	E31
C736	L631	L505	S376	P248	Q150	Q32
A738	L636	S510	VAL	H252	G158	K34
R739	D641	ALA	ASP	GLY	I162	L35
N745	L644	ALA	VAL	E255	A165	C36
L749	Q645	HIS	LVS	Q256	A165	M44
V754	T646	PHE	SER	R257	S170	L49
V755	B647	ALA	VAL	R258	E171	L49
I755	L648	ASP	ARG	T259	V175	V58
S756	V649	V517	GLY	V260	V175	R76
D760	N650	R520	S386	H261	D180	R76
V762	H651	E521	R389	E263	D180	N84
R769	V652	A522	K390	G264	S188	TTR
Q773	N658	L530	A391	L274	E189	VAL
Q776	G662	N531	L392	R281	R190	GLU
F776	SER	S532	M393	R281	Y191	LVS
F779	GLU	L533	H394	S285	L192	SER
F779	GLY	V534	G397	G286	Y196	GLU
F782	SER	E535	D400	I289	GLY	GLN
V791	ALA	R545	L403	R290	ASN	VAL
V792	TYR	L555	N404	R298	VAL	ASP
S795	G671	L559	L405	H299	L201	GLU
S795	K672	L562	R420	V300	A206	LVS
V800	E676	L562	F426	T301	F207	TTP
F802	L677	L565	F426	Y305	L211	LVS
L803	V673	L565	F426	Y305	W212	PHE
R804	V679	L572	I430	K312	N211	MET
				E212	E212	MET
				E212	E212	LVS
				E212	E212	TTR

ARG	E2253	ARG	E1516	GLU	HIS	VAL	E1189	GLU	D954	GLY	8805
ASP	L2254	GLY	A1522	PRO	LYS	PHE	L1190	VAL		ARG	
PRO	A2255	LEU	N1523	ALA	THR	ASP	K1193	CYS	A957	HIS	
SER	L2256	LEU	N1523		LYS	THR	K1193	GLY	GLU	GLY	
PRO	E2139	SER	P1541	V1441	ALA	GLN	P1203	THR	LVS	LEU	
THR	E2264	LEU	P1541	V1442	GLN	GLU	P1203	GLY	VAL	VAL	
SER	R2268	GLY	F1544	V1444	LYS	GLY	S1206	GLU	LVS	LVS	
SER	L2275	GLY	A1545	W1444	PRO	GLY	L1207	R1084	LVS	LVS	
LVS	L2275	SER	Q1554	W1444	ARG	ILE	G1208	F1085	LYS	LYS	
CYS	L2275	GLY	F1555	D1449	PRO	PRO	V1209	R1086	LYS	LYS	
PRO	R2275	GLY	F1555	D1449	GLY	GLY	K1219	I1087	PRO	PRO	
ASP	E2173	ASP	F1556	F1457	LYS	SER	K1219	F1088	LYS	LYS	
ASP	E2174	ASP	GLY	D1458	GLN	GLN	Y1236	F1089	ASN	ASN	
GLY	V2175	SER	ARG	L1459	ARG	PHE	A1240	A1090	Y970	Y970	
VAL	V2175	ASP	ILE	ASP	LEU	GLY	A1240	E1091			
VAL	E2481	LEU	LYS	VAL	LEU	LEU	Y1094	Y1094	Y976	Y976	
SER	GLY	GLY	ASN	ARG	ARG	LYS	M1244	E1104			
LYS	LVS	SER	VAL	THR	THR	ASN	R1245	E1104	P980	P980	
GLY	LVS	GLY	MET	V1465	THR	ASP	M1249				
GLY	GLY	GLY	PRO	L1465	LYS	ASP	M1249	D1112	1986	1986	
THR	GLY	GLY	LEU	L1469	PRO	GLY	W1250	M1113			
ASP	GLY	GLY	SER	G1470	ASP	ASP	L1251		P990	P990	
GLY	ILE	GLY	A1568	K1475	THR	THR	S1252	G1121			
ALA	ALA	ALA	G1569	V1476	ASP	ASP	K1253		R1009	R1009	
TRP	ASN	ASN	L1570	V1476	ALA	ALA		P1124	D1010	D1010	
ASN	P2293	ASN	H1575	I1480	SER	SER	F1258	L1128	R1011	R1011	
GLY	D2301	GLY	V1579	N1484	HIS	SER	E1266	E1132	Q1014	Q1014	
ASP	R2304	ASP	P1580	CYS	ALA	ALA	H1267	R1133	GLY	GLY	
LEU	L2326	SER	V1581	M1487	ARG	GLY	R1272	A1136	THR	THR	
GLY	P2329	SER	P1584	M1487	LEU	LEU	I1273	A1136	THR	THR	
GLY	E2330	GLY	R1585	M1488	GLY	GLY	I1274	F1137	GLY	GLY	
ILE	CYS	ILE	L1586	G1489	ASP	ASP	GLY	R1144	ILE	ILE	
HIS	GLY	HIS	H1587	GLY	VAL	THR	THR	W1145	GLN	GLN	
ALA	ALA	ALA	V1588	GLY	ALA	ALA	ILE	W1156	GLN	GLN	
ALA	ALA	ALA	Q1589	SER	ASP	HIS	SER		VAL	VAL	
ALA	ALA	ALA	F1590	MET	ASP	ASP	PRO	W1166	LYS	LYS	
ALA	ALA	ALA	H1593	PRO	ARG	HIS	THR	D1160	ASN	ASN	
ALA	ALA	ALA		GLY	ASP	ASP	CYS	D1160	ASN	ASN	
ALA	ALA	ALA	R1598	GLN	ASP	VAL	LEU	G1163	R1027	R1027	
ALA	ALA	ALA	M1599	GLY	THR	THR	LYS	C1164	L1032	L1032	
ALA	ALA	ALA	P1600	ARG	ASP	ARG	V1286	M1165			
ALA	ALA	ALA	M1601	ARG	VAL	VAL	T1286	G1059	G1059	G1059	
ALA	ALA	ALA	Q1602	M1501	LEU	LEU	LYS	E1170	Y1060	Y1060	
ALA	ALA	ALA		L1505	GLN	GLN	M1294	E1171	G1061	G1061	
ALA	ALA	ALA	K1605	E1506	THR	THR	M1300	T1172	I1066	I1066	
ALA	ALA	ALA	V1606	D1607	SER	SER	M1173	M1173	PRO	PRO	
ALA	ALA	ALA	D1607	G1508	T1425	T1425	M1174		ASP	ASP	
ALA	ALA	ALA	V1608	G1509	THR	THR	M1178		GLN	GLN	
ALA	ALA	ALA	S1609	V1510	LYS	LYS	M1178		ASP	ASP	
ALA	ALA	ALA	R1610	V1511	PRO	PRO	M1178		ASP	ASP	
ALA	ALA	ALA	I1611	ASP	GLY	GLY	D1184		HIS	HIS	
ALA	ALA	ALA	S1612	P1434	GLY	GLY	D1185		ALA	ALA	
ALA	ALA	ALA	E1613	ALA	GLY	GLY	S1186		ALA	ALA	
ALA	ALA	ALA	R1614	SER	GLN	GLN	S1188		ALA	ALA	
ASP	E2253	ARG	E2253	ASP	GLN	GLN	E2253	ASP	GLN	GLN	
GLY	L2254	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
PRO	A2255	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	L2256	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
PRO	E2139	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	E2264	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	R2268	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	L2275	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LVS	L2275	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
PRO	R2275	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2173	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E2174	ASP	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	V2175	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
VAL	E2481	LEU	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
SER	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
LYS	LVS	SER	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
GLY	LVS	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
THR	GLY	GLY	E2253	LEU	LEU	LEU	L2254	LEU	LEU	LEU	
ASP	E										

L3959	D3833	G3736	L3645	LEU	LEU	LYS	ASP	HIS	PRO	THR	ALA	F3061	ASP	VAL	P2668	L2528	I2439
Q3965	F3841	A3737	L3645	PHE	PHE	MET	TYR	LEU	GLY	THR	THR	F3061	GLY	SER	P2678	L2529	Q2442
L3968	G3950	M3740	P3648	HIS	HIS	SER	ARG	PRO	ALA	VAL	GLY	T3082	SER	ASP	P2679	THR	MET
E3971	D3854	V3741	ALA	GLN	GLN	ALA	ALA	LEU	MET	GLU	ASP	T3082	ARG	TYR	ALA	CYS	PRO
L3975	Y3858	L3742	VAL	LYS	LYS	VAL	TRP	GLY	GLY	CYS	VAL	T3082	SER	MET	P2534	ALA	ILE
M3982	T3875	S3748	PRO	SER	SER	ASP	LEU	LYS	THR	CYS	CYS	E2843	GLY	GLU	GLU	LYS	ALA
L3983	Y3878	E3751	GLU	THR	THR	ARG	LYS	LEU	LEU	THR	THR	K2857	HIS	ASN	TYR	ARG	ASP
E3988	L3879	P3754	ASP	ARG	ARG	ARG	ASN	LYS	ASN	ASN	PRO	L2861	PHE	VAL	VAL	LEU	ASN
G3989	Y3882	M3767	GLY	ARG	ARG	LYS	GLY	ALA	GLY	SER	SER	E2869	PRO	SER	SER	VAL	VAL
M3990	Y3882	K3768	THR	TYR	TYR	MET	ALA	MET	HIS	GLU	LEU	R2887	GLN	MET	MET	GLU	GLU
V3991	G3770	G3769	R3661	SER	SER	LYS	ASP	VAL	VAL	LEU	LEU	L2897	ILE	LYS	A2565	PRO	ASP
D4002	Y3892	G3770	L3665	LEU	LEU	GLY	PHE	GLY	GLY	LEU	GLY	G2901	PHE	GLN	D2568	MET	SER
M4003	Y3892	L3779	L3665	GLY	GLY	ASP	ARG	GLY	GLY	LEU	GLY	G2901	PHE	SER	S2576	SER	ALA
L4004	F3893	E3780	L3670	HIS	HIS	ARG	ARG	MET	ASP	GLY	ILE	V2904	ALA	MET	ILE	ILE	GLY
V4011	K3896	Y3781	R3674	PRO	PRO	TYR	VAL	VAL	HIS	ASN	VAL	G2907	VAL	ASP	CYS	F2461	F2461
I4014	L3899	L3782	R3674	GLN	GLN	SER	ALA	ALA	LEU	ASP	ASP	G2907	VAL	SER	GLY	C2462	C2462
L4015	Q3904	K3783	L3677	ARG	ARG	MET	VAL	VAL	LYS	LEU	LEU	F3118	VAL	GLY	GLY	D2463	D2463
R4016	R3905	F3791	L3688	LYS	LYS	THR	PHE	PHE	GLY	ILE	GLY	F3118	PRO	ASP	GLY	D2464	D2464
F4017	N3906	L3794	Y3689	ALA	ALA	SER	ILE	ILE	VAL	GLY	LEU	P3104	LEU	MET	GLY	H2465	H2465
F4018	F3907	L3797	M3690	VAL	VAL	TRP	TRP	TRP	ARG	TYR	LEU	P3104	ASP	SER	GLN	R2469	R2469
D4019	L3899	L3797	L3677	TRP	TRP	GLN	VAL	VAL	ASP	ASP	ASP	L3124	GLN	THR	Q2587	R2475	R2475
M4020	A3910	L3797	S3699	HIS	HIS	MET	ALA	ALA	LYS	SER	LEU	L3124	THR	THR	R2591	Y2476	Y2476
F4021	T3911	S3800	G3700	LYS	LYS	ALA	ALA	ALA	LYS	SER	GLY	S3144	PHE	PRO	L2738	Y2477	Y2477
L4022	A3914	G3801	HIS	LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	S3144	ILE	SER	L2738	GLY	GLY
S4030	F3917	S3802	ASP	LEU	LEU	LYS	ASP	ASP	ASN	ASN	ASN	L3144	ASN	ILE	W2742	ILE	ILE
D4031	Y3918	L3804	GLU	SER	SER	LYS	LEU	LEU	PHE	GLY	GLY	V3149	GLY	GLY	E2770	GLU	GLU
T4032	N3919	D3805	ASP	GLN	GLN	LEU	ARG	ARG	GLY	ALA	ALA	V3149	ARG	THR	GLY	VAL	VAL
S4045	T3920	R3811	ASP	ARG	ARG	ILE	GLY	GLY	TRP	TRP	MET	A3166	LEU	ARG	ALA	L2489	L2489
R4046	L3921	Q3812	GLY	LYS	LYS	ILE	GLN	GLN	LYS	LYS	VAL	A3166	ALA	ALA	R2605	GLU	GLU
A4052	T3922	N3813	ALA	ALA	ALA	ASN	ASN	ASN	ARG	ARG	VAL	P2990	THR	THR	R2606	VAL	VAL
H4056	Y3923	K3814	GLU	VAL	VAL	ILE	PHE	PHE	THR	THR	VAL	V3005	SER	ASP	P2607	G2492	G2492
T4060	T3925	ALA	VAL	VAL	VAL	ILE	VAL	VAL	THR	THR	VAL	A3170	THR	GLN	P2625	P2495	P2495
E4063	Q3926	GLY	LYS	CYS	CYS	CYS	VAL	VAL	THR	THR	PHE	A3170	SER	GLN	G2626	G2626	G2626
L4067	L3936	LEU	S3714	PHE	PHE	PRO	GLN	GLN	ALA	ALA	SER	S3183	LEU	GLN	G2627	TRP	ASP
L4068	R3940	GLY	L3726	ARG	ARG	ASN	ASN	ASN	ALA	ALA	SER	S3183	GLY	ILE	G2627	ALA	ALA
A4071	L3941	GLY	L3726	GLY	GLY	GLY	GLY	GLY	GLY	GLY	PRO	T3028	ASN	THR	GLY	THR	THR
T4073	F3948	GLY	Q3729	MET	MET	GLY	ILE	ILE	ASP	ASP	THR	T3028	THR	TYR	ASN	ALA	ALA
D4074	Y3952	LYS	A3730	ALA	ALA	GLN	ASN	ASN	ILE	ILE	ILE	T3028	VAL	VAL	GLY	ALA	ALA
T4078	M3955	VAL	R3731	LEU	LEU	LEU	GLY	GLY	THR	THR	THR	L3034	ASP	ASP	ALA	SER	SER
V4085	Y3625	LEU	L3732	ASP	ASP	LYS	ILE	ILE	THR	THR	THR	L3034	THR	THR	ARG	ALA	ALA
		GLN	R3733	ILE	ILE	ASN	ASP	ARG	THR	THR	THR	K3055	ALA	GLN	L2653	R2519	R2519
			D3734	ALA	ALA	ARG	THR	THR	THR	THR	THR	K3055	SER	THR	L2653	Y2658	Y2658
			R3735	VAL	VAL	PHE	LYS	LYS	PHE	PHE	PHE	K3055	LEU	GLU	GLN	L2521	L2521
						SER	SER	SER	VAL	VAL	VAL	K3055	ARG	SER	LYS	T2523	T2523

C4949	T4950	F4951	I4747	G4629	SER	ASP	ARG	LYS	LYS	L4207	K4086
W4950	F4952	F4953	K4752	Q4630	VAL	GLY	GLU	VAL	GLN	SER	R4087
F4952	F4953	F4954	K4753	W4631	VAL	GLU	GLY	GLU	MET	GLU	PHE
F4953	F4954	F4955	L4754	S4640	GLY	GLU	GLN	GLY	LYS	SER	HIS
F4955	F4956	F4957	L4755	F4641	GLY	GLU	TYR	LEU	VAL	ASP	E4090
F4956	F4957	F4958	L4756	P4642	GLU	LYS	LYS	ALA	LYS	LEU	L4102
F4957	F4958	F4959	L4757	N4643	LEU	ALA	LEU	ASN	LYS	ASN	L4102
F4958	F4959	F4960	L4758	W4646	PRO	ILE	ILE	MET	MET	ARG	T4114
F4959	F4960	F4961	Q4767	D4647	LYS	GLU	PRO	PRO	THR	ARG	R4115
F4960	F4961	F4962	L4770	ARG	THR	GLU	HIS	ASP	VAL	ALA	R4116
F4961	F4962	F4963	L4771	SER	ARG	LYS	ASN	PRO	ASP	ASN	Q4117
F4962	F4963	F4964	L4772	SER	SER	GLY	PRO	THR	ASP	LYS	L4122
F4963	F4964	F4965	L4773	V4650	SER	LYS	ASN	GLN	MET	GLU	L4122
F4964	F4965	F4966	Y4780	D4665	GLU	GLN	ALA	ASP	VAL	GLU	F4130
F4965	F4966	F4967	L4781	Y4668	ASN	LEU	LEU	VAL	ALA	GLU	L4134
F4966	F4967	F4968	Y4782	S4668	ASN	ARG	SER	ARG	PHE	LYS	L4134
F4967	F4968	F4969	Y4783	G4672	PHE	GLN	ASP	GLY	PHE	GLU	C4135
F4968	F4969	F4970	Y4784	MET	GLY	LEU	LEU	ASP	THR	LYS	R4136
F4969	F4970	F4971	F4789	ASP	SER	HIS	MET	MET	SER	PRO	I4137
F4970	F4971	F4972	F4790	ASP	LEU	HIS	SER	SER	THR	GLU	E4138
F4971	F4972	F4973	R4791	LYS	ALA	HIS	SER	GLU	TYR	GLU	I4139
F4972	F4973	F4974	R4792	ALA	SER	TYR	PRO	GLY	SER	GLN	Y4150
F4973	F4974	F4975	Y4794	LEU	SER	GLY	PRO	ARG	PHE	PRO	Y4150
F4974	F4975	F4976	N4795	ASP	PRO	GLU	ILE	LYS	MET	ARG	I4153
F4975	F4976	F4977	K4796	PHE	ARG	GLU	PRO	VAL	THR	MET	R4158
F4976	F4977	F4978	K4797	SER	ILE	VAL	VAL	GLU	LEU	GLY	PHE
F4977	F4978	F4979	G4800	ASP	ILE	VAL	GLN	GLY	HIS	PHE	W4161
F4978	F4979	F4980	G4801	ALA	ALA	PRO	GLU	THR	PHE	SER	E4162
F4979	F4980	F4981	D4804	ARG	GLU	GLU	LYS	LEU	ALA	LEU	K4163
F4980	F4981	F4982	C4807	H4559	SER	ALA	PHE	PRO	ALA	VAL	P4164
F4981	F4982	F4983	C4808	Y4560	ALA	PHE	GLN	SER	SER	THR	K4170
F4982	F4983	F4984	M4810	LYS	TRP	TRP	GLU	VAL	VAL	ARG	R4171
F4983	F4984	F4985	M4811	PRO	LYS	LYS	GLN	ASP	SER	ARG	K4171
F4984	F4985	F4986	H4812	LYS	ILE	ILE	LYS	THR	ARG	SER	I4174
F4985	F4986	F4987	M4813	ASP	ASP	GLY	LYS	ASP	PHE	ALA	I4174
F4986	F4987	F4988	SER	SER	SER	LYS	GLU	LEU	SER	LEU	N4179
F4987	F4988	F4989	G4821	R4498	GLU	R4499	GLU	LYS	ARG	ALA	G4182
F4988	F4989	F4990	V4822	N4499	LYS	F4500	LYS	LEU	ILE	ARG	E4183
F4989	F4990	F4991	R4823	F4501	GLU	R4502	GLU	THR	GLY	THR	K4184
F4990	F4991	F4992	A4824	R4503	LEU	R4504	LYS	GLU	GLY	ASN	E4185
F4991	F4992	F4993	G4825	S4696	ASP	R4505	LYS	SER	LEU	VAL	K4186
F4992	F4993	F4994	G4826	W4709	SER	R4506	GLU	ASP	LEU	THR	M4187
F4993	F4994	F4995	G4827	L4721	LEU	L4508	GLU	ASN	GLY	THR	E4188
F4994	F4995	F4996	I4828	L4722	PRO	K4610	ASN	LEU	GLY	MET	I4189
F4995	F4996	F4997	G4829	Y4726	LYS	L4611	LYS	LEU	GLY	ARG	F4190
F4996	F4997	F4998	E4831	W4727	ASP	E4612	SER	SER	ARG	VAL	V4191
F4997	F4998	F4999	I4832	M4727	SER	G4615	GLU	LEU	MET	LEU	N4192
F4998	F4999	F5000	P4835	L4732	LEU	N4616	PRO	ILE	VAL	LEU	F4193
F4999	F5000	F5001	E4836	G4733	GLU	L4617	GLU	PHE	GLU	SER	C4194
F5000	F5001	F5002	E4837	L4734	LEU	Y4735	LYS	ALA	GLY	LEU	E4195
F5001	F5002	F5003	E4838	Y4736	ASP	E4620	ALA	LEU	ALA	LYS	D4196
F5002	F5003	F5004	F4739	F4739	THR	I4627	GLU	ASP	LYS	SER	E4200
F5003	F5004	F5005	F4740	K4628	THR	K4628	GLU	LEU	LYS	LEU	E4200

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	133196	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	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	1.09	70/26752 (0.3%)	1.00	96/36151 (0.3%)
1	B	1.09	66/26752 (0.2%)	1.00	95/36151 (0.3%)
1	C	1.08	67/26752 (0.3%)	1.00	95/36151 (0.3%)
1	D	1.09	67/26752 (0.3%)	1.00	99/36151 (0.3%)
All	All	1.08	270/107008 (0.3%)	1.00	385/144604 (0.3%)

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
1	A	0	23
1	B	0	23
1	C	0	24
1	D	0	23
All	All	0	93

The worst 5 of 270 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3700	CYS	CB-SG	13.49	2.05	1.82
1	D	3700	CYS	CB-SG	13.43	2.05	1.82
1	A	3700	CYS	CB-SG	13.37	2.04	1.82
1	C	3700	CYS	CB-SG	13.08	2.04	1.82
1	B	3878	TYR	CG-CD1	-12.72	1.22	1.39

The worst 5 of 385 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	4948	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	D	4948	ARG	NE-CZ-NH2	13.25	126.92	120.30
1	B	4948	ARG	NE-CZ-NH2	13.09	126.84	120.30
1	C	4948	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	A	1089	ARG	NE-CZ-NH2	-9.54	115.53	120.30

There are no chirality outliers.

5 of 93 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	641	ASP	Peptide
1	A	686	VAL	Peptide
1	A	791	VAL	Peptide
1	A	818	GLY	Peptide
1	A	819	TYR	Peptide

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	26267	0	24896	381	0
1	B	26267	0	24897	372	0
1	C	26267	0	24897	370	0
1	D	26267	0	24896	377	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
All	All	105072	0	99586	1447	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 7.

The worst 5 of 1447 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (\AA)	Clash overlap (\AA)
1:D:4818:MET:SD	1:D:4818:MET:CG	2.01	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4818:MET:CG	1:C:4818:MET:SD	2.01	1.48
1:C:3700:CYS:SG	1:C:3700:CYS:CB	2.04	1.45
1:D:3700:CYS:SG	1:D:3700:CYS:CB	2.05	1.43
1:B:3700:CYS:CB	1:B:3700:CYS:SG	2.05	1.43

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	3289/4968 (66%)	2988 (91%)	279 (8%)	22 (1%)	26	71
1	B	3289/4968 (66%)	2994 (91%)	273 (8%)	22 (1%)	26	71
1	C	3289/4968 (66%)	2988 (91%)	280 (8%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2986 (91%)	282 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11956 (91%)	1114 (8%)	86 (1%)	31	71

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1737	THR
1	A	1756	SER
1	A	4071	ALA
1	B	1737	THR
1	B	1756	SER

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 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	2660/4355 (61%)	2616 (98%)	44 (2%)	68	88
1	B	2657/4355 (61%)	2617 (98%)	40 (2%)	72	89
1	C	2658/4355 (61%)	2615 (98%)	43 (2%)	70	88
1	D	2660/4355 (61%)	2616 (98%)	44 (2%)	68	88
All	All	10635/17420 (61%)	10464 (98%)	171 (2%)	72	88

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4187	MET
1	C	841	LYS
1	D	3990	ASN
1	B	4515	ASN
1	C	192	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4559	HIS
1	C	544	ASN
1	D	3954	HIS
1	B	4737	ASN
1	C	84	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.