



wwPDB EM Map/Model Validation Report ⓘ

Sep 5, 2016 – 02:40 PM EDT

PDB ID : 5J8V
EMDB ID: : EMD-8073
Title : Structure of rabbit ryanodine receptor RyR1 open state activated by calcium ion
Authors : Wang, X.; Wei, R.; Yin, C.; Sun, F.
Deposited on : 2016-04-08
Resolution : 4.90 Å(reported)
Based on PDB ID : 3J8H

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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-20027939

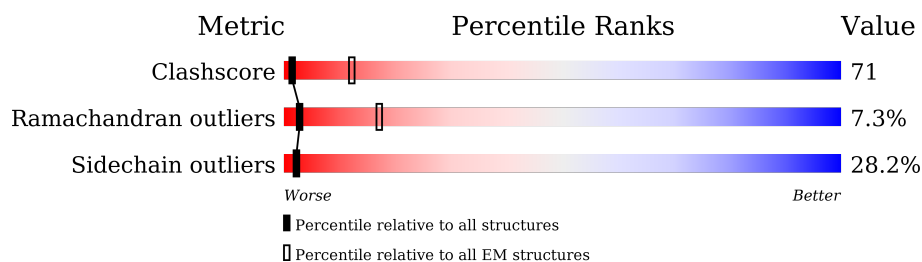
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 73616 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3453	Total 18404	C 11343	N 3553	O 3501	S 7	0	0
1	B	3453	Total 18404	C 11343	N 3553	O 3501	S 7	0	0
1	C	3453	Total 18404	C 11343	N 3553	O 3501	S 7	0	0
1	D	3453	Total 18404	C 11343	N 3553	O 3501	S 7	0	0




GLU	ALA	K3658	GLN	GLU	L3190	PHE	PHE	P3808	L2710	R2575	SER	GLU	ALA	ALA
GLU	GLU	W3661	THR	LEU	A3200	GLU	ALA	E2830	PRO	V2586	ALA	PRO	PRO	LYS
GLU	GLU	I3662	SER	VAL	MET	LEU	LYS	GLU	ASP	R2587	PHE	PRO	GLU	THR
VAL	GLU	E3665	ILE	VAL	VAL	LEU	ILE	GLU	TYR	R2588	ASP	TYR	GLU	PRO
GLU	VAL	D3666	ALA	GLU	A3204	LEU	LEU	ARG	VAL	R2589	ASN	ARG	ASN	ASP
GLU	VAL	H3667	PHE	GLU	P3208	PRO	PRO	THR	ASP	S2590	ARG	VAL	ARG	ILE
VAL	VAL	S3668	SER	ILE	P3208	LEU	LEU	THR	ALA	R2591	GLY	TRP	GLY	TRP
GLN	GLN	F3669	VAL	VAL	Y3213	LEU	ILE	LYS	SER	G2592	LYS	LEU	GLY	ASN
VAL	VAL	E3670	CYS	CYS	Y3213	GLN	GLN	LYS	TYR	L2595	HIS	HIS	ASN	P2325
ALA	ALA	D3671	ASP	ASP	S3217	TYR	PHE	ANG	SER	A2609	ALA	ALA	ALA	E2329
VAL	VAL	K3679	ASP	ASP	VAL	ASP	GLU	LYS	LYS	LEU	GLY	ILE	MET	F2340
GLY	GLY	K3760	GLN	ASP	THR	ARG	ARG	LYS	ALA	CYS	ILE	GLU	GLU	VAL
GLU	GLU	Q3761	ASP	GLU	THR	THR	THR	ILE	GLU	TRR	ILE	GLU	SER	W3441
L3762	L3762	R3762	THR	THR	THR	GLN	GLN	SER	LYS	ILE	GLU	GLU	GLU	I2342
L3763	L3763	R3763	GLN	GLN	THR	VAL	VAL	THR	ALA	ILE	ASN	GLN	GLN	G2343
L3764	L3764	R3764	LEU	LEU	VAL	SER	LEU	THR	THR	R2615	GLN	GLN	GLN	E2344
Y3765	Y3765	R3765	LEU	LEU	SER	ALA	ALA	ALA	THR	P2616	ASP	ASP	ASP	K2360
Q3766	Q3766	R3766	LEU	LEU	PRO	ALA	ARG	GLN	VAL	R2624	GLY	R2435	LEU	P2361
R3769	R3769	R3769	LYS	LYS	ARG	THR	THR	THR	ASP	GLY	LYS	ASP	LEU	E2362
R3773	R3773	R3773	THR	THR	ALA	VAL	VAL	VAL	GLY	I2634	LYS	I2443	GLY	C2363
A3785	A3785	C3786	LEU	LEU	ILE	GLY	GLY	GLN	THR	GLU	LYS	GLU	GLY	F2364
K3787	K3787	R3787	LEU	LEU	LEU	THR	THR	ALA	ALA	PHE	GLY	E2449	ALA	G3365
A3792	A3792	C3793	SER	SER	LEU	VAL	VAL	LEU	THR	GLU	ASP	A2450	ALA	P2366
Y3793	Y3793	R3793	LEU	LEU	GLY	VAL	VAL	LEU	VAL	TRP	GLY	A2451	LEU	LEU
D3695	D3695	L3696	LYS	LYS	GLY	GLN	GLN	LEU	P2737	K2638	P2528	D2529	ARG	R2452
D3696	D3696	L3697	LYS	LYS	GLY	GLN	GLN	LEU	R2738	P2639	M2530	R2531	GLY	I2453
L3698	L3698	R3698	LYS	LYS	GLY	GLN	GLN	LEU	P2739	P2640	A2532	R2454	GLY	R2454
S3795	S3795	R3795	LYS	LYS	GLY	GLN	GLN	LEU	V2740	GLU	A2533	A2455	GLY	GLY
Q3700	Q3700	R3701	LYS	LYS	GLY	GLN	GLN	LEU	L2743	GLU	A2534	A2456	GLY	GLY
L3701	L3701	R3702	LYS	LYS	GLY	GLN	GLN	LEU	I2734	PHE	S2522	S2459	SER	G2375
Y3702	Y3702	R3702	LYS	LYS	GLY	GLN	GLN	LEU	E2855	GLU	GLY	L2460	GLU	I2386
T3708	T3708	R3708	LYS	LYS	GLY	GLN	GLN	LEU	E2856	TRP	GLY	V2461	SER	SER
A3709	A3709	R3709	LYS	LYS	GLY	GLN	GLN	LEU	Y2857	P2658	TRP	P2462	ASP	GLU
L3710	L3710	R3710	LYS	LYS	GLY	GLN	GLN	LEU	R2858	GLY	ALA	D2463	ASP	GLU
L3710	L3710	R3710	LYS	LYS	GLY	GLN	GLN	LEU	G2887	TRP	ALA	D2464	ASP	GLU
D3717	D3717	R3717	LYS	LYS	GLY	GLN	GLN	LEU	R2888	ALA	ASN	V2467	PRO	PRO
E3718	E3718	R3718	LYS	LYS	GLY	GLN	GLN	LEU	K2897	PHE	GLY	M2546	ALA	ALA
D3719	D3719	R3719	LYS	LYS	GLY	GLN	GLN	LEU	VAL	VAL	VAL	A2549	ARG	ARG
L3721	L3721	R3721	LYS	LYS	GLY	GLN	GLN	LEU	H2902	G2667	VAL	L2550	ASP	ASP
Y3725	Y3725	R3725	LYS	LYS	GLY	GLN	GLN	LEU	P2903	K2677	GLY	L2556	GLY	GLY
E3734	E3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	L2904	F2677	THR	A2557	PRO	PRO
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	L2905	G2681	GLY	L2566	GLY	GLY
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	V2906	VAL	VAL	P2560	VAL	VAL
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	P2907	L2686	GLY	L2561	ARG	ARG
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	Y2777	ALA	LYS	I2562	ASP	ASP
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	E2779	ALA	LYS	L2562	ARG	ARG
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	K2786	LYS	LYS	ALA	ARG	ARG
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	T2787	LYS	LYS	ALA	ARG	ARG
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	H2788	ALA	LYS	VAL	GLU	GLU
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	P2789	Y2691	ALA	GLN	HIS	HIS
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	E2694	GLY	ALA	PRO	PHE	PHE
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	A2699	GLY	ALA	LYS	GLY	GLY
L3734	L3734	R3734	LYS	LYS	GLY	GLN	GLN	LEU	P2793	GLY	ALA	MET	GLU	GLU




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- Molecule 1: Ryanodine receptor 1

H151	P152	A153	G160	E161	K162	V163	R164	V165	G166	D167	D168	I169	I170	L171	V172	S173	V174	S175	S176	E177	R178	I179	L180	H181	L182	T183	T184	ALA	SER	GLY	LEU	GLN	VAL	ASP	ASP	GLN	ALA	SER	PHE	M196	W200	N203	E211	G212	Y213	V214	T215	H218	V219	L220	ARG	LEU	PHE	PHE	S205
S72	L73	S74	A77	D84	THR	VAL	VAL	GLU	ALA	GLY	VAL	GLU	SER	GLN	GLY	GLY	HIS	ARG	T100	Y103	H104	A106	R110	H111	A112	H113	S114	R115	H116	Y117	L118	S119	G120	L121	T122	T123	D129	K130	L131	A132	F133	G136	L137	A141	C146	W147	A148	T149	M150						
MET	GLY	ASP	GLY	GLY	GLY	GLU	GLY	GLU	ASP	GLU	VAL	VAL	Q12	R15	T16	D17	V20	V21	L22	Q23	C24	S25	A26	T27	V28	E31	Q32	L33	K34	L35	C36	L37	A38	A39	E40	G41	F42	G43	N44	C47	P51	A55	V58	P59	P60	L64	C65	C66	F67	T68	L69	E70	G71		

TYR	MET	VAL	TRP	GLY	GLY	ASP	PHE	THR	ILE	GLU	ALA	THR	ALA	F1245	F1246	MET	V1095	GLN	ASP	PHE	V789	GLY	G701	LEU	H596	Q460	PRO	V301	H226
VAL	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	E1246	E1247	SER	T1096	ASP	ILE	VAL	R790	GLY	G702	LEU	H597	H461	LYS	V302	H227
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	P1249	P1250	ASP	T1097	PRO	PRO	VAL	F791	GLY	G703	LEU	H598	E462	ALA	A304	D228
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	P1251	P1252	GLY	V1102	ALA	ALA	CYS	L792	GLY	G704	LEU	H599	E463	ALA	A305	D229
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1251	H1252	GLY	T1103	ALA	ALA	VAL	L793	GLY	G705	LEU	H600	F478	ARG	A306	D230
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1253	H1254	GLY	T1104	ALA	ALA	VAL	L794	GLY	G706	LEU	H601	G482	VAL	A307	D231
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1255	H1256	GLY	T1105	ALA	ALA	VAL	L795	GLY	G707	LEU	H602	M483	VAL	A308	D232
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1257	H1258	GLY	T1106	ALA	ALA	VAL	L796	GLY	G708	LEU	H603	G483	VAL	A309	D233
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1259	H1260	GLY	T1107	ALA	ALA	VAL	L797	GLY	G709	LEU	H604	M484	VAL	A310	D234
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1261	H1262	GLY	T1108	ALA	ALA	VAL	L798	GLY	G710	LEU	H605	M485	VAL	A311	D235
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1263	H1264	GLY	T1109	ALA	ALA	VAL	L799	GLY	G711	LEU	H606	M486	VAL	A312	D236
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1265	H1266	GLY	T1110	ALA	ALA	VAL	L800	GLY	G712	LEU	H607	M487	VAL	A313	D237
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1267	H1268	GLY	T1111	ALA	ALA	VAL	L801	GLY	G713	LEU	H608	M488	VAL	A314	D238
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1269	H1270	GLY	T1112	ALA	ALA	VAL	L802	GLY	G714	LEU	H609	M489	VAL	A315	D239
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1271	H1272	GLY	T1113	ALA	ALA	VAL	L803	GLY	G715	LEU	H610	M490	VAL	A316	D240
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1273	H1274	GLY	T1114	ALA	ALA	VAL	L804	GLY	G716	LEU	H611	M491	VAL	A317	D241
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1275	H1276	GLY	T1115	ALA	ALA	VAL	L805	GLY	G717	LEU	H612	M492	VAL	A318	D242
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1277	H1278	GLY	T1116	ALA	ALA	VAL	L806	GLY	G718	LEU	H613	M493	VAL	A319	D243
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1279	H1280	GLY	T1117	ALA	ALA	VAL	L807	GLY	G719	LEU	H614	M494	VAL	A320	D244
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1281	H1282	GLY	T1118	ALA	ALA	VAL	L808	GLY	G720	LEU	H615	M495	VAL	A321	D245
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1283	H1284	GLY	T1119	ALA	ALA	VAL	L809	GLY	G721	LEU	H616	M496	VAL	A322	D246
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1285	H1286	GLY	T1120	ALA	ALA	VAL	L810	GLY	G722	LEU	H617	M497	VAL	A323	D247
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1287	H1288	GLY	T1121	ALA	ALA	VAL	L811	GLY	G723	LEU	H618	M498	VAL	A324	D248
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1289	H1290	GLY	T1122	ALA	ALA	VAL	L812	GLY	G724	LEU	H619	M499	VAL	A325	D249
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1291	H1292	GLY	T1123	ALA	ALA	VAL	L813	GLY	G725	LEU	H620	M500	VAL	A326	D250
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1293	H1294	GLY	T1124	ALA	ALA	VAL	L814	GLY	G726	LEU	H621	M501	VAL	A327	D251
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1295	H1296	GLY	T1125	ALA	ALA	VAL	L815	GLY	G727	LEU	H622	M502	VAL	A328	D252
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1297	H1298	GLY	T1126	ALA	ALA	VAL	L816	GLY	G728	LEU	H623	M503	VAL	A329	D253
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1299	H1300	GLY	T1127	ALA	ALA	VAL	L817	GLY	G729	LEU	H624	M504	VAL	A330	D254
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1301	H1302	GLY	T1128	ALA	ALA	VAL	L818	GLY	G730	LEU	H625	M505	VAL	A331	D255
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1303	H1304	GLY	T1129	ALA	ALA	VAL	L819	GLY	G731	LEU	H626	M506	VAL	A332	D256
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1305	H1306	GLY	T1130	ALA	ALA	VAL	L820	GLY	G732	LEU	H627	M507	VAL	A333	D257
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1307	H1308	GLY	T1131	ALA	ALA	VAL	L821	GLY	G733	LEU	H628	M508	VAL	A334	D258
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1309	H1310	GLY	T1132	ALA	ALA	VAL	L822	GLY	G734	LEU	H629	M509	VAL	A335	D259
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1311	H1312	GLY	T1133	ALA	ALA	VAL	L823	GLY	G735	LEU	H630	M510	VAL	A336	D260
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1313	H1314	GLY	T1134	ALA	ALA	VAL	L824	GLY	G736	LEU	H631	M511	VAL	A337	D261
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1315	H1316	GLY	T1135	ALA	ALA	VAL	L825	GLY	G737	LEU	H632	M512	VAL	A338	D262
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1317	H1318	GLY	T1136	ALA	ALA	VAL	L826	GLY	G738	LEU	H633	M513	VAL	A339	D263
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1319	H1320	GLY	T1137	ALA	ALA	VAL	L827	GLY	G739	LEU	H634	M514	VAL	A340	D264
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1321	H1322	GLY	T1138	ALA	ALA	VAL	L828	GLY	G740	LEU	H635	M515	VAL	A341	D265
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1323	H1324	GLY	T1139	ALA	ALA	VAL	L829	GLY	G741	LEU	H636	M516	VAL	A342	D266
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1325	H1326	GLY	T1140	ALA	ALA	VAL	L830	GLY	G742	LEU	H637	M517	VAL	A343	D267
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1327	H1328	GLY	T1141	ALA	ALA	VAL	L831	GLY	G743	LEU	H638	M518	VAL	A344	D268
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1329	H1330	GLY	T1142	ALA	ALA	VAL	L832	GLY	G744	LEU	H639	M519	VAL	A345	D269
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1331	H1332	GLY	T1143	ALA	ALA	VAL	L833	GLY	G745	LEU	H640	M520	VAL	A346	D270
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1333	H1334	GLY	T1144	ALA	ALA	VAL	L834	GLY	G746	LEU	H641	M521	VAL	A347	D271
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1335	H1336	GLY	T1145	ALA	ALA	VAL	L835	GLY	G747	LEU	H642	M522	VAL	A348	D272
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1337	H1338	GLY	T1146	ALA	ALA	VAL	L836	GLY	G748	LEU	H643	M523	VAL	A349	D273
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1339	H1340	GLY	T1147	ALA	ALA	VAL	L837	GLY	G749	LEU	H644	M524	VAL	A350	D274
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1341	H1342	GLY	T1148	ALA	ALA	VAL	L838	GLY	G750	LEU	H645	M525	VAL	A351	D275
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1343	H1344	GLY	T1149	ALA	ALA	VAL	L839	GLY	G751	LEU	H646	M526	VAL	A352	D276
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1345	H1346	GLY	T1150	ALA	ALA	VAL	L840	GLY	G752	LEU	H647	M527	VAL	A353	D277
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1347	H1348	GLY	T1151	ALA	ALA	VAL	L841	GLY	G753	LEU	H648	M528	VAL	A354	D278
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1349	H1350	GLY	T1152	ALA	ALA	VAL	L842	GLY	G754	LEU	H649	M529	VAL	A355	D279
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1351	H1352	GLY	T1153	ALA	ALA	VAL	L843	GLY	G755	LEU	H650	M530	VAL	A356	D280
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1353	H1354	GLY	T1154	ALA	ALA	VAL	L844	GLY	G756	LEU	H651	M531	VAL	A357	D281
THR	TRP	GLY	GLY	THR	THR	ASP	THR	PRO	THR	ALA	PRO	LEU	PRO	H1355	H1356	GLY	T1155	ALA	ALA	VAL	L845	GLY	G757	LEU	H652	M532	VAL	A358	D282
THR	TRP	GLY	GLY	THR	THR	ASP	THR																						

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM




M5019	D5020	F5021	F5022	P5023	A5024	G5025	D5026	C5027	F5028	R5029	K5030	Q5031	Y5032	E5033	ASP	GLN	LEU	SER	M4954	M4955	F4956	T4957	F4958	F4959	I4960	C4961	G4964	S4965	D4966	Y4967	F4968	D4969	T4970	T4971	P4972	H4973	G4974	F4975	E4976	T4977	H4978	T4979	E4982	H4983	N4984	L4985	A4986	I4987	Y4988	F4989	F4990	F4991	Y4994	L4995	I4996	N4997	K4998	D4999	E5000	T5001	E5002	H5003	Q5006	E5007	S5008	Y5009	V5010	W5011	Y5014	Q5015	E5016	R5017	C5018																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
M4818	G4819	H4820	K4821	L4822	M4823	R4824	T4825	S4829	H4832	M4833	G4834	K4835	Q4836	L4837	V4838	M4839	L4840	G4841	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	41743	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)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.17	51/18508 (0.3%)	1.21	262/25601 (1.0%)
1	B	1.17	51/18508 (0.3%)	1.21	262/25601 (1.0%)
1	C	1.17	51/18508 (0.3%)	1.21	262/25601 (1.0%)
1	D	1.17	51/18508 (0.3%)	1.21	262/25601 (1.0%)
All	All	1.17	204/74032 (0.3%)	1.21	1048/102404 (1.0%)

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
1	A	1	3
1	B	1	3
1	C	1	3
1	D	1	3
All	All	4	12

The worst 5 of 204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4859	PHE	CA-CB	-43.48	0.58	1.53
1	B	4859	PHE	CA-CB	-43.48	0.58	1.53
1	C	4859	PHE	CA-CB	-43.48	0.58	1.53
1	D	4859	PHE	CA-CB	-43.48	0.58	1.53
1	A	4691	GLN	CA-CB	-40.95	0.63	1.53

The worst 5 of 1048 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2047	GLU	N-CA-CB	-38.23	41.78	110.60
1	C	2047	GLU	N-CA-CB	-38.23	41.78	110.60
1	D	2047	GLU	N-CA-CB	-38.23	41.78	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2047	GLU	N-CA-CB	-38.22	41.80	110.60
1	A	4168	GLU	N-CA-CB	-30.53	55.64	110.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4691	GLN	CA
1	B	4691	GLN	CA
1	C	4691	GLN	CA
1	D	4691	GLN	CA

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2192	TYR	Mainchain
1	A	2586	VAL	Peptide
1	A	4091	LYS	Peptide
1	B	2192	TYR	Mainchain
1	B	2586	VAL	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	18404	0	9770	2060	0
1	B	18404	0	9770	2067	0
1	C	18404	0	9770	2068	0
1	D	18404	0	9770	2069	0
All	All	73616	0	39080	8025	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 71.

The worst 5 of 8025 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4978:HIS:HE2	1:D:4983:HIS:CD2	1.11	1.67
1:A:4235:VAL:HG21	1:A:5019:TRP:CZ3	1.15	1.67
1:C:4115:SER:HA	1:C:4128:PHE:CZ	1.23	1.66
1:A:4978:HIS:HE2	1:A:4983:HIS:CD2	1.11	1.66
1:B:4978:HIS:HE2	1:B:4983:HIS:CD2	1.11	1.65

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	3311/5037 (66%)	2865 (86%)	203 (6%)	243 (7%)	1	21
1	B	3311/5037 (66%)	2865 (86%)	204 (6%)	242 (7%)	1	21
1	C	3311/5037 (66%)	2865 (86%)	203 (6%)	243 (7%)	1	21
1	D	3311/5037 (66%)	2864 (86%)	205 (6%)	242 (7%)	1	21
All	All	13244/20148 (66%)	11459 (86%)	815 (6%)	970 (7%)	3	21

5 of 970 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	25	SER
1	A	26	ALA
1	A	44	ASN
1	A	67	PHE

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	317/4276 (7%)	225 (71%)	92 (29%)	0	3
1	B	317/4276 (7%)	229 (72%)	88 (28%)	0	4
1	C	317/4276 (7%)	229 (72%)	88 (28%)	0	4
1	D	317/4276 (7%)	228 (72%)	89 (28%)	0	4
All	All	1268/17104 (7%)	911 (72%)	357 (28%)	2	4

5 of 357 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4931	ILE
1	C	4108	ILE
1	D	4916	PHE
1	B	4948	GLU
1	C	478	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4833	ASN
1	C	3833	GLN
1	D	4806	ASN
1	B	4857	ASN
1	C	1702	HIS

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 [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.