



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

Jan 30, 2017 – 11:01 AM EST

PDB ID : 5GO9  
EMDB ID: : EMD-9528  
Title : Cryo-EM structure of RyR2 in closed state  
Authors : Peng, W.; Wu, J.P.; Yan, N.  
Deposited on : 2016-07-26  
Resolution : 4.40 Å(reported)

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

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

---

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

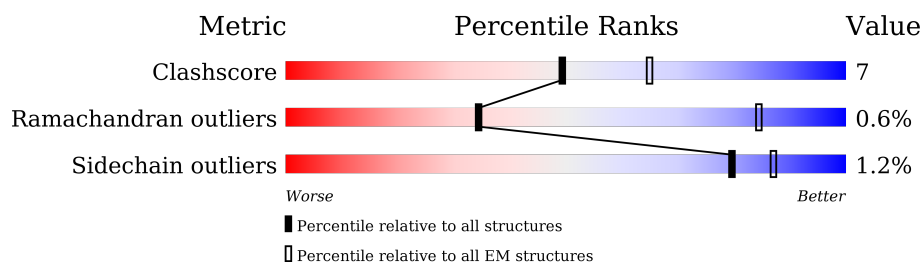
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	4968	
1	B	4968	
1	C	4968	
1	D	4968	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 105068 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
			26266	16740	4498	4874	154		
1	B	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	C	3423	Total	C	N	O	S	0	0
			26266	16740	4498	4874	154		
1	D	3423	Total	C	N	O	S	0	0
			26266	16740	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	



- Molecule 1: RyR2






WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

 **EMDataBank**  
Unified Data Resource for 3DEM

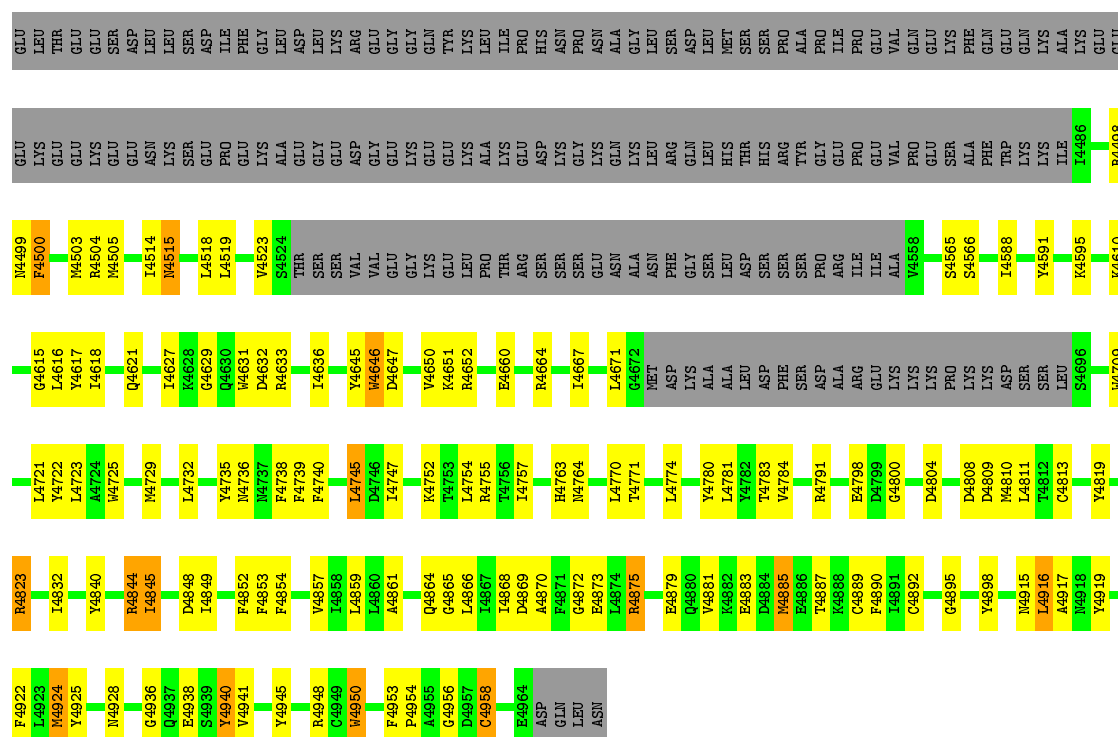




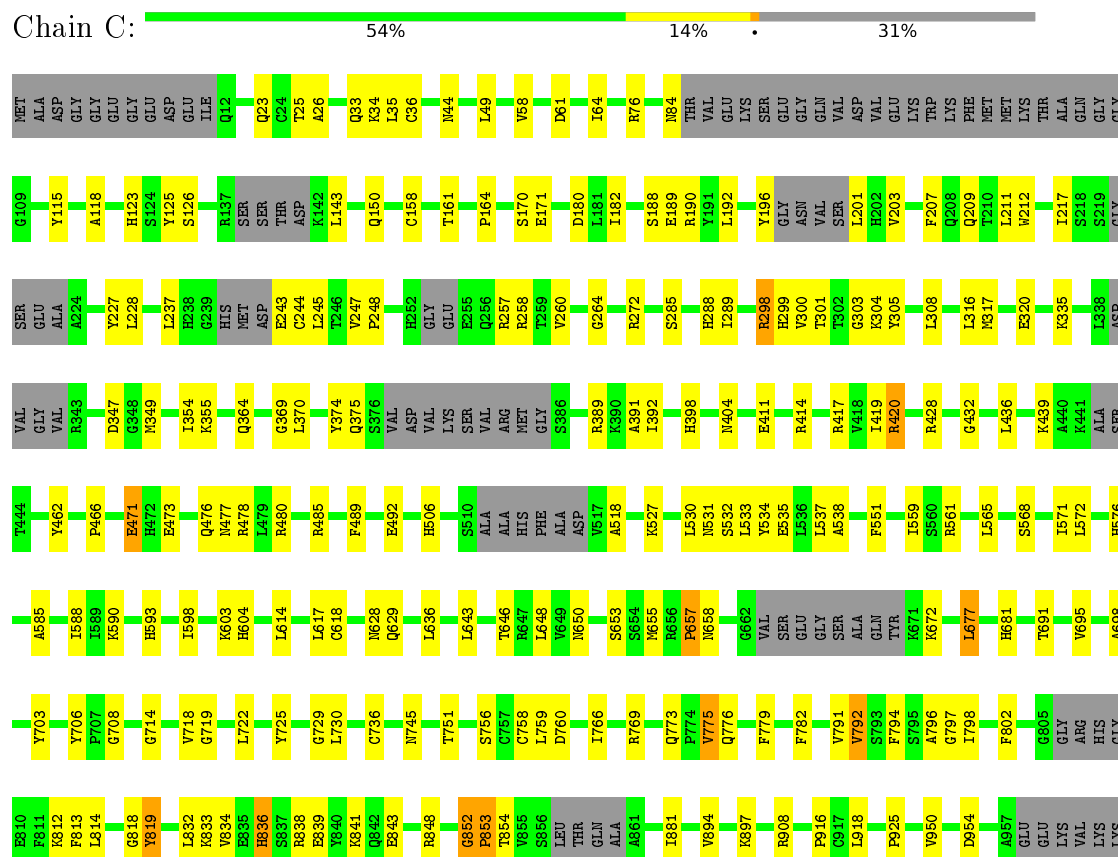








- Molecule 1: RyR2



[illegible]

K4086	V3945	N3813	GLU	LYS	ALA	THR	PHE	GLU	ILE	GLU	ILE	GLU	SER	GLU	SER	GLU	ASP	R2682	LEU
R4087	F3948	R3814	GLU	LYS	ILE	SER	ILE	VAL	TRP	GLY	TYR	ILE	GLY	ASP	GLY	ILE	ASP	P2583	
PHE		ALA	THR	VAL	TRP	ILE	TRP	ASP	GLN	ASP	ASN	ASN	GLY	THR	THR	THR	ASP	P2598	
E4090	F3952	GLY	VAL	TRP	GLN	VAL	SER	GLY	MET	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	P2601	
E4108	Q3961	LEU	ALA	ALA	ALA	ALA	HIS	SER	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
E4109	Q3971	GLY	LEU	LEU	LEU	LEU	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
M4110		MET	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	GLY	
V4126	L3975	THR	GLY	SER	ASP	GLY	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
ALA	Q3976	GLY	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	THR	GLY	
ASN	S3714	GLY	GLN	GLN	GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
F4130	V3980	SER	ASN	ASN	ASN	ASN	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	ILE	THR	GLY	
Q4131	K3722	GLY	THR	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
L4134	L3983	GLY	ALA	ALA	ALA	ALA	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	THR	GLY	
G4135	G4136	SER	VAL	VAL	VAL	VAL	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	PHE	THR	GLY	
R4136	R3986	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	GLY	
E4137		LEU	ALA	ALA	ALA	ALA	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	CYS	THR	GLY	
E4138	N3993	GLN	SER	SER	SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
E4139		D3833	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
M4140	I3996	LYS	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	GLY	
G4141		T3837	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	THR	GLY	
S4142	M4003	I3840	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
A4143	L4004	F3841	GLN	GLN	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
E4144																		GLY	
R4145	V4011	Q3845	ARG	ARG	ARG	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLY	
E4146	M4013		THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
S4157	L4014	I3859	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
R4158	L4015	I3871	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
PHE	F4016																	GLY	
SER	F4017	T3875	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	S4030	I3886	VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
THR	Y4036																	GLY	
ARG	K4170	Y3890	ARG	ARG	ARG	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
SER	R4171	W3891	ALA	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU			VAL	VAL	VAL	VAL	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	I4174	N3906	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
ALA	D4047	A3910	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	D4048	I3911	ASP	ASP	ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
ALA	F4049		GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	H4050	A3914	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
ARG	F4051		ASP	ASP	ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
TYR	A4052		GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
ASN	H4056	V3917	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
VAL	E4188	F3918	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	F4190	N3919	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
THR	V4191	T3920	ALA	ALA	ALA	ALA	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU		I4068	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
MET	C4194	S4069	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
MET		C4070	LEU	LEU	LEU	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
MET	A4071	I3921	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
MET	E4072	T3922	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	T4073	E3923	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
SER	D4074	I3924	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU		I3925	PRO	PRO	PRO	PRO	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	T4078	Q3926	GLN	GLN	GLN	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LYS		N3932	ARG	ARG	ARG	ARG	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
SER	A4204		ASP	ASP	ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	
LEU	A4205	Q3812	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	GLY	

Y4940	F4852	M4737	S4640	SER	GLU	LYS	ILE	LYS
F4941	F4853	F4738	F4738	VAL	ASP	GLU	VAL	LYS
W4942	F4854	F4739	F4739	GLY	GLY	GLY	GLY	GLN
Y4945	L4859	F4740	M4643	GLY	LYS	GLN	GLY	GLY
F4948	L4860	L4745	Y4645	LYS	GLU	GLY	LEU	LYS
W4949	A4861	L4747	W4646	GLU	GLU	TYR	LEU	VAL
W4950		L4747	D4647	LEU	ALA	LYS	ASN	LYS
F4953	Q4864	K4752	V4650	PRO	LYS	ILE	MET	LYS
F4954	G4865	L4753	K4651	THR	GLU	PRO	PRO	THR
A4955	L4866	L4754	R4652	ARG	ASP	HIS	ASP	VAL
G4956	I4867	R4755		SER	ASP	ASN	PRO	ARG
D4957	D4869	L4756	E4660	SER	LYS	ASN	THR	ASP
C4958	W4870	L4757	L4757	GLU	GLY	ASN	GLN	NET
	F4871	L4758	R4664	ASN	GLN	ALA	GLY	THR
K4861	G4872	S4759		ALA	LYS	GLY	GLU	THR
	E4873		I4667	ASN	LEU	LEU	VAL	ALA
E4964	L4874	H4763	L4671	PHE	GLN	SER	ARG	PHE
ASP	R4875	M4764	G4672	GLY	GLN	ASP	GLY	PHE
GLN				SER	LEU	ASP	GLY	THR
LEU				SER	LEU	NET	GLY	SER
ASN	E4879	T4771	ASP	ASP	THR	SER	ASP	TVR
	Q4880		LYS	SER	HIS	SER	GLY	TRP
	R4882	L4774	ALA	ARG	PRO	PRO	GLU	SER
	E4883		ALA	SER	HIS	ASN	GLY	SER
	D4884	Y4780	L4781	THR	TYR	ALA	GLU	VAL
	M4885	L4781	GLY	GLY	GLY	PRO	ARG	PHE
	F4886	Y4782	ASP	ARG	GLU	ILE	LYS	NET
	T4887	T4783	PHE	ILE	PRO	VAL	VAL	THR
	R4888	V4784	SER	ILE	GLU	GLY	LEU	LEU
	C4889		ASP	ALA	VAL	VAL	GLU	LEU
	F4890	R4791	ALA	ALA	PRO	GLN	GLY	HIS
	I4891	E4798	GLU	GLU	GLU	GLU	THR	PHE
	C4892	D4799	LYS	S4665	SER	LYS	LEU	ALA
	G4893	G4800	LYS	S4666	ALA	PHE	PRO	ALA
I4894			LYS		PHE	GLN	SER	SER
G4895			LYS	P4871	TRP	GLU	GLU	VAL
		D4804	PRO	LYS	LYS	GLN	ASP	SER
			LYS		LYS	LEU	LEU	ARG
			PRO		ILE	ALA	THR	GLY
	Y4898	D4808	LYS	L4888	ILE	LYS	ASP	PHE
	M4915	D4809	ASP			LYS	LEU	SER
L4916	L4916	M4810	SER	K4610		GLU	LEU	ARG
A4917	L4811	L4811	SER		R4498	GLU	LYS	ILE
M4918	T4812	T4812	LEU		M4499	GLU	GLU	ILE
Y4919	C4813	C4813	S4696		F4500	LYS	LEU	ILE
				G4615		GLU	THR	GLY
	Y4819	Y4819	W4709	L4616	M4503	GLU	GLU	GLY
				Y4617	M4504	GLY	GLU	LEU
				L4618	M4505	LYS	GLU	LEU
						ASN	ASP	GLY
				Q4621		L4514	LEU	GLY
						M4615	LEU	GLY
				L4627		L4518	ASP	LEU
				K4628		L4519	ASP	VAL
				G4629			ILE	PHE
				W4630			GLU	GLY
				W4631			PHE	GLY
				L4732			GLY	ALA
				L4732			ALA	LYS
				L4732			ASP	LYS
				W4725			THR	GLY
							GLY	LYS
				W4735			ASP	LYS
				M4736			LEU	LYS

- Molecule 1: RyR2

Chain D:  54% 14% 31%

H593	E471	D347	Y227	Y115	MET
I588	E472	G348	L228	G116	ALA
K603	E473	M349	L237	H123	ASP
H604	Q476	I354	H338	H124	GLY
V613	R477	K355	G239	Y125	GLU
L614	R478	Q364	HIS	S126	GLY
L617	R479	Q364	MET		GLU
C618	L480	G369	ASP	R137	ASP
N628	R485	E243	E243	SER	GLU
Q629	F489	C244	C244	SER	ILE
I632	R490	L370	L245	THR	Q12
L636	R485	Y374	T246	ASP	Q23
L643	F489	Q375	P247	L142	C24
T646	E492	VAL	P248	L143	T25
H657	E492	ASP	H252	Q150	A26
V649	H506	VAL	GLY	C158	Q33
N650	S510	LVS	E255		K34
M655	ALA	SER	E256	I162	L35
H656	ALA	ARG	R257	H163	C36
P657	ALA	HIS	R258	P164	
N658	HIS	MET	T259		M44
T662	PHE	GLY	V260	S170	
H666	ALA	S386	E171	D180	L49
V667	ASP	R389	G264	I181	V58
V669	V517	K390	R272		D61
N670	A518	A391	S285	S188	R76
M675	K527	H598	H289	E189	
H676	L530	M404	L289	R190	N84
P677	S531	E411	R298	Y191	THR
M678	S532	R414	H299	L192	VAL
L679	S533	R417	V300	Y196	GLU
V680	L537	R418	T301	GLY	LVS
V681	L537	R419	T302	ASN	SER
V682	L537	R420	G303	VAL	GLY
V683	F551	I419	K304	SER	GLN
V684	F551	R428	Y305	L201	VAL
V685	F559	R428	L308	T207	ASP
V686	S560	G432	L316	D208	VAL
V687	H561	L436	M317	D209	GLU
V688	L566	L436	E320	T210	LVS
V689	S568	L436	K335	L211	THR
V690	L571	K439	K335	W212	LVS
V691	L572	A440	K335	T217	PHE
V692	L576	K441	L338	S218	MET
V693	H576	ALA	ASP	S219	LVS
V694	SER	ALA	VAL	GLY	THR
V695	SER	T444	VAL	SER	ALA
V696	SER	T444	VAL	GLU	GLN
V697	SER	T444	VAL	GLU	GLY
V698	SER	T444	VAL	ALA	GLY
V699	SER	T444	VAL	A224	G109

P2293	G2181	LYS	LEU	GLU	G1747	M1551	Y1441	GLY	ALA	D1196	F1088	ASN	F813	Y706
D2301	GLY	THR	THR	GLU	D1640	Q1554	W1442	GLY	GLY	D1196	R1089	Y970	L814	F707
R2304	GLU	ALA	ALA	SER	I1641	F1555	W1443	GLY	GLY	P1203	A1090	P980	G818	G708
L2326	SER	LYS	ARG	ASP	L1642	F1556	G1444	ILE	ILE	S1206	E1091	Y1102	Y819	G714
P2329	LYS	LYS	LYS	THR	E1643	E1556	W1445	PRO	PRO	L14207	K1092	Y1094	L832	W718
E2330	VAL	THR	THR	GLU	L1644	LEU	D1449	ALA	ALA	D1220	T1093	P990	K833	G719
P2329	GLU	GLU	GLU	LYS	T1645	ARG	L1459	SER	SER	T1223	F1103	R1011	V834	L722
CYS	PRO	PHE	PHE	PRO	K1652	ILE	ASP	PHE	PHE	T1223	E1104	GLI014	H836	Y725
PHE	ASP	ARG	ARG	ASP	F1653	LYS	ASN	GLY	GLY	T1228	M1113	GLY	R838	G729
LYS	LYS	SER	SER	ALA	H1654	ASN	VAL	LEU	LEU	T1232	R1114	THR	E839	L730
LYS	LYS	SER	PRO	VAL	T1657	MET	ARG	LEU	PRO	T1232	R1119	GLY	Y840	H731
SER	GLU	GLU	GLN	PRO	V1664	PRO	THR	ASP	ASN	Y1236	P1120	THR	K841	
SER	ASP	SER	GLN	LEU	N1669	LEU	V1465	LEU	ASP	Y1236	G1121	GLY	Q842	C736
SER	ARG	ARG	ILE	ARG	V1672	SER	L1469	ASP	ASP	M1249	P1124	GLN	E843	
GLY	GLY	GLY	GLY	GLY	Y1778	K1576	E1472	THR	THR	W1250	P1124	GLN	Y737	A738
PRO	PRO	PRO	LEU	PRO	E1781	V1579	K1473	SER	ASP	L1251	L1128	ASP	R848	
ASN	ASN	ASN	ASN	ALA	F1782	P1580	G1474	THR	ALA	K1252	V1128	VAL	G852	N745
PHE	ALA	ALA	PHE	GLU	Q1683	Q1581	K1475	SER	ASP	K1253	L1128	LYS	P853	
LYS	LYS	LYS	LYS	GLU	L1685	Q1581	V1476	SER	SER	R1254	E1132	ASN	T854	S756
ASP	ASP	ASP	ASP	GLU	L1686	H1587	I1480	ALA	PHE	L1255	R1027	R1027	V855	C767
ASP	SER	SER	SER	SER	Y1687	V1588	M1484	GLY	GLY	P1256	R1028	R1028	S856	C758
LYS	LYS	LYS	LYS	LYS	K1692	Q1590	Y1486	VAL	VAL	F1257	M1029	M1029	LEU	L759
GLY	GLY	GLY	GLY	GLY	K1692	F1590	M1487	LEU	LEU	F1258	F1030	F1030	THR	D760
CYS	CYS	CYS	CYS	CYS	P1695	H1593	V1488	ASP	LYS	E1266	L1031	L1031	GLN	I766
PRO	PRO	PRO	PRO	ARG	R1699	S1597	C1489	VAL	THR	R1272	V1054	V1054	ALA	I766
CYS	CYS	CYS	CYS	CYS	R1699	R1598	A1490	LEU	LEU	I1273	W1145	W1145	A861	R769
PRO	PRO	PRO	PRO	PRO	V1703	M1599	GLY	ALA	HIS	D1274	H1146	H1146	I851	
GLU	GLU	GLU	GLU	GLU	L1706	P1600	GLU	ASP	HIS	GLY	G1059	G1059	K897	Q773
ILE	ILE	ILE	ILE	ILE	L1707	Q1602	SER	ARG	LEU	THR	Y1060	Y1060	Y775	P774
ASP	ASP	ASP	ASP	ASP	L1711	F1603	MET	ASP	VAL	ILE	G1061	G1061	Q776	Q775
ASP	ASP	ASP	ASP	ASP	T1716	F1604	SER	ASP	PRO	ASP	Y1062	Y1062	R908	
LEU	LEU	LEU	LEU	LEU	T1716	L1608	PRO	TYR	ASP	SER	A1066	A1066	P916	F779
D1999	D1999	D1999	D1999	D1999	L1719	V1608	GLY	GLY	VAL	SER	PRO	PRO	C917	F782
D2013	D2013	D2013	D2013	D2013	M1720	E1613	ARG	GLY	LYS	LYS	ASP	ASP	L918	
GLU	GLU	GLU	GLU	GLU	I1726	R1614	H1501	THR	THR	LYS	ASP	ASP	P925	V791
ASP	ASP	ASP	ASP	ASP	L1726	W1617	I1507	SER	GLY	V1285	H1173	H1173	W792	V791
SER	SER	SER	SER	SER	M1729	L1618	G1508	THR	GLU	T1297	T1172	T1172	S793	S793
ASN	ASN	ASN	ASN	ASN	T1733	L1622	C1509	THR	LYS	R1303	M1174	M1174	D854	A796
VAL	VAL	VAL	VAL	VAL	L1738	L1622	V1510	THR	LYS	L1304	L1177	L1177	A957	G797
MET	MET	MET	MET	MET	F1739	Q1626	V1511	THR	PRO	C1310	D1184	D1184	GLU	I798
GLN	GLN	GLN	GLN	GLN	P1740	F1739	ASP	PHE	PHE	GLY	D1185	D1185	GLU	F802
LYS	LYS	LYS	LYS	LYS	D1741	S1629	SER	ASN	ASN	ALA	S1186	S1186	VAL	G805
ASN	ASN	ASN	ASN	ASN	GLY	L1632	G1516	GLY	HIS	VAL	G1187	G1187	LYS	GLY
ALA	ALA	ALA	ALA	ALA	ASN	I1632	F1520	GLN	LYS	PHE	S1188	S1188	LYS	ARG
GLY	GLY	GLY	GLY	GLY	ASN	E1635	F1520	GLU	ASP	SER	L1190	L1190	MET	HIS
PRO	PRO	PRO	PRO	PRO	LYS	N1636	P1541	PRO	TYR	THR	A1191	A1191	LYS	GLY
ALA	ALA	ALA	ALA	ALA	HIS	R1637	P1541	ALA	ALA	THR	F1085	F1085	PRO	GLY
											R1087	R1087	LYS	H812

F3952	ALA	GLU	ALA	ARG	LEU	TYR	GLY	LEU	ARG	TYR	TRP	GLY	ASP	GLU	ALA	M2390
Q3961	GLY	ASP	TRP	GLN	VAL	SER	ASN	ASP	GLN	ASP	TRP	GLY	GLN	ASP	ALA	A2404
E3971	GLY	GLY	LYS	ALA	ALA	SER	GLY	THR	LYS	MET	LYS	ILE	PHE	PRO	GLU	PRO
I3975	VAL	GLU	LEU	TYR	LEU	GLY	ILE	ALA	ALA	GLY	GLY	GLN	MET	ILE	SER	GLU
Q3976	THR	GLU	SER	LYS	ARG	ASN	PRO	PRO	GLY	GLY	GLY	PRO	ASN	ILE	GLY	HIS
V3980	GLU	VAL	LYS	ASP	LEU	LYS	VAL	LEU	LEU	GLY	ARG	LYS	LEU	GLY	LEU	ILE
V3980	GLU	GLN	GLN	LEU	PRO	ARG	ILE	VAL	ALA	TRP	LEU	ARG	LEU	VAL	GLY	HIS
L3983	GLY	S3714	ARG	ASN	ILE	GLY	MET	GLY	GLY	GLY	GLY	PHE	GLY	VAL	ALA	ALA
L3983	SER	K3722	LYS	ARG	PRO	GLN	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
M3986	GLY	K3722	ARG	ARG	ILE	GLN	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
M3986	GLY	Q3729	VAL	GLY	LEU	PHE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
I3996	VAL	A3730	VAL	ASP	ILE	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
I3996	VAL	A3730	VAL	ASP	ILE	VAL	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
M4003	LEU	H3733	CYS	SER	ALA	GLN	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
L4004	GLN	D3833	CYS	SER	ALA	GLN	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
V4011	ASN	D3794	PHE	ASP	PRO	ASN	ASP	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA
M4013	GLY	R3735	ARG	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
L4014	LEU	G3736	MET	GLY	ASN	ASN	ILE	ILE	ILE	ILE	ILE	GLY	GLY	GLY	GLY	ALA
L4015	THR	A3737	PRO	THR	LEU	ASN	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
F4017	TYR	M3740	LEU	VAL	LEU	MET	ALA	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY	ALA
S4030	THR	Q3743	ASN	VAL	LEU	SER	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
Y4036	ASN	V3756	LEU	VAL	LYS	THR	ASP	LYS	LYS	LYS	LYS	GLY	GLY	GLY	GLY	ALA
S4045	GLY	T3759	ASN	ILE	ASN	ASP	ILE	ILE	ILE	ILE	ILE	GLY	GLY	GLY	GLY	ALA
R4047	VAL	G3763	ALA	VAL	LEU	SER	PHE	PHE	PHE	PHE	PHE	GLY	GLY	GLY	GLY	ALA
F4049	VAL	L3767	ALA	VAL	LEU	SER	PHE	PHE	PHE	PHE	PHE	GLY	GLY	GLY	GLY	ALA
K4051	PRO	G3770	VAL	HIS	ASP	LYS	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
A4052	GLY	M3778	THR	LEU	THR	LYS	ASP	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA
H4056	GLY	L3782	THR	SER	ARG	SER	THR	THR	THR	THR	THR	GLY	GLY	GLY	GLY	ALA
L4068	THR	K3783	CYS	THR	ARG	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
C4070	LYS	L3797	LYS	ARG	ASP	GLY	ILE	ILE	ILE	ILE	ILE	GLY	GLY	GLY	GLY	ALA
A4071	ARG	M3798	ARG	ARG	ARG	LYS	ARG	ARG	ARG	ARG	ARG	GLY	GLY	GLY	GLY	ALA
E4072	SER	Q3799	SER	LYS	SER	LYS	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
I4073	ASN	S3800	TYR	MET	ASN	MET	ALA	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY	ALA
D4074	TYR	T3922	TYR	TYR	ILE	LYS	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
T4078	LEU	S3802	SER	LEU	HIS	ARG	LEU	LEU	LEU	LEU	LEU	GLY	GLY	GLY	GLY	ALA
V4085	GLY	L3925	VAL	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA
R4086	THR	D3805	THR	ASP	LYS	ARG	ASP	ASP	ASP	ASP	ASP	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY	GLY	GLY	GLY	ALA
H4087	ASN	A3808	THR	VAL	LYS	MET	VAL	VAL	VAL	VAL	VAL	GLY				

G4956	D4869	R4755	E4660	PRO	ALA	LEU	ASN	LYS	GLU	E4108
D4957	A4870	T4756	E4660	THR	LYS	ILE	MET	MET	ARG	
C4958	F4871	I4757	R4664	ARG	GLU	PRO	PRO	THR	ALA	V4126
	G4872			SER	ASP	HIS	ASP	VAL	ASN	
K4961	E4873	H4763	I4667	SER	LYS	ASN	PRO	ARG	LYS	F4130
E4964	L4874	M4764		SER	GLY	PRO	THR	ASP	GLU	Q4131
ASP	R4875		L4671	GLU	LYS	ASN	GLN	MET	GLU	
GLN		T4771	G4672	ASN	GLN	ALA	ASP	VAL	GLU	L4134
LEU				ALA	LYS	ALA	GLY	ALA	SER	G4135
ASN		L4774	MET	ASP	ARG	LEU	VAL	ALA	GLU	R4136
			LYS	PHE	GLN	ASP	ARG	PHE	LYS	I4137
	K4882	Y4780	ALA	GLY	LEU	ASP	GLY	PHE	LYS	E4138
E4883	L4781		ALA	SER	LEU	LEU	ASP	THR	LYS	I4139
E4884	Y4782		ALA	LEU	HIS	MET	GLY	THR	LYS	I4139
M4885	T4783		THR	ASP	THR	SER	ASP	SER	PRO	M4140
E4886	V4784		ASP	SER	HIS	SER	GLY	TRP	GLU	G4141
T4887			PHE	SER	ARG	PRO	GLY	SER	GLN	S4142
K4888	R4791		SER	SER	TYR	ALA	GLY	VAL	GLY	A4143
C4889			ASP	PRO	GLY	PRO	ARG	PHE	PRO	K4144
F4890	E4798		ALA	ARG	GLU	ILE	LYS	MET	ARG	I4146
I4891	D4799		ARG	ILE	PRO	GLU	VAL	THR	MET	
C4892	G4800		ILE	ALA	VAL	VAL	GLU	LEU	PHE	S4157
G4893			LYS	ALA	PRO	GLN	GLY	LEU	GLY	R4158
I4894	D4804		LYS	GLY	PRO	GLU	THR	PHE	SER	
G4895			LYS	SER	SER	LYS	LEU	ALA	LEU	I4161
	D4808		PRO	S4865	ILE	LYS	ASP	ALA	VAL	E4162
Y4898	D4809		LYS	S4866	ALA	PHE	PRO	ALA	THR	R4163
	M4810		LYS	I4888	PHE	GLN	SER	SER	THR	R4164
N4915	L4811		ASP	K4610	TRP	GLU	GLY	VAL	VAL	
L4916	G4812		SER		LYS	GLN	ASP	SER	ARG	K4170
A4917	C4813		SER		LYS	LYS	LEU	ARG	SER	R4171
I4918			LEU		ILE	ALA	THR	GLY	ALA	
Y4919	Y4819		S4896	G4615		LYS	ASP	PHE	LEU	I4174
				L4616		GLU	LEU	SER	LEU	
F4922	R4823		W4709	Y4617	R4498	GLU	LYS	ARG	ALA	V4178
I4923				I4618	N4499	GLU	GLY	ILE	LEU	N4179
M4924	L4832		L4721		F4500	LYS	LEU	ILE	ARG	
Y4925			Y4722	Q4621		GLU	THR	GLY	TYR	M4187
	Y4840		L4723		M4503	GLU	GLY	GLY	ASN	E4188
			W4725	I4627	R4504	LYS	GLU	LEU	VAL	L4189
	R4844			K4628	M4505	GLU	SER	LEU	LEU	F4190
	I4845			G4629		GLU	ASP	THR	THR	V4191
E4931			M4729	Q4630	I4514	ASN	LEU	GLY	LEU	
	D4848			W4631	N4515	LYS	LEU	GLY	MET	C4194
G4936			L4732	D4632		SER	SER	SER	ARG	
Q4937				R4633	L4518	GLU	ASP	LEU	MET	T4197
E4938	F4852		Y4735		L4519	PRO	ILE	VAL	LEU	
S4939	F4853		N4736	I4636		GLU	PHE	GLU	SER	M4201
Y4940	F4854		N4737		V4523	LYS	GLY	GLY	LEU	Q4202
V4941			F4738	S4640	S4524	ALA	LEU	LYS	SER	I4203
W4942	V4857		F4739		THR	GLU	ASP	LYS	LEU	A4204
	I4858		F4740			GLY	LEU	LYS	LEU	A4205
Y4945	L4859			N4643	SER	ASP	LYS	ILE	LYS	Q4206
	L4860		L4745	Y4644	SER	GLY	GLY	LYS	LYS	
R4948	A4861		D4746	W4646	VAL	GLY	GLU	VAL	GLU	I4207
C4949			I4747	D4647	VAL	GLY	GLY	ALA	MET	SER
W4950	Q4864				GLY	LYS	GLY	GLU	LYS	GLU
	G4865				LYS	GLU	GLY	LEU	LYS	SER
F4953	L4866		K4752	V4650	GLY	GLU	GLY	LEU	ASP	GLU
P4954	I4867		T4753	K4651	LYS	GLU	TYR	LEU	VAL	LEU
A4955	I4868		L4754	R4652	LEU	LYS	LYS	ALA	LYS	ASN



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	48454	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	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	B	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	C	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
1	D	0.98	29/26751 (0.1%)	0.94	78/36149 (0.2%)
All	All	0.98	116/107004 (0.1%)	0.94	312/144596 (0.2%)

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	30
1	B	0	30
1	C	0	30
1	D	0	30
All	All	0	120

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	B	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	C	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	D	4945	TYR	CG-CD1	-10.60	1.25	1.39
1	A	4950	TRP	CE3-CZ3	-9.89	1.21	1.38

The worst 5 of 312 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	B	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	1089	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	4171	ARG	NE-CZ-NH2	-8.50	116.05	120.30

There are no chirality outliers.

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	471	GLU	Peptide
1	A	657	PRO	Peptide
1	A	729	GLY	Peptide
1	A	775	VAL	Peptide
1	A	791	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	26266	0	24898	409	0
1	B	26266	0	24898	421	0
1	C	26266	0	24898	414	0
1	D	26266	0	24898	401	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	105068	0	99592	1515	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 1515 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:A:4873:GLU:HA	1:B:4875:ARG:NH1	1.62	1.15

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4875:ARG:NH1	1:D:4873:GLU:HA	1.62	1.14
1:B:4873:GLU:HA	1:C:4875:ARG:NH1	1.62	1.13
1:C:4873:GLU:OE1	1:D:4875:ARG:HD3	1.49	1.12
1:C:4873:GLU:HA	1:D:4875:ARG:NH1	1.62	1.12

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%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	B	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	C	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
1	D	3289/4968 (66%)	2983 (91%)	285 (9%)	21 (1%)	30	74
All	All	13156/19872 (66%)	11932 (91%)	1140 (9%)	84 (1%)	34	74

5 of 84 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4071	ALA
1	B	4071	ALA
1	C	4071	ALA
1	D	4071	ALA
1	A	730	LEU

### 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	2659/4355 (61%)	2628 (99%)	31 (1%)	78	90
1	B	2658/4355 (61%)	2627 (99%)	31 (1%)	78	90
1	C	2659/4355 (61%)	2627 (99%)	32 (1%)	78	90
1	D	2660/4355 (61%)	2628 (99%)	32 (1%)	78	90
All	All	10636/17420 (61%)	10510 (99%)	126 (1%)	79	90

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4499	ASN
1	C	658	ASN
1	D	4136	ARG
1	B	4652	ARG
1	C	84	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3976	GLN
1	C	593	HIS
1	D	3916	GLN
1	B	4179	ASN
1	C	44	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.