



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:21 PM EDT

PDB ID : 5T9V
EMDB ID: : EMD-8376
Title : Structure of rabbit RyR1 (Caffeine/ATP/Ca²⁺ dataset, class 1)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-09
Resolution : 4.40 Å(reported)

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 : 1.7.1 (RC1), CSD as537be (2016)
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

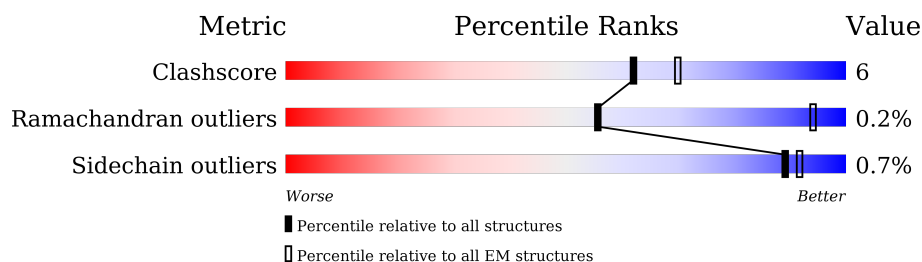
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

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

Mol	Chain	Length	Quality of chain
1	A	108	81% 18% .
1	F	108	81% 18% .
1	H	108	81% 18% .
1	J	108	81% 19% .
2	B	4416	83% 12% 5%
2	E	4416	83% 11% 5%
2	G	4416	83% 11% 5%
2	I	4416	83% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 121456 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

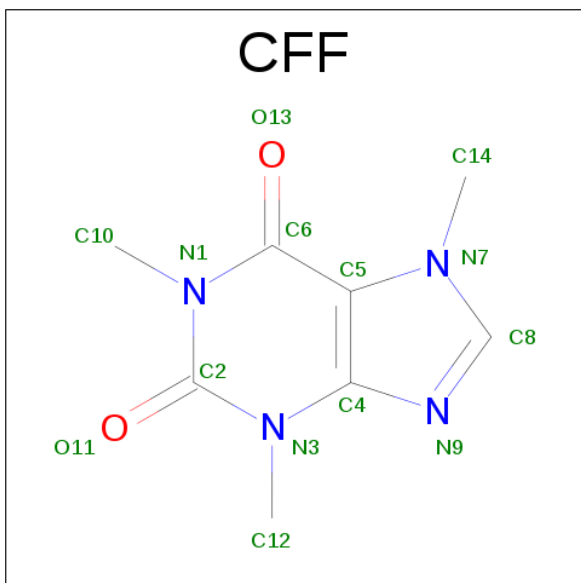
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total 31	C 10	N 5	O 13	P 3	0
3	G	1	Total 31	C 10	N 5	O 13	P 3	0
3	I	1	Total 31	C 10	N 5	O 13	P 3	0
3	E	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $\text{C}_8\text{H}_{10}\text{N}_4\text{O}_2$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	G	1	Total	C	N	O	0
			14	8	4	2	
4	I	1	Total	C	N	O	0
			14	8	4	2	
4	E	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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


- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	I	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 




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

Chain A: 




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

Chain H: 




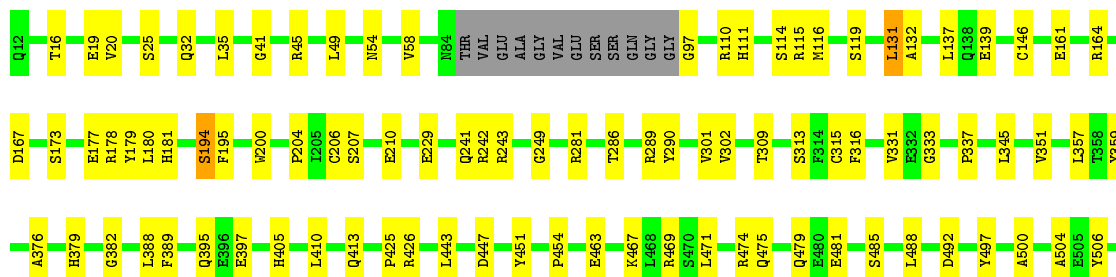
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 

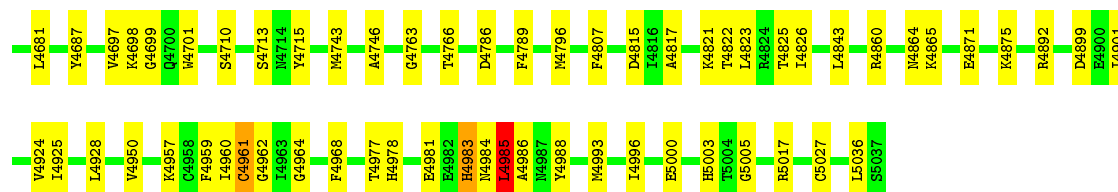


- Molecule 2: Ryanodine receptor 1

Chain B: 

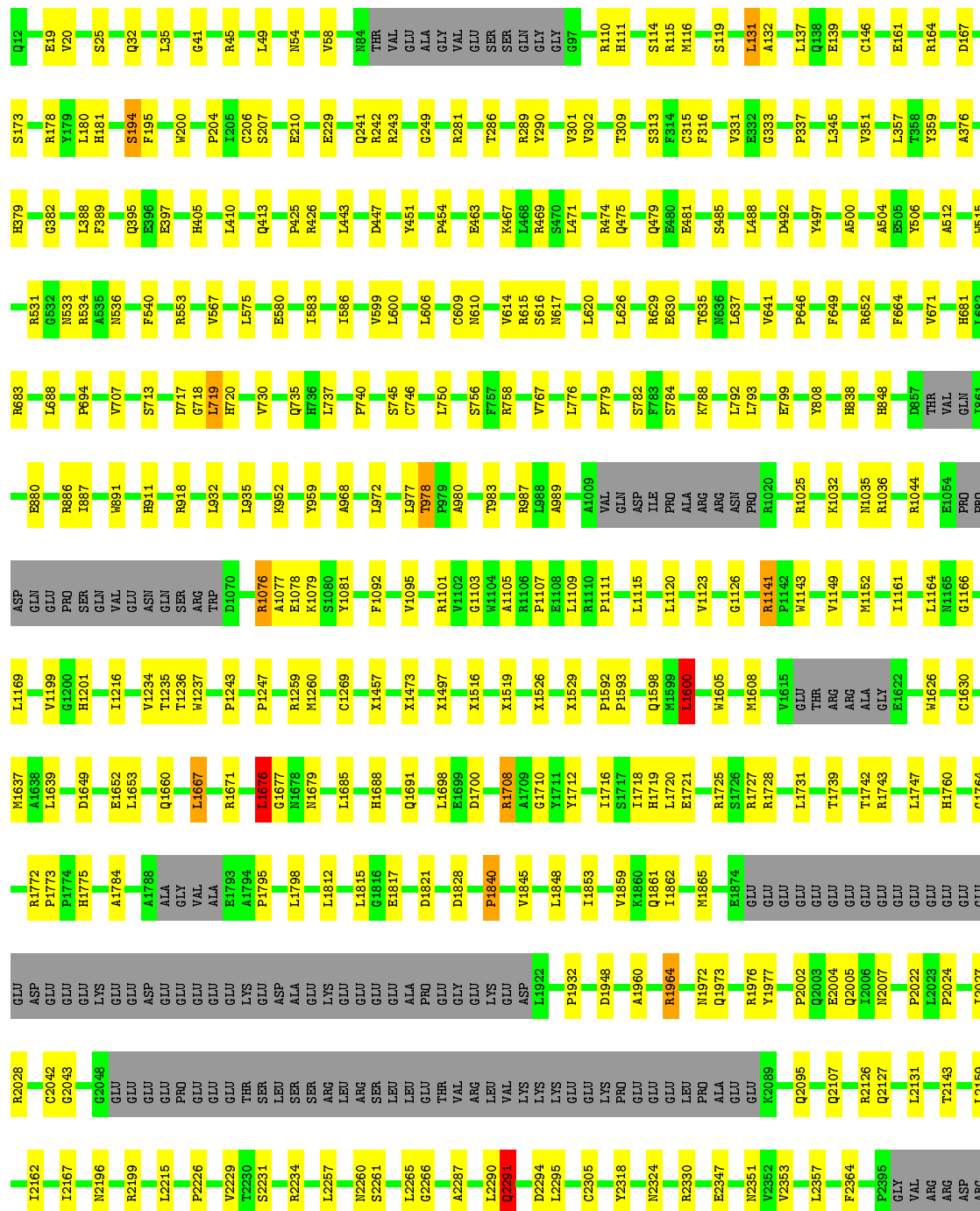





• Molecule 2: Ryanodine receptor 1

Chain G: 83% 11% 5%



ASP	LEU	I4088	L3890	I3674	GLU	ARG
ALA	GLY	T4104	L3891	I3680	LYS	ARG
ALA	GLY	I4816	N3896	A3680	LYS	GLU
GLY	ALA	G4105	N3897	G3681	THR	HIS
SER	SER	P4106	N3898	E3712	ARG	PHE
GLY	GLY	N4120	F3899	E3712	LYS	GLY
GLY	GLY	E4126	Q3900	I3728	GLU	GLU
GLY	GLY	E4126	N3901	I3728	PRO	GLU
SER	SER	N4130	L3903	C3733	THR	PRO
TRP	TRP	I4139	T3910	N3741	ALA	GLU
GLY	GLY	E4152	T3911	GLY	GLN	N2414
ALA	ALA	E4152	I3915	ALA	THR	
GLY	GLY	P4155	S3929	GLU	TYR	I2429
GLU	GLU	P4158	Y3937	GLU	ASP	I2430
GLU	GLU	R4159	Q3946	E3759	PRO	
ASP	GLY	R4161	N3950	R3762	ARG	P2438
ASP	ASP	L4166	Q3960	Q3766	GLY	
ASP	GLU	S4169	Q3960	T3772	GLY	R2452
GLU	GLU	R4180	E3967	R3773	GLY	I2453
M4639	M4639	R4192	G3971	Q3781		L2472
E4640	E4640	R4192	L3980	S3784		L2479
P4641	P4641	E4227	A3981	K3787		X2487
I4658	I4658	A4228	L3985	K3787		
R4673	R4673	M4231	V3986	S3803		X2502
E4674	E4674	E4232	H3994	I3804		P2737
L4681	L4681	N4559	H3994	L3805		R2738
Y4687	Y4687	R4563	H3998	N3809		P2739
V4697	V4697	F4571	K4002	V3812		P2748
K4698	K4698	F4575	L4017	K3815		L2751
G4699	G4699	F4575	E4032	F3816		L2755
Q4700	Q4700	V4582	G4033	L3817		
M4701	M4701	V4582	N4034	Q3830		W2775
Y4715	Y4715	P4587	V4049	Q3833		W2807
M4743	M4743	GLU	L4066	L3842		K2810
A4746	A4746	ASP	E4075	F3847		K2814
A4986	A4986	MET	Q4078	Q3850		I2823
N4987	N4987	GLY	V4081	A3853		
Y4988	Y4988	SER	V4085	Q3889		E2830
M4993	M4993	ALA				GLU
M4796	M4796	ALA				GLU
		GLY				ARG
						THR

• Molecule 2: Ryanodine receptor 1

Chain I:  83% 12% 5%

I887	S713	R553	L388	Q12
W891	D717	V567	F389	T16
T892	G718	L575	Q395	E19
R802	L719	E396	E397	V20
H911	H720	E580	H405	S25
R918	V730	I583	L410	Q32
M924	Q735	I586	Q413	L35
T928	H737	V599	P425	G41
L932	P740	L600	R426	R45
L935	S745	L606	L443	L49
K952	C746	C609	D447	N54
Y959	L750	W614	R242	V58
A968	S756	R615	Y451	N54
L972	F757	S616	P454	THR
L877	R767	L620	E463	VAL
T978	L776	L626	K467	GLU
P979	P779	P627	R469	ALA
A980	S782	G628	S470	GLY
T983	F783	R629	L471	GLU
R987	S784	E530	R474	SER
L988	K788	Q634	Q475	GLN
A989	L792	T635	E481	GLY
A1009	L793	N636	Q479	G97
VAL	E799	L637	E481	R110
GLU	Y808	V641	S485	H111
ASP	H838	P646	L488	S114
ILE	H838	P649	Y497	R115
PRO	H848	R652	A500	M116
ALA	D857	F664	A504	L131
ARG	THR	V671	E505	L137
ASU	VAL	H681	Y506	Q138
PRO	I861	R683	R631	E139
R1020	E876	G683	N533	R164
R1025	N877	L688	A535	D167
K1032	E880	P694	N536	S173
N1035	R886	F540		E177
R1036				R178
R1044				
T1045				
E1054				
PRO				
PRO				
ASP				
GLN				
GLU				
PRO				
SER				
GLN				
VAL				
GLU				
ASN				
GLN				
ARG				
THR				
D1070				
R1076				
E1078				
K1079				
S1080				
Y1081				
F1092				
V1095				
R1101				
V1102				
G1103				
A1105				
P1107				
E1108				
L1109				
R1110				
P1111				
L1115				
L1120				
V1123				
G1126				
R1141				
P1142				
W1143				
V1149				
M1152				
I1161				

L1164	M1637	H1760	P2024	R2126	F2364	K2810	X3552	K3815	K4002	F4575	Q4700	G4964
M1165	A1638	G1764	I2027	Q2127	P2395	K2814	X3556	M3816	L4017	V4582	W4701	F4968
G1166	L1639	R1772	R2028	L2131	GLY	L2823	N3651	L3817	E4032	V4587	Y4715	T4977
L1169	H1640	P1773	Q2029	T2143	ARG	E2830	K3658	Q3830	G4033	GLY	M4743	H4978
V1199	P1642	H1775	D2033	L2159	ASP	GLU	K3658	Q3833	N4034	GLU	A4746	E4981
H1200	D1649	A1784	F2034	I2162	ASP	THR	W3661	L3842	V4049	ASP	G4763	E4982
H1201	E1652	L1653	L2038	I2167	ARG	LYS	I3662	F3847	L4066	MET	T4766	H4983
I1216	L1653	A1788	C2042	L2196	GLU	THR	L3663	Q3850	E4075	GLY	D4786	A4985
V1234	Q1660	ALA	G2043	M2196	PHE	LYS	I3674	A3853	Q4078	SER	F4789	A4986
T1235	Q1667	GLY	G2043	R2199	GLY	LYS	L3677	Q3889	V4081	ALA	F4789	Y4988
T1236	L1667	VAL	G2043	R2199	GLU	THR	A3680	L3890	R4085	ASP	M4796	M4993
W1237	R1671	ALA	G2043	L2215	PRO	ILE	G3681	L3891	I4088	LEU	F4807	I4996
P1243	P1676	L1795	G2043	P2226	GLU	SER	L3698	L3891	T4104	ALA	D4815	K4997
P1247	M1679	L1798	G2043	V2229	GLU	THR	E3712	N3896	G4105	GLY	A4816	D4999
R1259	L1685	L1812	G2043	S2231	THR	ALA	I3728	D3898	P4106	SER	A4917	E5000
M1260	H1688	L1815	G2043	R2234	LEU	THR	C3733	Q3900	E4126	GLY	T4822	H5003
C1269	Q1691	G1816	G2043	L2257	SER	ASP	N3741	F3899	M4120	GLY	L4823	T5004
X1457	L1698	E1817	G2043	S2261	ARG	ARG	GLY	L3903	E4126	SER	R4824	G5005
X1497	E1693	D1821	G2043	I2260	LEU	GLY	ALA	L3903	E4126	TRP	I4826	Q5006
X1516	D1700	D1828	G2043	S2261	SER	GLY	GLU	T3910	M4130	GLY	L4843	E5007
X1519	R1708	P1840	G2043	G2266	LEU	S2868	GLU	I3915	I4139	ALA	R4860	R5017
X1526	G1710	P1840	G2043	G2266	THR	R2869	E3747	S3929	E4152	GLY	N4864	C5027
X1529	Y1711	V1845	G2043	A2287	VAL	Q2872	E3759	Y3937	P4155	ALA	K4865	L5036
P1593	I1716	L1848	G2043	L2290	ARG	N2884	R3762	Q3946	P4158	ALA	E4871	S5037
Q1598	S1717	I1853	G2043	Q2291	VAL	R2888	Q3766	N3950	R4159	GLY	K4875	R110
M1599	H1719	V1859	G2043	L2294	LYS	L2911	H3771	Q3960	L4160	ASP	R4892	S114
L1600	L1720	E1860	G2043	L2295	GLU	L2916	T3772	Q3967	L4166	ASP	D4899	R115
W1605	E1721	Q1861	G2043	C2305	GLU	K2916	R3773	E3971	S4169	GLU	E4900	M116
M1608	R1725	M1865	G2043	Y2318	LYS	L2930	G3774	G3971	R4180	GLU	I4901	L131
V1615	S1728	R1728	G2043	I2324	GLU	L2930	S3784	L3980	R4192	GLU	V4924	A132
GLU	R1728	GLU	G2043	R2330	LEU	X2950	K3787	A3981	E4227	M4639	I4925	L137
THR	L1731	GLU	G2043	E2347	PRO	X2950	S3803	R3984	A4228	E4640	L4928	Q138
ARG	T1739	GLU	G2043	I2351	GLU	X2954	L3804	L3985	E4674	P4641	K4957	E139
ALA	T1742	GLU	G2043	V2353	GLU	X3361	L3805	V3986	M4231	I4658	C4958	R164
GLY	R1743	GLU	G2043	L2357	GLU	X3362	N3809	H3994	E4232	Y4687	F4959	D167
E1622	L1747	GLU	G2043	L2357	GLU	X3365	V3812	H3998	R4563	V4697	I4960	S173
W1626	L1747	GLU	G2043	L2357	GLU	X3366	V3812	H3998	F4571	K4698	C4961	E177
C1630	L1747	GLU	G2043	L2357	GLU	X3366	V3812	H3998	F4571	G4699	G4962	Y178
												L180

• Molecule 2: Ryanodine receptor 1

Chain E: 83% 11% 5%

Q12	R110	S114	L131	L137	R164	D167	S173	E177	Y178	L180
E19	H111	R115	A132	Q138	L139	L143	L149	C4961	G4962	L180
V20		M116		E139						
S25										
Q32										
L35										
G41										
R45										
L49										
N54										
V58										
N84										
THR										
VAL										
GLU										
ALA										
GLY										
VAL										
GLU										
SER										
SER										
GLN										
GLY										
GLY										
G97										







4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, ZN, CA, ATP

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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	10/34534 (0.0%)
2	E	0.30	0/25428	0.54	10/34534 (0.0%)
2	G	0.30	0/25428	0.54	10/34534 (0.0%)
2	I	0.30	0/25428	0.54	10/34534 (0.0%)
All	All	0.30	0/105048	0.54	40/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	14
2	E	0	14
2	G	0	14
2	I	0	14
All	All	0	56

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	131	LEU	CA-CB-CG	7.69	132.98	115.30
2	B	131	LEU	CA-CB-CG	7.67	132.95	115.30
2	E	131	LEU	CA-CB-CG	7.67	132.93	115.30
2	G	131	LEU	CA-CB-CG	7.65	132.90	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4985	LEU	CA-CB-CG	6.48	130.20	115.30

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	194	SER	Peptide
2	B	694	PRO	Peptide
2	B	808	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	13	0
1	F	818	0	824	13	0
1	H	818	0	824	12	0
1	J	818	0	824	15	0
2	B	29499	0	24748	311	0
2	E	29499	0	24748	298	0
2	G	29499	0	24748	300	0
2	I	29499	0	24748	305	0
3	B	31	0	12	1	0
3	E	31	0	12	1	0
3	G	31	0	12	1	0
3	I	31	0	12	1	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
All	All	121456	0	102376	1234	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 6.

The worst 5 of 1234 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.64	0.86
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.64	0.86
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.64	0.85
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.64	0.85
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.81	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2890 (89%)	338 (10%)	7 (0%)	52	86
2	E	3235/4416 (73%)	2888 (89%)	340 (10%)	7 (0%)	52	86
2	G	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	52	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3235/4416 (73%)	2889 (89%)	339 (10%)	7 (0%)	52	86
All	All	13360/18096 (74%)	11932 (89%)	1400 (10%)	28 (0%)	56	86

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	I	1708	ARG
2	E	1708	ARG
2	E	4985	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	E	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	G	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
2	I	2493/3022 (82%)	2474 (99%)	19 (1%)	86	93
All	All	10324/12444 (83%)	10248 (99%)	76 (1%)	89	94

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	4120	ASN
2	I	1076	ARG
2	E	4034	ASN
2	G	4166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3946	GLN
2	I	111	HIS
2	E	3950	ASN
2	G	3960	GLN
2	G	4833	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	B	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.23	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	E	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.59	2 (7%)
4	CFF	E	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.22	1 (12%)
3	ATP	G	5101	-	26,33,33	0.92	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	G	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.23	1 (12%)
3	ATP	I	5101	-	26,33,33	0.91	1 (3%)	26,52,52	1.58	2 (7%)
4	CFF	I	5102	-	8,15,15	2.42	3 (37%)	8,23,23	1.22	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	B	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	E	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	G	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	0/0/0/0	0/2/2/2
3	ATP	I	5101	-	-	0/18/38/38	0/3/3/3
4	CFF	I	5102	-	-	0/0/0/0	0/2/2/2

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C4-N3	-4.43	1.34	1.39
4	B	5102	CFF	C4-N3	-4.42	1.34	1.39
4	I	5102	CFF	C4-N3	-4.42	1.34	1.39
4	G	5102	CFF	C4-N3	-4.39	1.34	1.39
4	G	5102	CFF	C6-N1	-4.10	1.32	1.38

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5101	ATP	N3-C2-N1	-5.95	124.20	128.87
3	B	5101	ATP	N3-C2-N1	-5.91	124.23	128.87
3	G	5101	ATP	N3-C2-N1	-5.89	124.25	128.87
3	I	5101	ATP	N3-C2-N1	-5.88	124.26	128.87
4	E	5102	CFF	C14-N7-C8	-2.56	111.94	125.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5101	ATP	1	0
3	E	5101	ATP	1	0
3	G	5101	ATP	1	0
3	I	5101	ATP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
2	I	14
2	E	14

The worst 5 of 56 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.47
1	G	4345:UNK	C	4540:PHE	N	73.47
1	I	4345:UNK	C	4540:PHE	N	73.47
1	E	4345:UNK	C	4540:PHE	N	73.47
1	B	3613:UNK	C	3639:THR	N	45.62