



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 08:31 PM EDT

PDB ID : 5TAY
EMDB ID: : EMD-8389
Title : Structure of rabbit RyR1 (ryanodine dataset, class 2)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.;
Frank, J.
Deposited on : 2016-09-10
Resolution : 4.60 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 : 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

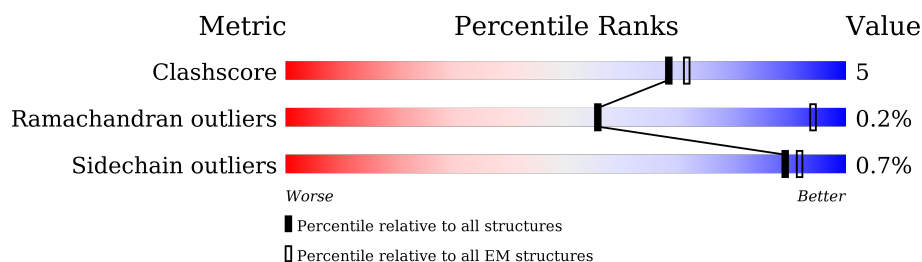
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 121276 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 ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

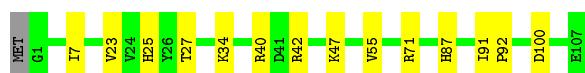
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0
4	E	1	Total 1	Ca 1	0

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: 




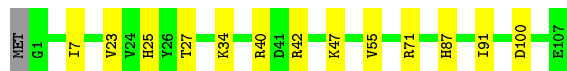
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



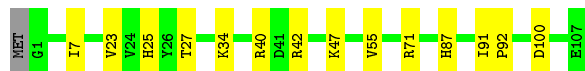
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




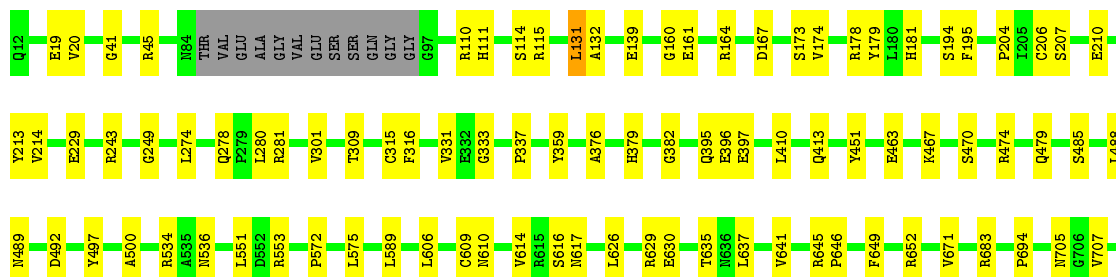
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryanodine receptor 1

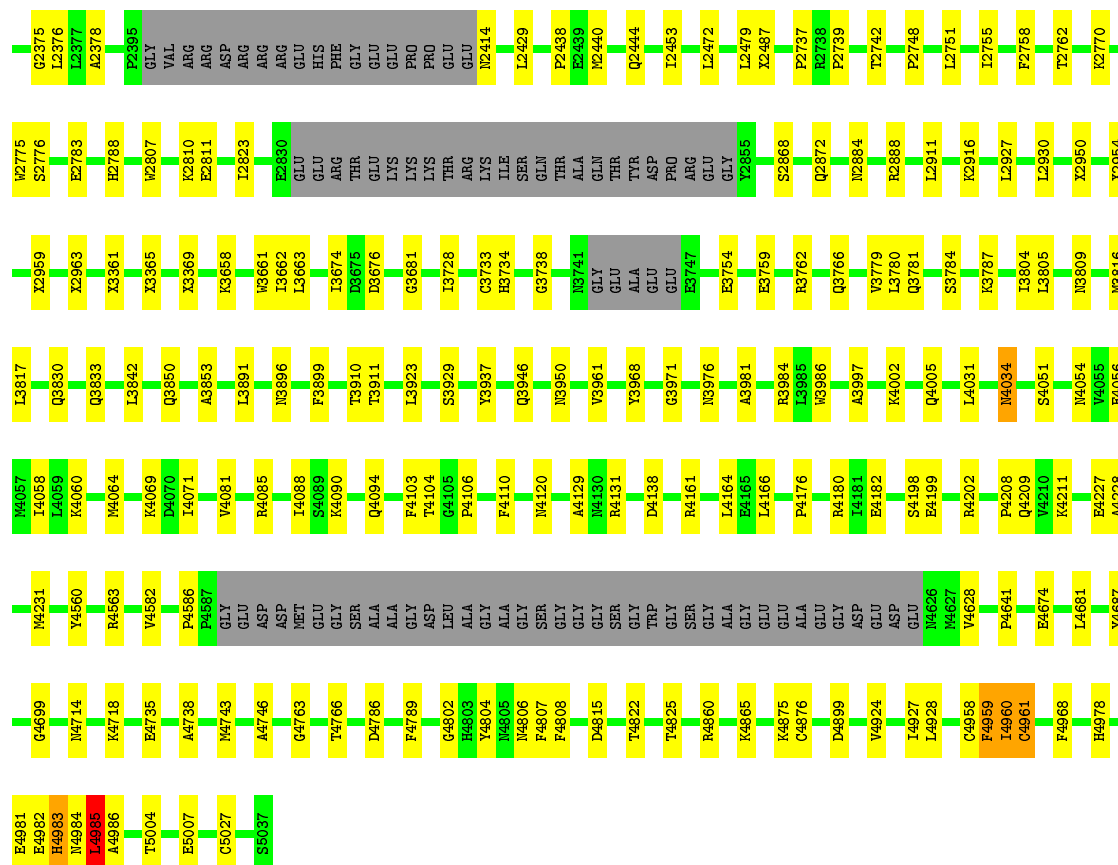
Chain B: 



T4825	ALA	L4166	G3971	E3754	I2884	P2739	I2351	I2167	I2188	I2185	I2167	I2131	I2107	I2006	I2005	I2004	I2003	I2002	GLU	GLU	I1695	H1260	E1054	I1053	P888	S713
R4860	GLY	P4176	I3976	E3759	I2888	I2742	V2352	I2308	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	D717
I4865	ASP	R4180	A3981	I3763	I2911	I2748	V2353	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	G718
K4875	GLU	R4181	A3981	I3763	I2911	I2748	V2353	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L720
C4876	ASP	R4182	A3986	I3766	I2916	I2751	V2358	I2308	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	H730
R4892	GLU	S4198	A3997	I3779	I2927	I2755	V2359	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	H735
V4914	GLU	E4199	K4002	I3780	I2927	I2758	V2364	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L737
V4924	GLU	R4202	Q4005	I3784	I2930	I2762	V2368	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	P740
L4928	GLU	P4208	I4031	I3787	I2950	I2770	V2376	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	V744
I4936	GLU	R4210	I4034	I3787	I2954	I2775	V2377	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L750
C4958	GLU	E4227	S4051	I3804	I2959	I2783	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	I789
F4959	GLU	R4228	I4054	I3809	I2963	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L776
I4960	GLU	R4231	I4055	I3816	I2964	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	P779
C4961	GLU	R4210	I4056	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	S782
F4968	GLU	R4210	I4057	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	K788
T4708	GLU	R4210	I4058	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L789
F4709	GLU	R4210	I4059	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	G794
I4714	GLU	R4210	I4060	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	H797
F4981	GLU	R4210	I4061	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	6798
F4982	GLU	R4210	I4062	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	L823
I4983	GLU	R4210	I4063	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	E824
I4984	GLU	R4210	I4064	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	6841
L4985	GLU	R4210	I4065	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	H848
A4986	GLU	R4210	I4066	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	P853
T5004	GLU	R4210	I4067	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	D857
E5007	GLU	R4210	I4068	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	VAL
C5027	GLU	R4210	I4069	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	VAL
S5037	GLU	R4210	I4070	I3817	I2965	I2788	V2395	I2309	I2048	I2043	I2042	I2041	I2040	I2039	I2038	I2037	I2036	I2035	I2034	GLU	GLU	L1698	C1269	E0890	Q889	GLN
																										T861
																										1870
																										K873
																										N877
																										R886
																										1887

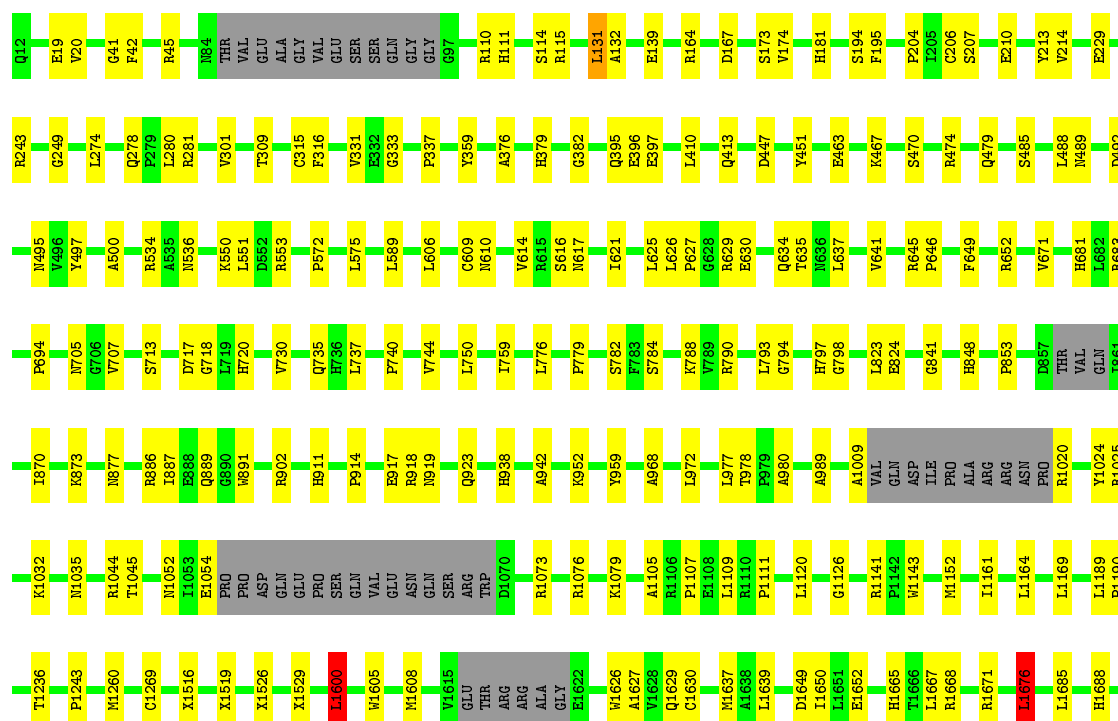
Chain G: 84% 10% 5%





• Molecule 2: Ryanodine receptor 1

Chain E: 84% 10% 5%



R4860	L4166	R3984	Q2872	E2738	F2340	Q2107	Q2005	GLU	Q1691
K4865	P4176	L3985	M2884	P2739	E2347	Q2127	I2006	GLU	L1695
K4875	R4180	W3986	R2888	T2742	E2347	Y2128	M2007	GLU	D1700
C4876	A3997	L3780	L2911	P2748	M2351	D2129	F2012	GLU	L1707
Y4888	E4181	Q3781	L2911	L2751	Y2352	L2131	P2022	GLU	R1708
V4924	E4182	K2916	K2916	L2755	V2353	E2132	P2023	GLU	A1709
L4928	S4198	K3787	K2916	L2755	L2357	E2133	P2024	GLU	G1710
C4958	E4199	K3787	L2927	F2758	L2358	L2144	R2028	ASP	Y1711
F4959	R4202	L3804	L2930	T2762	R2359	L2167	C2042	GLU	L1720
I4960	M4034	L3805	X2950	K2770	F2364	I2185	G2043	GLU	E1721
C4961	S4051	M3809	X2954	K2775	L2368	N2188	G2048	LYS	R1725
F4968	N4054	M3816	X2959	W2775	G2375	N2196	GLU	GLU	S1728
H4978	V4055	L3817	X2963	S2776	L2376	R2199	GLU	ASP	R1727
E4981	E4056	Q3830	X2963	E2783	L2377	L2215	GLU	GLU	R1728
E4982	E4057	Q3833	X3361	E2788	A2378	L2215	GLU	GLU	L1731
E4983	I4058	L3842	X3365	H2788	P2395	L2215	GLU	GLU	G1764
I4984	K4060	F3847	X3369	W2807	GLY	P2226	GLU	LYS	R1772
A4986	M4064	Q3850	X3369	K2810	VAL	V2229	THR	ASP	H1775
T5004	P4586	A3853	K3658	E2811	ARG	T2230	LEU	ALA	A1784
E5007	P4587	L3891	L3662	I2823	ARG	S2231	ARG	GLU	A1788
C5027	GLY	L3891	L3663	E2830	GLU	R2234	LEU	GLU	ALA
S5037	GLY	L3896	L3674	GLU	HIS	Q2247	ARG	GLU	GLY
	ASP	M3896	D3675	GLU	ARG	N2260	LEU	ALA	VAL
	ASP	F3899	D3676	THR	GLY	L2265	LEU	PRO	ALA
	GLY	T3910	G3681	GLU	GLU	L2265	THR	GLY	E1793
	ALA	T3911	I3728	LYS	PRO	T2271	VAL	GLY	A1794
	ALA	L3923	C3733	LYS	PRO	P2272	ARG	GLU	P1795
	ASP	S3929	H3734	THR	GLU	L2273	LEU	LYS	I1802
	LEU	Y3937	G3738	LYS	N2414	L2273	VAL	ASP	K1810
	ALA	Y3946	N3741	ILE	L2429	A2277	LYS	LYS	L1922
	GLY	Q3946	GLY	THR	L2429	E2285	GLU	LYS	P1932
	GLY	N3950	GLU	THR	A2437	L2290	LYS	GLU	D1828
	GLY	V3961	ALA	ASP	P2438	Q2291	LYS	GLU	P1840
	GLY	Y3968	GLU	THR	E2439	L2295	PRO	GLU	T1847
	TRP	G3971	E3747	THR	M2440	D2294	GLU	GLU	Y1865
	GLY	R4161	E3754	THR	Q2444	L2295	GLU	GLU	V1859
	GLY	L4164	E3759	ASP	I2453	Y2318	LEU	GLU	M1865
	ALA	E4165	R3762	ARG	L2472	C2326	PRO	GLU	E1874
				GLY	L2479	G2327	ALA	GLU	E1874
				Y2855	X2487	R2330	GLU	GLU	GLU
				S2868	P2737	F2337	R2089	GLU	GLU
							Q2095	GLU	GLU
								GLU	E2004

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: ZN, CA

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	0.30	0/834	0.53	0/1123
1	F	0.30	0/834	0.53	0/1123
1	H	0.30	0/834	0.53	0/1123
1	J	0.30	0/834	0.53	0/1123
2	B	0.30	0/25428	0.54	6/34534 (0.0%)
2	E	0.30	0/25428	0.54	6/34534 (0.0%)
2	G	0.30	0/25428	0.54	6/34534 (0.0%)
2	I	0.30	0/25428	0.54	6/34534 (0.0%)
All	All	0.30	0/105048	0.54	24/142628 (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	11
2	E	0	11
2	G	0	11
2	I	0	11
All	All	0	44

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	131	LEU	CA-CB-CG	7.94	133.56	115.30
2	I	131	LEU	CA-CB-CG	7.93	133.53	115.30
2	B	131	LEU	CA-CB-CG	7.92	133.53	115.30
2	G	131	LEU	CA-CB-CG	7.91	133.49	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1676	LEU	CA-CB-CG	6.62	130.52	115.30

There are no chirality outliers.

5 of 44 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	694	PRO	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	6	0
1	F	818	0	824	10	0
1	H	818	0	824	9	0
1	J	818	0	824	9	0
2	B	29499	0	24750	264	0
2	E	29499	0	24750	264	0
2	G	29499	0	24750	256	0
2	I	29499	0	24750	256	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	121276	0	102296	1050	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1050 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:B:4968:PHE:HE2	2:B:4978:HIS:CE1	1.29	1.49
2:E:4968:PHE:HE2	2:E:4978:HIS:CE1	1.29	1.48
2:I:4968:PHE:HE2	2:I:4978:HIS:CE1	1.29	1.48
2:G:4968:PHE:HE2	2:G:4978:HIS:CE1	1.29	1.48
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.09	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4416 (73%)	2892 (89%)	337 (10%)	6 (0%)	52	86
2	E	3235/4416 (73%)	2894 (90%)	335 (10%)	6 (0%)	52	86
2	G	3235/4416 (73%)	2895 (90%)	334 (10%)	6 (0%)	52	86
2	I	3235/4416 (73%)	2891 (89%)	338 (10%)	6 (0%)	52	86
All	All	13360/18096 (74%)	11944 (89%)	1392 (10%)	24 (0%)	56	86

5 of 24 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

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Mol	Chain	Res	Type
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	4959	PHE
2	I	1141	ARG
2	E	4120	ASN
2	G	4960	ILE
2	I	131	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	3960	GLN
2	I	383	HIS
2	E	3946	GLN
2	G	3994	HIS

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Mol	Chain	Res	Type
2	G	4806	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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14

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Mol	Chain	Number of breaks
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	73.85
1	G	4345:UNK	C	4540:PHE	N	73.85
1	I	4345:UNK	C	4540:PHE	N	73.85
1	E	4345:UNK	C	4540:PHE	N	73.85
1	B	3613:UNK	C	3639:THR	N	45.57