Integrative Structure Validation Report

February 18, 2025 - 08:38 AM PST

The following software was used in the production of this report:

Integrative Modeling Validation Version 2.0
Python-IHM Version 1.8
MolProbity Version 4.5.2

PDB ID	9A3W
PDB-Dev ID	PDBDEV_00000217
Structure Title	Structure of the phage immune evasion protein Gad1 bound to the Gabija GajAB complex
Structure Authors	Antine, S.P.; Johnson, A.G.; Mooney, S.E.; Mayer, M.L.; Kranzusch, P.J.
Deposited on	2023-10-26

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

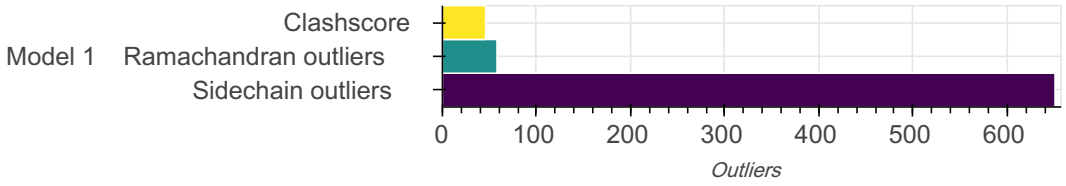
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: MolProbity Analysis



Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 1 model(s). A total of 4 datasets were used to build this entry.

Representation

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	Gabija protein GajA	A	626	-	1-626	100.00 / 100.00	Atomic
				B					
				C					
				D					
		2	Gabija protein GajB	E	493	-	1-493	100.00 / 100.00	Atomic
				F					
				G					
				H					
		3	Gabija anti-defense 1	I	295	-	1-295	100.00 / 100.00	Atomic
				J					
				K					
				L					
				M					
				N					
				O					
				P					

Datasets used for modeling

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	8U7I
2	Experimental model	PDB	8SM3
3	De Novo model	Not available	Not available
4	3DEM volume	EMDB	EMD-41983

Methodology and software

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	None	None	None	None	False	False
2	1	None	None	None	None	False	False

There are 3 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	Coot	0.8.9.3 EL	model building	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/
3	AlphaFold2	v2.2.4	model building	https://alphafold.ebi.ac.uk/
1	PHENIX	1.20.1-4487	refinement	https://phenix-online.org/

Data quality

3DEM volume

Validation for this section is under development.

Model quality

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Standard geometry: bond outliers

There are 114 bond length outliers in this entry (0.20% of 56306 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	57	GLU	CB-CG	58.25	3.27	1.52	1	1
L	57	GLU	CB-CG	58.24	3.27	1.52	1	1
I	57	GLU	CB-CG	58.24	3.27	1.52	1	1
K	57	GLU	CB-CG	58.24	3.27	1.52	1	1
L	131	LEU	C-N	38.92	1.87	1.33	1	1
I	131	LEU	C-N	35.90	1.83	1.33	1	1
K	57	GLU	CA-CB	15.96	1.85	1.53	1	1
I	57	GLU	CA-CB	15.95	1.85	1.53	1	1
L	57	GLU	CA-CB	15.95	1.85	1.53	1	1
J	57	GLU	CA-CB	15.92	1.85	1.53	1	1
L	56	ILE	N-CA	15.87	1.76	1.46	1	1
J	56	ILE	N-CA	15.86	1.76	1.46	1	1
I	56	ILE	N-CA	15.85	1.76	1.46	1	1
K	56	ILE	N-CA	15.85	1.76	1.46	1	1
K	56	ILE	CA-C	15.84	1.86	1.52	1	1
L	56	ILE	CA-C	15.84	1.86	1.52	1	1
I	56	ILE	CA-C	15.84	1.86	1.52	1	1
J	56	ILE	CA-C	15.82	1.86	1.52	1	1
I	54	SER	CA-C	15.20	1.84	1.52	1	1
J	54	SER	CA-C	15.19	1.84	1.52	1	1
K	54	SER	CA-C	15.18	1.84	1.52	1	1
L	54	SER	CA-C	15.17	1.84	1.52	1	1
L	127	ILE	C-N	14.60	1.53	1.33	1	1
J	127	ILE	C-N	14.58	1.53	1.33	1	1
I	127	ILE	C-N	14.56	1.53	1.33	1	1
K	127	ILE	C-N	14.53	1.53	1.33	1	1
J	55	VAL	N-CA	13.59	1.72	1.46	1	1
K	55	VAL	N-CA	13.58	1.72	1.46	1	1
L	55	VAL	N-CA	13.58	1.72	1.46	1	1
I	55	VAL	N-CA	13.57	1.72	1.46	1	1
L	57	GLU	N-CA	12.84	1.70	1.46	1	1
K	57	GLU	N-CA	12.81	1.70	1.46	1	1
I	57	GLU	N-CA	12.81	1.70	1.46	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	57	GLU	N-CA	12.80	1.70	1.46	1	1
K	55	VAL	CA-C	12.31	1.78	1.52	1	1
L	55	VAL	CA-C	12.29	1.78	1.52	1	1
I	55	VAL	CA-C	12.28	1.78	1.52	1	1
J	55	VAL	CA-C	12.26	1.78	1.52	1	1
N	129	GLY	C-N	10.94	1.48	1.33	1	1
P	129	GLY	C-N	10.91	1.48	1.33	1	1
O	129	GLY	C-N	10.90	1.48	1.33	1	1
M	129	GLY	C-N	10.88	1.48	1.33	1	1
L	53	PRO	C-N	9.60	1.46	1.33	1	1
K	53	PRO	C-N	9.59	1.46	1.33	1	1
I	53	PRO	C-N	9.57	1.46	1.33	1	1
J	53	PRO	C-N	9.56	1.46	1.33	1	1
M	58	LYS	C-N	9.06	1.46	1.33	1	1
O	58	LYS	C-N	9.00	1.46	1.33	1	1
P	58	LYS	C-N	9.00	1.45	1.33	1	1
N	58	LYS	C-N	8.99	1.45	1.33	1	1
J	54	SER	N-CA	8.78	1.62	1.46	1	1
L	54	SER	N-CA	8.78	1.62	1.46	1	1
K	54	SER	N-CA	8.78	1.62	1.46	1	1
I	54	SER	N-CA	8.77	1.62	1.46	1	1
J	55	VAL	C-N	8.70	1.45	1.33	1	1
I	55	VAL	C-N	8.69	1.45	1.33	1	1
L	55	VAL	C-N	8.69	1.45	1.33	1	1
K	55	VAL	C-N	8.65	1.45	1.33	1	1
L	54	SER	C-N	8.56	1.45	1.33	1	1
I	54	SER	C-N	8.53	1.45	1.33	1	1
K	54	SER	C-N	8.51	1.45	1.33	1	1
J	54	SER	C-N	8.49	1.45	1.33	1	1
J	56	ILE	C-N	8.29	1.45	1.33	1	1
I	56	ILE	C-N	8.24	1.44	1.33	1	1
L	56	ILE	C-N	8.23	1.44	1.33	1	1
K	56	ILE	C-N	8.21	1.44	1.33	1	1
P	40	GLU	C-N	6.30	1.24	1.33	1	1
O	40	GLU	C-N	6.30	1.24	1.33	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
M	40	GLU	C-N	6.29	1.24	1.33	1	1
N	40	GLU	C-N	6.25	1.24	1.33	1	1
K	40	GLU	C-N	6.12	1.24	1.33	1	1
I	40	GLU	C-N	6.12	1.24	1.33	1	1
L	40	GLU	C-N	6.11	1.24	1.33	1	1
J	40	GLU	C-N	6.11	1.24	1.33	1	1
P	53	PRO	N-CD	5.59	1.55	1.47	1	1
O	53	PRO	N-CD	5.57	1.55	1.47	1	1
N	53	PRO	N-CD	5.56	1.55	1.47	1	1
M	53	PRO	N-CD	5.53	1.55	1.47	1	1
I	53	PRO	N-CD	5.50	1.55	1.47	1	1
J	53	PRO	N-CD	5.48	1.55	1.47	1	1
K	53	PRO	N-CD	5.47	1.55	1.47	1	1
L	53	PRO	N-CD	5.45	1.55	1.47	1	1
L	109	GLU	C-N	5.33	1.40	1.33	1	1
I	109	GLU	C-N	5.32	1.40	1.33	1	1
N	123	VAL	C-N	5.32	1.25	1.33	1	1
K	109	GLU	C-N	5.31	1.40	1.33	1	1
P	123	VAL	C-N	5.28	1.26	1.33	1	1
J	109	GLU	C-N	5.28	1.40	1.33	1	1
O	123	VAL	C-N	5.25	1.26	1.33	1	1
M	123	VAL	C-N	5.18	1.26	1.33	1	1
L	123	VAL	C-N	5.14	1.26	1.33	1	1
I	123	VAL	C-N	5.11	1.26	1.33	1	1
J	123	VAL	C-N	5.11	1.26	1.33	1	1
K	123	VAL	C-N	5.10	1.26	1.33	1	1
M	130	GLU	C-N	4.88	1.40	1.33	1	1
P	130	GLU	C-N	4.84	1.40	1.33	1	1
O	130	GLU	C-N	4.82	1.40	1.33	1	1
N	130	GLU	C-N	4.80	1.40	1.33	1	1
P	126	GLU	C-N	4.47	1.27	1.33	1	1
N	126	GLU	C-N	4.46	1.27	1.33	1	1

Standard geometry: angle outliers

There are 135 bond angle outliers in this entry (0.18% of 75702 assessed bonds). A summary is provided below. The output is limited to 100 rows.

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	131	LEU	C-N-CA	32.75	62.75	121.70	1	1
I	131	LEU	C-N-CA	30.10	67.53	121.70	1	1
K	57	GLU	CA-CB-CG	22.34	158.79	114.10	1	1
I	57	GLU	CA-CB-CG	22.34	158.79	114.10	1	1
J	57	GLU	CA-CB-CG	22.34	158.79	114.10	1	1
L	57	GLU	CA-CB-CG	22.33	158.77	114.10	1	1
I	131	LEU	O-C-N	22.32	87.29	123.00	1	1
L	131	LEU	O-C-N	19.92	91.13	123.00	1	1
K	53	PRO	C-N-CA	17.06	152.40	121.70	1	1
L	53	PRO	C-N-CA	17.05	152.39	121.70	1	1
I	53	PRO	C-N-CA	17.05	152.38	121.70	1	1
J	53	PRO	C-N-CA	17.03	152.35	121.70	1	1
K	57	GLU	CB-CG-CD	16.72	141.03	112.60	1	1
I	57	GLU	CB-CG-CD	16.71	141.01	112.60	1	1
L	57	GLU	CB-CG-CD	16.70	141.00	112.60	1	1
J	57	GLU	CB-CG-CD	16.70	140.98	112.60	1	1
L	131	LEU	CA-C-N	15.25	85.70	116.20	1	1
I	131	LEU	CA-C-N	13.53	89.15	116.20	1	1
M	128	ASP	O-C-N	12.70	102.68	123.00	1	1
N	128	ASP	O-C-N	12.69	102.70	123.00	1	1
O	128	ASP	O-C-N	12.67	102.72	123.00	1	1
P	128	ASP	O-C-N	12.67	102.73	123.00	1	1
J	53	PRO	CA-C-N	11.16	93.88	116.20	1	1
K	53	PRO	CA-C-N	11.16	93.89	116.20	1	1
I	53	PRO	CA-C-N	11.15	93.89	116.20	1	1
L	53	PRO	CA-C-N	11.15	93.89	116.20	1	1
L	118	GLU	C-N-CA	10.73	141.02	121.70	1	1
I	118	GLU	C-N-CA	10.73	141.01	121.70	1	1
J	118	GLU	C-N-CA	10.72	140.99	121.70	1	1
K	118	GLU	C-N-CA	10.71	140.97	121.70	1	1
L	55	VAL	N-CA-C	9.99	138.97	111.00	1	1
K	55	VAL	N-CA-C	9.99	138.96	111.00	1	1
I	55	VAL	N-CA-C	9.98	138.94	111.00	1	1
J	55	VAL	N-CA-C	9.97	138.92	111.00	1	1
J	54	SER	CA-C-N	8.53	133.26	116.20	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
L	54	SER	CA-C-N	8.51	133.23	116.20	1	1
I	54	SER	CA-C-N	8.51	133.23	116.20	1	1
K	54	SER	CA-C-N	8.50	133.20	116.20	1	1
I	109	GLU	C-N-CA	8.35	106.66	121.70	1	1
L	109	GLU	C-N-CA	8.35	106.67	121.70	1	1
K	109	GLU	C-N-CA	8.34	106.68	121.70	1	1
J	109	GLU	C-N-CA	8.32	106.72	121.70	1	1
N	58	LYS	C-N-CA	7.97	136.04	121.70	1	1
P	58	LYS	C-N-CA	7.96	136.03	121.70	1	1
O	58	LYS	C-N-CA	7.95	136.02	121.70	1	1
M	58	LYS	C-N-CA	7.93	135.98	121.70	1	1
J	56	ILE	N-CA-C	7.63	132.35	111.00	1	1
K	56	ILE	N-CA-C	7.62	132.34	111.00	1	1
I	56	ILE	N-CA-C	7.62	132.34	111.00	1	1
L	56	ILE	N-CA-C	7.62	132.33	111.00	1	1
I	54	SER	N-CA-C	7.10	130.89	111.00	1	1
K	54	SER	N-CA-C	7.10	130.89	111.00	1	1
J	54	SER	N-CA-C	7.10	130.88	111.00	1	1
L	54	SER	N-CA-C	7.10	130.88	111.00	1	1
J	55	VAL	CA-C-N	6.56	129.33	116.20	1	1
I	55	VAL	CA-C-N	6.55	129.29	116.20	1	1
L	55	VAL	CA-C-N	6.54	129.27	116.20	1	1
K	55	VAL	CA-C-N	6.54	129.27	116.20	1	1
I	55	VAL	C-N-CA	6.29	133.03	121.70	1	1
J	55	VAL	C-N-CA	6.29	133.03	121.70	1	1
L	55	VAL	C-N-CA	6.28	133.01	121.70	1	1
K	55	VAL	C-N-CA	6.28	133.00	121.70	1	1
L	58	LYS	N-CA-CB	6.24	121.11	110.50	1	1
J	58	LYS	N-CA-CB	6.21	121.05	110.50	1	1
I	58	LYS	N-CA-CB	6.20	121.05	110.50	1	1
K	58	LYS	N-CA-CB	6.19	121.02	110.50	1	1
K	57	GLU	C-N-CA	6.17	132.80	121.70	1	1
I	57	GLU	C-N-CA	6.15	132.77	121.70	1	1
J	57	GLU	C-N-CA	6.14	132.75	121.70	1	1
L	57	GLU	C-N-CA	6.14	132.74	121.70	1	1

Chain	Res	Type	Atoms	|Z|	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
J	109	GLU	CA-C-O	6.02	110.57	120.80	1	1
I	109	GLU	CA-C-O	5.98	110.63	120.80	1	1
L	109	GLU	CA-C-O	5.98	110.63	120.80	1	1
K	109	GLU	CA-C-O	5.98	110.64	120.80	1	1
K	127	ILE	O-C-N	5.53	114.15	123.00	1	1
J	127	ILE	O-C-N	5.51	114.19	123.00	1	1
I	127	ILE	O-C-N	5.49	114.22	123.00	1	1
L	127	ILE	O-C-N	5.49	114.22	123.00	1	1
J	54	SER	CA-C-O	5.27	111.83	120.80	1	1
I	54	SER	CA-C-O	5.25	111.87	120.80	1	1
K	54	SER	CA-C-O	5.24	111.89	120.80	1	1
L	54	SER	CA-C-O	5.24	111.89	120.80	1	1
K	56	ILE	C-N-CA	5.17	131.00	121.70	1	1
L	56	ILE	C-N-CA	5.15	130.97	121.70	1	1
I	56	ILE	C-N-CA	5.15	130.97	121.70	1	1
J	56	ILE	C-N-CA	5.14	130.95	121.70	1	1
L	54	SER	O-C-N	5.08	114.88	123.00	1	1
I	54	SER	O-C-N	5.06	114.90	123.00	1	1
K	54	SER	O-C-N	5.06	114.91	123.00	1	1
J	54	SER	O-C-N	5.06	114.91	123.00	1	1
M	114	ASN	N-CA-C	4.85	124.57	111.00	1	1
O	114	ASN	N-CA-C	4.85	124.57	111.00	1	1
P	114	ASN	N-CA-C	4.85	124.57	111.00	1	1
N	114	ASN	N-CA-C	4.84	124.56	111.00	1	1
N	54	SER	N-CA-C	4.69	97.86	111.00	1	1
O	54	SER	N-CA-C	4.69	97.88	111.00	1	1
M	54	SER	N-CA-C	4.68	97.89	111.00	1	1
N	133	LEU	O-C-N	4.68	115.51	123.00	1	1
P	54	SER	N-CA-C	4.68	97.90	111.00	1	1
P	133	LEU	O-C-N	4.67	115.53	123.00	1	1

Too-close contacts

The following all-atom clashscore is based on a MolProbity analysis. All-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The table below contains clashscores for all atomic models in this entry.

Model ID	Clash score	Number of clashes
1	45.94	5088

There are 5088 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are >= 0.4 Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
M:33:PHE:HE1	M:53:PRO:CB	1.63	1	1
L:97:TYR:CZ	N:100:LYS:HE2	1.63	1	1
L:97:TYR:CE2	N:100:LYS:CE	1.62	1	1
P:33:PHE:HE1	P:53:PRO:CB	1.60	1	1
O:155:LEU:HG	O:255:LYS:CD	1.59	1	1
J:98:GLU:CA	P:99:VAL:HA	1.58	1	1
O:159:PRO:HG2	O:253:SER:CB	1.58	1	1
D:569:SER:HB3	K:23:TYR:CD2	1.58	1	1
K:42:TYR:CB	K:133:LEU:HD22	1.57	1	1
I:155:LEU:HG	N:136:HIS:CD2	1.57	1	1
M:37:ARG:CA	M:57:GLU:HG3	1.57	1	1
N:37:ARG:CA	N:57:GLU:HG3	1.57	1	1
O:33:PHE:HE1	O:53:PRO:CB	1.57	1	1
I:149:GLN:HB2	N:131:LEU:C	1.57	1	1
I:55:VAL:C	I:55:VAL:CA	1.56	1	1
N:33:PHE:HE1	N:53:PRO:CB	1.56	1	1
O:159:PRO:CD	O:253:SER:HA	1.56	1	1
L:55:VAL:C	L:55:VAL:CA	1.56	1	1
N:33:PHE:CE1	N:53:PRO:CB	1.56	1	1
B:569:SER:HB3	J:23:TYR:CD2	1.55	1	1
N:33:PHE:CE1	N:53:PRO:HB3	1.55	1	1
O:37:ARG:CA	O:57:GLU:HG3	1.55	1	1
I:57:GLU:CA	I:57:GLU:CB	1.55	1	1
J:57:GLU:CA	J:57:GLU:N	1.54	1	1
P:37:ARG:CA	P:57:GLU:HG3	1.54	1	1
L:57:GLU:CA	L:57:GLU:CB	1.54	1	1
J:97:TYR:CZ	P:100:LYS:HB3	1.54	1	1
O:33:PHE:CE1	O:53:PRO:HB3	1.54	1	1
M:149:GLN:HE21	N:215:MET:CE	1.54	1	1
K:57:GLU:CA	K:57:GLU:N	1.54	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
I:155:LEU:CG	N:136:HIS:CG	1.54	1	1
N:155:LEU:HG	N:255:LYS:CD	1.53	1	1
J:98:GLU:HA	P:99:VAL:CA	1.53	1	1
O:159:PRO:CG	O:253:SER:CA	1.53	1	1
P:33:PHE:CE1	P:53:PRO:HB3	1.53	1	1
K:149:GLN:HB2	P:131:LEU:C	1.52	1	1
M:33:PHE:CE1	M:53:PRO:HB3	1.52	1	1
P:37:ARG:N	P:57:GLU:CD	1.52	1	1
K:55:VAL:C	K:55:VAL:CA	1.51	1	1
I:57:GLU:CA	I:57:GLU:N	1.51	1	1
K:54:SER:C	K:54:SER:CA	1.51	1	1
M:37:ARG:N	M:57:GLU:CD	1.51	1	1
J:54:SER:C	J:54:SER:CA	1.50	1	1
J:57:GLU:CA	J:57:GLU:CB	1.50	1	1
J:55:VAL:C	J:55:VAL:CA	1.50	1	1
J:55:VAL:CA	J:55:VAL:N	1.50	1	1
O:155:LEU:HG	O:255:LYS:CE	1.50	1	1
L:142:TYR:CD2	O:138:PHE:O	1.49	1	1
K:57:GLU:CA	K:57:GLU:CB	1.49	1	1
K:92:GLU:CB	M:100:LYS:HZ1	1.49	1	1
L:57:GLU:CA	L:57:GLU:N	1.49	1	1
I:155:LEU:HG	N:136:HIS:CG	1.49	1	1
O:159:PRO:HB2	O:253:SER:C	1.49	1	1
I:155:LEU:CG	N:136:HIS:CB	1.49	1	1
K:92:GLU:HB3	M:100:LYS:NZ	1.49	1	1
L:54:SER:C	L:54:SER:CA	1.48	1	1
M:33:PHE:CE1	M:53:PRO:CB	1.48	1	1
P:37:ARG:CA	P:57:GLU:C	1.48	1	1
P:153:MET:O	P:161:TYR:CE2	1.48	1	1
M:37:ARG:CA	M:57:GLU:C	1.48	1	1
O:37:ARG:N	O:57:GLU:CD	1.48	1	1
L:55:VAL:CA	L:55:VAL:N	1.47	1	1
K:55:VAL:CA	K:55:VAL:N	1.47	1	1
M:149:GLN:CG	N:215:MET:HE1	1.47	1	1
N:40:GLU:CG	N:59:GLN:HE22	1.47	1	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:569:SER:HB3	L:23:TYR:CD2	1.47	1	1
I:55:VAL:CA	I:55:VAL:N	1.47	1	1
J:97:TYR:CE2	P:100:LYS:CB	1.47	1	1
O:40:GLU:CG	O:59:GLN:HE22	1.46	1	1
I:54:SER:C	I:54:SER:CA	1.46	1	1
I:155:LEU:CG	N:136:HIS:CD2	1.46	1	1
O:159:PRO:HG2	O:253:SER:CA	1.46	1	1
P:159:PRO:CD	P:161:TYR:HB3	1.46	1	1
J:98:GLU:HB2	P:102:LEU:CD2	1.46	1	1
O:159:PRO:HB3	O:254:GLY:CA	1.46	1	1
N:37:ARG:N	N:57:GLU:CD	1.46	1	1
M:36:LYS:CA	M:57:GLU:HG2	1.45	1	1
P:33:PHE:CE1	P:53:PRO:CB	1.45	1	1
O:36:LYS:CA	O:57:GLU:HG2	1.45	1	1
I:155:LEU:HD12	N:136:HIS:CA	1.45	1	1
J:98:GLU:CB	P:102:LEU:CB	1.45	1	1
J:98:GLU:CB	P:102:LEU:HB2	1.45	1	1
J:97:TYR:CZ	P:100:LYS:N	1.44	1	1
N:36:LYS:CA	N:57:GLU:HG2	1.44	1	1
O:150:THR:CB	O:160:CYS:SG	1.44	1	1
M:149:GLN:CG	N:215:MET:CE	1.44	1	1
P:154:LEU:HD13	P:160:CYS:CB	1.44	1	1
C:569:SER:HB3	I:23:TYR:CD2	1.43	1	1
J:97:TYR:CE2	P:100:LYS:HB3	1.43	1	1
P:36:LYS:CA	P:57:GLU:HG2	1.43	1	1
J:97:TYR:CE2	P:100:LYS:CA	1.43	1	1
L:125:GLU:CB	L:154:LEU:HD21	1.43	1	1
L:153:MET:C	O:136:HIS:CE1	1.43	1	1
N:36:LYS:CA	N:57:GLU:CG	1.43	1	1
O:36:LYS:CA	O:57:GLU:CG	1.43	1	1
L:155:LEU:CD1	O:136:HIS:HB2	1.42	1	1
K:98:GLU:OE1	M:102:LEU:CD2	1.42	1	1
L:142:TYR:CD2	O:138:PHE:C	1.42	1	1
L:98:GLU:HG2	N:102:LEU:N	1.42	1	1
I:154:LEU:N	N:136:HIS:CE1	1.42	1	1

Torsion angles: Protein backbone

In the following table, Ramachandran outliers are listed. The Analysed column shows the number of residues for which the backbone conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	6664	6398	208	58

There are 58 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	393	VAL	1
B	393	VAL	1
C	393	VAL	1
D	393	VAL	1
I	34	ASP	1
I	56	ILE	1
I	58	LYS	1
I	59	GLN	1
I	61	PRO	1
I	66	ASN	1
I	119	PHE	1
I	132	LYS	1
J	34	ASP	1
J	56	ILE	1
J	58	LYS	1
J	59	GLN	1
J	61	PRO	1
J	66	ASN	1
J	119	PHE	1
K	34	ASP	1
K	56	ILE	1
K	58	LYS	1
K	59	GLN	1
K	61	PRO	1
K	66	ASN	1
K	119	PHE	1
L	34	ASP	1
L	56	ILE	1
L	58	LYS	1

Chain	Res	Type	Models (Total)
L	59	GLN	1
L	61	PRO	1
L	66	ASN	1
L	119	PHE	1
L	132	LYS	1
M	28	LEU	1
M	34	ASP	1
M	59	GLN	1
M	135	SER	1
M	151	HIS	1
M	158	LYS	1
N	28	LEU	1
N	34	ASP	1
N	59	GLN	1
N	135	SER	1
N	151	HIS	1
N	158	LYS	1
O	28	LEU	1
O	34	ASP	1
O	59	GLN	1
O	135	SER	1
O	151	HIS	1
O	158	LYS	1
P	28	LEU	1
P	34	ASP	1
P	59	GLN	1
P	135	SER	1
P	151	HIS	1
P	158	LYS	1

Torsion angles : Protein sidechains

In the following table, sidechain rotameric outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analysed	Favored	Allowed	Outliers
1	6188	4335	1202	651

There are 651 unique sidechain outliers. Detailed list of outliers are tabulated below. The output is limited to 100

rows.

Chain	Res	Type	Models (Total)
A	1	VAL	1
A	271	SER	1
A	372	SER	1
A	389	SER	1
A	458	GLU	1
A	479	ILE	1
A	503	ARG	1
A	600	VAL	1
B	39	ASP	1
B	66	ASN	1
B	83	MET	1
B	118	THR	1
B	169	LYS	1
B	171	LEU	1
B	210	LEU	1
B	271	SER	1
B	364	LYS	1
B	372	SER	1
B	389	SER	1
B	397	SER	1
B	479	ILE	1
B	506	ASN	1
B	600	VAL	1
B	624	VAL	1
C	43	THR	1
C	51	THR	1
C	133	TYR	1
C	266	THR	1
C	271	SER	1
C	288	LYS	1
C	338	ILE	1
C	372	SER	1
C	389	SER	1
C	479	ILE	1

Chain	Res	Type	Models (Total)
C	503	ARG	1
C	600	VAL	1
D	1	VAL	1
D	5	ASP	1
D	43	THR	1
D	66	ASN	1
D	133	TYR	1
D	210	LEU	1
D	211	VAL	1
D	238	LEU	1
D	271	SER	1
D	277	VAL	1
D	364	LYS	1
D	372	SER	1
D	389	SER	1
D	397	SER	1
D	503	ARG	1
D	600	VAL	1
E	50	ASN	1
E	125	TYR	1
E	195	ILE	1
E	198	TRP	1
E	217	ASN	1
E	368	VAL	1
E	372	ASN	1
F	50	ASN	1
F	125	TYR	1
F	195	ILE	1
F	198	TRP	1
F	217	ASN	1
F	368	VAL	1
F	372	ASN	1
G	50	ASN	1
G	125	TYR	1
G	195	ILE	1

Chain	Res	Type	Models (Total)
G	198	TRP	1
G	217	ASN	1
G	368	VAL	1
G	372	ASN	1
H	50	ASN	1
H	125	TYR	1
H	195	ILE	1
H	198	TRP	1
H	217	ASN	1
H	368	VAL	1
H	372	ASN	1
I	2	LYS	1
I	4	ILE	1
I	6	ILE	1
I	8	THR	1
I	15	SER	1
I	16	ASP	1
I	18	ILE	1
I	19	GLU	1
I	22	ARG	1
I	23	TYR	1
I	26	SER	1
I	27	GLN	1
I	29	ASP	1
I	30	GLU	1
I	31	LEU	1
I	54	SER	1
I	55	VAL	1
I	56	ILE	1
I	57	GLU	1
I	58	LYS	1

Fit of model to data used for modeling ?

3DEM volume

Validation for this section is under development.

Fit of model to data used for validation

Validation for this section is under development.

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