

Integrative Structure Validation Report ?

July 30, 2026 - 09:05 AM PDT

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

IHMValidation Version 3.2
Python-IHM Version 2.9
MolProbity Version 4.5.2
PrISM Version db5a41
PyMOL Version 2.5.0

PDB ID	9AAD pdb_00009aad
Structure Title	Conformational ensemble of the PCASP and Ig3 domains of the Mucosa-associated lymphoid tissue lymphoma translocation protein 1 (MALT1(PCASP-Ig3)/339-719) at 298 K and 0.5 M NaCl
Structure Authors	Lesovoy, D.; Agback, P.; Han, X.; Roshchin, K.; Sandalova, T.; Achour, A.; Agback, T.; Orekhov, V.; Lomzov, A.
Deposited on	2025-12-22

This is a PDB-IHM Structure Validation Report.

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](#).

1. Overview ?

1.1. Summary ?

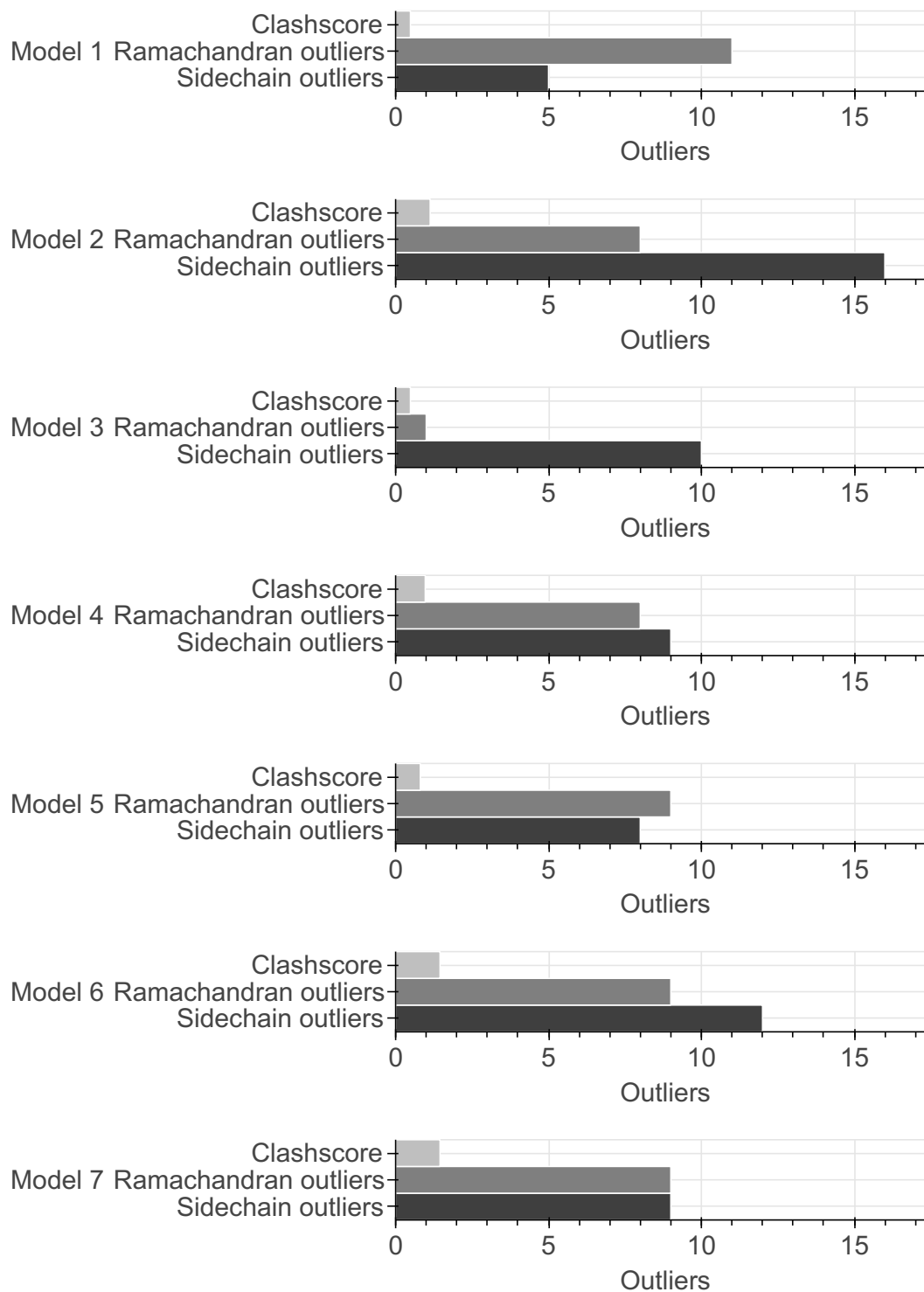
This entry consists of 20 model(s). A total of 2 dataset(s) were used to build this entry.

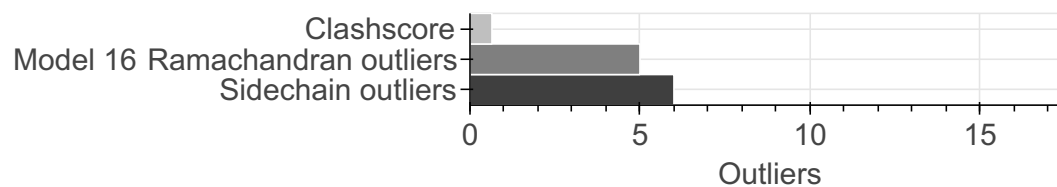
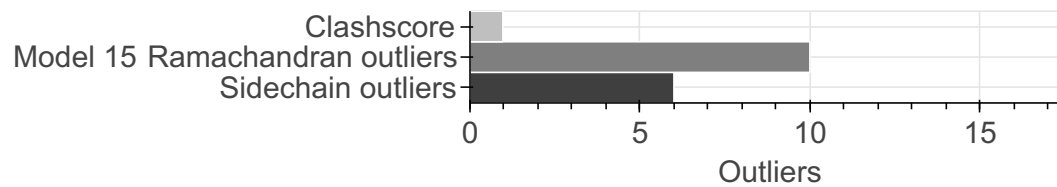
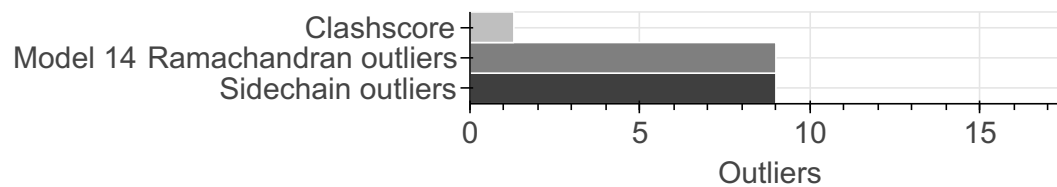
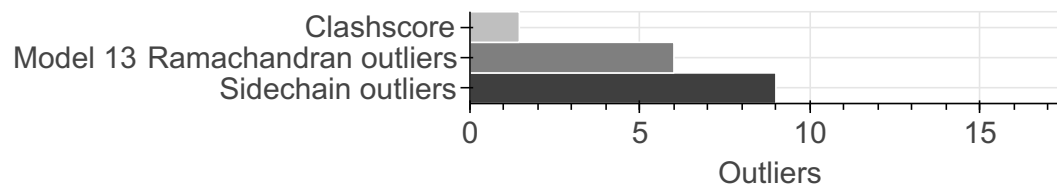
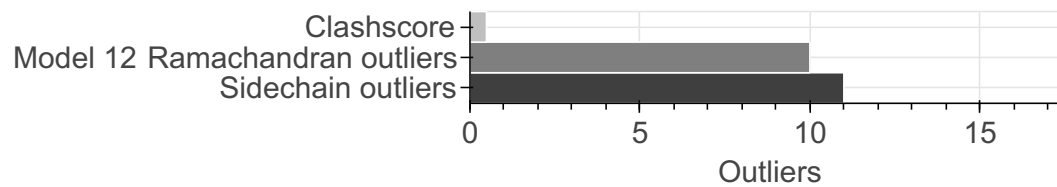
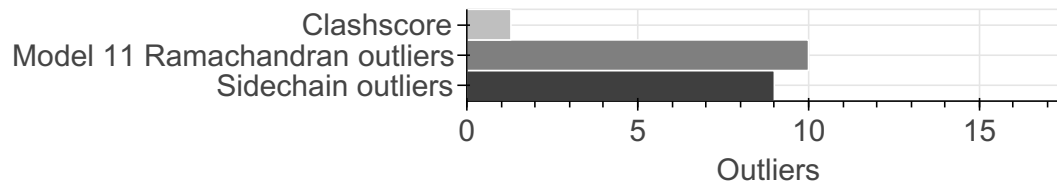
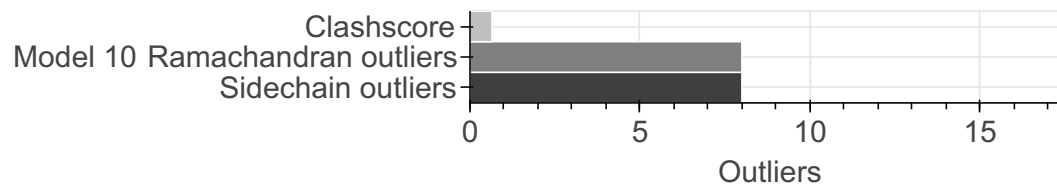
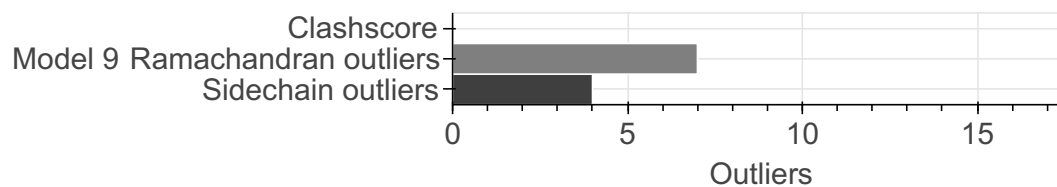
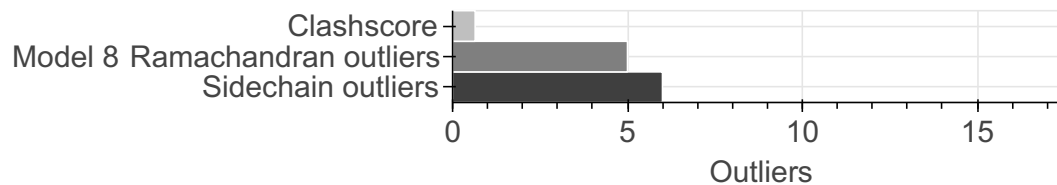
Name	Type	Count
NMR data	Experimental data	1
De Novo model	Starting model	1

1.2. 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 ?







2. Model Details ?

2.1. Ensemble information ?

This entry consists of 1 distinct ensemble(s).

2.2. 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	1-20	1	Mucosa-associated lymphoid tissue lymphoma translocation protein 1	A	388	-	1-388	100.00 / 100.00	Atomic

2.3. Datasets used for modeling ?

There are 2 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	De Novo model	Not available	Not available
2	NMR data	BMRB	52265

2.4. 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	Not available	Not available	Create starting structure	Not available	False	False
2	1	Not available	Not available	Full-atom molecular dynamics, Charmm36 force field with cutoff correction were performed. After minimization and NVT, free dynamics in the NPT ensemble was launched for 4 microseconds.	Not available	False	False
3	1	Not available	Not available	Relaxation parameters for the MD trajectory are calculated.	Not available	False	False
4	1	Not available	Not available	Relaxation parameters for the MD trajectory are calculated.	Not available	False	False
5	1	Not available	Not available	NMR data processed	Not available	False	False
6	1	Not available	Not available	NMR data analysis	Not available	False	False
7	1	Not available	Not available	NMR data analysis	Not available	False	False

There are 8 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
2	Gromacs	2022.40	model building	https://www.gromacs.org/
4	wolfram mathematica	Not available	data processing and validation	https://www.wolfram.com/mathematica/
1	AlphaFold	2	model building	https://alphafold.ebi.ac.uk/
3	Python	Not available	data processing	https://www.python.org/
5	TopSpin	4.3.0	data processing	https://www.bruker.com/en/products-and-solutions/mr/nmr-software/topspin.html
6	CcpNmr	2.4.2	other	https://ccpn.ac.uk/
7	Dynamics Center	2.8.4	other	https://www.bruker.com/en/products-and-solutions/mr/nmr-software/dynamics-center.html
8	MddNMR	Not available	other	http://mddnmr.spektrino.com/

3. Data quality ?

3.4. NMR ?

Validation for this section is under development.

4. 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.

4.1b. MolProbity Analysis ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Standard geometry: bond outliers ?

There are 1925 bond length outliers in this entry (3.05% of 63180 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)
A	386	HIS	CE1-NE2	12.62	1.45	1.32	20	7
A	322	VAL	C-N	11.14	1.48	1.33	4	6
A	167	SER	C-N	9.67	1.46	1.33	18	1
A	365	LYS	C-N	9.50	1.46	1.33	18	3
A	344	HIS	CE1-NE2	9.46	1.42	1.32	9	8
A	107	ASN	C-N	9.16	1.46	1.33	8	3
A	329	HIS	CE1-NE2	9.09	1.41	1.32	5	8
A	388	HIS	CE1-NE2	9.03	1.41	1.32	17	10
A	203	HIS	CE1-NE2	9.00	1.41	1.32	19	10
A	243	TRP	NE1-CE2	8.95	1.27	1.37	16	4
A	203	HIS	ND1-CE1	8.89	1.23	1.32	7	4
A	103	LEU	C-N	8.88	1.45	1.33	17	1
A	173	ILE	C-N	8.74	1.45	1.33	18	3
A	113	GLN	C-N	8.34	1.45	1.33	4	6
A	387	HIS	ND1-CE1	8.25	1.24	1.32	15	1
A	158	GLY	C-N	8.20	1.44	1.33	18	3
A	78	HIS	CB-CG	8.09	1.61	1.50	4	2
A	383	HIS	ND1-CE1	8.09	1.40	1.32	13	1
A	240	ASN	C-N	8.06	1.44	1.33	19	4
A	329	HIS	CG-ND1	8.05	1.47	1.38	7	5
A	17	ARG	CD-NE	8.02	1.57	1.46	16	7
A	19	HIS	ND1-CE1	7.99	1.40	1.32	5	5
A	383	HIS	CE1-NE2	7.93	1.40	1.32	17	6

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	385	HIS	CG-CD2	7.87	1.44	1.35	8	2
A	247	HIS	CD2-NE2	7.87	1.46	1.37	5	5
A	387	HIS	CE1-NE2	7.83	1.40	1.32	15	9
A	166	HIS	CE1-NE2	7.80	1.40	1.32	2	9
A	384	HIS	ND1-CE1	7.76	1.40	1.32	5	4
A	300	LEU	CA-CB	7.68	1.68	1.53	20	3
A	302	LEU	C-N	7.67	1.44	1.33	19	2
A	214	ARG	CD-NE	7.63	1.56	1.46	7	8
A	329	HIS	CD2-NE2	7.63	1.46	1.37	18	2
A	340	LYS	C-N	7.62	1.44	1.33	9	2
A	78	HIS	CE1-NE2	7.55	1.40	1.32	18	9
A	247	HIS	CE1-NE2	7.50	1.40	1.32	18	2
A	130	ARG	NE-CZ	7.50	1.24	1.33	3	2
A	63	LEU	CB-CG	7.48	1.68	1.53	14	1
A	360	ASP	C-N	7.47	1.43	1.33	5	4
A	280	SER	C-N	7.44	1.43	1.33	7	1
A	106	GLN	C-N	7.38	1.43	1.33	6	3
A	6	LYS	C-N	7.33	1.43	1.33	14	4
A	324	LYS	C-N	7.24	1.43	1.33	15	2
A	78	HIS	ND1-CE1	7.22	1.39	1.32	1	4
A	41	PHE	C-N	7.16	1.43	1.33	5	2
A	130	ARG	CD-NE	7.11	1.56	1.46	11	3
A	65	LEU	C-N	7.07	1.43	1.33	11	4
A	238	VAL	C-N	7.05	1.43	1.33	11	2
A	381	HIS	CE1-NE2	7.04	1.39	1.32	9	6
A	240	ASN	CA-CB	7.01	1.67	1.53	4	2
A	166	HIS	CB-CG	7.00	1.60	1.50	7	4
A	98	ARG	NE-CZ	7.00	1.25	1.33	20	3
A	19	HIS	CE1-NE2	6.99	1.39	1.32	17	6
A	374	LEU	C-N	6.97	1.43	1.33	19	2
A	309	ALA	C-N	6.97	1.43	1.33	13	6
A	97	TYR	C-N	6.95	1.43	1.33	6	4
A	203	HIS	CB-CG	6.92	1.59	1.50	11	2
A	202	CYS	C-N	6.92	1.43	1.33	10	2
A	386	HIS	ND1-CE1	6.91	1.39	1.32	2	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	273	ASN	C-N	6.89	1.43	1.33	13	1
A	337	SER	CA-CB	6.89	1.67	1.53	15	2
A	199	MET	C-N	6.87	1.43	1.33	1	5
A	388	HIS	CG-ND1	6.83	1.30	1.38	4	5
A	128	ARG	CD-NE	6.78	1.55	1.46	13	5
A	102	CYS	C-N	6.77	1.42	1.33	12	4
A	37	ARG	CD-NE	6.76	1.55	1.46	14	7
A	276	ILE	C-N	6.74	1.42	1.33	16	5
A	86	SER	C-N	6.73	1.42	1.33	2	5
A	251	GLU	C-N	6.73	1.42	1.33	9	4
A	283	TYR	CA-CB	6.72	1.66	1.53	5	2
A	310	ASN	C-N	6.72	1.42	1.33	11	3
A	104	CYS	C-N	6.71	1.42	1.33	3	4
A	166	HIS	CD2-NE2	6.70	1.45	1.37	5	4
A	385	HIS	CE1-NE2	6.70	1.39	1.32	16	9
A	98	ARG	CZ-NH2	6.68	1.24	1.33	4	3
A	214	ARG	NE-CZ	6.67	1.40	1.33	9	3
A	203	HIS	CG-ND1	6.62	1.45	1.38	13	2
A	299	PRO	N-CA	6.62	1.37	1.47	8	1
A	323	SER	C-N	6.59	1.42	1.33	15	4
A	98	ARG	CD-NE	6.58	1.55	1.46	2	6
A	24	ALA	C-N	6.54	1.45	1.34	13	4
A	221	ARG	C-N	6.53	1.42	1.33	1	4
A	368	VAL	CA-C	6.52	1.39	1.52	20	2
A	253	MET	C-N	6.52	1.42	1.33	6	2
A	35	LEU	C-N	6.51	1.42	1.33	16	2
A	381	HIS	C-N	6.51	1.42	1.33	7	4
A	162	PHE	C-N	6.50	1.42	1.33	5	2
A	270	GLU	CA-CB	6.49	1.66	1.53	15	1
A	384	HIS	C-N	6.48	1.42	1.33	9	4
A	384	HIS	CG-CD2	6.48	1.28	1.35	3	2
A	143	LEU	CA-CB	6.47	1.66	1.53	13	1
A	325	ASP	C-N	6.45	1.42	1.33	10	3
A	334	ARG	CD-NE	6.44	1.55	1.46	3	5
A	234	ALA	C-N	6.44	1.24	1.33	14	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	166	HIS	CG-CD2	6.43	1.42	1.35	14	2
A	39	LEU	C-N	6.42	1.42	1.33	19	3
A	220	LYS	C-N	6.40	1.42	1.33	2	3
A	385	HIS	CD2-NE2	6.39	1.30	1.37	10	3
A	54	MET	C-N	6.37	1.42	1.33	13	5
A	23	LYS	C-N	6.35	1.42	1.33	3	1
A	7	VAL	C-N	6.34	1.42	1.33	16	2

Standard geometry: angle outliers ?

There are 3817 bond angle outliers in this entry (4.47% of 85440 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)
A	240	ASN	CA-CB-CG	12.05	100.55	112.60	13	5
A	87	PHE	CA-CB-CG	11.20	102.60	113.80	18	8
A	382	ARG	NE-CZ-NH2	11.12	109.20	119.20	2	6
A	257	PHE	CA-CB-CG	10.78	103.02	113.80	4	7
A	305	ASP	CA-CB-CG	10.74	123.34	112.60	5	8
A	95	ASN	CA-CB-CG	10.54	123.14	112.60	3	6
A	344	HIS	CB-CG-CD2	10.45	117.61	131.20	16	4
A	360	ASP	CA-CB-CG	10.43	102.17	112.60	17	3
A	383	HIS	CA-CB-CG	10.25	124.05	113.80	18	7
A	258	ASP	CA-CB-CG	10.21	122.81	112.60	18	6
A	181	ARG	NE-CZ-NH2	10.11	110.10	119.20	8	5
A	95	ASN	CA-C-N	10.06	132.00	116.90	6	12
A	37	ARG	NE-CZ-NH2	10.02	110.18	119.20	19	4
A	344	HIS	CA-CB-CG	9.92	103.88	113.80	16	6
A	228	GLN	OE1-CD-NE2	9.91	112.69	122.60	1	7
A	78	HIS	ND1-CG-CD2	9.79	115.89	106.10	18	12
A	214	ARG	NE-CZ-NH1	9.67	131.17	121.50	12	11
A	122	PHE	CA-CB-CG	9.63	104.17	113.80	12	7
A	130	ARG	NE-CZ-NH2	9.62	127.86	119.20	17	8
A	24	ALA	CA-C-N	9.61	131.31	116.90	16	8
A	120	ASN	CA-CB-CG	9.58	103.02	112.60	16	9
A	17	ARG	NH1-CZ-NH2	9.57	106.85	119.30	16	7
A	134	ASP	CA-CB-CG	9.57	122.17	112.60	18	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	98	ARG	NE-CZ-NH2	9.40	110.74	119.20	8	11
A	92	ASP	CA-CB-CG	9.31	121.91	112.60	7	7
A	162	PHE	CA-CB-CG	9.27	104.53	113.80	20	8
A	107	ASN	CA-CB-CG	9.25	121.85	112.60	20	5
A	56	ASN	CA-CB-CG	9.24	103.36	112.60	1	7
A	384	HIS	CA-CB-CG	9.22	104.58	113.80	8	4
A	85	ASN	OD1-CG-ND2	9.11	113.49	122.60	18	5
A	267	PHE	CA-CB-CG	9.10	104.70	113.80	4	5
A	137	ILE	CA-C-N	8.94	130.31	116.90	15	7
A	221	ARG	NE-CZ-NH1	8.91	130.41	121.50	16	5
A	198	ASP	CA-CB-CG	8.85	121.45	112.60	2	3
A	303	ASP	CA-CB-CG	8.84	121.44	112.60	12	6
A	15	ASN	OD1-CG-ND2	8.79	113.81	122.60	12	7
A	128	ARG	NE-CZ-NH1	8.70	130.20	121.50	3	7
A	385	HIS	CA-CB-CG	8.68	122.48	113.80	5	4
A	273	ASN	CA-CB-CG	8.67	121.27	112.60	8	9
A	101	ASN	OD1-CG-ND2	8.64	113.96	122.60	13	6
A	269	ALA	N-CA-CB	8.63	123.34	110.40	3	4
A	203	HIS	CA-CB-CG	8.57	122.37	113.80	2	3
A	146	THR	CA-CB-OG1	8.55	122.42	109.60	16	3
A	148	ASN	CA-CB-CG	8.53	104.07	112.60	9	7
A	161	ALA	N-CA-CB	8.42	97.77	110.40	9	1
A	151	PHE	N-CA-CB	8.42	124.81	110.50	10	1
A	381	HIS	ND1-CE1-NE2	8.41	116.81	108.40	8	7
A	177	PHE	CA-CB-CG	8.41	105.39	113.80	5	9
A	17	ARG	NE-CZ-NH2	8.41	111.63	119.20	17	8
A	56	ASN	OD1-CG-ND2	8.37	114.23	122.60	20	5
A	19	HIS	ND1-CG-CD2	8.34	114.44	106.10	6	9
A	193	ASP	CA-CB-CG	8.33	120.93	112.60	8	6
A	125	ASP	CA-CB-CG	8.31	120.91	112.60	4	10
A	285	PRO	CA-C-N	8.29	129.33	116.90	19	12
A	13	ASN	CA-CB-CG	8.24	120.84	112.60	19	4
A	388	HIS	ND1-CG-CD2	8.24	114.34	106.10	4	11
A	131	ASN	OD1-CG-ND2	8.20	114.40	122.60	10	3
A	55	ARG	NE-CZ-NH1	8.19	129.69	121.50	13	4

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	155	THR	C-N-CA	8.17	136.40	121.70	19	8
A	305	ASP	CA-C-N	8.12	129.08	116.90	14	11
A	364	ASP	CA-CB-CG	8.09	120.69	112.60	4	10
A	180	ASP	CA-CB-CG	8.09	104.51	112.60	19	5
A	128	ARG	NE-CZ-NH2	8.06	126.46	119.20	11	8
A	98	ARG	NE-CZ-NH1	8.04	129.54	121.50	1	6
A	221	ARG	NE-CZ-NH2	8.00	126.40	119.20	5	5
A	171	ASN	C-CA-CB	8.00	94.90	110.10	2	2
A	155	THR	N-CA-CB	7.97	125.06	111.50	9	4
A	247	HIS	CA-CB-CG	7.94	105.86	113.80	19	7
A	17	ARG	NE-CZ-NH1	7.94	129.44	121.50	19	7
A	386	HIS	ND1-CE1-NE2	7.93	116.33	108.40	8	5
A	82	ASN	OD1-CG-ND2	7.93	114.67	122.60	2	7
A	40	ASP	C-CA-CB	7.92	125.15	110.10	13	2
A	334	ARG	NE-CZ-NH1	7.91	129.41	121.50	9	5
A	225	ASP	CA-C-N	7.85	128.68	116.90	1	7
A	135	ASP	CA-CB-CG	7.83	104.77	112.60	7	8
A	34	ASN	CA-CB-CG	7.83	104.77	112.60	20	7
A	15	ASN	CA-CB-CG	7.83	120.43	112.60	9	5
A	296	THR	CA-CB-OG1	7.83	121.34	109.60	18	3
A	242	GLN	CG-CD-NE2	7.77	128.05	116.40	19	1
A	13	ASN	OD1-CG-ND2	7.75	114.85	122.60	16	4
A	55	ARG	NE-CZ-NH2	7.70	112.27	119.20	1	5
A	166	HIS	ND1-CE1-NE2	7.70	116.10	108.40	4	8
A	372	LYS	CA-C-N	7.70	128.45	116.90	10	10
A	203	HIS	ND1-CE1-NE2	7.68	116.08	108.40	5	4
A	347	PHE	CA-CB-CG	7.66	121.46	113.80	18	7
A	181	ARG	NE-CZ-NH1	7.65	129.15	121.50	8	5
A	329	HIS	ND1-CG-CD2	7.62	113.72	106.10	5	8
A	388	HIS	CA-CB-CG	7.60	106.20	113.80	10	6
A	379	ASP	CA-CB-CG	7.59	120.19	112.60	14	6
A	28	ASP	CA-CB-CG	7.58	120.18	112.60	6	4
A	234	ALA	N-CA-CB	7.58	121.77	110.40	16	3
A	209	GLN	OE1-CD-NE2	7.55	115.05	122.60	12	6
A	188	ILE	C-N-CA	7.54	135.28	121.70	6	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	309	ALA	C-CA-CB	7.54	99.19	110.50	15	2
A	247	HIS	CD2-NE2-CE1	7.53	101.47	109.00	1	14
A	93	ALA	CA-C-N	7.49	128.13	116.90	15	6
A	239	ARG	NE-CZ-NH1	7.48	128.98	121.50	11	7
A	388	HIS	CB-CG-ND1	7.48	111.48	122.70	8	4
A	297	ASP	CA-CB-CG	7.47	105.13	112.60	17	6
A	249	LEU	CA-C-N	7.46	128.09	116.90	16	9

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	0.48	3
2	1.13	7
3	0.48	3
4	0.97	6
5	0.81	5
6	1.45	9
7	1.45	9
8	0.65	4
9	0.00	0
10	0.65	4
11	1.29	8
12	0.48	3
13	1.45	9
14	1.29	8
15	0.97	6
16	0.65	4
17	0.81	5
18	1.13	7
19	0.81	5
20	0.81	5

There are 110 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are ≥ 0.4 Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:189:THR:HG23	A:213:ILE:HD12	0.73	11	1
A:340:LYS:HA	A:381:HIS:CD2	0.65	16	4
A:275:MET:HB2	A:338:LEU:HD11	0.56	2	1
A:47:LEU:HD11	A:271:PHE:CE2	0.56	10	1
A:46:LEU:HB3	A:49:LEU:HD21	0.56	13	1
A:50:THR:HA	A:91:VAL:HG22	0.56	13	1
A:384:HIS:CG	A:385:HIS:N	0.56	18	1
A:384:HIS:CG	A:385:HIS:H	0.55	18	1
A:125:ASP:HA	A:154:ALA:HB3	0.55	14	1
A:263:ILE:HD11	A:351:LEU:HD13	0.54	18	2
A:166:HIS:CG	A:167:SER:H	0.54	7	2
A:185:ASP:HA	A:224:THR:HG21	0.53	6	1
A:267:PHE:CD1	A:277:ILE:HG22	0.52	2	1
A:6:LYS:HD3	A:41:PHE:CE1	0.51	4	1
A:32:LEU:HD22	A:175:MET:HE1	0.51	6	1
A:11:ILE:HD12	A:49:LEU:HD12	0.50	4	1
A:95:ASN:HA	A:96:PRO:C	0.50	3	2
A:154:ALA:HA	A:199:MET:HE1	0.50	5	1
A:384:HIS:CE1	A:386:HIS:HA	0.50	3	1
A:89:VAL:HG22	A:102:CYS:SG	0.50	11	2
A:150:VAL:HG11	A:192:LEU:HD12	0.50	10	1
A:340:LYS:HA	A:381:HIS:CG	0.49	16	3
A:302:LEU:HD22	A:338:LEU:HD23	0.48	17	1
A:55:ARG:HG3	A:103:LEU:HD21	0.48	7	1
A:10:LEU:HD11	A:36:LEU:HD12	0.48	5	1
A:57:ALA:HA	A:380:MET:HE1	0.48	2	1
A:46:LEU:HB3	A:49:LEU:HD11	0.47	14	1
A:261:VAL:HG22	A:284:LYS:HB2	0.47	14	1
A:36:LEU:HD11	A:72:LEU:HD22	0.47	14	1
A:162:PHE:CE2	A:205:THR:HG22	0.47	7	1
A:8:ALA:HB3	A:43:VAL:HG22	0.47	8	2
A:35:LEU:HD13	A:182:LEU:HD23	0.47	15	1
A:265:LEU:C	A:265:LEU:HD23	0.47	17	1
A:106:GLN:CD	A:106:GLN:H	0.47	4	1
A:214:ARG:HA	A:214:ARG:HE	0.47	6	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:352:SER:HA	A:363:GLU:HG3	0.47	7	1
A:22:LEU:HD22	A:78:HIS:CD2	0.47	17	1
A:254:CYS:HB2	A:264:GLN:HE22	0.46	2	1
A:299:PRO:HG2	A:302:LEU:HB2	0.46	19	1
A:144:LYS:HA	A:147:ALA:HB3	0.46	14	1
A:211:LEU:H	A:211:LEU:HD12	0.46	20	1
A:157:GLN:HE21	A:212:GLU:HB3	0.46	16	1
A:193:ASP:HA	A:213:ILE:HD11	0.46	17	1
A:16:TYR:CE2	A:91:VAL:HA	0.46	19	1
A:380:MET:HB3	A:380:MET:HE3	0.46	14	1
A:354:GLN:HG2	A:361:THR:HA	0.46	15	1
A:35:LEU:HD11	A:179:LYS:HA	0.46	13	1
A:49:LEU:HD22	A:53:GLU:HB3	0.46	4	1
A:166:HIS:CE1	A:171:ASN:H	0.46	6	1
A:157:GLN:CD	A:157:GLN:H	0.45	12	1
A:351:LEU:HD23	A:353:TYR:CE1	0.45	15	1
A:302:LEU:HD21	A:341:LEU:HB2	0.44	12	1
A:35:LEU:HB3	A:182:LEU:HD23	0.44	11	1
A:79:GLY:HA3	A:126:MET:HE3	0.44	19	1
A:28:ASP:OD1	A:171:ASN:HA	0.44	1	1
A:383:HIS:CG	A:384:HIS:H	0.44	8	1
A:65:LEU:HD13	A:112:MET:HG2	0.43	13	1
A:278:TYR:CZ	A:326:LEU:HD22	0.43	11	1
A:373:PRO:O	A:376:ALA:HB3	0.43	6	1
A:166:HIS:CG	A:167:SER:N	0.43	7	1
A:353:TYR:CE2	A:362:VAL:HG13	0.43	4	1
A:10:LEU:HD22	A:74:TYR:HB3	0.43	11	1
A:16:TYR:CD1	A:91:VAL:HA	0.43	12	1
A:10:LEU:HD22	A:32:LEU:HD23	0.43	13	1
A:328:LYS:O	A:329:HIS:HB2	0.43	20	1
A:47:LEU:HD12	A:274:VAL:HG21	0.42	13	1
A:326:LEU:HA	A:327:PRO:HD3	0.42	18	1
A:266:GLY:HA3	A:278:TYR:CE1	0.42	5	2
A:285:PRO:HA	A:286:PRO:HD3	0.42	15	1
A:276:ILE:HD12	A:319:SER:HB2	0.42	15	2

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:151:PHE:HB3	A:153:TYR:CZ	0.42	1	2
A:38:GLN:HB2	A:183:LEU:HD22	0.42	6	1
A:137:ILE:HD13	A:137:ILE:HG21	0.42	8	1
A:120:ASN:HB2	A:149:ILE:HG22	0.42	13	1
A:96:PRO:HB3	A:133:TYR:CD2	0.42	14	1
A:10:LEU:HD22	A:74:TYR:HB2	0.42	1	1
A:225:ASP:HA	A:226:PRO:HD3	0.41	2	1
A:275:MET:HB3	A:275:MET:HE2	0.41	2	1
A:119:LEU:HD22	A:221:ARG:HB3	0.41	20	1
A:166:HIS:CD2	A:170:ALA:HB2	0.41	8	1
A:10:LEU:HD23	A:32:LEU:HD23	0.41	10	1
A:46:LEU:HD23	A:273:ASN:HB3	0.41	18	1
A:47:LEU:H	A:273:ASN:HD21	0.41	3	1
A:243:TRP:C	A:243:TRP:CD2	0.41	4	1
A:383:HIS:HB3	A:384:HIS:CD2	0.41	11	1
A:61:PHE:CZ	A:112:MET:HE3	0.41	18	1
A:162:PHE:CE2	A:173:ILE:HD11	0.41	15	1
A:243:TRP:CZ2	A:247:HIS:CD2	0.41	5	1
A:157:GLN:HG3	A:210:ALA:O	0.41	7	1
A:203:HIS:O	A:206:LYS:HG2	0.41	17	1
A:383:HIS:CG	A:384:HIS:N	0.40	19	1
A:243:TRP:HA	A:246:ALA:HB3	0.40	13	1
A:270:GLU:HB3	A:271:PHE:CE1	0.40	6	1
A:53:GLU:CD	A:339:GLN:HE21	0.40	11	1
A:65:LEU:HD23	A:69:VAL:HG11	0.40	16	1
A:2:LEU:HD13	A:228:GLN:HA	0.40	7	1
A:276:ILE:HD11	A:332:TYR:HB3	0.40	10	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	386	360	15	11
2	386	352	26	8
3	386	366	19	1
4	386	355	23	8

Model ID	Analysed	Favored	Allowed	Outliers
5	386	357	20	9
6	386	356	21	9
7	386	347	30	9
8	386	349	32	5
9	386	354	25	7
10	386	360	18	8
11	386	350	26	10
12	386	360	16	10
13	386	359	21	6
14	386	359	18	9
15	386	353	23	10
16	386	357	24	5
17	386	356	26	4
18	386	350	29	7
19	386	346	30	10
20	386	357	21	8

There are 65 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	116	GLU	11
A	136	THR	11
A	337	SER	11
A	304	ILE	10
A	297	ASP	8
A	25	PRO	6
A	20	PRO	4
A	48	ASP	4
A	212	GLU	4
A	226	PRO	4
A	228	GLN	4
A	329	HIS	4
A	96	PRO	3
A	156	CYS	3
A	323	SER	3
A	387	HIS	3

Chain	Res	Type	Models (Total)
A	14	MET	2
A	21	LYS	2
A	40	ASP	2
A	117	THR	2
A	126	MET	2
A	166	HIS	2
A	203	HIS	2
A	220	LYS	2
A	250	PRO	2
A	299	PRO	2
A	373	PRO	2
A	374	LEU	2
A	2	LEU	1
A	22	LEU	1
A	23	LYS	1
A	42	LYS	1
A	67	LYS	1
A	83	PHE	1
A	90	PRO	1
A	94	PRO	1
A	100	GLU	1
A	119	LEU	1
A	129	LYS	1
A	137	ILE	1
A	138	PRO	1
A	147	ALA	1
A	185	ASP	1
A	202	CYS	1
A	209	GLN	1
A	210	ALA	1
A	211	LEU	1
A	213	ILE	1
A	225	ASP	1
A	230	THR	1
A	252	SER	1

Chain	Res	Type	Models (Total)
A	283	TYR	1
A	285	PRO	1
A	287	GLU	1
A	306	PRO	1
A	322	VAL	1
A	327	PRO	1
A	344	HIS	1
A	356	SER	1
A	375	ILE	1
A	379	ASP	1
A	382	ARG	1
A	384	HIS	1
A	385	HIS	1
A	386	HIS	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	345	322	18	5
2	345	306	23	16
3	345	311	24	10
4	345	310	26	9
5	345	313	24	8
6	345	303	30	12
7	345	317	19	9
8	345	318	21	6
9	345	322	19	4
10	345	310	27	8
11	345	318	18	9
12	345	312	22	11
13	345	308	28	9
14	345	303	33	9
15	345	317	22	6
16	345	318	21	6
17	345	325	17	3

Model ID	Analysed	Favored	Allowed	Outliers
18	345	309	27	9
19	345	320	16	9
20	345	314	24	7

There are 90 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	365	LYS	6
A	117	THR	5
A	189	THR	5
A	382	ARG	5
A	1	MET	4
A	20	PRO	4
A	23	LYS	4
A	25	PRO	4
A	224	THR	4
A	284	LYS	4
A	327	PRO	4
A	337	SER	4
A	126	MET	3
A	182	LEU	3
A	188	ILE	3
A	205	THR	3
A	228	GLN	3
A	307	LYS	3
A	314	PRO	3
A	322	VAL	3
A	22	LEU	2
A	44	VAL	2
A	94	PRO	2
A	95	ASN	2
A	137	ILE	2
A	144	LYS	2
A	146	THR	2
A	149	ILE	2
A	167	SER	2

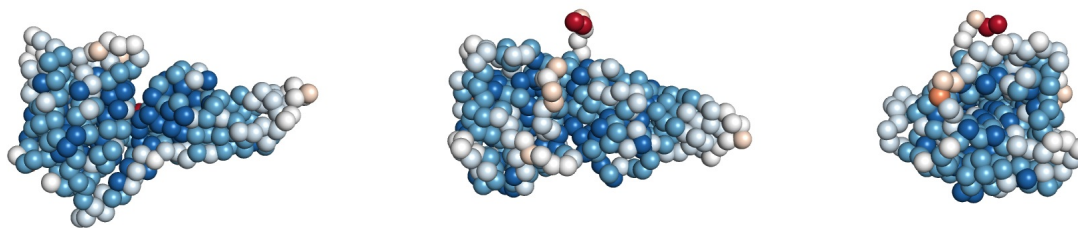
Chain	Res	Type	Models (Total)
A	230	THR	2
A	242	GLN	2
A	285	PRO	2
A	286	PRO	2
A	299	PRO	2
A	304	ILE	2
A	306	PRO	2
A	313	THR	2
A	375	ILE	2
A	10	LEU	1
A	14	MET	1
A	26	LEU	1
A	27	VAL	1
A	51	GLU	1
A	52	TYR	1
A	61	PHE	1
A	67	LYS	1
A	73	LEU	1
A	109	LEU	1
A	120	ASN	1
A	123	LEU	1
A	135	ASP	1
A	140	LEU	1
A	150	VAL	1
A	155	THR	1
A	156	CYS	1
A	157	GLN	1
A	164	ILE	1
A	175	MET	1
A	178	LEU	1
A	195	VAL	1
A	209	GLN	1
A	213	ILE	1
A	214	ARG	1
A	220	LYS	1

Chain	Res	Type	Models (Total)
A	226	PRO	1
A	233	SER	1
A	235	GLU	1
A	237	LEU	1
A	239	ARG	1
A	240	ASN	1
A	241	LEU	1
A	250	PRO	1
A	255	LEU	1
A	276	ILE	1
A	279	THR	1
A	281	ILE	1
A	289	ILE	1
A	294	TYR	1
A	297	ASP	1
A	300	LEU	1
A	301	ASP	1
A	305	ASP	1
A	317	THR	1
A	340	LYS	1
A	341	LEU	1
A	344	HIS	1
A	346	VAL	1
A	368	VAL	1
A	370	VAL	1
A	378	LEU	1

4.2. PrISM Precision Analysis

Regions of **low**  **high** precision, defined as the variability among the models that satisfy the input data and calculated as the density-weighted root mean-square fluctuation (RMSF) from the bead/atom center of density, annotated and visualized using PrISM. The per-bead precision is computed from the deposited ensemble of superposed integrative models. High- and low-precision regions are then determined by clustering beads of similar precision based on their proximity in the structure. Only coarse-grained beads (or CA atoms for atomic models) of deposited models are used for assessment and visualization, and three projections for each representative model are generated.

PrISM analysis for Ensemble 1 (models deposited/total: 20/1000).



5. Fit to Data Used for Modeling Assessment ?

5.4. NMR ?

Validation for this section is under development.

6. Fit to Data Used for Validation Assessment ?

Validation for this section is under development.

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