

Integrative Structure Validation Report ?

July 30, 2026 - 08:52 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	9AAC pdb_00009aac
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 0.06M NaCl
Structure Authors	Lesovoy, D.; Agback, P.; Han, X.; Roshchin, K.; Sandalova, T.; Achour, A.; Agback, T.; Orekhov, V.; Lomzov, A.
Deposited on	2025-07-22

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 ?

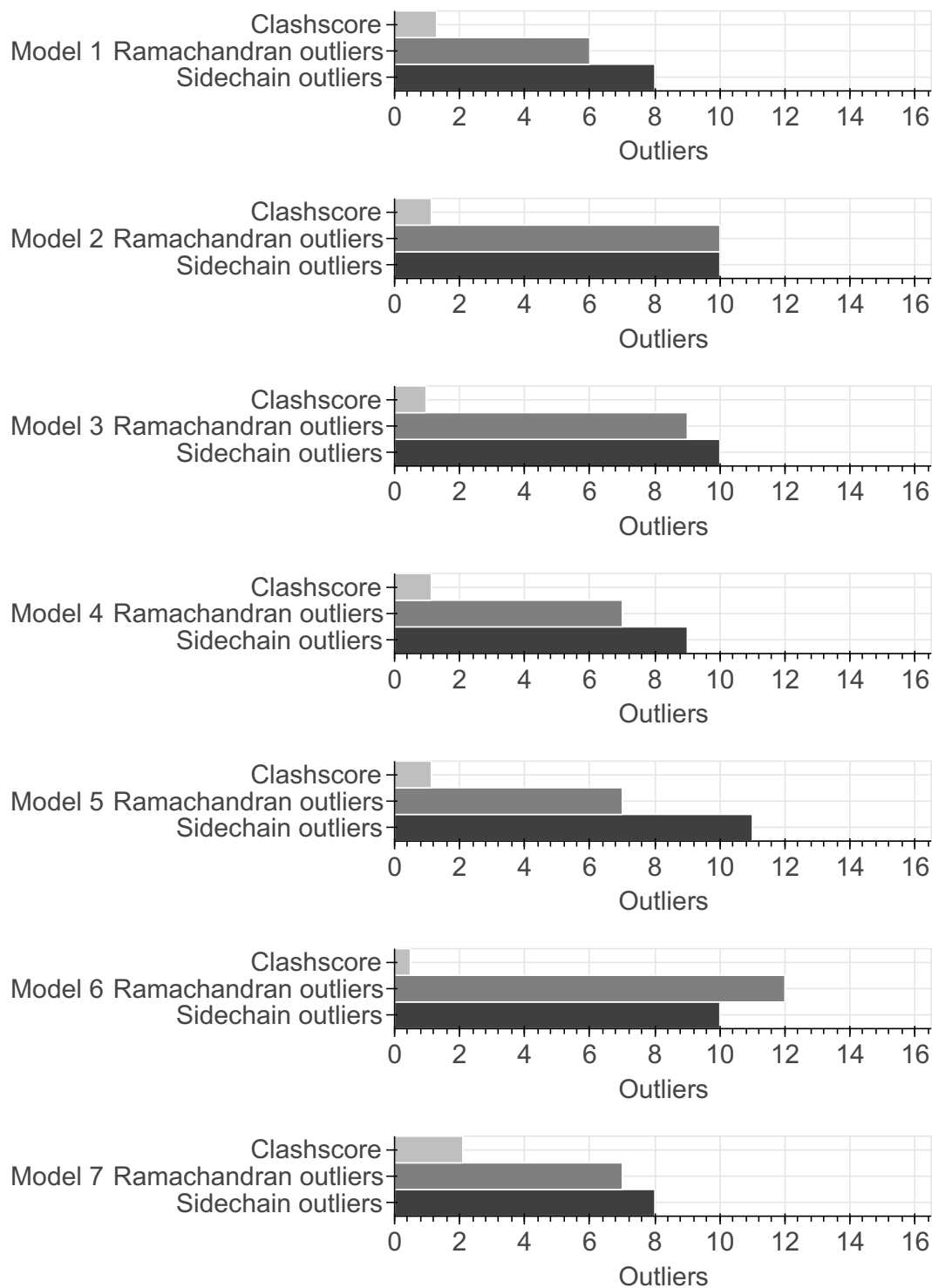
This entry consists of 20 model(s). A total of 2 dataset(s) were used to build this entry.

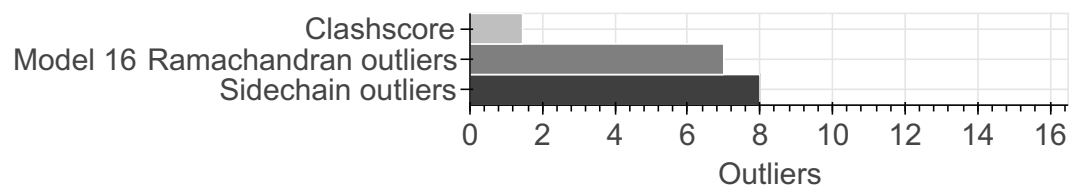
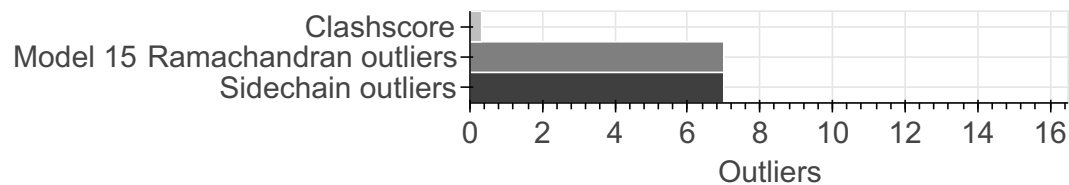
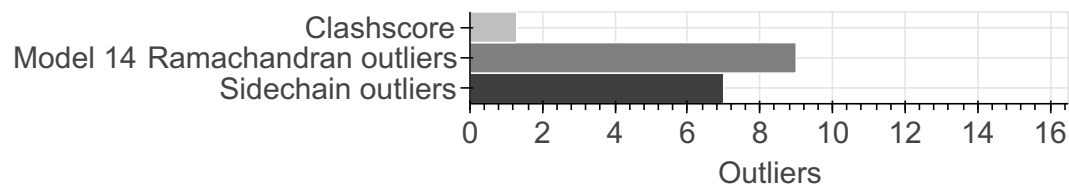
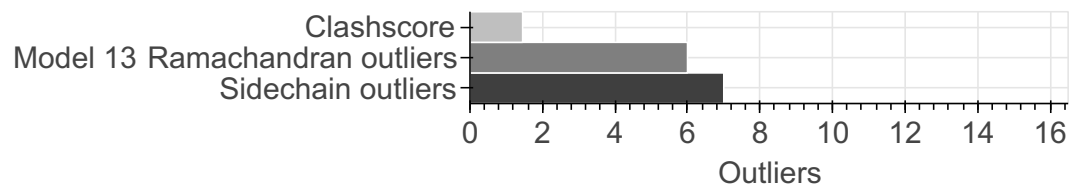
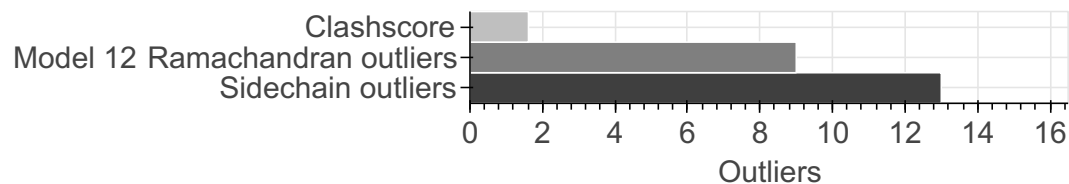
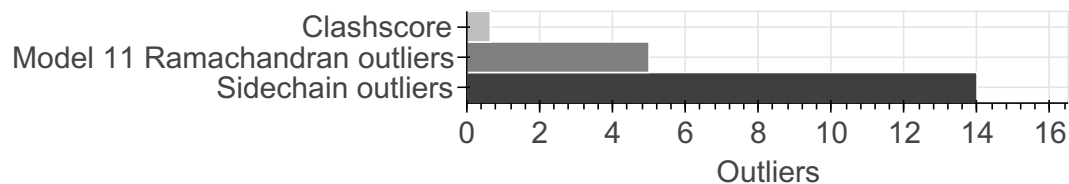
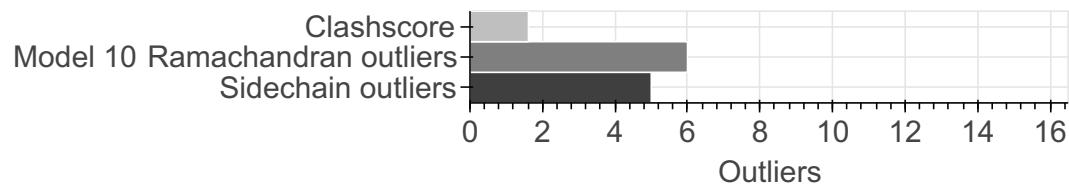
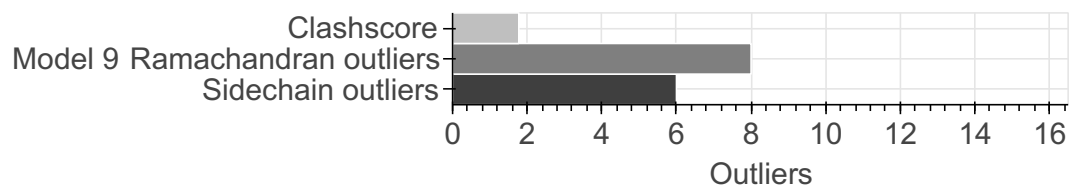
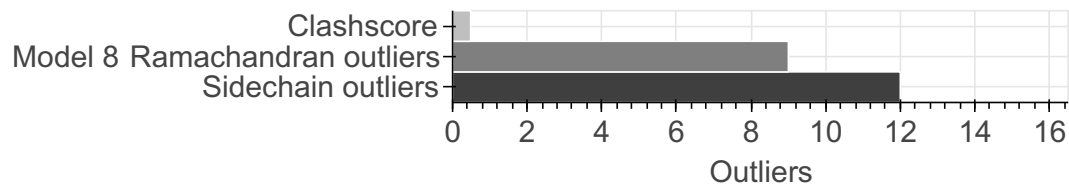
Name	Type	Count
NMR data	Experimental data	1
De Novo model	Starting model	1

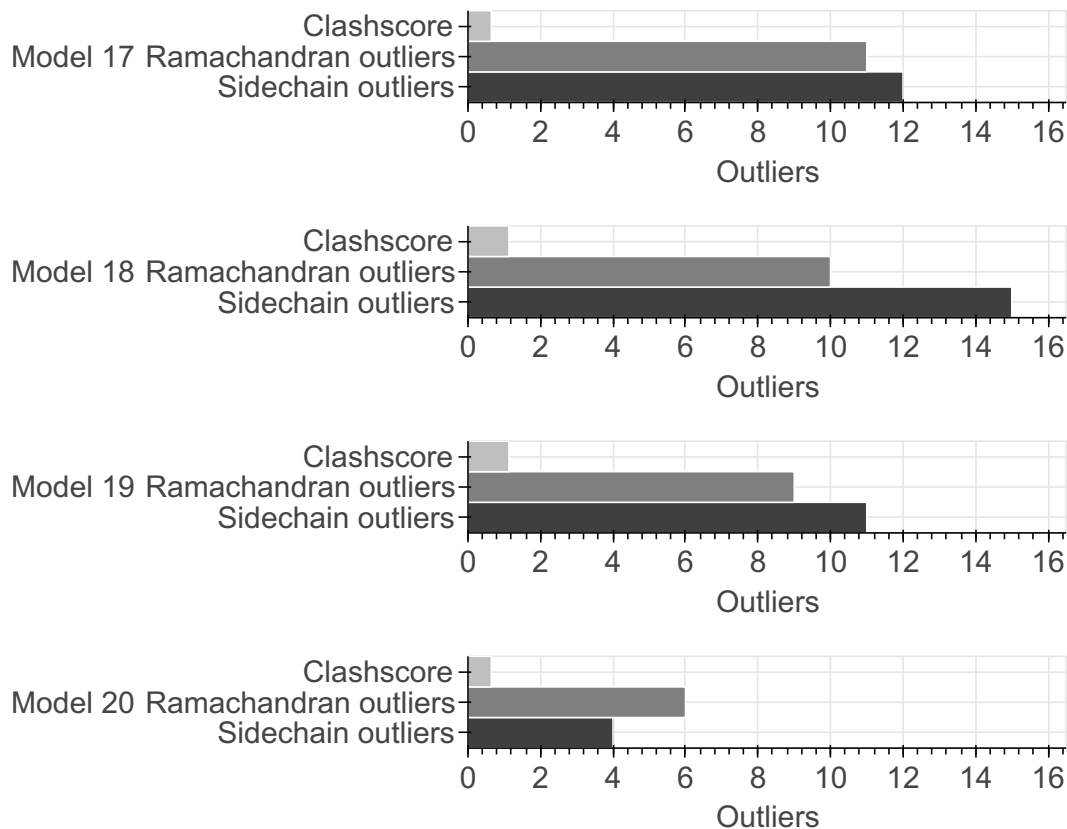
1.2. Overall quality ?

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 cuffix correction were performed. After minimization and NVT, free dynamics in the NPT ensemble was launched for 3 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 9 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
3	Gromacs	2022.40	model building	https://www.gromacs.org/
1	AlphaFold	3	model building	https://alphafold.ebi.ac.uk/
5	wolfram mathematica	Not available	data processing and validation	https://www.wolfram.com/mathematica/
4	Python	Not available	data processing	https://www.python.org/
6	TopSpin	4.3.0	data processing	https://www.bruker.com/en/products-and-solutions/mr/nmr-software/topspin.html
7	CcpNmr	2.4.2	other	https://ccpn.ac.uk/
8	Dynamics Center	2.8.4	other	https://www.bruker.com/en/products-and-solutions/mr/nmr-software/dynamics-center.html
2	pdbfixer	Not available	model building	https://github.com/openmm/pdbfixer
9	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 1945 bond length outliers in this entry (3.08% 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	381	HIS	CE1-NE2	10.62	1.43	1.32	6	11
A	385	HIS	CE1-NE2	10.24	1.42	1.32	3	8
A	329	HIS	CE1-NE2	9.97	1.42	1.32	18	13
A	344	HIS	CE1-NE2	9.81	1.42	1.32	10	9
A	384	HIS	ND1-CE1	9.61	1.42	1.32	14	12
A	181	ARG	CD-NE	9.54	1.59	1.46	16	5
A	19	HIS	CE1-NE2	9.42	1.42	1.32	16	8
A	55	ARG	C-N	9.08	1.46	1.33	5	5
A	386	HIS	CE1-NE2	8.78	1.41	1.32	6	6
A	344	HIS	CB-CG	8.76	1.62	1.50	15	4
A	125	ASP	CA-CB	8.70	1.70	1.53	6	3
A	316	GLU	C-N	8.63	1.45	1.33	5	4
A	151	PHE	C-N	8.62	1.45	1.33	12	5
A	375	ILE	C-N	8.56	1.45	1.33	18	1
A	203	HIS	CE1-NE2	8.47	1.41	1.32	1	7
A	214	ARG	CD-NE	8.46	1.58	1.46	20	5
A	364	ASP	C-N	8.38	1.45	1.33	2	1
A	70	TYR	C-N	8.34	1.45	1.33	14	2
A	370	VAL	C-N	8.23	1.44	1.33	5	3
A	311	LYS	C-N	8.15	1.44	1.33	6	6
A	37	ARG	CD-NE	8.07	1.57	1.46	17	6
A	243	TRP	NE1-CE2	8.06	1.46	1.37	8	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	188	ILE	C-N	7.94	1.44	1.33	3	1
A	221	ARG	C-N	7.93	1.44	1.33	7	1
A	387	HIS	CE1-NE2	7.84	1.40	1.32	3	8
A	351	LEU	CA-CB	7.79	1.69	1.53	9	3
A	216	SER	C-N	7.75	1.44	1.33	19	1
A	175	MET	C-N	7.70	1.44	1.33	2	2
A	59	ASP	C-N	7.65	1.44	1.33	12	3
A	166	HIS	CE1-NE2	7.50	1.40	1.32	10	9
A	147	ALA	C-N	7.46	1.43	1.33	5	3
A	285	PRO	N-CD	7.46	1.37	1.47	17	1
A	233	SER	CA-CB	7.45	1.68	1.53	3	4
A	272	SER	C-N	7.43	1.43	1.33	17	3
A	92	ASP	C-N	7.41	1.43	1.33	10	4
A	230	THR	C-N	7.34	1.43	1.33	16	2
A	334	ARG	CD-NE	7.32	1.56	1.46	17	3
A	388	HIS	CG-CD2	7.26	1.43	1.35	1	3
A	204	LEU	C-N	7.19	1.43	1.33	15	4
A	33	THR	C-N	7.15	1.43	1.33	11	3
A	169	LEU	C-N	7.14	1.43	1.33	13	5
A	385	HIS	CA-CB	7.13	1.67	1.53	10	3
A	78	HIS	ND1-CE1	7.12	1.25	1.32	1	3
A	155	THR	C-N	7.12	1.43	1.33	13	2
A	34	ASN	C-N	7.06	1.43	1.33	13	1
A	5	ASP	C-N	7.06	1.43	1.33	19	3
A	223	LEU	CA-CB	7.05	1.67	1.53	13	2
A	31	GLU	C-N	7.05	1.43	1.33	8	5
A	307	LYS	C-N	7.00	1.43	1.33	2	5
A	215	SER	C-N	7.00	1.43	1.33	17	2
A	382	ARG	CD-NE	7.00	1.56	1.46	1	5
A	315	GLU	C-N	7.00	1.43	1.33	19	4
A	388	HIS	CE1-NE2	6.98	1.39	1.32	17	8
A	376	ALA	C-N	6.98	1.43	1.33	1	2
A	13	ASN	C-N	6.96	1.43	1.33	4	2
A	284	LYS	C-N	6.94	1.23	1.34	13	2
A	178	LEU	C-N	6.91	1.43	1.33	16	3

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	161	ALA	C-N	6.90	1.43	1.33	4	4
A	46	LEU	C-N	6.88	1.43	1.33	17	3
A	61	PHE	CA-CB	6.88	1.67	1.53	14	1
A	242	GLN	C-N	6.87	1.43	1.33	9	2
A	26	LEU	C-N	6.83	1.42	1.33	1	3
A	287	GLU	C-N	6.83	1.23	1.33	20	3
A	291	CYS	C-N	6.77	1.42	1.33	17	2
A	344	HIS	CG-ND1	6.76	1.30	1.38	16	3
A	384	HIS	CE1-NE2	6.76	1.25	1.32	18	3
A	239	ARG	CD-NE	6.75	1.55	1.46	13	4
A	253	MET	C-N	6.74	1.42	1.33	1	2
A	78	HIS	CE1-NE2	6.74	1.39	1.32	6	11
A	113	GLN	C-N	6.73	1.42	1.33	13	4
A	322	VAL	C-N	6.73	1.42	1.33	3	4
A	329	HIS	CB-CG	6.71	1.40	1.50	9	3
A	74	TYR	C-N	6.70	1.42	1.33	4	2
A	159	ALA	C-N	6.69	1.42	1.33	10	4
A	32	LEU	C-N	6.67	1.42	1.33	7	2
A	80	TYR	C-N	6.66	1.42	1.33	14	2
A	203	HIS	CD2-NE2	6.64	1.45	1.37	14	3
A	106	GLN	CA-CB	6.63	1.66	1.53	13	1
A	384	HIS	CB-CG	6.59	1.59	1.50	3	5
A	118	GLY	C-N	6.59	1.42	1.33	10	1
A	157	GLN	C-N	6.58	1.42	1.33	9	4
A	292	ASP	C-N	6.57	1.42	1.33	9	2
A	137	ILE	C-N	6.56	1.45	1.34	11	3
A	162	PHE	C-N	6.53	1.42	1.33	13	3
A	139	ILE	C-N	6.52	1.42	1.33	13	2
A	119	LEU	CA-CB	6.51	1.66	1.53	13	3
A	92	ASP	CA-CB	6.50	1.66	1.53	12	1
A	368	VAL	C-N	6.50	1.42	1.33	16	1
A	381	HIS	ND1-CE1	6.49	1.26	1.32	5	2
A	206	LYS	C-N	6.48	1.42	1.33	17	4
A	264	GLN	C-N	6.45	1.42	1.33	9	2
A	330	CYS	C-N	6.44	1.42	1.33	3	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	216	SER	CA-C	6.43	1.39	1.52	12	2
A	195	VAL	C-N	6.43	1.42	1.33	12	4
A	211	LEU	CA-CB	6.42	1.66	1.53	10	2
A	348	THR	CA-C	6.42	1.66	1.52	6	1
A	366	GLN	C-N	6.42	1.42	1.33	4	2
A	127	CYS	C-N	6.42	1.42	1.33	17	2
A	193	ASP	C-N	6.41	1.42	1.33	1	1
A	76	ALA	C-N	6.40	1.42	1.33	13	2

Standard geometry: angle outliers ?

There are 3899 bond angle outliers in this entry (4.56% 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	193	ASP	CA-CB-CG	13.55	126.15	112.60	11	5
A	174	PHE	CA-CB-CG	12.50	126.30	113.80	14	8
A	354	GLN	OE1-CD-NE2	12.05	110.55	122.60	6	10
A	122	PHE	CA-CB-CG	11.36	125.16	113.80	9	7
A	382	ARG	NE-CZ-NH2	11.03	109.27	119.20	7	7
A	214	ARG	NE-CZ-NH2	10.82	128.94	119.20	11	6
A	381	HIS	CA-CB-CG	10.79	103.01	113.80	5	6
A	310	ASN	CA-CB-CG	10.63	101.97	112.60	15	6
A	273	ASN	CA-CB-CG	10.51	123.11	112.60	15	6
A	148	ASN	CA-CB-CG	10.33	122.93	112.60	2	6
A	55	ARG	NE-CZ-NH1	10.15	131.65	121.50	14	6
A	344	HIS	CB-CG-CD2	9.95	118.26	131.20	2	6
A	41	PHE	CA-CB-CG	9.91	103.89	113.80	7	3
A	95	ASN	OD1-CG-ND2	9.89	112.71	122.60	13	6
A	17	ARG	NE-CZ-NH2	9.86	110.33	119.20	1	9
A	381	HIS	ND1-CG-CD2	9.79	115.89	106.10	12	12
A	240	ASN	CA-CB-CG	9.72	102.88	112.60	15	9
A	369	ASN	CA-CB-CG	9.54	122.14	112.60	1	6
A	185	ASP	CA-CB-CG	9.51	103.09	112.60	12	4
A	257	PHE	CA-CB-CG	9.51	104.29	113.80	8	7
A	17	ARG	NE-CZ-NH1	9.44	130.94	121.50	10	6
A	308	ASP	CA-CB-CG	9.40	103.20	112.60	14	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	148	ASN	OD1-CG-ND2	9.38	113.22	122.60	20	8
A	278	TYR	CB-CG-CD1	9.36	106.77	120.80	11	1
A	37	ARG	NE-CZ-NH1	9.23	130.73	121.50	11	8
A	55	ARG	NE-CZ-NH2	9.19	110.93	119.20	16	8
A	19	HIS	CA-C-N	9.15	130.62	116.90	18	9
A	141	ASP	CA-CB-CG	9.14	121.74	112.60	12	6
A	15	ASN	OD1-CG-ND2	9.12	113.48	122.60	1	4
A	339	GLN	CB-CG-CD	9.12	128.10	112.60	8	2
A	313	THR	CA-C-N	9.09	130.54	116.90	7	6
A	197	GLU	O-C-N	9.06	108.51	123.00	19	3
A	38	GLN	OE1-CD-NE2	9.06	113.54	122.60	3	7
A	101	ASN	CA-CB-CG	8.94	103.66	112.60	12	5
A	15	ASN	CA-CB-CG	8.93	103.67	112.60	10	4
A	278	TYR	CB-CG-CD2	8.92	134.17	120.80	11	3
A	19	HIS	ND1-CG-CD2	8.91	115.01	106.10	10	9
A	55	ARG	NH1-CZ-NH2	8.91	107.72	119.30	18	6
A	298	PHE	CA-C-N	8.82	130.14	116.90	3	7
A	98	ARG	NE-CZ-NH1	8.78	130.28	121.50	11	7
A	334	ARG	NE-CZ-NH1	8.76	112.74	121.50	12	8
A	239	ARG	NE-CZ-NH1	8.68	130.18	121.50	14	9
A	98	ARG	NE-CZ-NH2	8.65	111.41	119.20	11	8
A	162	PHE	CA-CB-CG	8.61	122.41	113.80	6	8
A	166	HIS	CB-CG-ND1	8.60	109.79	122.70	6	8
A	166	HIS	ND1-CG-CD2	8.60	114.70	106.10	9	9
A	383	HIS	ND1-CG-CD2	8.58	114.68	106.10	15	9
A	334	ARG	NE-CZ-NH2	8.53	111.52	119.20	15	10
A	383	HIS	CA-CB-CG	8.53	122.33	113.80	12	7
A	355	TYR	N-CA-CB	8.53	125.00	110.50	12	2
A	240	ASN	OD1-CG-ND2	8.52	114.08	122.60	14	6
A	223	LEU	C-N-CA	8.52	137.03	121.70	11	8
A	383	HIS	ND1-CE1-NE2	8.51	116.91	108.40	20	4
A	101	ASN	OD1-CG-ND2	8.47	114.13	122.60	13	4
A	386	HIS	ND1-CG-CD2	8.45	114.55	106.10	3	9
A	78	HIS	ND1-CG-CD2	8.44	114.54	106.10	8	8
A	83	PHE	CA-CB-CG	8.39	122.19	113.80	5	5

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	381	HIS	CB-CG-ND1	8.35	110.18	122.70	14	6
A	56	ASN	CA-CB-CG	8.32	120.92	112.60	19	5
A	387	HIS	ND1-CG-CD2	8.17	114.27	106.10	18	11
A	344	HIS	CA-CB-CG	8.14	121.94	113.80	13	6
A	165	GLN	OE1-CD-NE2	8.13	114.47	122.60	4	7
A	78	HIS	ND1-CE1-NE2	8.10	116.50	108.40	8	8
A	203	HIS	CB-CG-CD2	8.08	120.70	131.20	15	5
A	85	ASN	CA-CB-CG	8.07	120.67	112.60	15	10
A	24	ALA	CA-C-N	8.07	129.01	116.90	9	7
A	95	ASN	CA-C-N	8.06	129.00	116.90	16	12
A	24	ALA	N-CA-CB	8.05	98.32	110.40	9	4
A	383	HIS	CD2-NE2-CE1	8.05	100.95	109.00	20	1
A	277	ILE	CA-CB-CG1	8.03	124.06	110.40	9	3
A	386	HIS	CA-CB-CG	8.03	105.77	113.80	14	4
A	130	ARG	NE-CZ-NH2	8.03	111.97	119.20	3	6
A	364	ASP	CA-CB-CG	8.02	120.62	112.60	10	6
A	222	ALA	N-CA-CB	8.02	98.36	110.40	17	3
A	214	ARG	NH1-CZ-NH2	7.98	108.93	119.30	11	3
A	37	ARG	NH1-CZ-NH2	7.95	108.96	119.30	5	5
A	203	HIS	ND1-CG-CD2	7.94	114.04	106.10	1	9
A	329	HIS	CD2-NE2-CE1	7.89	101.11	109.00	20	1
A	329	HIS	ND1-CG-CD2	7.88	113.98	106.10	15	13
A	107	ASN	CA-CB-CG	7.86	120.46	112.60	18	3
A	337	SER	N-CA-CB	7.86	123.86	110.50	5	9
A	329	HIS	CB-CG-CD2	7.85	120.99	131.20	7	3
A	247	HIS	CA-CB-CG	7.85	121.65	113.80	10	3
A	209	GLN	OE1-CD-NE2	7.83	114.77	122.60	20	6
A	181	ARG	NE-CZ-NH2	7.82	112.17	119.20	3	5
A	203	HIS	ND1-CE1-NE2	7.81	116.21	108.40	12	8
A	185	ASP	C-N-CA	7.79	135.72	121.70	2	3
A	181	ARG	NE-CZ-NH1	7.78	129.28	121.50	6	7
A	155	THR	CA-CB-OG1	7.76	121.24	109.60	14	6
A	57	ALA	C-CA-CB	7.73	98.90	110.50	18	3
A	385	HIS	CA-CB-CG	7.73	121.53	113.80	17	7
A	131	ASN	CA-CB-CG	7.70	104.90	112.60	8	6

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	267	PHE	CA-CB-CG	7.69	106.11	113.80	9	8
A	137	ILE	O-C-N	7.68	110.72	123.00	7	5
A	388	HIS	ND1-CG-CD2	7.67	113.77	106.10	11	14
A	135	ASP	CA-CB-CG	7.66	104.94	112.60	18	9
A	285	PRO	CA-C-N	7.66	128.38	116.90	12	6
A	17	ARG	CD-NE-CZ	7.65	135.12	124.40	14	6
A	386	HIS	CB-CG-CD2	7.64	121.26	131.20	18	4
A	283	TYR	C-CA-CB	7.64	124.62	110.10	14	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	1.29	8
2	1.13	7
3	0.97	6
4	1.13	7
5	1.13	7
6	0.48	3
7	2.10	13
8	0.48	3
9	1.77	11
10	1.61	10
11	0.65	4
12	1.61	10
13	1.45	9
14	1.29	8
15	0.32	2
16	1.45	9
17	0.65	4
18	1.13	7
19	1.13	7
20	0.65	4

There are 139 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)
A:261:VAL:HG22	A:285:PRO:HD2	0.68	4	1
A:249:LEU:HD12	A:250:PRO:HD2	0.66	2	1
A:177:PHE:HB2	A:195:VAL:HG13	0.62	4	1
A:205:THR:HG21	A:210:ALA:HB2	0.60	9	1
A:313:THR:HG23	A:316:GLU:HG3	0.59	13	1
A:263:ILE:HD11	A:351:LEU:HD13	0.58	7	2
A:64:LEU:HD11	A:240:ASN:HA	0.56	13	1
A:183:LEU:H	A:183:LEU:HD23	0.55	12	1
A:156:CYS:SG	A:204:LEU:HD23	0.55	18	1
A:42:LYS:HA	A:247:HIS:CE1	0.54	8	2
A:246:ALA:HB2	A:377:LYS:HB2	0.54	17	1
A:62:LEU:HD12	A:65:LEU:HD12	0.53	16	1
A:16:TYR:CE2	A:78:HIS:CD2	0.52	17	4
A:381:HIS:CG	A:382:ARG:N	0.52	7	1
A:166:HIS:CD2	A:168:GLY:H	0.52	3	2
A:302:LEU:HD13	A:335:LEU:HD22	0.52	13	1
A:87:PHE:CE2	A:104:CYS:HB2	0.52	2	1
A:382:ARG:HG2	A:385:HIS:CE1	0.51	19	1
A:166:HIS:CG	A:167:SER:H	0.51	7	1
A:296:THR:O	A:297:ASP:HB2	0.51	13	1
A:315:GLU:HG2	A:320:TYR:CE1	0.51	7	1
A:277:ILE:HD11	A:335:LEU:HD12	0.51	3	1
A:89:VAL:HG11	A:97:TYR:CE1	0.50	18	1
A:166:HIS:CG	A:167:SER:N	0.50	7	1
A:336:SER:O	A:337:SER:HB2	0.50	10	1
A:112:MET:HE2	A:120:ASN:HD21	0.50	16	2
A:302:LEU:HD11	A:345:LEU:HD13	0.49	9	1
A:64:LEU:HD22	A:243:TRP:CD2	0.49	1	1
A:19:HIS:CE1	A:97:TYR:CE1	0.49	10	1
A:49:LEU:HD22	A:53:GLU:HG2	0.49	3	1
A:62:LEU:HD13	A:111:LEU:HD13	0.48	10	1
A:88:MET:HE3	A:103:LEU:HD23	0.48	12	1
A:154:ALA:HB1	A:199:MET:HE1	0.48	14	1
A:295:VAL:HG22	A:349:VAL:HG22	0.47	19	1
A:14:MET:HG3	A:24:ALA:HB2	0.47	6	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:253:MET:HE1	A:370:VAL:HG12	0.47	7	1
A:340:LYS:O	A:385:HIS:CE1	0.47	18	1
A:31:GLU:CD	A:179:LYS:HZ2	0.46	17	1
A:338:LEU:HD22	A:373:PRO:HG2	0.46	9	1
A:154:ALA:HB2	A:211:LEU:HD13	0.46	14	2
A:385:HIS:CG	A:386:HIS:N	0.46	13	2
A:257:PHE:CE1	A:263:ILE:HD12	0.46	19	1
A:314:PRO:HD3	A:332:TYR:CE2	0.46	1	1
A:269:ALA:HB2	A:374:LEU:HD11	0.46	12	1
A:267:PHE:CD1	A:277:ILE:HG22	0.46	9	1
A:9:LEU:HD22	A:61:PHE:HB2	0.45	14	1
A:38:GLN:HG2	A:183:LEU:HD22	0.45	10	1
A:95:ASN:HA	A:96:PRO:C	0.45	18	1
A:191:LEU:O	A:195:VAL:HG23	0.45	4	2
A:270:GLU:HB3	A:321:LEU:HD12	0.45	4	1
A:2:LEU:C	A:2:LEU:HD12	0.45	7	1
A:8:ALA:HB3	A:43:VAL:HG13	0.45	18	1
A:370:VAL:O	A:370:VAL:HG12	0.45	1	3
A:112:MET:SD	A:122:PHE:CD2	0.45	12	1
A:173:ILE:HB	A:204:LEU:HD12	0.45	19	1
A:54:MET:HE1	A:75:TYR:CE1	0.45	9	1
A:64:LEU:CD1	A:240:ASN:HA	0.44	13	1
A:39:LEU:HD22	A:224:THR:HG22	0.44	1	1
A:354:GLN:HB2	A:361:THR:HG22	0.44	15	1
A:124:LEU:HD11	A:151:PHE:CE1	0.44	19	1
A:351:LEU:O	A:363:GLU:HA	0.44	8	1
A:383:HIS:CG	A:384:HIS:N	0.44	8	1
A:46:LEU:HB3	A:49:LEU:HD11	0.44	10	1
A:232:TYR:CD2	A:241:LEU:HD13	0.44	13	1
A:186:LYS:HB2	A:191:LEU:HD11	0.44	16	1
A:128:ARG:NH1	A:129:LYS:O	0.44	12	1
A:24:ALA:HB1	A:26:LEU:HG	0.43	3	1
A:42:LYS:HG3	A:247:HIS:CD2	0.43	2	1
A:73:LEU:HD23	A:122:PHE:CE1	0.43	14	1
A:6:LYS:HB3	A:41:PHE:HA	0.43	16	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:385:HIS:CE1	A:386:HIS:CD2	0.43	7	1
A:268:ALA:HB1	A:322:VAL:HG21	0.43	3	1
A:122:PHE:O	A:151:PHE:HA	0.43	15	1
A:64:LEU:HD22	A:243:TRP:CE3	0.43	1	1
A:382:ARG:HE	A:384:HIS:CD2	0.43	9	1
A:288:ILE:HD13	A:291:CYS:HB2	0.43	11	1
A:49:LEU:HB3	A:54:MET:HB2	0.43	20	1
A:328:LYS:C	A:329:HIS:CG	0.42	7	1
A:16:TYR:CD1	A:91:VAL:HA	0.42	9	1
A:177:PHE:CB	A:195:VAL:HG13	0.42	4	1
A:285:PRO:HD2	A:288:ILE:HD12	0.42	5	1
A:89:VAL:HA	A:90:PRO:HD3	0.42	6	1
A:385:HIS:CG	A:386:HIS:H	0.42	7	1
A:65:LEU:HB3	A:117:THR:CG2	0.42	7	1
A:93:ALA:HA	A:94:PRO:HD3	0.42	2	1
A:16:TYR:CD2	A:78:HIS:CD2	0.42	14	2
A:57:ALA:HA	A:380:MET:SD	0.42	14	1
A:2:LEU:HD23	A:226:PRO:HG2	0.42	19	1
A:173:ILE:HA	A:173:ILE:HD12	0.42	1	1
A:181:ARG:HB3	A:191:LEU:HD11	0.42	12	1
A:16:TYR:CD2	A:91:VAL:HA	0.42	16	1
A:49:LEU:HD22	A:53:GLU:HB3	0.42	17	1
A:386:HIS:CG	A:387:HIS:N	0.42	9	1
A:33:THR:HG23	A:43:VAL:HG11	0.42	1	1
A:80:TYR:HB3	A:87:PHE:HB2	0.42	5	1
A:298:PHE:CZ	A:333:THR:HG21	0.41	20	1
A:46:LEU:HD13	A:49:LEU:HD11	0.41	5	1
A:353:TYR:CD1	A:353:TYR:N	0.41	10	1
A:16:TYR:HB3	A:19:HIS:HB2	0.41	1	1
A:46:LEU:HD21	A:375:ILE:HD12	0.41	20	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	20	6

Model ID	Analysed	Favored	Allowed	Outliers
2	386	353	23	10
3	386	354	23	9
4	386	355	24	7
5	386	349	30	7
6	386	349	25	12
7	386	359	20	7
8	386	353	24	9
9	386	355	23	8
10	386	345	35	6
11	386	362	19	5
12	386	354	23	9
13	386	356	24	6
14	386	350	27	9
15	386	356	23	7
16	386	359	20	7
17	386	343	32	11
18	386	358	18	10
19	386	351	26	9
20	386	354	26	6

There are 61 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	304	ILE	15
A	297	ASP	11
A	134	ASP	9
A	337	SER	8
A	156	CYS	7
A	329	HIS	7
A	138	PRO	5
A	159	ALA	5
A	25	PRO	4
A	40	ASP	4
A	148	ASN	4
A	327	PRO	4
A	20	PRO	3

Chain	Res	Type	Models (Total)
A	117	THR	3
A	164	ILE	3
A	172	GLY	3
A	291	CYS	3
A	384	HIS	3
A	51	GLU	2
A	83	PHE	2
A	90	PRO	2
A	96	PRO	2
A	97	TYR	2
A	170	ALA	2
A	184	GLU	2
A	210	ALA	2
A	226	PRO	2
A	236	SER	2
A	237	LEU	2
A	310	ASN	2
A	373	PRO	2
A	374	LEU	2
A	381	HIS	2
A	386	HIS	2
A	48	ASP	1
A	50	THR	1
A	82	ASN	1
A	133	TYR	1
A	141	ASP	1
A	143	LEU	1
A	161	ALA	1
A	162	PHE	1
A	163	GLU	1
A	166	HIS	1
A	168	GLY	1
A	173	ILE	1
A	185	ASP	1
A	202	CYS	1

Chain	Res	Type	Models (Total)
A	206	LYS	1
A	229	GLY	1
A	230	THR	1
A	232	TYR	1
A	233	SER	1
A	235	GLU	1
A	250	PRO	1
A	252	SER	1
A	283	TYR	1
A	285	PRO	1
A	286	PRO	1
A	344	HIS	1
A	380	MET	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	317	20	8
2	345	310	25	10
3	345	320	15	10
4	345	311	25	9
5	345	318	16	11
6	345	315	20	10
7	345	313	24	8
8	345	300	33	12
9	345	312	27	6
10	345	310	30	5
11	345	308	23	14
12	345	299	33	13
13	345	305	33	7
14	345	313	25	7
15	345	310	28	7
16	345	314	23	8
17	345	308	25	12
18	345	304	26	15

Model ID	Analysed	Favored	Allowed	Outliers
19	345	307	27	11
20	345	321	20	4

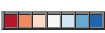
There are 98 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	117	THR	12
A	42	LYS	10
A	339	GLN	9
A	155	THR	7
A	307	LYS	5
A	1	MET	4
A	188	ILE	4
A	189	THR	4
A	230	THR	4
A	313	THR	4
A	179	LYS	3
A	247	HIS	3
A	276	ILE	3
A	279	THR	3
A	281	ILE	3
A	295	VAL	3
A	304	ILE	3
A	342	LYS	3
A	27	VAL	2
A	32	LEU	2
A	43	VAL	2
A	56	ASN	2
A	86	SER	2
A	99	SER	2
A	128	ARG	2
A	182	LEU	2
A	227	ILE	2
A	253	MET	2
A	264	GLN	2
A	282	VAL	2

Chain	Res	Type	Models (Total)
A	285	PRO	2
A	296	THR	2
A	299	PRO	2
A	301	ASP	2
A	327	PRO	2
A	368	VAL	2
A	370	VAL	2
A	375	ILE	2
A	10	LEU	1
A	11	ILE	1
A	25	PRO	1
A	26	LEU	1
A	30	TYR	1
A	47	LEU	1
A	51	GLU	1
A	58	VAL	1
A	62	LEU	1
A	72	LEU	1
A	73	LEU	1
A	81	GLU	1
A	82	ASN	1
A	83	PHE	1
A	85	ASN	1
A	94	PRO	1
A	100	GLU	1
A	106	GLN	1
A	107	ASN	1
A	121	VAL	1
A	124	LEU	1
A	130	ARG	1
A	135	ASP	1
A	136	THR	1
A	138	PRO	1
A	139	ILE	1
A	143	LEU	1

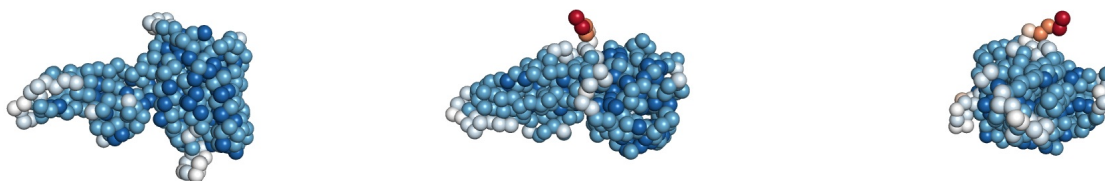
Chain	Res	Type	Models (Total)
A	145	VAL	1
A	148	ASN	1
A	151	PHE	1
A	160	GLU	1
A	162	PHE	1
A	190	VAL	1
A	191	LEU	1
A	206	LYS	1
A	208	LYS	1
A	209	GLN	1
A	213	ILE	1
A	224	THR	1
A	235	GLU	1
A	237	LEU	1
A	239	ARG	1
A	240	ASN	1
A	241	LEU	1
A	250	PRO	1
A	277	ILE	1
A	280	SER	1
A	289	ILE	1
A	290	MET	1
A	297	ASP	1
A	300	LEU	1
A	314	PRO	1
A	337	SER	1
A	348	THR	1
A	360	ASP	1
A	361	THR	1
A	362	VAL	1
A	372	LYS	1
A	382	ARG	1
A	383	HIS	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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