

# Integrative Structure Validation Report ?

February 18, 2025 - 08:37 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	9A3E
PDB-Dev ID	PDBDEV_00000199
Structure Title	Structure of SH3 domain from chicken alpha spectrin determined using restraints from solid-state NMR
Structure Authors	Soeldner B; Grohe K; Neidig P; Auch J; Blach S; Klein A; Vasa S K; Schafer L V; Linser R
Deposited on	2023-02-03

*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](mailto:helpdesk@pdb-ihm.org)*

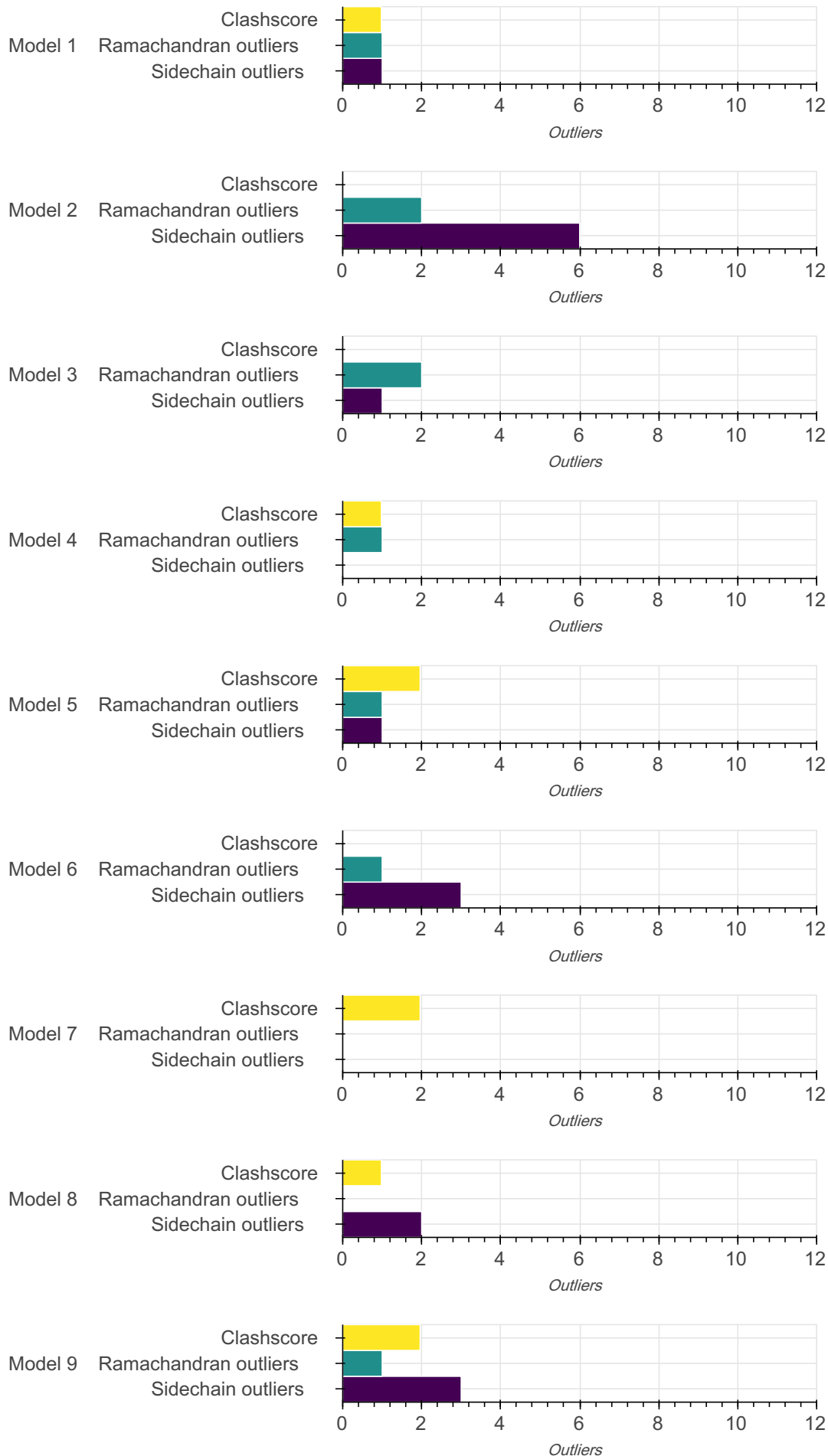
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

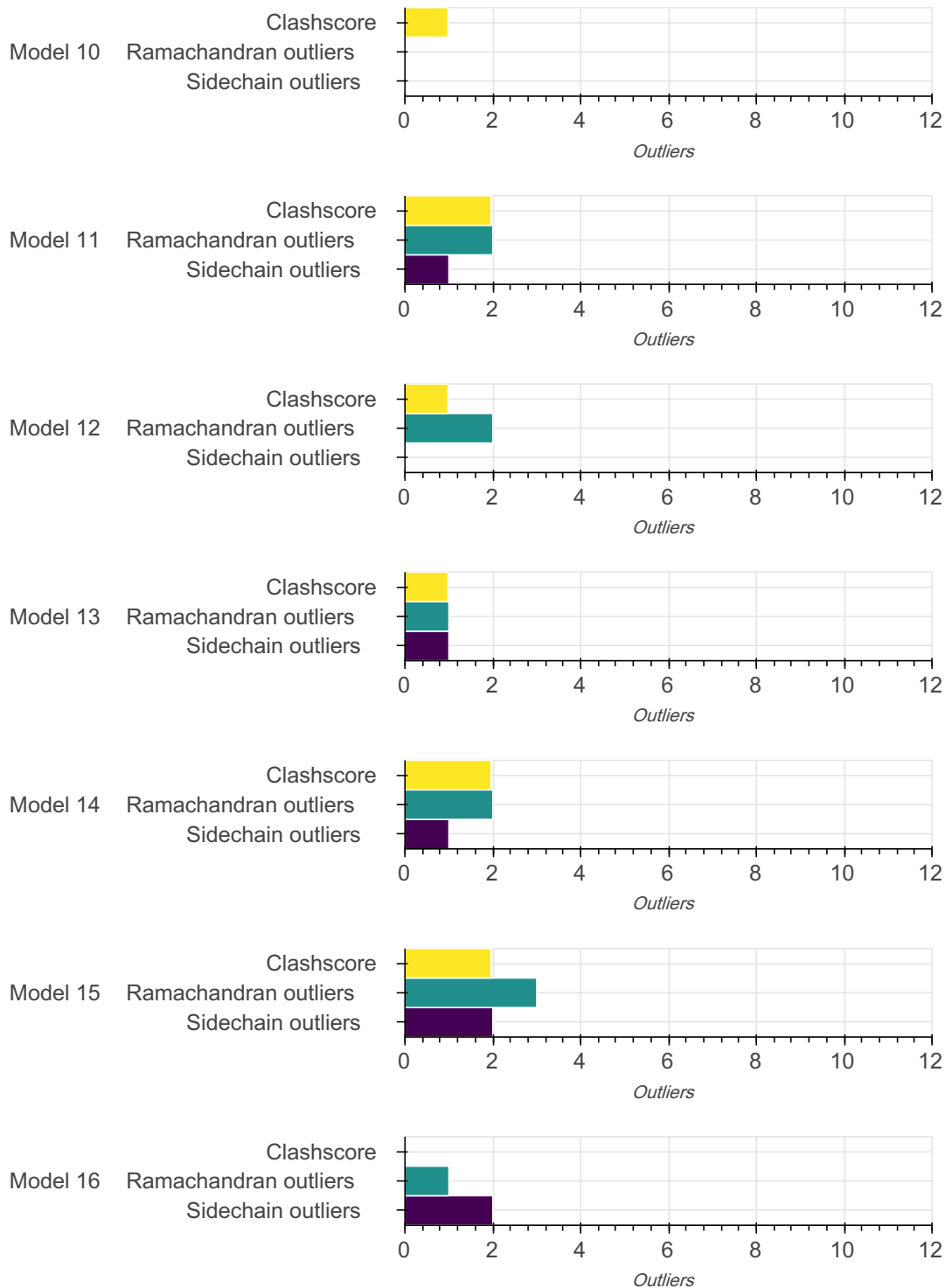
*List of references used to build this report is available [here](#).*

## 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 16 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	1-16	1	spectrin alpha chain	A	62	-	1-6, 7-61, 62	100.00 / 100.00	Atomic

## 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	<a href="#">2NUZ</a>
2	Experimental model	PDB	<a href="#">6SCW</a>
3	NMR data	BMRB	<a href="#">34785</a>
4	Experimental model	PDB	<a href="#">8CF4</a>

## 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	modeling	Restrained Molecular Dynamics Simulation	None	256000	False	False

*There is 1 software package reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">GROMACS</a>	2019.20	model building	<a href="http://www.gromacs.org">http://www.gromacs.org</a>

## Data quality ?

NMR

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 no bond length outliers.

### Standard geometry: angle outliers ?

There are 537 bond angle outliers in this entry (4.81% of 11168 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	16	GLN	OE1-CD-NE2	10.91	111.69	122.60	5	11
A	47	ASN	CA-CB-CG	10.76	101.84	112.60	9	7
A	49	ARG	NE-CZ-NH2	9.64	127.87	119.20	4	6
A	62	ASP	CA-CB-CG	9.03	121.63	112.60	7	7
A	29	ASP	CA-CB-CG	8.51	121.11	112.60	6	6
A	50	GLN	OE1-CD-NE2	8.42	114.18	122.60	9	10
A	14	ASP	CA-CB-CG	8.32	120.92	112.60	3	3
A	47	ASN	OD1-CG-ND2	8.26	114.34	122.60	10	9
A	52	PHE	CA-CB-CG	8.01	121.81	113.80	1	3
A	2	ASP	CA-CB-CG	7.76	120.36	112.60	16	6
A	41	TRP	CE2-CD2-CE3	7.59	111.21	118.80	5	4
A	40	ASP	CA-CB-CG	7.52	120.12	112.60	13	3
A	56	ALA	C-N-CA	7.51	135.23	121.70	15	2
A	21	ARG	NH1-CZ-NH2	7.42	109.65	119.30	2	2
A	47	ASN	C-N-CA	7.23	134.72	121.70	14	4
A	22	GLU	C-N-CA	7.15	134.57	121.70	10	1
A	58	VAL	CA-CB-CG2	7.10	122.47	110.40	6	4
A	9	VAL	CA-CB-CG2	7.08	122.43	110.40	16	6
A	24	THR	OG1-CB-CG2	7.08	95.14	109.30	8	1
A	55	ALA	N-CA-CB	7.04	99.84	110.40	12	3
A	49	ARG	NE-CZ-NH1	7.04	128.54	121.50	6	4
A	26	LYS	C-N-CA	7.01	134.32	121.70	12	3
A	4	THR	C-N-CA	6.82	133.98	121.70	8	2
A	38	ASN	OD1-CG-ND2	6.79	115.81	122.60	7	8

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	53	VAL	CA-CB-CG2	6.67	121.73	110.40	7	5
A	24	THR	CA-CB-OG1	6.51	99.84	109.60	15	2
A	23	VAL	CA-CB-CG1	6.50	121.45	110.40	1	2
A	48	ASP	CA-CB-CG	6.41	119.01	112.60	11	8
A	32	THR	CA-CB-OG1	6.38	100.04	109.60	9	4
A	47	ASN	C-CA-CB	6.37	122.20	110.10	13	4
A	51	GLY	O-C-N	6.35	112.84	123.00	6	1
A	46	VAL	C-N-CA	6.34	133.12	121.70	8	4
A	24	THR	CA-CB-CG2	6.33	121.25	110.50	4	4
A	46	VAL	O-C-N	6.22	113.05	123.00	4	1
A	7	GLU	C-CA-CB	6.16	121.81	110.10	2	1
A	24	THR	N-CA-CB	6.16	101.03	111.50	2	1
A	4	THR	O-C-N	6.13	113.20	123.00	2	2
A	7	GLU	N-CA-CB	6.07	100.18	110.50	3	1
A	20	PRO	N-CA-CB	6.06	109.66	103.00	4	4
A	33	LEU	C-N-CA	6.02	132.54	121.70	2	3
A	35	ASN	OD1-CG-ND2	6.00	116.60	122.60	12	6
A	54	PRO	N-CA-CB	5.99	109.59	103.00	12	3
A	21	ARG	CD-NE-CZ	5.94	132.72	124.40	11	2
A	31	LEU	N-CA-CB	5.93	100.43	110.50	5	1
A	30	ILE	C-N-CA	5.92	132.35	121.70	6	2
A	25	MET	CA-CB-CG	5.90	125.91	114.10	13	2
A	18	LYS	C-N-CA	5.90	132.32	121.70	8	4
A	11	ALA	N-CA-CB	5.89	101.57	110.40	4	2
A	55	ALA	C-CA-CB	5.88	119.32	110.50	3	2
A	35	ASN	C-N-CA	5.87	132.27	121.70	8	3
A	43	LYS	C-N-CA	5.87	132.27	121.70	2	3
A	19	SER	CA-C-N	5.86	125.69	116.90	7	6
A	41	TRP	CD2-CE3-CZ3	5.85	126.21	118.60	5	1
A	10	LEU	C-CA-CB	5.84	121.20	110.10	16	2
A	56	ALA	N-CA-C	5.78	127.18	111.00	5	1
A	25	MET	C-CA-CB	5.78	121.07	110.10	14	1
A	38	ASN	CA-CB-CG	5.77	118.37	112.60	5	1
A	8	LEU	C-N-CA	5.75	132.04	121.70	7	4
A	60	LYS	O-C-N	5.64	113.98	123.00	8	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	2	ASP	C-N-CA	5.59	131.77	121.70	7	5
A	56	ALA	N-CA-CB	5.59	102.01	110.40	14	2
A	15	TYR	C-N-CA	5.52	131.63	121.70	11	4
A	37	THR	CA-CB-OG1	5.48	117.83	109.60	11	2
A	21	ARG	NE-CZ-NH1	5.47	126.97	121.50	2	3
A	6	LYS	C-N-CA	5.46	131.52	121.70	6	1
A	42	TRP	CG-CD2-CE3	5.44	139.34	133.90	14	2
A	39	LYS	CG-CD-CE	5.43	123.78	111.30	9	1
A	3	GLU	CA-CB-CG	5.42	124.95	114.10	7	2
A	27	LYS	CG-CD-CE	5.40	123.73	111.30	2	2
A	47	ASN	CB-CG-ND2	5.40	124.50	116.40	2	5
A	14	ASP	C-N-CA	5.39	131.40	121.70	1	2
A	49	ARG	NH1-CZ-NH2	5.34	112.36	119.30	6	6
A	59	LYS	CA-C-O	5.34	111.72	120.80	10	1
A	52	PHE	C-N-CA	5.34	131.31	121.70	1	4
A	59	LYS	C-N-CA	5.30	131.23	121.70	16	2
A	25	MET	C-N-CA	5.27	131.18	121.70	9	2
A	42	TRP	CD2-CE2-NE1	5.27	100.55	107.40	11	5
A	52	PHE	C-CA-CB	5.26	120.10	110.10	1	2
A	3	GLU	N-CA-CB	5.25	101.58	110.50	4	3
A	18	LYS	CB-CG-CD	5.24	123.34	111.30	12	1
A	23	VAL	O-C-N	5.23	114.63	123.00	12	1
A	35	ASN	CA-CB-CG	5.21	117.81	112.60	16	1
A	56	ALA	C-CA-CB	5.20	102.70	110.50	15	1
A	27	LYS	N-CA-CB	5.19	101.68	110.50	1	2
A	27	LYS	C-N-CA	5.18	131.02	121.70	2	2
A	56	ALA	O-C-N	5.17	114.72	123.00	15	1
A	40	ASP	CA-C-O	5.17	112.01	120.80	6	2
A	19	SER	CA-CB-OG	5.12	121.35	111.10	1	1
A	49	ARG	CD-NE-CZ	5.12	131.56	124.40	7	2
A	50	GLN	CG-CD-NE2	5.11	124.06	116.40	5	1
A	42	TRP	CB-CG-CD2	5.10	133.94	126.80	1	2
A	29	ASP	C-CA-CB	5.10	119.78	110.10	16	2
A	39	LYS	CA-C-O	5.08	112.16	120.80	8	1
A	12	LEU	C-N-CA	5.07	130.83	121.70	7	2

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	42	TRP	CE2-CD2-CE3	5.04	113.76	118.80	14	4
A	19	SER	CA-C-O	5.03	112.24	120.80	1	2
A	60	LYS	C-N-CA	5.03	130.75	121.70	8	3
A	21	ARG	NE-CZ-NH2	5.03	123.73	119.20	10	3
A	49	ARG	C-N-CA	5.02	130.74	121.70	11	2
A	50	GLN	CB-CG-CD	5.02	121.13	112.60	12	2

### 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	0.98	1
2	0.00	0
3	0.00	0
4	0.98	1
5	1.96	2
6	0.00	0
7	1.96	2
8	0.98	1
9	1.96	2
10	0.98	1
11	1.96	2
12	0.98	1
13	0.98	1
14	1.96	2
15	1.96	2
16	0.00	0

There are 18 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:42:TRP:CH2	A:60:LYS:HE3	0.58	13	1
A:33:LEU:CD2	A:60:LYS:HE2	0.57	11	2
A:39:LYS:HE3	A:40:ASP:OD2	0.54	10	1
A:23:VAL:HG12	A:49:ARG:CZ	0.51	8	1
A:41:TRP:CZ3	A:54:PRO:HD3	0.49	12	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:25:MET:HE1	A:58:VAL:HG13	0.45	5	1
A:30:ILE:N	A:30:ILE:HD12	0.44	4	1
A:3:GLU:O	A:6:LYS:HE3	0.43	1	1
A:33:LEU:CD2	A:60:LYS:HE3	0.43	15	1
A:33:LEU:HD23	A:60:LYS:HE2	0.42	7	1
A:9:VAL:HG23	A:31:LEU:HB2	0.42	14	1
A:33:LEU:HD22	A:60:LYS:HE2	0.42	11	1
A:8:LEU:HD23	A:32:THR:HA	0.41	15	1
A:43:LYS:HE2	A:50:GLN:HB3	0.41	5	1
A:13:TYR:CG	A:14:ASP:N	0.41	9	1
A:22:GLU:HA	A:52:PHE:O	0.41	14	1
A:10:LEU:HB2	A:61:LEU:HD21	0.40	9	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	60	55	4	1
2	60	56	2	2
3	60	57	1	2
4	60	55	4	1
5	60	56	3	1
6	60	56	3	1
7	60	56	4	0
8	60	57	3	0
9	60	55	4	1
10	60	55	5	0
11	60	54	4	2
12	60	54	4	2
13	60	54	5	1
14	60	54	4	2
15	60	53	4	3
16	60	59	0	1

There are 5 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	47	ASN	11
A	20	PRO	3
A	14	ASP	2
A	48	ASP	2
A	56	ALA	2

### 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	56	51	4	1
2	56	49	1	6
3	56	50	5	1
4	56	51	5	0
5	56	50	5	1
6	56	48	5	3
7	56	53	3	0
8	56	49	5	2
9	56	53	0	3
10	56	54	2	0
11	56	54	1	1
12	56	53	3	0
13	56	50	5	1
14	56	51	4	1
15	56	51	3	2
16	56	49	5	2

*There are 17 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
A	3	GLU	3
A	58	VAL	3
A	1	MET	2
A	32	THR	2
A	37	THR	2
A	2	ASP	1
A	4	THR	1

Chain	Res	Type	Models (Total)
A	14	ASP	1
A	23	VAL	1
A	25	MET	1
A	27	LYS	1
A	30	ILE	1
A	31	LEU	1
A	38	ASN	1
A	40	ASP	1
A	46	VAL	1
A	48	ASP	1

### Fit of model to data used for modeling ?

#### NMR

Validation for this section is under development.

### Fit of model to data used for validation ?

Validation for this section is under development.

### *Acknowledgments*

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