

Integrative Structure Validation Report ?

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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

PDB ID	9A8V pdb_00009a8v
Structure Title	Integrative structure of Gaussia Luciferase "open" and "closed" structural states from NMR data
Structure Authors	Huang, Y.J.; Montelione, G.T.
Deposited on	2024-06-18

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 10 model(s). A total of 5 dataset(s) were used to build this entry.

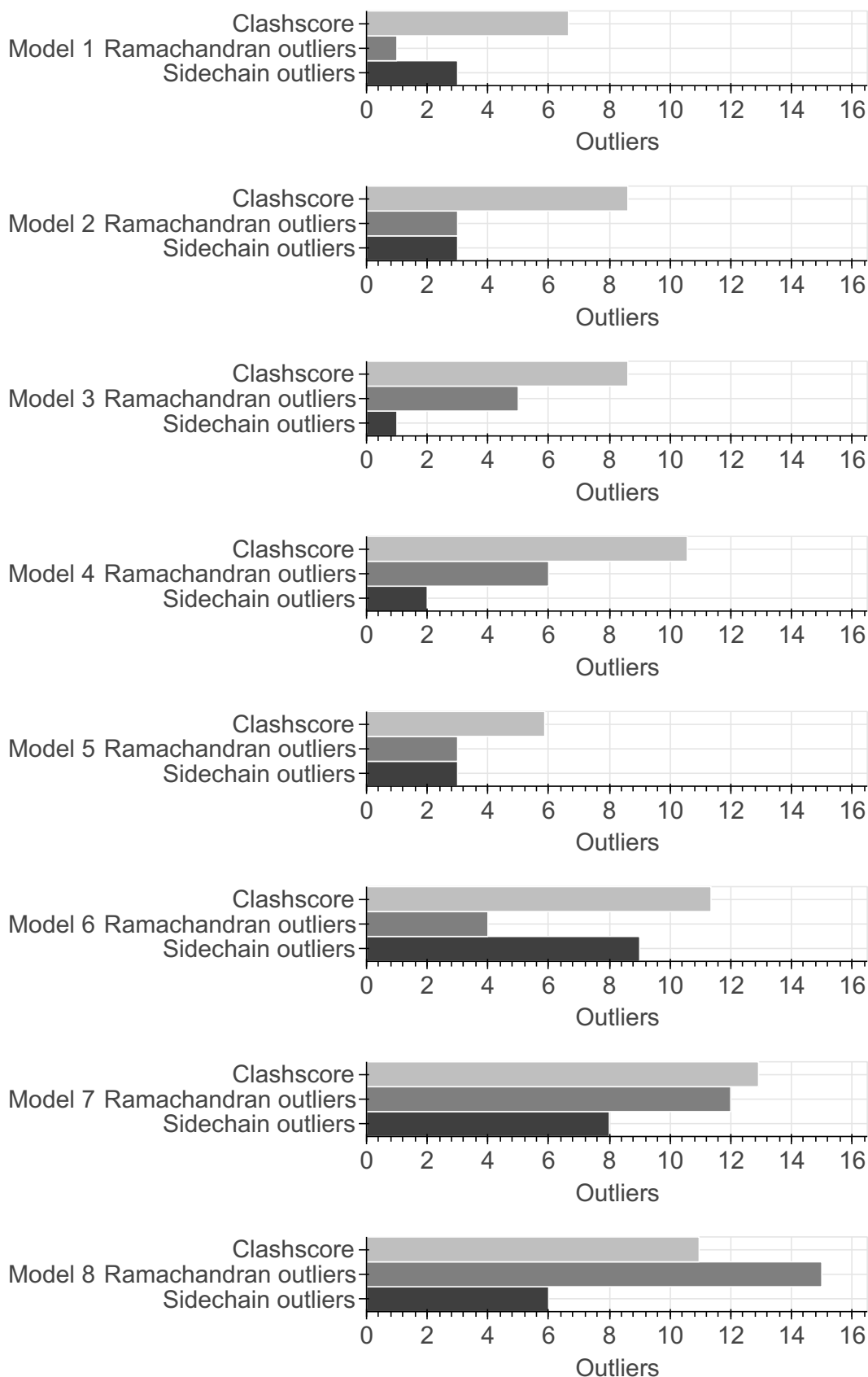
Name	Type	Count
NMR data	Experimental data	5

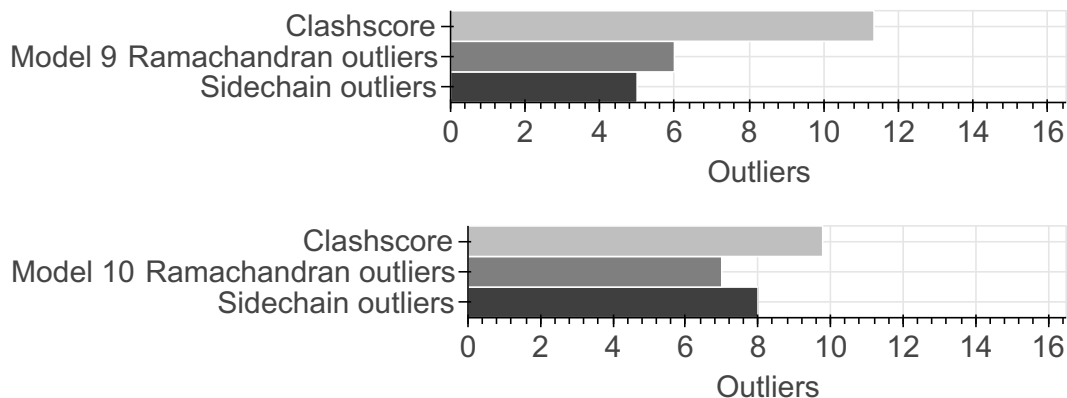
1.2. Overall quality ?

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 0 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	1-10	1	Luciferase	A	168	-	1-168	100.00 / 0.00	Atomic

2.3. Datasets used for modeling ?

There are 5 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	NMR data	BMRB	36385
2	NMR data	Zenodo	10.5281/zenodo.13831427
3	NMR data	Zenodo	10.5281/zenodo.13831427
4	NMR data	Zenodo	10.5281/zenodo.13831427
5	NMR data	Zenodo	10.5281/zenodo.13831427

2.4. Methodology and software ?

This entry is a result of 2 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
2	1	modeling	Not available	AFsample modeling calculations were carried out using modified version of AlphaFold v2.2.0. AFsample calculations, which use six different settings with network dropouts to create conformational heterogeneity, were carried out to generate ~6000 models	Not available	True	False
1	1	modeling	Not available	A modified version of AlphaFold v2.2.0 used by AFsample. AF2 was trained using the PDB database of 2018-04-30 and did not include any NMR structures in the training data.	Not available	True	False

There are 7 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
3	Protein Structure Validation Software	2.00	Validation	https://montelionelab.chem.rpi.edu/PSVS/PSVS2/
4	DoubleRecall	1.00	Validation	https://github.rpi.edu/RPIBioinformatics/AlphaFold-NMR
5	RPF server	ASDP ver 1.0	Validation	https://montelionelab.chem.rpi.edu/rpf/
6	AISAR	1.00	Model Selection	https://github.com/MontelioneLab/AISAR
2	AFsample	Not available	Enhanced Sampling	http://wallnerlab.org/AFsample
1	AlphaFold2	2.2.0	Model Building	https://github.com/google-deepmind/alphafold
7	RCI	Not available	Other	https://www.randomcoilindex.ca/cgi-bin/rci_cgi_current.py

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 1 bond length outliers in this entry (0.01% of 12930 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	76	ARG	CZ-NH2	4.76	1.27	1.33	1	1

Standard geometry: angle outliers ?

There are 87 bond angle outliers in this entry (0.50% of 17430 assessed bonds). A summary is provided below.

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	152	ALA	C-CA-CB	6.85	120.77	110.50	4	1
A	8	ASP	CA-CB-CG	6.74	105.86	112.60	10	2
A	78	HIS	CA-CB-CG	6.25	107.55	113.80	2	1
A	9	PHE	CA-CB-CG	6.14	107.66	113.80	9	4
A	151	PHE	CA-CB-CG	6.14	107.66	113.80	7	2
A	19	ALA	C-CA-CB	6.07	119.61	110.50	9	1
A	147	ARG	NE-CZ-NH2	5.95	124.56	119.20	4	1
A	18	PHE	CA-CB-CG	5.78	108.02	113.80	8	7
A	112	GLN	OE1-CD-NE2	5.72	116.88	122.60	8	9
A	10	ASN	OD1-CG-ND2	5.57	117.03	122.60	4	8
A	11	ILE	CA-CB-CG1	5.51	119.77	110.40	7	2
A	22	ASP	CA-CB-CG	5.48	107.12	112.60	9	2
A	78	HIS	CB-CG-CD2	5.47	124.09	131.20	2	2
A	21	THR	OG1-CB-CG2	5.37	98.56	109.30	1	1
A	156	GLN	OE1-CD-NE2	5.16	117.44	122.60	1	4
A	83	ASP	CA-CB-CG	5.13	107.47	112.60	3	3
A	164	GLY	C-N-CA	5.06	130.81	121.70	7	1
A	17	ASN	CA-CB-CG	5.05	107.55	112.60	6	3
A	88	GLN	OE1-CD-NE2	5.03	117.57	122.60	7	4
A	30	LEU	CA-C-N	5.02	124.43	116.90	4	1
A	76	ARG	NE-CZ-NH2	4.90	123.61	119.20	3	1
A	134	VAL	CA-CB-CG1	4.85	118.65	110.40	6	1
A	74	PRO	C-N-CA	4.82	130.37	121.70	8	1
A	5	ASN	OD1-CG-ND2	4.77	117.83	122.60	9	1
A	21	THR	C-N-CA	4.73	130.22	121.70	7	2
A	158	GLN	OE1-CD-NE2	4.72	117.88	122.60	3	2
A	34	LYS	CG-CD-CE	4.72	122.16	111.30	4	1
A	146	GLN	OE1-CD-NE2	4.72	117.88	122.60	2	1
A	65	CYS	CA-CB-SG	4.65	103.71	114.40	9	1

Chain	Res	Type	Atoms	Z	Observed (Å)	Ideal (Å)	Model ID (Worst)	Models (Total)
A	76	ARG	NE-CZ-NH1	4.61	126.11	121.50	1	1
A	91	ILE	CB-CG1-CD1	4.61	104.13	113.80	7	1
A	14	VAL	CA-CB-CG2	4.49	102.77	110.40	5	2
A	22	ASP	C-CA-CB	4.49	118.63	110.10	4	1
A	76	ARG	NH1-CZ-NH2	4.46	113.50	119.30	3	1
A	78	HIS	ND1-CE1-NE2	4.43	112.83	108.40	4	1
A	57	LEU	N-CA-CB	4.34	103.12	110.50	8	1
A	147	ARG	NH1-CZ-NH2	4.33	113.68	119.30	4	1
A	77	CYS	CA-CB-SG	4.32	104.46	114.40	10	1
A	22	ASP	N-CA-CB	4.23	103.31	110.50	10	1
A	31	PRO	N-CA-CB	4.20	107.62	103.00	4	1
A	168	ASP	CA-CB-CG	4.17	116.77	112.60	9	1
A	24	ASP	CA-CB-CG	4.10	108.50	112.60	9	1
A	14	VAL	CA-CB-CG1	4.09	117.35	110.40	5	1
A	28	GLY	N-CA-C	4.06	101.53	113.30	1	1
A	21	THR	CA-CB-CG2	4.00	103.69	110.50	4	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	6.65	17
2	8.61	22
3	8.61	22
4	10.57	27
5	5.87	15
6	11.35	29
7	12.92	33
8	10.96	28
9	11.35	29
10	9.78	25

There are 247 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:62:HIS:HA	A:91:ILE:HD11	0.90	10	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:40:LEU:HD22	A:88:GLN:HE22	0.87	5	5
A:23:LEU:HD23	A:30:LEU:HD11	0.84	7	1
A:23:LEU:HD21	A:147:ARG:CZ	0.77	4	1
A:20:THR:H	A:155:ILE:HD11	0.77	5	2
A:23:LEU:HD11	A:147:ARG:HH21	0.74	4	1
A:18:PHE:CE1	A:132:ALA:HB2	0.74	8	2
A:40:LEU:HD13	A:88:GLN:HE22	0.72	1	1
A:21:THR:HG21	A:150:THR:OG1	0.71	4	1
A:152:ALA:HB1	A:156:GLN:CD	0.71	4	1
A:23:LEU:HD22	A:30:LEU:HD21	0.69	7	1
A:18:PHE:CD1	A:132:ALA:HB3	0.69	10	1
A:132:ALA:HB1	A:159:VAL:HG21	0.69	2	1
A:19:ALA:HB2	A:151:PHE:CZ	0.69	1	3
A:19:ALA:HB3	A:147:ARG:CZ	0.68	9	3
A:40:LEU:HD13	A:88:GLN:NE2	0.66	1	5
A:23:LEU:CD2	A:30:LEU:HD11	0.66	7	1
A:133:ASN:HA	A:151:PHE:CZ	0.66	10	1
A:18:PHE:CZ	A:162:ILE:HD13	0.65	10	2
A:62:HIS:C	A:91:ILE:HD11	0.65	7	1
A:18:PHE:O	A:155:ILE:HD13	0.65	2	1
A:27:ARG:HA	A:30:LEU:HD13	0.65	7	1
A:19:ALA:HB2	A:151:PHE:CE1	0.64	1	1
A:64:LYS:HB2	A:95:ILE:HD11	0.64	10	1
A:40:LEU:CD1	A:88:GLN:HE22	0.64	1	1
A:9:PHE:CZ	A:57:LEU:HB3	0.64	10	3
A:18:PHE:CZ	A:132:ALA:HB2	0.64	9	2
A:20:THR:HG21	A:76:ARG:CD	0.63	6	1
A:23:LEU:HD21	A:147:ARG:NE	0.62	4	1
A:11:ILE:CG2	A:43:MET:HE3	0.62	7	1
A:27:ARG:CZ	A:75:GLY:HA2	0.62	8	1
A:16:SER:O	A:20:THR:HG23	0.62	9	1
A:118:ASP:HA	A:165:ALA:HB2	0.62	10	3
A:76:ARG:NH2	A:113:PHE:CE1	0.62	1	1
A:34:LYS:HE3	A:83:ASP:OD2	0.61	4	1
A:23:LEU:HD22	A:28:GLY:H	0.61	5	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:40:LEU:CD2	A:88:GLN:HE22	0.61	5	5
A:156:GLN:HA	A:159:VAL:HG22	0.60	4	1
A:9:PHE:CE2	A:57:LEU:HB3	0.60	10	5
A:16:SER:HA	A:147:ARG:HH22	0.60	8	1
A:155:ILE:O	A:159:VAL:HG23	0.59	3	2
A:20:THR:HG21	A:75:GLY:O	0.59	9	1
A:12:VAL:HG22	A:43:MET:HE1	0.59	6	1
A:132:ALA:C	A:151:PHE:CZ	0.59	8	4
A:21:THR:HG21	A:150:THR:CB	0.59	4	1
A:19:ALA:HB3	A:147:ARG:NH2	0.59	8	2
A:27:ARG:HH21	A:75:GLY:N	0.58	9	1
A:11:ILE:HG22	A:43:MET:HE3	0.57	7	1
A:23:LEU:HD11	A:147:ARG:NH2	0.57	4	1
A:129:LYS:HG3	A:159:VAL:HG21	0.56	7	1
A:6:ASN:HD21	A:58:ILE:HD11	0.56	6	1
A:22:ASP:HB3	A:25:ALA:HB3	0.56	2	1
A:76:ARG:NH2	A:113:PHE:CZ	0.56	1	1
A:132:ALA:HB1	A:159:VAL:HG22	0.55	3	1
A:11:ILE:HB	A:43:MET:HE3	0.55	8	2
A:27:ARG:HE	A:75:GLY:HA3	0.55	9	1
A:20:THR:HG21	A:76:ARG:HD3	0.54	6	1
A:22:ASP:CG	A:25:ALA:H	0.54	4	2
A:132:ALA:HB1	A:155:ILE:HG22	0.54	2	1
A:118:ASP:O	A:165:ALA:HB2	0.54	9	1
A:110:MET:HE2	A:158:GLN:OE1	0.53	4	1
A:133:ASN:HA	A:151:PHE:CE2	0.53	9	2
A:21:THR:C	A:23:LEU:H	0.53	8	3
A:159:VAL:HA	A:162:ILE:HD12	0.53	10	3
A:155:ILE:HG22	A:159:VAL:CG2	0.53	2	2
A:22:ASP:HA	A:75:GLY:HA3	0.53	4	1
A:19:ALA:CB	A:147:ARG:HE	0.52	2	3
A:15:ALA:C	A:147:ARG:NH2	0.52	3	1
A:9:PHE:CE2	A:11:ILE:HA	0.52	8	1
A:133:ASN:HA	A:151:PHE:CE1	0.52	7	1
A:35:LEU:HD22	A:39:VAL:HG11	0.52	3	1

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
A:104:PHE:HA	A:107:LEU:HD12	0.52	8	2
A:26:ASP:CG	A:146:GLN:H	0.51	4	1
A:64:LYS:CB	A:95:ILE:HD11	0.51	10	1
A:19:ALA:HB2	A:151:PHE:CE2	0.51	5	1
A:132:ALA:C	A:151:PHE:CE2	0.51	7	1
A:61:SER:O	A:91:ILE:HD11	0.50	9	1
A:4:GLU:C	A:6:ASN:H	0.50	5	3
A:21:THR:HB	A:23:LEU:HG	0.50	3	1
A:62:HIS:CA	A:91:ILE:HD11	0.50	7	1
A:28:GLY:H	A:146:GLN:HE22	0.49	1	1
A:132:ALA:O	A:151:PHE:CE2	0.49	7	1
A:31:PRO:C	A:33:LYS:H	0.49	9	3
A:5:ASN:C	A:7:GLU:H	0.49	4	5
A:20:THR:N	A:155:ILE:HD11	0.48	2	2
A:22:ASP:HA	A:75:GLY:CA	0.48	4	1
A:64:LYS:HG2	A:91:ILE:HG23	0.48	10	2
A:11:ILE:HD11	A:44:GLU:HG3	0.48	10	1
A:19:ALA:HA	A:147:ARG:NH2	0.48	7	1
A:147:ARG:HG2	A:151:PHE:CE2	0.48	1	1
A:22:ASP:H	A:150:THR:HG21	0.48	5	1
A:9:PHE:CZ	A:57:LEU:CB	0.48	7	1
A:20:THR:HG22	A:76:ARG:NH2	0.48	7	1
A:152:ALA:HB1	A:156:GLN:OE1	0.47	4	1
A:16:SER:HA	A:147:ARG:NH2	0.47	1	1
A:40:LEU:HD22	A:88:GLN:NE2	0.47	1	2
A:23:LEU:HD12	A:27:ARG:HH22	0.47	6	1
A:82:GLY:H	A:90:GLY:CA	0.47	8	3
A:151:PHE:CD1	A:155:ILE:HD12	0.47	6	1
A:82:GLY:H	A:90:GLY:HA2	0.47	8	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	166	149	16	1

Model ID	Analysed	Favored	Allowed	Outliers
2	166	155	8	3
3	166	152	9	5
4	166	152	8	6
5	166	148	15	3
6	166	144	18	4
7	166	134	20	12
8	166	140	11	15
9	166	147	13	6
10	166	140	19	7

There are 27 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	4	GLU	6
A	5	ASN	5
A	24	ASP	4
A	25	ALA	4
A	6	ASN	3
A	8	ASP	3
A	20	THR	3
A	22	ASP	3
A	30	LEU	3
A	33	LYS	3
A	87	ALA	3
A	134	VAL	3
A	26	ASP	2
A	28	GLY	2
A	82	GLY	2
A	88	GLN	2
A	7	GLU	1
A	10	ASN	1
A	29	LYS	1
A	32	GLY	1
A	74	PRO	1
A	76	ARG	1
A	132	ALA	1

Chain	Res	Type	Models (Total)
A	133	ASN	1
A	153	SER	1
A	165	ALA	1
A	167	GLY	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	138	127	8	3
2	138	132	3	3
3	138	131	6	1
4	138	129	7	2
5	138	130	5	3
6	138	122	7	9
7	138	120	10	8
8	138	119	13	6
9	138	122	11	5
10	138	111	19	8

There are 26 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
A	6	ASN	3
A	23	LEU	3
A	37	LEU	3
A	123	CYS	3
A	131	LEU	3
A	133	ASN	3
A	140	LEU	3
A	3	THR	2
A	4	GLU	2
A	26	ASP	2
A	77	CYS	2
A	79	THR	2
A	96	VAL	2
A	150	THR	2

Chain	Res	Type	Models (Total)
A	151	PHE	2
A	11	ILE	1
A	20	THR	1
A	21	THR	1
A	27	ARG	1
A	30	LEU	1
A	86	SER	1
A	95	ILE	1
A	122	ASP	1
A	155	ILE	1
A	156	GLN	1
A	159	VAL	1

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.

Acknowledgments

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