

# Integrative Structure Validation Report ?

March 20, 2025 - 08:41 AM PDT

*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	9A0Y
PDB-Dev ID	PDBDEV_00000070
Structure Title	USP7 TRAF domain in complex with DNA polymerase iota peptide 573-584
Structure Authors	Ashton NW; Valles GJ; Jaiswal N; Bezsonova I; Woodgate R
Deposited on	2020-12-11

*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)*

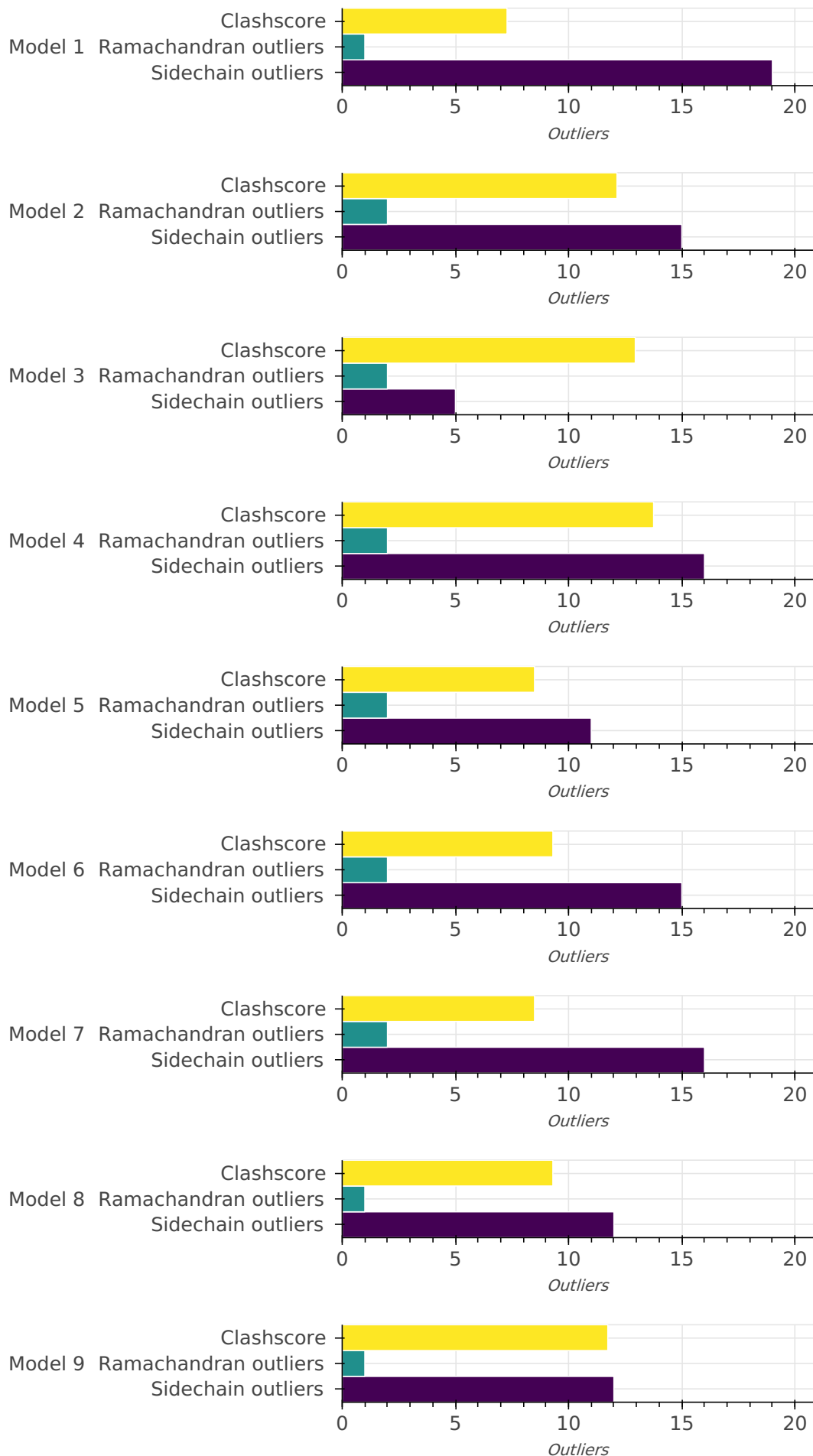
*A user guide is available at [https://pdb-ihm.org/validation\\_help.html](https://pdb-ihm.org/validation_help.html) with specific help available everywhere you see the ? symbol.*

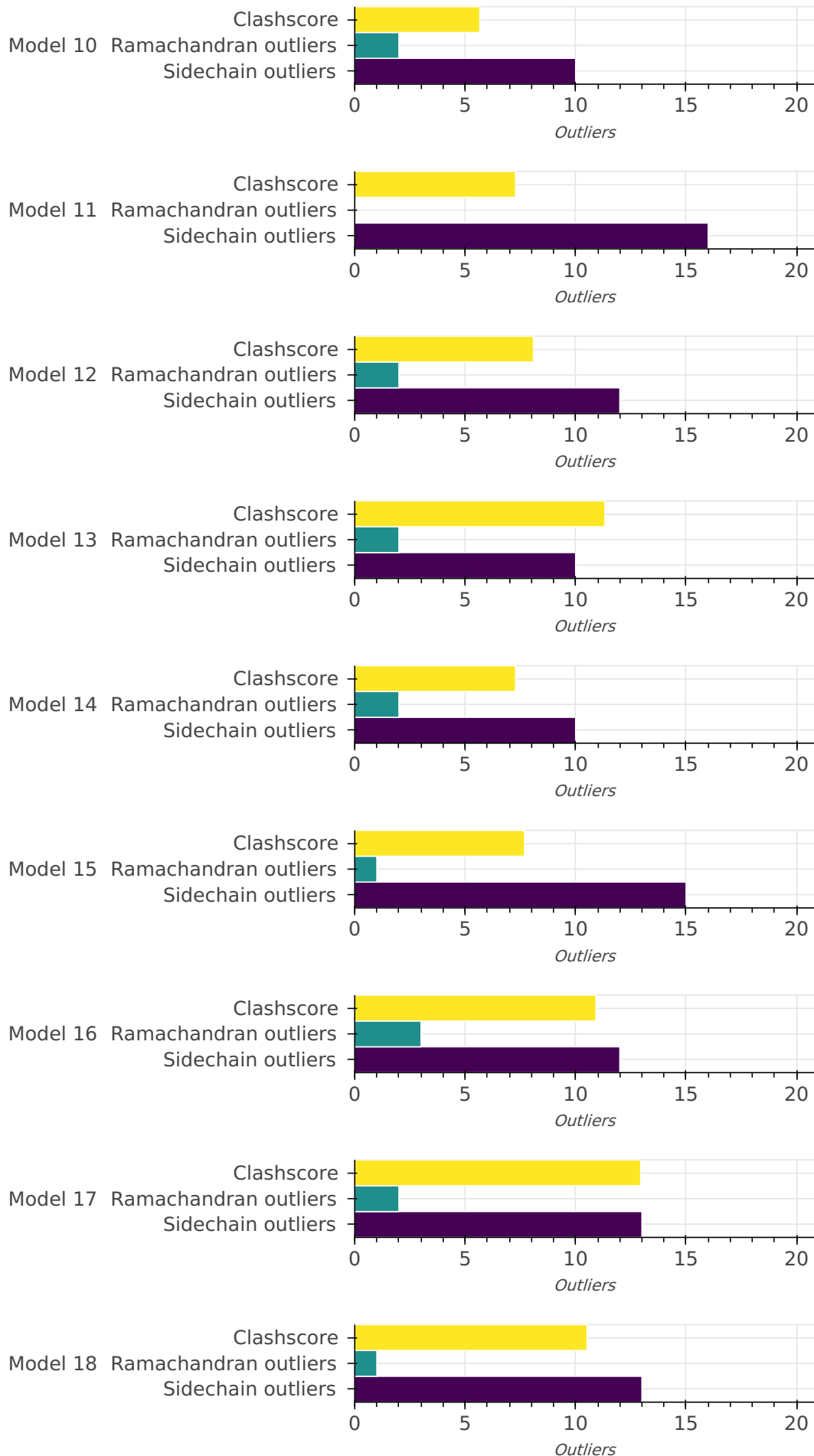
*List of references used to build this report is available [here](#).*

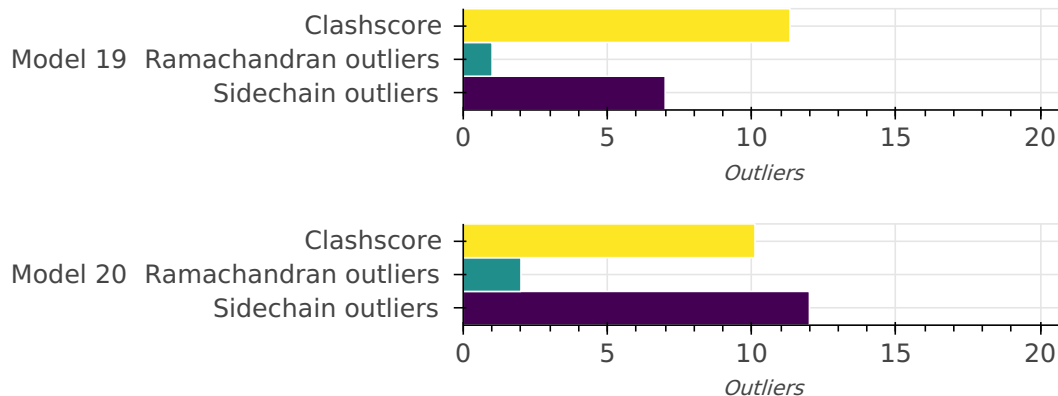
## Overall quality ?

*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 20 model(s). A total of 5 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	1-20	1	DNA polymerase iota peptide 573-584	A	12	1-12	-	100.00 / 100.00	Atomic
		2	USP7 TRAF domain	B	145	1-145	-	100.00 / 100.00	Atomic

### 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	Comparative model	Not available	Not available
2	Comparative model	Not available	Not available
3	Experimental model	PDB	<a href="#">2fop</a>
4	NMR data	BMRB	<a href="#">50080</a>
5	Mutagenesis data	Not available	<a href="#">10.1016/j.jmb.2020.166733</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	None	docking	None	–	False	False

*There are 3 software packages reported in this entry.*

ID	Software name	Software version	Software classification	Software location
1	<a href="#">MODELLER</a>	Not available	model building	<a href="https://salilab.org/modeller/">https://salilab.org/modeller/</a>
2	<a href="#">HADDOCK</a>	Not available	model building	<a href="http://haddock.science.uu.nl/services/HADDOCK/">http://haddock.science.uu.nl/services/HADDOCK/</a>
3	<a href="#">PYMOL</a>	Not available	model building	<a href="https://pymol.org/2/">https://pymol.org/2/</a>

## Data quality ?

### NMR

Validation for this section is under development.

### Mutagenesis

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 no bond angle outliers.

### 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	7.28	18
2	12.14	30
3	12.94	32
4	13.75	34
5	8.50	21
6	9.30	23
7	8.50	21
8	9.30	23
9	11.73	29
10	5.66	14
11	7.28	18
12	8.09	20
13	11.33	28
14	7.28	18
15	7.69	19
16	10.92	27
17	12.94	32
18	10.52	26
19	11.33	28
20	10.11	25

There are 486 clashes. The table below contains the detailed list of all clashes based on a MolProbity analysis. Bad clashes are  $\geq 0.4$  Angstrom. The output is limited to 100 rows.

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:39:ILE:HD11	B:133:VAL:HG21	0.82	18	5
B:29:PRO:HG3	B:38:LYS:HE3	0.80	19	1
B:35:LEU:HD21	B:143:VAL:HG11	0.80	1	5
B:72:CYS:HB3	B:140:PRO:HB3	0.77	13	8
B:111:MET:SD	B:116:VAL:HB	0.76	8	11
B:16:GLU:HG2	B:128:LYS:HE2	0.76	18	2
B:43:PRO:HB3	B:52:GLN:HG2	0.76	9	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:79:LYS:HB2	B:91:SER:HB3	0.75	8	7
B:84:ARG:HG3	B:122:GLY:HA3	0.74	11	13
B:100:HIS:HD2	B:101:LYS:HG2	0.72	17	6
B:10:THR:HB	B:134:PHE:HD1	0.72	9	10
B:7:SER:HA	B:33:ARG:HD3	0.71	18	6
B:43:PRO:HB2	B:52:GLN:HG2	0.70	16	3
B:124:ILE:HD11	B:127:ASP:HA	0.70	16	13
B:46:TYR:HB2	B:53:LYS:HB2	0.70	10	7
B:36:PRO:HD2	B:62:ASN:HB2	0.70	9	3
B:68:THR:HG22	B:100:HIS:HB2	0.69	12	2
B:27:SER:HB3	B:39:ILE:HB	0.69	2	4
B:78:LEU:HA	B:133:VAL:HG12	0.67	4	6
B:58:PHE:HA	B:106:GLY:HA3	0.67	20	5
B:16:GLU:HA	B:128:LYS:HG2	0.67	3	8
B:12:GLN:HG2	B:81:ILE:HD11	0.67	17	5
B:85:ASP:HB3	B:88:LYS:HG3	0.66	18	5
B:81:ILE:HD11	B:132:GLU:HB2	0.66	10	18
B:115:GLU:HG3	B:121:LYS:HE2	0.65	13	2
B:32:VAL:HB	B:37:TRP:CD1	0.65	12	13
B:85:ASP:HB3	B:88:LYS:HD3	0.64	15	1
B:27:SER:HB3	B:39:ILE:HG13	0.64	8	1
B:39:ILE:HD13	B:59:LEU:HG	0.64	13	1
B:58:PHE:HB3	B:104:ASP:OD1	0.63	13	3
B:73:HIS:HB2	B:97:LEU:HD12	0.63	7	2
B:20:ARG:HA	B:20:ARG:HE	0.62	2	2
A:7:THR:HG22	B:104:ASP:O	0.62	3	12
B:4:SER:HB3	B:31:PHE:HB3	0.62	17	1
B:20:ARG:HA	B:20:ARG:NE	0.62	2	15
B:14:THR:HG22	B:128:LYS:HG2	0.61	7	3
B:27:SER:CB	B:39:ILE:HB	0.61	2	5
B:29:PRO:HG3	B:38:LYS:HE2	0.60	4	1
B:70:TRP:HA	B:142:GLY:HA3	0.60	11	4
B:100:HIS:CD2	B:101:LYS:HG2	0.59	5	12
B:113:TRP:HA	B:116:VAL:HG12	0.59	3	3
B:99:PHE:HE2	B:101:LYS:HB2	0.59	15	4

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:16:GLU:HG2	B:128:LYS:HG2	0.58	10	2
B:17:ARG:HD2	B:20:ARG:HB2	0.58	9	1
B:17:ARG:HD3	B:127:ASP:OD2	0.57	3	5
B:78:LEU:HB2	B:110:PHE:HE2	0.57	3	1
B:126:ASP:HB3	B:128:LYS:HE2	0.57	19	2
B:17:ARG:HA	B:127:ASP:OD2	0.57	12	11
B:99:PHE:CE2	B:101:LYS:HB2	0.56	15	7
B:118:ASP:HB3	B:121:LYS:HG2	0.56	5	5
B:142:GLY:HA2	B:145:TRP:CZ2	0.56	17	3
B:71:SER:HB3	B:97:LEU:HD21	0.56	19	1
A:3:CYS:SG	B:109:ASN:HB2	0.55	2	3
A:11:ASN:HB3	B:101:LYS:HD2	0.55	8	1
B:21:LEU:HD23	B:113:TRP:HH2	0.55	12	10
B:39:ILE:HG21	B:133:VAL:HG11	0.55	11	1
B:12:GLN:HG3	B:132:GLU:HG3	0.54	4	1
B:46:TYR:CG	B:47:PRO:HD2	0.54	17	3
B:49:ARG:HG3	B:50:PRO:HD2	0.53	16	5
B:115:GLU:HG2	B:121:LYS:HE2	0.53	18	2
B:43:PRO:CB	B:52:GLN:HG2	0.53	16	2
B:32:VAL:HG12	B:33:ARG:HG2	0.52	12	1
B:118:ASP:OD2	B:120:GLU:HB2	0.52	8	2
B:83:TYR:CE2	B:125:ASP:HB2	0.52	4	2
B:11:PHE:HE2	B:39:ILE:HG12	0.52	3	1
B:98:PHE:HE1	B:105:TRP:HB3	0.51	17	1
A:8:SER:HB2	B:42:MET:HE1	0.51	2	1
B:60:GLN:HB3	B:104:ASP:HB2	0.51	13	1
B:80:ILE:O	B:89:SER:HB3	0.51	8	6
B:26:LEU:HB3	B:38:LYS:HD3	0.51	3	1
A:6:GLY:HA2	B:105:TRP:CZ3	0.51	13	1
A:5:PRO:HB2	B:105:TRP:HE1	0.50	19	2
B:70:TRP:HH2	B:103:ASN:HD22	0.50	16	1
B:37:TRP:HZ3	B:59:LEU:HD21	0.50	17	1
B:46:TYR:CD1	B:47:PRO:HD2	0.50	20	3
B:99:PHE:CZ	B:101:LYS:HB2	0.49	16	1
B:111:MET:HE3	B:115:GLU:HG2	0.49	9	1



Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:32:VAL:HB	B:37:TRP:NE1	0.49	14	5
B:82:ASN:HB3	B:85:ASP:O	0.48	4	8
B:29:PRO:HB3	B:38:LYS:HE3	0.48	5	2
B:74:ALA:HB3	B:98:PHE:HE2	0.48	17	1
B:71:SER:HB3	B:97:LEU:HD11	0.48	20	1
B:140:PRO:HB2	B:143:VAL:HG21	0.48	4	2
B:26:LEU:HA	B:39:ILE:O	0.48	19	2
B:99:PHE:HE1	B:101:LYS:HB2	0.48	3	2
B:44:ARG:HG3	B:108:SER:O	0.48	3	1
B:53:LYS:HG3	B:54:SER:OG	0.47	2	1
B:7:SER:HA	B:33:ARG:CD	0.47	5	3
B:55:VAL:HG22	B:113:TRP:CE3	0.47	5	2
B:62:ASN:ND2	B:65:SER:HB3	0.47	4	3
B:79:LYS:HE3	B:81:ILE:HG12	0.47	4	1
B:84:ARG:HD3	B:122:GLY:CA	0.47	5	1
B:84:ARG:NH2	B:88:LYS:HE2	0.47	17	1
B:17:ARG:HG3	B:20:ARG:HB2	0.47	5	1
B:126:ASP:O	B:128:LYS:HE2	0.46	14	1
B:76:ALA:HB2	B:135:VAL:HG23	0.46	13	6
B:6:ARG:O	B:33:ARG:HD2	0.46	5	1
B:118:ASP:HB3	B:121:LYS:CG	0.46	12	3
B:140:PRO:HB2	B:143:VAL:CG2	0.46	11	2
B:78:LEU:O	B:91:SER:HA	0.46	1	7

### 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	153	140	12	1
2	153	140	11	2
3	153	139	12	2
4	153	142	9	2
5	153	143	8	2
6	153	143	8	2
7	153	142	9	2
8	153	142	10	1

Model ID	Analysed	Favored	Allowed	Outliers
9	153	144	8	1
10	153	139	12	2
11	153	143	10	0
12	153	143	8	2
13	153	138	13	2
14	153	143	8	2
15	153	145	7	1
16	153	141	9	3
17	153	145	6	2
18	153	144	8	1
19	153	141	11	1
20	153	142	9	2

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

Chain	Res	Type	Models (Total)
B	47	PRO	19
B	48	ASP	8
B	53	LYS	4
B	62	ASN	1
B	101	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	142	108	15	19
2	142	111	16	15
3	142	112	25	5
4	142	108	18	16
5	142	107	24	11
6	142	111	16	15
7	142	106	20	16
8	142	111	19	12
9	142	111	19	12
10	142	113	19	10
11	142	108	18	16

Model ID	Analysed	Favored	Allowed	Outliers
12	142	110	20	12
13	142	110	22	10
14	142	113	19	10
15	142	110	17	15
16	142	113	17	12
17	142	108	21	13
18	142	113	16	13
19	142	112	23	7
20	142	112	18	12

*There are 60 unique sidechain outliers. Detailed list of outliers are tabulated below.*

Chain	Res	Type	Models (Total)
B	114	SER	16
B	108	SER	14
B	68	THR	13
B	91	SER	13
B	69	SER	11
B	111	MET	10
B	130	THR	10
B	49	ARG	9
B	51	HIS	9
B	4	SER	8
B	14	THR	8
B	24	SER	8
A	1	SER	7
A	12	SER	7
B	17	ARG	7
B	71	SER	7
A	7	THR	5
B	7	SER	5
B	66	ASP	5
B	20	ARG	4
B	23	GLU	4
B	54	SER	4
B	65	SER	4

Chain	Res	Type	Models (Total)
B	72	CYS	4
B	104	ASP	4
B	127	ASP	4
B	27	SER	3
B	67	SER	3
B	102	GLU	3
A	11	ASN	2
B	22	SER	2
B	39	ILE	2
B	40	MET	2
B	42	MET	2
B	60	GLN	2
B	78	LEU	2
B	80	ILE	2
B	133	VAL	2
B	138	ASP	2
B	141	HIS	2
A	8	SER	1
B	8	GLU	1
B	25	VAL	1
B	32	VAL	1
B	52	GLN	1
B	59	LEU	1
B	64	GLU	1
B	83	TYR	1
B	87	GLU	1
B	92	ARG	1
B	93	ARG	1
B	94	ILE	1
B	95	SER	1
B	107	PHE	1
B	109	ASN	1
B	115	GLU	1
B	117	THR	1
B	124	ILE	1

Chain	Res	Type	Models (Total)
B	128	LYS	1
B	143	VAL	1

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

#### NMR

Validation for this section is under development.

#### Mutagenesis

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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