

Integrative Structure Validation Report ?

March 20, 2025 - 08:35 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	9A0X
PDB-Dev ID	PDBDEV_00000069
Structure Title	USP7 UBL 1-2 domains in complex with DNA polymerase iota peptide 438-448
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

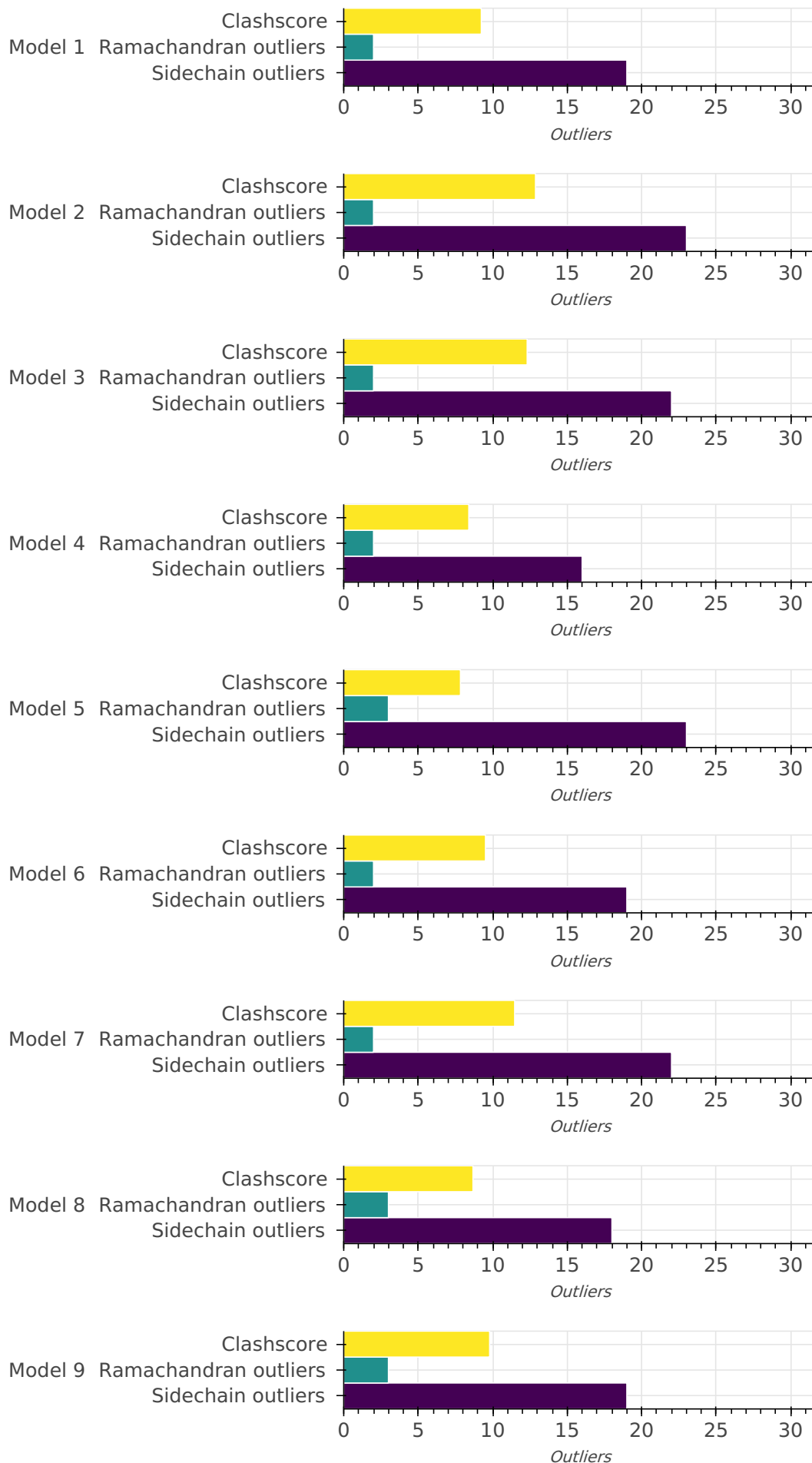
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

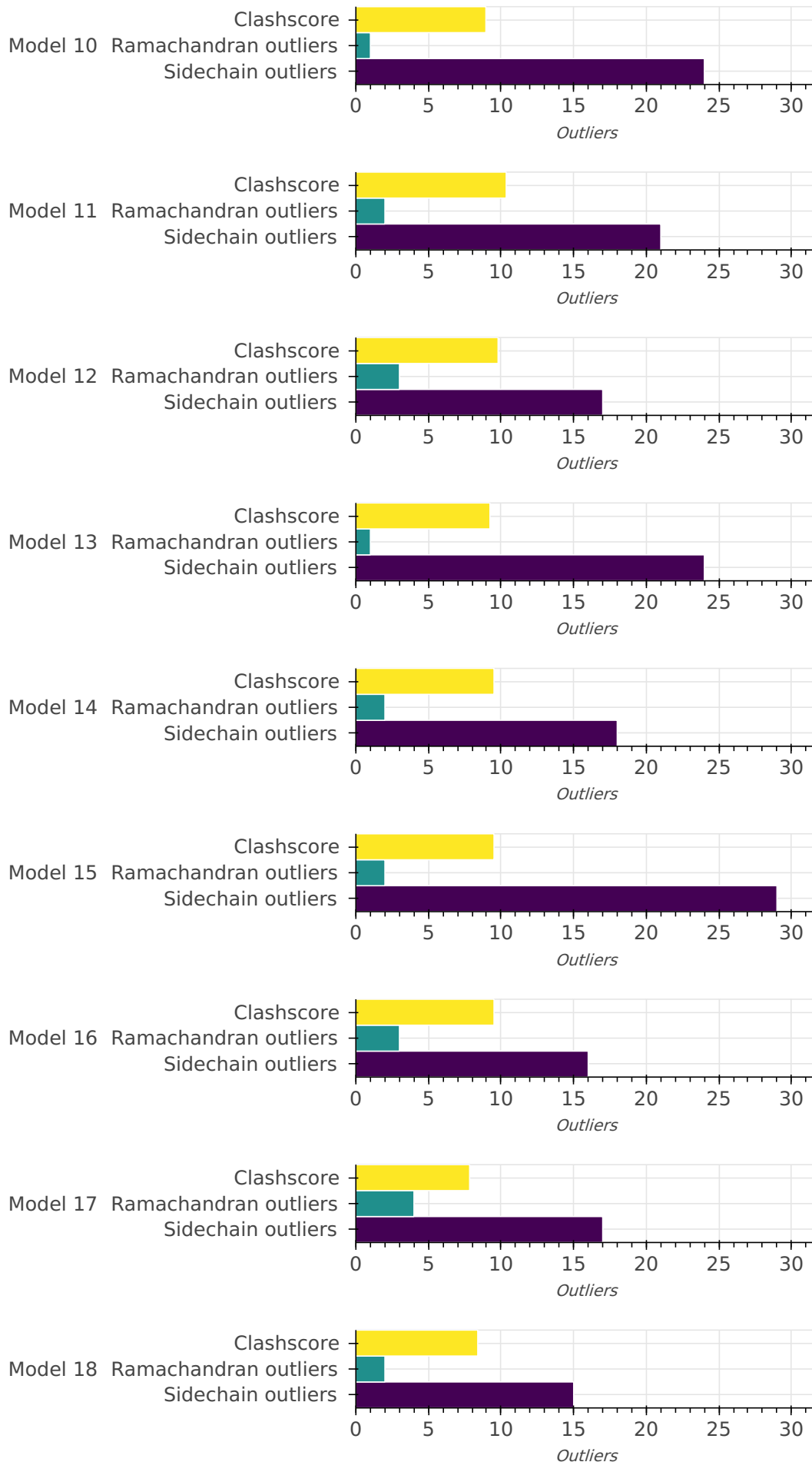
List of references used to build this report is available [here](#).

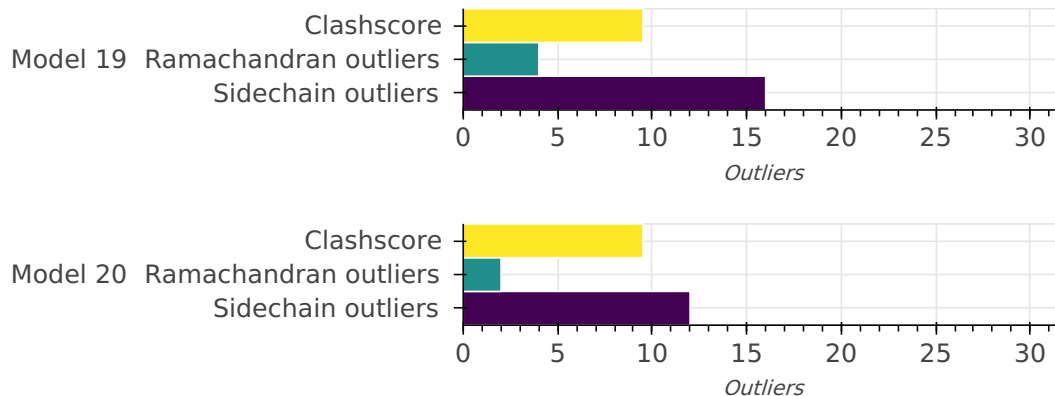
Overall quality ?

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 438-448	A	11	1-11	-	100.00 / 100.00	Atomic
		2	USP7 UBL 1-2 domains	B	214	1-214	-	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	5gg4
4	NMR data	BMRB	26782
5	Mutagenesis data	Not available	10.1016/j.jmb.2020.166733

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	MODELLER	Not available	model building	https://salilab.org/modeller/
2	HADDOCK	Not available	model building	http://haddock.science.uu.nl/services/HADDOCK/
3	PYMOL	Not available	model building	https://pymol.org/2/

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	9.23	33
2	12.87	46
3	12.31	44
4	8.39	30
5	7.83	28
6	9.51	34
7	11.47	41
8	8.67	31
9	9.79	35
10	8.95	32
11	10.35	37
12	9.79	35
13	9.23	33
14	9.51	34
15	9.51	34
16	9.51	34
17	7.83	28
18	8.39	30
19	9.51	34
20	9.51	34

There are 687 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)
B:119:ASP:HB3	B:122:HIS:HB2	0.99	3	2
A:9:LYS:HD2	B:177:VAL:HG11	0.89	18	2
B:103:THR:HG21	B:107:GLU:HG3	0.87	13	4
B:64:MET:HE3	B:100:PHE:HB2	0.83	14	6
B:37:LYS:HB3	B:88:ILE:HB	0.83	12	17
B:175:GLU:HB2	B:183:GLU:HB2	0.82	16	1
B:23:TYR:HB2	B:28:VAL:HG21	0.82	19	5

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:60:ARG:HB3	B:102:GLU:HB3	0.79	11	8
B:22:MET:HA	B:22:MET:HE3	0.78	14	11
B:159:MET:HE1	B:173:LEU:HD21	0.76	14	13
B:105:ASP:HB3	B:106:PRO:HD3	0.75	7	12
B:8:ILE:HB	B:31:THR:HB	0.75	8	9
B:141:CYS:HB3	B:162:ARG:HB3	0.74	10	7
B:82:ASP:HB3	B:85:LYS:HE2	0.74	7	2
B:11:GLU:HA	B:14:PHE:HD2	0.72	7	1
B:11:GLU:HG3	B:14:PHE:HD2	0.71	10	2
B:13:GLN:HB3	B:28:VAL:HG23	0.71	12	9
A:7:LYS:HG2	B:198:GLU:HG2	0.71	11	1
A:7:LYS:HE2	B:198:GLU:HB3	0.70	11	1
B:12:ASP:HB3	B:108:LEU:HD12	0.70	20	2
B:178:LYS:HE2	B:181:LEU:HD22	0.69	3	3
B:120:LYS:H	B:120:LYS:HD3	0.69	5	2
B:118:PHE:HB2	B:123:ASP:HB2	0.68	3	1
B:7:GLN:HG2	B:32:VAL:HG22	0.68	1	1
B:8:ILE:HD13	B:99:ILE:HB	0.68	17	8
B:148:ILE:HD13	B:199:LEU:HD21	0.68	5	1
B:45:VAL:HG12	B:56:GLN:HG2	0.68	15	8
B:12:ASP:HA	B:108:LEU:HB2	0.67	5	1
B:64:MET:HE2	B:100:PHE:HB2	0.67	7	11
B:127:PHE:HE2	B:202:GLY:HA2	0.67	11	8
B:11:GLU:HA	B:14:PHE:CD2	0.66	7	7
B:165:PHE:HE2	B:209:LYS:HD2	0.66	6	1
B:105:ASP:HA	B:112:GLY:HA3	0.65	3	2
B:21:ASP:HA	B:73:ARG:HH21	0.65	2	2
B:148:ILE:HA	B:192:LEU:HD11	0.65	3	1
B:170:SER:HB2	B:210:ASP:HB3	0.64	5	9
B:52:MET:HA	B:52:MET:HE2	0.64	9	3
B:129:LYS:HD3	B:204:ILE:HG21	0.64	19	1
B:24:ASP:HB3	B:27:LYS:HB3	0.64	11	6
B:104:VAL:HG13	B:105:ASP:H	0.63	3	6
B:21:ASP:HA	B:73:ARG:NH2	0.63	15	3
B:175:GLU:HB3	B:183:GLU:HB2	0.63	17	6

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:193:ASP:HA	B:199:LEU:HD22	0.62	8	1
B:86:THR:HB	B:89:GLU:HG3	0.62	20	7
A:10:ASP:HA	B:69:ASN:HA	0.62	12	1
B:41:LEU:HD12	B:85:LYS:HD2	0.61	2	4
B:175:GLU:HG3	B:185:ILE:HD11	0.61	11	2
B:66:ALA:HB2	B:72:LYS:HE2	0.61	16	1
B:107:GLU:HG2	B:108:LEU:H	0.60	9	4
B:4:MET:HB3	B:37:LYS:HG2	0.60	1	2
B:127:PHE:HB2	B:204:ILE:HG12	0.60	20	10
B:62:TRP:HB2	B:100:PHE:HB3	0.60	1	5
B:148:ILE:HA	B:192:LEU:HD12	0.60	4	2
B:9:VAL:HG22	B:100:PHE:HA	0.60	2	1
B:5:GLN:HB3	B:96:PRO:HB3	0.59	5	8
B:60:ARG:HH22	B:116:PRO:HG2	0.59	9	2
B:55:PRO:HG2	B:58:GLN:HB2	0.59	12	2
B:58:GLN:HB3	B:104:VAL:HB	0.59	14	4
B:156:LEU:HB2	B:157:PRO:HD3	0.59	15	15
B:163:ALA:HB2	B:207:PHE:HE2	0.59	16	5
B:146:THR:HG21	B:155:LEU:HD21	0.59	6	3
A:9:LYS:HD3	B:178:LYS:HD2	0.59	16	1
B:134:LYS:HE2	B:214:ASN:HA	0.58	7	1
B:175:GLU:HB2	B:185:ILE:HD11	0.58	15	2
B:63:PRO:HA	B:99:ILE:HD13	0.58	12	15
B:163:ALA:HB2	B:207:PHE:HZ	0.58	2	1
B:62:TRP:HB3	B:74:PRO:HB2	0.58	10	2
B:156:LEU:HB3	B:157:PRO:HD3	0.57	7	1
B:171:LEU:HD23	B:209:LYS:HA	0.57	13	14
B:174:TYR:HB3	B:182:THR:HG22	0.57	7	6
B:155:LEU:HD11	B:192:LEU:HD21	0.57	5	3
B:64:MET:HB2	B:98:THR:HB	0.57	1	6
B:190:VAL:HG23	B:195:ALA:HB2	0.57	1	1
B:9:VAL:HG22	B:30:TYR:HB3	0.57	13	1
B:119:ASP:H	B:123:ASP:HB2	0.57	17	2
B:174:TYR:HB2	B:206:VAL:HB	0.56	1	2
B:12:ASP:HA	B:108:LEU:HD12	0.56	7	3

Atom 1	Atom 2	Clash(Å)	Model ID (Worst)	Models (Total)
B:37:LYS:HD3	B:88:ILE:HD12	0.56	13	1
B:82:ASP:HB2	B:85:LYS:HD3	0.56	15	2
B:105:ASP:H	B:106:PRO:HD2	0.56	15	8
B:13:GLN:HB3	B:28:VAL:HG13	0.56	2	2
B:8:ILE:HD11	B:44:PHE:HZ	0.55	8	3
B:59:ILE:HB	B:101:LEU:HD12	0.55	5	1
B:60:ARG:H	B:102:GLU:HB3	0.55	1	1
B:48:LEU:HD21	B:101:LEU:HD11	0.55	4	1
B:128:LEU:HB2	B:141:CYS:HB2	0.55	2	3
B:4:MET:SD	B:37:LYS:HA	0.55	15	5
A:4:HIS:HB2	B:200:MET:HE2	0.55	20	3
B:123:ASP:HA	B:147:PRO:HA	0.55	18	3
B:211:ASP:HB3	B:214:ASN:ND2	0.55	19	3
B:56:GLN:HA	B:59:ILE:HG12	0.55	10	4
B:127:PHE:HE1	B:202:GLY:HA2	0.55	8	2
B:48:LEU:HD21	B:101:LEU:HG	0.55	3	1
B:178:LYS:HG2	B:181:LEU:HD22	0.54	12	1
B:127:PHE:CE1	B:202:GLY:HA2	0.54	19	1
B:129:LYS:HE3	B:204:ILE:HG21	0.53	20	2
B:129:LYS:O	B:206:VAL:HA	0.53	6	7
B:73:ARG:HD3	B:202:GLY:O	0.53	7	2
B:41:LEU:HB2	B:85:LYS:HE3	0.53	6	1
B:86:THR:O	B:90:LEU:HG	0.53	7	2

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	221	204	15	2
2	221	205	14	2
3	221	206	13	2
4	221	206	13	2
5	221	209	9	3
6	221	210	9	2
7	221	207	12	2
8	221	208	10	3

Model ID	Analysed	Favored	Allowed	Outliers
9	221	205	13	3
10	221	211	9	1
11	221	205	14	2
12	221	211	7	3
13	221	208	12	1
14	221	209	10	2
15	221	208	11	2
16	221	208	10	3
17	221	203	14	4
18	221	209	10	2
19	221	206	11	4
20	221	207	12	2

There are 9 unique backbone outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	82	ASP	19
B	105	ASP	19
B	27	LYS	2
B	81	ALA	2
A	9	LYS	1
B	21	ASP	1
B	107	GLU	1
B	112	GLY	1
B	202	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	205	163	23	19
2	205	160	22	23
3	205	162	21	22
4	205	167	22	16
5	205	157	25	23
6	205	163	23	19
7	205	160	23	22

Model ID	Analysed	Favored	Allowed	Outliers
8	205	168	19	18
9	205	165	21	19
10	205	166	15	24
11	205	158	26	21
12	205	168	20	17
13	205	167	14	24
14	205	164	23	18
15	205	158	18	29
16	205	166	23	16
17	205	168	20	17
18	205	165	25	15
19	205	159	30	16
20	205	168	25	12

There are 88 unique sidechain outliers. Detailed list of outliers are tabulated below.

Chain	Res	Type	Models (Total)
B	135	THR	19
B	146	THR	17
B	149	SER	16
B	98	THR	14
B	101	LEU	14
B	103	THR	14
B	114	THR	14
B	86	THR	12
B	107	GLU	12
B	41	LEU	11
B	182	THR	11
B	191	SER	11
B	82	ASP	10
B	31	THR	9
B	40	SER	9
B	68	SER	9
B	27	LYS	8
B	104	VAL	8
B	92	ASP	7

Chain	Res	Type	Models (Total)
A	1	SER	6
B	12	ASP	6
B	170	SER	6
B	189	ASP	6
B	5	GLN	5
B	21	ASP	5
B	30	TYR	5
B	49	SER	5
B	57	ASP	5
B	186	GLN	5
B	9	VAL	4
B	22	MET	4
B	79	ASN	4
B	154	ASP	4
B	201	ASP	4
A	5	SER	3
A	9	LYS	3
A	10	ASP	3
A	11	THR	3
B	39	SER	3
B	71	THR	3
B	93	ASN	3
B	111	SER	3
B	117	LYS	3
B	177	VAL	3
B	198	GLU	3
B	203	ASP	3
B	11	GLU	2
B	26	GLU	2
B	51	THR	2
B	61	LEU	2
B	78	ASP	2
B	108	LEU	2
B	120	LYS	2
B	123	ASP	2

Chain	Res	Type	Models (Total)
B	166	ILE	2
B	176	GLU	2
B	178	LYS	2
B	205	ILE	2
B	211	ASP	2
A	8	MET	1
B	20	ASN	1
B	25	GLU	1
B	33	PHE	1
B	43	GLU	1
B	46	GLN	1
B	48	LEU	1
B	52	MET	1
B	54	PHE	1
B	60	ARG	1
B	64	MET	1
B	65	GLN	1
B	72	LYS	1
B	73	ARG	1
B	77	LEU	1
B	84	ASN	1
B	115	LEU	1
B	136	ARG	1
B	139	ASN	1
B	141	CYS	1
B	144	ILE	1
B	156	LEU	1
B	175	GLU	1
B	180	ASN	1
B	181	LEU	1
B	184	ARG	1
B	192	LEU	1
B	204	ILE	1
B	208	GLN	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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