Integrative Structure Validation Report

July 22, 2024 - 04:18 PM PDT

The following software was used in the production of this report:

Python-IHM Version 1.3
MolProbity Version 4.5.2
Integrative Modeling Validation Version 1.2

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

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

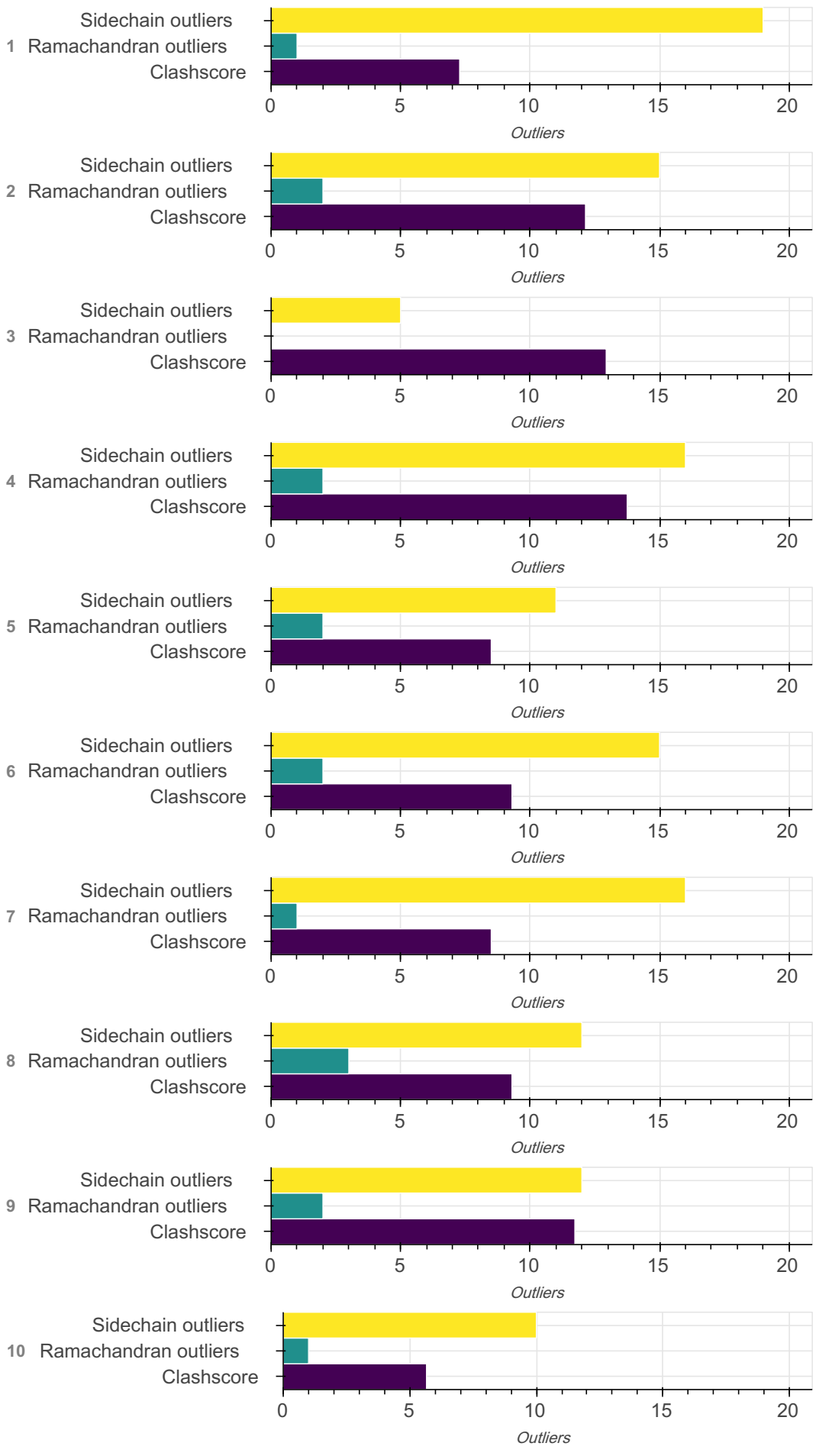
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

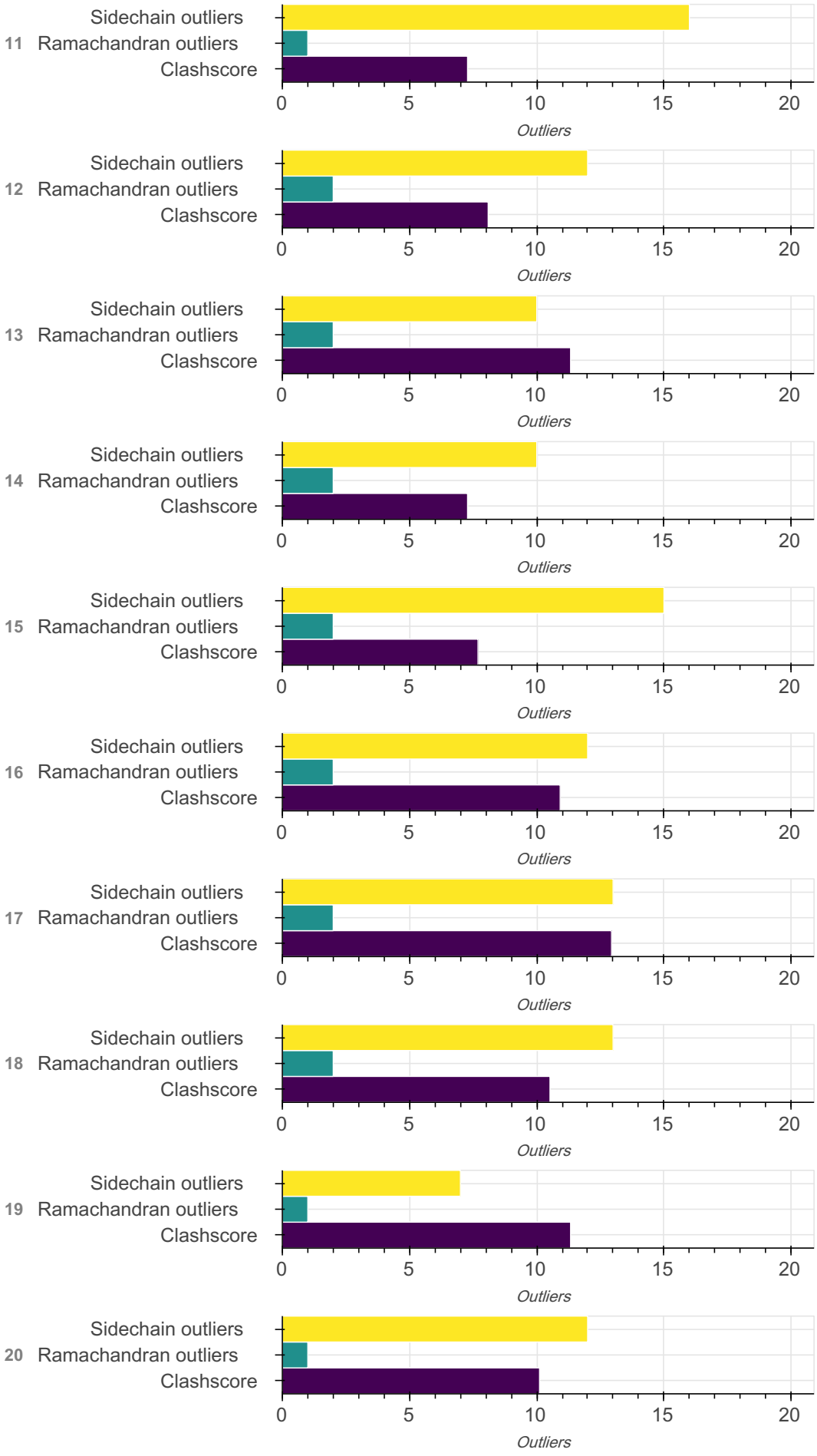
List of references used to build this report is available here.

Overall quality

This validation report contains model quality assessments for all structures, data quality assessment for SAS datasets and fit to model assessments for SAS 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


1
2
3
4
5
6
7
8
9
10
Sidechain outliers
Ramachandran outliers
Clashscore
0
5
10
15
20
Outliers


11
12
13
14
15
16
17
18
19
20
Sidechain outliers
Ramachandran outliers
Clashscore
0
5
10
15
20
Outliers

Ensemble information

This entry consists of 0 distinct ensemble(s).

Summary

This entry consists of 20 unique models, with 2 subunits in each model. A total of 5 datasets or restraints were used to build this entry. Each model is represented by 2 rigid bodies and 0 flexible or non-rigid units.

Entry composition

There are 20 unique types of models in this entry.These models are titled None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None, None respectively.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	DNA polymerase iota peptide 573-584	A	A	12
1	2	2	USP7 TRAF domain	B	B	145
2	1	1	DNA polymerase iota peptide 573-584	A	A	12
2	2	2	USP7 TRAF domain	B	B	145
3	1	1	DNA polymerase iota peptide 573-584	A	A	12
3	2	2	USP7 TRAF domain	B	B	145
4	1	1	DNA polymerase iota peptide 573-584	A	A	12
4	2	2	USP7 TRAF domain	B	B	145
5	1	1	DNA polymerase iota peptide 573-584	A	A	12
5	2	2	USP7 TRAF domain	B	B	145

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
6	1	1	DNA polymerase iota peptide 573-584	A	A	12
6	2	2	USP7 TRAF domain	B	B	145
7	1	1	DNA polymerase iota peptide 573-584	A	A	12
7	2	2	USP7 TRAF domain	B	B	145
8	1	1	DNA polymerase iota peptide 573-584	A	A	12
8	2	2	USP7 TRAF domain	B	B	145
9	1	1	DNA polymerase iota peptide 573-584	A	A	12
9	2	2	USP7 TRAF domain	B	B	145
10	1	1	DNA polymerase iota peptide 573-584	A	A	12
10	2	2	USP7 TRAF domain	B	B	145
11	1	1	DNA polymerase iota peptide 573-584	A	A	12
11	2	2	USP7 TRAF domain	B	B	145
12	1	1	DNA polymerase iota peptide 573-584	A	A	12
12	2	2	USP7 TRAF domain	B	B	145
13	1	1	DNA polymerase iota peptide 573-584	A	A	12
13	2	2	USP7 TRAF domain	B	B	145
14	1	1	DNA polymerase iota peptide 573-584	A	A	12
14	2	2	USP7 TRAF domain	B	B	145

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
15	1	1	DNA polymerase iota peptide 573-584	A	A	12
15	2	2	USP7 TRAF domain	B	B	145
16	1	1	DNA polymerase iota peptide 573-584	A	A	12
16	2	2	USP7 TRAF domain	B	B	145
17	1	1	DNA polymerase iota peptide 573-584	A	A	12
17	2	2	USP7 TRAF domain	B	B	145
18	1	1	DNA polymerase iota peptide 573-584	A	A	12
18	2	2	USP7 TRAF domain	B	B	145
19	1	1	DNA polymerase iota peptide 573-584	A	A	12
19	2	2	USP7 TRAF domain	B	B	145
20	1	1	DNA polymerase iota peptide 573-584	A	A	12
20	2	2	USP7 TRAF domain	B	B	145

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	2fop
4	NMR data	BMRB	50080

ID	Dataset type	Database name	Data access code
5	Mutagenesis data	File	10.1016/j.jmb.2020.166733

Representation

This entry has only one representation and includes 2 rigid bodies and 0 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	1-12	-
B	1-145	-

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	docking	None	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

Bond length outliers can not be evaluated for this model

Standard geometry: angle outliers

Bond angle outliers do not exist or can not be evaluated for this model

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 the 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

Model ID	Clash score	Number of clashes
16	10.92	27
17	12.94	32
18	10.52	26
19	11.33	28
20	10.11	25

All 486 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Model ID	Atom-1	Atom-2	Clash overlap (Å)
1	B:25:ASP:HB3	B:28:LYS:HG3	0.467
1	B:64:ILE:HD11	B:67:ASP:HA	0.462
1	B:18:LEU:O	B:31:SER:HA	0.460
1	B:16:ALA:HB2	B:75:VAL:HG23	0.444
1	B:18:LEU:HA	B:73:VAL:HG12	0.430
1	B:40:HIS:HD2	B:41:LYS:HG2	0.428
1	B:12:CYS:HB3	B:80:PRO:HB3	0.427
1	B:24:ARG:HG3	B:62:GLY:HA3	0.425
1	B:41:LYS:HA	B:41:LYS:HD2	0.424
1	B:79:ALA:HA	B:80:PRO:HD3	0.415
1	B:21:ILE:HD11	B:72:GLU:HB2	0.405
2	B:39:PHE:CE2	B:41:LYS:HB2	0.555
2	B:21:ILE:HD11	B:72:GLU:HB2	0.531
2	B:24:ARG:HG3	B:62:GLY:HA3	0.507
2	B:12:CYS:HB3	B:80:PRO:HB3	0.496
2	B:80:PRO:HB2	B:83:VAL:HG21	0.476

Model ID	Atom-1	Atom-2	Clash overlap (Å)
2	B:2:ASN:ND2	B:5:SER:HB3	0.467
2	B:20:ILE:O	B:29:SER:HB3	0.467
2	B:53:TRP:HA	B:56:VAL:HG12	0.462
2	B:64:ILE:HD11	B:67:ASP:HA	0.460
2	B:39:PHE:HE2	B:41:LYS:HB2	0.453
2	B:18:LEU:O	B:31:SER:HA	0.443
2	B:79:ALA:HA	B:80:PRO:HD3	0.440
2	B:41:LYS:HA	B:41:LYS:HD3	0.410
3	B:21:ILE:HD11	B:72:GLU:HB2	0.631
3	B:10:TRP:HA	B:82:GLY:HA3	0.596
3	B:53:TRP:HA	B:56:VAL:HG12	0.593
3	B:18:LEU:HA	B:73:VAL:HG12	0.580
3	B:18:LEU:HB2	B:50:PHE:HE2	0.570
3	B:8:THR:HG22	B:40:HIS:HB2	0.565
3	B:51:MET:SD	B:56:VAL:HB	0.479
3	B:39:PHE:HE2	B:41:LYS:HB2	0.478
3	B:20:ILE:O	B:29:SER:HB3	0.477
3	B:58:ASP:OD1	B:60:GLU:HB2	0.436
3	B:22:ASN:HB3	B:25:ASP:O	0.408
3	B:21:ILE:CD1	B:72:GLU:HB2	0.401
4	B:18:LEU:HA	B:73:VAL:HG12	0.674
4	B:51:MET:SD	B:56:VAL:HB	0.653
4	B:40:HIS:HD2	B:41:LYS:HG2	0.611

Model ID	Atom-1	Atom-2	Clash overlap (Å)
4	B:40:HIS:CD2	B:41:LYS:HG2	0.528
4	B:23:TYR:CE2	B:65:ASP:HB2	0.520
4	B:22:ASN:HB3	B:25:ASP:O	0.481
4	B:80:PRO:HB2	B:83:VAL:HG21	0.478
4	B:24:ARG:HG3	B:62:GLY:HA3	0.477
4	B:2:ASN:ND2	B:5:SER:HB3	0.471
4	B:19:LYS:HE3	B:21:ILE:HG12	0.470
4	B:66:ASP:HB3	B:68:LYS:HE2	0.466
4	B:19:LYS:HE3	B:21:ILE:CG1	0.455
4	B:82:GLY:HA2	B:85:TRP:CZ2	0.452
4	B:13:HIS:HA	B:37:LEU:HA	0.438
4	B:80:PRO:HB2	B:83:VAL:CG2	0.409
4	B:18:LEU:O	B:31:SER:HA	0.401
5	B:40:HIS:CD2	B:41:LYS:HG2	0.594
5	B:58:ASP:HB3	B:61:LYS:HG2	0.560
5	B:19:LYS:HB2	B:31:SER:HB3	0.479
5	B:24:ARG:HD3	B:62:GLY:CA	0.470
5	B:39:PHE:HE2	B:41:LYS:HB2	0.435
5	B:64:ILE:HD11	B:67:ASP:HA	0.421
5	B:21:ILE:HD11	B:72:GLU:HB2	0.420
5	B:21:ILE:CG1	B:72:GLU:HB2	0.411
5	B:24:ARG:HD3	B:62:GLY:HA3	0.411
5	B:18:LEU:HA	B:73:VAL:HG12	0.403

Model ID	Atom-1	Atom-2	Clash overlap (Å)
6	B:25:ASP:HB3	B:28:LYS:HG3	0.588
6	B:21:ILE:HD11	B:72:GLU:HB2	0.582
6	B:51:MET:SD	B:56:VAL:HB	0.488
6	B:10:TRP:HA	B:82:GLY:HA3	0.472
6	B:64:ILE:HD11	B:67:ASP:HA	0.450
6	B:21:ILE:HD12	B:70:THR:HB	0.427
6	B:40:HIS:CD2	B:41:LYS:HG2	0.425
6	B:24:ARG:HG3	B:62:GLY:HA3	0.416
7	B:13:HIS:HB2	B:37:LEU:HD12	0.629
7	B:39:PHE:CE2	B:41:LYS:HB2	0.545
7	B:21:ILE:HD11	B:72:GLU:HB2	0.519
7	B:32:ARG:HB2	B:50:PHE:CE2	0.452
7	B:16:ALA:HB2	B:75:VAL:HG23	0.449
7	B:39:PHE:HE2	B:41:LYS:HB2	0.447
7	B:22:ASN:HB3	B:25:ASP:O	0.436
7	B:58:ASP:HA	B:59:PRO:HD3	0.403
7	B:11:SER:HB2	B:37:LEU:HD21	0.401
7	B:64:ILE:HD11	B:67:ASP:HA	0.400
8	B:51:MET:SD	B:56:VAL:HB	0.758
8	B:19:LYS:HB2	B:31:SER:HB3	0.751
8	B:24:ARG:HG3	B:62:GLY:HA3	0.631
8	B:21:ILE:HD11	B:72:GLU:HB2	0.523
8	B:58:ASP:OD1	B:60:GLU:HB2	0.523

Model ID	Atom-1	Atom-2	Clash overlap (Å)
8	B:39:PHE:CE2	B:41:LYS:HB2	0.519
8	B:20:ILE:O	B:29:SER:HB3	0.510
8	B:12:CYS:HB3	B:80:PRO:HB3	0.472
8	B:22:ASN:HB3	B:25:ASP:O	0.426
9	B:64:ILE:HD11	B:67:ASP:HA	0.569
9	B:40:HIS:CD2	B:41:LYS:HG2	0.520
9	B:51:MET:HE3	B:55:GLU:HG2	0.489
9	B:21:ILE:HD11	B:72:GLU:HB2	0.458
9	B:12:CYS:HB3	B:80:PRO:HB3	0.451
9	B:22:ASN:HB3	B:25:ASP:O	0.450
9	B:2:ASN:ND2	B:5:SER:HB3	0.419
9	B:58:ASP:HB3	B:61:LYS:CG	0.412
9	B:58:ASP:HB3	B:61:LYS:HG3	0.402
9	B:32:ARG:HB2	B:50:PHE:CE2	0.400
10	B:21:ILE:HD11	B:72:GLU:HB2	0.656
10	B:18:LEU:HA	B:73:VAL:HG12	0.616
10	B:40:HIS:CD2	B:41:LYS:HG2	0.544
10	B:51:MET:SD	B:56:VAL:HB	0.500
10	B:58:ASP:HB3	B:61:LYS:HG2	0.417
11	B:24:ARG:HG3	B:62:GLY:HA3	0.739
11	B:10:TRP:HA	B:82:GLY:HA3	0.598
11	B:40:HIS:CD2	B:41:LYS:HG2	0.590
11	B:64:ILE:HD11	B:67:ASP:HA	0.566

Model ID	Atom-1	Atom-2	Clash overlap (Å)
11	B:40:HIS:HD2	B:41:LYS:HG2	0.538
11	B:51:MET:SD	B:56:VAL:HB	0.485
11	B:80:PRO:HB2	B:83:VAL:CG2	0.461
11	B:16:ALA:HB2	B:75:VAL:HG23	0.454
11	B:21:ILE:HD11	B:72:GLU:HB2	0.427
11	B:68:LYS:HB2	B:68:LYS:HE3	0.422
11	B:10:TRP:HB2	B:83:VAL:HG13	0.413
11	B:58:ASP:HB3	B:61:LYS:HB2	0.408
11	B:79:ALA:HA	B:80:PRO:HD3	0.401
12	B:8:THR:HG22	B:40:HIS:HB2	0.695
12	B:51:MET:SD	B:56:VAL:HB	0.638
12	B:64:ILE:HD11	B:67:ASP:HA	0.627
12	B:21:ILE:HD11	B:72:GLU:HB2	0.562
12	B:58:ASP:HB3	B:61:LYS:HG2	0.516
12	B:58:ASP:HB3	B:61:LYS:CG	0.463
12	B:16:ALA:HB2	B:75:VAL:HG23	0.427
12	B:21:ILE:HD12	B:70:THR:HG22	0.413
12	B:24:ARG:HG3	B:62:GLY:HA3	0.412
12	B:20:ILE:H	B:20:ILE:HG13	0.403
13	B:12:CYS:HB3	B:80:PRO:HB3	0.772
13	B:55:GLU:HG3	B:61:LYS:HE2	0.654
13	B:19:LYS:HB2	B:31:SER:HB3	0.627
13	B:40:HIS:CD2	B:41:LYS:HG2	0.553

Model ID	Atom-1	Atom-2	Clash overlap (Å)
13	B:24:ARG:HG3	B:62:GLY:HA3	0.472
13	B:16:ALA:HB2	B:75:VAL:HG23	0.463
13	B:58:ASP:HB3	B:61:LYS:HG2	0.443
13	B:40:HIS:HD2	B:41:LYS:HG2	0.440
13	B:58:ASP:HB3	B:61:LYS:CG	0.439
13	B:50:PHE:HD1	B:51:MET:HG2	0.424
13	B:21:ILE:HD11	B:72:GLU:HB2	0.423
13	B:64:ILE:HD11	B:67:ASP:HA	0.421
13	B:18:LEU:O	B:31:SER:HA	0.403
14	B:51:MET:SD	B:56:VAL:HB	0.665
14	B:55:GLU:HG3	B:61:LYS:HE2	0.584
14	B:21:ILE:HD11	B:72:GLU:HB2	0.547
14	B:64:ILE:HD11	B:67:ASP:HA	0.520
14	B:24:ARG:HG3	B:62:GLY:HA3	0.518
14	B:19:LYS:HB2	B:31:SER:HB3	0.512
14	B:20:ILE:O	B:29:SER:HB3	0.482
14	B:66:ASP:O	B:68:LYS:HE2	0.464
15	B:25:ASP:HB3	B:28:LYS:HD3	0.638
15	B:39:PHE:HE2	B:41:LYS:HB2	0.591
15	B:39:PHE:CE2	B:41:LYS:HB2	0.560
15	B:21:ILE:HD11	B:72:GLU:HB2	0.531
15	B:40:HIS:CD2	B:41:LYS:HG2	0.531
15	B:64:ILE:HD11	B:67:ASP:HA	0.507

Model ID	Atom-1	Atom-2	Clash overlap (Å)
15	B:24:ARG:HG3	B:62:GLY:HA3	0.488
15	B:12:CYS:HB3	B:80:PRO:HB3	0.440
15	B:51:MET:SD	B:56:VAL:HB	0.439
15	B:55:GLU:HG2	B:61:LYS:HE2	0.419
15	B:18:LEU:O	B:31:SER:HA	0.404
16	B:64:ILE:HD11	B:67:ASP:HA	0.700
16	B:24:ARG:HG3	B:62:GLY:HA3	0.627
16	B:51:MET:SD	B:56:VAL:HB	0.542
16	B:21:ILE:HD11	B:72:GLU:HB2	0.522
16	B:10:TRP:HH2	B:43:ASN:HD22	0.499
16	B:39:PHE:CZ	B:41:LYS:HB2	0.494
16	B:23:TYR:CE2	B:65:ASP:HB2	0.463
16	B:25:ASP:OD2	B:27:GLU:HB2	0.449
16	B:25:ASP:HB3	B:28:LYS:HG3	0.444
16	B:40:HIS:CD2	B:41:LYS:HG2	0.413
16	B:58:ASP:HA	B:59:PRO:HD3	0.402
17	B:40:HIS:HD2	B:41:LYS:HG2	0.725
17	B:82:GLY:HA2	B:85:TRP:CZ2	0.559
17	B:64:ILE:HD11	B:67:ASP:HA	0.551
17	B:40:HIS:CD2	B:41:LYS:HG2	0.545
17	B:25:ASP:HB3	B:28:LYS:HG3	0.521
17	B:38:PHE:HE2	B:45:TRP:HB3	0.514
17	B:14:ALA:HB3	B:38:PHE:HE1	0.481

Model ID	Atom-1	Atom-2	Clash overlap (Å)
17	B:24:ARG:NH2	B:28:LYS:HE2	0.468
17	B:19:LYS:HB2	B:31:SER:HB3	0.448
17	B:12:CYS:HB3	B:80:PRO:HB3	0.438
17	B:10:TRP:HA	B:82:GLY:HA3	0.427
17	B:58:ASP:HB3	B:61:LYS:HG2	0.425
17	B:24:ARG:HG3	B:62:GLY:HA3	0.419
17	B:20:ILE:O	B:29:SER:HB3	0.402
17	B:79:ALA:HA	B:80:PRO:HD3	0.401
18	B:25:ASP:HB3	B:28:LYS:HG3	0.657
18	B:21:ILE:HD11	B:72:GLU:HB2	0.571
18	B:55:GLU:HG2	B:61:LYS:HE2	0.532
18	B:20:ILE:O	B:29:SER:HB3	0.471
18	B:40:HIS:HD2	B:41:LYS:HG2	0.470
18	B:40:HIS:CD2	B:41:LYS:HG2	0.451
18	B:39:PHE:CE2	B:41:LYS:HB2	0.450
18	B:18:LEU:O	B:31:SER:HA	0.437
18	B:22:ASN:HB3	B:25:ASP:O	0.430
18	B:12:CYS:HB3	B:80:PRO:HB3	0.428
18	B:18:LEU:N	B:18:LEU:HD12	0.428
18	B:51:MET:SD	B:56:VAL:HB	0.417
18	B:20:ILE:HD12	B:51:MET:HE3	0.410
18	B:25:ASP:HB3	B:28:LYS:CG	0.400
19	B:13:HIS:HB2	B:37:LEU:HD12	0.582

Model ID	Atom-1	Atom-2	Clash overlap (Å)
19	B:66:ASP:HB3	B:68:LYS:HE2	0.567
19	B:11:SER:HB3	B:37:LEU:HD21	0.558
19	B:19:LYS:HB2	B:31:SER:HB3	0.507
19	B:39:PHE:CE2	B:41:LYS:HB2	0.491
19	B:21:ILE:HD11	B:72:GLU:HB2	0.482
19	B:82:GLY:HA2	B:85:TRP:CZ2	0.455
19	B:18:LEU:HA	B:73:VAL:HG12	0.441
19	B:16:ALA:HB2	B:75:VAL:HG23	0.427
19	B:56:VAL:HG23	B:63:PHE:HB3	0.425
19	B:18:LEU:O	B:31:SER:HA	0.423
19	B:79:ALA:HA	B:80:PRO:HD3	0.418
19	B:22:ASN:HB3	B:25:ASP:O	0.417
20	B:24:ARG:HG3	B:62:GLY:HA3	0.671
20	B:21:ILE:HD11	B:72:GLU:HB2	0.605
20	B:39:PHE:CE2	B:41:LYS:HB2	0.544
20	B:39:PHE:HE2	B:41:LYS:HB2	0.535
20	B:53:TRP:HA	B:56:VAL:HG12	0.506
20	B:11:SER:HB3	B:37:LEU:HD11	0.479
20	B:22:ASN:HB3	B:25:ASP:O	0.452
20	B:19:LYS:HB2	B:31:SER:HB3	0.410
20	B:40:HIS:CD2	B:41:LYS:HG2	0.408
20	B:24:ARG:HG3	B:62:GLY:CA	0.404

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	Analyzed	Favored	Allowed	Outliers
1	153	140	12	1
2	153	139	12	2
3	153	143	10	0
4	153	143	8	2
5	153	138	13	2
6	153	143	8	2
7	153	145	7	1
8	153	141	9	3
9	153	145	6	2
10	153	144	8	1
11	153	141	11	1
12	153	140	11	2
13	153	142	9	2
14	153	139	12	2
15	153	142	9	2
16	153	143	8	2
17	153	143	8	2
18	153	142	9	2
19	153	142	10	1
20	153	144	8	1

Detailed list of outliers are tabulated below.

Torsion angles: Protein sidechains

In the following table, sidechain outliers are listed. The Analysed column shows the number of residues for which the sidechain conformation was analysed.

Model ID	Analyzed	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
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

Detailed list of outliers are tabulated below.

Model ID	Chain	Residue ID	Residue type
1	B	8	THR

Model ID	Chain	Residue ID	Residue type
1	B	9	SER
1	B	11	SER
1	B	42	GLU
1	B	48	SER
1	B	49	ASN
1	B	51	MET
1	B	54	SER
1	B	67	ASP
1	B	68	LYS
1	B	73	VAL
2	B	4	GLU
2	B	8	THR
2	B	9	SER
2	B	42	GLU
2	B	48	SER
2	B	51	MET
2	B	54	SER
2	B	70	THR
2	B	78	ASP
3	B	31	SER
3	B	51	MET
3	B	54	SER
4	B	5	SER

Model ID	Chain	Residue ID	Residue type
4	B	8	THR
4	B	9	SER
4	B	11	SER
4	B	34	ILE
4	B	44	ASP
4	B	48	SER
4	B	51	MET
4	B	54	SER
4	B	70	THR
5	B	6	ASP
5	B	31	SER
5	B	33	ARG
5	B	54	SER
5	B	67	ASP
5	B	70	THR
6	B	6	ASP
6	B	8	THR
6	B	9	SER
6	B	31	SER
6	B	48	SER
6	B	51	MET
6	B	54	SER
6	B	67	ASP

Model ID	Chain	Residue ID	Residue type
6	B	70	THR
6	B	78	ASP
6	B	81	HIS
7	B	8	THR
7	B	9	SER
7	B	11	SER
7	B	12	CYS
7	B	18	LEU
7	B	20	ILE
7	B	31	SER
7	B	48	SER
7	B	57	THR
7	B	70	THR
8	B	6	ASP
8	B	7	SER
8	B	12	CYS
8	B	47	PHE
8	B	48	SER
8	B	51	MET
8	B	54	SER
8	B	70	THR
9	B	9	SER
9	B	11	SER

Model ID	Chain	Residue ID	Residue type
9	B	31	SER
9	B	48	SER
9	B	54	SER
9	B	55	GLU
10	B	7	SER
10	B	8	THR
10	B	11	SER
10	B	31	SER
10	B	48	SER
10	B	51	MET
10	B	54	SER
10	B	64	ILE
11	B	6	ASP
11	B	8	THR
11	B	11	SER
11	B	70	THR
11	B	73	VAL
12	B	8	THR
12	B	12	CYS
12	B	18	LEU
12	B	20	ILE
12	B	31	SER
12	B	32	ARG

Model ID	Chain	Residue ID	Residue type
12	B	51	MET
12	B	54	SER
13	B	7	SER
13	B	8	THR
13	B	31	SER
13	B	42	GLU
13	B	44	ASP
13	B	48	SER
13	B	54	SER
14	B	9	SER
14	B	31	SER
14	B	51	MET
14	B	54	SER
15	B	5	SER
15	B	6	ASP
15	B	8	THR
15	B	9	SER
15	B	31	SER
15	B	48	SER
15	B	54	SER
15	B	81	HIS
16	B	5	SER
16	B	8	THR

Model ID	Chain	Residue ID	Residue type
16	B	9	SER
16	B	48	SER
16	B	51	MET
16	B	70	THR
17	B	9	SER
17	B	11	SER
17	B	31	SER
17	B	48	SER
17	B	70	THR
17	B	83	VAL
18	B	8	THR
18	B	12	CYS
18	B	31	SER
18	B	44	ASP
18	B	48	SER
18	B	54	SER
19	B	9	SER
19	B	31	SER
19	B	35	SER
19	B	48	SER
19	B	54	SER
19	B	67	ASP
20	B	5	SER

Model ID	Chain	Residue ID	Residue type
20	B	8	THR
20	B	23	TYR
20	B	27	GLU
20	B	44	ASP
20	B	54	SER
20	B	70	THR

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.

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