



Full wwPDB NMR Structure Validation Report ⓘ

Nov 6, 2017 – 07:17 PM EST

PDB ID : 2KQW
Title : SARS coronavirus-unique domain (SUD): Three-domain molecular architecture in solution and RNA binding. II: Structure of the SUD-C domain of SUD-MC
Authors : Johnson, M.A.; Chatterjee, A.; Wuthrich, K.; Joint Center for Structural Genomics (JCSG)
Deposited on : unknown

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20030345
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

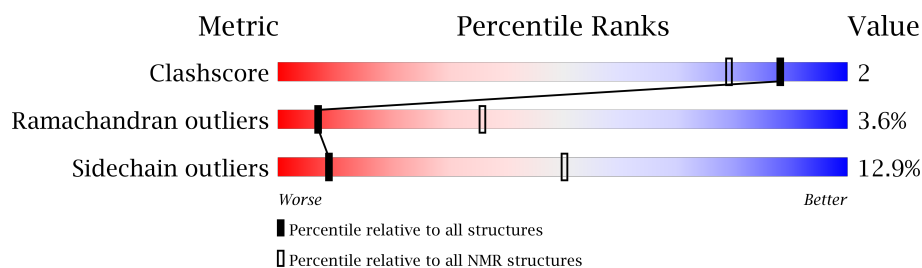
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	198	<div> <div style="width: 30%; background-color: green;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 66%; background-color: grey;"></div> </div> <div> <div style="width: 30%;"></div> <div style="width: 5%; text-align: center;">. .</div> <div style="width: 66%;"></div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:132-A:198 (67)	0.41	10

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 6, 9, 12, 13, 16, 17, 20
2	4, 5, 10, 11, 14, 18, 19
3	1, 2, 7
4	8, 15

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1062 atoms, of which 523 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-structural protein 3.

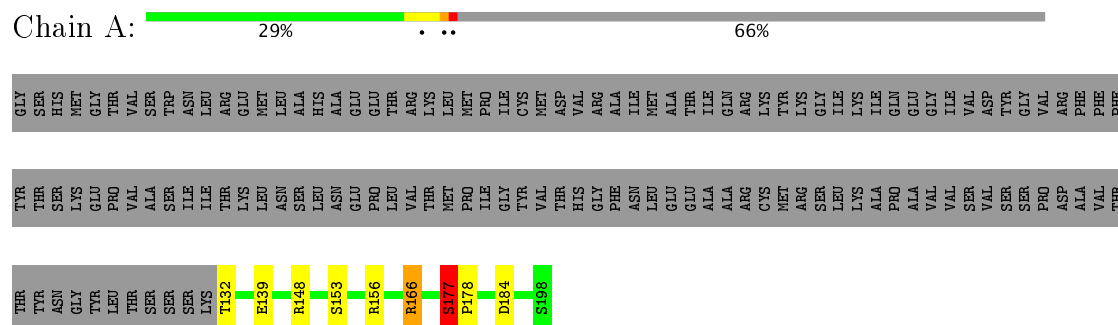
Mol	Chain	Residues	Atoms					Trace
1	A	67	Total	C	H	N	O	0
			1062	343	523	88	108	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P0C6U8
A	2	SER	-	EXPRESSION TAG	UNP P0C6U8
A	3	HIS	-	EXPRESSION TAG	UNP P0C6U8
A	4	MET	-	EXPRESSION TAG	UNP P0C6U8

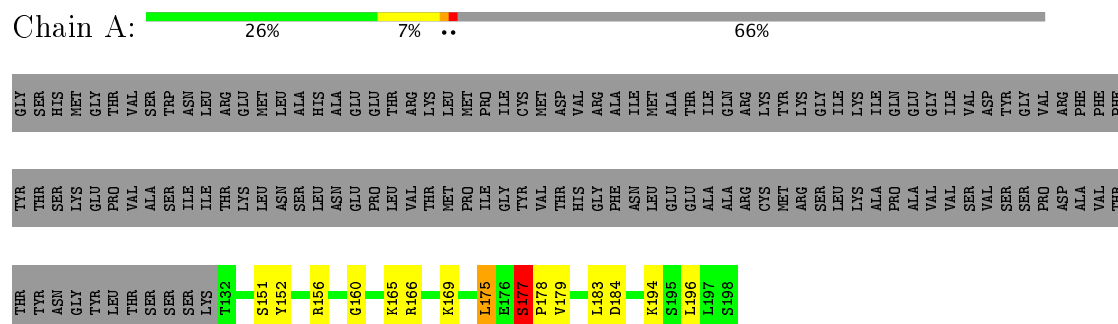
4.2.2 Score per residue for model 2

- Molecule 1: Non-structural protein 3



4.2.3 Score per residue for model 3

- Molecule 1: Non-structural protein 3



4.2.4 Score per residue for model 4

- Molecule 1: Non-structural protein 3



4.2.5 Score per residue for model 5

- Molecule 1: Non-structural protein 3



GLY SER HIS MET GLY THR VAL SER TRP ASN LEU ARG GLU MET LEU ALA HIS ALA GLU GLU THR LYS ARG LEU MET PRO ILE TYR CYS MET ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS ILE GLN GLY VAL ASP TYR VAL ARG PHE PHE

TYR THR SER LYS GLY PRO VAL ALA SER SER ILE LEU THR LYS LEU ASN SER LEU ASN PRO VAL THR LYS MET PRO ILE GLY THR VAL MET THR HIS GLY PHE ASN ILE MET LEU GLU ALA THR ILE ALA ARG CYS MET ARG SER LEU LYS SER VAL ASP TYR SER PRO ASP VAL THR

THR TYR ASN GLY TYR LEU THR SER SER LYS T132 S133 E134 E135 V141 F163 L164 R165 R166 K169 S177 S189 L190 D191 K192 K193 R194 S195 L196 L197 S198

4.2.6 Score per residue for model 6

- Molecule 1: Non-structural protein 3



GLY SER HIS MET GLY THR VAL SER TRP ASN LEU ARG GLU MET LEU ALA HIS ALA GLU GLU THR LYS ARG LEU MET PRO ILE TYR CYS MET ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS ILE GLN GLY VAL ASP TYR VAL ARG PHE PHE

TYR THR SER LYS GLY PRO VAL ALA SER SER ILE LEU THR LYS LEU ASN SER LEU ASN PRO VAL THR LYS MET PRO ILE GLY TYR VAL THR HIS GLY PHE ASN ILE MET LEU GLU ALA THR ILE ALA ARG CYS MET ARG SER LEU LYS SER VAL ASP TYR SER PRO ASP VAL THR

THR TYR ASN GLY TYR LEU THR SER SER LYS T132 R186 H173 S177 P178 V179 D184 S195 L196 L197 S198

4.2.7 Score per residue for model 7

- Molecule 1: Non-structural protein 3



GLY SER HIS MET GLY THR VAL SER TRP ASN LEU ARG GLU MET LEU ALA HIS ALA GLU GLU THR LYS ARG LEU MET PRO ILE TYR CYS MET ASP VAL ARG ALA ILE MET LEU ALA THR ILE GLN ARG LYS TYR LYS ILE GLN GLY VAL ASP TYR VAL ARG PHE PHE

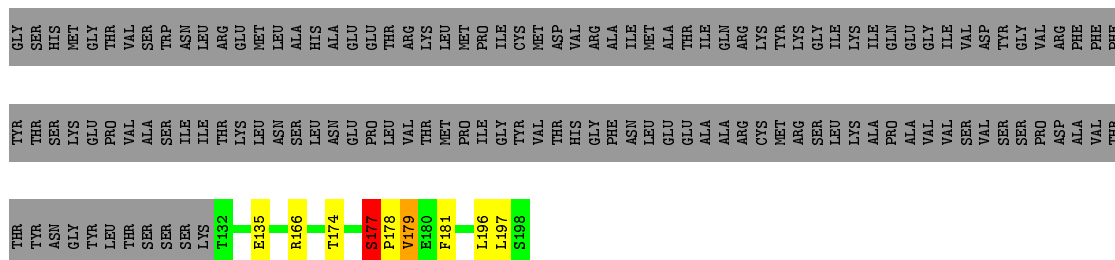
TYR THR SER LYS GLY PRO VAL ALA SER SER ILE LEU THR LYS LEU ASN SER LEU ASN PRO VAL THR LYS MET PRO ILE GLY TYR VAL THR HIS GLY PHE ASN ILE MET LEU GLU ALA THR ILE ALA ARG CYS MET ARG SER LEU LYS SER VAL ASP TYR SER PRO ASP VAL THR

THR TYR ASN GLY TYR LEU THR SER SER LYS T132 S146 Y147 R148 S153 G154 Q155 R156 R166 H173 T174 L175 E176 S177 P178 H182 L190 S195 L196 L197 S198

4.2.8 Score per residue for model 8

- Molecule 1: Non-structural protein 3

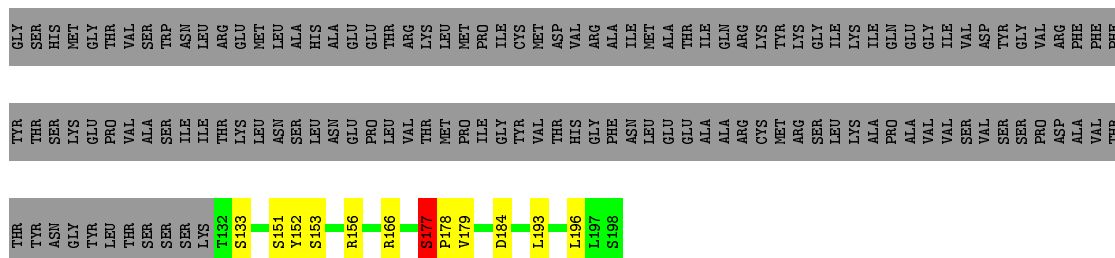




4.2.9 Score per residue for model 9

- Molecule 1: Non-structural protein 3

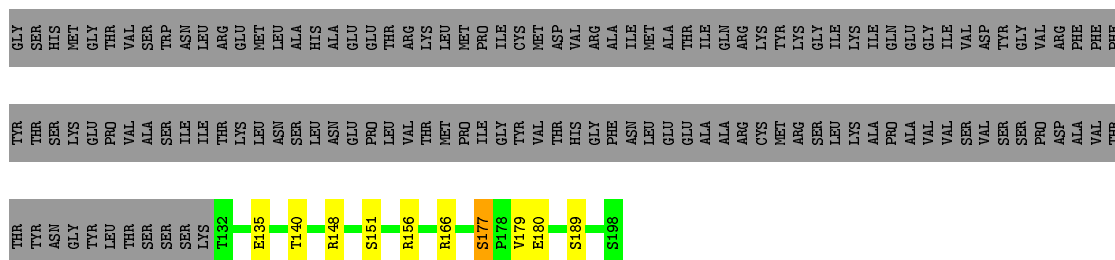
Chain A: 28% 6% . 66%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Non-structural protein 3

Chain A: 29% 5% . 66%

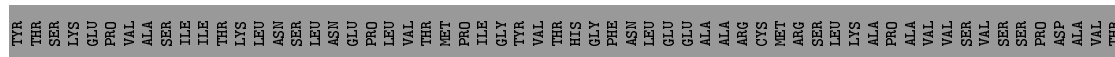


4.2.11 Score per residue for model 11

- Molecule 1: Non-structural protein 3

Chain A: 27% 6% .. 66%

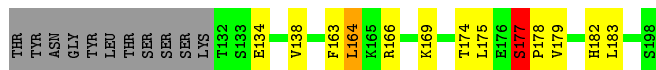






4.2.15 Score per residue for model 15

- Molecule 1: Non-structural protein 3



4.2.16 Score per residue for model 16

- Molecule 1: Non-structural protein 3



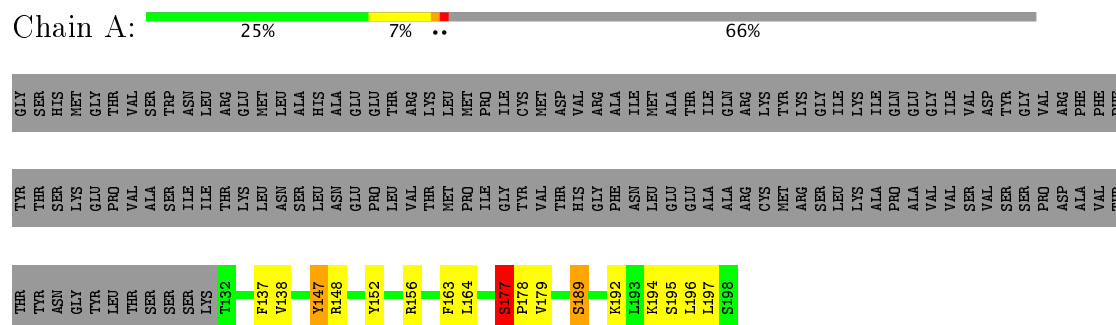
4.2.17 Score per residue for model 17

- Molecule 1: Non-structural protein 3



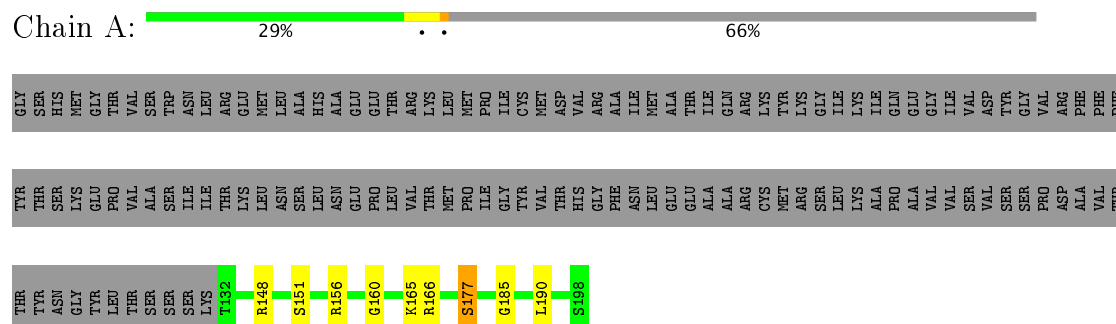
4.2.18 Score per residue for model 18

- Molecule 1: Non-structural protein 3



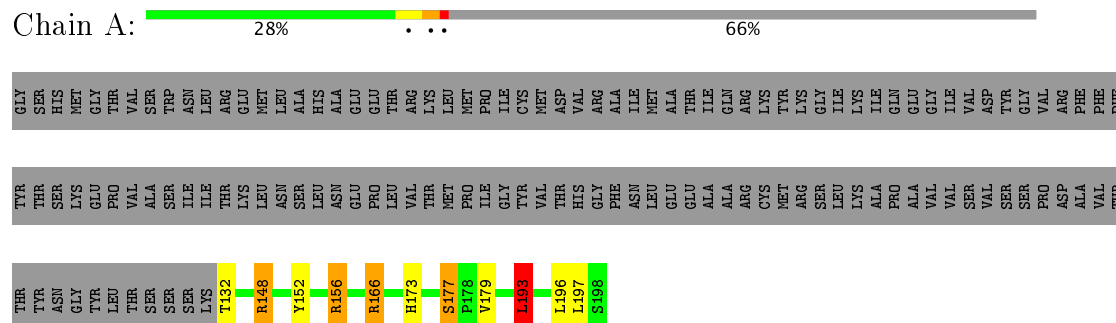
4.2.19 Score per residue for model 19

- Molecule 1: Non-structural protein 3



4.2.20 Score per residue for model 20

- Molecule 1: Non-structural protein 3



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
UNIO	refinement	
CANDID	refinement	
OpalP	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.62±0.01	0±0/550 (0.0±0.0%)	1.10±0.05	1±1/742 (0.1±0.1%)
All	All	0.62	0/11000 (0.0%)	1.10	16/14840 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.0±1.0
All	All	0	20

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	197	LEU	CB-CG-CD2	8.44	125.34	111.00	8	2
1	A	166	ARG	NE-CZ-NH2	-6.36	117.12	120.30	7	2
1	A	193	LEU	CD1-CG-CD2	6.13	128.89	110.50	16	3
1	A	197	LEU	CD1-CG-CD2	6.08	128.75	110.50	17	1
1	A	148	ARG	NE-CZ-NH2	-6.03	117.29	120.30	20	1
1	A	173	HIS	CA-CB-CG	5.42	122.81	113.60	17	2
1	A	156	ARG	NE-CZ-NH2	-5.28	117.66	120.30	11	1
1	A	147	TYR	CB-CG-CD2	-5.26	117.84	121.00	18	1
1	A	152	TYR	CB-CG-CD2	-5.24	117.86	121.00	12	1
1	A	148	ARG	NE-CZ-NH1	5.18	122.89	120.30	14	1
1	A	166	ARG	NE-CZ-NH1	5.06	122.83	120.30	7	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	166	ARG	Sidechain	6
1	A	148	ARG	Sidechain	6
1	A	152	TYR	Sidechain	4
1	A	156	ARG	Sidechain	3
1	A	163	PHE	Sidechain	1

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	539	523	522	2±2
All	All	10780	10460	10440	46

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:HD13	1:A:184:ASP:HB3	0.64	1.67	12	1
1:A:193:LEU:CD1	1:A:197:LEU:HD21	0.57	2.29	20	3
1:A:182:HIS:CD2	1:A:187:VAL:HG22	0.57	2.35	12	2
1:A:141:VAL:HG11	1:A:164:LEU:HD11	0.56	1.77	4	1
1:A:174:THR:HG23	1:A:180:GLU:OE1	0.55	2.02	14	1
1:A:174:THR:HG23	1:A:180:GLU:CD	0.54	2.23	14	1
1:A:163:PHE:CD2	1:A:164:LEU:HD23	0.52	2.38	5	3
1:A:188:LEU:HD12	1:A:196:LEU:HD11	0.48	1.85	13	1
1:A:175:LEU:H	1:A:175:LEU:HD22	0.48	1.69	11	1
1:A:197:LEU:HD22	1:A:197:LEU:H	0.47	1.70	17	1
1:A:141:VAL:HG11	1:A:164:LEU:HD21	0.47	1.86	5	1
1:A:163:PHE:CG	1:A:164:LEU:HD23	0.47	2.45	5	1
1:A:138:VAL:HA	1:A:163:PHE:CZ	0.46	2.45	14	5
1:A:188:LEU:CD1	1:A:196:LEU:HD11	0.46	2.40	13	1
1:A:193:LEU:O	1:A:197:LEU:HD22	0.46	2.10	13	2
1:A:194:LYS:HA	1:A:197:LEU:CD2	0.46	2.41	17	1
1:A:169:LYS:HB3	1:A:183:LEU:HD11	0.44	1.90	15	2
1:A:177:SER:N	1:A:178:PRO:HA	0.43	2.28	12	12
1:A:197:LEU:H	1:A:197:LEU:HD22	0.42	1.75	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:PHE:CE2	1:A:164:LEU:CD2	0.41	3.02	15	1
1:A:137:PHE:CD1	1:A:194:LYS:HE2	0.41	2.49	18	1
1:A:190:LEU:HD11	1:A:194:LYS:HE3	0.41	1.92	12	1
1:A:160:GLY:HA2	1:A:175:LEU:HD21	0.41	1.92	3	1
1:A:179:VAL:HG12	1:A:181:PHE:CZ	0.40	2.51	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	65/198 (33%)	55±2 (85±3%)	8±2 (12±3%)	2±1 (4±1%)	7	36
All	All	1300/3960 (33%)	1099 (85%)	154 (12%)	47 (4%)	7	36

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	177	SER	20
1	A	179	VAL	15
1	A	174	THR	4
1	A	148	ARG	2
1	A	134	GLU	1
1	A	168	ASP	1
1	A	160	GLY	1
1	A	153	SER	1
1	A	189	SER	1
1	A	185	GLY	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	61/174 (35%)	53±3 (87±4%)	8±3 (13±4%)	9	50
All	All	1220/3480 (35%)	1063 (87%)	157 (13%)	9	50

All 37 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	177	SER	20
1	A	156	ARG	14
1	A	196	LEU	13
1	A	166	ARG	8
1	A	132	THR	8
1	A	151	SER	7
1	A	184	ASP	7
1	A	195	SER	7
1	A	193	LEU	6
1	A	175	LEU	6
1	A	164	LEU	4
1	A	189	SER	4
1	A	169	LYS	4
1	A	135	GLU	4
1	A	180	GLU	4
1	A	153	SER	4
1	A	190	LEU	3
1	A	149	ASP	3
1	A	191	ASP	3
1	A	182	HIS	2
1	A	173	HIS	2
1	A	155	GLN	2
1	A	168	ASP	2
1	A	198	SER	2
1	A	133	SER	2
1	A	165	LYS	2
1	A	140	THR	2
1	A	146	SER	2
1	A	194	LYS	2
1	A	148	ARG	1
1	A	147	TYR	1
1	A	139	GLU	1
1	A	152	TYR	1
1	A	192	LYS	1
1	A	183	LEU	1
1	A	197	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	158	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided