Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 09:33 AM EDT

PDB ID	:	2L38
Title	:	R29Q Sticholysin II mutant
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Deposited on	:	2010-09-10

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

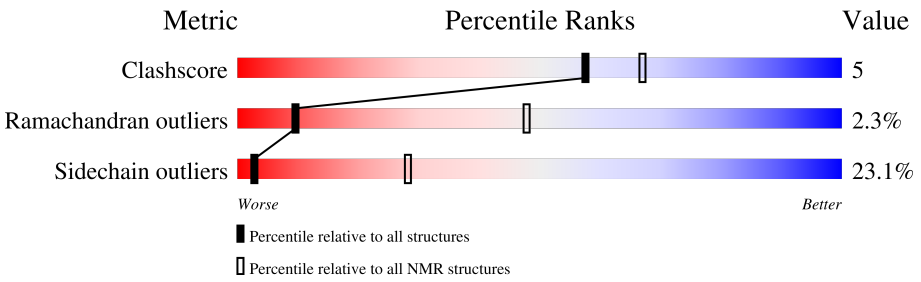
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	175	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:2-A:24, A:30-A:74, A:84-A:105, A:113-A:175 (153)	0.86	15

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2689 atoms, of which 1330 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sticholysin-2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	175	2689	870	1330	227	256	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLN	ARG	engineered mutation	UNP P07845

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Sticholysin-2

Chain A: 66% 20% • 13%

A1 I7 L17 D18 K19 V20 L21 G25 K26 V27 S28 Q29 K30 I31 A32 V33 S39 L46 F50 R51 L69 L70 Y71 R74 K75 D76 T77 G78 P79 V80 A81 T82 G83 A86 A89 Y90 T97 L98 G99 V100 M101 F102 F106 D107 Y108 N109 W110 Y111

S112 R125 D133 N144 K149 L155 R156 M157 K158 G159 I160 M161 K168 I173 S174 R175

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Sticholysin-2

Chain A: 61% 21% 5% 13%

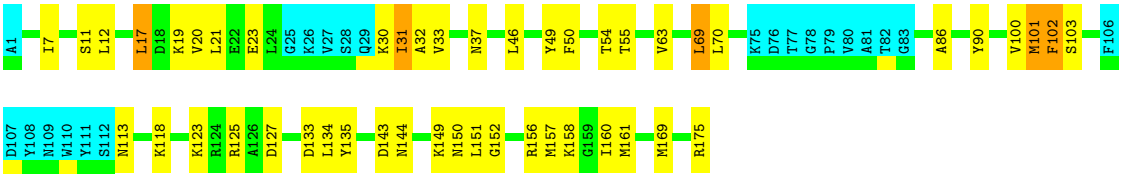
A1 I6 T13 L17 D18 K19 V20 L21 E22 G25 K26 V27 S28 Q29 K30 I31 A32 V33 N37 E38 S39 W43 T44 A45 L46 Y49 T55 P60 L69 L70 Y71 K75 D76 T77 G78 P79 V80 A81 T82 G83 A84 A89 Y90 Y91 M92 S93 S94

T97 V100 M101 F102 F106 D107 Y108 N109 W110 Y111 S112 N113 V117 K123 R124 R125 D133 L134 Y135 R141 N144 G145 W146 Y153 M157 K158 G159 I160 M161 M169 K172 I173 S174 R175

4.2.2 Score per residue for model 2

• Molecule 1: Sticholysin-2

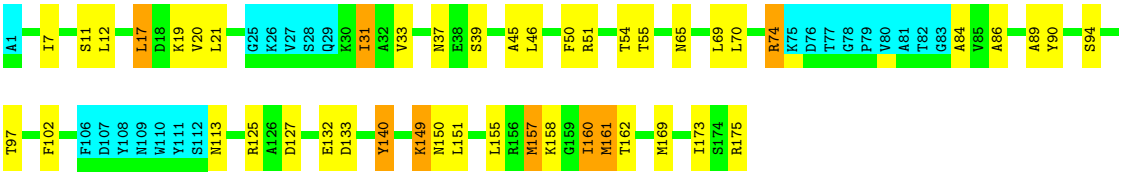
Chain A: 60% 25% • 13%



4.2.3 Score per residue for model 3

- Molecule 1: Sticholysin-2

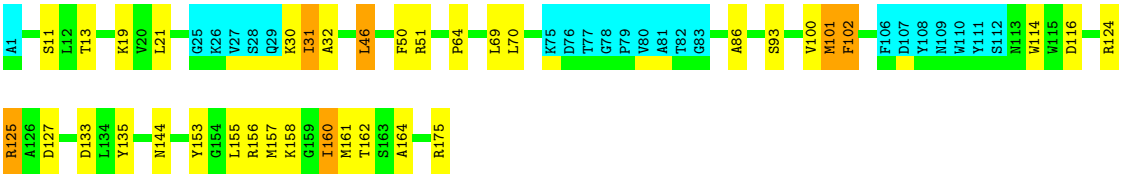
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Sticholysin-2

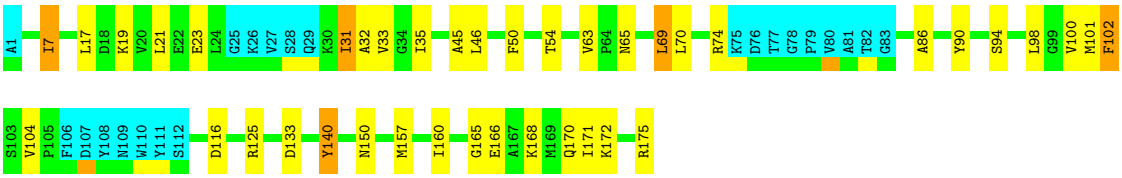
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Sticholysin-2

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Sticholysin-2

Chain A: 60% 24% • 13%

A1 L2 I7 A8 G9 A10 S11 L12 L17 D18 K19 V20 G25 K26 V27 S28 Q29 K30 I31 A32 V33 G34 I35 S39 A45 L46 F50 R51 S52 L59 P60 V63 L69 L70 Y71 K75 D76 T77 G78 P79 V80 A81 T82 G83 Y90 L98 G99 V100

M101 F102 F106 D107 Y108 N109 W110 Y111 S112 W115 K118 R125 A126 D127 Q128 D133 N144 G145 W146 H147 E148 K149 L155 K158 A164 G165 K168 M169 Q170 I171 K172 I173 S174 R175

4.2.7 Score per residue for model 7

- Molecule 1: Sticholysin-2

Chain A: 56% 27% 5% 13%

A1 L2 I7 L12 T13 L17 D18 K19 V20 L21 L24 G25 K26 V27 S28 Q29 K30 I31 A32 V33 N37 E38 W43 T44 A45 L46 N47 R51 P60 N65 L69 L70 K75 D76 T77 G78 P79 V80 A81 T82 G83 A84 V85 A86 A89 Y90 T97

V100 M101 F102 S103 F106 D107 Y108 N109 W110 Y111 S112 D116 V117 K118 I119 Y120 S121 G122 K123 R124 R125 D133 L134 Y135 K149 N150 L151 G152 Y153 G154 L155 R156 M157 K158 G159 I160 M161 T162 S163 A164 G165 K168 I173 S174 R175

4.2.8 Score per residue for model 8

- Molecule 1: Sticholysin-2

Chain A: 62% 23% • 13%

A1 L2 A3 I7 S11 L12 T13 L17 D18 K19 V20 L21 E22 E23 L24 G25 K26 V27 S28 Q29 K30 I31 A32 S39 A45 L46 G53 T54 V57 N65 L69 L70 K75 D76 T77 G78 P79 V80 A81 T82 G83 A84 V85 A86 A89 Y90 T97

V100 M101 F102 F106 D107 Y108 N109 W110 Y111 S112 N113 R125 M130 D133 L134 R141 N144 L151 G152 Y153 R156 M157 K158 I173 S174 R175

4.2.9 Score per residue for model 9

- Molecule 1: Sticholysin-2

Chain A: 64% 22% • 13%

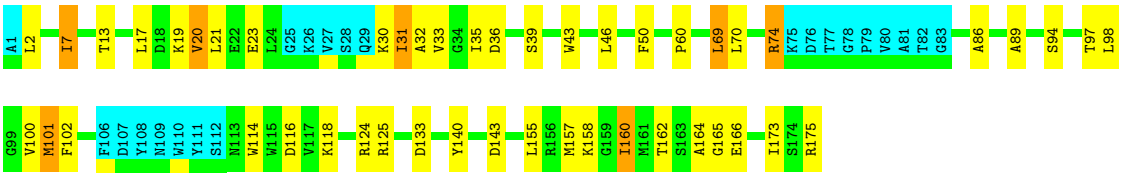
A1 L2 I7 L17 D18 K19 V20 L21 G25 K26 V27 S28 Q29 K30 I31 A32 I35 D36 N37 L46 F50 T54 V57 V63 P64 L69 L70 Y71 K75 D76 T77 G78 P79 V80 A81 T82 G83 A86 M92 S93 S94 L98 G99 V100 M101 F102

S103 V104 P105 F106 D107 Y108 N109 W110 Y111 S112 R125 D133 L134 Y135 N138 R141 G142 D143 L151 M157 I160 M161 T162 K168 M169 R175

4.2.10 Score per residue for model 10

- Molecule 1: Sticholysin-2

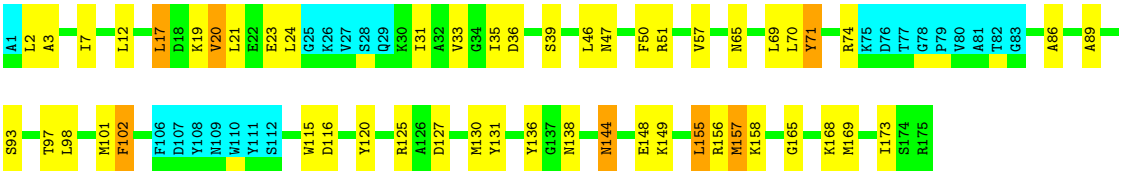
Chain A: 60% 23% • 13%



4.2.11 Score per residue for model 11

- Molecule 1: Sticholysin-2

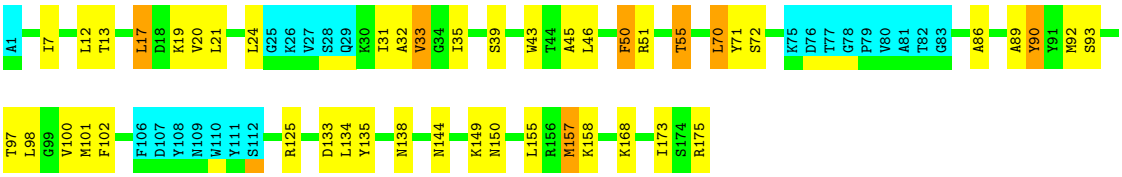
Chain A: 58% 26% • 13%



4.2.12 Score per residue for model 12

- Molecule 1: Sticholysin-2

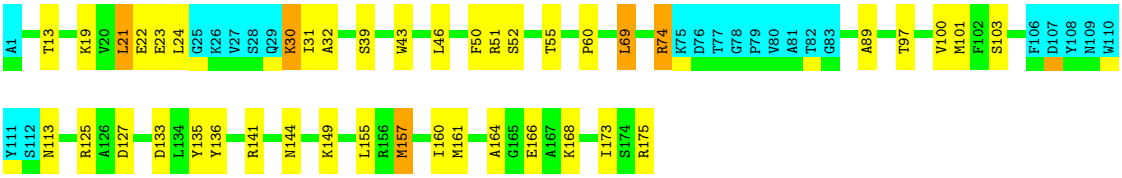
Chain A: 61% 22% • 13%



4.2.13 Score per residue for model 13

- Molecule 1: Sticholysin-2

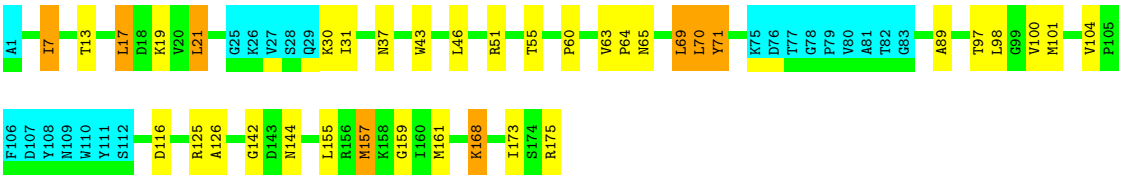
Chain A: 63% 21% • 13%



4.2.14 Score per residue for model 14

- Molecule 1: Sticholysin-2

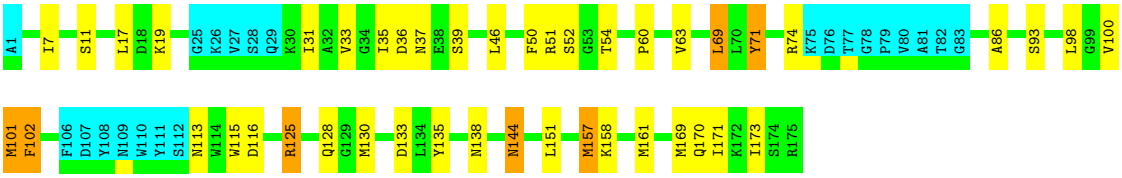
Chain A: 66% 17% 5% 13%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Sticholysin-2

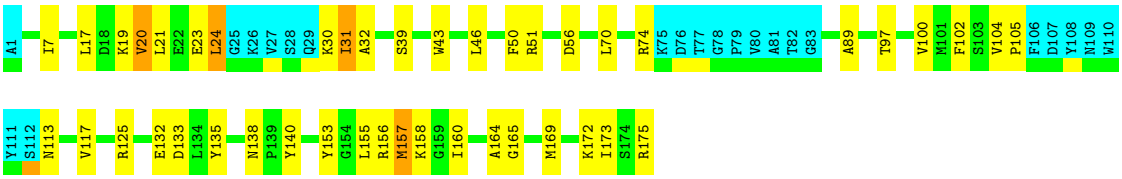
Chain A: 62% 21% • 13%



4.2.16 Score per residue for model 16

- Molecule 1: Sticholysin-2

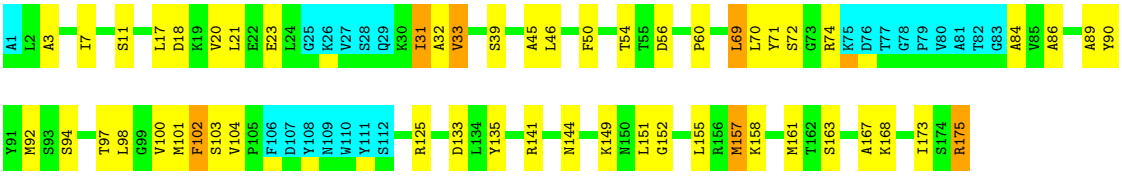
Chain A: 62% 23% • 13%



4.2.17 Score per residue for model 17

- Molecule 1: Sticholysin-2

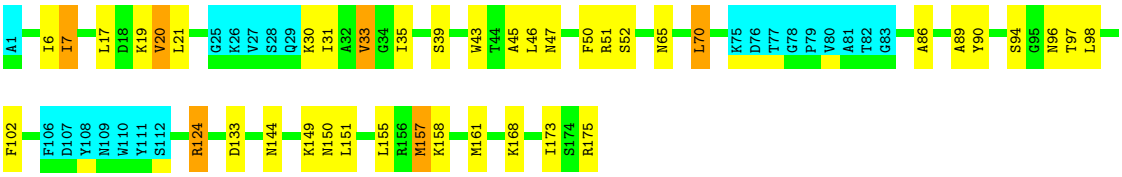
Chain A: 57% 27% • 13%



4.2.18 Score per residue for model 18

- Molecule 1: Sticholysin-2

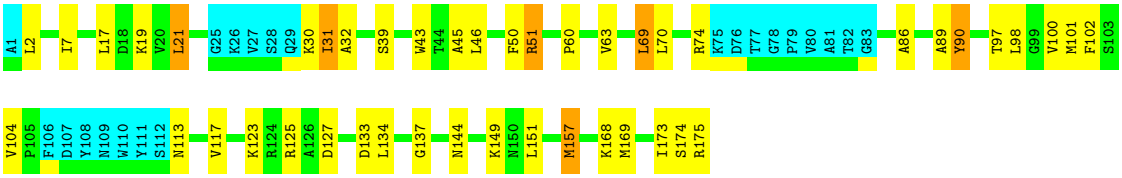
Chain A: 64% 20% • 13%



4.2.19 Score per residue for model 19

- Molecule 1: Sticholysin-2

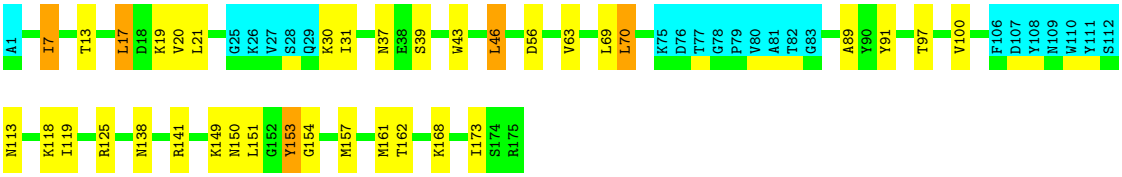
Chain A: 62% 22% • 13%



4.2.20 Score per residue for model 20

- Molecule 1: Sticholysin-2

Chain A: 67% 18% • 13%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure solution	

No chemical shift data was provided.

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	0.76±0.05	0±1/1217 (0.0± 0.1%)	1.06±0.02	1±1/1644 (0.1± 0.1%)
All	All	0.76	3/24340 (0.0%)	1.06	21/32880 (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	1.1±0.8
All	All	0	21

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	159	GLY	CA-C	6.52	1.62	1.51	14	1
1	A	126	ALA	N-CA	-6.14	1.34	1.46	14	1
1	A	126	ALA	CA-CB	5.24	1.63	1.52	14	1

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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	136	TYR	CB-CG-CD1	-8.40	115.96	121.00	11	1
1	A	124	ARG	NE-CZ-NH1	7.85	124.22	120.30	18	2
1	A	156	ARG	NE-CZ-NH2	-6.50	117.05	120.30	2	1
1	A	51	ARG	NE-CZ-NH1	6.02	123.31	120.30	16	2
1	A	140	TYR	CB-CG-CD2	-5.83	117.50	121.00	3	2
1	A	136	TYR	CB-CG-CD2	5.80	124.48	121.00	11	1
1	A	156	ARG	NE-CZ-NH1	5.72	123.16	120.30	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	125	ARG	NE-CZ-NH1	5.62	123.11	120.30	15	2
1	A	74	ARG	NE-CZ-NH1	5.44	123.02	120.30	3	3
1	A	156	ARG	CD-NE-CZ	5.37	131.11	123.60	2	1
1	A	20	VAL	CA-CB-CG1	5.35	118.92	110.90	11	4
1	A	175	ARG	NE-CZ-NH1	5.14	122.87	120.30	17	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	102	PHE	Sidechain	7
1	A	153	TYR	Sidechain	5
1	A	135	TYR	Sidechain	3
1	A	120	TYR	Sidechain	2
1	A	49	TYR	Sidechain	1
1	A	140	TYR	Sidechain	1
1	A	74	ARG	Sidechain	1
1	A	90	TYR	Sidechain	1

6.2 Too-close contacts (i)

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	1190	1175	1174	12±3
All	All	23800	23500	23480	237

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD11	1:A:17:LEU:HD23	0.76	1.56	11	2
1:A:35:ILE:HG21	1:A:98:LEU:HD21	0.74	1.59	15	5
1:A:63:VAL:HG21	1:A:69:LEU:HD13	0.74	1.58	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD11	1:A:32:ALA:HB2	0.74	1.59	17	4
1:A:33:VAL:HG11	1:A:102:PHE:CG	0.68	2.23	18	2
1:A:86:ALA:HB3	1:A:102:PHE:CZ	0.67	2.24	18	12
1:A:21:LEU:HD22	1:A:32:ALA:HB2	0.67	1.65	9	4
1:A:45:ALA:HB2	1:A:90:TYR:CZ	0.63	2.28	6	2
1:A:104:VAL:HG22	1:A:168:LYS:HE2	0.63	1.70	5	2
1:A:17:LEU:HD21	1:A:70:LEU:CD1	0.63	2.24	11	5
1:A:43:TRP:CZ2	1:A:173:ILE:HD11	0.62	2.29	20	10
1:A:33:VAL:HG11	1:A:102:PHE:CD1	0.62	2.29	7	2
1:A:45:ALA:HB2	1:A:90:TYR:CE1	0.61	2.29	18	2
1:A:45:ALA:HB2	1:A:90:TYR:CE2	0.59	2.33	19	6
1:A:119:ILE:HD12	1:A:153:TYR:CZ	0.58	2.33	7	1
1:A:69:LEU:HD11	1:A:90:TYR:CE2	0.57	2.34	6	1
1:A:89:ALA:HB2	1:A:124:ARG:HH22	0.57	1.59	18	1
1:A:151:LEU:HD13	1:A:157:MET:SD	0.57	2.39	19	3
1:A:55:THR:HG21	1:A:71:TYR:CZ	0.56	2.35	14	1
1:A:60:PRO:CG	1:A:69:LEU:HD12	0.56	2.31	10	7
1:A:60:PRO:HG2	1:A:69:LEU:HD12	0.56	1.77	15	7
1:A:74:ARG:NH1	1:A:104:VAL:HG11	0.55	2.16	16	1
1:A:89:ALA:HB1	1:A:97:THR:HG22	0.55	1.78	20	6
1:A:157:MET:CB	1:A:173:ILE:HG22	0.55	2.31	17	7
1:A:157:MET:HB3	1:A:173:ILE:HG22	0.55	1.77	8	8
1:A:31:ILE:HG21	1:A:84:ALA:HB3	0.55	1.77	1	2
1:A:101:MET:HB3	1:A:134:LEU:HD13	0.55	1.79	2	2
1:A:21:LEU:CB	1:A:32:ALA:HB2	0.55	2.32	19	1
1:A:21:LEU:HD11	1:A:30:LYS:CB	0.53	2.34	14	1
1:A:54:THR:HG22	1:A:74:ARG:O	0.53	2.04	17	1
1:A:86:ALA:HB3	1:A:102:PHE:CE2	0.53	2.39	12	5
1:A:46:LEU:HD12	1:A:125:ARG:HA	0.53	1.80	4	1
1:A:160:ILE:HD11	1:A:162:THR:HG23	0.52	1.80	10	3
1:A:33:VAL:HG11	1:A:102:PHE:CE2	0.52	2.40	12	2
1:A:12:LEU:HD13	1:A:17:LEU:HD23	0.52	1.80	6	1
1:A:17:LEU:HD13	1:A:21:LEU:HD23	0.52	1.81	9	1
1:A:33:VAL:HG11	1:A:102:PHE:CE1	0.52	2.40	6	2
1:A:35:ILE:HD11	1:A:100:VAL:HB	0.52	1.82	6	1
1:A:31:ILE:HD11	1:A:102:PHE:CD2	0.51	2.41	6	2
1:A:35:ILE:HG23	1:A:171:ILE:O	0.51	2.06	5	1
1:A:35:ILE:HG21	1:A:98:LEU:CD2	0.51	2.36	11	4
1:A:31:ILE:HD11	1:A:102:PHE:CD1	0.50	2.41	16	3
1:A:63:VAL:HG21	1:A:69:LEU:HD22	0.50	1.83	2	1
1:A:157:MET:HB2	1:A:173:ILE:HG22	0.49	1.84	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ARG:CZ	1:A:104:VAL:HG11	0.49	2.37	16	1
1:A:6:ILE:HD11	1:A:70:LEU:HG	0.49	1.84	1	1
1:A:89:ALA:HB1	1:A:97:THR:CG2	0.49	2.38	13	9
1:A:155:LEU:HD11	1:A:173:ILE:HB	0.49	1.84	6	1
1:A:31:ILE:HD13	1:A:32:ALA:N	0.49	2.23	5	4
1:A:98:LEU:HD22	1:A:173:ILE:HD13	0.49	1.85	19	2
1:A:21:LEU:HB2	1:A:32:ALA:HB2	0.48	1.84	19	1
1:A:101:MET:HB2	1:A:134:LEU:HD13	0.48	1.85	12	2
1:A:17:LEU:HD11	1:A:70:LEU:HD13	0.48	1.85	14	1
1:A:33:VAL:HG13	1:A:71:TYR:HB3	0.48	1.85	1	5
1:A:7:ILE:HD13	1:A:11:SER:OG	0.48	2.09	6	1
1:A:118:LYS:HA	1:A:151:LEU:HD21	0.47	1.85	20	1
1:A:33:VAL:C	1:A:70:LEU:HD23	0.47	2.30	5	1
1:A:24:LEU:HD11	1:A:30:LYS:HD2	0.47	1.86	13	1
1:A:12:LEU:CD1	1:A:17:LEU:HD23	0.47	2.39	7	3
1:A:155:LEU:HD12	1:A:156:ARG:N	0.47	2.25	11	1
1:A:98:LEU:HD13	1:A:173:ILE:HG21	0.47	1.87	11	2
1:A:32:ALA:HB1	1:A:70:LEU:HD21	0.47	1.86	12	1
1:A:160:ILE:HD13	1:A:161:MET:N	0.46	2.26	9	2
1:A:6:ILE:HD11	1:A:70:LEU:CG	0.46	2.41	1	1
1:A:117:VAL:HG11	1:A:157:MET:SD	0.45	2.51	1	1
1:A:85:VAL:HG22	1:A:103:SER:HA	0.45	1.87	7	1
1:A:37:ASN:HB3	1:A:43:TRP:CZ2	0.45	2.46	7	2
1:A:32:ALA:HB3	1:A:168:LYS:HG2	0.45	1.87	19	2
1:A:33:VAL:HG21	1:A:102:PHE:CD2	0.45	2.47	3	1
1:A:101:MET:CB	1:A:134:LEU:HD13	0.45	2.42	2	2
1:A:114:TRP:CZ2	1:A:135:TYR:CE2	0.45	3.04	4	1
1:A:117:VAL:O	1:A:151:LEU:HD11	0.45	2.11	19	1
1:A:101:MET:SD	1:A:114:TRP:CZ3	0.45	3.10	10	1
1:A:24:LEU:C	1:A:24:LEU:HD12	0.44	2.33	16	1
1:A:149:LYS:CE	1:A:151:LEU:HD12	0.44	2.42	3	1
1:A:32:ALA:HB1	1:A:70:LEU:HD11	0.44	1.90	8	1
1:A:170:GLN:C	1:A:171:ILE:HD12	0.44	2.33	6	3
1:A:57:VAL:HG23	1:A:71:TYR:CE1	0.44	2.48	11	2
1:A:46:LEU:HD11	1:A:91:TYR:HB2	0.44	1.88	20	1
1:A:101:MET:SD	1:A:114:TRP:CH2	0.44	3.11	4	1
1:A:37:ASN:HB3	1:A:43:TRP:CH2	0.43	2.47	7	1
1:A:146:TRP:CE3	1:A:158:LYS:CG	0.43	3.02	1	1
1:A:119:ILE:HD12	1:A:151:LEU:HD22	0.43	1.91	20	1
1:A:146:TRP:CE3	1:A:158:LYS:HG3	0.43	2.49	1	2
1:A:32:ALA:HB1	1:A:70:LEU:CD2	0.43	2.44	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ILE:CD1	1:A:102:PHE:CD2	0.43	3.02	6	1
1:A:50:PHE:CZ	1:A:55:THR:HG23	0.43	2.49	12	1
1:A:17:LEU:HD11	1:A:70:LEU:HD11	0.42	1.90	1	2
1:A:21:LEU:HD11	1:A:30:LYS:HB2	0.42	1.91	14	1
1:A:31:ILE:CD1	1:A:102:PHE:CD1	0.42	3.01	16	1
1:A:149:LYS:HE3	1:A:151:LEU:HD12	0.42	1.92	18	2
1:A:151:LEU:HD22	1:A:153:TYR:CE2	0.42	2.49	7	1
1:A:35:ILE:HG12	1:A:98:LEU:HD21	0.42	1.92	6	1
1:A:115:TRP:CE3	1:A:171:ILE:HD11	0.42	2.50	6	1
1:A:84:ALA:H	1:A:104:VAL:CG2	0.42	2.27	17	1
1:A:101:MET:SD	1:A:115:TRP:HA	0.42	2.54	15	2
1:A:89:ALA:HB2	1:A:130:MET:CE	0.41	2.44	8	1
1:A:33:VAL:HG21	1:A:102:PHE:CD1	0.41	2.50	10	1
1:A:160:ILE:CD1	1:A:162:THR:HG23	0.41	2.45	10	1
1:A:21:LEU:CD2	1:A:32:ALA:HB2	0.41	2.44	16	1
1:A:146:TRP:CE3	1:A:160:ILE:HB	0.41	2.50	1	1
1:A:7:ILE:HD12	1:A:9:GLY:H	0.41	1.75	6	1
1:A:24:LEU:CD1	1:A:72:SER:HB2	0.41	2.44	12	1
1:A:21:LEU:C	1:A:21:LEU:HD12	0.41	2.35	14	1
1:A:31:ILE:CG2	1:A:84:ALA:HB3	0.41	2.46	3	1
1:A:3:ALA:HB3	1:A:57:VAL:HG11	0.41	1.91	8	1
1:A:6:ILE:HD11	1:A:70:LEU:HD12	0.41	1.93	18	1
1:A:17:LEU:HD21	1:A:70:LEU:HD11	0.41	1.93	3	1
1:A:12:LEU:HD21	1:A:17:LEU:HD23	0.41	1.93	12	1
1:A:105:PRO:CG	1:A:164:ALA:HB2	0.40	2.46	16	1
1:A:21:LEU:HD22	1:A:31:ILE:O	0.40	2.16	1	1
1:A:86:ALA:HB3	1:A:102:PHE:CE1	0.40	2.50	11	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	152/175 (87%)	132±4 (87±3%)	17±4 (11±3%)	4±2 (2±1%)	9	48
All	All	3040/3500 (87%)	2639 (87%)	331 (11%)	70 (2%)	9	48

All 22 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	7	ILE	15
1	A	144	ASN	11
1	A	165	GLY	6
1	A	116	ASP	5
1	A	164	ALA	5
1	A	152	GLY	3
1	A	65	ASN	3
1	A	64	PRO	3
1	A	54	THR	3
1	A	123	LYS	2
1	A	3	ALA	2
1	A	138	ASN	2
1	A	143	ASP	1
1	A	52	SER	1
1	A	122	GLY	1
1	A	53	GLY	1
1	A	142	GLY	1
1	A	56	ASP	1
1	A	167	ALA	1
1	A	137	GLY	1
1	A	153	TYR	1
1	A	154	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	121/138 (88%)	93±3 (77±3%)	28±3 (23±3%)	3 28
All	All	2420/2760 (88%)	1862 (77%)	558 (23%)	3 28

All 84 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	31	ILE	20
1	A	19	LYS	19

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Mol	Chain	Res	Type	Models (Total)
1	A	46	LEU	19
1	A	125	ARG	19
1	A	157	MET	19
1	A	17	LEU	17
1	A	69	LEU	17
1	A	133	ASP	17
1	A	100	VAL	16
1	A	50	PHE	15
1	A	39	SER	14
1	A	175	ARG	14
1	A	101	MET	12
1	A	20	VAL	12
1	A	158	LYS	12
1	A	70	LEU	11
1	A	161	MET	11
1	A	30	LYS	11
1	A	21	LEU	11
1	A	51	ARG	11
1	A	155	LEU	11
1	A	160	ILE	10
1	A	149	LYS	10
1	A	13	THR	9
1	A	113	ASN	9
1	A	169	MET	9
1	A	168	LYS	9
1	A	23	GLU	8
1	A	37	ASN	7
1	A	94	SER	7
1	A	127	ASP	7
1	A	7	ILE	7
1	A	2	LEU	7
1	A	135	TYR	6
1	A	141	ARG	6
1	A	11	SER	6
1	A	150	ASN	6
1	A	74	ARG	6
1	A	63	VAL	6
1	A	33	VAL	5
1	A	55	THR	5
1	A	93	SER	5
1	A	71	TYR	5
1	A	144	ASN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	92	MET	4
1	A	172	LYS	4
1	A	103	SER	4
1	A	118	LYS	4
1	A	156	ARG	4
1	A	65	ASN	4
1	A	138	ASN	4
1	A	54	THR	3
1	A	90	TYR	3
1	A	151	LEU	3
1	A	140	TYR	3
1	A	166	GLU	3
1	A	24	LEU	3
1	A	47	ASN	3
1	A	162	THR	3
1	A	36	ASP	3
1	A	52	SER	3
1	A	22	GLU	2
1	A	123	LYS	2
1	A	132	GLU	2
1	A	128	GLN	2
1	A	148	GLU	2
1	A	143	ASP	2
1	A	116	ASP	2
1	A	130	MET	2
1	A	56	ASP	2
1	A	49	TYR	1
1	A	124	ARG	1
1	A	59	LEU	1
1	A	38	GLU	1
1	A	153	TYR	1
1	A	104	VAL	1
1	A	131	TYR	1
1	A	136	TYR	1
1	A	117	VAL	1
1	A	18	ASP	1
1	A	72	SER	1
1	A	163	SER	1
1	A	96	ASN	1
1	A	174	SER	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 monosaccharides 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 (i)

No chemical shift data were provided