



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:46 pm BST

PDB ID : 2KXS
Title : ZO1 ZU5 domain in complex with GRINL1A peptide
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Deposited on : 2010-05-12

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 ⓘ 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

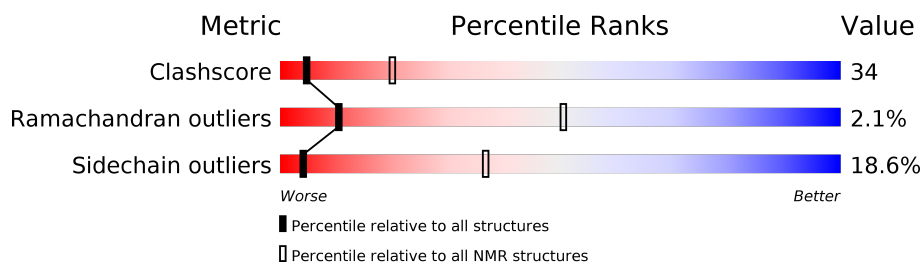
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	146	<div> <div></div> <div>36%</div> <div>39%</div> <div>5%</div> <div>20%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 16 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:3-A:101, A:124-A:132, A:138-A:146 (117)	0.17	16

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2199 atoms, of which 1108 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	146	2199	694	1108	187	204	6	0

There are 18 discrepancies between the modelled and reference sequences:

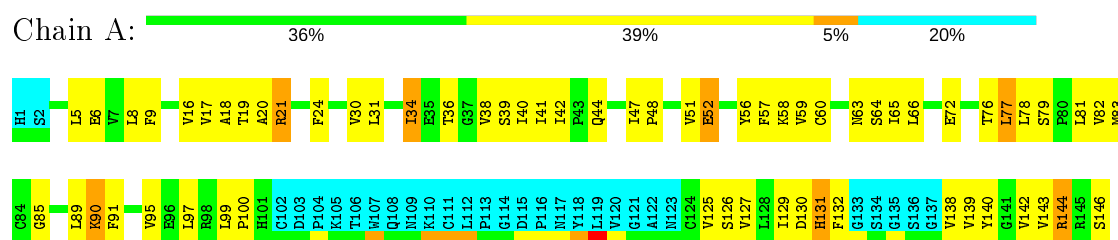
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	EXPRESSION TAG	UNP Q07157
A	2	SER	-	EXPRESSION TAG	UNP Q07157
A	3	SER	-	EXPRESSION TAG	UNP Q07157
A	4	GLY	-	EXPRESSION TAG	UNP Q07157
A	5	LEU	-	EXPRESSION TAG	UNP Q07157
A	6	GLU	-	EXPRESSION TAG	UNP Q07157
A	7	VAL	-	EXPRESSION TAG	UNP Q07157
A	8	LEU	-	EXPRESSION TAG	UNP Q07157
A	9	PHE	-	EXPRESSION TAG	UNP Q07157
A	10	GLN	-	EXPRESSION TAG	UNP Q07157
A	11	GLY	-	EXPRESSION TAG	UNP Q07157
A	12	PRO	-	EXPRESSION TAG	UNP Q07157
A	13	GLY	-	EXPRESSION TAG	UNP Q07157
A	14	SER	-	EXPRESSION TAG	UNP Q07157
A	133	GLY	-	LINKER	UNP D2E9U7
A	134	SER	-	LINKER	UNP D2E9U7
A	135	GLY	-	LINKER	UNP D2E9U7
A	136	SER	-	LINKER	UNP D2E9U7

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein

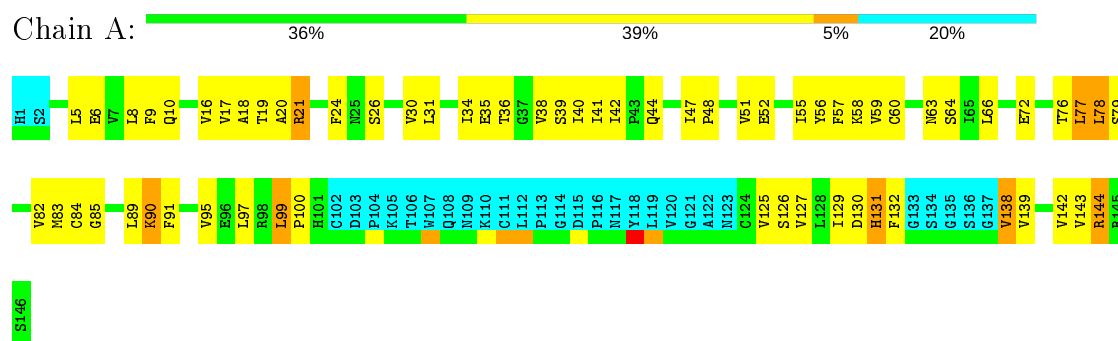


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

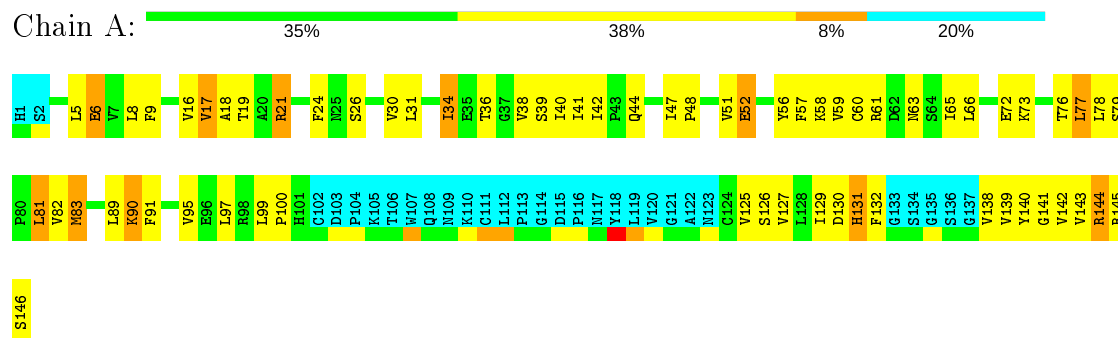
4.2.1 Score per residue for model 1

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



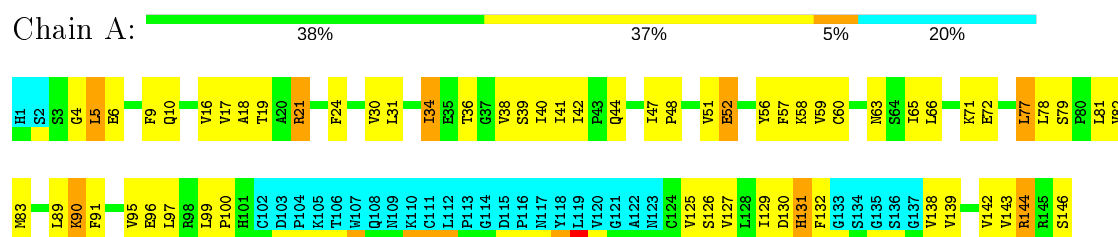
4.2.2 Score per residue for model 2

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



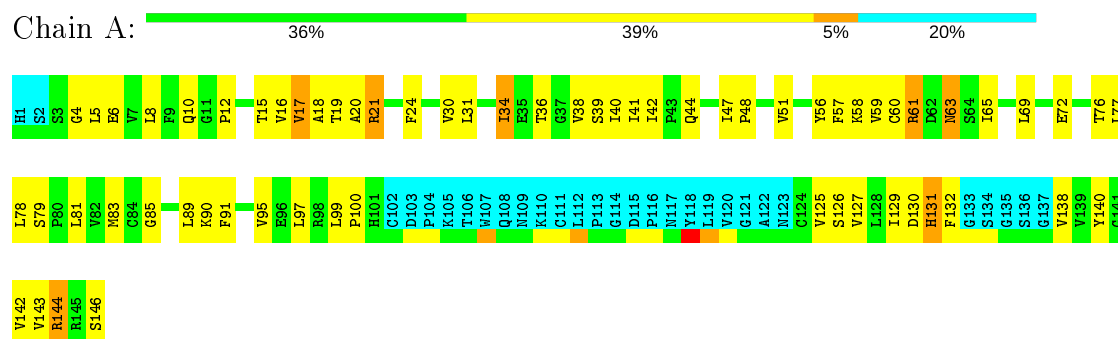
4.2.3 Score per residue for model 3

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



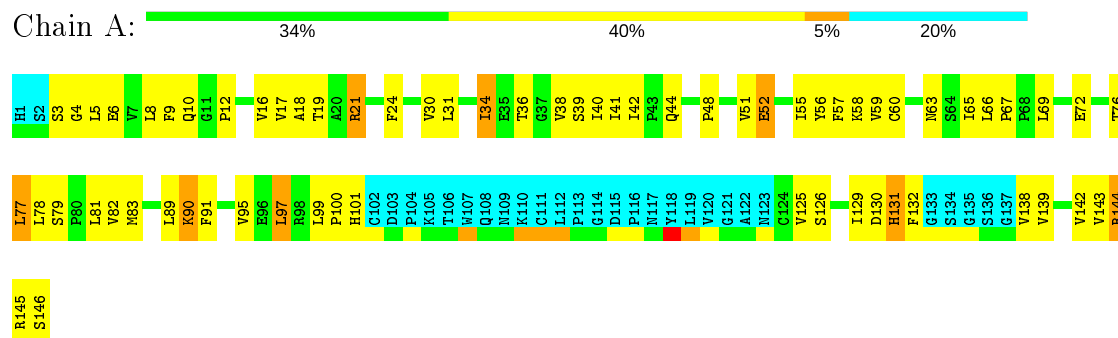
4.2.4 Score per residue for model 4

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



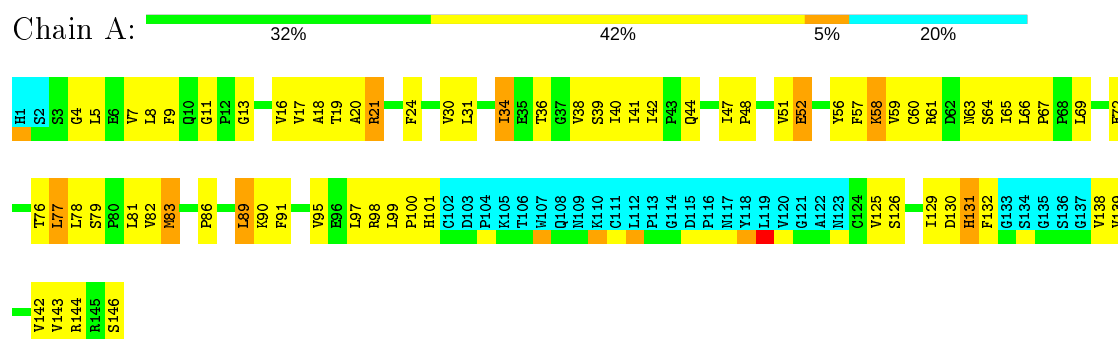
4.2.5 Score per residue for model 5

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



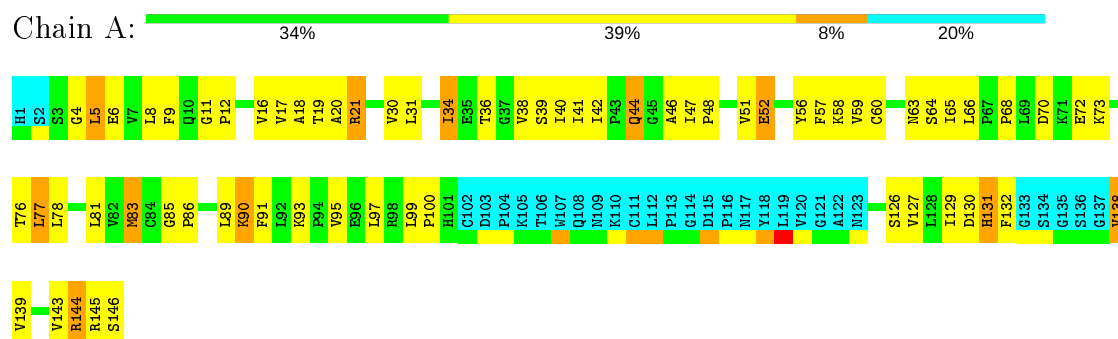
4.2.6 Score per residue for model 6

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



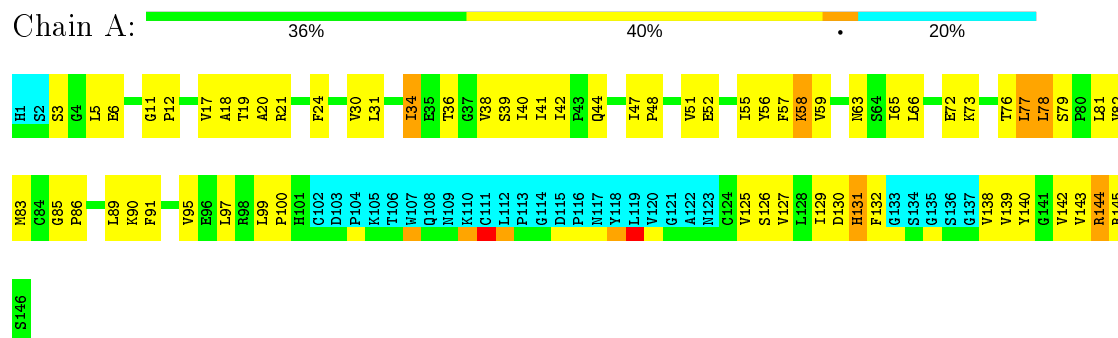
4.2.7 Score per residue for model 7

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



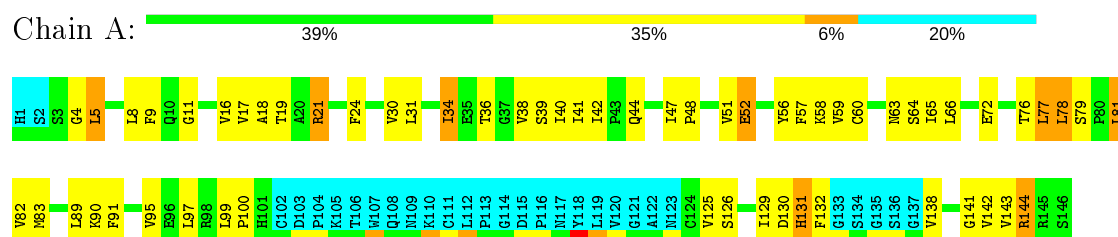
4.2.8 Score per residue for model 8

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



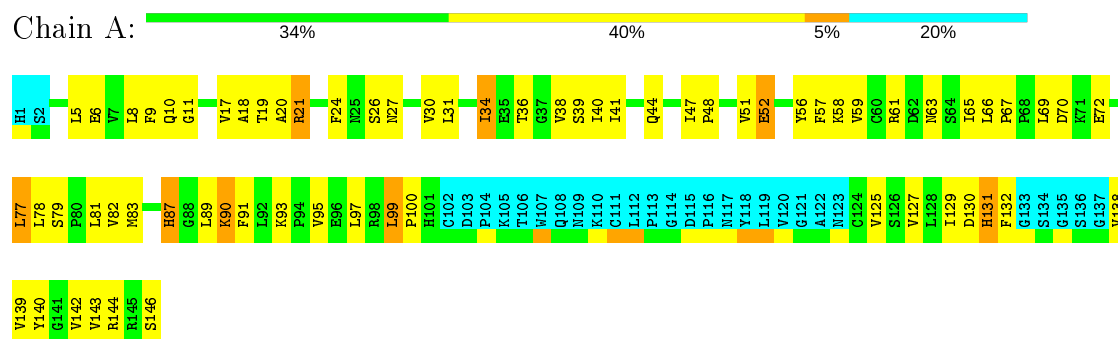
4.2.9 Score per residue for model 9

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



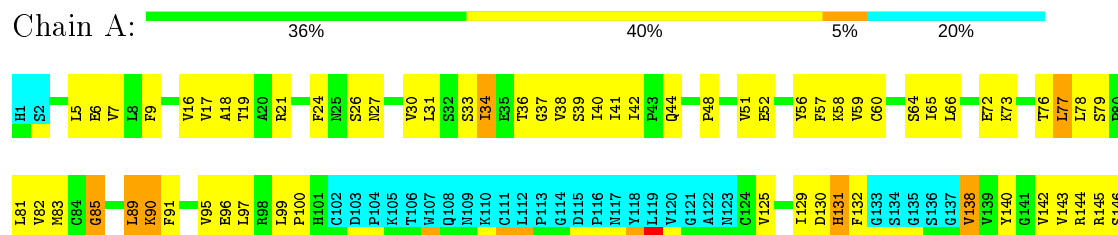
4.2.10 Score per residue for model 10

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



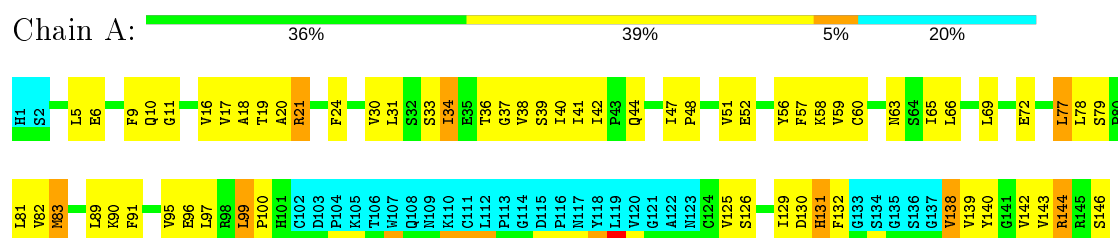
4.2.11 Score per residue for model 11

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



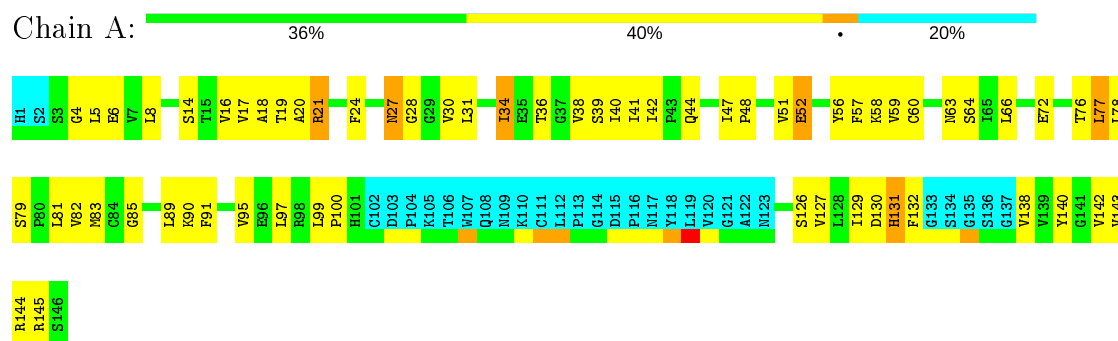
4.2.12 Score per residue for model 12

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



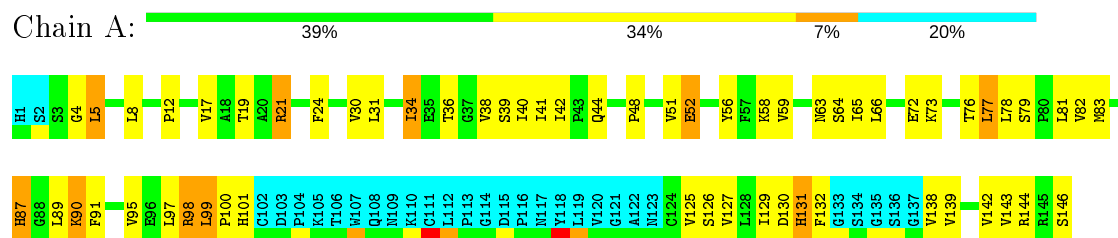
4.2.13 Score per residue for model 13

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



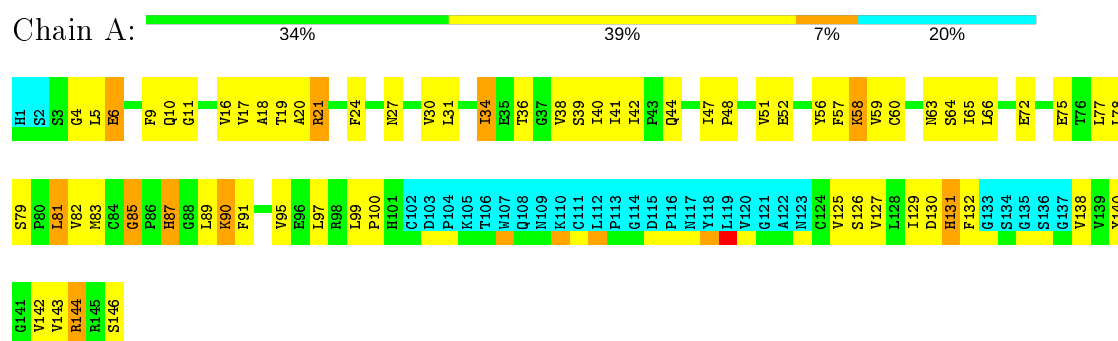
4.2.14 Score per residue for model 14

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



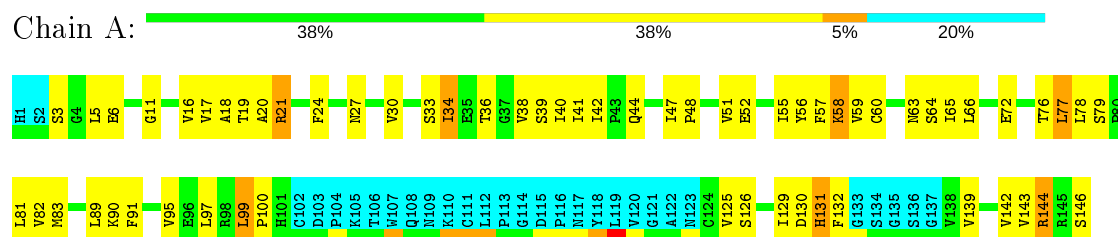
4.2.15 Score per residue for model 15

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



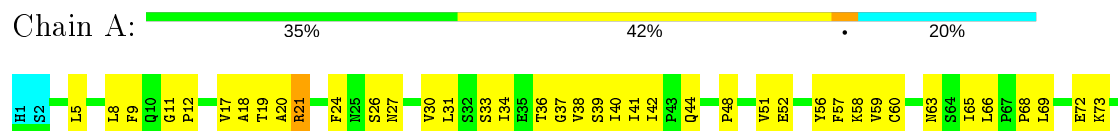
4.2.16 Score per residue for model 16 (medoid)

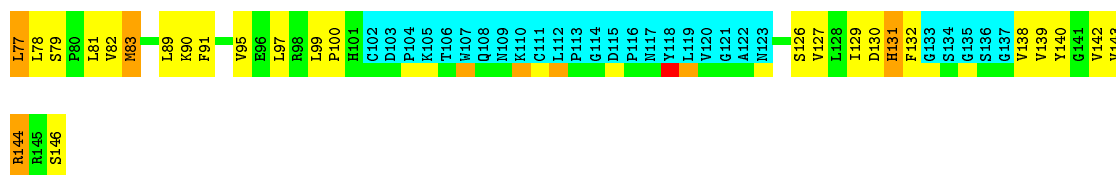
- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



4.2.17 Score per residue for model 17

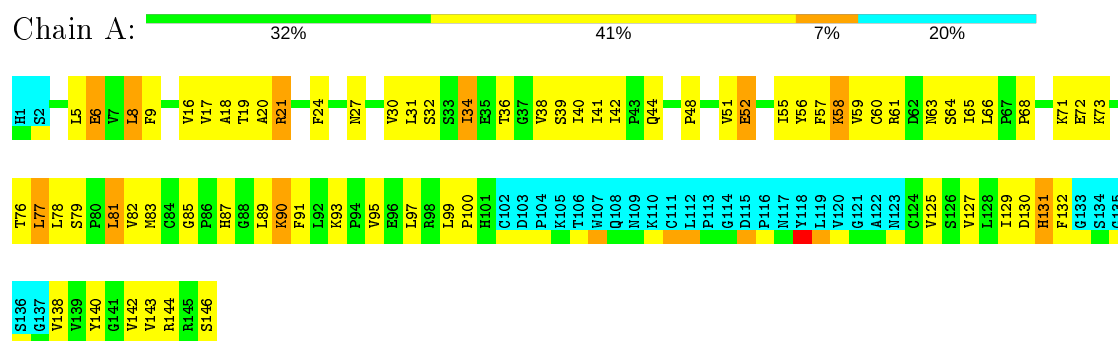
- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein





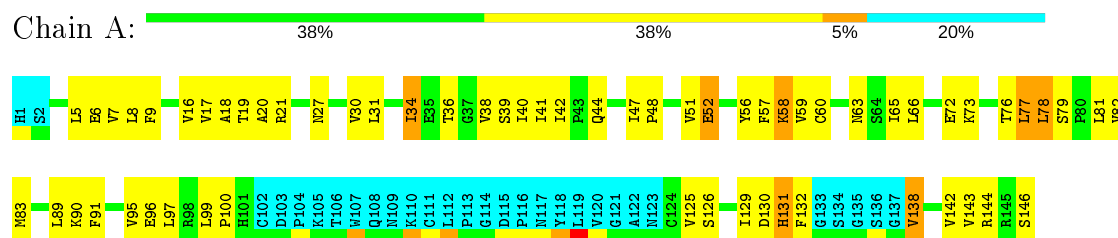
4.2.18 Score per residue for model 18

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



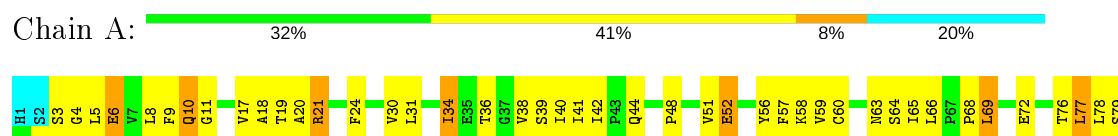
4.2.19 Score per residue for model 19

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



4.2.20 Score per residue for model 20

- Molecule 1: Tight junction protein ZO-1, LINKER, peptide of Myocardium-enriched Zo-associated protein



V142	R80
V143	L81
R144	L82
R145	M83
S146	G84
	G85
	R86
	R87
	G88
	L89
	K90
	F91
	V95
	E96
	L97
	R98
	L99
	P100
	H101
	G102
	D103
	P104
	K105
	T106
	W107
	G108
	M109
	K110
	G111
	L112
	P113
	G114
	D115
	P116
	W117
	Y118
	L119
	V120
	G121
	A122
	M123
	G124
	V125
	S126
	V127
	L128
	L129
	D130
	H131
	F132
	G133
	S134
	G135
	S136
	G137
	V138
	V139
	Y140
	G141

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 200 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
CNS	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

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	882	915	912	61±4
All	All	17640	18300	18240	1211

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:THR:HG21	1:A:59:VAL:HG11	1.03	1.27	4	20
1:A:5:LEU:HD23	1:A:125:VAL:HG11	0.91	1.40	8	16
1:A:31:LEU:HD12	1:A:57:PHE:CE2	0.86	2.06	10	1
1:A:129:ILE:HD13	1:A:132:PHE:CZ	0.85	2.06	13	20
1:A:129:ILE:HG21	1:A:132:PHE:CD1	0.85	2.07	8	11
1:A:36:THR:HG21	1:A:59:VAL:CG1	0.83	2.03	4	19
1:A:129:ILE:HG21	1:A:132:PHE:CE1	0.83	2.09	8	10
1:A:86:PRO:CG	1:A:89:LEU:HD12	0.77	2.10	8	3
1:A:127:VAL:HG11	1:A:140:TYR:CE1	0.77	2.14	20	1
1:A:5:LEU:HD13	1:A:6:GLU:N	0.77	1.94	18	16
1:A:8:LEU:HD11	1:A:77:LEU:HD11	0.77	1.56	13	2
1:A:65:ILE:HG21	1:A:81:LEU:HG	0.76	1.58	8	8
1:A:65:ILE:HG21	1:A:81:LEU:CD1	0.75	2.11	3	6
1:A:59:VAL:HG22	1:A:82:VAL:HG22	0.74	1.58	8	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:HD11	1:A:144:ARG:HG3	0.73	1.58	6	15
1:A:18:ALA:HB3	1:A:59:VAL:HB	0.73	1.61	2	19
1:A:10:GLN:OE1	1:A:65:ILE:HG22	0.73	1.84	12	4
1:A:19:THR:HG23	1:A:58:LYS:HG3	0.72	1.60	1	20
1:A:19:THR:HG22	1:A:21:ARG:HD2	0.72	1.62	12	12
1:A:86:PRO:HG2	1:A:89:LEU:HD12	0.72	1.62	7	2
1:A:65:ILE:HG21	1:A:81:LEU:HD13	0.71	1.61	9	3
1:A:89:LEU:HD13	1:A:91:PHE:CZ	0.71	2.20	11	1
1:A:78:LEU:HD11	1:A:144:ARG:CG	0.71	2.15	17	6
1:A:36:THR:CG2	1:A:59:VAL:HG11	0.70	2.12	5	18
1:A:83:MET:HA	1:A:139:VAL:HG12	0.70	1.64	6	3
1:A:82:VAL:O	1:A:139:VAL:HG23	0.70	1.87	10	1
1:A:76:THR:HG22	1:A:144:ARG:HD3	0.70	1.62	18	1
1:A:9:PHE:CZ	1:A:138:VAL:HG12	0.69	2.22	7	15
1:A:19:THR:HG23	1:A:58:LYS:CG	0.69	2.18	1	20
1:A:97:LEU:HD22	1:A:127:VAL:CG1	0.68	2.18	13	1
1:A:77:LEU:HD23	1:A:79:SER:O	0.68	1.88	6	10
1:A:65:ILE:HG21	1:A:81:LEU:HD22	0.68	1.64	2	1
1:A:48:PRO:HG2	1:A:51:VAL:HG11	0.67	1.65	2	20
1:A:59:VAL:HG13	1:A:81:LEU:O	0.67	1.89	15	2
1:A:129:ILE:HD13	1:A:132:PHE:HZ	0.66	1.51	13	18
1:A:101:HIS:ND1	1:A:142:VAL:HG21	0.66	2.05	6	1
1:A:4:GLY:O	1:A:143:VAL:HG12	0.66	1.91	14	10
1:A:20:ALA:HB1	1:A:31:LEU:HD11	0.66	1.67	10	1
1:A:65:ILE:HG21	1:A:81:LEU:CD2	0.66	2.21	2	1
1:A:5:LEU:HD23	1:A:127:VAL:HB	0.66	1.66	17	1
1:A:97:LEU:HD23	1:A:98:ARG:N	0.65	2.05	20	2
1:A:77:LEU:C	1:A:78:LEU:HD13	0.65	2.12	1	3
1:A:31:LEU:HD23	1:A:57:PHE:CD2	0.65	2.26	7	3
1:A:101:HIS:CD2	1:A:142:VAL:HG21	0.65	2.27	14	2
1:A:78:LEU:HD13	1:A:78:LEU:N	0.65	2.06	1	3
1:A:48:PRO:O	1:A:51:VAL:HG12	0.65	1.91	4	20
1:A:40:ILE:HG12	1:A:97:LEU:HD12	0.64	1.68	14	2
1:A:127:VAL:HG21	1:A:140:TYR:CE2	0.64	2.26	8	3
1:A:66:LEU:O	1:A:66:LEU:HD23	0.64	1.92	19	6
1:A:66:LEU:HD23	1:A:66:LEU:O	0.64	1.92	2	9
1:A:31:LEU:HD12	1:A:57:PHE:CZ	0.64	2.28	10	1
1:A:65:ILE:CD1	1:A:77:LEU:HD13	0.64	2.23	5	7
1:A:101:HIS:CE1	1:A:142:VAL:HG21	0.64	2.28	6	1
1:A:42:ILE:HG23	1:A:95:VAL:HG12	0.63	1.70	6	19
1:A:65:ILE:HD13	1:A:81:LEU:HD11	0.63	1.70	16	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LYS:CG	1:A:131:HIS:HB2	0.63	2.23	11	20
1:A:76:THR:HG22	1:A:144:ARG:HD2	0.63	1.70	19	4
1:A:34:ILE:O	1:A:34:ILE:HD13	0.62	1.94	18	8
1:A:16:VAL:HG22	1:A:60:CYS:SG	0.62	2.34	11	15
1:A:76:THR:HG23	1:A:78:LEU:CD1	0.62	2.24	8	3
1:A:8:LEU:HD23	1:A:68:PRO:HD2	0.61	1.71	18	2
1:A:20:ALA:HB3	1:A:57:PHE:CE1	0.61	2.31	16	4
1:A:36:THR:HG21	1:A:59:VAL:CB	0.60	2.27	17	16
1:A:129:ILE:HG21	1:A:132:PHE:CD2	0.59	2.32	11	3
1:A:41:ILE:HD12	1:A:41:ILE:N	0.59	2.12	14	12
1:A:95:VAL:HG22	1:A:129:ILE:O	0.58	1.99	8	19
1:A:34:ILE:HD13	1:A:34:ILE:O	0.58	1.98	5	10
1:A:20:ALA:HB1	1:A:31:LEU:CD1	0.58	2.27	10	1
1:A:127:VAL:HG21	1:A:140:TYR:HE2	0.58	1.58	8	7
1:A:65:ILE:HD13	1:A:81:LEU:HD21	0.57	1.74	2	1
1:A:8:LEU:HD12	1:A:141:GLY:HA3	0.57	1.76	9	1
1:A:89:LEU:HD23	1:A:90:LYS:N	0.57	2.14	7	2
1:A:31:LEU:HD23	1:A:57:PHE:CE2	0.57	2.34	7	3
1:A:82:VAL:O	1:A:139:VAL:HG12	0.57	2.00	16	9
1:A:78:LEU:HD21	1:A:144:ARG:HD2	0.57	1.77	13	3
1:A:40:ILE:HD12	1:A:57:PHE:CD1	0.57	2.34	18	14
1:A:138:VAL:O	1:A:138:VAL:HG23	0.57	2.00	19	12
1:A:89:LEU:HD21	1:A:91:PHE:CE1	0.57	2.35	20	14
1:A:97:LEU:C	1:A:97:LEU:HD23	0.56	2.21	3	10
1:A:57:PHE:HB2	1:A:82:VAL:HG13	0.56	1.77	6	10
1:A:97:LEU:HD23	1:A:97:LEU:C	0.55	2.22	9	7
1:A:41:ILE:N	1:A:41:ILE:HD12	0.55	2.16	5	8
1:A:40:ILE:HD12	1:A:57:PHE:CD2	0.55	2.36	8	5
1:A:17:VAL:HG11	1:A:61:ARG:HD3	0.55	1.77	4	2
1:A:5:LEU:HD23	1:A:125:VAL:CG1	0.55	2.32	11	10
1:A:78:LEU:HD21	1:A:144:ARG:HB2	0.55	1.77	8	3
1:A:8:LEU:HD12	1:A:8:LEU:N	0.55	2.17	14	2
1:A:138:VAL:HG23	1:A:138:VAL:O	0.55	2.02	11	6
1:A:91:PHE:N	1:A:130:ASP:O	0.54	2.41	15	20
1:A:21:ARG:CB	1:A:56:TYR:HB3	0.54	2.32	19	3
1:A:21:ARG:HG3	1:A:56:TYR:HB2	0.54	1.78	7	12
1:A:97:LEU:HB3	1:A:127:VAL:HG13	0.53	1.79	13	9
1:A:78:LEU:HD22	1:A:78:LEU:H	0.53	1.62	1	1
1:A:90:LYS:HG3	1:A:131:HIS:HB2	0.53	1.79	11	1
1:A:21:ARG:HB3	1:A:56:TYR:CB	0.52	2.34	16	3
1:A:77:LEU:HD22	1:A:81:LEU:CD2	0.52	2.35	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:LEU:HD23	1:A:57:PHE:CE1	0.52	2.39	4	8
1:A:78:LEU:HD21	1:A:144:ARG:CG	0.52	2.34	9	1
1:A:10:GLN:HG2	1:A:139:VAL:HG11	0.52	1.81	10	1
1:A:5:LEU:HD11	1:A:140:TYR:CD2	0.52	2.39	13	3
1:A:97:LEU:HD21	1:A:99:LEU:HG	0.52	1.80	15	15
1:A:38:VAL:HG22	1:A:100:PRO:CD	0.52	2.35	14	20
1:A:10:GLN:NE2	1:A:139:VAL:HG11	0.51	2.20	1	2
1:A:7:VAL:O	1:A:7:VAL:HG13	0.51	2.04	19	1
1:A:89:LEU:HD23	1:A:90:LYS:H	0.51	1.66	7	2
1:A:78:LEU:H	1:A:78:LEU:HD22	0.51	1.66	8	2
1:A:7:VAL:HG13	1:A:7:VAL:O	0.51	2.06	6	1
1:A:38:VAL:CG2	1:A:99:LEU:HD23	0.51	2.35	11	6
1:A:129:ILE:HG21	1:A:132:PHE:CE2	0.50	2.41	11	2
1:A:78:LEU:HD21	1:A:144:ARG:CB	0.50	2.36	8	3
1:A:97:LEU:CD2	1:A:99:LEU:HD11	0.50	2.36	5	1
1:A:38:VAL:HG22	1:A:100:PRO:HD2	0.50	1.84	15	20
1:A:76:THR:HG22	1:A:144:ARG:CD	0.50	2.36	20	5
1:A:18:ALA:CB	1:A:36:THR:HG23	0.50	2.37	15	2
1:A:143:VAL:HG13	1:A:143:VAL:O	0.50	2.07	11	10
1:A:7:VAL:HG22	1:A:140:TYR:CE1	0.50	2.41	11	1
1:A:8:LEU:HD22	1:A:68:PRO:HD3	0.50	1.82	17	1
1:A:10:GLN:CG	1:A:139:VAL:HG11	0.50	2.37	3	2
1:A:143:VAL:O	1:A:143:VAL:HG13	0.49	2.08	18	9
1:A:24:PHE:HZ	1:A:31:LEU:HD23	0.49	1.67	10	1
1:A:41:ILE:CD1	1:A:41:ILE:N	0.49	2.76	14	2
1:A:41:ILE:HD13	1:A:98:ARG:HG3	0.49	1.85	14	1
1:A:76:THR:HG23	1:A:78:LEU:CD2	0.49	2.37	16	1
1:A:47:ILE:HG23	1:A:48:PRO:HD2	0.49	1.85	7	14
1:A:8:LEU:HD13	1:A:141:GLY:HA3	0.48	1.84	2	1
1:A:5:LEU:HD11	1:A:140:TYR:HD1	0.48	1.68	20	2
1:A:97:LEU:HD22	1:A:99:LEU:CD1	0.48	2.38	20	2
1:A:90:LYS:HG2	1:A:131:HIS:HB2	0.48	1.84	2	20
1:A:19:THR:HG22	1:A:21:ARG:CD	0.48	2.36	9	4
1:A:86:PRO:CB	1:A:89:LEU:HD12	0.48	2.39	8	1
1:A:129:ILE:HD13	1:A:132:PHE:CE1	0.47	2.43	8	3
1:A:20:ALA:CB	1:A:31:LEU:HD11	0.47	2.37	10	1
1:A:79:SER:CB	1:A:142:VAL:CG1	0.47	2.93	3	17
1:A:79:SER:N	1:A:142:VAL:HG12	0.47	2.25	19	10
1:A:78:LEU:HD11	1:A:144:ARG:HG2	0.46	1.86	17	1
1:A:34:ILE:C	1:A:34:ILE:HD13	0.46	2.30	18	11
1:A:40:ILE:CD1	1:A:57:PHE:CD2	0.46	2.98	19	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:CB	1:A:57:PHE:CE1	0.46	2.99	16	3
1:A:78:LEU:HD11	1:A:144:ARG:CD	0.46	2.41	10	2
1:A:40:ILE:CD1	1:A:57:PHE:CD1	0.46	2.98	9	11
1:A:87:HIS:CD2	1:A:87:HIS:O	0.46	2.68	14	2
1:A:20:ALA:CB	1:A:57:PHE:CZ	0.46	2.99	18	6
1:A:34:ILE:HD13	1:A:34:ILE:C	0.46	2.30	20	7
1:A:65:ILE:CG2	1:A:81:LEU:HD13	0.46	2.39	9	2
1:A:87:HIS:O	1:A:87:HIS:CD2	0.46	2.69	20	2
1:A:89:LEU:O	1:A:132:PHE:N	0.45	2.49	16	19
1:A:65:ILE:HG21	1:A:81:LEU:HD11	0.45	1.87	3	1
1:A:87:HIS:N	1:A:87:HIS:CD2	0.45	2.84	18	1
1:A:84:CYS:SG	1:A:138:VAL:HG23	0.45	2.51	1	1
1:A:99:LEU:HD12	1:A:125:VAL:HB	0.45	1.88	14	1
1:A:89:LEU:CD2	1:A:91:PHE:CZ	0.45	2.99	18	4
1:A:51:VAL:HG22	1:A:52:GLU:N	0.45	2.27	9	17
1:A:57:PHE:CD1	1:A:57:PHE:O	0.45	2.70	7	4
1:A:24:PHE:CZ	1:A:31:LEU:HB2	0.45	2.47	14	16
1:A:56:TYR:CE2	1:A:85:GLY:CA	0.45	3.00	7	1
1:A:9:PHE:CZ	1:A:138:VAL:CG1	0.45	3.00	7	1
1:A:38:VAL:CG2	1:A:100:PRO:CD	0.45	2.95	18	17
1:A:15:THR:O	1:A:60:CYS:HA	0.44	2.12	4	1
1:A:31:LEU:CD2	1:A:57:PHE:CE2	0.44	3.00	7	1
1:A:20:ALA:HB3	1:A:57:PHE:CE2	0.44	2.47	13	4
1:A:79:SER:N	1:A:142:VAL:CG1	0.44	2.80	17	16
1:A:21:ARG:HB3	1:A:56:TYR:HB2	0.44	1.89	8	2
1:A:5:LEU:HD13	1:A:5:LEU:C	0.44	2.33	10	2
1:A:83:MET:CA	1:A:139:VAL:HG12	0.44	2.43	17	2
1:A:79:SER:N	1:A:142:VAL:HG11	0.44	2.28	17	1
1:A:97:LEU:HD21	1:A:99:LEU:HD11	0.43	1.90	5	1
1:A:129:ILE:HD13	1:A:132:PHE:CE2	0.43	2.45	11	1
1:A:89:LEU:HD13	1:A:91:PHE:CE1	0.43	2.48	11	1
1:A:76:THR:HG22	1:A:144:ARG:HE	0.43	1.74	5	1
1:A:21:ARG:CB	1:A:56:TYR:CB	0.43	2.96	8	2
1:A:90:LYS:CD	1:A:131:HIS:HB2	0.43	2.44	19	11
1:A:79:SER:HB2	1:A:142:VAL:HG12	0.43	1.90	8	2
1:A:8:LEU:CD1	1:A:77:LEU:HD11	0.43	2.42	19	1
1:A:90:LYS:HG2	1:A:131:HIS:CD2	0.43	2.49	6	3
1:A:79:SER:CB	1:A:142:VAL:HB	0.43	2.44	16	3
1:A:78:LEU:HD22	1:A:78:LEU:N	0.43	2.27	1	1
1:A:24:PHE:HD2	1:A:55:ILE:HD12	0.43	1.74	8	2
1:A:41:ILE:N	1:A:96:GLU:O	0.43	2.52	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:LEU:HD12	1:A:89:LEU:C	0.43	2.34	4	1
1:A:8:LEU:HD23	1:A:67:PRO:HA	0.43	1.91	6	3
1:A:57:PHE:O	1:A:57:PHE:CD1	0.43	2.72	19	1
1:A:8:LEU:HD23	1:A:68:PRO:CD	0.43	2.44	20	1
1:A:97:LEU:HD21	1:A:99:LEU:CG	0.42	2.45	12	3
1:A:65:ILE:CD1	1:A:77:LEU:CD1	0.42	2.96	20	1
1:A:5:LEU:C	1:A:5:LEU:HD13	0.42	2.33	1	2
1:A:21:ARG:HA	1:A:56:TYR:HB3	0.42	1.91	5	5
1:A:77:LEU:HD22	1:A:81:LEU:HD22	0.42	1.91	7	2
1:A:20:ALA:HB2	1:A:33:SER:HB2	0.42	1.90	16	1
1:A:20:ALA:O	1:A:57:PHE:N	0.42	2.52	8	3
1:A:90:LYS:HG2	1:A:131:HIS:CG	0.42	2.50	4	1
1:A:21:ARG:CD	1:A:56:TYR:CB	0.42	2.97	4	1
1:A:78:LEU:N	1:A:78:LEU:HD22	0.42	2.30	8	1
1:A:5:LEU:HD11	1:A:140:TYR:CD1	0.42	2.49	20	1
1:A:20:ALA:O	1:A:56:TYR:CA	0.42	2.68	1	2
1:A:56:TYR:O	1:A:85:GLY:N	0.42	2.53	8	3
1:A:24:PHE:CZ	1:A:31:LEU:HD22	0.42	2.49	9	3
1:A:57:PHE:HB2	1:A:82:VAL:CG1	0.42	2.45	10	1
1:A:38:VAL:HG21	1:A:99:LEU:HD23	0.42	1.90	11	1
1:A:89:LEU:HD23	1:A:91:PHE:CZ	0.42	2.50	18	1
1:A:63:ASN:N	1:A:63:ASN:ND2	0.42	2.66	4	1
1:A:42:ILE:CG2	1:A:46:ALA:HB3	0.42	2.45	7	1
1:A:79:SER:HB2	1:A:142:VAL:CG1	0.42	2.45	8	2
1:A:21:ARG:CD	1:A:21:ARG:N	0.42	2.82	10	1
1:A:48:PRO:O	1:A:51:VAL:CG1	0.42	2.68	14	2
1:A:33:SER:O	1:A:37:GLY:N	0.41	2.48	11	3
1:A:76:THR:HG22	1:A:144:ARG:NE	0.41	2.31	6	1
1:A:82:VAL:H	1:A:139:VAL:HG23	0.41	1.76	10	1
1:A:97:LEU:HD23	1:A:127:VAL:CG2	0.41	2.46	14	1
1:A:41:ILE:N	1:A:41:ILE:CD1	0.41	2.83	18	1
1:A:27:ASN:ND2	1:A:28:GLY:O	0.41	2.53	13	1
1:A:97:LEU:CD2	1:A:99:LEU:CD1	0.41	2.98	3	5
1:A:97:LEU:HD23	1:A:99:LEU:HD11	0.41	1.92	14	1
1:A:20:ALA:O	1:A:56:TYR:HA	0.41	2.16	20	1
1:A:83:MET:CG	1:A:139:VAL:CG1	0.41	2.98	7	3
1:A:24:PHE:CE2	1:A:55:ILE:HB	0.41	2.51	18	3
1:A:69:LEU:HD13	1:A:76:THR:N	0.41	2.31	20	1
1:A:79:SER:HB2	1:A:142:VAL:HB	0.41	1.91	9	1
1:A:77:LEU:CD2	1:A:79:SER:O	0.41	2.69	20	1
1:A:51:VAL:CG2	1:A:52:GLU:N	0.40	2.84	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:O	1:A:59:VAL:N	0.40	2.54	15	1
1:A:21:ARG:HD2	1:A:56:TYR:CG	0.40	2.52	20	2
1:A:78:LEU:CD1	1:A:78:LEU:N	0.40	2.78	9	1
1:A:5:LEU:HB2	1:A:125:VAL:HG11	0.40	1.93	14	1
1:A:75:GLU:HA	1:A:144:ARG:O	0.40	2.16	15	1
1:A:56:TYR:CD1	1:A:56:TYR:N	0.40	2.89	16	1
1:A:56:TYR:CE1	1:A:85:GLY:CA	0.40	3.03	18	1
1:A:83:MET:CG	1:A:139:VAL:HG12	0.40	2.47	7	1
1:A:56:TYR:O	1:A:85:GLY:CA	0.40	2.69	15	1
1:A:76:THR:CG2	1:A:78:LEU:HD21	0.40	2.47	16	1
1:A:85:GLY:O	1:A:87:HIS:CD2	0.40	2.74	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	116/146 (79%)	101±2 (87±1%)	13±2 (11±1%)	2±1 (2±1%)	10	50
All	All	2320/2920 (79%)	2018 (87%)	253 (11%)	49 (2%)	10	50

All 7 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	44	GLN	20
1	A	11	GLY	10
1	A	12	PRO	6
1	A	85	GLY	6
1	A	138	VAL	5
1	A	13	GLY	1
1	A	63	ASN	1

6.3.2 Protein sidechains ⓘ

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	101/124 (81%)	82±2 (81±2%)	19±2 (19±2%)	4	37
All	All	2020/2480 (81%)	1644 (81%)	376 (19%)	4	37

All 44 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	131	HIS	20
1	A	77	LEU	20
1	A	72	GLU	20
1	A	83	MET	20
1	A	34	ILE	20
1	A	17	VAL	20
1	A	39	SER	20
1	A	30	VAL	20
1	A	21	ARG	18
1	A	63	ASN	18
1	A	126	SER	17
1	A	146	SER	16
1	A	52	GLU	14
1	A	144	ARG	12
1	A	90	LYS	11
1	A	64	SER	11
1	A	73	LYS	8
1	A	27	ASN	8
1	A	69	LEU	7
1	A	145	ARG	6
1	A	58	LYS	6
1	A	26	SER	5
1	A	81	LEU	5
1	A	99	LEU	5
1	A	87	HIS	4
1	A	6	GLU	4
1	A	78	LEU	4
1	A	66	LEU	4
1	A	3	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	5	LEU	4
1	A	61	ARG	4
1	A	93	LYS	3
1	A	71	LYS	2
1	A	89	LEU	2
1	A	98	ARG	2
1	A	8	LEU	2
1	A	60	CYS	2
1	A	70	ASP	2
1	A	14	SER	1
1	A	44	GLN	1
1	A	32	SER	1
1	A	35	GLU	1
1	A	10	GLN	1
1	A	97	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided