



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:57 pm GMT

PDB ID : 1ZUB
Title : Solution Structure of the RIM1alpha PDZ Domain in Complex with an ELKS1b C-terminal Peptide
Authors : Lu, J.; Li, H.; Wang, Y.; Sudhof, T.C.; Rizo, J.
Deposited on : 2005-05-30

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 : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

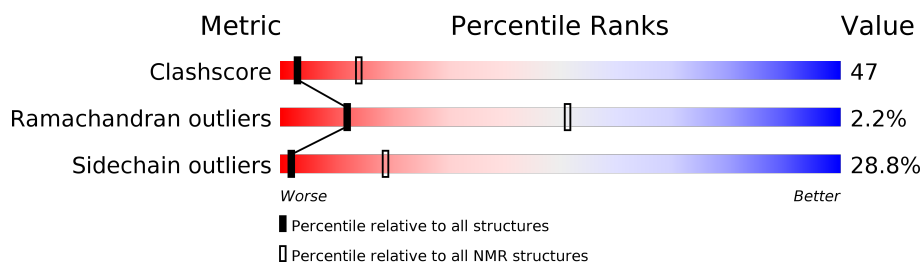
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

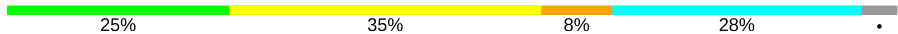

The overall completeness of chemical shifts assignment was not calculated.

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	114	
2	B	11	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:612-A:618, A:629-A:638, A:645-A:704, B:945-B:948 (81)	0.15	3

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 and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1800 atoms, of which 917 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regulating synaptic membrane exocytosis protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	109	Total	C	H	N	O	S	0
			1709	527	876	149	155	2	

There are 5 discrepancies between the modelled and reference sequences:

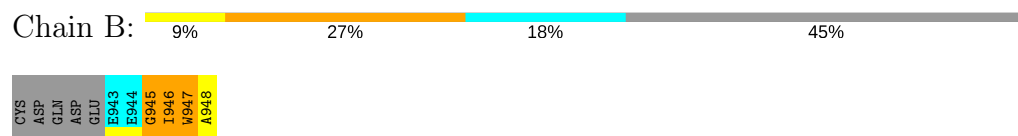
Chain	Residue	Modelled	Actual	Comment	Reference
A	592	GLY	-	CLONING ARTIFACT	UNP Q9JIR4
A	593	SER	-	CLONING ARTIFACT	UNP Q9JIR4
A	594	PRO	-	CLONING ARTIFACT	UNP Q9JIR4
A	595	GLY	-	CLONING ARTIFACT	UNP Q9JIR4
A	596	SER	-	CLONING ARTIFACT	UNP Q9JIR4

- Molecule 2 is a protein called ELKS1b.

Mol	Chain	Residues	Atoms					Trace
2	B	6	Total	C	H	N	O	0
			91	32	41	7	11	

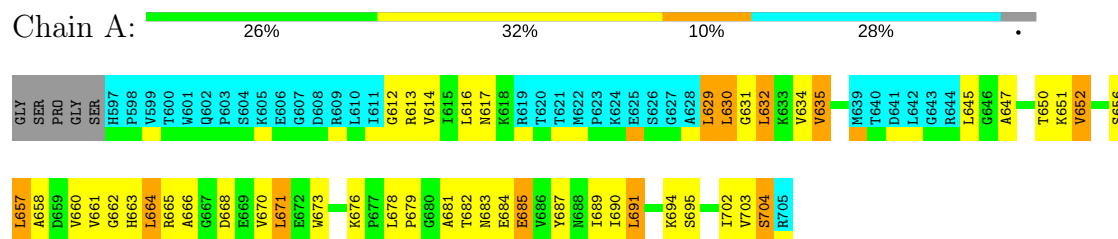
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	938	CYS	-	CLONING ARTIFACT	UNP Q811U3

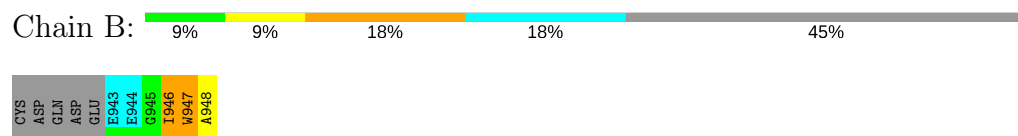


4.2.2 Score per residue for model 2

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

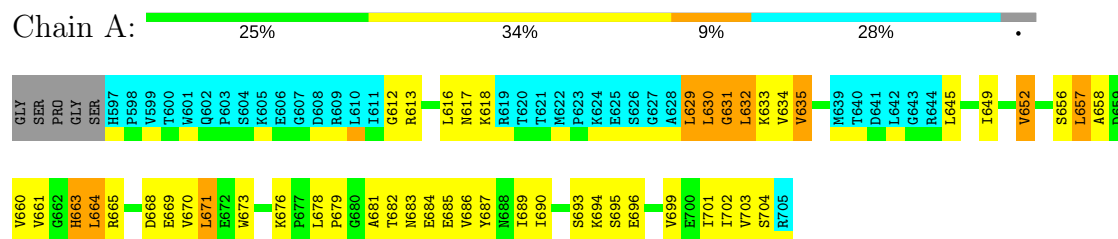


- Molecule 2: ELKS1b

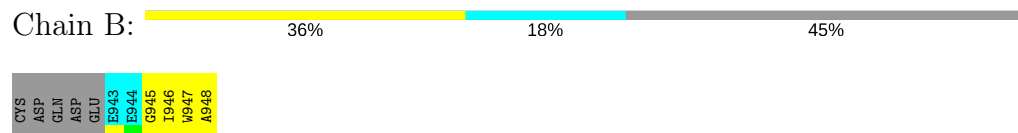


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

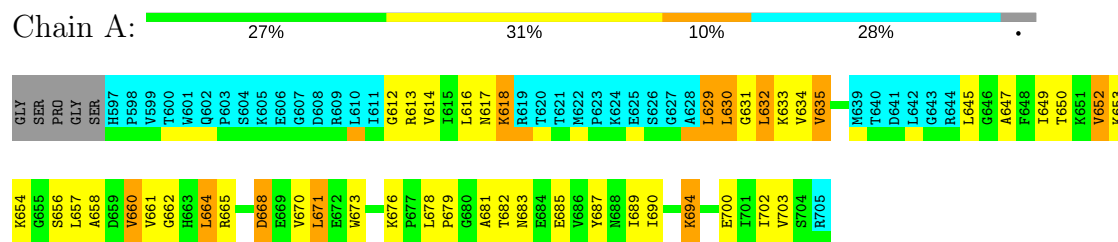


- Molecule 2: ELKS1b

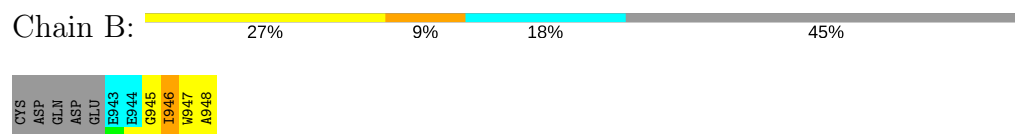


4.2.4 Score per residue for model 4

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

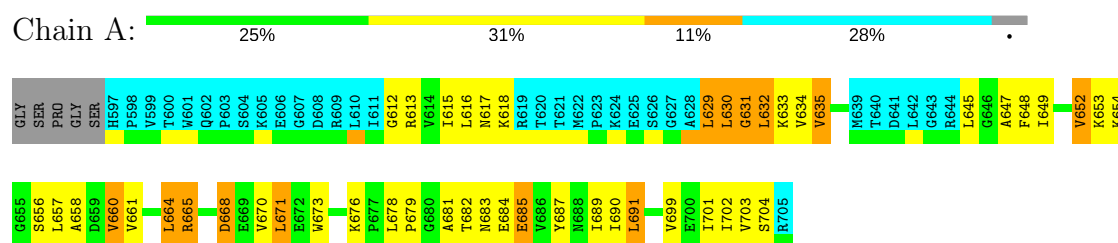


- Molecule 2: ELKS1b

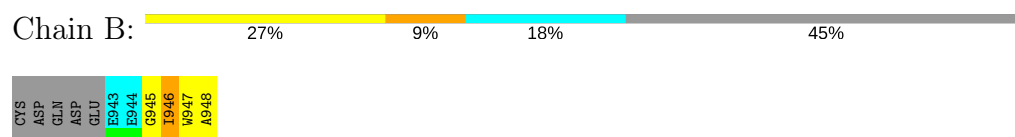


4.2.5 Score per residue for model 5

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

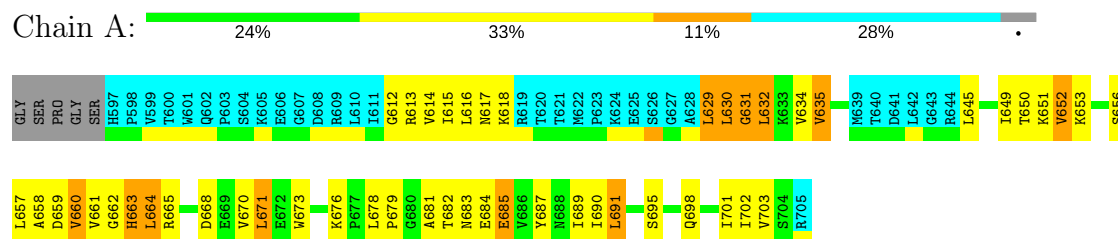


- Molecule 2: ELKS1b

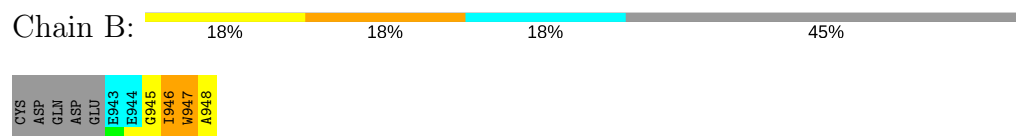


4.2.6 Score per residue for model 6

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

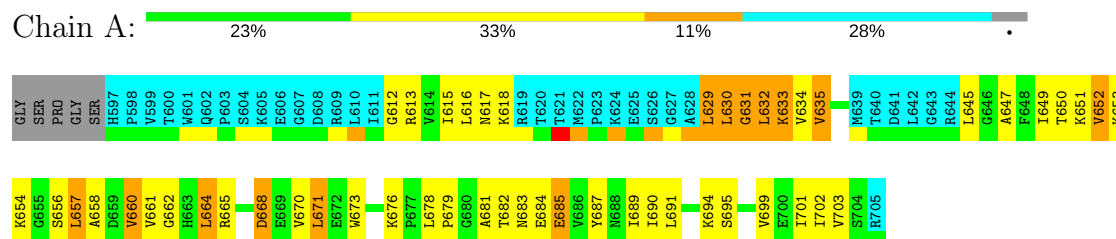


- Molecule 2: ELKS1b

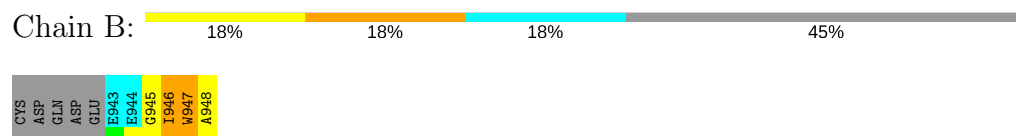


4.2.7 Score per residue for model 7

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

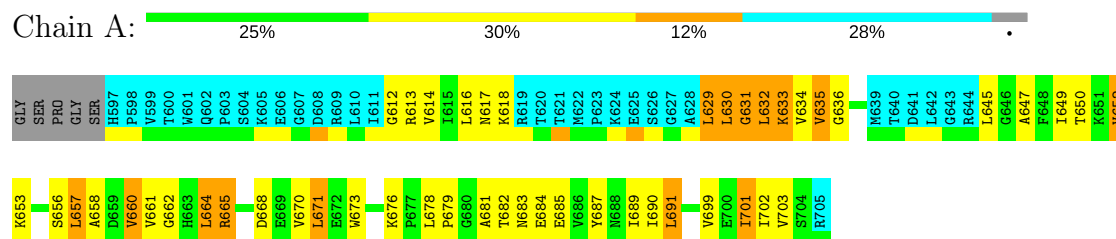


- Molecule 2: ELKS1b

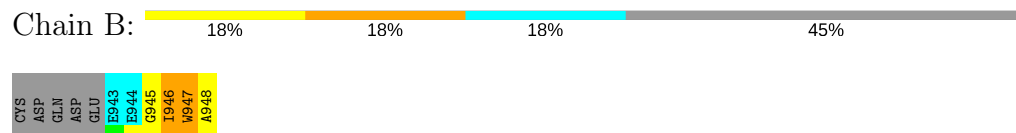


4.2.8 Score per residue for model 8

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

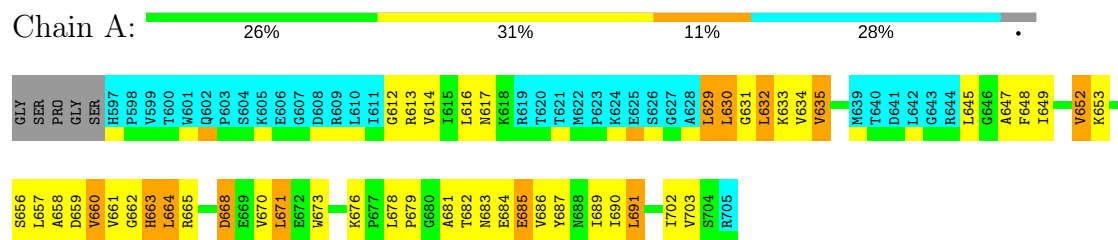


- Molecule 2: ELKS1b

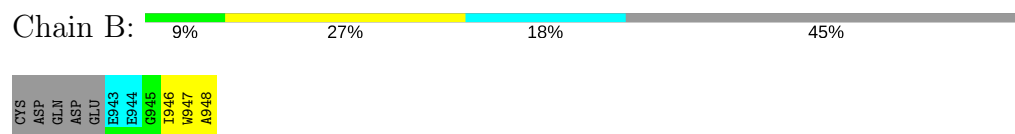


4.2.9 Score per residue for model 9

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

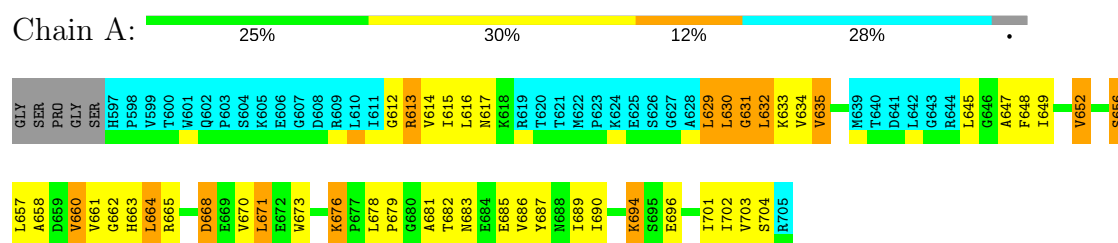


- Molecule 2: ELKS1b

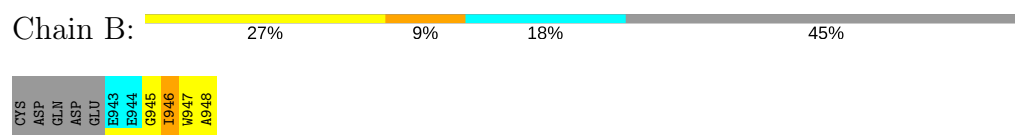


4.2.10 Score per residue for model 10

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

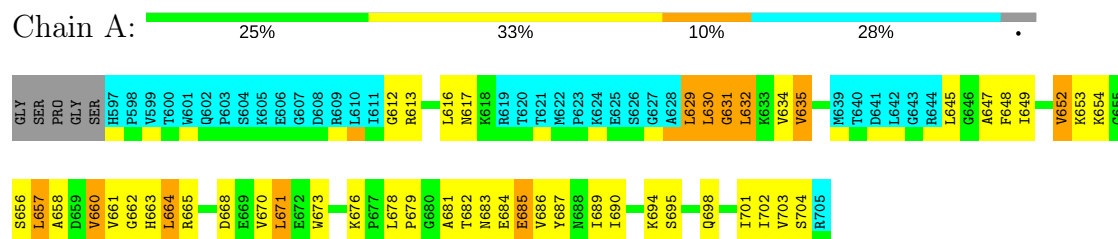


- Molecule 2: ELKS1b

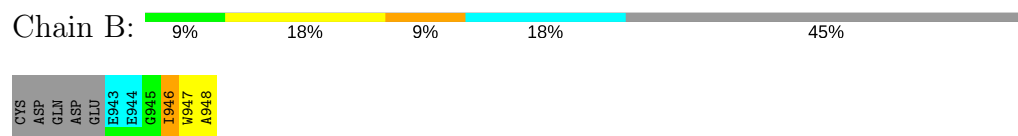


4.2.11 Score per residue for model 11

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

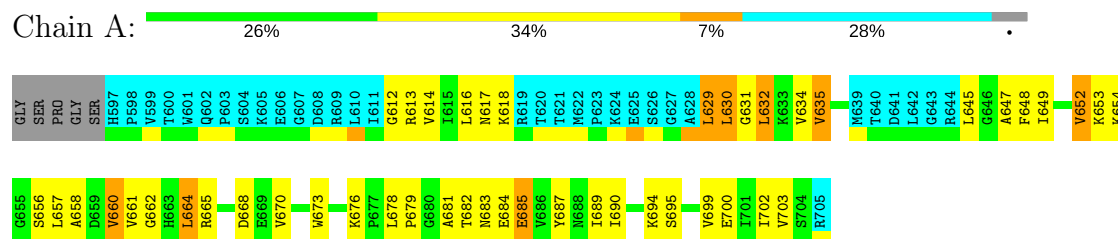


- Molecule 2: ELKS1b

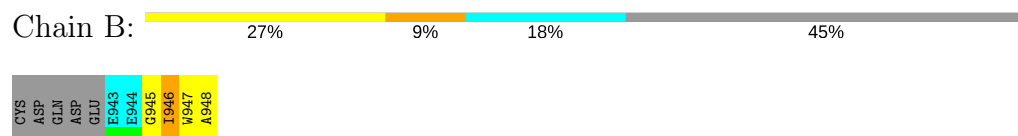


4.2.12 Score per residue for model 12

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

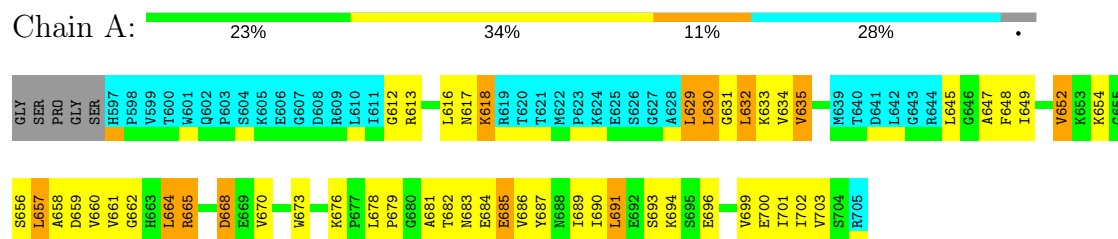


- Molecule 2: ELKS1b

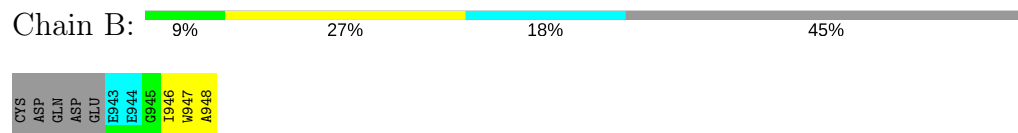


4.2.13 Score per residue for model 13

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

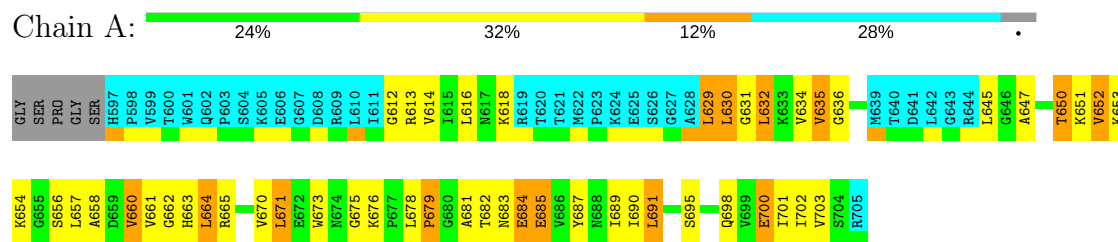


- Molecule 2: ELKS1b

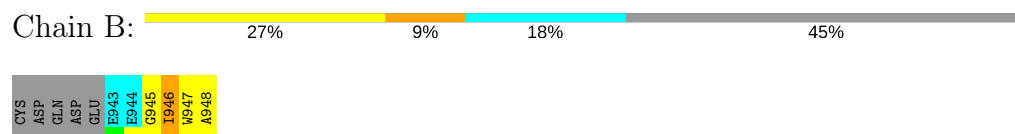


4.2.14 Score per residue for model 14

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

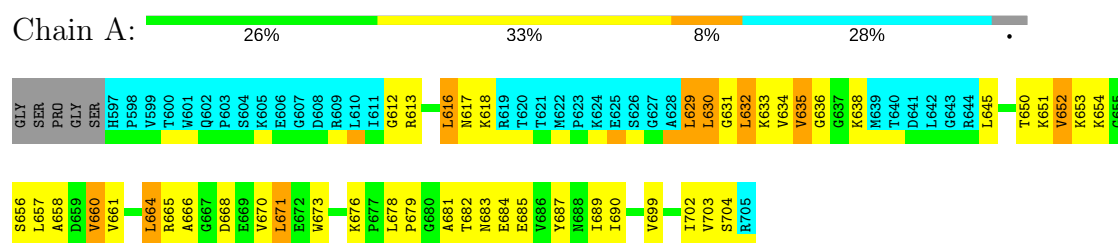


- Molecule 2: ELKS1b

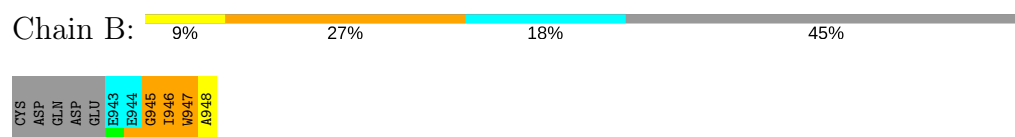


4.2.15 Score per residue for model 15

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

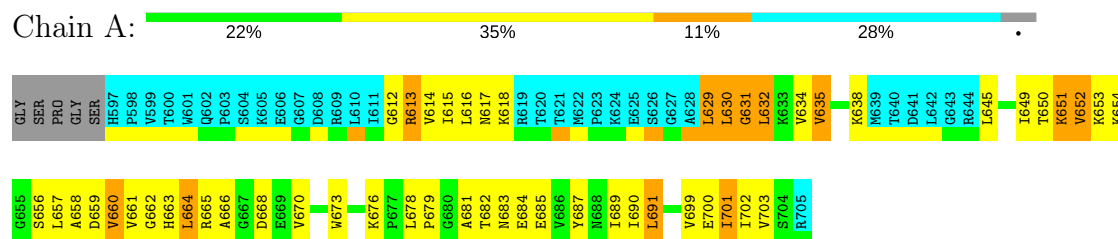


- Molecule 2: ELKS1b

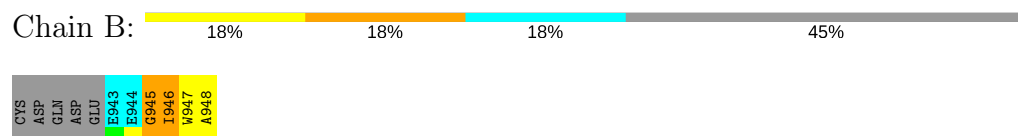


4.2.16 Score per residue for model 16

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

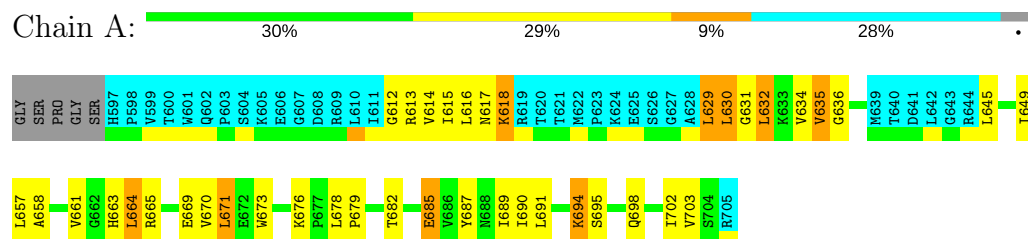


- Molecule 2: ELKS1b

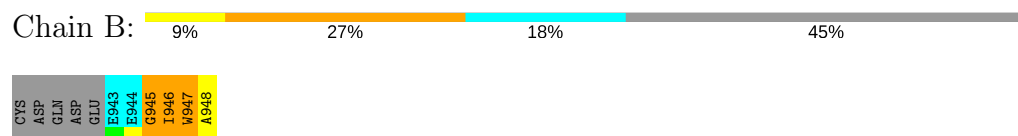


4.2.17 Score per residue for model 17

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

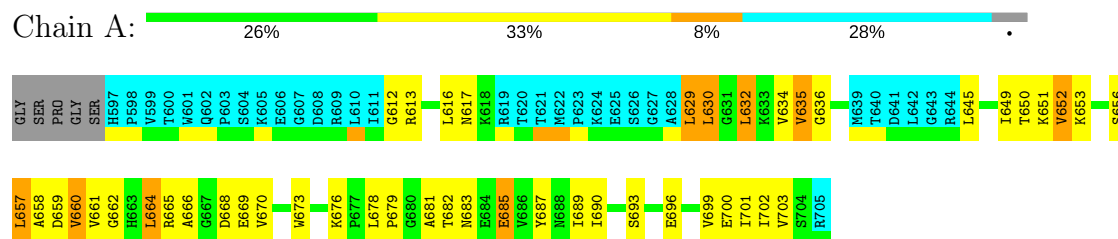


- Molecule 2: ELKS1b

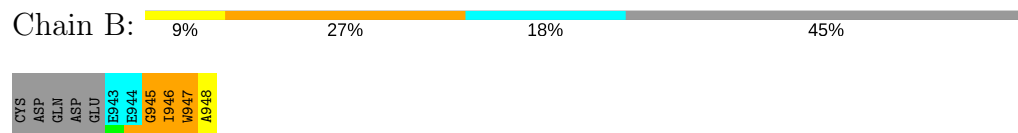


4.2.18 Score per residue for model 18

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

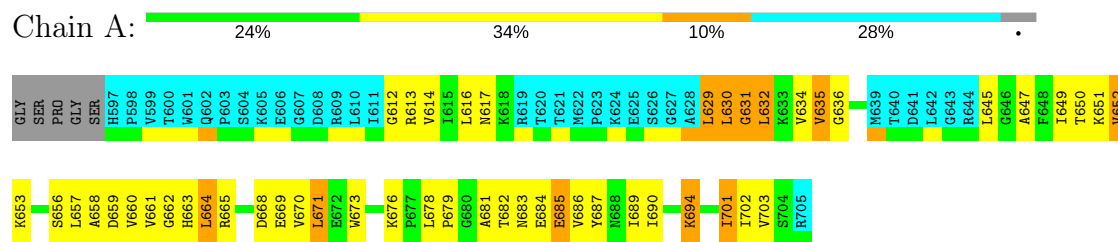


- Molecule 2: ELKS1b

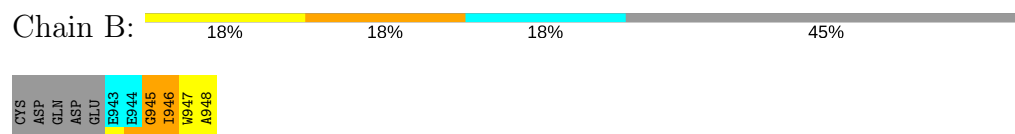


4.2.19 Score per residue for model 19

- Molecule 1: Regulating synaptic membrane exocytosis protein 1

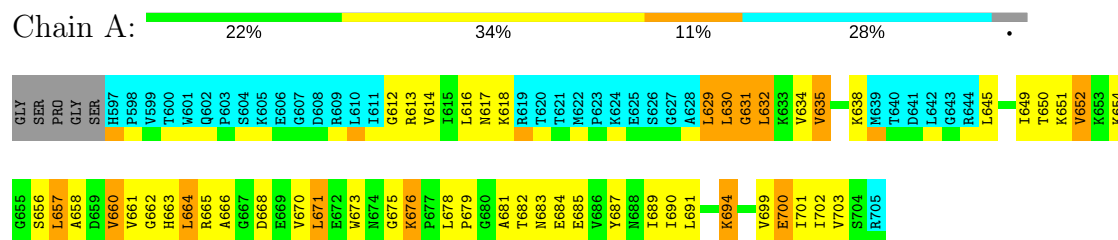


- Molecule 2: ELKS1b

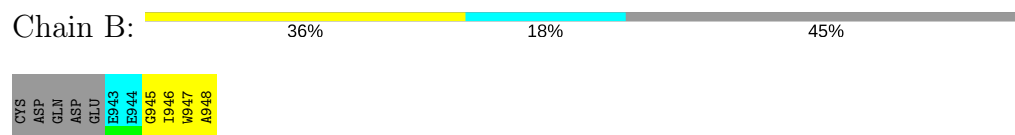


4.2.20 Score per residue for model 20

- Molecule 1: Regulating synaptic membrane exocytosis protein 1



- Molecule 2: ELKS1b



5 Refinement protocol and experimental data overview ⓘ

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

Of the 1000 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	1.1

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	578	619	618	59±5
2	B	32	29	29	10±2
All	All	12200	12960	12940	1183

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 47.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:690:ILE:HD12	2:B:946:ILE:HD12	1.10	1.15	13	9
1:A:690:ILE:HD12	2:B:946:ILE:HG13	0.93	1.41	17	7
1:A:690:ILE:HD13	2:B:946:ILE:HG13	0.91	1.42	19	2
1:A:629:LEU:HD23	2:B:948:ALA:OXT	0.86	1.69	2	7
1:A:616:LEU:HD21	1:A:658:ALA:N	0.85	1.87	12	19
1:A:681:ALA:HB1	1:A:685:GLU:HB3	0.84	1.47	19	19
1:A:616:LEU:HD13	1:A:630:LEU:HD12	0.84	1.47	4	12
1:A:629:LEU:HD23	2:B:948:ALA:O	0.84	1.73	10	12
1:A:632:LEU:HD23	1:A:632:LEU:O	0.83	1.73	17	7
1:A:690:ILE:CD1	2:B:946:ILE:HD12	0.83	2.03	3	7
1:A:681:ALA:HB1	1:A:685:GLU:CB	0.82	2.05	16	17
1:A:656:SER:O	1:A:660:VAL:HG22	0.79	1.78	3	19
1:A:690:ILE:HD12	2:B:946:ILE:CD1	0.78	2.06	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:616:LEU:HD11	1:A:658:ALA:CB	0.78	2.09	12	17
1:A:612:GLY:O	1:A:702:ILE:HG23	0.77	1.79	13	20
1:A:685:GLU:O	1:A:689:ILE:HD12	0.76	1.81	16	18
1:A:671:LEU:HD21	1:A:704:SER:OG	0.75	1.80	5	3
1:A:632:LEU:O	1:A:632:LEU:HD23	0.75	1.79	6	4
1:A:632:LEU:HD12	1:A:658:ALA:CB	0.75	2.11	15	9
1:A:632:LEU:HD22	1:A:632:LEU:O	0.75	1.80	15	5
1:A:632:LEU:HD13	2:B:948:ALA:OXT	0.75	1.80	15	7
1:A:630:LEU:HG	2:B:948:ALA:O	0.75	1.80	6	7
1:A:617:ASN:O	1:A:657:LEU:HD13	0.74	1.82	20	18
1:A:678:LEU:N	1:A:679:PRO:HD2	0.74	1.98	11	20
1:A:657:LEU:O	1:A:661:VAL:HG12	0.74	1.81	19	19
1:A:632:LEU:O	1:A:632:LEU:HD22	0.73	1.83	14	4
1:A:616:LEU:HD13	1:A:630:LEU:HB2	0.72	1.62	2	8
1:A:673:TRP:HB2	1:A:678:LEU:HD11	0.72	1.60	11	16
1:A:614:VAL:HG13	1:A:662:GLY:HA2	0.70	1.63	12	12
1:A:616:LEU:HD11	1:A:658:ALA:HA	0.70	1.64	15	14
1:A:629:LEU:N	1:A:629:LEU:HD22	0.69	2.03	11	12
1:A:645:LEU:HD13	1:A:682:THR:HA	0.69	1.63	19	20
1:A:686:VAL:HA	1:A:689:ILE:HD13	0.68	1.65	10	3
1:A:635:VAL:HG23	2:B:945:GLY:N	0.68	2.04	4	1
1:A:664:LEU:HD13	1:A:664:LEU:N	0.68	2.03	10	11
1:A:615:ILE:HD12	1:A:700:GLU:HG3	0.68	1.66	16	1
2:B:945:GLY:C	2:B:946:ILE:HD13	0.67	2.10	1	6
1:A:681:ALA:HB1	1:A:685:GLU:HB2	0.67	1.66	16	6
1:A:664:LEU:N	1:A:664:LEU:HD13	0.67	2.05	2	9
1:A:616:LEU:HD13	1:A:630:LEU:CD1	0.66	2.21	13	8
1:A:616:LEU:HD21	1:A:658:ALA:CA	0.66	2.21	19	18
1:A:676:LYS:HD3	1:A:689:ILE:HG12	0.66	1.68	9	2
1:A:682:THR:HG23	1:A:684:GLU:HG3	0.66	1.67	14	1
1:A:682:THR:HG23	1:A:684:GLU:HG2	0.65	1.69	11	8
1:A:632:LEU:HD22	1:A:632:LEU:C	0.65	2.11	16	6
1:A:687:TYR:O	1:A:691:LEU:HD22	0.65	1.91	2	8
1:A:632:LEU:C	1:A:632:LEU:HD22	0.65	2.11	12	3
1:A:618:LYS:HG2	1:A:630:LEU:HD22	0.64	1.70	3	2
1:A:616:LEU:HD11	1:A:658:ALA:HB2	0.64	1.69	14	14
1:A:618:LYS:HG2	1:A:630:LEU:HD23	0.63	1.69	13	2
1:A:630:LEU:O	1:A:657:LEU:HD12	0.63	1.94	7	4
1:A:670:VAL:O	1:A:678:LEU:HD12	0.63	1.94	10	8
1:A:632:LEU:HD12	1:A:658:ALA:HB2	0.62	1.70	15	7
1:A:670:VAL:HG22	1:A:703:VAL:CG1	0.62	2.24	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:632:LEU:CD2	1:A:634:VAL:HG23	0.62	2.24	2	9
1:A:629:LEU:N	1:A:629:LEU:HD13	0.62	2.10	13	3
1:A:630:LEU:HG	2:B:948:ALA:OXT	0.61	1.94	16	12
1:A:616:LEU:CD1	1:A:630:LEU:HD12	0.61	2.25	4	4
1:A:618:LYS:NZ	1:A:699:VAL:HG21	0.61	2.10	16	1
1:A:629:LEU:HD22	1:A:629:LEU:N	0.61	2.10	19	7
1:A:616:LEU:HD21	1:A:658:ALA:HA	0.60	1.72	9	16
1:A:629:LEU:HD13	1:A:629:LEU:N	0.60	2.11	15	4
1:A:690:ILE:HD13	2:B:946:ILE:CG1	0.60	2.26	10	1
1:A:630:LEU:HD23	1:A:630:LEU:N	0.60	2.11	18	5
1:A:678:LEU:N	1:A:679:PRO:CD	0.60	2.64	17	20
1:A:634:VAL:HG21	1:A:673:TRP:HZ3	0.59	1.57	9	20
1:A:630:LEU:HG	2:B:948:ALA:C	0.59	2.17	5	11
1:A:632:LEU:O	2:B:948:ALA:C	0.58	2.41	20	20
1:A:615:ILE:HD12	1:A:615:ILE:N	0.58	2.14	5	1
1:A:618:LYS:HZ3	1:A:699:VAL:HG21	0.58	1.58	16	1
1:A:629:LEU:HB2	2:B:948:ALA:O	0.58	1.99	13	2
1:A:682:THR:HG23	1:A:684:GLU:CG	0.57	2.29	13	5
1:A:632:LEU:HD13	2:B:948:ALA:O	0.57	1.98	2	2
1:A:634:VAL:CG1	1:A:647:ALA:HB1	0.57	2.30	12	9
1:A:630:LEU:N	1:A:630:LEU:HD23	0.57	2.14	3	3
1:A:629:LEU:HD22	1:A:629:LEU:H	0.56	1.61	13	5
1:A:687:TYR:CD1	2:B:946:ILE:CD1	0.55	2.89	1	11
1:A:632:LEU:O	2:B:948:ALA:HB3	0.55	2.01	17	6
1:A:632:LEU:HD12	1:A:649:ILE:CD1	0.55	2.32	18	7
1:A:616:LEU:HD22	1:A:630:LEU:HB2	0.55	1.78	15	2
1:A:631:GLY:HA3	1:A:658:ALA:HB3	0.55	1.79	19	3
1:A:629:LEU:H	1:A:629:LEU:HD22	0.55	1.62	2	7
1:A:613:ARG:HA	1:A:702:ILE:HD12	0.54	1.78	13	20
1:A:649:ILE:HD12	1:A:668:ASP:HB2	0.54	1.79	16	10
1:A:632:LEU:HD23	2:B:948:ALA:OXT	0.54	2.02	7	3
1:A:682:THR:HG22	1:A:685:GLU:OE2	0.54	2.02	11	2
1:A:616:LEU:HD11	1:A:658:ALA:CA	0.54	2.33	5	18
1:A:693:SER:OG	1:A:699:VAL:HG22	0.54	2.03	3	2
1:A:652:VAL:HG21	1:A:665:ARG:HA	0.54	1.80	1	20
1:A:645:LEU:HD13	1:A:682:THR:CA	0.53	2.33	14	4
1:A:615:ILE:HG21	1:A:698:GLN:NE2	0.53	2.19	6	1
1:A:634:VAL:CG1	1:A:635:VAL:N	0.53	2.72	4	20
1:A:671:LEU:HD13	1:A:671:LEU:N	0.53	2.19	2	1
1:A:638:LYS:HG3	1:A:638:LYS:O	0.53	2.03	16	1
1:A:651:LYS:HA	1:A:666:ALA:HB2	0.53	1.81	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:616:LEU:HD13	1:A:630:LEU:HD13	0.53	1.81	13	1
1:A:632:LEU:HD12	1:A:658:ALA:HB1	0.52	1.81	12	7
1:A:632:LEU:HD12	1:A:649:ILE:HD13	0.52	1.80	11	6
1:A:631:GLY:O	1:A:658:ALA:HB3	0.52	2.04	5	3
1:A:673:TRP:CE2	1:A:690:ILE:HG13	0.52	2.40	19	2
1:A:634:VAL:HG21	1:A:673:TRP:CZ3	0.52	2.39	4	11
1:A:632:LEU:HD23	1:A:632:LEU:C	0.52	2.25	8	7
1:A:673:TRP:CZ2	1:A:690:ILE:HD13	0.52	2.39	1	11
1:A:632:LEU:O	2:B:948:ALA:OXT	0.51	2.28	7	13
1:A:616:LEU:HB3	1:A:630:LEU:HD13	0.51	1.82	15	1
1:A:669:GLU:OE1	1:A:671:LEU:HD11	0.51	2.05	3	1
1:A:616:LEU:HD12	1:A:701:ILE:HD11	0.51	1.82	3	7
1:A:673:TRP:HB3	1:A:689:ILE:HG21	0.51	1.80	10	2
1:A:635:VAL:O	1:A:647:ALA:HA	0.51	2.06	10	8
1:A:686:VAL:HG12	2:B:946:ILE:HD11	0.51	1.82	13	3
1:A:629:LEU:HD23	2:B:947:TRP:CE3	0.51	2.41	15	1
1:A:682:THR:HG22	1:A:685:GLU:OE1	0.50	2.07	14	2
1:A:629:LEU:C	1:A:630:LEU:HD23	0.50	2.26	1	4
1:A:687:TYR:CE1	2:B:946:ILE:CD1	0.50	2.95	19	4
1:A:673:TRP:CE2	1:A:690:ILE:HD13	0.49	2.42	11	2
1:A:629:LEU:CD2	2:B:947:TRP:CE3	0.49	2.96	15	1
1:A:687:TYR:CE1	2:B:946:ILE:HD13	0.49	2.42	15	7
1:A:616:LEU:CD1	1:A:658:ALA:HB2	0.49	2.38	1	8
1:A:617:ASN:O	1:A:657:LEU:HD22	0.49	2.08	13	1
1:A:671:LEU:N	1:A:671:LEU:HD13	0.49	2.23	5	2
1:A:632:LEU:C	1:A:632:LEU:CD2	0.48	2.81	16	5
1:A:686:VAL:HG12	1:A:690:ILE:HD12	0.48	1.84	10	1
1:A:673:TRP:CD1	1:A:689:ILE:HG22	0.48	2.44	10	1
1:A:682:THR:OG1	1:A:683:ASN:N	0.48	2.47	16	18
1:A:671:LEU:HD22	1:A:671:LEU:H	0.48	1.68	2	7
1:A:670:VAL:HG22	1:A:703:VAL:HG13	0.47	1.86	19	16
1:A:629:LEU:HB2	2:B:948:ALA:C	0.47	2.30	18	1
1:A:671:LEU:HD21	1:A:704:SER:HB2	0.47	1.85	2	1
1:A:629:LEU:N	1:A:629:LEU:CD2	0.47	2.75	11	4
1:A:669:GLU:CD	1:A:671:LEU:HD11	0.47	2.29	17	2
1:A:686:VAL:HG12	1:A:690:ILE:CD1	0.47	2.40	10	1
1:A:632:LEU:CD2	1:A:632:LEU:C	0.47	2.82	9	4
1:A:631:GLY:C	1:A:658:ALA:HB3	0.46	2.30	3	7
1:A:673:TRP:CE2	1:A:690:ILE:CG1	0.46	2.98	19	1
1:A:664:LEU:N	1:A:664:LEU:CD1	0.46	2.77	2	7
1:A:632:LEU:C	1:A:632:LEU:HD23	0.46	2.31	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:664:LEU:CD1	1:A:664:LEU:N	0.46	2.77	15	2
1:A:629:LEU:HG	2:B:947:TRP:C	0.46	2.31	15	6
1:A:635:VAL:CG2	2:B:945:GLY:N	0.46	2.79	5	2
1:A:671:LEU:HD21	1:A:704:SER:HB3	0.46	1.87	15	1
1:A:657:LEU:C	1:A:661:VAL:HG12	0.46	2.30	13	3
1:A:616:LEU:CD2	1:A:657:LEU:HB2	0.46	2.41	13	1
1:A:614:VAL:HG13	1:A:662:GLY:CA	0.46	2.39	12	1
1:A:616:LEU:HD21	1:A:657:LEU:C	0.45	2.31	14	14
1:A:690:ILE:CD1	2:B:946:ILE:HG13	0.45	2.41	11	2
1:A:675:GLY:N	1:A:700:GLU:CG	0.45	2.79	20	2
1:A:632:LEU:HD13	1:A:632:LEU:N	0.45	2.27	1	2
1:A:616:LEU:O	1:A:699:VAL:N	0.45	2.49	7	7
1:A:690:ILE:HD12	2:B:946:ILE:CG1	0.45	2.41	8	2
1:A:662:GLY:C	1:A:664:LEU:HD13	0.45	2.32	18	5
1:A:671:LEU:H	1:A:671:LEU:HD22	0.45	1.72	20	9
1:A:615:ILE:HD12	1:A:700:GLU:CG	0.45	2.39	16	1
1:A:687:TYR:CD1	2:B:946:ILE:HD12	0.45	2.47	1	1
1:A:615:ILE:N	1:A:615:ILE:HD12	0.44	2.26	6	1
1:A:673:TRP:CZ2	1:A:690:ILE:HG23	0.44	2.47	1	1
1:A:632:LEU:HD23	1:A:634:VAL:HG23	0.44	1.89	19	2
1:A:673:TRP:CB	1:A:678:LEU:HD11	0.44	2.40	9	1
1:A:614:VAL:C	1:A:615:ILE:HD13	0.44	2.33	16	1
1:A:638:LYS:N	1:A:645:LEU:HD22	0.43	2.28	15	1
1:A:618:LYS:NZ	1:A:630:LEU:HD21	0.43	2.28	3	2
1:A:683:ASN:O	1:A:687:TYR:CD1	0.43	2.71	16	7
1:A:645:LEU:CD1	1:A:682:THR:HB	0.43	2.44	15	1
1:A:633:LYS:CG	2:B:947:TRP:CE3	0.43	3.01	8	1
1:A:616:LEU:HD22	1:A:657:LEU:HB2	0.43	1.90	7	1
1:A:618:LYS:HB3	1:A:630:LEU:HD23	0.43	1.89	8	1
1:A:686:VAL:HG12	1:A:690:ILE:CG1	0.43	2.44	11	1
1:A:635:VAL:CG1	1:A:636:GLY:N	0.42	2.82	18	7
1:A:618:LYS:CB	1:A:629:LEU:O	0.42	2.67	14	2
1:A:618:LYS:CD	1:A:694:LYS:O	0.42	2.68	17	1
1:A:663:HIS:C	1:A:664:LEU:HD13	0.42	2.34	6	3
1:A:701:ILE:C	1:A:702:ILE:HD13	0.42	2.35	6	2
1:A:678:LEU:HD21	1:A:689:ILE:HG21	0.42	1.90	3	1
1:A:635:VAL:N	1:A:648:PHE:O	0.42	2.52	11	6
1:A:633:LYS:HG2	2:B:947:TRP:CE3	0.42	2.50	8	2
1:A:683:ASN:O	1:A:687:TYR:CG	0.42	2.73	13	7
1:A:690:ILE:O	1:A:694:LYS:N	0.42	2.53	10	4
1:A:633:LYS:O	1:A:650:THR:N	0.42	2.53	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:634:VAL:HG13	1:A:647:ALA:HB1	0.42	1.91	9	1
1:A:691:LEU:O	1:A:694:LYS:CG	0.42	2.68	17	2
1:A:629:LEU:HG	2:B:947:TRP:O	0.42	2.15	16	1
1:A:631:GLY:CA	1:A:658:ALA:HB3	0.42	2.45	3	1
1:A:617:ASN:O	1:A:657:LEU:CD2	0.41	2.67	13	1
1:A:686:VAL:HG12	2:B:946:ILE:CD1	0.41	2.45	13	1
1:A:632:LEU:N	1:A:632:LEU:HD13	0.41	2.30	10	2
1:A:632:LEU:N	1:A:632:LEU:CD1	0.41	2.83	1	1
1:A:691:LEU:CD1	2:B:946:ILE:CG2	0.41	2.98	1	1
1:A:685:GLU:O	1:A:689:ILE:CD1	0.41	2.68	12	5
1:A:618:LYS:NZ	1:A:630:LEU:CD2	0.41	2.83	8	1
1:A:634:VAL:HG11	1:A:647:ALA:HB1	0.41	1.91	12	1
1:A:658:ALA:O	1:A:663:HIS:N	0.41	2.53	10	1
1:A:631:GLY:CA	1:A:656:SER:OG	0.41	2.69	11	1
1:A:661:VAL:CG1	1:A:662:GLY:N	0.41	2.83	12	1
1:A:632:LEU:HB2	1:A:652:VAL:HG13	0.41	1.92	18	2
1:A:629:LEU:CD2	1:A:629:LEU:N	0.41	2.77	3	3
1:A:615:ILE:N	1:A:615:ILE:CD1	0.41	2.83	5	1
1:A:676:LYS:CD	1:A:689:ILE:CG1	0.41	2.99	10	1
1:A:690:ILE:HG21	2:B:946:ILE:CG2	0.41	2.46	4	1
1:A:687:TYR:CZ	2:B:945:GLY:O	0.41	2.73	19	1
1:A:615:ILE:HG21	1:A:698:GLN:HE21	0.41	1.76	17	1
1:A:699:VAL:CG1	1:A:700:GLU:N	0.41	2.84	18	1
1:A:630:LEU:CD2	1:A:630:LEU:N	0.41	2.83	2	1
1:A:683:ASN:OD1	1:A:687:TYR:CE1	0.41	2.74	7	1
1:A:673:TRP:CE3	1:A:701:ILE:HG21	0.41	2.51	8	1
1:A:618:LYS:CE	1:A:630:LEU:CD2	0.40	2.99	1	1
1:A:671:LEU:HD22	1:A:671:LEU:N	0.40	2.32	3	1
1:A:632:LEU:HB2	1:A:652:VAL:CG1	0.40	2.46	20	1
1:A:630:LEU:N	1:A:630:LEU:CD2	0.40	2.83	15	1
1:A:616:LEU:CD2	1:A:657:LEU:CB	0.40	3.00	18	1
1:A:616:LEU:CD2	1:A:658:ALA:N	0.40	2.79	19	1
1:A:687:TYR:CE1	2:B:945:GLY:O	0.40	2.75	1	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	77/114 (68%)	69±1 (89±2%)	7±1 (10±1%)	1±0 (1±1%)	18	63
2	B	3/11 (27%)	2±0 (67±0%)	0±0 (12±16%)	1±0 (22±16%)	0	2
All	All	1600/2500 (64%)	1410 (88%)	155 (10%)	35 (2%)	12	51

All 4 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	631	GLY	19
2	B	945	GLY	13
1	A	654	LYS	2
1	A	679	PRO	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	63/94 (67%)	46±2 (73±3%)	17±2 (27±3%)	2	22
2	B	2/9 (22%)	0±0 (12±22%)	2±0 (88±22%)	0	0
All	All	1300/2060 (63%)	925 (71%)	375 (29%)	2	19

All 38 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	652	VAL	20
1	A	632	LEU	20
1	A	630	LEU	20
1	A	664	LEU	20
1	A	635	VAL	20
1	A	629	LEU	20
2	B	947	TRP	19
1	A	676	LYS	19
1	A	671	LEU	16
2	B	946	ILE	16

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Mol	Chain	Res	Type	Models (Total)
1	A	653	LYS	15
1	A	660	VAL	15
1	A	668	ASP	13
1	A	685	GLU	12
1	A	663	HIS	11
1	A	633	LYS	10
1	A	694	LYS	10
1	A	618	LYS	9
1	A	691	LEU	9
1	A	695	SER	8
1	A	654	LYS	8
1	A	657	LEU	8
1	A	701	ILE	8
1	A	684	GLU	7
1	A	651	LYS	6
1	A	650	THR	6
1	A	659	ASP	6
1	A	700	GLU	5
1	A	696	GLU	4
1	A	613	ARG	3
1	A	665	ARG	3
1	A	615	ILE	2
1	A	698	GLN	2
1	A	704	SER	1
1	A	693	SER	1
1	A	616	LEU	1
1	A	656	SER	1
1	A	638	LYS	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