



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 05:48 AM UTC

PDB ID : 2N64 / pdb_00002n64
BMRB ID : 25750
Title : NMR Structure of the C-terminal Coiled-Coil Domain of CIN85
Authors : Habeck, M.; Becker, S.; Griesinger, C.; Wong, L.E.
Deposited on : 2015-08-11

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

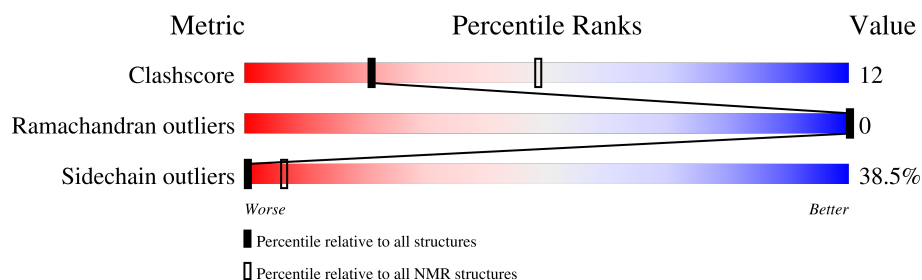
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 20%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	75	
1	B	75	
1	C	75	

2 Ensemble composition and analysis

This entry contains 30 models. Model 20 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:605-A:664, B:605-B:664, C:605-C:665 (181)	0.73	20

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 6 clusters and 1 single-model cluster was found.

Cluster number	Models
1	2, 4, 5, 6, 8, 9, 10, 11, 13, 15, 18, 19, 20, 21, 24
2	22, 27, 28, 30
3	12, 14, 16
4	7, 23, 25
5	1, 3
6	26, 29
Single-model clusters	17

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3771 atoms, of which 1944 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SH3 domain-containing kinase-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	75	Total	C	H	N	O	S	0
			1257	373	648	113	119	4	
1	B	75	Total	C	H	N	O	S	0
			1257	373	648	113	119	4	
1	C	75	Total	C	H	N	O	S	0
			1257	373	648	113	119	4	

There are 9 discrepancies between the modelled and reference sequences:

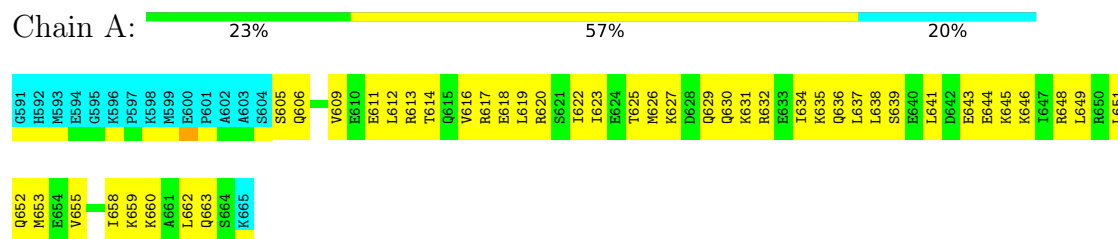
Chain	Residue	Modelled	Actual	Comment	Reference
A	591	GLY	-	expression tag	UNP Q96B97
A	592	HIS	-	expression tag	UNP Q96B97
A	593	MET	-	expression tag	UNP Q96B97
B	591	GLY	-	expression tag	UNP Q96B97
B	592	HIS	-	expression tag	UNP Q96B97
B	593	MET	-	expression tag	UNP Q96B97
C	591	GLY	-	expression tag	UNP Q96B97
C	592	HIS	-	expression tag	UNP Q96B97
C	593	MET	-	expression tag	UNP Q96B97

4 Residue-property plots [i](#)

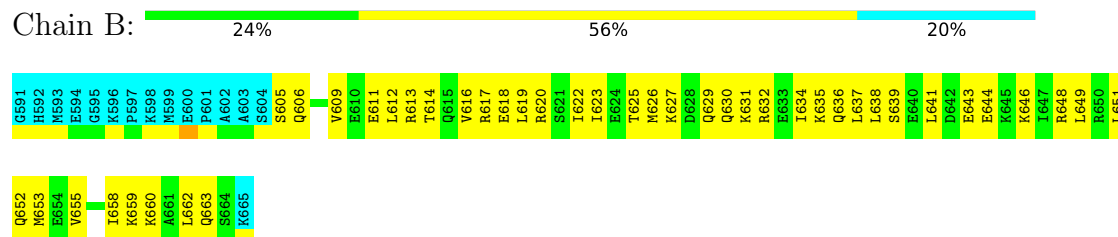
4.1 Average score per residue in the NMR ensemble

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.

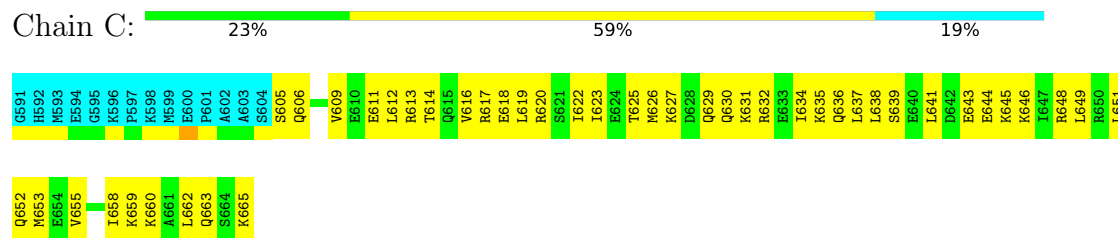
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1



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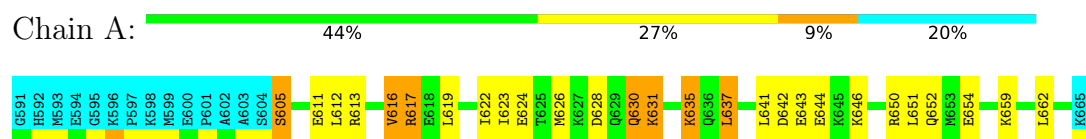


4.2 Scores per residue for each member of the ensemble

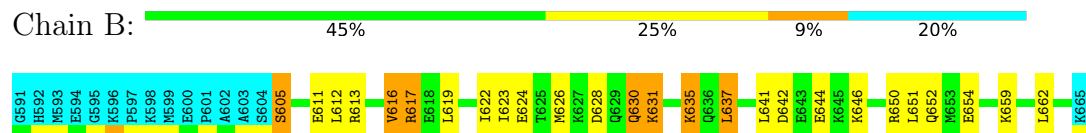
Colouring as in section [4.1](#) above.

4.2.1 Score per residue for model 1

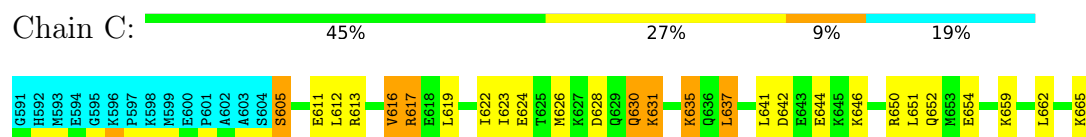
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

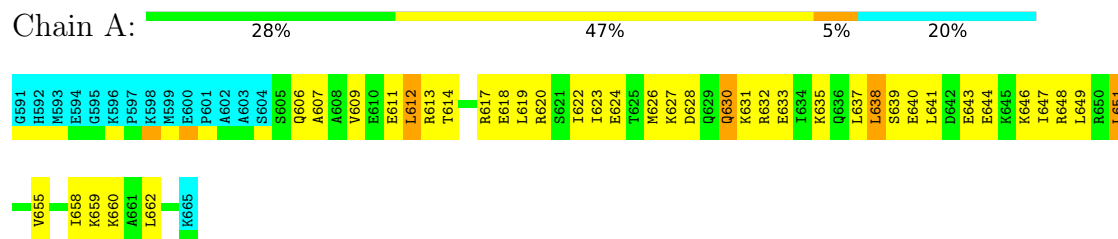


- Molecule 1: SH3 domain-containing kinase-binding protein 1

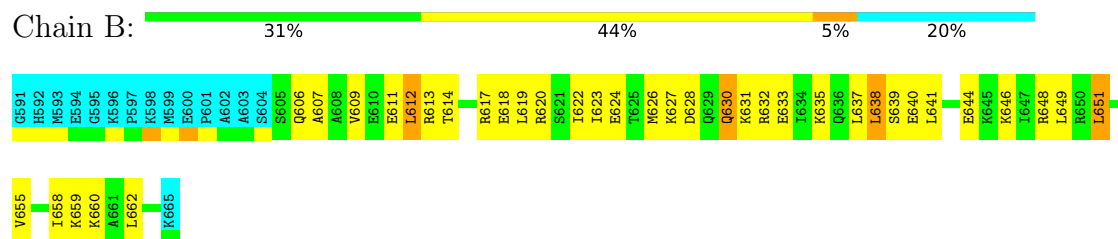


4.2.2 Score per residue for model 2

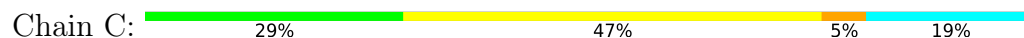
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

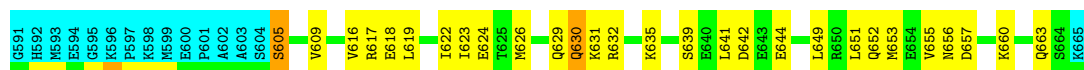




4.2.3 Score per residue for model 3

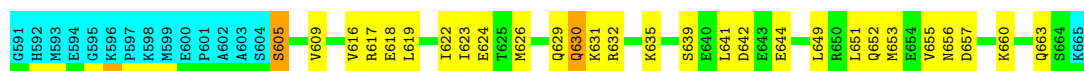
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 43% 35% 20%



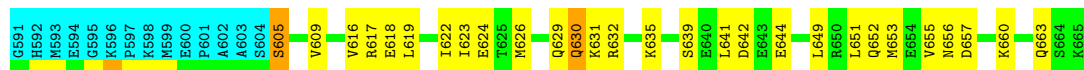
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 43% 35% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

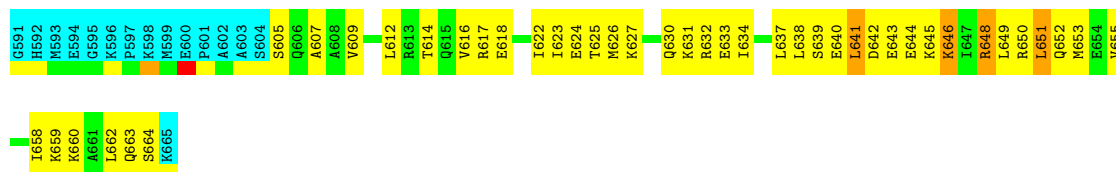
Chain C: 44% 35% 19%



4.2.4 Score per residue for model 4

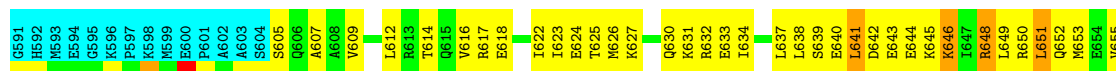
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 24% 51% 5% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

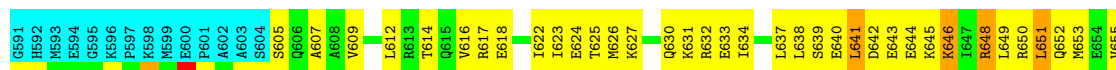
Chain B: 24% 51% 5% 20%





- Molecule 1: SH3 domain-containing kinase-binding protein 1

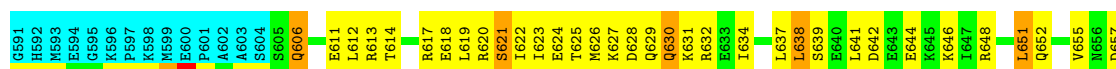
Chain C: 24% 52% 5% 19%



4.2.5 Score per residue for model 5

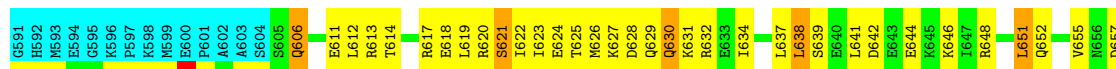
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 31% 43% 7% 20%



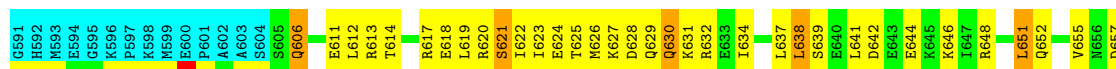
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 31% 43% 7% 20%



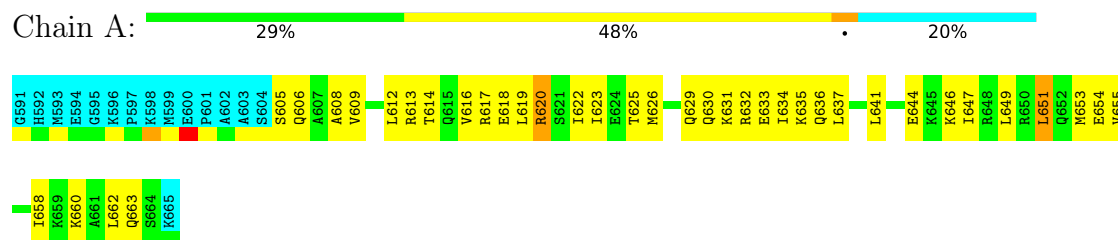
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 31% 44% 7% 19%

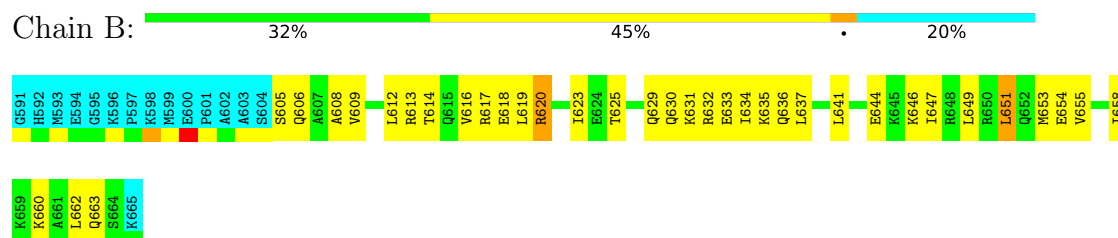


4.2.6 Score per residue for model 6

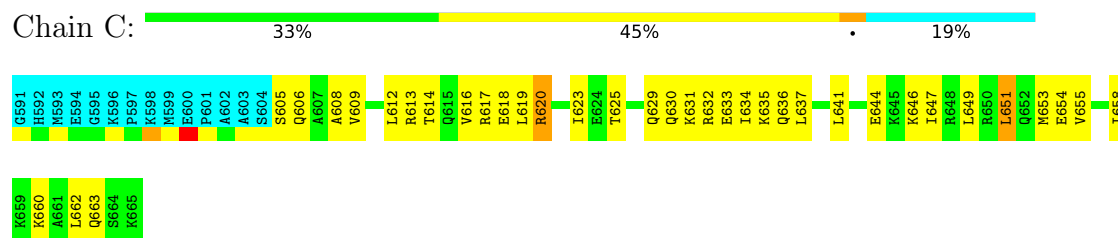
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

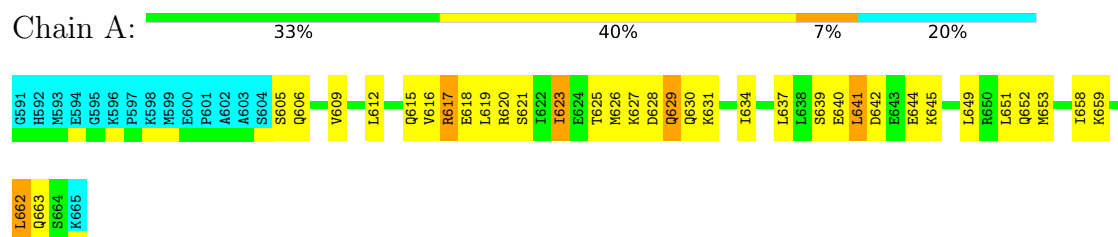


- Molecule 1: SH3 domain-containing kinase-binding protein 1

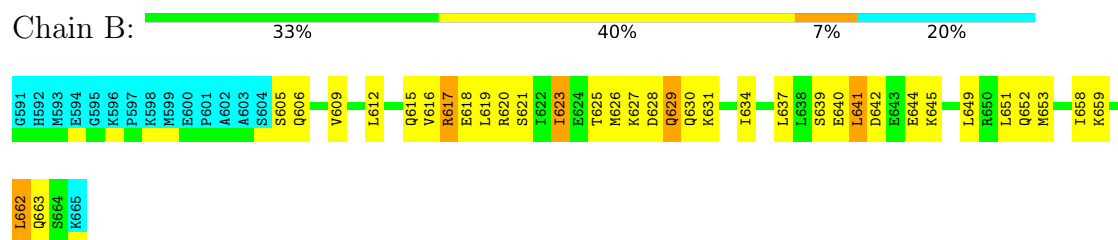


4.2.7 Score per residue for model 7

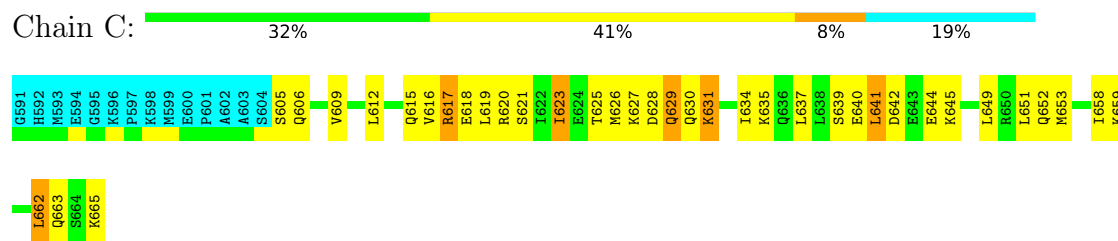
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

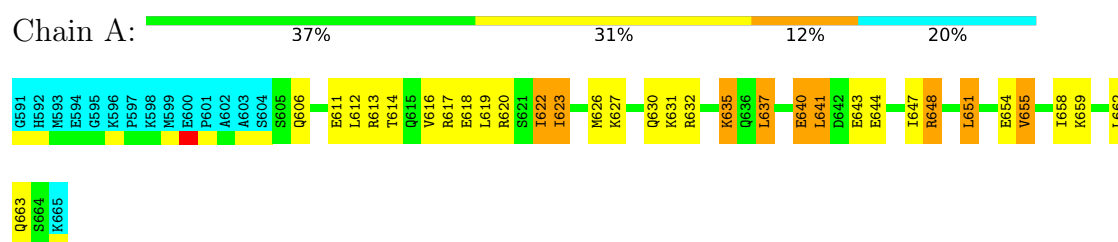


- Molecule 1: SH3 domain-containing kinase-binding protein 1

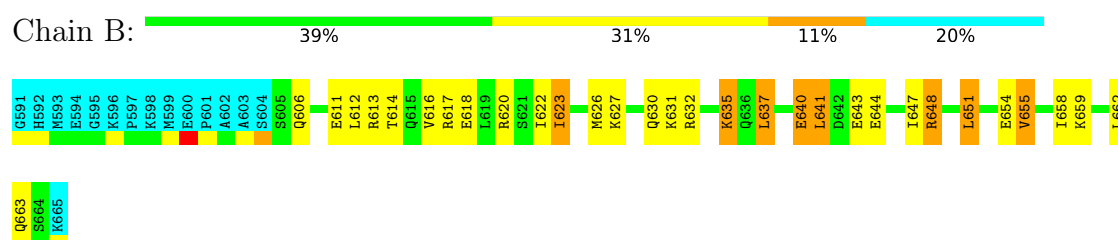


4.2.8 Score per residue for model 8

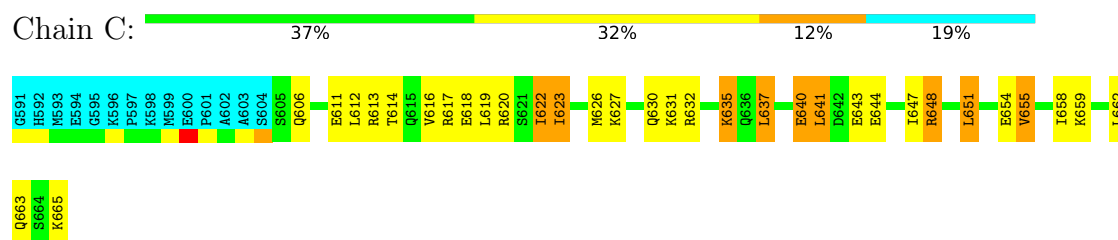
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1



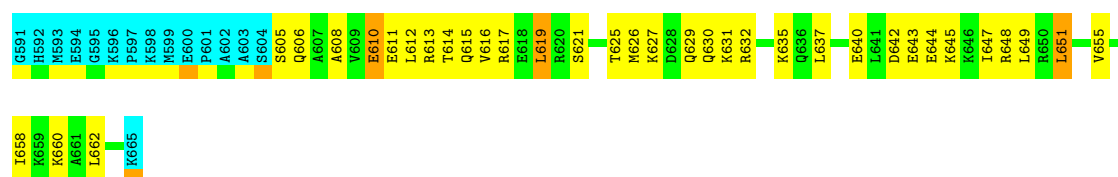
- Molecule 1: SH3 domain-containing kinase-binding protein 1



4.2.9 Score per residue for model 9

- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 33% 43% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 33% 43% 5% 19%



4.2.10 Score per residue for model 10

- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 40% 35% 5% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 40% 35% 5% 20%



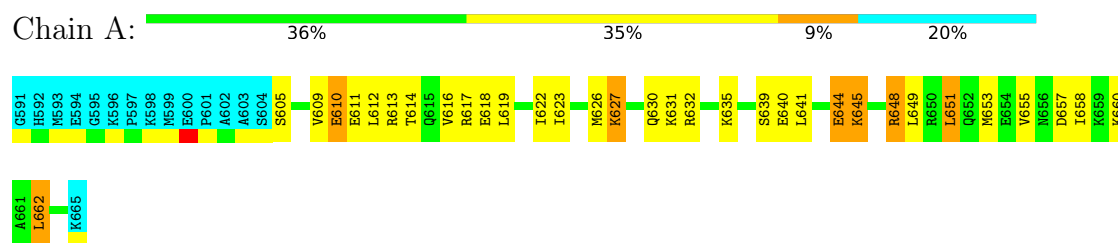
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 40% 36% 5% 19%

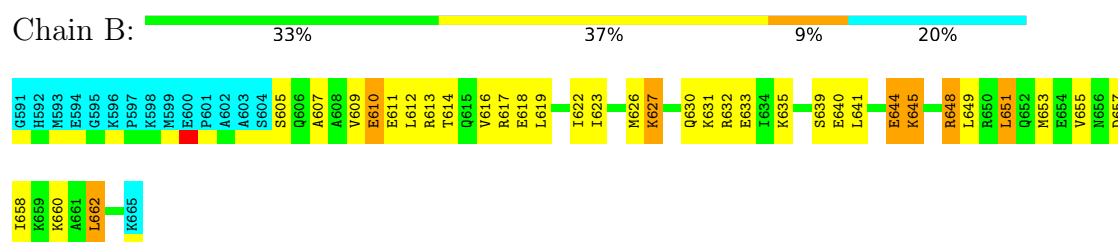


4.2.11 Score per residue for model 11

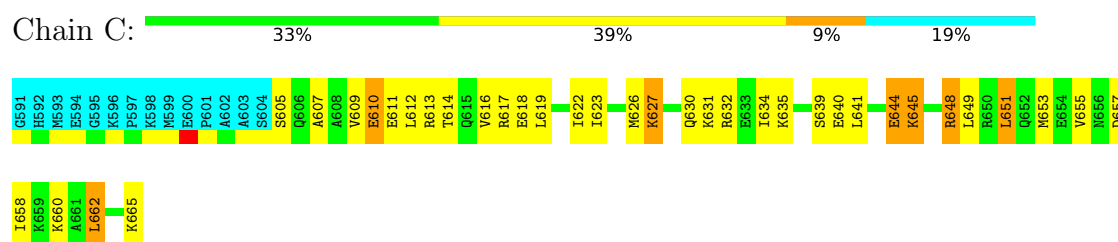
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

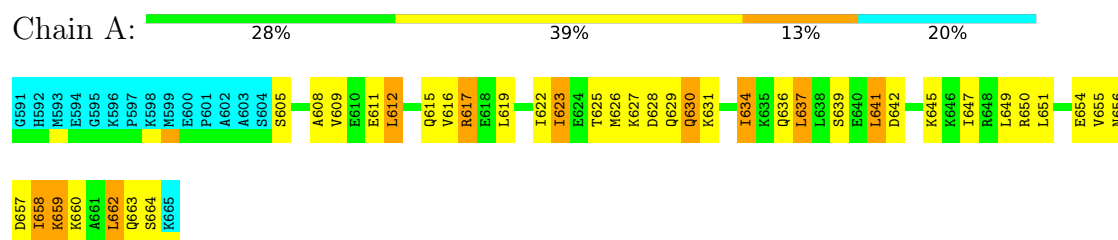


- Molecule 1: SH3 domain-containing kinase-binding protein 1



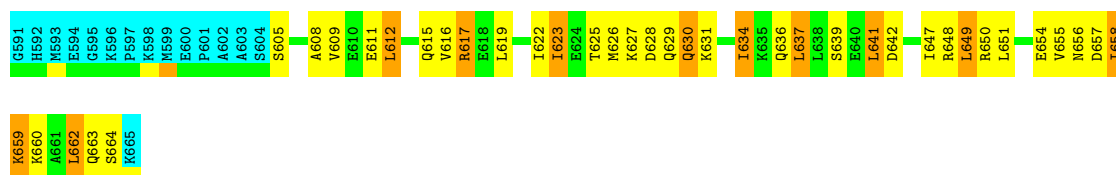
4.2.12 Score per residue for model 12

- Molecule 1: SH3 domain-containing kinase-binding protein 1



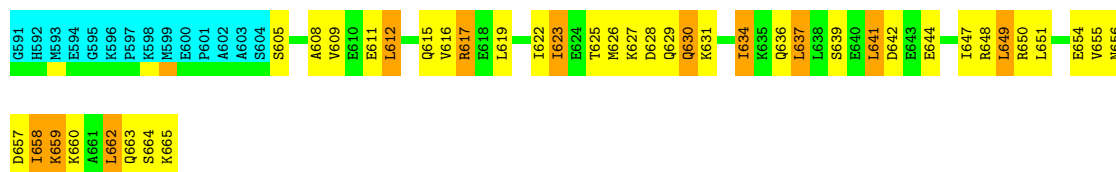
- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

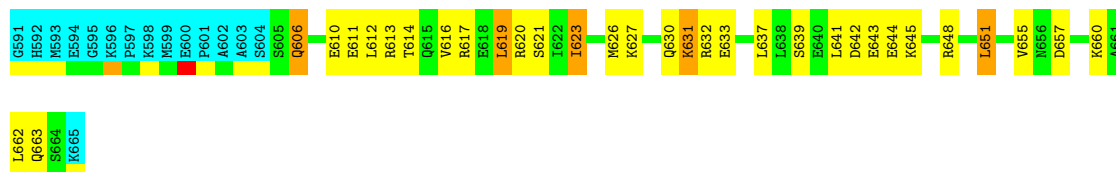
Chain C: 27% 40% 15% 19%



4.2.13 Score per residue for model 13

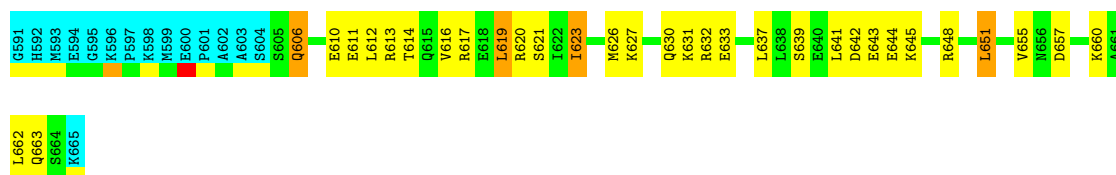
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 37% 36% 7% 20%



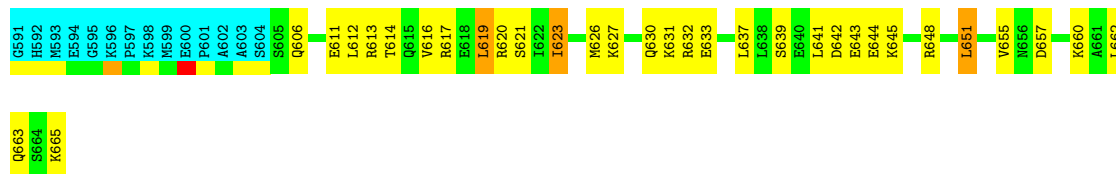
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 37% 37% 5% 20%



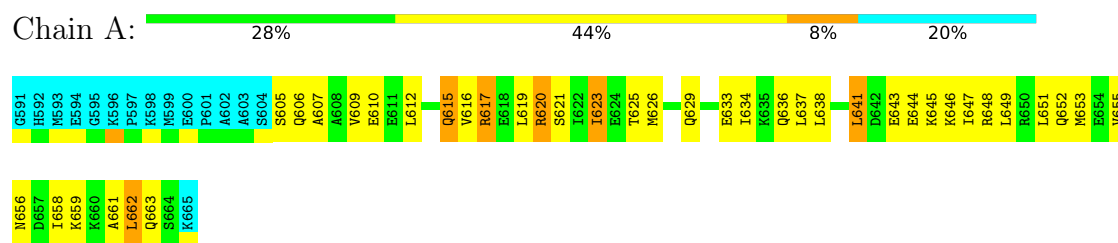
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 39% 39% 19%

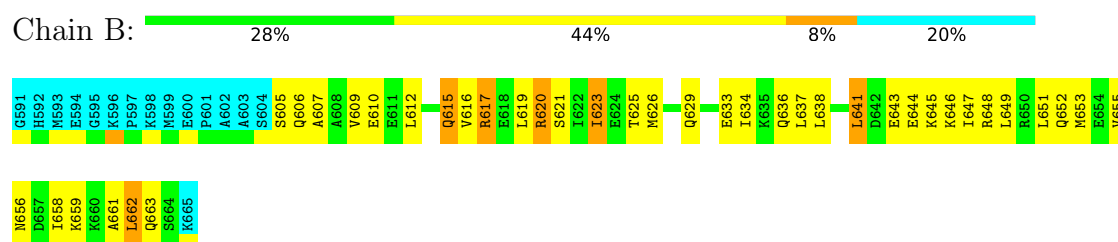


4.2.14 Score per residue for model 14

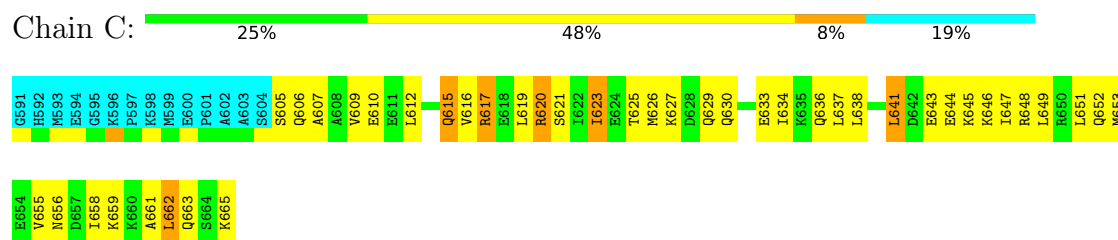
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

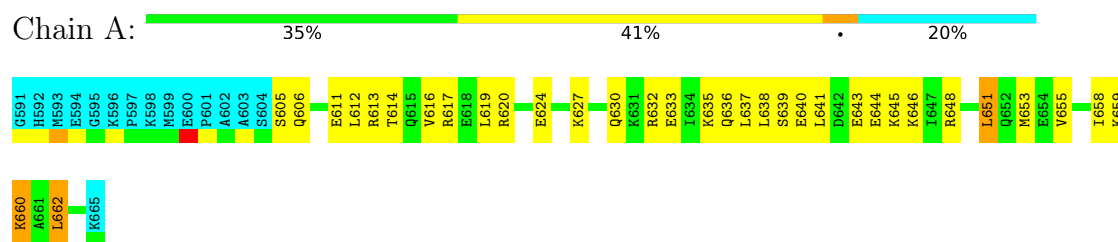


- Molecule 1: SH3 domain-containing kinase-binding protein 1



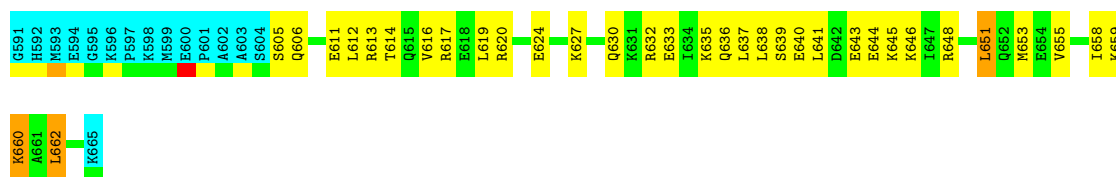
4.2.15 Score per residue for model 15

- Molecule 1: SH3 domain-containing kinase-binding protein 1

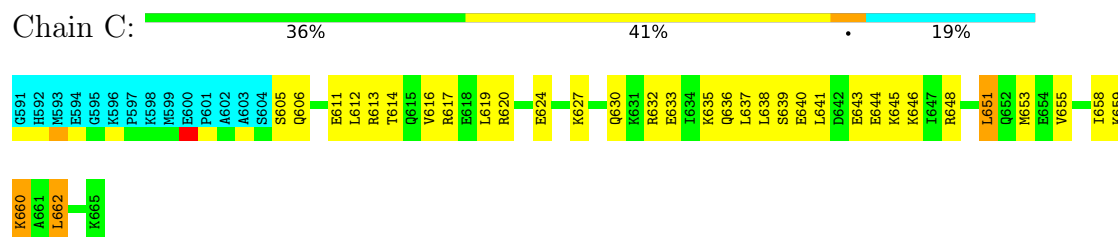


- Molecule 1: SH3 domain-containing kinase-binding protein 1



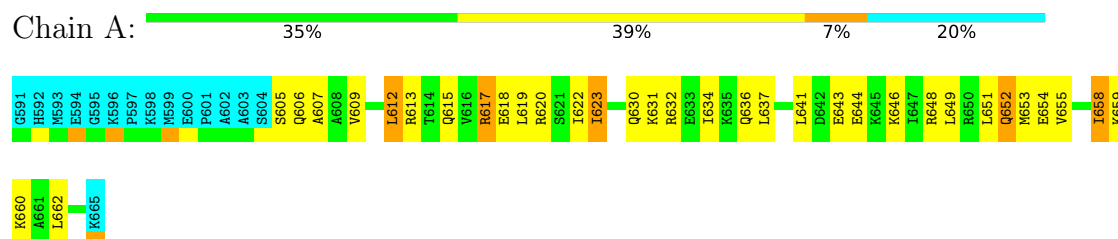


- Molecule 1: SH3 domain-containing kinase-binding protein 1

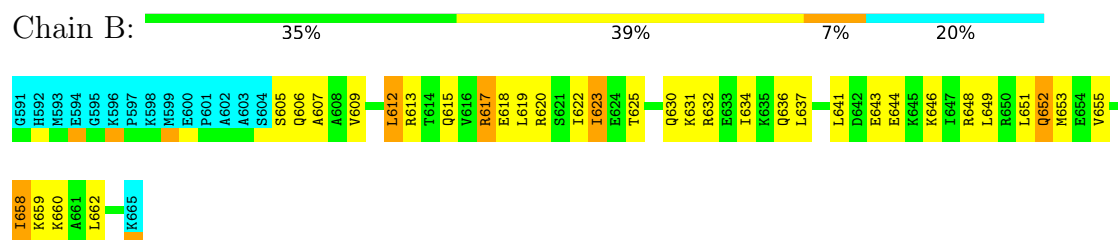


4.2.16 Score per residue for model 16

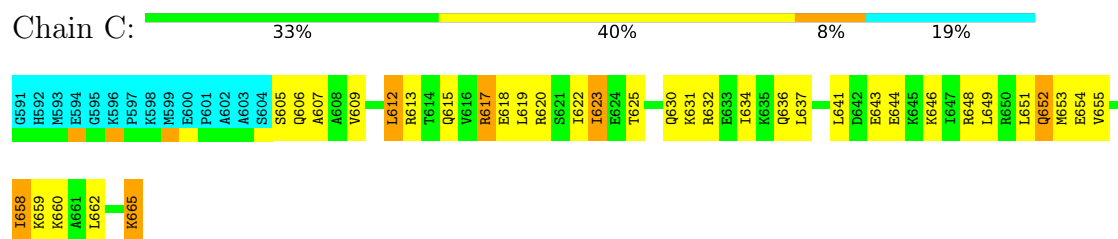
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

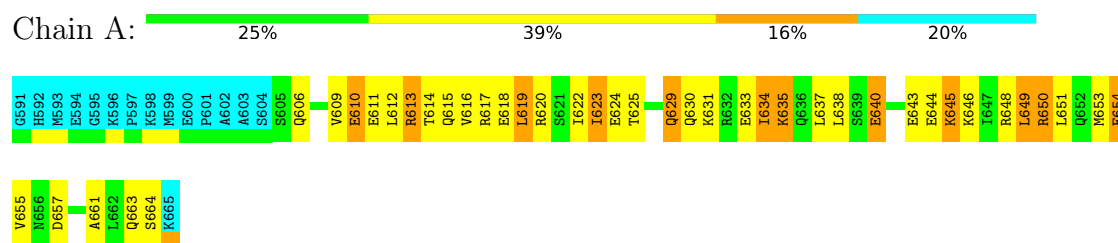


- Molecule 1: SH3 domain-containing kinase-binding protein 1

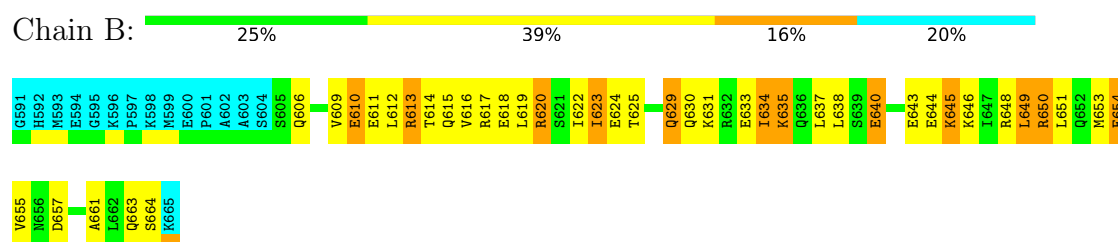


4.2.17 Score per residue for model 17

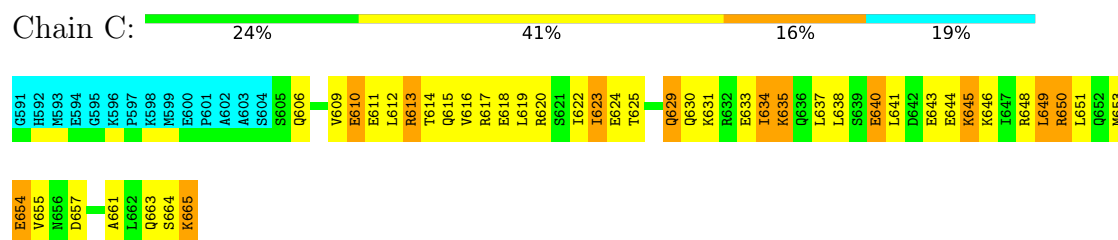
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

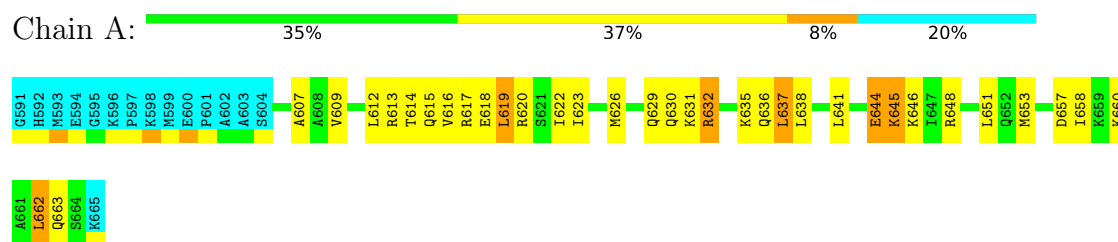


- Molecule 1: SH3 domain-containing kinase-binding protein 1



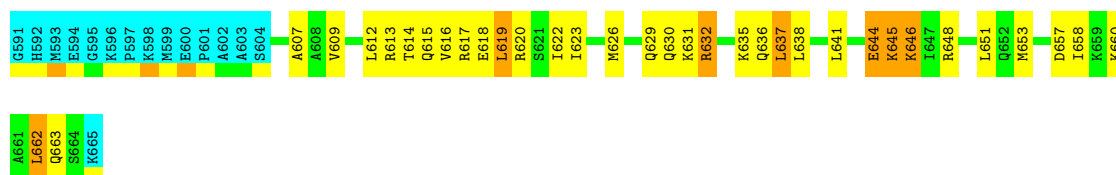
4.2.18 Score per residue for model 18

- Molecule 1: SH3 domain-containing kinase-binding protein 1



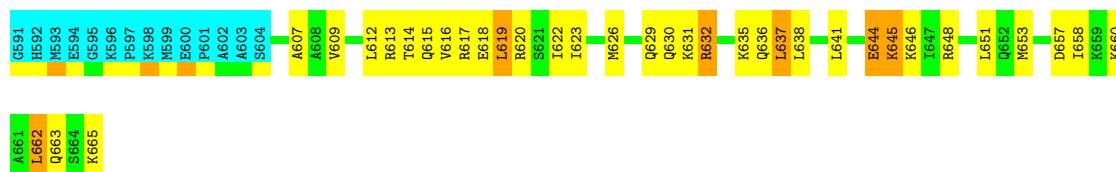
- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

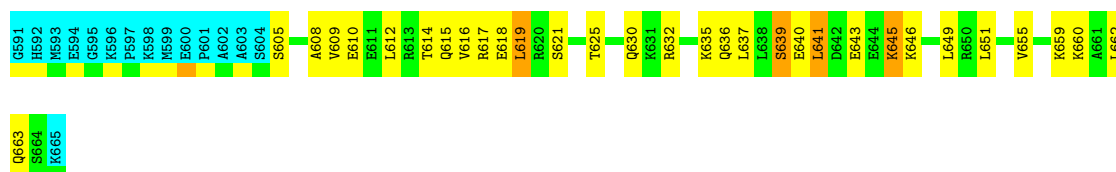
Chain C: 35% 39% 8% 19%



4.2.19 Score per residue for model 19

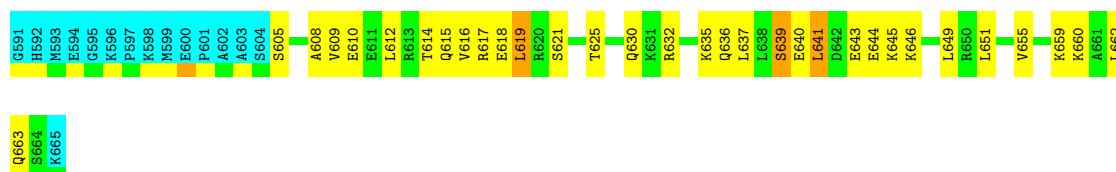
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 39% 36% 5% 20%



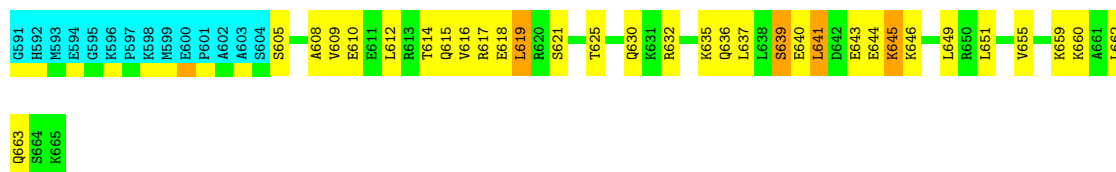
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 37% 39% 20%



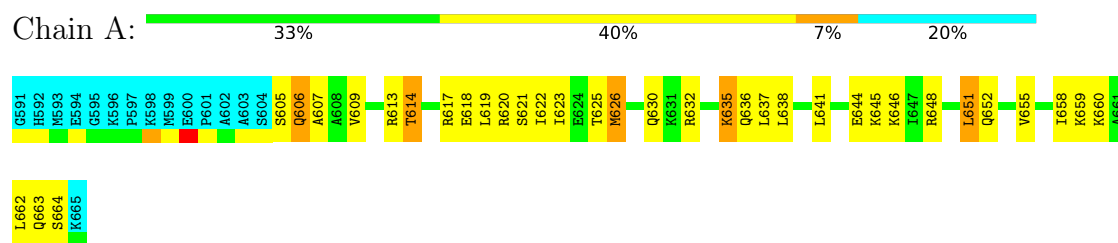
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 39% 37% 5% 19%

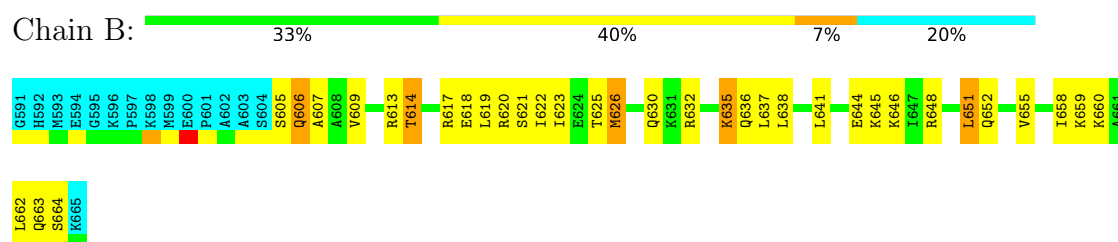


4.2.20 Score per residue for model 20 (medoid)

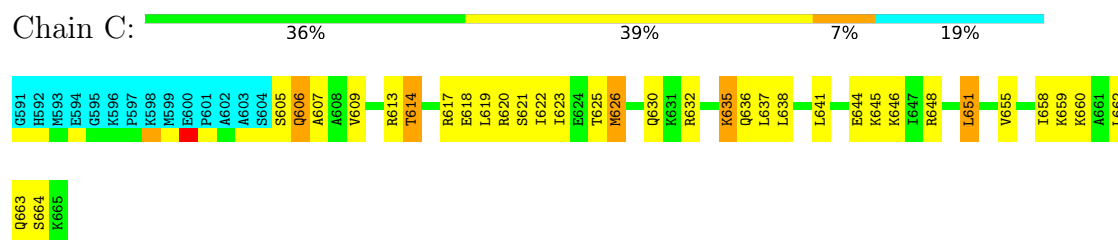
- Molecule 1: SH3 domain-containing kinase-binding protein 1



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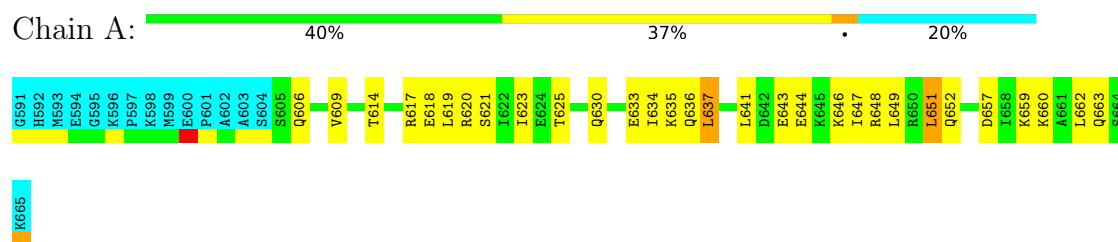


- Molecule 1: SH3 domain-containing kinase-binding protein 1



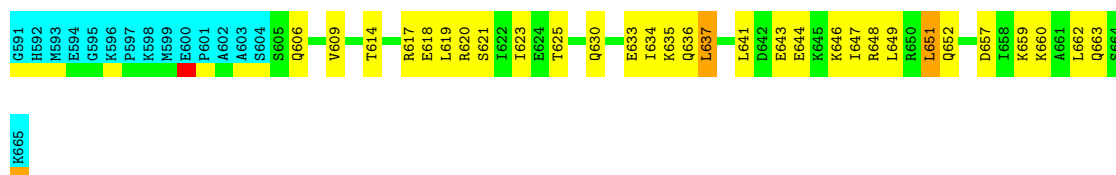
4.2.21 Score per residue for model 21

- Molecule 1: SH3 domain-containing kinase-binding protein 1



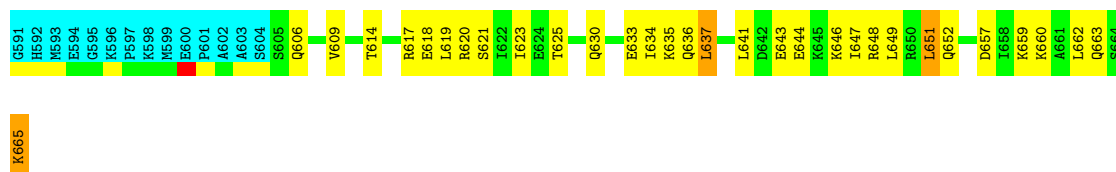
- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

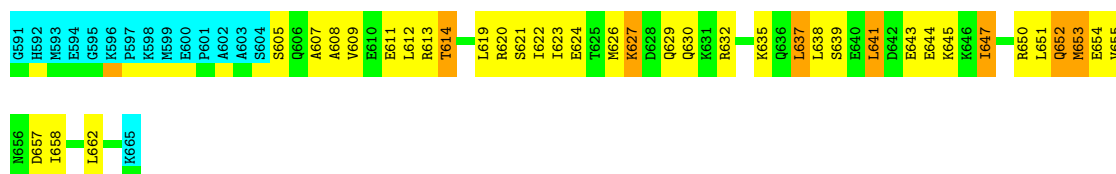
Chain C: 40% 37% 19%



4.2.22 Score per residue for model 22

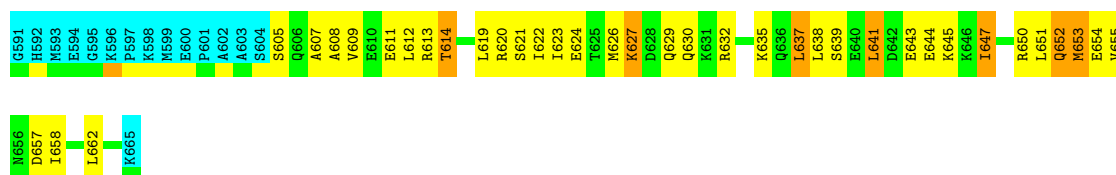
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 31% 40% 9% 20%



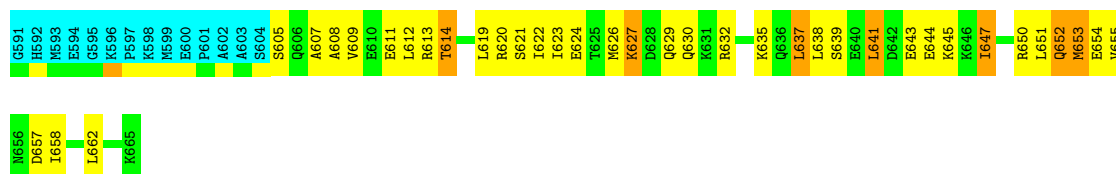
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 31% 40% 9% 20%



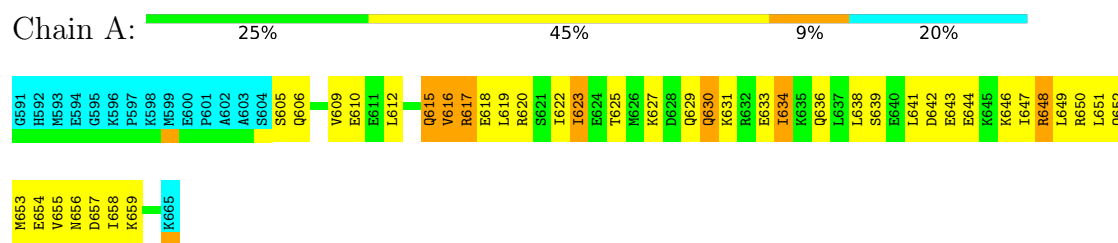
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 32% 40% 9% 19%

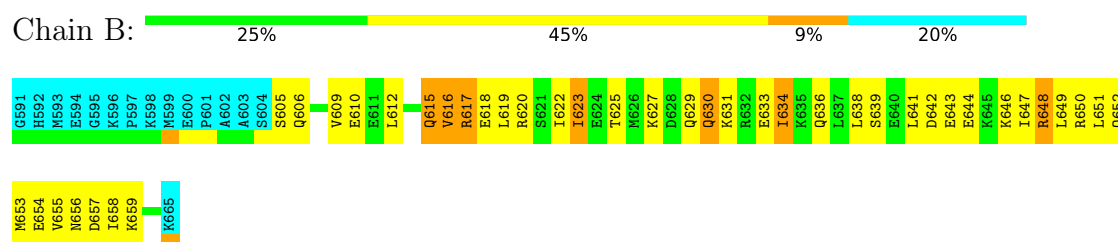


4.2.23 Score per residue for model 23

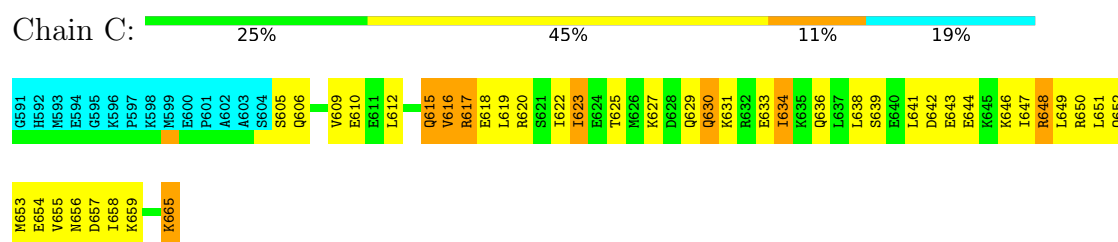
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

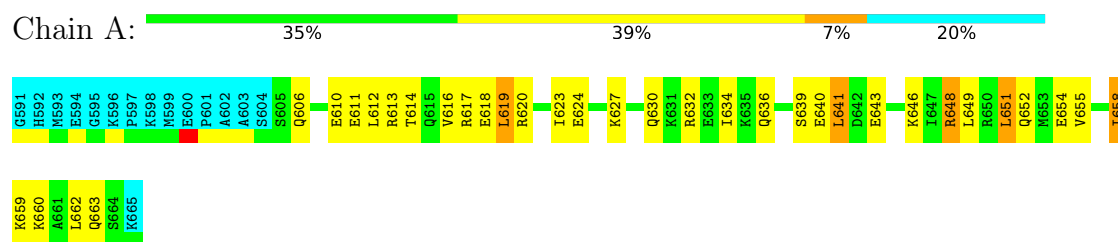


- Molecule 1: SH3 domain-containing kinase-binding protein 1



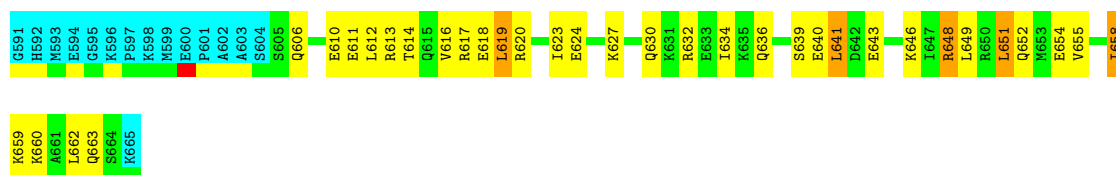
4.2.24 Score per residue for model 24

- Molecule 1: SH3 domain-containing kinase-binding protein 1



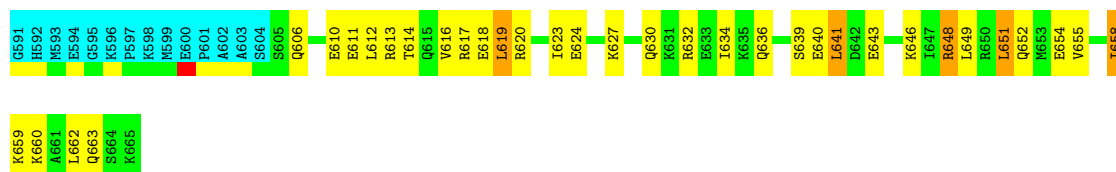
- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

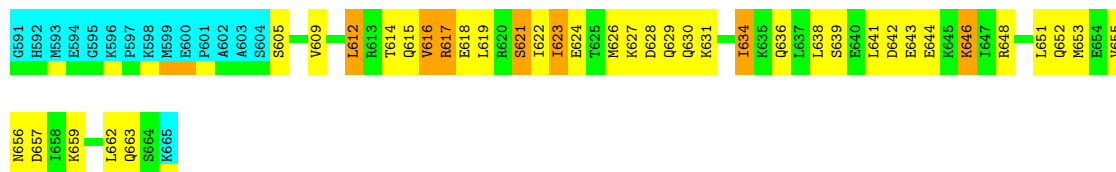
Chain C: 36% 39% 7% 19%



4.2.25 Score per residue for model 25

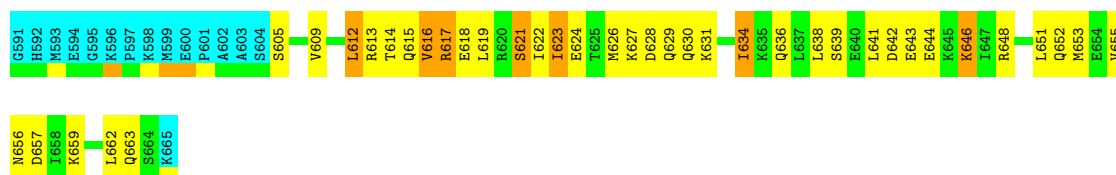
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 29% 41% 9% 20%



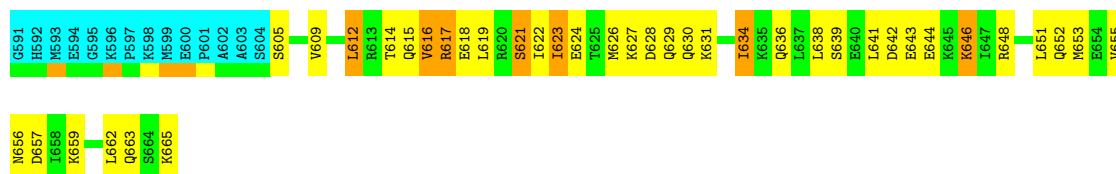
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 28% 43% 9% 20%



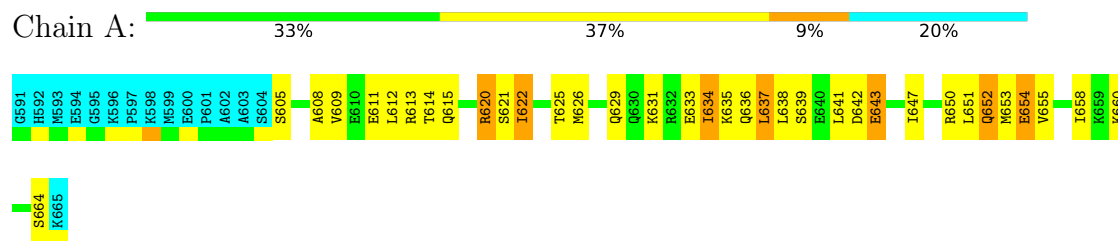
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 29% 43% 9% 19%

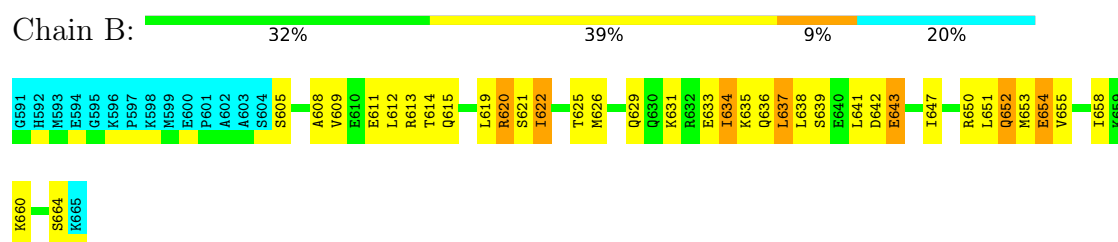


4.2.26 Score per residue for model 26

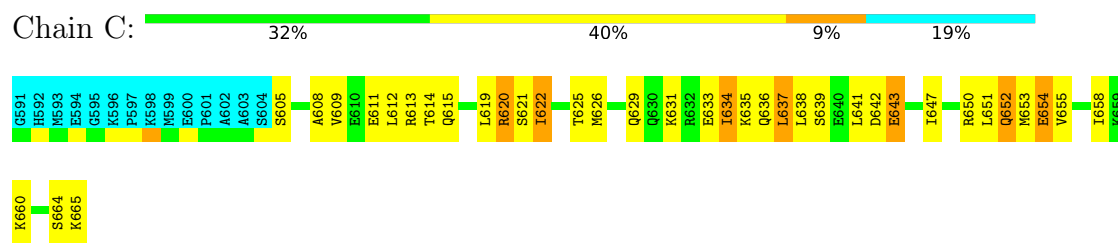
- Molecule 1: SH3 domain-containing kinase-binding protein 1



- Molecule 1: SH3 domain-containing kinase-binding protein 1

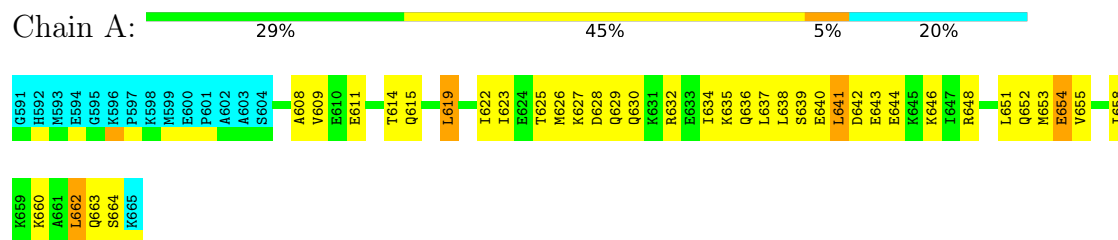


- Molecule 1: SH3 domain-containing kinase-binding protein 1



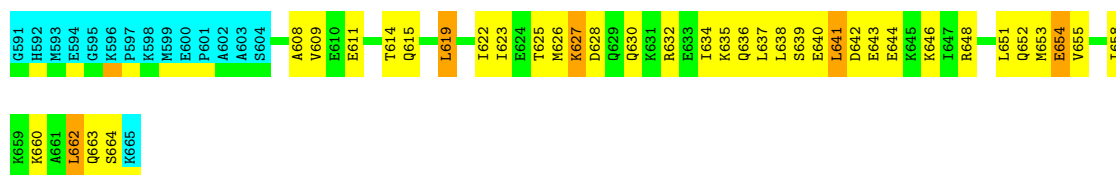
4.2.27 Score per residue for model 27

- Molecule 1: SH3 domain-containing kinase-binding protein 1



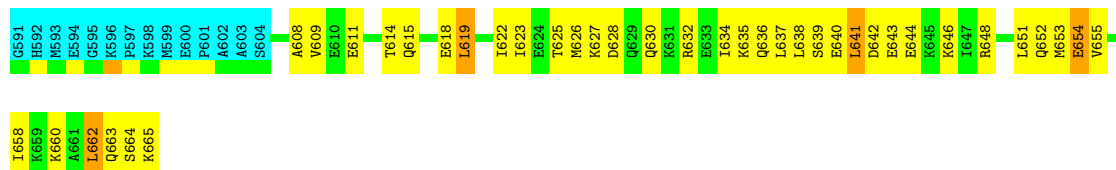
- Molecule 1: SH3 domain-containing kinase-binding protein 1





- Molecule 1: SH3 domain-containing kinase-binding protein 1

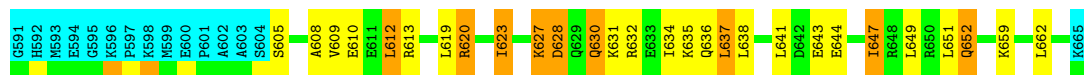
Chain C: 29% 47% 5% 19%



4.2.28 Score per residue for model 28

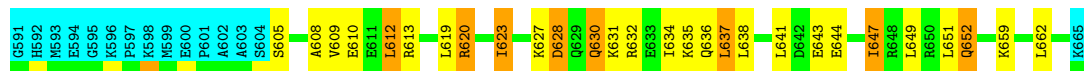
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 43% 25% 12% 20%



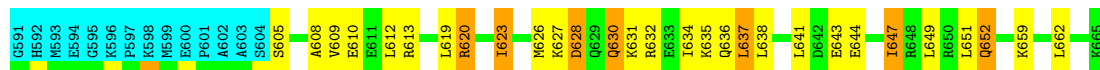
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 43% 27% 11% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

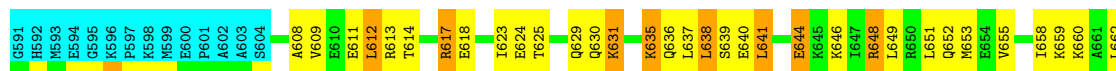
Chain C: 43% 29% 9% 19%



4.2.29 Score per residue for model 29

- Molecule 1: SH3 domain-containing kinase-binding protein 1

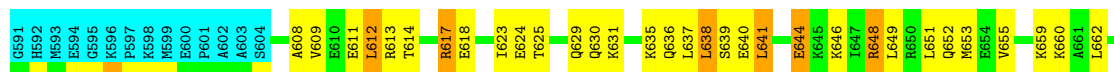
Chain A: 36% 33% 11% 20%





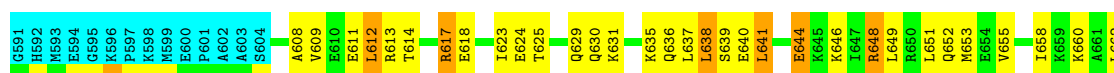
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 37% 35% 8% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

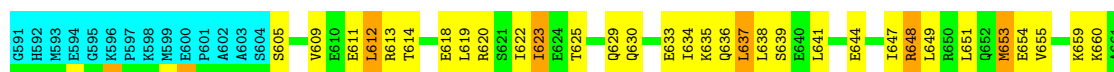
Chain C: 37% 36% 8% 19%



4.2.30 Score per residue for model 30

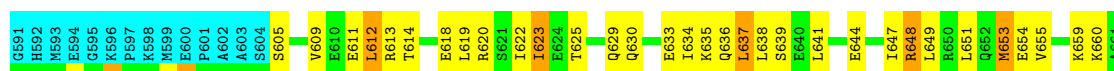
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain A: 33% 40% 7% 20%



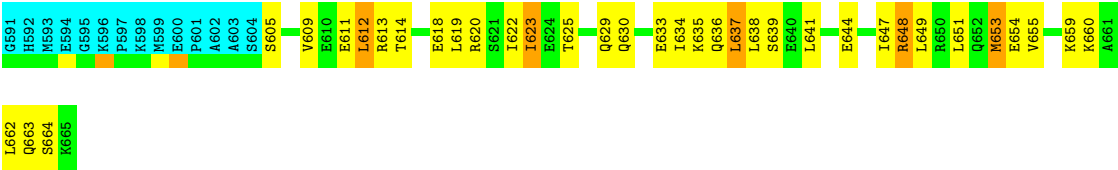
- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain B: 33% 40% 7% 20%



- Molecule 1: SH3 domain-containing kinase-binding protein 1

Chain C: 35% 40% 7% 19%



5 Refinement protocol and experimental data overview

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

Of the 2440 calculated structures, 30 were deposited, based on the following criterion: *every 84th structure after convergence*.

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

Software name	Classification	Version
ISD (Inferential structure determination)	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	20%

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	499	534	534	18±5
1	B	499	534	534	18±5
1	C	509	547	547	19±5
All	All	45210	48450	48450	1113

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:609:VAL:HG11	1:C:608:ALA:HB1	0.86	1.47	29	6
1:A:662:LEU:HD22	1:C:658:ILE:HG13	0.85	1.48	20	3
1:B:608:ALA:HB1	1:C:609:VAL:HG11	0.84	1.47	29	6
1:A:608:ALA:HB1	1:B:609:VAL:HG11	0.84	1.47	29	6
1:A:658:ILE:HG13	1:B:662:LEU:HD22	0.83	1.49	20	3
1:B:658:ILE:HG13	1:C:662:LEU:HD22	0.82	1.49	20	3
1:B:612:LEU:HD21	1:C:613:ARG:HA	0.81	1.53	8	10
1:B:651:LEU:O	1:B:655:VAL:HG23	0.81	1.76	27	21
1:A:651:LEU:O	1:A:655:VAL:HG23	0.80	1.76	27	21
1:C:651:LEU:O	1:C:655:VAL:HG23	0.80	1.76	27	21
1:B:619:LEU:HA	1:B:622:ILE:HD12	0.80	1.52	23	10
1:A:612:LEU:HD21	1:B:613:ARG:HA	0.80	1.53	8	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:619:LEU:HA	1:A:622:ILE:HD12	0.80	1.52	23	10
1:C:619:LEU:HA	1:C:622:ILE:HD12	0.80	1.52	23	10
1:A:613:ARG:HA	1:C:612:LEU:HD21	0.78	1.53	8	10
1:C:665:LYS:OXT	1:C:665:LYS:HG3	0.78	1.75	8	6
1:A:612:LEU:O	1:A:616:VAL:HG23	0.74	1.82	19	15
1:C:612:LEU:O	1:C:616:VAL:HG23	0.74	1.82	19	15
1:B:612:LEU:O	1:B:616:VAL:HG23	0.73	1.82	19	15
1:A:620:ARG:HA	1:A:623:ILE:HD12	0.73	1.61	20	7
1:B:620:ARG:HA	1:B:623:ILE:HD12	0.71	1.61	20	7
1:C:620:ARG:HA	1:C:623:ILE:HD12	0.71	1.61	20	7
1:A:645:LYS:O	1:A:649:LEU:HD12	0.71	1.85	17	1
1:B:645:LYS:O	1:B:649:LEU:HD12	0.71	1.85	17	1
1:C:645:LYS:O	1:C:649:LEU:HD12	0.70	1.85	17	1
1:A:655:VAL:HG21	1:C:651:LEU:HD11	0.69	1.64	30	6
1:C:605:SER:O	1:C:609:VAL:HG23	0.68	1.88	14	13
1:B:619:LEU:O	1:B:623:ILE:HD12	0.68	1.88	7	6
1:A:605:SER:O	1:A:609:VAL:HG23	0.68	1.88	14	13
1:A:619:LEU:O	1:A:623:ILE:HD12	0.68	1.88	7	6
1:B:605:SER:O	1:B:609:VAL:HG23	0.68	1.88	4	13
1:A:615:GLN:O	1:A:619:LEU:HD12	0.68	1.89	9	1
1:A:635:LYS:HA	1:A:638:LEU:HD12	0.68	1.66	20	1
1:C:615:GLN:O	1:C:619:LEU:HD12	0.67	1.89	9	1
1:A:651:LEU:HD11	1:B:655:VAL:HG21	0.67	1.64	30	6
1:C:635:LYS:HA	1:C:638:LEU:HD12	0.67	1.66	20	1
1:B:651:LEU:HD11	1:C:655:VAL:HG21	0.67	1.64	30	6
1:C:634:ILE:HA	1:C:637:LEU:HD12	0.67	1.67	17	1
1:B:615:GLN:O	1:B:619:LEU:HD12	0.67	1.89	9	2
1:B:634:ILE:HA	1:B:637:LEU:HD12	0.67	1.67	17	1
1:B:635:LYS:HA	1:B:638:LEU:HD12	0.67	1.66	20	1
1:A:662:LEU:HD11	1:C:662:LEU:HG	0.66	1.67	22	2
1:B:619:LEU:HD21	1:C:620:ARG:HG3	0.66	1.68	2	3
1:B:662:LEU:HG	1:C:662:LEU:HD11	0.66	1.67	22	2
1:C:619:LEU:O	1:C:623:ILE:HD12	0.66	1.88	7	5
1:B:606:GLN:HA	1:B:606:GLN:OE1	0.65	1.91	20	1
1:A:606:GLN:OE1	1:A:606:GLN:HA	0.65	1.91	20	1
1:A:634:ILE:HA	1:A:637:LEU:HD12	0.65	1.67	17	1
1:A:620:ARG:HG3	1:C:619:LEU:HD21	0.64	1.68	2	3
1:A:662:LEU:HG	1:B:662:LEU:HD11	0.64	1.67	22	2
1:C:606:GLN:HA	1:C:606:GLN:OE1	0.64	1.91	20	1
1:B:612:LEU:HD22	1:C:616:VAL:HG21	0.64	1.69	24	4
1:A:619:LEU:HD21	1:B:620:ARG:HG3	0.64	1.68	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:605:SER:O	1:A:609:VAL:HG22	0.64	1.92	3	1
1:A:612:LEU:HD22	1:B:616:VAL:HG21	0.63	1.69	24	4
1:C:665:LYS:OXT	1:C:665:LYS:CG	0.63	2.47	8	8
1:C:605:SER:O	1:C:609:VAL:HG22	0.63	1.92	3	1
1:A:661:ALA:HB3	1:B:662:LEU:HD21	0.63	1.71	14	1
1:B:605:SER:O	1:B:609:VAL:HG22	0.63	1.92	3	1
1:A:651:LEU:HD22	1:B:652:GLN:HG2	0.63	1.71	1	6
1:B:661:ALA:HB3	1:C:662:LEU:HD21	0.63	1.71	14	1
1:A:623:ILE:HD13	1:C:619:LEU:HD21	0.63	1.71	25	1
1:A:616:VAL:HG21	1:C:612:LEU:HD22	0.63	1.69	24	4
1:A:619:LEU:HD23	1:B:623:ILE:HD11	0.63	1.71	13	3
1:C:634:ILE:O	1:C:638:LEU:HD12	0.62	1.94	26	4
1:A:641:LEU:HD21	1:C:641:LEU:HA	0.62	1.71	27	5
1:B:641:LEU:HA	1:C:641:LEU:HD21	0.62	1.71	27	5
1:A:651:LEU:HD13	1:B:652:GLN:HG3	0.62	1.71	28	2
1:B:651:LEU:HD22	1:C:652:GLN:HG2	0.62	1.71	1	6
1:A:641:LEU:HA	1:B:641:LEU:HD21	0.62	1.71	27	5
1:A:634:ILE:O	1:A:638:LEU:HD12	0.62	1.94	26	4
1:A:662:LEU:HD21	1:C:661:ALA:HB3	0.62	1.71	14	1
1:B:651:LEU:HD13	1:C:652:GLN:HG3	0.62	1.71	28	2
1:A:618:GLU:O	1:A:622:ILE:HG13	0.62	1.95	17	3
1:B:619:LEU:HD23	1:C:623:ILE:HD11	0.61	1.71	13	3
1:A:613:ARG:HG2	1:C:612:LEU:HD21	0.61	1.72	26	3
1:A:652:GLN:HG2	1:C:651:LEU:HD22	0.61	1.71	1	6
1:B:634:ILE:O	1:B:638:LEU:HD12	0.61	1.94	26	4
1:A:652:GLN:HG3	1:C:651:LEU:HD13	0.61	1.71	28	2
1:B:618:GLU:O	1:B:622:ILE:HG13	0.61	1.95	17	3
1:C:621:SER:O	1:C:625:THR:HG23	0.61	1.96	26	3
1:A:621:SER:O	1:A:625:THR:HG23	0.61	1.96	26	3
1:A:619:LEU:HD21	1:B:623:ILE:HD13	0.61	1.71	25	1
1:B:619:LEU:HD21	1:C:623:ILE:HD13	0.61	1.71	25	1
1:A:623:ILE:HD11	1:C:619:LEU:HD23	0.61	1.71	13	3
1:A:612:LEU:HD21	1:B:613:ARG:HG2	0.61	1.72	26	3
1:B:621:SER:O	1:B:625:THR:HG23	0.60	1.96	26	3
1:B:662:LEU:HD12	1:C:662:LEU:CD1	0.60	2.26	11	1
1:C:618:GLU:O	1:C:622:ILE:HG13	0.60	1.95	17	3
1:B:612:LEU:HD21	1:C:613:ARG:HG2	0.60	1.72	26	3
1:B:653:MET:HE3	1:B:653:MET:HA	0.60	1.72	30	1
1:A:662:LEU:HD12	1:B:662:LEU:CD1	0.60	2.26	11	1
1:A:653:MET:HE3	1:A:653:MET:HA	0.60	1.72	30	1
1:A:662:LEU:CD1	1:C:662:LEU:HD12	0.60	2.26	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:653:MET:HE3	1:C:653:MET:HA	0.59	1.72	30	1
1:A:626:MET:SD	1:B:623:ILE:HG22	0.58	2.39	13	4
1:A:637:LEU:HB2	1:C:637:LEU:HD22	0.58	1.75	17	1
1:A:616:VAL:HG11	1:C:615:GLN:HB3	0.58	1.75	14	2
1:B:615:GLN:HB3	1:C:616:VAL:HG11	0.58	1.75	23	2
1:A:609:VAL:HG11	1:C:608:ALA:CB	0.58	2.27	29	2
1:B:626:MET:SD	1:C:623:ILE:HG22	0.58	2.39	13	4
1:B:613:ARG:O	1:B:617:ARG:HD2	0.58	1.99	1	1
1:B:635:LYS:HE3	1:B:635:LYS:HA	0.57	1.77	8	1
1:A:615:GLN:HB3	1:B:616:VAL:HG11	0.57	1.75	23	2
1:B:608:ALA:CB	1:C:609:VAL:HG11	0.57	2.27	29	3
1:A:613:ARG:O	1:A:617:ARG:HD2	0.57	1.99	1	1
1:B:622:ILE:HG22	1:C:623:ILE:HG21	0.57	1.76	1	2
1:C:613:ARG:O	1:C:617:ARG:HD2	0.57	1.99	1	1
1:A:634:ILE:HG21	1:C:633:GLU:HB3	0.57	1.77	30	6
1:A:623:ILE:HD11	1:C:623:ILE:HD11	0.57	1.77	12	3
1:A:623:ILE:HG22	1:C:626:MET:SD	0.57	2.38	13	4
1:A:635:LYS:HE3	1:A:635:LYS:HA	0.57	1.76	8	1
1:B:637:LEU:HD22	1:C:637:LEU:HB2	0.57	1.75	17	1
1:A:623:ILE:HD11	1:B:623:ILE:HD11	0.57	1.77	12	3
1:B:623:ILE:HD11	1:C:623:ILE:HD11	0.57	1.77	12	3
1:A:633:GLU:HB3	1:B:634:ILE:HG21	0.57	1.77	30	6
1:A:623:ILE:HG21	1:C:622:ILE:HG22	0.56	1.76	1	2
1:A:662:LEU:HD22	1:C:658:ILE:HG23	0.56	1.77	12	1
1:A:658:ILE:HG23	1:B:662:LEU:HD22	0.56	1.77	12	1
1:A:623:ILE:HG12	1:B:623:ILE:HD13	0.56	1.77	24	2
1:A:622:ILE:HG22	1:B:623:ILE:HG21	0.56	1.76	1	2
1:A:637:LEU:HD22	1:B:637:LEU:HB2	0.56	1.75	17	1
1:B:623:ILE:HG12	1:C:623:ILE:HD13	0.56	1.77	24	2
1:A:608:ALA:CB	1:B:609:VAL:HG11	0.56	2.27	29	3
1:A:631:LYS:O	1:A:635:LYS:HD2	0.56	2.01	1	2
1:C:631:LYS:O	1:C:635:LYS:HD2	0.56	2.01	1	1
1:B:637:LEU:HD12	1:C:634:ILE:HG23	0.56	1.78	21	4
1:A:658:ILE:HD12	1:B:659:LYS:HA	0.56	1.78	20	2
1:C:654:GLU:O	1:C:658:ILE:HG13	0.56	2.01	23	5
1:C:635:LYS:HE3	1:C:635:LYS:HA	0.55	1.77	8	1
1:C:643:GLU:O	1:C:647:ILE:HG13	0.55	2.02	21	3
1:A:643:GLU:O	1:A:647:ILE:HG13	0.55	2.02	21	3
1:B:654:GLU:O	1:B:658:ILE:HG13	0.55	2.01	23	4
1:B:633:GLU:HB3	1:C:634:ILE:HG21	0.55	1.77	30	7
1:A:654:GLU:O	1:A:658:ILE:HG13	0.55	2.01	23	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:645:LYS:HE3	1:C:644:GLU:HG2	0.55	1.79	17	1
1:B:622:ILE:HG22	1:B:626:MET:SD	0.55	2.42	27	5
1:B:625:THR:O	1:B:629:GLN:HB2	0.55	2.02	14	3
1:A:637:LEU:HD12	1:B:634:ILE:HG23	0.55	1.78	21	4
1:B:658:ILE:HD12	1:C:659:LYS:HA	0.55	1.78	20	2
1:A:625:THR:O	1:A:629:GLN:HB2	0.55	2.02	14	3
1:C:625:THR:O	1:C:629:GLN:HB2	0.55	2.02	14	3
1:B:644:GLU:HG2	1:C:645:LYS:HE3	0.55	1.79	17	1
1:A:655:VAL:HG21	1:C:651:LEU:HD21	0.55	1.79	19	1
1:C:611:GLU:O	1:C:614:THR:HG22	0.55	2.02	26	1
1:B:631:LYS:O	1:B:635:LYS:HD2	0.54	2.01	1	1
1:B:658:ILE:HG23	1:C:662:LEU:HD22	0.54	1.77	12	1
1:A:634:ILE:HG23	1:C:637:LEU:HD12	0.54	1.78	21	4
1:A:623:ILE:HD13	1:C:623:ILE:HG12	0.54	1.77	24	2
1:C:659:LYS:HG2	1:C:663:GLN:NE2	0.54	2.17	30	1
1:B:643:GLU:O	1:B:647:ILE:HG13	0.54	2.02	21	3
1:B:659:LYS:HG2	1:B:663:GLN:NE2	0.54	2.17	30	1
1:A:651:LEU:HD21	1:B:655:VAL:HG21	0.54	1.79	19	1
1:A:622:ILE:HG22	1:A:626:MET:SD	0.54	2.43	20	5
1:B:644:GLU:HA	1:B:647:ILE:HD12	0.53	1.80	30	1
1:C:622:ILE:HG22	1:C:626:MET:SD	0.53	2.42	27	5
1:B:611:GLU:O	1:B:614:THR:HG22	0.53	2.02	26	1
1:A:644:GLU:HA	1:A:647:ILE:HD12	0.53	1.80	30	1
1:C:648:ARG:CZ	1:C:648:ARG:HB3	0.53	2.32	23	4
1:A:659:LYS:HA	1:C:658:ILE:HD12	0.53	1.78	20	2
1:B:651:LEU:HD21	1:C:655:VAL:HG21	0.53	1.79	19	1
1:A:659:LYS:HG2	1:A:663:GLN:NE2	0.53	2.17	30	1
1:B:648:ARG:CZ	1:B:648:ARG:HB3	0.53	2.32	23	4
1:B:658:ILE:CG1	1:C:662:LEU:HD13	0.53	2.34	11	1
1:A:644:GLU:HG2	1:B:645:LYS:HE3	0.53	1.79	17	1
1:A:640:GLU:HB3	1:B:641:LEU:HD13	0.53	1.81	27	3
1:A:637:LEU:HD11	1:B:638:LEU:HD12	0.53	1.81	2	1
1:C:627:LYS:O	1:C:630:GLN:HG3	0.53	2.04	25	2
1:A:648:ARG:CZ	1:A:648:ARG:HB3	0.53	2.32	23	4
1:B:640:GLU:HB3	1:C:641:LEU:HD13	0.53	1.81	27	3
1:C:644:GLU:HA	1:C:647:ILE:HD12	0.52	1.80	30	1
1:B:637:LEU:HD11	1:C:638:LEU:HD12	0.52	1.81	2	1
1:A:658:ILE:CG1	1:B:662:LEU:HD13	0.52	2.34	11	1
1:A:645:LYS:HG2	1:C:644:GLU:HG3	0.52	1.81	18	3
1:A:611:GLU:O	1:A:614:THR:HG22	0.52	2.02	26	1
1:B:627:LYS:O	1:B:630:GLN:HG3	0.52	2.04	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:641:LEU:HD13	1:C:640:GLU:HB3	0.52	1.81	27	3
1:B:644:GLU:HG3	1:C:645:LYS:HG2	0.52	1.81	18	3
1:A:638:LEU:HD12	1:C:637:LEU:HD11	0.52	1.81	2	1
1:A:662:LEU:HD13	1:C:658:ILE:CG1	0.52	2.34	11	1
1:C:622:ILE:CG2	1:C:626:MET:SD	0.52	2.98	27	1
1:A:640:GLU:O	1:A:644:GLU:HG3	0.52	2.05	17	1
1:A:644:GLU:HG3	1:B:645:LYS:HG2	0.51	1.81	18	2
1:A:627:LYS:O	1:A:630:GLN:HG3	0.51	2.05	23	2
1:A:622:ILE:CG2	1:A:626:MET:SD	0.51	2.98	27	1
1:B:622:ILE:CG2	1:B:626:MET:SD	0.51	2.98	27	1
1:C:640:GLU:O	1:C:644:GLU:HG3	0.51	2.05	17	1
1:B:640:GLU:O	1:B:644:GLU:HG3	0.51	2.05	17	1
1:B:629:GLN:O	1:B:633:GLU:HB2	0.51	2.06	17	1
1:B:640:GLU:HG2	1:C:641:LEU:HD22	0.51	1.82	27	2
1:A:655:VAL:HA	1:A:658:ILE:HD12	0.51	1.83	12	1
1:B:631:LYS:O	1:B:634:ILE:HG13	0.51	2.05	23	4
1:C:631:LYS:O	1:C:634:ILE:HG13	0.51	2.05	23	4
1:A:641:LEU:HD22	1:C:640:GLU:HG2	0.51	1.82	27	1
1:B:644:GLU:HG2	1:C:645:LYS:HD3	0.50	1.82	11	1
1:C:629:GLN:O	1:C:633:GLU:HB2	0.50	2.06	17	1
1:C:613:ARG:HB2	1:C:613:ARG:NH1	0.50	2.21	6	1
1:A:640:GLU:HG2	1:B:641:LEU:HD22	0.50	1.82	27	1
1:A:644:GLU:HG2	1:B:645:LYS:HD3	0.50	1.82	11	1
1:B:655:VAL:HA	1:B:658:ILE:HD12	0.50	1.83	12	1
1:B:613:ARG:HB2	1:B:613:ARG:NH1	0.50	2.21	6	1
1:C:643:GLU:O	1:C:647:ILE:HD12	0.50	2.06	26	4
1:A:631:LYS:O	1:A:634:ILE:HG13	0.50	2.05	23	4
1:A:654:GLU:OE2	1:A:658:ILE:HD11	0.50	2.07	26	1
1:B:619:LEU:HD11	1:C:616:VAL:HG13	0.50	1.84	3	1
1:B:654:GLU:OE2	1:B:658:ILE:HD11	0.50	2.07	26	1
1:A:613:ARG:HB2	1:A:613:ARG:NH1	0.50	2.21	6	1
1:A:643:GLU:O	1:A:647:ILE:HD12	0.50	2.06	26	4
1:B:643:GLU:O	1:B:647:ILE:HD12	0.50	2.06	26	4
1:A:629:GLN:O	1:A:633:GLU:HB2	0.50	2.06	17	1
1:A:613:ARG:HB2	1:A:613:ARG:HH11	0.49	1.67	6	1
1:A:662:LEU:HD12	1:B:662:LEU:HD11	0.49	1.84	11	1
1:B:613:ARG:HB2	1:B:613:ARG:HH11	0.49	1.67	6	1
1:A:626:MET:HG2	1:B:627:LYS:HE2	0.49	1.84	9	1
1:A:619:LEU:HD11	1:B:616:VAL:HG13	0.49	1.84	3	1
1:A:645:LYS:HD3	1:C:644:GLU:HG2	0.49	1.82	11	1
1:C:630:GLN:HG2	1:C:631:LYS:N	0.49	2.21	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:623:ILE:CG2	1:A:624:GLU:N	0.49	2.75	17	1
1:C:661:ALA:O	1:C:665:LYS:HG2	0.49	2.07	17	1
1:B:658:ILE:HG13	1:C:662:LEU:HD13	0.49	1.85	9	2
1:B:630:GLN:HG2	1:B:631:LYS:N	0.49	2.21	12	1
1:C:654:GLU:OE2	1:C:658:ILE:HD11	0.49	2.07	26	1
1:C:655:VAL:HA	1:C:658:ILE:HD12	0.49	1.83	12	1
1:A:660:LYS:HZ2	1:A:660:LYS:HA	0.49	1.68	15	1
1:B:640:GLU:OE1	1:C:641:LEU:HD13	0.49	2.08	24	1
1:A:616:VAL:HG13	1:C:619:LEU:HD11	0.49	1.84	3	1
1:B:662:LEU:HD12	1:C:662:LEU:HD11	0.49	1.84	11	1
1:A:609:VAL:HG13	1:C:612:LEU:HD23	0.49	1.84	29	1
1:A:651:LEU:HD21	1:B:652:GLN:HA	0.49	1.85	21	5
1:B:626:MET:HG2	1:C:627:LYS:HE2	0.49	1.84	9	1
1:A:644:GLU:OE2	1:B:645:LYS:HA	0.49	2.08	13	1
1:A:645:LYS:HA	1:C:644:GLU:OE2	0.49	2.08	13	1
1:C:623:ILE:CG2	1:C:624:GLU:N	0.49	2.75	17	1
1:C:613:ARG:HB2	1:C:613:ARG:HH11	0.48	1.67	6	1
1:A:630:GLN:HG2	1:A:631:LYS:N	0.48	2.21	12	1
1:A:644:GLU:HB2	1:B:645:LYS:HE2	0.48	1.85	14	2
1:A:612:LEU:HG	1:B:612:LEU:HB3	0.48	1.85	30	4
1:B:612:LEU:HD23	1:C:609:VAL:HG13	0.48	1.84	29	1
1:A:641:LEU:HD13	1:C:640:GLU:OE1	0.48	2.08	24	1
1:B:611:GLU:O	1:B:615:GLN:HG3	0.48	2.08	27	1
1:A:640:GLU:OE1	1:B:641:LEU:HD13	0.48	2.08	24	1
1:C:642:ASP:O	1:C:646:LYS:HD2	0.48	2.09	1	1
1:A:662:LEU:HD13	1:C:658:ILE:HG13	0.48	1.85	9	2
1:A:622:ILE:CG2	1:A:626:MET:HE3	0.48	2.39	22	2
1:B:644:GLU:HB2	1:C:645:LYS:HE2	0.48	1.85	14	2
1:A:611:GLU:O	1:A:615:GLN:HG3	0.48	2.08	27	1
1:A:662:LEU:HD11	1:C:662:LEU:HD12	0.48	1.84	11	1
1:B:644:GLU:OE2	1:C:645:LYS:HA	0.48	2.08	13	1
1:B:623:ILE:CG2	1:B:624:GLU:N	0.48	2.75	17	1
1:B:622:ILE:CG2	1:B:626:MET:HE3	0.48	2.39	22	1
1:B:651:LEU:HD21	1:C:652:GLN:HA	0.48	1.85	21	4
1:B:612:LEU:HG	1:C:612:LEU:HB3	0.48	1.86	30	3
1:C:622:ILE:CG2	1:C:626:MET:HE3	0.48	2.39	22	1
1:C:611:GLU:O	1:C:615:GLN:HG3	0.48	2.08	27	1
1:C:665:LYS:OXT	1:C:665:LYS:HG2	0.47	2.08	21	2
1:A:658:ILE:HG13	1:B:662:LEU:HD13	0.47	1.85	9	2
1:A:652:GLN:HA	1:C:651:LEU:HD21	0.47	1.85	21	5
1:A:627:LYS:HE2	1:C:626:MET:HG2	0.47	1.84	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:654:GLU:HB3	1:B:655:VAL:HG11	0.47	1.86	17	1
1:B:626:MET:SD	1:C:627:LYS:HG3	0.47	2.50	11	2
1:A:612:LEU:HB3	1:C:612:LEU:HG	0.47	1.85	30	3
1:A:651:LEU:HD11	1:B:655:VAL:CG2	0.47	2.40	27	5
1:A:655:VAL:CG2	1:C:651:LEU:HD11	0.47	2.38	30	5
1:B:651:LEU:HD11	1:C:655:VAL:CG2	0.47	2.40	27	5
1:A:612:LEU:HD23	1:B:609:VAL:HG13	0.47	1.84	29	1
1:A:642:ASP:O	1:A:646:LYS:HD2	0.47	2.09	1	1
1:A:637:LEU:HD23	1:B:641:LEU:HD12	0.47	1.86	12	4
1:A:627:LYS:HG3	1:C:626:MET:SD	0.47	2.50	11	2
1:A:651:LEU:HD11	1:B:652:GLN:HB2	0.47	1.86	21	1
1:B:630:GLN:HA	1:B:630:GLN:OE1	0.47	2.10	28	1
1:A:646:LYS:O	1:A:650:ARG:HG3	0.47	2.10	4	2
1:A:619:LEU:HD13	1:B:620:ARG:HD2	0.47	1.86	7	2
1:B:622:ILE:HG23	1:B:626:MET:SD	0.47	2.50	26	1
1:A:630:GLN:OE1	1:A:630:GLN:HA	0.47	2.10	28	1
1:B:642:ASP:O	1:B:646:LYS:HD2	0.47	2.09	1	1
1:A:641:LEU:HD12	1:C:637:LEU:HD23	0.47	1.87	22	4
1:A:626:MET:SD	1:B:627:LYS:HG3	0.47	2.50	11	2
1:B:643:GLU:O	1:B:647:ILE:HG22	0.47	2.10	14	1
1:C:630:GLN:HA	1:C:630:GLN:OE1	0.47	2.10	28	1
1:B:646:LYS:O	1:B:650:ARG:HG3	0.47	2.10	4	2
1:B:612:LEU:HD21	1:C:613:ARG:HB2	0.47	1.87	16	1
1:C:639:SER:O	1:C:643:GLU:HG2	0.47	2.10	19	1
1:A:623:ILE:HG12	1:B:623:ILE:HG12	0.47	1.87	18	3
1:A:652:GLN:HB2	1:C:651:LEU:HD11	0.47	1.86	21	1
1:A:623:ILE:HG12	1:C:623:ILE:HG12	0.47	1.87	8	3
1:B:619:LEU:HD13	1:C:620:ARG:HD2	0.47	1.86	7	2
1:A:643:GLU:O	1:A:647:ILE:HG22	0.47	2.10	14	1
1:B:639:SER:O	1:B:643:GLU:HG2	0.47	2.10	19	1
1:A:620:ARG:HB2	1:A:620:ARG:HH11	0.47	1.70	26	1
1:C:646:LYS:O	1:C:650:ARG:HG3	0.46	2.10	4	2
1:B:622:ILE:O	1:B:626:MET:HG3	0.46	2.10	4	1
1:A:613:ARG:CA	1:C:612:LEU:HD21	0.46	2.39	5	2
1:A:655:VAL:HG11	1:C:654:GLU:HB3	0.46	1.86	17	1
1:C:620:ARG:HH11	1:C:620:ARG:HB2	0.46	1.70	26	1
1:A:620:ARG:HD2	1:C:619:LEU:HD13	0.46	1.86	7	2
1:A:622:ILE:HG23	1:A:626:MET:SD	0.46	2.50	26	1
1:C:622:ILE:HG23	1:C:626:MET:SD	0.46	2.50	26	1
1:B:623:ILE:HG12	1:C:623:ILE:HG12	0.46	1.87	8	3
1:A:637:LEU:HG	1:B:638:LEU:HG	0.46	1.87	26	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:630:GLN:HG2	1:C:630:GLN:HB3	0.46	1.88	1	1
1:A:622:ILE:O	1:A:626:MET:HG3	0.46	2.10	4	2
1:C:622:ILE:O	1:C:626:MET:HG3	0.46	2.10	4	1
1:B:654:GLU:HB3	1:C:655:VAL:HG11	0.46	1.86	17	1
1:A:645:LYS:HE2	1:C:644:GLU:HB2	0.46	1.85	14	2
1:B:611:GLU:O	1:B:614:THR:HG23	0.46	2.11	22	1
1:B:637:LEU:HD23	1:C:641:LEU:HD12	0.46	1.86	12	4
1:A:613:ARG:HB2	1:C:612:LEU:HD21	0.46	1.87	16	1
1:A:611:GLU:O	1:A:614:THR:HG23	0.46	2.11	22	1
1:A:612:LEU:HD21	1:B:613:ARG:CA	0.46	2.39	5	1
1:A:638:LEU:HG	1:C:637:LEU:HG	0.46	1.88	18	3
1:B:637:LEU:HG	1:C:638:LEU:HG	0.46	1.87	26	3
1:B:620:ARG:HB2	1:B:620:ARG:HH11	0.46	1.70	26	1
1:B:662:LEU:HD23	1:B:663:GLN:HE21	0.46	1.70	4	1
1:A:630:GLN:HG2	1:B:630:GLN:HB3	0.46	1.88	1	1
1:C:640:GLU:HA	1:C:643:GLU:OE1	0.46	2.11	17	1
1:B:629:GLN:O	1:B:633:GLU:HG3	0.46	2.11	23	1
1:A:651:LEU:HD22	1:B:651:LEU:HD22	0.45	1.88	10	1
1:A:651:LEU:HD22	1:C:651:LEU:HD22	0.45	1.88	10	1
1:C:643:GLU:O	1:C:647:ILE:HG22	0.45	2.10	14	1
1:A:630:GLN:HB3	1:C:630:GLN:HG2	0.45	1.88	1	1
1:B:651:LEU:HD22	1:C:651:LEU:HD22	0.45	1.88	10	1
1:A:639:SER:O	1:A:643:GLU:HG2	0.45	2.10	19	1
1:A:623:ILE:HD13	1:C:619:LEU:HD22	0.45	1.88	5	1
1:B:616:VAL:HA	1:B:619:LEU:HD12	0.45	1.87	1	1
1:C:611:GLU:O	1:C:614:THR:HG23	0.45	2.11	22	1
1:C:629:GLN:O	1:C:633:GLU:HG3	0.45	2.11	23	1
1:A:662:LEU:HD23	1:A:663:GLN:HE21	0.45	1.70	4	1
1:A:623:ILE:CG1	1:B:623:ILE:HD13	0.45	2.41	24	1
1:A:651:LEU:HD21	1:B:652:GLN:CA	0.45	2.41	5	1
1:B:627:LYS:O	1:B:630:GLN:HG2	0.45	2.12	7	1
1:B:649:LEU:HA	1:B:652:GLN:HG3	0.45	1.89	7	1
1:A:612:LEU:HD21	1:B:613:ARG:HB2	0.45	1.87	16	1
1:A:631:LYS:O	1:A:635:LYS:HB2	0.45	2.12	17	1
1:B:651:LEU:HD11	1:C:652:GLN:HB2	0.45	1.86	21	1
1:C:642:ASP:O	1:C:646:LYS:HG3	0.45	2.12	10	1
1:A:649:LEU:HA	1:A:652:GLN:HG3	0.45	1.89	7	1
1:B:623:ILE:CG1	1:C:623:ILE:HD13	0.45	2.41	24	1
1:B:611:GLU:O	1:B:615:GLN:HG2	0.45	2.12	26	1
1:A:626:MET:HE2	1:B:627:LYS:CB	0.45	2.42	5	1
1:A:627:LYS:O	1:A:630:GLN:HG2	0.45	2.12	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:645:LYS:O	1:C:649:LEU:HG	0.45	2.12	9	1
1:B:646:LYS:HB3	1:B:650:ARG:NH1	0.45	2.27	17	1
1:A:627:LYS:CB	1:C:626:MET:HE2	0.45	2.42	5	1
1:A:652:GLN:CA	1:C:651:LEU:HD21	0.45	2.41	5	1
1:A:623:ILE:HD13	1:C:623:ILE:CG1	0.45	2.41	24	1
1:A:654:GLU:O	1:A:658:ILE:HG22	0.45	2.12	24	1
1:B:654:GLU:O	1:B:658:ILE:HG22	0.45	2.12	24	1
1:B:626:MET:HE2	1:C:627:LYS:CB	0.44	2.42	5	1
1:B:645:LYS:O	1:B:649:LEU:HG	0.44	2.12	9	1
1:A:642:ASP:O	1:A:646:LYS:HG3	0.44	2.12	10	1
1:B:640:GLU:HA	1:B:643:GLU:OE1	0.44	2.11	17	1
1:C:662:LEU:HA	1:C:665:LYS:HD3	0.44	1.88	21	1
1:C:611:GLU:O	1:C:615:GLN:HG2	0.44	2.12	26	1
1:C:616:VAL:HA	1:C:619:LEU:HD12	0.44	1.87	1	1
1:C:662:LEU:HD23	1:C:663:GLN:HE21	0.44	1.70	4	1
1:B:630:GLN:NE2	1:C:630:GLN:HB3	0.44	2.27	5	1
1:C:631:LYS:O	1:C:635:LYS:HB2	0.44	2.12	17	2
1:A:626:MET:HG2	1:B:630:GLN:NE2	0.44	2.27	25	2
1:C:627:LYS:O	1:C:630:GLN:HG2	0.44	2.12	7	2
1:A:640:GLU:HA	1:A:643:GLU:OE1	0.44	2.11	17	1
1:A:611:GLU:O	1:A:615:GLN:HG2	0.44	2.12	26	1
1:A:616:VAL:HA	1:A:619:LEU:HD12	0.44	1.87	1	1
1:A:619:LEU:HD22	1:B:623:ILE:HD13	0.44	1.88	5	1
1:B:642:ASP:O	1:B:646:LYS:HG3	0.44	2.12	10	1
1:A:648:ARG:HH11	1:A:652:GLN:HG3	0.44	1.72	14	1
1:B:655:VAL:O	1:B:659:LYS:HB2	0.44	2.13	15	1
1:B:637:LEU:HD21	1:C:638:LEU:HA	0.44	1.89	15	2
1:B:651:LEU:HD21	1:C:652:GLN:CA	0.44	2.41	5	1
1:A:645:LYS:O	1:A:649:LEU:HG	0.44	2.12	9	1
1:A:627:LYS:HZ1	1:C:629:GLN:HB3	0.44	1.72	22	1
1:C:654:GLU:O	1:C:658:ILE:HG22	0.44	2.12	24	1
1:A:630:GLN:NE2	1:B:630:GLN:HB3	0.44	2.27	5	1
1:A:630:GLN:HB3	1:C:630:GLN:NE2	0.44	2.27	5	1
1:A:630:GLN:NE2	1:C:626:MET:HG2	0.44	2.27	25	2
1:A:659:LYS:HD2	1:A:663:GLN:HE21	0.44	1.73	12	1
1:B:631:LYS:O	1:B:635:LYS:HB2	0.44	2.12	17	1
1:C:646:LYS:HB3	1:C:650:ARG:NH1	0.44	2.27	17	1
1:B:626:MET:HG2	1:C:630:GLN:NE2	0.44	2.28	7	2
1:A:629:GLN:O	1:A:633:GLU:HG3	0.44	2.11	23	1
1:C:628:ASP:HB3	1:C:632:ARG:NH2	0.44	2.28	28	1
1:C:619:LEU:O	1:C:623:ILE:HG13	0.44	2.13	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:659:LYS:HD2	1:C:663:GLN:HE21	0.44	1.73	12	1
1:B:619:LEU:O	1:B:623:ILE:HG13	0.43	2.13	2	2
1:C:648:ARG:HH11	1:C:652:GLN:HG3	0.43	1.72	14	1
1:A:655:VAL:O	1:A:659:LYS:HB2	0.43	2.13	15	1
1:C:656:ASN:O	1:C:660:LYS:HG3	0.43	2.13	3	1
1:B:637:LEU:HD22	1:C:637:LEU:CB	0.43	2.43	17	1
1:B:615:GLN:HG2	1:B:619:LEU:CD1	0.43	2.44	19	1
1:A:629:GLN:HB3	1:B:627:LYS:HZ1	0.43	1.72	22	1
1:A:619:LEU:O	1:A:623:ILE:HG13	0.43	2.13	2	3
1:B:612:LEU:HD21	1:C:613:ARG:CA	0.43	2.39	5	1
1:B:659:LYS:HD2	1:B:663:GLN:HE21	0.43	1.73	12	1
1:A:646:LYS:HB3	1:A:650:ARG:NH1	0.43	2.27	17	1
1:B:651:LEU:CD2	1:C:655:VAL:HG21	0.43	2.43	19	1
1:C:615:GLN:HG2	1:C:619:LEU:CD1	0.43	2.44	19	1
1:A:628:ASP:HB3	1:A:632:ARG:NH2	0.43	2.28	28	1
1:A:658:ILE:HD11	1:B:659:LYS:HG2	0.43	1.90	12	1
1:B:651:LEU:HG	1:C:652:GLN:HG3	0.43	1.91	24	1
1:C:649:LEU:HA	1:C:652:GLN:HG3	0.43	1.89	7	1
1:A:627:LYS:HG3	1:C:626:MET:HG3	0.43	1.91	12	1
1:B:648:ARG:HA	1:C:648:ARG:HD3	0.43	1.91	11	1
1:A:626:MET:HG3	1:B:627:LYS:HG3	0.43	1.91	12	1
1:A:659:LYS:HG2	1:C:658:ILE:HD11	0.43	1.90	12	1
1:B:628:ASP:HB3	1:B:632:ARG:NH2	0.43	2.28	28	1
1:B:656:ASN:O	1:B:660:LYS:HG3	0.43	2.13	3	1
1:A:655:VAL:HG21	1:C:651:LEU:CD2	0.43	2.43	19	1
1:B:619:LEU:HD22	1:C:623:ILE:HD13	0.43	1.88	5	1
1:B:648:ARG:HH11	1:B:652:GLN:HG3	0.43	1.72	14	1
1:A:632:ARG:NE	1:A:632:ARG:HA	0.43	2.29	18	1
1:A:651:LEU:CD2	1:B:655:VAL:HG21	0.43	2.43	19	1
1:A:619:LEU:HD22	1:B:620:ARG:HD2	0.43	1.91	14	1
1:A:637:LEU:HD21	1:B:638:LEU:HA	0.43	1.90	15	2
1:A:649:LEU:O	1:A:653:MET:HG2	0.43	2.14	23	1
1:A:630:GLN:HG2	1:B:630:GLN:HG2	0.43	1.91	2	2
1:A:656:ASN:O	1:A:660:LYS:HG3	0.43	2.13	3	1
1:A:648:ARG:HD3	1:C:648:ARG:HA	0.43	1.90	11	1
1:C:655:VAL:O	1:C:659:LYS:HB2	0.43	2.13	15	1
1:A:615:GLN:HG2	1:A:619:LEU:CD1	0.43	2.44	19	1
1:C:632:ARG:NE	1:C:632:ARG:HA	0.42	2.29	18	1
1:B:630:GLN:HG2	1:C:630:GLN:HG2	0.42	1.91	2	2
1:A:623:ILE:CG2	1:C:626:MET:SD	0.42	3.08	4	1
1:A:638:LEU:HA	1:C:637:LEU:HD21	0.42	1.90	29	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:631:LYS:HZ1	1:C:629:GLN:HG3	0.42	1.75	18	1
1:B:632:ARG:NE	1:B:632:ARG:HA	0.42	2.29	18	1
1:B:649:LEU:O	1:B:653:MET:HG2	0.42	2.14	23	1
1:A:652:GLN:HG3	1:C:651:LEU:HG	0.42	1.91	24	1
1:B:658:ILE:HD11	1:C:659:LYS:HG2	0.42	1.90	12	1
1:A:631:LYS:HA	1:A:631:LYS:HD3	0.42	1.56	13	1
1:A:637:LEU:CB	1:C:637:LEU:HD22	0.42	2.43	17	1
1:C:649:LEU:O	1:C:653:MET:HG2	0.42	2.14	23	1
1:A:651:LEU:HG	1:B:652:GLN:HG3	0.42	1.91	24	1
1:A:630:GLN:HG2	1:C:630:GLN:HG2	0.42	1.91	2	2
1:A:645:LYS:HE3	1:C:640:GLU:HG2	0.42	1.92	7	1
1:B:626:MET:HG3	1:C:627:LYS:HG3	0.42	1.91	12	1
1:C:660:LYS:HA	1:C:660:LYS:HZ2	0.42	1.73	15	1
1:B:652:GLN:HB3	1:B:653:MET:HE2	0.42	1.90	22	1
1:C:622:ILE:HG23	1:C:626:MET:HE3	0.42	1.91	22	1
1:A:648:ARG:HD3	1:C:644:GLU:HG2	0.42	1.92	27	1
1:A:626:MET:SD	1:B:623:ILE:CG2	0.42	3.07	4	1
1:B:622:ILE:HG23	1:B:626:MET:HE3	0.42	1.91	22	1
1:A:655:VAL:HG21	1:C:651:LEU:CD1	0.42	2.44	27	1
1:A:641:LEU:O	1:A:645:LYS:HG3	0.42	2.15	7	2
1:A:620:ARG:HD2	1:C:619:LEU:HD22	0.42	1.91	14	1
1:B:660:LYS:HZ2	1:B:660:LYS:HA	0.42	1.74	15	1
1:A:658:ILE:HD11	1:B:655:VAL:HG13	0.42	1.90	16	1
1:B:611:GLU:O	1:B:614:THR:CG2	0.42	2.68	29	1
1:C:643:GLU:HG2	1:C:647:ILE:HD11	0.42	1.92	2	1
1:A:662:LEU:HD13	1:C:658:ILE:CG2	0.42	2.45	7	1
1:B:643:GLU:OE1	1:B:643:GLU:HA	0.42	2.14	15	1
1:B:658:ILE:HD11	1:C:655:VAL:HG13	0.42	1.90	16	1
1:A:659:LYS:HE3	1:C:658:ILE:HB	0.42	1.92	20	1
1:A:652:GLN:HB3	1:A:653:MET:HE2	0.42	1.90	22	1
1:B:619:LEU:HD11	1:C:620:ARG:HB2	0.42	1.92	24	1
1:C:611:GLU:O	1:C:614:THR:CG2	0.42	2.68	29	1
1:C:641:LEU:O	1:C:645:LYS:HG3	0.42	2.14	4	2
1:A:648:ARG:HA	1:B:648:ARG:HD3	0.42	1.91	11	1
1:C:644:GLU:HA	1:C:647:ILE:CG2	0.42	2.45	14	1
1:C:644:GLU:O	1:C:648:ARG:HB2	0.42	2.15	29	1
1:B:626:MET:SD	1:C:623:ILE:CG2	0.42	3.07	4	1
1:B:629:GLN:HG3	1:C:631:LYS:HZ1	0.42	1.75	18	1
1:A:658:ILE:HB	1:B:659:LYS:HE3	0.42	1.92	20	1
1:A:622:ILE:HG23	1:A:626:MET:HE3	0.42	1.91	22	1
1:B:641:LEU:O	1:B:645:LYS:HG3	0.41	2.15	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:619:LEU:O	1:A:622:ILE:HB	0.41	2.15	8	1
1:A:648:ARG:NH2	1:C:647:ILE:HD13	0.41	2.30	8	1
1:A:658:ILE:CG2	1:B:662:LEU:HD13	0.41	2.45	7	1
1:B:619:LEU:HD11	1:C:623:ILE:HD13	0.41	1.92	12	2
1:B:647:ILE:HD13	1:C:648:ARG:NH2	0.41	2.31	8	1
1:B:658:ILE:HB	1:C:659:LYS:HE3	0.41	1.92	20	1
1:A:620:ARG:HB2	1:C:619:LEU:HD11	0.41	1.92	24	1
1:B:658:ILE:CG2	1:C:662:LEU:HD13	0.41	2.45	7	1
1:B:629:GLN:HB3	1:C:627:LYS:HZ1	0.41	1.74	22	1
1:B:651:LEU:CD1	1:C:655:VAL:HG21	0.41	2.44	27	1
1:A:623:ILE:HD13	1:C:619:LEU:HD11	0.41	1.92	12	2
1:B:644:GLU:HA	1:B:647:ILE:CG2	0.41	2.45	14	1
1:A:611:GLU:O	1:A:614:THR:CG2	0.41	2.68	29	1
1:A:644:GLU:O	1:A:648:ARG:HB2	0.41	2.15	29	1
1:A:644:GLU:HA	1:A:647:ILE:CG2	0.41	2.45	14	1
1:B:619:LEU:HD22	1:C:620:ARG:HD2	0.41	1.91	14	1
1:A:647:ILE:HG22	1:B:652:GLN:HE22	0.41	1.75	26	1
1:A:644:GLU:HG2	1:B:648:ARG:HD3	0.41	1.92	27	1
1:B:640:GLU:HG2	1:C:645:LYS:HE3	0.41	1.92	7	1
1:B:654:GLU:OE2	1:C:655:VAL:HG12	0.41	2.16	23	1
1:A:629:GLN:HB3	1:B:627:LYS:HZ3	0.41	1.75	27	1
1:B:644:GLU:O	1:B:648:ARG:HB2	0.41	2.15	29	1
1:A:640:GLU:HG2	1:B:645:LYS:HE3	0.41	1.92	7	1
1:A:637:LEU:CD2	1:B:637:LEU:HB3	0.41	2.46	1	1
1:B:648:ARG:HH12	1:B:649:LEU:HD12	0.41	1.76	12	1
1:B:606:GLN:O	1:B:610:GLU:HG2	0.41	2.16	13	1
1:B:646:LYS:HA	1:B:646:LYS:HE2	0.41	1.93	18	1
1:C:652:GLN:HB3	1:C:653:MET:HE2	0.41	1.90	22	1
1:A:638:LEU:HG	1:C:637:LEU:CG	0.41	2.46	26	1
1:B:637:LEU:CD2	1:C:637:LEU:HB3	0.41	2.46	1	1
1:A:643:GLU:HG2	1:A:647:ILE:HD11	0.41	1.92	2	1
1:C:612:LEU:HD12	1:C:612:LEU:HA	0.41	1.72	12	1
1:A:606:GLN:O	1:A:610:GLU:HG2	0.41	2.16	13	1
1:A:643:GLU:OE1	1:A:643:GLU:HA	0.41	2.14	15	1
1:C:643:GLU:OE1	1:C:643:GLU:HA	0.41	2.14	15	1
1:A:629:GLN:HG3	1:B:631:LYS:HZ1	0.41	1.75	18	1
1:A:654:GLU:OE2	1:B:655:VAL:HG12	0.41	2.16	23	1
1:A:655:VAL:HG12	1:C:654:GLU:OE2	0.41	2.16	23	1
1:A:642:ASP:O	1:A:646:LYS:HD3	0.41	2.15	25	1
1:C:619:LEU:O	1:C:622:ILE:HB	0.41	2.15	8	1
1:A:645:LYS:HD3	1:C:644:GLU:HG3	0.41	1.93	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:637:LEU:HD22	1:B:637:LEU:CB	0.41	2.43	17	1
1:A:644:GLU:OE2	1:B:644:GLU:HB2	0.41	2.16	17	1
1:C:642:ASP:O	1:C:646:LYS:HD3	0.41	2.15	25	1
1:A:652:GLN:HE22	1:C:647:ILE:HG22	0.41	1.75	26	1
1:C:615:GLN:O	1:C:619:LEU:HG	0.40	2.17	26	1
1:B:644:GLU:HG2	1:C:648:ARG:HD3	0.40	1.92	27	1
1:B:648:ARG:NH1	1:B:648:ARG:HB3	0.40	2.31	27	1
1:A:647:ILE:HD13	1:B:648:ARG:NH2	0.40	2.31	8	1
1:A:655:VAL:HG13	1:C:658:ILE:HD11	0.40	1.90	16	1
1:A:644:GLU:HB2	1:C:644:GLU:OE2	0.40	2.16	17	1
1:C:665:LYS:HG3	1:C:665:LYS:OXT	0.40	2.16	18	1
1:A:637:LEU:HB3	1:C:637:LEU:CD2	0.40	2.46	1	1
1:A:637:LEU:CG	1:B:638:LEU:HG	0.40	2.46	26	1
1:B:637:LEU:CG	1:C:638:LEU:HG	0.40	2.46	26	1
1:C:648:ARG:NH1	1:C:648:ARG:HB3	0.40	2.32	27	1
1:B:633:GLU:HB2	1:C:634:ILE:HD13	0.40	1.93	30	1
1:A:643:GLU:HA	1:A:646:LYS:HE2	0.40	1.94	10	1
1:A:662:LEU:HD21	1:C:661:ALA:CB	0.40	2.45	14	1
1:A:619:LEU:HG	1:B:620:ARG:HD2	0.40	1.94	17	1
1:A:619:LEU:HD11	1:B:620:ARG:HB2	0.40	1.92	24	1
1:B:615:GLN:O	1:B:619:LEU:HG	0.40	2.16	26	1
1:A:629:GLN:HB3	1:B:627:LYS:NZ	0.40	2.31	27	1
1:A:659:LYS:HD2	1:C:658:ILE:HD11	0.40	1.94	29	1
1:A:643:GLU:HA	1:A:646:LYS:HD2	0.40	1.94	1	1
1:C:648:ARG:HH12	1:C:649:LEU:HD12	0.40	1.76	12	1
1:A:612:LEU:HD22	1:B:613:ARG:HE	0.40	1.77	25	1
1:B:642:ASP:O	1:B:646:LYS:HD3	0.40	2.15	25	1
1:A:648:ARG:HB3	1:A:648:ARG:NH1	0.40	2.32	27	1
1:A:658:ILE:HD11	1:B:659:LYS:HD2	0.40	1.94	29	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	60/75 (80%)	60±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	60/75 (80%)	60±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	C	60/75 (80%)	60±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	5400/6750 (80%)	5394 (100%)	6 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	57/68 (84%)	35±3 (62±5%)	22±3 (38±5%)	0	7
1	B	57/68 (84%)	35±3 (62±5%)	22±3 (38±5%)	0	7
1	C	58/68 (85%)	36±3 (61±5%)	22±3 (39±5%)	0	6
All	All	5160/6120 (84%)	3175 (62%)	1985 (38%)	0	6

All 172 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	641	LEU	28
1	B	641	LEU	28
1	C	641	LEU	28
1	A	630	GLN	26
1	B	630	GLN	26
1	C	630	GLN	26
1	A	617	ARG	25
1	B	617	ARG	25
1	C	617	ARG	25
1	A	635	LYS	20
1	B	635	LYS	20
1	C	635	LYS	20
1	A	644	GLU	19
1	A	662	LEU	19
1	B	644	GLU	19
1	B	662	LEU	19

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Mol	Chain	Res	Type	Models (Total)
1	C	644	GLU	19
1	C	662	LEU	19
1	A	648	ARG	19
1	B	648	ARG	19
1	C	648	ARG	19
1	A	637	LEU	18
1	B	637	LEU	18
1	C	637	LEU	18
1	A	632	ARG	18
1	A	639	SER	18
1	A	660	LYS	18
1	B	632	ARG	18
1	B	639	SER	18
1	B	660	LYS	18
1	C	632	ARG	18
1	C	639	SER	18
1	C	660	LYS	18
1	A	614	THR	17
1	B	614	THR	17
1	C	614	THR	17
1	A	636	GLN	17
1	B	636	GLN	17
1	C	636	GLN	17
1	A	606	GLN	16
1	A	646	LYS	16
1	B	606	GLN	16
1	B	646	LYS	16
1	C	606	GLN	16
1	C	646	LYS	16
1	A	653	MET	16
1	B	653	MET	16
1	C	653	MET	16
1	A	631	LYS	15
1	B	631	LYS	15
1	C	631	LYS	15
1	A	649	LEU	15
1	A	651	LEU	15
1	B	649	LEU	15
1	B	651	LEU	15
1	C	649	LEU	15
1	C	651	LEU	15
1	A	623	ILE	15

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Mol	Chain	Res	Type	Models (Total)
1	B	623	ILE	15
1	C	623	ILE	15
1	A	659	LYS	14
1	B	659	LYS	14
1	C	659	LYS	14
1	A	618	GLU	14
1	B	618	GLU	14
1	C	618	GLU	14
1	A	663	GLN	14
1	B	663	GLN	14
1	C	663	GLN	14
1	C	665	LYS	14
1	A	619	LEU	13
1	B	619	LEU	13
1	C	619	LEU	13
1	A	611	GLU	11
1	B	611	GLU	11
1	C	611	GLU	11
1	A	642	ASP	11
1	A	657	ASP	11
1	B	642	ASP	11
1	B	657	ASP	11
1	C	642	ASP	11
1	C	657	ASP	11
1	A	612	LEU	10
1	A	624	GLU	10
1	B	612	LEU	10
1	B	624	GLU	10
1	C	612	LEU	10
1	C	624	GLU	10
1	A	627	LYS	10
1	A	638	LEU	10
1	B	627	LYS	10
1	B	638	LEU	10
1	C	627	LYS	10
1	C	638	LEU	10
1	A	629	GLN	10
1	B	629	GLN	10
1	C	629	GLN	10
1	A	625	THR	10
1	B	625	THR	10
1	C	625	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	621	SER	10
1	B	621	SER	10
1	C	621	SER	10
1	A	640	GLU	9
1	B	640	GLU	9
1	C	640	GLU	9
1	A	628	ASP	8
1	A	654	GLU	8
1	B	628	ASP	8
1	B	654	GLU	8
1	C	628	ASP	8
1	C	654	GLU	8
1	A	643	GLU	8
1	A	664	SER	8
1	B	643	GLU	8
1	B	664	SER	8
1	C	643	GLU	8
1	C	664	SER	8
1	A	620	ARG	8
1	B	620	ARG	8
1	C	620	ARG	8
1	A	615	GLN	8
1	B	615	GLN	8
1	C	615	GLN	8
1	A	605	SER	7
1	B	605	SER	7
1	C	605	SER	7
1	A	658	ILE	7
1	B	658	ILE	7
1	C	658	ILE	7
1	A	634	ILE	7
1	B	634	ILE	7
1	C	634	ILE	7
1	A	652	GLN	7
1	B	652	GLN	7
1	C	652	GLN	7
1	A	610	GLU	6
1	B	610	GLU	6
1	C	610	GLU	6
1	A	609	VAL	5
1	B	609	VAL	5
1	C	609	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	647	ILE	5
1	B	647	ILE	5
1	C	647	ILE	5
1	A	645	LYS	5
1	B	645	LYS	5
1	C	645	LYS	5
1	A	650	ARG	5
1	B	650	ARG	5
1	C	650	ARG	5
1	A	626	MET	4
1	B	626	MET	4
1	C	626	MET	4
1	A	656	ASN	4
1	B	656	ASN	4
1	C	656	ASN	4
1	A	616	VAL	3
1	B	616	VAL	3
1	C	616	VAL	3
1	A	633	GLU	3
1	B	633	GLU	3
1	C	633	GLU	3
1	A	622	ILE	2
1	B	622	ILE	2
1	C	622	ILE	2
1	A	655	VAL	1
1	B	655	VAL	1
1	C	655	VAL	1
1	A	613	ARG	1
1	B	613	ARG	1
1	C	613	ARG	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 [i](#)

There are no oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 20% for the well-defined parts and 20% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	657
Number of shifts mapped to atoms	657
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	73	-0.45 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	71	0.88 ± 0.14	Should be checked
$^{13}\text{C}'$	71	2.56 ± 0.05	Should be applied
^{15}N	71	-0.30 ± 0.18	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 20%, i.e. 553 atoms were assigned a chemical shift out of a possible 2736. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	238/905 (26%)	60/362 (17%)	118/362 (33%)	60/181 (33%)
Sidechain	315/1831 (17%)	191/1169 (16%)	116/562 (21%)	8/100 (8%)

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	Total	¹H	¹³C	¹⁵N
Overall	553/2736 (20%)	251/1531 (16%)	234/924 (25%)	68/281 (24%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 20%, i.e. 657 atoms were assigned a chemical shift out of a possible 3276. 0 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	286/1119 (26%)	71/450 (16%)	144/450 (32%)	71/219 (32%)
Sidechain	371/2133 (17%)	230/1365 (17%)	133/660 (20%)	8/108 (7%)
Aromatic	0/24 (0%)	0/12 (0%)	0/6 (0%)	0/6 (0%)
Overall	657/3276 (20%)	301/1827 (16%)	277/1116 (25%)	79/333 (24%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

