



# Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2020 – 03:05 pm BST

PDB ID : 2LCT  
Title : Solution structure of the Vav1 SH2 domain complexed with a Syk-derived doubly phosphorylated peptide  
Authors : Chen, C.; Gorenstein, N.; Post, C.  
Deposited on : 2011-05-09

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

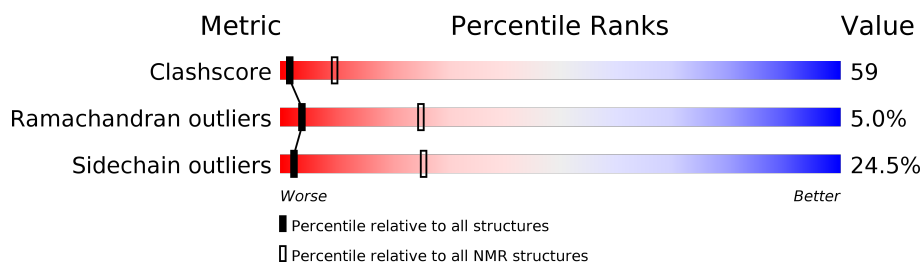
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	107	
2	B	13	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:666-A:696, A:705-A:766 (93)	0.17	2

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 1 single-model cluster was found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1940 atoms, of which 957 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Proto-oncogene vav.

Mol	Chain	Residues	Atoms						Trace
1	A	107	Total	C	H	N	O	S	0
			1741	555	873	149	160	4	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	661	GLY	-	EXPRESSION TAG	UNP P15498
A	662	HIS	-	EXPRESSION TAG	UNP P15498
A	663	MET	-	EXPRESSION TAG	UNP P15498

- Molecule 2 is a protein called Tyrosine-protein kinase SYK.

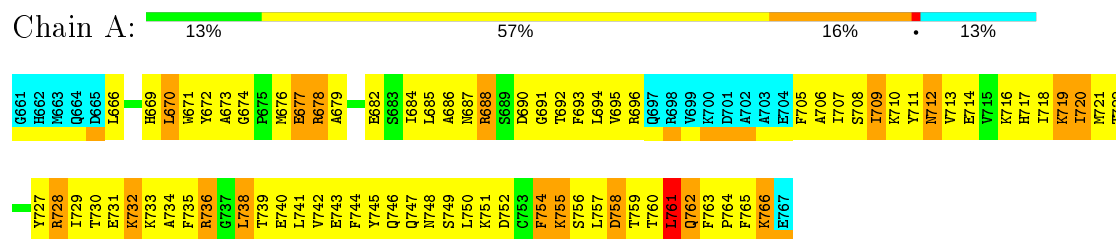
Mol	Chain	Residues	Atoms						Trace
2	B	13	Total	C	H	N	O	P	0
			199	66	84	13	34	2	

## 4 Residue-property plots [i](#)

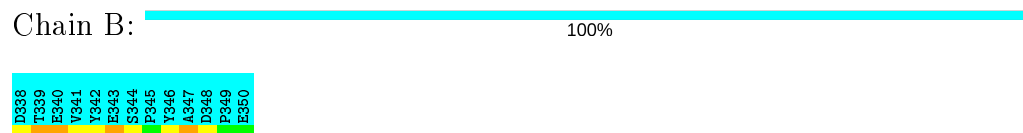
### 4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Proto-oncogene vav



- Molecule 2: Tyrosine-protein kinase SYK

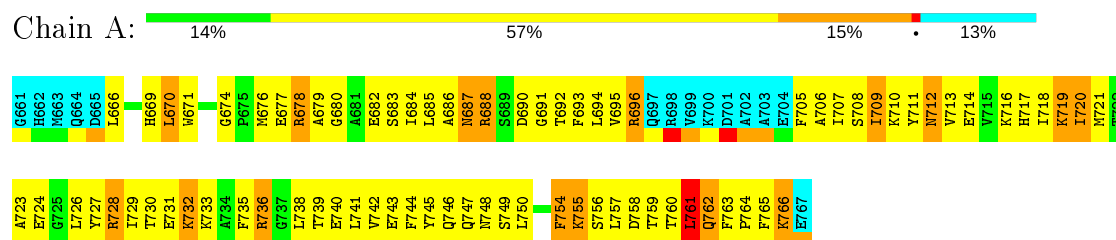


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

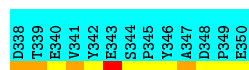
#### 4.2.1 Score per residue for model 1

- Molecule 1: Proto-oncogene vav




- Molecule 2: Tyrosine-protein kinase SYK

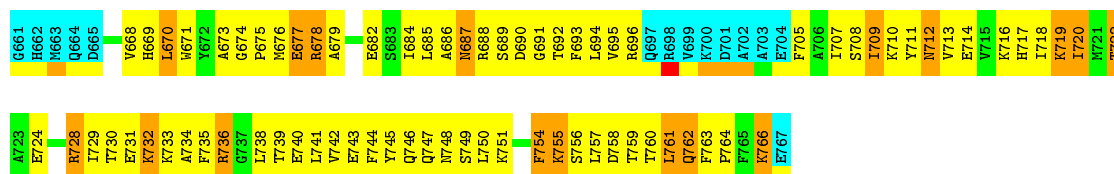
Chain B:  100%



#### 4.2.2 Score per residue for model 2 (medoid)

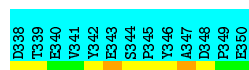
- Molecule 1: Proto-oncogene vav

Chain A:  16% 55% 16% 13%




- Molecule 2: Tyrosine-protein kinase SYK

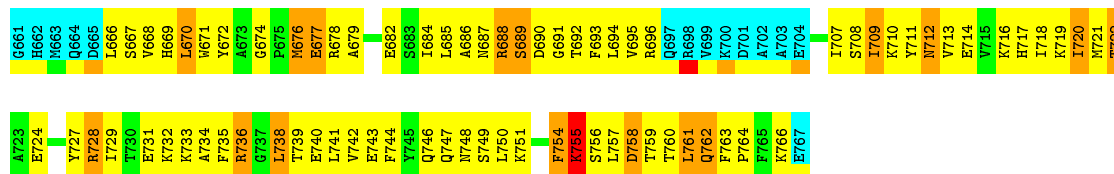
Chain B:  100%



#### 4.2.3 Score per residue for model 3

- Molecule 1: Proto-oncogene vav

Chain A:  16% 55% 15% 13%



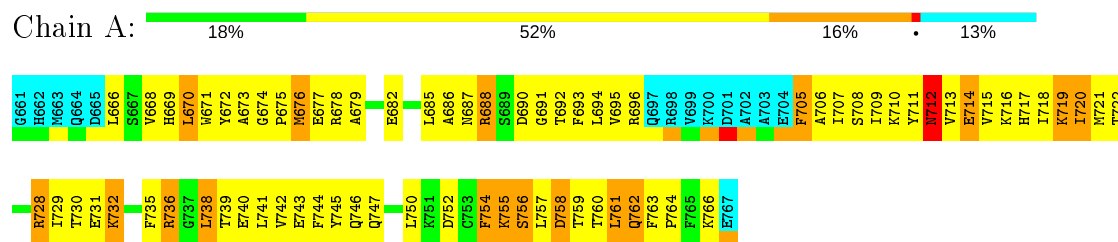
- Molecule 2: Tyrosine-protein kinase SYK

Chain B:  100%

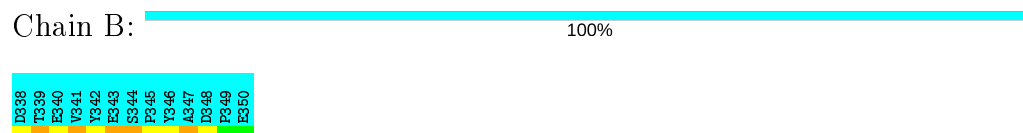


#### 4.2.4 Score per residue for model 4

- Molecule 1: Proto-oncogene vav

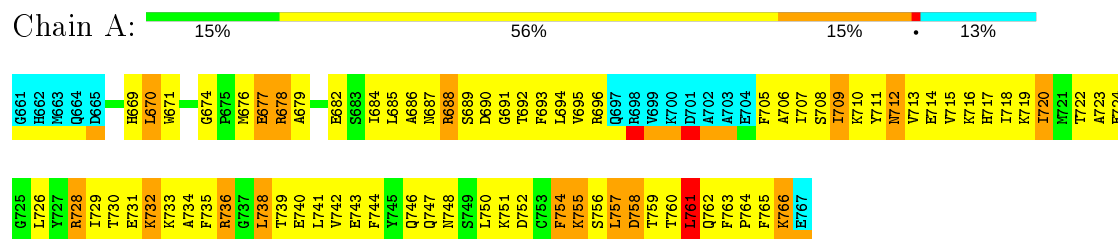


- Molecule 2: Tyrosine-protein kinase SYK

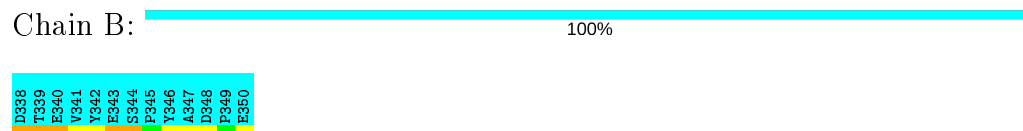


#### 4.2.5 Score per residue for model 5

- Molecule 1: Proto-oncogene vav

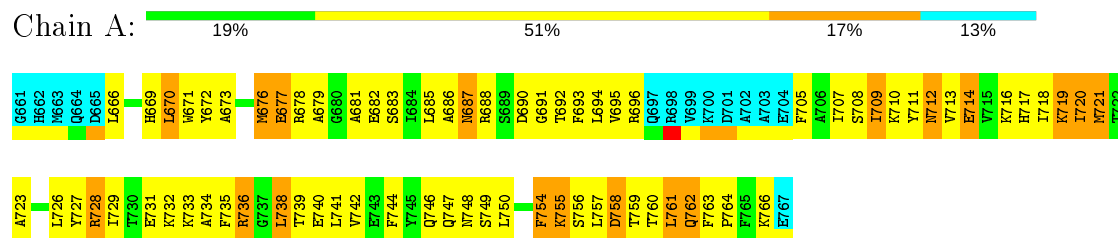


- Molecule 2: Tyrosine-protein kinase SYK



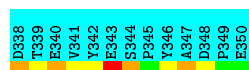
#### 4.2.6 Score per residue for model 6

- Molecule 1: Proto-oncogene vav



- Molecule 2: Tyrosine-protein kinase SYK

Chain B:  100%



#### 4.2.7 Score per residue for model 7

- Molecule 1: Proto-oncogene vav

Chain A:  16% 58% 13% 13%




- Molecule 2: Tyrosine-protein kinase SYK

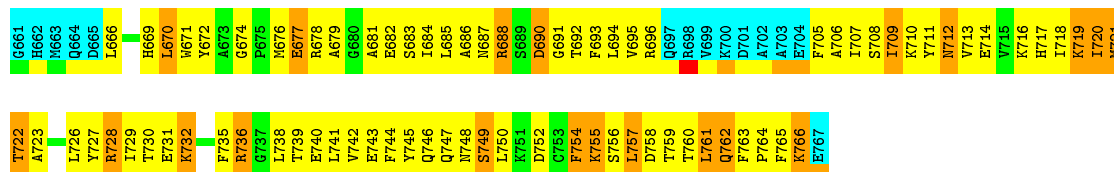
Chain B:  100%



#### 4.2.8 Score per residue for model 8

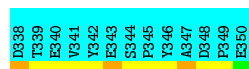
- Molecule 1: Proto-oncogene vav

Chain A:  13% 55% 19% 13%



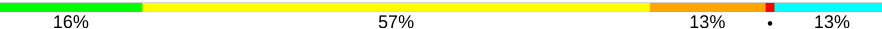
- Molecule 2: Tyrosine-protein kinase SYK

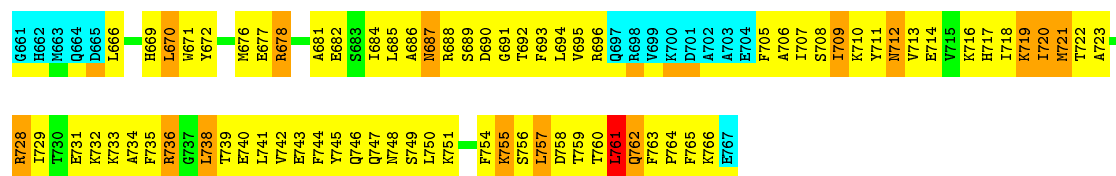
Chain B:  100%



#### 4.2.9 Score per residue for model 9

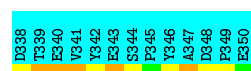
- Molecule 1: Proto-oncogene vav

Chain A: 




- Molecule 2: Tyrosine-protein kinase SYK

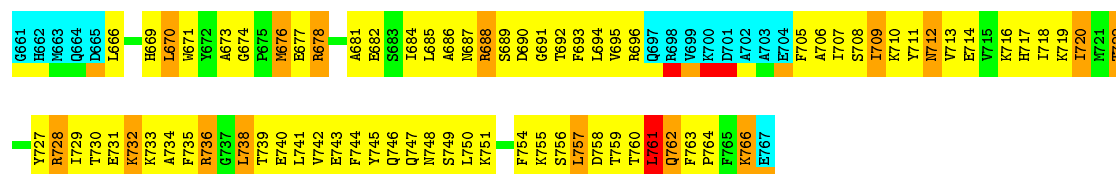
Chain B: 



#### 4.2.10 Score per residue for model 10

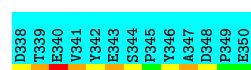
- Molecule 1: Proto-oncogene vav

Chain A: 




- Molecule 2: Tyrosine-protein kinase SYK

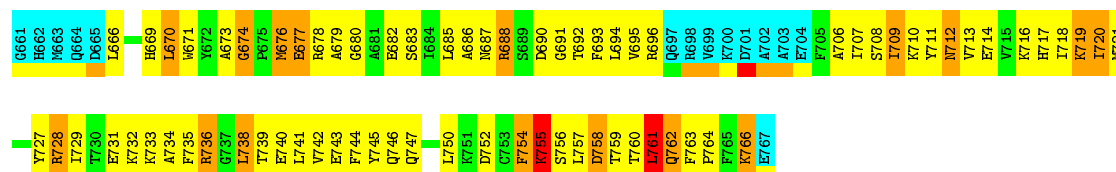
Chain B: 



#### 4.2.11 Score per residue for model 11

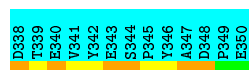
- Molecule 1: Proto-oncogene vav

Chain A: 




- Molecule 2: Tyrosine-protein kinase SYK

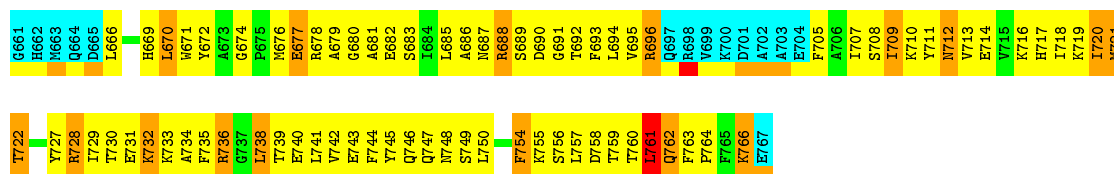
Chain B:  100%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Proto-oncogene vav

Chain A:  15% 56% 15% 13%




- Molecule 2: Tyrosine-protein kinase SYK

Chain B:  100%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Proto-oncogene vav

Chain A:  14% 57% 15% 13%



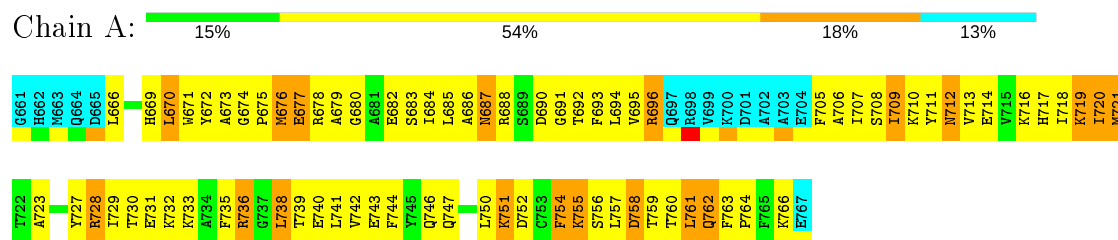
- Molecule 2: Tyrosine-protein kinase SYK

Chain B:  100%

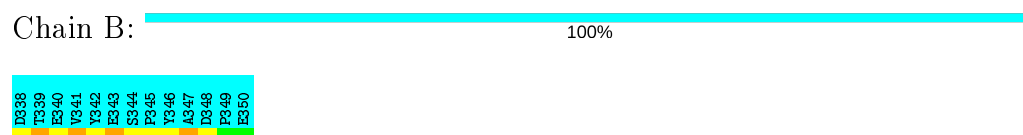


#### 4.2.14 Score per residue for model 14

- Molecule 1: Proto-oncogene vav

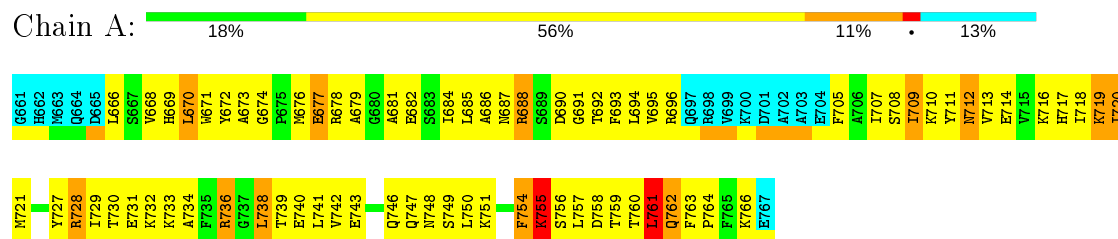


- Molecule 2: Tyrosine-protein kinase SYK

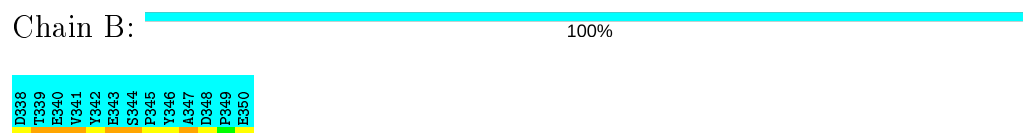


#### 4.2.15 Score per residue for model 15

- Molecule 1: Proto-oncogene vav

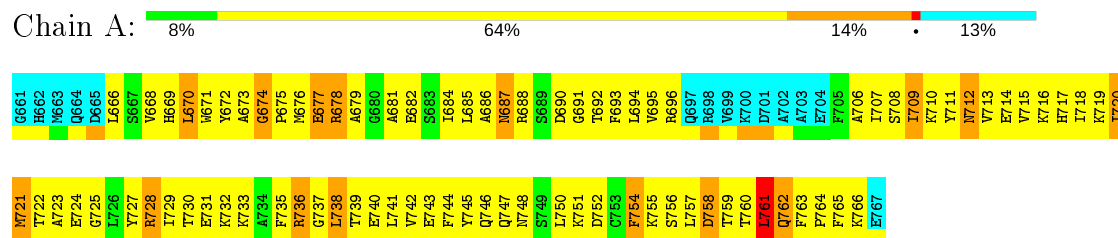


- Molecule 2: Tyrosine-protein kinase SYK



#### 4.2.16 Score per residue for model 16

- Molecule 1: Proto-oncogene vav



- Molecule 2: Tyrosine-protein kinase SYK

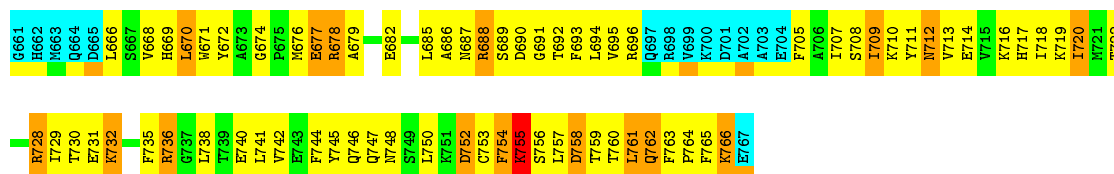
Chain B:  100%



#### 4.2.17 Score per residue for model 17

- Molecule 1: Proto-oncogene vav

Chain A:  21% 50% 15% 13%



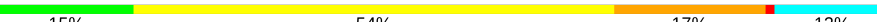
- Molecule 2: Tyrosine-protein kinase SYK

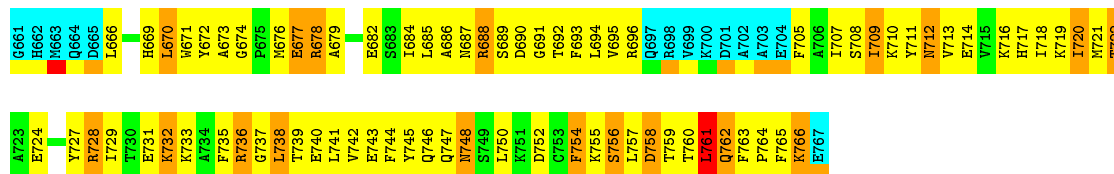
Chain B:  100%



#### 4.2.18 Score per residue for model 18

- Molecule 1: Proto-oncogene vav

Chain A:  15% 54% 17% 13%



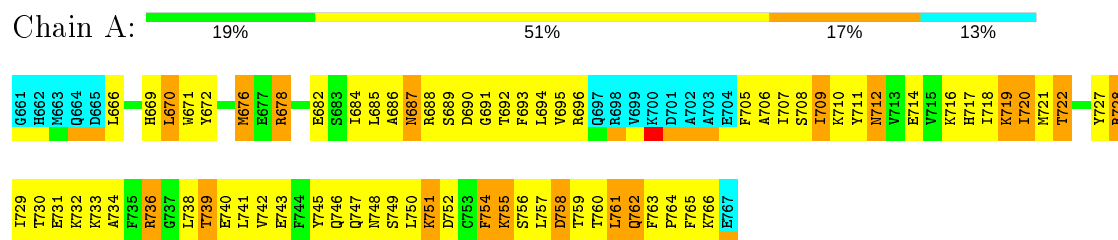
- Molecule 2: Tyrosine-protein kinase SYK

Chain B:  100%

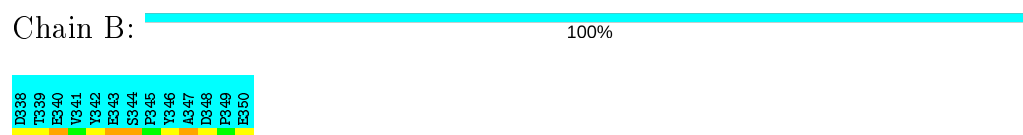


#### 4.2.19 Score per residue for model 19

- Molecule 1: Proto-oncogene vav

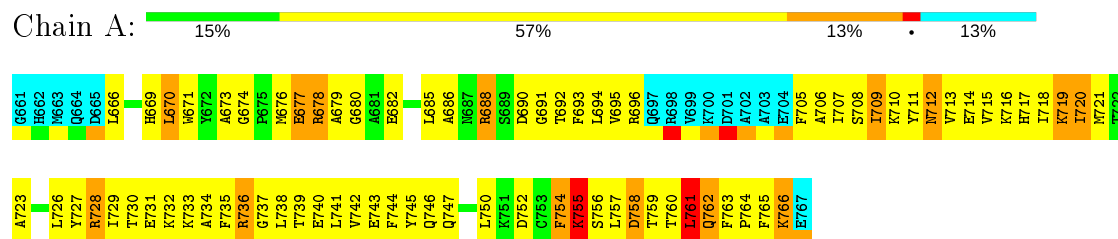


- Molecule 2: Tyrosine-protein kinase SYK

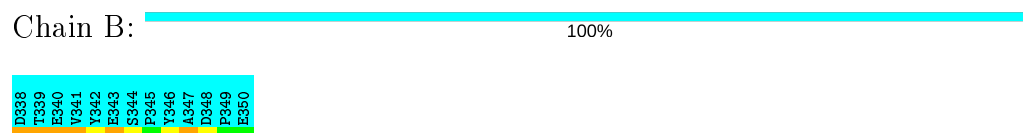


#### 4.2.20 Score per residue for model 20

- Molecule 1: Proto-oncogene vav



- Molecule 2: Tyrosine-protein kinase SYK



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	
X-PLOR NIH	structure solution	
X-PLOR NIH	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1221
Number of shifts mapped to atoms	1221
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

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	756	770	768	90±6
2	B	0	0	0	0±0
All	All	15120	15400	15360	1795

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 59.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:670:LEU:HD23	1:A:670:LEU:N	0.96	1.75	1	15
1:A:670:LEU:N	1:A:670:LEU:HD23	0.96	1.75	17	5
1:A:707:ILE:HD13	1:A:729:ILE:HG23	0.95	1.36	14	20
1:A:685:LEU:HD13	1:A:694:LEU:HD23	0.84	1.49	16	20
1:A:670:LEU:HD23	1:A:670:LEU:H	0.83	1.32	10	12
1:A:666:LEU:HD13	1:A:738:LEU:HD12	0.81	1.52	17	4
1:A:693:PHE:HB3	1:A:709:ILE:HG23	0.80	1.51	6	19
1:A:670:LEU:H	1:A:670:LEU:HD23	0.78	1.36	8	8
1:A:729:ILE:HG13	1:A:741:LEU:HD11	0.77	1.55	10	20
1:A:693:PHE:CD1	1:A:761:LEU:HD12	0.77	2.15	2	18
1:A:729:ILE:CG1	1:A:741:LEU:HD11	0.77	2.10	10	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:694:LEU:HD12	1:A:695:VAL:N	0.76	1.95	4	19
1:A:696:ARG:HG3	1:A:706:ALA:HB3	0.76	1.56	1	7
1:A:670:LEU:N	1:A:670:LEU:CD2	0.75	2.50	17	6
1:A:670:LEU:CD2	1:A:670:LEU:N	0.74	2.50	8	14
1:A:707:ILE:HD11	1:A:720:ILE:HG13	0.73	1.59	13	20
1:A:705:PHE:CD2	1:A:738:LEU:HD11	0.72	2.19	1	2
1:A:720:ILE:HD11	1:A:741:LEU:HD12	0.72	1.62	14	16
1:A:755:LYS:NZ	1:A:756:SER:OG	0.72	2.22	4	19
1:A:693:PHE:CD2	1:A:761:LEU:HD12	0.72	2.19	15	2
1:A:696:ARG:CG	1:A:706:ALA:HB3	0.72	2.15	10	8
1:A:739:THR:HG22	1:A:743:GLU:HG3	0.72	1.60	19	1
1:A:695:VAL:HG21	1:A:742:VAL:HG21	0.71	1.61	1	19
1:A:669:HIS:CD2	1:A:671:TRP:CZ2	0.71	2.78	7	20
1:A:688:ARG:O	1:A:710:LYS:NZ	0.71	2.24	2	20
1:A:685:LEU:CD1	1:A:694:LEU:HD23	0.70	2.16	4	14
1:A:693:PHE:N	1:A:763:PHE:O	0.69	2.25	20	20
1:A:676:MET:O	1:A:696:ARG:NE	0.69	2.25	11	16
1:A:677:GLU:OE1	1:A:679:ALA:HB3	0.69	1.87	13	15
1:A:669:HIS:NE2	1:A:739:THR:OG1	0.69	2.24	9	17
1:A:716:LYS:HD2	1:A:757:LEU:HD21	0.68	1.63	10	19
1:A:686:ALA:O	1:A:710:LYS:NZ	0.68	2.26	3	20
1:A:750:LEU:HD22	1:A:754:PHE:CZ	0.67	2.24	20	10
1:A:708:SER:OG	1:A:717:HIS:ND1	0.66	2.22	6	20
1:A:707:ILE:HD12	1:A:707:ILE:H	0.66	1.49	1	9
1:A:750:LEU:HD22	1:A:754:PHE:CE1	0.66	2.25	14	12
1:A:751:LYS:NZ	1:A:758:ASP:OD1	0.65	2.30	16	8
1:A:729:ILE:HD12	1:A:745:TYR:CD2	0.65	2.26	18	9
1:A:707:ILE:H	1:A:707:ILE:HD12	0.65	1.51	3	11
1:A:714:GLU:OE2	1:A:716:LYS:NZ	0.65	2.30	16	17
1:A:761:LEU:CD2	1:A:761:LEU:N	0.65	2.60	10	8
1:A:730:THR:HG23	1:A:732:LYS:H	0.65	1.52	4	13
1:A:707:ILE:HD11	1:A:720:ILE:CG1	0.65	2.22	18	20
1:A:750:LEU:HD13	1:A:754:PHE:CE2	0.65	2.27	10	5
1:A:705:PHE:CG	1:A:738:LEU:HD11	0.64	2.26	1	2
1:A:666:LEU:HD22	1:A:738:LEU:HB2	0.64	1.69	19	3
1:A:692:THR:O	1:A:710:LYS:N	0.64	2.27	20	20
1:A:733:LYS:NZ	1:A:734:ALA:O	0.64	2.31	7	13
1:A:761:LEU:N	1:A:761:LEU:CD2	0.64	2.61	20	12
1:A:695:VAL:HG11	1:A:738:LEU:HD11	0.63	1.70	3	9
1:A:760:THR:O	1:A:762:GLN:N	0.63	2.31	5	20
1:A:705:PHE:O	1:A:720:ILE:N	0.63	2.28	14	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:687:ASN:OD1	1:A:688:ARG:NH1	0.62	2.27	4	12
1:A:688:ARG:NH2	1:A:765:PHE:O	0.62	2.25	18	7
1:A:694:LEU:C	1:A:694:LEU:HD12	0.62	2.15	5	11
1:A:707:ILE:HD11	1:A:720:ILE:CD1	0.62	2.25	4	7
1:A:714:GLU:OE1	1:A:716:LYS:NZ	0.62	2.30	11	3
1:A:741:LEU:C	1:A:741:LEU:HD13	0.62	2.15	13	14
1:A:736:ARG:NH1	1:A:740:GLU:OE1	0.62	2.30	8	11
1:A:692:THR:HG23	1:A:764:PRO:O	0.61	1.96	20	9
1:A:694:LEU:HD12	1:A:694:LEU:C	0.61	2.15	7	7
1:A:759:THR:OG1	1:A:762:GLN:NE2	0.61	2.31	12	1
1:A:714:GLU:CD	1:A:716:LYS:NZ	0.61	2.54	19	3
1:A:728:ARG:NE	1:A:731:GLU:HA	0.61	2.11	7	20
1:A:682:GLU:OE1	1:A:717:HIS:NE2	0.61	2.34	11	20
1:A:729:ILE:HG21	1:A:754:PHE:CZ	0.59	2.32	9	6
1:A:719:LYS:NZ	1:A:731:GLU:OE2	0.59	2.33	20	9
1:A:676:MET:O	1:A:696:ARG:NH2	0.59	2.33	17	2
1:A:718:ILE:CD1	1:A:754:PHE:CE2	0.59	2.85	6	13
1:A:707:ILE:HD12	1:A:718:ILE:O	0.59	1.98	9	7
1:A:684:ILE:HG22	1:A:688:ARG:CD	0.59	2.28	18	2
1:A:685:LEU:O	1:A:710:LYS:NZ	0.58	2.30	20	20
1:A:750:LEU:O	1:A:754:PHE:N	0.58	2.35	10	16
1:A:676:MET:O	1:A:696:ARG:NH1	0.58	2.35	3	2
1:A:707:ILE:HD12	1:A:707:ILE:N	0.58	2.14	20	7
1:A:738:LEU:O	1:A:742:VAL:N	0.58	2.31	17	18
1:A:707:ILE:N	1:A:707:ILE:HD12	0.58	2.14	4	13
1:A:678:ARG:NH1	1:A:682:GLU:OE2	0.57	2.33	16	5
1:A:670:LEU:CD1	1:A:764:PRO:HG3	0.57	2.28	16	20
1:A:724:GLU:N	1:A:724:GLU:CD	0.57	2.55	2	3
1:A:728:ARG:NH2	1:A:731:GLU:OE1	0.57	2.31	13	14
1:A:707:ILE:N	1:A:718:ILE:O	0.57	2.35	10	10
1:A:741:LEU:HD13	1:A:741:LEU:C	0.57	2.20	17	6
1:A:728:ARG:CD	1:A:731:GLU:HA	0.57	2.30	1	20
1:A:750:LEU:HD22	1:A:754:PHE:CE2	0.56	2.35	12	4
1:A:693:PHE:CB	1:A:709:ILE:HG23	0.56	2.30	5	2
1:A:673:ALA:N	1:A:695:VAL:O	0.56	2.35	14	12
1:A:733:LYS:NZ	1:A:748:ASN:OD1	0.56	2.29	18	2
1:A:671:TRP:O	1:A:695:VAL:N	0.56	2.38	1	16
1:A:674:GLY:O	1:A:676:MET:N	0.56	2.34	14	16
1:A:761:LEU:N	1:A:761:LEU:HD22	0.56	2.15	7	9
1:A:677:GLU:OE2	1:A:679:ALA:HB3	0.56	2.00	17	2
1:A:678:ARG:NE	1:A:682:GLU:OE1	0.55	2.29	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:672:TYR:O	1:A:766:LYS:NZ	0.55	2.27	14	11
1:A:761:LEU:HD22	1:A:761:LEU:N	0.55	2.16	4	11
1:A:669:HIS:CD2	1:A:671:TRP:CH2	0.55	2.95	5	7
1:A:711:TYR:O	1:A:712:ASN:CB	0.54	2.55	20	20
1:A:691:GLY:CA	1:A:762:GLN:HB2	0.54	2.32	19	19
1:A:736:ARG:NH2	1:A:740:GLU:OE2	0.54	2.34	1	6
1:A:723:ALA:O	1:A:726:LEU:N	0.54	2.35	13	7
1:A:741:LEU:HD13	1:A:741:LEU:O	0.53	2.03	17	4
1:A:666:LEU:HD13	1:A:738:LEU:CD1	0.53	2.29	17	3
1:A:670:LEU:CB	1:A:766:LYS:HB2	0.53	2.33	17	7
1:A:677:GLU:O	1:A:681:ALA:N	0.53	2.34	10	6
1:A:707:ILE:HG22	1:A:708:SER:N	0.53	2.18	4	7
1:A:707:ILE:HG22	1:A:708:SER:H	0.53	1.62	14	7
1:A:711:TYR:O	1:A:712:ASN:HB3	0.53	2.04	1	16
1:A:684:ILE:HG22	1:A:688:ARG:NE	0.52	2.20	18	2
1:A:741:LEU:O	1:A:741:LEU:HD13	0.52	2.04	1	4
1:A:729:ILE:HG12	1:A:741:LEU:HD11	0.52	1.81	14	3
1:A:736:ARG:NH2	1:A:740:GLU:OE1	0.52	2.34	20	3
1:A:754:PHE:CD1	1:A:754:PHE:N	0.52	2.78	20	10
1:A:718:ILE:HG21	1:A:729:ILE:O	0.52	2.04	6	6
1:A:752:ASP:CG	1:A:753:CYS:N	0.52	2.63	17	1
1:A:719:LYS:O	1:A:719:LYS:NZ	0.52	2.34	14	2
1:A:755:LYS:HG2	1:A:756:SER:N	0.52	2.19	18	13
1:A:666:LEU:HA	1:A:669:HIS:CD2	0.51	2.41	1	11
1:A:691:GLY:N	1:A:710:LYS:O	0.51	2.32	19	5
1:A:724:GLU:CD	1:A:724:GLU:N	0.51	2.61	1	3
1:A:666:LEU:HD13	1:A:738:LEU:HD13	0.51	1.82	13	2
1:A:707:ILE:HD11	1:A:720:ILE:HD12	0.51	1.81	4	4
1:A:759:THR:OG1	1:A:760:THR:N	0.51	2.44	8	18
1:A:754:PHE:N	1:A:754:PHE:CD1	0.51	2.74	9	9
1:A:709:ILE:N	1:A:709:ILE:HD12	0.51	2.20	7	1
1:A:708:SER:HA	1:A:716:LYS:O	0.51	2.06	12	11
1:A:677:GLU:HA	1:A:696:ARG:NH2	0.51	2.21	17	6
1:A:696:ARG:HH11	1:A:706:ALA:HB3	0.51	1.66	4	1
1:A:666:LEU:HB2	1:A:672:TYR:CD2	0.51	2.41	3	3
1:A:720:ILE:HD13	1:A:738:LEU:HG	0.51	1.82	13	1
1:A:761:LEU:CD2	1:A:761:LEU:H	0.50	2.20	18	13
1:A:739:THR:O	1:A:743:GLU:N	0.50	2.35	19	13
1:A:761:LEU:H	1:A:761:LEU:CD2	0.50	2.19	4	7
1:A:735:PHE:CE2	1:A:744:PHE:CG	0.50	3.00	17	2
1:A:684:ILE:HD13	1:A:765:PHE:CD2	0.50	2.41	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:711:TYR:CD2	1:A:757:LEU:HD13	0.50	2.41	10	4
1:A:761:LEU:HD23	1:A:761:LEU:H	0.50	1.66	10	4
1:A:693:PHE:CD2	1:A:763:PHE:O	0.50	2.65	1	18
1:A:669:HIS:O	1:A:766:LYS:NZ	0.50	2.29	10	6
1:A:751:LYS:NZ	1:A:758:ASP:CG	0.50	2.65	9	5
1:A:761:LEU:H	1:A:761:LEU:HD23	0.50	1.66	12	2
1:A:709:ILE:HD12	1:A:716:LYS:O	0.50	2.07	7	6
1:A:693:PHE:CD1	1:A:761:LEU:CD1	0.49	2.95	5	5
1:A:693:PHE:CD2	1:A:761:LEU:CD1	0.49	2.95	10	1
1:A:671:TRP:NE1	1:A:743:GLU:OE2	0.49	2.39	13	12
1:A:735:PHE:CZ	1:A:744:PHE:CG	0.49	3.01	16	15
1:A:711:TYR:CE1	1:A:759:THR:HB	0.49	2.42	1	9
1:A:718:ILE:HD11	1:A:754:PHE:CE2	0.49	2.41	3	7
1:A:750:LEU:HD13	1:A:754:PHE:CD2	0.49	2.43	10	2
1:A:695:VAL:HG22	1:A:707:ILE:HG23	0.48	1.85	13	4
1:A:672:TYR:CZ	1:A:674:GLY:CA	0.48	2.96	13	3
1:A:712:ASN:O	1:A:713:VAL:HG22	0.48	2.08	15	17
1:A:682:GLU:O	1:A:686:ALA:N	0.48	2.37	4	8
1:A:722:THR:OG1	1:A:722:THR:O	0.48	2.30	19	4
1:A:755:LYS:HZ3	1:A:756:SER:CB	0.48	2.21	11	3
1:A:724:GLU:N	1:A:724:GLU:OE2	0.48	2.47	16	1
1:A:755:LYS:O	1:A:756:SER:OG	0.47	2.32	9	1
1:A:751:LYS:CB	1:A:757:LEU:O	0.47	2.62	19	4
1:A:721:MET:O	1:A:727:TYR:HA	0.47	2.10	16	7
1:A:748:ASN:O	1:A:760:THR:HG22	0.47	2.09	5	2
1:A:666:LEU:HD22	1:A:738:LEU:HB3	0.47	1.87	13	4
1:A:682:GLU:HB3	1:A:717:HIS:CE1	0.47	2.44	13	4
1:A:671:TRP:CB	1:A:693:PHE:CE1	0.47	2.98	5	11
1:A:678:ARG:NH1	1:A:682:GLU:CD	0.47	2.68	16	1
1:A:707:ILE:O	1:A:708:SER:OG	0.47	2.33	11	7
1:A:670:LEU:HD12	1:A:764:PRO:CG	0.47	2.40	4	12
1:A:760:THR:OG1	1:A:762:GLN:NE2	0.47	2.45	5	1
1:A:741:LEU:CD2	1:A:745:TYR:CE1	0.46	2.98	18	2
1:A:722:THR:O	1:A:722:THR:OG1	0.46	2.32	2	3
1:A:677:GLU:HA	1:A:696:ARG:CZ	0.46	2.40	11	2
1:A:721:MET:SD	1:A:723:ALA:N	0.46	2.88	8	4
1:A:695:VAL:HG11	1:A:738:LEU:CD1	0.46	2.41	5	3
1:A:668:VAL:HG23	1:A:669:HIS:CE1	0.46	2.45	17	1
1:A:694:LEU:N	1:A:708:SER:O	0.46	2.47	17	10
1:A:682:GLU:O	1:A:686:ALA:CB	0.46	2.64	15	5
1:A:687:ASN:C	1:A:687:ASN:HD22	0.46	2.14	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:736:ARG:HE	1:A:740:GLU:CD	0.46	2.12	1	8
1:A:693:PHE:CD1	1:A:763:PHE:O	0.46	2.69	15	2
1:A:762:GLN:HB3	1:A:763:PHE:CD2	0.46	2.46	5	1
1:A:693:PHE:CG	1:A:761:LEU:HD12	0.46	2.46	19	5
1:A:727:TYR:CD2	1:A:738:LEU:N	0.46	2.84	10	4
1:A:689:SER:O	1:A:692:THR:OG1	0.45	2.26	5	7
1:A:686:ALA:C	1:A:710:LYS:NZ	0.45	2.69	14	17
1:A:679:ALA:O	1:A:683:SER:OG	0.45	2.25	8	2
1:A:709:ILE:HD12	1:A:709:ILE:N	0.45	2.27	8	5
1:A:688:ARG:NH1	1:A:765:PHE:O	0.45	2.49	7	1
1:A:682:GLU:HB3	1:A:715:VAL:HB	0.45	1.87	16	2
1:A:709:ILE:N	1:A:716:LYS:O	0.45	2.45	20	1
1:A:670:LEU:O	1:A:766:LYS:HG3	0.45	2.12	5	8
1:A:751:LYS:CB	1:A:751:LYS:NZ	0.45	2.77	14	2
1:A:712:ASN:O	1:A:713:VAL:CG2	0.45	2.64	10	19
1:A:709:ILE:O	1:A:716:LYS:N	0.45	2.45	20	1
1:A:733:LYS:O	1:A:745:TYR:OH	0.45	2.31	16	2
1:A:718:ILE:CD1	1:A:754:PHE:CZ	0.45	3.00	3	1
1:A:736:ARG:NE	1:A:740:GLU:OE1	0.45	2.32	13	4
1:A:682:GLU:CB	1:A:715:VAL:HB	0.44	2.42	5	2
1:A:695:VAL:HG21	1:A:742:VAL:CG2	0.44	2.39	1	2
1:A:680:GLY:O	1:A:683:SER:OG	0.44	2.29	12	4
1:A:712:ASN:O	1:A:712:ASN:ND2	0.44	2.45	4	1
1:A:739:THR:O	1:A:743:GLU:CG	0.44	2.65	19	1
1:A:737:GLY:O	1:A:741:LEU:HB2	0.44	2.13	18	2
1:A:694:LEU:CD1	1:A:694:LEU:C	0.44	2.84	7	2
1:A:676:MET:HG3	1:A:677:GLU:N	0.44	2.28	2	1
1:A:694:LEU:C	1:A:694:LEU:CD1	0.44	2.85	17	2
1:A:720:ILE:HD11	1:A:741:LEU:CD1	0.44	2.43	13	2
1:A:678:ARG:HG3	1:A:717:HIS:CD2	0.44	2.48	7	1
1:A:754:PHE:CD2	1:A:757:LEU:HG	0.44	2.47	15	2
1:A:678:ARG:HG2	1:A:717:HIS:CD2	0.43	2.48	19	2
1:A:678:ARG:HH12	1:A:682:GLU:CD	0.43	2.13	16	1
1:A:671:TRP:CB	1:A:693:PHE:CE2	0.43	3.01	10	2
1:A:694:LEU:O	1:A:708:SER:N	0.43	2.43	13	2
1:A:688:ARG:N	1:A:688:ARG:HH11	0.43	2.11	3	1
1:A:686:ALA:C	1:A:710:LYS:HZ1	0.43	2.13	11	1
1:A:695:VAL:CG2	1:A:742:VAL:HG21	0.43	2.42	5	2
1:A:754:PHE:HD1	1:A:754:PHE:N	0.43	2.11	9	1
1:A:696:ARG:O	1:A:706:ALA:N	0.43	2.39	4	4
1:A:709:ILE:O	1:A:715:VAL:HA	0.43	2.12	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:685:LEU:HD21	1:A:693:PHE:HA	0.43	1.90	11	1
1:A:685:LEU:HD11	1:A:765:PHE:HB3	0.43	1.90	20	1
1:A:671:TRP:CZ3	1:A:738:LEU:HD22	0.43	2.48	13	1
1:A:755:LYS:C	1:A:757:LEU:H	0.43	2.16	12	3
1:A:745:TYR:O	1:A:760:THR:HB	0.43	2.13	11	6
1:A:707:ILE:O	1:A:717:HIS:HA	0.43	2.13	2	3
1:A:694:LEU:HB2	1:A:765:PHE:CD1	0.43	2.49	9	3
1:A:721:MET:SD	1:A:728:ARG:CZ	0.43	3.07	9	1
1:A:722:THR:HG23	1:A:722:THR:O	0.42	2.12	5	2
1:A:720:ILE:HD13	1:A:738:LEU:CD2	0.42	2.45	19	1
1:A:666:LEU:HD22	1:A:738:LEU:CB	0.42	2.44	6	1
1:A:676:MET:CG	1:A:677:GLU:N	0.42	2.83	17	2
1:A:751:LYS:HE2	1:A:758:ASP:CG	0.42	2.35	14	1
1:A:678:ARG:O	1:A:682:GLU:HG2	0.42	2.14	8	1
1:A:735:PHE:CZ	1:A:744:PHE:CD1	0.42	3.08	16	1
1:A:670:LEU:CD1	1:A:764:PRO:CG	0.42	2.98	16	4
1:A:750:LEU:HD12	1:A:759:THR:HG23	0.42	1.92	16	1
1:A:749:SER:OG	1:A:752:ASP:OD2	0.42	2.31	8	1
1:A:666:LEU:C	1:A:668:VAL:H	0.42	2.18	4	1
1:A:759:THR:O	1:A:760:THR:CG2	0.42	2.67	7	2
1:A:671:TRP:O	1:A:694:LEU:HA	0.42	2.15	20	1
1:A:676:MET:C	1:A:696:ARG:HE	0.42	2.15	6	1
1:A:717:HIS:C	1:A:718:ILE:HG13	0.41	2.36	13	2
1:A:741:LEU:HD21	1:A:745:TYR:CE1	0.41	2.50	18	1
1:A:666:LEU:HB3	1:A:672:TYR:CG	0.41	2.50	18	1
1:A:759:THR:O	1:A:760:THR:HG23	0.41	2.15	1	2
1:A:669:HIS:CE1	1:A:739:THR:HG23	0.41	2.51	14	1
1:A:707:ILE:CD1	1:A:729:ILE:HG23	0.41	2.27	19	1
1:A:692:THR:CG2	1:A:764:PRO:O	0.41	2.68	17	2
1:A:730:THR:C	1:A:731:GLU:CG	0.41	2.89	8	1
1:A:695:VAL:HA	1:A:706:ALA:O	0.41	2.15	20	1
1:A:733:LYS:HE2	1:A:735:PHE:CE2	0.41	2.50	14	1
1:A:669:HIS:CE1	1:A:739:THR:CG2	0.41	3.04	6	1
1:A:705:PHE:H	1:A:720:ILE:HG22	0.41	1.74	20	1
1:A:693:PHE:CG	1:A:761:LEU:CD1	0.41	3.03	8	1
1:A:726:LEU:HA	1:A:735:PHE:O	0.41	2.14	13	1
1:A:750:LEU:HG	1:A:760:THR:HA	0.41	1.93	5	1
1:A:682:GLU:HB2	1:A:715:VAL:HG21	0.41	1.92	4	1
1:A:723:ALA:HB2	1:A:728:ARG:NH1	0.41	2.31	16	1
1:A:691:GLY:O	1:A:762:GLN:HB2	0.41	2.15	5	1
1:A:724:GLU:OE2	1:A:724:GLU:N	0.41	2.54	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:676:MET:O	1:A:696:ARG:HD2	0.41	2.16	12	1
1:A:727:TYR:O	1:A:735:PHE:N	0.40	2.52	13	1
1:A:723:ALA:C	1:A:725:GLY:N	0.40	2.75	16	1
1:A:728:ARG:NH2	1:A:731:GLU:HB3	0.40	2.31	1	1
1:A:765:PHE:CZ	1:A:766:LYS:HG2	0.40	2.51	5	2
1:A:671:TRP:CZ2	1:A:739:THR:HA	0.40	2.51	7	1
1:A:666:LEU:C	1:A:668:VAL:N	0.40	2.74	4	1
1:A:687:ASN:ND2	1:A:687:ASN:C	0.40	2.75	14	1
1:A:720:ILE:HG23	1:A:721:MET:N	0.40	2.31	4	1
1:A:677:GLU:CD	1:A:680:GLY:H	0.40	2.19	20	1
1:A:751:LYS:NZ	1:A:751:LYS:HB2	0.40	2.32	14	1
1:A:730:THR:C	1:A:732:LYS:H	0.40	2.20	5	1
1:A:681:ALA:HB1	1:A:694:LEU:HD21	0.40	1.93	12	1
1:A:695:VAL:HG11	1:A:738:LEU:HD21	0.40	1.94	20	1
1:A:727:TYR:CD1	1:A:727:TYR:N	0.40	2.88	15	1
1:A:690:ASP:OD2	1:A:712:ASN:N	0.40	2.37	8	1
1:A:737:GLY:O	1:A:741:LEU:CB	0.40	2.70	16	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	93/107 (87%)	76±2 (81±2%)	13±2 (14±2%)	5±1 (5±1%)	4	25
2	B	0	-	-	-	-	-
All	All	1860/2400 (78%)	1512 (81%)	255 (14%)	93 (5%)	4	25

All 8 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	712	ASN	20
1	A	761	LEU	20
1	A	754	PHE	18
1	A	755	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	758	ASP	11
1	A	675	PRO	5
1	A	674	GLY	3
1	A	705	PHE	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	81/92 (88%)	61±2 (75±2%)	20±2 (25±2%)	<b>2</b> 25
2	B	0	-	-	-
All	All	1620/2040 (79%)	1223 (75%)	397 (25%)	<b>2</b> 25

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

Mol	Chain	Res	Type	Models (Total)
1	A	736	ARG	20
1	A	670	LEU	20
1	A	746	GLN	20
1	A	747	GLN	20
1	A	728	ARG	20
1	A	720	ILE	20
1	A	690	ASP	20
1	A	762	GLN	19
1	A	709	ILE	19
1	A	738	LEU	15
1	A	719	LYS	14
1	A	688	ARG	14
1	A	758	ASP	14
1	A	677	GLU	13
1	A	748	ASN	13
1	A	687	ASN	12
1	A	678	ARG	11
1	A	761	LEU	11
1	A	749	SER	11
1	A	722	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	766	LYS	10
1	A	752	ASP	10
1	A	684	ILE	10
1	A	732	LYS	10
1	A	721	MET	8
1	A	676	MET	7
1	A	755	LYS	6
1	A	757	LEU	4
1	A	696	ARG	3
1	A	689	SER	3
1	A	751	LYS	2
1	A	756	SER	2
1	A	714	GLU	2
1	A	730	THR	1
1	A	712	ASN	1
1	A	667	SER	1
1	A	739	THR	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	PTR	B	342	2	15,16,17	1.05±0.05	0±0 (0±0%)
2	PTR	B	346	2	15,16,17	1.09±0.05	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types,

if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	PTR	B	342	2	19,22,24	0.93±0.05	0±0 (0±0%)
2	PTR	B	346	2	19,22,24	0.95±0.04	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	B	342	2	-	0±0,10,11,13	0±0,1,1,1
2	PTR	B	346	2	-	0±0,10,11,13	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 80% for the well-defined parts and 72% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	1221
Number of shifts mapped to atoms	1221
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	98	$-0.03 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	93	$-0.02 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	95	$0.59 \pm 0.26$	Should be applied

#### 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 80%, i.e. 960 atoms were assigned a chemical shift out of a possible 1199. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	364/461 (79%)	182/184 (99%)	92/186 (49%)	90/91 (99%)
Sidechain	500/615 (81%)	308/361 (85%)	192/225 (85%)	0/29 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	96/123 (78%)	49/65 (75%)	47/53 (89%)	0/5 (0%)
Overall	960/1199 (80%)	539/610 (88%)	331/464 (71%)	90/125 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1068 atoms were assigned a chemical shift out of a possible 1484. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	405/582 (70%)	212/232 (91%)	98/236 (42%)	95/114 (83%)
Sidechain	563/771 (73%)	361/452 (80%)	202/284 (71%)	0/35 (0%)
Aromatic	100/131 (76%)	51/69 (74%)	49/55 (89%)	0/7 (0%)
Overall	1068/1484 (72%)	624/753 (83%)	349/575 (61%)	95/156 (61%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

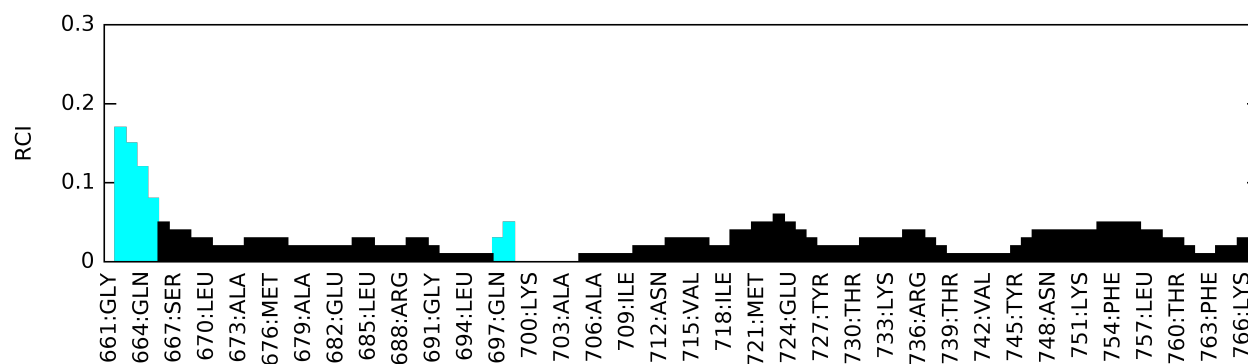
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	669	HIS	HB3	0.79	5.00 – 1.10	-5.8
1	A	766	LYS	HG3	-0.15	2.76 – -0.04	-5.4

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

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:

