



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 13, 2026 – 10:32 AM EDT

PDB ID : 12KL / pdb\_000012kl  
BMRB ID : 31301  
Title : SSNMR Structure of Anti-necroptosis Viral:Human Functional Hetero-amyloid M45:RIPK3  
Authors : He, C.; Varghese, N.R.; Keeler, E.G.; Pham, C.L.; Xie, T.; Williams, B.; Tetter, S.; Semaan, C.; Wilde, K.L.; Brown, S.H.J.; Bouwer, J.C.; Gambin, Y.; Sierecki, E.; Steain, M.; Zhou, R.; Sunde, M.; McDermott, A.E.  
Deposited on : 2026-04-09

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.

The types of validation reports are described at

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

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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  
BMRB Restraints Analysis : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

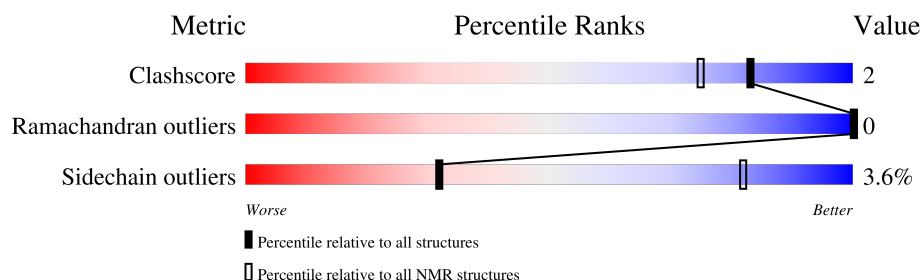
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLID-STATE NMR*

The overall completeness of chemical shifts assignment is 9%.

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  $\geq 3$ , 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	133	18% 80%
1	C	133	17% 80%
1	E	133	17% 80%
1	G	133	19% 80%
2	B	92	27% 70%
2	D	92	24% 70%
2	F	92	27% 70%
2	H	92	27% 70%

## 2 Ensemble composition and analysis

This entry contains 10 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:448-A:471, C:447-C:471, E:447-E:471, G:447-G:471, (199)	B:51-B:75, D:51-D:75, F:51-F:75, H:51-H:75	0.96	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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 7, 8, 9
2	6, 10
Single-model clusters	4

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3292 atoms, of which 1628 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Receptor-interacting serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms						Trace
1	A	27	Total	C	H	N	O	S	0
			409	127	201	37	42	2	
1	C	27	Total	C	H	N	O	S	0
			409	127	201	37	42	2	
1	E	27	Total	C	H	N	O	S	0
			409	127	201	37	42	2	
1	G	27	Total	C	H	N	O	S	0
			409	127	201	37	42	2	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	GLY	-	expression tag	UNP Q9Y572
A	387	SER	-	expression tag	UNP Q9Y572
C	386	GLY	-	expression tag	UNP Q9Y572
C	387	SER	-	expression tag	UNP Q9Y572
E	386	GLY	-	expression tag	UNP Q9Y572
E	387	SER	-	expression tag	UNP Q9Y572
G	386	GLY	-	expression tag	UNP Q9Y572
G	387	SER	-	expression tag	UNP Q9Y572

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase large subunit-like protein.

Mol	Chain	Residues	Atoms						Trace
2	B	28	Total	C	H	N	O	S	0
			414	130	206	38	37	3	
2	D	28	Total	C	H	N	O	S	0
			414	130	206	38	37	3	
2	F	28	Total	C	H	N	O	S	0
			414	130	206	38	37	3	
2	H	28	Total	C	H	N	O	S	0
			414	130	206	38	37	3	

There are 8 discrepancies between the modelled and reference sequences:

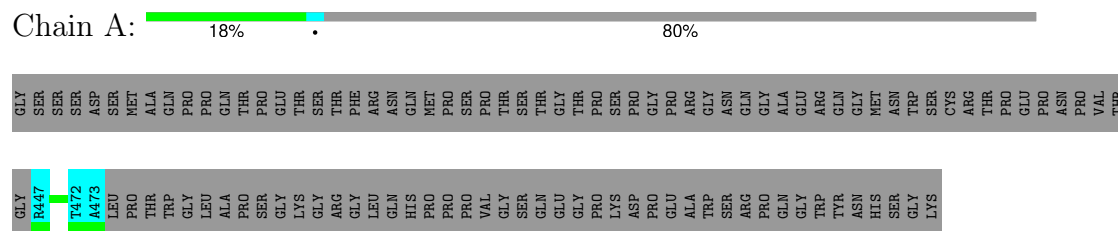
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP H2A2P4
B	0	SER	-	expression tag	UNP H2A2P4
D	-1	GLY	-	expression tag	UNP H2A2P4
D	0	SER	-	expression tag	UNP H2A2P4
F	-1	GLY	-	expression tag	UNP H2A2P4
F	0	SER	-	expression tag	UNP H2A2P4
H	-1	GLY	-	expression tag	UNP H2A2P4
H	0	SER	-	expression tag	UNP H2A2P4

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

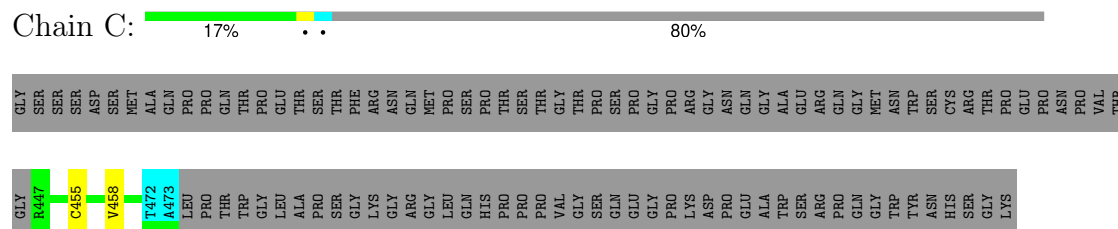
### 4.1 Average score per residue in the NMR ensemble

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.

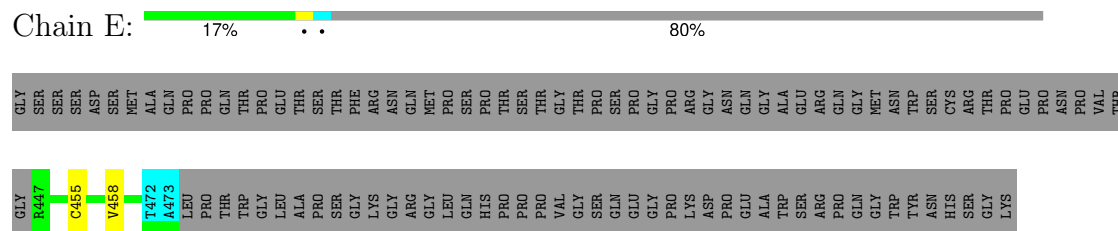
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



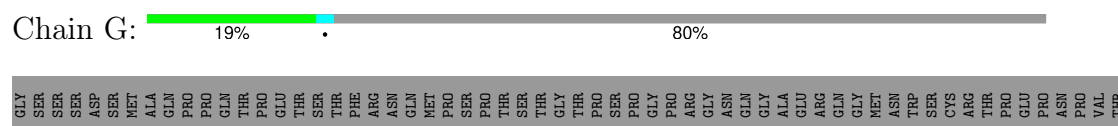
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

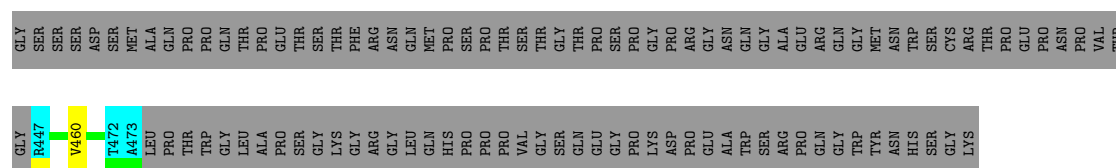


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



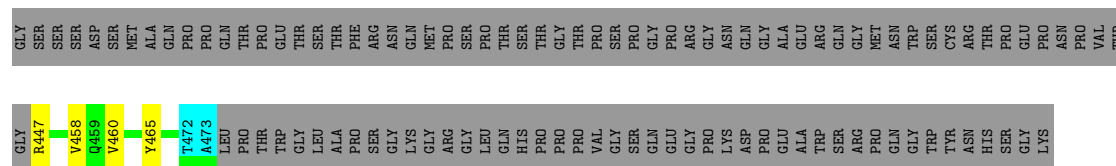


Chain A:  17% 80%



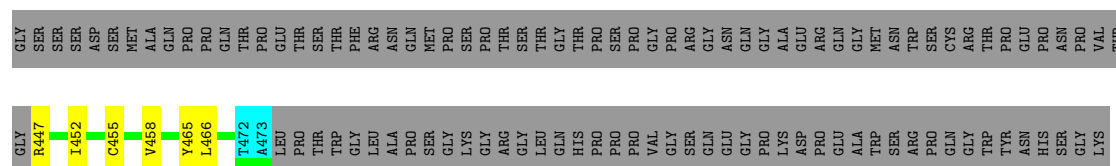
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  16% 80%



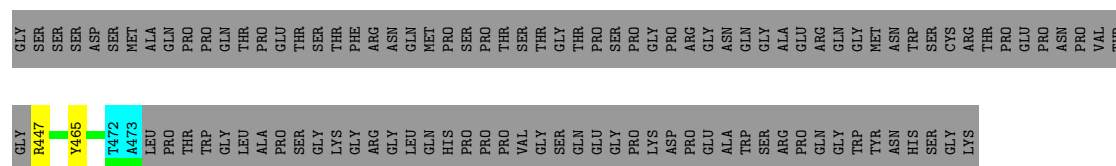
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain E:  14% 80%



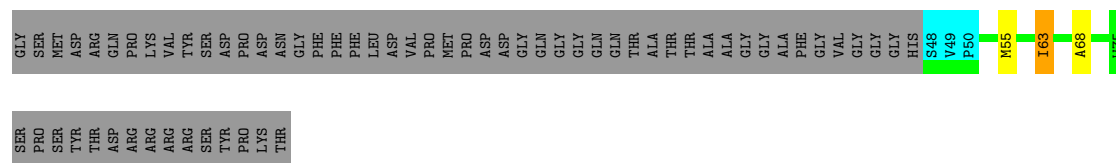
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G:  17% 80%



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

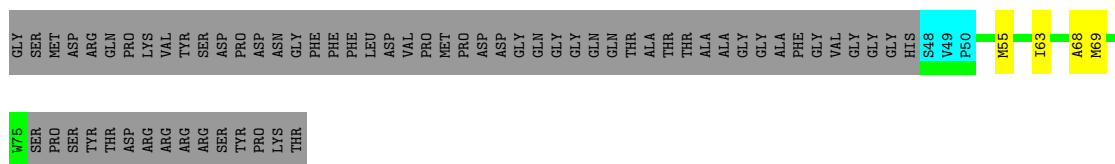
Chain B:  24% 70%



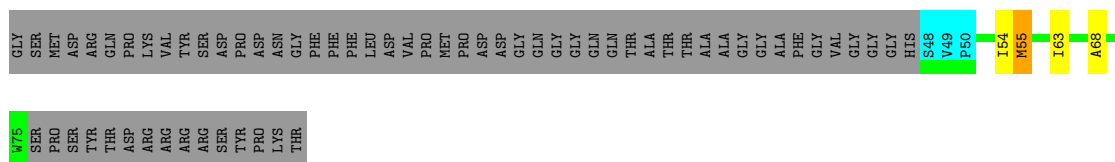
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain D:  23% 70%

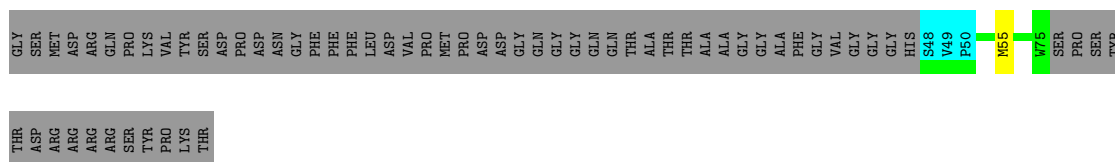




- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

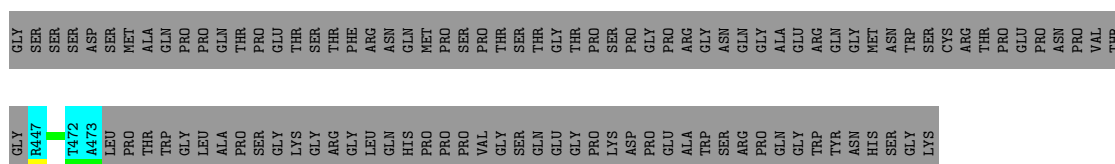


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

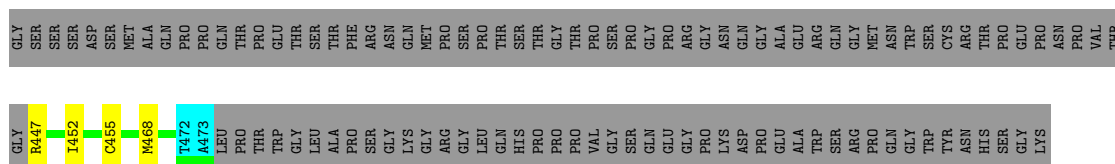


#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



GLY SER SER SER ASP SER MET ALA GLN PRO PRO GLN THR PRO GLU THR SER THR PHE ARG ASN ASN GLN MET MET PRO PRO SER PRO PRO THR THR GLY THR THR PRO SER SER PRO GLY PRO GLY ARG GLY ASN GLN GLY ALA GLU ARG GLN MET MET ASN TRP SER CYS ARG THR PRO GLU PRO ASN PRO VAL THR

GLY R447 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS SER GLY ARG GLY LEU GLN HIS PRO PRO VAL GLY SER SER GLN GLY THR THR PRO LYS ASP PRO GLU ALA TRP SER ARG GLY ASN GLN PRO GLY ALA GLN GLY TRP TYR ASN HIS SER GLY LYS

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G: 17% 80%

GLY SER SER SER ASP SER MET ALA GLN PRO PRO GLN THR PRO GLU THR SER THR PHE ARG ASN ASN GLN MET MET PRO PRO SER PRO PRO THR THR GLY THR THR PRO SER SER PRO GLY LYS ASP PRO GLU ALA TRP SER ARG GLY ASN GLN GLY ALA GLN GLY TRP TYR ASN HIS SER GLY LYS

GLY R447 V458 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS SER GLY ARG GLY LEU GLN HIS PRO PRO VAL GLY SER SER GLN GLY THR THR PRO LYS ASP PRO GLU ALA TRP SER ARG GLY ASN GLN GLY TRP TYR ASN HIS SER GLY LYS

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain B: 25% 70%

GLY SER MET ASP ARG GLN PRO LYS VAL TYR SER ASP ASP ASP ASN PHE PHE LEU ASP VAL PRO MET MET PRO ASP ASP ASP GLN GLY THR THR THR ALA ALA GLY GLY PHE VAL GLY GLY HIS S48 V49 P50 M55 I61 W75 PRO

SER TYR THR ASP ARG ARG ARG ARG SER TYR PRO LYS THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain D: 23% 70%

GLY SER MET ASP ARG GLN PRO LYS VAL TYR SER ASP ASP ASP ASN PHE PHE LEU ASP VAL PRO MET MET PRO ASP ASP ASP GLN GLY THR THR THR ALA ALA GLY GLY PHE VAL GLY GLY HIS S48 V49 P50 M55 I61 W62 I63 I71

W75 SER PRO ASP TYR THR ARG ARG ARG ARG SER TYR PRO LYS THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain F: 24% 70%

GLY SER MET ASP ARG GLN PRO LYS VAL TYR SER ASP ASP ASP ASN PHE PHE LEU ASP VAL PRO MET MET PRO ASP ASP ASP GLN GLY THR THR THR ALA ALA GLY GLY PHE VAL GLY GLY HIS S48 V49 P50 I61 M69 S70 I71 W75

SER PRO SER TYR THR ARG ARG ARG ARG SER TYR PRO LYS THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain H: 27% 70%

GLY SER MET ASP ARG GLN PRO LYS VAL TYR SER ASP ASP ASP ASN PHE PHE LEU ASP VAL PRO MET MET PRO ASP ASP ASP GLN GLY THR THR THR ALA ALA GLY GLY PHE VAL GLY GLY HIS S48 V49 P50 W75 SER PRO SER TYR THR ASP

ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

### 4.2.3 Score per residue for model 3

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A:  18% 80%

GLY SER SER SER ASP SER MET ALA PRO PRO GLN THR PRO GLU THR SER THR PHE ARG GLN HIS GLN MET MET PRO PRO SER PRO THR THR GLY THR PRO PRO LYS SER ASP PRO GLU ALA ARG GLY ASN GLN GLY ALA ALA GLU ARG GLN GLN TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

GLY R447 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS THR SER ARG GLY PHE LEU GLN HIS GLN MET PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  17% 80%

GLY SER SER SER ASP SER MET ALA GLN PRO PRO GLN THR PRO GLU THR SER THR PHE ARG GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

GLY R447 C455 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS THR SER ARG GLY PHE LEU GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain E:  17% 80%

GLY SER SER SER ASP SER MET ALA GLN PRO PRO GLN THR PRO GLU THR SER THR PHE ARG GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

GLY R447 C455 V458 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS THR SER ARG GLY PHE LEU GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G:  18% 80%

GLY SER SER SER ASP SER MET ALA GLN PRO PRO GLN THR PRO GLU THR SER THR PHE ARG GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

GLY R447 T472 A473 LEU PRO THR TRP GLY LEU ALA PRO SER GLY LYS THR SER ARG GLY PHE LEU GLN HIS GLN MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain B:  24% 70%

GLY SER MET ASP ARG GLN PRO LYS VAL TYR SER ASP PRO ASP ASN PHE PHE LEU ASP VAL VAL MET MET PRO PRO THR THR GLY THR THR PRO SER SER PRO PRO VAL GLY GLN GLY THR PRO LYS SER ASP PRO GLU ALA TRP SER ASN GLN GLY ALA GLU TRP TYR ASN HIS MET SER ASN TRP SER CYS THR THR PRO GLU PRO ASN PRO VAL THR

SER  
TYR  
THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain D:  25% .. 70%

[illegible]

SER  
TYR  
THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain F:  25% • • 70%

GLY	SER	MET	ASP	ARG	GLN	PRO	LYS	VAL	TYR	SER	ASP	PRO	ASP	ASN	GLY	PHE	PHE	PHE	LEU	ASP	VAL	ASP	PRO	MET	PRO	ASP	ASP	GLY	GLN	GLY	GLY	GLN	GLN	THR	THR	ALA	ALA	THR	THR	ALA	ALA	GLY	GLY	GLY	ALA	ALA	PHE	GLY	VAL	VAL	GLY	GLY	GLY	GLY	HIS	S48	V49	P50	M56	W75	SER	PRO	PRO	SER	SER	TYR
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THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain H:  26% 70%

GLY	SER	ASP	ARG	GLN	PRO	LYS	VAL	TYR	SER	ASP	PRO	ASP	ASN	GLY	PHE	PHE	LEU	ASP	VAL	PRO	MET	PRO	ASP	ASP	GLY	GLN	GLY	GLY	GLN	GLN	THR	THR	ALA	ALA	ALA	GLY	GLY	ALA	PHE	GLY	VAL	GLY	GLY	GLY	GLY	HIS	S48	V49	P50	N56	W75	SER	PRO	PRO	SER	TYR
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THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

#### 4.2.4 Score per residue for model 4

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A: 

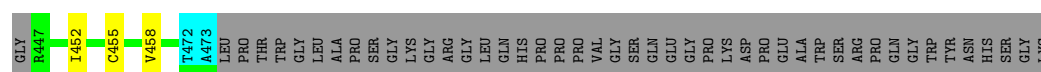
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	GLY	R447	I452	C455	T472	A473	LEU	PRO	THR	TRP	GLY	LYS	GLY	ARG	GLY	LEU	GLN	HIS	PRO	PRO	VAL	GLY	SER	GLN	GLN	GLY	ASP	PRO	ALA	TRP	SER	ARG	PRO	GLN	GLN	GLY	TRP	TYP	ASN	HIS	SER	GLY	LYS
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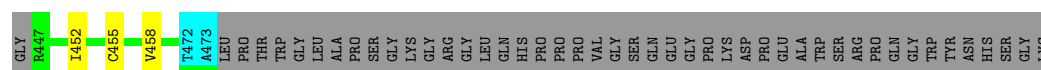
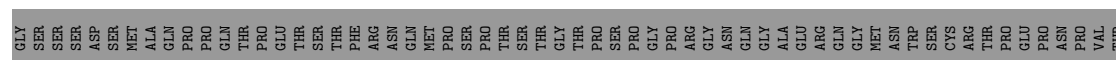
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  17% 80%

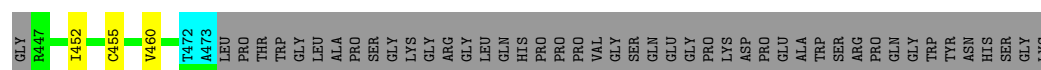
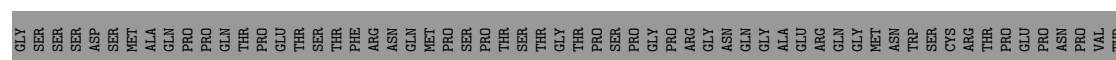
GLY	SER	SER	SER	ASP	SER	MET	ALA	GLN	PRO	PRO	PRO	THR	THR	GLU	GLY	THR	THR	THR	THR	GLY	THR	THR	THR	THR	PRO	SER	SER	PRO	PRO	SER	PRO	PRO	GLY	ARG	ARG	ASN	GLN	GLY	GLN	ALA	ALA	GLU	GLU	ARG	ARG	GLN	GLY	GLN	MET	MET	ASN	TRP	SER	CYS	THR	THR	PRO	PRO	GLU	PRO	PRO	ASN	ASN	PRO	PRO	VAL	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



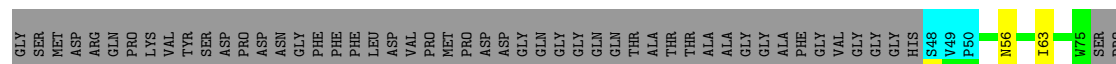
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



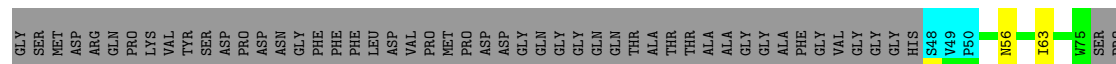
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



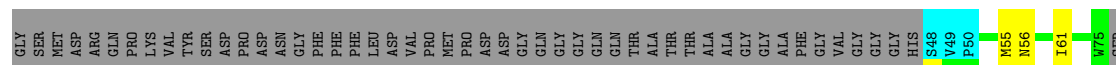
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

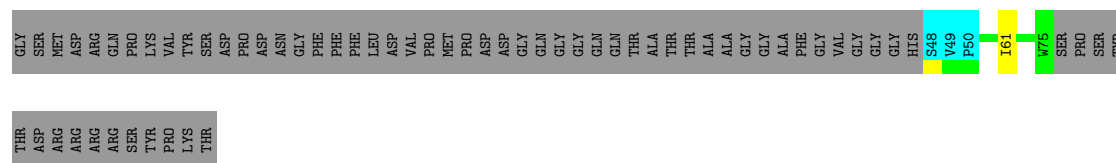


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

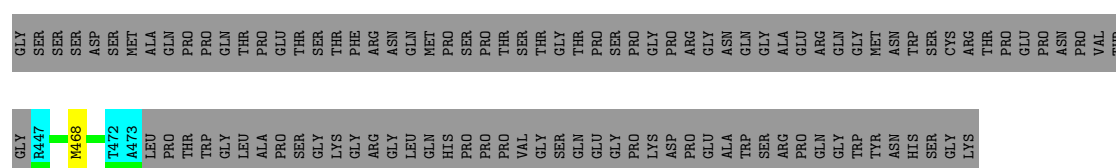
Chain H:  26% . . 70%



#### 4.2.5 Score per residue for model 5

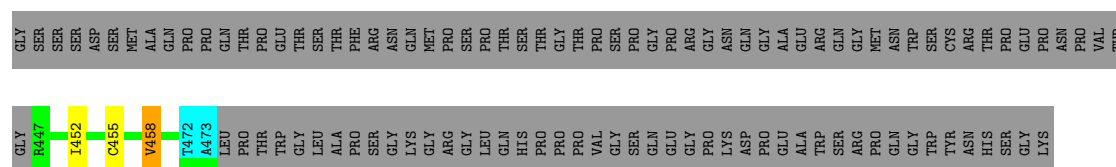
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A:  17% 2% 80%



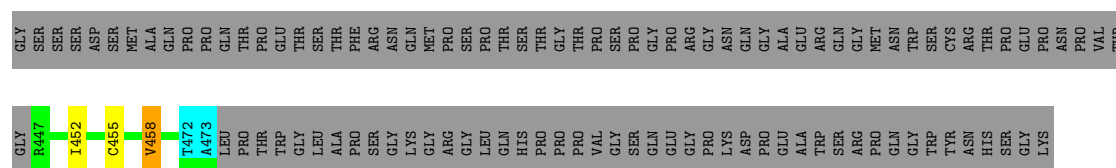
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  17% ... 80%



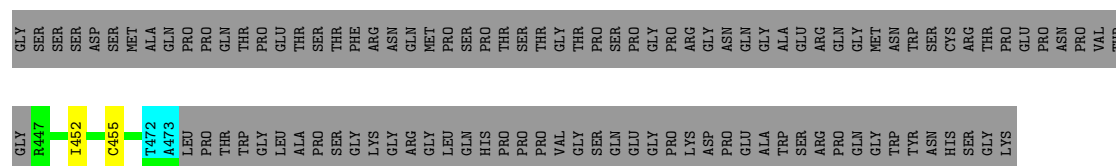
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain E:  17% ... 80%

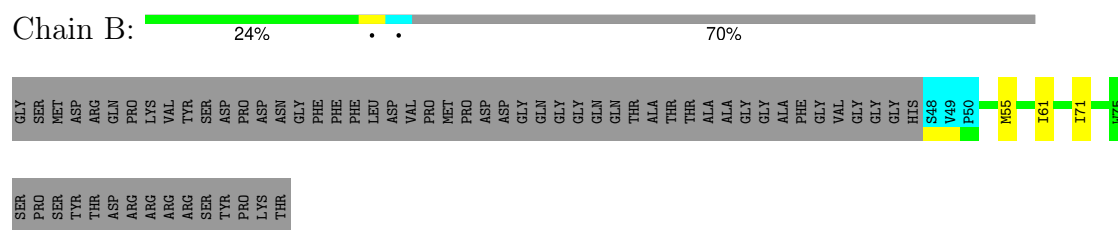


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

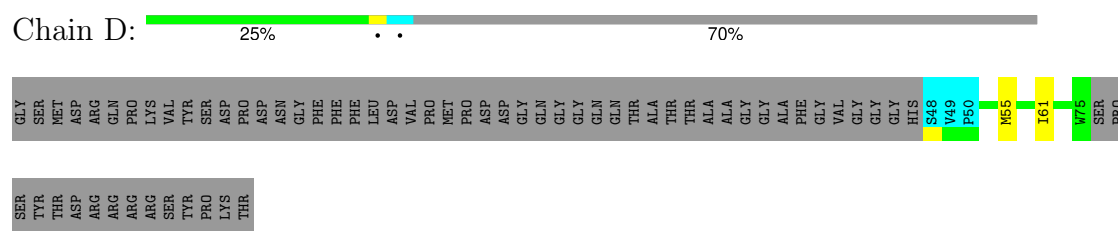
Chain G:  17% 80%



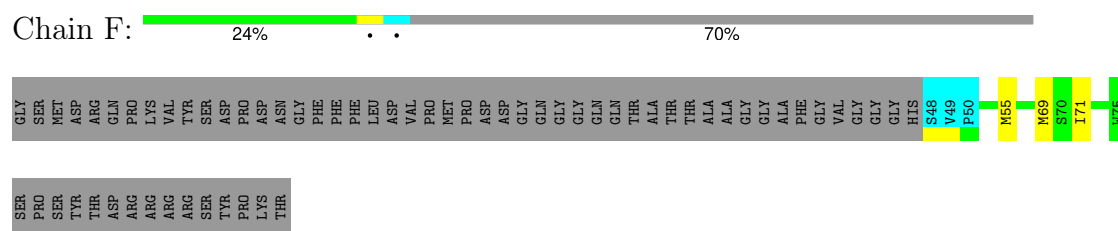
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



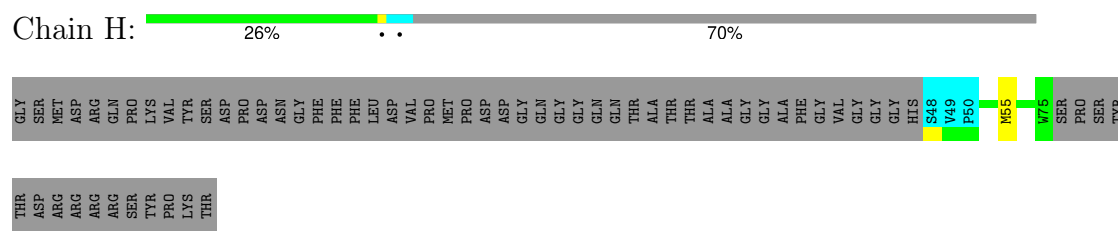
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

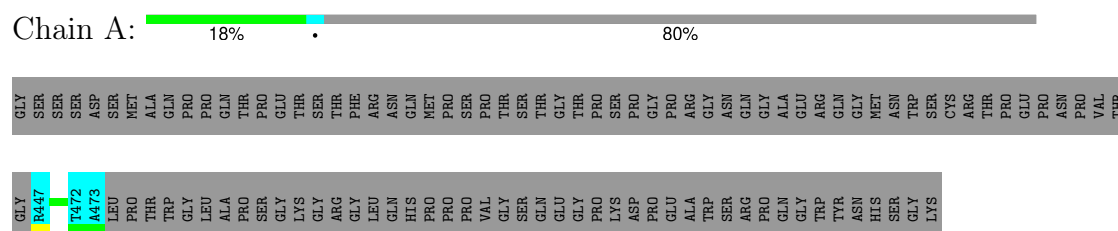


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

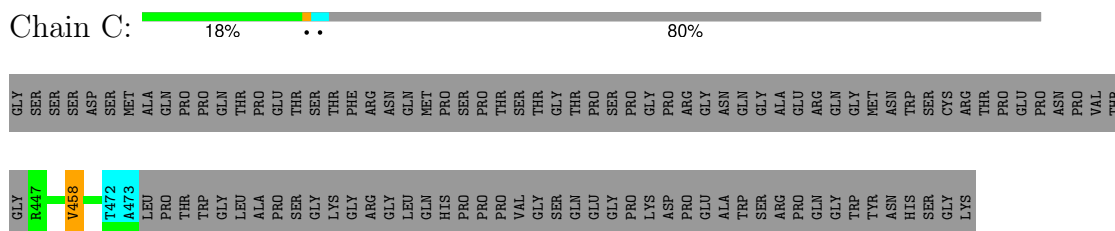


#### 4.2.6 Score per residue for model 6

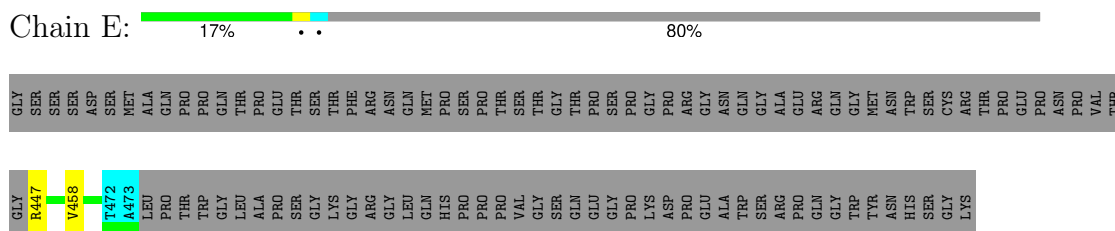
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



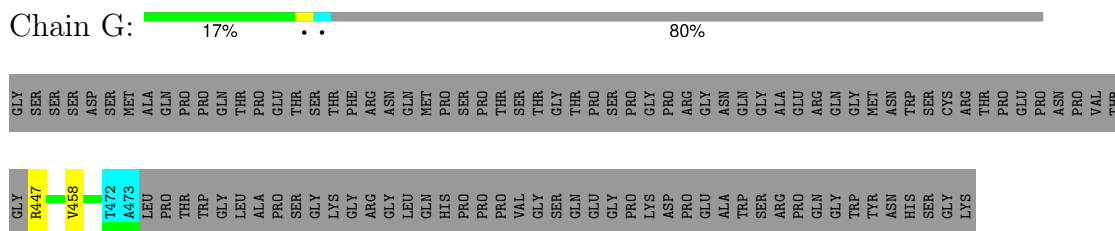
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



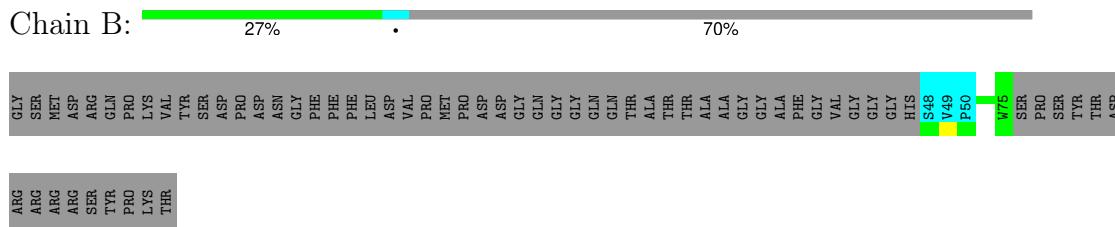
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



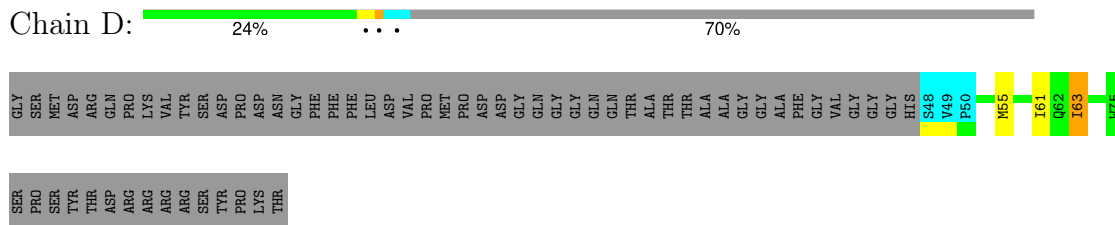
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

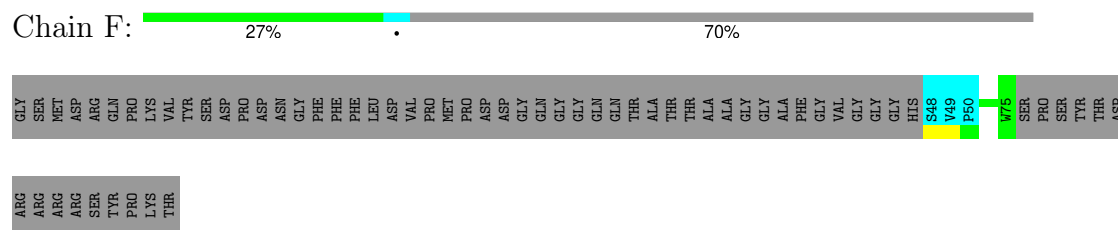


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

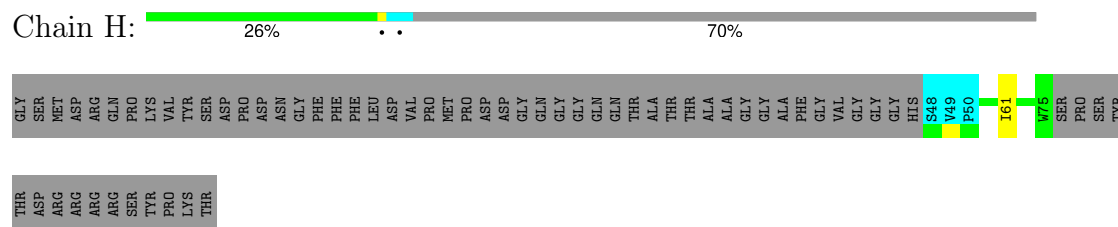


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



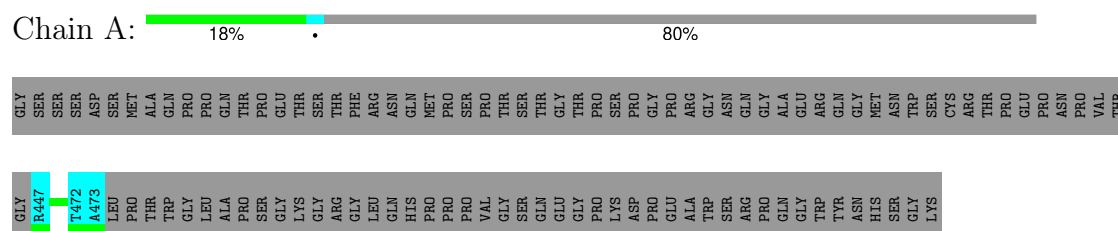


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

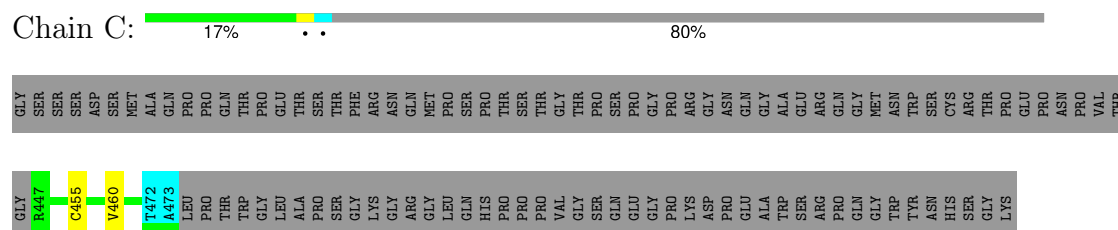


#### 4.2.7 Score per residue for model 7

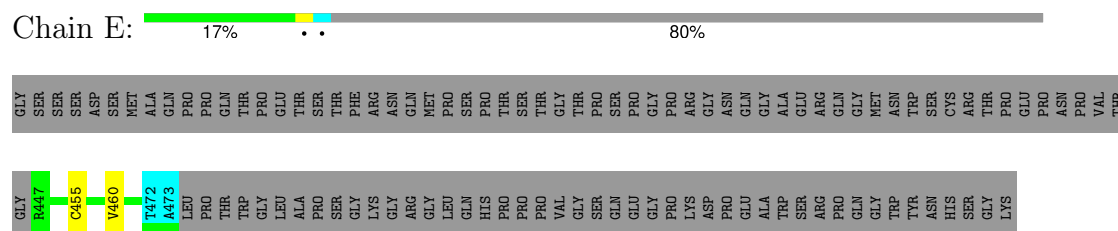
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

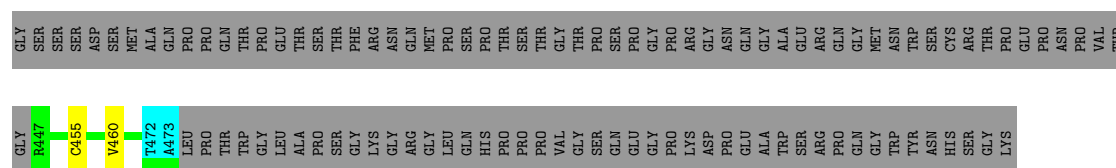


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



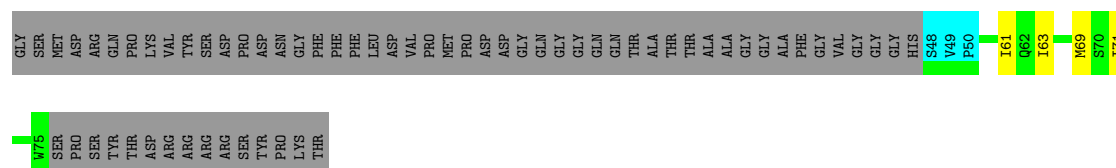
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G:  17% 80%



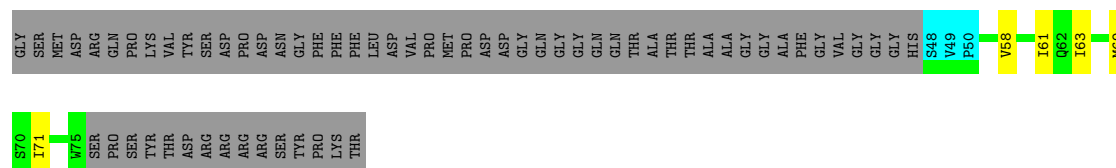
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain B:  23% 70%



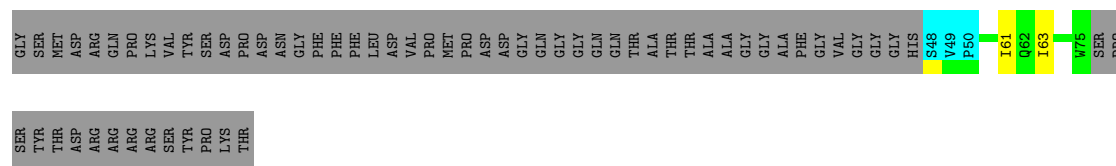
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain D:  22% 5% 70%



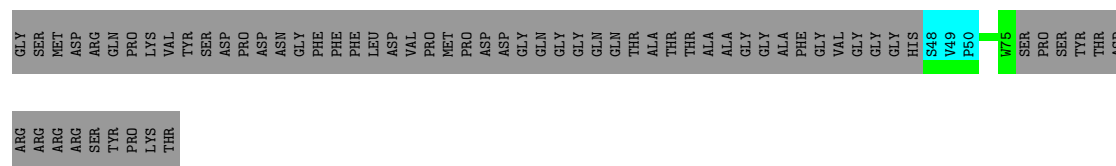
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain F:  25% 70%



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

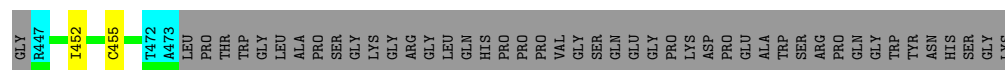
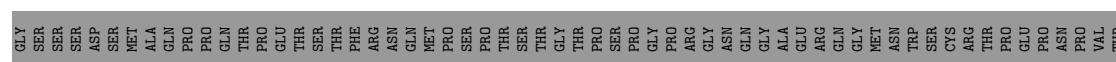
Chain H:  27% 70%



## 4.2.8 Score per residue for model 8

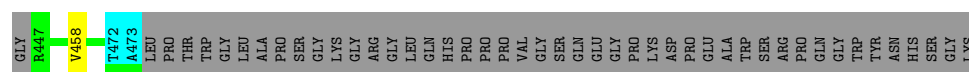
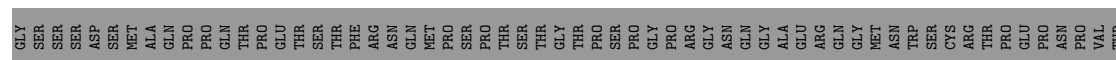
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A:  17% 2% 3% 80%



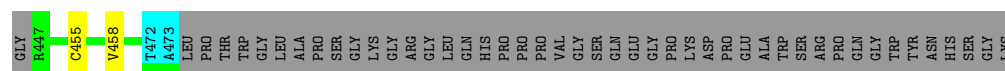
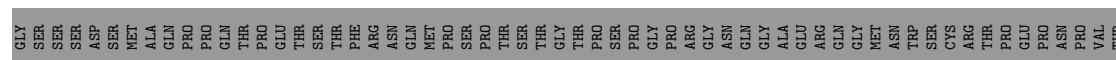
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  18% .. 80%



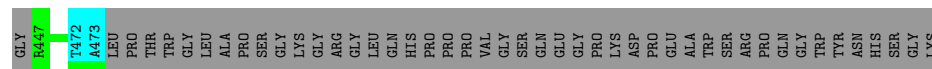
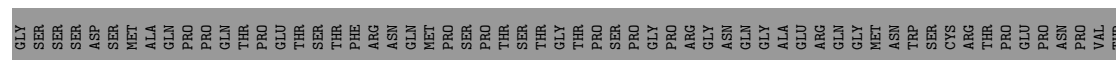
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain E:  17% 2% 81%



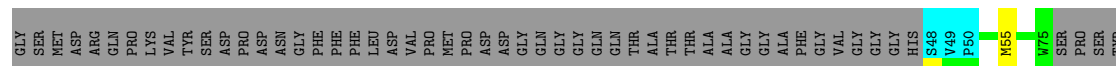
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G:  19% 80%



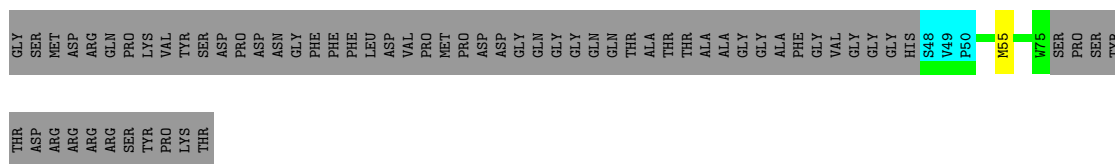
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain B:  26%  $\dots$  70%



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain D: 



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



#### 4.2.9 Score per residue for model 9

- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

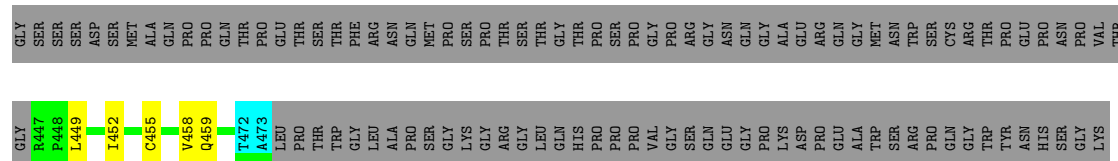


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

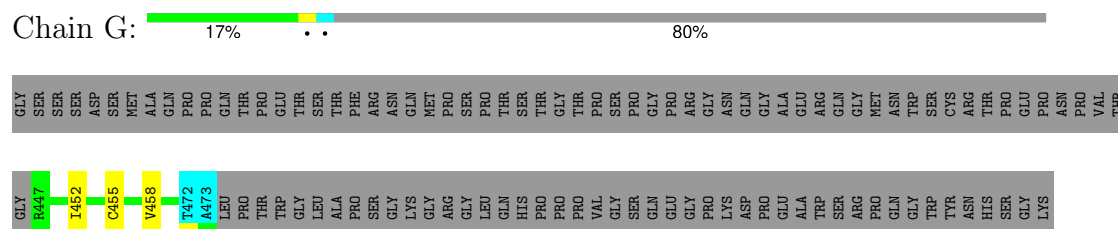


- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

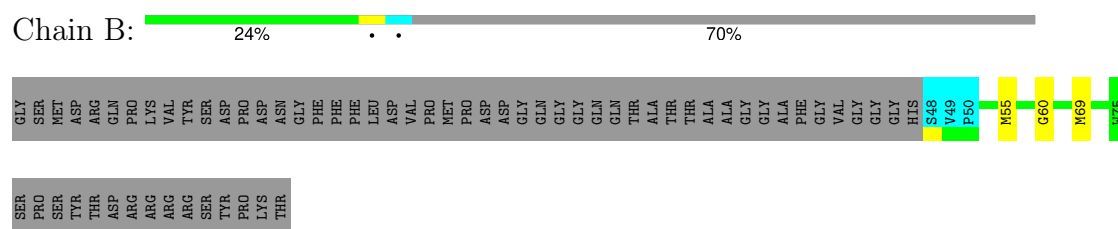




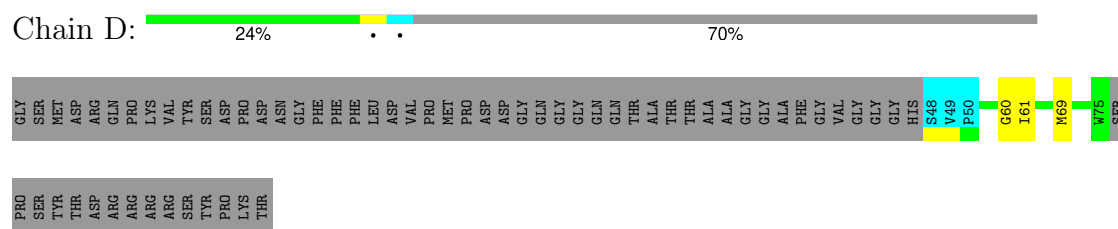
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3



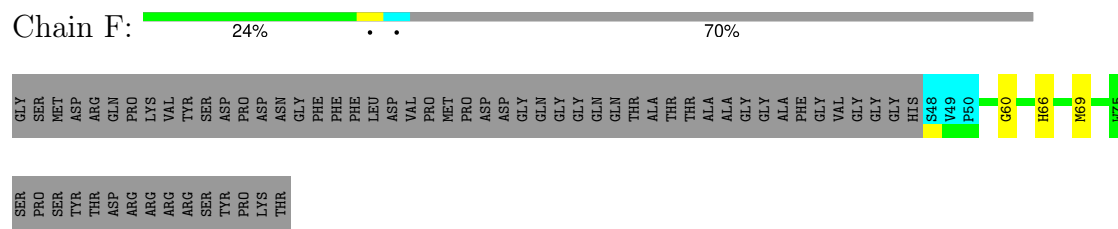
- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

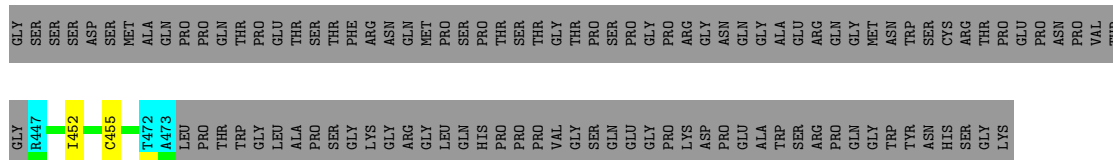


- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

#### 4.2.10 Score per residue for model 10

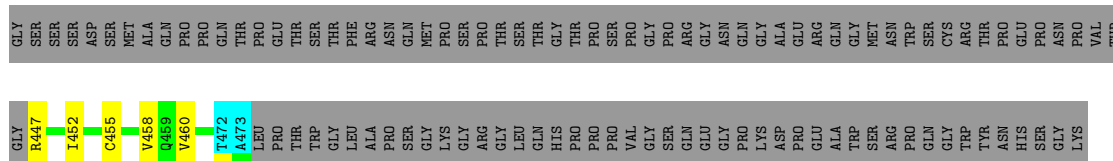
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain A: 



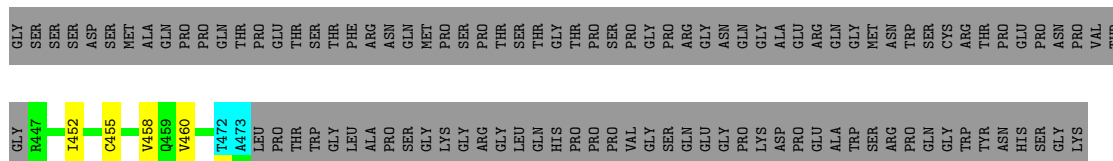
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain C:  15% 80%



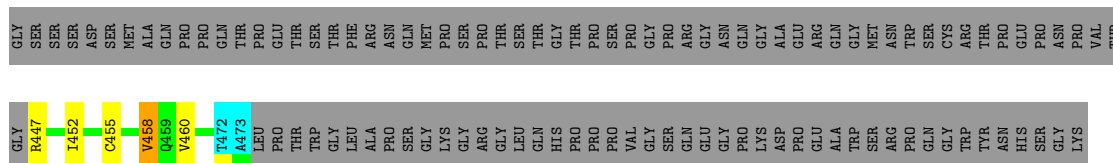
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain E:  16% . . 80%



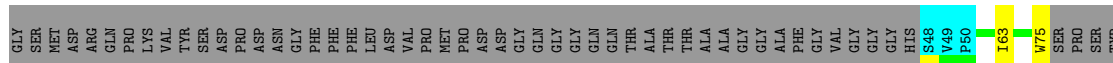
- Molecule 1: Receptor-interacting serine/threonine-protein kinase 3

Chain G:  15% ... 80%



- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein

Chain B: 



THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



GLY  
SER  
MET  
ASP  
ARG  
GLN  
PRO  
LYS  
VAL  
TYR  
SER  
SER  
ASP  
PRO  
ASP  
ASN  
GLY  
PHE  
PHE  
PHE  
LEU  
ASP  
VAL  
PRO  
MET  
PRO  
ASP  
ASP  
GLY  
GLN  
GLY  
GLY  
GLN  
GLN  
THR  
ALA  
THR  
THR  
THR  
ALA  
ALA  
GLY  
GLY  
PHE  
GLY  
VAL  
GLY  
GLY  
GLY  
GLY  
HIS  
S48  
V49  
P50  
M55  
I63  
W75  
SER  
PRO

SER  
TYR  
THR  
ASP  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



GLY  
SER  
MET  
ASP  
ARG  
GLN  
PRO  
LYS  
VAL  
TYR  
SER  
SER  
ASP  
PRO  
ASP  
ASN  
GLY  
PHE  
PHE  
PHE  
LEU  
ASP  
VAL  
PRO  
MET  
PRO  
ASP  
ASP  
GLY  
GLN  
GLY  
GLY  
GLN  
GLN  
THR  
ALA  
THR  
THR  
THR  
ALA  
ALA  
GLY  
GLY  
PHE  
GLY  
VAL  
GLY  
GLY  
GLY  
GLY  
HIS  
S48  
V49  
P50  
W75  
SER  
PRO  
SER  
TYR  
THR  
ASP

ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

- Molecule 2: Ribonucleoside-diphosphate reductase large subunit-like protein



GLY  
SER  
MET  
ASP  
ARG  
GLN  
PRO  
LYS  
VAL  
TYR  
SER  
SER  
ASP  
PRO  
ASP  
ASN  
GLY  
PHE  
PHE  
PHE  
LEU  
ASP  
VAL  
PRO  
MET  
PRO  
ASP  
ASP  
GLY  
GLN  
GLY  
GLY  
GLN  
GLN  
THR  
ALA  
THR  
THR  
THR  
ALA  
ALA  
GLY  
GLY  
PHE  
GLY  
VAL  
GLY  
GLY  
GLY  
GLY  
HIS  
S48  
V49  
P50  
I61  
W75  
SER  
PRO  
PRO  
SER  
TYR

THR  
ASP  
ARG  
ARG  
ARG  
ARG  
ARG  
SER  
TYR  
PRO  
LYS  
THR

## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 10 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
X-PLOR NIH	structure calculation	
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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	277
Number of shifts mapped to atoms	277
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.



## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.65±0.04	0±0/188 ( 0.0± 0.0%)	1.08±0.03	0±0/257 ( 0.0± 0.0%)
1	C	0.71±0.03	0±0/199 ( 0.0± 0.0%)	1.13±0.03	0±0/272 ( 0.0± 0.0%)
1	E	0.69±0.03	0±0/199 ( 0.0± 0.0%)	1.12±0.02	0±0/272 ( 0.0± 0.0%)
1	G	0.68±0.02	0±0/199 ( 0.0± 0.0%)	1.12±0.03	0±0/272 ( 0.0± 0.0%)
2	B	0.73±0.02	0±0/191 ( 0.0± 0.0%)	1.17±0.02	0±0/257 ( 0.0± 0.0%)
2	D	0.72±0.04	0±0/191 ( 0.0± 0.0%)	1.17±0.03	0±0/257 ( 0.0± 0.0%)
2	F	0.70±0.03	0±0/191 ( 0.0± 0.0%)	1.17±0.03	0±0/257 ( 0.0± 0.1%)
2	H	0.70±0.04	0±0/191 ( 0.0± 0.0%)	1.18±0.03	0±0/257 ( 0.0± 0.1%)
All	All	0.70	0/15490 ( 0.0%)	1.14	2/21010 ( 0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	F	66	HIS	CA-CB-CG	-5.72	108.08	113.80	9	1
2	H	66	HIS	CA-CB-CG	-5.26	108.54	113.80	9	1

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	185	176	176	1±0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	196	189	188	2±1
1	E	196	189	188	2±1
1	G	196	189	188	2±2
2	B	188	185	184	1±1
2	D	188	185	184	2±1
2	F	188	185	184	1±1
2	H	188	185	184	1±2
All	All	15250	14830	14760	73

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:G:458:VAL:HG13	2:H:61:ILE:HD12	0.70	1.63	10	2
2:D:63:ILE:HD11	1:E:460:VAL:HG22	0.69	1.64	7	1
1:G:460:VAL:CG2	2:H:61:ILE:HD11	0.64	2.22	10	2
1:E:452:ILE:HD11	1:E:455:CYS:SG	0.62	2.33	4	5
1:G:460:VAL:HG21	2:H:61:ILE:HD11	0.62	1.71	4	2
1:C:460:VAL:CG2	2:D:63:ILE:HG22	0.61	2.26	1	1
2:D:61:ILE:HG22	1:E:455:CYS:SG	0.60	2.37	3	2
1:A:460:VAL:CG2	2:B:63:ILE:HG22	0.58	2.28	1	1
2:D:69:MET:SD	1:E:466:LEU:HD22	0.58	2.38	1	1
1:G:458:VAL:CG1	2:H:61:ILE:HD12	0.57	2.30	10	2
1:G:452:ILE:HD11	1:G:455:CYS:SG	0.56	2.41	5	4
2:B:63:ILE:HD11	1:C:460:VAL:HG22	0.56	1.77	7	1
2:F:69:MET:HE2	2:F:71:ILE:CG1	0.56	2.31	5	2
2:D:55:MET:SD	2:D:61:ILE:HD11	0.55	2.41	2	1
2:D:60:GLY:O	2:D:69:MET:HE1	0.52	2.04	9	1
1:A:452:ILE:HD11	1:A:455:CYS:SG	0.51	2.46	4	2
2:B:61:ILE:HG22	1:C:455:CYS:SG	0.50	2.46	3	2
1:C:468:MET:SD	2:D:71:ILE:HD12	0.50	2.46	2	1
2:F:63:ILE:HD11	1:G:460:VAL:HG22	0.50	1.81	7	1
2:B:60:GLY:O	2:B:69:MET:HE1	0.49	2.07	9	1
1:C:452:ILE:HD11	1:C:455:CYS:SG	0.49	2.47	5	3
2:D:61:ILE:O	1:E:458:VAL:HG23	0.48	2.08	5	1
2:B:55:MET:SD	2:B:61:ILE:HD11	0.48	2.48	2	1
2:B:68:ALA:HB3	1:C:465:TYR:CD2	0.47	2.43	1	1
1:E:452:ILE:HD11	1:E:455:CYS:CB	0.47	2.39	4	2
2:H:60:GLY:O	2:H:69:MET:HE1	0.47	2.09	9	1
2:F:69:MET:HE2	2:F:71:ILE:HD11	0.47	1.85	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:68:ALA:HB3	1:C:465:TYR:HD2	0.46	1.69	1	1
1:E:455:CYS:H	2:F:58:VAL:HG12	0.46	1.69	8	1
2:B:61:ILE:O	1:C:458:VAL:HG23	0.45	2.11	5	1
2:F:60:GLY:O	2:F:69:MET:HE1	0.45	2.12	9	1
1:C:452:ILE:HD11	1:C:455:CYS:CB	0.45	2.42	5	3
2:D:69:MET:HE2	2:D:71:ILE:CG1	0.44	2.43	7	1
2:F:61:ILE:HG22	1:G:455:CYS:SG	0.44	2.52	7	1
2:F:68:ALA:HB3	1:G:465:TYR:CD2	0.44	2.46	1	1
2:F:54:ILE:N	2:F:55:MET:HE3	0.44	2.28	1	1
2:D:55:MET:HE1	2:D:63:ILE:CD1	0.44	2.43	2	1
2:D:63:ILE:CG2	1:E:460:VAL:HG22	0.43	2.43	10	1
1:A:468:MET:HG2	2:B:71:ILE:HD12	0.43	1.90	5	1
2:B:63:ILE:CG2	1:C:460:VAL:HG22	0.43	2.44	10	1
1:G:460:VAL:HG23	2:H:61:ILE:HD11	0.42	1.89	10	1
2:F:69:MET:HE2	2:F:71:ILE:CD1	0.42	2.44	5	1
2:D:58:VAL:O	1:E:455:CYS:SG	0.41	2.78	7	1
2:F:55:MET:SD	2:F:61:ILE:HD13	0.41	2.55	4	1
2:D:55:MET:HE1	2:D:63:ILE:HB	0.41	1.93	6	1
1:A:452:ILE:HD11	1:A:455:CYS:CB	0.41	2.45	8	1
2:F:61:ILE:HG23	1:G:458:VAL:HG23	0.41	1.93	2	1
2:D:68:ALA:HB3	1:E:465:TYR:CD2	0.41	2.50	1	1
1:G:452:ILE:HD11	1:G:455:CYS:CB	0.41	2.46	5	1
1:C:458:VAL:HG13	2:D:61:ILE:HD12	0.41	1.92	6	2
2:B:69:MET:HE2	2:B:71:ILE:CG1	0.40	2.46	7	1
1:A:460:VAL:HG11	2:B:55:MET:HE1	0.40	1.92	9	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	24/133 (18%)	24±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	C	24/133 (18%)	24±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
1	E	24/133 (18%)	24±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	24/133 (18%)	24±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
2	B	24/92 (26%)	24±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
2	D	24/92 (26%)	24±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
2	F	24/92 (26%)	24±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
2	H	24/92 (26%)	24±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
All	All	1920/9000 (21%)	1903 (99%)	17 (1%)	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	22/111 (20%)	22±0 (100±1%)	0±0 (0±1%)	78	96
1	C	23/111 (21%)	22±1 (95±2%)	1±1 (5±2%)	24	75
1	E	23/111 (21%)	22±1 (95±3%)	1±1 (5±3%)	22	72
1	G	23/111 (21%)	22±1 (97±3%)	1±1 (3±3%)	37	85
2	B	20/72 (28%)	19±1 (96±4%)	1±1 (4±4%)	26	77
2	D	20/72 (28%)	19±1 (96±4%)	1±1 (4±4%)	26	77
2	F	20/72 (28%)	19±1 (96±4%)	1±1 (4±4%)	29	79
2	H	20/72 (28%)	20±0 (98±2%)	0±0 (2±2%)	42	88
All	All	1710/7320 (23%)	1648 (96%)	62 (4%)	32	82

All 24 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	E	458	VAL	8
1	C	458	VAL	6
1	G	447	ARG	5
1	C	447	ARG	4
2	D	55	MET	4

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Mol	Chain	Res	Type	Models (Total)
2	B	55	MET	3
1	E	447	ARG	3
2	F	55	MET	3
2	H	55	MET	3
2	B	63	ILE	2
2	B	56	ASN	2
2	B	75	TRP	2
2	D	56	ASN	2
2	F	56	ASN	2
2	F	75	TRP	2
2	D	63	ILE	2
1	G	458	VAL	2
2	F	63	ILE	1
2	H	56	ASN	1
1	A	459	GLN	1
1	C	459	GLN	1
1	E	459	GLN	1
2	D	75	TRP	1
2	H	75	TRP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 6.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 6.7 Other polymers ⓘ

There are no such molecules in this entry.

## 6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name: *assigned\_chemical\_shifts\_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	277
Number of shifts mapped to atoms	277
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
$^{13}\text{C}_\alpha$	52	$0.00 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	49	$-0.87 \pm 0.27$	Should be checked
$^{13}\text{C}'$	49	$0.40 \pm 0.23$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	50	$-0.61 \pm 0.38$	None needed (imprecise)

#### 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 9%, i.e. 245 atoms were assigned a chemical shift out of a possible 2625. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	137/1007 (14%)	0/414 (0%)	92/398 (23%)	45/195 (23%)
Sidechain	99/1430 (7%)	0/937 (0%)	94/428 (22%)	5/65 (8%)

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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	9/188 (5%)	0/88 (0%)	9/88 (10%)	0/12 (0%)
Overall	245/2625 (9%)	0/1439 (0%)	195/914 (21%)	50/272 (18%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 270 atoms were assigned a chemical shift out of a possible 2868. 0 out of 32 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	149/1104 (13%)	0/452 (0%)	101/440 (23%)	48/212 (23%)
Sidechain	112/1576 (7%)	0/1036 (0%)	107/472 (23%)	5/68 (7%)
Aromatic	9/188 (5%)	0/88 (0%)	9/88 (10%)	0/12 (0%)
Overall	270/2868 (9%)	0/1576 (0%)	217/1000 (22%)	53/292 (18%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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

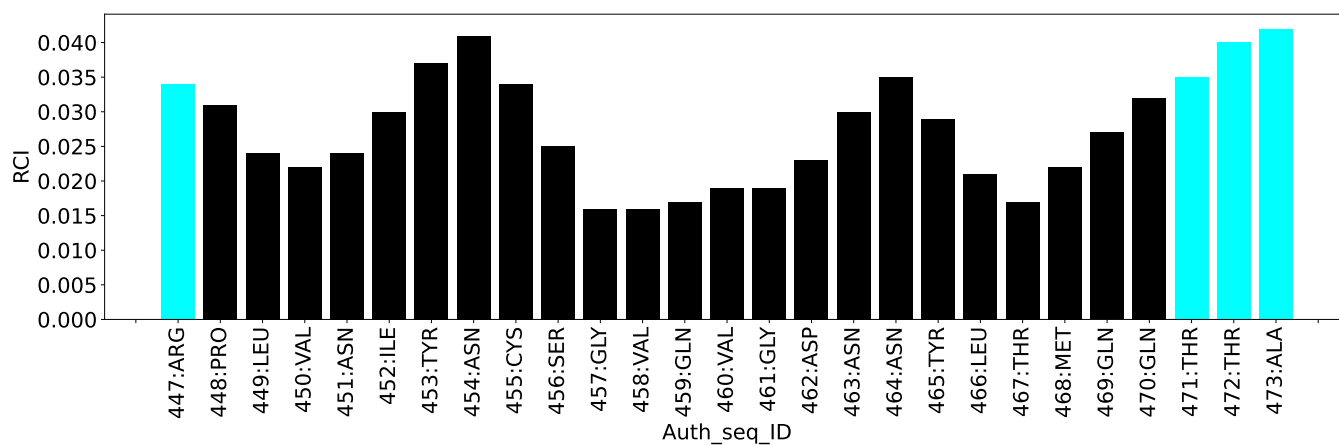
There are no statistically unusual chemical shifts.

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

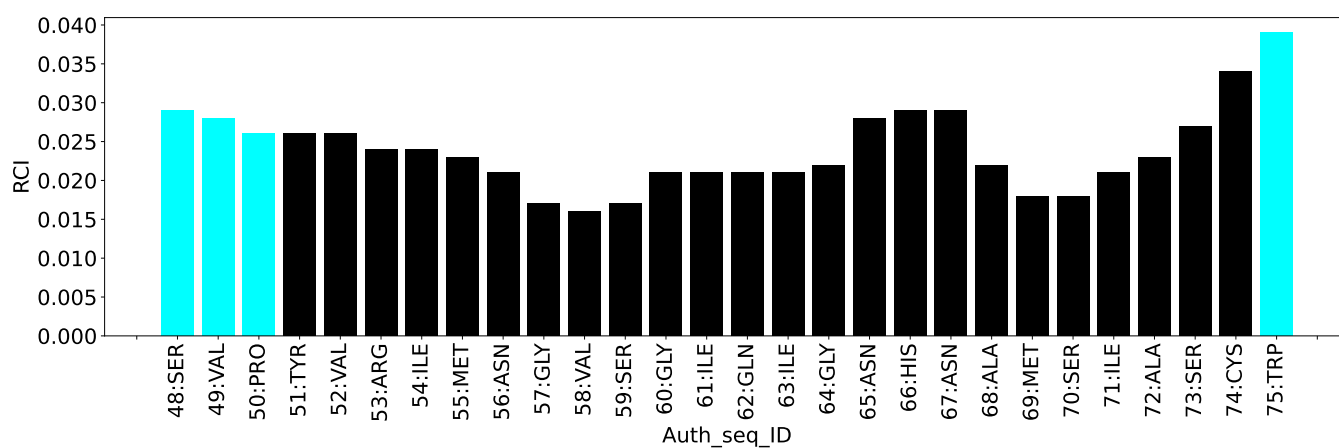
The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted 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:





Random coil index (RCI) for chain B:



## 8 NMR restraints analysis

### 8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	71
Intra-residue ( $ i-j =0$ )	0
Sequential ( $ i-j =1$ )	1
Medium range ( $ i-j >1$ and $ i-j <5$ )	26
Long range ( $ i-j \geq 5$ )	22
Inter-chain	22
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	62
Number of unmapped restraints	0
Number of restraints per residue	0.1
Number of long range restraints per residue <sup>1</sup>	0.0

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

### 8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

#### 8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	1.5	0.19
0.2-0.5 (Medium)	2.1	0.49
>0.5 (Large)	6.5	4.69

### 8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	0.5	5.73
10.0-20.0 (Medium)	0.1	14.6
>20.0 (Large)	0.1	23.41

## 9 Distance violation analysis ⓘ

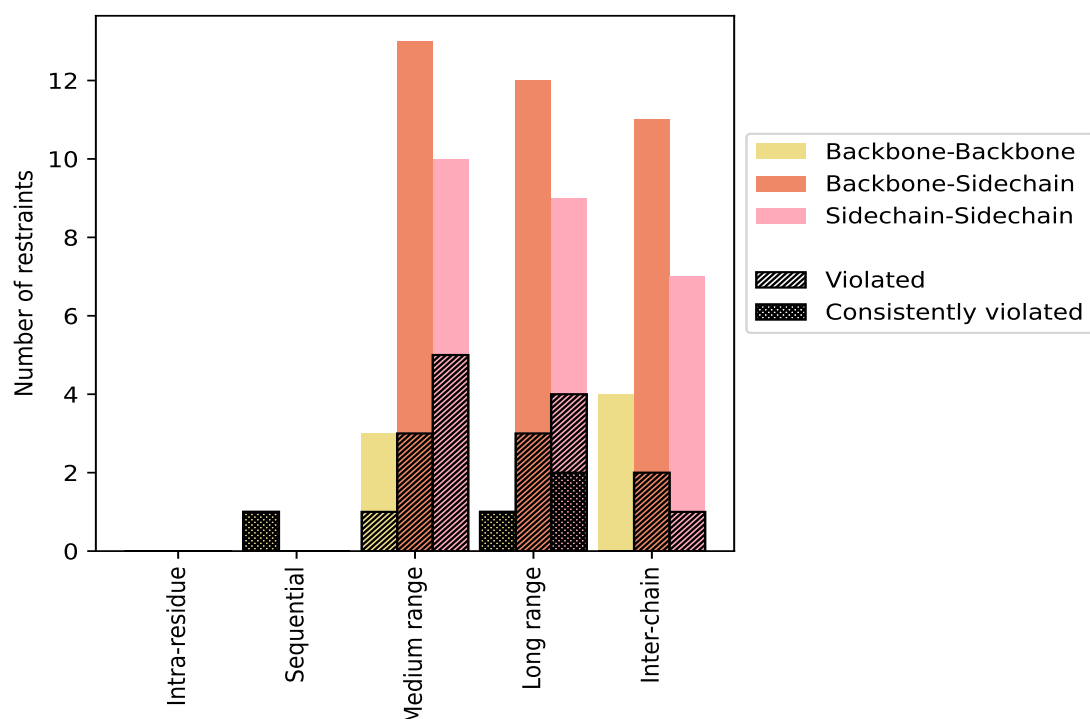
### 9.1 Summary of distance violations ⓘ

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
Intra-residue ( $ i-j =0$ )	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ( $ i-j =1$ )	1	1.4	1	100.0	1.4	1	100.0	1.4
Backbone-Backbone	1	1.4	1	100.0	1.4	1	100.0	1.4
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ( $ i-j >1$ & $ i-j <5$ )	26	36.6	9	34.6	12.7	0	0.0	0.0
Backbone-Backbone	3	4.2	1	33.3	1.4	0	0.0	0.0
Backbone-Sidechain	13	18.3	3	23.1	4.2	0	0.0	0.0
Sidechain-Sidechain	10	14.1	5	50.0	7.0	0	0.0	0.0
Long range ( $ i-j \geq 5$ )	22	31.0	8	36.4	11.3	3	13.6	4.2
Backbone-Backbone	1	1.4	1	100.0	1.4	1	100.0	1.4
Backbone-Sidechain	12	16.9	3	25.0	4.2	0	0.0	0.0
Sidechain-Sidechain	9	12.7	4	44.4	5.6	2	22.2	2.8
Inter-chain	22	31.0	3	13.6	4.2	0	0.0	0.0
Backbone-Backbone	4	5.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	11	15.5	2	18.2	2.8	0	0.0	0.0
Sidechain-Sidechain	7	9.9	1	14.3	1.4	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	71	100.0	21	29.6	29.6	4	5.6	5.6
Backbone-Backbone	9	12.7	3	33.3	4.2	2	22.2	2.8
Backbone-Sidechain	36	50.7	8	22.2	11.3	0	0.0	0.0
Sidechain-Sidechain	26	36.6	10	38.5	14.1	2	7.7	2.8

<sup>1</sup> percentage calculated with respect to the total number of distance restraints, <sup>2</sup> percentage calculated with respect to the number of restraints in a particular restraint category, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

### 9.1.1 Bar chart : Distribution of distance restraints and violations [i](#)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

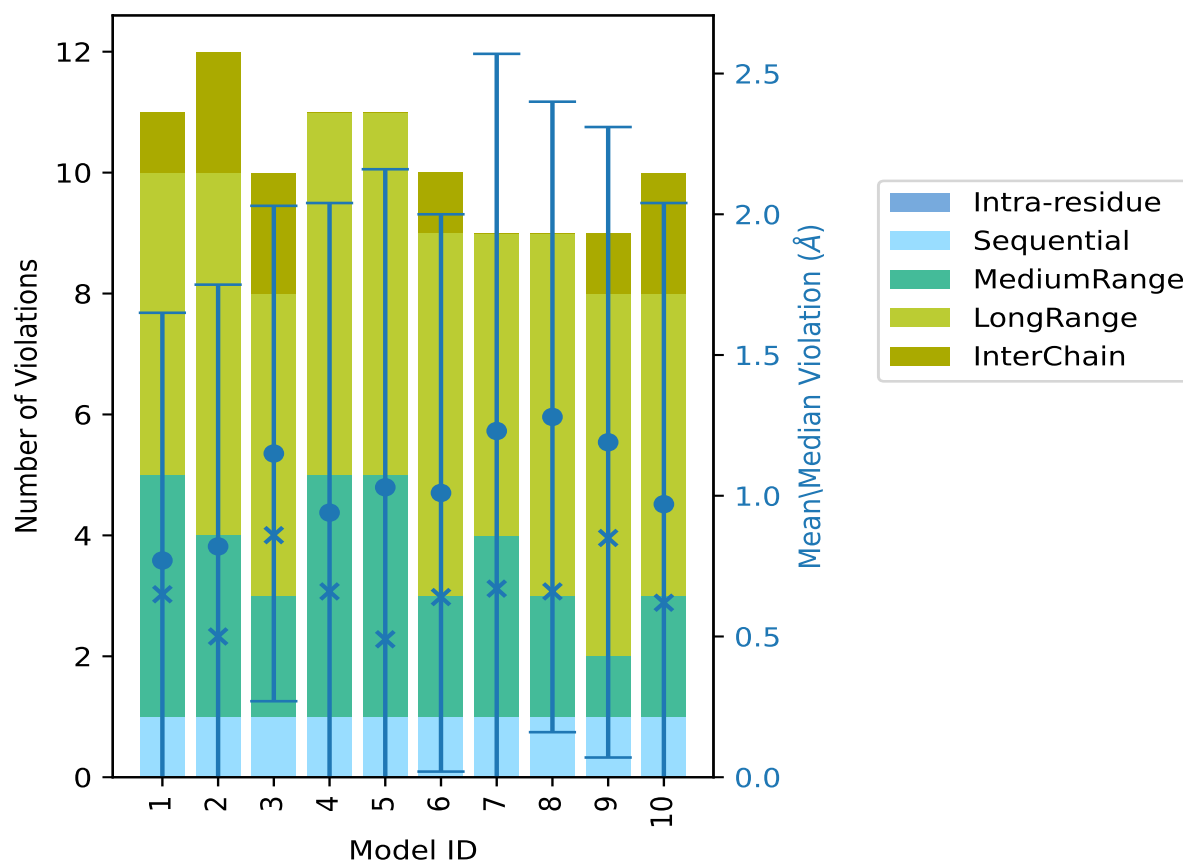
## 9.2 Distance violation statistics for each model [i](#)

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD <sup>6</sup> (Å)	Median (Å)
	IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total				
1	0	1	4	5	1	11	0.77	3.35	0.88	0.65
2	0	1	3	6	2	12	0.82	3.7	0.93	0.5
3	0	1	2	5	2	10	1.15	3.17	0.88	0.86
4	0	1	4	6	0	11	0.94	4.17	1.1	0.66
5	0	1	4	6	0	11	1.03	3.73	1.13	0.49
6	0	1	2	6	1	10	1.01	3.59	0.99	0.64
7	0	1	3	5	0	9	1.23	4.69	1.34	0.67
8	0	1	2	6	0	9	1.28	3.79	1.12	0.66
9	0	1	1	6	1	9	1.19	4.07	1.12	0.85
10	0	1	2	5	2	10	0.97	3.92	1.07	0.62

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup>Standard deviation

### 9.2.1 Bar graph : Distance Violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

### 9.3 Distance violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 50(IR:0, SQ:0, MR:17, LR:14, IC:19) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	5	1	0	6	1	10.0
0	0	0	1	1	2	2	20.0
0	0	0	0	1	1	3	30.0

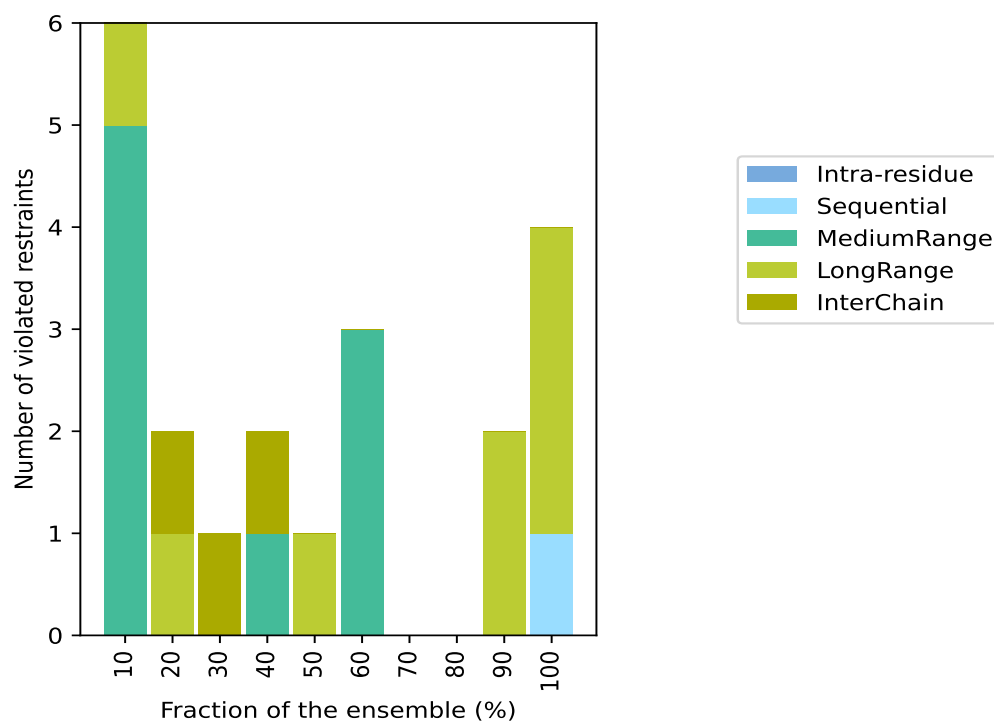
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Number of violated restraints						Fraction of the ensemble	
IR <sup>1</sup>	SQ <sup>2</sup>	MR <sup>3</sup>	LR <sup>4</sup>	IC <sup>5</sup>	Total	Count <sup>6</sup>	%
0	0	1	0	1	2	4	40.0
0	0	0	1	0	1	5	50.0
0	0	3	0	0	3	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	2	0	2	9	90.0
0	1	0	3	0	4	10	100.0

<sup>1</sup>Intra-residue restraints, <sup>2</sup>Sequential restraints, <sup>3</sup>Medium range restraints, <sup>4</sup>Long range restraints, <sup>5</sup>Inter-chain restraints, <sup>6</sup> Number of models with violations

### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

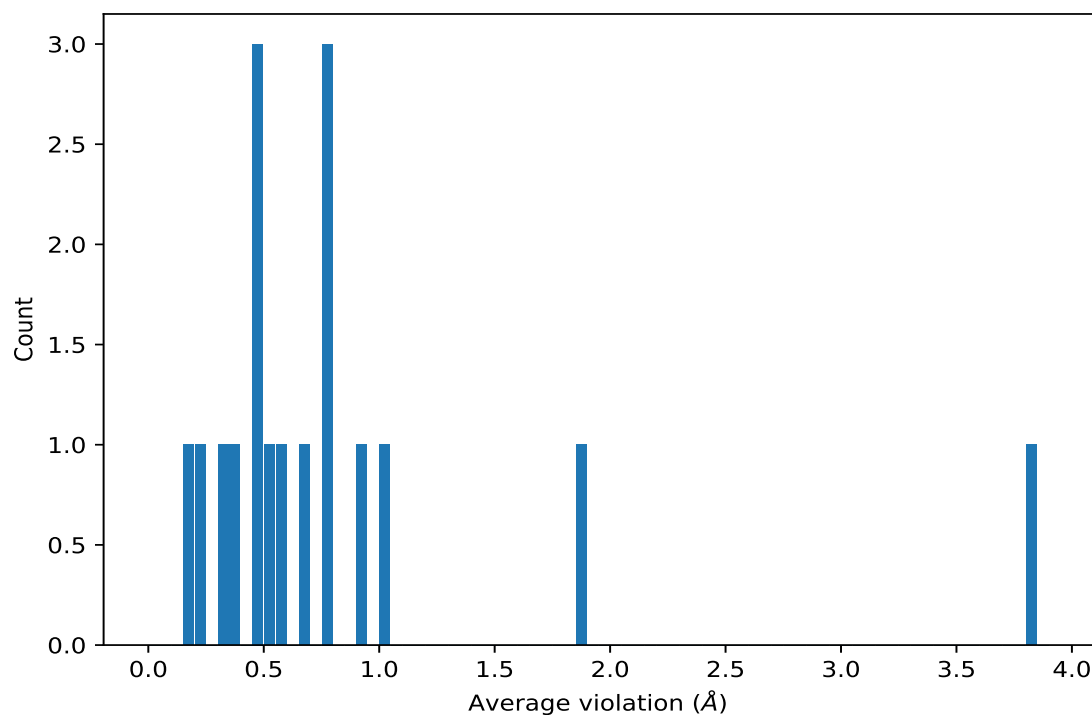


## 9.4 Most violated distance restraints in the ensemble ⓘ

### 9.4.1 Histogram : Distribution of mean distance violations ⓘ

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models

in the ensemble



#### 9.4.2 Table: Most violated distance restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	10	3.82	0.41	3.76
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	10	1.86	0.45	1.88
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	10	0.67	0.0	0.67
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	10	0.49	0.19	0.48
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	9	1.02	0.29	0.84
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	9	0.91	0.57	0.8
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	6	0.55	0.2	0.64
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	6	0.53	0.16	0.46
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	6	0.24	0.16	0.2
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	5	0.31	0.26	0.19
(1,16)	2:63:B:ILE:CD1	1:461:C:GLY:N	4	0.49	0.36	0.3
(1,16)	2:63:B:ILE:CD1	1:461:A:GLY:N	4	0.49	0.36	0.3
(1,45)	2:65:B:ASN:CB	2:63:B:ILE:N	4	0.16	0.06	0.15
(1,10)	2:63:B:ILE:CD1	1:461:A:GLY:CA	3	0.78	0.53	0.6
(1,10)	2:63:B:ILE:CD1	1:461:C:GLY:CA	3	0.78	0.53	0.6

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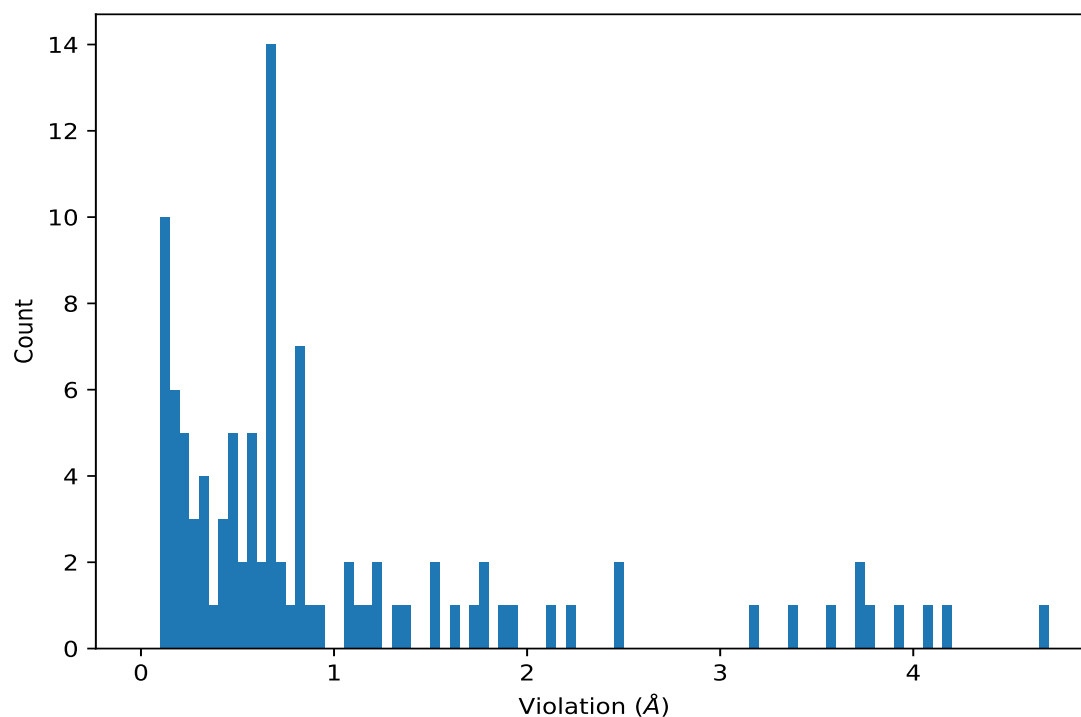
Key	Atom-1	Atom-2	Models <sup>1</sup>	Mean (Å)	SD <sup>1</sup> (Å)	Median (Å)
(1,50)	1:456:A:SER:CB	1:468:A:MET:CE	2	0.76	0.17	0.76
(2,1)	2:53:B:ARG:NH1	1:462:A:ASP:OD1	2	0.36	0.22	0.36

<sup>1</sup>Number of violated models, <sup>2</sup>Standard deviation

## 9.5 All violated distance restraints [i](#)

### 9.5.1 Histogram : Distribution of distance violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



### 9.5.2 Table : All distance violations [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	7	4.69
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	4	4.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	9	4.07
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	10	3.92
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	8	3.79
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	5	3.73
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	2	3.7
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	6	3.59
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	1	3.35
(1,54)	1:457:A:GLY:CA	1:469:A:GLN:C	3	3.17
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	5	2.46
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	8	2.46
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	3	2.23
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	7	2.11
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	6	1.91
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	9	1.85
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	8	1.76
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	5	1.75
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	10	1.71
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	2	1.61
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	4	1.51
(1,10)	2:63:B:ILE:CD1	1:461:C:GLY:CA	3	1.5
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	5	1.35
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	6	1.31
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	7	1.23
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	1	1.21
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	9	1.19
(1,16)	2:63:B:ILE:CD1	1:461:C:GLY:N	3	1.11
(1,24)	2:59:B:SER:CB	2:71:B:ILE:CG1	4	1.07
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	8	1.05
(1,50)	1:456:A:SER:CB	1:468:A:MET:CE	9	0.92
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	3	0.89
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	9	0.85
(1,58)	1:447:A:ARG:CA	1:449:A:LEU:CD1	4	0.84
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	3	0.84
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	10	0.83
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	7	0.82
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	1	0.81
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	3	0.8
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	9	0.79
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	1	0.71
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	4	0.71
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	2	0.68
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	6	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	1	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	2	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	3	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	5	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	6	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	7	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	9	0.67
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	10	0.67
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	10	0.66
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	4	0.66
(1,1)	1:457:C:GLY:C	1:458:C:VAL:N	8	0.66
(1,47)	1:452:A:ILE:CG1	1:457:A:GLY:C	1	0.65
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	8	0.62
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	6	0.61
(1,10)	2:63:B:ILE:CD1	1:461:C:GLY:CA	2	0.6
(2,1)	2:53:B:ARG:NH1	1:462:A:ASP:OD1	6	0.59
(1,50)	1:456:A:SER:CB	1:468:A:MET:CE	8	0.59
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	10	0.58
(1,51)	1:457:A:GLY:CA	1:466:A:LEU:CB	2	0.55
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	10	0.54
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	8	0.51
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	5	0.49
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	7	0.48
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	7	0.47
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	4	0.45
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	1	0.45
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	2	0.44
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	7	0.42
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	2	0.4
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	6	0.39
(1,44)	2:71:B:ILE:CG1	2:73:B:SER:CB	5	0.35
(1,34)	2:54:B:ILE:CG1	2:56:B:ASN:CB	2	0.35
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	2	0.34
(1,16)	2:63:B:ILE:CD1	1:461:C:GLY:N	10	0.32
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	4	0.27
(1,16)	2:63:B:ILE:CD1	1:461:C:GLY:N	2	0.27
(1,45)	2:65:B:ASN:CB	2:63:B:ILE:N	2	0.25
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	6	0.24
(1,16)	2:63:B:ILE:CD1	1:461:A:GLY:N	9	0.24
(1,10)	2:63:B:ILE:CD1	1:461:A:GLY:CA	10	0.24
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	4	0.23
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	4	0.19
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	1	0.19
(1,25)	2:59:B:SER:CB	2:71:B:ILE:CD1	10	0.18
(1,45)	2:65:B:ASN:CB	2:63:B:ILE:N	3	0.17
(1,65)	1:466:A:LEU:CB	1:468:A:MET:CG	3	0.16
(1,40)	2:62:B:GLN:CA	2:64:B:GLY:C	7	0.16
(1,23)	2:59:B:SER:CB	2:69:B:MET:CE	9	0.15
(2,1)	2:53:B:ARG:NH1	1:462:A:ASP:OD1	1	0.14
(1,33)	2:53:B:ARG:CB	2:55:B:MET:CB	5	0.14
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	5	0.14
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	6	0.12
(1,45)	2:65:B:ASN:CB	2:63:B:ILE:N	1	0.12
(1,39)	2:61:B:ILE:CD1	2:63:B:ILE:CG1	1	0.12
(1,46)	1:452:A:ILE:CD1	1:457:A:GLY:C	5	0.11
(1,45)	2:65:B:ASN:CB	2:63:B:ILE:N	5	0.11
(1,32)	2:50:B:PRO:CD	2:52:B:VAL:CA	8	0.1

## 10 Dihedral-angle violation analysis [i](#)

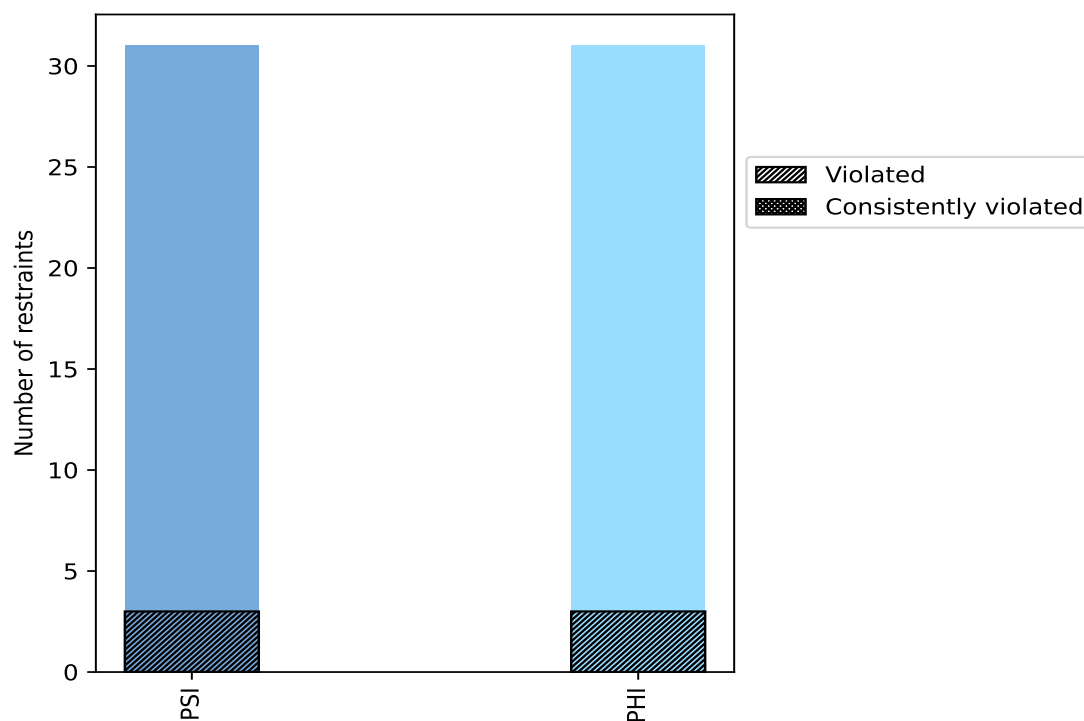
### 10.1 Summary of dihedral-angle violations [i](#)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	% <sup>1</sup>	Violated <sup>3</sup>			Consistently Violated <sup>4</sup>		
			Count	% <sup>2</sup>	% <sup>1</sup>	Count	% <sup>2</sup>	% <sup>1</sup>
PSI	31	50.0	3	9.7	4.8	0	0.0	0.0
PHI	31	50.0	3	9.7	4.8	0	0.0	0.0
Total	62	100.0	6	9.7	9.7	0	0.0	0.0

<sup>1</sup> percentage calculated with respect to total number of dihedral-angle restraints, <sup>2</sup> percentage calculated with respect to number of restraints in a particular dihedral-angle type, <sup>3</sup> violated in at least one model, <sup>4</sup> violated in all the models

#### 10.1.1 Bar chart : Distribution of dihedral-angles and violations [i](#)



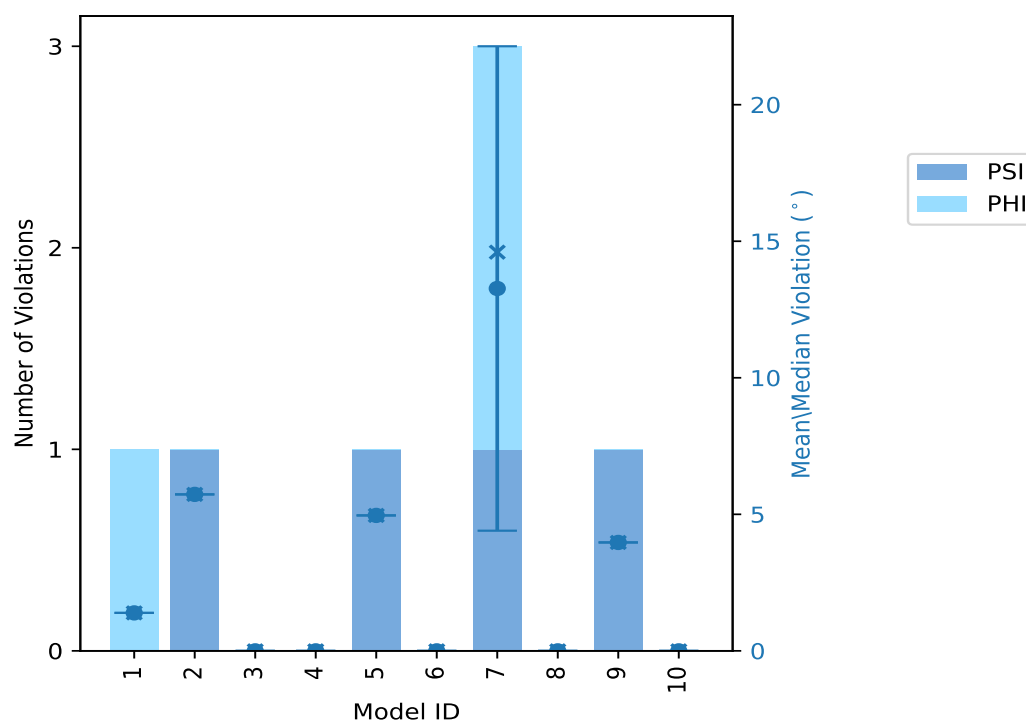
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

## 10.2 Dihedral-angle violation statistics for each model [i](#)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than 1° are not included in the statistics.

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	1	1	1.39	1.39	0.0	1.39
2	1	0	1	5.73	5.73	0.0	5.73
3	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0.0	0.0	0.0	0.0
5	1	0	1	4.96	4.96	0.0	4.96
6	0	0	0	0.0	0.0	0.0	0.0
7	1	2	3	13.27	23.41	8.87	14.6
8	0	0	0	0.0	0.0	0.0	0.0
9	1	0	1	3.97	3.97	0.0	3.97
10	0	0	0	0.0	0.0	0.0	0.0

### 10.2.1 Bar graph : Dihedral violation statistics for each model [i](#)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

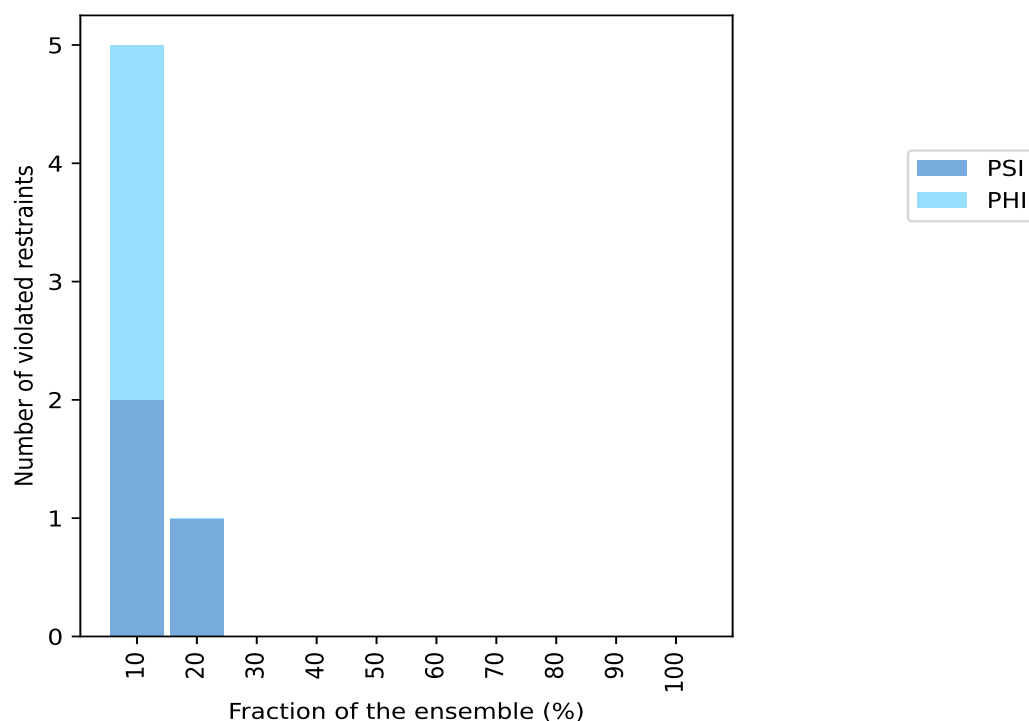
### 10.3 Dihedral-angle violation statistics for the ensemble [i](#)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count <sup>1</sup>	%
2	3	5	1	10.0
1	0	1	2	20.0
0	0	0	3	30.0
0	0	0	4	40.0
0	0	0	5	50.0
0	0	0	6	60.0
0	0	0	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
0	0	0	10	100.0

<sup>1</sup> Number of models with violations

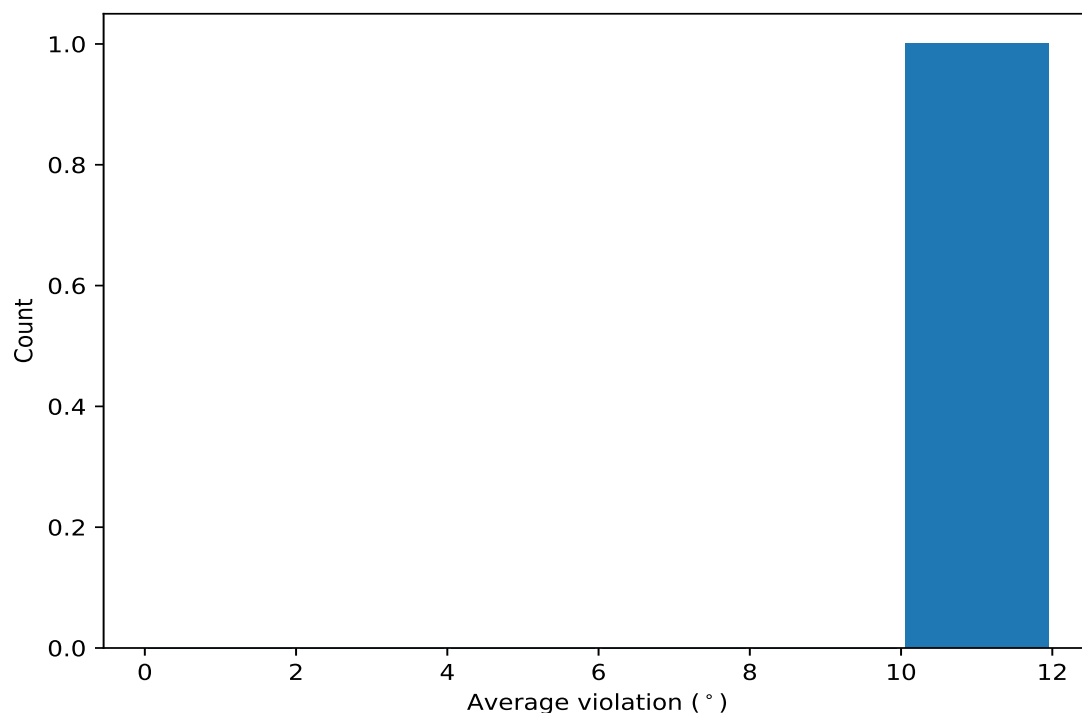
#### 10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



## 10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

### 10.4.1 Histogram : Distribution of mean dihedral-angle violations [i](#)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



### 10.4.2 Table: Most violated dihedral-angle restraints [i](#)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models <sup>1</sup>	Mean	SD <sup>2</sup>	Median
(1,6)	2:53:B:ARG:N	2:53:B:ARG:CA	2:53:B:ARG:C	2:54:B:ILE:N	2	10.16	4.43	10.16

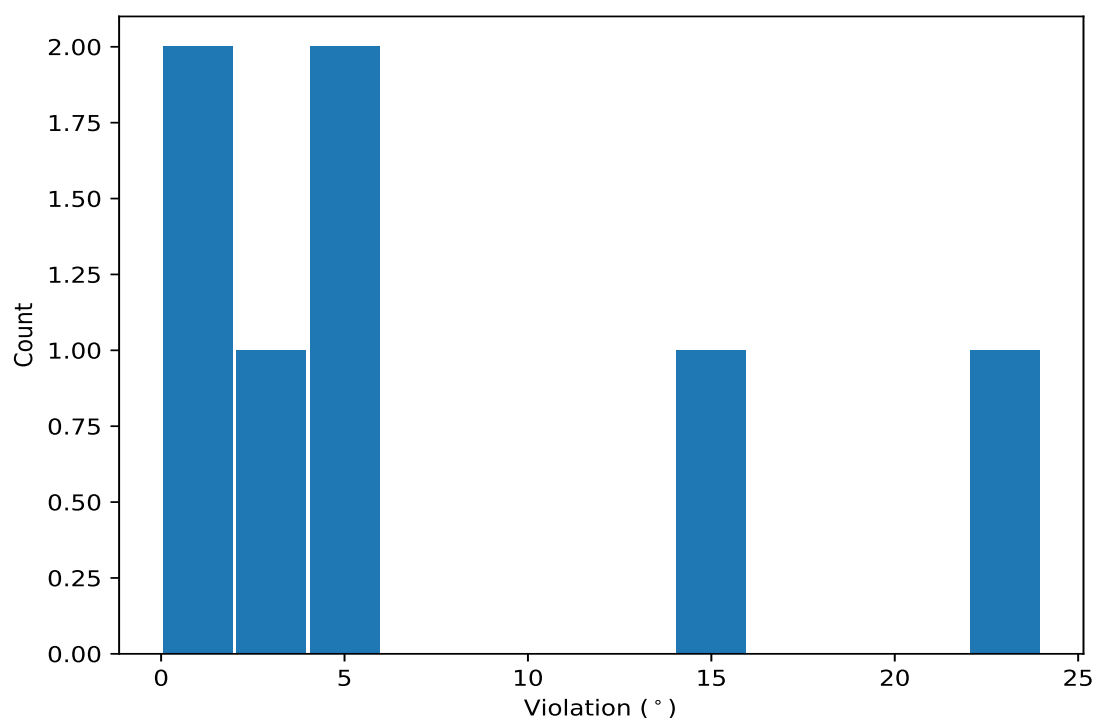
<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

## 10.5 All violated dihedral-angle restraints [i](#)

### 10.5.1 Histogram : Distribution of violations [i](#)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.





### 10.5.2 Table: All violated dihedral-angle restraints [i](#)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,45)	1:457:A:GLY:C	1:458:A:VAL:N	1:458:A:VAL:CA	1:458:A:VAL:C	7	23.41
(1,6)	2:53:B:ARG:N	2:53:B:ARG:CA	2:53:B:ARG:C	2:54:B:ILE:N	7	14.6
(1,6)	2:53:B:ARG:N	2:53:B:ARG:CA	2:53:B:ARG:C	2:54:B:ILE:N	2	5.73
(1,38)	1:451:A:ASN:N	1:451:A:ASN:CA	1:451:A:ASN:C	1:452:A:ILE:N	5	4.96
(1,22)	2:65:B:ASN:N	2:65:B:ASN:CA	2:65:B:ASN:C	2:66:B:HIS:N	9	3.97
(1,15)	2:60:B:GLY:C	2:61:B:ILE:N	2:61:B:ILE:CA	2:61:B:ILE:C	7	1.81
(1,7)	2:53:B:ARG:C	2:54:B:ILE:N	2:54:B:ILE:CA	2:54:B:ILE:C	1	1.39