



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 02:52 PM UTC

PDB ID : 2RSV / pdb_00002rsv
BMRB ID : 11506
Title : Solution structure of human full-length vaccinia related kinase 1 (VRK1)
Authors : Koshiba, S.; Tochio, N.; Yokoyama, J.; Kigawa, T.
Deposited on : 2012-07-12

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
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

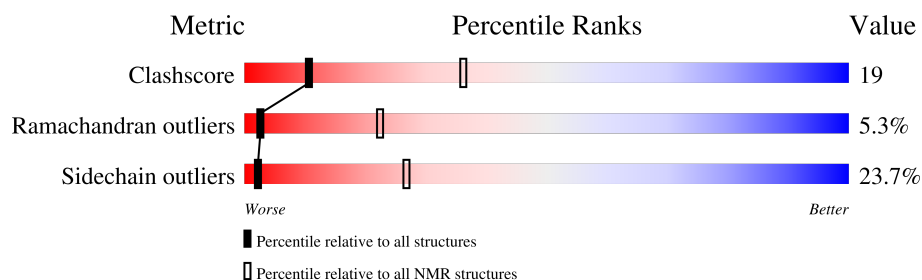
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 52%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	403	33% 35% . 29%

2 Ensemble composition and analysis

This entry contains 18 models. Model 13 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:24-A:44, A:50-A:204, A:223-A:309, A:315-A:336 (285)	1.50	13

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 7 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6497 atoms, of which 3260 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Serine/threonine-protein kinase VRK1.

Mol	Chain	Residues	Atoms						Trace
1	A	403	Total	C	H	N	O	S	0
			6497	2043	3260	571	609	14	

There are 7 discrepancies between the modelled and reference sequences:

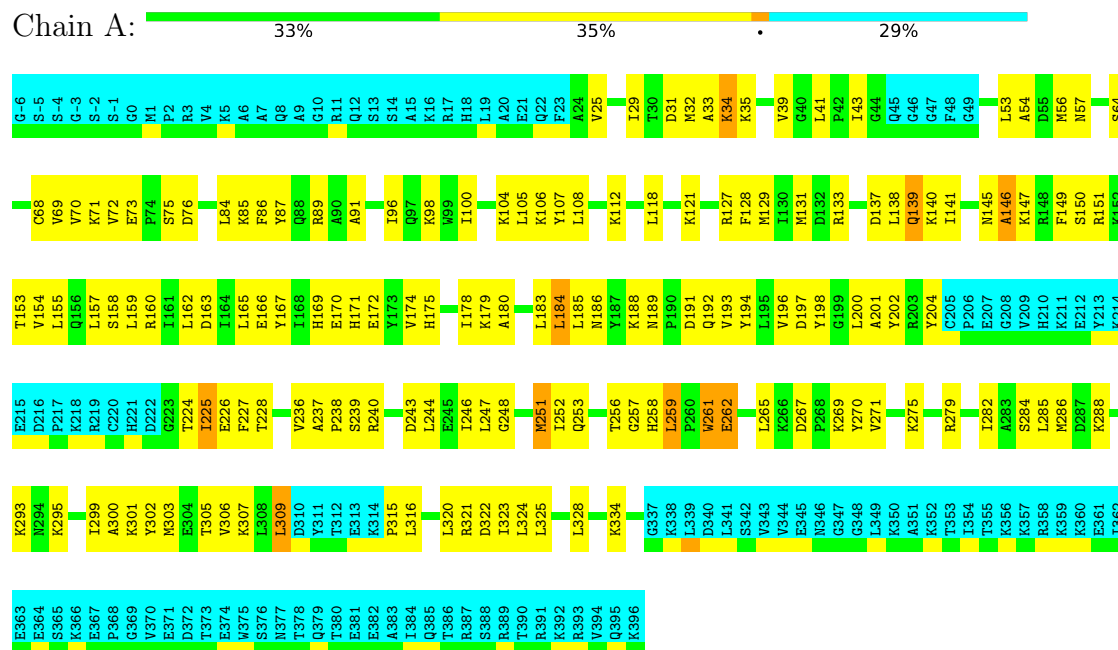
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q99986
A	-5	SER	-	expression tag	UNP Q99986
A	-4	SER	-	expression tag	UNP Q99986
A	-3	GLY	-	expression tag	UNP Q99986
A	-2	SER	-	expression tag	UNP Q99986
A	-1	SER	-	expression tag	UNP Q99986
A	0	GLY	-	expression tag	UNP Q99986

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: Serine/threonine-protein kinase VRK1

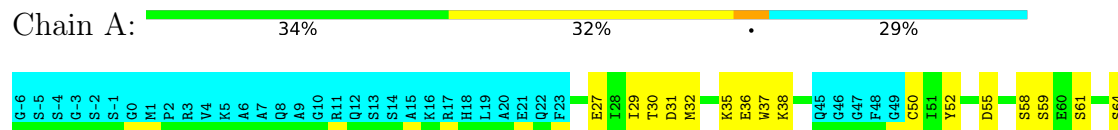


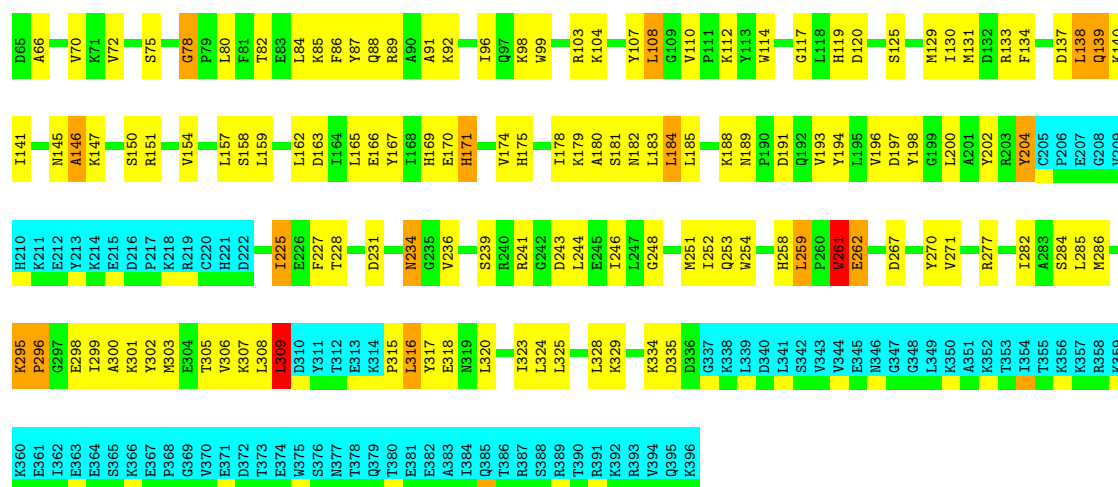
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Serine/threonine-protein kinase VRK1

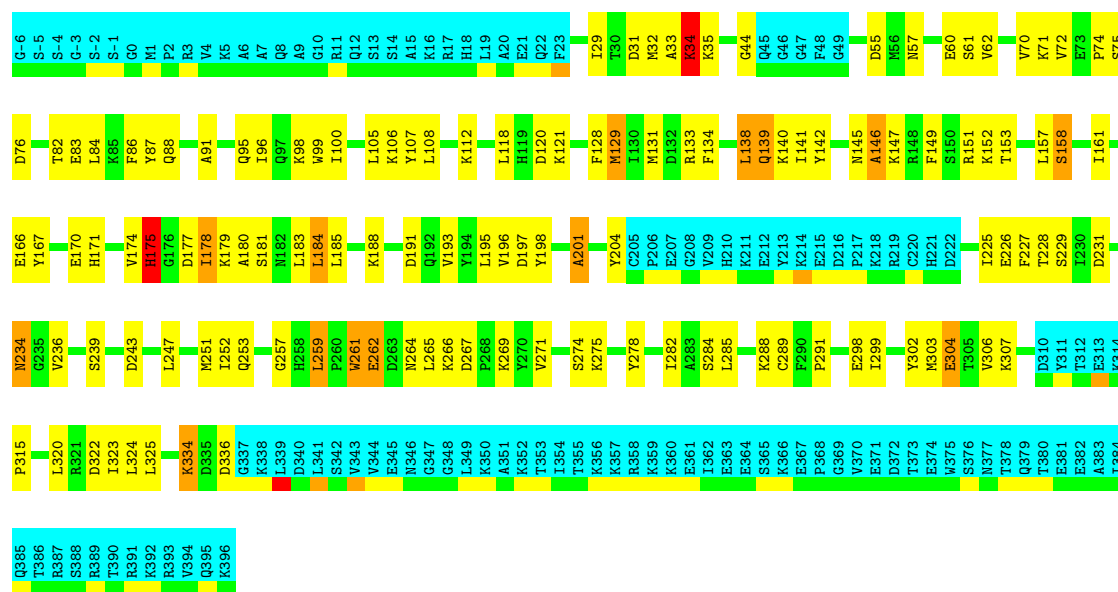




4.2.2 Score per residue for model 2

- Molecule 1: Serine/threonine-protein kinase VRK1

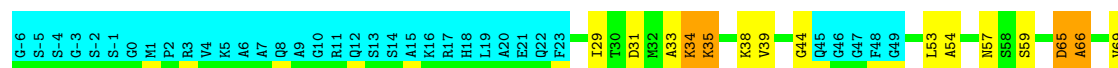
Chain A: 39% 28% 29%

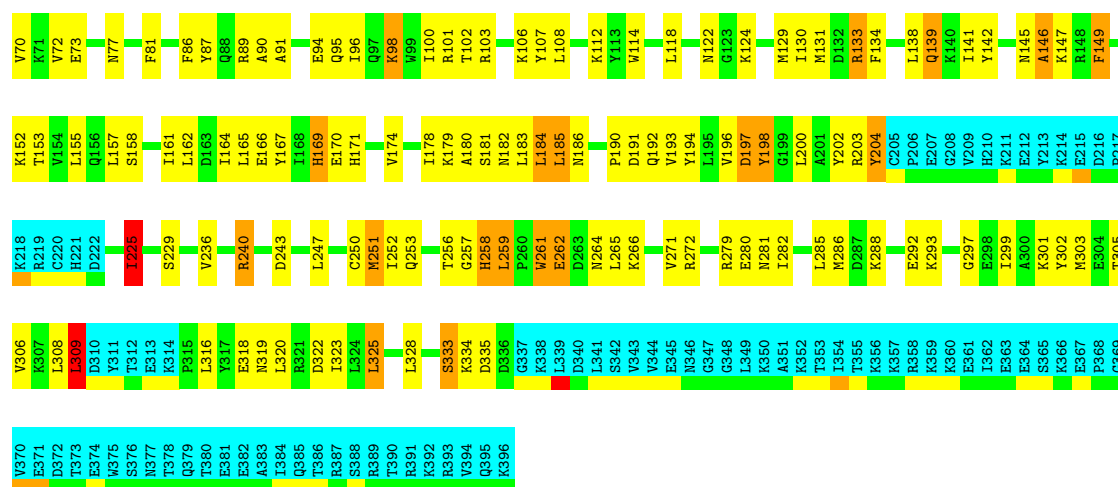


4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase VRK1

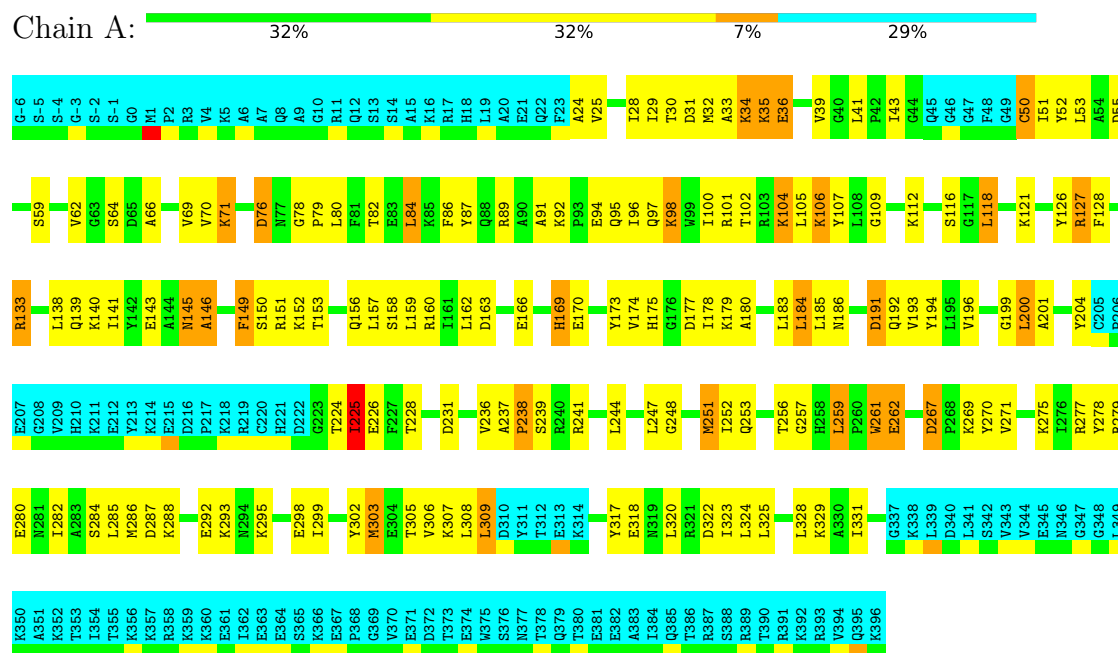
Chain A: 36% 29% 6% 29%





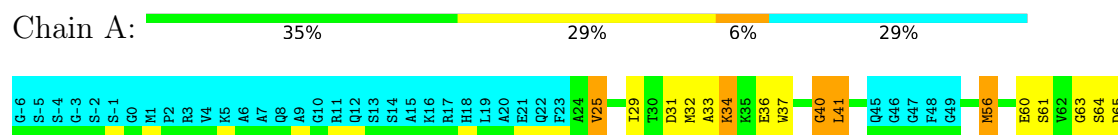
4.2.4 Score per residue for model 4

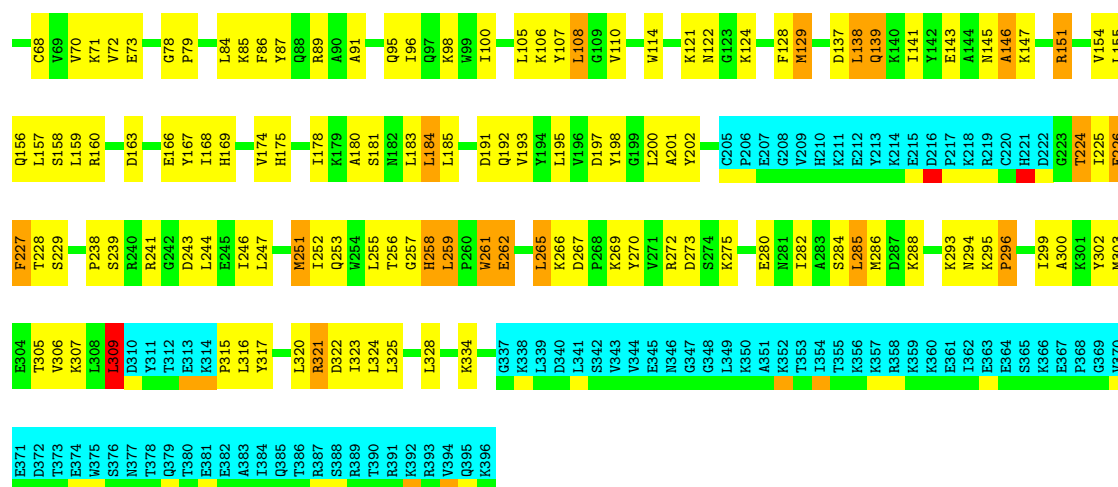
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.5 Score per residue for model 5

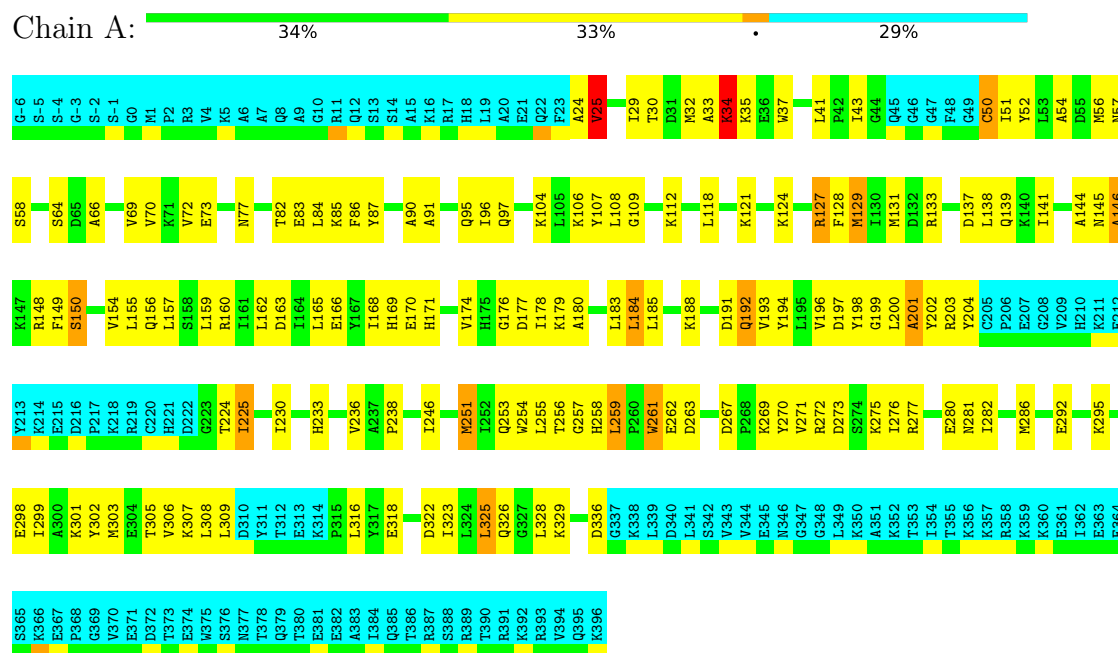
- Molecule 1: Serine/threonine-protein kinase VRK1





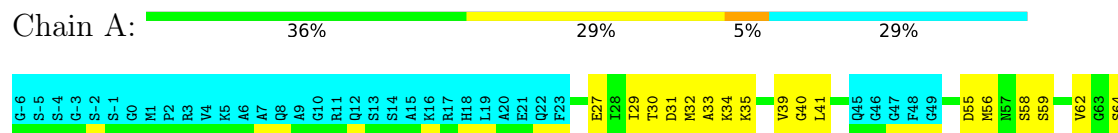
4.2.6 Score per residue for model 6

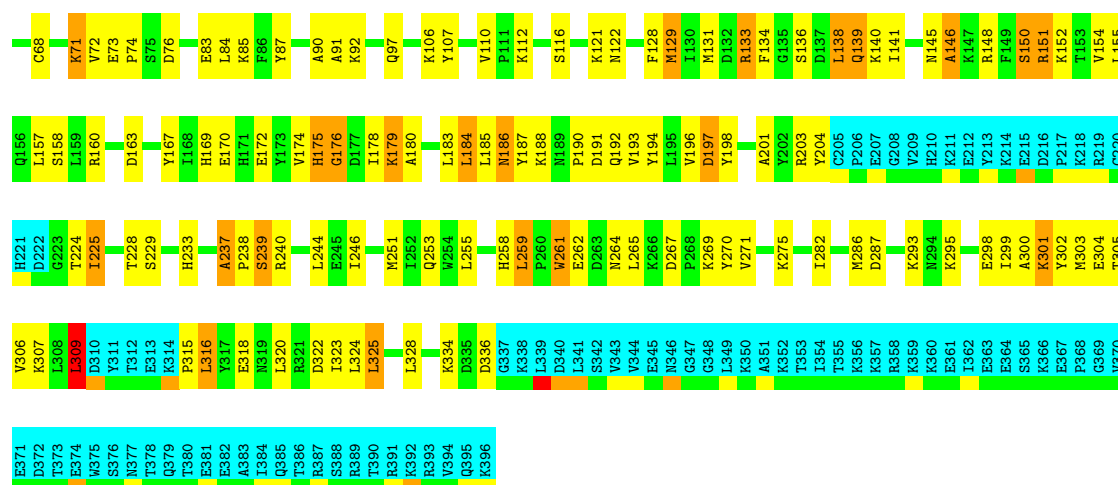
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.7 Score per residue for model 7

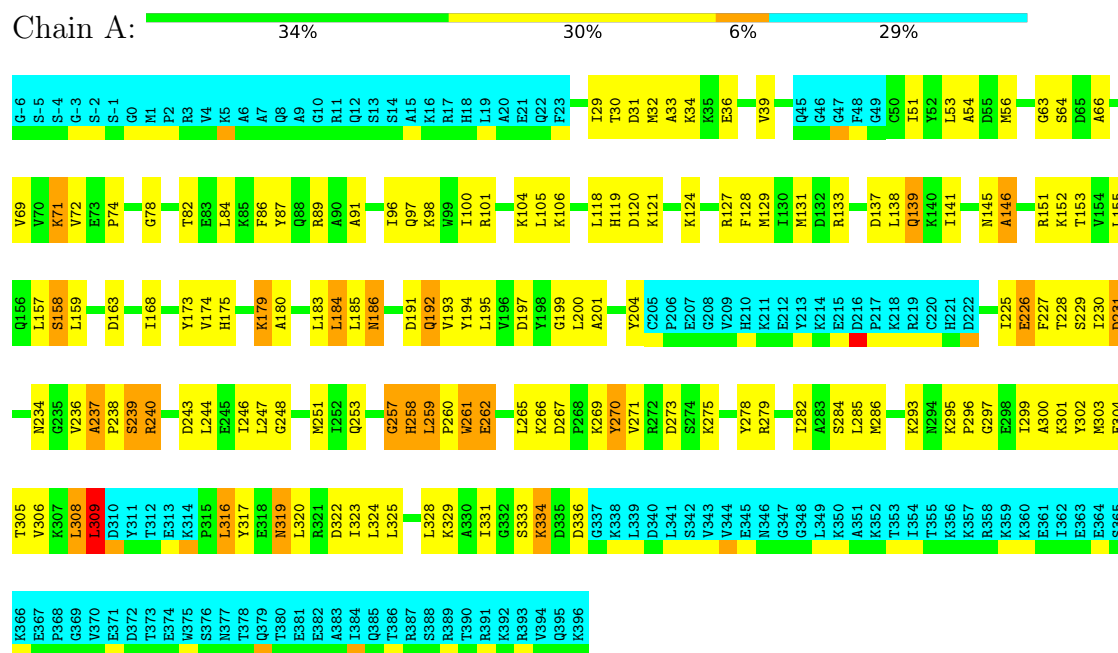
- Molecule 1: Serine/threonine-protein kinase VRK1





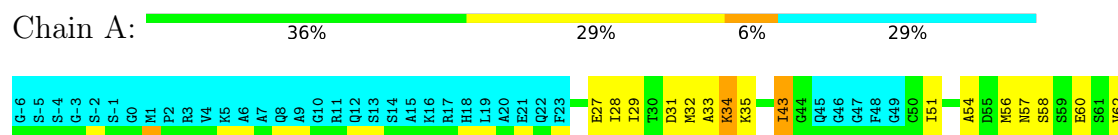
4.2.8 Score per residue for model 8

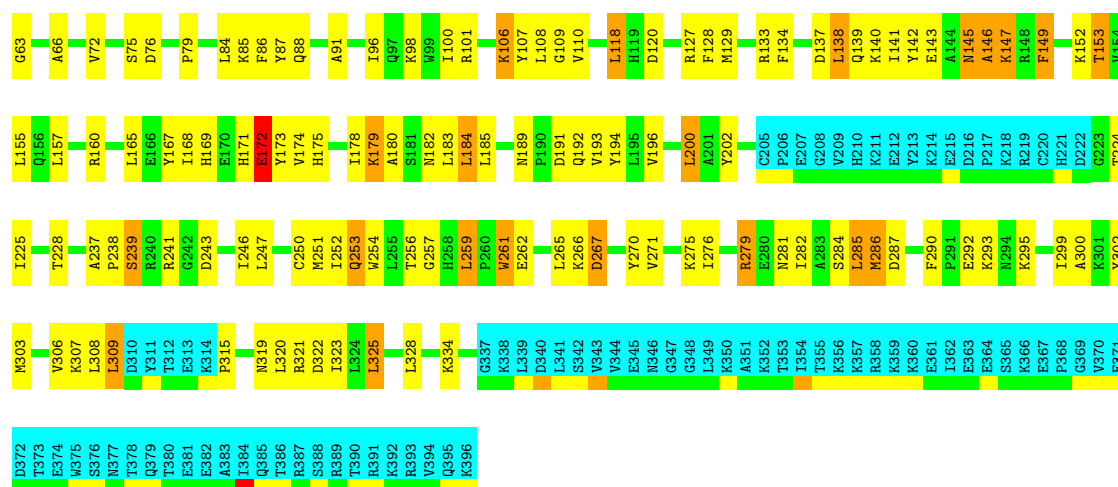
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.9 Score per residue for model 9

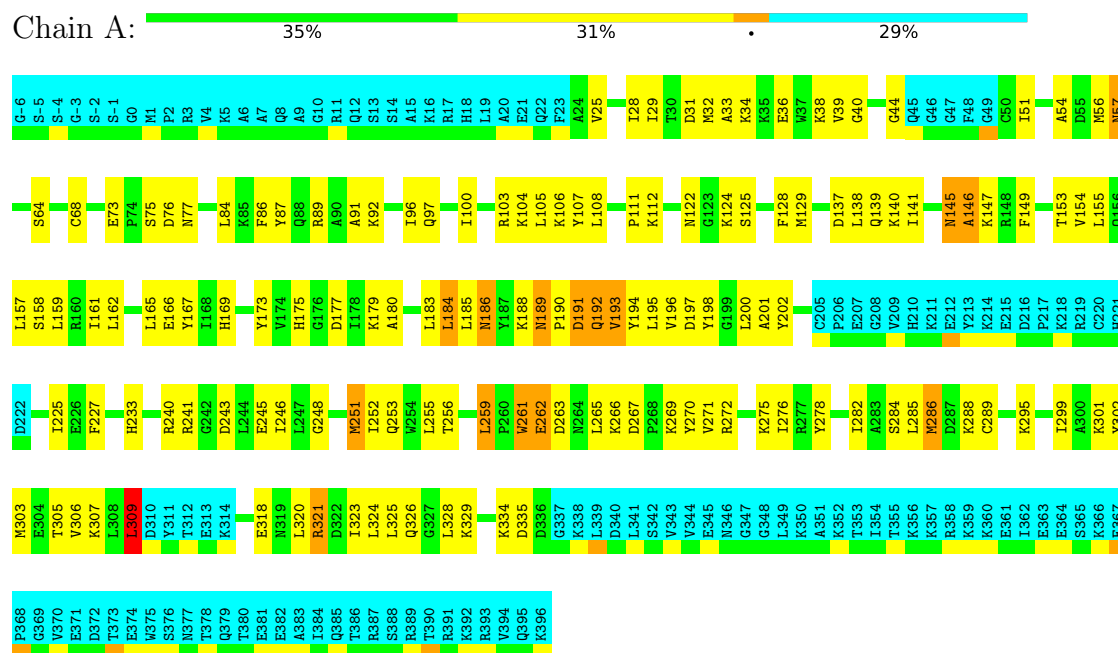
- Molecule 1: Serine/threonine-protein kinase VRK1





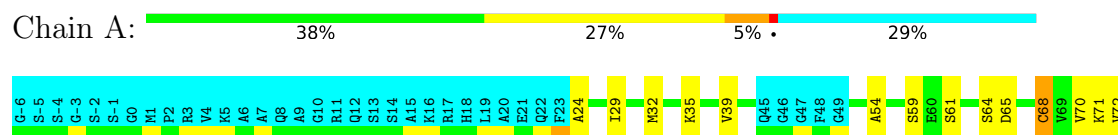
4.2.10 Score per residue for model 10

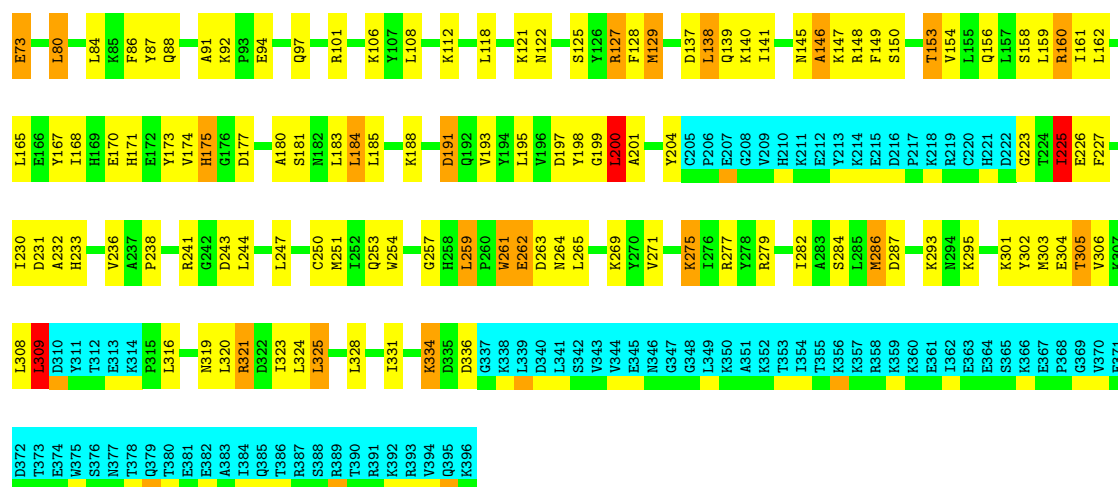
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.11 Score per residue for model 11

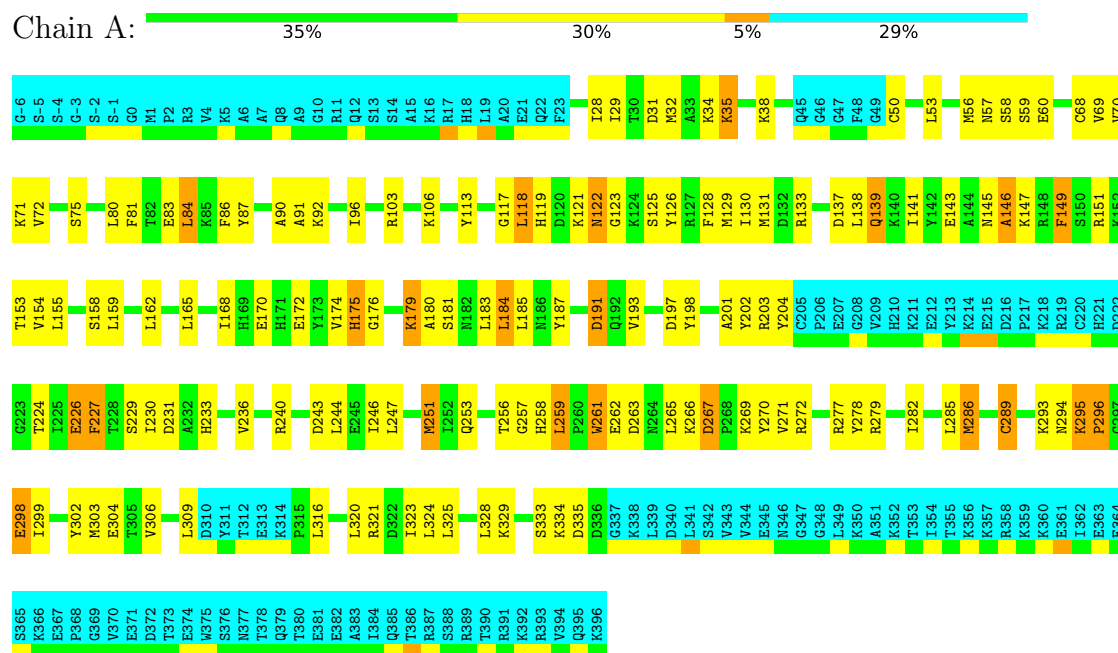
- Molecule 1: Serine/threonine-protein kinase VRK1





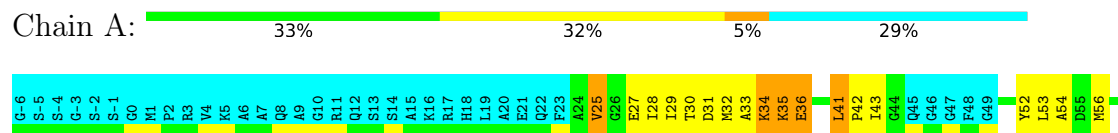
4.2.12 Score per residue for model 12

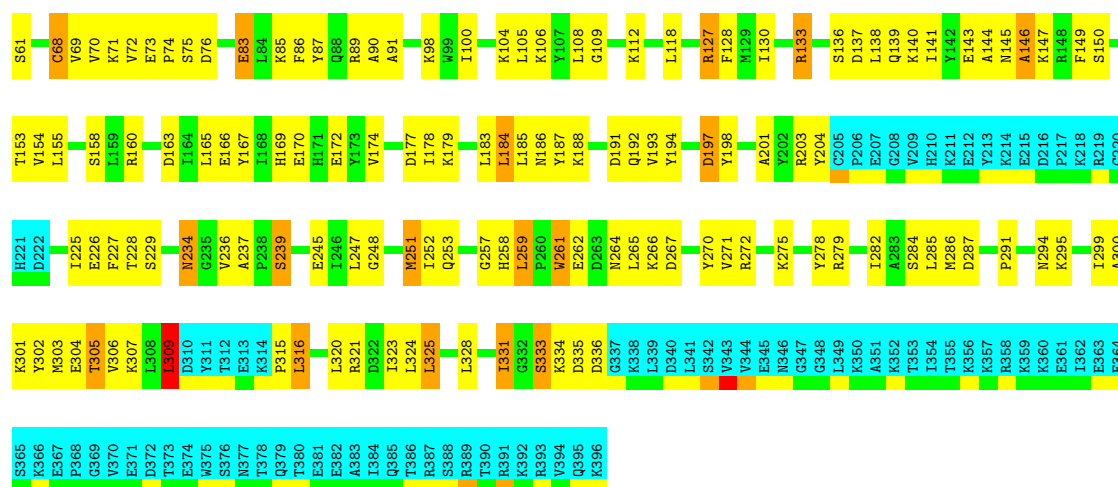
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.13 Score per residue for model 13 (medoid)

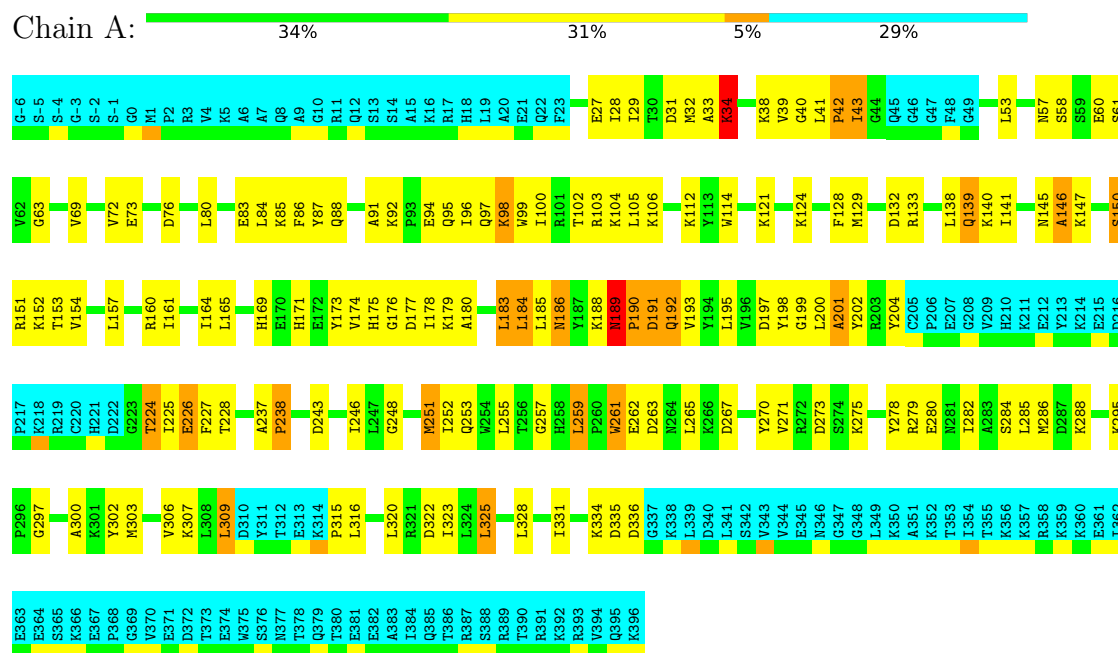
- Molecule 1: Serine/threonine-protein kinase VRK1





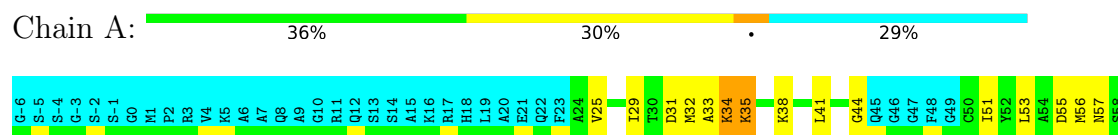
4.2.14 Score per residue for model 14

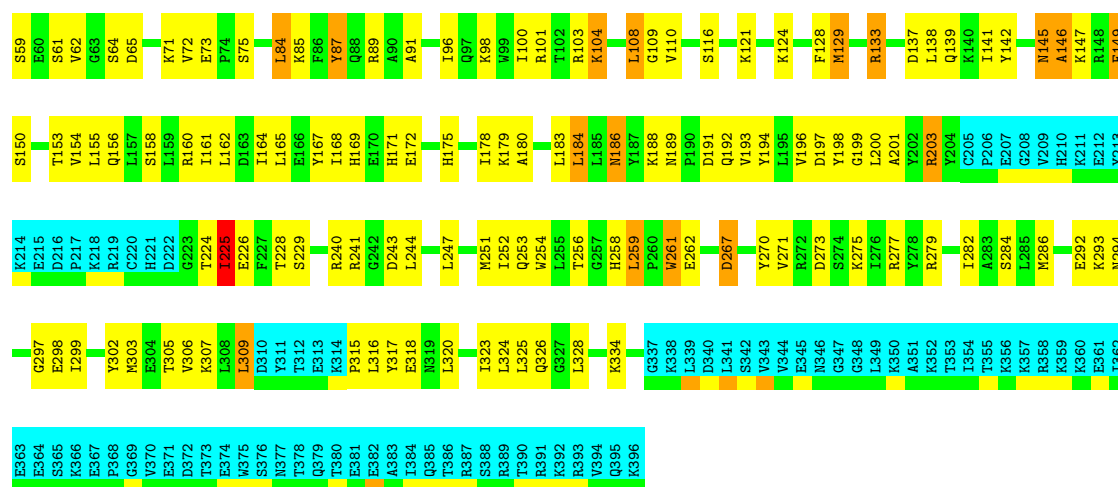
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.15 Score per residue for model 15

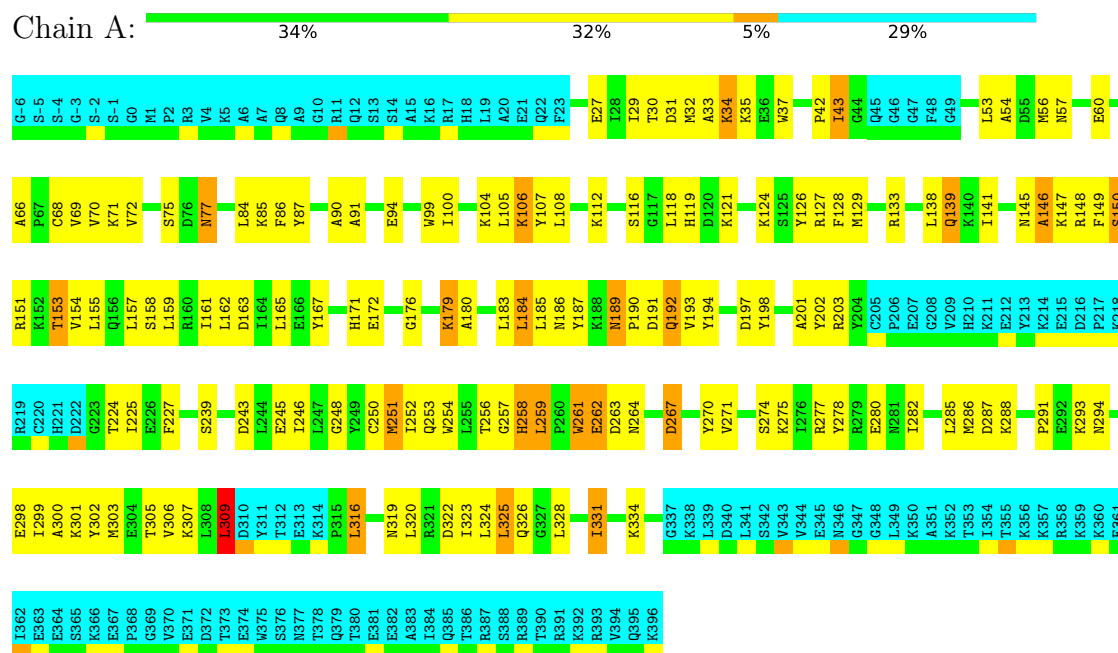
- Molecule 1: Serine/threonine-protein kinase VRK1





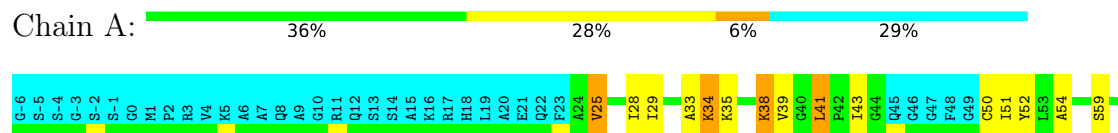
4.2.16 Score per residue for model 16

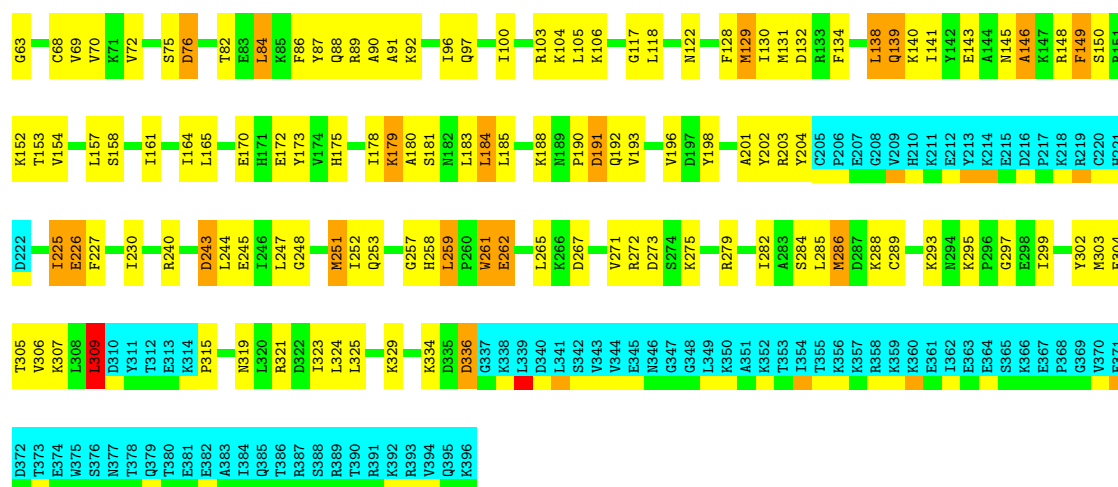
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.17 Score per residue for model 17

- Molecule 1: Serine/threonine-protein kinase VRK1

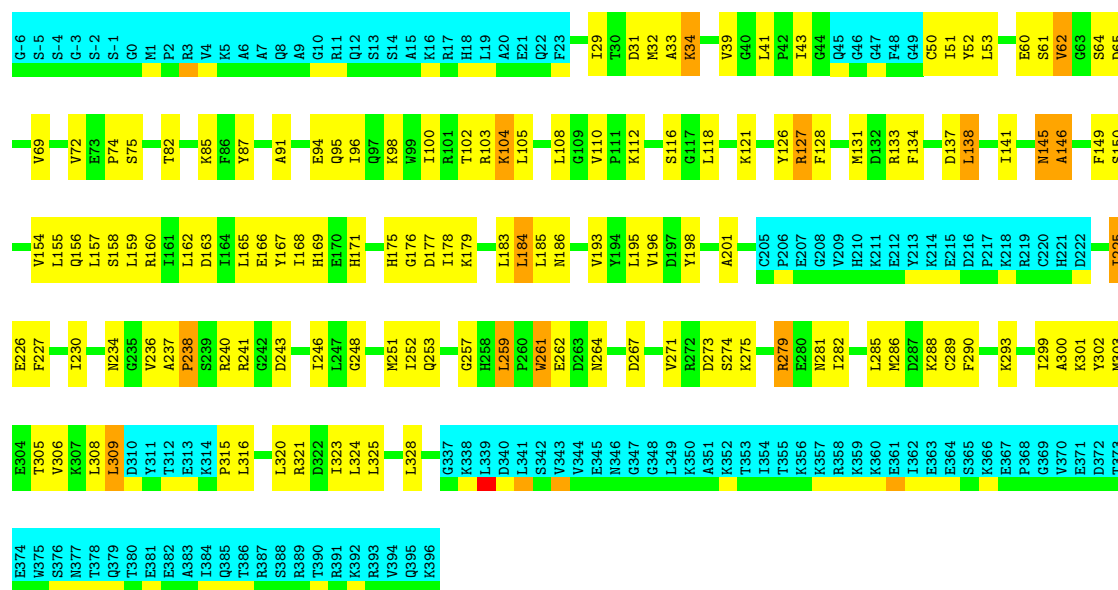




4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein kinase VRK1

Chain A: 37% 30% 29%



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 18 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	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	2601
Number of shifts mapped to atoms	2601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2313	2336	2330	87±7
All	All	41634	42048	41940	1565

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:309:LEU:HD21	1:A:316:LEU:HD22	0.93	1.40	7	1
1:A:141:ILE:HD11	1:A:185:LEU:HD11	0.91	1.37	1	10
1:A:259:LEU:HD22	1:A:261:TRP:CH2	0.89	2.02	2	18
1:A:278:TYR:CD1	1:A:285:LEU:HD12	0.85	2.06	16	3
1:A:29:ILE:HD12	1:A:128:PHE:CZ	0.84	2.06	9	14
1:A:259:LEU:HD13	1:A:261:TRP:CZ2	0.84	2.07	18	18
1:A:305:THR:HG21	1:A:323:ILE:HD11	0.82	1.49	11	2
1:A:29:ILE:HD12	1:A:128:PHE:CE1	0.82	2.10	4	14
1:A:183:LEU:C	1:A:184:LEU:HD23	0.82	2.00	11	17
1:A:37:TRP:CZ3	1:A:56:MET:HE2	0.81	2.09	5	1
1:A:252:ILE:O	1:A:256:THR:HG22	0.80	1.77	9	3
1:A:72:VAL:HG22	1:A:128:PHE:CB	0.79	2.07	17	12
1:A:150:SER:O	1:A:154:VAL:HG23	0.79	1.78	7	10
1:A:183:LEU:O	1:A:184:LEU:HD23	0.79	1.77	18	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:302:TYR:O	1:A:306:VAL:HG23	0.79	1.78	15	14
1:A:302:TYR:CE2	1:A:324:LEU:HD11	0.78	2.13	8	1
1:A:110:VAL:HG21	1:A:167:TYR:CE2	0.77	2.15	1	2
1:A:259:LEU:HD13	1:A:261:TRP:CE2	0.77	2.14	2	13
1:A:137:ASP:OD1	1:A:184:LEU:HD22	0.77	1.80	9	5
1:A:247:LEU:HD23	1:A:302:TYR:OH	0.76	1.81	5	10
1:A:305:THR:O	1:A:309:LEU:HD12	0.76	1.79	3	4
1:A:105:LEU:HD13	1:A:108:LEU:HD13	0.76	1.55	2	4
1:A:86:PHE:CZ	1:A:168:ILE:HG22	0.76	2.15	9	1
1:A:149:PHE:CE1	1:A:153:THR:HG21	0.76	2.16	4	3
1:A:174:VAL:HG13	1:A:204:TYR:CD1	0.76	2.16	2	6
1:A:259:LEU:HD22	1:A:261:TRP:CZ2	0.75	2.16	14	11
1:A:237:ALA:HB3	1:A:238:PRO:HD3	0.75	1.58	7	5
1:A:184:LEU:C	1:A:193:VAL:HG23	0.74	2.06	3	5
1:A:286:MET:HE1	1:A:303:MET:SD	0.74	2.22	9	4
1:A:108:LEU:HD21	1:A:167:TYR:CE2	0.74	2.18	9	2
1:A:137:ASP:CG	1:A:184:LEU:HD22	0.73	2.07	11	9
1:A:87:TYR:HA	1:A:91:ALA:HB3	0.73	1.58	2	16
1:A:325:LEU:HD23	1:A:328:LEU:HD12	0.73	1.58	9	6
1:A:202:TYR:CZ	1:A:237:ALA:HB1	0.73	2.18	14	1
1:A:320:LEU:HA	1:A:323:ILE:HD12	0.72	1.61	14	15
1:A:96:ILE:HG22	1:A:100:ILE:HD11	0.72	1.61	10	4
1:A:118:LEU:HD23	1:A:126:TYR:O	0.72	1.84	4	4
1:A:138:LEU:HA	1:A:141:ILE:HD12	0.72	1.61	1	9
1:A:225:ILE:HD11	1:A:271:VAL:CG1	0.72	2.14	17	8
1:A:78:GLY:O	1:A:82:THR:HG23	0.72	1.85	8	2
1:A:54:ALA:HB3	1:A:68:CYS:HB3	0.72	1.62	10	4
1:A:158:SER:OG	1:A:324:LEU:HD13	0.72	1.84	18	6
1:A:177:ASP:OD1	1:A:195:LEU:HD21	0.71	1.84	2	1
1:A:155:LEU:HB3	1:A:328:LEU:HD21	0.71	1.62	15	12
1:A:91:ALA:HA	1:A:96:ILE:HD11	0.71	1.59	9	9
1:A:282:ILE:HD13	1:A:303:MET:CB	0.71	2.16	14	14
1:A:286:MET:HE3	1:A:303:MET:SD	0.71	2.26	13	4
1:A:225:ILE:HG23	1:A:265:LEU:HD22	0.71	1.63	14	7
1:A:108:LEU:HD21	1:A:167:TYR:CG	0.71	2.21	15	4
1:A:84:LEU:HD21	1:A:129:MET:HB2	0.70	1.61	8	11
1:A:182:ASN:O	1:A:196:VAL:HG22	0.70	1.85	9	3
1:A:198:TYR:HB3	1:A:201:ALA:HB3	0.70	1.62	16	2
1:A:286:MET:HE1	1:A:299:ILE:HB	0.70	1.60	6	6
1:A:175:HIS:CD2	1:A:195:LEU:HD21	0.70	2.21	18	3
1:A:162:LEU:HA	1:A:165:LEU:HD12	0.70	1.64	15	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:LEU:HD11	1:A:325:LEU:HA	0.69	1.63	1	4
1:A:139:GLN:CA	1:A:180:ALA:HB1	0.69	2.17	4	14
1:A:69:VAL:HG13	1:A:133:ARG:HD2	0.69	1.64	8	1
1:A:138:LEU:HD21	1:A:193:VAL:HG21	0.68	1.65	5	8
1:A:278:TYR:CG	1:A:285:LEU:HD12	0.68	2.22	16	3
1:A:50:CYS:HB3	1:A:51:ILE:HD12	0.68	1.66	6	1
1:A:149:PHE:CD1	1:A:153:THR:HG21	0.68	2.23	10	2
1:A:306:VAL:HA	1:A:309:LEU:HD12	0.68	1.64	13	10
1:A:316:LEU:HD22	1:A:319:ASN:HB2	0.68	1.66	8	1
1:A:244:LEU:HD13	1:A:320:LEU:CD1	0.68	2.19	15	2
1:A:251:MET:O	1:A:255:LEU:HD12	0.68	1.89	14	1
1:A:243:ASP:HA	1:A:246:ILE:HD12	0.67	1.66	16	7
1:A:253:GLN:HB2	1:A:259:LEU:HD11	0.67	1.66	10	11
1:A:69:VAL:HG13	1:A:133:ARG:CG	0.67	2.20	13	3
1:A:230:ILE:HD11	1:A:275:LYS:HG3	0.67	1.67	6	1
1:A:117:GLY:O	1:A:118:LEU:HD23	0.67	1.89	17	1
1:A:84:LEU:HD22	1:A:129:MET:HE2	0.66	1.65	2	1
1:A:179:LYS:O	1:A:183:LEU:HD12	0.66	1.90	9	10
1:A:139:GLN:N	1:A:180:ALA:HB1	0.66	2.04	11	12
1:A:174:VAL:HG21	1:A:240:ARG:HG3	0.66	1.68	3	1
1:A:244:LEU:HD13	1:A:320:LEU:HD11	0.66	1.68	7	5
1:A:309:LEU:HD21	1:A:315:PRO:HA	0.66	1.66	17	1
1:A:302:TYR:CE1	1:A:320:LEU:HD22	0.65	2.26	2	2
1:A:230:ILE:HD11	1:A:275:LYS:HB3	0.65	1.67	8	1
1:A:155:LEU:HD12	1:A:331:ILE:HD11	0.65	1.68	16	2
1:A:154:VAL:HG21	1:A:255:LEU:HG	0.65	1.69	10	2
1:A:100:ILE:HG23	1:A:105:LEU:C	0.65	2.17	14	1
1:A:174:VAL:HG13	1:A:204:TYR:CE1	0.65	2.27	8	5
1:A:244:LEU:HD21	1:A:317:TYR:CE2	0.64	2.27	8	2
1:A:226:GLU:HG3	1:A:265:LEU:HD11	0.64	1.68	8	1
1:A:227:PHE:HB3	1:A:246:ILE:HG23	0.64	1.70	18	4
1:A:154:VAL:HG11	1:A:251:MET:HB3	0.64	1.69	12	4
1:A:176:GLY:HA3	1:A:246:ILE:HD13	0.64	1.68	14	1
1:A:50:CYS:O	1:A:51:ILE:HD13	0.64	1.93	4	1
1:A:199:GLY:C	1:A:200:LEU:HD22	0.64	2.17	8	1
1:A:108:LEU:HD21	1:A:167:TYR:CD1	0.64	2.28	11	2
1:A:286:MET:HE1	1:A:300:ALA:N	0.64	2.07	13	2
1:A:302:TYR:HA	1:A:323:ILE:HD13	0.64	1.68	5	9
1:A:134:PHE:CE2	1:A:196:VAL:HG11	0.63	2.28	18	2
1:A:69:VAL:HG13	1:A:133:ARG:HG3	0.63	1.70	13	2
1:A:195:LEU:HD23	1:A:198:TYR:CZ	0.63	2.28	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:259:LEU:HD22	1:A:261:TRP:CZ3	0.63	2.27	1	2
1:A:69:VAL:HG13	1:A:133:ARG:HB3	0.63	1.70	18	1
1:A:252:ILE:CD1	1:A:285:LEU:HD21	0.63	2.23	18	1
1:A:139:GLN:HA	1:A:180:ALA:HB1	0.63	1.69	2	12
1:A:185:LEU:HD23	1:A:193:VAL:HB	0.63	1.68	3	6
1:A:51:ILE:HG23	1:A:71:LYS:HD2	0.63	1.70	8	1
1:A:225:ILE:HD12	1:A:271:VAL:HG11	0.62	1.71	15	2
1:A:309:LEU:HG	1:A:316:LEU:HD22	0.62	1.70	5	2
1:A:108:LEU:HD21	1:A:167:TYR:CD2	0.62	2.29	13	4
1:A:118:LEU:HD23	1:A:127:ARG:HA	0.62	1.70	11	5
1:A:199:GLY:C	1:A:200:LEU:HD12	0.62	2.20	6	2
1:A:299:ILE:HG22	1:A:303:MET:CG	0.62	2.24	5	11
1:A:158:SER:OG	1:A:247:LEU:HD11	0.62	1.95	2	3
1:A:96:ILE:HG22	1:A:100:ILE:CD1	0.62	2.24	3	5
1:A:253:GLN:HG3	1:A:259:LEU:HD11	0.62	1.70	14	2
1:A:286:MET:SD	1:A:300:ALA:HB2	0.62	2.33	1	4
1:A:178:ILE:CG2	1:A:183:LEU:HD11	0.62	2.23	9	4
1:A:151:ARG:HA	1:A:255:LEU:HD21	0.62	1.72	7	2
1:A:286:MET:HE3	1:A:300:ALA:HA	0.62	1.72	18	3
1:A:72:VAL:HG22	1:A:128:PHE:HB3	0.62	1.70	18	12
1:A:253:GLN:HB3	1:A:259:LEU:HD11	0.62	1.71	18	2
1:A:225:ILE:HD13	1:A:226:GLU:HG2	0.62	1.71	4	2
1:A:173:TYR:CE1	1:A:201:ALA:HB1	0.61	2.30	14	1
1:A:199:GLY:O	1:A:200:LEU:HD12	0.61	1.95	4	3
1:A:86:PHE:CE2	1:A:91:ALA:HB2	0.61	2.30	8	1
1:A:173:TYR:CD1	1:A:201:ALA:HB1	0.61	2.30	14	1
1:A:159:LEU:HD12	1:A:328:LEU:HD11	0.61	1.71	4	4
1:A:259:LEU:HD12	1:A:262:GLU:HG2	0.61	1.72	10	2
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.61	1.69	13	3
1:A:309:LEU:O	1:A:316:LEU:HD22	0.61	1.95	11	1
1:A:30:THR:HG22	1:A:36:GLU:HG2	0.61	1.70	1	1
1:A:253:GLN:CG	1:A:259:LEU:HD11	0.61	2.25	14	3
1:A:225:ILE:CG2	1:A:265:LEU:HD11	0.60	2.26	5	1
1:A:248:GLY:C	1:A:303:MET:HE1	0.60	2.21	16	3
1:A:165:LEU:HD21	1:A:178:ILE:HD11	0.60	1.72	9	3
1:A:96:ILE:HG23	1:A:108:LEU:HD23	0.60	1.73	1	1
1:A:43:ILE:HG13	1:A:51:ILE:HG22	0.60	1.73	9	2
1:A:145:ASN:O	1:A:146:ALA:HB3	0.60	1.97	10	18
1:A:302:TYR:CE1	1:A:306:VAL:HG21	0.60	2.32	11	4
1:A:302:TYR:CE2	1:A:320:LEU:HD22	0.59	2.32	3	4
1:A:28:ILE:HD11	1:A:38:LYS:HE3	0.59	1.73	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:SER:HB3	1:A:324:LEU:HD13	0.59	1.75	2	3
1:A:138:LEU:HD22	1:A:141:ILE:HD12	0.59	1.75	11	4
1:A:225:ILE:HG13	1:A:271:VAL:HG11	0.59	1.73	9	3
1:A:52:TYR:O	1:A:70:VAL:HG12	0.59	1.97	13	5
1:A:184:LEU:HD11	1:A:196:VAL:HG21	0.59	1.74	4	4
1:A:299:ILE:HG22	1:A:303:MET:HG2	0.59	1.75	5	6
1:A:259:LEU:HD13	1:A:261:TRP:CH2	0.59	2.32	1	1
1:A:309:LEU:HD21	1:A:315:PRO:O	0.59	1.97	1	1
1:A:161:ILE:HA	1:A:164:ILE:HD12	0.59	1.73	3	3
1:A:176:GLY:HA2	1:A:246:ILE:HD13	0.59	1.73	18	1
1:A:169:HIS:CD2	1:A:174:VAL:HG12	0.59	2.33	9	3
1:A:253:GLN:HB2	1:A:259:LEU:HD21	0.59	1.74	14	5
1:A:244:LEU:HD13	1:A:316:LEU:HD11	0.59	1.75	7	1
1:A:159:LEU:CD1	1:A:328:LEU:HD11	0.58	2.28	1	3
1:A:252:ILE:HD13	1:A:285:LEU:HD11	0.58	1.74	18	2
1:A:165:LEU:HD22	1:A:243:ASP:HB3	0.58	1.75	1	2
1:A:325:LEU:HD23	1:A:325:LEU:O	0.58	1.96	1	5
1:A:331:ILE:HD12	1:A:331:ILE:O	0.58	1.97	16	2
1:A:100:ILE:HG23	1:A:106:LYS:H	0.58	1.59	16	4
1:A:251:MET:HG3	1:A:299:ILE:HD12	0.58	1.74	12	1
1:A:225:ILE:HD12	1:A:228:THR:HG22	0.58	1.75	8	3
1:A:226:GLU:HB3	1:A:265:LEU:HD11	0.58	1.74	12	2
1:A:131:MET:HE1	1:A:196:VAL:CG1	0.58	2.29	6	1
1:A:155:LEU:CB	1:A:328:LEU:HD21	0.58	2.28	15	3
1:A:189:ASN:CB	1:A:190:PRO:CD	0.58	2.82	16	1
1:A:159:LEU:HD21	1:A:321:ARG:HG2	0.57	1.76	11	1
1:A:184:LEU:HD23	1:A:184:LEU:N	0.57	2.14	11	4
1:A:185:LEU:HA	1:A:192:GLN:O	0.57	1.99	16	2
1:A:302:TYR:CD1	1:A:320:LEU:HD22	0.57	2.35	14	2
1:A:301:LYS:HD2	1:A:323:ILE:HG23	0.57	1.76	7	1
1:A:169:HIS:CG	1:A:174:VAL:HG12	0.57	2.34	9	1
1:A:90:ALA:HB1	1:A:171:HIS:CE1	0.57	2.35	3	1
1:A:174:VAL:HG11	1:A:239:SER:HB3	0.57	1.75	8	1
1:A:55:ASP:CB	1:A:62:VAL:HG13	0.57	2.30	2	1
1:A:40:GLY:CA	1:A:62:VAL:HG11	0.57	2.29	7	1
1:A:261:TRP:HB2	1:A:271:VAL:HG22	0.57	1.76	14	6
1:A:159:LEU:HD22	1:A:321:ARG:HG2	0.57	1.77	18	2
1:A:225:ILE:HD11	1:A:271:VAL:HG12	0.57	1.76	3	2
1:A:25:VAL:HG22	1:A:40:GLY:O	0.57	1.99	5	2
1:A:302:TYR:CD2	1:A:324:LEU:HD21	0.56	2.35	1	1
1:A:54:ALA:O	1:A:66:ALA:HB1	0.56	1.99	3	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:175:HIS:NE2	1:A:228:THR:HG23	0.56	2.15	1	1
1:A:261:TRP:O	1:A:271:VAL:HG22	0.56	2.00	4	4
1:A:248:GLY:O	1:A:252:ILE:HD12	0.56	2.00	4	6
1:A:174:VAL:HG11	1:A:239:SER:O	0.56	2.01	5	2
1:A:141:ILE:HG22	1:A:149:PHE:CE1	0.56	2.36	3	2
1:A:316:LEU:HD23	1:A:317:TYR:N	0.56	2.15	15	1
1:A:145:ASN:O	1:A:146:ALA:CB	0.56	2.53	10	15
1:A:33:ALA:O	1:A:34:LYS:HB2	0.56	2.00	8	5
1:A:305:THR:HB	1:A:316:LEU:HD21	0.56	1.76	13	1
1:A:159:LEU:HD11	1:A:325:LEU:CA	0.56	2.31	10	5
1:A:252:ILE:HG22	1:A:259:LEU:HD23	0.56	1.78	3	2
1:A:118:LEU:HD21	1:A:127:ARG:HG3	0.56	1.77	18	2
1:A:100:ILE:HD13	1:A:105:LEU:HD12	0.56	1.78	13	1
1:A:202:TYR:CE1	1:A:237:ALA:HB1	0.56	2.35	14	1
1:A:155:LEU:HD13	1:A:328:LEU:HD23	0.56	1.78	18	2
1:A:37:TRP:CE2	1:A:56:MET:HE3	0.56	2.35	16	1
1:A:53:LEU:HB3	1:A:66:ALA:HB3	0.56	1.78	8	2
1:A:108:LEU:HG	1:A:110:VAL:HG23	0.56	1.77	9	2
1:A:152:LYS:CB	1:A:331:ILE:HD13	0.56	2.30	14	1
1:A:33:ALA:HB3	1:A:35:LYS:HD2	0.56	1.76	3	2
1:A:237:ALA:HB1	1:A:238:PRO:HD2	0.56	1.78	8	1
1:A:237:ALA:HB3	1:A:238:PRO:CD	0.55	2.30	9	3
1:A:158:SER:HB2	1:A:324:LEU:HD13	0.55	1.76	17	2
1:A:178:ILE:HG23	1:A:183:LEU:HD11	0.55	1.78	9	7
1:A:98:LYS:O	1:A:102:THR:HG23	0.55	2.02	4	3
1:A:225:ILE:CG1	1:A:271:VAL:HG11	0.55	2.31	11	3
1:A:234:ASN:HB3	1:A:236:VAL:HG23	0.55	1.79	13	5
1:A:79:PRO:O	1:A:82:THR:HG22	0.55	2.01	4	1
1:A:161:ILE:HG21	1:A:178:ILE:HG21	0.55	1.79	15	1
1:A:231:ASP:OD2	1:A:236:VAL:HG11	0.55	2.02	8	1
1:A:189:ASN:CB	1:A:190:PRO:HD2	0.55	2.31	16	1
1:A:282:ILE:HD13	1:A:303:MET:HB2	0.54	1.77	1	13
1:A:261:TRP:HB2	1:A:271:VAL:HG13	0.54	1.77	8	2
1:A:325:LEU:C	1:A:325:LEU:HD23	0.54	2.27	4	5
1:A:309:LEU:HD21	1:A:316:LEU:HA	0.54	1.78	15	1
1:A:176:GLY:O	1:A:246:ILE:HD13	0.54	2.01	16	3
1:A:285:LEU:HD12	1:A:285:LEU:C	0.54	2.28	1	8
1:A:96:ILE:HG22	1:A:100:ILE:CG1	0.54	2.33	5	1
1:A:138:LEU:N	1:A:138:LEU:HD23	0.54	2.17	5	3
1:A:25:VAL:HG22	1:A:41:LEU:HA	0.54	1.80	17	5
1:A:73:GLU:HG3	1:A:80:LEU:HD23	0.54	1.79	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:325:LEU:HD23	1:A:325:LEU:C	0.54	2.28	1	1
1:A:168:ILE:HG21	1:A:198:TYR:OH	0.54	2.03	6	1
1:A:151:ARG:CA	1:A:255:LEU:HD21	0.54	2.32	7	1
1:A:168:ILE:HD11	1:A:175:HIS:CE1	0.54	2.38	18	2
1:A:111:PRO:HG3	1:A:196:VAL:HG12	0.54	1.79	10	1
1:A:244:LEU:HD22	1:A:320:LEU:CD1	0.54	2.33	7	2
1:A:100:ILE:HG23	1:A:105:LEU:O	0.54	2.03	14	1
1:A:225:ILE:CD1	1:A:271:VAL:HG11	0.54	2.32	2	9
1:A:175:HIS:CE1	1:A:228:THR:HG23	0.54	2.38	1	1
1:A:184:LEU:O	1:A:193:VAL:HG23	0.53	2.02	3	2
1:A:152:LYS:HG2	1:A:331:ILE:HD12	0.53	1.80	4	2
1:A:157:LEU:HD22	1:A:193:VAL:HG11	0.53	1.79	16	8
1:A:302:TYR:CZ	1:A:320:LEU:HD22	0.53	2.39	15	3
1:A:231:ASP:OD1	1:A:236:VAL:HG21	0.53	2.02	4	1
1:A:137:ASP:HB3	1:A:184:LEU:HD22	0.53	1.79	5	2
1:A:198:TYR:CB	1:A:201:ALA:HB2	0.53	2.33	15	4
1:A:230:ILE:HD13	1:A:279:ARG:HE	0.53	1.63	17	2
1:A:165:LEU:HD22	1:A:243:ASP:CG	0.53	2.29	17	2
1:A:230:ILE:HD11	1:A:275:LYS:CB	0.53	2.33	8	1
1:A:82:THR:HB	1:A:201:ALA:HB3	0.53	1.81	2	2
1:A:134:PHE:CD2	1:A:184:LEU:HD12	0.53	2.39	9	5
1:A:141:ILE:CD1	1:A:185:LEU:HD11	0.53	2.34	10	6
1:A:282:ILE:HD13	1:A:303:MET:HB3	0.53	1.81	15	3
1:A:261:TRP:C	1:A:261:TRP:CD1	0.53	2.87	1	2
1:A:309:LEU:HD22	1:A:316:LEU:HD12	0.53	1.81	15	1
1:A:156:GLN:OE1	1:A:328:LEU:HD13	0.53	2.03	6	1
1:A:39:VAL:HG13	1:A:53:LEU:O	0.53	2.02	18	1
1:A:87:TYR:O	1:A:91:ALA:HB3	0.52	2.04	15	11
1:A:54:ALA:HB3	1:A:68:CYS:CB	0.52	2.32	10	2
1:A:86:PHE:CZ	1:A:198:TYR:CE2	0.52	2.97	12	3
1:A:43:ILE:HD11	1:A:69:VAL:HG12	0.52	1.80	17	1
1:A:286:MET:HE2	1:A:300:ALA:N	0.52	2.19	9	1
1:A:244:LEU:HD21	1:A:317:TYR:CE1	0.52	2.40	1	1
1:A:328:LEU:HD12	1:A:335:ASP:OD2	0.52	2.04	12	1
1:A:100:ILE:HD11	1:A:108:LEU:HB2	0.52	1.82	16	1
1:A:37:TRP:CZ2	1:A:56:MET:HE3	0.52	2.40	6	1
1:A:251:MET:SD	1:A:299:ILE:HD12	0.52	2.44	3	2
1:A:79:PRO:HG3	1:A:200:LEU:HD12	0.52	1.82	9	1
1:A:41:LEU:HD23	1:A:42:PRO:HD2	0.52	1.82	13	1
1:A:158:SER:CB	1:A:324:LEU:HD13	0.51	2.36	12	7
1:A:24:ALA:C	1:A:25:VAL:HG23	0.51	2.30	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LYS:O	1:A:123:GLY:N	0.51	2.41	12	1
1:A:80:LEU:HG	1:A:84:LEU:HD23	0.51	1.82	14	4
1:A:285:LEU:HD12	1:A:286:MET:N	0.51	2.20	1	1
1:A:134:PHE:CZ	1:A:196:VAL:HG11	0.51	2.40	2	1
1:A:165:LEU:HD23	1:A:168:ILE:HD11	0.51	1.82	11	1
1:A:175:HIS:NE2	1:A:195:LEU:HD21	0.51	2.21	11	1
1:A:278:TYR:CE1	1:A:285:LEU:HD12	0.51	2.40	16	1
1:A:230:ILE:HD13	1:A:279:ARG:NE	0.51	2.20	17	1
1:A:86:PHE:CZ	1:A:198:TYR:CE1	0.51	2.99	14	1
1:A:224:THR:HG22	1:A:226:GLU:HG2	0.51	1.82	14	1
1:A:55:ASP:HB2	1:A:62:VAL:HG13	0.51	1.83	7	2
1:A:174:VAL:HG22	1:A:202:TYR:O	0.51	2.06	6	2
1:A:86:PHE:CE1	1:A:173:TYR:CD2	0.51	2.98	17	1
1:A:42:PRO:O	1:A:43:ILE:HG23	0.51	2.05	16	2
1:A:225:ILE:HD12	1:A:228:THR:CG2	0.51	2.35	14	3
1:A:190:PRO:O	1:A:191:ASP:CB	0.51	2.59	16	2
1:A:175:HIS:CE1	1:A:198:TYR:CD1	0.51	2.99	2	2
1:A:301:LYS:HG2	1:A:323:ILE:HG23	0.51	1.83	16	1
1:A:53:LEU:HD23	1:A:69:VAL:HG12	0.51	1.83	18	1
1:A:302:TYR:N	1:A:323:ILE:HG21	0.50	2.21	15	8
1:A:236:VAL:HG12	1:A:238:PRO:HD2	0.50	1.82	18	1
1:A:226:GLU:CG	1:A:265:LEU:HD11	0.50	2.36	8	1
1:A:168:ILE:HD13	1:A:175:HIS:NE2	0.50	2.22	15	1
1:A:86:PHE:CD1	1:A:198:TYR:CD2	0.50	2.99	16	1
1:A:86:PHE:CE1	1:A:198:TYR:CD2	0.50	3.00	1	1
1:A:225:ILE:O	1:A:265:LEU:HD22	0.50	2.06	3	3
1:A:43:ILE:CD1	1:A:51:ILE:HG22	0.50	2.35	4	1
1:A:286:MET:HE1	1:A:299:ILE:CB	0.50	2.34	6	3
1:A:69:VAL:HG13	1:A:133:ARG:HG2	0.50	1.83	4	1
1:A:96:ILE:CG2	1:A:100:ILE:HD11	0.50	2.37	3	3
1:A:84:LEU:HG	1:A:129:MET:HE2	0.50	1.83	11	2
1:A:152:LYS:HB3	1:A:331:ILE:HD13	0.50	1.84	14	1
1:A:244:LEU:CD1	1:A:316:LEU:HD11	0.50	2.37	7	1
1:A:33:ALA:O	1:A:34:LYS:CB	0.50	2.60	6	11
1:A:25:VAL:HG22	1:A:41:LEU:HG	0.50	1.83	15	1
1:A:261:TRP:CD1	1:A:262:GLU:N	0.49	2.80	9	17
1:A:282:ILE:HG21	1:A:304:GLU:CG	0.49	2.37	2	1
1:A:141:ILE:HG22	1:A:149:PHE:CZ	0.49	2.42	9	2
1:A:225:ILE:HD13	1:A:225:ILE:C	0.49	2.32	15	2
1:A:175:HIS:CE1	1:A:198:TYR:CZ	0.49	2.99	7	1
1:A:159:LEU:HD22	1:A:321:ARG:CG	0.49	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:HD23	1:A:324:LEU:HD22	0.49	1.84	7	3
1:A:159:LEU:HD11	1:A:325:LEU:HG	0.49	1.84	16	1
1:A:253:GLN:CB	1:A:259:LEU:HD11	0.49	2.38	18	4
1:A:28:ILE:HG21	1:A:36:GLU:HB3	0.49	1.84	4	3
1:A:86:PHE:CZ	1:A:198:TYR:CZ	0.49	3.00	12	1
1:A:150:SER:HB2	1:A:153:THR:HG23	0.49	1.84	13	1
1:A:86:PHE:CE1	1:A:90:ALA:HB3	0.49	2.41	17	1
1:A:175:HIS:CD2	1:A:198:TYR:CE1	0.49	3.00	10	1
1:A:309:LEU:HD11	1:A:320:LEU:HD11	0.49	1.82	18	1
1:A:138:LEU:HD21	1:A:193:VAL:CG2	0.49	2.37	11	17
1:A:168:ILE:CD1	1:A:175:HIS:CD2	0.49	2.96	5	3
1:A:158:SER:OG	1:A:247:LEU:HD21	0.49	2.08	8	1
1:A:257:GLY:O	1:A:258:HIS:CG	0.49	2.65	8	2
1:A:261:TRP:HB2	1:A:271:VAL:HA	0.49	1.84	11	4
1:A:53:LEU:HD21	1:A:133:ARG:CZ	0.49	2.38	15	1
1:A:247:LEU:HD23	1:A:302:TYR:CZ	0.49	2.43	4	1
1:A:286:MET:HE1	1:A:299:ILE:CG2	0.49	2.38	15	3
1:A:261:TRP:HA	1:A:270:TYR:CD1	0.48	2.43	16	3
1:A:149:PHE:CG	1:A:153:THR:HG21	0.48	2.43	10	1
1:A:70:VAL:HG23	1:A:130:ILE:HD13	0.48	1.84	12	2
1:A:296:PRO:HB3	1:A:300:ALA:HB2	0.48	1.84	5	1
1:A:159:LEU:HD11	1:A:325:LEU:N	0.48	2.23	6	1
1:A:108:LEU:HD11	1:A:167:TYR:CG	0.48	2.43	1	1
1:A:256:THR:HG23	1:A:289:CYS:O	0.48	2.09	10	2
1:A:86:PHE:CD1	1:A:201:ALA:HB1	0.48	2.42	5	1
1:A:105:LEU:HD11	1:A:167:TYR:CE1	0.48	2.44	18	1
1:A:225:ILE:HD11	1:A:271:VAL:HG11	0.48	1.85	17	3
1:A:252:ILE:HG21	1:A:289:CYS:SG	0.48	2.49	18	3
1:A:276:ILE:HG23	1:A:279:ARG:NH1	0.48	2.23	9	1
1:A:158:SER:O	1:A:162:LEU:HD12	0.48	2.08	4	1
1:A:72:VAL:HG22	1:A:128:PHE:HB2	0.48	1.84	12	1
1:A:154:VAL:HG11	1:A:251:MET:HA	0.48	1.85	13	3
1:A:267:ASP:CB	1:A:270:TYR:CE2	0.48	2.97	15	6
1:A:69:VAL:HG13	1:A:133:ARG:CB	0.48	2.38	18	2
1:A:175:HIS:O	1:A:200:LEU:HD22	0.48	2.09	4	1
1:A:175:HIS:CE1	1:A:246:ILE:HD11	0.48	2.43	9	1
1:A:130:ILE:N	1:A:130:ILE:HD12	0.48	2.24	1	1
1:A:175:HIS:CE1	1:A:198:TYR:CE1	0.48	3.02	7	2
1:A:40:GLY:HA2	1:A:62:VAL:HG11	0.48	1.85	7	1
1:A:176:GLY:C	1:A:246:ILE:HD13	0.47	2.34	6	1
1:A:159:LEU:HD13	1:A:159:LEU:O	0.47	2.09	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:TYR:CE1	1:A:254:TRP:CD1	0.47	3.02	15	1
1:A:43:ILE:HG21	1:A:53:LEU:HD21	0.47	1.85	13	2
1:A:110:VAL:HG22	1:A:164:ILE:HG23	0.47	1.86	15	1
1:A:261:TRP:O	1:A:271:VAL:HG13	0.47	2.10	1	2
1:A:53:LEU:HD22	1:A:66:ALA:HB3	0.47	1.86	3	1
1:A:72:VAL:HG22	1:A:128:PHE:CG	0.47	2.45	17	3
1:A:325:LEU:HD21	1:A:335:ASP:CB	0.47	2.39	3	1
1:A:272:ARG:NH1	1:A:276:ILE:HD11	0.47	2.25	6	1
1:A:175:HIS:CE1	1:A:198:TYR:CE2	0.47	3.01	7	1
1:A:272:ARG:O	1:A:276:ILE:HD12	0.47	2.08	10	1
1:A:159:LEU:HD11	1:A:325:LEU:CB	0.47	2.39	18	1
1:A:244:LEU:HD21	1:A:317:TYR:CZ	0.47	2.44	4	1
1:A:149:PHE:HE1	1:A:153:THR:HG21	0.47	1.70	9	1
1:A:110:VAL:HG21	1:A:167:TYR:CD2	0.47	2.44	7	3
1:A:252:ILE:HG12	1:A:285:LEU:HD13	0.47	1.87	10	1
1:A:165:LEU:HD22	1:A:243:ASP:OD2	0.47	2.10	14	1
1:A:230:ILE:HD12	1:A:279:ARG:HG3	0.47	1.86	18	1
1:A:154:VAL:HG21	1:A:255:LEU:CG	0.47	2.39	6	1
1:A:251:MET:SD	1:A:299:ILE:HG23	0.47	2.50	4	1
1:A:295:LYS:N	1:A:296:PRO:HD2	0.47	2.25	12	1
1:A:150:SER:HB3	1:A:153:THR:HG23	0.47	1.86	17	1
1:A:226:GLU:O	1:A:227:PHE:HB2	0.47	2.10	17	1
1:A:296:PRO:CB	1:A:300:ALA:HB2	0.46	2.40	5	1
1:A:159:LEU:HD11	1:A:325:LEU:HB2	0.46	1.85	18	1
1:A:78:GLY:N	1:A:79:PRO:CD	0.46	2.78	5	2
1:A:186:ASN:ND2	1:A:194:TYR:CE1	0.46	2.83	16	3
1:A:30:THR:HA	1:A:35:LYS:O	0.46	2.11	4	3
1:A:299:ILE:O	1:A:303:MET:HG2	0.46	2.11	15	4
1:A:69:VAL:HG13	1:A:133:ARG:HB2	0.46	1.86	14	1
1:A:133:ARG:NH1	1:A:187:TYR:CE2	0.46	2.83	7	3
1:A:224:THR:HG22	1:A:226:GLU:CG	0.46	2.41	14	1
1:A:316:LEU:HD23	1:A:317:TYR:CG	0.46	2.45	15	1
1:A:175:HIS:ND1	1:A:198:TYR:CG	0.46	2.84	2	1
1:A:100:ILE:HG23	1:A:105:LEU:HB2	0.46	1.87	8	3
1:A:168:ILE:CD1	1:A:175:HIS:CE1	0.46	2.99	18	2
1:A:227:PHE:CB	1:A:246:ILE:HG23	0.46	2.40	18	1
1:A:252:ILE:HD11	1:A:285:LEU:HD21	0.46	1.86	18	1
1:A:174:VAL:HG21	1:A:239:SER:O	0.46	2.11	1	2
1:A:108:LEU:HD21	1:A:167:TYR:CZ	0.46	2.46	9	2
1:A:230:ILE:HD11	1:A:275:LYS:CG	0.46	2.40	6	1
1:A:55:ASP:CG	1:A:62:VAL:HG13	0.46	2.35	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ILE:CG1	1:A:51:ILE:HG22	0.46	2.41	4	1
1:A:200:LEU:HD22	1:A:200:LEU:N	0.46	2.25	8	1
1:A:107:TYR:CD2	1:A:108:LEU:O	0.46	2.69	10	1
1:A:114:TRP:CD1	1:A:114:TRP:N	0.46	2.85	3	4
1:A:325:LEU:HD21	1:A:335:ASP:HB2	0.46	1.88	3	1
1:A:174:VAL:CG1	1:A:204:TYR:CD1	0.46	2.99	12	3
1:A:175:HIS:CD2	1:A:195:LEU:CD2	0.46	2.98	18	2
1:A:53:LEU:HD23	1:A:68:CYS:O	0.46	2.11	12	1
1:A:316:LEU:HD23	1:A:319:ASN:HB3	0.46	1.88	16	1
1:A:139:GLN:HB2	1:A:180:ALA:O	0.45	2.11	2	2
1:A:189:ASN:CB	1:A:190:PRO:HD3	0.45	2.41	14	1
1:A:87:TYR:CA	1:A:91:ALA:HB3	0.45	2.41	4	5
1:A:282:ILE:HD13	1:A:303:MET:C	0.45	2.36	7	8
1:A:244:LEU:HD12	1:A:309:LEU:CD1	0.45	2.42	4	1
1:A:174:VAL:HG21	1:A:204:TYR:HB3	0.45	1.88	14	2
1:A:301:LYS:HB2	1:A:323:ILE:HG23	0.45	1.87	6	1
1:A:86:PHE:CE2	1:A:173:TYR:CD1	0.45	3.05	10	1
1:A:70:VAL:CG2	1:A:128:PHE:CD1	0.45	2.99	11	2
1:A:86:PHE:O	1:A:90:ALA:HB3	0.45	2.12	12	1
1:A:251:MET:CG	1:A:299:ILE:HD12	0.45	2.41	12	1
1:A:282:ILE:HG21	1:A:304:GLU:HG2	0.45	1.89	2	1
1:A:261:TRP:HA	1:A:270:TYR:CZ	0.45	2.46	8	1
1:A:305:THR:O	1:A:309:LEU:HA	0.45	2.11	7	5
1:A:159:LEU:HD21	1:A:321:ARG:O	0.45	2.12	10	1
1:A:302:TYR:CE2	1:A:306:VAL:HG21	0.45	2.46	2	1
1:A:282:ILE:CD1	1:A:303:MET:HB3	0.45	2.41	15	6
1:A:302:TYR:HB2	1:A:323:ILE:HG21	0.45	1.88	3	1
1:A:253:GLN:NE2	1:A:254:TRP:CD1	0.45	2.85	16	2
1:A:182:ASN:OD1	1:A:196:VAL:HG23	0.45	2.12	3	1
1:A:62:VAL:HG13	1:A:66:ALA:HB2	0.45	1.88	9	1
1:A:259:LEU:HD12	1:A:262:GLU:HB3	0.45	1.89	12	1
1:A:202:TYR:CD1	1:A:202:TYR:C	0.45	2.94	17	3
1:A:108:LEU:HD21	1:A:167:TYR:CE1	0.44	2.46	5	1
1:A:286:MET:HG3	1:A:300:ALA:HB2	0.44	1.88	8	1
1:A:62:VAL:HG12	1:A:62:VAL:O	0.44	2.12	18	1
1:A:72:VAL:HG13	1:A:128:PHE:HB3	0.44	1.90	9	3
1:A:175:HIS:CE1	1:A:198:TYR:CG	0.44	3.06	2	1
1:A:261:TRP:CD1	1:A:261:TRP:C	0.44	2.96	4	4
1:A:86:PHE:CE2	1:A:90:ALA:CB	0.44	3.01	6	1
1:A:267:ASP:O	1:A:271:VAL:HG23	0.44	2.12	8	1
1:A:228:THR:HG23	1:A:228:THR:O	0.44	2.12	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:ASN:CB	1:A:190:PRO:HB2	0.44	2.42	14	2
1:A:28:ILE:HD13	1:A:38:LYS:HG3	0.44	1.88	12	1
1:A:133:ARG:CD	1:A:187:TYR:CD2	0.44	3.00	12	1
1:A:149:PHE:CE2	1:A:153:THR:CG2	0.44	3.00	12	1
1:A:175:HIS:CD2	1:A:175:HIS:N	0.44	2.85	12	1
1:A:55:ASP:HB2	1:A:66:ALA:HB2	0.44	1.88	1	1
1:A:295:LYS:N	1:A:296:PRO:CD	0.44	2.81	1	1
1:A:225:ILE:HG22	1:A:265:LEU:HD11	0.44	1.88	5	1
1:A:252:ILE:CG2	1:A:259:LEU:HD23	0.44	2.43	5	1
1:A:161:ILE:HG21	1:A:178:ILE:HG12	0.44	1.88	17	2
1:A:41:LEU:H	1:A:53:LEU:HD12	0.44	1.73	4	1
1:A:83:GLU:CG	1:A:87:TYR:CE1	0.44	3.00	6	2
1:A:162:LEU:CD1	1:A:324:LEU:HD12	0.44	2.43	11	2
1:A:159:LEU:HD22	1:A:321:ARG:HG3	0.44	1.90	5	1
1:A:31:ASP:OD1	1:A:34:LYS:N	0.44	2.50	13	2
1:A:141:ILE:HD11	1:A:185:LEU:CD1	0.44	2.43	10	2
1:A:86:PHE:CD1	1:A:173:TYR:CD2	0.44	3.06	9	1
1:A:271:VAL:HG12	1:A:275:LYS:CD	0.44	2.43	17	2
1:A:305:THR:CG2	1:A:323:ILE:HD11	0.44	2.33	11	1
1:A:316:LEU:HD23	1:A:316:LEU:N	0.44	2.27	12	1
1:A:31:ASP:HA	1:A:117:GLY:CA	0.43	2.43	12	2
1:A:70:VAL:O	1:A:70:VAL:HG13	0.43	2.12	2	3
1:A:174:VAL:HG13	1:A:204:TYR:HD1	0.43	1.68	2	1
1:A:158:SER:CB	1:A:247:LEU:HD11	0.43	2.43	5	1
1:A:27:GLU:O	1:A:28:ILE:HD13	0.43	2.13	9	2
1:A:226:GLU:O	1:A:227:PHE:CG	0.43	2.71	5	3
1:A:43:ILE:CD1	1:A:69:VAL:HG12	0.43	2.43	4	2
1:A:253:GLN:HB3	1:A:259:LEU:HD21	0.43	1.91	9	1
1:A:290:PHE:N	1:A:290:PHE:CD1	0.43	2.86	18	1
1:A:62:VAL:CG1	1:A:66:ALA:HB2	0.43	2.43	4	1
1:A:96:ILE:HG22	1:A:100:ILE:HG12	0.43	1.89	5	1
1:A:169:HIS:CE1	1:A:174:VAL:HG12	0.43	2.47	14	2
1:A:286:MET:HE3	1:A:300:ALA:CA	0.43	2.40	18	1
1:A:86:PHE:C	1:A:86:PHE:CD1	0.43	2.97	12	3
1:A:236:VAL:HG12	1:A:237:ALA:N	0.43	2.29	13	1
1:A:175:HIS:CE1	1:A:195:LEU:HD21	0.43	2.48	5	1
1:A:152:LYS:CG	1:A:331:ILE:HD12	0.43	2.43	4	1
1:A:278:TYR:CD2	1:A:285:LEU:HB3	0.43	2.48	4	1
1:A:158:SER:OG	1:A:251:MET:HE1	0.43	2.14	10	1
1:A:259:LEU:HD12	1:A:262:GLU:CG	0.43	2.41	10	1
1:A:138:LEU:HD13	1:A:141:ILE:HD12	0.43	1.90	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:PHE:CZ	1:A:90:ALA:CB	0.43	3.01	6	1
1:A:198:TYR:CB	1:A:201:ALA:HB3	0.43	2.39	16	2
1:A:305:THR:HG23	1:A:316:LEU:HD23	0.43	1.89	1	1
1:A:282:ILE:CD1	1:A:303:MET:CB	0.43	2.96	13	4
1:A:175:HIS:CE1	1:A:198:TYR:CD2	0.43	3.06	7	1
1:A:278:TYR:CD1	1:A:285:LEU:HB3	0.43	2.48	13	3
1:A:126:TYR:CD1	1:A:126:TYR:N	0.43	2.86	12	1
1:A:68:CYS:SG	1:A:130:ILE:HG22	0.43	2.54	17	1
1:A:305:THR:CG2	1:A:316:LEU:HD23	0.43	2.43	1	1
1:A:185:LEU:HD23	1:A:193:VAL:CB	0.43	2.43	5	1
1:A:267:ASP:O	1:A:270:TYR:CE1	0.43	2.72	9	2
1:A:259:LEU:CD2	1:A:261:TRP:CH2	0.43	2.99	15	1
1:A:138:LEU:N	1:A:138:LEU:CD2	0.42	2.82	5	2
1:A:174:VAL:HG22	1:A:204:TYR:CD1	0.42	2.48	13	1
1:A:305:THR:HG22	1:A:309:LEU:CD1	0.42	2.44	15	1
1:A:155:LEU:CD1	1:A:328:LEU:HD23	0.42	2.44	18	1
1:A:130:ILE:N	1:A:130:ILE:CD1	0.42	2.83	1	1
1:A:86:PHE:CD1	1:A:86:PHE:C	0.42	2.97	11	4
1:A:252:ILE:HD11	1:A:303:MET:SD	0.42	2.54	2	1
1:A:286:MET:HE1	1:A:299:ILE:HG22	0.42	1.91	8	1
1:A:138:LEU:HD23	1:A:183:LEU:O	0.42	2.14	10	1
1:A:183:LEU:HA	1:A:194:TYR:O	0.42	2.14	13	2
1:A:176:GLY:CA	1:A:246:ILE:HD13	0.42	2.44	12	1
1:A:24:ALA:O	1:A:39:VAL:HG12	0.42	2.13	4	1
1:A:141:ILE:CG2	1:A:149:PHE:CE1	0.42	3.02	3	1
1:A:82:THR:OG1	1:A:201:ALA:HB3	0.42	2.13	4	1
1:A:225:ILE:HG12	1:A:225:ILE:O	0.42	2.15	5	1
1:A:109:GLY:HA3	1:A:164:ILE:HD11	0.42	1.90	15	1
1:A:320:LEU:HD23	1:A:323:ILE:HD12	0.42	1.92	16	1
1:A:309:LEU:HD21	1:A:316:LEU:H	0.42	1.75	18	1
1:A:86:PHE:CD1	1:A:173:TYR:CZ	0.42	3.08	4	1
1:A:200:LEU:N	1:A:200:LEU:CD2	0.42	2.83	8	1
1:A:177:ASP:CG	1:A:195:LEU:HD21	0.42	2.38	2	1
1:A:267:ASP:HB3	1:A:270:TYR:CE2	0.42	2.50	6	7
1:A:128:PHE:CD1	1:A:128:PHE:C	0.42	2.97	13	5
1:A:39:VAL:HG12	1:A:40:GLY:N	0.42	2.29	14	1
1:A:71:LYS:O	1:A:128:PHE:HA	0.42	2.14	4	1
1:A:138:LEU:C	1:A:180:ALA:HB1	0.42	2.39	11	1
1:A:198:TYR:HB3	1:A:201:ALA:HB2	0.42	1.90	15	1
1:A:305:THR:HG22	1:A:309:LEU:HD12	0.42	1.92	15	1
1:A:90:ALA:HB1	1:A:167:TYR:CE2	0.42	2.49	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:305:THR:O	1:A:309:LEU:CA	0.42	2.68	17	1
1:A:204:TYR:CE2	1:A:240:ARG:NH2	0.42	2.88	3	1
1:A:200:LEU:HD23	1:A:200:LEU:O	0.42	2.14	9	1
1:A:158:SER:HA	1:A:161:ILE:HD12	0.42	1.92	16	2
1:A:175:HIS:CD2	1:A:198:TYR:O	0.42	2.73	14	1
1:A:305:THR:O	1:A:309:LEU:N	0.42	2.53	17	1
1:A:37:TRP:CD1	1:A:37:TRP:N	0.41	2.88	1	1
1:A:174:VAL:HG23	1:A:202:TYR:HB3	0.41	1.90	1	1
1:A:71:LYS:NZ	1:A:131:MET:HE3	0.41	2.30	8	1
1:A:51:ILE:HD12	1:A:71:LYS:CG	0.41	2.45	15	1
1:A:244:LEU:CD1	1:A:320:LEU:HD11	0.41	2.40	15	1
1:A:90:ALA:CB	1:A:171:HIS:CE1	0.41	3.02	3	1
1:A:302:TYR:C	1:A:302:TYR:CD1	0.41	2.98	3	1
1:A:251:MET:HE3	1:A:299:ILE:HD12	0.41	1.92	13	2
1:A:226:GLU:O	1:A:227:PHE:CD2	0.41	2.73	12	2
1:A:100:ILE:O	1:A:104:LYS:N	0.41	2.54	4	5
1:A:224:THR:O	1:A:228:THR:HG23	0.41	2.14	5	1
1:A:71:LYS:HE3	1:A:131:MET:HE3	0.41	1.92	7	1
1:A:86:PHE:CE1	1:A:198:TYR:CZ	0.41	3.08	11	1
1:A:226:GLU:HB2	1:A:271:VAL:CG1	0.41	2.45	15	1
1:A:51:ILE:O	1:A:52:TYR:CD1	0.41	2.73	18	2
1:A:53:LEU:HD22	1:A:65:ASP:O	0.41	2.15	3	1
1:A:244:LEU:HD12	1:A:309:LEU:HD11	0.41	1.92	4	1
1:A:107:TYR:CG	1:A:108:LEU:N	0.41	2.88	6	1
1:A:226:GLU:C	1:A:227:PHE:CG	0.41	2.99	8	1
1:A:165:LEU:O	1:A:169:HIS:CG	0.41	2.73	13	2
1:A:278:TYR:CD2	1:A:285:LEU:CB	0.41	3.04	4	1
1:A:139:GLN:N	1:A:180:ALA:O	0.41	2.54	8	2
1:A:286:MET:HE3	1:A:290:PHE:HE2	0.41	1.76	9	1
1:A:241:ARG:HB3	1:A:309:LEU:HD22	0.41	1.93	11	1
1:A:69:VAL:O	1:A:130:ILE:HG23	0.41	2.15	13	1
1:A:267:ASP:HB2	1:A:270:TYR:CE2	0.41	2.51	1	2
1:A:141:ILE:CG2	1:A:149:PHE:CZ	0.41	3.04	3	1
1:A:302:TYR:CD1	1:A:302:TYR:C	0.41	2.98	10	3
1:A:253:GLN:OE1	1:A:254:TRP:CD1	0.41	2.73	11	2
1:A:29:ILE:HG23	1:A:39:VAL:CG2	0.41	2.45	10	2
1:A:165:LEU:O	1:A:169:HIS:CD2	0.41	2.74	15	1
1:A:261:TRP:O	1:A:271:VAL:CG2	0.41	2.69	1	1
1:A:226:GLU:O	1:A:227:PHE:CD1	0.41	2.74	2	1
1:A:282:ILE:HD12	1:A:303:MET:CB	0.41	2.46	2	2
1:A:186:ASN:OD1	1:A:194:TYR:CE1	0.41	2.73	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:TYR:CZ	1:A:237:ALA:O	0.41	2.74	9	1
1:A:54:ALA:HB3	1:A:68:CYS:HB2	0.41	1.91	16	1
1:A:109:GLY:O	1:A:194:TYR:CD2	0.41	2.74	13	4
1:A:169:HIS:CD2	1:A:204:TYR:OH	0.41	2.74	7	1
1:A:309:LEU:CD2	1:A:316:LEU:HD22	0.41	2.29	7	1
1:A:100:ILE:O	1:A:104:LYS:HA	0.41	2.15	18	1
1:A:96:ILE:HG23	1:A:108:LEU:CD2	0.41	2.46	1	1
1:A:86:PHE:CD1	1:A:173:TYR:CE1	0.41	3.08	4	1
1:A:250:CYS:O	1:A:254:TRP:CG	0.41	2.74	9	1
1:A:157:LEU:O	1:A:161:ILE:HD12	0.41	2.15	10	1
1:A:227:PHE:CD1	1:A:262:GLU:OE1	0.41	2.73	11	1
1:A:113:TYR:CD1	1:A:113:TYR:C	0.41	2.99	12	1
1:A:204:TYR:CE2	1:A:239:SER:OG	0.41	2.74	13	1
1:A:328:LEU:HD13	1:A:335:ASP:HB3	0.41	1.93	13	1
1:A:309:LEU:HD23	1:A:315:PRO:HA	0.41	1.91	18	1
1:A:227:PHE:CE2	1:A:262:GLU:OE2	0.41	2.74	1	1
1:A:83:GLU:OE1	1:A:198:TYR:CD2	0.41	2.74	2	1
1:A:107:TYR:CD1	1:A:192:GLN:OE1	0.41	2.75	3	1
1:A:86:PHE:O	1:A:90:ALA:N	0.41	2.52	6	1
1:A:202:TYR:CE1	1:A:203:ARG:O	0.41	2.74	6	1
1:A:107:TYR:CG	1:A:192:GLN:NE2	0.41	2.89	9	1
1:A:172:GLU:O	1:A:173:TYR:CG	0.41	2.74	9	1
1:A:89:ARG:O	1:A:171:HIS:CE1	0.40	2.74	1	1
1:A:194:TYR:N	1:A:194:TYR:CD1	0.40	2.89	1	1
1:A:274:SER:O	1:A:278:TYR:CD2	0.40	2.74	2	1
1:A:260:PRO:O	1:A:261:TRP:HB3	0.40	2.16	8	1
1:A:142:TYR:CE1	1:A:147:LYS:O	0.40	2.74	9	1
1:A:155:LEU:HD11	1:A:298:GLU:HG3	0.40	1.93	12	1
1:A:252:ILE:HD11	1:A:303:MET:HE1	0.40	1.92	13	1
1:A:118:LEU:HD21	1:A:127:ARG:CG	0.40	2.46	18	1
1:A:142:TYR:CZ	1:A:147:LYS:O	0.40	2.75	2	2
1:A:175:HIS:O	1:A:175:HIS:CD2	0.40	2.74	7	1
1:A:83:GLU:O	1:A:87:TYR:CD1	0.40	2.74	13	2
1:A:174:VAL:HG22	1:A:204:TYR:HD1	0.40	1.76	13	1
1:A:168:ILE:HD13	1:A:175:HIS:CD2	0.40	2.50	15	1
1:A:134:PHE:HE2	1:A:196:VAL:HG11	0.40	1.72	18	1
1:A:252:ILE:HD11	1:A:303:MET:HE2	0.40	1.93	18	1
1:A:225:ILE:HD12	1:A:271:VAL:CG1	0.40	2.47	4	1
1:A:244:LEU:HD21	1:A:317:TYR:CD2	0.40	2.52	5	1
1:A:301:LYS:HB3	1:A:323:ILE:HG23	0.40	1.91	7	1
1:A:202:TYR:CE1	1:A:237:ALA:O	0.40	2.74	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:ASP:O	1:A:198:TYR:CG	0.40	2.75	3	1
1:A:305:THR:HG21	1:A:323:ILE:CD1	0.40	2.34	11	1
1:A:134:PHE:CZ	1:A:196:VAL:CG1	0.40	3.05	2	1
1:A:244:LEU:HB2	1:A:306:VAL:HG13	0.40	1.94	17	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	285/403 (71%)	237±3 (83±1%)	33±3 (12±1%)	15±3 (5±1%)	2	22
All	All	5130/7254 (71%)	4259 (83%)	600 (12%)	271 (5%)	2	22

All 66 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	146	ALA	18
1	A	261	TRP	18
1	A	197	ASP	14
1	A	257	GLY	13
1	A	191	ASP	12
1	A	258	HIS	11
1	A	309	LEU	11
1	A	34	LYS	9
1	A	225	ILE	8
1	A	201	ALA	8
1	A	107	TYR	6
1	A	334	LYS	6
1	A	336	ASP	6
1	A	57	ASN	6
1	A	238	PRO	6
1	A	74	PRO	5
1	A	178	ILE	5
1	A	297	GLY	5

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Mol	Chain	Res	Type	Models (Total)
1	A	76	ASP	5
1	A	63	GLY	5
1	A	43	ILE	5
1	A	75	SER	4
1	A	296	PRO	4
1	A	44	GLY	4
1	A	190	PRO	4
1	A	25	VAL	4
1	A	240	ARG	4
1	A	203	ARG	4
1	A	61	SER	3
1	A	175	HIS	3
1	A	291	PRO	3
1	A	294	ASN	3
1	A	224	THR	3
1	A	108	LEU	2
1	A	333	SER	2
1	A	64	SER	2
1	A	106	LYS	2
1	A	227	PHE	2
1	A	58	SER	2
1	A	90	ALA	2
1	A	237	ALA	2
1	A	77	ASN	2
1	A	189	ASN	2
1	A	59	SER	2
1	A	149	PHE	2
1	A	50	CYS	2
1	A	78	GLY	1
1	A	134	PHE	1
1	A	204	TYR	1
1	A	315	PRO	1
1	A	66	ALA	1
1	A	198	TYR	1
1	A	105	LEU	1
1	A	40	GLY	1
1	A	293	LYS	1
1	A	176	GLY	1
1	A	239	SER	1
1	A	172	GLU	1
1	A	295	LYS	1
1	A	24	ALA	1

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Mol	Chain	Res	Type	Models (Total)
1	A	200	LEU	1
1	A	35	LYS	1
1	A	122	ASN	1
1	A	42	PRO	1
1	A	60	GLU	1
1	A	62	VAL	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	250/349 (72%)	191±5 (76±2%)	59±5 (24±2%)	2	27
All	All	4500/6282 (72%)	3432 (76%)	1068 (24%)	2	27

All 171 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	184	LEU	18
1	A	251	MET	18
1	A	259	LEU	18
1	A	32	MET	16
1	A	309	LEU	15
1	A	307	LYS	13
1	A	35	LYS	12
1	A	112	LYS	12
1	A	284	SER	12
1	A	295	LYS	12
1	A	334	LYS	12
1	A	179	LYS	12
1	A	275	LYS	12
1	A	106	LYS	12
1	A	325	LEU	12
1	A	98	LYS	11
1	A	139	GLN	11
1	A	31	ASP	11
1	A	121	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	293	LYS	11
1	A	85	LYS	10
1	A	140	LYS	10
1	A	147	LYS	10
1	A	170	GLU	10
1	A	188	LYS	10
1	A	262	GLU	10
1	A	149	PHE	10
1	A	322	ASP	10
1	A	192	GLN	10
1	A	104	LYS	9
1	A	151	ARG	9
1	A	163	ASP	9
1	A	166	GLU	9
1	A	171	HIS	9
1	A	71	LYS	9
1	A	129	MET	9
1	A	267	ASP	9
1	A	269	LYS	9
1	A	288	LYS	9
1	A	73	GLU	9
1	A	279	ARG	9
1	A	64	SER	8
1	A	92	LYS	8
1	A	103	ARG	8
1	A	133	ARG	8
1	A	138	LEU	8
1	A	298	GLU	8
1	A	301	LYS	8
1	A	191	ASP	8
1	A	229	SER	8
1	A	266	LYS	8
1	A	89	ARG	8
1	A	124	LYS	8
1	A	97	GLN	8
1	A	186	ASN	8
1	A	56	MET	8
1	A	160	ARG	8
1	A	181	SER	7
1	A	241	ARG	7
1	A	277	ARG	7
1	A	308	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	316	LEU	7
1	A	318	GLU	7
1	A	329	LYS	7
1	A	34	LYS	7
1	A	95	GLN	7
1	A	264	ASN	7
1	A	304	GLU	7
1	A	122	ASN	7
1	A	177	ASP	7
1	A	226	GLU	7
1	A	273	ASP	7
1	A	172	GLU	7
1	A	38	LYS	6
1	A	59	SER	6
1	A	88	GLN	6
1	A	131	MET	6
1	A	169	HIS	6
1	A	189	ASN	6
1	A	200	LEU	6
1	A	60	GLU	6
1	A	75	SER	6
1	A	94	GLU	6
1	A	101	ARG	6
1	A	280	GLU	6
1	A	127	ARG	6
1	A	143	GLU	6
1	A	224	THR	6
1	A	239	SER	6
1	A	287	ASP	6
1	A	305	THR	6
1	A	41	LEU	6
1	A	321	ARG	6
1	A	263	ASP	6
1	A	231	ASP	5
1	A	61	SER	5
1	A	76	ASP	5
1	A	118	LEU	5
1	A	152	LYS	5
1	A	153	THR	5
1	A	65	ASP	5
1	A	225	ILE	5
1	A	240	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	272	ARG	5
1	A	292	GLU	5
1	A	319	ASN	5
1	A	84	LEU	5
1	A	116	SER	5
1	A	145	ASN	5
1	A	150	SER	5
1	A	156	GLN	5
1	A	148	ARG	5
1	A	233	HIS	5
1	A	286	MET	5
1	A	27	GLU	4
1	A	50	CYS	4
1	A	58	SER	4
1	A	99	TRP	4
1	A	119	HIS	4
1	A	120	ASP	4
1	A	125	SER	4
1	A	57	ASN	4
1	A	243	ASP	4
1	A	203	ARG	4
1	A	256	THR	4
1	A	281	ASN	4
1	A	333	SER	4
1	A	36	GLU	4
1	A	228	THR	4
1	A	68	CYS	4
1	A	326	GLN	4
1	A	245	GLU	4
1	A	234	ASN	3
1	A	335	ASP	3
1	A	175	HIS	3
1	A	77	ASN	3
1	A	250	CYS	3
1	A	30	THR	3
1	A	253	GLN	3
1	A	331	ILE	3
1	A	336	ASP	3
1	A	204	TYR	2
1	A	158	SER	2
1	A	81	PHE	2
1	A	202	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	258	HIS	2
1	A	285	LEU	2
1	A	83	GLU	2
1	A	136	SER	2
1	A	197	ASP	2
1	A	173	TYR	2
1	A	294	ASN	2
1	A	132	ASP	2
1	A	274	SER	2
1	A	82	THR	2
1	A	261	TRP	1
1	A	185	LEU	1
1	A	55	ASP	1
1	A	303	MET	1
1	A	265	LEU	1
1	A	25	VAL	1
1	A	270	TYR	1
1	A	193	VAL	1
1	A	80	LEU	1
1	A	230	ILE	1
1	A	289	CYS	1
1	A	183	LEU	1
1	A	87	TYR	1
1	A	108	LEU	1
1	A	196	VAL	1
1	A	102	THR	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 52% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: working_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	2601
Number of shifts mapped to atoms	2601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	363	0.11 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	325	1.09 ± 0.09	Should be checked
$^{13}\text{C}'$	363	-0.01 ± 0.05	None needed (< 0.5 ppm)
^{15}N	343	-0.15 ± 0.15	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 2114 atoms were assigned a chemical shift out of a possible 4029. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1092/1419 (77%)	266/577 (46%)	560/570 (98%)	266/272 (98%)
Sidechain	896/2270 (39%)	474/1471 (32%)	422/707 (60%)	0/92 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	126/340 (37%)	63/161 (39%)	58/162 (36%)	5/17 (29%)
Overall	2114/4029 (52%)	803/2209 (36%)	1040/1439 (72%)	271/381 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 2601 atoms were assigned a chemical shift out of a possible 5602. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1412/2013 (70%)	343/821 (42%)	726/806 (90%)	343/386 (89%)
Sidechain	1049/3175 (33%)	534/2043 (26%)	515/988 (52%)	0/144 (0%)
Aromatic	140/414 (34%)	70/197 (36%)	64/193 (33%)	6/24 (25%)
Overall	2601/5602 (46%)	947/3061 (31%)	1305/1987 (66%)	349/554 (63%)

7.1.4 Statistically unusual chemical shifts ⓘ

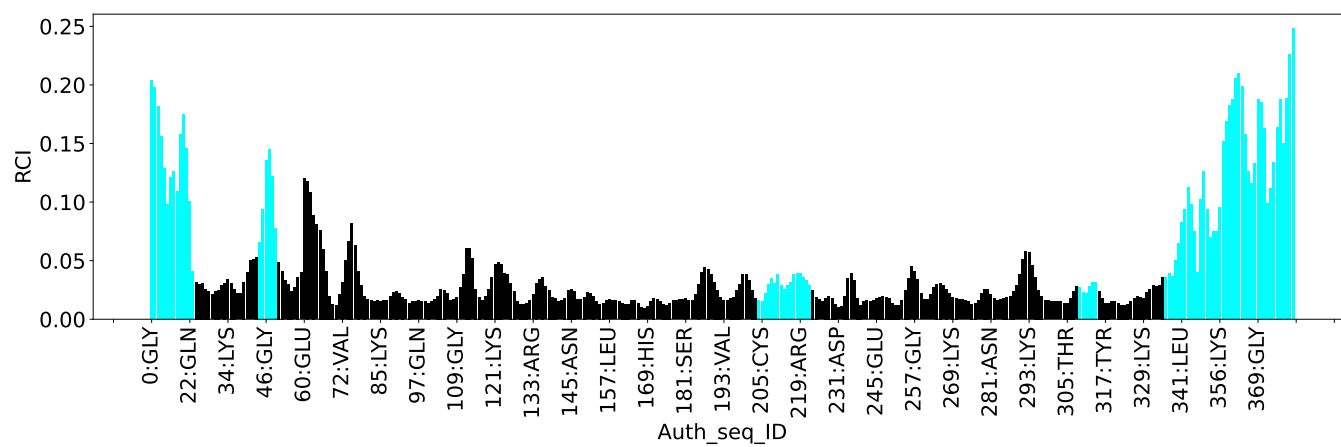
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	ILE	HD11	-0.81	-0.72 – 2.09	-5.3
1	A	29	ILE	HD12	-0.81	-0.72 – 2.09	-5.3
1	A	29	ILE	HD13	-0.81	-0.72 – 2.09	-5.3
1	A	29	ILE	HG21	-0.64	-0.56 – 2.11	-5.3
1	A	29	ILE	HG22	-0.64	-0.56 – 2.11	-5.3
1	A	29	ILE	HG23	-0.64	-0.56 – 2.11	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:



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	3061
Intra-residue ($ i-j =0$)	440
Sequential ($ i-j =1$)	710
Medium range ($ i-j >1$ and $ i-j <5$)	599
Long range ($ i-j \geq 5$)	1224
Inter-chain	0
Hydrogen bond restraints	88
Disulfide bond restraints	0
Total dihedral-angle restraints	322
Number of unmapped restraints	0
Number of restraints per residue	8.4
Number of long range restraints per residue ¹	3.1

¹Long 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)	0.8	0.14
0.2-0.5 (Medium)	None	None
>0.5 (Large)	None	None

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)	0.1	1.13
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

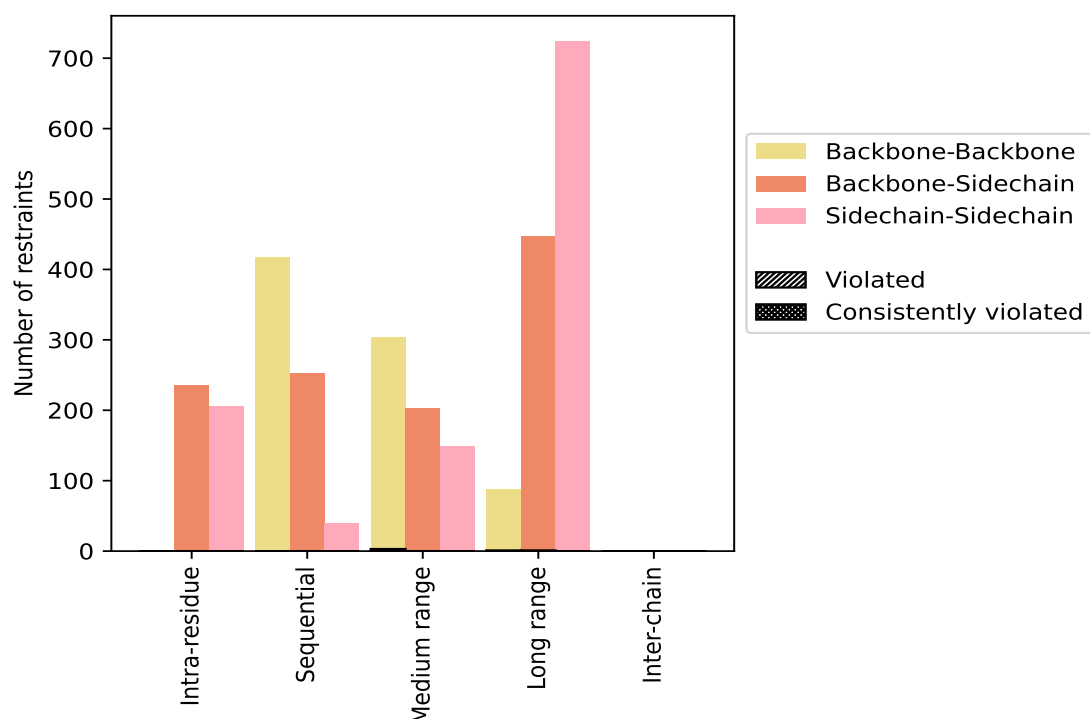
9.1 Summary of distance violations ⓘ

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	440	14.4	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	235	7.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	205	6.7	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	710	23.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	417	13.6	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	253	8.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	40	1.3	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	599	19.6	3	0.5	0.1	0	0.0	0.0
Backbone-Backbone	303	9.9	3	1.0	0.1	0	0.0	0.0
Backbone-Sidechain	148	4.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	148	4.8	0	0.0	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	1224	40.0	2	0.2	0.1	0	0.0	0.0
Backbone-Backbone	87	2.8	1	1.1	0.0	0	0.0	0.0
Backbone-Sidechain	413	13.5	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	724	23.7	0	0.0	0.0	0	0.0	0.0
Inter-chain	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
Hydrogen bond	88	2.9	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	3061	100.0	5	0.2	0.2	0	0.0	0.0
Backbone-Backbone	807	26.4	4	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	1137	37.1	1	0.1	0.0	0	0.0	0.0
Sidechain-Sidechain	1117	36.5	0	0.0	0.0	0	0.0	0.0

¹ percentage calculated with respect to the total number of distance restraints, ² percentage calculated with respect to the number of restraints in a particular restraint category, ³ violated in at least one model, ⁴ 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 ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	1	1	0	2	0.1	0.1	0.0	0.1
3	0	0	1	0	0	1	0.1	0.1	0.0	0.1
4	0	0	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	1	0	0	1	0.13	0.13	0.0	0.13
6	0	0	1	0	0	1	0.12	0.12	0.0	0.12
7	0	0	1	1	0	2	0.12	0.12	0.0	0.12
8	0	0	1	0	0	1	0.11	0.11	0.0	0.11
9	0	0	1	0	0	1	0.13	0.13	0.0	0.13
10	0	0	2	0	0	2	0.12	0.13	0.01	0.12

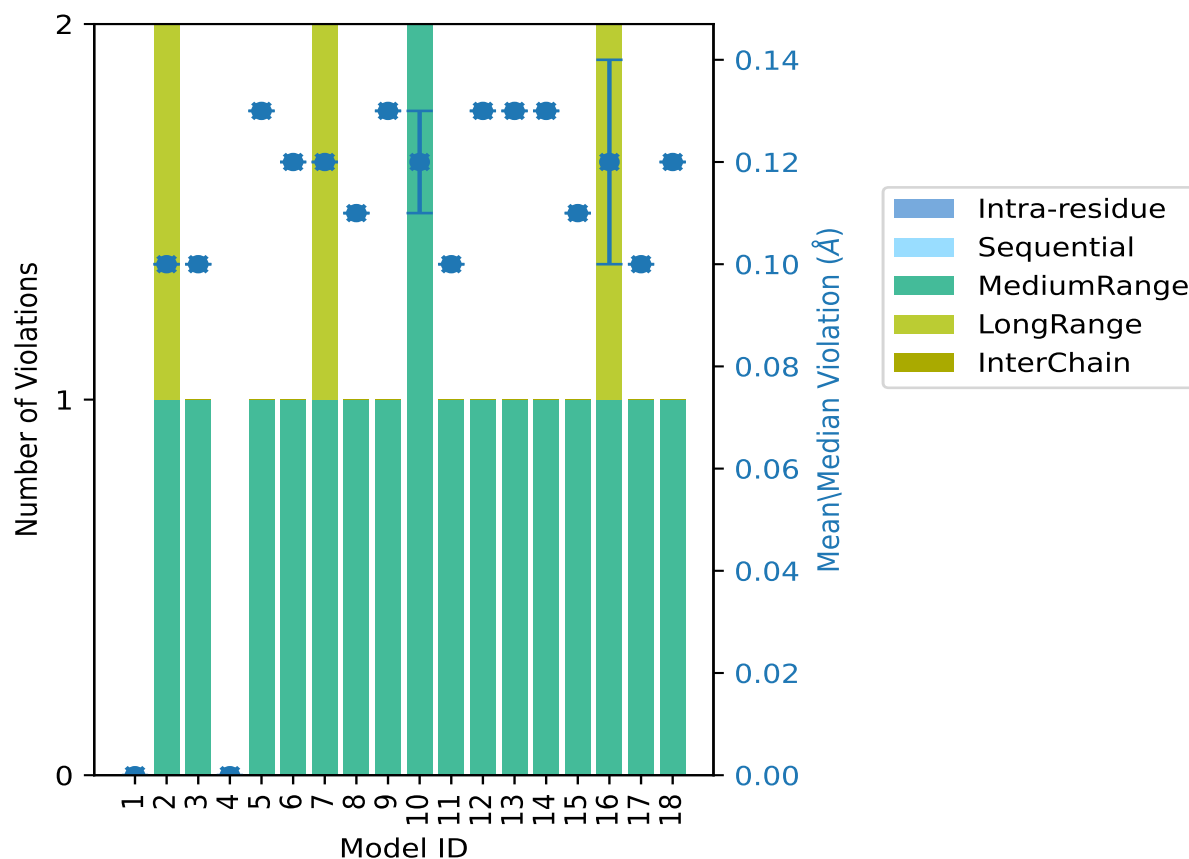
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	0	1	0	0	1	0.1	0.1	0.0	0.1
12	0	0	1	0	0	1	0.13	0.13	0.0	0.13
13	0	0	1	0	0	1	0.13	0.13	0.0	0.13
14	0	0	1	0	0	1	0.13	0.13	0.0	0.13
15	0	0	1	0	0	1	0.11	0.11	0.0	0.11
16	0	0	1	1	0	2	0.12	0.14	0.02	0.12
17	0	0	1	0	0	1	0.1	0.1	0.0	0.1
18	0	0	1	0	0	1	0.12	0.12	0.0	0.12

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

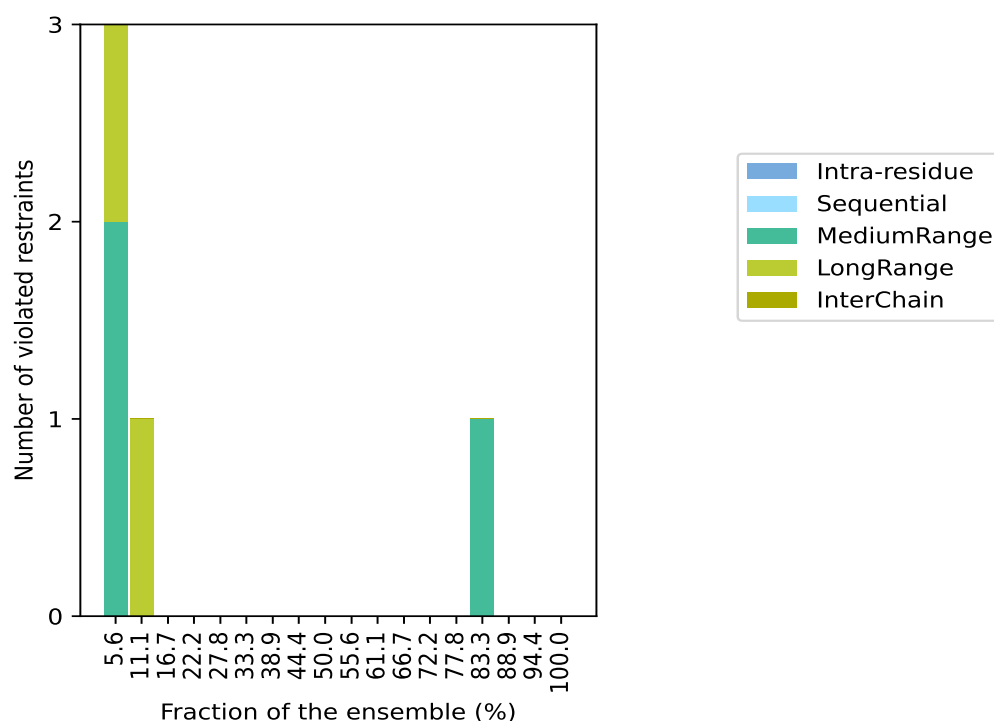
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2968(IR:440, SQ:710, MR:596, LR:1222, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	2	1	0	3	1	5.6
0	0	0	1	0	1	2	11.1
0	0	0	0	0	0	3	16.7
0	0	0	0	0	0	4	22.2
0	0	0	0	0	0	5	27.8
0	0	0	0	0	0	6	33.3
0	0	0	0	0	0	7	38.9
0	0	0	0	0	0	8	44.4
0	0	0	0	0	0	9	50.0
0	0	0	0	0	0	10	55.6
0	0	0	0	0	0	11	61.1
0	0	0	0	0	0	12	66.7
0	0	0	0	0	0	13	72.2
0	0	0	0	0	0	14	77.8
0	0	1	0	0	1	15	83.3
0	0	0	0	0	0	16	88.9
0	0	0	0	0	0	17	94.4
0	0	0	0	0	0	18	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

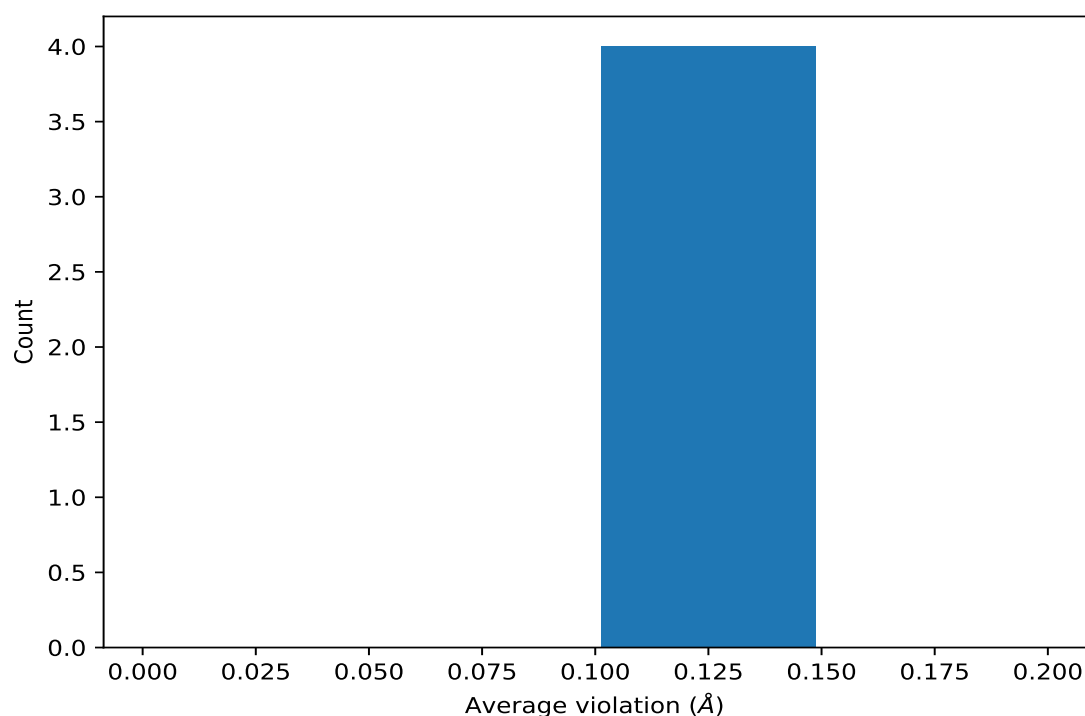
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



9.4 Most violated distance restraints in the ensemble [i](#)

9.4.1 Histogram : Distribution of mean distance 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



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.

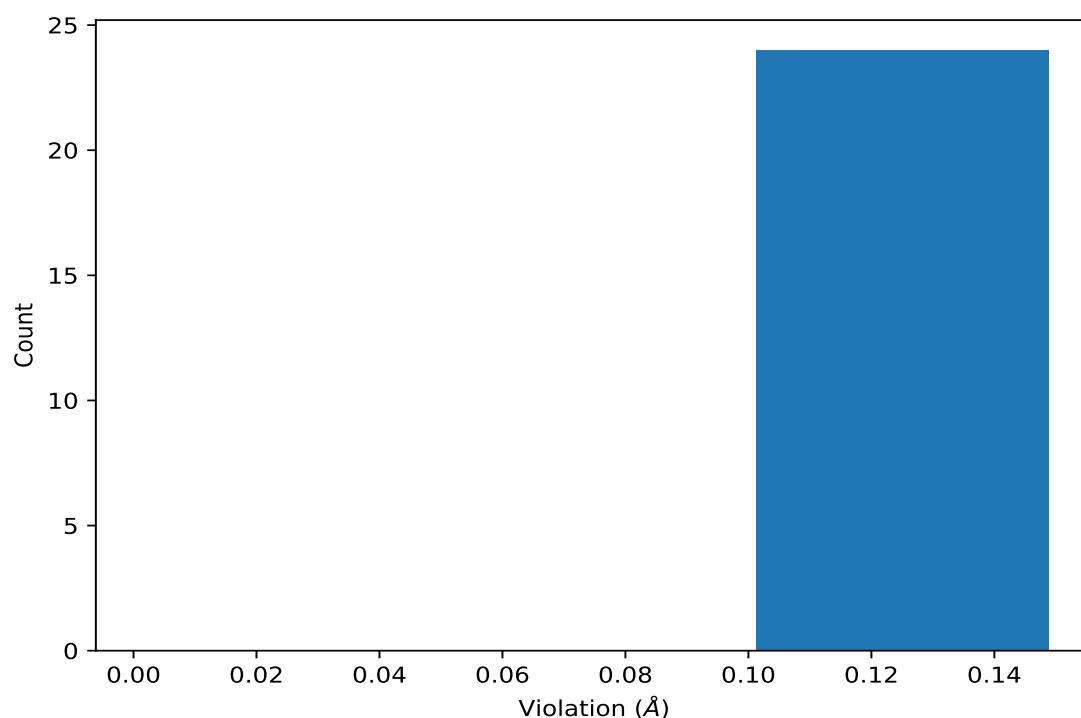
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	15	0.12	0.01	0.12
(1,1335)	1:138:A:LEU:HD11	1:194:A:TYR:H	2	0.11	0.0	0.11
(1,1335)	1:138:A:LEU:HD12	1:194:A:TYR:H	2	0.11	0.0	0.11
(1,1335)	1:138:A:LEU:HD13	1:194:A:TYR:H	2	0.11	0.0	0.11

¹Number of violated models, ²Standard 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)
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	16	0.14
(1,1089)	1:121:A:LYS:H	1:123:A:GLY:H	12	0.13
(1,818)	1:189:A:ASN:H	1:187:A:TYR:H	10	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	5	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	9	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	13	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	14	0.13
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	6	0.12
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	7	0.12
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	10	0.12
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	18	0.12
(1,1335)	1:138:A:LEU:HD11	1:194:A:TYR:H	7	0.11
(1,1335)	1:138:A:LEU:HD12	1:194:A:TYR:H	7	0.11
(1,1335)	1:138:A:LEU:HD13	1:194:A:TYR:H	7	0.11
(1,1140)	1:186:A:ASN:H	1:191:A:ASP:H	16	0.11
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	15	0.11
(1,1335)	1:138:A:LEU:HD11	1:194:A:TYR:H	2	0.1
(1,1335)	1:138:A:LEU:HD12	1:194:A:TYR:H	2	0.1
(1,1335)	1:138:A:LEU:HD13	1:194:A:TYR:H	2	0.1
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	2	0.1
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	3	0.1
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	11	0.1
(1,649)	1:264:A:ASN:H	1:266:A:LYS:H	17	0.1

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

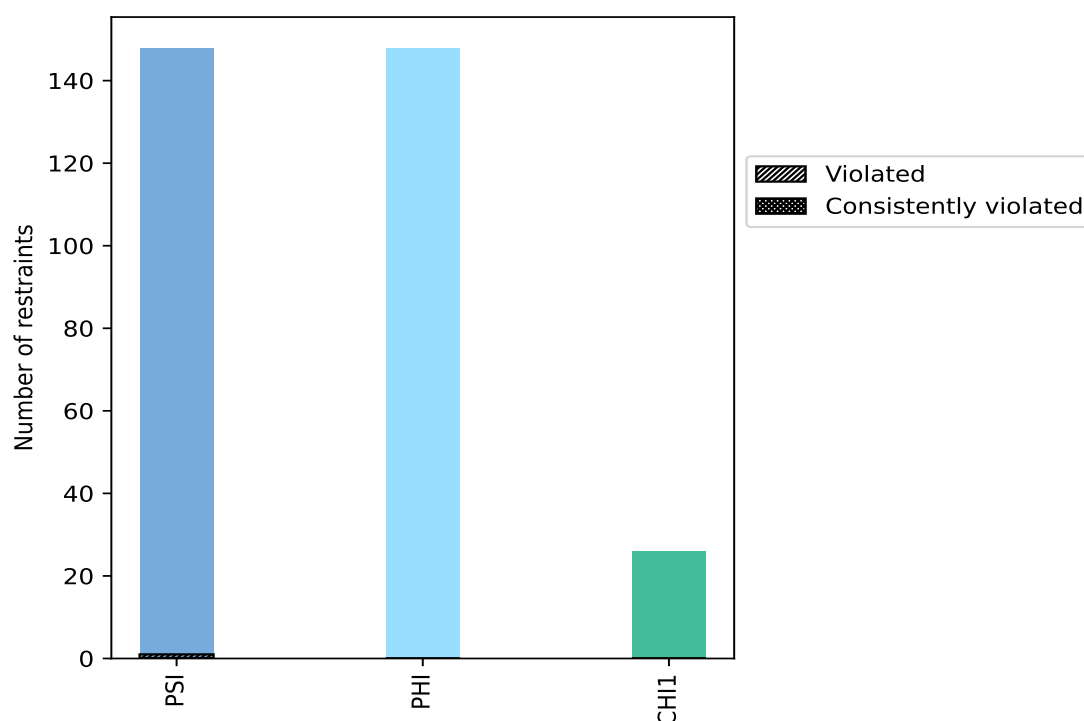
10.1 Summary of dihedral-angle violations [i](#)

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	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	148	46.0	1	0.7	0.3	0	0.0	0.0
PHI	148	46.0	0	0.0	0.0	0	0.0	0.0
CHI1	26	8.1	0	0.0	0.0	0	0.0	0.0
Total	322	100.0	1	0.3	0.3	0	0.0	0.0

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

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



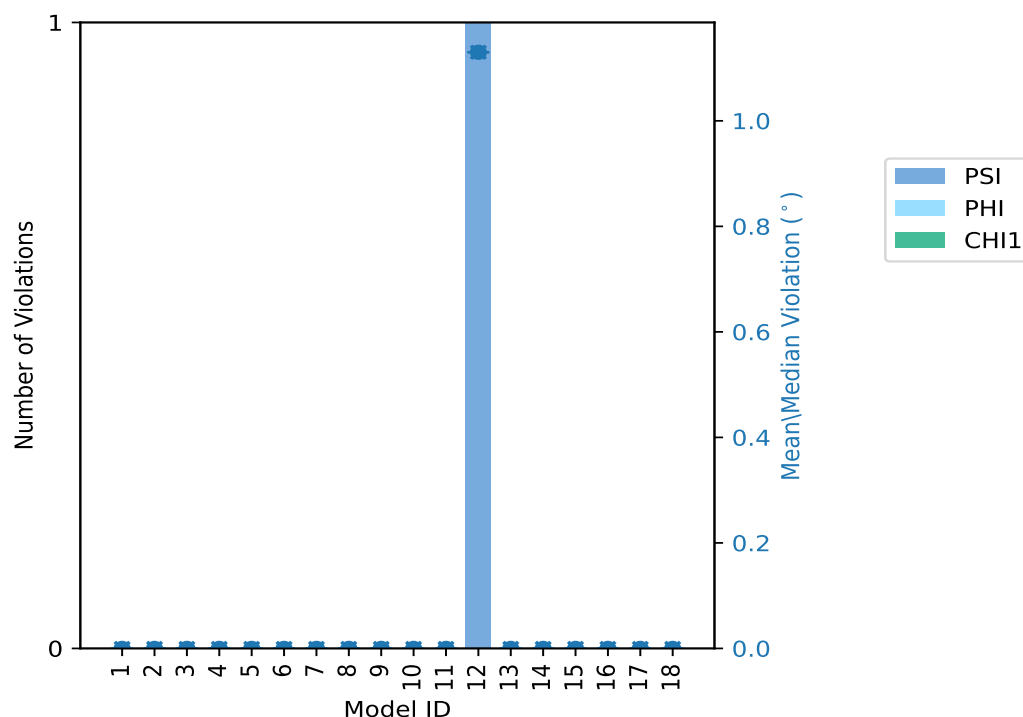
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	CHI1	Total				
1	0	0	0	0	0.0	0.0	0.0	0.0
2	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	0	0	0.0	0.0	0.0	0.0
4	0	0	0	0	0.0	0.0	0.0	0.0
5	0	0	0	0	0.0	0.0	0.0	0.0
6	0	0	0	0	0.0	0.0	0.0	0.0
7	0	0	0	0	0.0	0.0	0.0	0.0
8	0	0	0	0	0.0	0.0	0.0	0.0
9	0	0	0	0	0.0	0.0	0.0	0.0
10	0	0	0	0	0.0	0.0	0.0	0.0
11	0	0	0	0	0.0	0.0	0.0	0.0
12	1	0	0	1	1.13	1.13	0.0	1.13
13	0	0	0	0	0.0	0.0	0.0	0.0
14	0	0	0	0	0.0	0.0	0.0	0.0
15	0	0	0	0	0.0	0.0	0.0	0.0
16	0	0	0	0	0.0	0.0	0.0	0.0
17	0	0	0	0	0.0	0.0	0.0	0.0
18	0	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	CHI1	Total	Count ¹	%
1	0	0	1	1	5.6
0	0	0	0	2	11.1
0	0	0	0	3	16.7
0	0	0	0	4	22.2
0	0	0	0	5	27.8
0	0	0	0	6	33.3
0	0	0	0	7	38.9
0	0	0	0	8	44.4
0	0	0	0	9	50.0
0	0	0	0	10	55.6
0	0	0	0	11	61.1

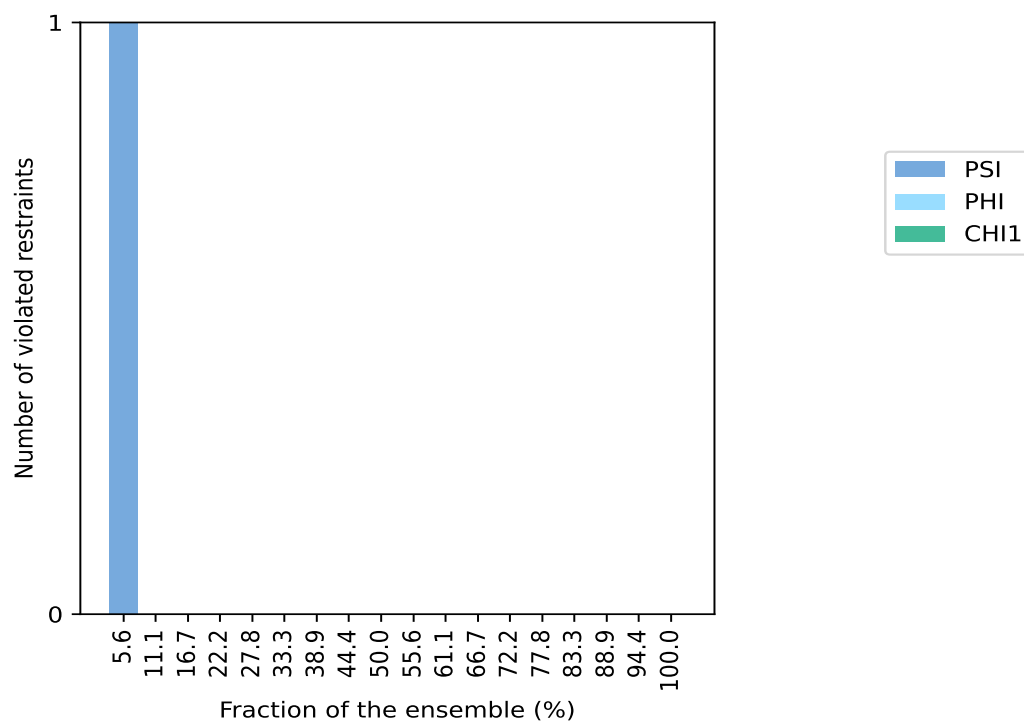
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Number of violated restraints				Fraction of the ensemble	
PSI	PHI	CHI1	Total	Count ¹	%
0	0	0	0	12	66.7
0	0	0	0	13	72.2
0	0	0	0	14	77.8
0	0	0	0	15	83.3
0	0	0	0	16	88.9
0	0	0	0	17	94.4
0	0	0	0	18	100.0

¹ 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](#)

No violations found

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.

Data insufficient to plot histogram

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 (°)
(1,82)	1:121:A:LYS:N	1:121:A:LYS:CA	1:121:A:LYS:C	1:122:A:ASN:N	12	1.13