



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 01:35 am BST

PDB ID : 2RSV
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

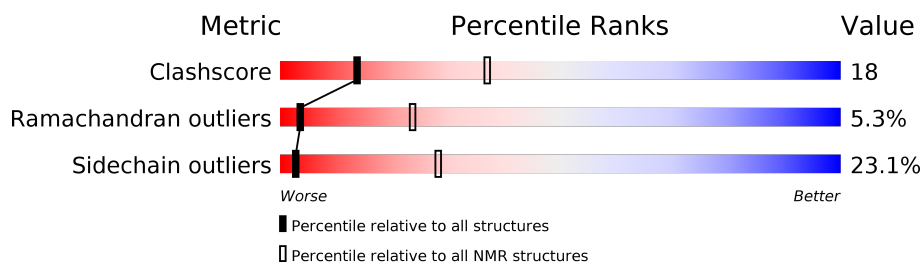
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 50%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	

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)	0.86	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:

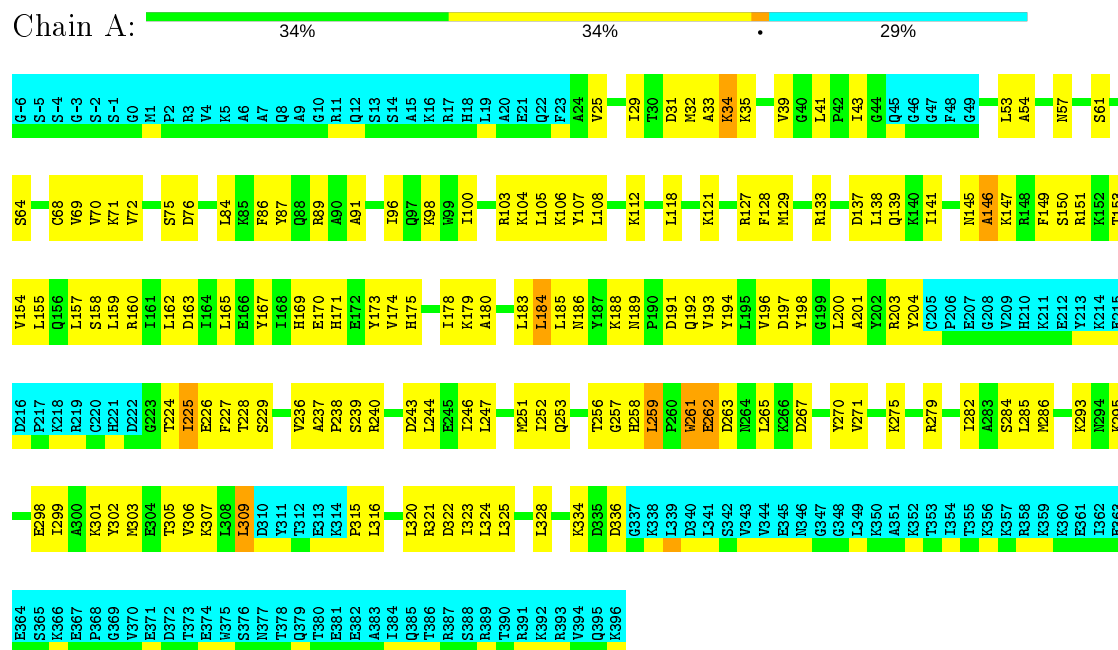
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP Q99986
A	-5	SER	-	EXPRESSION TAG	UNP Q99986
A	-4	SER	-	EXPRESSION TAG	UNP Q99986
A	-3	GLY	-	EXPRESSION TAG	UNP Q99986
A	-2	SER	-	EXPRESSION TAG	UNP Q99986
A	-1	SER	-	EXPRESSION TAG	UNP Q99986
A	0	GLY	-	EXPRESSION TAG	UNP Q99986

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Serine/threonine-protein kinase VRK1

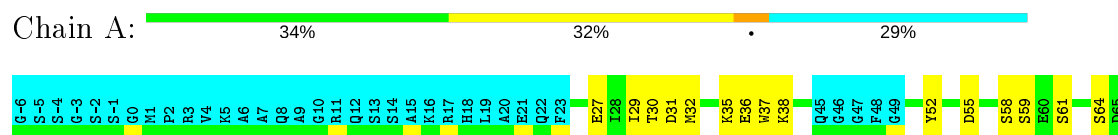


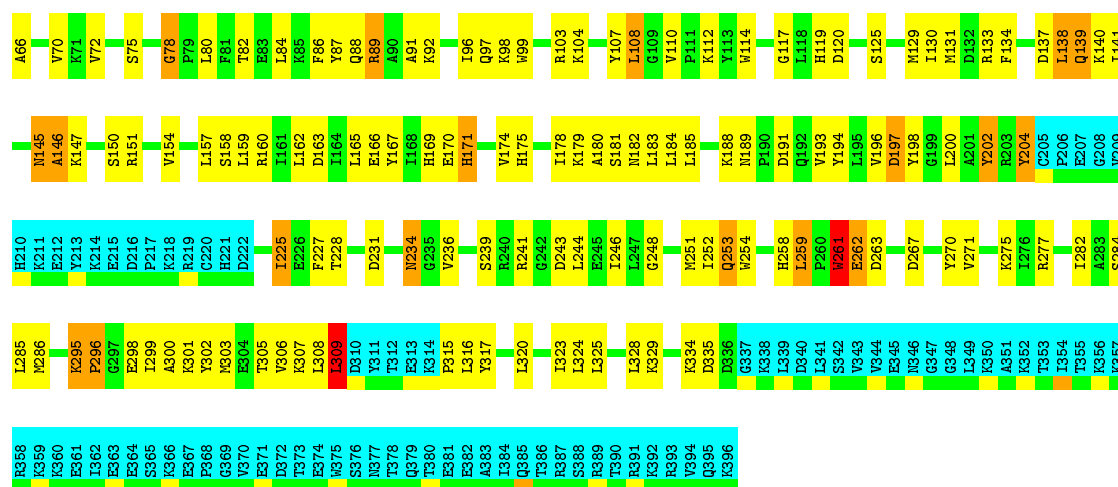
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

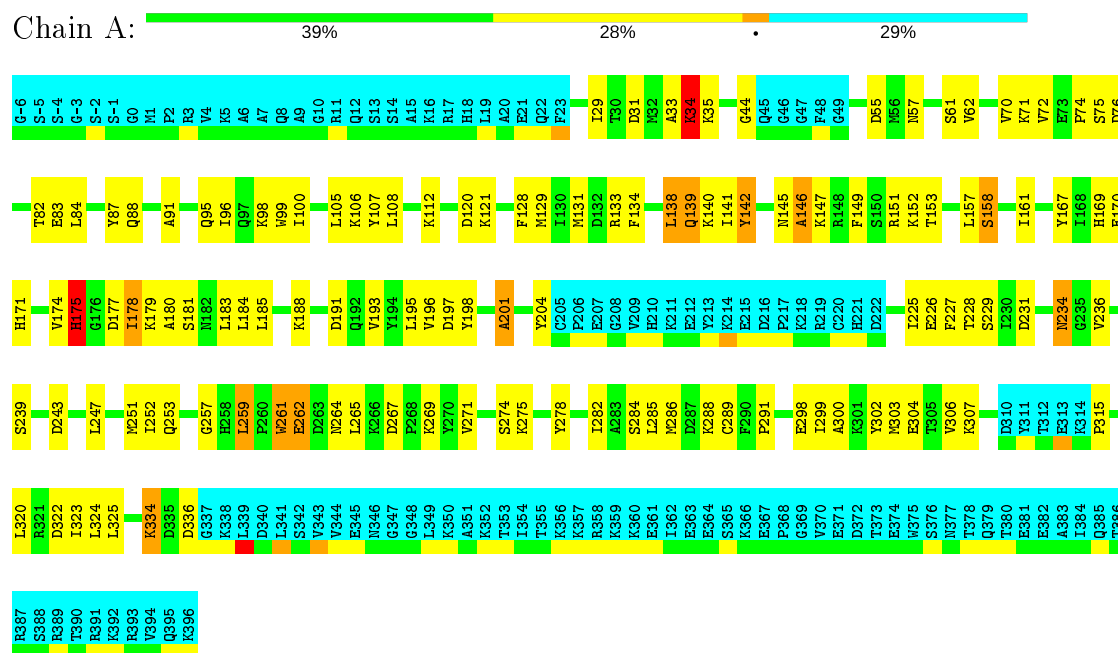
- Molecule 1: Serine/threonine-protein kinase VRK1





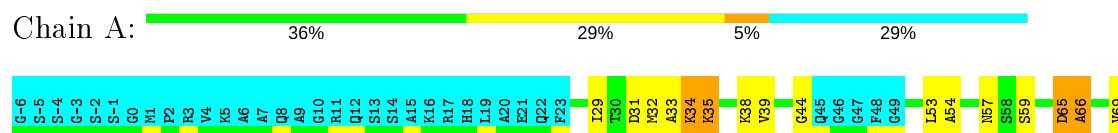
4.2.2 Score per residue for model 2

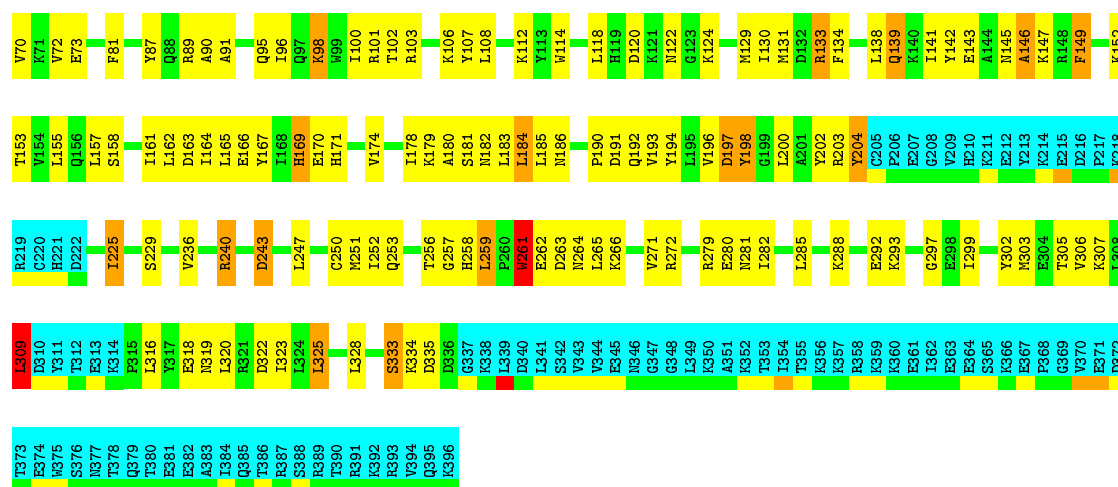
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.3 Score per residue for model 3

- Molecule 1: Serine/threonine-protein kinase VRK1

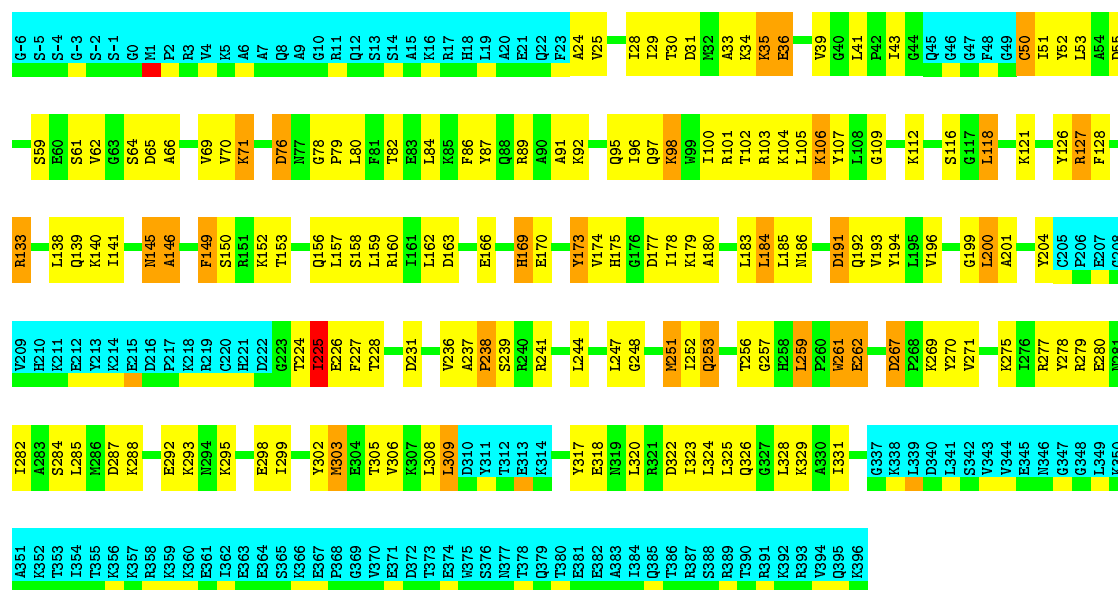




4.2.4 Score per residue for model 4

- Molecule 1: Serine/threonine-protein kinase VRK1

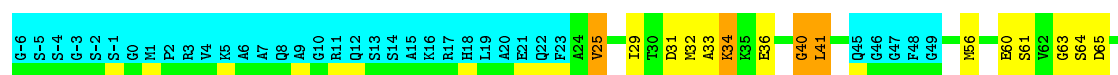
Chain A: 32% 32% 7% 29%

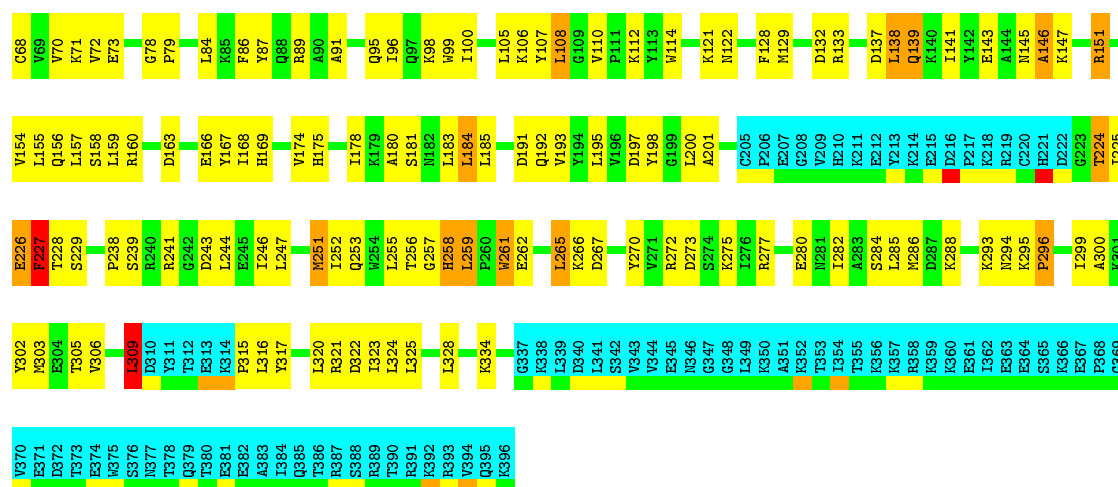


4.2.5 Score per residue for model 5

- Molecule 1: Serine/threonine-protein kinase VRK1

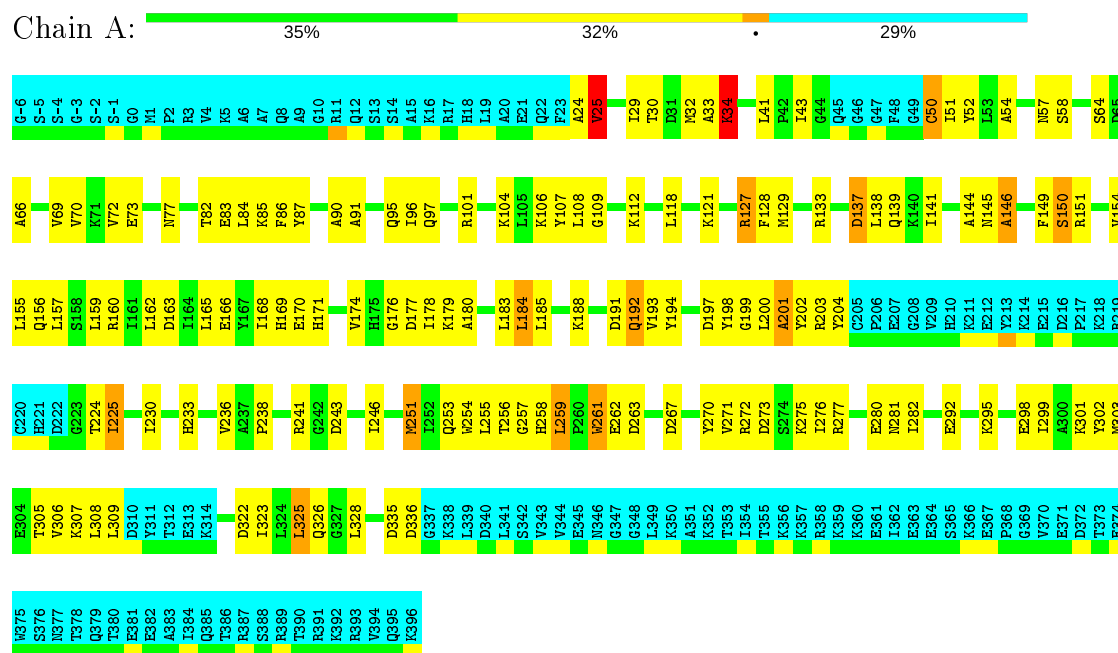
Chain A: 36% 30% 29%





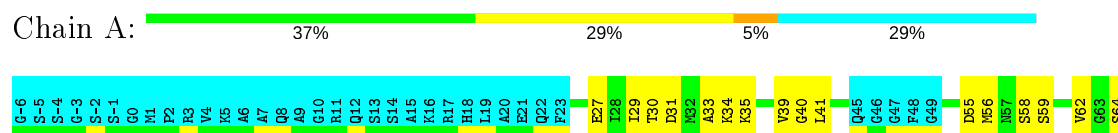
4.2.6 Score per residue for model 6

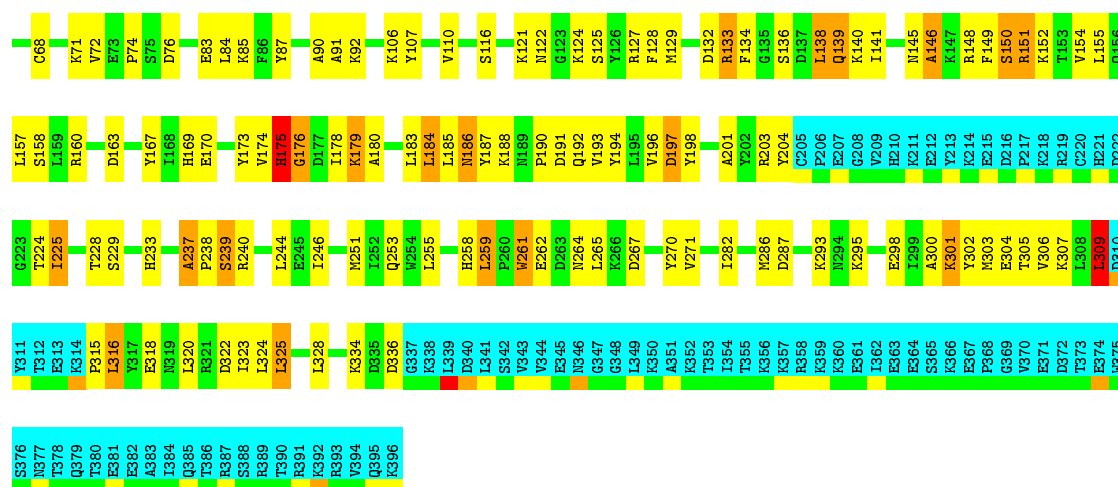
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.7 Score per residue for model 7

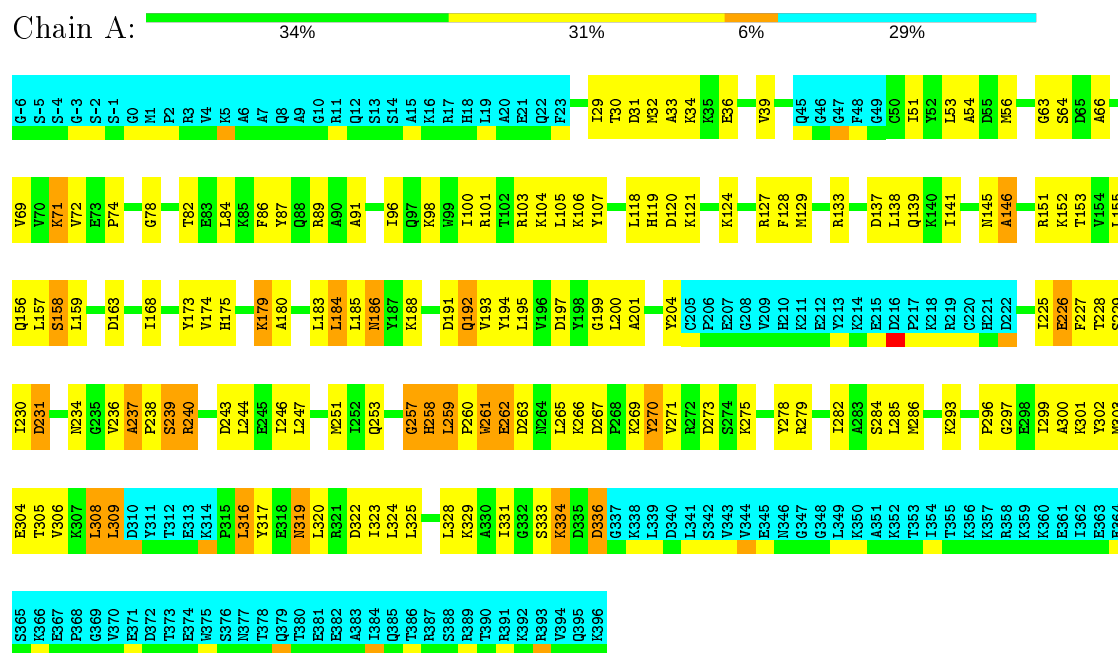
- Molecule 1: Serine/threonine-protein kinase VRK1





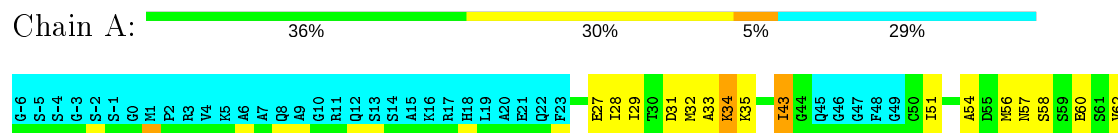
4.2.8 Score per residue for model 8

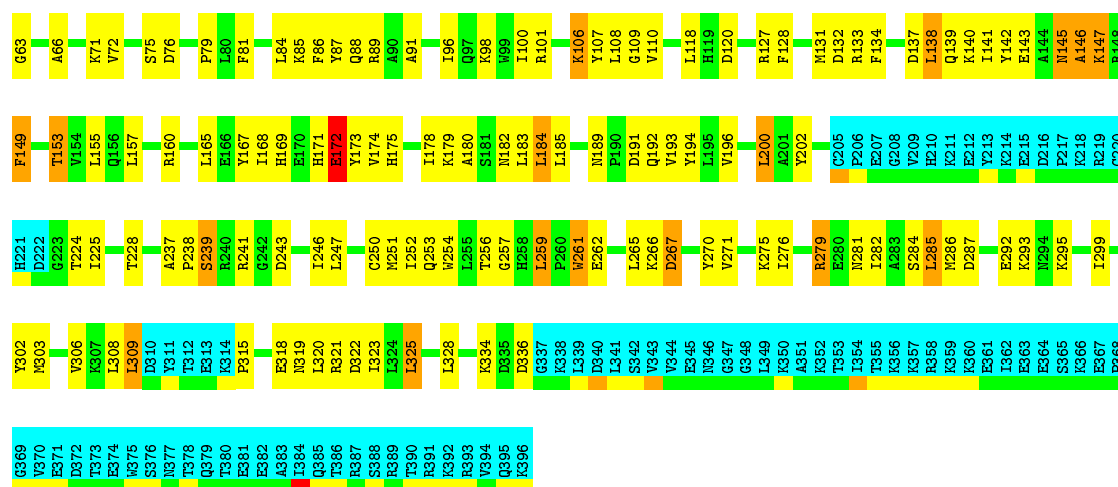
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.9 Score per residue for model 9

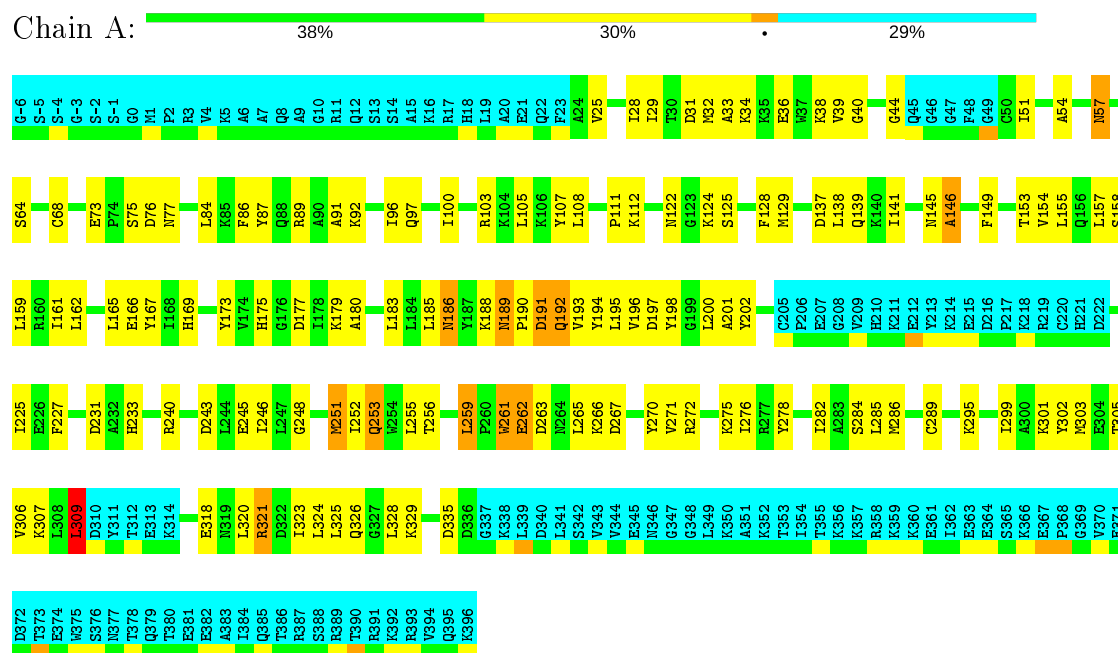
- Molecule 1: Serine/threonine-protein kinase VRK1





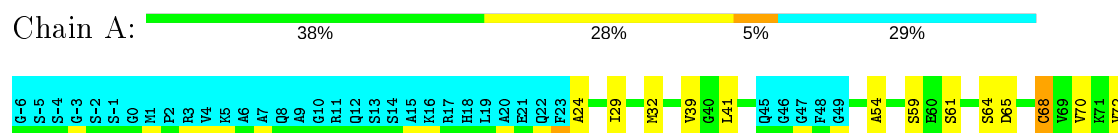
4.2.10 Score per residue for model 10

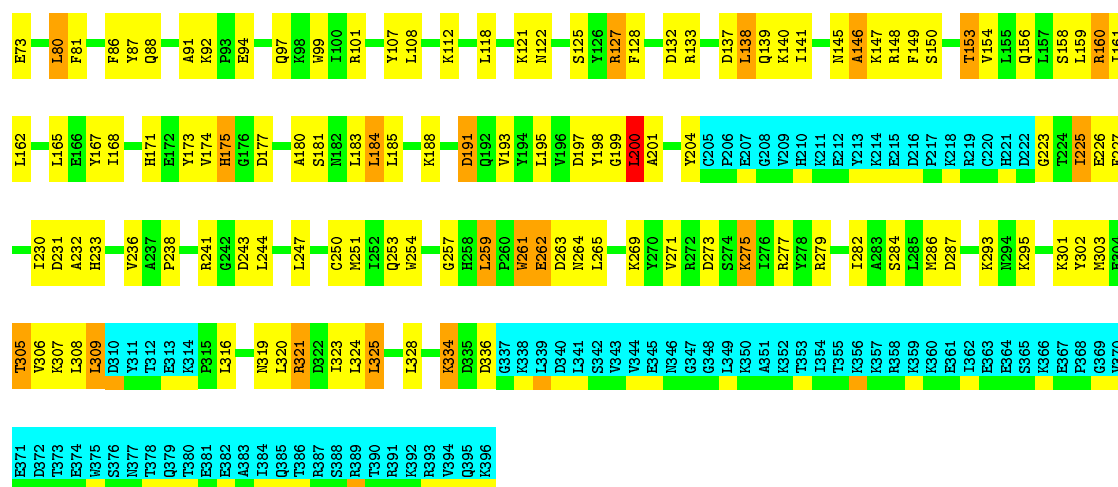
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.11 Score per residue for model 11

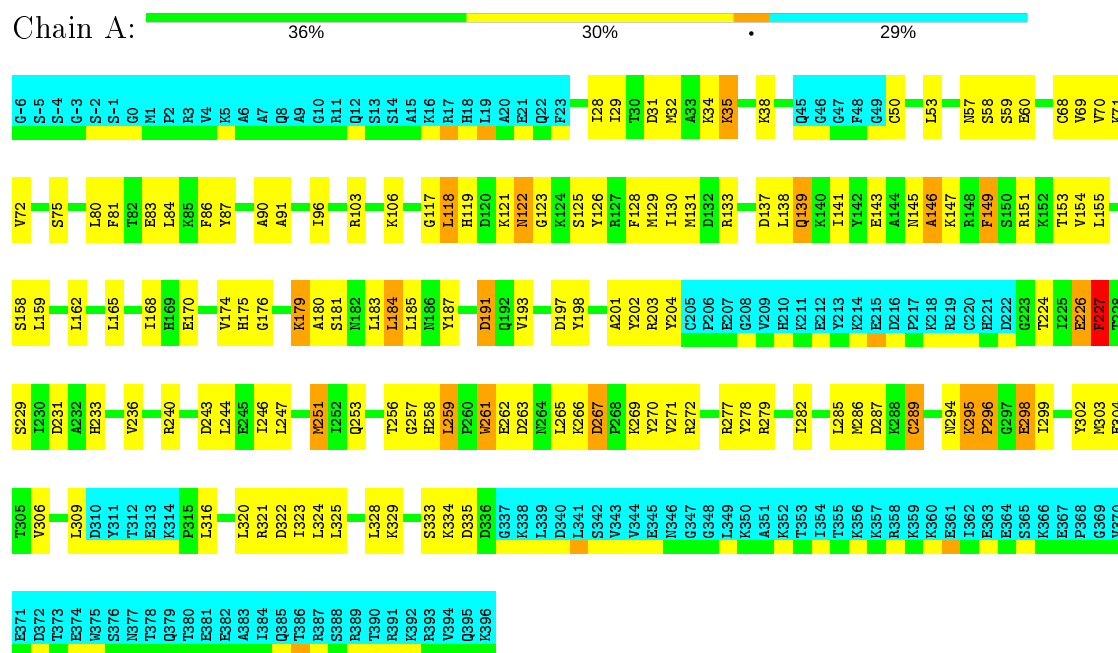
- Molecule 1: Serine/threonine-protein kinase VRK1





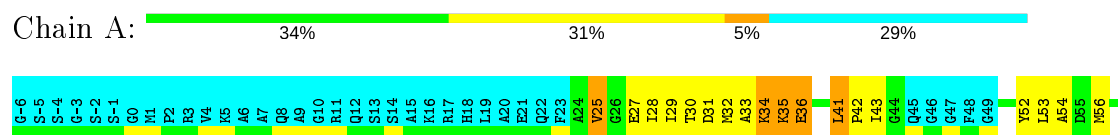
4.2.12 Score per residue for model 12

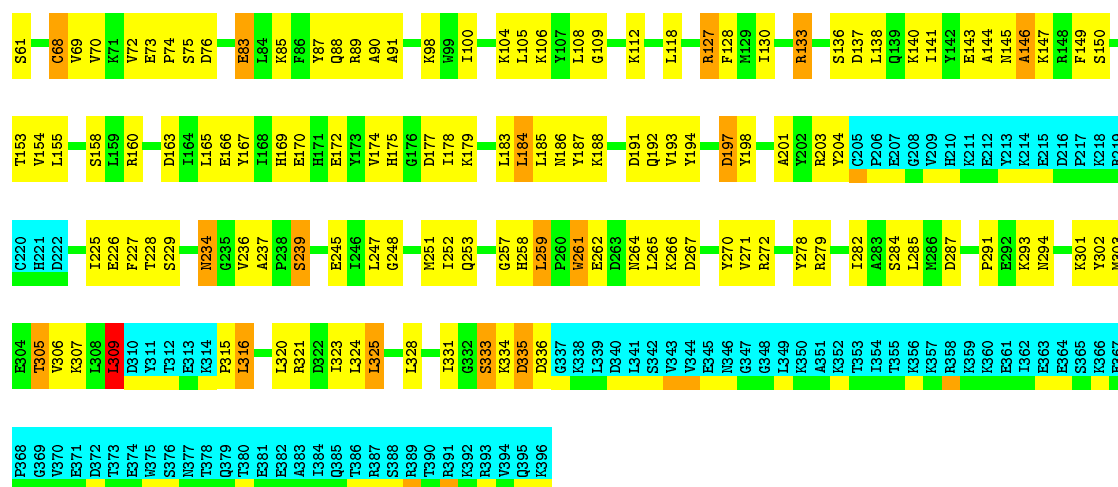
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.13 Score per residue for model 13 (medoid)

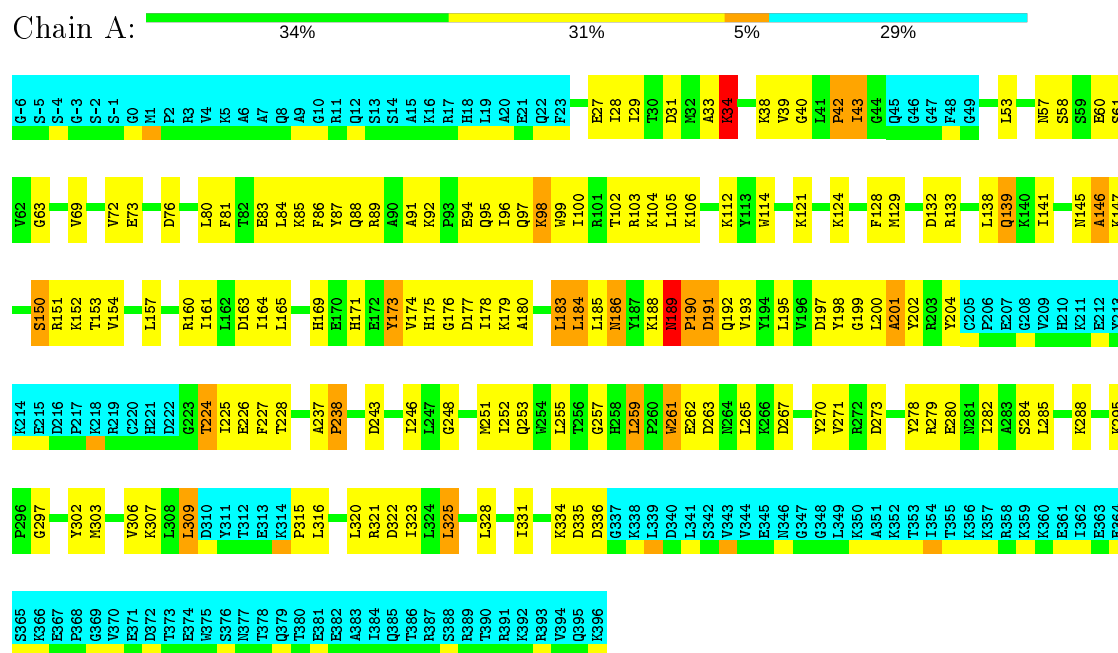
- Molecule 1: Serine/threonine-protein kinase VRK1





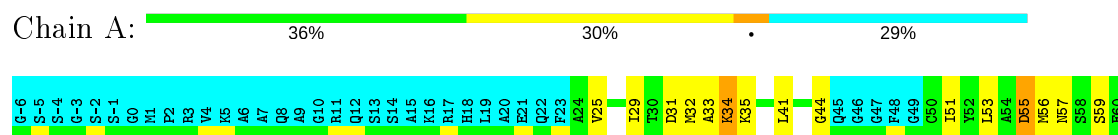
4.2.14 Score per residue for model 14

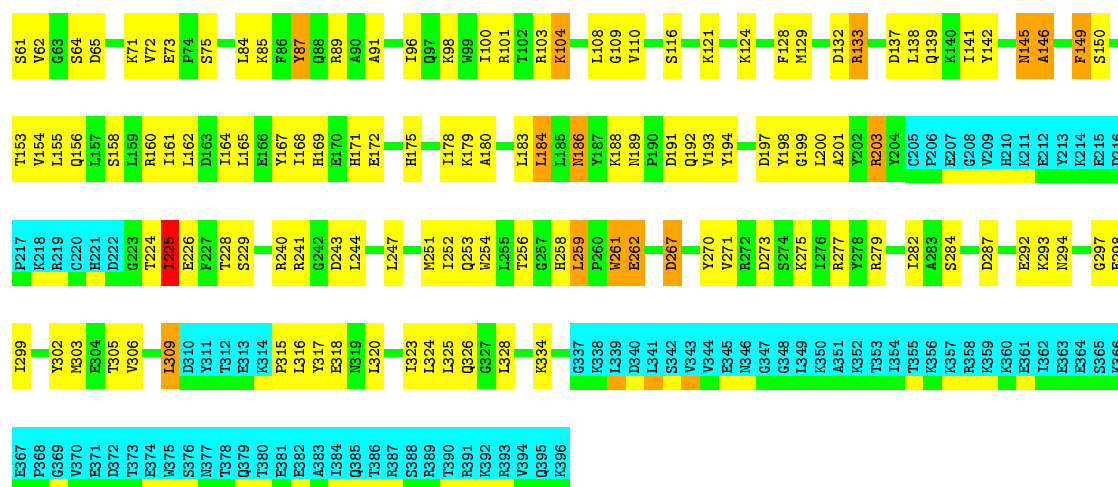
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.15 Score per residue for model 15

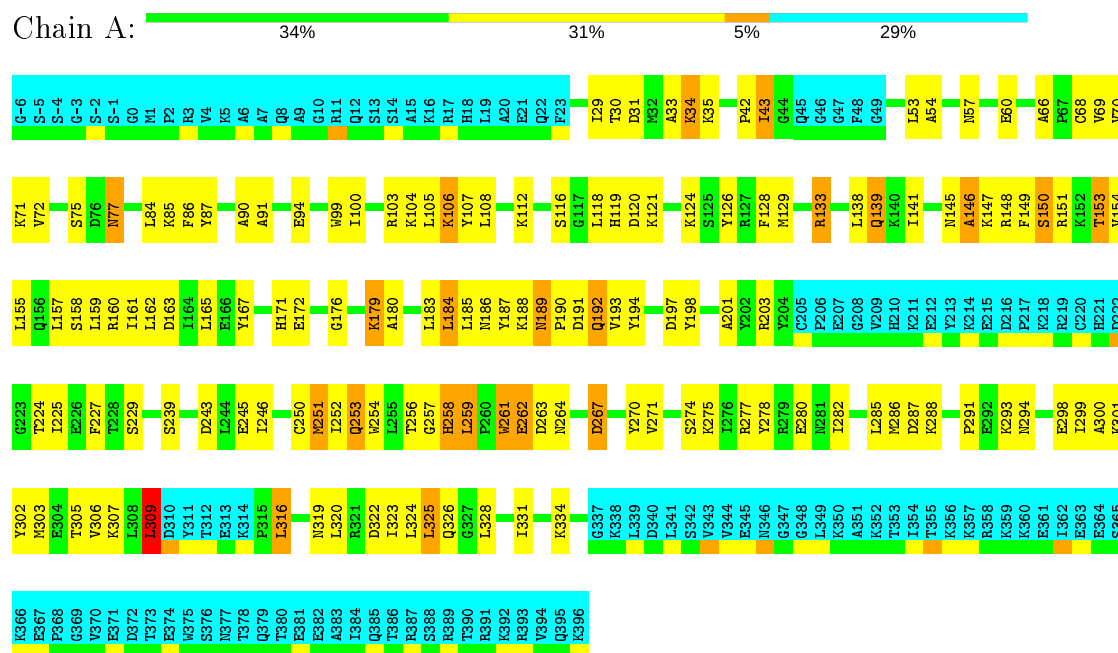
- Molecule 1: Serine/threonine-protein kinase VRK1





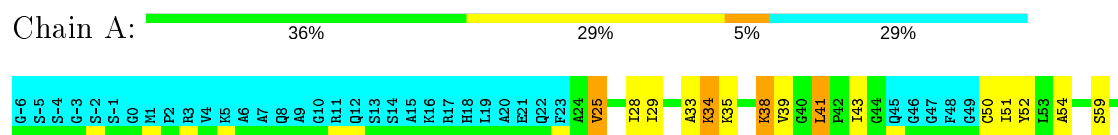
4.2.16 Score per residue for model 16

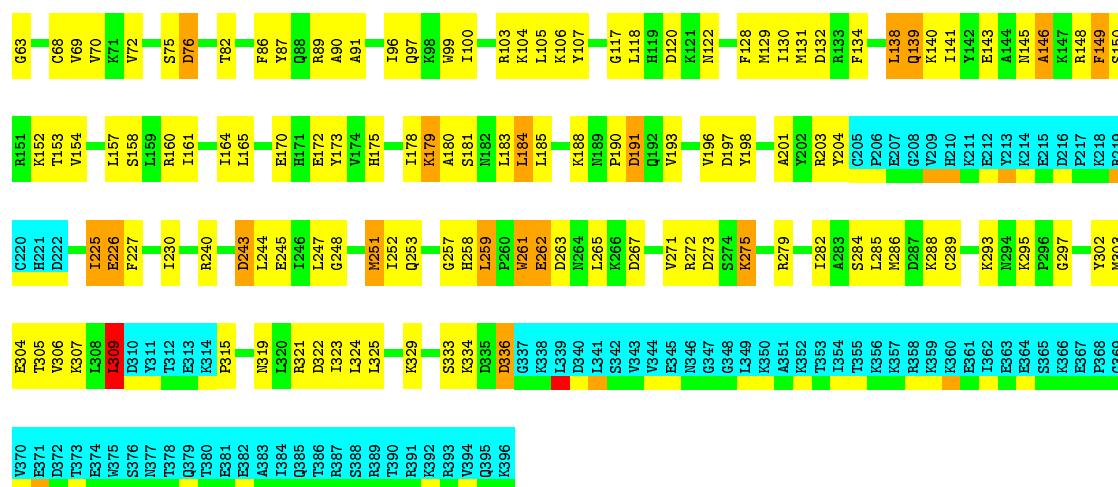
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.17 Score per residue for model 17

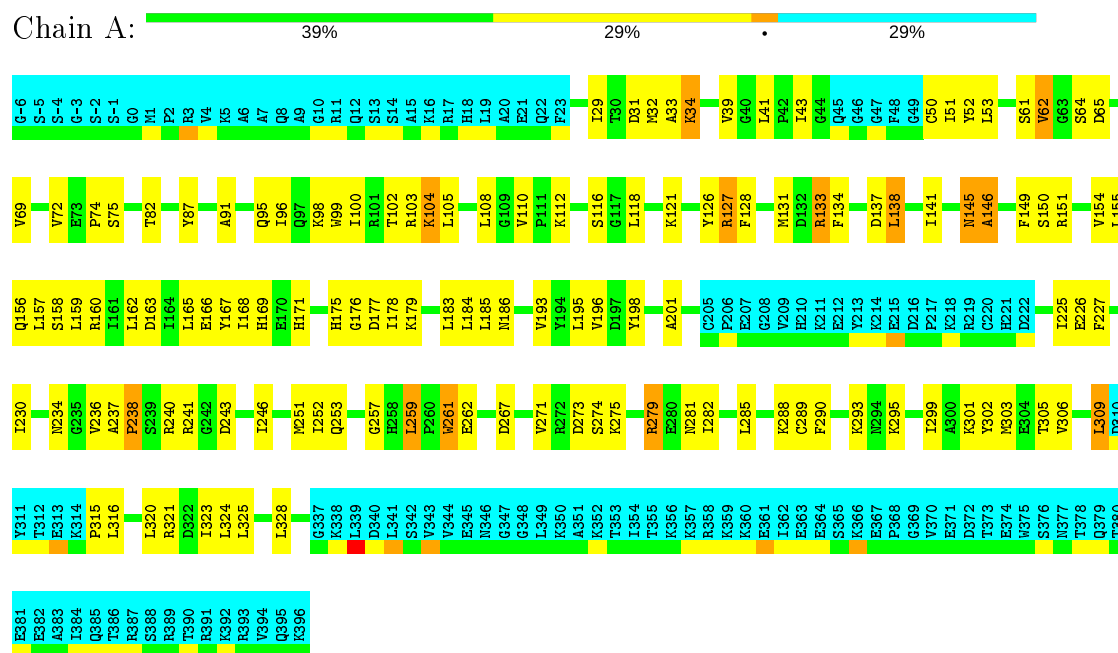
- Molecule 1: Serine/threonine-protein kinase VRK1





4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein kinase VRK1



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)	input_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)	50%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	2313	2336	2330	83±7
All	All	41634	42048	41940	1486

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 18.

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: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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:VAL:HG21	1:A:167:TYR:CE2	0.77	2.15	1	2
1:A:183:LEU:C	1:A:184:LEU:HD23	0.77	2.00	11	16
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:108:LEU:HD21	1:A:167:TYR:CE2	0.74	2.18	9	2
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: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:182:ASN:O	1:A:196:VAL:HG22	0.70	1.85	9	3
1:A:84:LEU:HD21	1:A:129:MET:HB2	0.70	1.61	8	11
1:A:198:TYR:HB3	1:A:201:ALA:HB3	0.70	1.62	16	2
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
1:A:159:LEU:HD11	1:A:325:LEU:HA	0.69	1.63	1	4
1:A:184:LEU:C	1:A:193:VAL:HG23	0.69	2.06	3	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:137:ASP:CG	1:A:184:LEU:HD22	0.69	2.07	11	8
1:A:138:LEU:HD21	1:A:193:VAL:HG21	0.68	1.65	5	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:108:LEU:HD21	1:A:167:TYR:CD1	0.64	2.28	11	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
1:A:259:LEU:HD22	1:A:261:TRP:CZ3	0.63	2.27	1	2
1:A:252:ILE:CD1	1:A:285:LEU:HD21	0.63	2.23	18	1
1:A:69:VAL:HG13	1:A:133:ARG:HB3	0.63	1.70	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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: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:100:ILE:HG23	1:A:105:LEU:C	0.60	2.17	14	1
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
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:199:GLY:C	1:A:200:LEU:HD22	0.59	2.17	8	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
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: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:199:GLY:C	1:A:200:LEU:HD12	0.57	2.20	6	2
1:A:159:LEU:HD21	1:A:321:ARG:HG2	0.57	1.76	11	1
1:A:184:LEU:N	1:A:184:LEU:HD23	0.57	2.14	11	3
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:184:LEU:O	1:A:193:VAL:HG23	0.55	2.02	3	2
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: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:138:LEU:N	1:A:138:LEU:HD23	0.54	2.17	5	1
1:A:96:ILE:HG22	1:A:100:ILE:CG1	0.54	2.33	5	1
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
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: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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:325:LEU:O	1:A:325:LEU:HD23	0.53	2.04	2	3
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: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: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:138:LEU:HD23	1:A:138:LEU:N	0.51	2.19	9	2
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:224:THR:HG22	1:A:226:GLU:HG2	0.51	1.82	14	1
1:A:86:PHE:CZ	1:A:198:TYR:CE1	0.51	2.99	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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: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:325:LEU:C	1:A:325:LEU:HD23	0.50	2.27	4	3
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:285:LEU:C	1:A:285:LEU:HD12	0.49	2.28	13	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
1:A:285:LEU:HD12	1:A:285:LEU:C	0.49	2.28	1	4
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:325:LEU:HD23	1:A:325:LEU:C	0.49	2.28	1	3
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:184:LEU:HD23	1:A:184:LEU:N	0.49	2.21	6	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:165:LEU:HD22	1:A:243:ASP:CG	0.48	2.29	17	2
1:A:261:TRP:C	1:A:261:TRP:CD1	0.48	2.87	1	2
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:HD12	1:A:130:ILE:N	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:159:LEU:HD13	1:A:159:LEU:O	0.47	2.09	11	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:286:MET:HE1	1:A:300:ALA:N	0.47	2.25	16	2
1:A:296:PRO:CB	1:A:300:ALA:HB2	0.46	2.40	5	1
1:A:24:ALA:C	1:A:25:VAL:HG23	0.46	2.30	6	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:43:ILE:CG1	1:A:51:ILE:HG22	0.46	2.41	4	1
1:A:200:LEU:N	1:A:200:LEU:HD22	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:N	1:A:114:TRP:CD1	0.46	2.85	3	2
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:114:TRP:CD1	1:A:114:TRP:N	0.45	2.84	5	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:LEU:HD12	1:A:309:LEU:CD1	0.45	2.42	4	1
1:A:301:LYS:HB2	1:A:323:ILE:HG23	0.45	1.87	6	1
1:A:174:VAL:HG21	1:A:204:TYR:HB3	0.45	1.88	14	2
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:251:MET:CG	1:A:299:ILE:HD12	0.45	2.41	12	1
1:A:86:PHE:O	1:A:90:ALA:HB3	0.45	2.12	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:302:TYR:HB2	1:A:323:ILE:HG21	0.45	1.88	3	1
1:A:282:ILE:CD1	1:A:303:MET:HB3	0.45	2.41	15	6
1:A:225:ILE:HD13	1:A:225:ILE:C	0.45	2.32	15	2
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: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:O	1:A:62:VAL:HG12	0.44	2.12	18	1
1:A:175:HIS:CE1	1:A:198:TYR:CG	0.44	3.06	2	1
1:A:72:VAL:HG13	1:A:128:PHE:HB3	0.44	1.90	9	3
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:186:ASN:CB	1:A:190:PRO:HB2	0.44	2.42	14	2
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:N	1:A:175:HIS:CD2	0.44	2.85	12	1
1:A:28:ILE:HD13	1:A:38:LYS:HG3	0.44	1.88	12	1
1:A:228:THR:HG23	1:A:228:THR:O	0.44	2.12	14	1
1:A:295:LYS:N	1:A:296:PRO:CD	0.44	2.81	1	1
1:A:55:ASP:HB2	1:A:66:ALA:HB2	0.44	1.88	1	1
1:A:252:ILE:CG2	1:A:259:LEU:HD23	0.44	2.43	5	1
1:A:225:ILE:HG22	1:A:265:LEU:HD11	0.44	1.88	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:305:THR:CG2	1:A:323:ILE:HD11	0.44	2.33	11	1
1:A:271:VAL:HG12	1:A:275:LYS:CD	0.44	2.43	17	2
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:174:VAL:HG13	1:A:204:TYR:HD1	0.43	1.68	2	1
1:A:70:VAL:HG13	1:A:70:VAL:O	0.43	2.12	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:CD1	1:A:290:PHE:N	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: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:278:TYR:CD2	1:A:285:LEU:HB3	0.43	2.48	4	1
1:A:152:LYS:CG	1:A:331:ILE:HD12	0.43	2.43	4	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
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:N	1:A:126:TYR:CD1	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	1
1:A:176:GLY:C	1:A:246:ILE:HD13	0.42	2.34	6	1
1:A:228:THR:O	1:A:228:THR:HG23	0.42	2.14	9	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:LEU:CD1	1:A:328:LEU:HD23	0.42	2.44	18	1
1:A:130:ILE:CD1	1:A:130:ILE:N	0.42	2.83	1	1
1:A:252:ILE:HD11	1:A:303:MET:SD	0.42	2.54	2	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:O	1:A:225:ILE:HG12	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:CD2	1:A:200:LEU:N	0.42	2.83	8	1
1:A:227:PHE:CG	1:A:227:PHE:O	0.42	2.73	4	1
1:A:267:ASP:HB3	1:A:270:TYR:CE2	0.42	2.50	6	7
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: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
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:O	1:A:200:LEU:HD23	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:174:VAL:HG23	1:A:202:TYR:HB3	0.41	1.90	1	1
1:A:37:TRP:N	1:A:37:TRP:CD1	0.41	2.88	1	1
1:A:244:LEU:CD1	1:A:320:LEU:HD11	0.41	2.40	15	1
1:A:51:ILE:HD12	1:A:71:LYS:CG	0.41	2.45	15	1
1:A:90:ALA:CB	1:A:171:HIS:CE1	0.41	3.02	3	1
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: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:70:VAL:O	1:A:70:VAL:HG13	0.41	2.16	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	2
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: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: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:55:ASP:CG	1:A:62:VAL:HG13	0.41	2.35	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
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:282:ILE:HD13	1:A:303:MET:C	0.41	2.36	11	3
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:138:LEU:CD2	1:A:138:LEU:N	0.41	2.84	9	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:328:LEU:HD13	1:A:335:ASP:HB3	0.41	1.93	13	1
1:A:204:TYR:CE2	1:A:239:SER:OG	0.41	2.74	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:202:TYR:CE1	1:A:203:ARG:O	0.41	2.74	6	1
1:A:86:PHE:O	1:A:90:ALA:N	0.41	2.52	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:194:TYR:CD1	1:A:194:TYR:N	0.40	2.89	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ARG:O	1:A:171:HIS:CE1	0.40	2.74	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: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:174:VAL:HG22	1:A:204:TYR:HD1	0.40	1.76	13	1
1:A:83:GLU:O	1:A:87:TYR:CD1	0.40	2.74	13	2
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: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
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%)	3	23
All	All	5130/7254 (71%)	4259 (83%)	600 (12%)	271 (5%)	3	23

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	261	TRP	18
1	A	146	ALA	18

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Mol	Chain	Res	Type	Models (Total)
1	A	197	ASP	14
1	A	257	GLY	13
1	A	191	ASP	12
1	A	309	LEU	11
1	A	258	HIS	11
1	A	34	LYS	9
1	A	225	ILE	8
1	A	201	ALA	8
1	A	57	ASN	6
1	A	334	LYS	6
1	A	336	ASP	6
1	A	107	TYR	6
1	A	238	PRO	6
1	A	297	GLY	5
1	A	43	ILE	5
1	A	178	ILE	5
1	A	76	ASP	5
1	A	63	GLY	5
1	A	74	PRO	5
1	A	240	ARG	4
1	A	25	VAL	4
1	A	203	ARG	4
1	A	44	GLY	4
1	A	296	PRO	4
1	A	190	PRO	4
1	A	75	SER	4
1	A	61	SER	3
1	A	294	ASN	3
1	A	224	THR	3
1	A	175	HIS	3
1	A	291	PRO	3
1	A	108	LEU	2
1	A	333	SER	2
1	A	90	ALA	2
1	A	59	SER	2
1	A	64	SER	2
1	A	189	ASN	2
1	A	237	ALA	2
1	A	50	CYS	2
1	A	58	SER	2
1	A	106	LYS	2
1	A	77	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	227	PHE	2
1	A	149	PHE	2
1	A	134	PHE	1
1	A	42	PRO	1
1	A	66	ALA	1
1	A	60	GLU	1
1	A	204	TYR	1
1	A	172	GLU	1
1	A	122	ASN	1
1	A	293	LYS	1
1	A	176	GLY	1
1	A	62	VAL	1
1	A	35	LYS	1
1	A	315	PRO	1
1	A	40	GLY	1
1	A	198	TYR	1
1	A	78	GLY	1
1	A	239	SER	1
1	A	105	LEU	1
1	A	24	ALA	1
1	A	295	LYS	1
1	A	200	LEU	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%)	192±6 (77±2%)	58±6 (23±2%)	3	28
All	All	4500/6282 (72%)	3459 (77%)	1041 (23%)	3	28

All 169 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	259	LEU	18
1	A	251	MET	15
1	A	184	LEU	14

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Mol	Chain	Res	Type	Models (Total)
1	A	309	LEU	13
1	A	284	SER	12
1	A	133	ARG	12
1	A	322	ASP	12
1	A	325	LEU	12
1	A	188	LYS	12
1	A	112	LYS	12
1	A	32	MET	12
1	A	293	LYS	11
1	A	89	ARG	11
1	A	121	LYS	11
1	A	179	LYS	11
1	A	295	LYS	11
1	A	98	LYS	11
1	A	334	LYS	11
1	A	275	LYS	11
1	A	160	ARG	11
1	A	307	LYS	11
1	A	163	ASP	11
1	A	149	PHE	11
1	A	31	ASP	11
1	A	103	ARG	11
1	A	106	LYS	10
1	A	151	ARG	10
1	A	263	ASP	10
1	A	229	SER	9
1	A	262	GLU	9
1	A	139	GLN	9
1	A	279	ARG	9
1	A	267	ASP	9
1	A	171	HIS	9
1	A	170	GLU	9
1	A	35	LYS	9
1	A	166	GLU	8
1	A	191	ASP	8
1	A	287	ASP	8
1	A	273	ASP	8
1	A	288	LYS	8
1	A	186	ASN	8
1	A	64	SER	8
1	A	192	GLN	8
1	A	140	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	99	TRP	8
1	A	277	ARG	8
1	A	138	LEU	8
1	A	147	LYS	8
1	A	298	GLU	8
1	A	181	SER	7
1	A	169	HIS	7
1	A	266	LYS	7
1	A	131	MET	7
1	A	241	ARG	7
1	A	97	GLN	7
1	A	122	ASN	7
1	A	95	GLN	7
1	A	124	LYS	7
1	A	104	LYS	7
1	A	301	LYS	7
1	A	101	ARG	7
1	A	85	LYS	7
1	A	177	ASP	7
1	A	73	GLU	7
1	A	120	ASP	7
1	A	71	LYS	7
1	A	132	ASP	7
1	A	61	SER	6
1	A	65	ASP	6
1	A	318	GLU	6
1	A	88	GLN	6
1	A	189	ASN	6
1	A	59	SER	6
1	A	280	GLU	6
1	A	253	GLN	6
1	A	75	SER	6
1	A	264	ASN	6
1	A	156	GLN	6
1	A	329	LYS	6
1	A	239	SER	6
1	A	226	GLU	6
1	A	321	ARG	6
1	A	92	LYS	6
1	A	224	THR	6
1	A	143	GLU	6
1	A	243	ASP	6

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Mol	Chain	Res	Type	Models (Total)
1	A	231	ASP	6
1	A	200	LEU	6
1	A	127	ARG	6
1	A	56	MET	6
1	A	34	LYS	6
1	A	305	THR	6
1	A	41	LEU	6
1	A	38	LYS	5
1	A	319	ASN	5
1	A	240	ARG	5
1	A	173	TYR	5
1	A	333	SER	5
1	A	292	GLU	5
1	A	81	PHE	5
1	A	233	HIS	5
1	A	153	THR	5
1	A	308	LEU	5
1	A	326	GLN	5
1	A	76	ASP	5
1	A	125	SER	5
1	A	272	ARG	5
1	A	172	GLU	5
1	A	269	LYS	5
1	A	116	SER	5
1	A	150	SER	5
1	A	286	MET	5
1	A	145	ASN	5
1	A	316	LEU	5
1	A	335	ASP	5
1	A	336	ASP	5
1	A	57	ASN	4
1	A	152	LYS	4
1	A	304	GLU	4
1	A	60	GLU	4
1	A	256	THR	4
1	A	281	ASN	4
1	A	119	HIS	4
1	A	203	ARG	4
1	A	148	ARG	4
1	A	58	SER	4
1	A	197	ASP	4
1	A	36	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	228	THR	4
1	A	68	CYS	4
1	A	175	HIS	4
1	A	245	GLU	4
1	A	30	THR	3
1	A	27	GLU	3
1	A	202	TYR	3
1	A	118	LEU	3
1	A	94	GLU	3
1	A	250	CYS	3
1	A	50	CYS	3
1	A	234	ASN	3
1	A	129	MET	2
1	A	285	LEU	2
1	A	204	TYR	2
1	A	225	ILE	2
1	A	55	ASP	2
1	A	83	GLU	2
1	A	158	SER	2
1	A	274	SER	2
1	A	107	TYR	2
1	A	82	THR	2
1	A	137	ASP	2
1	A	294	ASN	2
1	A	136	SER	2
1	A	261	TRP	2
1	A	77	ASN	2
1	A	227	PHE	2
1	A	80	LEU	1
1	A	270	TYR	1
1	A	25	VAL	1
1	A	183	LEU	1
1	A	87	TYR	1
1	A	265	LEU	1
1	A	84	LEU	1
1	A	142	TYR	1
1	A	303	MET	1
1	A	258	HIS	1
1	A	289	CYS	1
1	A	102	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 50% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	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 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	325	1.09 ± 0.10	Should be applied
$^{13}\text{C}'$	363	-0.01 ± 0.07	None needed (< 0.5 ppm)
^{15}N	343	-0.14 ± 0.16	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 50%, i.e. 1827 atoms were assigned a chemical shift out of a possible 3660. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1092/1399 (78%)	266/557 (48%)	560/570 (98%)	266/272 (98%)
Sidechain	609/1946 (31%)	187/1147 (16%)	422/707 (60%)	0/92 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	126/315 (40%)	63/161 (39%)	58/137 (42%)	5/17 (29%)
Overall	1827/3660 (50%)	516/1865 (28%)	1040/1414 (74%)	271/381 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 2275 atoms were assigned a chemical shift out of a possible 5133. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1412/1981 (71%)	343/789 (43%)	726/806 (90%)	343/386 (89%)
Sidechain	723/2767 (26%)	208/1635 (13%)	515/988 (52%)	0/144 (0%)
Aromatic	140/385 (36%)	70/197 (36%)	64/164 (39%)	6/24 (25%)
Overall	2275/5133 (44%)	621/2621 (24%)	1305/1958 (67%)	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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	29	ILE	HG23	-0.64	2.13 – -0.57	-5.3
1	A	29	ILE	HG21	-0.64	2.13 – -0.57	-5.3
1	A	29	ILE	HG22	-0.64	2.13 – -0.57	-5.3
1	A	29	ILE	HD11	-0.81	2.13 – -0.77	-5.1
1	A	29	ILE	HD12	-0.81	2.13 – -0.77	-5.1
1	A	29	ILE	HD13	-0.81	2.13 – -0.77	-5.1

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.

Random coil index (RCI) for chain A:

