



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:57 pm BST

PDB ID : 2KUL
Title : Solution structure of human vaccinia related kinase 1(VRK1)
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Deposited on : 2010-02-19

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

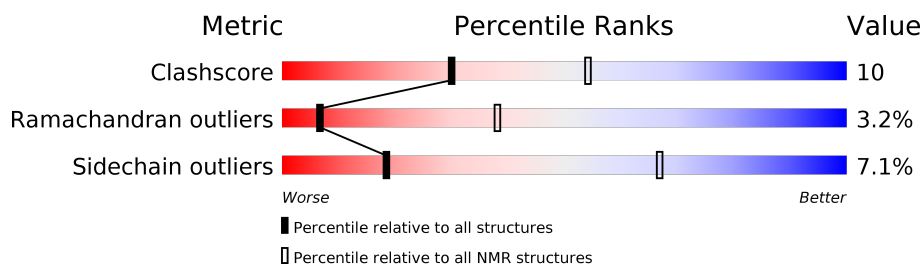
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 72%.

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	368	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:25-A:59, A:66-A:217, A:222-A:338, A:352-A:356 (309)	0.98	1

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5844 atoms, of which 2943 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	360	Total	C	H	N	O	S	0
			5844	1848	2943	508	531	14	

There are 8 discrepancies between the modelled and reference sequences:

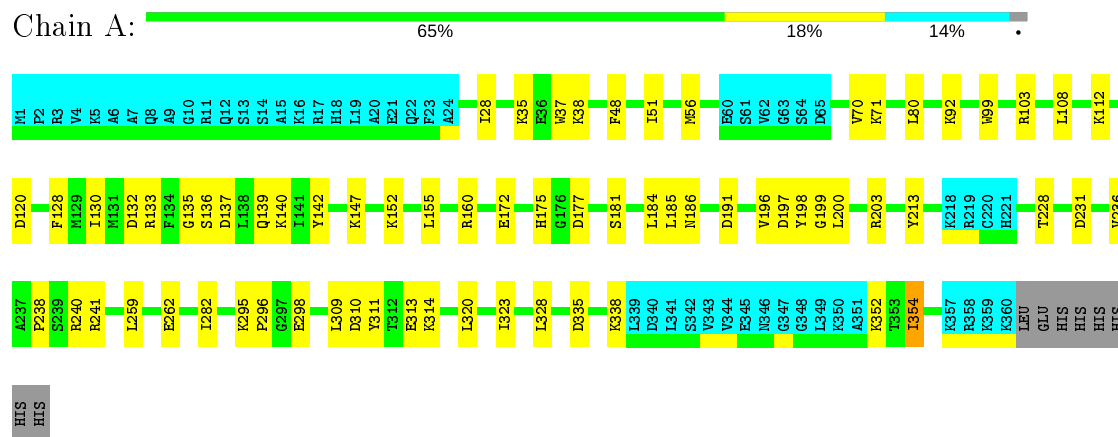
Chain	Residue	Modelled	Actual	Comment	Reference
A	361	LEU	-	expression tag	UNP Q99986
A	362	GLU	-	expression tag	UNP Q99986
A	363	HIS	-	expression tag	UNP Q99986
A	364	HIS	-	expression tag	UNP Q99986
A	365	HIS	-	expression tag	UNP Q99986
A	366	HIS	-	expression tag	UNP Q99986
A	367	HIS	-	expression tag	UNP Q99986
A	368	HIS	-	expression tag	UNP Q99986

4 Residue-property plots

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

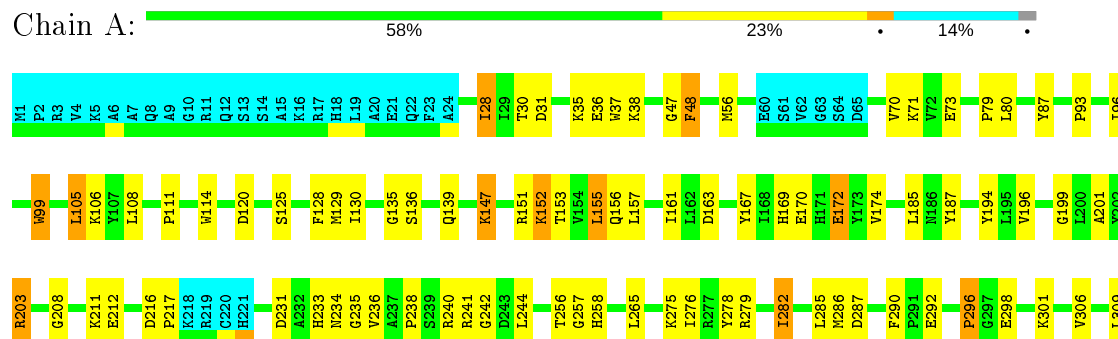


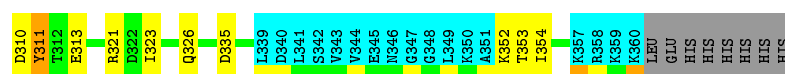
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

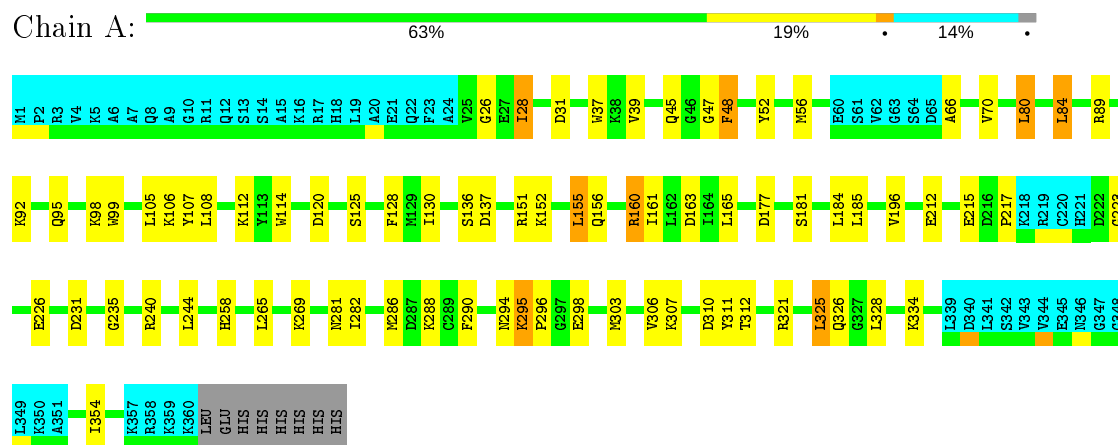
- Molecule 1: Serine/threonine-protein kinase VRK1





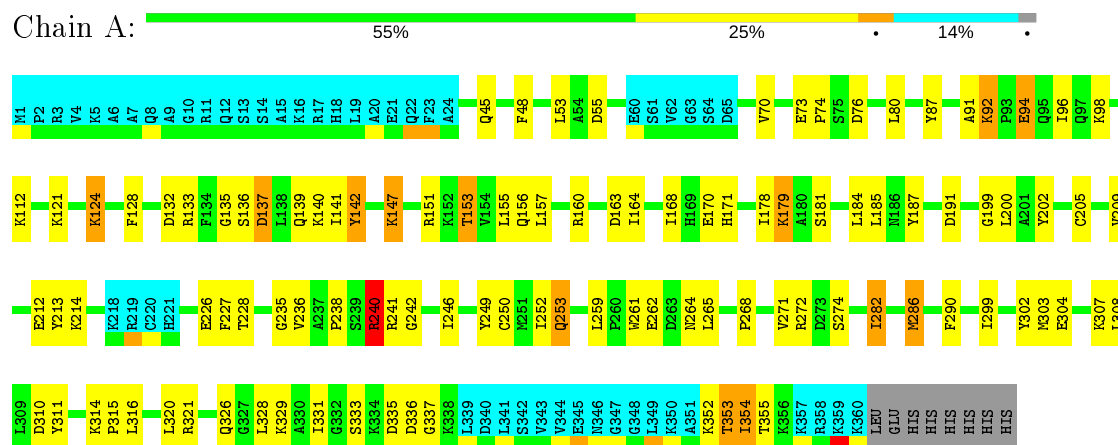
4.2.2 Score per residue for model 2

- Molecule 1: Serine/threonine-protein kinase VRK1



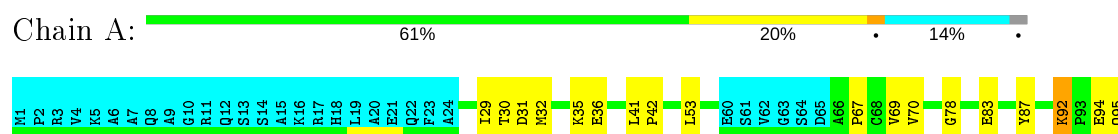
4.2.3 Score per residue for model 3

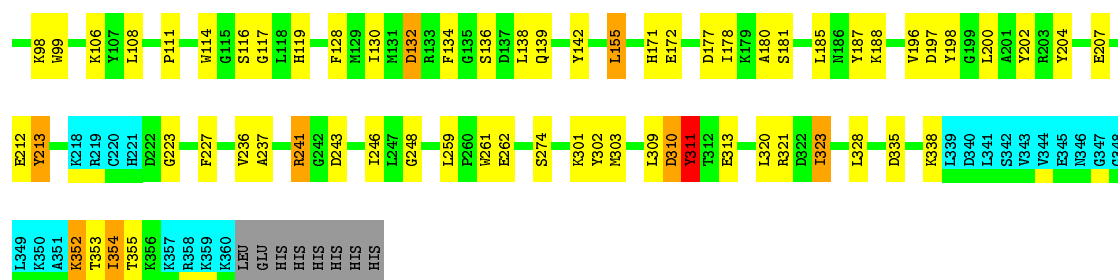
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.4 Score per residue for model 4

- Molecule 1: Serine/threonine-protein kinase VRK1

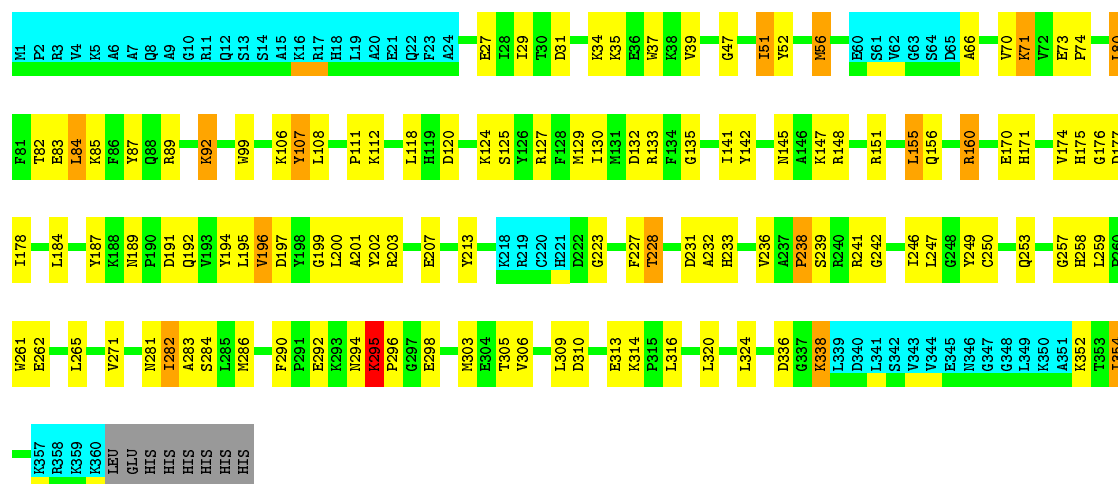




4.2.5 Score per residue for model 5

- Molecule 1: Serine/threonine-protein kinase VRK1

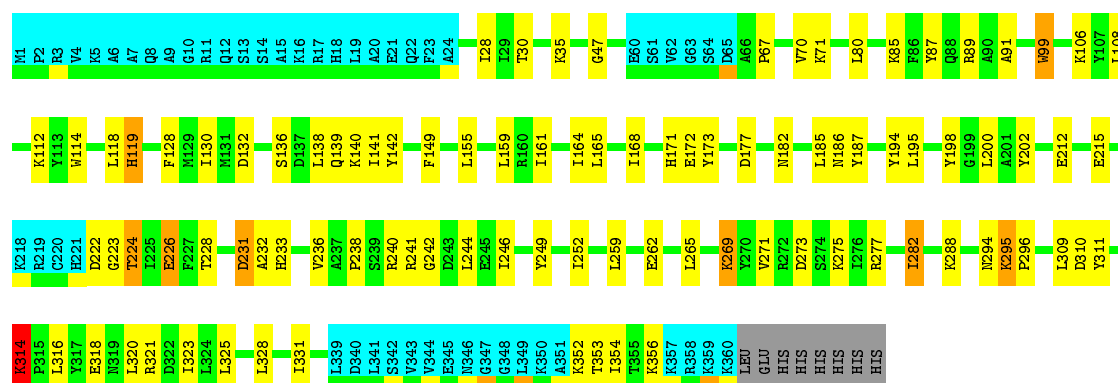
Chain A: 51% 28% 14%



4.2.6 Score per residue for model 6

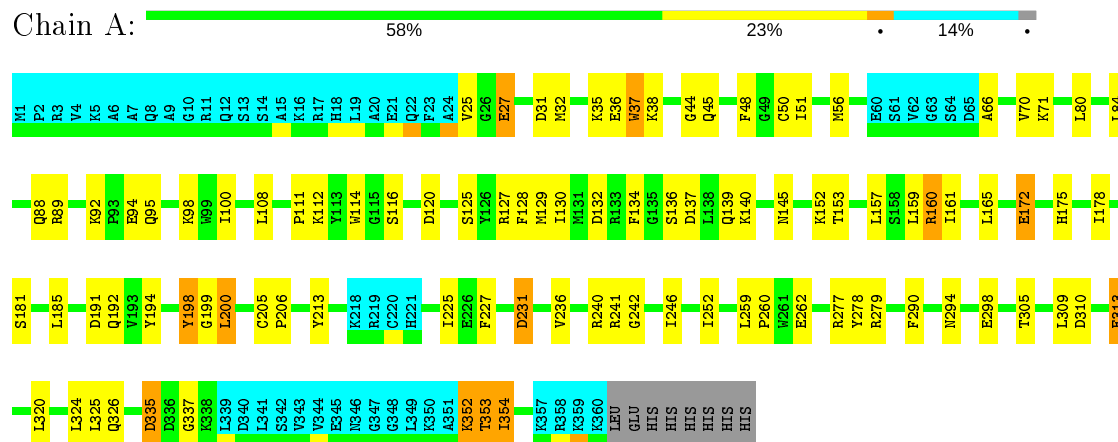
- Molecule 1: Serine/threonine-protein kinase VRK1

Chain A: 58% 24% 14%



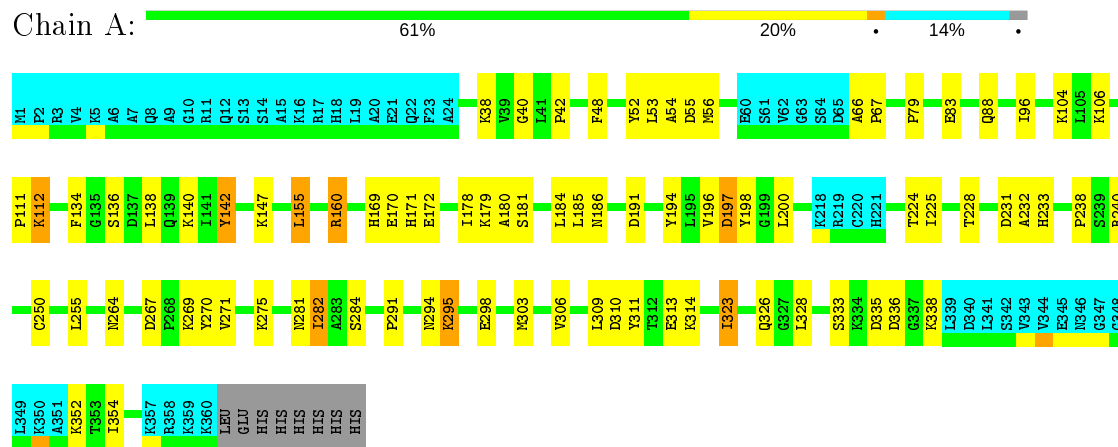
4.2.7 Score per residue for model 7

- Molecule 1: Serine/threonine-protein kinase VRK1



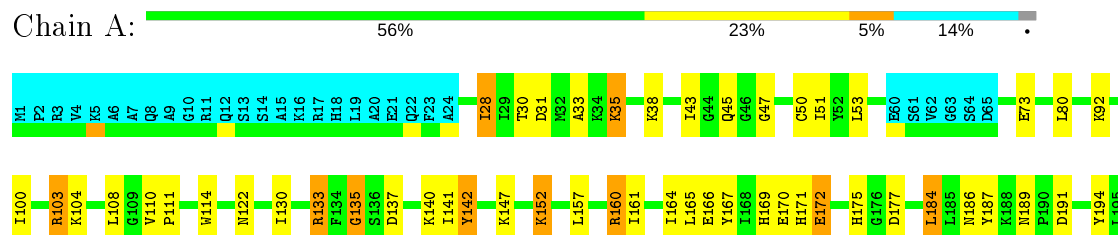
4.2.8 Score per residue for model 8

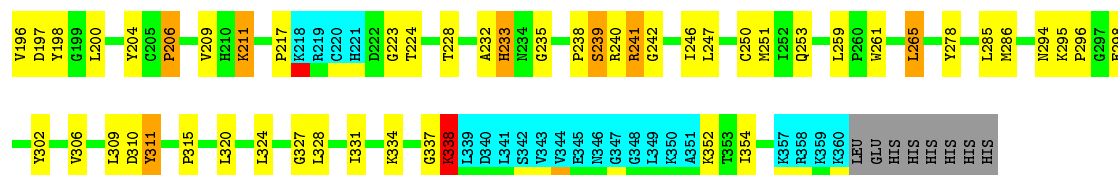
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.9 Score per residue for model 9

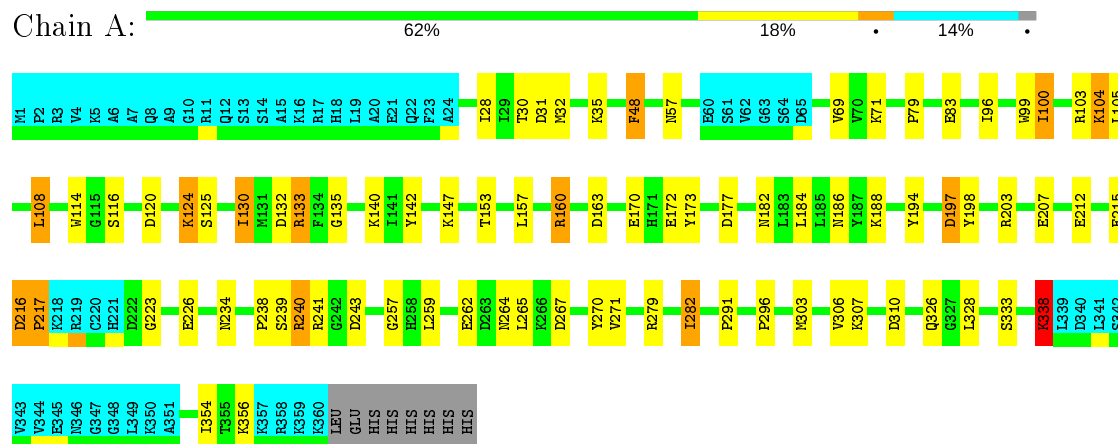
- Molecule 1: Serine/threonine-protein kinase VRK1





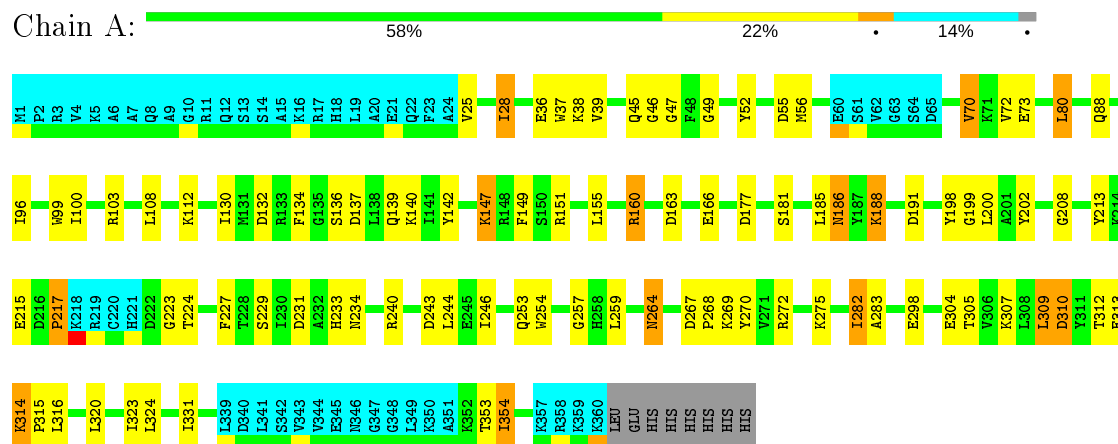
4.2.10 Score per residue for model 10

- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.11 Score per residue for model 11

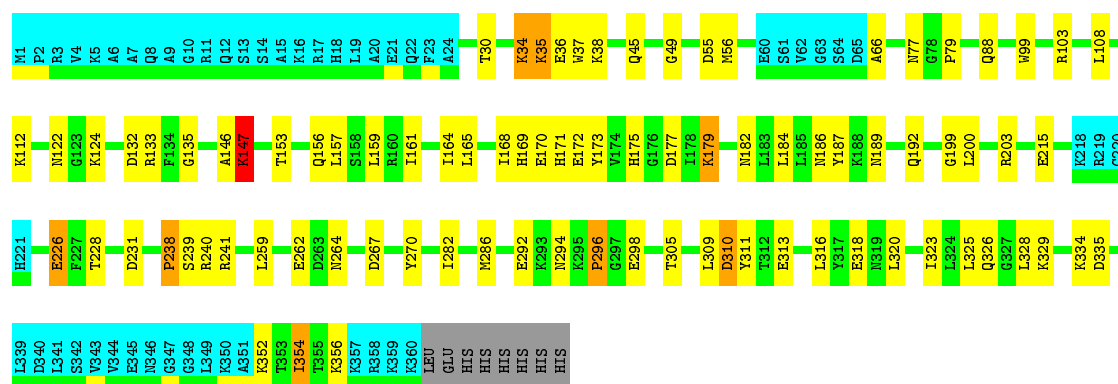
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.12 Score per residue for model 12

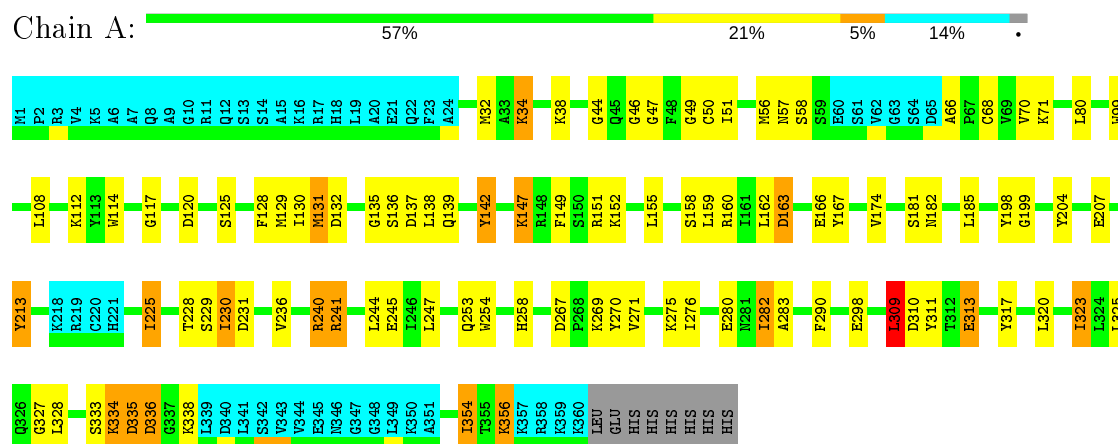
- Molecule 1: Serine/threonine-protein kinase VRK1





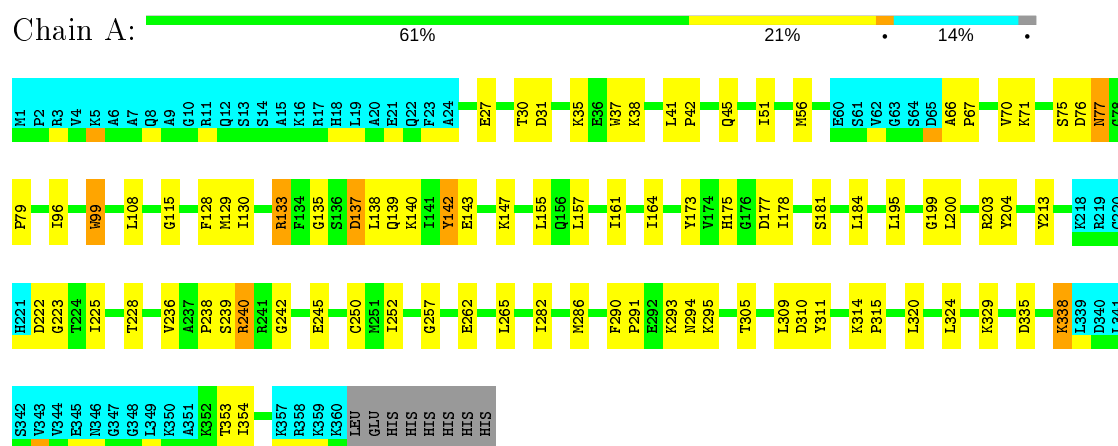
4.2.13 Score per residue for model 13

- Molecule 1: Serine/threonine-protein kinase VRK1



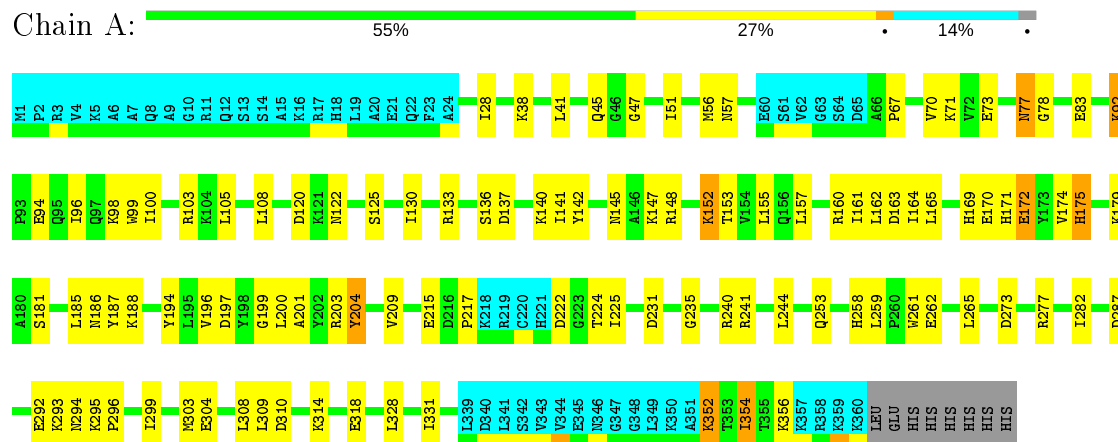
4.2.14 Score per residue for model 14

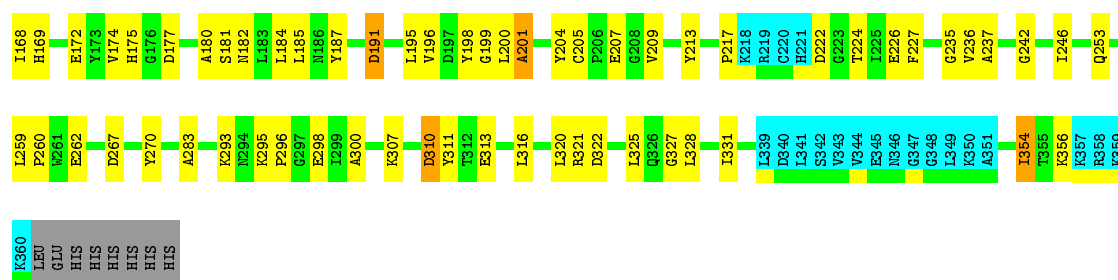
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.15 Score per residue for model 15

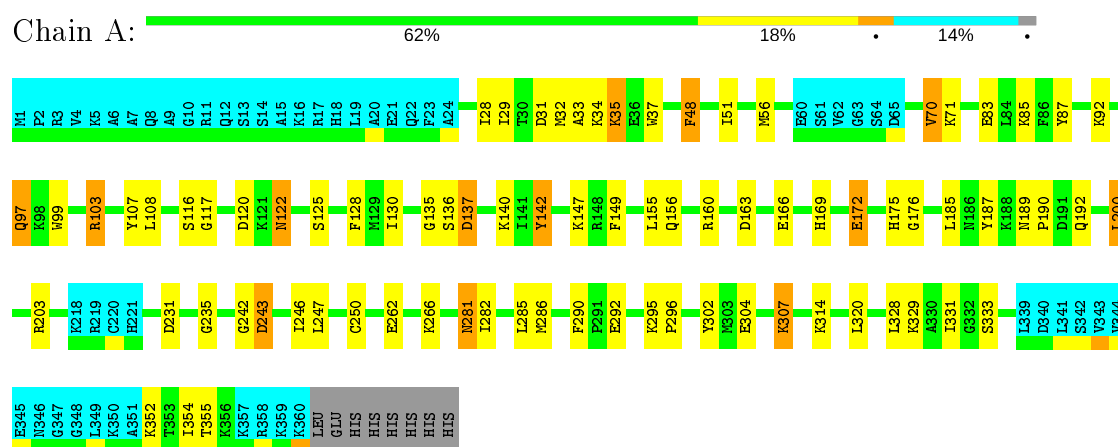
- Molecule 1: Serine/threonine-protein kinase VRK1





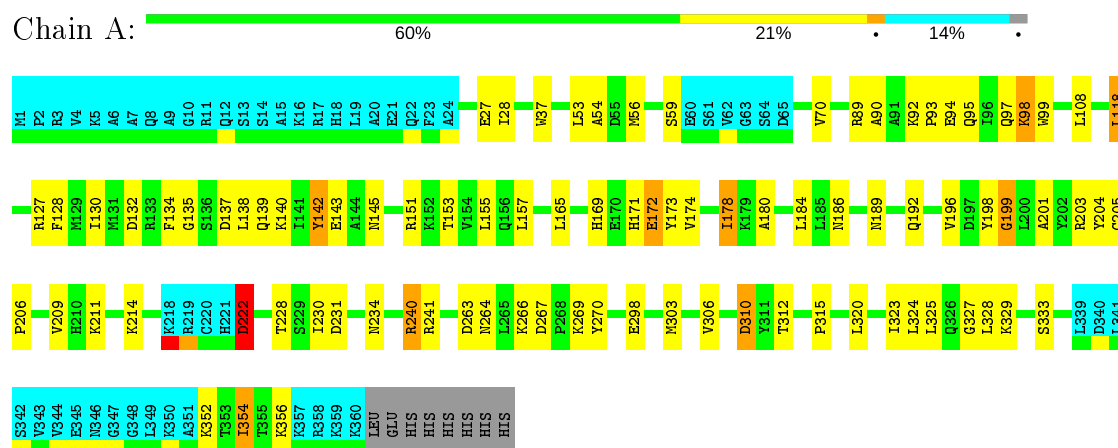
4.2.18 Score per residue for model 18

- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.19 Score per residue for model 19

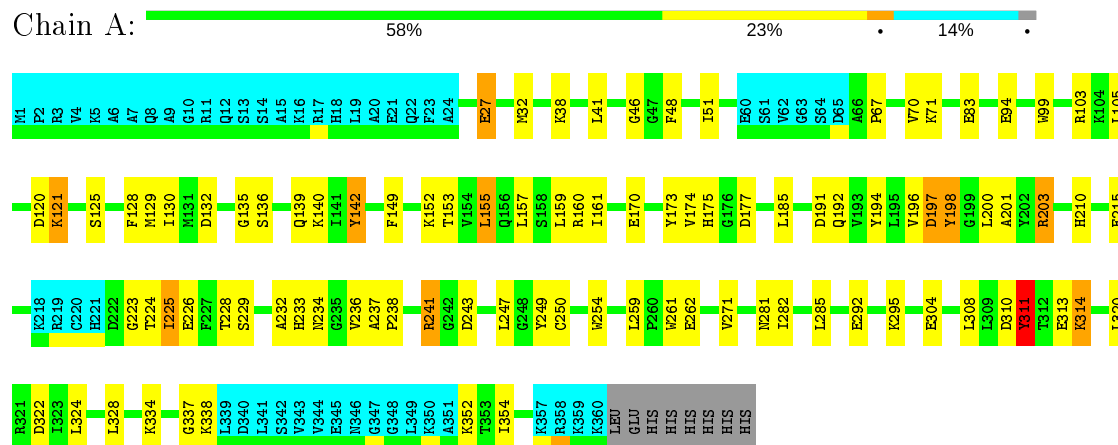
- Molecule 1: Serine/threonine-protein kinase VRK1



4.2.20 Score per residue for model 20

- Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS, simulated annealing, TORSION ANGLE DYNAMICS*.

Of the 200 calculated structures, 20 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	refinement	1.1

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	3545
Number of shifts mapped to atoms	3545
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	72%

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	2512	2531	2524	51±7
All	All	50240	50620	50480	1011

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ASP:HB2	1:A:223:GLY:HA3	0.92	1.38	10	5
1:A:175:HIS:HB2	1:A:201:ALA:HA	0.88	1.41	15	1
1:A:136:SER:HB2	1:A:185:LEU:HB2	0.87	1.46	6	14
1:A:215:GLU:HB2	1:A:236:VAL:HA	0.87	1.46	20	1
1:A:112:LYS:HB3	1:A:132:ASP:HB2	0.84	1.47	12	8
1:A:104:LYS:HE3	1:A:104:LYS:HA	0.83	1.49	10	1
1:A:177:ASP:HB2	1:A:223:GLY:HA2	0.82	1.51	14	3
1:A:241:ARG:HG3	1:A:311:TYR:HA	0.81	1.53	1	4
1:A:205:CYS:HB2	1:A:209:VAL:HA	0.81	1.50	17	2
1:A:73:GLU:HG2	1:A:80:LEU:HB2	0.81	1.50	1	1
1:A:37:TRP:HB3	1:A:56:MET:HG2	0.80	1.51	14	1
1:A:139:GLN:HB3	1:A:181:SER:HA	0.79	1.55	13	4
1:A:310:ASP:HB3	1:A:313:GLU:HB2	0.79	1.53	13	2
1:A:124:LYS:HA	1:A:124:LYS:HE3	0.78	1.53	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:ARG:HD2	1:A:188:LYS:HB2	0.78	1.55	15	1
1:A:35:LYS:HG3	1:A:36:GLU:HG3	0.78	1.56	17	2
1:A:176:GLY:HA2	1:A:243:ASP:HB3	0.78	1.55	18	1
1:A:309:LEU:HG	1:A:310:ASP:H	0.77	1.36	4	1
1:A:227:PHE:HB3	1:A:246:ILE:HG23	0.77	1.57	4	3
1:A:328:LEU:HD11	1:A:334:LYS:HA	0.75	1.59	12	1
1:A:253:GLN:HE21	1:A:259:LEU:HG	0.75	1.40	17	1
1:A:120:ASP:HA	1:A:125:SER:HA	0.74	1.58	13	10
1:A:137:ASP:HB3	1:A:139:GLN:HG2	0.73	1.60	7	1
1:A:259:LEU:HB2	1:A:262:GLU:HB2	0.72	1.59	10	5
1:A:213:TYR:HB2	1:A:236:VAL:HG21	0.72	1.60	17	1
1:A:290:PHE:HB3	1:A:296:PRO:HB3	0.72	1.60	2	1
1:A:200:LEU:HD11	1:A:352:LYS:HD2	0.72	1.60	9	1
1:A:200:LEU:HA	1:A:354:ILE:HB	0.71	1.62	3	2
1:A:298:GLU:HG3	1:A:327:GLY:HA3	0.71	1.61	9	4
1:A:278:TYR:HA	1:A:285:LEU:HG	0.71	1.60	9	2
1:A:241:ARG:HD3	1:A:311:TYR:HD1	0.71	1.46	3	1
1:A:37:TRP:HA	1:A:56:MET:SD	0.71	2.24	7	3
1:A:79:PRO:HB3	1:A:199:GLY:HA2	0.71	1.60	14	1
1:A:31:ASP:HB3	1:A:37:TRP:CZ2	0.71	2.21	7	2
1:A:213:TYR:HA	1:A:236:VAL:HG21	0.70	1.63	4	2
1:A:87:TYR:HE1	1:A:111:PRO:HG2	0.70	1.45	1	1
1:A:138:LEU:HA	1:A:141:ILE:HB	0.70	1.62	6	1
1:A:45:GLN:H	1:A:49:GLY:HA2	0.70	1.47	11	2
1:A:121:LYS:HE2	1:A:121:LYS:HA	0.69	1.64	20	1
1:A:28:ILE:HB	1:A:36:GLU:HG2	0.69	1.62	1	1
1:A:139:GLN:HB2	1:A:181:SER:HA	0.69	1.62	4	1
1:A:179:LYS:HE3	1:A:224:THR:HG21	0.69	1.64	15	1
1:A:248:GLY:HA3	1:A:303:MET:SD	0.69	2.28	4	1
1:A:104:LYS:HE2	1:A:104:LYS:HA	0.69	1.63	8	1
1:A:259:LEU:HB2	1:A:262:GLU:HG3	0.68	1.64	16	1
1:A:200:LEU:HD11	1:A:352:LYS:HA	0.68	1.65	3	1
1:A:156:GLN:HE21	1:A:335:ASP:HB2	0.68	1.48	12	1
1:A:240:ARG:HG2	1:A:315:PRO:HB3	0.68	1.65	11	1
1:A:142:TYR:HD1	1:A:147:LYS:HB3	0.67	1.48	8	2
1:A:38:LYS:HG2	1:A:56:MET:HA	0.67	1.66	16	2
1:A:42:PRO:HA	1:A:52:TYR:HD1	0.67	1.48	8	2
1:A:186:ASN:HB3	1:A:189:ASN:HB3	0.67	1.65	12	2
1:A:152:LYS:HG2	1:A:335:ASP:HA	0.67	1.67	7	1
1:A:217:PRO:HA	1:A:235:GLY:HA3	0.67	1.67	17	1
1:A:215:GLU:HA	1:A:234:ASN:HB3	0.67	1.67	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:GLN:HA	1:A:142:TYR:HD2	0.66	1.49	14	1
1:A:264:ASN:HB3	1:A:270:TYR:HB3	0.65	1.67	19	5
1:A:38:LYS:HG2	1:A:57:ASN:HB2	0.65	1.67	15	1
1:A:70:VAL:HB	1:A:130:ILE:HD13	0.65	1.69	1	9
1:A:160:ARG:HA	1:A:160:ARG:HE	0.65	1.51	10	1
1:A:301:LYS:HA	1:A:301:LYS:HE2	0.65	1.68	1	1
1:A:309:LEU:O	1:A:313:GLU:HB2	0.65	1.92	5	2
1:A:51:ILE:HD12	1:A:71:LYS:HA	0.65	1.68	13	3
1:A:173:TYR:HA	1:A:203:ARG:HA	0.64	1.68	10	1
1:A:47:GLY:HA3	1:A:51:ILE:HD11	0.64	1.67	13	1
1:A:47:GLY:HA3	1:A:196:VAL:HG11	0.64	1.68	1	1
1:A:142:TYR:CE1	1:A:147:LYS:HD3	0.64	2.28	16	1
1:A:137:ASP:HB3	1:A:184:LEU:HD13	0.64	1.69	19	1
1:A:137:ASP:HB3	1:A:139:GLN:HG3	0.64	1.69	11	2
1:A:124:LYS:HE2	1:A:124:LYS:HA	0.64	1.70	3	1
1:A:165:LEU:O	1:A:169:HIS:HB3	0.63	1.94	12	1
1:A:51:ILE:HG23	1:A:71:LYS:HB3	0.63	1.69	15	1
1:A:37:TRP:HA	1:A:56:MET:HA	0.63	1.70	11	2
1:A:67:PRO:HA	1:A:133:ARG:HG2	0.63	1.68	16	1
1:A:201:ALA:H	1:A:354:ILE:HG22	0.62	1.54	5	1
1:A:142:TYR:HB2	1:A:147:LYS:HA	0.62	1.69	15	1
1:A:41:LEU:HB3	1:A:53:LEU:HD12	0.62	1.70	4	1
1:A:35:LYS:HE2	1:A:35:LYS:HA	0.62	1.71	6	1
1:A:73:GLU:HB3	1:A:74:PRO:HD2	0.62	1.71	5	2
1:A:138:LEU:HB3	1:A:180:ALA:O	0.62	1.95	4	2
1:A:267:ASP:HB2	1:A:270:TYR:CD1	0.62	2.30	11	1
1:A:177:ASP:HB3	1:A:200:LEU:HB2	0.62	1.72	12	1
1:A:186:ASN:HB2	1:A:194:TYR:HE1	0.61	1.55	15	4
1:A:287:ASP:HA	1:A:296:PRO:HB2	0.61	1.72	15	1
1:A:240:ARG:HD3	1:A:315:PRO:HG3	0.61	1.69	14	1
1:A:169:HIS:CE1	1:A:174:VAL:HG12	0.61	2.30	1	1
1:A:178:ILE:HB	1:A:250:CYS:SG	0.61	2.35	8	1
1:A:35:LYS:H	1:A:37:TRP:HZ3	0.61	1.37	18	1
1:A:73:GLU:OE1	1:A:77:ASN:HA	0.61	1.96	15	1
1:A:110:VAL:HG22	1:A:111:PRO:HD2	0.61	1.72	9	1
1:A:200:LEU:HD21	1:A:352:LYS:HB3	0.60	1.72	6	1
1:A:83:GLU:HG3	1:A:198:TYR:HB2	0.60	1.73	4	2
1:A:271:VAL:O	1:A:275:LYS:HG2	0.60	1.96	6	2
1:A:31:ASP:HB3	1:A:37:TRP:HZ2	0.60	1.56	7	1
1:A:172:GLU:HB3	1:A:203:ARG:HB2	0.60	1.72	10	1
1:A:140:LYS:HE3	1:A:140:LYS:HA	0.60	1.71	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:LYS:HE2	1:A:106:LYS:HA	0.60	1.71	6	1
1:A:229:SER:HA	1:A:275:LYS:HE2	0.60	1.73	11	1
1:A:179:LYS:HZ2	1:A:179:LYS:HB3	0.60	1.54	12	1
1:A:200:LEU:HD21	1:A:352:LYS:HE3	0.60	1.73	8	1
1:A:155:LEU:HD22	1:A:328:LEU:HG	0.60	1.72	15	1
1:A:92:LYS:HB3	1:A:94:GLU:HG2	0.60	1.72	15	1
1:A:160:ARG:HE	1:A:160:ARG:HA	0.60	1.57	13	2
1:A:242:GLY:O	1:A:246:ILE:HG13	0.60	1.97	7	8
1:A:159:LEU:HG	1:A:321:ARG:HD2	0.59	1.73	6	1
1:A:48:PHE:HZ	1:A:199:GLY:HA3	0.59	1.55	3	1
1:A:267:ASP:OD1	1:A:269:LYS:HG2	0.59	1.97	13	3
1:A:33:ALA:HB3	1:A:35:LYS:HE2	0.59	1.74	9	1
1:A:226:GLU:HG3	1:A:265:LEU:HG	0.59	1.72	3	1
1:A:85:LYS:HA	1:A:85:LYS:HE2	0.59	1.72	18	2
1:A:198:TYR:HB2	1:A:201:ALA:HB2	0.59	1.75	17	1
1:A:329:LYS:HA	1:A:333:SER:O	0.59	1.97	3	2
1:A:165:LEU:O	1:A:169:HIS:HB2	0.59	1.97	19	2
1:A:204:TYR:HB2	1:A:209:VAL:HG12	0.59	1.74	15	1
1:A:71:LYS:HE3	1:A:129:MET:HB3	0.58	1.75	5	1
1:A:155:LEU:HB3	1:A:328:LEU:HD22	0.58	1.75	16	1
1:A:45:GLN:HB2	1:A:51:ILE:HG12	0.58	1.76	7	2
1:A:138:LEU:O	1:A:142:TYR:HB3	0.58	1.98	13	3
1:A:156:GLN:O	1:A:160:ARG:HG2	0.58	1.99	18	4
1:A:240:ARG:HD2	1:A:315:PRO:HG3	0.58	1.75	3	1
1:A:320:LEU:O	1:A:323:ILE:HG13	0.58	1.99	6	1
1:A:211:LYS:HE2	1:A:211:LYS:HA	0.58	1.75	9	1
1:A:43:ILE:HG22	1:A:45:GLN:HG2	0.58	1.74	17	1
1:A:142:TYR:HA	1:A:149:PHE:CZ	0.58	2.34	6	2
1:A:85:LYS:HA	1:A:85:LYS:HE3	0.58	1.76	16	1
1:A:309:LEU:HG	1:A:310:ASP:N	0.57	2.13	4	1
1:A:160:ARG:NH1	1:A:160:ARG:HA	0.57	2.13	5	1
1:A:265:LEU:HA	1:A:271:VAL:CG1	0.57	2.29	5	1
1:A:133:ARG:HG3	1:A:187:TYR:HB3	0.57	1.75	15	1
1:A:335:ASP:HB3	1:A:338:LYS:HB2	0.57	1.75	4	1
1:A:142:TYR:CE1	1:A:147:LYS:HB3	0.57	2.34	17	3
1:A:295:LYS:HD3	1:A:331:ILE:HD12	0.57	1.76	18	1
1:A:338:LYS:HB3	1:A:338:LYS:NZ	0.57	2.15	10	1
1:A:48:PHE:HB2	1:A:71:LYS:HE3	0.57	1.75	18	1
1:A:140:LYS:HE2	1:A:140:LYS:HA	0.57	1.75	20	1
1:A:155:LEU:HG	1:A:328:LEU:HB2	0.57	1.76	20	3
1:A:175:HIS:CE1	1:A:200:LEU:HB2	0.57	2.35	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:334:LYS:HD2	1:A:336:ASP:HB2	0.57	1.75	13	1
1:A:172:GLU:HB2	1:A:206:PRO:HA	0.57	1.76	19	1
1:A:153:THR:O	1:A:157:LEU:HG	0.57	1.99	12	4
1:A:48:PHE:CE2	1:A:198:TYR:HA	0.57	2.33	7	1
1:A:191:ASP:CB	1:A:338:LYS:HB3	0.57	2.30	8	1
1:A:111:PRO:HD3	1:A:194:TYR:HB3	0.57	1.75	1	1
1:A:92:LYS:HB3	1:A:95:GLN:HE21	0.57	1.59	4	1
1:A:169:HIS:CD2	1:A:170:GLU:HG3	0.57	2.35	12	1
1:A:328:LEU:HG	1:A:333:SER:O	0.57	2.00	13	3
1:A:191:ASP:HB3	1:A:338:LYS:HB2	0.56	1.77	9	1
1:A:200:LEU:HA	1:A:354:ILE:HG23	0.56	1.77	9	2
1:A:295:LYS:HA	1:A:295:LYS:HE3	0.56	1.76	5	3
1:A:139:GLN:HA	1:A:142:TYR:HD1	0.56	1.60	19	1
1:A:304:GLU:O	1:A:308:LEU:HG	0.56	2.01	3	3
1:A:156:GLN:NE2	1:A:335:ASP:HB2	0.56	2.15	12	1
1:A:261:TRP:HB2	1:A:271:VAL:HA	0.56	1.78	3	2
1:A:155:LEU:HG	1:A:328:LEU:HD22	0.56	1.76	6	2
1:A:112:LYS:HE3	1:A:112:LYS:HA	0.56	1.77	8	1
1:A:199:GLY:HA3	1:A:352:LYS:O	0.56	2.01	19	3
1:A:281:ASN:HD22	1:A:285:LEU:HD23	0.56	1.60	20	1
1:A:89:ARG:HA	1:A:89:ARG:NE	0.56	2.16	2	1
1:A:160:ARG:NE	1:A:160:ARG:HA	0.56	2.16	15	2
1:A:229:SER:HA	1:A:275:LYS:CD	0.56	2.31	13	1
1:A:142:TYR:HE1	1:A:147:LYS:HD3	0.56	1.60	16	2
1:A:99:TRP:HH2	1:A:163:ASP:HB2	0.56	1.61	13	2
1:A:152:LYS:HD2	1:A:335:ASP:HB2	0.56	1.76	13	1
1:A:99:TRP:HZ2	1:A:108:LEU:HD22	0.56	1.59	6	4
1:A:142:TYR:HA	1:A:149:PHE:HZ	0.56	1.61	18	3
1:A:200:LEU:HA	1:A:354:ILE:HA	0.55	1.77	17	1
1:A:199:GLY:HA3	1:A:354:ILE:CG2	0.55	2.31	15	1
1:A:179:LYS:HG3	1:A:227:PHE:CE2	0.55	2.37	3	1
1:A:179:LYS:HD2	1:A:224:THR:OG1	0.55	2.01	8	1
1:A:83:GLU:HB2	1:A:198:TYR:HD2	0.55	1.60	8	1
1:A:252:ILE:HD12	1:A:286:MET:SD	0.55	2.41	14	2
1:A:199:GLY:HA3	1:A:352:LYS:HB2	0.55	1.78	12	1
1:A:32:MET:HG2	1:A:116:SER:O	0.55	2.01	10	3
1:A:147:LYS:HD3	1:A:257:GLY:O	0.55	2.01	10	2
1:A:118:LEU:HB3	1:A:127:ARG:HG3	0.55	1.79	19	1
1:A:213:TYR:HD1	1:A:236:VAL:HB	0.55	1.60	16	2
1:A:31:ASP:HB3	1:A:37:TRP:CH2	0.55	2.37	18	1
1:A:237:ALA:HB3	1:A:238:PRO:HD3	0.55	1.79	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:GLU:HG2	1:A:207:GLU:H	0.55	1.62	17	1
1:A:227:PHE:HZ	1:A:253:GLN:HG3	0.55	1.61	5	1
1:A:187:TYR:CE2	1:A:188:LYS:HE2	0.55	2.36	4	1
1:A:52:TYR:HE1	1:A:72:VAL:HB	0.55	1.62	11	1
1:A:38:LYS:HE3	1:A:56:MET:HB3	0.55	1.77	17	1
1:A:94:GLU:HG2	1:A:98:LYS:HE3	0.55	1.79	4	1
1:A:192:GLN:HB3	1:A:194:TYR:CE2	0.55	2.37	5	3
1:A:135:GLY:HA3	1:A:187:TYR:HD1	0.54	1.62	9	3
1:A:241:ARG:HD3	1:A:310:ASP:O	0.54	2.03	19	2
1:A:169:HIS:HD2	1:A:240:ARG:HD3	0.54	1.61	1	1
1:A:268:PRO:O	1:A:272:ARG:HG3	0.54	2.02	11	2
1:A:255:LEU:HD11	1:A:294:ASN:HD21	0.54	1.62	8	1
1:A:151:ARG:NH2	1:A:295:LYS:HB3	0.54	2.17	2	1
1:A:121:LYS:HG2	1:A:122:ASN:HD22	0.54	1.62	17	1
1:A:199:GLY:O	1:A:354:ILE:HB	0.54	2.02	13	1
1:A:352:LYS:HE3	1:A:353:THR:O	0.54	2.03	16	1
1:A:309:LEU:HD22	1:A:314:LYS:O	0.54	2.02	15	1
1:A:71:LYS:HE2	1:A:129:MET:SD	0.54	2.42	1	1
1:A:159:LEU:HD21	1:A:325:LEU:HD11	0.54	1.79	6	1
1:A:40:GLY:HA3	1:A:55:ASP:HB2	0.54	1.79	8	1
1:A:282:ILE:HG13	1:A:303:MET:HB2	0.54	1.80	10	1
1:A:188:LYS:HE3	1:A:188:LYS:HA	0.54	1.78	11	1
1:A:103:ARG:HG3	1:A:105:LEU:HD13	0.54	1.79	20	1
1:A:259:LEU:HB2	1:A:262:GLU:HB3	0.54	1.79	20	1
1:A:166:GLU:HA	1:A:169:HIS:HB2	0.53	1.77	18	1
1:A:325:LEU:O	1:A:329:LYS:HG3	0.53	2.03	19	1
1:A:99:TRP:CH2	1:A:108:LEU:HD22	0.53	2.38	1	1
1:A:305:THR:O	1:A:309:LEU:HG	0.53	2.02	5	4
1:A:133:ARG:HD3	1:A:133:ARG:H	0.53	1.63	10	1
1:A:105:LEU:HG	1:A:163:ASP:OD1	0.53	2.03	1	1
1:A:32:MET:HB2	1:A:117:GLY:HA2	0.53	1.81	13	1
1:A:216:ASP:HB3	1:A:236:VAL:HB	0.53	1.78	1	1
1:A:151:ARG:NH1	1:A:331:ILE:HB	0.53	2.18	3	1
1:A:231:ASP:O	1:A:236:VAL:HG12	0.53	2.04	6	1
1:A:28:ILE:HD13	1:A:28:ILE:H	0.53	1.62	1	1
1:A:38:LYS:HB3	1:A:56:MET:HA	0.53	1.79	1	1
1:A:197:ASP:HB2	1:A:198:TYR:CD2	0.53	2.38	10	1
1:A:198:TYR:HD2	1:A:200:LEU:H	0.53	1.45	6	2
1:A:173:TYR:CD1	1:A:203:ARG:HA	0.53	2.39	12	1
1:A:281:ASN:ND2	1:A:284:SER:HB2	0.53	2.19	5	1
1:A:295:LYS:HE3	1:A:331:ILE:HG21	0.53	1.81	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:GLN:HA	1:A:98:LYS:HE3	0.53	1.80	19	1
1:A:156:GLN:NE2	1:A:335:ASP:HA	0.53	2.18	1	1
1:A:316:LEU:O	1:A:320:LEU:HG	0.53	2.04	12	6
1:A:182:ASN:ND2	1:A:195:LEU:HD22	0.53	2.19	6	1
1:A:320:LEU:O	1:A:324:LEU:HG	0.53	2.03	9	6
1:A:147:LYS:HG3	1:A:257:GLY:HA2	0.53	1.79	16	1
1:A:105:LEU:HG	1:A:163:ASP:HB2	0.52	1.79	15	1
1:A:147:LYS:HD3	1:A:253:GLN:HG2	0.52	1.79	15	1
1:A:47:GLY:O	1:A:48:PHE:HB2	0.52	2.05	17	2
1:A:48:PHE:HA	1:A:352:LYS:HD2	0.52	1.80	3	1
1:A:204:TYR:CE1	1:A:239:SER:HA	0.52	2.39	14	1
1:A:37:TRP:CE3	1:A:56:MET:HB2	0.52	2.40	5	1
1:A:172:GLU:HB2	1:A:205:CYS:O	0.52	2.04	7	1
1:A:47:GLY:HA2	1:A:181:SER:O	0.52	2.04	15	1
1:A:241:ARG:HG3	1:A:311:TYR:HD1	0.52	1.65	6	1
1:A:67:PRO:O	1:A:133:ARG:HB3	0.52	2.05	14	1
1:A:96:ILE:HA	1:A:99:TRP:CZ3	0.52	2.40	1	2
1:A:169:HIS:HE1	1:A:174:VAL:HG12	0.52	1.65	17	2
1:A:97:GLN:HA	1:A:97:GLN:HE21	0.52	1.65	18	1
1:A:352:LYS:O	1:A:353:THR:HG22	0.52	2.05	7	1
1:A:124:LYS:HE3	1:A:124:LYS:HA	0.52	1.81	12	1
1:A:172:GLU:O	1:A:203:ARG:HA	0.52	2.05	15	1
1:A:354:ILE:HG13	1:A:356:LYS:HD3	0.52	1.82	12	1
1:A:147:LYS:HE3	1:A:253:GLN:HB3	0.52	1.82	9	1
1:A:46:GLY:O	1:A:71:LYS:HE2	0.52	2.05	13	1
1:A:89:ARG:HG3	1:A:173:TYR:CE2	0.51	2.40	6	1
1:A:228:THR:O	1:A:232:ALA:HB3	0.51	2.05	20	2
1:A:186:ASN:HB2	1:A:194:TYR:CE1	0.51	2.40	15	1
1:A:114:TRP:CD1	1:A:130:ILE:HG22	0.51	2.40	1	3
1:A:352:LYS:O	1:A:353:THR:HB	0.51	2.05	4	2
1:A:47:GLY:HA2	1:A:71:LYS:HE3	0.51	1.82	16	1
1:A:178:ILE:HB	1:A:246:ILE:HG22	0.51	1.81	7	2
1:A:69:VAL:HG22	1:A:132:ASP:O	0.51	2.06	10	1
1:A:56:MET:HA	1:A:56:MET:CE	0.51	2.35	17	1
1:A:94:GLU:HG2	1:A:98:LYS:HE2	0.51	1.82	19	1
1:A:273:ASP:O	1:A:277:ARG:HB2	0.51	2.05	15	1
1:A:39:VAL:HG23	1:A:52:TYR:CD2	0.51	2.40	11	1
1:A:160:ARG:HA	1:A:160:ARG:NE	0.51	2.21	13	1
1:A:157:LEU:O	1:A:161:ILE:HG12	0.51	2.06	7	5
1:A:147:LYS:O	1:A:257:GLY:HA2	0.51	2.05	11	1
1:A:99:TRP:CZ3	1:A:108:LEU:HD13	0.51	2.40	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HG2	1:A:56:MET:O	0.51	2.06	14	1
1:A:108:LEU:HD23	1:A:108:LEU:H	0.51	1.66	5	2
1:A:231:ASP:OD2	1:A:238:PRO:HA	0.51	2.06	12	2
1:A:147:LYS:HG3	1:A:253:GLN:HE22	0.51	1.66	11	1
1:A:290:PHE:HB3	1:A:294:ASN:O	0.51	2.06	14	1
1:A:161:ILE:O	1:A:165:LEU:HB2	0.51	2.05	12	3
1:A:167:TYR:O	1:A:171:HIS:HB2	0.51	2.06	9	1
1:A:107:TYR:HE2	1:A:160:ARG:HD3	0.51	1.66	18	1
1:A:47:GLY:HA3	1:A:196:VAL:CG1	0.51	2.34	1	1
1:A:179:LYS:HG3	1:A:227:PHE:HE2	0.51	1.65	3	1
1:A:212:GLU:CD	1:A:212:GLU:H	0.51	2.09	10	1
1:A:175:HIS:HB3	1:A:198:TYR:HD2	0.51	1.66	17	1
1:A:302:TYR:CD1	1:A:320:LEU:HD12	0.51	2.41	9	2
1:A:306:VAL:HA	1:A:309:LEU:HB2	0.51	1.82	16	1
1:A:200:LEU:HB3	1:A:222:ASP:HB3	0.50	1.84	14	1
1:A:215:GLU:O	1:A:216:ASP:HB2	0.50	2.07	10	1
1:A:142:TYR:CD1	1:A:147:LYS:HB3	0.50	2.42	3	5
1:A:267:ASP:HB3	1:A:270:TYR:HD2	0.50	1.67	12	2
1:A:174:VAL:O	1:A:201:ALA:HA	0.50	2.05	20	3
1:A:67:PRO:O	1:A:132:ASP:HA	0.50	2.07	20	2
1:A:90:ALA:HA	1:A:99:TRP:CH2	0.50	2.41	19	1
1:A:244:LEU:HG	1:A:320:LEU:HD21	0.50	1.83	11	1
1:A:338:LYS:NZ	1:A:338:LYS:HB3	0.50	2.21	9	1
1:A:238:PRO:HG2	1:A:242:GLY:HA3	0.50	1.84	14	1
1:A:32:MET:HA	1:A:32:MET:CE	0.50	2.37	18	2
1:A:240:ARG:HG2	1:A:312:THR:HG23	0.50	1.83	19	1
1:A:44:GLY:HA2	1:A:50:CYS:HA	0.50	1.83	7	2
1:A:155:LEU:HG	1:A:328:LEU:HG	0.50	1.82	8	2
1:A:259:LEU:HB2	1:A:262:GLU:CG	0.50	2.36	16	1
1:A:205:CYS:CB	1:A:209:VAL:HA	0.50	2.31	17	1
1:A:196:VAL:HG13	1:A:197:ASP:N	0.50	2.21	20	1
1:A:202:TYR:HD1	1:A:354:ILE:HD11	0.50	1.66	3	1
1:A:314:LYS:HD2	1:A:314:LYS:H	0.50	1.66	5	1
1:A:314:LYS:N	1:A:314:LYS:HD2	0.50	2.21	5	1
1:A:104:LYS:NZ	1:A:104:LYS:HB2	0.50	2.22	9	1
1:A:222:ASP:OD1	1:A:228:THR:HG21	0.50	2.06	19	1
1:A:169:HIS:HA	1:A:174:VAL:HG12	0.50	1.84	15	1
1:A:31:ASP:OD1	1:A:35:LYS:HE3	0.49	2.07	9	1
1:A:105:LEU:HG	1:A:163:ASP:OD2	0.49	2.08	2	1
1:A:27:GLU:O	1:A:38:LYS:HA	0.49	2.06	20	2
1:A:26:GLY:HA2	1:A:56:MET:SD	0.49	2.48	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:PRO:HB3	1:A:134:PHE:HE2	0.49	1.67	7	1
1:A:94:GLU:O	1:A:98:LYS:HG2	0.49	2.08	7	1
1:A:111:PRO:HG3	1:A:196:VAL:HG12	0.49	1.83	9	1
1:A:267:ASP:O	1:A:271:VAL:HG23	0.49	2.08	10	1
1:A:169:HIS:HD2	1:A:170:GLU:HG3	0.49	1.66	12	1
1:A:142:TYR:CE2	1:A:143:GLU:HG3	0.49	2.42	14	1
1:A:238:PRO:HB2	1:A:242:GLY:HA3	0.49	1.84	1	1
1:A:106:LYS:HG3	1:A:107:TYR:CD1	0.49	2.42	2	1
1:A:259:LEU:O	1:A:262:GLU:HG3	0.49	2.07	7	2
1:A:196:VAL:HG22	1:A:197:ASP:H	0.49	1.68	4	1
1:A:30:THR:HA	1:A:35:LYS:O	0.49	2.08	9	5
1:A:200:LEU:HG	1:A:353:THR:HA	0.49	1.84	7	1
1:A:48:PHE:HZ	1:A:79:PRO:HB2	0.49	1.68	8	1
1:A:155:LEU:HD22	1:A:328:LEU:HD22	0.49	1.83	13	2
1:A:70:VAL:CG2	1:A:128:PHE:HB2	0.49	2.37	18	12
1:A:164:ILE:O	1:A:168:ILE:HG12	0.49	2.08	3	4
1:A:83:GLU:O	1:A:87:TYR:HB2	0.49	2.08	5	2
1:A:106:LYS:HD2	1:A:107:TYR:CD1	0.49	2.43	5	1
1:A:253:GLN:HG2	1:A:259:LEU:HG	0.49	1.85	11	1
1:A:197:ASP:O	1:A:200:LEU:HG	0.49	2.07	4	1
1:A:133:ARG:HD2	1:A:187:TYR:CD1	0.49	2.42	12	1
1:A:107:TYR:CE2	1:A:160:ARG:HD3	0.49	2.43	18	1
1:A:287:ASP:HA	1:A:296:PRO:CB	0.49	2.37	15	1
1:A:328:LEU:O	1:A:331:ILE:HG22	0.49	2.08	6	4
1:A:151:ARG:HD2	1:A:298:GLU:OE2	0.49	2.07	13	2
1:A:354:ILE:H	1:A:354:ILE:HD13	0.49	1.68	7	2
1:A:328:LEU:HB3	1:A:333:SER:O	0.49	2.08	8	1
1:A:240:ARG:CZ	1:A:241:ARG:HA	0.49	2.38	13	1
1:A:192:GLN:OE1	1:A:192:GLN:HA	0.49	2.08	19	1
1:A:259:LEU:HB2	1:A:262:GLU:CB	0.49	2.37	20	1
1:A:35:LYS:HZ1	1:A:114:TRP:HB3	0.49	1.68	7	1
1:A:261:TRP:O	1:A:265:LEU:HB3	0.49	2.08	15	2
1:A:241:ARG:HG2	1:A:311:TYR:O	0.49	2.08	12	1
1:A:51:ILE:HD12	1:A:71:LYS:HB3	0.49	1.85	17	2
1:A:53:LEU:HD13	1:A:54:ALA:N	0.49	2.23	8	1
1:A:239:SER:O	1:A:240:ARG:HB2	0.49	2.07	12	1
1:A:47:GLY:HA3	1:A:196:VAL:CG2	0.49	2.37	17	1
1:A:34:LYS:O	1:A:35:LYS:HE2	0.49	2.08	18	1
1:A:287:ASP:HA	1:A:296:PRO:HG2	0.49	1.84	1	1
1:A:241:ARG:HB2	1:A:310:ASP:O	0.48	2.08	5	2
1:A:114:TRP:HB2	1:A:130:ILE:CG2	0.48	2.37	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:203:ARG:HD2	1:A:215:GLU:OE2	0.48	2.08	12	1
1:A:162:LEU:HB3	1:A:317:TYR:CE1	0.48	2.43	13	1
1:A:79:PRO:HG3	1:A:353:THR:HA	0.48	1.85	14	1
1:A:282:ILE:HD13	1:A:282:ILE:H	0.48	1.68	8	5
1:A:38:LYS:O	1:A:55:ASP:HB3	0.48	2.08	12	1
1:A:28:ILE:HG22	1:A:38:LYS:HG2	0.48	1.85	11	1
1:A:179:LYS:HZ2	1:A:227:PHE:HD2	0.48	1.50	16	1
1:A:38:LYS:HG2	1:A:56:MET:SD	0.48	2.48	8	1
1:A:160:ARG:HA	1:A:163:ASP:OD2	0.48	2.07	11	1
1:A:34:LYS:O	1:A:35:LYS:HB3	0.48	2.09	12	2
1:A:37:TRP:HB2	1:A:56:MET:O	0.48	2.07	19	1
1:A:228:THR:CG2	1:A:232:ALA:HB3	0.48	2.39	6	1
1:A:273:ASP:O	1:A:277:ARG:HG2	0.48	2.07	6	1
1:A:28:ILE:H	1:A:28:ILE:HD13	0.48	1.67	9	2
1:A:299:ILE:H	1:A:299:ILE:HD12	0.48	1.69	15	1
1:A:290:PHE:HE2	1:A:294:ASN:HB3	0.48	1.67	16	3
1:A:282:ILE:HG12	1:A:283:ALA:N	0.48	2.23	5	4
1:A:158:SER:O	1:A:162:LEU:HG	0.48	2.09	13	1
1:A:309:LEU:O	1:A:310:ASP:HB2	0.48	2.09	12	3
1:A:269:LYS:HB2	1:A:269:LYS:NZ	0.48	2.23	6	1
1:A:149:PHE:HD2	1:A:254:TRP:HB3	0.48	1.69	13	2
1:A:99:TRP:O	1:A:103:ARG:HB2	0.48	2.08	16	1
1:A:47:GLY:N	1:A:184:LEU:HD11	0.48	2.23	17	1
1:A:53:LEU:HD23	1:A:69:VAL:HG12	0.48	1.86	4	1
1:A:31:ASP:HA	1:A:117:GLY:HA3	0.48	1.86	18	2
1:A:159:LEU:HD21	1:A:325:LEU:HD21	0.48	1.85	13	2
1:A:200:LEU:HG	1:A:353:THR:O	0.48	2.08	11	1
1:A:83:GLU:HB3	1:A:197:ASP:O	0.48	2.09	15	1
1:A:87:TYR:CE1	1:A:111:PRO:HG2	0.48	2.35	1	2
1:A:90:ALA:HA	1:A:99:TRP:HH2	0.48	1.69	17	1
1:A:290:PHE:CE2	1:A:292:GLU:HB2	0.48	2.44	18	1
1:A:294:ASN:O	1:A:295:LYS:HB2	0.47	2.09	2	4
1:A:177:ASP:CB	1:A:223:GLY:HA3	0.47	2.27	10	1
1:A:241:ARG:NH2	1:A:279:ARG:HD2	0.47	2.24	10	1
1:A:326:GLN:HA	1:A:329:LYS:HE2	0.47	1.84	12	1
1:A:70:VAL:HA	1:A:129:MET:O	0.47	2.09	14	4
1:A:204:TYR:CE1	1:A:237:ALA:HB3	0.47	2.44	17	1
1:A:186:ASN:ND2	1:A:194:TYR:HE1	0.47	2.06	10	1
1:A:178:ILE:O	1:A:178:ILE:HG12	0.47	2.09	14	1
1:A:42:PRO:HA	1:A:52:TYR:CD1	0.47	2.44	17	1
1:A:262:GLU:O	1:A:265:LEU:HD22	0.47	2.08	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:ILE:HA	1:A:37:TRP:O	0.47	2.10	2	1
1:A:89:ARG:HA	1:A:89:ARG:HE	0.47	1.66	2	2
1:A:87:TYR:O	1:A:91:ALA:HB3	0.47	2.09	6	2
1:A:310:ASP:HB3	1:A:313:GLU:OE1	0.47	2.09	4	1
1:A:121:LYS:O	1:A:121:LYS:HD3	0.47	2.09	3	1
1:A:114:TRP:HB2	1:A:130:ILE:HG22	0.47	1.86	6	5
1:A:184:LEU:CD1	1:A:194:TYR:HB2	0.47	2.40	10	1
1:A:310:ASP:HB3	1:A:313:GLU:HB3	0.47	1.87	11	1
1:A:265:LEU:HA	1:A:271:VAL:CG2	0.47	2.39	6	1
1:A:47:GLY:CA	1:A:71:LYS:HE3	0.47	2.40	16	1
1:A:70:VAL:HB	1:A:130:ILE:CD1	0.47	2.39	16	10
1:A:145:ASN:OD1	1:A:148:ARG:HB2	0.47	2.10	5	1
1:A:137:ASP:O	1:A:141:ILE:HG13	0.47	2.10	9	1
1:A:96:ILE:O	1:A:100:ILE:HD13	0.47	2.09	10	1
1:A:51:ILE:HD12	1:A:71:LYS:HG3	0.47	1.86	14	1
1:A:259:LEU:O	1:A:262:GLU:HB2	0.47	2.10	17	1
1:A:152:LYS:HD3	1:A:153:THR:N	0.47	2.24	1	1
1:A:106:LYS:HB3	1:A:106:LYS:HZ2	0.47	1.70	4	1
1:A:111:PRO:HB3	1:A:134:PHE:HZ	0.47	1.70	4	1
1:A:171:HIS:C	1:A:172:GLU:HG3	0.47	2.30	4	1
1:A:106:LYS:HD2	1:A:107:TYR:HD1	0.47	1.70	5	1
1:A:224:THR:HB	1:A:226:GLU:OE1	0.47	2.09	6	1
1:A:100:ILE:HG13	1:A:105:LEU:HB2	0.47	1.86	17	1
1:A:137:ASP:HB2	1:A:140:LYS:HG3	0.47	1.86	11	2
1:A:197:ASP:HB2	1:A:198:TYR:CE2	0.47	2.45	10	1
1:A:175:HIS:HE1	1:A:200:LEU:HB2	0.47	1.70	20	1
1:A:204:TYR:HB2	1:A:237:ALA:HB1	0.46	1.87	4	1
1:A:241:ARG:HB2	1:A:311:TYR:O	0.46	2.11	4	1
1:A:165:LEU:HD13	1:A:175:HIS:CD2	0.46	2.45	7	1
1:A:196:VAL:HG23	1:A:198:TYR:CE2	0.46	2.46	19	1
1:A:205:CYS:SG	1:A:211:LYS:HB2	0.46	2.50	19	1
1:A:173:TYR:HB3	1:A:201:ALA:HB1	0.46	1.86	20	1
1:A:309:LEU:HA	1:A:313:GLU:HB3	0.46	1.87	8	1
1:A:276:ILE:HG12	1:A:279:ARG:HH21	0.46	1.70	1	1
1:A:256:THR:HG22	1:A:290:PHE:HB2	0.46	1.86	1	1
1:A:240:ARG:O	1:A:244:LEU:HD23	0.46	2.10	15	1
1:A:232:ALA:HB2	1:A:238:PRO:HG3	0.46	1.87	16	2
1:A:263:ASP:O	1:A:266:LYS:HD2	0.46	2.09	19	1
1:A:152:LYS:N	1:A:152:LYS:HD2	0.46	2.25	15	1
1:A:303:MET:HA	1:A:306:VAL:HG22	0.46	1.87	2	5
1:A:240:ARG:O	1:A:244:LEU:HG	0.46	2.10	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PRO:HB3	1:A:187:TYR:OH	0.46	2.11	4	1
1:A:310:ASP:CG	1:A:311:TYR:H	0.46	2.12	14	1
1:A:41:LEU:HD22	1:A:42:PRO:HD2	0.46	1.86	14	1
1:A:241:ARG:HD3	1:A:306:VAL:O	0.46	2.10	1	1
1:A:137:ASP:OD1	1:A:181:SER:HA	0.46	2.11	2	1
1:A:176:GLY:O	1:A:246:ILE:HD13	0.46	2.11	5	1
1:A:288:LYS:NZ	1:A:288:LYS:HB3	0.46	2.25	6	1
1:A:227:PHE:O	1:A:246:ILE:HG12	0.46	2.10	11	3
1:A:66:ALA:N	1:A:67:PRO:HD2	0.46	2.25	14	2
1:A:151:ARG:O	1:A:155:LEU:HB2	0.46	2.11	1	1
1:A:112:LYS:HD2	1:A:114:TRP:CE2	0.46	2.46	2	1
1:A:282:ILE:H	1:A:282:ILE:HD13	0.46	1.71	6	3
1:A:264:ASN:CB	1:A:270:TYR:HB3	0.46	2.41	11	1
1:A:230:ILE:HD13	1:A:230:ILE:H	0.46	1.69	13	1
1:A:271:VAL:HG13	1:A:275:LYS:HZ2	0.46	1.71	13	1
1:A:173:TYR:HB3	1:A:203:ARG:HA	0.46	1.86	14	1
1:A:313:GLU:O	1:A:314:LYS:HD3	0.46	2.11	20	1
1:A:110:VAL:CG2	1:A:111:PRO:HD2	0.46	2.40	9	1
1:A:139:GLN:HA	1:A:142:TYR:HB3	0.46	1.87	11	1
1:A:31:ASP:HA	1:A:128:PHE:HZ	0.46	1.71	16	1
1:A:99:TRP:HH2	1:A:108:LEU:HD22	0.46	1.70	1	1
1:A:173:TYR:HB3	1:A:203:ARG:HD2	0.46	1.87	16	1
1:A:174:VAL:HG13	1:A:204:TYR:HE2	0.46	1.69	19	1
1:A:259:LEU:HD13	1:A:261:TRP:CZ2	0.46	2.46	15	2
1:A:133:ARG:O	1:A:133:ARG:HG2	0.46	2.10	9	1
1:A:175:HIS:HB3	1:A:177:ASP:OD1	0.46	2.11	12	1
1:A:302:TYR:CD1	1:A:320:LEU:HD22	0.45	2.47	18	2
1:A:100:ILE:HD11	1:A:108:LEU:HG	0.45	1.86	7	2
1:A:186:ASN:HD21	1:A:194:TYR:HE1	0.45	1.52	10	1
1:A:48:PHE:CZ	1:A:79:PRO:HG2	0.45	2.46	10	1
1:A:38:LYS:HB2	1:A:56:MET:HA	0.45	1.88	13	1
1:A:267:ASP:OD1	1:A:269:LYS:HE3	0.45	2.11	16	1
1:A:354:ILE:HD13	1:A:354:ILE:H	0.45	1.71	16	1
1:A:321:ARG:O	1:A:325:LEU:HB2	0.45	2.11	2	1
1:A:104:LYS:HE3	1:A:104:LYS:CA	0.45	2.33	10	1
1:A:320:LEU:O	1:A:323:ILE:HG22	0.45	2.11	13	1
1:A:231:ASP:HB3	1:A:238:PRO:HA	0.45	1.86	16	1
1:A:85:LYS:O	1:A:89:ARG:HG2	0.45	2.11	6	1
1:A:225:ILE:HA	1:A:228:THR:OG1	0.45	2.10	14	1
1:A:139:GLN:HA	1:A:142:TYR:CD2	0.45	2.47	20	2
1:A:66:ALA:HB3	1:A:67:PRO:HD3	0.45	1.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:TYR:CD2	1:A:201:ALA:HB1	0.45	2.47	19	1
1:A:199:GLY:O	1:A:354:ILE:HA	0.45	2.11	19	1
1:A:290:PHE:CE2	1:A:294:ASN:HB3	0.45	2.47	2	2
1:A:92:LYS:HG2	1:A:94:GLU:OE2	0.45	2.11	3	1
1:A:295:LYS:HA	1:A:295:LYS:CE	0.45	2.41	14	1
1:A:35:LYS:HB2	1:A:37:TRP:CZ3	0.45	2.47	18	1
1:A:152:LYS:HG3	1:A:153:THR:N	0.45	2.26	20	1
1:A:269:LYS:HB3	1:A:269:LYS:NZ	0.45	2.26	2	1
1:A:252:ILE:HB	1:A:299:ILE:HG21	0.45	1.87	3	1
1:A:106:LYS:HG2	1:A:321:ARG:NH2	0.45	2.27	4	1
1:A:174:VAL:HG11	1:A:203:ARG:NH1	0.45	2.27	20	1
1:A:184:LEU:HD23	1:A:196:VAL:HG22	0.45	1.87	2	1
1:A:205:CYS:HB2	1:A:209:VAL:O	0.45	2.12	3	1
1:A:175:HIS:CE1	1:A:200:LEU:HB3	0.45	2.47	18	1
1:A:135:GLY:HA3	1:A:187:TYR:CD1	0.45	2.44	9	2
1:A:83:GLU:HA	1:A:198:TYR:HB2	0.45	1.88	10	1
1:A:175:HIS:CB	1:A:201:ALA:HA	0.45	2.28	15	1
1:A:152:LYS:CG	1:A:335:ASP:HA	0.45	2.38	7	1
1:A:43:ILE:HD11	1:A:53:LEU:HD12	0.45	1.88	9	1
1:A:99:TRP:CE2	1:A:103:ARG:HG3	0.45	2.46	11	1
1:A:304:GLU:O	1:A:307:LYS:HG3	0.45	2.11	18	1
1:A:147:LYS:O	1:A:147:LYS:HG2	0.45	2.12	12	1
1:A:103:ARG:HD3	1:A:103:ARG:O	0.44	2.12	9	1
1:A:92:LYS:O	1:A:96:ILE:HG13	0.44	2.11	3	1
1:A:199:GLY:O	1:A:354:ILE:HG23	0.44	2.12	7	2
1:A:48:PHE:CZ	1:A:79:PRO:HB2	0.44	2.46	8	1
1:A:137:ASP:HA	1:A:184:LEU:HA	0.44	1.89	9	1
1:A:206:PRO:HG2	1:A:209:VAL:HG23	0.44	1.89	9	1
1:A:200:LEU:HD13	1:A:352:LYS:HZ3	0.44	1.71	15	1
1:A:147:LYS:HG3	1:A:253:GLN:OE1	0.44	2.12	3	1
1:A:249:TYR:O	1:A:253:GLN:HB2	0.44	2.12	3	1
1:A:157:LEU:O	1:A:160:ARG:HG3	0.44	2.13	7	1
1:A:66:ALA:O	1:A:133:ARG:HG3	0.44	2.13	12	1
1:A:178:ILE:HG23	1:A:250:CYS:SG	0.44	2.52	14	1
1:A:175:HIS:CE1	1:A:177:ASP:HB3	0.44	2.47	16	1
1:A:303:MET:O	1:A:306:VAL:HG22	0.44	2.12	16	1
1:A:191:ASP:CB	1:A:338:LYS:HA	0.44	2.42	20	1
1:A:191:ASP:HB2	1:A:338:LYS:HD3	0.44	1.89	5	1
1:A:51:ILE:CD1	1:A:71:LYS:HB3	0.44	2.43	5	1
1:A:84:LEU:HD22	1:A:127:ARG:HD3	0.44	1.89	7	1
1:A:142:TYR:HD1	1:A:147:LYS:HB2	0.44	1.72	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:PHE:HD2	1:A:153:THR:HG21	0.44	1.71	17	1
1:A:84:LEU:O	1:A:88:GLN:HG2	0.44	2.12	17	1
1:A:103:ARG:HG2	1:A:105:LEU:HD13	0.44	1.90	15	1
1:A:32:MET:CE	1:A:32:MET:HA	0.44	2.43	7	1
1:A:139:GLN:HG2	1:A:181:SER:HA	0.44	1.87	11	1
1:A:149:PHE:HB2	1:A:254:TRP:HB3	0.44	1.90	20	1
1:A:246:ILE:O	1:A:249:TYR:HB2	0.44	2.13	5	1
1:A:89:ARG:HG3	1:A:173:TYR:HE2	0.44	1.73	6	1
1:A:68:CYS:HA	1:A:131:MET:O	0.44	2.12	16	2
1:A:67:PRO:CA	1:A:133:ARG:HG2	0.44	2.42	16	1
1:A:191:ASP:HB2	1:A:338:LYS:HA	0.44	1.89	20	1
1:A:265:LEU:HD13	1:A:265:LEU:O	0.44	2.12	10	1
1:A:241:ARG:CG	1:A:311:TYR:HA	0.44	2.36	1	1
1:A:133:ARG:HE	1:A:187:TYR:HE1	0.44	1.55	5	1
1:A:213:TYR:HA	1:A:236:VAL:HG23	0.44	1.90	14	1
1:A:213:TYR:CD1	1:A:236:VAL:HB	0.44	2.45	16	1
1:A:195:LEU:HD23	1:A:196:VAL:N	0.44	2.28	5	1
1:A:231:ASP:HB3	1:A:238:PRO:HB3	0.44	1.90	5	1
1:A:240:ARG:HD2	1:A:311:TYR:O	0.44	2.13	8	1
1:A:298:GLU:HA	1:A:323:ILE:CD1	0.44	2.42	8	1
1:A:225:ILE:O	1:A:225:ILE:HD13	0.44	2.13	13	2
1:A:99:TRP:CZ2	1:A:108:LEU:HD22	0.44	2.47	14	2
1:A:210:HIS:HB2	1:A:238:PRO:HB2	0.44	1.90	20	1
1:A:178:ILE:HG22	1:A:178:ILE:O	0.43	2.13	19	2
1:A:80:LEU:HD12	1:A:127:ARG:HE	0.43	1.73	5	1
1:A:247:LEU:O	1:A:251:MET:HG3	0.43	2.13	9	1
1:A:226:GLU:HG3	1:A:226:GLU:H	0.43	1.41	12	1
1:A:328:LEU:HD21	1:A:334:LYS:HA	0.43	1.90	13	1
1:A:177:ASP:HB3	1:A:199:GLY:HA3	0.43	1.89	17	1
1:A:321:ARG:HG3	1:A:322:ASP:N	0.43	2.28	17	1
1:A:171:HIS:CD2	1:A:172:GLU:HG2	0.43	2.48	19	1
1:A:275:LYS:O	1:A:279:ARG:HG3	0.43	2.12	1	1
1:A:189:ASN:HB3	1:A:191:ASP:OD1	0.43	2.13	5	1
1:A:337:GLY:C	1:A:338:LYS:HD2	0.43	2.33	9	1
1:A:226:GLU:HA	1:A:265:LEU:HD21	0.43	1.89	10	1
1:A:137:ASP:HA	1:A:184:LEU:HD13	0.43	1.90	14	1
1:A:281:ASN:HB3	1:A:285:LEU:HD23	0.43	1.90	18	1
1:A:137:ASP:HB3	1:A:184:LEU:HB3	0.43	1.90	9	1
1:A:224:THR:O	1:A:228:THR:HB	0.43	2.13	20	1
1:A:39:VAL:HG12	1:A:52:TYR:CE1	0.43	2.48	2	1
1:A:29:ILE:HB	1:A:128:PHE:CZ	0.43	2.47	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:GLU:O	1:A:98:LYS:HG3	0.43	2.13	4	1
1:A:182:ASN:CG	1:A:198:TYR:HB3	0.43	2.34	13	1
1:A:147:LYS:HZ1	1:A:262:GLU:CD	0.43	2.17	14	1
1:A:106:LYS:HB2	1:A:321:ARG:HH22	0.43	1.74	1	1
1:A:124:LYS:HA	1:A:124:LYS:CE	0.43	2.35	10	1
1:A:137:ASP:OD1	1:A:140:LYS:HG2	0.43	2.14	18	1
1:A:80:LEU:O	1:A:84:LEU:HB2	0.43	2.14	2	2
1:A:247:LEU:HD12	1:A:250:CYS:SG	0.43	2.54	5	2
1:A:157:LEU:O	1:A:161:ILE:HB	0.43	2.14	12	1
1:A:309:LEU:HD13	1:A:315:PRO:HA	0.43	1.91	14	1
1:A:306:VAL:O	1:A:309:LEU:HG	0.43	2.13	1	1
1:A:178:ILE:HB	1:A:246:ILE:CG2	0.43	2.44	3	1
1:A:30:THR:HG23	1:A:35:LYS:HB2	0.43	1.89	4	1
1:A:31:ASP:HB2	1:A:116:SER:O	0.43	2.14	10	1
1:A:316:LEU:O	1:A:320:LEU:HD13	0.43	2.14	11	1
1:A:309:LEU:HD22	1:A:315:PRO:HA	0.43	1.90	14	1
1:A:155:LEU:O	1:A:159:LEU:HG	0.43	2.14	20	2
1:A:203:ARG:NH2	1:A:207:GLU:H	0.43	2.12	5	1
1:A:31:ASP:OD2	1:A:115:GLY:HA3	0.43	2.13	14	1
1:A:132:ASP:HB2	1:A:134:PHE:CE1	0.43	2.48	19	1
1:A:229:SER:HA	1:A:249:TYR:CE2	0.43	2.49	20	1
1:A:177:ASP:HB2	1:A:223:GLY:CA	0.43	2.44	11	2
1:A:200:LEU:HG	1:A:353:THR:CA	0.43	2.44	7	1
1:A:77:ASN:OD1	1:A:79:PRO:HD2	0.43	2.13	12	1
1:A:147:LYS:HG3	1:A:257:GLY:O	0.43	2.14	1	2
1:A:51:ILE:HD11	1:A:71:LYS:HD2	0.43	1.91	18	1
1:A:167:TYR:HA	1:A:170:GLU:OE2	0.43	2.14	1	1
1:A:172:GLU:HG2	1:A:203:ARG:HB2	0.43	1.90	1	1
1:A:45:GLN:HB2	1:A:137:ASP:OD2	0.43	2.13	15	1
1:A:95:GLN:O	1:A:98:LYS:HB3	0.42	2.14	2	1
1:A:178:ILE:HG22	1:A:250:CYS:SG	0.42	2.54	3	1
1:A:160:ARG:HH21	1:A:164:ILE:HG21	0.42	1.74	9	1
1:A:133:ARG:HG2	1:A:133:ARG:O	0.42	2.13	10	1
1:A:262:GLU:O	1:A:265:LEU:HG	0.42	2.14	14	1
1:A:145:ASN:O	1:A:148:ARG:HG2	0.42	2.14	15	1
1:A:39:VAL:HG22	1:A:52:TYR:CE1	0.42	2.49	5	1
1:A:298:GLU:CD	1:A:298:GLU:H	0.42	2.17	12	5
1:A:177:ASP:HB2	1:A:182:ASN:ND2	0.42	2.29	12	1
1:A:37:TRP:CZ3	1:A:56:MET:HG2	0.42	2.49	12	1
1:A:191:ASP:HB2	1:A:338:LYS:HB3	0.42	1.91	8	1
1:A:43:ILE:HB	1:A:51:ILE:O	0.42	2.14	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:HD12	1:A:42:PRO:HD2	0.42	1.90	4	1
1:A:281:ASN:ND2	1:A:284:SER:HB3	0.42	2.29	8	1
1:A:152:LYS:HE2	1:A:152:LYS:O	0.42	2.15	9	1
1:A:153:THR:O	1:A:157:LEU:HD13	0.42	2.15	10	1
1:A:335:ASP:CG	1:A:336:ASP:H	0.42	2.18	3	1
1:A:174:VAL:HG13	1:A:204:TYR:CD1	0.42	2.48	13	1
1:A:33:ALA:HB3	1:A:37:TRP:CH2	0.42	2.49	18	1
1:A:175:HIS:CE1	1:A:178:ILE:HD13	0.42	2.49	5	1
1:A:294:ASN:O	1:A:295:LYS:HB3	0.42	2.15	8	1
1:A:160:ARG:HD2	1:A:160:ARG:O	0.42	2.15	11	1
1:A:164:ILE:HD13	1:A:195:LEU:HB3	0.42	1.91	14	1
1:A:138:LEU:HB3	1:A:180:ALA:HB1	0.42	1.92	19	2
1:A:202:TYR:HB2	1:A:222:ASP:HB3	0.42	1.91	6	1
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.42	1.92	8	1
1:A:302:TYR:O	1:A:306:VAL:HG13	0.42	2.15	9	1
1:A:146:ALA:C	1:A:147:LYS:HD3	0.42	2.35	12	1
1:A:276:ILE:O	1:A:280:GLU:HG3	0.42	2.15	13	1
1:A:43:ILE:HD11	1:A:53:LEU:HB2	0.42	1.91	16	1
1:A:53:LEU:HD23	1:A:54:ALA:N	0.42	2.30	17	2
1:A:240:ARG:HG2	1:A:315:PRO:HG3	0.42	1.91	9	1
1:A:170:GLU:O	1:A:207:GLU:HA	0.42	2.14	10	1
1:A:96:ILE:O	1:A:100:ILE:HG13	0.42	2.15	11	2
1:A:199:GLY:HA3	1:A:352:LYS:CB	0.42	2.44	12	1
1:A:38:LYS:CB	1:A:56:MET:HA	0.42	2.45	13	1
1:A:155:LEU:CB	1:A:328:LEU:HD22	0.42	2.43	16	1
1:A:224:THR:OG1	1:A:226:GLU:HG2	0.42	2.14	17	1
1:A:103:ARG:HG3	1:A:103:ARG:O	0.42	2.13	18	1
1:A:240:ARG:HG3	1:A:315:PRO:HG3	0.42	1.91	19	1
1:A:200:LEU:HD13	1:A:352:LYS:NZ	0.42	2.30	15	1
1:A:213:TYR:HA	1:A:236:VAL:CG2	0.42	2.45	3	3
1:A:182:ASN:O	1:A:195:LEU:HA	0.42	2.15	6	2
1:A:226:GLU:HG2	1:A:265:LEU:HD13	0.42	1.91	2	1
1:A:261:TRP:HB3	1:A:274:SER:CB	0.42	2.44	4	1
1:A:93:PRO:O	1:A:97:GLN:HG3	0.42	2.14	19	1
1:A:282:ILE:HB	1:A:304:GLU:HG2	0.42	1.91	15	1
1:A:67:PRO:HA	1:A:133:ARG:CZ	0.42	2.44	15	1
1:A:354:ILE:HD13	1:A:355:THR:N	0.41	2.30	3	2
1:A:200:LEU:HD21	1:A:352:LYS:HB2	0.41	1.92	5	1
1:A:196:VAL:O	1:A:197:ASP:HB3	0.41	2.15	8	2
1:A:99:TRP:CE3	1:A:108:LEU:HG	0.41	2.50	10	1
1:A:325:LEU:O	1:A:329:LYS:HG2	0.41	2.15	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:240:ARG:HH21	1:A:244:LEU:HB2	0.41	1.75	13	1
1:A:177:ASP:CB	1:A:199:GLY:HA3	0.41	2.45	17	1
1:A:293:LYS:HD3	1:A:293:LYS:O	0.41	2.15	15	1
1:A:70:VAL:HB	1:A:130:ILE:HG12	0.41	1.91	5	1
1:A:96:ILE:HD12	1:A:112:LYS:NZ	0.41	2.30	8	1
1:A:73:GLU:HB2	1:A:80:LEU:HG	0.41	1.91	9	1
1:A:46:GLY:HA3	1:A:137:ASP:OD2	0.41	2.15	11	1
1:A:30:THR:HA	1:A:35:LYS:HA	0.41	1.90	12	1
1:A:34:LYS:O	1:A:34:LYS:HD3	0.41	2.15	13	1
1:A:47:GLY:HA2	1:A:71:LYS:CE	0.41	2.43	16	1
1:A:286:MET:HE2	1:A:303:MET:HG3	0.41	1.91	3	1
1:A:73:GLU:OE1	1:A:80:LEU:HB2	0.41	2.16	3	2
1:A:176:GLY:O	1:A:228:THR:HA	0.41	2.15	16	2
1:A:111:PRO:HG3	1:A:134:PHE:HZ	0.41	1.74	8	1
1:A:83:GLU:HG2	1:A:87:TYR:CE2	0.41	2.50	18	1
1:A:121:LYS:HE2	1:A:121:LYS:CA	0.41	2.43	20	1
1:A:261:TRP:HB3	1:A:274:SER:HB2	0.41	1.92	3	1
1:A:204:TYR:OH	1:A:239:SER:HA	0.41	2.14	9	1
1:A:151:ARG:HG2	1:A:331:ILE:HD13	0.41	1.92	11	1
1:A:305:THR:O	1:A:309:LEU:HB2	0.41	2.14	12	1
1:A:51:ILE:CD1	1:A:71:LYS:HG3	0.41	2.46	14	1
1:A:241:ARG:HD2	1:A:310:ASP:O	0.41	2.15	16	1
1:A:229:SER:HA	1:A:249:TYR:HE2	0.41	1.75	20	1
1:A:151:ARG:HH11	1:A:331:ILE:HB	0.41	1.74	3	1
1:A:71:LYS:O	1:A:128:PHE:HA	0.41	2.15	6	1
1:A:80:LEU:HD13	1:A:80:LEU:O	0.41	2.14	6	1
1:A:173:TYR:CB	1:A:203:ARG:HA	0.41	2.46	14	1
1:A:293:LYS:HB3	1:A:293:LYS:NZ	0.41	2.30	17	1
1:A:249:TYR:CZ	1:A:275:LYS:HD2	0.41	2.50	6	1
1:A:51:ILE:CD1	1:A:71:LYS:HD3	0.41	2.45	7	1
1:A:295:LYS:HE2	1:A:331:ILE:HA	0.41	1.92	9	1
1:A:79:PRO:O	1:A:83:GLU:HG2	0.41	2.15	10	1
1:A:73:GLU:HB2	1:A:80:LEU:HB2	0.41	1.92	11	1
1:A:29:ILE:HG12	1:A:37:TRP:O	0.41	2.14	18	1
1:A:259:LEU:O	1:A:262:GLU:HG2	0.41	2.16	15	1
1:A:142:TYR:CZ	1:A:147:LYS:HE3	0.41	2.50	5	1
1:A:155:LEU:HD21	1:A:324:LEU:HB3	0.41	1.93	5	1
1:A:314:LYS:HD2	1:A:314:LYS:N	0.41	2.31	6	1
1:A:103:ARG:HA	1:A:103:ARG:NE	0.41	2.30	12	1
1:A:104:LYS:HD2	1:A:104:LYS:N	0.41	2.31	16	1
1:A:122:ASN:HD22	1:A:122:ASN:N	0.41	2.14	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ILE:HA	1:A:164:ILE:HG22	0.41	1.91	15	1
1:A:53:LEU:HD12	1:A:133:ARG:HH21	0.41	1.74	3	1
1:A:95:GLN:HA	1:A:95:GLN:OE1	0.41	2.16	7	1
1:A:169:HIS:CD2	1:A:240:ARG:HD3	0.41	2.47	1	1
1:A:151:ARG:HD3	1:A:294:ASN:HD21	0.41	1.76	5	1
1:A:261:TRP:HB2	1:A:271:VAL:HG12	0.41	1.93	5	1
1:A:169:HIS:HE1	1:A:240:ARG:HA	0.41	1.76	8	1
1:A:253:GLN:HG3	1:A:259:LEU:CD1	0.41	2.46	9	1
1:A:247:LEU:HA	1:A:250:CYS:SG	0.41	2.55	18	2
1:A:100:ILE:HG22	1:A:105:LEU:HB2	0.41	1.92	10	1
1:A:313:GLU:OE1	1:A:314:LYS:HG2	0.41	2.16	11	1
1:A:204:TYR:HA	1:A:237:ALA:HB1	0.41	1.92	16	1
1:A:200:LEU:CD1	1:A:352:LYS:HZ3	0.41	2.29	15	1
1:A:174:VAL:HG22	1:A:202:TYR:O	0.41	2.16	5	1
1:A:116:SER:HB3	1:A:129:MET:HG3	0.41	1.93	7	1
1:A:260:PRO:HG2	1:A:278:TYR:HE1	0.41	1.76	7	1
1:A:282:ILE:N	1:A:282:ILE:HD13	0.41	2.31	11	1
1:A:166:GLU:HG3	1:A:167:TYR:N	0.41	2.30	13	1
1:A:283:ALA:HA	1:A:300:ALA:HB1	0.41	1.93	17	1
1:A:172:GLU:OE2	1:A:203:ARG:HD3	0.41	2.16	18	1
1:A:238:PRO:HB3	1:A:242:GLY:HA3	0.40	1.93	3	1
1:A:352:LYS:HG3	1:A:353:THR:H	0.40	1.76	6	1
1:A:134:PHE:HD1	1:A:186:ASN:HA	0.40	1.75	11	1
1:A:189:ASN:HB3	1:A:192:GLN:HG3	0.40	1.92	18	1
1:A:99:TRP:HZ2	1:A:108:LEU:HD11	0.40	1.75	2	1
1:A:301:LYS:HB3	1:A:323:ILE:HD11	0.40	1.93	4	1
1:A:199:GLY:O	1:A:354:ILE:HG22	0.40	2.16	11	1
1:A:310:ASP:HB3	1:A:313:GLU:HG2	0.40	1.92	17	1
1:A:118:LEU:HD23	1:A:119:HIS:N	0.40	2.31	6	1
1:A:267:ASP:HB3	1:A:270:TYR:CD1	0.40	2.51	13	1
1:A:352:LYS:HG2	1:A:353:THR:N	0.40	2.31	16	1
1:A:161:ILE:O	1:A:165:LEU:HG	0.40	2.17	15	1
1:A:225:ILE:HB	1:A:265:LEU:HD12	0.40	1.93	15	1
1:A:119:HIS:HB2	1:A:128:PHE:HE2	0.40	1.76	4	1
1:A:186:ASN:HB3	1:A:189:ASN:O	0.40	2.16	9	1
1:A:294:ASN:O	1:A:296:PRO:HD3	0.40	2.17	12	1
1:A:202:TYR:HB2	1:A:354:ILE:HG13	0.40	1.92	4	1
1:A:171:HIS:O	1:A:172:GLU:HB2	0.40	2.16	6	1
1:A:217:PRO:HD3	1:A:234:ASN:O	0.40	2.16	10	1
1:A:36:GLU:O	1:A:56:MET:HG2	0.40	2.17	11	1
1:A:240:ARG:HH11	1:A:309:LEU:HD11	0.40	1.75	13	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	309/368 (84%)	264±5 (85±2%)	36±4 (12±1%)	10±2 (3±1%)	7	38
All	All	6180/7360 (84%)	5270 (85%)	712 (12%)	198 (3%)	7	38

All 73 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	310	ASP	14
1	A	135	GLY	11
1	A	296	PRO	9
1	A	92	LYS	9
1	A	231	ASP	9
1	A	172	GLU	8
1	A	295	LYS	7
1	A	48	PHE	6
1	A	314	LYS	6
1	A	217	PRO	5
1	A	335	ASP	5
1	A	240	ARG	4
1	A	356	LYS	4
1	A	66	ALA	4
1	A	338	LYS	4
1	A	238	PRO	4
1	A	337	GLY	3
1	A	147	LYS	3
1	A	313	GLU	3
1	A	47	GLY	3
1	A	311	TYR	3
1	A	197	ASP	3
1	A	239	SER	3
1	A	215	GLU	3
1	A	78	GLY	2
1	A	36	GLU	2
1	A	35	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	207	GLU	2
1	A	208	GLY	2
1	A	334	LYS	2
1	A	291	PRO	2
1	A	198	TYR	2
1	A	309	LEU	2
1	A	34	LYS	2
1	A	206	PRO	2
1	A	292	GLU	2
1	A	214	LYS	2
1	A	294	ASN	2
1	A	122	ASN	2
1	A	336	ASP	2
1	A	107	TYR	1
1	A	216	ASP	1
1	A	203	ARG	1
1	A	200	LEU	1
1	A	222	ASP	1
1	A	211	LYS	1
1	A	352	LYS	1
1	A	57	ASN	1
1	A	120	ASP	1
1	A	210	HIS	1
1	A	196	VAL	1
1	A	293	LYS	1
1	A	199	GLY	1
1	A	46	GLY	1
1	A	55	ASP	1
1	A	76	ASP	1
1	A	179	LYS	1
1	A	353	THR	1
1	A	312	THR	1
1	A	177	ASP	1
1	A	171	HIS	1
1	A	178	ILE	1
1	A	228	THR	1
1	A	175	HIS	1
1	A	133	ARG	1
1	A	49	GLY	1
1	A	212	GLU	1
1	A	201	ALA	1
1	A	50	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	75	SER	1
1	A	56	MET	1
1	A	204	TYR	1
1	A	123	GLY	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	271/319 (85%)	252±5 (93±2%)	19±5 (7±2%)	18	67
All	All	5420/6380 (85%)	5034 (93%)	386 (7%)	18	67

All 142 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	354	ILE	18
1	A	282	ILE	14
1	A	142	TYR	11
1	A	28	ILE	10
1	A	155	LEU	9
1	A	160	ARG	8
1	A	323	ILE	7
1	A	147	LYS	7
1	A	286	MET	7
1	A	80	LEU	6
1	A	307	LYS	6
1	A	170	GLU	6
1	A	326	GLN	6
1	A	311	TYR	5
1	A	99	TRP	5
1	A	258	HIS	5
1	A	241	ARG	5
1	A	243	ASP	5
1	A	27	GLU	5
1	A	240	ARG	4
1	A	228	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	89	ARG	4
1	A	103	ARG	4
1	A	352	LYS	4
1	A	88	GLN	4
1	A	108	LEU	4
1	A	338	LYS	4
1	A	212	GLU	4
1	A	225	ILE	4
1	A	226	GLU	4
1	A	35	LYS	4
1	A	171	HIS	4
1	A	133	ARG	3
1	A	356	LYS	3
1	A	298	GLU	3
1	A	213	TYR	3
1	A	309	LEU	3
1	A	152	LYS	3
1	A	31	ASP	3
1	A	163	ASP	3
1	A	290	PHE	3
1	A	318	GLU	3
1	A	181	SER	3
1	A	231	ASP	3
1	A	269	LYS	3
1	A	137	ASP	3
1	A	98	LYS	3
1	A	92	LYS	3
1	A	222	ASP	3
1	A	184	LEU	3
1	A	224	THR	3
1	A	264	ASN	3
1	A	140	LYS	2
1	A	313	GLU	2
1	A	162	LEU	2
1	A	124	LYS	2
1	A	353	THR	2
1	A	245	GLU	2
1	A	188	LYS	2
1	A	77	ASN	2
1	A	187	TYR	2
1	A	211	LYS	2
1	A	325	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	230	ILE	2
1	A	34	LYS	2
1	A	94	GLU	2
1	A	85	LYS	2
1	A	70	VAL	2
1	A	151	ARG	2
1	A	234	ASN	2
1	A	84	LEU	2
1	A	122	ASN	2
1	A	186	ASN	2
1	A	57	ASN	2
1	A	314	LYS	2
1	A	292	GLU	2
1	A	191	ASP	2
1	A	197	ASP	2
1	A	281	ASN	2
1	A	265	LEU	2
1	A	253	GLN	2
1	A	334	LYS	2
1	A	166	GLU	2
1	A	252	ILE	2
1	A	56	MET	2
1	A	200	LEU	2
1	A	153	THR	2
1	A	203	ARG	2
1	A	233	HIS	2
1	A	118	LEU	2
1	A	71	LYS	2
1	A	322	ASP	1
1	A	107	TYR	1
1	A	336	ASP	1
1	A	145	ASN	1
1	A	262	GLU	1
1	A	32	MET	1
1	A	291	PRO	1
1	A	179	LYS	1
1	A	273	ASP	1
1	A	41	LEU	1
1	A	51	ILE	1
1	A	202	TYR	1
1	A	172	GLU	1
1	A	159	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	121	LYS	1
1	A	38	LYS	1
1	A	279	ARG	1
1	A	328	LEU	1
1	A	76	ASP	1
1	A	303	MET	1
1	A	131	MET	1
1	A	182	ASN	1
1	A	266	LYS	1
1	A	198	TYR	1
1	A	329	LYS	1
1	A	112	LYS	1
1	A	247	LEU	1
1	A	55	ASP	1
1	A	277	ARG	1
1	A	312	THR	1
1	A	119	HIS	1
1	A	304	GLU	1
1	A	106	LYS	1
1	A	215	GLU	1
1	A	288	LYS	1
1	A	321	ARG	1
1	A	82	THR	1
1	A	79	PRO	1
1	A	97	GLN	1
1	A	105	LEU	1
1	A	37	TRP	1
1	A	130	ILE	1
1	A	100	ILE	1
1	A	295	LYS	1
1	A	192	GLN	1
1	A	93	PRO	1
1	A	104	LYS	1
1	A	29	ILE	1
1	A	214	LYS	1
1	A	175	HIS	1
1	A	132	ASP	1

6.3.3 RNA ⓘ

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 72% for the well-defined parts and 69% 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 [i](#)

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	3545
Number of shifts mapped to atoms	3545
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	354	0.10 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	317	0.61 ± 0.08	Should be applied
$^{13}\text{C}'$	343	0.18 ± 0.09	None needed (< 0.5 ppm)
^{15}N	327	-0.41 ± 0.21	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 72%, i.e. 2857 atoms were assigned a chemical shift out of a possible 3972. 34 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1477/1515 (97%)	577/603 (96%)	612/618 (99%)	288/294 (98%)
Sidechain	1264/2109 (60%)	850/1245 (68%)	409/765 (53%)	5/99 (5%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	116/348 (33%)	111/178 (62%)	0/151 (0%)	5/19 (26%)
Overall	2857/3972 (72%)	1538/2026 (76%)	1021/1534 (67%)	298/412 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 69%, i.e. 3200 atoms were assigned a chemical shift out of a possible 4615. 40 out of 53 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	1674/1768 (95%)	650/704 (92%)	697/720 (97%)	327/344 (95%)
Sidechain	1406/2474 (57%)	935/1462 (64%)	466/887 (53%)	5/125 (4%)
Aromatic	120/373 (32%)	115/191 (60%)	0/159 (0%)	5/23 (22%)
Overall	3200/4615 (69%)	1700/2357 (72%)	1163/1766 (66%)	337/492 (68%)

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	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HG22	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HG21	-0.80	2.13 – -0.57	-5.8
1	A	29	ILE	HD11	-0.94	2.13 – -0.77	-5.6
1	A	29	ILE	HD12	-0.94	2.13 – -0.77	-5.6
1	A	29	ILE	HD13	-0.94	2.13 – -0.77	-5.6
1	A	130	ILE	HG22	-0.62	2.13 – -0.57	-5.2
1	A	130	ILE	HG23	-0.62	2.13 – -0.57	-5.2
1	A	130	ILE	HG21	-0.62	2.13 – -0.57	-5.2

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:

