Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 05:14 PM EDT

PDB ID	:	2KTY
BMRB ID	:	16715
Title	:	Solution Structure of human Vaccinia Related Kinase-1
Authors	:	Shin, J.; Yoon, H.
Deposited on	:	2010-02-10

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

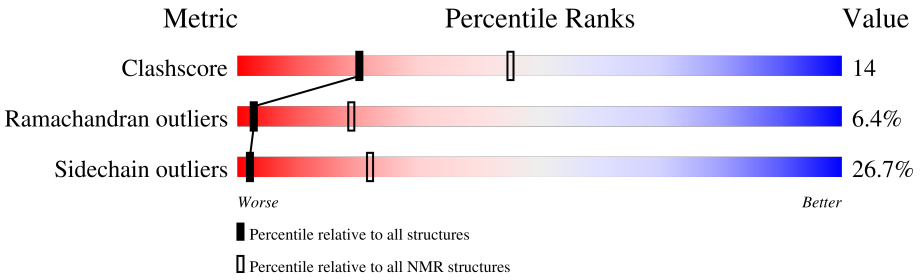
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	368	45% 39% • 12% •

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:25-A:56, A:66-A:335, A:339-A:345, A:350-A:356 (316)	1.45	4

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5833 atoms, of which 2932 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	360	5833	1848	2932	508	531	14	0

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

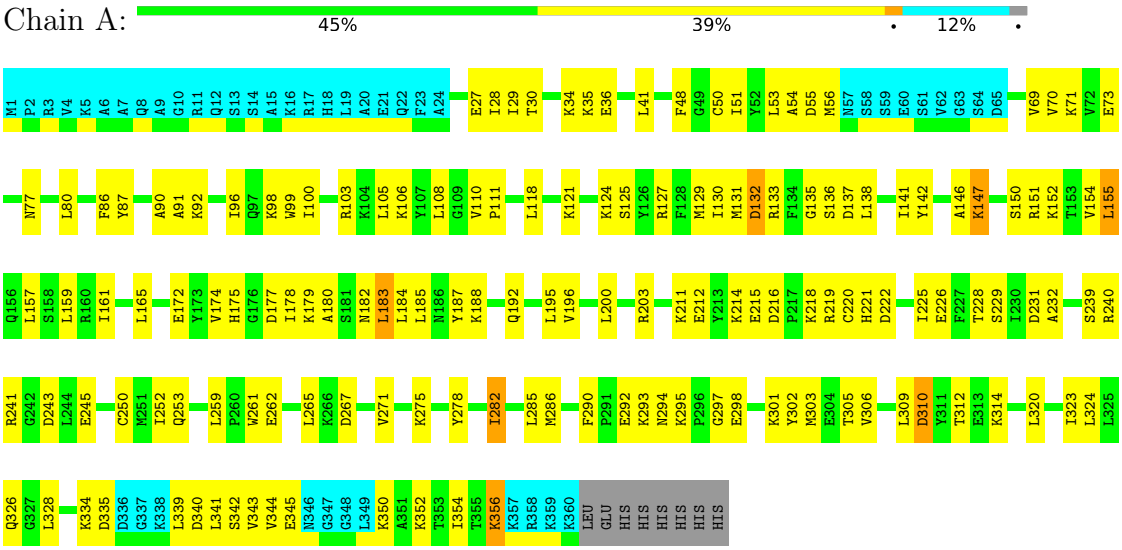
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:



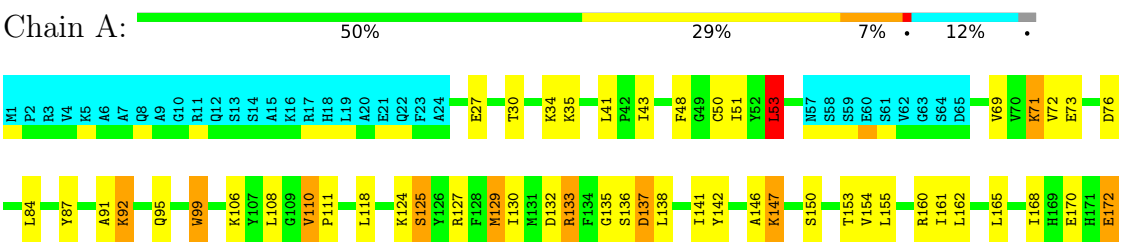
4.2 Scores per residue for each member of the ensemble

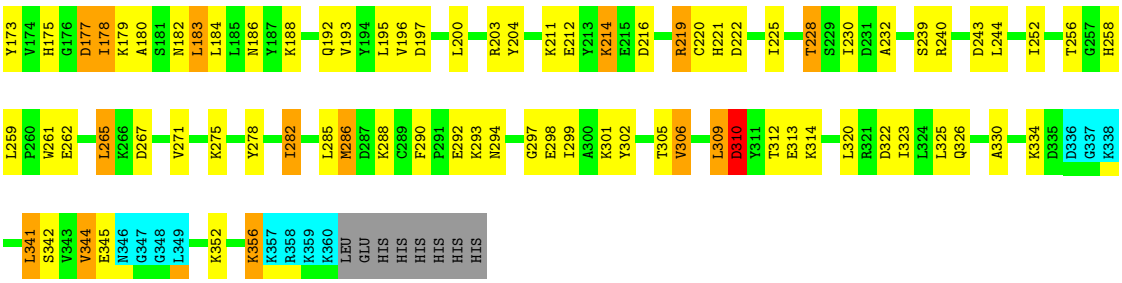
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Serine/threonine-protein kinase VRK1

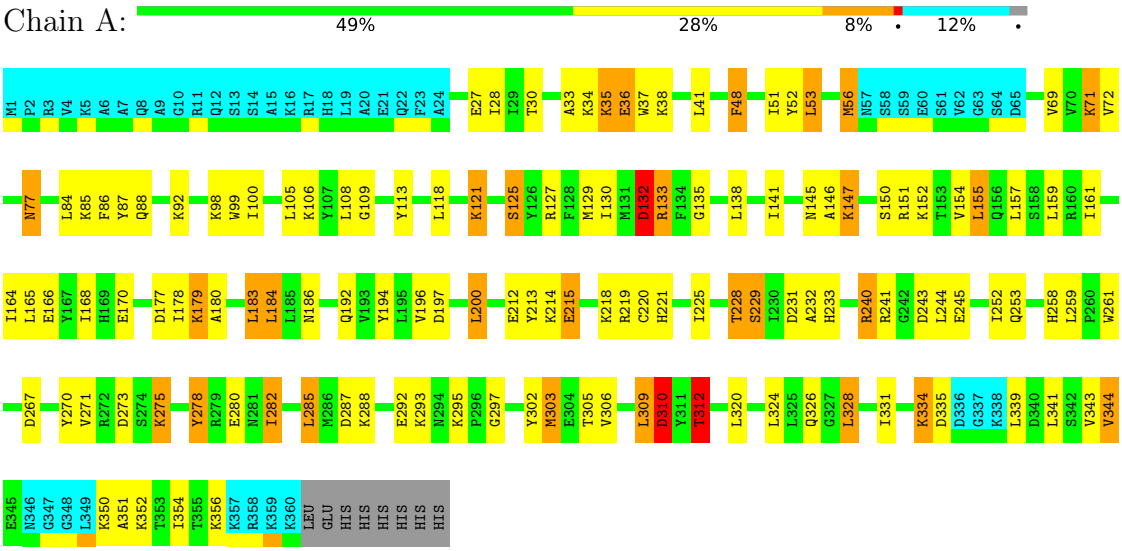
Chain A:





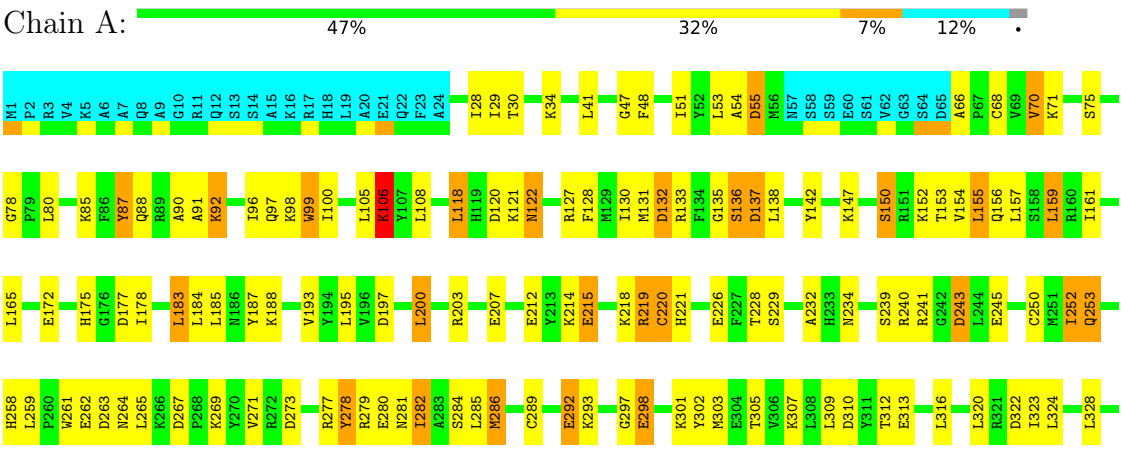
4.2.2 Score per residue for model 2

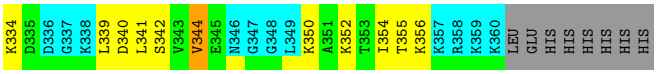
• Molecule 1: Serine/threonine-protein kinase VRK1



4.2.3 Score per residue for model 3

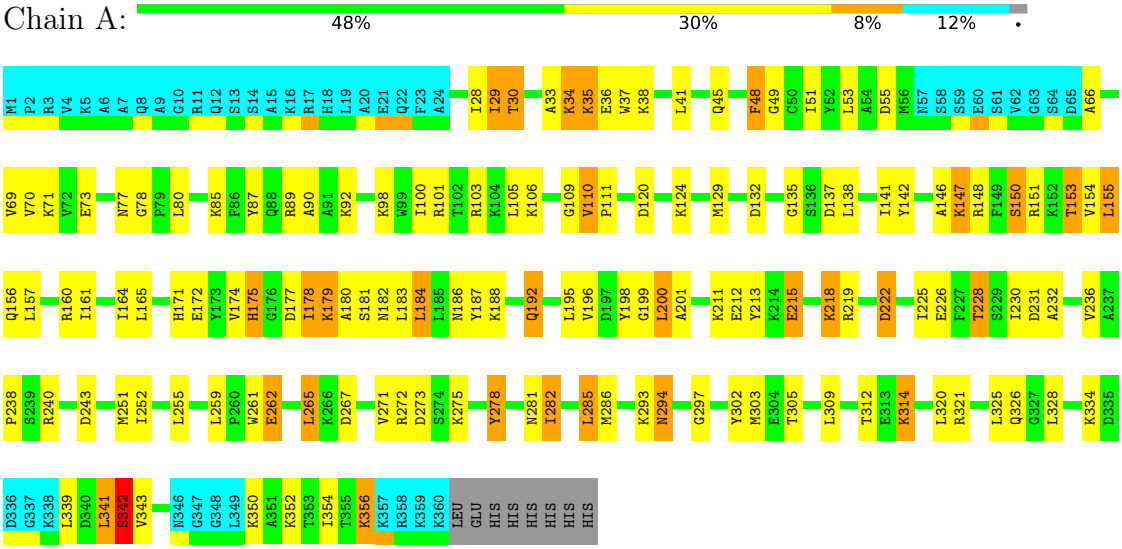
• Molecule 1: Serine/threonine-protein kinase VRK1





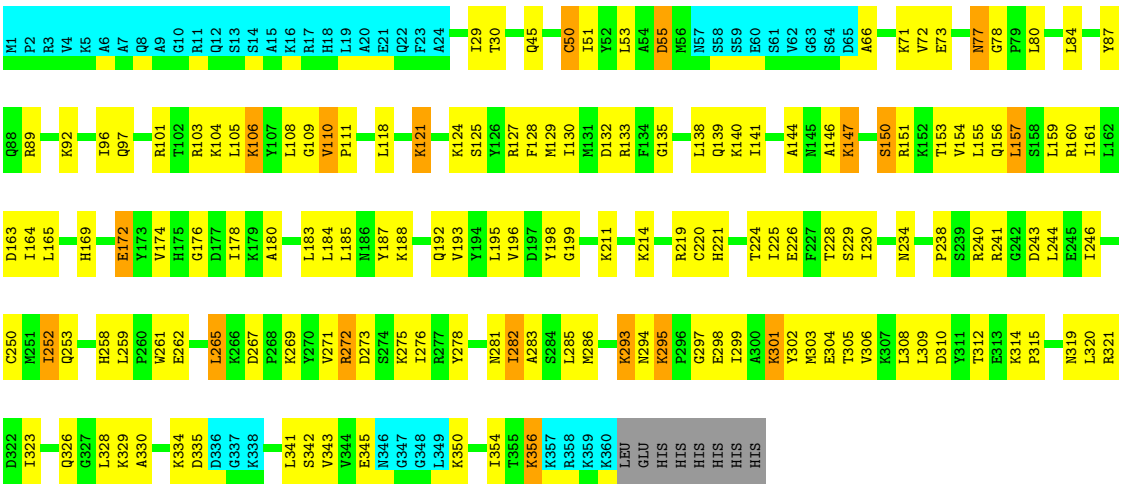
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Serine/threonine-protein kinase VRK1



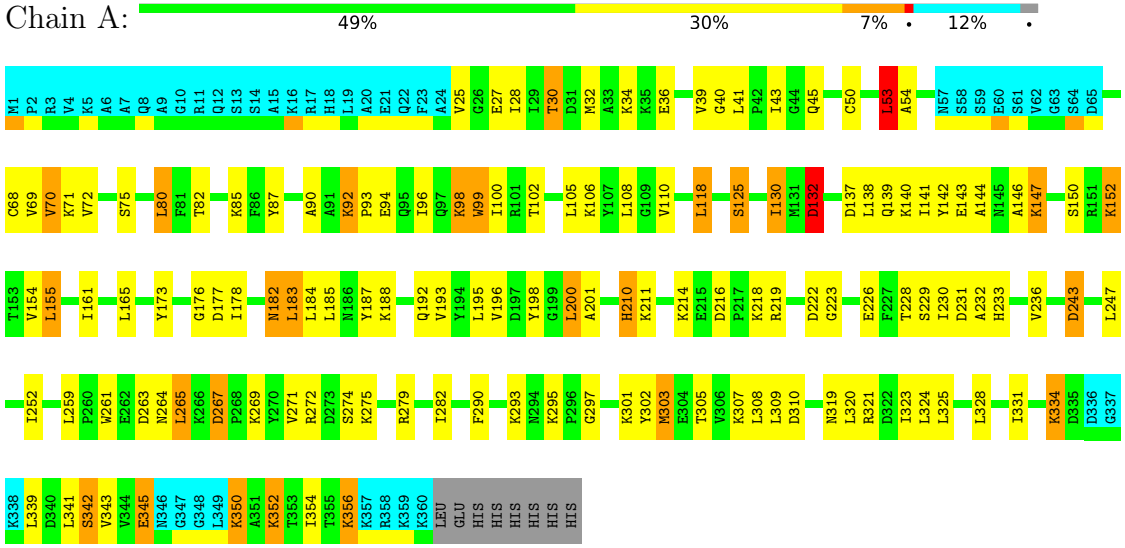
4.2.5 Score per residue for model 5

• Molecule 1: Serine/threonine-protein kinase VRK1



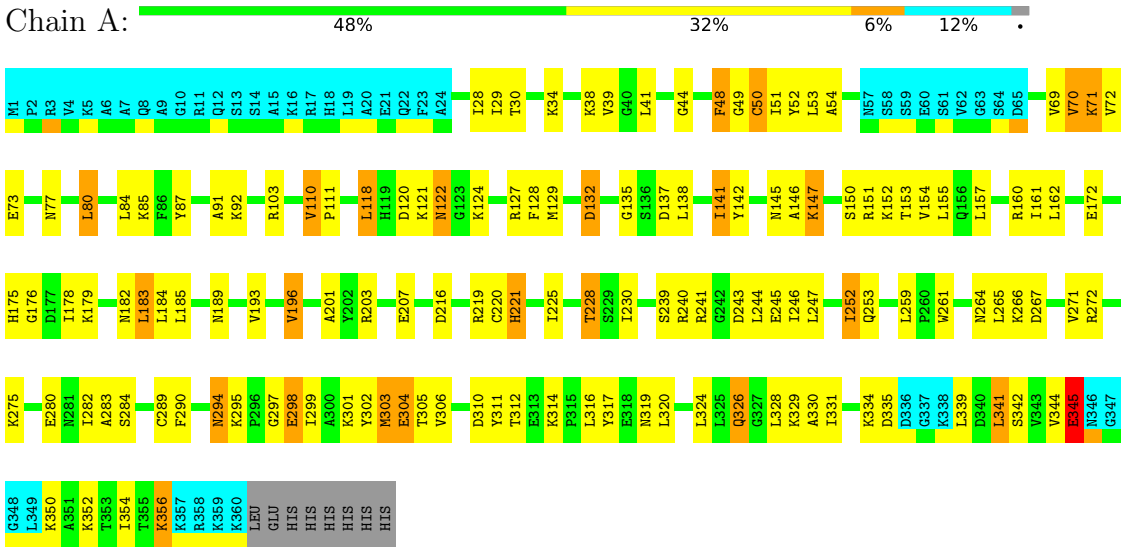
4.2.6 Score per residue for model 6

• Molecule 1: Serine/threonine-protein kinase VRK1



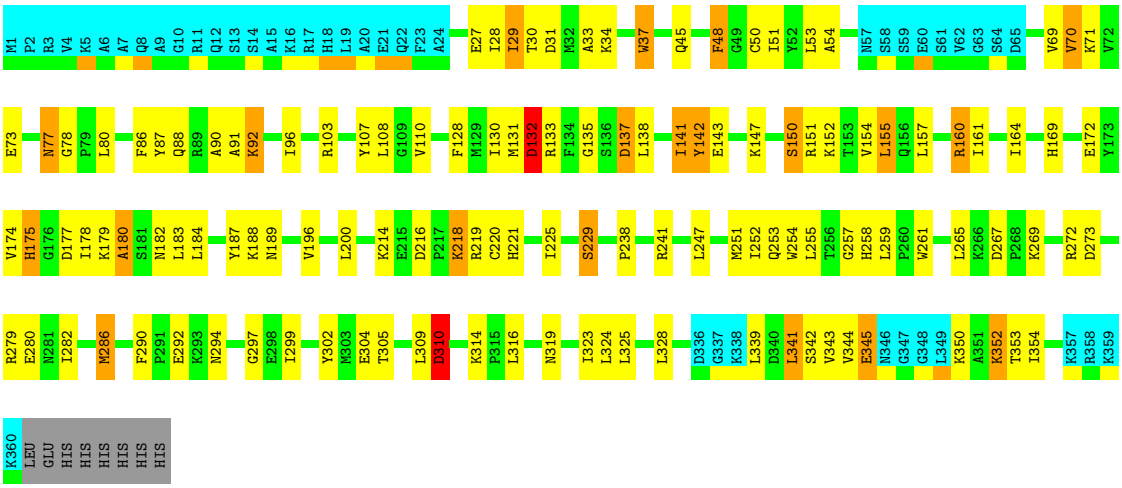
4.2.7 Score per residue for model 7

• Molecule 1: Serine/threonine-protein kinase VRK1



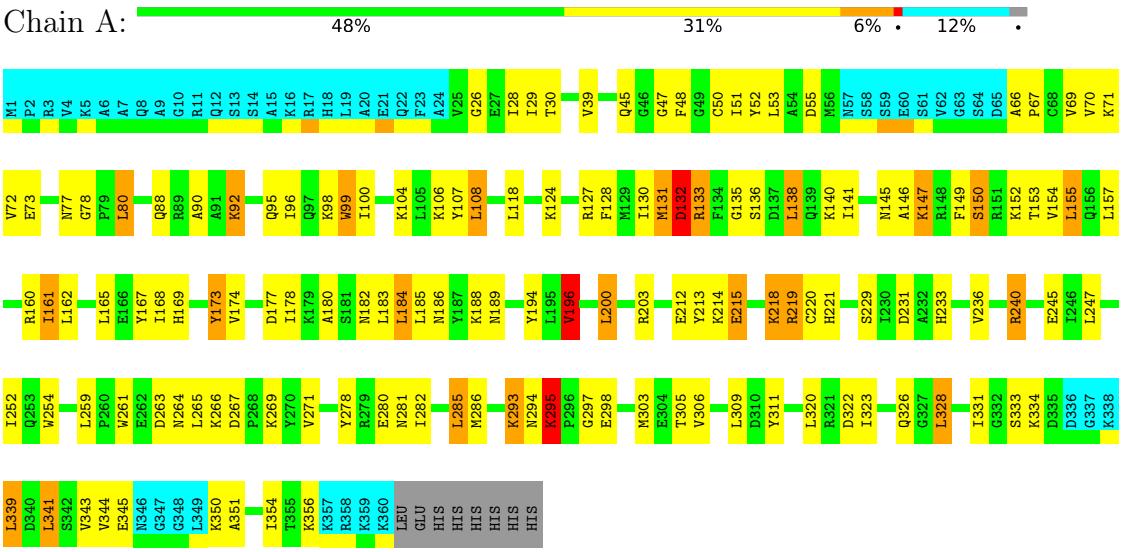
4.2.8 Score per residue for model 8

• Molecule 1: Serine/threonine-protein kinase VRK1



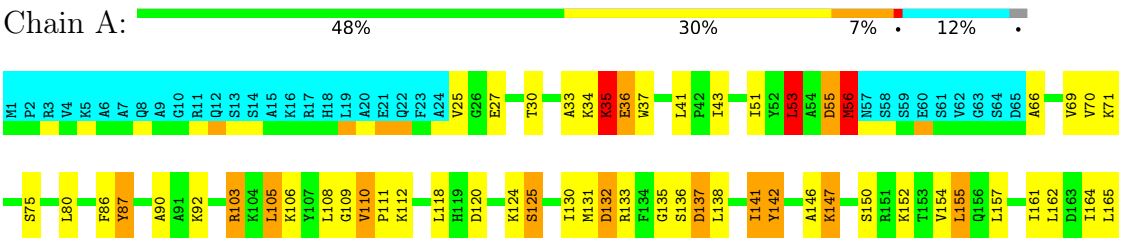
4.2.9 Score per residue for model 9

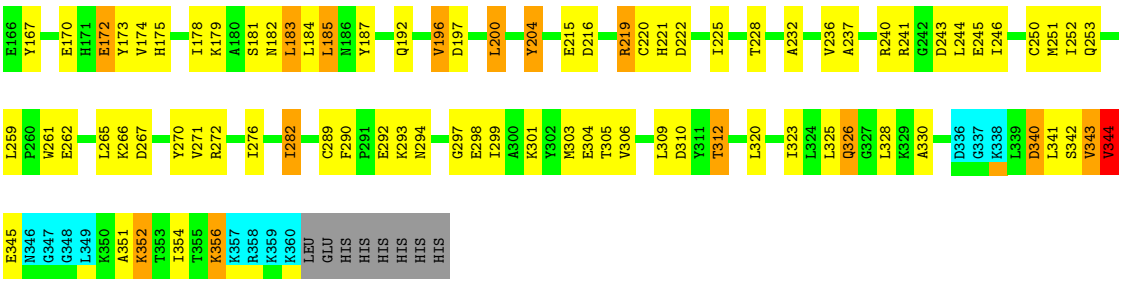
• Molecule 1: Serine/threonine-protein kinase VRK1



4.2.10 Score per residue for model 10

• Molecule 1: Serine/threonine-protein kinase VRK1

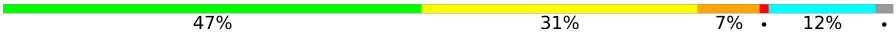


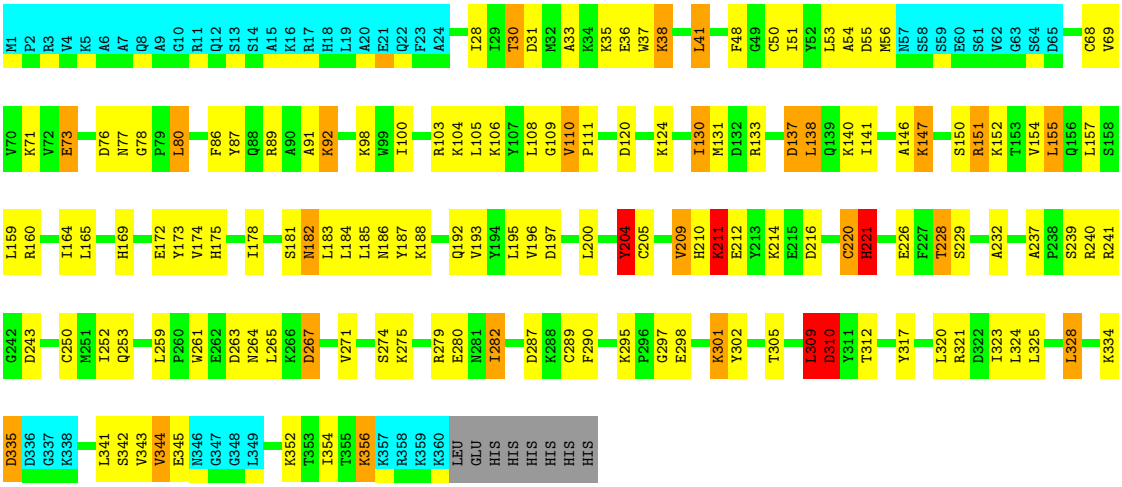


4.2.11 Score per residue for model 11

• Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:

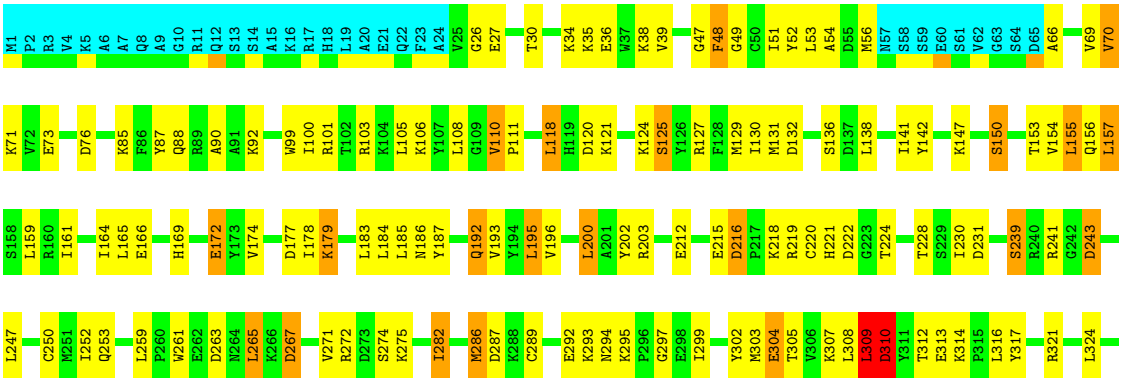


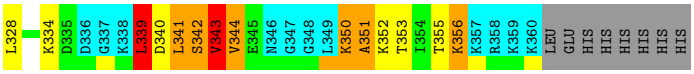


4.2.12 Score per residue for model 12

• Molecule 1: Serine/threonine-protein kinase VRK1

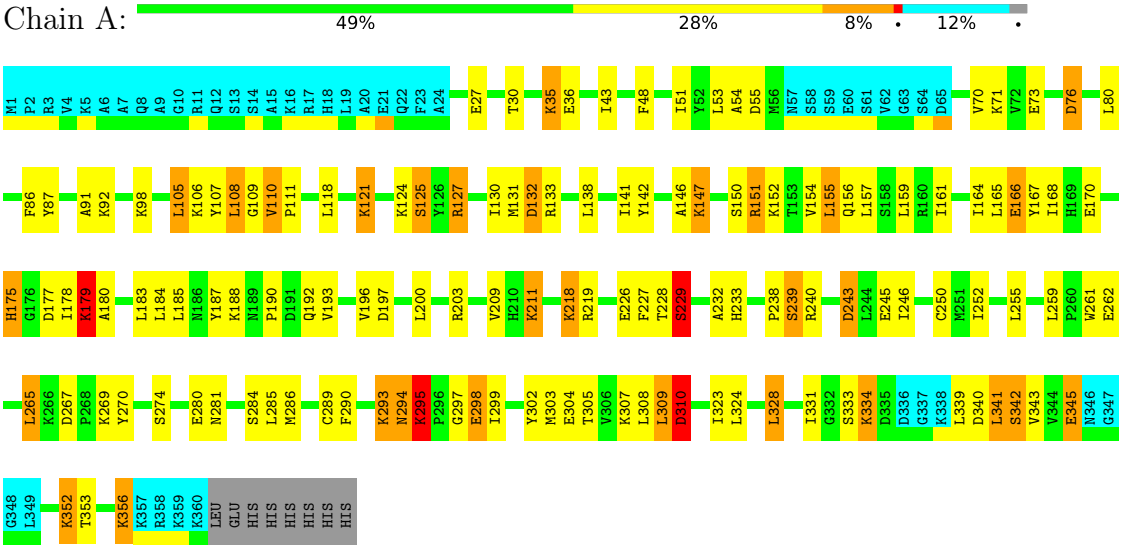
Chain A:





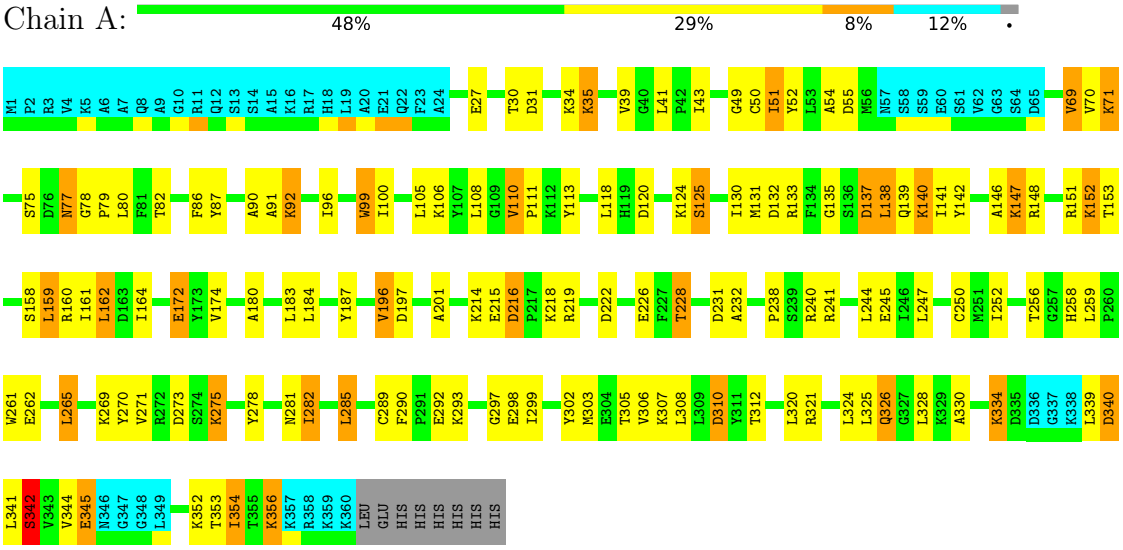
4.2.13 Score per residue for model 13

• Molecule 1: Serine/threonine-protein kinase VRK1



4.2.14 Score per residue for model 14

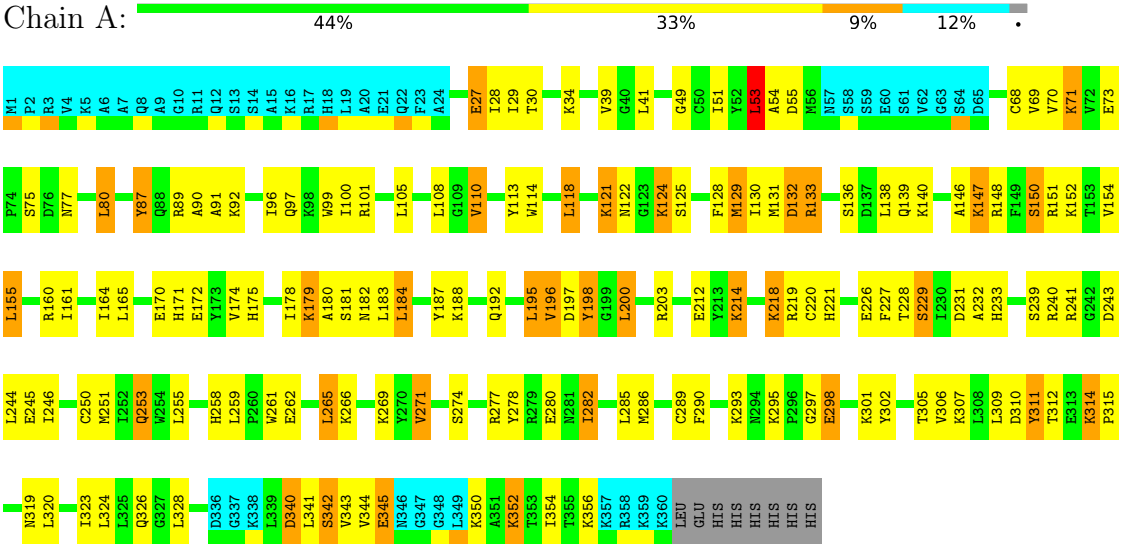
• Molecule 1: Serine/threonine-protein kinase VRK1



4.2.15 Score per residue for model 15

• Molecule 1: Serine/threonine-protein kinase VRK1

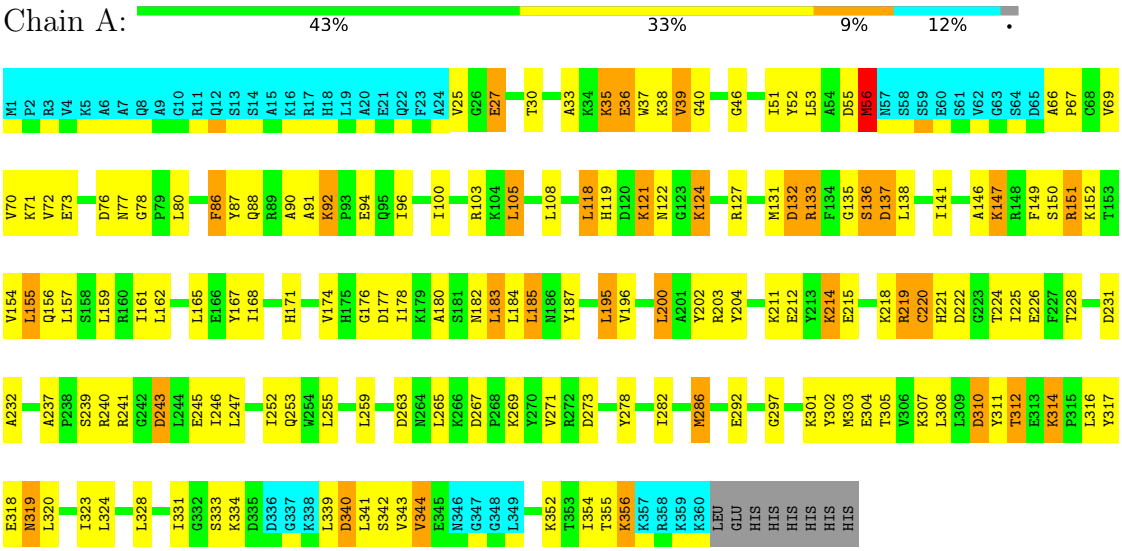
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Serine/threonine-protein kinase VRK1

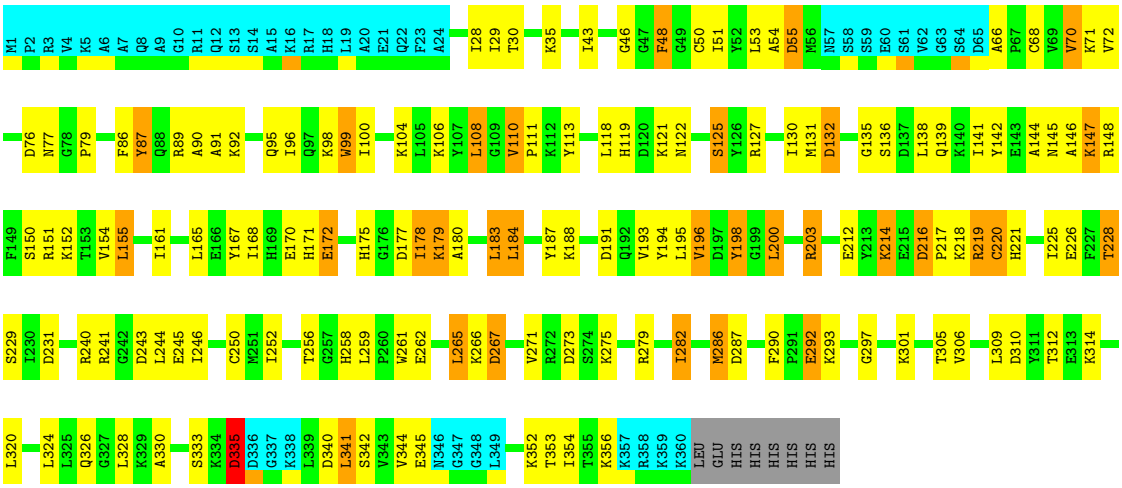
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Serine/threonine-protein kinase VRK1

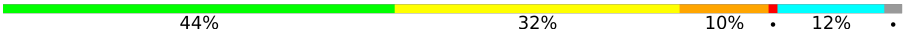
Chain A:

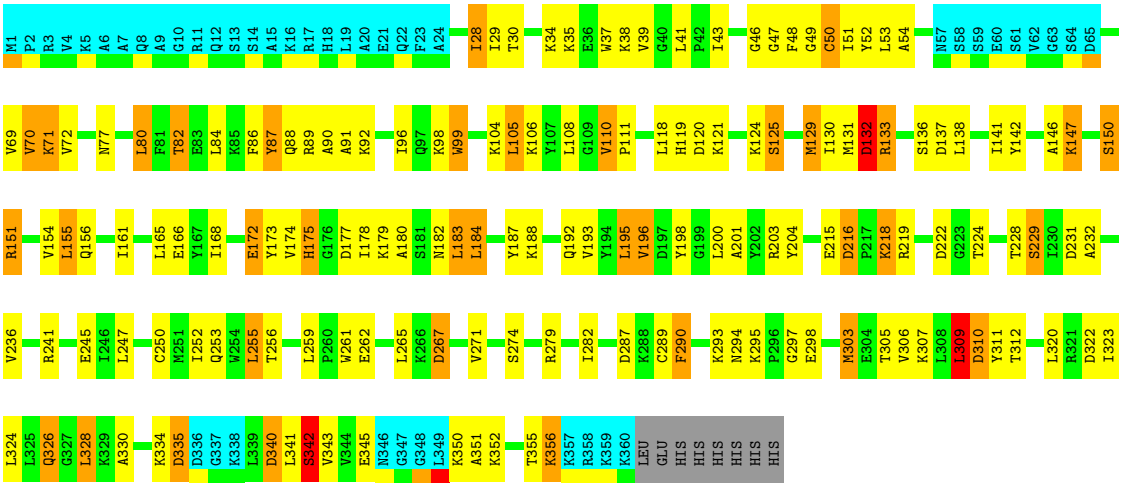


4.2.18 Score per residue for model 18

• Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:

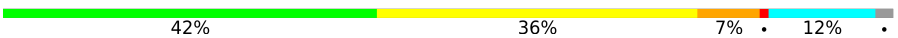


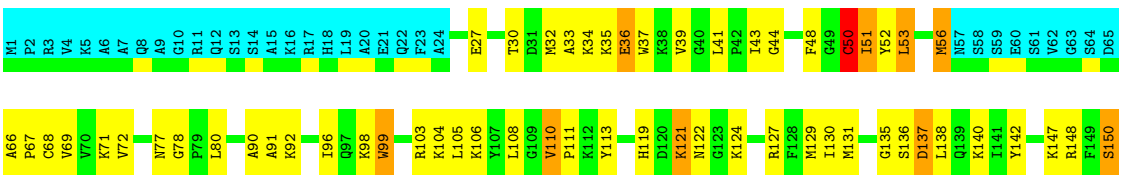


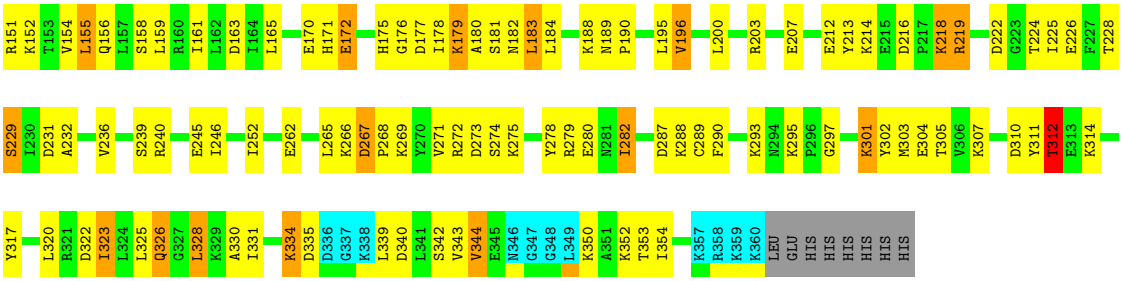
4.2.19 Score per residue for model 19

• Molecule 1: Serine/threonine-protein kinase VRK1

Chain A:



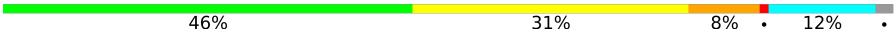


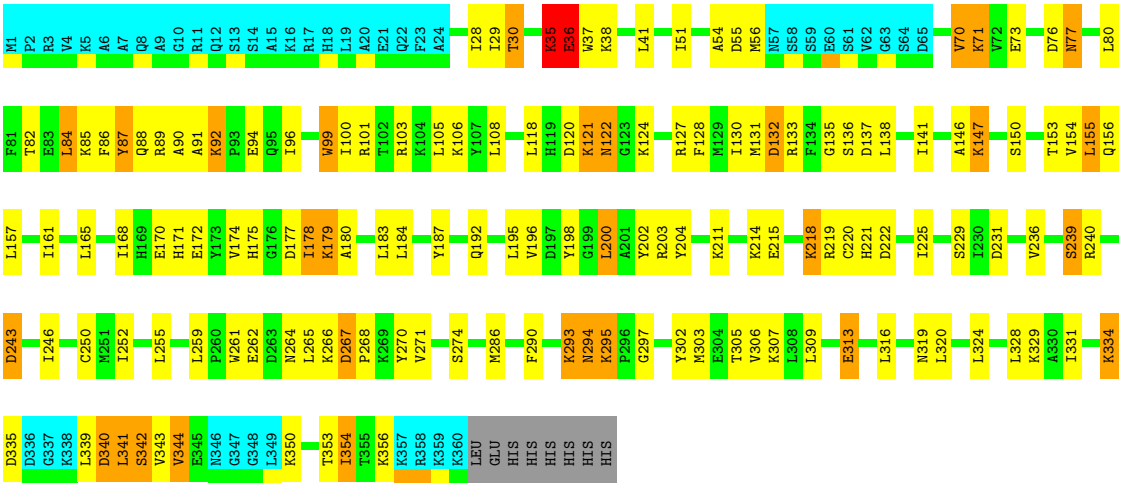


4.2.20 Score per residue for model 20

• 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*.

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
CYANA	refinement	

No chemical shift data was provided.

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	2574	2599	2599	71±9
All	All	51480	51980	51980	1420

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:LEU:HD11	1:A:341:LEU:HD22	0.95	1.36	6	2
1:A:138:LEU:HD22	1:A:183:LEU:HD22	0.85	1.46	5	4
1:A:184:LEU:HD23	1:A:196:VAL:HG22	0.84	1.49	16	5
1:A:141:ILE:HD13	1:A:341:LEU:HD23	0.83	1.50	11	4
1:A:141:ILE:HG21	1:A:341:LEU:HD23	0.83	1.50	6	3
1:A:110:VAL:HG23	1:A:164:ILE:HD11	0.83	1.46	12	3
1:A:200:LEU:HD22	1:A:200:LEU:O	0.82	1.74	4	1
1:A:161:ILE:HG21	1:A:178:ILE:HD11	0.81	1.51	4	5
1:A:43:ILE:HD11	1:A:53:LEU:HD12	0.80	1.50	10	2
1:A:96:ILE:HG23	1:A:108:LEU:HD12	0.78	1.54	8	3
1:A:157:LEU:HD23	1:A:193:VAL:HG11	0.77	1.55	11	2
1:A:161:ILE:HG23	1:A:195:LEU:HD11	0.76	1.57	20	2
1:A:155:LEU:HD23	1:A:328:LEU:HD13	0.75	1.58	11	2
1:A:278:TYR:CG	1:A:285:LEU:HD22	0.74	2.17	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:ILE:HG23	1:A:108:LEU:HD22	0.73	1.61	3	7
1:A:30:THR:HG23	1:A:35:LYS:HG3	0.73	1.61	13	3
1:A:141:ILE:HD11	1:A:344:VAL:HG22	0.73	1.60	12	2
1:A:225:ILE:HG21	1:A:271:VAL:HG21	0.73	1.58	17	1
1:A:118:LEU:C	1:A:118:LEU:HD22	0.72	2.05	6	3
1:A:141:ILE:HG21	1:A:341:LEU:HD22	0.72	1.62	2	2
1:A:184:LEU:HD21	1:A:196:VAL:HG12	0.71	1.61	17	4
1:A:51:ILE:HD12	1:A:71:LYS:CB	0.71	2.15	18	12
1:A:138:LEU:HB3	1:A:180:ALA:HB1	0.71	1.61	15	11
1:A:138:LEU:HD22	1:A:183:LEU:HD13	0.71	1.60	14	7
1:A:184:LEU:HD23	1:A:196:VAL:HG13	0.71	1.61	19	1
1:A:225:ILE:HG23	1:A:265:LEU:HD21	0.70	1.63	10	2
1:A:141:ILE:HG23	1:A:343:VAL:HG21	0.70	1.61	2	2
1:A:184:LEU:HD21	1:A:196:VAL:CG1	0.70	2.15	15	5
1:A:184:LEU:HD21	1:A:196:VAL:HG13	0.70	1.62	15	2
1:A:29:ILE:HD11	1:A:37:TRP:CH2	0.69	2.22	8	1
1:A:259:LEU:HD13	1:A:261:TRP:CZ2	0.69	2.23	15	17
1:A:99:TRP:CZ3	1:A:108:LEU:HD13	0.69	2.23	2	3
1:A:200:LEU:HD12	1:A:352:LYS:HG2	0.69	1.64	10	1
1:A:224:THR:HG23	1:A:351:ALA:HB2	0.69	1.65	12	1
1:A:90:ALA:HB1	1:A:110:VAL:HG21	0.67	1.66	12	3
1:A:118:LEU:HD21	1:A:125:SER:HB3	0.67	1.67	14	4
1:A:161:ILE:HG21	1:A:178:ILE:CD1	0.67	2.20	17	4
1:A:155:LEU:HG	1:A:328:LEU:HD22	0.67	1.66	11	7
1:A:183:LEU:C	1:A:184:LEU:HD13	0.67	2.11	15	2
1:A:48:PHE:CE2	1:A:351:ALA:HB1	0.66	2.24	2	2
1:A:265:LEU:HA	1:A:271:VAL:HG23	0.66	1.67	15	1
1:A:56:MET:HG2	1:A:66:ALA:HB2	0.66	1.66	16	1
1:A:78:GLY:N	1:A:79:PRO:HD2	0.66	2.06	14	1
1:A:168:ILE:HG22	1:A:173:TYR:O	0.66	1.91	18	1
1:A:177:ASP:CB	1:A:200:LEU:HD23	0.65	2.22	1	1
1:A:302:TYR:CE2	1:A:320:LEU:HD22	0.65	2.26	11	8
1:A:99:TRP:CD1	1:A:99:TRP:C	0.65	2.70	1	9
1:A:155:LEU:HB2	1:A:328:LEU:HD13	0.65	1.68	4	5
1:A:298:GLU:HG2	1:A:324:LEU:HD23	0.65	1.69	18	1
1:A:259:LEU:HD22	1:A:261:TRP:CZ3	0.65	2.27	12	6
1:A:161:ILE:HG21	1:A:247:LEU:HD13	0.65	1.67	9	7
1:A:182:ASN:ND2	1:A:195:LEU:HD22	0.65	2.07	6	1
1:A:182:ASN:OD1	1:A:183:LEU:HD12	0.65	1.91	1	2
1:A:183:LEU:O	1:A:184:LEU:HD23	0.65	1.92	20	1
1:A:118:LEU:HD11	1:A:125:SER:HB2	0.64	1.66	1	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:LEU:HD11	1:A:341:LEU:HD13	0.64	1.68	12	1
1:A:66:ALA:HB3	1:A:67:PRO:HD3	0.64	1.67	9	3
1:A:204:TYR:CB	1:A:209:VAL:HG23	0.64	2.22	11	1
1:A:222:ASP:CB	1:A:232:ALA:HB1	0.64	2.22	4	2
1:A:252:ILE:HD13	1:A:286:MET:CE	0.64	2.22	3	1
1:A:204:TYR:O	1:A:237:ALA:HB1	0.64	1.93	16	1
1:A:141:ILE:HD13	1:A:341:LEU:HD22	0.64	1.69	20	1
1:A:228:THR:HG23	1:A:232:ALA:HB3	0.64	1.70	14	5
1:A:165:LEU:HD21	1:A:243:ASP:OD2	0.64	1.93	2	2
1:A:54:ALA:HB2	1:A:70:VAL:CG1	0.64	2.23	6	1
1:A:244:LEU:HD22	1:A:320:LEU:HD13	0.63	1.70	1	1
1:A:157:LEU:CD2	1:A:193:VAL:HG11	0.63	2.23	5	3
1:A:141:ILE:CD1	1:A:344:VAL:HG22	0.63	2.22	12	2
1:A:157:LEU:O	1:A:161:ILE:HD12	0.63	1.94	20	8
1:A:184:LEU:HD11	1:A:196:VAL:HG22	0.63	1.68	4	1
1:A:302:TYR:CD2	1:A:320:LEU:HD22	0.63	2.28	4	8
1:A:282:ILE:HG21	1:A:303:MET:HB3	0.63	1.71	18	2
1:A:165:LEU:HD13	1:A:243:ASP:OD2	0.63	1.93	6	1
1:A:184:LEU:O	1:A:185:LEU:HD23	0.63	1.94	10	3
1:A:225:ILE:HD13	1:A:268:PRO:HA	0.62	1.71	20	1
1:A:183:LEU:HD23	1:A:193:VAL:HG21	0.62	1.71	6	2
1:A:278:TYR:CD2	1:A:285:LEU:HD22	0.62	2.29	2	1
1:A:155:LEU:HD22	1:A:328:LEU:HD22	0.62	1.71	17	1
1:A:265:LEU:O	1:A:265:LEU:HD13	0.62	1.93	10	6
1:A:253:GLN:OE1	1:A:259:LEU:HD11	0.62	1.94	8	1
1:A:28:ILE:HD12	1:A:38:LYS:HG3	0.62	1.71	18	1
1:A:278:TYR:CZ	1:A:285:LEU:HD12	0.62	2.29	3	1
1:A:174:VAL:HG21	1:A:238:PRO:HG2	0.62	1.70	8	2
1:A:69:VAL:HG22	1:A:132:ASP:O	0.62	1.93	8	9
1:A:90:ALA:O	1:A:96:ILE:HD11	0.62	1.94	6	7
1:A:50:CYS:O	1:A:72:VAL:HG12	0.62	1.95	5	7
1:A:157:LEU:HD23	1:A:254:TRP:CH2	0.62	2.30	8	2
1:A:309:LEU:HD13	1:A:309:LEU:O	0.62	1.95	10	1
1:A:138:LEU:HD22	1:A:183:LEU:CB	0.62	2.23	4	11
1:A:141:ILE:HG21	1:A:341:LEU:HG	0.62	1.72	11	2
1:A:298:GLU:CG	1:A:324:LEU:HD23	0.62	2.25	3	2
1:A:230:ILE:HD11	1:A:275:LYS:CB	0.62	2.25	6	2
1:A:137:ASP:O	1:A:141:ILE:HD12	0.61	1.94	6	7
1:A:73:GLU:CG	1:A:80:LEU:HD13	0.61	2.25	4	1
1:A:184:LEU:HD23	1:A:196:VAL:CG2	0.61	2.25	12	3
1:A:225:ILE:HA	1:A:228:THR:HG22	0.61	1.71	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:ARG:O	1:A:164:ILE:HG22	0.61	1.95	8	3
1:A:253:GLN:HB2	1:A:259:LEU:HD21	0.61	1.72	11	7
1:A:200:LEU:HD12	1:A:352:LYS:CG	0.61	2.25	10	1
1:A:118:LEU:HD11	1:A:125:SER:CB	0.61	2.26	12	5
1:A:183:LEU:C	1:A:184:LEU:HD22	0.61	2.14	16	12
1:A:55:ASP:HB2	1:A:66:ALA:HB3	0.61	1.70	3	3
1:A:150:SER:O	1:A:154:VAL:HG23	0.61	1.94	11	19
1:A:73:GLU:HG3	1:A:80:LEU:HD23	0.61	1.72	11	2
1:A:141:ILE:HG21	1:A:341:LEU:CD2	0.61	2.25	18	5
1:A:278:TYR:CE2	1:A:285:LEU:HD12	0.61	2.31	3	3
1:A:155:LEU:HG	1:A:324:LEU:HD22	0.61	1.73	2	1
1:A:177:ASP:CG	1:A:200:LEU:HD13	0.61	2.16	12	4
1:A:53:LEU:HD13	1:A:68:CYS:O	0.61	1.95	11	1
1:A:82:THR:HG21	1:A:201:ALA:HB3	0.61	1.71	14	1
1:A:328:LEU:O	1:A:331:ILE:HG22	0.61	1.96	6	4
1:A:185:LEU:HD11	1:A:341:LEU:HD23	0.61	1.73	9	2
1:A:51:ILE:HG23	1:A:71:LYS:HA	0.61	1.72	3	13
1:A:220:CYS:O	1:A:355:THR:HG21	0.61	1.96	3	1
1:A:136:SER:OG	1:A:344:VAL:HG11	0.61	1.96	12	1
1:A:154:VAL:HG21	1:A:255:LEU:CD1	0.61	2.26	16	1
1:A:136:SER:CB	1:A:344:VAL:HG21	0.61	2.25	20	1
1:A:281:ASN:O	1:A:285:LEU:HD12	0.60	1.95	14	3
1:A:176:GLY:O	1:A:246:ILE:HG21	0.60	1.96	5	2
1:A:53:LEU:HD23	1:A:68:CYS:O	0.60	1.96	6	2
1:A:228:THR:CG2	1:A:232:ALA:HB3	0.60	2.27	3	3
1:A:184:LEU:HD21	1:A:196:VAL:HG23	0.60	1.71	4	1
1:A:222:ASP:HB2	1:A:232:ALA:HB1	0.60	1.73	14	2
1:A:185:LEU:HD11	1:A:341:LEU:CD2	0.60	2.26	7	2
1:A:228:THR:O	1:A:232:ALA:HB3	0.60	1.96	15	7
1:A:177:ASP:HB2	1:A:200:LEU:HD22	0.60	1.72	3	4
1:A:264:ASN:O	1:A:271:VAL:HG13	0.60	1.96	3	2
1:A:184:LEU:HD23	1:A:196:VAL:HG12	0.60	1.70	7	4
1:A:141:ILE:HG23	1:A:342:SER:HB2	0.60	1.72	4	3
1:A:66:ALA:HB3	1:A:67:PRO:CD	0.60	2.27	9	2
1:A:30:THR:HG23	1:A:35:LYS:CG	0.60	2.26	14	3
1:A:200:LEU:HD21	1:A:222:ASP:O	0.60	1.97	10	1
1:A:225:ILE:CG2	1:A:271:VAL:HG21	0.60	2.26	17	3
1:A:220:CYS:O	1:A:221:HIS:C	0.60	2.38	11	11
1:A:103:ARG:HB3	1:A:105:LEU:HD23	0.60	1.74	10	1
1:A:200:LEU:HD11	1:A:352:LYS:HD3	0.60	1.72	6	1
1:A:225:ILE:HG23	1:A:265:LEU:CD2	0.60	2.27	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:ARG:HG3	1:A:328:LEU:HD11	0.60	1.73	11	2
1:A:141:ILE:CG1	1:A:344:VAL:HG22	0.60	2.26	20	1
1:A:155:LEU:CB	1:A:328:LEU:HD13	0.59	2.27	12	4
1:A:244:LEU:HD21	1:A:317:TYR:CE1	0.59	2.32	7	1
1:A:155:LEU:HD22	1:A:328:LEU:CD2	0.59	2.27	17	1
1:A:240:ARG:NH2	1:A:312:THR:HG22	0.59	2.12	2	1
1:A:252:ILE:HG22	1:A:299:ILE:HG21	0.59	1.72	14	1
1:A:262:GLU:O	1:A:265:LEU:HD22	0.59	1.97	15	1
1:A:213:TYR:HB2	1:A:236:VAL:HG21	0.59	1.74	19	1
1:A:96:ILE:HG22	1:A:100:ILE:HD12	0.59	1.73	6	6
1:A:165:LEU:HD13	1:A:243:ASP:OD1	0.59	1.98	20	2
1:A:136:SER:HB3	1:A:344:VAL:HG11	0.59	1.73	16	1
1:A:190:PRO:HB3	1:A:344:VAL:HG21	0.59	1.74	19	1
1:A:342:SER:O	1:A:344:VAL:HG23	0.59	1.97	3	2
1:A:184:LEU:HD12	1:A:194:TYR:O	0.59	1.98	9	3
1:A:118:LEU:HD21	1:A:125:SER:CB	0.59	2.28	14	1
1:A:309:LEU:HD12	1:A:310:ASP:O	0.59	1.98	8	2
1:A:86:PHE:CE1	1:A:168:ILE:HG22	0.59	2.32	13	2
1:A:51:ILE:HD12	1:A:71:LYS:HB3	0.59	1.73	14	6
1:A:259:LEU:HD22	1:A:261:TRP:CH2	0.59	2.32	9	10
1:A:155:LEU:HD11	1:A:325:LEU:HD22	0.59	1.74	10	1
1:A:306:VAL:HG23	1:A:320:LEU:HD21	0.59	1.74	1	1
1:A:54:ALA:HB2	1:A:70:VAL:HG12	0.59	1.73	15	9
1:A:118:LEU:HD11	1:A:125:SER:HB3	0.58	1.74	5	1
1:A:155:LEU:CD2	1:A:328:LEU:HD13	0.58	2.28	11	3
1:A:182:ASN:O	1:A:195:LEU:HD23	0.58	1.97	15	3
1:A:137:ASP:OD1	1:A:184:LEU:HD22	0.58	1.98	20	1
1:A:43:ILE:CD1	1:A:53:LEU:HD12	0.58	2.27	10	2
1:A:265:LEU:HD23	1:A:266:LYS:N	0.58	2.13	15	1
1:A:175:HIS:CE1	1:A:195:LEU:HD13	0.58	2.33	4	1
1:A:138:LEU:HD12	1:A:341:LEU:HD21	0.58	1.76	10	3
1:A:185:LEU:HD12	1:A:193:VAL:HG23	0.58	1.74	13	1
1:A:30:THR:HG23	1:A:35:LYS:HB2	0.58	1.75	2	2
1:A:298:GLU:HB3	1:A:324:LEU:HD23	0.58	1.74	7	3
1:A:28:ILE:HD12	1:A:35:LYS:HG3	0.58	1.76	20	1
1:A:29:ILE:HD12	1:A:128:PHE:CD2	0.58	2.34	5	1
1:A:184:LEU:HD22	1:A:184:LEU:N	0.58	2.13	15	15
1:A:105:LEU:HD11	1:A:166:GLU:OE2	0.58	1.98	13	1
1:A:39:VAL:HG23	1:A:52:TYR:CD1	0.58	2.34	7	1
1:A:141:ILE:HG23	1:A:343:VAL:CG2	0.58	2.29	2	1
1:A:252:ILE:HD12	1:A:286:MET:CE	0.58	2.29	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:221:HIS:CG	1:A:221:HIS:O	0.58	2.56	10	3
1:A:225:ILE:HG12	1:A:271:VAL:HG11	0.58	1.75	1	2
1:A:178:ILE:O	1:A:178:ILE:HG22	0.58	1.99	13	10
1:A:69:VAL:HG13	1:A:132:ASP:O	0.58	1.99	9	1
1:A:144:ALA:HB1	1:A:345:GLU:OE2	0.58	1.99	17	1
1:A:90:ALA:CB	1:A:110:VAL:HG21	0.58	2.29	6	2
1:A:174:VAL:HG21	1:A:238:PRO:CG	0.57	2.29	14	1
1:A:100:ILE:HD11	1:A:108:LEU:HD13	0.57	1.75	6	1
1:A:244:LEU:CD2	1:A:320:LEU:HD21	0.57	2.28	17	1
1:A:255:LEU:HD21	1:A:294:ASN:OD1	0.57	1.99	4	2
1:A:185:LEU:HD23	1:A:193:VAL:HG23	0.57	1.76	5	3
1:A:151:ARG:CG	1:A:328:LEU:HD11	0.57	2.29	13	2
1:A:136:SER:CB	1:A:344:VAL:HG11	0.57	2.29	12	1
1:A:141:ILE:HG23	1:A:342:SER:CB	0.57	2.30	18	2
1:A:99:TRP:CH2	1:A:108:LEU:HD13	0.57	2.35	12	2
1:A:138:LEU:HD22	1:A:183:LEU:HB2	0.57	1.76	2	4
1:A:152:LYS:HA	1:A:328:LEU:HD11	0.57	1.77	19	2
1:A:252:ILE:HD11	1:A:290:PHE:CE1	0.57	2.35	7	1
1:A:204:TYR:HB3	1:A:209:VAL:HG23	0.57	1.75	11	1
1:A:138:LEU:CD2	1:A:183:LEU:HD22	0.57	2.27	5	1
1:A:226:GLU:N	1:A:265:LEU:HD21	0.57	2.15	6	1
1:A:39:VAL:HG23	1:A:52:TYR:CD2	0.57	2.35	14	4
1:A:262:GLU:O	1:A:265:LEU:HD23	0.57	1.99	4	4
1:A:138:LEU:HD22	1:A:183:LEU:HB3	0.57	1.77	17	1
1:A:118:LEU:O	1:A:118:LEU:HD23	0.56	2.00	7	2
1:A:309:LEU:HD22	1:A:314:LYS:O	0.56	2.00	15	2
1:A:247:LEU:HD23	1:A:302:TYR:OH	0.56	2.00	12	2
1:A:301:LYS:HB3	1:A:323:ILE:HD13	0.56	1.76	10	3
1:A:52:TYR:CE2	1:A:72:VAL:HG21	0.56	2.35	16	2
1:A:28:ILE:HG23	1:A:38:LYS:CE	0.56	2.31	4	1
1:A:73:GLU:HB2	1:A:80:LEU:HD22	0.56	1.77	20	3
1:A:309:LEU:HD13	1:A:315:PRO:HA	0.56	1.76	15	2
1:A:198:TYR:O	1:A:200:LEU:HD12	0.56	1.99	6	1
1:A:175:HIS:NE2	1:A:201:ALA:HB2	0.56	2.15	7	1
1:A:73:GLU:CD	1:A:80:LEU:HD23	0.56	2.20	9	1
1:A:265:LEU:HD12	1:A:265:LEU:O	0.56	2.00	17	5
1:A:153:THR:O	1:A:157:LEU:HD12	0.56	2.01	5	2
1:A:43:ILE:HD12	1:A:69:VAL:HG11	0.56	1.77	19	2
1:A:53:LEU:HD11	1:A:133:ARG:NE	0.56	2.16	18	1
1:A:53:LEU:HD21	1:A:133:ARG:NE	0.56	2.15	1	3
1:A:151:ARG:NH2	1:A:331:ILE:HG21	0.56	2.16	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLY:O	1:A:164:ILE:HD12	0.56	2.01	4	4
1:A:80:LEU:O	1:A:80:LEU:HD13	0.56	2.01	13	8
1:A:43:ILE:HD11	1:A:53:LEU:HB2	0.56	1.75	13	2
1:A:165:LEU:HD11	1:A:243:ASP:OD1	0.56	2.01	4	1
1:A:283:ALA:HB2	1:A:304:GLU:HB2	0.56	1.75	5	2
1:A:256:THR:HG22	1:A:290:PHE:CD2	0.56	2.36	18	1
1:A:153:THR:HG22	1:A:339:LEU:HD13	0.56	1.77	20	1
1:A:309:LEU:HD13	1:A:314:LYS:O	0.56	2.01	17	1
1:A:177:ASP:HB2	1:A:200:LEU:HD23	0.56	1.76	1	1
1:A:29:ILE:HD12	1:A:128:PHE:CE2	0.56	2.35	5	3
1:A:55:ASP:CB	1:A:66:ALA:HB3	0.56	2.31	5	2
1:A:90:ALA:HB2	1:A:167:TYR:OH	0.56	1.99	9	3
1:A:240:ARG:CD	1:A:312:THR:HG22	0.56	2.31	19	1
1:A:271:VAL:HG12	1:A:275:LYS:CD	0.56	2.30	2	1
1:A:165:LEU:HD22	1:A:243:ASP:OD2	0.56	2.01	13	2
1:A:161:ILE:HD11	1:A:183:LEU:HD21	0.56	1.78	12	4
1:A:78:GLY:N	1:A:79:PRO:CD	0.56	2.69	14	1
1:A:182:ASN:ND2	1:A:195:LEU:HD11	0.55	2.16	1	3
1:A:244:LEU:HD22	1:A:320:LEU:HD21	0.55	1.77	17	3
1:A:306:VAL:HG12	1:A:320:LEU:HD21	0.55	1.78	18	3
1:A:185:LEU:CD1	1:A:341:LEU:HD22	0.55	2.22	6	1
1:A:55:ASP:C	1:A:56:MET:HG3	0.55	2.21	10	1
1:A:161:ILE:CG2	1:A:178:ILE:HD11	0.55	2.32	15	1
1:A:255:LEU:HD11	1:A:294:ASN:CG	0.55	2.22	4	1
1:A:182:ASN:ND2	1:A:195:LEU:HD21	0.55	2.17	16	1
1:A:302:TYR:CD1	1:A:320:LEU:HD22	0.55	2.37	6	1
1:A:165:LEU:HD21	1:A:243:ASP:HB3	0.55	1.78	11	1
1:A:252:ILE:CG2	1:A:299:ILE:HG21	0.55	2.32	14	1
1:A:138:LEU:CD2	1:A:183:LEU:HD13	0.55	2.32	10	7
1:A:259:LEU:HD13	1:A:261:TRP:CH2	0.55	2.36	12	3
1:A:342:SER:O	1:A:343:VAL:HG13	0.55	2.02	12	1
1:A:108:LEU:HD21	1:A:167:TYR:CD2	0.55	2.36	13	1
1:A:161:ILE:HG12	1:A:183:LEU:HD21	0.55	1.79	4	1
1:A:298:GLU:HB3	1:A:324:LEU:HD12	0.55	1.78	13	2
1:A:43:ILE:HD11	1:A:53:LEU:HD22	0.55	1.77	18	1
1:A:317:TYR:HA	1:A:320:LEU:HD12	0.55	1.79	11	2
1:A:141:ILE:CG1	1:A:344:VAL:HG13	0.55	2.32	16	1
1:A:252:ILE:HB	1:A:299:ILE:HG21	0.55	1.79	1	5
1:A:93:PRO:HA	1:A:96:ILE:HD12	0.55	1.78	6	1
1:A:278:TYR:CD2	1:A:285:LEU:HD13	0.55	2.36	2	1
1:A:176:GLY:HA2	1:A:246:ILE:HD13	0.55	1.77	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:LEU:HD21	1:A:157:LEU:HD21	0.55	1.79	8	1
1:A:343:VAL:HG22	1:A:344:VAL:HG22	0.55	1.79	10	1
1:A:138:LEU:CB	1:A:180:ALA:HB1	0.55	2.30	15	1
1:A:282:ILE:HG21	1:A:303:MET:CG	0.54	2.32	9	1
1:A:161:ILE:HG23	1:A:195:LEU:CD1	0.54	2.31	20	2
1:A:184:LEU:HD11	1:A:196:VAL:CG2	0.54	2.33	4	1
1:A:66:ALA:N	1:A:67:PRO:HD2	0.54	2.15	19	3
1:A:149:PHE:CE1	1:A:341:LEU:HD11	0.54	2.38	9	1
1:A:175:HIS:ND1	1:A:201:ALA:HB2	0.54	2.18	18	1
1:A:56:MET:CG	1:A:66:ALA:HB2	0.54	2.31	16	1
1:A:28:ILE:HG22	1:A:35:LYS:HG2	0.54	1.79	2	1
1:A:200:LEU:C	1:A:200:LEU:HD13	0.54	2.23	4	1
1:A:82:THR:HG22	1:A:198:TYR:O	0.54	2.03	20	1
1:A:165:LEU:HD11	1:A:243:ASP:CG	0.54	2.23	4	2
1:A:174:VAL:HG11	1:A:238:PRO:CG	0.54	2.32	4	2
1:A:51:ILE:HG23	1:A:71:LYS:CA	0.54	2.32	17	6
1:A:184:LEU:HD11	1:A:196:VAL:HG12	0.54	1.79	2	2
1:A:29:ILE:HD12	1:A:128:PHE:CE1	0.54	2.37	20	3
1:A:244:LEU:HD22	1:A:320:LEU:CD2	0.54	2.32	7	2
1:A:41:LEU:O	1:A:53:LEU:HD23	0.54	2.03	11	1
1:A:256:THR:HG22	1:A:290:PHE:CE2	0.54	2.38	1	2
1:A:73:GLU:HG3	1:A:80:LEU:HD13	0.54	1.78	4	1
1:A:222:ASP:HB3	1:A:232:ALA:HB1	0.54	1.78	4	1
1:A:183:LEU:O	1:A:184:LEU:HD13	0.54	2.03	5	3
1:A:173:TYR:CD1	1:A:201:ALA:HB1	0.54	2.37	6	1
1:A:251:MET:CE	1:A:324:LEU:HD21	0.54	2.32	8	1
1:A:53:LEU:HD13	1:A:56:MET:CE	0.54	2.32	19	1
1:A:298:GLU:HG3	1:A:324:LEU:HD23	0.54	1.79	3	1
1:A:53:LEU:HD12	1:A:69:VAL:HG12	0.54	1.79	4	2
1:A:142:TYR:CD1	1:A:142:TYR:C	0.54	2.81	8	2
1:A:168:ILE:HG13	1:A:174:VAL:HG12	0.54	1.80	9	1
1:A:100:ILE:HG23	1:A:105:LEU:HB2	0.53	1.79	4	2
1:A:226:GLU:HG3	1:A:265:LEU:HD22	0.53	1.78	4	3
1:A:328:LEU:O	1:A:328:LEU:HD13	0.53	2.03	8	1
1:A:39:VAL:HG23	1:A:52:TYR:CB	0.53	2.32	9	1
1:A:177:ASP:OD1	1:A:200:LEU:HD22	0.53	2.03	2	1
1:A:70:VAL:HG12	1:A:130:ILE:HD11	0.53	1.79	6	1
1:A:267:ASP:O	1:A:271:VAL:HG23	0.53	2.03	11	7
1:A:155:LEU:HD22	1:A:324:LEU:HD22	0.53	1.80	12	1
1:A:43:ILE:CD1	1:A:69:VAL:HG11	0.53	2.33	19	1
1:A:99:TRP:CZ2	1:A:108:LEU:HD13	0.53	2.38	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:VAL:HG12	1:A:275:LYS:HD2	0.53	1.78	19	3
1:A:153:THR:HG22	1:A:339:LEU:HG	0.53	1.77	12	1
1:A:151:ARG:NE	1:A:331:ILE:HD13	0.53	2.17	16	1
1:A:225:ILE:HD13	1:A:268:PRO:CA	0.53	2.33	20	1
1:A:182:ASN:O	1:A:196:VAL:HG22	0.53	2.03	19	1
1:A:109:GLY:CA	1:A:164:ILE:HD11	0.53	2.34	2	1
1:A:316:LEU:HD23	1:A:319:ASN:CG	0.53	2.24	16	2
1:A:157:LEU:HD23	1:A:254:TRP:CZ3	0.53	2.39	9	1
1:A:174:VAL:HG22	1:A:202:TYR:O	0.53	2.04	20	3
1:A:175:HIS:NE2	1:A:200:LEU:HD12	0.53	2.19	13	1
1:A:91:ALA:HB1	1:A:113:TYR:CD1	0.53	2.39	14	1
1:A:157:LEU:HD22	1:A:183:LEU:HD22	0.53	1.81	16	1
1:A:176:GLY:O	1:A:200:LEU:HD22	0.53	2.04	6	1
1:A:91:ALA:HB1	1:A:113:TYR:CB	0.53	2.34	19	1
1:A:161:ILE:HD12	1:A:195:LEU:HD11	0.53	1.79	19	1
1:A:51:ILE:HD12	1:A:71:LYS:HB2	0.53	1.80	18	4
1:A:138:LEU:HD22	1:A:183:LEU:CD2	0.53	2.30	5	1
1:A:178:ILE:CG2	1:A:246:ILE:HG22	0.53	2.34	15	3
1:A:209:VAL:HG12	1:A:211:LYS:HG2	0.53	1.80	13	1
1:A:162:LEU:HD22	1:A:317:TYR:CE2	0.53	2.37	16	1
1:A:109:GLY:HA3	1:A:164:ILE:HD11	0.52	1.81	2	1
1:A:343:VAL:HG22	1:A:343:VAL:O	0.52	2.04	18	3
1:A:25:VAL:HG22	1:A:40:GLY:C	0.52	2.25	16	1
1:A:213:TYR:OH	1:A:312:THR:HG21	0.52	2.04	2	1
1:A:177:ASP:CB	1:A:200:LEU:HD13	0.52	2.34	13	4
1:A:178:ILE:O	1:A:179:LYS:C	0.52	2.45	13	10
1:A:161:ILE:CD1	1:A:195:LEU:HD13	0.52	2.34	5	1
1:A:301:LYS:HG2	1:A:323:ILE:HG21	0.52	1.81	15	1
1:A:252:ILE:HD12	1:A:286:MET:HG3	0.52	1.80	1	2
1:A:155:LEU:HD11	1:A:324:LEU:HB3	0.52	1.80	3	4
1:A:230:ILE:HD11	1:A:275:LYS:HD2	0.52	1.81	5	2
1:A:165:LEU:HD13	1:A:243:ASP:CG	0.52	2.24	6	1
1:A:197:ASP:O	1:A:198:TYR:C	0.52	2.47	15	1
1:A:226:GLU:HG2	1:A:265:LEU:HD21	0.52	1.82	16	1
1:A:252:ILE:HD12	1:A:286:MET:SD	0.52	2.44	20	3
1:A:196:VAL:HG13	1:A:197:ASP:CG	0.52	2.25	10	1
1:A:229:SER:HB2	1:A:246:ILE:HD11	0.52	1.82	13	1
1:A:353:THR:HG22	1:A:354:ILE:HD13	0.52	1.81	20	2
1:A:240:ARG:NH1	1:A:309:LEU:HD12	0.52	2.20	20	1
1:A:138:LEU:CD1	1:A:341:LEU:HD21	0.52	2.35	6	2
1:A:184:LEU:C	1:A:185:LEU:HD23	0.52	2.25	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ALA:HB3	1:A:37:TRP:HE1	0.52	1.65	11	5
1:A:177:ASP:CB	1:A:200:LEU:HD22	0.52	2.34	13	1
1:A:152:LYS:HD2	1:A:153:THR:HG23	0.51	1.81	14	1
1:A:265:LEU:HD12	1:A:271:VAL:CG2	0.51	2.35	16	1
1:A:302:TYR:CE2	1:A:320:LEU:HD23	0.51	2.40	14	3
1:A:226:GLU:CA	1:A:265:LEU:HD21	0.51	2.35	6	2
1:A:265:LEU:HD22	1:A:271:VAL:HG11	0.51	1.82	10	1
1:A:161:ILE:HG22	1:A:165:LEU:CD1	0.51	2.35	17	2
1:A:27:GLU:O	1:A:39:VAL:HG23	0.51	2.05	6	2
1:A:302:TYR:HB2	1:A:323:ILE:HD11	0.51	1.82	13	2
1:A:110:VAL:HG23	1:A:164:ILE:CD1	0.51	2.28	12	3
1:A:184:LEU:HD23	1:A:196:VAL:CG1	0.51	2.35	19	2
1:A:311:TYR:O	1:A:312:THR:HG23	0.51	2.06	19	3
1:A:306:VAL:CG1	1:A:320:LEU:HD21	0.51	2.35	18	1
1:A:118:LEU:HD22	1:A:118:LEU:O	0.51	2.05	15	3
1:A:111:PRO:HG3	1:A:196:VAL:HG12	0.51	1.81	12	1
1:A:198:TYR:HB2	1:A:200:LEU:HD12	0.51	1.82	4	1
1:A:103:ARG:CB	1:A:105:LEU:HD13	0.51	2.36	5	1
1:A:161:ILE:HG21	1:A:178:ILE:HD12	0.51	1.82	13	3
1:A:110:VAL:HG22	1:A:111:PRO:HD2	0.51	1.83	13	12
1:A:86:PHE:CE1	1:A:90:ALA:HB2	0.51	2.41	10	1
1:A:253:GLN:CB	1:A:259:LEU:HD21	0.51	2.36	11	1
1:A:165:LEU:HD11	1:A:243:ASP:HB3	0.51	1.82	15	1
1:A:225:ILE:HG22	1:A:271:VAL:HG21	0.51	1.83	2	1
1:A:204:TYR:CZ	1:A:237:ALA:HB3	0.51	2.41	11	1
1:A:159:LEU:HD23	1:A:160:ARG:N	0.51	2.21	14	1
1:A:161:ILE:CG1	1:A:183:LEU:HD21	0.50	2.37	4	1
1:A:118:LEU:C	1:A:118:LEU:CD2	0.50	2.78	16	3
1:A:136:SER:OG	1:A:344:VAL:HG22	0.50	2.06	3	1
1:A:141:ILE:CD1	1:A:185:LEU:HD11	0.50	2.36	16	1
1:A:100:ILE:HG23	1:A:105:LEU:CB	0.50	2.37	12	4
1:A:141:ILE:HG21	1:A:341:LEU:HD21	0.50	1.82	9	1
1:A:154:VAL:HG21	1:A:255:LEU:HD13	0.50	1.81	16	1
1:A:91:ALA:HB1	1:A:113:TYR:CD2	0.50	2.41	17	1
1:A:43:ILE:HG22	1:A:45:GLN:CG	0.50	2.36	6	1
1:A:308:LEU:HD12	1:A:308:LEU:O	0.50	2.06	16	1
1:A:29:ILE:HG22	1:A:37:TRP:O	0.50	2.06	18	1
1:A:84:LEU:HD13	1:A:129:MET:CG	0.50	2.37	2	1
1:A:141:ILE:HG12	1:A:343:VAL:HG22	0.50	1.84	11	1
1:A:261:TRP:CD1	1:A:271:VAL:HG13	0.50	2.41	11	1
1:A:252:ILE:HD12	1:A:286:MET:HE2	0.50	1.83	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:LEU:HD21	1:A:352:LYS:HB3	0.50	1.84	11	1
1:A:53:LEU:HD12	1:A:54:ALA:N	0.50	2.21	13	1
1:A:341:LEU:O	1:A:342:SER:CB	0.50	2.60	6	1
1:A:52:TYR:CD1	1:A:70:VAL:HG13	0.50	2.41	7	1
1:A:161:ILE:HD12	1:A:178:ILE:HD12	0.50	1.84	8	1
1:A:153:THR:HA	1:A:339:LEU:HD22	0.50	1.82	9	1
1:A:282:ILE:HG21	1:A:303:MET:HG2	0.50	1.83	9	1
1:A:100:ILE:HD11	1:A:108:LEU:HB2	0.50	1.84	11	1
1:A:159:LEU:HD12	1:A:325:LEU:HD21	0.50	1.83	14	1
1:A:226:GLU:HA	1:A:265:LEU:HD11	0.50	1.84	19	3
1:A:272:ARG:O	1:A:276:ILE:HD12	0.50	2.06	5	2
1:A:146:ALA:O	1:A:147:LYS:C	0.49	2.48	14	16
1:A:196:VAL:HG13	1:A:197:ASP:N	0.49	2.21	10	2
1:A:165:LEU:HD23	1:A:168:ILE:HD11	0.49	1.83	16	4
1:A:183:LEU:HD23	1:A:193:VAL:CG2	0.49	2.37	3	5
1:A:96:ILE:CG2	1:A:108:LEU:HD22	0.49	2.35	3	5
1:A:198:TYR:O	1:A:198:TYR:CG	0.49	2.65	17	1
1:A:53:LEU:HD13	1:A:69:VAL:HG12	0.49	1.84	18	1
1:A:239:SER:HB3	1:A:312:THR:HG23	0.49	1.84	1	1
1:A:239:SER:O	1:A:240:ARG:HB3	0.49	2.07	20	2
1:A:184:LEU:HD21	1:A:196:VAL:CG2	0.49	2.36	4	1
1:A:328:LEU:HD11	1:A:335:ASP:HA	0.49	1.83	17	1
1:A:138:LEU:HD21	1:A:157:LEU:CD2	0.49	2.38	4	1
1:A:168:ILE:HG22	1:A:173:TYR:C	0.49	2.28	18	1
1:A:282:ILE:HD11	1:A:304:GLU:OE2	0.49	2.08	19	1
1:A:137:ASP:C	1:A:141:ILE:HD12	0.49	2.28	18	3
1:A:200:LEU:HD13	1:A:201:ALA:N	0.49	2.23	4	1
1:A:226:GLU:HA	1:A:265:LEU:HD21	0.49	1.84	6	2
1:A:304:GLU:OE2	1:A:308:LEU:HD11	0.49	2.08	13	1
1:A:103:ARG:HB2	1:A:105:LEU:HD13	0.49	1.85	5	1
1:A:141:ILE:CG2	1:A:341:LEU:HD23	0.49	2.33	6	1
1:A:141:ILE:CD1	1:A:341:LEU:HD23	0.49	2.33	11	1
1:A:90:ALA:O	1:A:110:VAL:HG21	0.49	2.07	15	1
1:A:149:PHE:CE1	1:A:341:LEU:HD12	0.49	2.42	16	1
1:A:220:CYS:SG	1:A:355:THR:HG21	0.49	2.47	16	1
1:A:35:LYS:O	1:A:36:GLU:CB	0.49	2.60	10	7
1:A:185:LEU:HD23	1:A:193:VAL:HA	0.49	1.83	6	1
1:A:90:ALA:HB3	1:A:110:VAL:HG11	0.49	1.85	8	1
1:A:138:LEU:HD11	1:A:341:LEU:HD21	0.49	1.84	12	1
1:A:80:LEU:HD12	1:A:127:ARG:CD	0.49	2.38	13	1
1:A:226:GLU:CG	1:A:265:LEU:HD22	0.49	2.38	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:ILE:CG2	1:A:247:LEU:HD13	0.49	2.38	16	1
1:A:136:SER:HB3	1:A:344:VAL:HG21	0.49	1.83	20	1
1:A:141:ILE:HD13	1:A:341:LEU:CD2	0.49	2.36	1	2
1:A:155:LEU:HD13	1:A:328:LEU:HD23	0.49	1.84	2	1
1:A:53:LEU:HD11	1:A:55:ASP:OD2	0.49	2.08	17	1
1:A:295:LYS:HG2	1:A:331:ILE:HG21	0.48	1.85	9	1
1:A:255:LEU:HD12	1:A:255:LEU:O	0.48	2.07	13	1
1:A:30:THR:HG23	1:A:35:LYS:HB3	0.48	1.84	10	4
1:A:165:LEU:HD21	1:A:243:ASP:CB	0.48	2.37	12	2
1:A:230:ILE:HD11	1:A:275:LYS:CD	0.48	2.38	7	1
1:A:73:GLU:CG	1:A:80:LEU:HD23	0.48	2.38	7	3
1:A:52:TYR:CD2	1:A:70:VAL:HG13	0.48	2.43	18	1
1:A:165:LEU:HD12	1:A:165:LEU:O	0.48	2.09	19	1
1:A:73:GLU:CB	1:A:80:LEU:HD22	0.48	2.38	20	1
1:A:87:TYR:O	1:A:91:ALA:HB2	0.48	2.09	17	10
1:A:153:THR:HA	1:A:339:LEU:HD23	0.48	1.84	7	1
1:A:220:CYS:HB3	1:A:355:THR:HG21	0.48	1.83	12	1
1:A:298:GLU:OE1	1:A:328:LEU:HD12	0.48	2.09	13	1
1:A:87:TYR:C	1:A:87:TYR:CD1	0.48	2.86	15	1
1:A:309:LEU:HD12	1:A:310:ASP:N	0.48	2.23	17	2
1:A:282:ILE:N	1:A:282:ILE:HD13	0.48	2.23	5	12
1:A:244:LEU:HB3	1:A:306:VAL:HG11	0.48	1.86	7	3
1:A:343:VAL:O	1:A:344:VAL:HG13	0.48	2.08	10	1
1:A:174:VAL:O	1:A:174:VAL:HG23	0.48	2.08	11	1
1:A:96:ILE:HG12	1:A:108:LEU:HD23	0.48	1.85	15	1
1:A:155:LEU:HD21	1:A:324:LEU:HB3	0.48	1.84	15	1
1:A:310:ASP:HB2	1:A:312:THR:HG22	0.48	1.84	17	1
1:A:35:LYS:O	1:A:36:GLU:HB2	0.48	2.09	4	4
1:A:25:VAL:HG13	1:A:40:GLY:O	0.48	2.09	6	1
1:A:241:ARG:HA	1:A:244:LEU:HD12	0.48	1.85	7	3
1:A:99:TRP:CD1	1:A:100:ILE:N	0.48	2.82	9	2
1:A:96:ILE:CG2	1:A:108:LEU:HD12	0.48	2.38	17	1
1:A:165:LEU:HD13	1:A:175:HIS:CE1	0.48	2.44	19	1
1:A:106:LYS:HD3	1:A:159:LEU:HD23	0.47	1.86	3	1
1:A:53:LEU:HD21	1:A:55:ASP:OD2	0.47	2.10	5	1
1:A:177:ASP:HB2	1:A:200:LEU:HD13	0.47	1.86	13	3
1:A:265:LEU:HD23	1:A:271:VAL:HG21	0.47	1.86	9	1
1:A:158:SER:O	1:A:162:LEU:HD12	0.47	2.08	14	1
1:A:165:LEU:HD12	1:A:175:HIS:NE2	0.47	2.24	15	1
1:A:29:ILE:HD12	1:A:128:PHE:CZ	0.47	2.43	7	1
1:A:53:LEU:HD22	1:A:69:VAL:HG12	0.47	1.86	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:LEU:HD21	1:A:133:ARG:HE	0.47	1.69	11	2
1:A:304:GLU:CD	1:A:308:LEU:HD12	0.47	2.30	12	1
1:A:100:ILE:HG23	1:A:105:LEU:HB3	0.47	1.86	14	2
1:A:216:ASP:N	1:A:217:PRO:HD2	0.47	2.24	17	1
1:A:70:VAL:HG12	1:A:130:ILE:CG1	0.47	2.39	6	1
1:A:316:LEU:HD23	1:A:319:ASN:HB2	0.47	1.85	20	2
1:A:141:ILE:HG23	1:A:342:SER:HB3	0.47	1.84	12	3
1:A:155:LEU:CD2	1:A:324:LEU:HD22	0.47	2.39	15	1
1:A:175:HIS:CE1	1:A:178:ILE:HD13	0.47	2.45	15	1
1:A:252:ILE:HD13	1:A:286:MET:HE2	0.47	1.84	3	2
1:A:153:THR:HG22	1:A:339:LEU:HD22	0.47	1.86	4	1
1:A:28:ILE:HD13	1:A:38:LYS:HG3	0.47	1.87	2	1
1:A:53:LEU:HA	1:A:69:VAL:HG12	0.47	1.86	2	1
1:A:178:ILE:HG21	1:A:250:CYS:SG	0.47	2.49	3	3
1:A:29:ILE:HD13	1:A:37:TRP:O	0.47	2.10	4	1
1:A:251:MET:HE3	1:A:324:LEU:HD21	0.47	1.87	8	1
1:A:87:TYR:OH	1:A:196:VAL:HG23	0.47	2.09	10	1
1:A:175:HIS:O	1:A:175:HIS:CG	0.47	2.67	10	1
1:A:165:LEU:HD11	1:A:178:ILE:HD11	0.47	1.85	13	1
1:A:96:ILE:O	1:A:100:ILE:HG12	0.47	2.10	15	1
1:A:155:LEU:CB	1:A:328:LEU:HD12	0.47	2.40	19	1
1:A:106:LYS:CD	1:A:159:LEU:HD23	0.47	2.40	3	1
1:A:55:ASP:O	1:A:56:MET:C	0.47	2.53	10	1
1:A:204:TYR:CD1	1:A:237:ALA:HB1	0.47	2.45	10	1
1:A:227:PHE:O	1:A:246:ILE:HD12	0.47	2.10	13	1
1:A:226:GLU:HA	1:A:265:LEU:HD12	0.47	1.87	15	1
1:A:80:LEU:HD11	1:A:129:MET:CE	0.47	2.40	15	1
1:A:244:LEU:HD23	1:A:306:VAL:HG12	0.47	1.87	15	1
1:A:84:LEU:HD13	1:A:129:MET:HG2	0.47	1.85	2	2
1:A:137:ASP:OD1	1:A:184:LEU:HD12	0.47	2.09	3	2
1:A:33:ALA:HB1	1:A:36:GLU:OE2	0.46	2.10	2	1
1:A:96:ILE:HG12	1:A:108:LEU:HD12	0.46	1.85	5	1
1:A:244:LEU:HD21	1:A:317:TYR:CZ	0.46	2.45	7	1
1:A:211:LYS:HG2	1:A:312:THR:HG21	0.46	1.86	11	1
1:A:190:PRO:HB3	1:A:343:VAL:HG22	0.46	1.85	13	1
1:A:161:ILE:CG2	1:A:195:LEU:HD11	0.46	2.37	20	1
1:A:230:ILE:HG23	1:A:275:LYS:HD2	0.46	1.86	1	1
1:A:224:THR:O	1:A:228:THR:N	0.46	2.48	5	1
1:A:141:ILE:HG21	1:A:341:LEU:CG	0.46	2.40	4	3
1:A:118:LEU:HD23	1:A:125:SER:HB3	0.46	1.86	6	1
1:A:53:LEU:HD13	1:A:133:ARG:HD2	0.46	1.86	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LYS:O	1:A:36:GLU:CG	0.46	2.63	20	1
1:A:196:VAL:HG23	1:A:197:ASP:CG	0.46	2.31	1	1
1:A:69:VAL:HG13	1:A:133:ARG:HA	0.46	1.86	9	2
1:A:161:ILE:HD11	1:A:195:LEU:HD13	0.46	1.87	5	1
1:A:108:LEU:HD11	1:A:167:TYR:CD2	0.46	2.46	10	1
1:A:46:GLY:O	1:A:51:ILE:HG21	0.46	2.11	17	1
1:A:66:ALA:N	1:A:67:PRO:CD	0.46	2.79	19	1
1:A:138:LEU:HD22	1:A:183:LEU:CD1	0.46	2.40	20	1
1:A:153:THR:HG22	1:A:339:LEU:HA	0.46	1.87	3	1
1:A:28:ILE:HG23	1:A:38:LYS:HE3	0.46	1.88	4	1
1:A:226:GLU:HA	1:A:265:LEU:HD22	0.46	1.88	11	1
1:A:185:LEU:CD2	1:A:193:VAL:HG23	0.46	2.41	12	1
1:A:331:ILE:HD11	1:A:333:SER:CB	0.46	2.39	13	1
1:A:222:ASP:OD1	1:A:232:ALA:HB1	0.46	2.11	16	2
1:A:328:LEU:HD13	1:A:334:LYS:HA	0.46	1.87	19	1
1:A:140:LYS:CE	1:A:144:ALA:HB2	0.46	2.41	6	1
1:A:155:LEU:CD2	1:A:325:LEU:HD22	0.46	2.40	19	1
1:A:138:LEU:C	1:A:180:ALA:HB1	0.46	2.31	16	3
1:A:55:ASP:HB3	1:A:66:ALA:HB3	0.46	1.86	5	1
1:A:196:VAL:HG22	1:A:197:ASP:H	0.46	1.70	10	1
1:A:121:LYS:O	1:A:122:ASN:C	0.45	2.55	20	3
1:A:43:ILE:HG22	1:A:45:GLN:HG2	0.45	1.88	6	1
1:A:155:LEU:CG	1:A:328:LEU:HD13	0.45	2.41	12	2
1:A:165:LEU:HD22	1:A:243:ASP:HB2	0.45	1.88	20	2
1:A:118:LEU:HD12	1:A:127:ARG:HG3	0.45	1.88	17	1
1:A:301:LYS:HB2	1:A:323:ILE:HD11	0.45	1.87	19	1
1:A:343:VAL:O	1:A:344:VAL:C	0.45	2.55	11	3
1:A:177:ASP:HB3	1:A:200:LEU:HD13	0.45	1.88	20	1
1:A:344:VAL:HG22	1:A:344:VAL:O	0.45	2.11	2	2
1:A:151:ARG:HG2	1:A:328:LEU:HD12	0.45	1.87	4	1
1:A:175:HIS:CD2	1:A:201:ALA:HB2	0.45	2.46	7	1
1:A:137:ASP:OD2	1:A:184:LEU:HD12	0.45	2.11	11	1
1:A:27:GLU:N	1:A:39:VAL:HG12	0.45	2.27	15	1
1:A:175:HIS:NE2	1:A:195:LEU:HD22	0.45	2.25	20	1
1:A:53:LEU:HD21	1:A:133:ARG:CZ	0.45	2.42	1	1
1:A:66:ALA:CB	1:A:67:PRO:CD	0.45	2.94	9	1
1:A:161:ILE:HG12	1:A:178:ILE:HD12	0.45	1.87	9	1
1:A:155:LEU:CG	1:A:328:LEU:HD22	0.45	2.40	11	2
1:A:226:GLU:CG	1:A:265:LEU:HD21	0.45	2.42	16	1
1:A:321:ARG:O	1:A:325:LEU:HD23	0.45	2.11	14	3
1:A:169:HIS:ND1	1:A:174:VAL:HG22	0.45	2.27	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:SER:CB	1:A:185:LEU:HD12	0.45	2.42	10	1
1:A:86:PHE:CZ	1:A:168:ILE:HD11	0.45	2.46	18	1
1:A:82:THR:HG21	1:A:198:TYR:OH	0.45	2.11	18	1
1:A:178:ILE:O	1:A:178:ILE:CG2	0.45	2.64	13	3
1:A:151:ARG:NH1	1:A:255:LEU:HD21	0.45	2.27	15	1
1:A:262:GLU:HG2	1:A:265:LEU:HD23	0.45	1.87	1	1
1:A:70:VAL:HG12	1:A:130:ILE:CD1	0.45	2.42	6	1
1:A:316:LEU:HD23	1:A:319:ASN:CB	0.45	2.41	7	1
1:A:157:LEU:HD21	1:A:193:VAL:HG21	0.45	1.87	12	1
1:A:341:LEU:O	1:A:344:VAL:HG23	0.45	2.11	8	1
1:A:252:ILE:HD13	1:A:286:MET:HE3	0.45	1.87	3	1
1:A:157:LEU:HD21	1:A:193:VAL:HG11	0.45	1.89	5	1
1:A:98:LYS:O	1:A:102:THR:HG23	0.45	2.12	6	1
1:A:255:LEU:HD21	1:A:294:ASN:HD21	0.45	1.72	13	1
1:A:196:VAL:HG23	1:A:198:TYR:H	0.45	1.71	15	2
1:A:48:PHE:CZ	1:A:351:ALA:HB1	0.44	2.47	18	1
1:A:200:LEU:HD22	1:A:200:LEU:C	0.44	2.32	4	1
1:A:108:LEU:HD22	1:A:110:VAL:HG23	0.44	1.89	8	1
1:A:174:VAL:HG21	1:A:204:TYR:HB2	0.44	1.88	10	1
1:A:155:LEU:HD23	1:A:328:LEU:HD23	0.44	1.90	18	1
1:A:49:GLY:H	1:A:51:ILE:HD11	0.44	1.71	4	1
1:A:138:LEU:HD12	1:A:341:LEU:HD22	0.44	1.89	11	1
1:A:309:LEU:HD23	1:A:310:ASP:N	0.44	2.27	11	2
1:A:156:GLN:CB	1:A:339:LEU:HD11	0.44	2.43	13	1
1:A:229:SER:HB2	1:A:246:ILE:HD13	0.44	1.89	17	1
1:A:182:ASN:CG	1:A:195:LEU:HD11	0.44	2.32	1	1
1:A:198:TYR:O	1:A:199:GLY:C	0.44	2.56	4	2
1:A:225:ILE:HD13	1:A:271:VAL:HG21	0.44	1.88	10	1
1:A:137:ASP:HA	1:A:184:LEU:HD13	0.44	1.89	16	1
1:A:214:LYS:HA	1:A:236:VAL:HG22	0.44	1.90	6	1
1:A:155:LEU:CD1	1:A:325:LEU:HD22	0.44	2.41	10	1
1:A:204:TYR:CE1	1:A:237:ALA:HB3	0.44	2.46	11	1
1:A:244:LEU:HD22	1:A:320:LEU:CD1	0.44	2.41	1	1
1:A:281:ASN:O	1:A:285:LEU:HD23	0.44	2.13	13	2
1:A:331:ILE:HD11	1:A:333:SER:HB3	0.44	1.89	13	1
1:A:105:LEU:HD21	1:A:166:GLU:OE1	0.44	2.12	18	1
1:A:161:ILE:O	1:A:165:LEU:HD13	0.44	2.13	10	2
1:A:200:LEU:HD11	1:A:352:LYS:CB	0.43	2.43	1	1
1:A:309:LEU:O	1:A:310:ASP:CB	0.43	2.65	13	2
1:A:174:VAL:HG21	1:A:238:PRO:HG3	0.43	1.87	14	1
1:A:244:LEU:HB3	1:A:306:VAL:HG21	0.43	1.90	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:271:VAL:HG12	1:A:275:LYS:HD3	0.43	1.88	2	1
1:A:286:MET:SD	1:A:299:ILE:HG22	0.43	2.53	12	1
1:A:155:LEU:HD22	1:A:328:LEU:HD12	0.43	1.90	19	1
1:A:161:ILE:CD1	1:A:183:LEU:HD21	0.43	2.43	12	1
1:A:225:ILE:HD11	1:A:268:PRO:HB3	0.43	1.88	19	1
1:A:168:ILE:HD11	1:A:175:HIS:CE1	0.43	2.47	1	1
1:A:34:LYS:O	1:A:35:LYS:CG	0.43	2.66	4	3
1:A:152:LYS:CD	1:A:153:THR:HG23	0.43	2.43	14	1
1:A:100:ILE:HD13	1:A:100:ILE:N	0.43	2.29	15	1
1:A:114:TRP:CD1	1:A:114:TRP:N	0.43	2.87	15	1
1:A:177:ASP:OD2	1:A:200:LEU:HD13	0.43	2.12	12	1
1:A:140:LYS:CE	1:A:344:VAL:HG11	0.43	2.43	14	1
1:A:151:ARG:HH12	1:A:255:LEU:HD21	0.43	1.72	15	1
1:A:227:PHE:HB3	1:A:246:ILE:HG23	0.43	1.91	15	1
1:A:79:PRO:HB3	1:A:353:THR:HG23	0.43	1.89	17	1
1:A:84:LEU:HD22	1:A:129:MET:SD	0.43	2.53	2	2
1:A:54:ALA:HB1	1:A:130:ILE:HD11	0.43	1.89	11	1
1:A:141:ILE:HG12	1:A:344:VAL:HG13	0.43	1.90	16	1
1:A:174:VAL:HG13	1:A:243:ASP:OD2	0.43	2.13	4	3
1:A:253:GLN:HB2	1:A:259:LEU:HD11	0.43	1.89	10	2
1:A:323:ILE:HD12	1:A:324:LEU:N	0.43	2.29	8	2
1:A:241:ARG:NH2	1:A:309:LEU:HD13	0.43	2.28	18	1
1:A:240:ARG:HD3	1:A:312:THR:HG22	0.43	1.91	19	1
1:A:326:GLN:O	1:A:330:ALA:HB2	0.43	2.14	18	8
1:A:141:ILE:HD12	1:A:345:GLU:HB3	0.43	1.90	7	1
1:A:301:LYS:HG2	1:A:323:ILE:HD13	0.43	1.91	11	1
1:A:157:LEU:CD2	1:A:193:VAL:HG21	0.43	2.44	12	1
1:A:87:TYR:O	1:A:91:ALA:N	0.43	2.51	15	1
1:A:141:ILE:HG12	1:A:344:VAL:HG22	0.43	1.91	16	1
1:A:184:LEU:CD2	1:A:196:VAL:HG22	0.42	2.34	1	1
1:A:84:LEU:HD12	1:A:129:MET:SD	0.42	2.54	7	1
1:A:49:GLY:O	1:A:50:CYS:CB	0.42	2.66	18	2
1:A:184:LEU:HD13	1:A:184:LEU:N	0.42	2.29	15	1
1:A:304:GLU:O	1:A:308:LEU:HD23	0.42	2.13	16	1
1:A:175:HIS:CD2	1:A:195:LEU:HD23	0.42	2.49	3	1
1:A:197:ASP:OD2	1:A:200:LEU:HD12	0.42	2.14	3	1
1:A:243:ASP:HA	1:A:246:ILE:HD12	0.42	1.90	16	2
1:A:255:LEU:HD23	1:A:299:ILE:CD1	0.42	2.44	8	1
1:A:71:LYS:O	1:A:128:PHE:HA	0.42	2.15	9	1
1:A:131:MET:O	1:A:132:ASP:O	0.42	2.38	9	1
1:A:50:CYS:O	1:A:72:VAL:HG22	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:GLY:C	1:A:164:ILE:HD12	0.42	2.35	11	1
1:A:26:GLY:N	1:A:39:VAL:HG13	0.42	2.29	12	1
1:A:84:LEU:HD12	1:A:127:ARG:HD3	0.42	1.89	20	1
1:A:176:GLY:CA	1:A:246:ILE:HD13	0.42	2.44	7	1
1:A:253:GLN:O	1:A:257:GLY:HA2	0.42	2.15	8	1
1:A:25:VAL:HG22	1:A:40:GLY:O	0.42	2.14	16	1
1:A:176:GLY:O	1:A:246:ILE:HD13	0.42	2.15	19	1
1:A:165:LEU:C	1:A:165:LEU:HD13	0.42	2.35	5	1
1:A:140:LYS:HE3	1:A:144:ALA:HB2	0.42	1.91	6	1
1:A:99:TRP:CZ3	1:A:108:LEU:HD22	0.42	2.50	12	1
1:A:302:TYR:O	1:A:306:VAL:HG13	0.42	2.15	14	2
1:A:55:ASP:O	1:A:56:MET:CB	0.42	2.66	16	1
1:A:328:LEU:HD12	1:A:333:SER:HB3	0.42	1.91	16	1
1:A:29:ILE:HD12	1:A:128:PHE:CD1	0.42	2.49	20	1
1:A:265:LEU:HD13	1:A:265:LEU:C	0.42	2.35	7	1
1:A:80:LEU:HD23	1:A:127:ARG:HB2	0.42	1.91	16	1
1:A:91:ALA:O	1:A:92:LYS:CB	0.42	2.68	1	1
1:A:153:THR:HG21	1:A:341:LEU:HD12	0.42	1.91	4	1
1:A:26:GLY:H	1:A:39:VAL:HG13	0.42	1.75	12	2
1:A:172:GLU:O	1:A:173:TYR:CG	0.42	2.73	11	1
1:A:48:PHE:O	1:A:51:ILE:HD11	0.42	2.15	18	1
1:A:151:ARG:CD	1:A:255:LEU:HD11	0.42	2.45	18	1
1:A:328:LEU:HD13	1:A:328:LEU:C	0.41	2.35	10	2
1:A:238:PRO:O	1:A:239:SER:CB	0.41	2.68	13	1
1:A:295:LYS:NZ	1:A:331:ILE:HD13	0.41	2.29	13	1
1:A:80:LEU:HD21	1:A:127:ARG:HG2	0.41	1.91	3	1
1:A:328:LEU:C	1:A:328:LEU:HD13	0.41	2.36	7	1
1:A:31:ASP:OD2	1:A:33:ALA:HB3	0.41	2.15	8	1
1:A:218:LYS:O	1:A:219:ARG:C	0.41	2.59	17	1
1:A:138:LEU:HD13	1:A:183:LEU:HB3	0.41	1.92	20	1
1:A:69:VAL:HG13	1:A:133:ARG:HG2	0.41	1.92	2	1
1:A:80:LEU:HD13	1:A:80:LEU:C	0.41	2.35	10	2
1:A:96:ILE:HG23	1:A:108:LEU:CD1	0.41	2.37	8	1
1:A:196:VAL:O	1:A:197:ASP:CB	0.41	2.69	14	1
1:A:252:ILE:O	1:A:256:THR:HG23	0.41	2.16	14	1
1:A:216:ASP:CB	1:A:217:PRO:CD	0.41	2.98	17	1
1:A:244:LEU:HD13	1:A:306:VAL:HB	0.41	1.92	2	1
1:A:213:TYR:HB2	1:A:236:VAL:HG23	0.41	1.91	4	2
1:A:144:ALA:CB	1:A:343:VAL:HG12	0.41	2.45	5	1
1:A:155:LEU:HD23	1:A:328:LEU:CD1	0.41	2.36	11	1
1:A:77:ASN:HB3	1:A:80:LEU:CB	0.41	2.44	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:TYR:O	1:A:91:ALA:HB3	0.41	2.16	7	1
1:A:282:ILE:HG21	1:A:303:MET:SD	0.41	2.55	7	1
1:A:200:LEU:HD23	1:A:352:LYS:CB	0.41	2.46	15	1
1:A:157:LEU:C	1:A:161:ILE:HD12	0.41	2.35	20	1
1:A:220:CYS:O	1:A:221:HIS:CD2	0.41	2.73	1	1
1:A:303:MET:O	1:A:306:VAL:HG22	0.41	2.15	2	1
1:A:53:LEU:HD12	1:A:68:CYS:O	0.41	2.16	3	1
1:A:174:VAL:HG11	1:A:238:PRO:HG3	0.41	1.93	4	1
1:A:265:LEU:HA	1:A:271:VAL:HG11	0.41	1.93	7	1
1:A:239:SER:HB2	1:A:312:THR:HG23	0.41	1.91	12	1
1:A:230:ILE:HG23	1:A:275:LYS:HG3	0.41	1.91	4	1
1:A:165:LEU:HD21	1:A:243:ASP:CG	0.41	2.36	5	2
1:A:231:ASP:O	1:A:236:VAL:HG12	0.41	2.15	9	1
1:A:298:GLU:CD	1:A:328:LEU:HD12	0.41	2.35	11	1
1:A:53:LEU:HD21	1:A:133:ARG:CD	0.41	2.46	15	1
1:A:184:LEU:O	1:A:193:VAL:HG23	0.41	2.16	17	1
1:A:177:ASP:HB2	1:A:200:LEU:HD21	0.41	1.92	4	1
1:A:30:THR:HG23	1:A:36:GLU:HG2	0.41	1.93	6	1
1:A:160:ARG:NE	1:A:193:VAL:HG13	0.41	2.31	7	1
1:A:185:LEU:HD11	1:A:341:LEU:CD1	0.41	2.41	12	1
1:A:165:LEU:HD21	1:A:175:HIS:HB3	0.41	1.93	20	1
1:A:255:LEU:HD11	1:A:294:ASN:ND2	0.40	2.30	4	1
1:A:86:PHE:CE2	1:A:168:ILE:HG21	0.40	2.51	2	1
1:A:82:THR:CG2	1:A:201:ALA:HB3	0.40	2.46	6	1
1:A:84:LEU:HD13	1:A:129:MET:SD	0.40	2.56	18	1
1:A:179:LYS:O	1:A:180:ALA:HB2	0.40	2.16	8	1
1:A:28:ILE:HD13	1:A:38:LYS:HB3	0.40	1.93	11	1
1:A:155:LEU:HG	1:A:328:LEU:HD13	0.40	1.93	16	1
1:A:47:GLY:HA3	1:A:351:ALA:HB3	0.40	1.92	18	1
1:A:176:GLY:C	1:A:246:ILE:HD13	0.40	2.36	19	1
1:A:282:ILE:HA	1:A:285:LEU:HD21	0.40	1.91	2	1
1:A:343:VAL:C	1:A:344:VAL:HG22	0.40	2.37	10	1
1:A:161:ILE:HG22	1:A:165:LEU:HD12	0.40	1.94	17	1
1:A:173:TYR:O	1:A:174:VAL:HG13	0.40	2.16	18	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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	316/368 (86%)	250±4 (79±1%)	46±4 (14±1%)	20±4 (6±1%)	3 19
All	All	6320/7360 (86%)	5002 (79%)	913 (14%)	405 (6%)	3 19

All 71 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	297	GLY	20
1	A	356	LYS	17
1	A	219	ARG	15
1	A	135	GLY	14
1	A	172	GLU	14
1	A	218	LYS	14
1	A	92	LYS	13
1	A	310	ASP	12
1	A	344	VAL	12
1	A	77	ASN	11
1	A	334	LYS	11
1	A	340	ASP	11
1	A	132	ASP	10
1	A	342	SER	10
1	A	192	GLN	8
1	A	229	SER	8
1	A	312	THR	8
1	A	339	LEU	8
1	A	78	GLY	8
1	A	294	ASN	8
1	A	345	GLU	8
1	A	214	LYS	7
1	A	121	LYS	7
1	A	55	ASP	7
1	A	215	GLU	6
1	A	179	LYS	6
1	A	295	LYS	6
1	A	292	GLU	5
1	A	48	PHE	5
1	A	293	LYS	5
1	A	239	SER	5
1	A	352	LYS	5
1	A	196	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	309	LEU	5
1	A	343	VAL	5
1	A	53	LEU	4
1	A	35	LYS	4
1	A	106	LYS	4
1	A	221	HIS	4
1	A	335	ASP	4
1	A	56	MET	3
1	A	240	ARG	3
1	A	47	GLY	3
1	A	120	ASP	3
1	A	122	ASN	3
1	A	211	LYS	3
1	A	124	LYS	3
1	A	175	HIS	3
1	A	353	THR	3
1	A	351	ALA	3
1	A	50	CYS	3
1	A	49	GLY	3
1	A	76	ASP	3
1	A	216	ASP	3
1	A	36	GLU	2
1	A	105	LEU	2
1	A	313	GLU	2
1	A	44	GLY	2
1	A	314	LYS	2
1	A	341	LEU	2
1	A	46	GLY	2
1	A	210	HIS	1
1	A	223	GLY	1
1	A	350	LYS	1
1	A	180	ALA	1
1	A	173	TYR	1
1	A	66	ALA	1
1	A	204	TYR	1
1	A	212	GLU	1
1	A	222	ASP	1
1	A	203	ARG	1

6.3.2 Protein sidechains (i)

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	278/319 (87%)	204±7 (73±2%)	74±7 (27±2%)	2 22
All	All	5560/6380 (87%)	4074 (73%)	1486 (27%)	2 22

All 225 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	147	LYS	20
1	A	305	THR	20
1	A	155	LEU	19
1	A	267	ASP	18
1	A	130	ILE	17
1	A	132	ASP	16
1	A	354	ILE	16
1	A	293	LYS	15
1	A	92	LYS	15
1	A	187	TYR	15
1	A	106	LYS	14
1	A	124	LYS	14
1	A	282	ILE	14
1	A	303	MET	14
1	A	131	MET	14
1	A	30	THR	13
1	A	41	LEU	13
1	A	110	VAL	13
1	A	142	TYR	13
1	A	188	LYS	13
1	A	310	ASP	13
1	A	356	LYS	13
1	A	152	LYS	13
1	A	350	LYS	13
1	A	70	VAL	13
1	A	48	PHE	12
1	A	133	ARG	12
1	A	203	ARG	12
1	A	200	LEU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	245	GLU	12
1	A	352	LYS	12
1	A	34	LYS	11
1	A	183	LEU	11
1	A	216	ASP	11
1	A	240	ARG	11
1	A	341	LEU	11
1	A	87	TYR	11
1	A	231	ASP	11
1	A	342	SER	11
1	A	27	GLU	10
1	A	53	LEU	10
1	A	125	SER	10
1	A	212	GLU	10
1	A	214	LYS	10
1	A	219	ARG	10
1	A	334	LYS	10
1	A	345	GLU	10
1	A	98	LYS	10
1	A	229	SER	10
1	A	295	LYS	10
1	A	269	LYS	10
1	A	289	CYS	10
1	A	307	LYS	10
1	A	151	ARG	10
1	A	290	PHE	10
1	A	71	LYS	9
1	A	99	TRP	9
1	A	137	ASP	9
1	A	265	LEU	9
1	A	286	MET	9
1	A	301	LYS	9
1	A	121	LYS	9
1	A	159	LEU	9
1	A	241	ARG	9
1	A	252	ILE	9
1	A	273	ASP	9
1	A	280	GLU	9
1	A	326	GLN	9
1	A	150	SER	9
1	A	103	ARG	9
1	A	35	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	127	ARG	8
1	A	136	SER	8
1	A	170	GLU	8
1	A	172	GLU	8
1	A	228	THR	8
1	A	258	HIS	8
1	A	298	GLU	8
1	A	314	LYS	8
1	A	88	GLN	8
1	A	215	GLU	8
1	A	28	ILE	8
1	A	118	LEU	8
1	A	156	GLN	8
1	A	243	ASP	8
1	A	262	GLU	8
1	A	218	LYS	8
1	A	250	CYS	8
1	A	105	LEU	8
1	A	274	SER	8
1	A	73	GLU	7
1	A	129	MET	7
1	A	309	LEU	7
1	A	56	MET	7
1	A	77	ASN	7
1	A	85	LYS	7
1	A	278	TYR	7
1	A	328	LEU	7
1	A	335	ASP	7
1	A	220	CYS	7
1	A	279	ARG	7
1	A	89	ARG	7
1	A	182	ASN	7
1	A	272	ARG	7
1	A	80	LEU	7
1	A	196	VAL	7
1	A	186	ASN	6
1	A	192	GLN	6
1	A	211	LYS	6
1	A	184	LEU	6
1	A	287	ASP	6
1	A	263	ASP	6
1	A	292	GLU	6

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Mol	Chain	Res	Type	Models (Total)
1	A	120	ASP	6
1	A	171	HIS	6
1	A	104	LYS	6
1	A	140	LYS	6
1	A	266	LYS	6
1	A	86	PHE	6
1	A	340	ASP	6
1	A	76	ASP	5
1	A	160	ARG	5
1	A	162	LEU	5
1	A	204	TYR	5
1	A	222	ASP	5
1	A	322	ASP	5
1	A	323	ILE	5
1	A	179	LYS	5
1	A	233	HIS	5
1	A	270	TYR	5
1	A	312	THR	5
1	A	75	SER	5
1	A	101	ARG	5
1	A	148	ARG	5
1	A	50	CYS	5
1	A	139	GLN	5
1	A	38	LYS	5
1	A	195	LEU	5
1	A	178	ILE	4
1	A	294	ASN	4
1	A	145	ASN	4
1	A	275	LYS	4
1	A	285	LEU	4
1	A	253	GLN	4
1	A	45	GLN	4
1	A	175	HIS	4
1	A	181	SER	4
1	A	319	ASN	4
1	A	264	ASN	4
1	A	141	ILE	4
1	A	189	ASN	4
1	A	304	GLU	4
1	A	311	TYR	4
1	A	169	HIS	4
1	A	36	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	122	ASN	4
1	A	119	HIS	4
1	A	95	GLN	3
1	A	173	TYR	3
1	A	288	LYS	3
1	A	313	GLU	3
1	A	325	LEU	3
1	A	37	TRP	3
1	A	166	GLU	3
1	A	197	ASP	3
1	A	97	GLN	3
1	A	207	GLU	3
1	A	284	SER	3
1	A	29	ILE	3
1	A	251	MET	3
1	A	157	LEU	3
1	A	308	LEU	3
1	A	321	ARG	3
1	A	329	LYS	3
1	A	94	GLU	3
1	A	107	TYR	3
1	A	108	LEU	3
1	A	138	LEU	3
1	A	55	ASP	3
1	A	185	LEU	3
1	A	236	VAL	3
1	A	239	SER	3
1	A	51	ILE	3
1	A	224	THR	3
1	A	153	THR	2
1	A	177	ASP	2
1	A	113	TYR	2
1	A	234	ASN	2
1	A	277	ARG	2
1	A	316	LEU	2
1	A	84	LEU	2
1	A	163	ASP	2
1	A	32	MET	2
1	A	143	GLU	2
1	A	210	HIS	2
1	A	343	VAL	2
1	A	333	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	A	31	ASP	2
1	A	198	TYR	2
1	A	68	CYS	2
1	A	306	VAL	1
1	A	281	ASN	1
1	A	161	ILE	1
1	A	25	VAL	1
1	A	112	LYS	1
1	A	344	VAL	1
1	A	205	CYS	1
1	A	209	VAL	1
1	A	221	HIS	1
1	A	317	TYR	1
1	A	339	LEU	1
1	A	69	VAL	1
1	A	271	VAL	1
1	A	39	VAL	1
1	A	225	ILE	1
1	A	318	GLU	1
1	A	191	ASP	1
1	A	226	GLU	1
1	A	324	LEU	1
1	A	82	THR	1
1	A	165	LEU	1
1	A	255	LEU	1
1	A	355	THR	1
1	A	158	SER	1
1	A	246	ILE	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided