



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:02 am BST

PDB ID : 2MBG
Title : Rlip76 (gap-gbd)
Authors : Rajasekar, K.V.; Campbell, L.J.; Nietlispach, D.; Owen, D.; Mott, H.R.
Deposited on : 2013-07-30

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

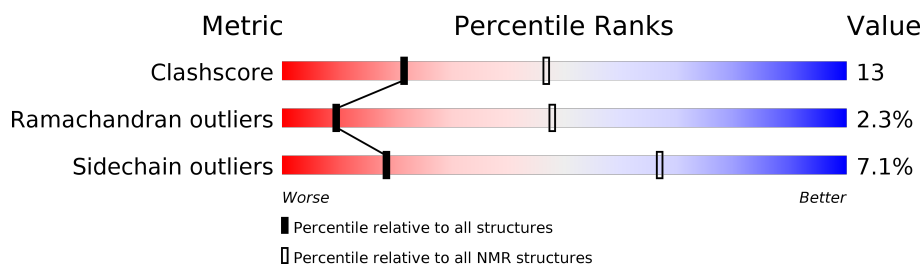
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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	265	

2 Ensemble composition and analysis ⓘ

This entry contains 35 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:189-A:380, A:390-A:446 (249)	0.51	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 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 8, 9, 11, 12, 13, 14, 15, 17, 18, 19, 20, 24, 25, 28, 29, 30, 31, 32, 34
2	7, 23, 26, 35
3	16, 27
4	22, 33
Single-model clusters	10; 21

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4406 atoms, of which 2234 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RalA-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	265	Total	C	H	N	O	S	0
			4406	1385	2234	373	399	15	

There are 2 discrepancies between the modelled and reference sequences:

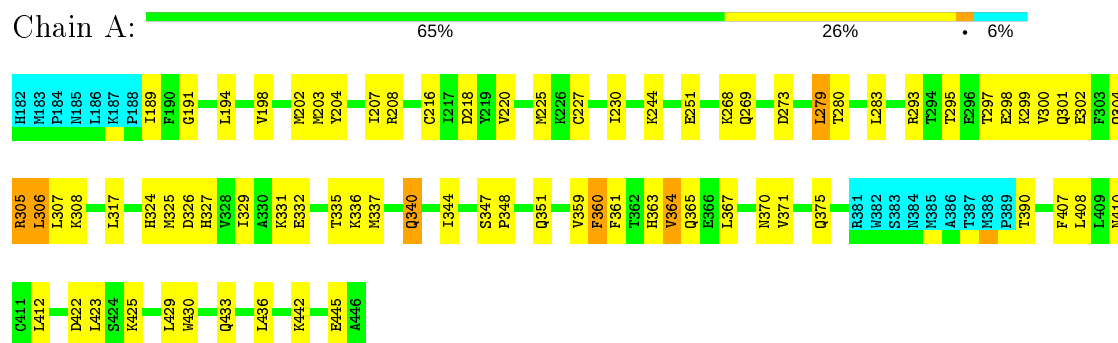
Chain	Residue	Modelled	Actual	Comment	Reference
A	182	HIS	-	EXPRESSION TAG	UNP Q15311
A	183	MET	-	EXPRESSION TAG	UNP Q15311

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RalA-binding protein 1

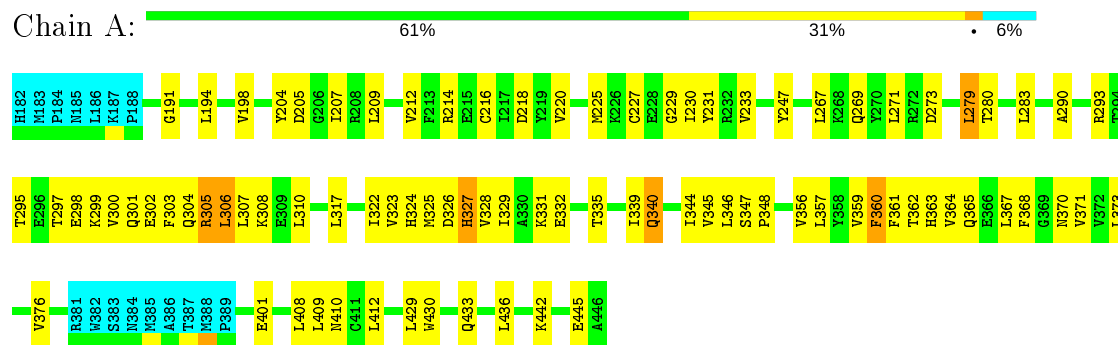


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

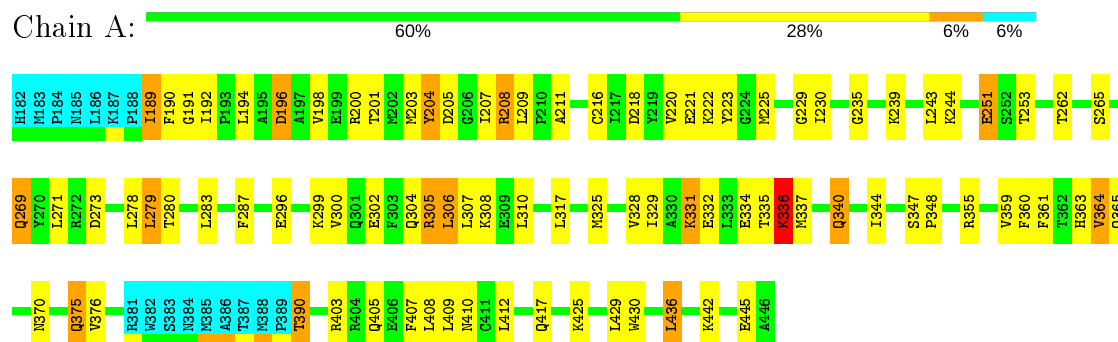
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: RalA-binding protein 1



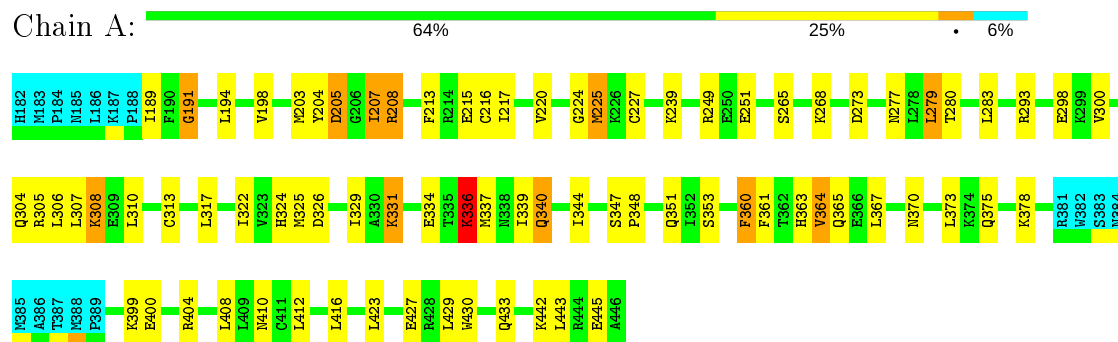
4.2.2 Score per residue for model 2

- Molecule 1: RalA-binding protein 1



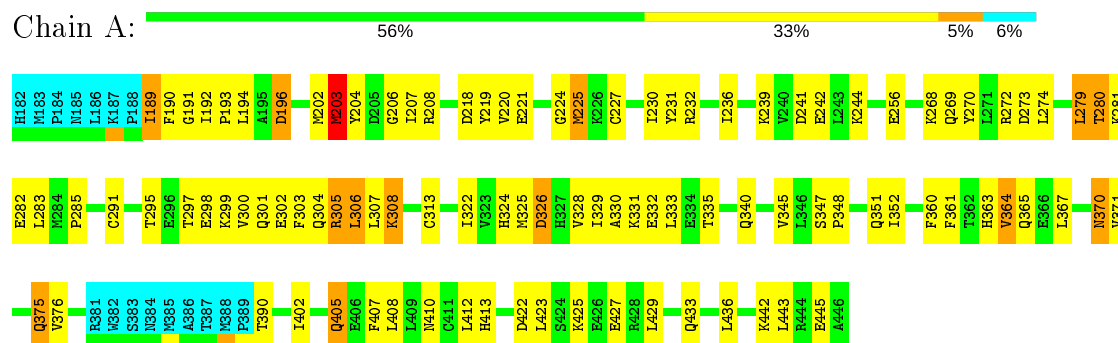
4.2.3 Score per residue for model 3

- Molecule 1: RalA-binding protein 1



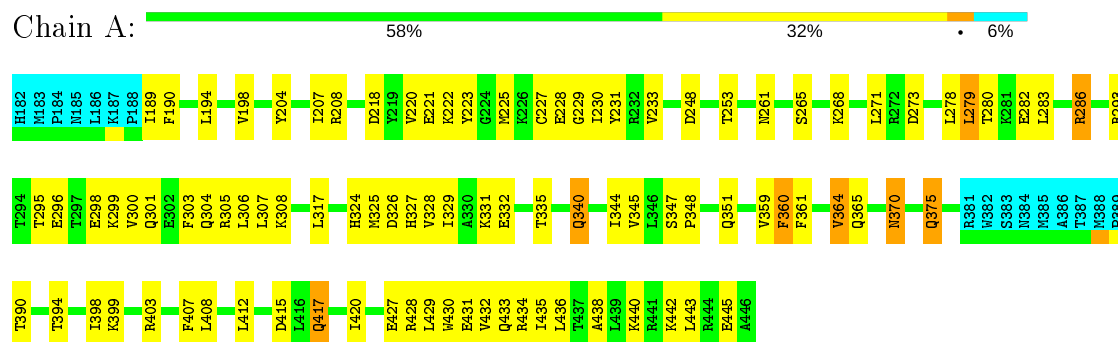
4.2.4 Score per residue for model 4

- Molecule 1: RalA-binding protein 1



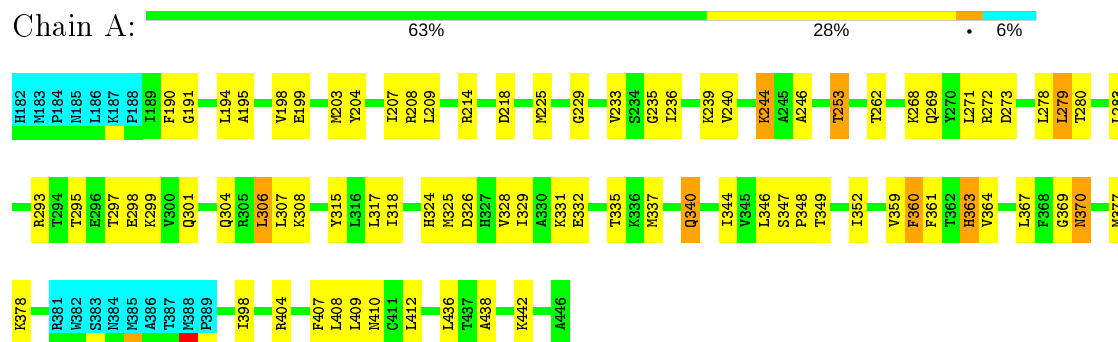
4.2.5 Score per residue for model 5

- Molecule 1: RalA-binding protein 1



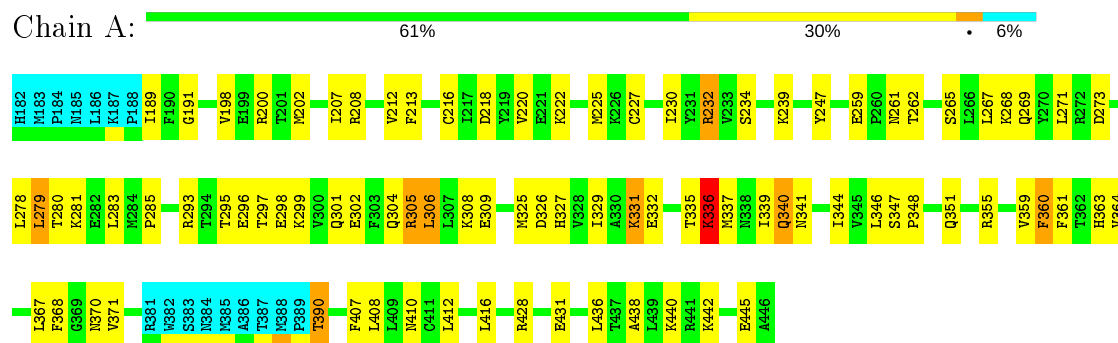
4.2.6 Score per residue for model 6

- Molecule 1: RalA-binding protein 1



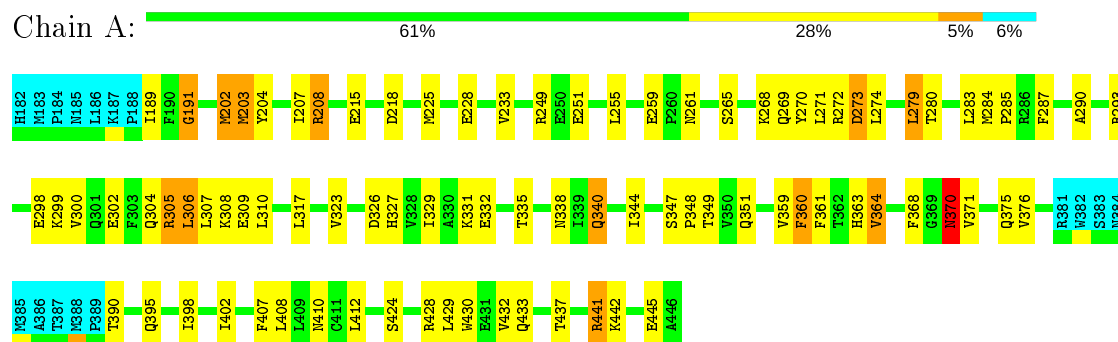
4.2.7 Score per residue for model 7

- Molecule 1: RalA-binding protein 1



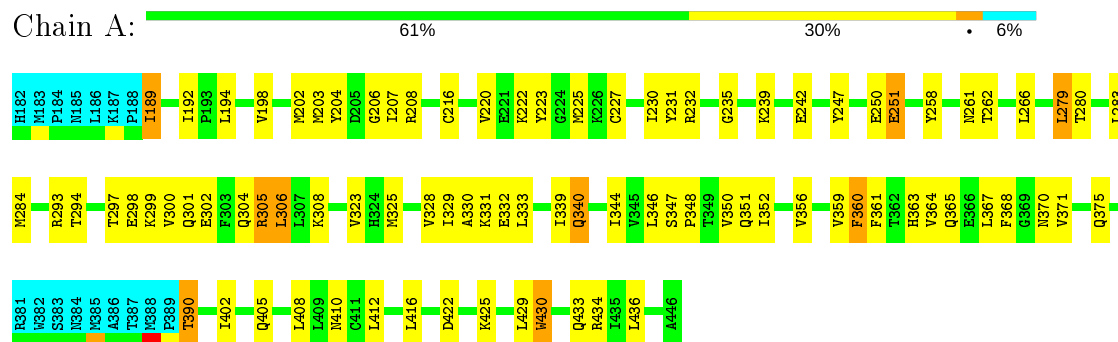
4.2.8 Score per residue for model 8

- Molecule 1: RalA-binding protein 1



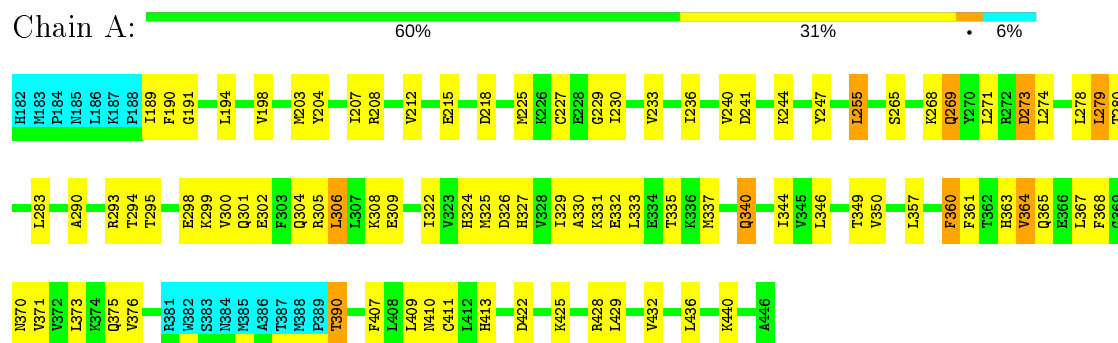
4.2.9 Score per residue for model 9

- Molecule 1: RalA-binding protein 1



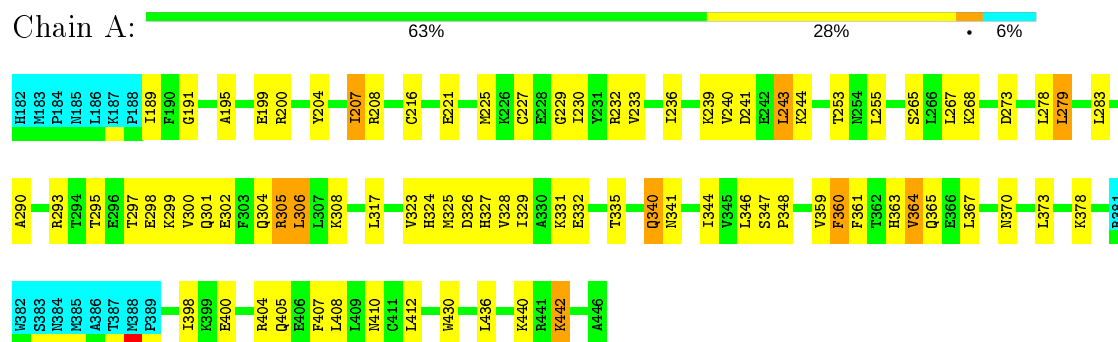
4.2.10 Score per residue for model 10

- Molecule 1: RalA-binding protein 1



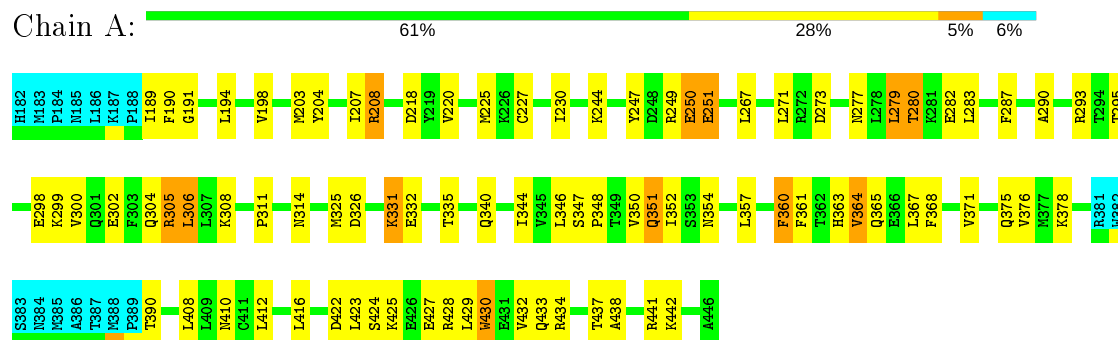
4.2.11 Score per residue for model 11

- Molecule 1: RalA-binding protein 1



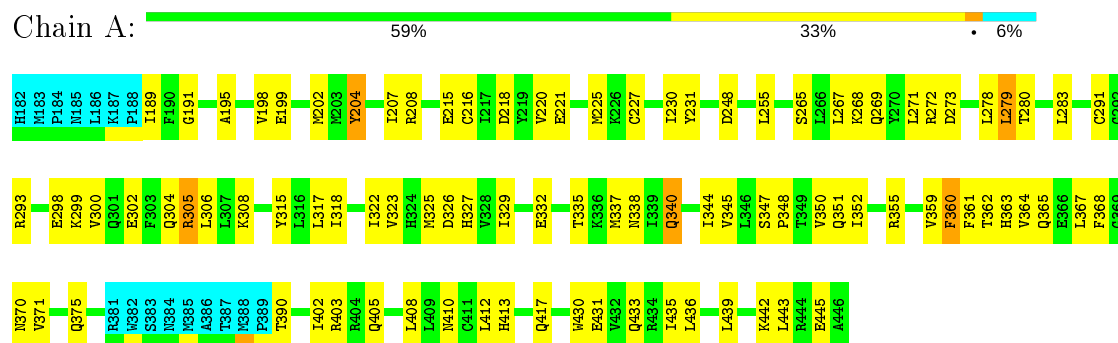
4.2.12 Score per residue for model 12

- Molecule 1: RalA-binding protein 1



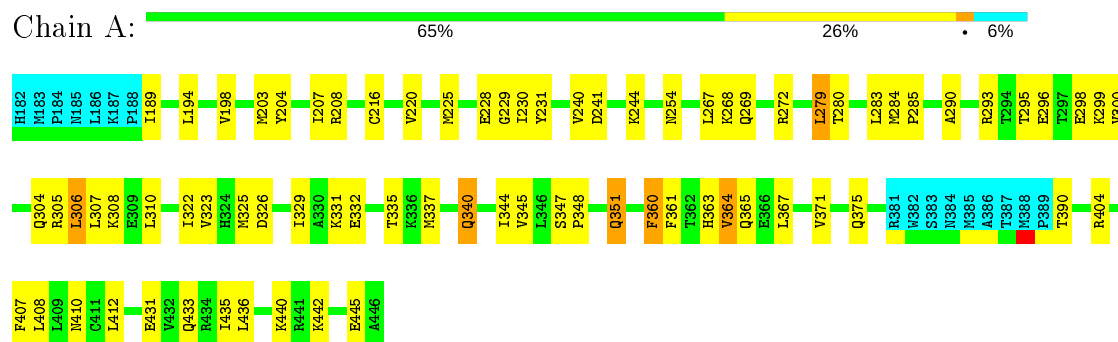
4.2.13 Score per residue for model 13

- Molecule 1: RalA-binding protein 1



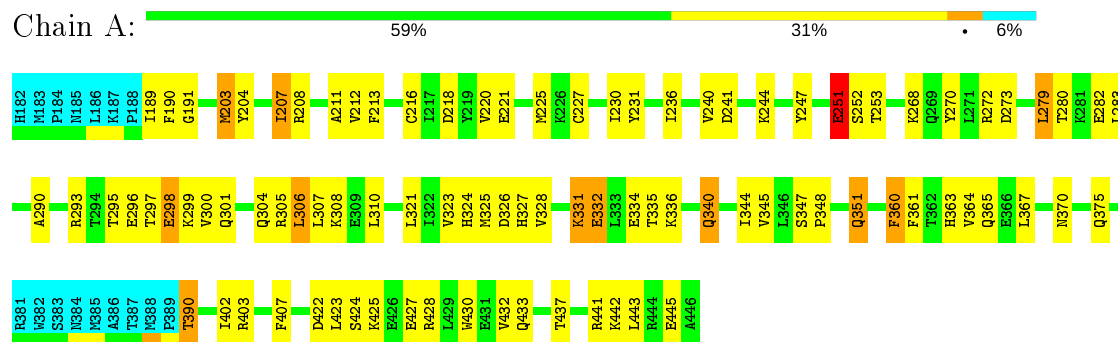
4.2.14 Score per residue for model 14

- Molecule 1: RalA-binding protein 1



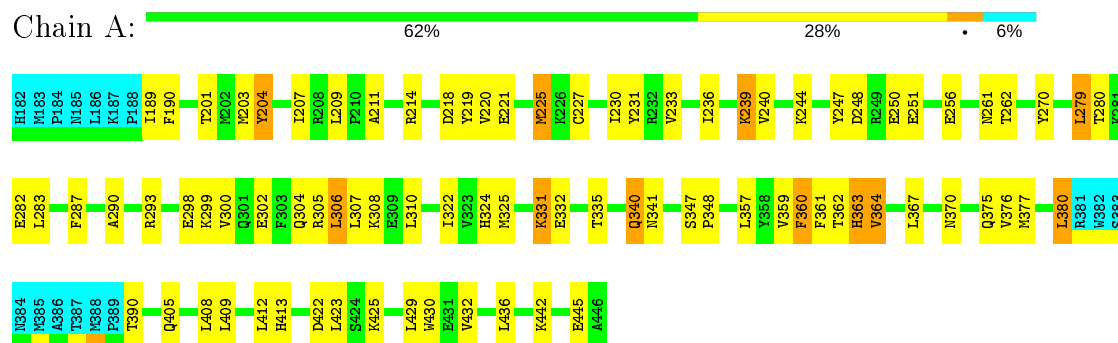
4.2.15 Score per residue for model 15

- Molecule 1: RalA-binding protein 1



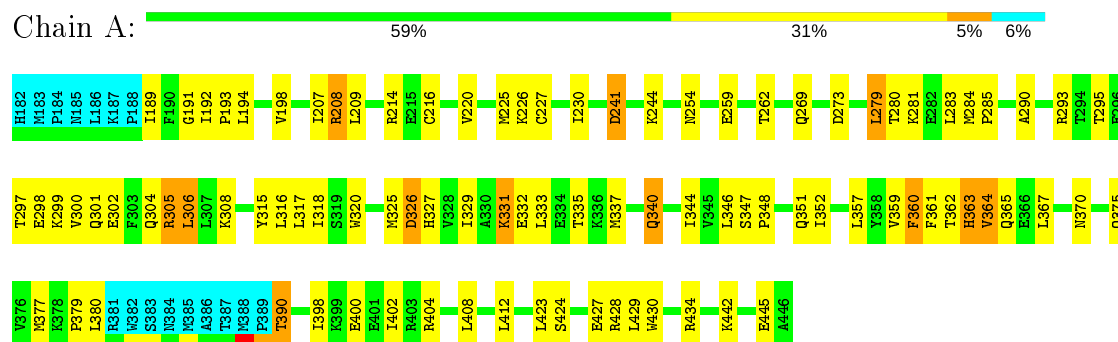
4.2.16 Score per residue for model 16

- Molecule 1: RalA-binding protein 1



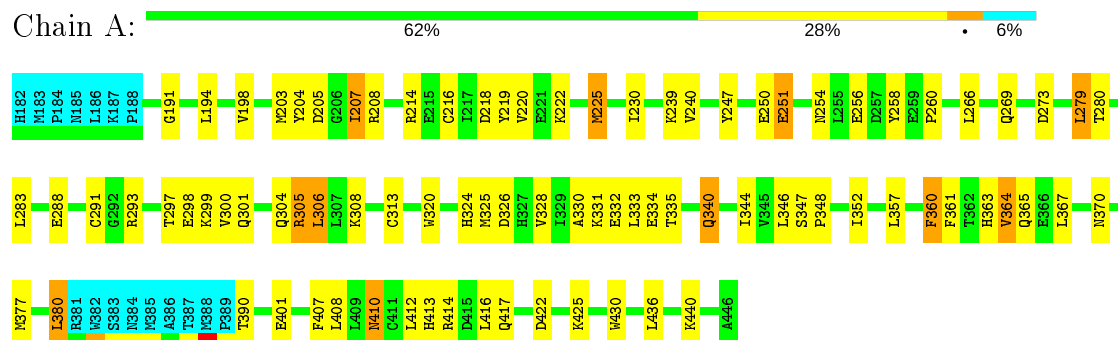
4.2.17 Score per residue for model 17

- Molecule 1: RalA-binding protein 1



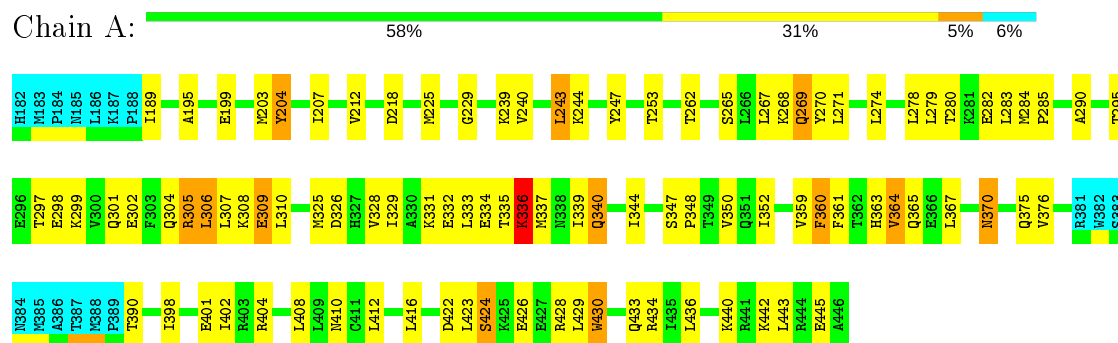
4.2.18 Score per residue for model 18

- Molecule 1: RalA-binding protein 1



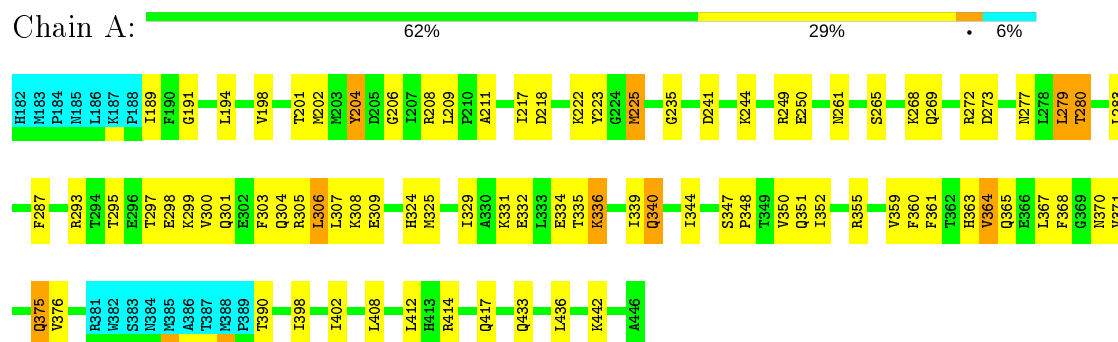
4.2.19 Score per residue for model 19

- Molecule 1: RalA-binding protein 1



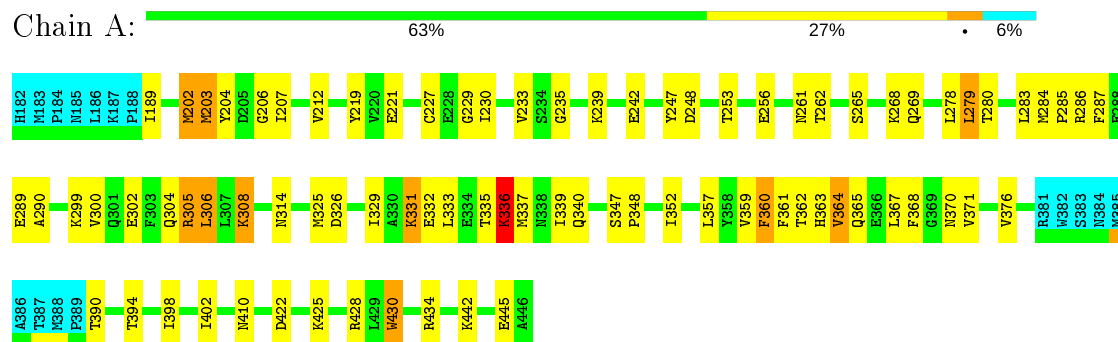
4.2.20 Score per residue for model 20

- Molecule 1: RalA-binding protein 1



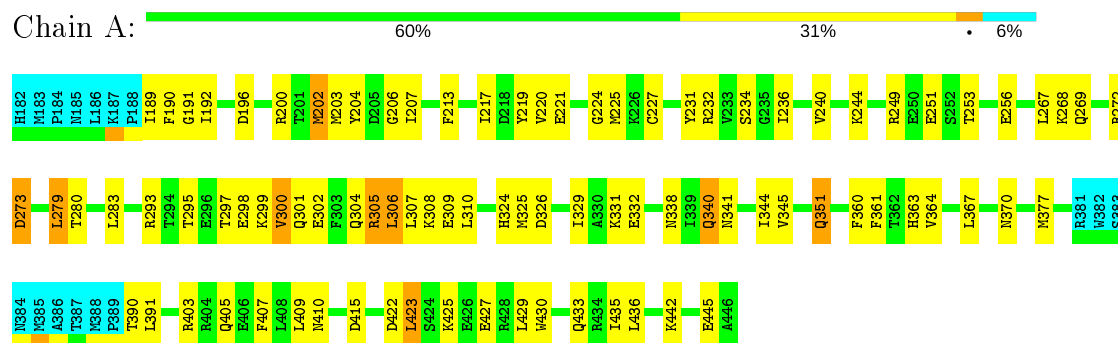
4.2.21 Score per residue for model 21

- Molecule 1: RalA-binding protein 1



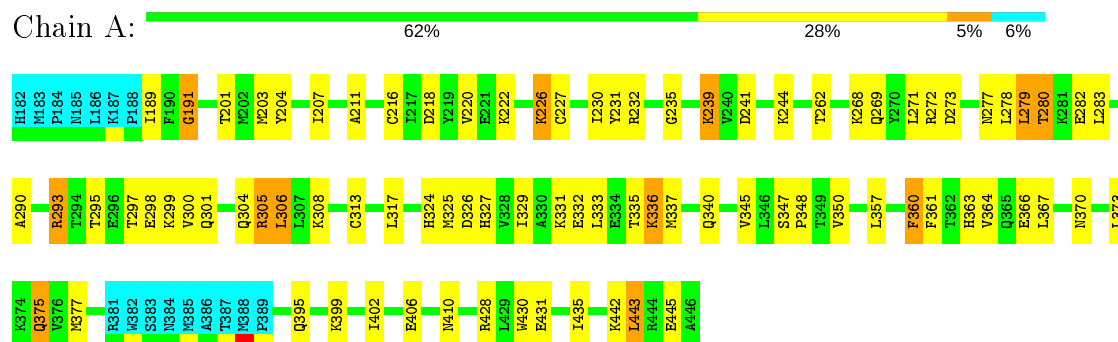
4.2.22 Score per residue for model 22

- Molecule 1: RalA-binding protein 1



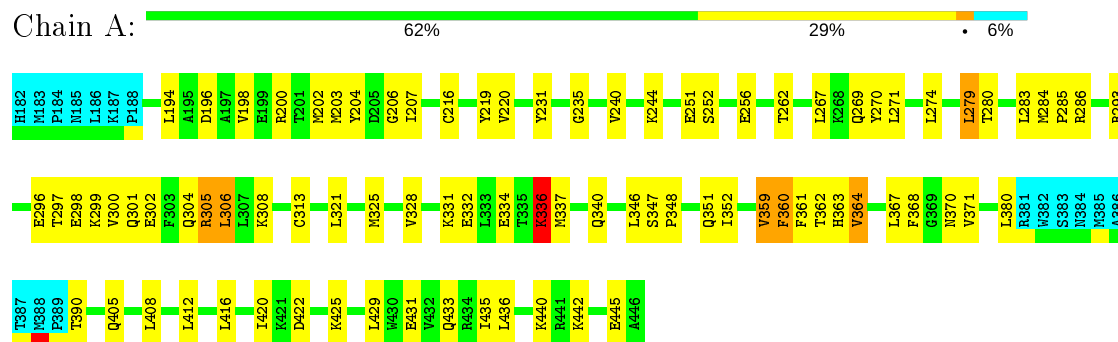
4.2.23 Score per residue for model 23

- Molecule 1: RalA-binding protein 1



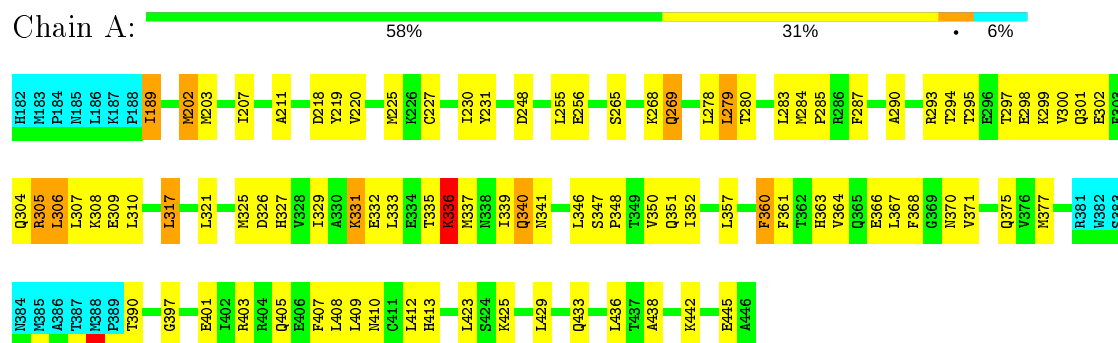
4.2.24 Score per residue for model 24

- Molecule 1: RalA-binding protein 1



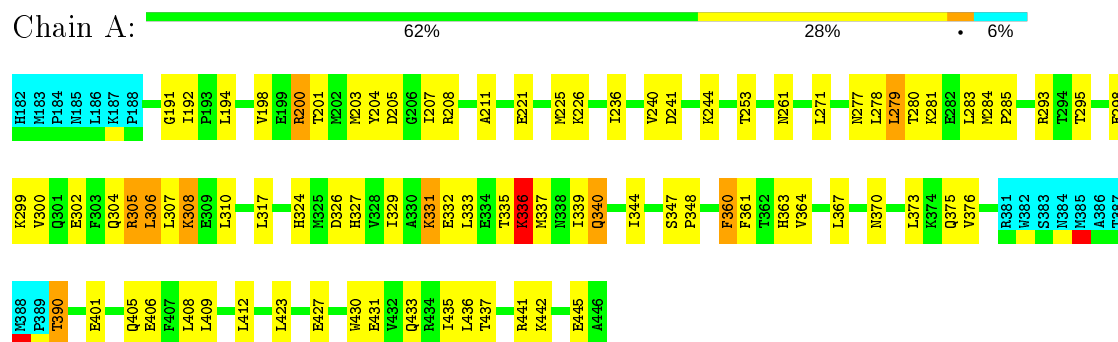
4.2.25 Score per residue for model 25

- Molecule 1: RalA-binding protein 1



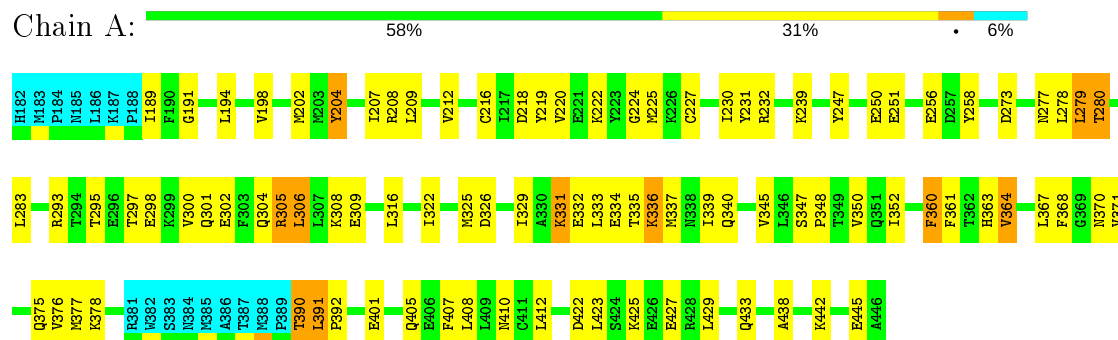
4.2.26 Score per residue for model 26

- Molecule 1: RalA-binding protein 1



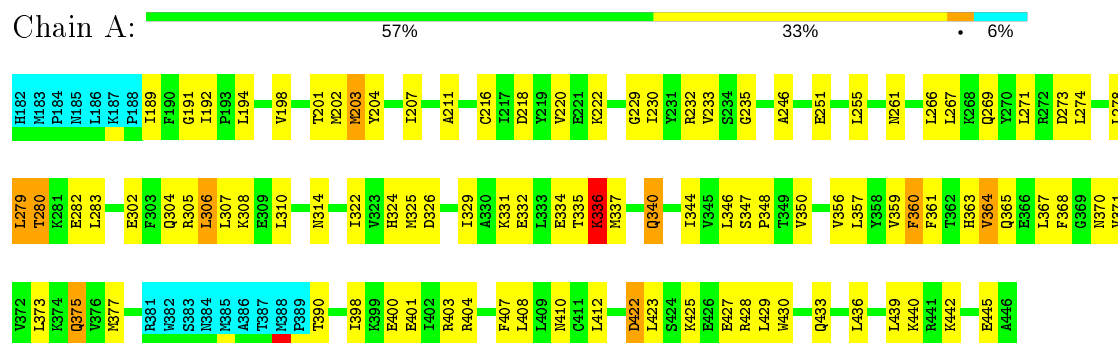
4.2.27 Score per residue for model 27

- Molecule 1: RalA-binding protein 1



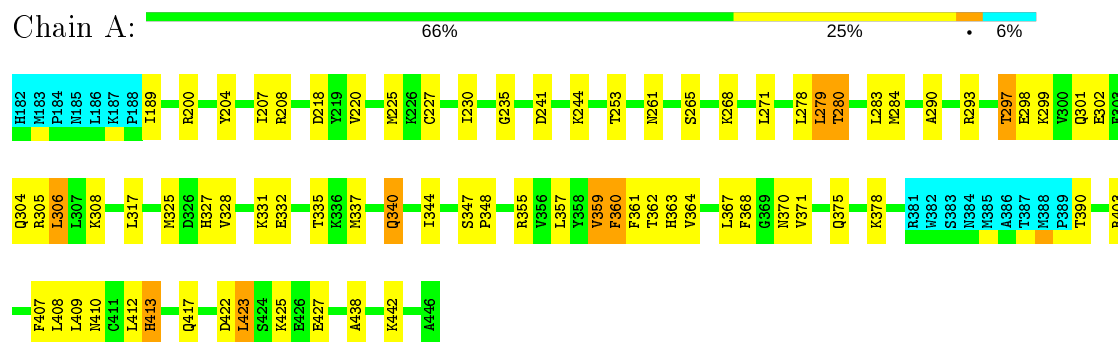
4.2.28 Score per residue for model 28

- Molecule 1: RalA-binding protein 1



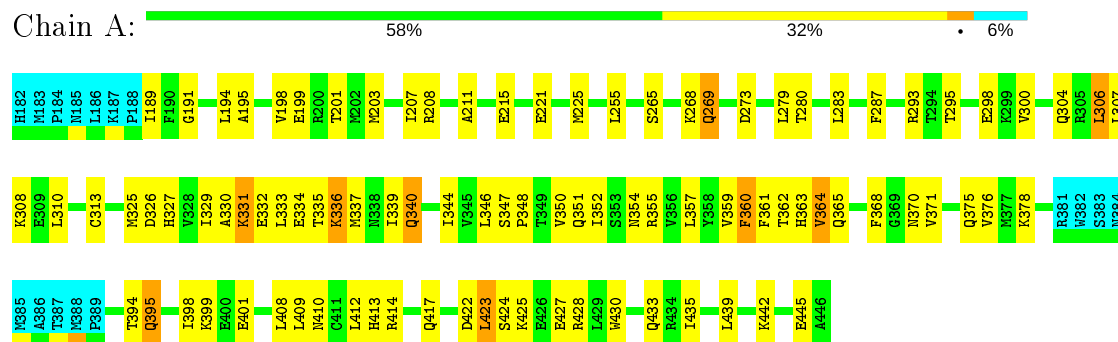
4.2.29 Score per residue for model 29

- Molecule 1: RalA-binding protein 1



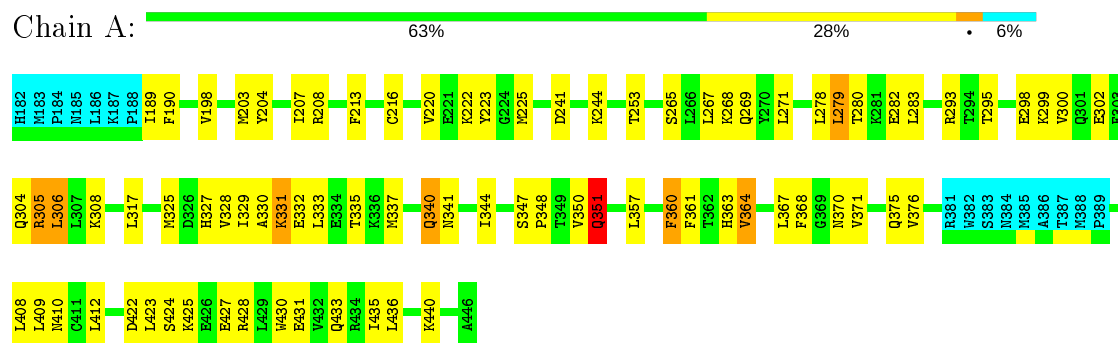
4.2.30 Score per residue for model 30

- Molecule 1: RalA-binding protein 1



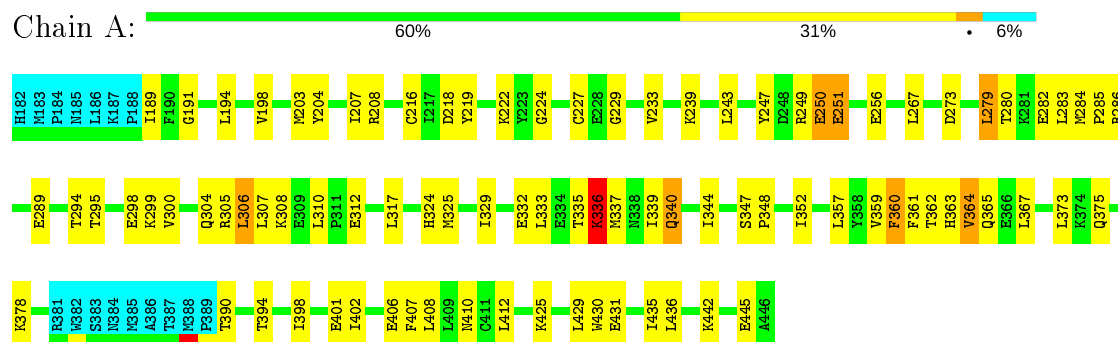
4.2.31 Score per residue for model 31

- Molecule 1: RalA-binding protein 1



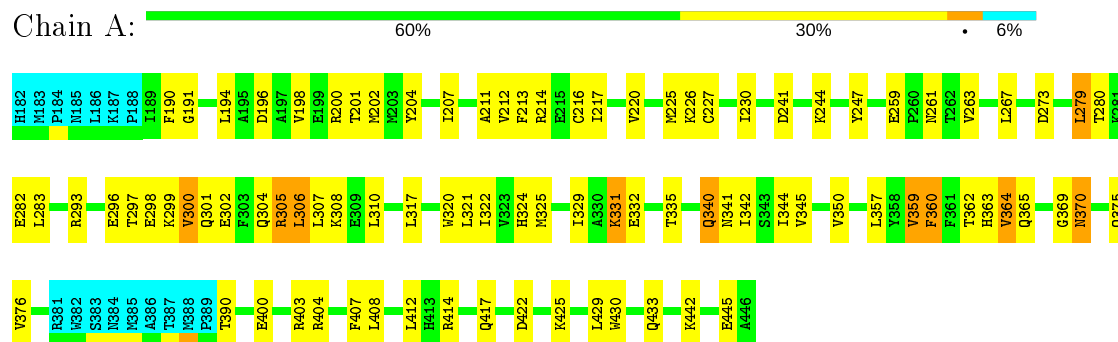
4.2.32 Score per residue for model 32

- Molecule 1: RalA-binding protein 1



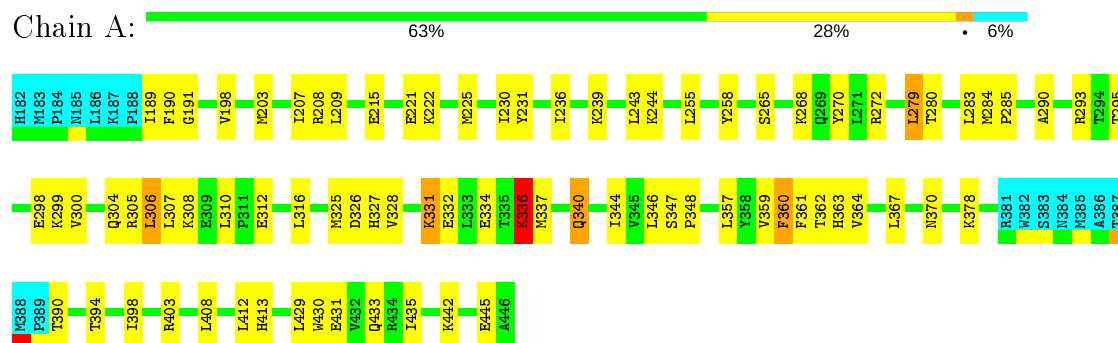
4.2.33 Score per residue for model 33

- Molecule 1: RalA-binding protein 1



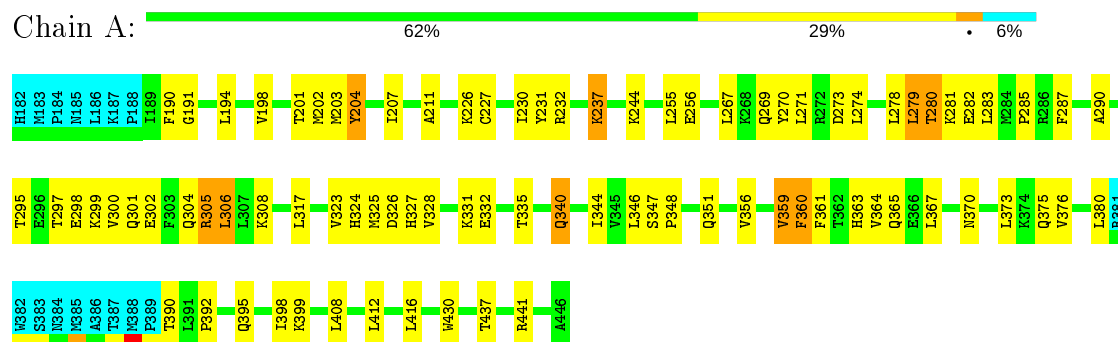
4.2.34 Score per residue for model 34

- Molecule 1: RalA-binding protein 1



4.2.35 Score per residue for model 35

- Molecule 1: RalA-binding protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 35 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	

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	3262
Number of shifts mapped to atoms	3262
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	2041	2100	2096	54±5
All	All	71435	73500	73360	1881

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:TYR:HA	1:A:251:GLU:HB3	0.90	1.44	32	6
1:A:241:ASP:HA	1:A:244:LYS:HE2	0.89	1.43	14	5
1:A:295:THR:HB	1:A:298:GLU:HG2	0.88	1.46	12	22
1:A:225:MET:HG3	1:A:331:LYS:HG3	0.86	1.45	14	11
1:A:300:VAL:HG12	1:A:363:HIS:HB2	0.86	1.48	17	13
1:A:332:GLU:HB2	1:A:337:MET:HB2	0.83	1.48	10	6
1:A:225:MET:SD	1:A:331:LYS:HG2	0.81	2.15	2	1
1:A:324:HIS:HD2	1:A:373:LEU:HG	0.78	1.39	23	7
1:A:225:MET:SD	1:A:331:LYS:HG3	0.77	2.19	31	10
1:A:293:ARG:HB2	1:A:299:LYS:HG2	0.77	1.57	33	19
1:A:377:MET:SD	1:A:405:GLN:HA	0.76	2.21	16	1
1:A:331:LYS:HA	1:A:331:LYS:HE3	0.76	1.58	25	5
1:A:332:GLU:HA	1:A:335:THR:OG1	0.75	1.81	35	26
1:A:408:LEU:O	1:A:412:LEU:HG	0.75	1.80	29	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:422:ASP:HB2	1:A:425:LYS:HG2	0.75	1.57	22	12
1:A:331:LYS:HE3	1:A:331:LYS:HA	0.74	1.58	17	4
1:A:347:SER:HB3	1:A:348:PRO:HD3	0.73	1.60	6	32
1:A:239:LYS:HE2	1:A:239:LYS:HA	0.72	1.59	3	4
1:A:219:TYR:CE1	1:A:256:GLU:HA	0.71	2.20	18	9
1:A:360:PHE:HA	1:A:363:HIS:CE1	0.71	2.21	21	6
1:A:331:LYS:HA	1:A:334:GLU:HG2	0.71	1.62	24	7
1:A:329:ILE:O	1:A:332:GLU:HG2	0.70	1.86	13	6
1:A:360:PHE:O	1:A:364:VAL:HB	0.70	1.86	29	33
1:A:325:MET:HB3	1:A:361:PHE:HE1	0.70	1.47	24	21
1:A:442:LYS:HA	1:A:445:GLU:HB3	0.70	1.64	26	11
1:A:363:HIS:O	1:A:367:LEU:HG	0.70	1.86	11	17
1:A:329:ILE:HG21	1:A:339:ILE:HG12	0.69	1.63	1	6
1:A:239:LYS:HA	1:A:239:LYS:HE2	0.69	1.65	2	1
1:A:189:ILE:HD11	1:A:200:ARG:HG2	0.68	1.63	7	2
1:A:265:SER:HA	1:A:268:LYS:HE3	0.68	1.66	8	3
1:A:290:ALA:HA	1:A:293:ARG:HG2	0.68	1.66	14	7
1:A:283:LEU:HD12	1:A:306:LEU:HD12	0.67	1.67	28	34
1:A:293:ARG:HB3	1:A:298:GLU:HB2	0.67	1.64	3	20
1:A:220:VAL:HG12	1:A:225:MET:SD	0.67	2.29	9	2
1:A:329:ILE:HA	1:A:332:GLU:HG2	0.67	1.66	10	3
1:A:237:LYS:H	1:A:237:LYS:HD3	0.67	1.49	35	1
1:A:225:MET:HB3	1:A:331:LYS:HE2	0.67	1.64	1	1
1:A:241:ASP:HA	1:A:244:LYS:HD2	0.66	1.66	15	1
1:A:203:MET:HE3	1:A:211:ALA:HA	0.66	1.68	15	1
1:A:204:TYR:HE2	1:A:376:VAL:HA	0.65	1.51	2	1
1:A:202:MET:SD	1:A:206:GLY:HA2	0.65	2.32	4	4
1:A:190:PHE:HE1	1:A:270:TYR:HA	0.65	1.51	16	1
1:A:221:GLU:HA	1:A:225:MET:SD	0.65	2.30	15	3
1:A:363:HIS:CD2	1:A:367:LEU:HD22	0.65	2.26	12	2
1:A:239:LYS:HA	1:A:239:LYS:HE3	0.65	1.67	23	1
1:A:213:PHE:O	1:A:217:ILE:HG12	0.65	1.91	3	1
1:A:279:LEU:HD23	1:A:352:ILE:HD11	0.65	1.67	12	12
1:A:204:TYR:HE1	1:A:376:VAL:HG13	0.65	1.49	33	2
1:A:241:ASP:HA	1:A:244:LYS:HD3	0.65	1.68	20	5
1:A:279:LEU:HG	1:A:287:PHE:CE1	0.65	2.27	25	4
1:A:218:ASP:O	1:A:222:LYS:HG2	0.64	1.92	27	1
1:A:304:GLN:O	1:A:308:LYS:HG2	0.64	1.93	34	35
1:A:324:HIS:CD2	1:A:373:LEU:HG	0.64	2.26	23	5
1:A:196:ASP:O	1:A:200:ARG:HG2	0.64	1.92	33	3
1:A:297:THR:O	1:A:301:GLN:HG2	0.64	1.93	11	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:326:ASP:HA	1:A:329:ILE:HG12	0.64	1.69	25	9
1:A:203:MET:HE3	1:A:376:VAL:HG21	0.63	1.69	16	4
1:A:307:LEU:HA	1:A:310:LEU:HG	0.63	1.69	33	13
1:A:271:LEU:HD11	1:A:278:LEU:HD21	0.63	1.70	26	9
1:A:402:ILE:HD12	1:A:443:LEU:HD12	0.63	1.68	13	2
1:A:271:LEU:HD21	1:A:278:LEU:HD11	0.63	1.69	10	3
1:A:233:VAL:HG23	1:A:261:ASN:HB3	0.63	1.71	5	4
1:A:335:THR:O	1:A:336:LYS:HB3	0.62	1.94	2	2
1:A:240:VAL:HG22	1:A:262:THR:HG23	0.62	1.72	16	1
1:A:331:LYS:HE3	1:A:331:LYS:C	0.62	2.15	2	1
1:A:344:ILE:HA	1:A:354:ASN:OD1	0.61	1.95	12	1
1:A:325:MET:HB3	1:A:361:PHE:CE1	0.61	2.29	21	30
1:A:300:VAL:HB	1:A:367:LEU:HD11	0.61	1.71	4	3
1:A:322:ILE:HB	1:A:364:VAL:HG21	0.61	1.70	28	8
1:A:190:PHE:O	1:A:273:ASP:HB2	0.61	1.96	6	1
1:A:413:HIS:CD2	1:A:429:LEU:HD21	0.61	2.31	34	1
1:A:302:GLU:O	1:A:305:ARG:HG3	0.61	1.96	31	7
1:A:336:LYS:HD3	1:A:337:MET:HG3	0.61	1.71	28	5
1:A:442:LYS:HA	1:A:445:GLU:CB	0.60	2.25	26	19
1:A:230:ILE:HD11	1:A:260:PRO:HB2	0.60	1.70	18	1
1:A:203:MET:SD	1:A:376:VAL:HB	0.60	2.36	21	2
1:A:336:LYS:HD3	1:A:337:MET:N	0.60	2.10	25	5
1:A:191:GLY:HA2	1:A:273:ASP:O	0.60	1.96	7	23
1:A:360:PHE:HA	1:A:363:HIS:CD2	0.60	2.32	31	5
1:A:193:PRO:HG2	1:A:196:ASP:HB2	0.59	1.73	4	1
1:A:205:ASP:HB2	1:A:207:ILE:HG23	0.59	1.72	3	1
1:A:286:ARG:HA	1:A:286:ARG:HE	0.59	1.55	5	2
1:A:208:ARG:HB2	1:A:316:LEU:HD12	0.59	1.74	27	1
1:A:268:LYS:O	1:A:272:ARG:HG3	0.59	1.98	13	10
1:A:228:GLU:HA	1:A:335:THR:HB	0.59	1.74	14	2
1:A:398:ILE:HG23	1:A:439:LEU:HD12	0.59	1.74	28	1
1:A:361:PHE:O	1:A:364:VAL:HG12	0.59	1.97	25	31
1:A:442:LYS:HA	1:A:445:GLU:HB2	0.59	1.75	7	14
1:A:198:VAL:O	1:A:202:MET:HG3	0.59	1.98	13	6
1:A:203:MET:HG3	1:A:204:TYR:H	0.59	1.58	16	2
1:A:198:VAL:HG21	1:A:208:ARG:O	0.59	1.98	20	1
1:A:328:VAL:HG13	1:A:331:LYS:HE2	0.59	1.74	31	1
1:A:203:MET:SD	1:A:376:VAL:HG21	0.59	2.38	26	4
1:A:232:ARG:HD3	1:A:337:MET:SD	0.58	2.38	27	1
1:A:300:VAL:HB	1:A:367:LEU:HD21	0.58	1.74	27	5
1:A:340:GLN:O	1:A:344:ILE:HG13	0.58	1.98	2	27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:PHE:CZ	1:A:244:LYS:HG2	0.58	2.34	10	3
1:A:227:CYS:O	1:A:230:ILE:HB	0.58	1.98	4	18
1:A:204:TYR:HB2	1:A:376:VAL:HG13	0.58	1.74	27	1
1:A:254:ASN:HB2	1:A:380:LEU:HG	0.58	1.75	17	1
1:A:235:GLY:HA3	1:A:262:THR:HA	0.58	1.76	6	5
1:A:340:GLN:HE21	1:A:341:ASN:N	0.57	1.96	31	5
1:A:405:GLN:HE22	1:A:439:LEU:HD12	0.57	1.60	13	1
1:A:400:GLU:O	1:A:404:ARG:HG2	0.57	1.98	17	3
1:A:423:LEU:O	1:A:427:GLU:HG3	0.57	1.99	31	12
1:A:300:VAL:HG12	1:A:363:HIS:HB3	0.57	1.77	25	5
1:A:224:GLY:HA2	1:A:227:CYS:SG	0.57	2.40	32	5
1:A:359:VAL:HA	1:A:362:THR:OG1	0.57	2.00	32	11
1:A:422:ASP:HB2	1:A:425:LYS:CG	0.56	2.31	21	7
1:A:363:HIS:O	1:A:367:LEU:HD13	0.56	2.01	7	3
1:A:331:LYS:O	1:A:334:GLU:HG2	0.56	2.00	18	1
1:A:363:HIS:HD2	1:A:367:LEU:HD22	0.56	1.60	12	1
1:A:429:LEU:HG	1:A:433:GLN:NE2	0.56	2.16	28	10
1:A:331:LYS:HE3	1:A:332:GLU:N	0.56	2.16	2	1
1:A:290:ALA:O	1:A:299:LYS:HG2	0.56	2.01	10	12
1:A:194:LEU:HD23	1:A:274:LEU:HD22	0.55	1.78	28	1
1:A:241:ASP:HA	1:A:244:LYS:CE	0.55	2.31	10	2
1:A:405:GLN:HB2	1:A:436:LEU:HD21	0.55	1.78	4	1
1:A:239:LYS:HD2	1:A:258:TYR:CE2	0.55	2.37	34	2
1:A:325:MET:HG2	1:A:346:LEU:HD11	0.55	1.79	7	13
1:A:296:GLU:O	1:A:300:VAL:HG13	0.55	2.02	5	2
1:A:216:CYS:SG	1:A:267:LEU:HD13	0.55	2.42	14	4
1:A:229:GLY:HA2	1:A:337:MET:SD	0.55	2.42	14	4
1:A:247:TYR:HA	1:A:251:GLU:CB	0.55	2.29	15	3
1:A:209:LEU:HB3	1:A:214:ARG:NH2	0.55	2.17	16	1
1:A:214:ARG:HG2	1:A:320:TRP:HZ3	0.55	1.60	33	2
1:A:222:LYS:HZ1	1:A:378:LYS:HB3	0.55	1.61	34	1
1:A:272:ARG:HG2	1:A:351:GLN:HE22	0.55	1.62	8	1
1:A:218:ASP:OD1	1:A:375:GLN:HB2	0.55	2.02	29	12
1:A:293:ARG:HB2	1:A:299:LYS:CG	0.55	2.32	15	4
1:A:229:GLY:HA3	1:A:233:VAL:HG23	0.55	1.78	10	2
1:A:300:VAL:HG22	1:A:363:HIS:HB2	0.55	1.79	10	1
1:A:189:ILE:CG1	1:A:248:ASP:HA	0.55	2.32	21	2
1:A:220:VAL:O	1:A:225:MET:HG2	0.54	2.02	13	6
1:A:281:LYS:O	1:A:285:PRO:HD3	0.54	2.02	7	5
1:A:277:ASN:HB2	1:A:280:THR:HA	0.54	1.77	20	3
1:A:401:GLU:HA	1:A:401:GLU:OE1	0.54	2.03	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:THR:HB	1:A:282:GLU:OE1	0.54	2.02	12	2
1:A:270:TYR:O	1:A:274:LEU:HG	0.54	2.01	35	5
1:A:332:GLU:OE2	1:A:338:ASN:HA	0.54	2.02	13	3
1:A:241:ASP:HA	1:A:244:LYS:HE3	0.54	1.79	29	1
1:A:329:ILE:CG2	1:A:339:ILE:HG12	0.54	2.32	1	8
1:A:212:VAL:HG22	1:A:247:TYR:CD1	0.54	2.38	15	3
1:A:328:VAL:O	1:A:331:LYS:HE3	0.54	2.02	31	1
1:A:251:GLU:OE2	1:A:253:THR:HG22	0.54	2.03	2	1
1:A:254:ASN:HB2	1:A:380:LEU:HB2	0.54	1.79	18	1
1:A:278:LEU:HD11	1:A:317:LEU:HD12	0.54	1.78	25	1
1:A:235:GLY:HA2	1:A:261:ASN:HD22	0.54	1.63	29	3
1:A:208:ARG:HD2	1:A:208:ARG:N	0.54	2.18	8	1
1:A:425:LYS:O	1:A:429:LEU:HG	0.54	2.02	16	5
1:A:265:SER:HA	1:A:268:LYS:HG2	0.54	1.79	13	9
1:A:282:GLU:HB2	1:A:283:LEU:HD22	0.53	1.79	5	7
1:A:398:ILE:HD13	1:A:442:LYS:HB3	0.53	1.80	20	3
1:A:424:SER:O	1:A:428:ARG:HD3	0.53	2.03	12	1
1:A:437:THR:O	1:A:441:ARG:HG2	0.53	2.03	12	3
1:A:324:HIS:O	1:A:328:VAL:HG23	0.53	2.03	5	8
1:A:225:MET:O	1:A:331:LYS:HG2	0.53	2.03	31	1
1:A:279:LEU:H	1:A:279:LEU:HD22	0.53	1.63	35	19
1:A:290:ALA:HB2	1:A:302:GLU:HG2	0.53	1.80	25	1
1:A:296:GLU:HA	1:A:299:LYS:HD2	0.53	1.81	7	3
1:A:249:ARG:O	1:A:250:GLU:HB2	0.53	2.04	32	2
1:A:215:GLU:HB3	1:A:255:LEU:HD11	0.53	1.80	30	1
1:A:239:LYS:HB2	1:A:262:THR:HG21	0.53	1.80	7	2
1:A:391:LEU:HD13	1:A:442:LYS:HD2	0.53	1.80	27	1
1:A:194:LEU:O	1:A:198:VAL:HG23	0.53	2.03	3	18
1:A:231:TYR:O	1:A:345:VAL:HG21	0.53	2.04	13	6
1:A:239:LYS:HE3	1:A:262:THR:OG1	0.53	2.03	16	1
1:A:300:VAL:O	1:A:304:GLN:HG3	0.53	2.04	26	12
1:A:302:GLU:O	1:A:306:LEU:HD22	0.53	2.04	11	17
1:A:232:ARG:HA	1:A:345:VAL:HG11	0.53	1.81	4	2
1:A:405:GLN:HE22	1:A:435:ILE:HB	0.53	1.62	22	1
1:A:201:THR:O	1:A:211:ALA:HB2	0.52	2.03	20	9
1:A:430:TRP:O	1:A:434:ARG:HG3	0.52	2.04	12	4
1:A:350:VAL:O	1:A:351:GLN:HG2	0.52	2.04	12	1
1:A:300:VAL:HG12	1:A:363:HIS:CG	0.52	2.39	2	7
1:A:226:LYS:HB3	1:A:331:LYS:HD3	0.52	1.79	33	2
1:A:435:ILE:O	1:A:439:LEU:HG	0.52	2.04	30	1
1:A:198:VAL:HG11	1:A:208:ARG:HA	0.52	1.81	13	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:226:LYS:HB2	1:A:335:THR:CG2	0.52	2.35	23	1
1:A:424:SER:HA	1:A:427:GLU:OE2	0.52	2.05	31	1
1:A:403:ARG:HG2	1:A:407:PHE:CE2	0.52	2.39	15	7
1:A:414:ARG:HA	1:A:417:GLN:OE1	0.52	2.04	30	4
1:A:230:ILE:HG13	1:A:231:TYR:HD1	0.52	1.63	9	1
1:A:225:MET:CG	1:A:331:LYS:HG3	0.52	2.34	15	4
1:A:239:LYS:HD2	1:A:258:TYR:CD2	0.52	2.40	27	2
1:A:400:GLU:HB3	1:A:404:ARG:NH1	0.52	2.20	11	2
1:A:325:MET:O	1:A:328:VAL:HB	0.52	2.05	31	2
1:A:209:LEU:HD23	1:A:214:ARG:HD3	0.52	1.82	6	1
1:A:232:ARG:HG3	1:A:337:MET:SD	0.52	2.45	7	2
1:A:239:LYS:HD3	1:A:258:TYR:CE2	0.51	2.40	9	2
1:A:363:HIS:CD2	1:A:367:LEU:HD11	0.51	2.40	10	2
1:A:299:LYS:HB3	1:A:363:HIS:HE1	0.51	1.66	7	1
1:A:422:ASP:HB3	1:A:425:LYS:HG2	0.51	1.80	28	1
1:A:368:PHE:HB3	1:A:371:VAL:HG23	0.51	1.81	13	15
1:A:408:LEU:O	1:A:412:LEU:HD13	0.51	2.05	4	14
1:A:198:VAL:HG21	1:A:313:CYS:SG	0.51	2.45	24	1
1:A:267:LEU:O	1:A:271:LEU:HG	0.51	2.05	19	5
1:A:279:LEU:N	1:A:279:LEU:HD22	0.51	2.21	21	23
1:A:208:ARG:HD2	1:A:313:CYS:SG	0.51	2.45	4	1
1:A:279:LEU:O	1:A:283:LEU:HB2	0.51	2.05	17	12
1:A:217:ILE:HG13	1:A:324:HIS:CG	0.51	2.41	33	3
1:A:356:VAL:HA	1:A:359:VAL:HG12	0.51	1.82	9	3
1:A:401:GLU:O	1:A:405:GLN:HG2	0.51	2.05	27	2
1:A:305:ARG:CD	1:A:306:LEU:HD13	0.51	2.36	2	2
1:A:230:ILE:HG22	1:A:331:LYS:HZ3	0.51	1.65	2	1
1:A:363:HIS:NE2	1:A:367:LEU:HD22	0.51	2.21	16	2
1:A:190:PHE:CZ	1:A:244:LYS:HA	0.51	2.40	6	3
1:A:429:LEU:O	1:A:433:GLN:HG2	0.51	2.06	8	2
1:A:225:MET:HA	1:A:230:ILE:HG12	0.51	1.83	15	1
1:A:191:GLY:O	1:A:192:ILE:HG23	0.51	2.06	26	1
1:A:290:ALA:HB2	1:A:302:GLU:CG	0.51	2.36	1	1
1:A:190:PHE:CD2	1:A:244:LYS:HE3	0.51	2.40	12	2
1:A:284:MET:HB3	1:A:285:PRO:HD3	0.51	1.81	25	7
1:A:220:VAL:HG12	1:A:225:MET:HB3	0.51	1.82	15	4
1:A:370:ASN:HD22	1:A:370:ASN:N	0.51	2.03	33	1
1:A:218:ASP:O	1:A:222:LYS:HD3	0.50	2.06	7	1
1:A:235:GLY:HA3	1:A:262:THR:OG1	0.50	2.07	24	1
1:A:431:GLU:O	1:A:435:ILE:HG12	0.50	2.07	31	9
1:A:330:ALA:O	1:A:333:LEU:HB3	0.50	2.06	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:332:GLU:HB3	1:A:337:MET:HB2	0.50	1.82	26	1
1:A:222:LYS:HE2	1:A:223:TYR:CE2	0.50	2.40	31	4
1:A:300:VAL:HG13	1:A:367:LEU:CD2	0.50	2.37	21	1
1:A:190:PHE:CE1	1:A:244:LYS:HA	0.50	2.41	35	1
1:A:295:THR:O	1:A:299:LYS:HG3	0.50	2.06	6	7
1:A:377:MET:HE3	1:A:401:GLU:O	0.50	2.06	18	1
1:A:216:CYS:O	1:A:220:VAL:HG22	0.50	2.07	2	8
1:A:398:ILE:O	1:A:402:ILE:HG12	0.50	2.07	32	4
1:A:425:LYS:O	1:A:428:ARG:HB3	0.50	2.06	21	1
1:A:402:ILE:HG23	1:A:436:LEU:HD11	0.50	1.81	9	3
1:A:305:ARG:HD3	1:A:306:LEU:HD13	0.50	1.83	27	2
1:A:336:LYS:CD	1:A:337:MET:HG3	0.50	2.37	24	2
1:A:321:LEU:HD21	1:A:346:LEU:HD11	0.50	1.84	25	1
1:A:296:GLU:OE2	1:A:299:LYS:HD2	0.49	2.07	2	2
1:A:189:ILE:HG13	1:A:248:ASP:HA	0.49	1.82	16	1
1:A:239:LYS:HA	1:A:239:LYS:CE	0.49	2.37	18	1
1:A:305:ARG:HD3	1:A:305:ARG:C	0.49	2.28	12	8
1:A:190:PHE:HB3	1:A:273:ASP:HB3	0.49	1.84	5	1
1:A:255:LEU:HD23	1:A:378:LYS:HZ1	0.49	1.67	11	1
1:A:254:ASN:OD1	1:A:256:GLU:HG2	0.49	2.06	18	1
1:A:436:LEU:HD11	1:A:440:LYS:HE3	0.49	1.84	19	3
1:A:405:GLN:HA	1:A:405:GLN:HE21	0.49	1.65	4	1
1:A:279:LEU:HD22	1:A:279:LEU:H	0.49	1.68	28	9
1:A:202:MET:HG2	1:A:206:GLY:HA3	0.49	1.84	9	1
1:A:335:THR:C	1:A:336:LYS:HG3	0.49	2.27	19	2
1:A:412:LEU:HB2	1:A:429:LEU:HD21	0.49	1.84	17	1
1:A:225:MET:HB3	1:A:331:LYS:HD3	0.49	1.85	12	1
1:A:409:LEU:HD22	1:A:436:LEU:HD23	0.49	1.83	25	1
1:A:204:TYR:CE2	1:A:376:VAL:HA	0.49	2.36	2	1
1:A:304:GLN:HG2	1:A:367:LEU:HG	0.49	1.85	7	6
1:A:278:LEU:HA	1:A:314:ASN:OD1	0.49	2.07	28	2
1:A:327:HIS:O	1:A:331:LYS:HG2	0.49	2.07	23	5
1:A:428:ARG:O	1:A:432:VAL:HG23	0.49	2.08	15	4
1:A:236:ILE:HB	1:A:239:LYS:HG2	0.49	1.85	11	2
1:A:218:ASP:OD2	1:A:222:LYS:HD2	0.49	2.08	23	2
1:A:332:GLU:HA	1:A:335:THR:HG1	0.49	1.66	14	4
1:A:329:ILE:O	1:A:333:LEU:HG	0.49	2.07	23	4
1:A:220:VAL:HG11	1:A:231:TYR:HE2	0.49	1.68	22	3
1:A:325:MET:O	1:A:329:ILE:HG12	0.48	2.08	33	2
1:A:407:PHE:HA	1:A:410:ASN:ND2	0.48	2.23	10	10
1:A:279:LEU:HD22	1:A:279:LEU:N	0.48	2.23	4	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:280:THR:HB	1:A:282:GLU:OE2	0.48	2.07	23	3
1:A:283:LEU:HD22	1:A:306:LEU:HD12	0.48	1.84	11	1
1:A:249:ARG:O	1:A:250:GLU:HB3	0.48	2.09	12	1
1:A:278:LEU:HD12	1:A:350:VAL:HG12	0.48	1.84	28	3
1:A:278:LEU:HD12	1:A:350:VAL:HG23	0.48	1.85	19	1
1:A:220:VAL:HG11	1:A:231:TYR:CE2	0.48	2.43	25	1
1:A:300:VAL:HB	1:A:367:LEU:CD1	0.48	2.39	3	2
1:A:332:GLU:OE1	1:A:337:MET:HB2	0.48	2.09	21	2
1:A:328:VAL:O	1:A:332:GLU:HG2	0.48	2.09	6	5
1:A:195:ALA:O	1:A:199:GLU:HG2	0.48	2.08	6	5
1:A:332:GLU:CB	1:A:337:MET:HB2	0.48	2.36	31	1
1:A:438:ALA:O	1:A:442:LYS:HG3	0.48	2.09	7	4
1:A:225:MET:HG3	1:A:331:LYS:CG	0.48	2.38	15	1
1:A:363:HIS:HA	1:A:366:GLU:HB2	0.48	1.86	25	2
1:A:265:SER:HA	1:A:268:LYS:HE2	0.47	1.86	7	3
1:A:208:ARG:HB3	1:A:313:CYS:SG	0.47	2.49	18	2
1:A:401:GLU:CD	1:A:439:LEU:HD22	0.47	2.29	30	1
1:A:401:GLU:HG2	1:A:439:LEU:HD13	0.47	1.85	30	1
1:A:204:TYR:CE1	1:A:408:LEU:HD12	0.47	2.44	13	1
1:A:271:LEU:HD23	1:A:349:THR:O	0.47	2.09	6	2
1:A:259:GLU:HB3	1:A:261:ASN:OD1	0.47	2.09	7	2
1:A:249:ARG:HD2	1:A:251:GLU:OE2	0.47	2.09	22	3
1:A:203:MET:HE3	1:A:376:VAL:HG11	0.47	1.86	31	1
1:A:190:PHE:HE2	1:A:269:GLN:HG3	0.47	1.70	22	1
1:A:331:LYS:HD2	1:A:335:THR:OG1	0.47	2.09	31	1
1:A:278:LEU:HD11	1:A:317:LEU:HD22	0.47	1.86	11	1
1:A:298:GLU:HA	1:A:301:GLN:NE2	0.47	2.24	10	2
1:A:259:GLU:HB2	1:A:262:THR:OG1	0.47	2.10	17	1
1:A:346:LEU:HB2	1:A:357:LEU:HG	0.47	1.86	17	1
1:A:305:ARG:C	1:A:305:ARG:HD3	0.47	2.29	7	7
1:A:412:LEU:O	1:A:416:LEU:HG	0.47	2.09	9	3
1:A:291:CYS:SG	1:A:355:ARG:HG3	0.47	2.49	13	1
1:A:230:ILE:HG13	1:A:231:TYR:CD2	0.47	2.45	35	3
1:A:370:ASN:N	1:A:370:ASN:HD22	0.47	2.08	6	1
1:A:323:VAL:HG22	1:A:365:GLN:NE2	0.47	2.25	13	6
1:A:436:LEU:O	1:A:440:LYS:HG2	0.47	2.09	5	7
1:A:442:LYS:HE3	1:A:445:GLU:OE2	0.47	2.10	28	1
1:A:329:ILE:O	1:A:332:GLU:HB2	0.47	2.09	5	4
1:A:190:PHE:CZ	1:A:244:LYS:HB2	0.47	2.44	16	1
1:A:363:HIS:HA	1:A:366:GLU:CG	0.47	2.40	25	1
1:A:364:VAL:HG13	1:A:365:GLN:HE21	0.46	1.70	4	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:329:ILE:HD12	1:A:339:ILE:HA	0.46	1.87	20	1
1:A:213:PHE:O	1:A:217:ILE:HD13	0.46	2.10	33	2
1:A:332:GLU:OE2	1:A:337:MET:HB2	0.46	2.10	30	1
1:A:328:VAL:O	1:A:331:LYS:HG3	0.46	2.10	2	1
1:A:236:ILE:O	1:A:240:VAL:HG23	0.46	2.10	15	5
1:A:307:LEU:HA	1:A:310:LEU:CD1	0.46	2.40	25	5
1:A:300:VAL:HG13	1:A:367:LEU:HD21	0.46	1.86	21	1
1:A:357:LEU:HA	1:A:360:PHE:HB2	0.46	1.87	30	11
1:A:226:LYS:HB3	1:A:331:LYS:HB3	0.46	1.86	23	1
1:A:192:ILE:O	1:A:274:LEU:HD23	0.46	2.10	28	1
1:A:370:ASN:HD22	1:A:371:VAL:N	0.46	2.08	8	2
1:A:221:GLU:HA	1:A:225:MET:CG	0.46	2.41	26	2
1:A:335:THR:C	1:A:336:LYS:HD2	0.46	2.31	26	1
1:A:409:LEU:HD11	1:A:433:GLN:HG3	0.46	1.86	26	2
1:A:230:ILE:HG13	1:A:231:TYR:CD1	0.46	2.46	9	1
1:A:280:THR:O	1:A:284:MET:HB2	0.46	2.10	26	4
1:A:361:PHE:HA	1:A:364:VAL:HG22	0.46	1.86	22	1
1:A:230:ILE:CD1	1:A:260:PRO:HB2	0.46	2.40	18	1
1:A:279:LEU:HD12	1:A:352:ILE:HD11	0.46	1.88	20	1
1:A:346:LEU:HD23	1:A:357:LEU:HD12	0.46	1.88	1	1
1:A:212:VAL:HG22	1:A:247:TYR:CD2	0.46	2.45	7	2
1:A:427:GLU:O	1:A:431:GLU:HG3	0.46	2.11	5	1
1:A:222:LYS:HE3	1:A:223:TYR:CE2	0.46	2.46	5	1
1:A:424:SER:O	1:A:428:ARG:HG2	0.46	2.11	19	2
1:A:363:HIS:ND1	1:A:367:LEU:HD22	0.46	2.25	31	2
1:A:307:LEU:HD22	1:A:367:LEU:HD23	0.45	1.86	14	1
1:A:203:MET:CE	1:A:376:VAL:HG21	0.45	2.41	16	1
1:A:331:LYS:HE3	1:A:331:LYS:CA	0.45	2.38	30	1
1:A:265:SER:O	1:A:269:GLN:HB2	0.45	2.11	10	5
1:A:240:VAL:O	1:A:244:LYS:HB3	0.45	2.10	6	1
1:A:215:GLU:HB3	1:A:255:LEU:HD21	0.45	1.88	34	2
1:A:232:ARG:HD2	1:A:341:ASN:HB3	0.45	1.87	11	1
1:A:190:PHE:CE1	1:A:270:TYR:HA	0.45	2.46	15	1
1:A:424:SER:HA	1:A:427:GLU:OE1	0.45	2.11	15	1
1:A:377:MET:HE1	1:A:405:GLN:HB2	0.45	1.87	22	1
1:A:409:LEU:HD12	1:A:436:LEU:HD12	0.45	1.89	31	1
1:A:229:GLY:O	1:A:233:VAL:HG22	0.45	2.12	5	4
1:A:428:ARG:NH2	1:A:431:GLU:HG3	0.45	2.26	7	1
1:A:208:ARG:HG3	1:A:313:CYS:SG	0.45	2.52	3	1
1:A:295:THR:O	1:A:298:GLU:HG2	0.45	2.12	15	1
1:A:213:PHE:HE1	1:A:321:LEU:HD23	0.45	1.71	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:329:ILE:HA	1:A:332:GLU:CG	0.45	2.40	6	2
1:A:229:GLY:O	1:A:233:VAL:HG23	0.45	2.11	6	1
1:A:321:LEU:O	1:A:325:MET:HB2	0.45	2.10	24	1
1:A:415:ASP:OD2	1:A:420:ILE:HD11	0.45	2.11	5	1
1:A:315:TYR:O	1:A:318:ILE:HG22	0.45	2.12	6	3
1:A:406:GLU:HG2	1:A:436:LEU:HD21	0.45	1.88	26	2
1:A:422:ASP:CB	1:A:425:LYS:HG2	0.45	2.41	4	4
1:A:288:GLU:HA	1:A:291:CYS:SG	0.45	2.52	18	1
1:A:416:LEU:HA	1:A:420:ILE:HB	0.45	1.88	24	1
1:A:409:LEU:HD11	1:A:433:GLN:CG	0.45	2.41	26	1
1:A:329:ILE:CA	1:A:332:GLU:HG2	0.45	2.40	10	1
1:A:239:LYS:O	1:A:243:LEU:HD22	0.45	2.12	11	2
1:A:290:ALA:HA	1:A:293:ARG:CG	0.45	2.40	14	3
1:A:209:LEU:HB2	1:A:316:LEU:HD23	0.45	1.87	17	2
1:A:422:ASP:OD1	1:A:425:LYS:HG2	0.44	2.11	9	1
1:A:311:PRO:HG2	1:A:314:ASN:OD1	0.44	2.11	12	1
1:A:229:GLY:HA2	1:A:233:VAL:HG23	0.44	1.89	28	1
1:A:239:LYS:O	1:A:243:LEU:HG	0.44	2.12	32	2
1:A:240:VAL:O	1:A:244:LYS:HG3	0.44	2.12	19	5
1:A:218:ASP:OD2	1:A:378:LYS:HE3	0.44	2.12	12	1
1:A:332:GLU:HB3	1:A:337:MET:C	0.44	2.32	28	1
1:A:299:LYS:HB3	1:A:363:HIS:CE1	0.44	2.47	7	1
1:A:220:VAL:HG11	1:A:231:TYR:HE1	0.44	1.73	9	1
1:A:277:ASN:HB2	1:A:280:THR:CA	0.44	2.42	12	3
1:A:279:LEU:HB3	1:A:287:PHE:CE1	0.44	2.48	35	3
1:A:331:LYS:HE2	1:A:334:GLU:OE1	0.44	2.13	15	2
1:A:192:ILE:HB	1:A:193:PRO:HD2	0.44	1.89	17	1
1:A:395:GLN:O	1:A:399:LYS:HG2	0.44	2.11	35	2
1:A:412:LEU:HD21	1:A:428:ARG:HE	0.44	1.72	31	1
1:A:355:ARG:O	1:A:359:VAL:HG23	0.44	2.13	2	3
1:A:189:ILE:HA	1:A:192:ILE:HD11	0.44	1.89	9	2
1:A:360:PHE:CD1	1:A:363:HIS:HE1	0.44	2.30	18	2
1:A:215:GLU:HB3	1:A:255:LEU:CD1	0.44	2.43	13	1
1:A:213:PHE:HA	1:A:267:LEU:CD2	0.44	2.42	7	1
1:A:216:CYS:SG	1:A:267:LEU:HD22	0.44	2.53	33	3
1:A:213:PHE:HA	1:A:267:LEU:HD21	0.44	1.89	22	1
1:A:359:VAL:HB	1:A:363:HIS:CD2	0.44	2.47	30	1
1:A:218:ASP:O	1:A:222:LYS:HG3	0.44	2.13	18	4
1:A:304:GLN:CG	1:A:367:LEU:HG	0.44	2.43	14	1
1:A:218:ASP:OD2	1:A:375:GLN:HB2	0.44	2.12	8	2
1:A:200:ARG:CZ	1:A:200:ARG:HA	0.44	2.43	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:204:TYR:CE2	1:A:408:LEU:HB2	0.44	2.48	29	1
1:A:300:VAL:HG12	1:A:363:HIS:CB	0.44	2.40	31	2
1:A:350:VAL:HG13	1:A:352:ILE:HG13	0.44	1.89	13	1
1:A:331:LYS:HE2	1:A:334:GLU:OE2	0.44	2.11	27	1
1:A:331:LYS:HA	1:A:331:LYS:HE2	0.44	1.88	5	1
1:A:409:LEU:HD22	1:A:436:LEU:CD1	0.44	2.43	6	2
1:A:329:ILE:HG23	1:A:339:ILE:HG12	0.44	1.89	9	2
1:A:207:ILE:O	1:A:208:ARG:HD2	0.44	2.13	11	1
1:A:429:LEU:O	1:A:432:VAL:HG22	0.44	2.13	12	1
1:A:363:HIS:O	1:A:366:GLU:HB2	0.44	2.12	25	1
1:A:236:ILE:HD12	1:A:239:LYS:NZ	0.44	2.28	34	1
1:A:221:GLU:HB2	1:A:324:HIS:NE2	0.44	2.27	16	1
1:A:255:LEU:HD12	1:A:378:LYS:HE3	0.44	1.89	30	1
1:A:207:ILE:HG13	1:A:207:ILE:O	0.43	2.12	2	1
1:A:394:THR:O	1:A:398:ILE:HG13	0.43	2.13	30	3
1:A:369:GLY:O	1:A:370:ASN:HB2	0.43	2.12	6	2
1:A:225:MET:CB	1:A:331:LYS:HG3	0.43	2.43	11	1
1:A:404:ARG:HA	1:A:407:PHE:CD2	0.43	2.48	14	1
1:A:307:LEU:HA	1:A:310:LEU:CG	0.43	2.43	33	1
1:A:341:ASN:O	1:A:345:VAL:HG13	0.43	2.14	33	1
1:A:399:LYS:HE3	1:A:443:LEU:HD21	0.43	1.89	3	2
1:A:409:LEU:O	1:A:413:HIS:HB2	0.43	2.14	29	4
1:A:323:VAL:HG21	1:A:371:VAL:HG21	0.43	1.89	14	1
1:A:279:LEU:CD1	1:A:352:ILE:HD11	0.43	2.43	19	2
1:A:305:ARG:O	1:A:309:GLU:HG2	0.43	2.13	27	2
1:A:328:VAL:HG13	1:A:331:LYS:CE	0.43	2.43	31	1
1:A:216:CYS:SG	1:A:267:LEU:HB2	0.43	2.54	32	1
1:A:301:GLN:O	1:A:304:GLN:HB2	0.43	2.12	27	1
1:A:405:GLN:HB3	1:A:436:LEU:HG	0.43	1.89	2	1
1:A:229:GLY:CA	1:A:337:MET:SD	0.43	3.07	6	1
1:A:405:GLN:CB	1:A:436:LEU:HD13	0.43	2.43	25	1
1:A:350:VAL:O	1:A:351:GLN:HB2	0.43	2.14	20	4
1:A:205:ASP:OD1	1:A:207:ILE:HG12	0.43	2.13	2	2
1:A:401:GLU:OE1	1:A:404:ARG:HD2	0.43	2.14	28	2
1:A:325:MET:HA	1:A:328:VAL:HG23	0.43	1.90	35	1
1:A:332:GLU:CD	1:A:338:ASN:HA	0.43	2.33	8	1
1:A:216:CYS:O	1:A:220:VAL:HG23	0.43	2.13	18	4
1:A:350:VAL:HG23	1:A:352:ILE:HG13	0.43	1.90	9	1
1:A:204:TYR:HE1	1:A:376:VAL:HG23	0.43	1.74	20	1
1:A:190:PHE:CE1	1:A:244:LYS:HB2	0.43	2.49	34	2
1:A:399:LYS:HE2	1:A:443:LEU:HD21	0.43	1.89	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:MET:O	1:A:211:ALA:HB2	0.43	2.14	25	1
1:A:268:LYS:HB2	1:A:349:THR:OG1	0.43	2.13	10	1
1:A:407:PHE:O	1:A:410:ASN:ND2	0.43	2.52	18	1
1:A:303:PHE:O	1:A:307:LEU:HG	0.43	2.12	5	4
1:A:438:ALA:O	1:A:442:LYS:HG2	0.43	2.14	12	3
1:A:203:MET:O	1:A:412:LEU:HD21	0.43	2.14	16	1
1:A:429:LEU:HB3	1:A:433:GLN:NE2	0.42	2.29	4	1
1:A:422:ASP:CG	1:A:425:LYS:HG2	0.42	2.34	15	1
1:A:203:MET:HA	1:A:428:ARG:HH22	0.42	1.74	28	2
1:A:208:ARG:O	1:A:209:LEU:HG	0.42	2.13	27	2
1:A:415:ASP:HA	1:A:417:GLN:NE2	0.42	2.29	5	1
1:A:402:ILE:HG13	1:A:443:LEU:HD12	0.42	1.91	19	1
1:A:209:LEU:N	1:A:209:LEU:HD12	0.42	2.29	20	1
1:A:313:CYS:O	1:A:317:LEU:HB2	0.42	2.14	23	1
1:A:300:VAL:HB	1:A:367:LEU:CD2	0.42	2.44	26	1
1:A:213:PHE:HA	1:A:267:LEU:CD1	0.42	2.44	31	1
1:A:350:VAL:HG11	1:A:357:LEU:HD11	0.42	1.90	33	2
1:A:357:LEU:O	1:A:360:PHE:HB2	0.42	2.14	28	4
1:A:437:THR:O	1:A:441:ARG:HG3	0.42	2.13	15	2
1:A:363:HIS:HA	1:A:366:GLU:HG3	0.42	1.92	25	1
1:A:328:VAL:O	1:A:332:GLU:N	0.42	2.51	24	4
1:A:405:GLN:HG2	1:A:436:LEU:HD13	0.42	1.91	16	1
1:A:259:GLU:H	1:A:259:GLU:CD	0.42	2.18	8	1
1:A:364:VAL:HG22	1:A:368:PHE:CD2	0.42	2.49	8	1
1:A:235:GLY:HA2	1:A:261:ASN:ND2	0.42	2.30	28	2
1:A:430:TRP:N	1:A:430:TRP:CD1	0.42	2.84	23	1
1:A:218:ASP:OD2	1:A:378:LYS:HE2	0.42	2.15	32	1
1:A:324:HIS:HD1	1:A:373:LEU:HG	0.42	1.75	35	1
1:A:330:ALA:O	1:A:333:LEU:HB2	0.42	2.15	9	2
1:A:350:VAL:C	1:A:351:GLN:HE21	0.42	2.17	12	1
1:A:345:VAL:O	1:A:348:PRO:HD2	0.42	2.15	14	1
1:A:201:THR:HB	1:A:211:ALA:HB3	0.42	1.90	16	1
1:A:214:ARG:HG2	1:A:320:TRP:CZ3	0.42	2.49	17	1
1:A:328:VAL:O	1:A:332:GLU:HG3	0.42	2.14	18	1
1:A:295:THR:HB	1:A:298:GLU:CG	0.42	2.33	20	1
1:A:331:LYS:HB3	1:A:331:LYS:HE3	0.42	1.66	31	1
1:A:409:LEU:CD1	1:A:436:LEU:HD12	0.42	2.45	1	1
1:A:208:ARG:HD3	1:A:208:ARG:N	0.42	2.29	17	1
1:A:360:PHE:HA	1:A:363:HIS:ND1	0.42	2.29	18	2
1:A:208:ARG:HG3	1:A:312:GLU:CD	0.42	2.34	32	1
1:A:321:LEU:O	1:A:325:MET:HG2	0.42	2.15	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:ILE:HD12	1:A:196:ASP:HB3	0.42	1.92	2	1
1:A:298:GLU:HA	1:A:301:GLN:HE21	0.42	1.74	5	1
1:A:225:MET:O	1:A:331:LYS:HB3	0.42	2.15	10	1
1:A:286:ARG:HA	1:A:286:ARG:NE	0.42	2.30	24	1
1:A:293:ARG:NE	1:A:293:ARG:HA	0.42	2.30	3	1
1:A:204:TYR:CE1	1:A:376:VAL:HG13	0.41	2.50	1	1
1:A:203:MET:HE1	1:A:376:VAL:HG11	0.41	1.92	4	1
1:A:271:LEU:HD12	1:A:274:LEU:HD12	0.41	1.92	10	1
1:A:225:MET:HB2	1:A:331:LYS:HG3	0.41	1.91	11	1
1:A:215:GLU:OE2	1:A:378:LYS:HE3	0.41	2.14	3	1
1:A:305:ARG:HD2	1:A:306:LEU:HD13	0.41	1.90	2	1
1:A:346:LEU:CB	1:A:357:LEU:HG	0.41	2.45	34	1
1:A:239:LYS:O	1:A:242:GLU:HB2	0.41	2.15	4	1
1:A:405:GLN:CB	1:A:436:LEU:HD21	0.41	2.45	4	1
1:A:370:ASN:HD22	1:A:370:ASN:C	0.41	2.17	5	1
1:A:246:ALA:HB3	1:A:253:THR:HG23	0.41	1.91	6	1
1:A:218:ASP:OD2	1:A:378:LYS:HG3	0.41	2.15	6	1
1:A:335:THR:O	1:A:336:LYS:CB	0.41	2.66	2	1
1:A:405:GLN:NE2	1:A:432:VAL:HB	0.41	2.29	16	1
1:A:359:VAL:HG23	1:A:363:HIS:CE1	0.41	2.51	19	1
1:A:221:GLU:HG2	1:A:225:MET:HE3	0.41	1.92	22	1
1:A:322:ILE:HG22	1:A:364:VAL:HG11	0.41	1.92	33	1
1:A:377:MET:SD	1:A:404:ARG:HB3	0.41	2.55	6	1
1:A:293:ARG:HD2	1:A:298:GLU:HB3	0.41	1.92	10	1
1:A:379:PRO:O	1:A:380:LEU:HB2	0.41	2.16	17	1
1:A:279:LEU:HD22	1:A:287:PHE:CZ	0.41	2.51	20	1
1:A:293:ARG:CD	1:A:298:GLU:HB3	0.41	2.45	29	1
1:A:355:ARG:O	1:A:359:VAL:HG13	0.41	2.16	29	2
1:A:279:LEU:HD12	1:A:287:PHE:CZ	0.41	2.51	21	2
1:A:212:VAL:HG12	1:A:247:TYR:CD1	0.41	2.50	19	1
1:A:299:LYS:CB	1:A:363:HIS:HE1	0.41	2.29	20	1
1:A:356:VAL:O	1:A:359:VAL:HG22	0.41	2.15	35	1
1:A:392:PRO:HB2	1:A:398:ILE:CG1	0.41	2.46	35	1
1:A:209:LEU:HB3	1:A:214:ARG:NH1	0.41	2.30	1	1
1:A:191:GLY:HA2	1:A:273:ASP:C	0.41	2.36	6	1
1:A:212:VAL:HB	1:A:247:TYR:CE1	0.41	2.51	10	1
1:A:201:THR:HB	1:A:211:ALA:CB	0.41	2.45	16	1
1:A:278:LEU:HD21	1:A:317:LEU:HD22	0.41	1.91	35	1
1:A:331:LYS:CA	1:A:331:LYS:HE2	0.41	2.46	5	1
1:A:208:ARG:N	1:A:208:ARG:HD3	0.41	2.31	12	1
1:A:402:ILE:O	1:A:406:GLU:HG3	0.41	2.16	23	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:ILE:HG12	1:A:248:ASP:HA	0.41	1.93	5	2
1:A:347:SER:CB	1:A:348:PRO:HD3	0.41	2.41	6	2
1:A:356:VAL:HA	1:A:359:VAL:CG1	0.41	2.46	9	1
1:A:290:ALA:HB2	1:A:302:GLU:HB3	0.41	1.92	11	1
1:A:322:ILE:HG23	1:A:361:PHE:CD1	0.41	2.50	14	1
1:A:203:MET:HG3	1:A:204:TYR:N	0.41	2.31	18	1
1:A:202:MET:O	1:A:203:MET:HB2	0.41	2.15	21	2
1:A:398:ILE:O	1:A:402:ILE:HG13	0.41	2.15	21	1
1:A:342:ILE:HA	1:A:345:VAL:HG22	0.41	1.92	33	1
1:A:412:LEU:O	1:A:416:LEU:HD23	0.41	2.15	7	1
1:A:430:TRP:CD1	1:A:430:TRP:N	0.41	2.88	21	1
1:A:293:ARG:HB3	1:A:298:GLU:CB	0.41	2.43	3	1
1:A:215:GLU:OE1	1:A:255:LEU:HD21	0.41	2.16	8	1
1:A:212:VAL:HB	1:A:247:TYR:CE2	0.41	2.51	27	1
1:A:326:ASP:HB2	1:A:361:PHE:HB3	0.40	1.92	4	1
1:A:331:LYS:HE2	1:A:331:LYS:HA	0.40	1.91	14	1
1:A:404:ARG:HA	1:A:407:PHE:HD2	0.40	1.74	14	1
1:A:230:ILE:O	1:A:231:TYR:HB2	0.40	2.16	34	2
1:A:416:LEU:HB2	1:A:417:GLN:NE2	0.40	2.31	18	1
1:A:227:CYS:HB2	1:A:230:ILE:HB	0.40	1.93	25	1
1:A:323:VAL:HG21	1:A:371:VAL:HB	0.40	1.92	8	1
1:A:331:LYS:CA	1:A:334:GLU:HG2	0.40	2.42	2	1
1:A:291:CYS:O	1:A:299:LYS:HE3	0.40	2.16	4	1
1:A:331:LYS:HE2	1:A:331:LYS:HB3	0.40	1.62	18	1
1:A:340:GLN:HE21	1:A:340:GLN:C	0.40	2.20	22	1
1:A:347:SER:HA	1:A:357:LEU:HD21	0.40	1.93	25	1
1:A:204:TYR:HA	1:A:408:LEU:HD12	0.40	1.93	31	1
1:A:286:ARG:O	1:A:289:GLU:HB2	0.40	2.16	32	1
1:A:255:LEU:HD22	1:A:255:LEU:H	0.40	1.76	34	1
1:A:189:ILE:O	1:A:192:ILE:HG12	0.40	2.15	4	1
1:A:402:ILE:HD12	1:A:443:LEU:CD1	0.40	2.46	15	1
1:A:422:ASP:O	1:A:426:GLU:HG3	0.40	2.17	19	1
1:A:332:GLU:OE2	1:A:337:MET:HE2	0.40	2.16	29	1
1:A:324:HIS:HB2	1:A:373:LEU:CD1	0.40	2.46	32	1
1:A:259:GLU:O	1:A:263:VAL:HG23	0.40	2.16	33	1
1:A:196:ASP:O	1:A:200:ARG:HG3	0.40	2.17	2	1
1:A:409:LEU:HD13	1:A:436:LEU:HD12	0.40	1.91	2	1
1:A:405:GLN:HB3	1:A:436:LEU:HD21	0.40	1.93	11	1
1:A:284:MET:N	1:A:285:PRO:HD2	0.40	2.32	19	1
1:A:286:ARG:HD3	1:A:289:GLU:HG3	0.40	1.93	21	1
1:A:295:THR:CB	1:A:298:GLU:HG2	0.40	2.36	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:LEU:O	1:A:198:VAL:HG12	0.40	2.16	32	1
1:A:307:LEU:CA	1:A:310:LEU:HG	0.40	2.45	33	1
1:A:217:ILE:HG23	1:A:324:HIS:CD2	0.40	2.52	3	1
1:A:405:GLN:OE1	1:A:405:GLN:HA	0.40	2.16	9	1
1:A:215:GLU:HB3	1:A:255:LEU:CD2	0.40	2.46	10	1
1:A:207:ILE:O	1:A:208:ARG:HB2	0.40	2.16	15	1
1:A:430:TRP:O	1:A:434:ARG:HG2	0.40	2.16	17	1
1:A:240:VAL:HG13	1:A:266:LEU:HD23	0.40	1.92	18	1
1:A:397:GLY:O	1:A:401:GLU:HB2	0.40	2.17	25	1
1:A:246:ALA:HA	1:A:251:GLU:OE2	0.40	2.17	28	1
1:A:297:THR:HG22	1:A:301:GLN:CD	0.40	2.37	33	1
1:A:213:PHE:CE2	1:A:320:TRP:HB3	0.40	2.51	33	1
1:A:208:ARG:HE	1:A:312:GLU:CD	0.40	2.20	34	1
1:A:305:ARG:HD3	1:A:306:LEU:N	0.40	2.32	27	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	248/265 (94%)	226±3 (91±1%)	16±3 (7±1%)	6±2 (2±1%)	9	48
All	All	8680/9275 (94%)	7914 (91%)	566 (7%)	200 (2%)	9	48

All 24 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	207	ILE	33
1	A	280	THR	31
1	A	390	THR	25
1	A	204	TYR	22
1	A	189	ILE	21
1	A	336	LYS	15
1	A	251	GLU	7
1	A	203	MET	7

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Mol	Chain	Res	Type	Models (Total)
1	A	309	GLU	6
1	A	250	GLU	6
1	A	191	GLY	4
1	A	202	MET	4
1	A	351	GLN	4
1	A	226	LYS	3
1	A	370	ASN	2
1	A	380	LEU	2
1	A	354	ASN	1
1	A	230	ILE	1
1	A	392	PRO	1
1	A	225	MET	1
1	A	236	ILE	1
1	A	206	GLY	1
1	A	208	ARG	1
1	A	252	SER	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	228/243 (94%)	212±3 (93±1%)	16±3 (7±1%)	18	67
All	All	7980/8505 (94%)	7414 (93%)	566 (7%)	18	67

All 86 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	340	GLN	35
1	A	279	LEU	33
1	A	360	PHE	33
1	A	370	ASN	32
1	A	305	ARG	32
1	A	306	LEU	32
1	A	430	TRP	22
1	A	364	VAL	22
1	A	269	GLN	21

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Mol	Chain	Res	Type	Models (Total)
1	A	326	ASP	19
1	A	375	GLN	18
1	A	336	LYS	16
1	A	331	LYS	15
1	A	410	ASN	15
1	A	351	GLN	14
1	A	317	LEU	14
1	A	327	HIS	13
1	A	253	THR	10
1	A	203	MET	9
1	A	359	VAL	8
1	A	433	GLN	7
1	A	208	ARG	7
1	A	225	MET	6
1	A	423	LEU	6
1	A	377	MET	5
1	A	221	GLU	5
1	A	413	HIS	5
1	A	255	LEU	4
1	A	417	GLN	4
1	A	308	LYS	4
1	A	294	THR	4
1	A	232	ARG	4
1	A	333	LEU	4
1	A	204	TYR	4
1	A	363	HIS	4
1	A	403	ARG	3
1	A	205	ASP	3
1	A	395	GLN	3
1	A	273	ASP	3
1	A	243	LEU	3
1	A	424	SER	3
1	A	196	ASP	2
1	A	218	ASP	2
1	A	194	LEU	2
1	A	300	VAL	2
1	A	200	ARG	2
1	A	266	LEU	2
1	A	189	ILE	2
1	A	405	GLN	2
1	A	277	ASN	2
1	A	251	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	394	THR	2
1	A	239	LYS	2
1	A	261	ASN	2
1	A	242	GLU	2
1	A	234	SER	2
1	A	416	LEU	2
1	A	378	LYS	2
1	A	307	LEU	1
1	A	202	MET	1
1	A	415	ASP	1
1	A	428	ARG	1
1	A	244	LYS	1
1	A	332	GLU	1
1	A	442	LYS	1
1	A	270	TYR	1
1	A	309	GLU	1
1	A	262	THR	1
1	A	256	GLU	1
1	A	228	GLU	1
1	A	353	SER	1
1	A	411	CYS	1
1	A	297	THR	1
1	A	436	LEU	1
1	A	401	GLU	1
1	A	441	ARG	1
1	A	293	ARG	1
1	A	286	ARG	1
1	A	391	LEU	1
1	A	252	SER	1
1	A	241	ASP	1
1	A	380	LEU	1
1	A	237	LYS	1
1	A	298	GLU	1
1	A	443	LEU	1
1	A	422	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 84% for the well-defined parts and 83% 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	3262
Number of shifts mapped to atoms	3262
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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
$^{13}\text{C}_\alpha$	254	-0.51 ± 0.10	Should be applied
$^{13}\text{C}_\beta$	242	0.23 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	232	-0.37 ± 0.09	None needed (< 0.5 ppm)
^{15}N	246	0.97 ± 0.20	Should be applied

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 84%, i.e. 2732 atoms were assigned a chemical shift out of a possible 3263. 1 out of 51 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	1185/1227 (97%)	480/489 (98%)	467/498 (94%)	238/240 (99%)
Sidechain	1388/1836 (76%)	852/1073 (79%)	518/674 (77%)	18/89 (20%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	159/200 (80%)	88/104 (85%)	69/86 (80%)	2/10 (20%)
Overall	2732/3263 (84%)	1420/1666 (85%)	1054/1258 (84%)	258/339 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 2873 atoms were assigned a chemical shift out of a possible 3477. 1 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	1232/1301 (95%)	500/518 (97%)	486/530 (92%)	246/253 (97%)
Sidechain	1469/1956 (75%)	905/1147 (79%)	544/714 (76%)	20/95 (21%)
Aromatic	172/220 (78%)	95/114 (83%)	74/93 (80%)	3/13 (23%)
Overall	2873/3477 (83%)	1500/1779 (84%)	1104/1337 (83%)	269/361 (75%)

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	271	LEU	CG	66.14	32.55 – 21.05	34.2
1	A	244	LYS	HG2	-0.54	2.67 – 0.07	-7.3
1	A	209	LEU	HD11	-0.90	2.16 – -0.64	-5.9
1	A	209	LEU	HD13	-0.90	2.16 – -0.64	-5.9
1	A	209	LEU	HD12	-0.90	2.16 – -0.64	-5.9

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:

