



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:17 pm GMT

PDB ID : 2KR6
Title : Solution structure of presenilin-1 CTF subunit
Authors : Doetsch, V.
Deposited on : 2009-12-04

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

<http://wwpdb.org/validation/2016/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	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

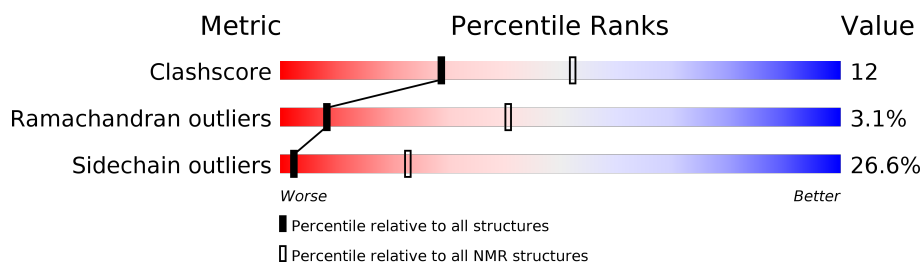
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	176	

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:356-A:368, A:383-A:427, A:437-A:461 (83)	0.69	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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2701 atoms, of which 1331 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Presenilin-1.

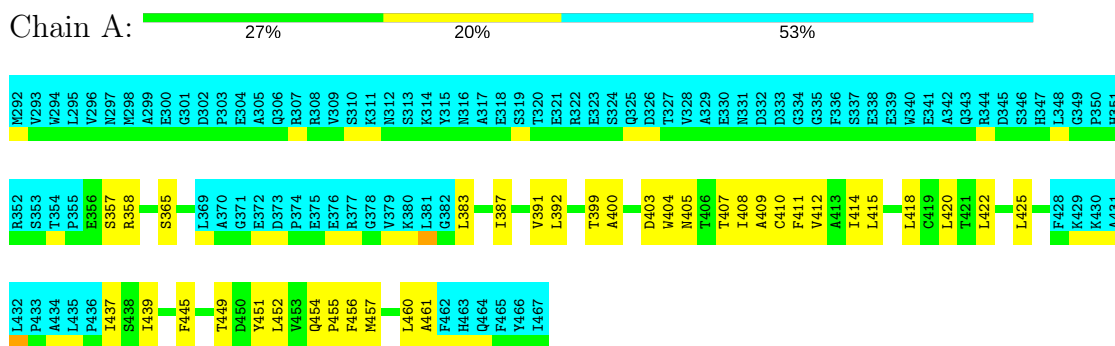
Mol	Chain	Residues	Atoms						Trace
1	A	176	Total	C	H	N	O	S	0
			2701	876	1331	224	265	5	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Presenilin-1

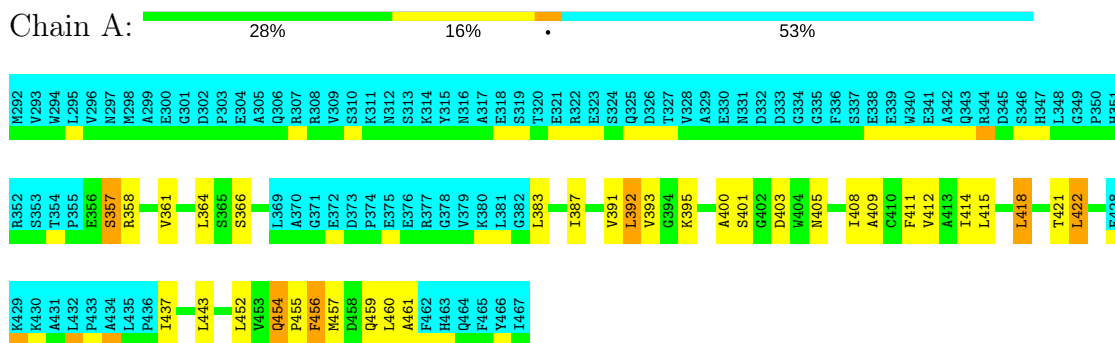


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

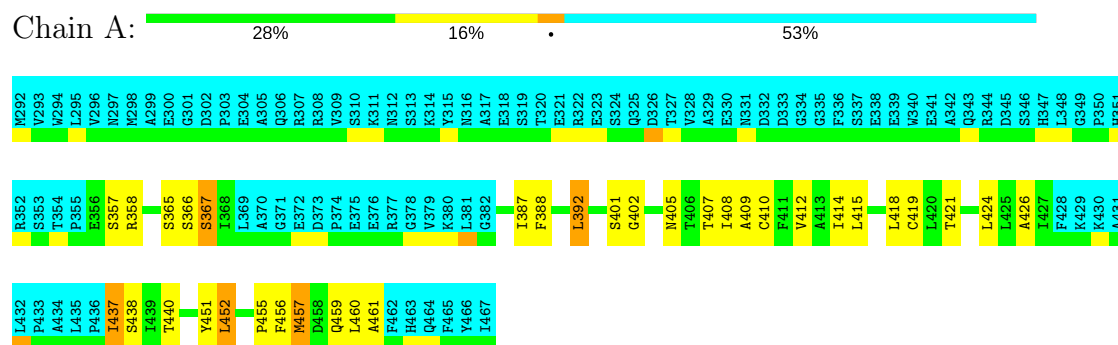
4.2.1 Score per residue for model 1

- Molecule 1: Presenilin-1



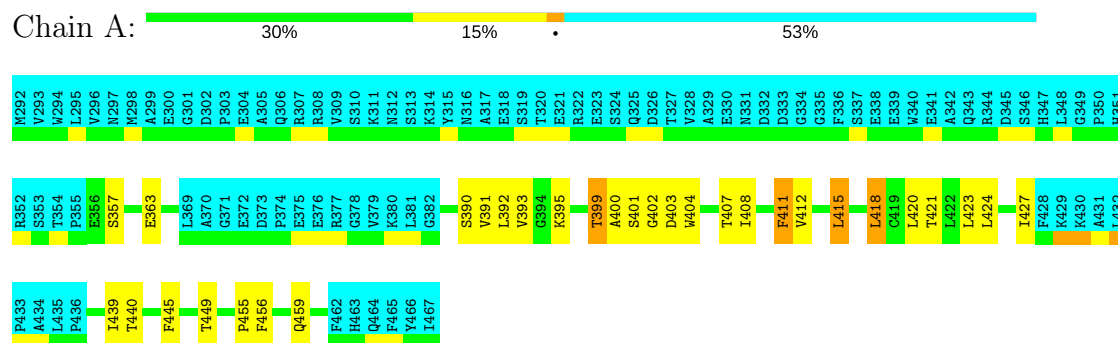
4.2.2 Score per residue for model 2

• Molecule 1: Presenilin-1



4.2.3 Score per residue for model 3

• Molecule 1: Presenilin-1



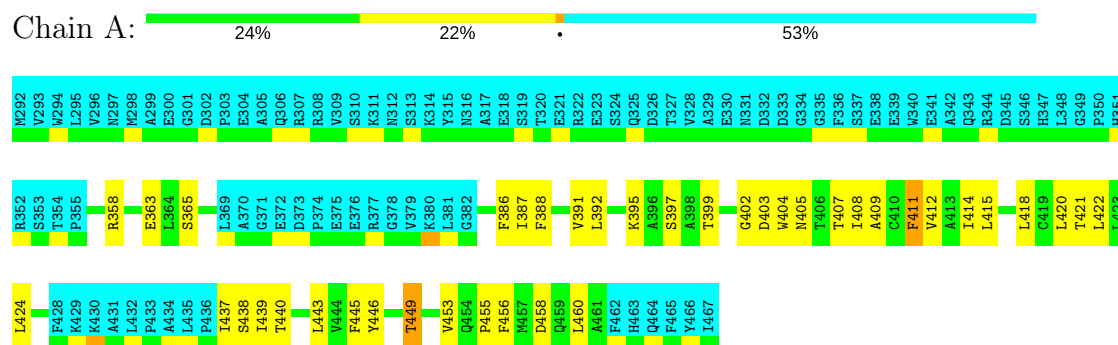
4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Presenilin-1



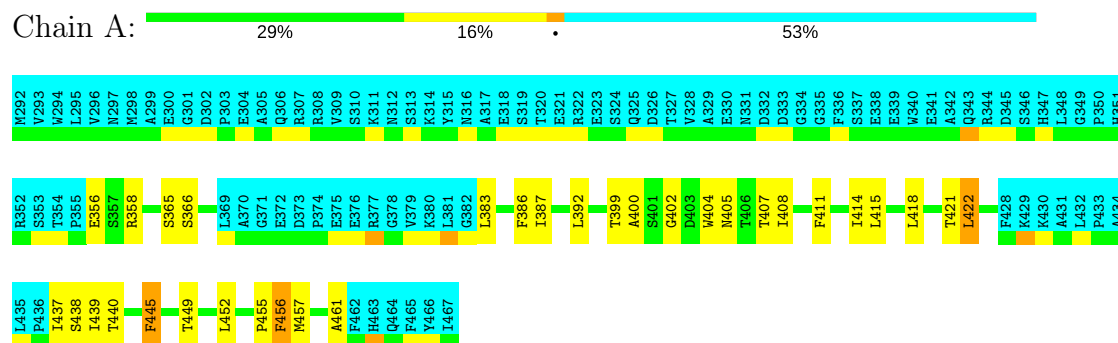
4.2.5 Score per residue for model 5

• Molecule 1: Presenilin-1



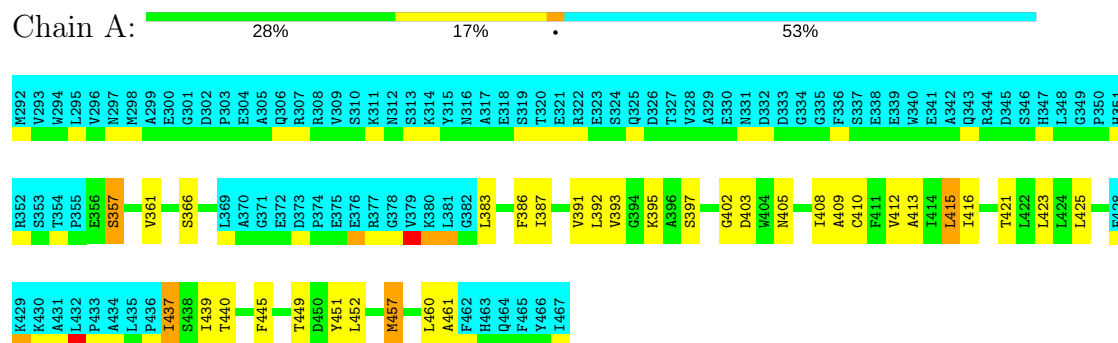
4.2.6 Score per residue for model 6

• Molecule 1: Presenilin-1



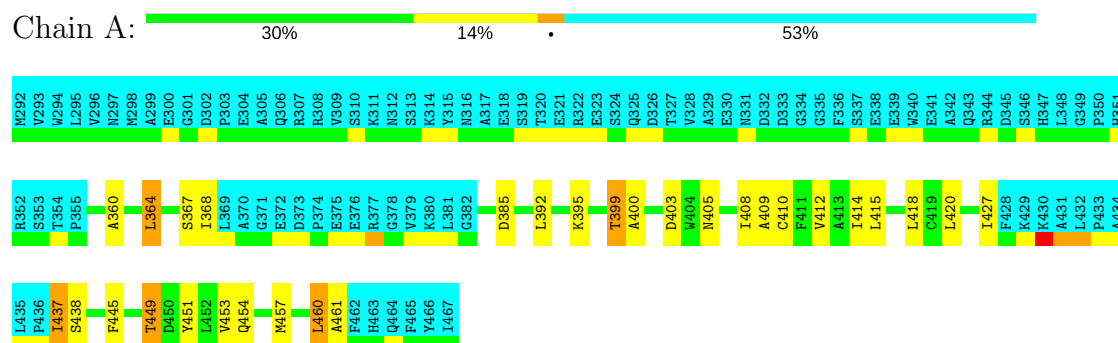
4.2.7 Score per residue for model 7

• Molecule 1: Presenilin-1



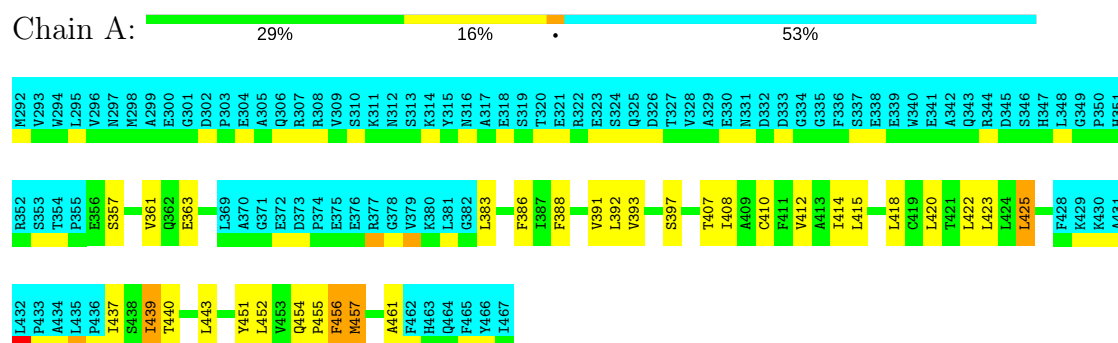
4.2.11 Score per residue for model 11

• Molecule 1: Presenilin-1



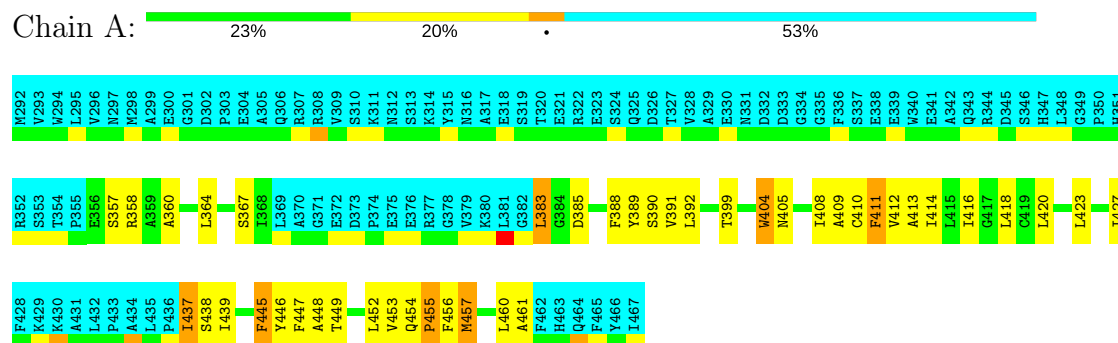
4.2.12 Score per residue for model 12

• Molecule 1: Presenilin-1



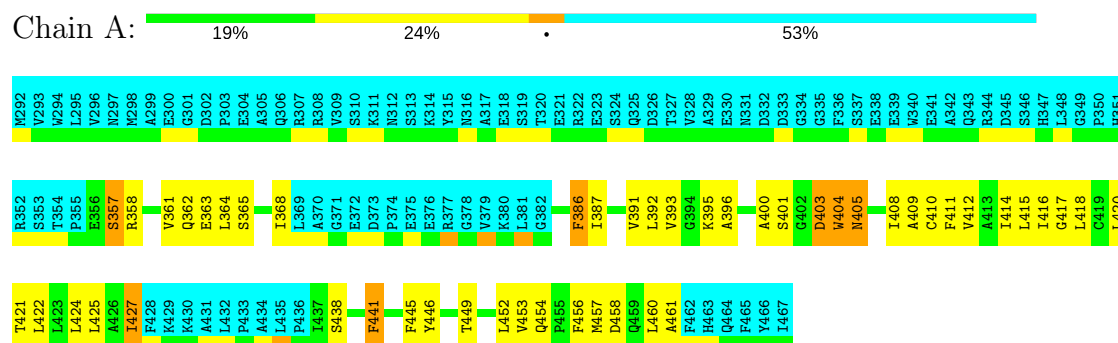
4.2.13 Score per residue for model 13

• Molecule 1: Presenilin-1



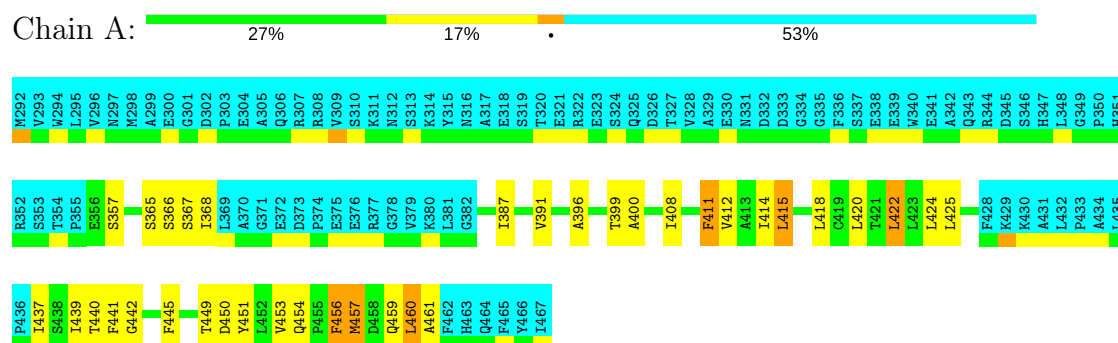
4.2.14 Score per residue for model 14

• Molecule 1: Presenilin-1



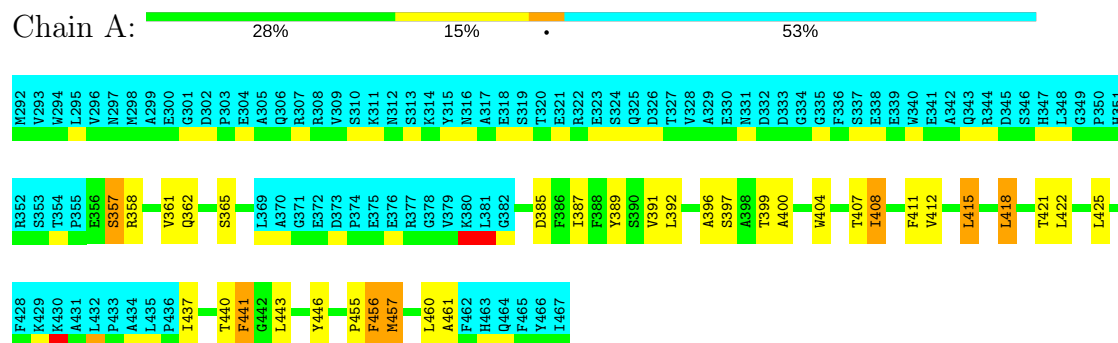
4.2.15 Score per residue for model 15

• Molecule 1: Presenilin-1



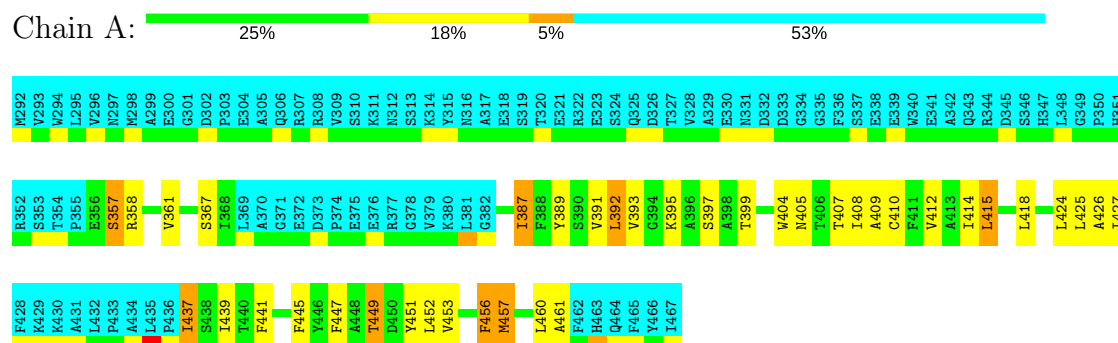
4.2.16 Score per residue for model 16

• Molecule 1: Presenilin-1



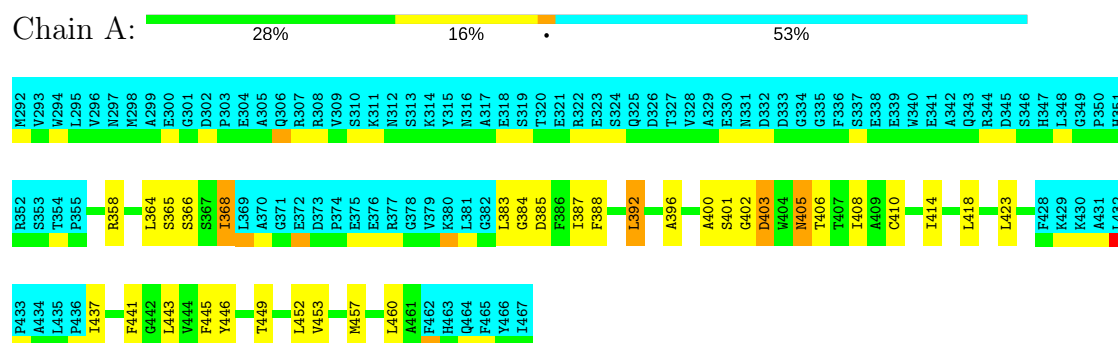
4.2.17 Score per residue for model 17

• Molecule 1: Presenilin-1



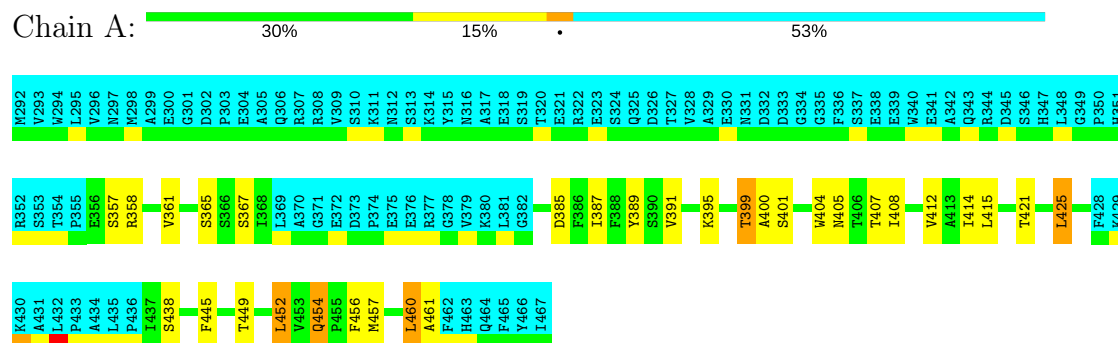
4.2.18 Score per residue for model 18

• Molecule 1: Presenilin-1



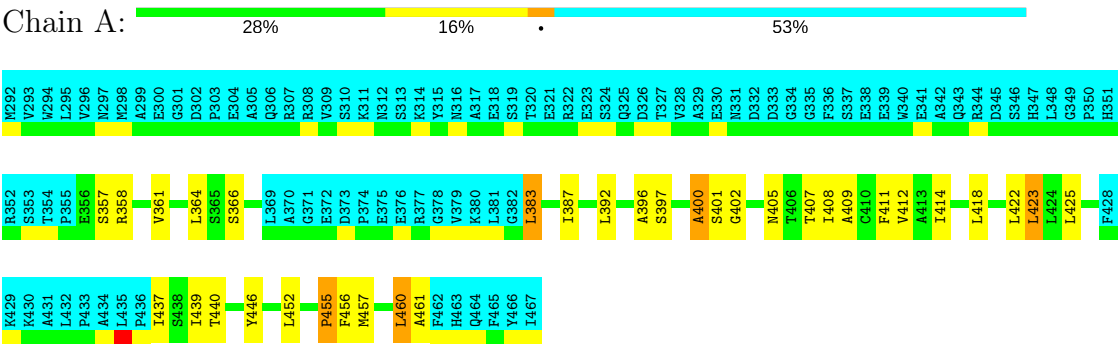
4.2.19 Score per residue for model 19

• Molecule 1: Presenilin-1



4.2.20 Score per residue for model 20

● Molecule 1: Presenilin-1



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	3.0

No chemical shift data was provided. 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	629	642	642	15±5
All	All	12580	12840	12840	299

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:414:ILE:HG21	1:A:460:LEU:HD22	0.88	1.43	13	1
1:A:387:ILE:HG23	1:A:415:LEU:HD12	0.84	1.47	15	1
1:A:392:LEU:HD22	1:A:408:ILE:HD12	0.80	1.51	10	2
1:A:392:LEU:HD12	1:A:408:ILE:HG23	0.76	1.54	6	1
1:A:387:ILE:HD13	1:A:415:LEU:HD22	0.76	1.57	14	2
1:A:414:ILE:HD11	1:A:460:LEU:HD22	0.75	1.59	4	2
1:A:405:ASN:O	1:A:409:ALA:HB3	0.73	1.83	10	10
1:A:392:LEU:HD23	1:A:408:ILE:HG21	0.73	1.59	4	1
1:A:392:LEU:HD22	1:A:408:ILE:HG22	0.67	1.65	12	1
1:A:408:ILE:O	1:A:412:VAL:HG23	0.66	1.91	1	18
1:A:392:LEU:HD12	1:A:408:ILE:HD12	0.66	1.67	7	1
1:A:391:VAL:HG11	1:A:411:PHE:HB2	0.64	1.69	5	1
1:A:387:ILE:HG21	1:A:415:LEU:HD13	0.64	1.68	9	1
1:A:404:TRP:O	1:A:408:ILE:HD13	0.64	1.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:387:ILE:CG1	1:A:415:LEU:HD13	0.63	2.24	4	1
1:A:414:ILE:HG23	1:A:456:PHE:HB2	0.63	1.71	8	5
1:A:387:ILE:HD13	1:A:415:LEU:CD2	0.63	2.24	5	2
1:A:388:PHE:CE1	1:A:408:ILE:HD11	0.63	2.29	2	1
1:A:392:LEU:CD1	1:A:408:ILE:HD12	0.62	2.24	7	2
1:A:391:VAL:HG13	1:A:411:PHE:CB	0.62	2.24	15	3
1:A:418:LEU:HD12	1:A:455:PRO:CB	0.62	2.24	3	2
1:A:387:ILE:O	1:A:391:VAL:HG23	0.62	1.95	7	6
1:A:413:ALA:HA	1:A:416:ILE:HD12	0.61	1.72	7	4
1:A:357:SER:O	1:A:361:VAL:HG23	0.61	1.95	14	9
1:A:414:ILE:HD12	1:A:456:PHE:CG	0.61	2.30	20	1
1:A:414:ILE:HG23	1:A:456:PHE:CB	0.60	2.26	6	7
1:A:392:LEU:HD11	1:A:403:ASP:HB3	0.60	1.71	10	1
1:A:445:PHE:O	1:A:449:THR:HG22	0.60	1.96	9	3
1:A:392:LEU:HD11	1:A:403:ASP:CB	0.60	2.26	10	1
1:A:392:LEU:HD13	1:A:408:ILE:HB	0.60	1.74	10	1
1:A:387:ILE:CG1	1:A:415:LEU:HD11	0.60	2.27	2	1
1:A:392:LEU:HB2	1:A:408:ILE:HD12	0.60	1.74	14	1
1:A:418:LEU:HD13	1:A:455:PRO:HB3	0.59	1.75	5	1
1:A:389:TYR:O	1:A:393:VAL:HG22	0.59	1.98	9	1
1:A:412:VAL:HA	1:A:415:LEU:HD23	0.58	1.74	9	1
1:A:392:LEU:HD13	1:A:408:ILE:HD11	0.58	1.75	11	1
1:A:414:ILE:CG2	1:A:460:LEU:HD22	0.58	2.26	13	2
1:A:405:ASN:O	1:A:408:ILE:HG22	0.58	1.99	9	1
1:A:387:ILE:HG13	1:A:415:LEU:HD11	0.58	1.74	2	1
1:A:388:PHE:O	1:A:392:LEU:HD12	0.58	1.99	4	1
1:A:383:LEU:HD22	1:A:423:LEU:HD13	0.57	1.75	13	1
1:A:451:TYR:O	1:A:452:LEU:HD22	0.57	1.99	9	4
1:A:414:ILE:HG21	1:A:457:MET:CG	0.57	2.30	10	1
1:A:392:LEU:HD12	1:A:408:ILE:HG12	0.56	1.76	17	1
1:A:391:VAL:HG11	1:A:411:PHE:CB	0.56	2.31	13	2
1:A:456:PHE:HB2	1:A:460:LEU:HD12	0.56	1.77	16	1
1:A:391:VAL:HG13	1:A:411:PHE:HB2	0.56	1.78	4	3
1:A:399:THR:HG21	1:A:407:THR:HG21	0.56	1.77	16	1
1:A:418:LEU:HD22	1:A:456:PHE:CZ	0.55	2.36	16	1
1:A:392:LEU:HD13	1:A:408:ILE:HG21	0.55	1.78	18	1
1:A:364:LEU:O	1:A:368:ILE:HG23	0.55	2.01	14	1
1:A:449:THR:HG22	1:A:453:VAL:HG21	0.55	1.79	5	3
1:A:449:THR:HG22	1:A:453:VAL:CG2	0.55	2.31	5	3
1:A:418:LEU:HD12	1:A:456:PHE:HB2	0.55	1.77	15	1
1:A:414:ILE:HD13	1:A:460:LEU:HG	0.54	1.78	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:414:ILE:HD12	1:A:460:LEU:CB	0.54	2.32	15	1
1:A:387:ILE:HG23	1:A:415:LEU:CD1	0.54	2.26	15	1
1:A:449:THR:CG2	1:A:453:VAL:HG13	0.54	2.33	15	1
1:A:383:LEU:CD2	1:A:423:LEU:HD13	0.54	2.33	13	1
1:A:364:LEU:O	1:A:368:ILE:HG22	0.53	2.03	18	1
1:A:457:MET:O	1:A:461:ALA:HB3	0.53	2.03	1	13
1:A:414:ILE:HD12	1:A:456:PHE:HB3	0.53	1.78	13	1
1:A:387:ILE:HD13	1:A:439:ILE:CG1	0.53	2.33	20	1
1:A:422:LEU:HD13	1:A:422:LEU:O	0.53	2.03	4	3
1:A:391:VAL:HG13	1:A:411:PHE:HB3	0.53	1.80	15	2
1:A:418:LEU:HD12	1:A:456:PHE:CG	0.52	2.39	15	1
1:A:384:GLY:O	1:A:387:ILE:HG22	0.52	2.05	10	2
1:A:414:ILE:HD11	1:A:457:MET:N	0.52	2.20	2	1
1:A:391:VAL:HG11	1:A:412:VAL:HG23	0.52	1.80	15	2
1:A:388:PHE:CE2	1:A:412:VAL:HG21	0.52	2.39	2	1
1:A:392:LEU:HD13	1:A:408:ILE:CG2	0.52	2.33	18	1
1:A:392:LEU:HD23	1:A:393:VAL:N	0.52	2.20	17	4
1:A:392:LEU:HD13	1:A:408:ILE:HD12	0.51	1.80	2	1
1:A:411:PHE:O	1:A:415:LEU:HD23	0.51	2.05	15	3
1:A:392:LEU:HD13	1:A:408:ILE:CD1	0.51	2.36	11	1
1:A:387:ILE:HD11	1:A:415:LEU:HD22	0.51	1.83	4	1
1:A:392:LEU:CB	1:A:408:ILE:HD12	0.51	2.35	14	1
1:A:405:ASN:HA	1:A:408:ILE:HG23	0.51	1.82	10	1
1:A:414:ILE:HG13	1:A:460:LEU:HD13	0.51	1.82	13	1
1:A:386:PHE:CE2	1:A:439:ILE:HG22	0.50	2.41	4	2
1:A:418:LEU:HD23	1:A:455:PRO:HB3	0.50	1.82	2	1
1:A:414:ILE:O	1:A:418:LEU:HD23	0.50	2.06	14	1
1:A:387:ILE:HD11	1:A:415:LEU:HD12	0.50	1.83	17	1
1:A:392:LEU:HD23	1:A:408:ILE:HG13	0.50	1.83	13	1
1:A:383:LEU:HD13	1:A:439:ILE:CG2	0.49	2.38	9	1
1:A:392:LEU:HD12	1:A:408:ILE:CG2	0.49	2.32	6	1
1:A:396:ALA:HA	1:A:400:ALA:HB3	0.49	1.83	20	1
1:A:396:ALA:HB1	1:A:402:GLY:O	0.49	2.08	18	1
1:A:457:MET:HG3	1:A:461:ALA:HB3	0.49	1.84	2	1
1:A:402:GLY:C	1:A:408:ILE:HD11	0.49	2.28	6	1
1:A:405:ASN:HB3	1:A:407:THR:HG22	0.49	1.85	6	1
1:A:387:ILE:HG13	1:A:415:LEU:HD13	0.49	1.84	4	1
1:A:445:PHE:O	1:A:449:THR:HG23	0.49	2.07	7	2
1:A:418:LEU:HD12	1:A:455:PRO:CG	0.48	2.37	20	3
1:A:396:ALA:HB1	1:A:401:SER:O	0.48	2.08	9	1
1:A:396:ALA:HB1	1:A:402:GLY:C	0.48	2.28	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:418:LEU:HD23	1:A:418:LEU:O	0.48	2.07	15	1
1:A:414:ILE:HG21	1:A:460:LEU:CD2	0.48	2.28	13	1
1:A:399:THR:O	1:A:400:ALA:HB3	0.48	2.09	3	7
1:A:415:LEU:O	1:A:415:LEU:HD13	0.47	2.09	7	2
1:A:383:LEU:HA	1:A:439:ILE:HG21	0.47	1.86	20	2
1:A:392:LEU:O	1:A:396:ALA:HB2	0.47	2.09	18	3
1:A:392:LEU:HD23	1:A:393:VAL:HG23	0.47	1.87	1	1
1:A:423:LEU:O	1:A:427:ILE:HG22	0.47	2.09	13	2
1:A:387:ILE:CG2	1:A:415:LEU:HD13	0.47	2.40	9	1
1:A:360:ALA:O	1:A:364:LEU:HD23	0.47	2.10	13	2
1:A:422:LEU:O	1:A:422:LEU:HD13	0.47	2.10	6	2
1:A:414:ILE:HG21	1:A:457:MET:HG2	0.46	1.86	10	1
1:A:392:LEU:HD23	1:A:393:VAL:CG2	0.46	2.41	1	1
1:A:405:ASN:HD22	1:A:407:THR:HG23	0.46	1.71	20	1
1:A:360:ALA:O	1:A:364:LEU:HD13	0.46	2.11	8	1
1:A:414:ILE:HG22	1:A:418:LEU:HD12	0.46	1.87	9	1
1:A:457:MET:O	1:A:461:ALA:HB2	0.46	2.10	14	3
1:A:418:LEU:HD22	1:A:455:PRO:HB3	0.46	1.88	10	3
1:A:392:LEU:HD22	1:A:408:ILE:CD1	0.46	2.39	9	1
1:A:449:THR:HG22	1:A:453:VAL:HG13	0.46	1.87	15	1
1:A:414:ILE:HG23	1:A:456:PHE:HB3	0.46	1.87	17	3
1:A:414:ILE:HD12	1:A:460:LEU:HB3	0.45	1.87	15	1
1:A:418:LEU:HD22	1:A:455:PRO:CB	0.45	2.42	5	1
1:A:414:ILE:HG23	1:A:456:PHE:CD2	0.45	2.46	20	1
1:A:424:LEU:O	1:A:424:LEU:HD23	0.45	2.12	9	1
1:A:392:LEU:HD23	1:A:408:ILE:CG2	0.45	2.39	4	1
1:A:386:PHE:CE2	1:A:439:ILE:HD12	0.44	2.47	6	1
1:A:426:ALA:HB1	1:A:437:ILE:HG21	0.44	1.88	2	1
1:A:456:PHE:O	1:A:460:LEU:HD12	0.44	2.13	20	1
1:A:418:LEU:HD13	1:A:455:PRO:HA	0.44	1.89	12	1
1:A:357:SER:O	1:A:361:VAL:HG12	0.44	2.12	17	1
1:A:408:ILE:HG23	1:A:409:ALA:H	0.43	1.72	10	1
1:A:453:VAL:O	1:A:454:GLN:C	0.43	2.57	14	3
1:A:390:SER:HA	1:A:393:VAL:HG12	0.43	1.90	3	1
1:A:418:LEU:HD21	1:A:455:PRO:CB	0.43	2.43	1	1
1:A:418:LEU:HD12	1:A:455:PRO:HG3	0.43	1.90	4	3
1:A:414:ILE:HD11	1:A:460:LEU:HD13	0.43	1.90	11	1
1:A:391:VAL:CG2	1:A:415:LEU:HD12	0.43	2.44	4	1
1:A:408:ILE:HG23	1:A:409:ALA:N	0.43	2.29	20	4
1:A:387:ILE:O	1:A:391:VAL:HG13	0.43	2.13	1	1
1:A:423:LEU:O	1:A:423:LEU:HD13	0.42	2.13	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:418:LEU:HD13	1:A:418:LEU:C	0.42	2.35	2	1
1:A:391:VAL:HG11	1:A:415:LEU:HD23	0.42	1.90	12	1
1:A:405:ASN:CA	1:A:408:ILE:HG23	0.42	2.44	10	1
1:A:387:ILE:HG12	1:A:415:LEU:HD11	0.42	1.90	1	1
1:A:387:ILE:CD1	1:A:439:ILE:HD11	0.42	2.45	20	1
1:A:418:LEU:HD12	1:A:456:PHE:CB	0.42	2.43	15	1
1:A:423:LEU:C	1:A:423:LEU:HD13	0.42	2.35	12	2
1:A:396:ALA:O	1:A:400:ALA:HB2	0.42	2.15	15	1
1:A:392:LEU:HD22	1:A:408:ILE:HG13	0.42	1.92	20	1
1:A:437:ILE:O	1:A:437:ILE:HG23	0.42	2.15	11	1
1:A:418:LEU:HD13	1:A:455:PRO:CA	0.42	2.43	12	1
1:A:387:ILE:HD13	1:A:439:ILE:HG13	0.42	1.91	20	1
1:A:446:TYR:OH	1:A:460:LEU:HD13	0.41	2.15	16	1
1:A:439:ILE:O	1:A:439:ILE:HG23	0.41	2.15	3	2
1:A:411:PHE:CD1	1:A:411:PHE:C	0.41	2.93	5	1
1:A:386:PHE:CD2	1:A:439:ILE:HD12	0.41	2.51	12	1
1:A:391:VAL:HG11	1:A:408:ILE:O	0.41	2.16	15	1
1:A:457:MET:HG2	1:A:461:ALA:HB3	0.41	1.92	13	1
1:A:439:ILE:HG21	1:A:445:PHE:HA	0.41	1.92	17	1
1:A:427:ILE:HG23	1:A:427:ILE:O	0.41	2.15	14	1
1:A:414:ILE:HG22	1:A:418:LEU:CD1	0.41	2.46	9	1
1:A:388:PHE:HE1	1:A:392:LEU:HD11	0.41	1.76	12	1
1:A:392:LEU:O	1:A:392:LEU:HD22	0.41	2.15	13	1
1:A:391:VAL:HG12	1:A:395:LYS:HG3	0.41	1.92	5	1
1:A:414:ILE:HD12	1:A:456:PHE:CD1	0.41	2.50	20	1
1:A:392:LEU:HD12	1:A:393:VAL:N	0.41	2.30	3	1
1:A:445:PHE:CZ	1:A:449:THR:HG21	0.41	2.51	19	1
1:A:414:ILE:HD12	1:A:415:LEU:N	0.41	2.31	5	1
1:A:418:LEU:HD23	1:A:419:CYS:N	0.41	2.31	4	1
1:A:386:PHE:CD2	1:A:439:ILE:HG22	0.40	2.51	5	1
1:A:414:ILE:HD11	1:A:457:MET:CA	0.40	2.46	2	1
1:A:405:ASN:OD1	1:A:407:THR:HG23	0.40	2.16	19	1
1:A:388:PHE:CZ	1:A:408:ILE:HD11	0.40	2.51	2	1
1:A:383:LEU:HA	1:A:387:ILE:HD13	0.40	1.92	6	1
1:A:416:ILE:HD12	1:A:417:GLY:N	0.40	2.30	14	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	83/176 (47%)	67±3 (81±4%)	14±3 (16±3%)	3±1 (3±1%)	8	41
All	All	1660/3520 (47%)	1339 (81%)	270 (16%)	51 (3%)	8	41

All 15 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	437	ILE	13
1	A	454	GLN	5
1	A	400	ALA	4
1	A	402	GLY	4
1	A	405	ASN	3
1	A	455	PRO	3
1	A	368	ILE	3
1	A	427	ILE	3
1	A	441	PHE	3
1	A	404	TRP	2
1	A	443	LEU	2
1	A	403	ASP	2
1	A	439	ILE	2
1	A	442	GLY	1
1	A	401	SER	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	68/146 (47%)	50±4 (73±5%)	18±4 (27±5%)	2	23
All	All	1360/2920 (47%)	998 (73%)	362 (27%)	2	23

All 59 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	358	ARG	13
1	A	460	LEU	13
1	A	357	SER	12
1	A	420	LEU	11
1	A	365	SER	11
1	A	456	PHE	11
1	A	410	CYS	11
1	A	404	TRP	11
1	A	415	LEU	10
1	A	422	LEU	10
1	A	438	SER	10
1	A	403	ASP	10
1	A	421	THR	10
1	A	452	LEU	9
1	A	457	MET	9
1	A	425	LEU	9
1	A	395	LYS	8
1	A	440	THR	8
1	A	366	SER	8
1	A	424	LEU	8
1	A	445	PHE	8
1	A	411	PHE	8
1	A	407	THR	7
1	A	446	TYR	7
1	A	418	LEU	7
1	A	397	SER	7
1	A	399	THR	6
1	A	383	LEU	6
1	A	459	GLN	6
1	A	392	LEU	6
1	A	385	ASP	6
1	A	451	TYR	6
1	A	449	THR	6
1	A	401	SER	6
1	A	363	GLU	5
1	A	388	PHE	5
1	A	364	LEU	4
1	A	441	PHE	4
1	A	423	LEU	4
1	A	454	GLN	4
1	A	367	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	443	LEU	4
1	A	389	TYR	3
1	A	405	ASN	3
1	A	406	THR	3
1	A	408	ILE	3
1	A	387	ILE	3
1	A	458	ASP	2
1	A	386	PHE	2
1	A	356	GLU	2
1	A	362	GLN	2
1	A	437	ILE	2
1	A	450	ASP	2
1	A	447	PHE	2
1	A	391	VAL	1
1	A	368	ILE	1
1	A	419	CYS	1
1	A	427	ILE	1
1	A	390	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided