



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 12:29 AM UTC

PDB ID : 1TKN / pdb_00001tkn
Title : Solution structure of CAPPD*, an independently folded extracellular domain
of human Amyloid-beta Precursor Protein
Authors : Dulubova, I.; Ho, A.; Huryeva, I.; Sudhof, T.C.; Rizo, J.
Deposited on : 2004-06-08

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

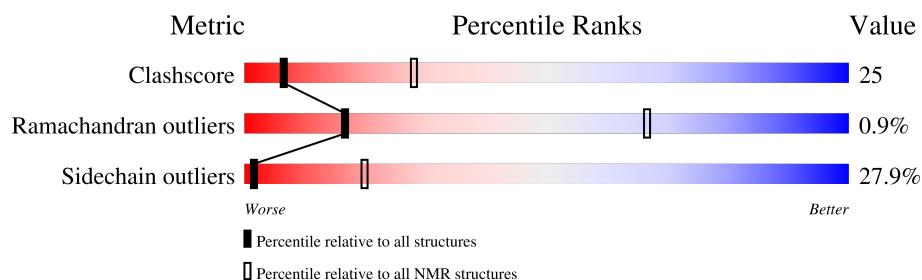
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	110	47% 39% 12% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:462-A:569 (108)	0.79	2

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1875 atoms, of which 953 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid beta A4 protein.

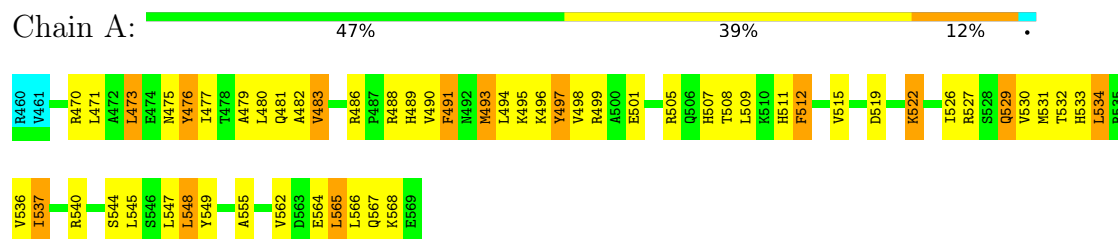
Mol	Chain	Residues	Atoms						Trace
1	A	110	Total	C	H	N	O	S	0
			1875	577	953	176	164	5	

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: Amyloid beta A4 protein

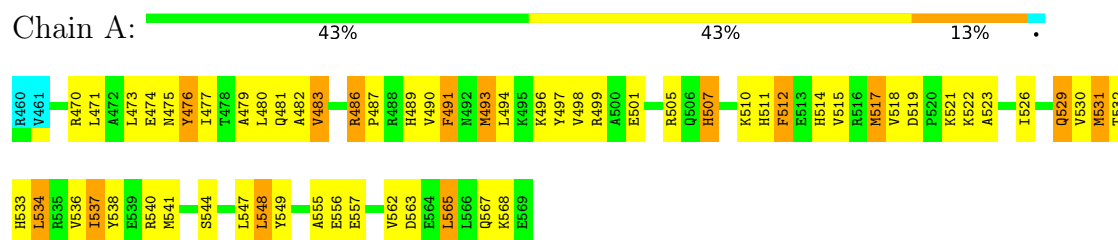


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

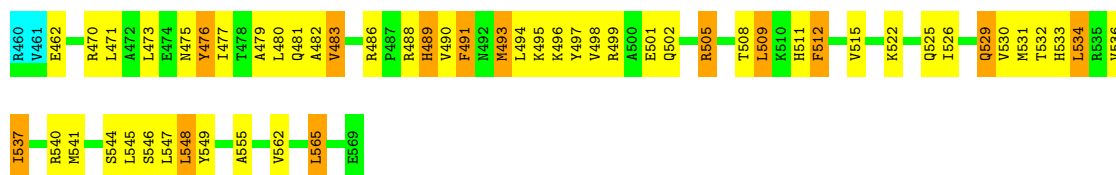
- Molecule 1: Amyloid beta A4 protein



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: Amyloid beta A4 protein

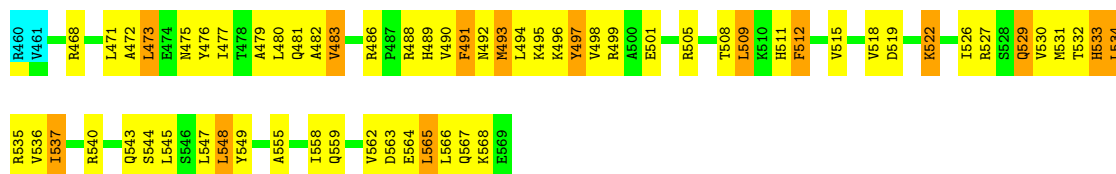




4.2.3 Score per residue for model 3

- Molecule 1: Amyloid beta A4 protein

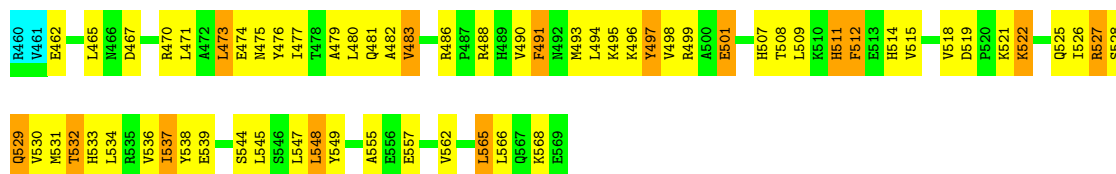
Chain A: 41% 45% 13%



4.2.4 Score per residue for model 4

- Molecule 1: Amyloid beta A4 protein

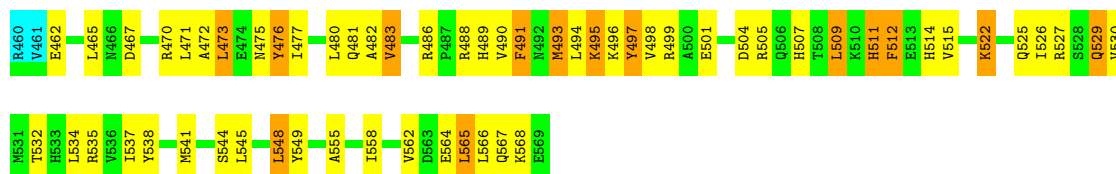
Chain A: 41% 45% 13%



4.2.5 Score per residue for model 5

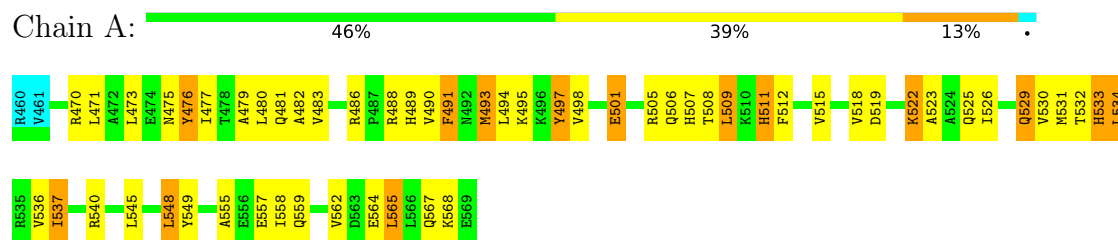
- Molecule 1: Amyloid beta A4 protein

Chain A: 45% 41% 13%



4.2.6 Score per residue for model 6

- Molecule 1: Amyloid beta A4 protein



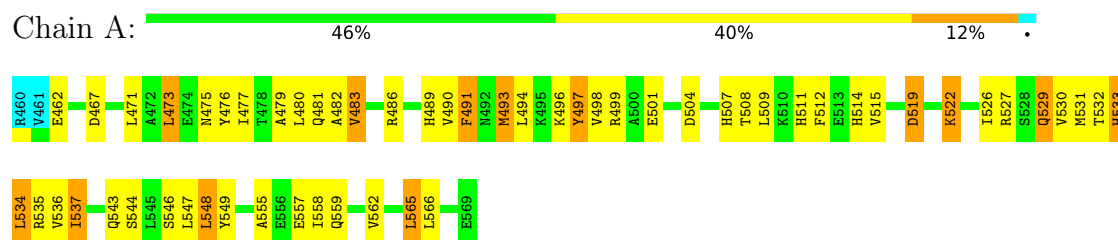
4.2.7 Score per residue for model 7

- Molecule 1: Amyloid beta A4 protein



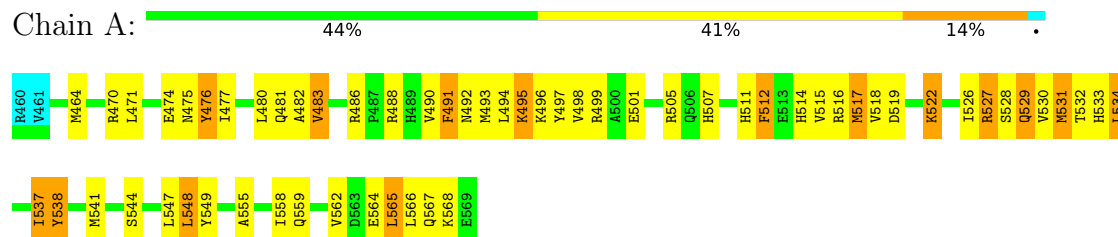
4.2.8 Score per residue for model 8

- Molecule 1: Amyloid beta A4 protein



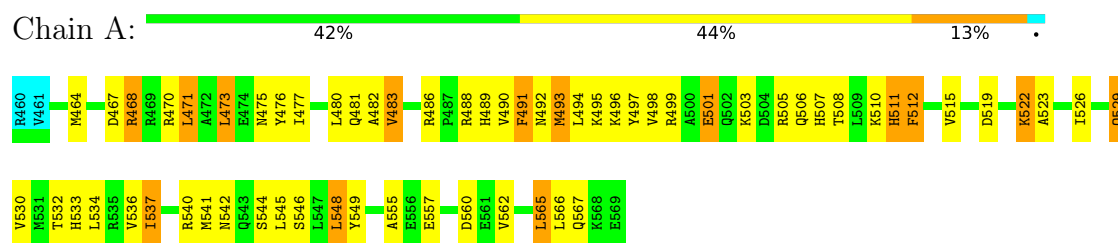
4.2.9 Score per residue for model 9

- Molecule 1: Amyloid beta A4 protein



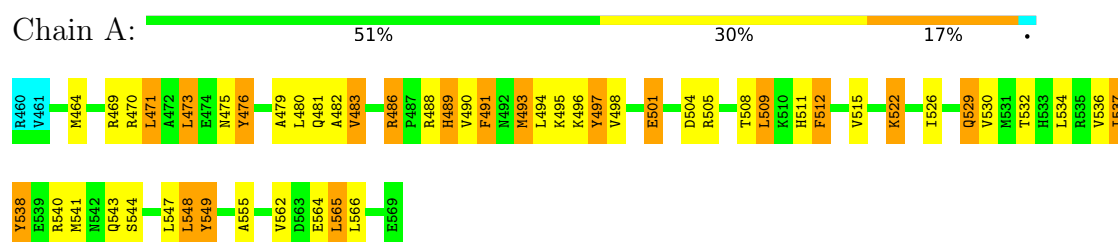
4.2.10 Score per residue for model 10

- Molecule 1: Amyloid beta A4 protein



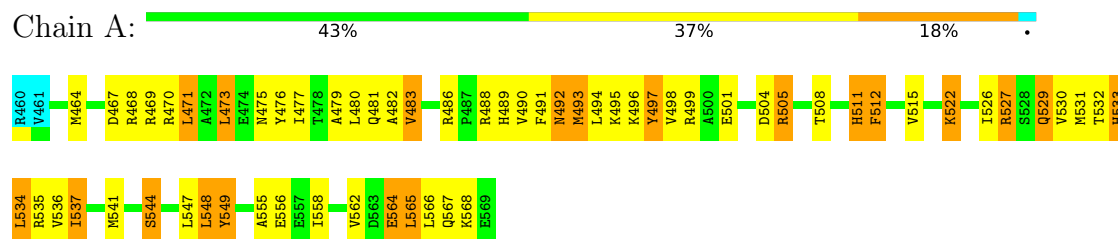
4.2.11 Score per residue for model 11

- Molecule 1: Amyloid beta A4 protein



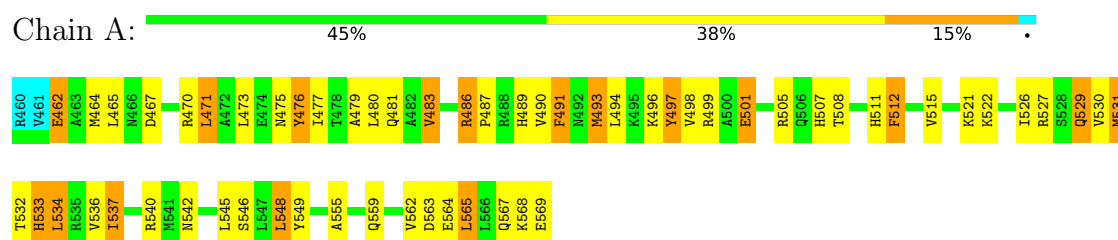
4.2.12 Score per residue for model 12

- Molecule 1: Amyloid beta A4 protein



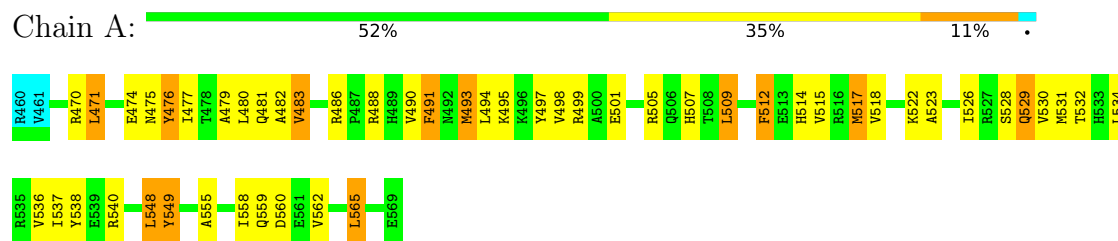
4.2.13 Score per residue for model 13

- Molecule 1: Amyloid beta A4 protein



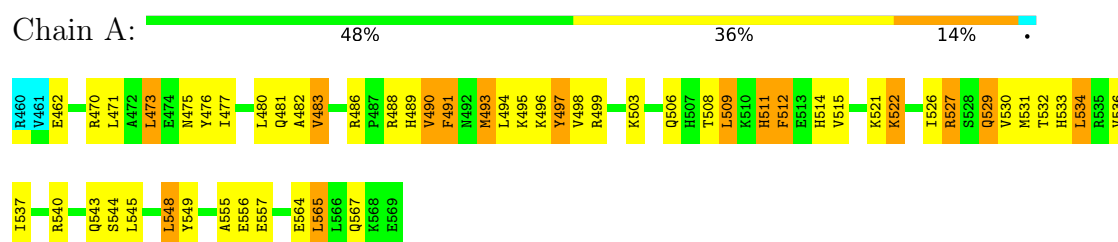
4.2.14 Score per residue for model 14

- Molecule 1: Amyloid beta A4 protein



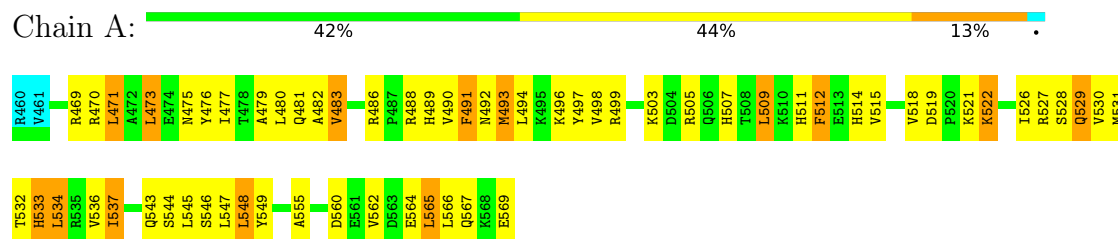
4.2.15 Score per residue for model 15

- Molecule 1: Amyloid beta A4 protein



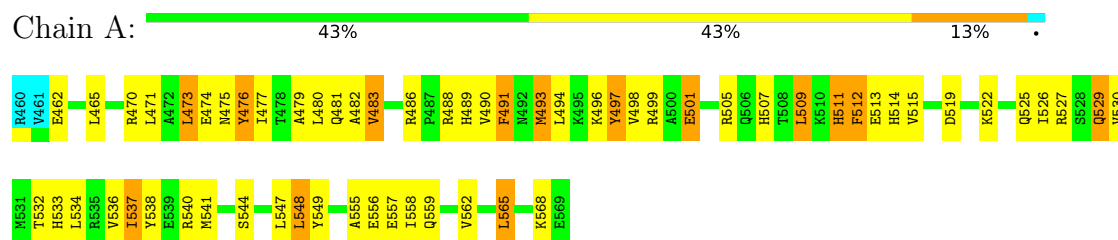
4.2.16 Score per residue for model 16

- Molecule 1: Amyloid beta A4 protein



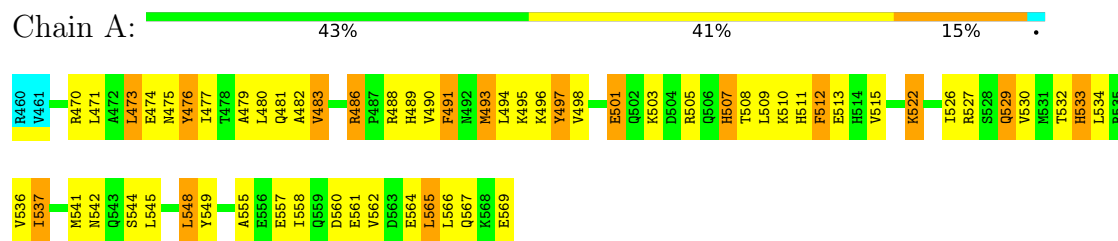
4.2.17 Score per residue for model 17

- Molecule 1: Amyloid beta A4 protein



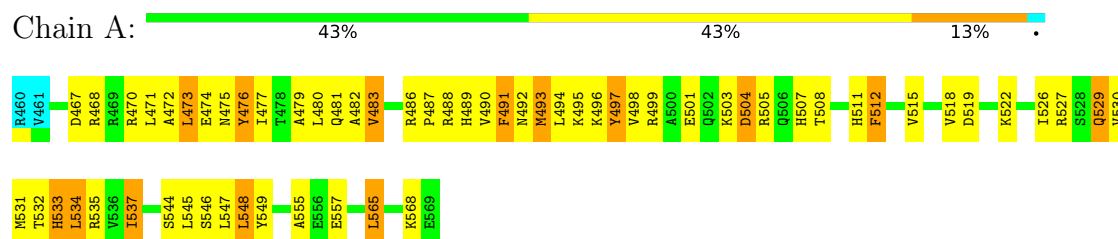
4.2.18 Score per residue for model 18

- Molecule 1: Amyloid beta A4 protein



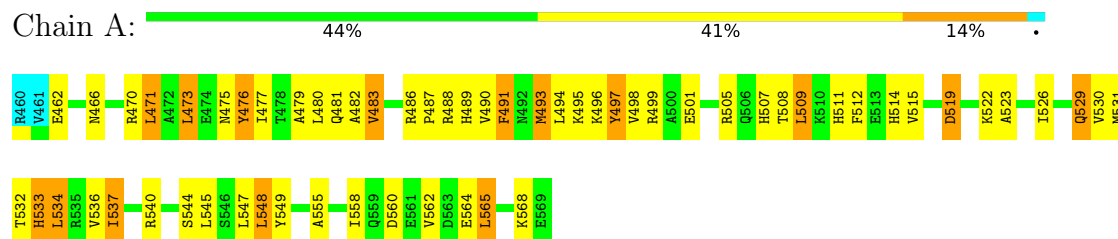
4.2.19 Score per residue for model 19

- Molecule 1: Amyloid beta A4 protein



4.2.20 Score per residue for model 20

- Molecule 1: Amyloid beta A4 protein



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 1000 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1
CNS	refinement	1

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	904	929	924	46±4
All	All	18080	18580	18480	921

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:515:VAL:HG11	1:A:526:ILE:HD11	1.08	1.21	11	20
1:A:508:THR:HG22	1:A:530:VAL:HG13	0.91	1.39	18	2
1:A:548:LEU:HD22	1:A:548:LEU:O	0.84	1.73	14	20
1:A:548:LEU:HD13	1:A:549:TYR:N	0.83	1.89	16	20
1:A:515:VAL:HG11	1:A:526:ILE:CD1	0.81	2.05	13	14
1:A:486:ARG:O	1:A:490:VAL:HG13	0.81	1.75	11	20
1:A:529:GLN:O	1:A:532:THR:HG22	0.77	1.80	3	20
1:A:494:LEU:O	1:A:498:VAL:HG23	0.76	1.81	18	16
1:A:498:VAL:HG11	1:A:566:LEU:CD2	0.76	2.11	10	7
1:A:533:HIS:O	1:A:537:ILE:HD12	0.76	1.80	3	10
1:A:498:VAL:HG11	1:A:566:LEU:HD21	0.75	1.56	9	3
1:A:562:VAL:HA	1:A:565:LEU:HD23	0.75	1.59	8	13
1:A:508:THR:HG21	1:A:533:HIS:HB3	0.74	1.57	18	3
1:A:498:VAL:HG13	1:A:541:MET:HE1	0.74	1.58	2	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:511:HIS:O	1:A:515:VAL:HG12	0.74	1.83	7	17
1:A:473:LEU:HD23	1:A:497:TYR:CD1	0.74	2.18	19	2
1:A:490:VAL:O	1:A:494:LEU:HD23	0.73	1.83	8	11
1:A:548:LEU:HD21	1:A:555:ALA:HA	0.72	1.61	13	20
1:A:481:GLN:O	1:A:483:VAL:HG23	0.72	1.85	20	19
1:A:491:PHE:CE1	1:A:565:LEU:HD22	0.72	2.20	1	11
1:A:473:LEU:HD23	1:A:497:TYR:CD2	0.71	2.20	18	2
1:A:473:LEU:HD21	1:A:544:SER:OG	0.71	1.86	11	3
1:A:512:PHE:CD2	1:A:530:VAL:HG11	0.71	2.21	7	7
1:A:501:GLU:OE1	1:A:541:MET:HE3	0.70	1.87	17	2
1:A:544:SER:HA	1:A:547:LEU:HD12	0.69	1.64	4	12
1:A:473:LEU:HD23	1:A:497:TYR:CE1	0.69	2.22	19	7
1:A:495:LYS:HB2	1:A:565:LEU:HD11	0.69	1.63	5	3
1:A:532:THR:O	1:A:536:VAL:HG23	0.68	1.89	4	15
1:A:562:VAL:O	1:A:566:LEU:HD12	0.68	1.89	16	8
1:A:477:ILE:HD13	1:A:480:LEU:HD12	0.68	1.66	5	15
1:A:512:PHE:CD1	1:A:530:VAL:HG21	0.68	2.24	19	4
1:A:473:LEU:HD23	1:A:497:TYR:CE2	0.68	2.24	15	4
1:A:479:ALA:CB	1:A:490:VAL:HG12	0.67	2.19	11	13
1:A:465:LEU:HD13	1:A:504:ASP:OD1	0.67	1.90	5	1
1:A:480:LEU:HD11	1:A:548:LEU:HB2	0.67	1.67	16	15
1:A:473:LEU:HD21	1:A:544:SER:HB2	0.67	1.66	7	3
1:A:479:ALA:HB1	1:A:490:VAL:HG12	0.66	1.68	7	4
1:A:548:LEU:HD13	1:A:548:LEU:C	0.65	2.16	13	20
1:A:508:THR:HG21	1:A:534:LEU:HB2	0.65	1.68	10	3
1:A:512:PHE:HB2	1:A:530:VAL:HG11	0.64	1.69	18	1
1:A:548:LEU:HD22	1:A:548:LEU:C	0.62	2.20	16	20
1:A:512:PHE:CB	1:A:530:VAL:HG11	0.61	2.26	18	1
1:A:495:LYS:CB	1:A:565:LEU:HD11	0.61	2.25	2	5
1:A:515:VAL:HG21	1:A:522:LYS:HD2	0.61	1.72	3	7
1:A:476:TYR:CD2	1:A:494:LEU:HD21	0.61	2.31	17	2
1:A:491:PHE:CD1	1:A:565:LEU:HD22	0.61	2.31	1	11
1:A:479:ALA:HB3	1:A:490:VAL:HG12	0.60	1.73	2	9
1:A:512:PHE:HD1	1:A:530:VAL:HG21	0.59	1.58	19	3
1:A:471:LEU:HD12	1:A:475:ASN:ND2	0.58	2.14	16	19
1:A:473:LEU:HD22	1:A:476:TYR:CE2	0.58	2.34	8	2
1:A:498:VAL:HG11	1:A:566:LEU:HD22	0.58	1.75	10	3
1:A:495:LYS:CD	1:A:565:LEU:HD13	0.57	2.28	15	4
1:A:473:LEU:HD21	1:A:544:SER:HB3	0.57	1.76	8	2
1:A:495:LYS:HG3	1:A:565:LEU:HD13	0.57	1.75	9	1
1:A:471:LEU:HD12	1:A:475:ASN:HD22	0.56	1.61	20	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:476:TYR:CD1	1:A:494:LEU:HD21	0.55	2.36	13	7
1:A:514:HIS:O	1:A:518:VAL:HG22	0.55	2.01	16	2
1:A:505:ARG:HA	1:A:537:ILE:HD13	0.55	1.77	1	11
1:A:565:LEU:C	1:A:565:LEU:HD12	0.55	2.27	15	3
1:A:495:LYS:CE	1:A:565:LEU:HD13	0.55	2.32	15	3
1:A:473:LEU:C	1:A:473:LEU:HD12	0.54	2.27	16	3
1:A:526:ILE:HD12	1:A:530:VAL:CG2	0.54	2.33	19	2
1:A:508:THR:HG22	1:A:530:VAL:CG1	0.53	2.25	18	3
1:A:473:LEU:HD22	1:A:476:TYR:HE2	0.53	1.64	15	2
1:A:531:MET:HA	1:A:534:LEU:HD12	0.53	1.80	7	13
1:A:515:VAL:HG11	1:A:526:ILE:HD13	0.53	1.78	13	1
1:A:498:VAL:HG13	1:A:541:MET:CE	0.52	2.33	18	2
1:A:476:TYR:C	1:A:476:TYR:CD1	0.52	2.87	8	4
1:A:536:VAL:HG13	1:A:540:ARG:HG3	0.51	1.82	6	6
1:A:473:LEU:HD12	1:A:473:LEU:O	0.51	2.05	16	3
1:A:487:PRO:O	1:A:558:ILE:HG22	0.51	2.05	20	1
1:A:514:HIS:HA	1:A:517:MET:HE2	0.51	1.82	1	1
1:A:526:ILE:O	1:A:530:VAL:HG23	0.51	2.06	20	4
1:A:505:ARG:HD3	1:A:537:ILE:HG21	0.51	1.82	19	1
1:A:514:HIS:HD2	1:A:517:MET:HE2	0.50	1.66	14	1
1:A:509:LEU:HD12	1:A:509:LEU:O	0.50	2.06	6	5
1:A:491:PHE:CD1	1:A:491:PHE:C	0.50	2.90	8	17
1:A:491:PHE:HE1	1:A:565:LEU:HD22	0.50	1.64	17	7
1:A:505:ARG:CG	1:A:537:ILE:HG21	0.50	2.36	19	1
1:A:508:THR:HG22	1:A:530:VAL:HG12	0.50	1.83	7	2
1:A:504:ASP:OD1	1:A:537:ILE:HD11	0.49	2.07	12	2
1:A:477:ILE:O	1:A:480:LEU:HB2	0.49	2.07	7	19
1:A:548:LEU:HD21	1:A:555:ALA:CA	0.49	2.35	13	9
1:A:477:ILE:CD1	1:A:480:LEU:HD12	0.49	2.37	13	2
1:A:512:PHE:HB2	1:A:530:VAL:HG21	0.49	1.83	18	1
1:A:509:LEU:C	1:A:509:LEU:HD12	0.49	2.32	20	2
1:A:498:VAL:HG22	1:A:541:MET:CE	0.49	2.38	10	3
1:A:473:LEU:HD13	1:A:476:TYR:CZ	0.49	2.43	15	2
1:A:514:HIS:CD2	1:A:517:MET:HE2	0.49	2.43	14	1
1:A:519:ASP:O	1:A:523:ALA:HB2	0.49	2.08	1	4
1:A:491:PHE:HB2	1:A:562:VAL:HG23	0.49	1.84	18	7
1:A:508:THR:CG2	1:A:530:VAL:HG13	0.48	2.26	18	6
1:A:495:LYS:HB3	1:A:565:LEU:HD11	0.48	1.83	12	1
1:A:558:ILE:O	1:A:562:VAL:HG23	0.48	2.09	20	3
1:A:481:GLN:O	1:A:482:ALA:C	0.48	2.56	19	19
1:A:505:ARG:CD	1:A:537:ILE:HG21	0.48	2.38	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:509:LEU:HD12	1:A:509:LEU:C	0.47	2.34	6	3
1:A:534:LEU:HD13	1:A:534:LEU:O	0.47	2.09	5	2
1:A:515:VAL:CG1	1:A:526:ILE:HD11	0.47	2.35	2	2
1:A:491:PHE:CD1	1:A:492:ASN:N	0.47	2.83	3	4
1:A:489:HIS:O	1:A:493:MET:CE	0.47	2.63	18	16
1:A:548:LEU:C	1:A:548:LEU:CD1	0.47	2.86	13	14
1:A:534:LEU:C	1:A:534:LEU:HD13	0.47	2.34	11	3
1:A:498:VAL:HG12	1:A:502:GLN:HE21	0.47	1.69	2	1
1:A:505:ARG:HG2	1:A:534:LEU:HD21	0.46	1.86	5	1
1:A:495:LYS:CG	1:A:565:LEU:HD22	0.46	2.40	15	1
1:A:501:GLU:CD	1:A:541:MET:HE3	0.46	2.35	17	1
1:A:512:PHE:CD1	1:A:530:VAL:HG11	0.46	2.45	17	2
1:A:490:VAL:HG21	1:A:558:ILE:HG21	0.46	1.85	8	4
1:A:476:TYR:CG	1:A:494:LEU:CD2	0.46	2.99	2	1
1:A:476:TYR:CD2	1:A:494:LEU:CD2	0.46	2.99	17	1
1:A:522:LYS:O	1:A:526:ILE:HG23	0.45	2.10	12	5
1:A:468:ARG:O	1:A:472:ALA:HB2	0.45	2.11	19	2
1:A:472:ALA:HB1	1:A:497:TYR:HB2	0.45	1.89	5	1
1:A:536:VAL:HG13	1:A:540:ARG:CG	0.45	2.41	15	5
1:A:498:VAL:HG22	1:A:541:MET:HE2	0.45	1.88	1	3
1:A:495:LYS:CG	1:A:565:LEU:HD13	0.45	2.42	7	1
1:A:512:PHE:CD2	1:A:530:VAL:CG1	0.45	2.99	4	2
1:A:497:TYR:CD1	1:A:498:VAL:N	0.45	2.85	8	1
1:A:498:VAL:O	1:A:501:GLU:CG	0.45	2.64	10	1
1:A:526:ILE:O	1:A:529:GLN:N	0.45	2.50	15	5
1:A:490:VAL:CG2	1:A:558:ILE:HG21	0.44	2.42	8	1
1:A:473:LEU:HD22	1:A:544:SER:OG	0.44	2.12	10	1
1:A:548:LEU:C	1:A:548:LEU:CD2	0.44	2.89	18	15
1:A:462:GLU:HA	1:A:465:LEU:HD12	0.44	1.88	13	4
1:A:562:VAL:CA	1:A:565:LEU:HD23	0.44	2.39	9	1
1:A:512:PHE:CE1	1:A:527:ARG:HA	0.44	2.46	12	3
1:A:512:PHE:CE1	1:A:530:VAL:HB	0.44	2.47	3	1
1:A:473:LEU:HD21	1:A:544:SER:CB	0.44	2.42	5	1
1:A:512:PHE:HE1	1:A:527:ARG:HA	0.44	1.71	9	1
1:A:476:TYR:CD1	1:A:477:ILE:N	0.44	2.86	10	3
1:A:505:ARG:CA	1:A:537:ILE:HD13	0.44	2.43	13	1
1:A:542:ASN:HA	1:A:545:LEU:HD12	0.44	1.88	13	1
1:A:491:PHE:CE2	1:A:565:LEU:HD22	0.44	2.48	10	1
1:A:487:PRO:HA	1:A:490:VAL:HG22	0.43	1.90	1	4
1:A:558:ILE:HD12	1:A:559:GLN:N	0.43	2.27	8	5
1:A:476:TYR:CD1	1:A:494:LEU:CD2	0.43	3.01	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:545:LEU:O	1:A:549:TYR:CD2	0.43	2.71	15	12
1:A:495:LYS:HE3	1:A:565:LEU:HD13	0.43	1.90	15	2
1:A:505:ARG:HG2	1:A:537:ILE:HD13	0.43	1.89	19	1
1:A:509:LEU:N	1:A:509:LEU:CD2	0.43	2.82	17	5
1:A:486:ARG:C	1:A:490:VAL:HG13	0.43	2.38	7	1
1:A:564:GLU:HA	1:A:567:GLN:HG3	0.43	1.91	16	8
1:A:476:TYR:OH	1:A:548:LEU:HB3	0.43	2.14	13	2
1:A:468:ARG:HA	1:A:471:LEU:HD23	0.43	1.91	10	1
1:A:508:THR:HG21	1:A:534:LEU:HG	0.42	1.91	7	1
1:A:501:GLU:CD	1:A:541:MET:HE2	0.42	2.40	5	1
1:A:501:GLU:HG3	1:A:541:MET:HE2	0.42	1.92	7	1
1:A:497:TYR:CD1	1:A:497:TYR:C	0.42	2.98	15	2
1:A:522:LYS:HD2	1:A:526:ILE:HD13	0.42	1.91	9	1
1:A:473:LEU:O	1:A:476:TYR:CD2	0.42	2.72	16	1
1:A:476:TYR:OH	1:A:548:LEU:CB	0.42	2.67	18	3
1:A:518:VAL:HG23	1:A:519:ASP:N	0.42	2.29	4	7
1:A:563:ASP:O	1:A:567:GLN:CG	0.42	2.68	13	3
1:A:564:GLU:HA	1:A:567:GLN:HG2	0.42	1.90	7	2
1:A:565:LEU:HG	1:A:566:LEU:N	0.42	2.29	7	2
1:A:476:TYR:CD2	1:A:494:LEU:HD22	0.42	2.49	12	1
1:A:514:HIS:CD2	1:A:517:MET:HE3	0.42	2.49	1	1
1:A:490:VAL:CG2	1:A:491:PHE:N	0.42	2.82	14	2
1:A:497:TYR:CE2	1:A:501:GLU:OE2	0.42	2.72	11	2
1:A:515:VAL:HG13	1:A:523:ALA:CB	0.42	2.44	14	2
1:A:532:THR:HA	1:A:535:ARG:CD	0.42	2.45	8	3
1:A:512:PHE:CE1	1:A:527:ARG:HG2	0.42	2.50	16	1
1:A:517:MET:CG	1:A:518:VAL:N	0.42	2.82	9	3
1:A:522:LYS:CE	1:A:526:ILE:CG2	0.42	2.98	8	2
1:A:512:PHE:CE1	1:A:527:ARG:HG3	0.42	2.50	9	1
1:A:473:LEU:HD13	1:A:476:TYR:CE2	0.42	2.50	15	1
1:A:476:TYR:CB	1:A:493:MET:HB3	0.41	2.45	14	1
1:A:515:VAL:O	1:A:519:ASP:N	0.41	2.50	20	5
1:A:505:ARG:NH1	1:A:534:LEU:HD11	0.41	2.29	14	1
1:A:497:TYR:CZ	1:A:501:GLU:OE2	0.41	2.74	6	4
1:A:490:VAL:O	1:A:494:LEU:CD2	0.41	2.68	5	1
1:A:473:LEU:HA	1:A:476:TYR:CE2	0.41	2.51	12	1
1:A:508:THR:CG2	1:A:530:VAL:CG1	0.41	2.99	12	2
1:A:473:LEU:C	1:A:473:LEU:CD1	0.41	2.93	16	1
1:A:512:PHE:CD1	1:A:512:PHE:C	0.41	2.98	18	1
1:A:508:THR:HG21	1:A:533:HIS:CB	0.41	2.45	13	2
1:A:509:LEU:CD2	1:A:534:LEU:CD2	0.41	2.99	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:497:TYR:OH	1:A:544:SER:CB	0.41	2.69	15	1
1:A:504:ASP:HB3	1:A:537:ILE:HD11	0.41	1.92	19	1
1:A:512:PHE:CZ	1:A:530:VAL:HB	0.41	2.51	1	1
1:A:497:TYR:CE1	1:A:501:GLU:OE2	0.41	2.74	13	1
1:A:492:ASN:O	1:A:495:LYS:CG	0.40	2.69	12	1
1:A:537:ILE:HG22	1:A:538:TYR:N	0.40	2.30	11	2
1:A:491:PHE:CD2	1:A:561:GLU:OE1	0.40	2.74	18	1
1:A:508:THR:HG23	1:A:530:VAL:HG13	0.40	1.93	3	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	107/110 (97%)	103±1 (96±1%)	3±1 (3±1%)	1±0 (1±0%)	16	66
All	All	2140/2200 (97%)	2064 (96%)	56 (3%)	20 (1%)	16	66

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	483	VAL	20

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	99/101 (98%)	71±2 (72±2%)	28±2 (28±2%)	1	20
All	All	1980/2020 (98%)	1427 (72%)	553 (28%)	1	20

All 67 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	491	PHE	20
1	A	493	MET	20
1	A	497	TYR	20
1	A	512	PHE	20
1	A	522	LYS	20
1	A	529	GLN	20
1	A	537	ILE	20
1	A	548	LEU	20
1	A	565	LEU	20
1	A	473	LEU	18
1	A	496	LYS	18
1	A	470	ARG	17
1	A	499	ARG	17
1	A	488	ARG	16
1	A	476	TYR	15
1	A	501	GLU	15
1	A	534	LEU	15
1	A	507	HIS	14
1	A	533	HIS	13
1	A	509	LEU	12
1	A	527	ARG	12
1	A	568	LYS	11
1	A	511	HIS	10
1	A	557	GLU	9
1	A	474	GLU	8
1	A	471	LEU	8
1	A	538	TYR	7
1	A	467	ASP	7
1	A	531	MET	6
1	A	525	GLN	6
1	A	546	SER	6
1	A	543	GLN	6
1	A	514	HIS	6
1	A	495	LYS	6
1	A	560	ASP	6
1	A	521	LYS	5
1	A	462	GLU	5
1	A	464	MET	5
1	A	503	LYS	5
1	A	486	ARG	4
1	A	510	LYS	4
1	A	556	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	505	ARG	4
1	A	528	SER	4
1	A	506	GLN	4
1	A	517	MET	3
1	A	489	HIS	3
1	A	468	ARG	3
1	A	504	ASP	3
1	A	469	ARG	3
1	A	549	TYR	3
1	A	564	GLU	3
1	A	569	GLU	3
1	A	535	ARG	2
1	A	567	GLN	2
1	A	519	ASP	2
1	A	559	GLN	2
1	A	542	ASN	2
1	A	492	ASN	2
1	A	513	GLU	2
1	A	540	ARG	1
1	A	532	THR	1
1	A	539	GLU	1
1	A	516	ARG	1
1	A	544	SER	1
1	A	490	VAL	1
1	A	466	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides 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