



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 04:01 AM UTC

PDB ID : 2RP5 / pdb_00002rp5
Title : Solution structure of the oligomerization domain in CEP-1
Authors : Ou, H.D.; Doetsch, V.
Deposited on : 2008-05-01

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

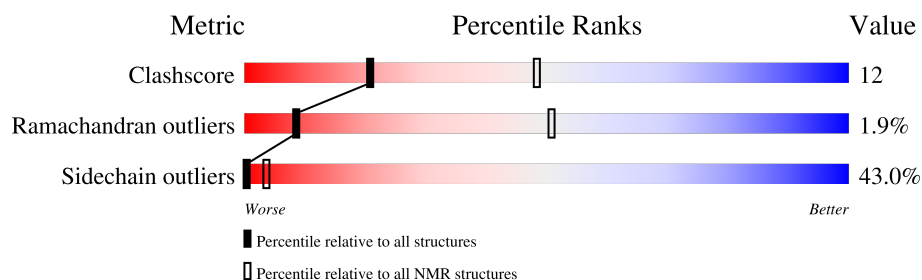
1 Overall quality at a glance

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	136	
1	B	136	

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:530-A:643, B:530-B:644 (229)	1.19	19

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3844 atoms, of which 1922 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative uncharacterized protein cep-1.

Mol	Chain	Residues	Atoms						Trace
1	A	117	Total	C	H	N	O	S	0
			1922	622	961	159	177	3	
1	B	117	Total	C	H	N	O	S	0
			1922	622	961	159	177	3	

There are 10 discrepancies between the modelled and reference sequences:

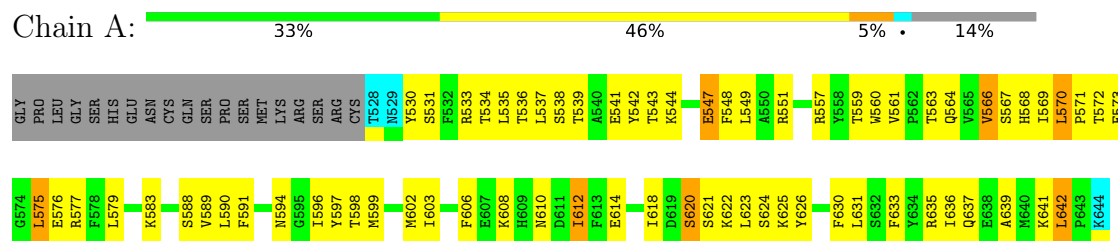
Chain	Residue	Modelled	Actual	Comment	Reference
A	509	GLY	-	expression tag	UNP Q20646
A	510	PRO	-	expression tag	UNP Q20646
A	511	LEU	-	expression tag	UNP Q20646
A	512	GLY	-	expression tag	UNP Q20646
A	513	SER	-	expression tag	UNP Q20646
B	509	GLY	-	expression tag	UNP Q20646
B	510	PRO	-	expression tag	UNP Q20646
B	511	LEU	-	expression tag	UNP Q20646
B	512	GLY	-	expression tag	UNP Q20646
B	513	SER	-	expression tag	UNP Q20646

4 Residue-property plots

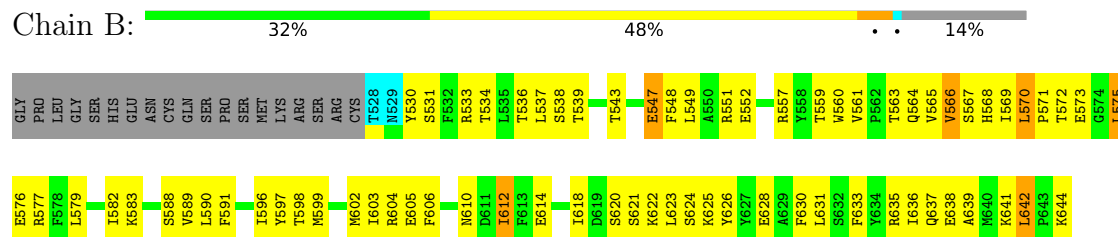
4.1 Average score per residue in the NMR ensemble

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: Putative uncharacterized protein cep-1



- Molecule 1: Putative uncharacterized protein cep-1

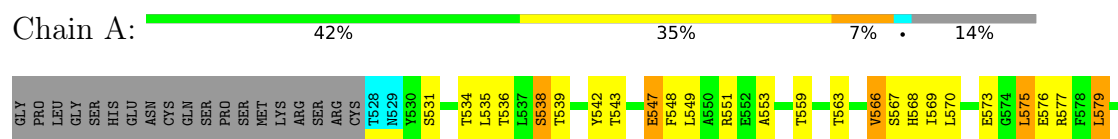


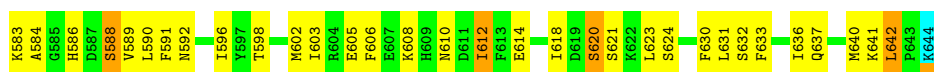
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

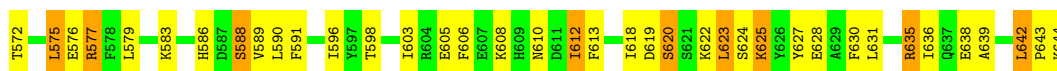
- Molecule 1: Putative uncharacterized protein cep-1





- Molecule 1: Putative uncharacterized protein cep-1

Chain B: 35% 38% 11% 14%



4.2.2 Score per residue for model 2

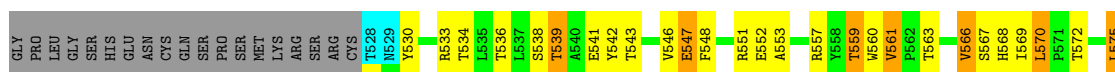
- Molecule 1: Putative uncharacterized protein cep-1

Chain A: 38% 39% 7% 14%



- Molecule 1: Putative uncharacterized protein cep-1

Chain B: 40% 37% 8% 14%



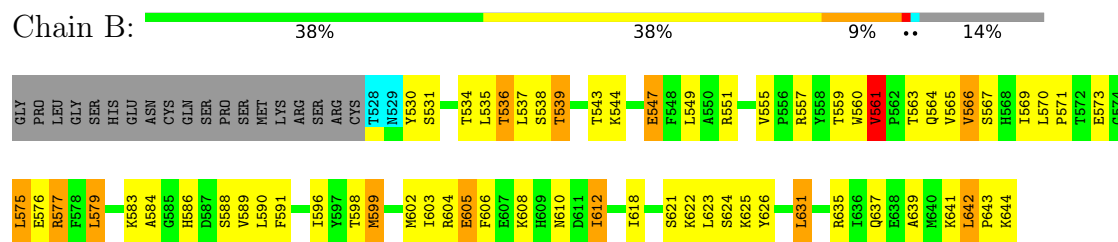
4.2.3 Score per residue for model 3

- Molecule 1: Putative uncharacterized protein cep-1

Chain A: 37% 38% 8% 14%

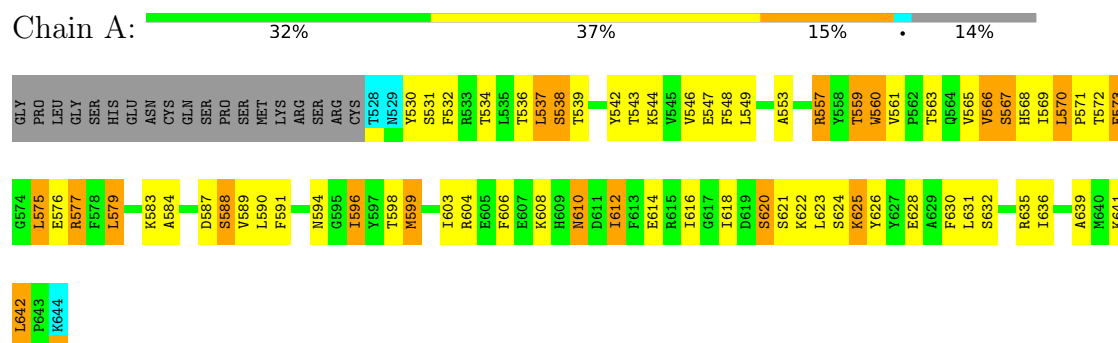


- Molecule 1: Putative uncharacterized protein cep-1

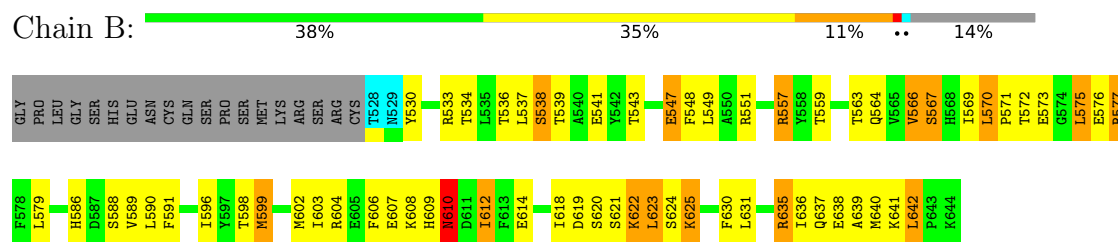


4.2.4 Score per residue for model 4

- Molecule 1: Putative uncharacterized protein cep-1

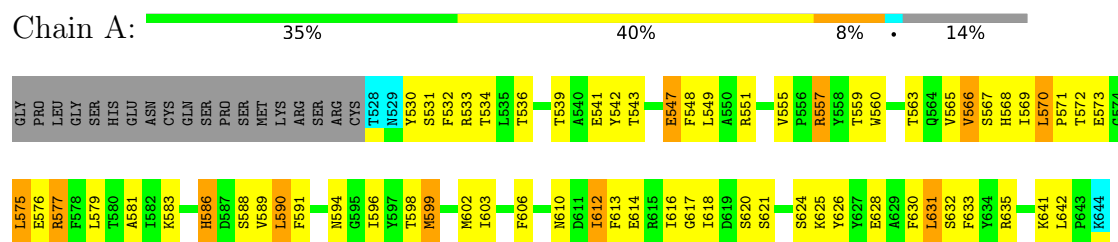


- Molecule 1: Putative uncharacterized protein cep-1



4.2.5 Score per residue for model 5

- Molecule 1: Putative uncharacterized protein cep-1



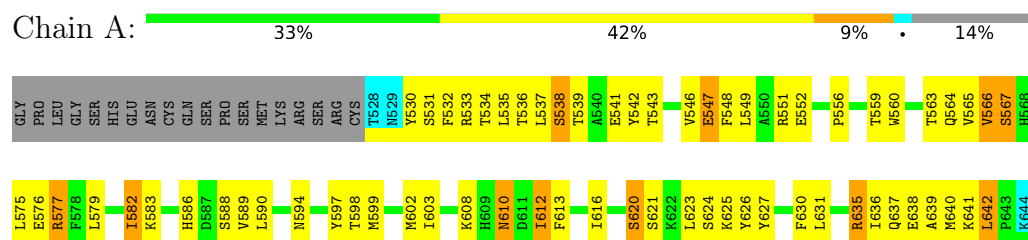
- Molecule 1: Putative uncharacterized protein cep-1



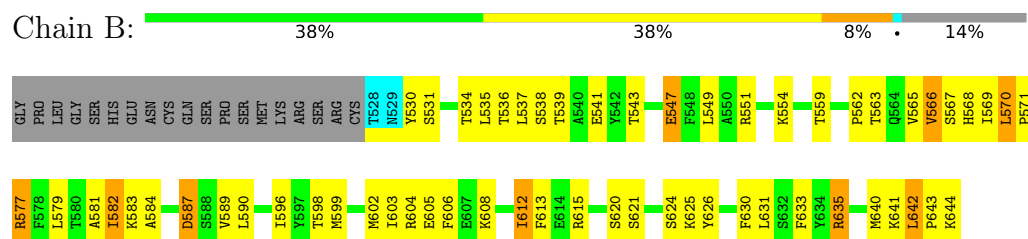


4.2.6 Score per residue for model 6

- Molecule 1: Putative uncharacterized protein cep-1

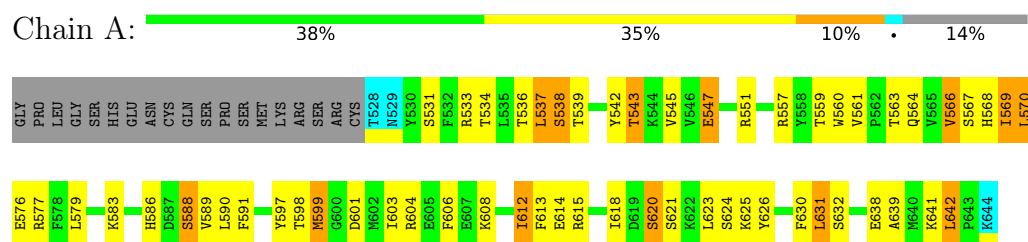


- Molecule 1: Putative uncharacterized protein cep-1

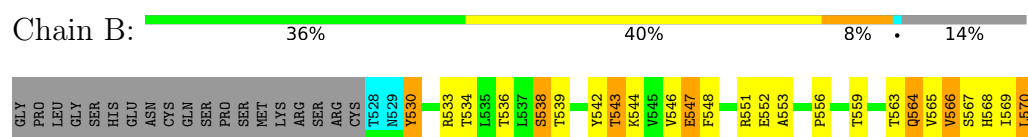


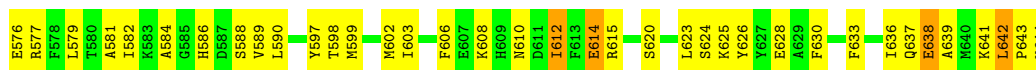
4.2.7 Score per residue for model 7

- Molecule 1: Putative uncharacterized protein cep-1



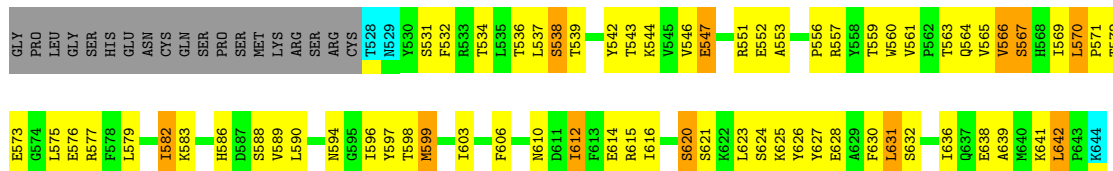
- Molecule 1: Putative uncharacterized protein cep-1



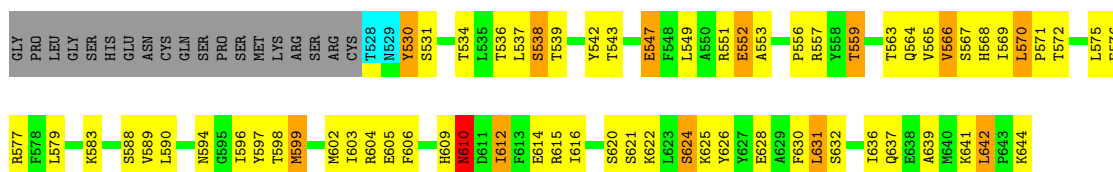


4.2.8 Score per residue for model 8

- Molecule 1: Putative uncharacterized protein cep-1

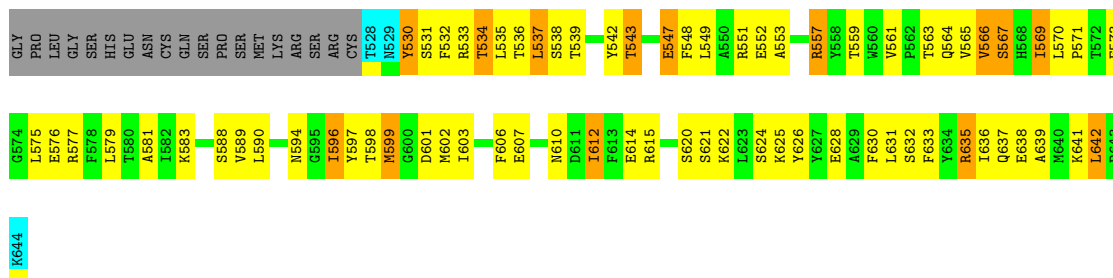


- Molecule 1: Putative uncharacterized protein cep-1



4.2.9 Score per residue for model 9

- Molecule 1: Putative uncharacterized protein cep-1



- Molecule 1: Putative uncharacterized protein cep-1

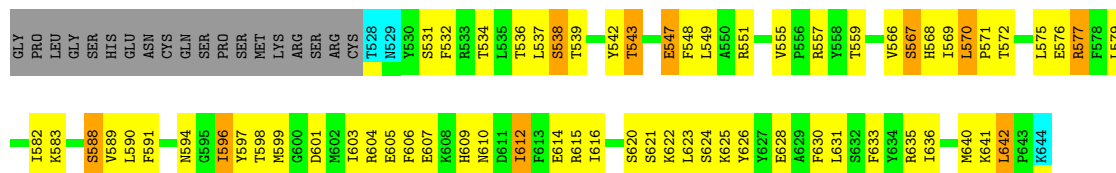




4.2.10 Score per residue for model 10

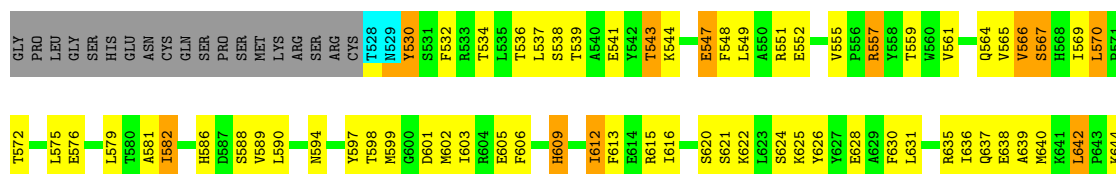
- Molecule 1: Putative uncharacterized protein cep-1

Chain A: 35% 41% 7% • 14%



- Molecule 1: Putative uncharacterized protein cep-1

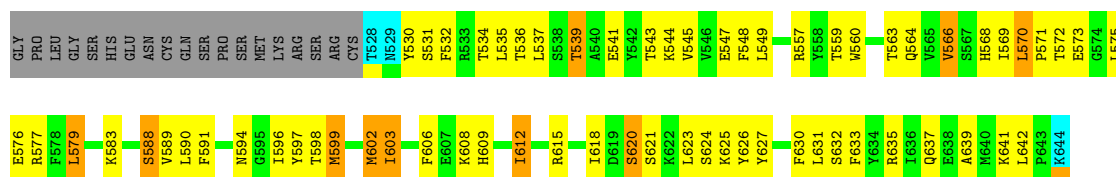
Chain B: 36% 40% 8% • 14%



4.2.11 Score per residue for model 11

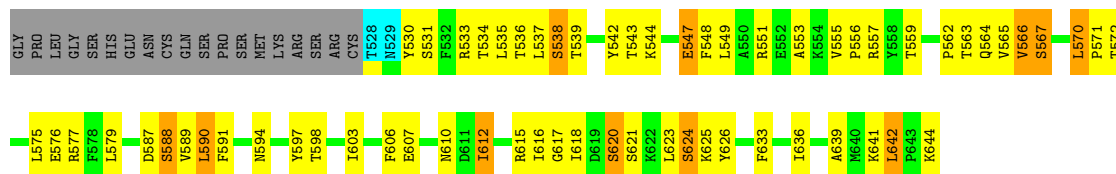
- Molecule 1: Putative uncharacterized protein cep-1

Chain A: 36% 40% 7% • 14%



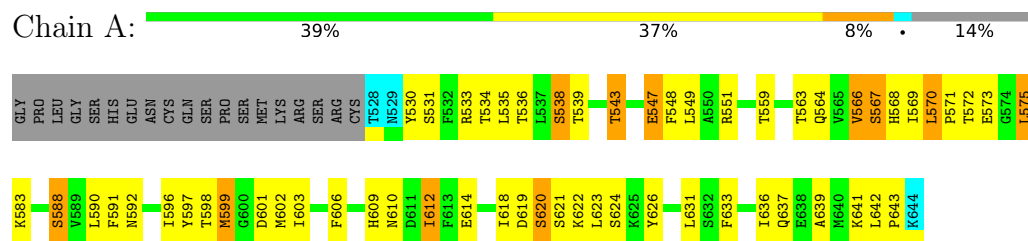
- Molecule 1: Putative uncharacterized protein cep-1

Chain B: 38% 38% 8% • 14%

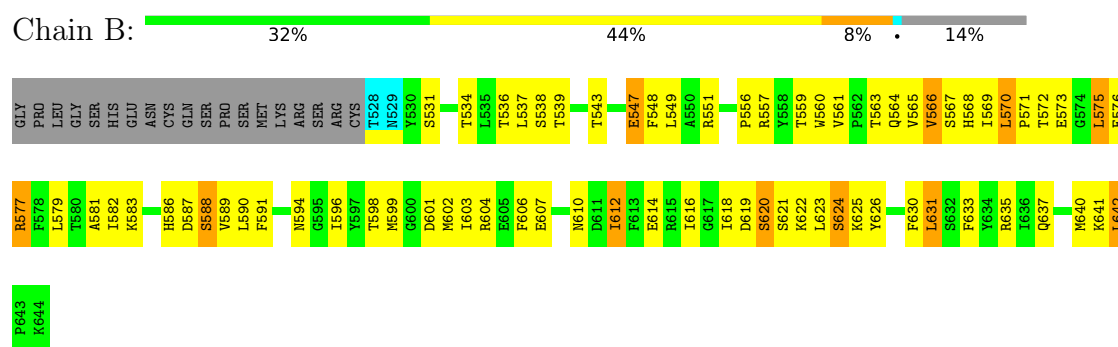


4.2.12 Score per residue for model 12

- Molecule 1: Putative uncharacterized protein cep-1

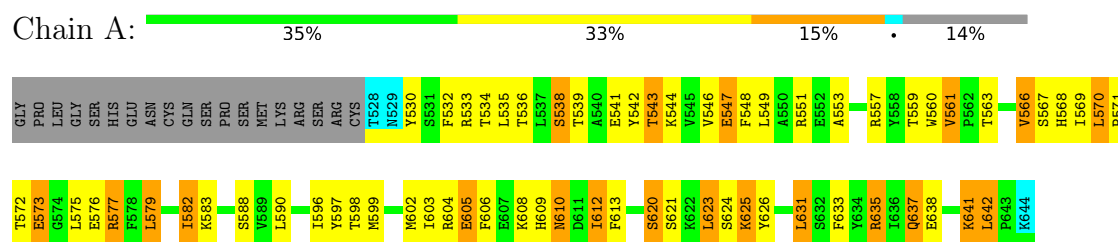


- Molecule 1: Putative uncharacterized protein cep-1

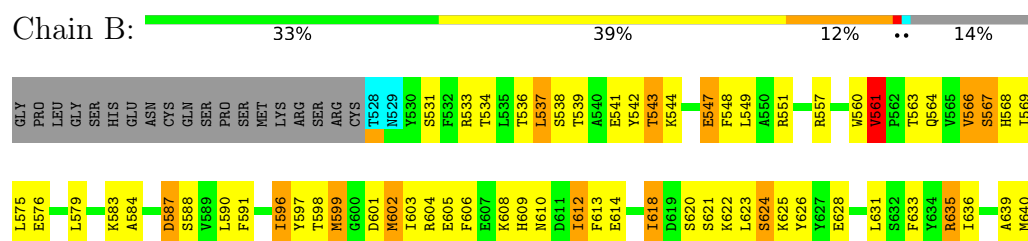


4.2.13 Score per residue for model 13

- Molecule 1: Putative uncharacterized protein cep-1

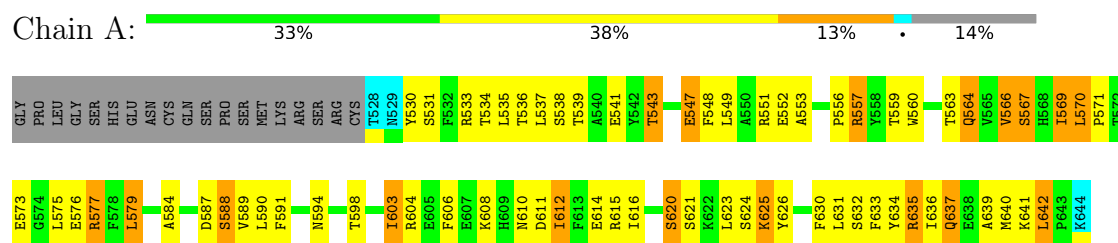


- Molecule 1: Putative uncharacterized protein cep-1

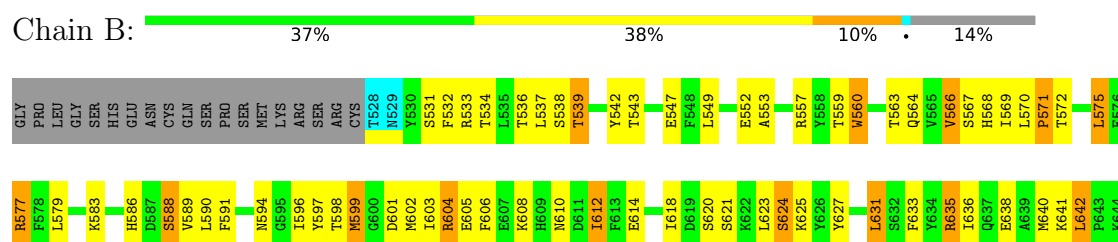


4.2.14 Score per residue for model 14

- Molecule 1: Putative uncharacterized protein cep-1

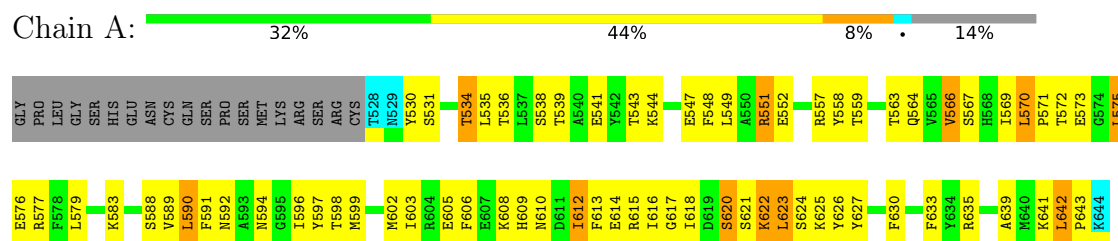


- Molecule 1: Putative uncharacterized protein cep-1

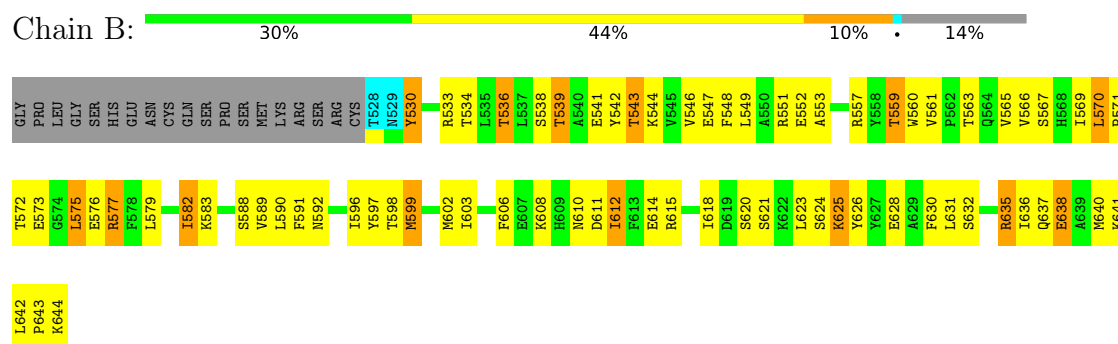


4.2.15 Score per residue for model 15

- Molecule 1: Putative uncharacterized protein cep-1

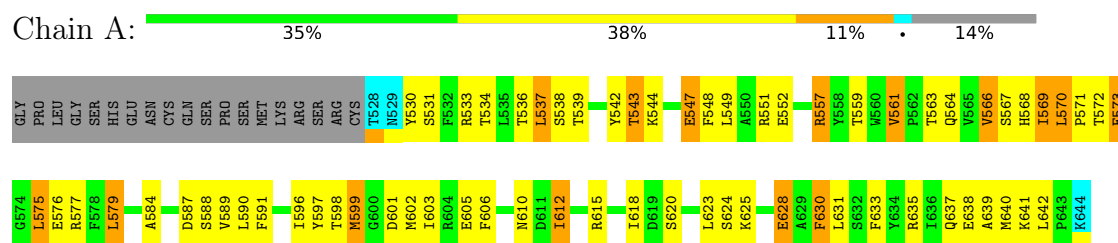


- Molecule 1: Putative uncharacterized protein cep-1

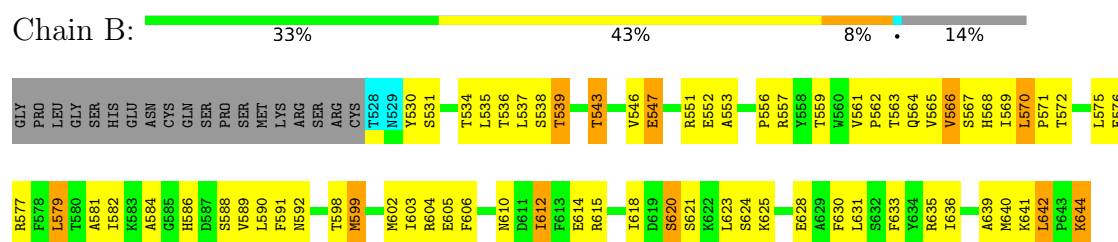


4.2.16 Score per residue for model 16

- Molecule 1: Putative uncharacterized protein cep-1

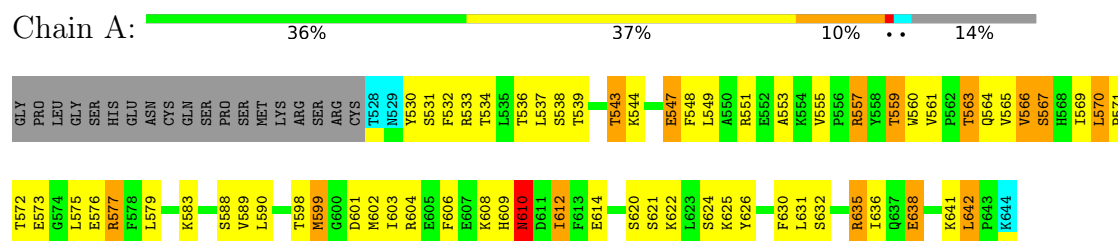


- Molecule 1: Putative uncharacterized protein cep-1

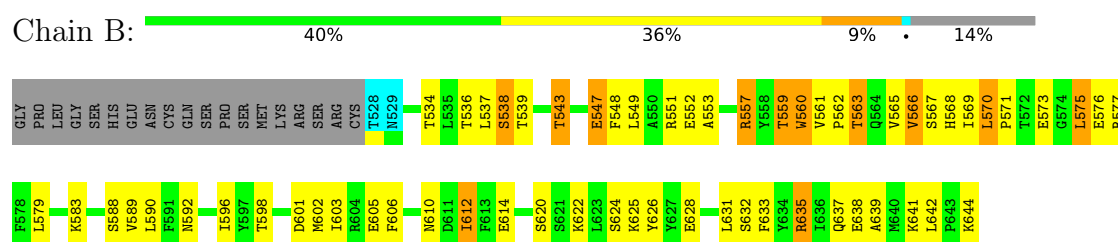


4.2.17 Score per residue for model 17

- Molecule 1: Putative uncharacterized protein cep-1

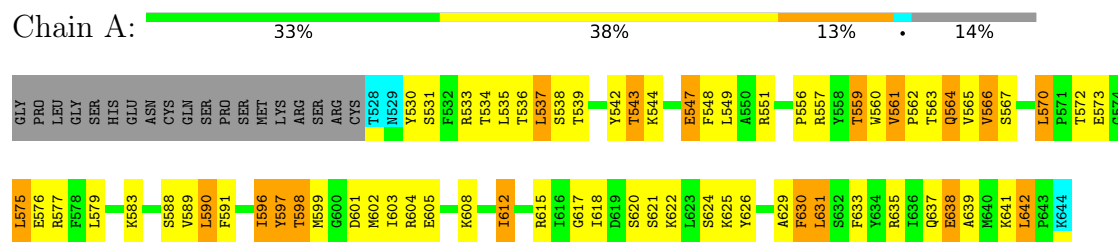


- Molecule 1: Putative uncharacterized protein cep-1

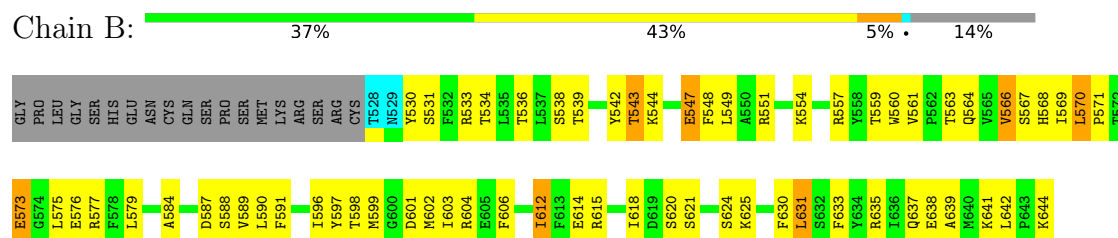


4.2.18 Score per residue for model 18

- Molecule 1: Putative uncharacterized protein cep-1

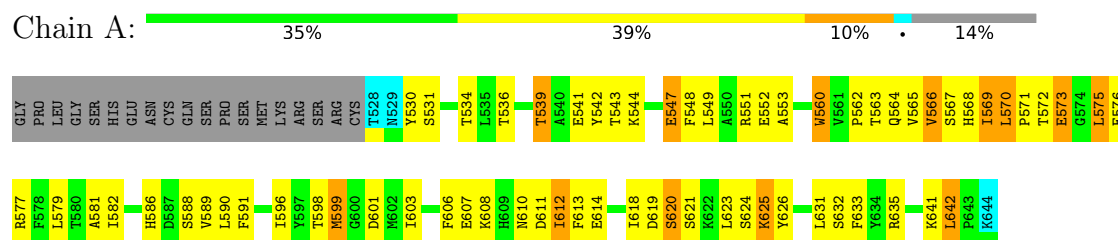


- Molecule 1: Putative uncharacterized protein cep-1

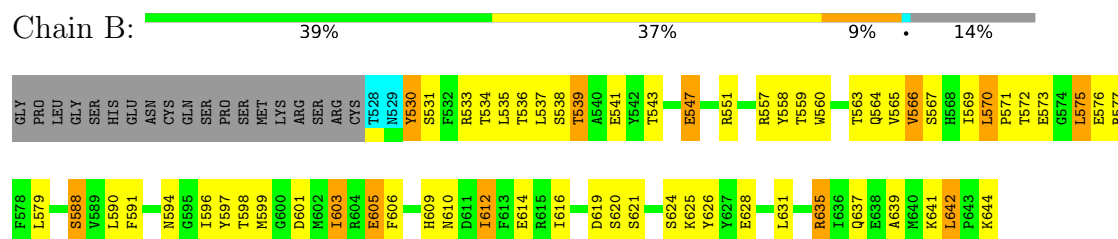


4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: Putative uncharacterized protein cep-1

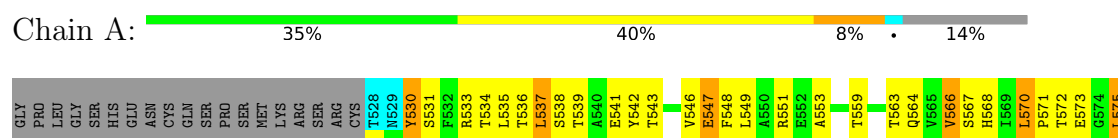


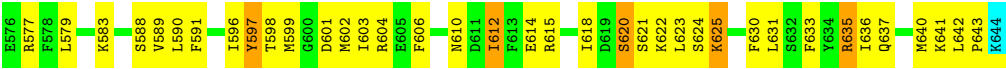
- Molecule 1: Putative uncharacterized protein cep-1



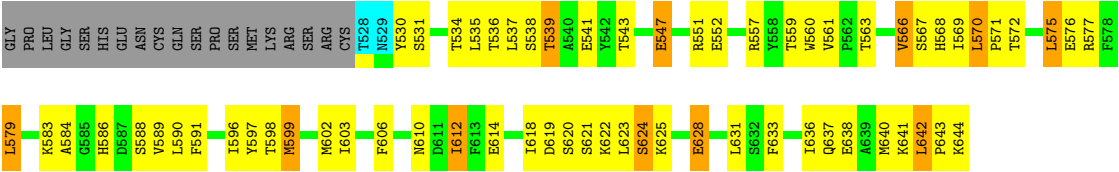
4.2.20 Score per residue for model 20

- Molecule 1: Putative uncharacterized protein cep-1





● Molecule 1: Putative uncharacterized protein cep-1



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 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
ARIA	refinement	1.2
TALOS	geometry optimization	

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	936	935	932	24±4
1	B	946	948	945	24±4
All	All	37640	37660	37540	903

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:543:THR:HG22	1:A:642:LEU:HG	0.90	1.42	10	20
1:B:543:THR:HG22	1:B:642:LEU:HG	0.84	1.49	2	19
1:B:556:PRO:HG3	1:B:564:GLN:HB2	0.84	1.49	16	1
1:A:606:PHE:HA	1:A:612:ILE:HD11	0.75	1.58	12	18
1:B:606:PHE:HA	1:B:612:ILE:HD11	0.75	1.56	4	19
1:B:552:GLU:HA	1:B:557:ARG:HH12	0.73	1.43	9	1
1:B:549:LEU:HB2	1:B:635:ARG:HG2	0.72	1.61	17	4
1:B:549:LEU:HB3	1:B:635:ARG:HD3	0.72	1.60	3	1
1:B:566:VAL:HA	1:B:569:ILE:HD12	0.68	1.64	19	11
1:B:556:PRO:HD3	1:B:564:GLN:HG3	0.68	1.66	9	1
1:A:566:VAL:HA	1:A:569:ILE:HD12	0.68	1.66	3	9
1:B:572:THR:HA	1:B:599:MET:HB2	0.67	1.66	19	1
1:B:635:ARG:HA	1:B:635:ARG:NE	0.67	2.05	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:561:VAL:HG11	1:B:628:GLU:HG2	0.67	1.64	15	2
1:B:594:ASN:HB2	1:B:616:ILE:HG22	0.66	1.66	2	7
1:A:531:SER:HB2	1:B:539:THR:HG23	0.66	1.67	15	1
1:B:547:GLU:O	1:B:551:ARG:HG2	0.65	1.90	20	17
1:B:569:ILE:HG12	1:B:577:ARG:HD2	0.65	1.69	12	6
1:A:620:SER:HA	1:A:623:LEU:HB2	0.65	1.69	7	12
1:A:572:THR:HA	1:A:599:MET:HB2	0.64	1.70	12	4
1:A:538:SER:HB3	1:B:530:TYR:CE2	0.64	2.28	10	1
1:B:562:PRO:HG2	1:B:582:ILE:HA	0.64	1.70	16	1
1:A:530:TYR:HB2	1:B:539:THR:OG1	0.64	1.93	19	6
1:A:612:ILE:HD13	1:A:630:PHE:HE2	0.63	1.52	2	11
1:A:547:GLU:O	1:A:551:ARG:HG2	0.63	1.94	3	18
1:A:639:ALA:HA	1:A:642:LEU:HB2	0.63	1.70	15	12
1:A:579:LEU:HD12	1:A:584:ALA:HB3	0.63	1.70	4	5
1:B:639:ALA:HA	1:B:642:LEU:HB2	0.62	1.70	7	13
1:B:570:LEU:HD12	1:B:571:PRO:HD2	0.62	1.70	14	1
1:A:571:PRO:HA	1:A:599:MET:SD	0.62	2.34	11	1
1:A:538:SER:HB3	1:B:530:TYR:CE1	0.62	2.29	7	1
1:A:534:THR:HG23	1:B:536:THR:HG23	0.61	1.72	9	3
1:B:556:PRO:HD3	1:B:564:GLN:HB2	0.61	1.72	8	1
1:B:594:ASN:HD22	1:B:596:ILE:HD11	0.61	1.54	19	2
1:B:547:GLU:HG3	1:B:644:LYS:HE3	0.61	1.72	8	1
1:A:582:ILE:HD12	1:A:626:TYR:HD1	0.61	1.56	13	2
1:B:572:THR:HA	1:B:599:MET:SD	0.60	2.36	7	2
1:B:619:ASP:HB3	1:B:622:LYS:HD2	0.60	1.71	12	1
1:A:631:LEU:O	1:A:635:ARG:HD2	0.60	1.95	13	1
1:A:570:LEU:HD13	1:A:571:PRO:HD2	0.60	1.70	19	14
1:B:567:SER:HB3	1:B:636:ILE:HD13	0.60	1.72	10	6
1:B:571:PRO:O	1:B:599:MET:HB2	0.60	1.96	14	9
1:B:571:PRO:HA	1:B:599:MET:HG3	0.59	1.73	20	1
1:A:553:ALA:HB1	1:A:636:ILE:HD11	0.59	1.73	14	3
1:A:570:LEU:HD12	1:A:571:PRO:HD2	0.59	1.74	3	1
1:B:620:SER:HA	1:B:623:LEU:HB2	0.59	1.73	20	6
1:A:605:GLU:HB3	1:A:612:ILE:HG12	0.59	1.74	1	1
1:A:571:PRO:O	1:A:599:MET:HB2	0.59	1.98	9	7
1:B:549:LEU:HD13	1:B:635:ARG:HD2	0.58	1.75	1	1
1:B:612:ILE:HD13	1:B:630:PHE:HE2	0.58	1.59	5	9
1:B:530:TYR:CD1	1:B:624:SER:HA	0.58	2.33	8	1
1:A:549:LEU:HB2	1:A:635:ARG:HG2	0.58	1.74	17	5
1:B:565:VAL:HG13	1:B:581:ALA:HB1	0.58	1.73	6	7
1:B:579:LEU:HD12	1:B:584:ALA:HB3	0.58	1.76	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:543:THR:HA	1:B:642:LEU:HD21	0.58	1.75	9	7
1:A:594:ASN:HB2	1:A:616:ILE:HG22	0.58	1.76	3	9
1:A:584:ALA:HB1	1:A:587:ASP:HB2	0.58	1.73	16	3
1:B:605:GLU:HB3	1:B:612:ILE:HG12	0.58	1.76	19	1
1:A:569:ILE:HG12	1:A:577:ARG:HD2	0.57	1.76	17	7
1:B:566:VAL:HG13	1:B:633:PHE:HD1	0.57	1.60	5	10
1:B:532:PHE:HZ	1:B:631:LEU:HD21	0.57	1.59	1	2
1:A:622:LYS:HE2	1:A:626:TYR:OH	0.57	2.00	9	4
1:A:565:VAL:HG13	1:A:581:ALA:HB1	0.56	1.77	5	3
1:A:570:LEU:O	1:A:573:GLU:HG3	0.56	2.00	4	3
1:A:567:SER:HB3	1:A:636:ILE:HD13	0.56	1.76	10	9
1:A:530:TYR:CD1	1:B:538:SER:HB2	0.56	2.35	9	1
1:A:622:LYS:HB3	1:A:626:TYR:CE1	0.55	2.36	9	6
1:A:622:LYS:HB3	1:A:625:LYS:HD3	0.55	1.77	20	1
1:A:553:ALA:HB2	1:A:632:SER:HB3	0.55	1.78	4	3
1:B:530:TYR:OH	1:B:611:ASP:HA	0.55	2.00	15	1
1:A:543:THR:HA	1:A:642:LEU:HD21	0.55	1.78	4	6
1:B:605:GLU:O	1:B:609:HIS:HB2	0.55	2.02	10	3
1:B:603:ILE:HG12	1:B:637:GLN:HG2	0.55	1.79	19	1
1:A:582:ILE:HD12	1:A:626:TYR:CD1	0.55	2.36	6	3
1:A:566:VAL:HG13	1:A:633:PHE:HD2	0.54	1.61	15	3
1:A:566:VAL:HG13	1:A:633:PHE:HD1	0.54	1.62	3	11
1:B:622:LYS:HB3	1:B:625:LYS:HE2	0.54	1.78	13	1
1:B:562:PRO:HB2	1:B:565:VAL:HG12	0.54	1.79	6	3
1:A:561:VAL:HG21	1:A:629:ALA:HB2	0.54	1.78	18	1
1:B:575:LEU:HD21	1:B:596:ILE:HG22	0.54	1.80	6	1
1:B:530:TYR:CE2	1:B:627:TYR:HB3	0.54	2.38	1	1
1:A:539:THR:OG1	1:B:530:TYR:HB2	0.54	2.02	2	3
1:B:552:GLU:HA	1:B:557:ARG:NH1	0.54	2.16	9	1
1:A:619:ASP:HB3	1:A:622:LYS:HD3	0.54	1.80	3	1
1:A:570:LEU:O	1:A:573:GLU:HG2	0.54	2.02	13	2
1:A:532:PHE:CZ	1:A:631:LEU:HD21	0.53	2.37	13	3
1:B:543:THR:HB	1:B:644:LYS:HG3	0.53	1.81	13	2
1:A:538:SER:HB2	1:B:530:TYR:CE1	0.53	2.39	20	1
1:B:560:TRP:CZ3	1:B:625:LYS:HA	0.53	2.38	1	1
1:B:553:ALA:HB1	1:B:636:ILE:HD11	0.53	1.79	8	7
1:B:530:TYR:CD2	1:B:627:TYR:HB3	0.53	2.39	1	1
1:B:532:PHE:CZ	1:B:631:LEU:HD21	0.53	2.39	1	3
1:A:542:TYR:CE1	1:B:535:LEU:HD13	0.52	2.39	3	8
1:B:566:VAL:HG13	1:B:633:PHE:HD2	0.52	1.63	20	2
1:A:535:LEU:HD13	1:B:542:TYR:HE1	0.52	1.64	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:570:LEU:HD13	1:B:571:PRO:HD2	0.52	1.81	9	12
1:A:538:SER:O	1:A:542:TYR:HB2	0.52	2.05	10	4
1:B:556:PRO:HD3	1:B:564:GLN:HG2	0.52	1.80	11	1
1:B:622:LYS:HB3	1:B:625:LYS:HD3	0.52	1.80	4	1
1:B:584:ALA:HB1	1:B:587:ASP:HB2	0.52	1.82	18	1
1:A:631:LEU:O	1:A:635:ARG:HD3	0.51	2.04	3	3
1:B:613:PHE:CE2	1:B:626:TYR:HB3	0.51	2.40	10	4
1:A:532:PHE:HE1	1:A:627:TYR:HB3	0.51	1.66	8	1
1:A:594:ASN:HD22	1:A:596:ILE:HD11	0.51	1.65	15	2
1:B:588:SER:HA	1:B:591:PHE:HD1	0.51	1.66	11	5
1:B:638:GLU:HA	1:B:638:GLU:OE1	0.51	2.06	2	1
1:A:605:GLU:O	1:A:609:HIS:HB2	0.51	2.05	10	4
1:A:556:PRO:HD3	1:A:564:GLN:HB2	0.51	1.81	18	2
1:B:631:LEU:O	1:B:635:ARG:HG2	0.51	2.05	19	2
1:B:560:TRP:HH2	1:B:624:SER:HB2	0.51	1.65	20	2
1:A:575:LEU:CD2	1:A:596:ILE:HG22	0.50	2.36	3	9
1:B:614:GLU:HG3	1:B:623:LEU:HD11	0.50	1.81	13	1
1:A:545:VAL:HG22	1:B:548:PHE:HE2	0.50	1.66	11	2
1:B:631:LEU:HB3	1:B:635:ARG:NH1	0.50	2.20	10	1
1:B:548:PHE:CD2	1:B:549:LEU:HG	0.50	2.41	4	10
1:B:570:LEU:C	1:B:572:THR:H	0.50	2.14	7	17
1:A:556:PRO:HG3	1:A:564:GLN:HB2	0.50	1.82	8	1
1:A:631:LEU:HG	1:B:538:SER:OG	0.50	2.06	1	4
1:B:565:VAL:O	1:B:569:ILE:HG13	0.50	2.07	9	8
1:B:588:SER:HA	1:B:591:PHE:CD1	0.50	2.42	11	6
1:A:570:LEU:C	1:A:572:THR:H	0.50	2.14	4	14
1:B:538:SER:O	1:B:542:TYR:HB2	0.50	2.07	8	2
1:B:575:LEU:HD22	1:B:602:MET:SD	0.50	2.47	20	1
1:B:549:LEU:CB	1:B:635:ARG:HG2	0.50	2.35	17	1
1:B:560:TRP:CE3	1:B:561:VAL:HG23	0.50	2.42	17	1
1:A:569:ILE:HG21	1:A:577:ARG:HB3	0.49	1.84	14	1
1:A:638:GLU:OE1	1:A:638:GLU:HA	0.49	2.06	17	2
1:B:584:ALA:HB1	1:B:587:ASP:OD2	0.49	2.07	13	1
1:A:548:PHE:CD2	1:A:549:LEU:HG	0.49	2.41	11	18
1:A:635:ARG:HH11	1:A:635:ARG:HG3	0.49	1.66	13	1
1:B:571:PRO:HA	1:B:599:MET:SD	0.49	2.48	13	1
1:B:553:ALA:HB2	1:B:632:SER:HB3	0.49	1.84	17	2
1:A:612:ILE:HD13	1:A:630:PHE:CE2	0.49	2.40	2	1
1:A:562:PRO:HB2	1:A:565:VAL:HG12	0.49	1.85	18	1
1:B:622:LYS:HE2	1:B:626:TYR:OH	0.49	2.08	8	3
1:A:538:SER:HB3	1:B:530:TYR:HE2	0.49	1.65	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:553:ALA:O	1:A:563:THR:HB	0.49	2.07	17	2
1:A:565:VAL:O	1:A:569:ILE:HG13	0.49	2.08	6	6
1:B:635:ARG:NE	1:B:635:ARG:CA	0.48	2.76	16	1
1:B:591:PHE:CE1	1:B:618:ILE:HD11	0.48	2.44	11	11
1:B:560:TRP:CH2	1:B:624:SER:HB2	0.48	2.43	14	2
1:A:566:VAL:HA	1:A:569:ILE:CD1	0.48	2.38	2	12
1:A:609:HIS:O	1:A:610:ASN:HB2	0.48	2.07	12	1
1:A:591:PHE:CE1	1:A:618:ILE:HD11	0.48	2.44	16	11
1:A:625:LYS:HD3	1:A:626:TYR:CE1	0.48	2.43	14	1
1:A:549:LEU:HD13	1:A:635:ARG:HD3	0.48	1.85	15	1
1:B:606:PHE:HA	1:B:612:ILE:CD1	0.48	2.38	5	2
1:B:636:ILE:O	1:B:640:MET:HG3	0.48	2.08	13	3
1:B:549:LEU:HB3	1:B:635:ARG:NE	0.48	2.23	18	1
1:B:609:HIS:O	1:B:610:ASN:HB3	0.48	2.07	4	2
1:A:552:GLU:HA	1:A:557:ARG:NH1	0.48	2.23	16	1
1:B:575:LEU:CD2	1:B:596:ILE:HG22	0.48	2.39	2	11
1:A:631:LEU:O	1:A:635:ARG:HG2	0.48	2.09	10	2
1:B:599:MET:O	1:B:599:MET:HG2	0.48	2.09	5	1
1:B:584:ALA:HB1	1:B:587:ASP:OD1	0.48	2.09	13	2
1:A:613:PHE:CD2	1:A:626:TYR:HB3	0.48	2.44	7	1
1:A:569:ILE:HG23	1:A:577:ARG:HH11	0.48	1.69	13	1
1:B:530:TYR:OH	1:B:628:GLU:HA	0.47	2.09	1	1
1:A:537:LEU:HD12	1:A:542:TYR:HA	0.47	1.84	16	6
1:B:549:LEU:HA	1:B:552:GLU:HG3	0.47	1.86	8	1
1:A:535:LEU:HD13	1:B:542:TYR:CE1	0.47	2.43	14	3
1:B:530:TYR:OH	1:B:624:SER:HA	0.47	2.09	11	1
1:A:571:PRO:HG3	1:A:637:GLN:HG3	0.47	1.86	14	1
1:A:553:ALA:CB	1:A:636:ILE:HD11	0.47	2.39	4	3
1:B:566:VAL:HA	1:B:569:ILE:CD1	0.47	2.39	18	11
1:B:584:ALA:HB1	1:B:587:ASP:CG	0.47	2.34	13	1
1:B:555:VAL:HB	1:B:557:ARG:NH1	0.47	2.24	11	1
1:B:639:ALA:HA	1:B:642:LEU:HD22	0.47	1.86	19	2
1:A:565:VAL:CG1	1:A:581:ALA:HB1	0.47	2.40	5	1
1:B:532:PHE:HE1	1:B:631:LEU:HD21	0.47	1.70	10	1
1:A:571:PRO:HB3	1:A:633:PHE:HE1	0.47	1.70	11	2
1:B:591:PHE:HA	1:B:596:ILE:HD12	0.47	1.87	13	1
1:B:560:TRP:CH2	1:B:625:LYS:HB2	0.47	2.44	15	1
1:A:588:SER:HA	1:A:591:PHE:CD1	0.47	2.45	12	7
1:A:560:TRP:CZ3	1:A:625:LYS:HA	0.47	2.45	4	2
1:A:571:PRO:HB3	1:A:633:PHE:HE2	0.47	1.70	13	1
1:A:532:PHE:HZ	1:A:627:TYR:HB3	0.46	1.69	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:620:SER:HA	1:A:623:LEU:CB	0.46	2.40	15	1
1:A:549:LEU:HB3	1:A:635:ARG:NE	0.46	2.25	3	1
1:B:622:LYS:HB3	1:B:626:TYR:CE1	0.46	2.45	17	3
1:B:582:ILE:HD12	1:B:626:TYR:HD1	0.46	1.71	10	1
1:B:613:PHE:O	1:B:618:ILE:HB	0.46	2.10	13	1
1:A:552:GLU:HA	1:A:557:ARG:HH12	0.46	1.70	16	1
1:A:560:TRP:O	1:A:561:VAL:HB	0.46	2.10	3	1
1:A:613:PHE:CE2	1:A:626:TYR:HB3	0.46	2.46	13	3
1:A:532:PHE:CE1	1:B:538:SER:HB3	0.46	2.46	11	2
1:A:579:LEU:HD12	1:A:584:ALA:CB	0.46	2.40	4	5
1:B:605:GLU:HA	1:B:605:GLU:OE1	0.46	2.11	3	1
1:B:532:PHE:CE1	1:B:631:LEU:HD21	0.46	2.45	10	1
1:B:565:VAL:CG1	1:B:581:ALA:HB1	0.46	2.40	9	3
1:A:556:PRO:HG3	1:A:564:GLN:HB3	0.46	1.87	14	1
1:B:560:TRP:CZ3	1:B:625:LYS:HB2	0.45	2.45	15	2
1:B:604:ARG:NH2	1:B:605:GLU:HG2	0.45	2.26	8	1
1:A:609:HIS:O	1:A:610:ASN:HB3	0.45	2.12	10	1
1:A:613:PHE:HB2	1:A:627:TYR:CZ	0.45	2.46	15	2
1:B:614:GLU:HG2	1:B:623:LEU:HD11	0.45	1.88	7	1
1:B:556:PRO:HD3	1:B:564:GLN:CG	0.45	2.40	11	1
1:B:560:TRP:CZ3	1:B:561:VAL:HG23	0.45	2.46	13	1
1:A:612:ILE:O	1:A:615:ARG:HG2	0.45	2.11	18	1
1:A:588:SER:HA	1:A:591:PHE:HD1	0.45	1.72	12	1
1:B:638:GLU:OE1	1:B:638:GLU:HA	0.45	2.10	15	1
1:B:582:ILE:HD12	1:B:626:TYR:CD1	0.45	2.47	6	4
1:A:633:PHE:HA	1:A:636:ILE:HD12	0.45	1.86	14	2
1:B:571:PRO:HB3	1:B:633:PHE:HE1	0.45	1.71	11	1
1:B:619:ASP:OD2	1:B:622:LYS:HG3	0.45	2.12	1	1
1:A:542:TYR:O	1:A:546:VAL:HG23	0.45	2.12	6	5
1:B:560:TRP:CE3	1:B:561:VAL:HG13	0.45	2.47	1	1
1:A:532:PHE:HE2	1:A:631:LEU:HD21	0.45	1.71	10	2
1:A:544:LYS:HD2	1:B:548:PHE:HZ	0.45	1.72	2	1
1:A:631:LEU:HD12	1:A:635:ARG:NH2	0.45	2.27	6	1
1:A:635:ARG:HG3	1:A:635:ARG:NH1	0.45	2.27	13	1
1:A:575:LEU:HD11	1:A:597:TYR:HA	0.45	1.88	18	2
1:A:572:THR:HA	1:A:599:MET:CG	0.45	2.42	19	1
1:A:532:PHE:HE1	1:B:538:SER:HB3	0.44	1.72	11	1
1:A:530:TYR:HE1	1:B:538:SER:HB3	0.44	1.72	4	1
1:B:549:LEU:HD13	1:B:635:ARG:NH1	0.44	2.27	4	1
1:B:570:LEU:O	1:B:573:GLU:HG2	0.44	2.12	6	1
1:B:602:MET:HG2	1:B:603:ILE:N	0.44	2.27	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:559:THR:O	1:B:560:TRP:HB3	0.44	2.12	15	1
1:B:631:LEU:HD12	1:B:635:ARG:NH2	0.44	2.27	15	3
1:A:538:SER:OG	1:B:631:LEU:HG	0.44	2.13	12	4
1:A:606:PHE:HA	1:A:609:HIS:O	0.44	2.12	11	1
1:A:575:LEU:HD21	1:A:596:ILE:HG22	0.44	1.90	1	3
1:B:553:ALA:CB	1:B:636:ILE:HD11	0.44	2.42	15	2
1:A:532:PHE:CE2	1:A:631:LEU:HD21	0.44	2.46	13	2
1:A:544:LYS:HD2	1:B:548:PHE:CZ	0.44	2.48	2	1
1:B:579:LEU:HD12	1:B:584:ALA:CB	0.44	2.41	5	1
1:A:599:MET:O	1:A:599:MET:HG3	0.44	2.11	12	1
1:A:636:ILE:O	1:A:640:MET:HG3	0.44	2.12	14	1
1:B:569:ILE:HG12	1:B:577:ARG:HB3	0.44	1.88	14	1
1:A:637:GLN:O	1:A:641:LYS:HG2	0.43	2.13	13	1
1:B:606:PHE:HB2	1:B:630:PHE:CZ	0.43	2.48	10	1
1:B:555:VAL:HB	1:B:557:ARG:HH11	0.43	1.73	11	1
1:A:560:TRP:CD1	1:A:560:TRP:H	0.43	2.30	7	2
1:A:599:MET:O	1:A:599:MET:HG2	0.43	2.14	17	1
1:A:575:LEU:HD22	1:A:596:ILE:HG22	0.43	1.90	4	2
1:B:631:LEU:O	1:B:635:ARG:HD3	0.43	2.13	18	1
1:A:556:PRO:HD3	1:A:564:GLN:HB3	0.43	1.90	2	1
1:A:543:THR:HG22	1:A:642:LEU:CG	0.43	2.33	9	2
1:B:543:THR:HG22	1:B:642:LEU:CG	0.43	2.37	7	1
1:B:553:ALA:HA	1:B:563:THR:HG22	0.43	1.90	17	1
1:A:530:TYR:CE1	1:B:538:SER:HB3	0.43	2.49	4	1
1:A:571:PRO:HB3	1:A:633:PHE:CE1	0.43	2.49	15	1
1:A:572:THR:HA	1:A:599:MET:HG3	0.42	1.91	4	2
1:A:562:PRO:HG2	1:A:582:ILE:HA	0.42	1.89	19	1
1:A:579:LEU:O	1:A:582:ILE:HG12	0.42	2.14	13	1
1:B:613:PHE:HB2	1:B:627:TYR:CE2	0.42	2.48	1	1
1:A:585:GLY:O	1:A:586:HIS:HB3	0.42	2.13	2	1
1:B:591:PHE:HB3	1:B:596:ILE:HB	0.42	1.91	2	1
1:A:591:PHE:HB3	1:A:596:ILE:O	0.42	2.15	5	1
1:A:552:GLU:HA	1:A:557:ARG:HD2	0.42	1.90	14	1
1:A:606:PHE:HA	1:A:612:ILE:CD1	0.42	2.43	16	2
1:B:546:VAL:HG11	1:B:638:GLU:HB3	0.42	1.90	7	1
1:A:639:ALA:HA	1:A:642:LEU:HD22	0.42	1.91	8	1
1:A:572:THR:HA	1:A:599:MET:CB	0.42	2.44	12	2
1:B:546:VAL:HG22	1:B:635:ARG:NH1	0.42	2.29	16	1
1:B:619:ASP:HB3	1:B:622:LYS:HE2	0.42	1.91	20	1
1:B:633:PHE:HA	1:B:636:ILE:HD12	0.42	1.92	9	1
1:A:561:VAL:HG11	1:A:628:GLU:HG2	0.42	1.91	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:570:LEU:O	1:B:573:GLU:HG3	0.42	2.13	18	1
1:B:542:TYR:O	1:B:546:VAL:HG23	0.42	2.14	15	3
1:B:612:ILE:HD12	1:B:612:ILE:H	0.42	1.75	5	1
1:B:637:GLN:HA	1:B:640:MET:HE3	0.42	1.91	15	1
1:B:571:PRO:HG3	1:B:637:GLN:OE1	0.42	2.15	17	1
1:B:556:PRO:HB3	1:B:564:GLN:HG2	0.42	1.92	7	1
1:A:596:ILE:C	1:A:598:THR:H	0.42	2.22	18	1
1:A:532:PHE:HB2	1:A:610:ASN:ND2	0.41	2.30	6	1
1:A:602:MET:HG2	1:A:603:ILE:N	0.41	2.30	11	1
1:A:591:PHE:HB3	1:A:596:ILE:HB	0.41	1.91	4	3
1:B:562:PRO:HB2	1:B:565:VAL:CG1	0.41	2.45	11	1
1:B:618:ILE:HG23	1:B:626:TYR:CE2	0.41	2.51	13	1
1:B:601:ASP:OD1	1:B:604:ARG:HD3	0.41	2.15	14	1
1:A:549:LEU:HD21	1:B:544:LYS:HD3	0.41	1.91	5	1
1:A:590:LEU:HG	1:A:617:GLY:C	0.41	2.40	15	3
1:B:626:TYR:N	1:B:626:TYR:CD1	0.41	2.89	15	1
1:A:572:THR:CA	1:A:599:MET:HB2	0.41	2.46	19	1
1:B:594:ASN:HB3	1:B:596:ILE:HG13	0.41	1.91	9	1
1:B:560:TRP:O	1:B:561:VAL:HB	0.41	2.16	3	1
1:B:582:ILE:HD11	1:B:626:TYR:CE1	0.41	2.51	12	1
1:B:584:ALA:HB2	1:B:626:TYR:HE1	0.41	1.74	7	1
1:B:537:LEU:HD12	1:B:542:TYR:HA	0.41	1.92	13	1
1:A:641:LYS:N	1:A:641:LYS:HD3	0.41	2.31	8	1
1:B:537:LEU:HB3	1:B:542:TYR:HD1	0.41	1.75	9	1
1:B:561:VAL:HG21	1:B:628:GLU:HB3	0.41	1.92	17	1
1:A:599:MET:C	1:A:601:ASP:H	0.41	2.24	19	1
1:A:613:PHE:HB3	1:A:618:ILE:HG13	0.41	1.93	19	1
1:A:560:TRP:CZ3	1:A:625:LYS:HB2	0.41	2.51	13	1
1:B:590:LEU:O	1:B:616:ILE:HB	0.40	2.16	2	1
1:B:599:MET:HG3	1:B:602:MET:HE1	0.40	1.93	13	1
1:A:541:GLU:O	1:A:545:VAL:HG23	0.40	2.16	2	1
1:B:576:GLU:HG3	1:B:577:ARG:N	0.40	2.32	4	1
1:A:538:SER:CB	1:B:530:TYR:CE2	0.40	3.04	1	1
1:A:631:LEU:HD22	1:A:631:LEU:HA	0.40	1.79	7	1
1:A:603:ILE:HA	1:A:634:TYR:OH	0.40	2.16	14	1
1:B:559:THR:HB	1:B:560:TRP:CD1	0.40	2.51	2	1
1:B:609:HIS:HB3	1:B:610:ASN:H	0.40	1.44	8	1
1:B:556:PRO:HB3	1:B:564:GLN:HB3	0.40	1.92	12	1
1:A:566:VAL:HG13	1:A:633:PHE:CD1	0.40	2.51	14	1
1:B:631:LEU:O	1:B:635:ARG:HG3	0.40	2.16	3	1
1:A:594:ASN:HB3	1:A:596:ILE:HG13	0.40	1.94	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:532:PHE:HE2	1:B:631:LEU:HD21	0.40	1.75	9	1
1:A:579:LEU:HD23	1:A:588:SER:HB3	0.40	1.92	11	1
1:B:590:LEU:HG	1:B:617:GLY:C	0.40	2.41	11	1
1:A:609:HIS:HB3	1:A:610:ASN:H	0.40	1.47	17	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	114/136 (84%)	106±2 (93±2%)	6±1 (5±1%)	2±2 (2±1%)	9	52
1	B	114/136 (84%)	105±2 (92±2%)	6±1 (6±1%)	2±1 (2±1%)	8	48
All	All	4560/5440 (84%)	4225 (93%)	248 (5%)	87 (2%)	8	51

All 19 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	610	ASN	9
1	B	643	PRO	8
1	B	586	HIS	8
1	A	597	TYR	8
1	B	610	ASN	7
1	A	557	ARG	6
1	B	557	ARG	6
1	B	597	TYR	6
1	A	596	ILE	5
1	B	596	ILE	5
1	A	559	THR	4
1	B	561	VAL	3
1	A	643	PRO	3
1	A	561	VAL	2
1	A	586	HIS	2
1	B	559	THR	2
1	B	571	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	560	TRP	1
1	B	560	TRP	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	101/121 (83%)	57±4 (56±4%)	44±4 (44±4%)	0	3
1	B	102/121 (84%)	59±3 (58±3%)	43±3 (42±3%)	0	4
All	All	4060/4840 (84%)	2316 (57%)	1744 (43%)	0	3

All 152 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	534	THR	20
1	A	536	THR	20
1	A	539	THR	20
1	A	566	VAL	20
1	A	575	LEU	20
1	A	577	ARG	20
1	A	579	LEU	20
1	A	588	SER	20
1	A	590	LEU	20
1	A	598	THR	20
1	A	603	ILE	20
1	A	612	ILE	20
1	A	624	SER	20
1	B	534	THR	20
1	B	536	THR	20
1	B	539	THR	20
1	B	547	GLU	20
1	B	566	VAL	20
1	B	567	SER	20
1	B	575	LEU	20
1	B	579	LEU	20
1	B	590	LEU	20

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Mol	Chain	Res	Type	Models (Total)
1	B	598	THR	20
1	B	603	ILE	20
1	B	612	ILE	20
1	B	624	SER	20
1	A	547	GLU	19
1	A	567	SER	19
1	A	570	LEU	19
1	A	620	SER	19
1	A	621	SER	19
1	A	641	LYS	19
1	B	538	SER	19
1	B	559	THR	19
1	B	563	THR	19
1	B	570	LEU	19
1	B	588	SER	19
1	B	625	LYS	19
1	A	531	SER	18
1	A	563	THR	18
1	A	576	GLU	18
1	A	589	VAL	18
1	B	576	GLU	18
1	B	577	ARG	18
1	B	589	VAL	18
1	A	625	LYS	18
1	A	559	THR	17
1	A	573	GLU	17
1	B	620	SER	17
1	B	621	SER	17
1	A	599	MET	17
1	A	583	LYS	16
1	B	537	LEU	16
1	B	602	MET	16
1	B	641	LYS	16
1	A	538	SER	15
1	A	642	LEU	15
1	B	644	LYS	15
1	A	614	GLU	14
1	B	557	ARG	14
1	B	642	LEU	14
1	B	614	GLU	14
1	A	568	HIS	13
1	A	602	MET	13

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Mol	Chain	Res	Type	Models (Total)
1	B	568	HIS	13
1	A	537	LEU	13
1	B	599	MET	13
1	B	531	SER	13
1	A	608	LYS	12
1	B	533	ARG	12
1	B	583	LYS	12
1	A	533	ARG	12
1	A	557	ARG	12
1	A	564	GLN	12
1	A	631	LEU	12
1	A	637	GLN	11
1	B	635	ARG	11
1	B	638	GLU	11
1	A	544	LYS	11
1	B	631	LEU	11
1	B	573	GLU	11
1	A	541	GLU	10
1	B	604	ARG	10
1	B	637	GLN	10
1	B	530	TYR	10
1	A	635	ARG	10
1	A	530	TYR	10
1	B	615	ARG	10
1	B	541	GLU	9
1	B	561	VAL	9
1	B	610	ASN	9
1	B	552	GLU	9
1	A	561	VAL	9
1	A	604	ARG	9
1	A	543	THR	9
1	A	615	ARG	9
1	A	610	ASN	8
1	B	605	GLU	8
1	B	608	LYS	8
1	B	544	LYS	8
1	B	564	GLN	8
1	A	630	PHE	8
1	A	638	GLU	8
1	A	601	ASP	8
1	A	632	SER	7
1	A	560	TRP	7

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Mol	Chain	Res	Type	Models (Total)
1	B	601	ASP	7
1	A	569	ILE	7
1	B	543	THR	7
1	B	628	GLU	7
1	B	623	LEU	6
1	B	640	MET	6
1	A	628	GLU	6
1	A	535	LEU	6
1	B	597	TYR	6
1	A	586	HIS	5
1	A	640	MET	5
1	A	552	GLU	5
1	B	582	ILE	5
1	A	555	VAL	4
1	B	607	GLU	4
1	A	582	ILE	4
1	A	597	TYR	4
1	B	587	ASP	4
1	B	630	PHE	4
1	A	592	ASN	3
1	B	554	LYS	3
1	A	623	LEU	3
1	A	607	GLU	3
1	A	626	TYR	3
1	A	605	GLU	3
1	B	560	TRP	3
1	B	592	ASN	3
1	B	586	HIS	2
1	B	555	VAL	2
1	A	596	ILE	2
1	B	619	ASP	2
1	B	622	LYS	2
1	B	626	TYR	2
1	A	619	ASP	2
1	A	622	LYS	2
1	A	611	ASP	2
1	B	611	ASP	1
1	B	632	SER	1
1	B	609	HIS	1
1	B	535	LEU	1
1	B	618	ILE	1
1	A	551	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	558	TYR	1
1	B	551	ARG	1
1	B	558	TYR	1
1	B	569	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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

No chemical shift data were provided