Full wwPDB NMR Structure Validation Report (i)

Mar 6, 2022 – 05:24 PM EST

PDB ID	:	2RP5
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 (i) symbol.

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

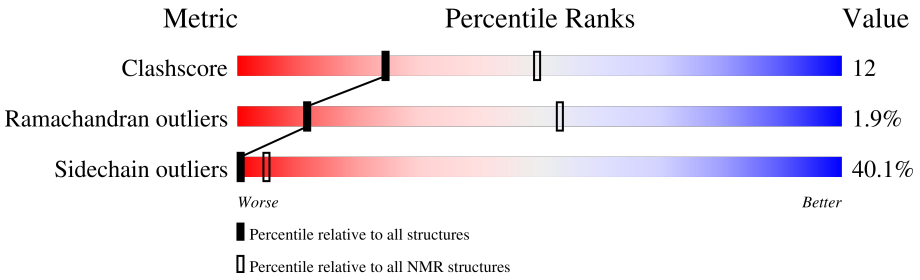
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	136	36% 43% • • 14%
1	B	136	36% 46% • • 14%

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)	0.68	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 (i)

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

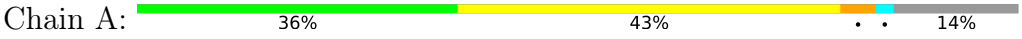
4 Residue-property plots

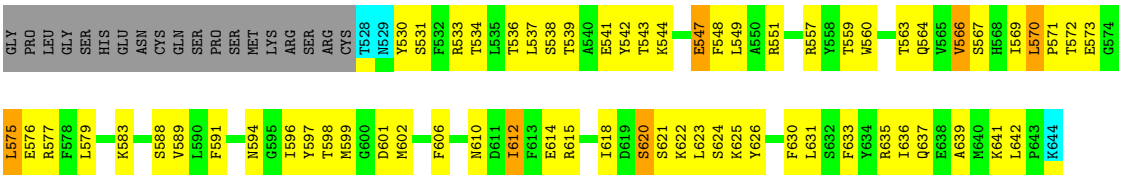
4.1 Average score per residue in the NMR ensemble

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

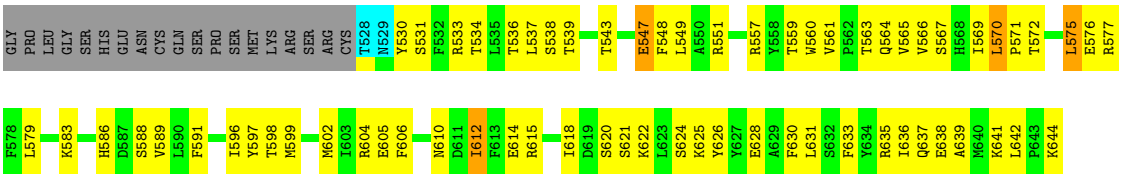
Chain A:





• Molecule 1: Putative uncharacterized protein cep-1

Chain B:



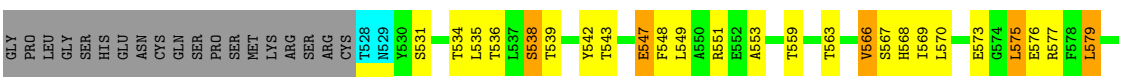
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

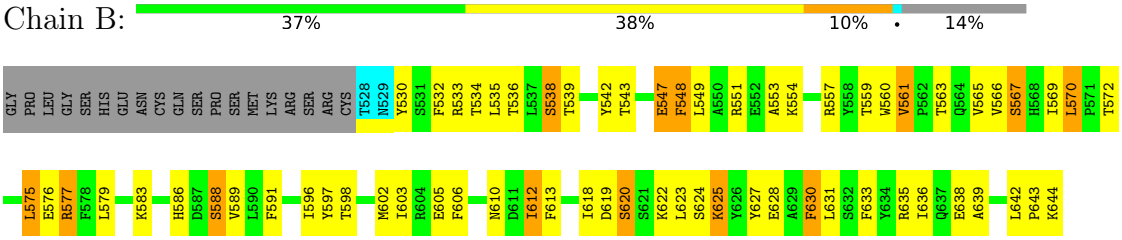
4.2.1 Score per residue for model 1

• Molecule 1: Putative uncharacterized protein cep-1

Chain A:

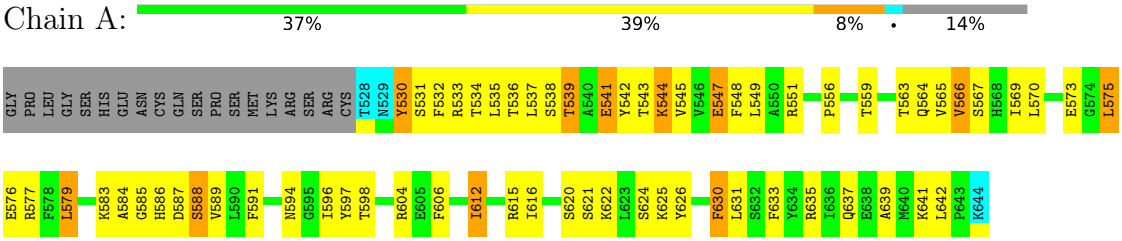


• Molecule 1: Putative uncharacterized protein cep-1

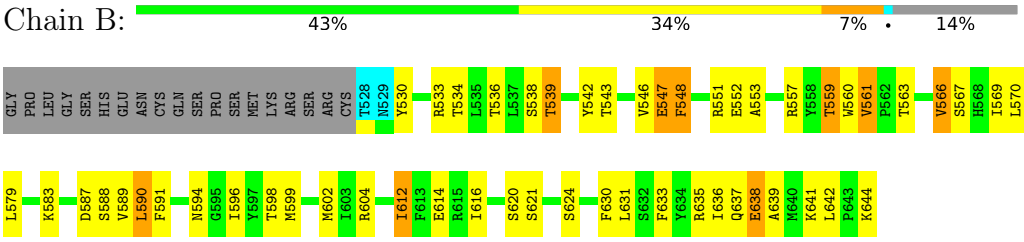


4.2.2 Score per residue for model 2

• Molecule 1: Putative uncharacterized protein cep-1

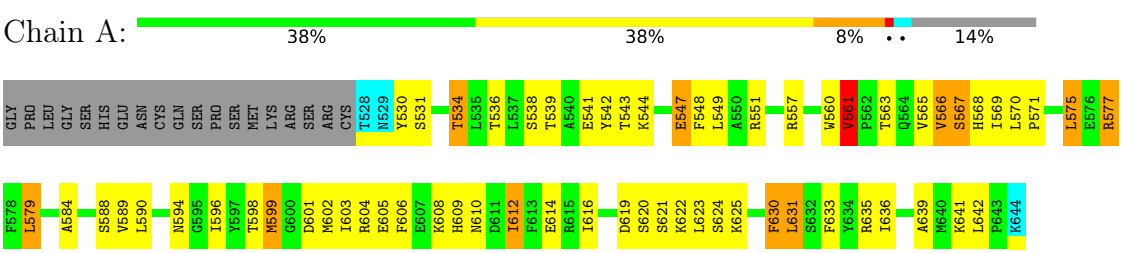


• Molecule 1: Putative uncharacterized protein cep-1



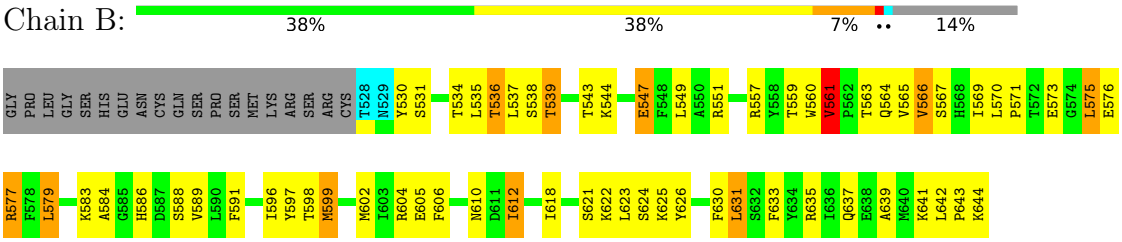
4.2.3 Score per residue for model 3

• Molecule 1: Putative uncharacterized protein cep-1



• Molecule 1: Putative uncharacterized protein cep-1

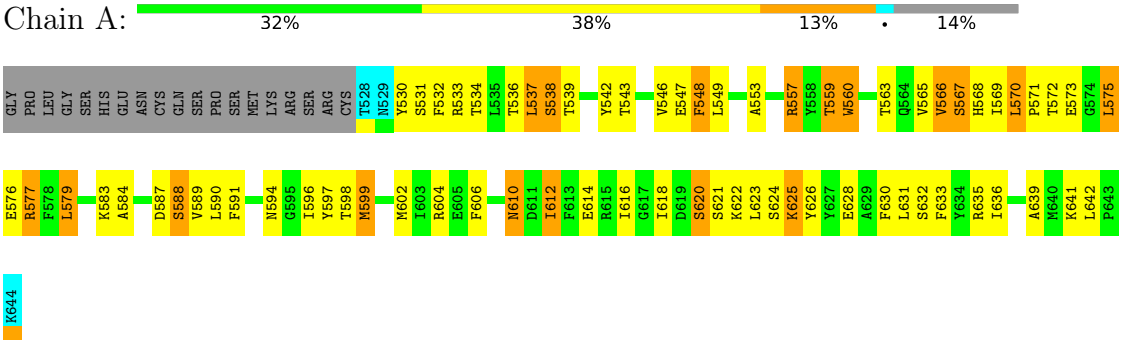
Chain B:



4.2.4 Score per residue for model 4

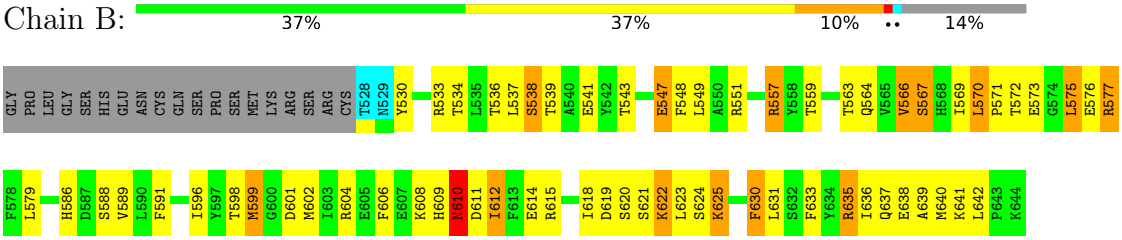
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

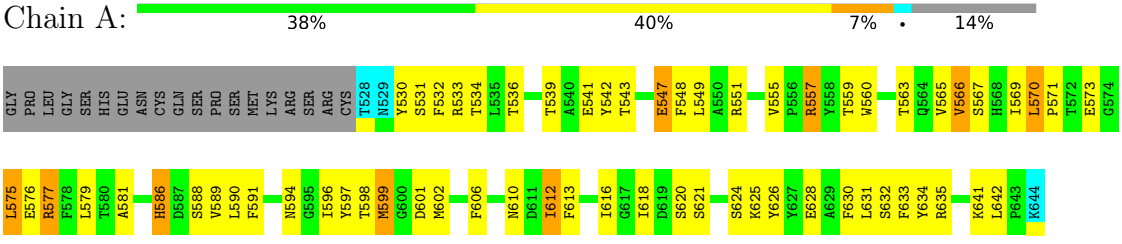
Chain B:



4.2.5 Score per residue for model 5

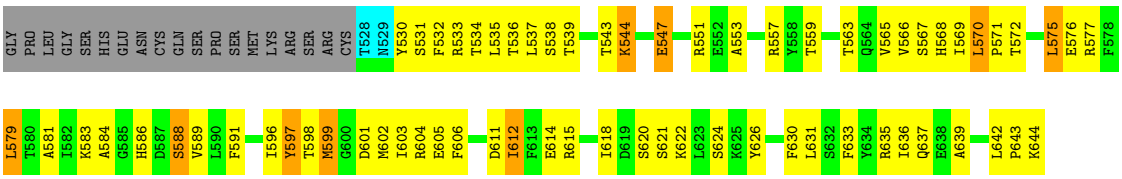
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

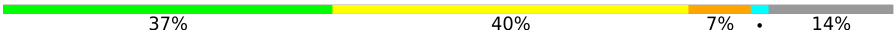
Chain B:

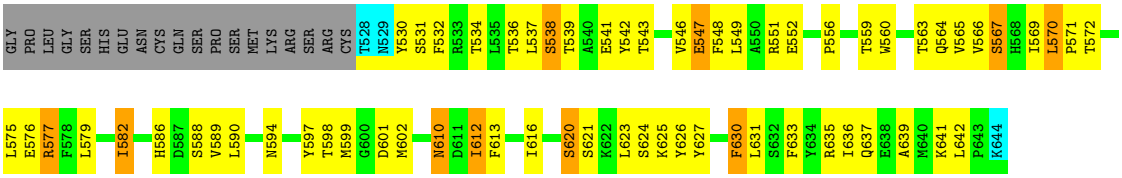


4.2.6 Score per residue for model 6

• Molecule 1: Putative uncharacterized protein cep-1

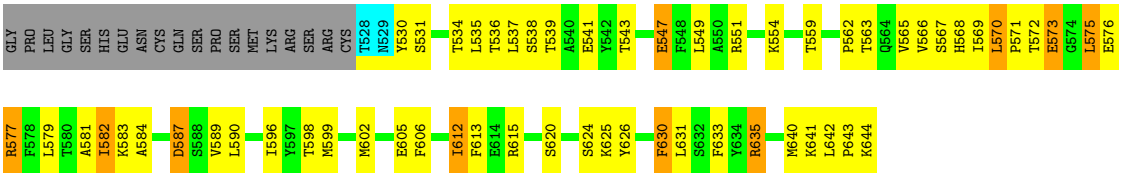
Chain A:





• Molecule 1: Putative uncharacterized protein cep-1

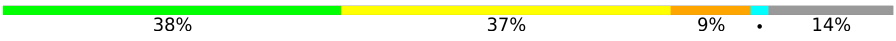
Chain B:

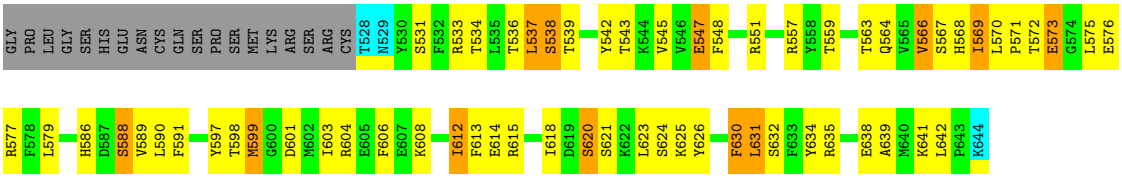


4.2.7 Score per residue for model 7

• Molecule 1: Putative uncharacterized protein cep-1

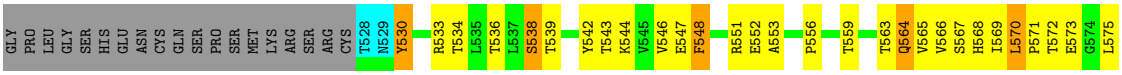
Chain A:

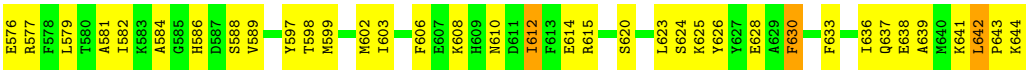




• Molecule 1: Putative uncharacterized protein cep-1

Chain B:

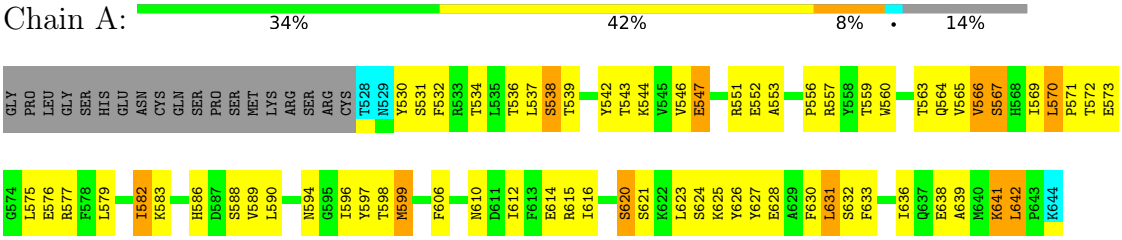




4.2.8 Score per residue for model 8

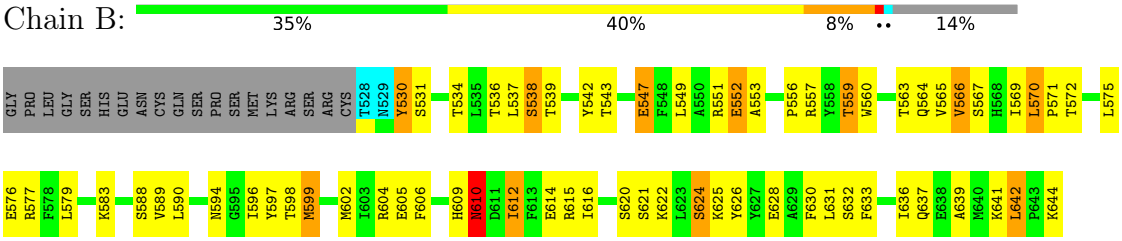
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

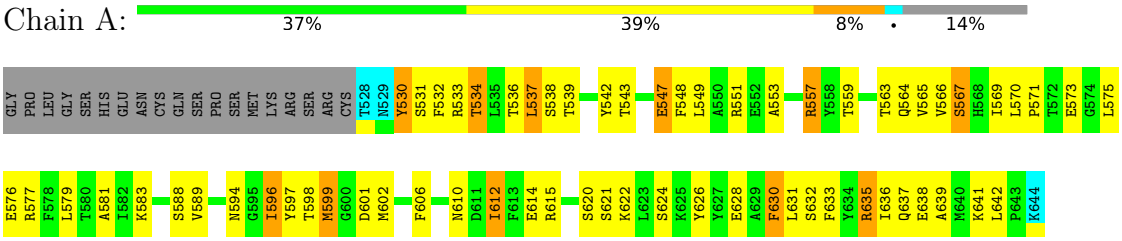
Chain B:



4.2.9 Score per residue for model 9

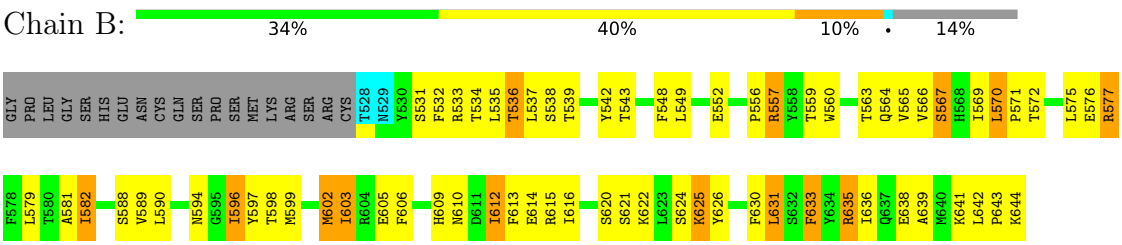
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

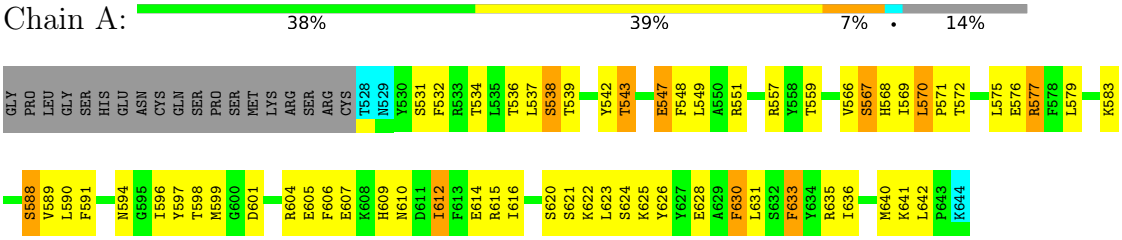
Chain B:



4.2.10 Score per residue for model 10

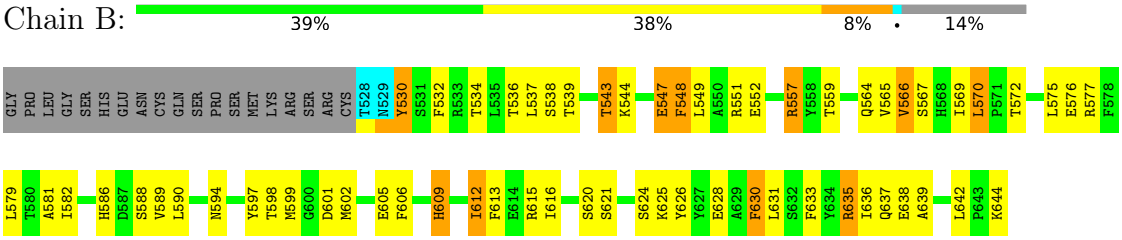
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

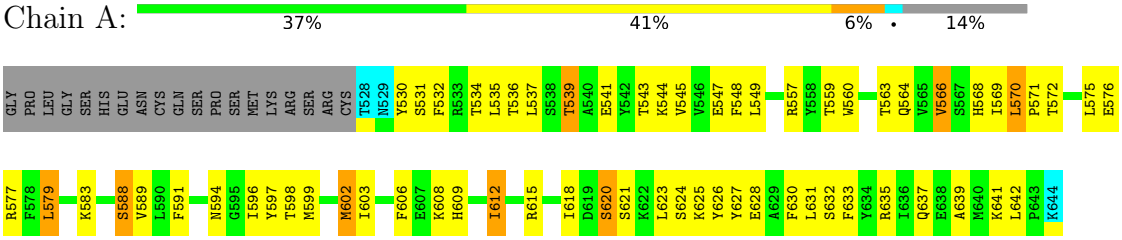
Chain B:



4.2.11 Score per residue for model 11

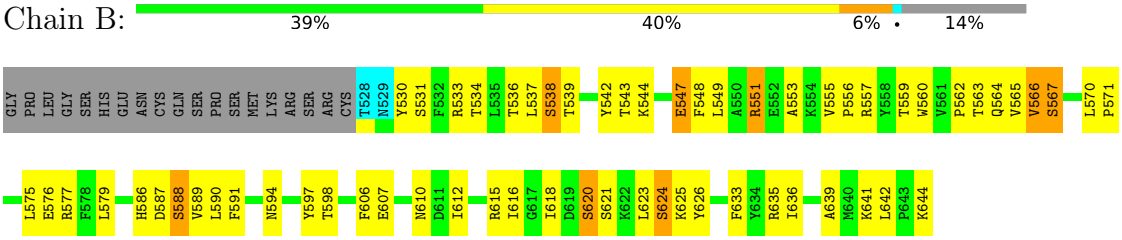
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:



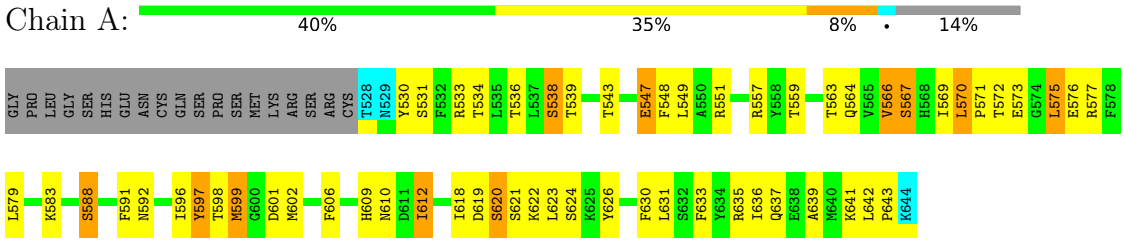
• Molecule 1: Putative uncharacterized protein cep-1

Chain B:

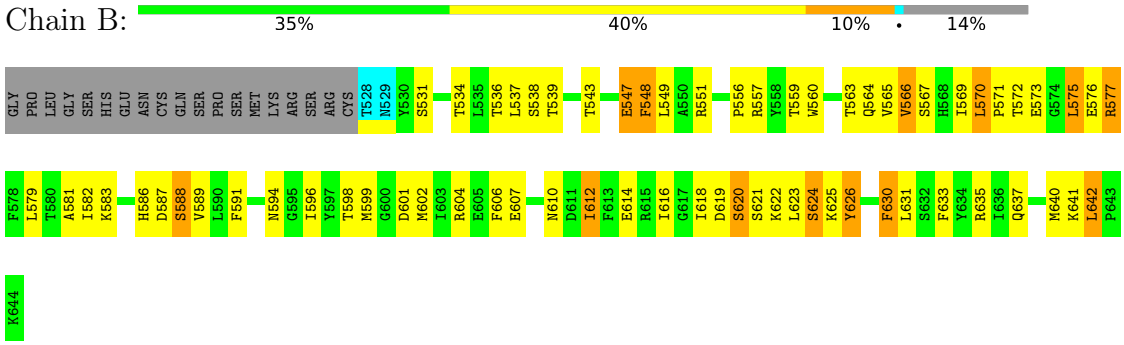


4.2.12 Score per residue for model 12

• Molecule 1: Putative uncharacterized protein cep-1

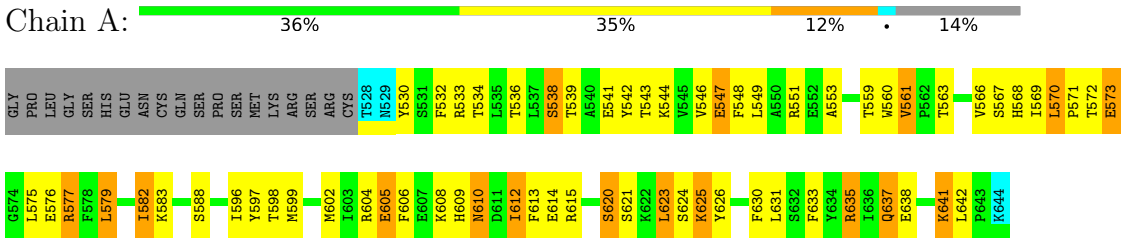


• Molecule 1: Putative uncharacterized protein cep-1

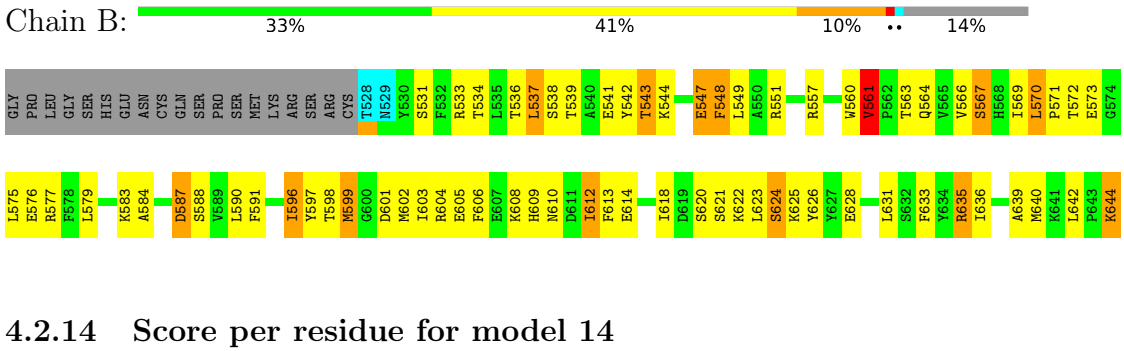


4.2.13 Score per residue for model 13

• Molecule 1: Putative uncharacterized protein cep-1

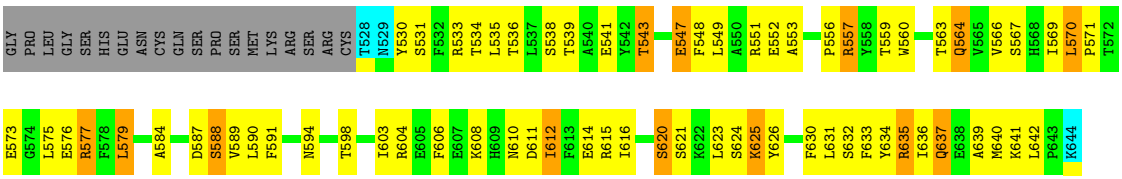


• Molecule 1: Putative uncharacterized protein cep-1



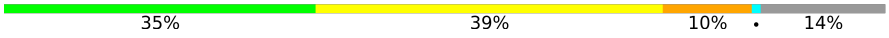
4.2.14 Score per residue for model 14

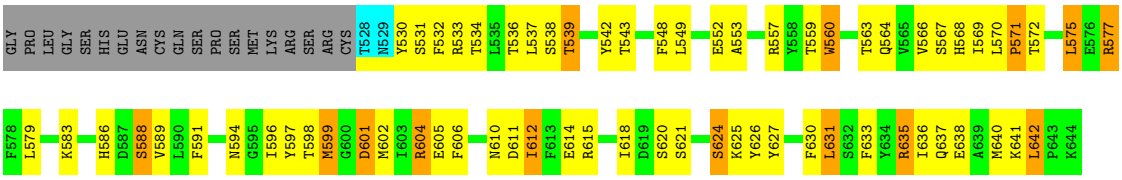
• Molecule 1: Putative uncharacterized protein cep-1



• Molecule 1: Putative uncharacterized protein cep-1

Chain B:

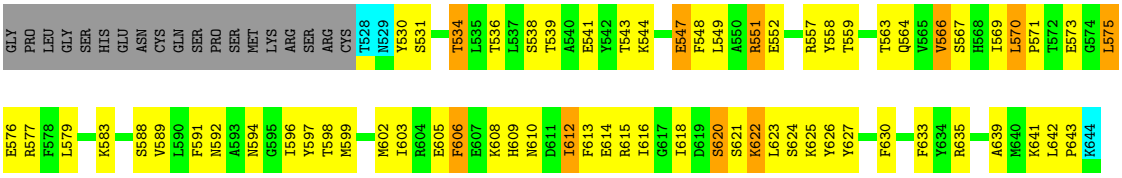




4.2.15 Score per residue for model 15

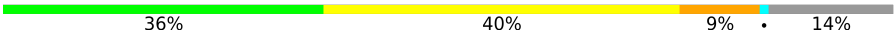
• Molecule 1: Putative uncharacterized protein cep-1

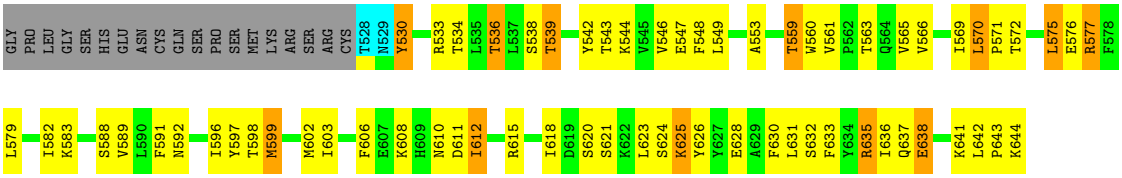
Chain A:



• Molecule 1: Putative uncharacterized protein cep-1

Chain B:





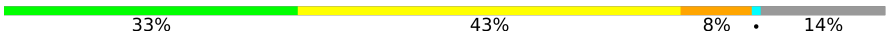
4.2.16 Score per residue for model 16

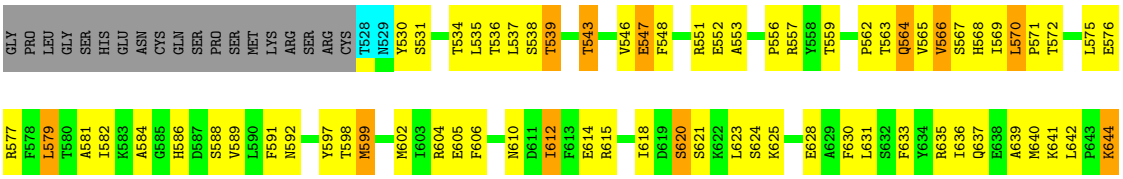
• Molecule 1: Putative uncharacterized protein cep-1

Chain A:

• Molecule 1: Putative uncharacterized protein cep-1

Chain B:

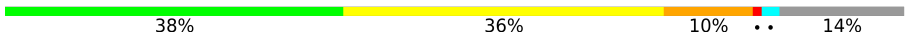


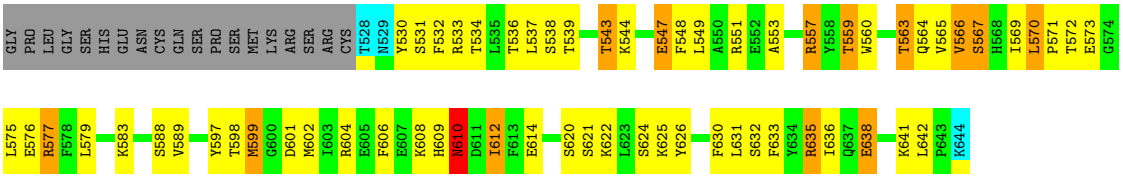


4.2.17 Score per residue for model 17

• Molecule 1: Putative uncharacterized protein cep-1

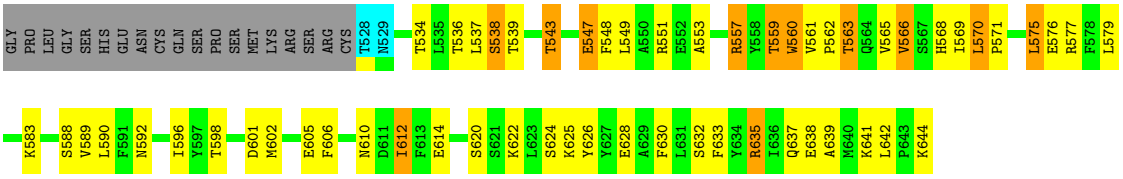
Chain A:





• Molecule 1: Putative uncharacterized protein cep-1

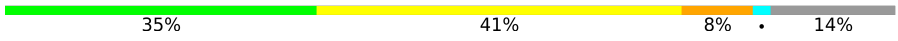
Chain B:

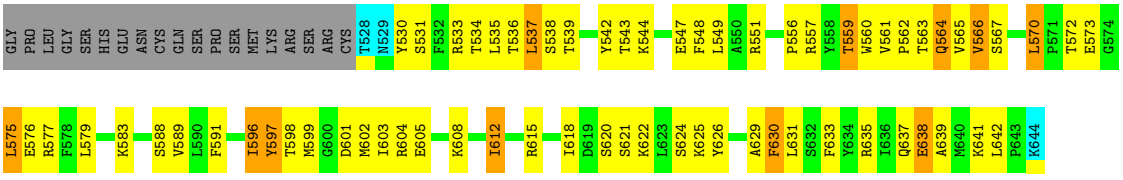


4.2.18 Score per residue for model 18

• Molecule 1: Putative uncharacterized protein cep-1

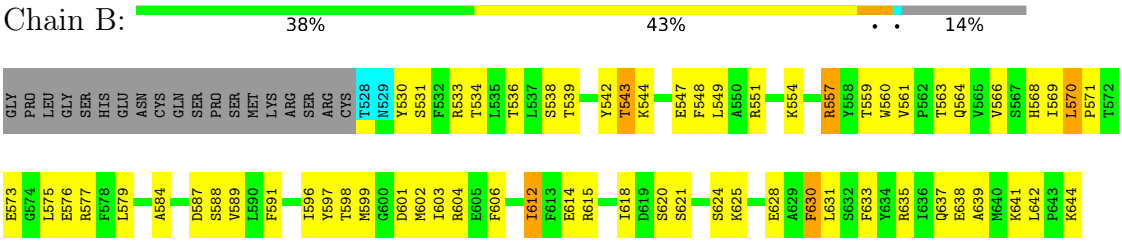
Chain A:





• Molecule 1: Putative uncharacterized protein cep-1

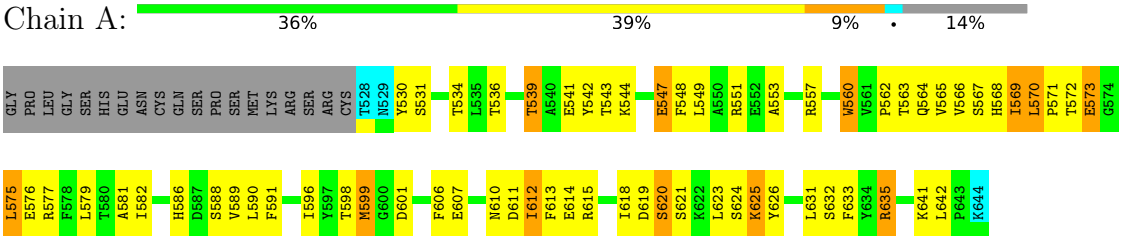
Chain B:



4.2.19 Score per residue for model 19 (medoid)

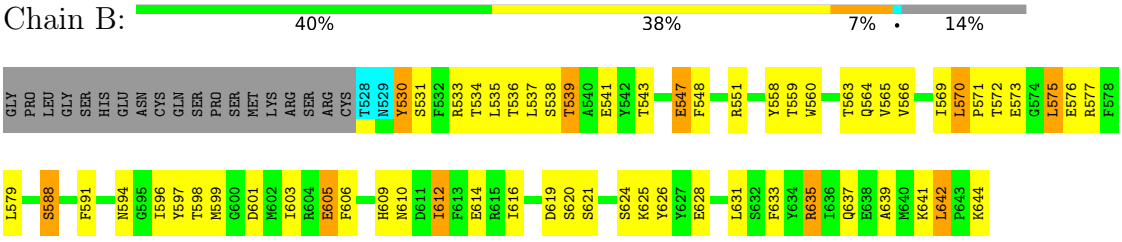
- Molecule 1: Putative uncharacterized protein cep-1

Chain A:



- Molecule 1: Putative uncharacterized protein cep-1

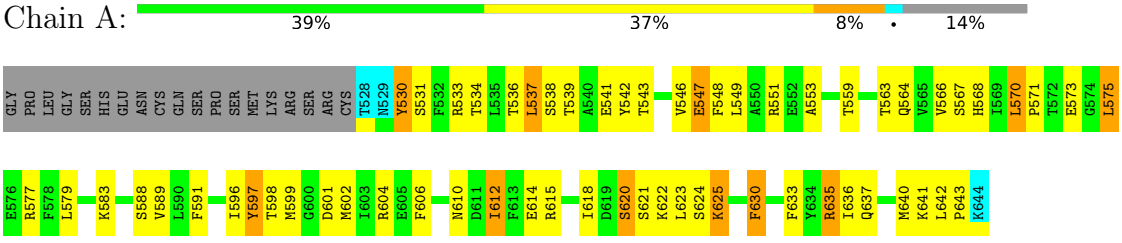
Chain B:



4.2.20 Score per residue for model 20

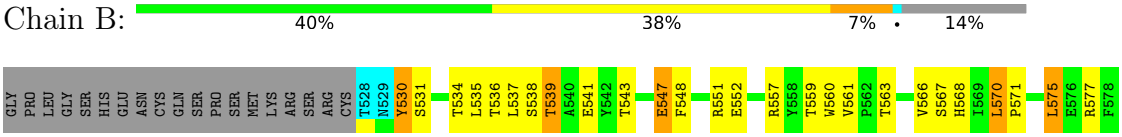
- Molecule 1: Putative uncharacterized protein cep-1

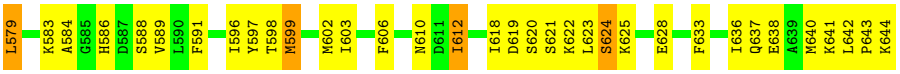
Chain A:



- Molecule 1: Putative uncharacterized protein cep-1

Chain B:




L579
K583
A584
G585
H586
D587
S588
V589
L590
F591
I596
Y597
T598
M599
M602
I603
F606
N610
D611
I612
I618
D619
S620
S621
K622
L623
S624
K625
E628
F633
I636
Q637
E638
A639
M640
K641
L642
P643
K644

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	23±4
All	All	37640	37660	37540	886

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: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: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:HA	1:A:638:GLU:OE1	0.49	2.06	17	1
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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:A:638:GLU:OE1	1:A:638:GLU:HA	0.46	2.10	18	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:570:LEU:C	1:B:572:THR:H	0.45	2.14	7	14
1:B:560:TRP:CZ3	1:B:625:LYS:HB2	0.45	2.45	15	2
1:A:570:LEU:C	1:A:572:THR:H	0.45	2.14	4	10
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:599:MET:HG3	1:A:599:MET:O	0.45	2.11	12	1
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:602:MET:HG2	1:B:603:ILE:N	0.44	2.27	9	1
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: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: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:584:ALA:HB1	1:B:587:ASP:CG	0.42	2.34	13	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: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: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: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: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: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
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:A:609:HIS:HB3	1:A:610:ASN:H	0.40	1.47	17	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	114/136 (84%)	106±2 (93±2%)	6±1 (5±1%)	2±2 (2±1%)	12	54
1	B	114/136 (84%)	105±2 (92±2%)	6±1 (6±1%)	2±1 (2±1%)	10	50
All	All	4560/5440 (84%)	4225 (93%)	248 (5%)	87 (2%)	11	53

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
1	A	560	TRP	1
1	B	560	TRP	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	101/121 (83%)	60±3 (59±3%)	41±3 (41±3%)	0 4
1	B	102/121 (84%)	62±3 (60±3%)	40±3 (40±3%)	0 5
All	All	4060/4840 (84%)	2430 (60%)	1630 (40%)	0 5

All 153 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	575	LEU	20
1	A	577	ARG	20
1	A	579	LEU	20
1	A	588	SER	20
1	A	598	THR	20
1	A	624	SER	20
1	A	641	LYS	20
1	B	534	THR	20
1	B	536	THR	20
1	B	539	THR	20
1	B	575	LEU	20
1	B	577	ARG	20
1	B	579	LEU	20
1	B	598	THR	20
1	B	624	SER	20
1	A	547	GLU	19
1	A	612	ILE	19
1	A	620	SER	19
1	A	621	SER	19
1	B	538	SER	19
1	B	559	THR	19
1	B	563	THR	19
1	B	588	SER	19
1	B	612	ILE	19
1	A	531	SER	18
1	A	563	THR	18
1	A	567	SER	18
1	A	570	LEU	18
1	A	576	GLU	18
1	A	589	VAL	18
1	A	625	LYS	18

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Mol	Chain	Res	Type	Models (Total)
1	A	630	PHE	18
1	B	570	LEU	18
1	B	589	VAL	18
1	A	559	THR	17
1	B	576	GLU	17
1	B	602	MET	17
1	B	620	SER	17
1	B	625	LYS	17
1	B	547	GLU	16
1	B	644	LYS	16
1	B	621	SER	16
1	B	641	LYS	16
1	A	599	MET	16
1	A	538	SER	15
1	A	573	GLU	15
1	B	567	SER	15
1	A	602	MET	14
1	B	630	PHE	14
1	B	537	LEU	14
1	A	566	VAL	13
1	A	583	LYS	13
1	A	601	ASP	13
1	A	614	GLU	13
1	A	615	ARG	13
1	B	557	ARG	13
1	A	530	TYR	13
1	B	599	MET	13
1	B	637	GLN	13
1	A	557	ARG	13
1	B	530	TYR	13
1	B	531	SER	13
1	B	533	ARG	12
1	B	583	LYS	12
1	A	533	ARG	12
1	A	537	LEU	12
1	A	635	ARG	12
1	B	615	ARG	12
1	B	635	ARG	12
1	A	597	TYR	11
1	A	637	GLN	11
1	B	614	GLU	11
1	A	564	GLN	11

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Mol	Chain	Res	Type	Models (Total)
1	A	568	HIS	10
1	B	548	PHE	10
1	B	597	TYR	10
1	B	638	GLU	10
1	A	541	GLU	10
1	A	544	LYS	10
1	A	604	ARG	10
1	B	566	VAL	10
1	B	610	ASN	9
1	B	604	ARG	9
1	A	590	LEU	9
1	B	564	GLN	9
1	B	601	ASP	9
1	A	610	ASN	8
1	B	603	ILE	8
1	B	633	PHE	8
1	B	590	LEU	8
1	A	608	LYS	8
1	A	631	LEU	8
1	B	544	LYS	8
1	A	560	TRP	8
1	B	568	HIS	8
1	A	632	SER	7
1	B	605	GLU	7
1	B	552	GLU	7
1	B	573	GLU	7
1	A	628	GLU	7
1	A	638	GLU	7
1	B	628	GLU	7
1	A	586	HIS	5
1	A	603	ILE	5
1	B	561	VAL	5
1	B	587	ASP	5
1	B	631	LEU	5
1	A	633	PHE	5
1	B	541	GLU	5
1	A	569	ILE	5
1	B	642	LEU	5
1	B	560	TRP	5
1	B	543	THR	5
1	A	640	MET	4
1	B	608	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	B	640	MET	4
1	B	626	TYR	4
1	A	592	ASN	3
1	B	554	LYS	3
1	B	586	HIS	3
1	B	611	ASP	3
1	A	552	GLU	3
1	A	582	ILE	3
1	B	582	ILE	3
1	A	543	THR	3
1	A	626	TYR	3
1	A	605	GLU	3
1	B	592	ASN	3
1	A	561	VAL	2
1	A	623	LEU	2
1	B	623	LEU	2
1	A	548	PHE	2
1	B	619	ASP	2
1	A	634	TYR	2
1	A	607	GLU	2
1	B	607	GLU	2
1	A	619	ASP	2
1	A	622	LYS	2
1	A	611	ASP	2
1	A	587	ASP	1
1	B	622	LYS	1
1	A	555	VAL	1
1	A	642	LEU	1
1	B	632	SER	1
1	B	609	HIS	1
1	B	551	ARG	1
1	A	551	ARG	1
1	A	558	TYR	1
1	A	606	PHE	1
1	B	558	TYR	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided