



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:19 pm BST

PDB ID : 2LSL
Title : Solution structure of the C-terminal domain of Tetrahymena telomerase protein p65
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Deposited on : 2012-05-01

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

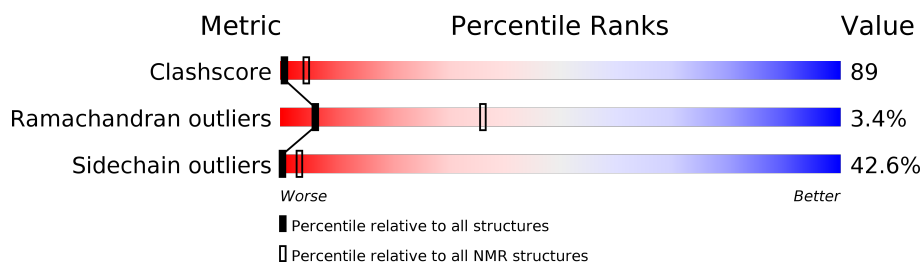
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	137	<div> <div></div> <div>9%</div> <div>31%</div> <div>23%</div> <div>31%</div> <div>5%</div> </div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:376-A:410, A:461-A:479, A:487-A:519 (87)	0.16	11

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 12 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2138 atoms, of which 1068 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Telomerase associated protein p65.

Mol	Chain	Residues	Atoms						Trace
1	A	130	Total	C	H	N	O	S	0
			2138	671	1068	187	208	4	

There are 30 discrepancies between the modelled and reference sequences:

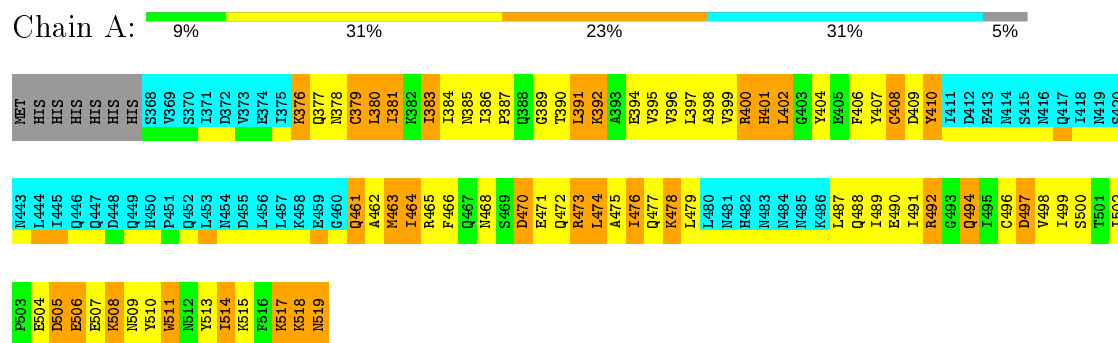
Chain	Residue	Modelled	Actual	Comment	Reference
A	361	MET	-	EXPRESSION TAG	UNP Q6JXI6
A	362	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	363	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	364	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	365	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	366	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	367	HIS	-	EXPRESSION TAG	UNP Q6JXI6
A	368	SER	-	EXPRESSION TAG	UNP Q6JXI6
A	?	-	ASN	DELETION	UNP Q6JXI6
A	?	-	LYS	DELETION	UNP Q6JXI6
A	?	-	ILE	DELETION	UNP Q6JXI6
A	?	-	SER	DELETION	UNP Q6JXI6
A	?	-	LEU	DELETION	UNP Q6JXI6
A	?	-	SER	DELETION	UNP Q6JXI6
A	?	-	THR	DELETION	UNP Q6JXI6
A	?	-	GLN	DELETION	UNP Q6JXI6
A	?	-	GLN	DELETION	UNP Q6JXI6
A	?	-	GLN	DELETION	UNP Q6JXI6
A	?	-	ASN	DELETION	UNP Q6JXI6
A	?	-	THR	DELETION	UNP Q6JXI6
A	?	-	ALA	DELETION	UNP Q6JXI6
A	?	-	GLN	DELETION	UNP Q6JXI6
A	?	-	CYS	DELETION	UNP Q6JXI6
A	?	-	SER	DELETION	UNP Q6JXI6
A	?	-	ASN	DELETION	UNP Q6JXI6
A	?	-	ILE	DELETION	UNP Q6JXI6
A	?	-	GLN	DELETION	UNP Q6JXI6
A	?	-	ILE	DELETION	UNP Q6JXI6
A	?	-	GLU	DELETION	UNP Q6JXI6
A	?	-	ASN	DELETION	UNP Q6JXI6

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Telomerase associated protein p65

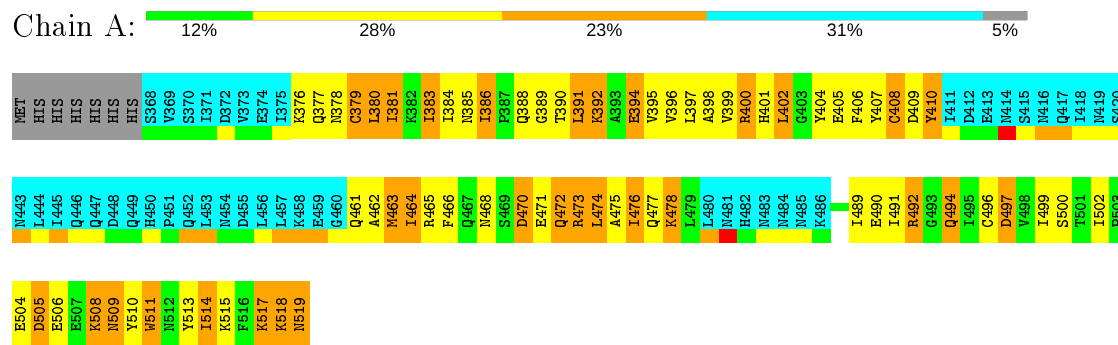


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

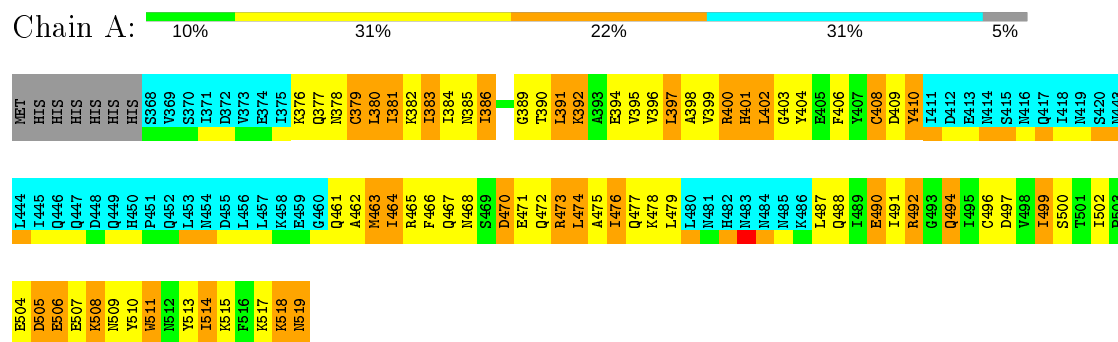
4.2.1 Score per residue for model 1

- Molecule 1: Telomerase associated protein p65



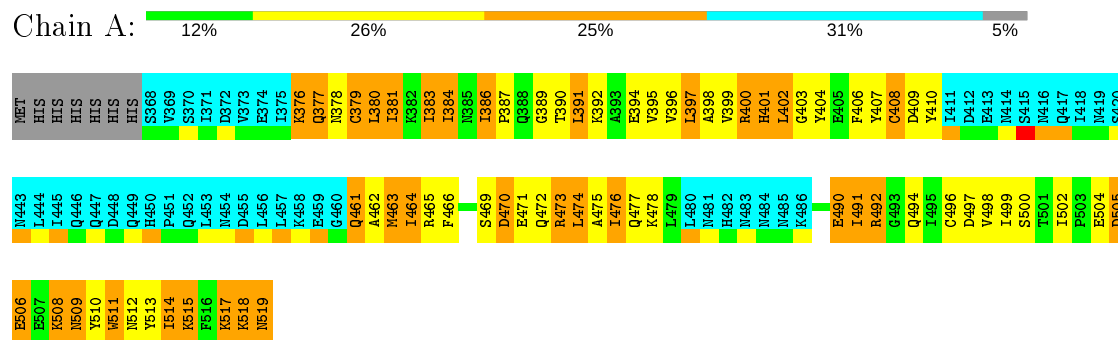
4.2.2 Score per residue for model 2

- Molecule 1: Telomerase associated protein p65



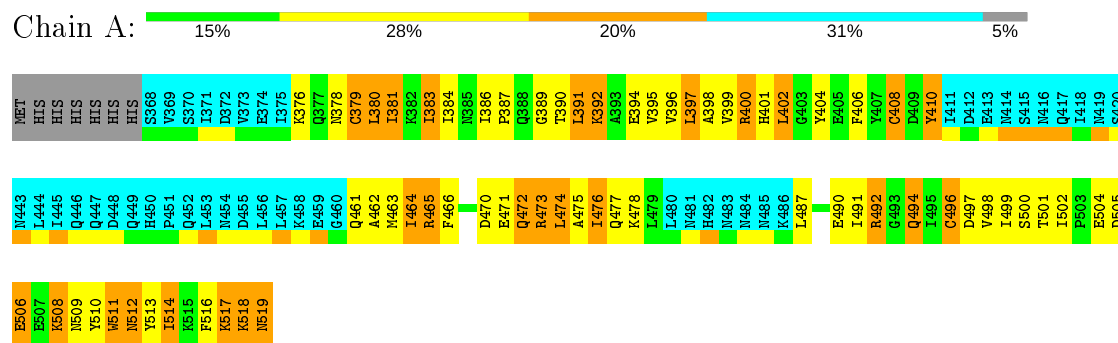
4.2.3 Score per residue for model 3

- Molecule 1: Telomerase associated protein p65



4.2.4 Score per residue for model 4

- Molecule 1: Telomerase associated protein p65



4.2.5 Score per residue for model 5

- Molecule 1: Telomerase associated protein p65

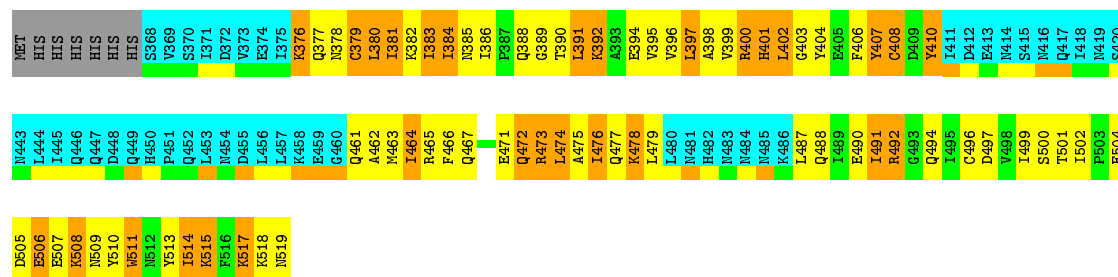
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Telomerase associated protein p65

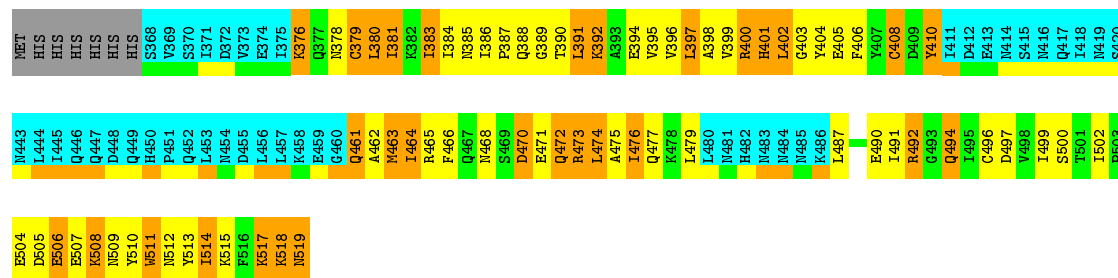
Chain A: 



4.2.7 Score per residue for model 7

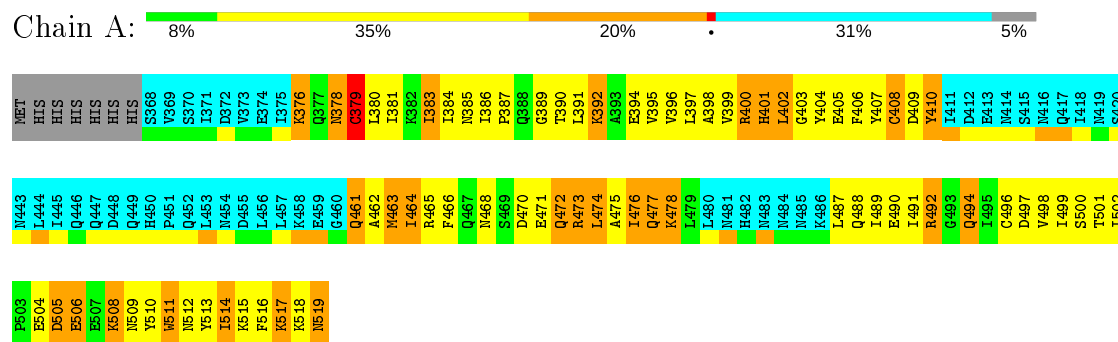
- Molecule 1: Telomerase associated protein p65

Chain A:  12% 30% 22% 31% 5%



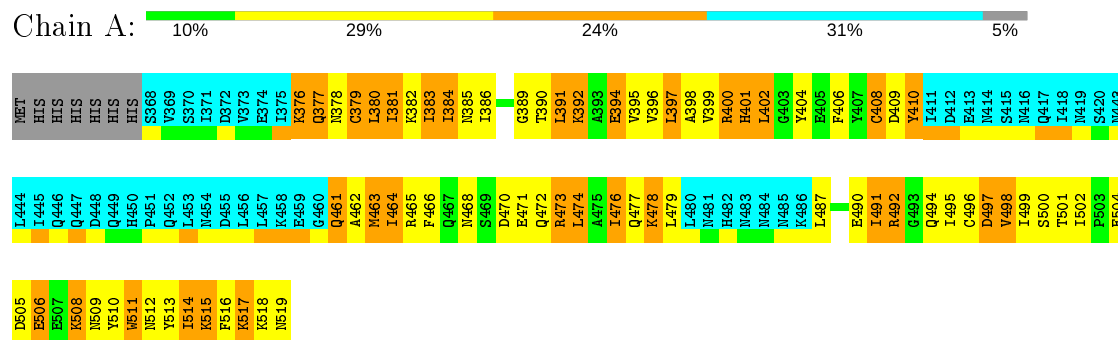
4.2.8 Score per residue for model 8

- Molecule 1: Telomerase associated protein p65



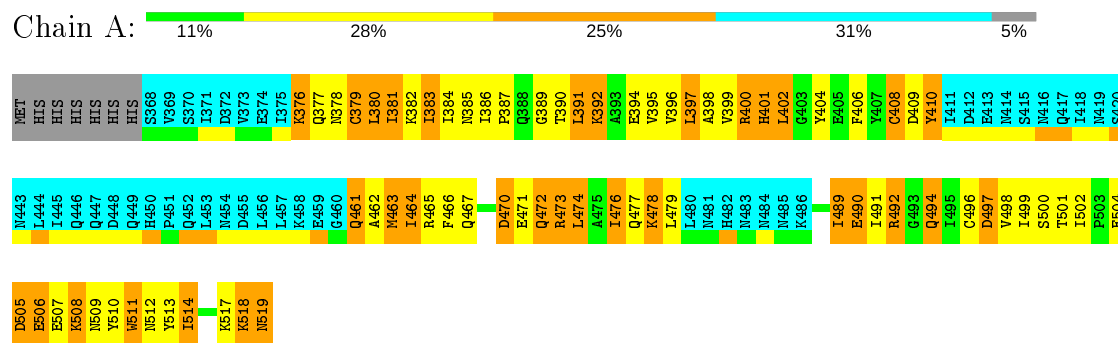
4.2.9 Score per residue for model 9

- Molecule 1: Telomerase associated protein p65



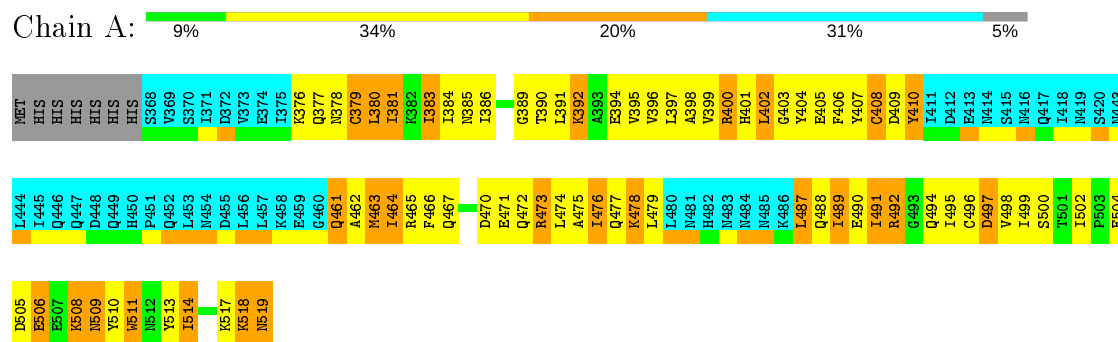
4.2.10 Score per residue for model 10

- Molecule 1: Telomerase associated protein p65



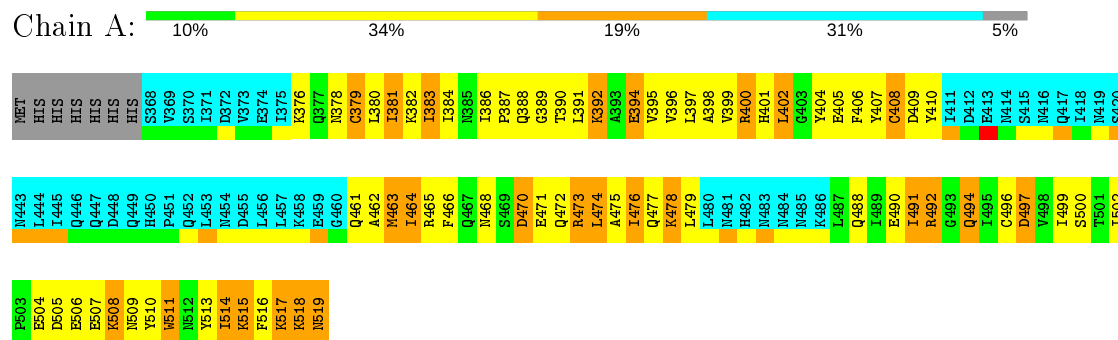
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Telomerase associated protein p65



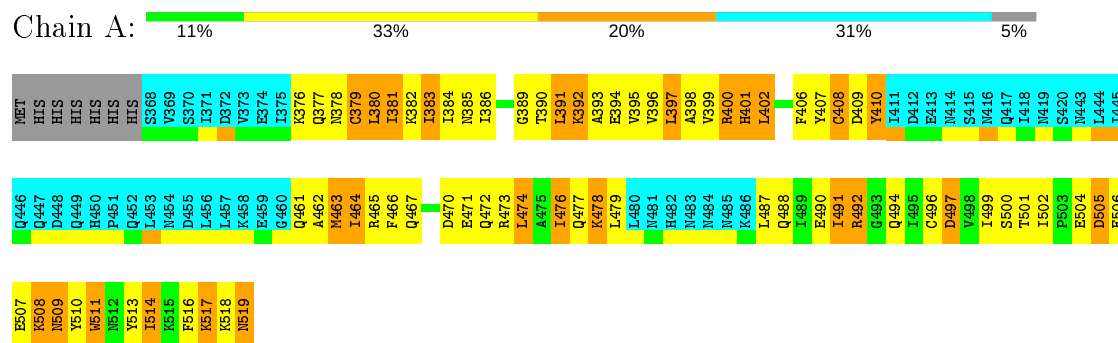
4.2.12 Score per residue for model 12

- Molecule 1: Telomerase associated protein p65



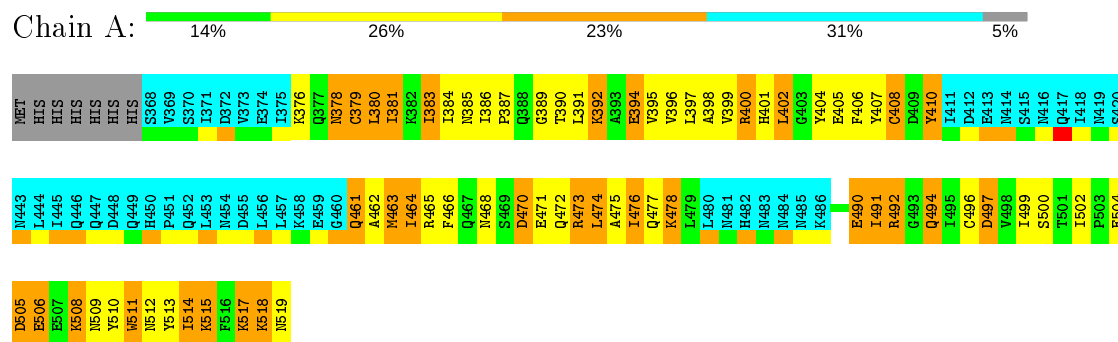
4.2.13 Score per residue for model 13

- Molecule 1: Telomerase associated protein p65



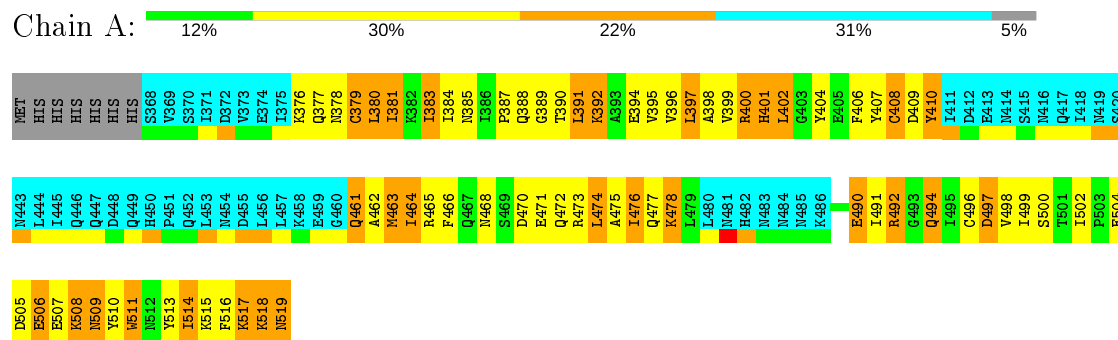
4.2.14 Score per residue for model 14

- Molecule 1: Telomerase associated protein p65



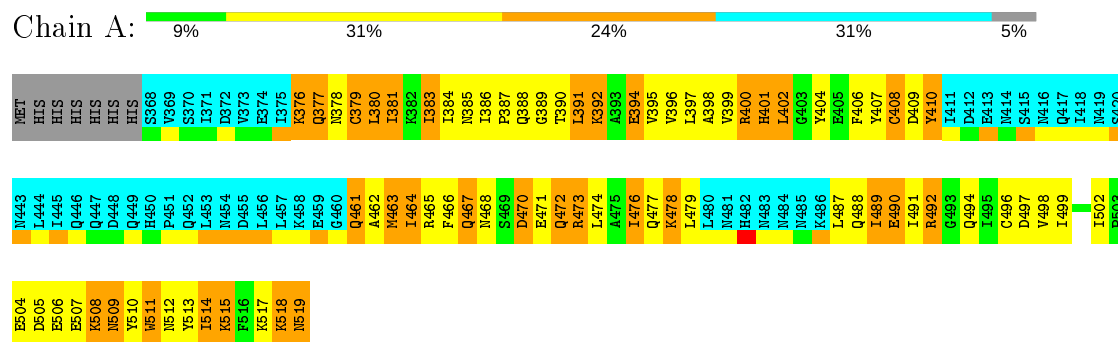
4.2.15 Score per residue for model 15

- Molecule 1: Telomerase associated protein p65



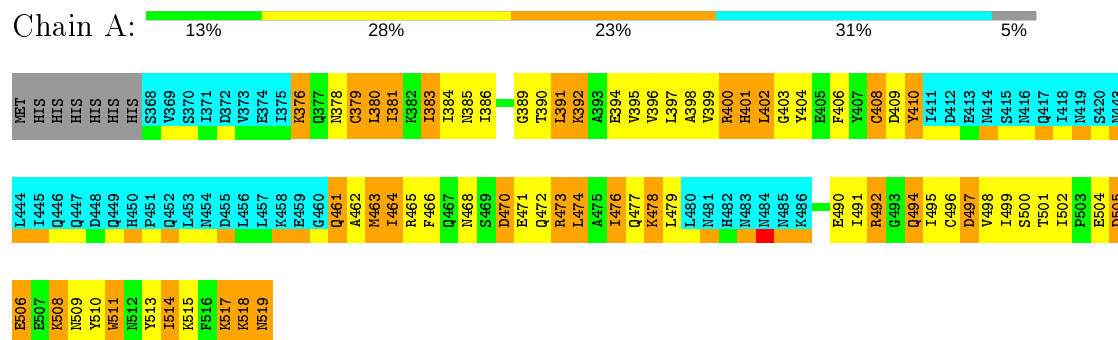
4.2.17 Score per residue for model 17

- Molecule 1: Telomerase associated protein p65



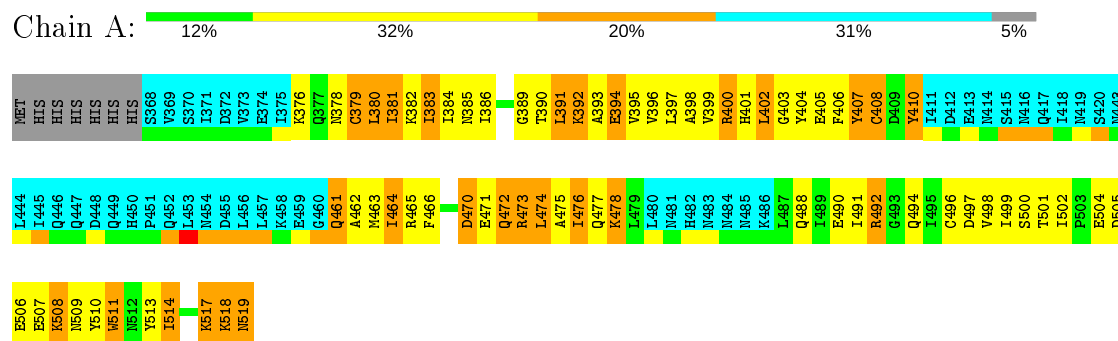
4.2.18 Score per residue for model 18

- Molecule 1: Telomerase associated protein p65



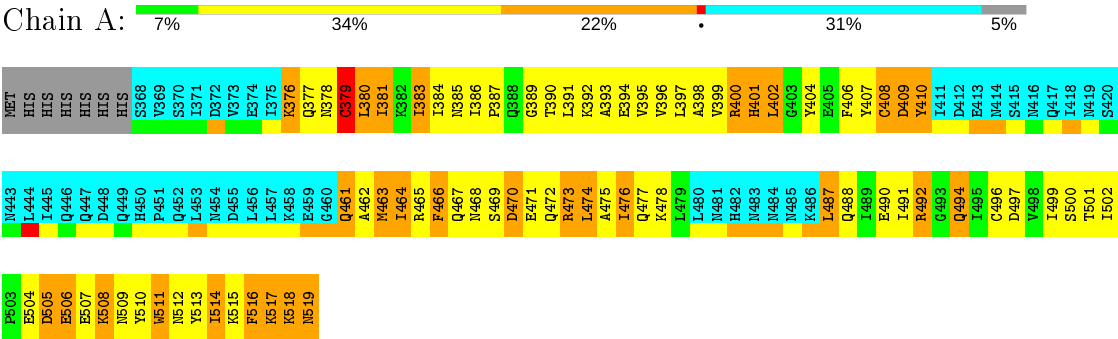
4.2.19 Score per residue for model 19

- Molecule 1: Telomerase associated protein p65



4.2.20 Score per residue for model 20

- Molecule 1: Telomerase associated protein p65



5 Refinement protocol and experimental data overview

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

Of the 200 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
CYANA	structure solution	2.1
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1449
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	727	740	739	131±9
All	All	14540	14800	14780	2619

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 89.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:406:PHE:CD1	1:A:464:ILE:HD13	1.07	1.83	8	1
1:A:398:ALA:CB	1:A:491:ILE:HG22	1.03	1.83	10	20
1:A:406:PHE:CD1	1:A:464:ILE:HD11	0.96	1.96	17	19
1:A:489:ILE:HD13	1:A:490:GLU:N	0.93	1.78	10	3
1:A:396:VAL:HG13	1:A:408:CYS:SG	0.92	2.05	1	20
1:A:398:ALA:HB3	1:A:491:ILE:HG22	0.92	1.41	4	9
1:A:464:ILE:HD11	1:A:466:PHE:CE1	0.90	2.01	8	1
1:A:392:LYS:O	1:A:396:VAL:HG23	0.88	1.68	1	19
1:A:464:ILE:HD12	1:A:466:PHE:CE1	0.86	2.06	15	18
1:A:404:TYR:OH	1:A:474:LEU:HD22	0.84	1.72	8	12
1:A:383:ILE:HD12	1:A:498:VAL:HG22	0.82	1.52	9	1
1:A:397:LEU:O	1:A:397:LEU:HD22	0.81	1.76	3	5
1:A:391:LEU:N	1:A:391:LEU:HD13	0.80	1.92	7	7
1:A:390:THR:HG23	1:A:394:GLU:CG	0.79	2.08	14	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:389:GLY:O	1:A:391:LEU:HD13	0.79	1.78	19	12
1:A:391:LEU:HD13	1:A:391:LEU:N	0.78	1.93	4	5
1:A:402:LEU:HD22	1:A:479:LEU:HD21	0.77	1.56	11	4
1:A:390:THR:HG22	1:A:394:GLU:HG3	0.75	1.57	16	2
1:A:387:PRO:HG3	1:A:491:ILE:HD11	0.75	1.58	16	3
1:A:396:VAL:HG22	1:A:408:CYS:HB2	0.75	1.58	9	19
1:A:476:ILE:HD11	1:A:500:SER:HB2	0.74	1.58	1	17
1:A:395:VAL:HG11	1:A:462:ALA:HB3	0.73	1.60	6	20
1:A:406:PHE:CD1	1:A:464:ILE:CD1	0.73	2.72	17	20
1:A:406:PHE:CD2	1:A:466:PHE:CE2	0.72	2.78	4	20
1:A:383:ILE:HD12	1:A:498:VAL:CG2	0.72	2.14	4	2
1:A:397:LEU:C	1:A:397:LEU:HD13	0.71	2.06	20	7
1:A:404:TYR:OH	1:A:474:LEU:HD13	0.71	1.86	20	4
1:A:464:ILE:HD11	1:A:466:PHE:CD1	0.71	2.20	8	1
1:A:381:ILE:CG1	1:A:464:ILE:HG23	0.71	2.15	8	1
1:A:397:LEU:HD13	1:A:397:LEU:C	0.70	2.06	16	9
1:A:398:ALA:HB2	1:A:491:ILE:HG22	0.70	1.63	7	4
1:A:383:ILE:HD12	1:A:498:VAL:HG23	0.70	1.62	4	2
1:A:389:GLY:O	1:A:391:LEU:HD23	0.70	1.86	9	1
1:A:406:PHE:CD2	1:A:466:PHE:CD2	0.69	2.80	7	19
1:A:470:ASP:O	1:A:474:LEU:HD12	0.69	1.87	2	8
1:A:381:ILE:HD13	1:A:498:VAL:HG13	0.69	1.63	4	1
1:A:406:PHE:CD2	1:A:466:PHE:CZ	0.69	2.80	17	1
1:A:398:ALA:HB1	1:A:491:ILE:HG22	0.69	1.63	8	16
1:A:464:ILE:HD12	1:A:465:ARG:N	0.69	2.03	8	1
1:A:396:VAL:HG22	1:A:408:CYS:SG	0.69	2.28	11	13
1:A:381:ILE:HG12	1:A:464:ILE:HG22	0.68	1.65	12	18
1:A:502:ILE:HG23	1:A:506:GLU:HB3	0.68	1.65	4	20
1:A:377:GLN:O	1:A:380:LEU:HD12	0.68	1.89	20	6
1:A:464:ILE:HD13	1:A:464:ILE:C	0.68	2.09	15	11
1:A:464:ILE:C	1:A:464:ILE:HD13	0.68	2.09	5	8
1:A:402:LEU:HD21	1:A:475:ALA:O	0.67	1.88	11	9
1:A:402:LEU:HD22	1:A:479:LEU:CD2	0.67	2.20	11	5
1:A:406:PHE:CE1	1:A:464:ILE:HG13	0.67	2.24	1	19
1:A:381:ILE:CD1	1:A:464:ILE:HG21	0.67	2.19	18	17
1:A:395:VAL:HG11	1:A:462:ALA:CB	0.67	2.20	20	20
1:A:381:ILE:HG13	1:A:464:ILE:HG22	0.67	1.65	4	1
1:A:390:THR:HG22	1:A:394:GLU:CG	0.66	2.19	16	1
1:A:406:PHE:CE1	1:A:464:ILE:CG1	0.66	2.79	9	19
1:A:464:ILE:CD1	1:A:466:PHE:CE1	0.66	2.79	15	18
1:A:406:PHE:CG	1:A:464:ILE:HD11	0.65	2.26	16	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:380:LEU:HD23	1:A:465:ARG:HG3	0.65	1.65	5	9
1:A:387:PRO:CG	1:A:491:ILE:HD11	0.65	2.21	20	6
1:A:510:TYR:CE2	1:A:514:ILE:CD1	0.64	2.80	12	20
1:A:384:ILE:HD12	1:A:385:ASN:ND2	0.64	2.06	18	2
1:A:406:PHE:CD1	1:A:464:ILE:CG1	0.64	2.81	12	19
1:A:464:ILE:HD13	1:A:465:ARG:N	0.64	2.08	17	19
1:A:466:PHE:CE1	1:A:472:GLN:NE2	0.64	2.66	17	1
1:A:390:THR:HG23	1:A:394:GLU:HG3	0.64	1.69	12	13
1:A:391:LEU:HD22	1:A:391:LEU:H	0.63	1.54	15	5
1:A:383:ILE:CD1	1:A:498:VAL:HG22	0.63	2.23	9	2
1:A:466:PHE:CE1	1:A:472:GLN:CG	0.63	2.82	5	12
1:A:381:ILE:CG1	1:A:464:ILE:CG2	0.62	2.77	4	7
1:A:380:LEU:HD11	1:A:507:GLU:HG3	0.62	1.71	7	8
1:A:391:LEU:H	1:A:391:LEU:HD22	0.62	1.54	2	7
1:A:397:LEU:O	1:A:397:LEU:HD13	0.62	1.94	16	2
1:A:476:ILE:HG22	1:A:477:GLN:N	0.62	2.08	7	20
1:A:499:ILE:HG22	1:A:501:THR:HG22	0.62	1.70	9	2
1:A:396:VAL:HG22	1:A:408:CYS:CB	0.62	2.25	9	17
1:A:464:ILE:HD12	1:A:464:ILE:C	0.62	2.14	8	1
1:A:404:TYR:CD2	1:A:475:ALA:HB2	0.61	2.30	11	1
1:A:398:ALA:CB	1:A:491:ILE:CG2	0.61	2.78	5	17
1:A:406:PHE:CE1	1:A:464:ILE:HD13	0.61	2.28	8	1
1:A:381:ILE:HD13	1:A:464:ILE:HG21	0.61	1.73	6	17
1:A:476:ILE:HD11	1:A:500:SER:CB	0.61	2.26	16	15
1:A:466:PHE:CZ	1:A:472:GLN:OE1	0.60	2.55	4	5
1:A:383:ILE:HG22	1:A:462:ALA:O	0.60	1.97	10	19
1:A:402:LEU:HD23	1:A:479:LEU:HD23	0.60	1.72	5	1
1:A:472:GLN:NE2	1:A:476:ILE:CD1	0.60	2.65	14	16
1:A:472:GLN:OE1	1:A:472:GLN:HA	0.59	1.97	4	2
1:A:383:ILE:HD12	1:A:498:VAL:HB	0.59	1.73	5	8
1:A:466:PHE:CE1	1:A:472:GLN:HG2	0.59	2.33	12	12
1:A:410:TYR:O	1:A:410:TYR:CD1	0.59	2.56	17	4
1:A:513:TYR:CZ	1:A:517:LYS:HD2	0.59	2.32	12	20
1:A:390:THR:HG21	1:A:492:ARG:CB	0.59	2.27	16	1
1:A:381:ILE:CD1	1:A:464:ILE:CG2	0.59	2.81	18	10
1:A:472:GLN:CA	1:A:472:GLN:OE1	0.58	2.51	6	5
1:A:510:TYR:CZ	1:A:514:ILE:HD12	0.58	2.34	1	12
1:A:384:ILE:HD12	1:A:385:ASN:HD22	0.58	1.57	9	3
1:A:472:GLN:HA	1:A:472:GLN:OE1	0.58	1.99	6	4
1:A:472:GLN:OE1	1:A:472:GLN:CA	0.58	2.52	4	1
1:A:386:ILE:HD13	1:A:387:PRO:N	0.58	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:479:LEU:HB3	1:A:487:LEU:HD22	0.58	1.74	7	1
1:A:510:TYR:CZ	1:A:514:ILE:CD1	0.57	2.88	1	15
1:A:402:LEU:HD23	1:A:475:ALA:HB1	0.57	1.75	6	9
1:A:401:HIS:O	1:A:401:HIS:CD2	0.57	2.57	18	2
1:A:391:LEU:CD1	1:A:391:LEU:N	0.56	2.67	6	3
1:A:383:ILE:CG2	1:A:462:ALA:O	0.56	2.53	9	20
1:A:378:ASN:CB	1:A:472:GLN:NE2	0.56	2.69	8	1
1:A:463:MET:SD	1:A:510:TYR:CZ	0.56	2.98	14	4
1:A:510:TYR:CD2	1:A:514:ILE:CD1	0.56	2.88	12	20
1:A:391:LEU:O	1:A:395:VAL:HG23	0.56	2.00	9	3
1:A:381:ILE:HG12	1:A:464:ILE:HG23	0.56	1.76	8	1
1:A:392:LYS:O	1:A:396:VAL:CG2	0.56	2.54	20	3
1:A:502:ILE:HG22	1:A:502:ILE:O	0.56	2.01	14	4
1:A:396:VAL:O	1:A:399:VAL:CG2	0.56	2.53	16	13
1:A:464:ILE:HD11	1:A:466:PHE:CZ	0.56	2.36	8	1
1:A:383:ILE:O	1:A:461:GLN:CB	0.56	2.54	20	20
1:A:466:PHE:CZ	1:A:472:GLN:CD	0.56	2.79	19	5
1:A:389:GLY:O	1:A:391:LEU:CD1	0.56	2.54	17	11
1:A:487:LEU:N	1:A:487:LEU:HD23	0.56	2.16	11	1
1:A:463:MET:SD	1:A:510:TYR:CE1	0.56	2.99	2	5
1:A:465:ARG:NH1	1:A:511:TRP:CD1	0.56	2.74	13	1
1:A:510:TYR:O	1:A:514:ILE:CD1	0.55	2.55	18	20
1:A:376:LYS:CB	1:A:379:CYS:SG	0.55	2.94	20	17
1:A:390:THR:HG21	1:A:492:ARG:HB3	0.55	1.78	16	1
1:A:471:GLU:O	1:A:474:LEU:N	0.55	2.38	8	1
1:A:387:PRO:HG2	1:A:390:THR:HG21	0.55	1.77	20	5
1:A:391:LEU:N	1:A:391:LEU:CD1	0.55	2.65	7	1
1:A:466:PHE:CE1	1:A:472:GLN:CD	0.55	2.80	1	6
1:A:476:ILE:CG2	1:A:477:GLN:N	0.55	2.70	7	20
1:A:406:PHE:CB	1:A:466:PHE:HA	0.55	2.32	15	20
1:A:378:ASN:O	1:A:472:GLN:NE2	0.55	2.40	14	12
1:A:472:GLN:NE2	1:A:476:ILE:HD12	0.55	2.16	4	2
1:A:465:ARG:CZ	1:A:511:TRP:CD1	0.55	2.89	13	1
1:A:381:ILE:HG12	1:A:464:ILE:CG2	0.55	2.32	4	20
1:A:397:LEU:HD13	1:A:398:ALA:N	0.55	2.16	3	3
1:A:381:ILE:HG13	1:A:464:ILE:HG23	0.55	1.78	8	1
1:A:406:PHE:O	1:A:406:PHE:CD1	0.55	2.60	5	7
1:A:514:ILE:O	1:A:518:LYS:CG	0.54	2.55	7	3
1:A:513:TYR:CZ	1:A:517:LYS:CD	0.54	2.89	12	5
1:A:390:THR:HG23	1:A:394:GLU:HG2	0.54	1.80	4	5
1:A:406:PHE:CD1	1:A:406:PHE:O	0.54	2.60	16	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:492:ARG:O	1:A:492:ARG:NE	0.54	2.41	7	6
1:A:403:GLY:O	1:A:404:TYR:CD1	0.54	2.61	8	2
1:A:378:ASN:O	1:A:472:GLN:CG	0.54	2.55	6	6
1:A:518:LYS:O	1:A:519:ASN:CB	0.54	2.56	18	19
1:A:492:ARG:O	1:A:492:ARG:CD	0.54	2.56	16	10
1:A:492:ARG:CD	1:A:492:ARG:O	0.54	2.56	5	10
1:A:381:ILE:HB	1:A:499:ILE:O	0.54	2.03	10	20
1:A:515:LYS:O	1:A:519:ASN:CB	0.54	2.56	6	11
1:A:501:THR:HG23	1:A:501:THR:O	0.54	2.03	9	3
1:A:376:LYS:CG	1:A:379:CYS:SG	0.54	2.96	17	3
1:A:473:ARG:O	1:A:476:ILE:N	0.54	2.41	18	18
1:A:464:ILE:HD12	1:A:466:PHE:CZ	0.53	2.38	19	9
1:A:404:TYR:OH	1:A:474:LEU:CB	0.53	2.56	17	13
1:A:381:ILE:HD13	1:A:464:ILE:CG2	0.53	2.33	18	9
1:A:380:LEU:O	1:A:381:ILE:HG22	0.53	2.03	8	4
1:A:390:THR:HG23	1:A:394:GLU:HB2	0.53	1.80	13	2
1:A:513:TYR:CE2	1:A:517:LYS:CD	0.53	2.91	18	1
1:A:492:ARG:O	1:A:492:ARG:CG	0.53	2.56	4	1
1:A:491:ILE:HG13	1:A:491:ILE:O	0.53	2.04	5	6
1:A:518:LYS:O	1:A:519:ASN:ND2	0.53	2.42	17	8
1:A:407:TYR:N	1:A:407:TYR:CD1	0.53	2.76	3	5
1:A:472:GLN:OE1	1:A:476:ILE:HD13	0.53	2.04	15	8
1:A:381:ILE:CG1	1:A:464:ILE:HG22	0.53	2.34	4	1
1:A:398:ALA:HB3	1:A:491:ILE:CG2	0.53	2.32	19	9
1:A:490:GLU:HA	1:A:494:GLN:O	0.53	2.04	16	20
1:A:381:ILE:HD11	1:A:498:VAL:CG2	0.53	2.33	10	3
1:A:475:ALA:O	1:A:479:LEU:HD12	0.53	2.03	7	1
1:A:381:ILE:HD12	1:A:498:VAL:HG23	0.53	1.80	8	1
1:A:384:ILE:CD1	1:A:385:ASN:ND2	0.53	2.71	11	1
1:A:397:LEU:HD13	1:A:397:LEU:O	0.53	2.04	8	5
1:A:394:GLU:CA	1:A:394:GLU:OE1	0.53	2.57	1	4
1:A:409:ASP:O	1:A:463:MET:N	0.53	2.41	8	13
1:A:402:LEU:C	1:A:402:LEU:CD1	0.53	2.77	5	1
1:A:381:ILE:CD1	1:A:498:VAL:HG13	0.52	2.34	4	1
1:A:377:GLN:O	1:A:380:LEU:CD1	0.52	2.58	20	1
1:A:395:VAL:O	1:A:399:VAL:HG22	0.52	2.05	5	15
1:A:383:ILE:CD1	1:A:498:VAL:CG2	0.52	2.87	11	2
1:A:492:ARG:NE	1:A:492:ARG:O	0.52	2.42	2	5
1:A:472:GLN:NE2	1:A:476:ILE:HD13	0.52	2.19	10	3
1:A:390:THR:OG1	1:A:492:ARG:CD	0.52	2.57	8	6
1:A:387:PRO:CB	1:A:494:GLN:OE1	0.52	2.58	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:515:LYS:NZ	1:A:515:LYS:O	0.52	2.42	3	1
1:A:376:LYS:CD	1:A:376:LYS:N	0.52	2.72	10	1
1:A:397:LEU:C	1:A:397:LEU:CD1	0.52	2.78	16	7
1:A:402:LEU:HD23	1:A:479:LEU:CD2	0.52	2.35	5	1
1:A:383:ILE:O	1:A:461:GLN:CA	0.51	2.58	20	1
1:A:400:ARG:O	1:A:402:LEU:N	0.51	2.43	6	19
1:A:515:LYS:O	1:A:515:LYS:CE	0.51	2.59	3	3
1:A:378:ASN:O	1:A:472:GLN:HG2	0.51	2.06	19	5
1:A:402:LEU:C	1:A:402:LEU:HD13	0.51	2.24	5	1
1:A:470:ASP:N	1:A:470:ASP:OD1	0.51	2.44	18	4
1:A:519:ASN:ND2	1:A:519:ASN:OXT	0.51	2.43	1	1
1:A:381:ILE:CD1	1:A:498:VAL:CG2	0.51	2.88	10	1
1:A:504:GLU:O	1:A:508:LYS:HG3	0.51	2.06	4	20
1:A:504:GLU:O	1:A:508:LYS:CG	0.51	2.59	4	18
1:A:505:ASP:O	1:A:508:LYS:HD2	0.51	2.05	5	20
1:A:394:GLU:N	1:A:394:GLU:OE1	0.51	2.44	9	1
1:A:513:TYR:CE2	1:A:517:LYS:HD2	0.51	2.41	18	1
1:A:513:TYR:O	1:A:517:LYS:HG2	0.51	2.05	13	20
1:A:472:GLN:CD	1:A:476:ILE:CD1	0.51	2.80	15	11
1:A:378:ASN:HB2	1:A:472:GLN:NE2	0.51	2.20	8	1
1:A:387:PRO:CG	1:A:494:GLN:OE1	0.51	2.58	12	2
1:A:491:ILE:HG12	1:A:496:CYS:SG	0.50	2.46	19	18
1:A:491:ILE:O	1:A:491:ILE:HG13	0.50	2.06	9	14
1:A:470:ASP:OD1	1:A:470:ASP:N	0.50	2.43	7	3
1:A:464:ILE:C	1:A:464:ILE:CD1	0.50	2.80	5	10
1:A:384:ILE:HD11	1:A:497:ASP:HB2	0.50	1.81	11	2
1:A:463:MET:SD	1:A:510:TYR:CE2	0.50	3.04	1	1
1:A:479:LEU:HB2	1:A:487:LEU:CD2	0.50	2.37	2	2
1:A:390:THR:OG1	1:A:492:ARG:NE	0.50	2.43	8	2
1:A:387:PRO:CA	1:A:494:GLN:NE2	0.50	2.75	10	1
1:A:472:GLN:O	1:A:472:GLN:OE1	0.50	2.30	6	4
1:A:519:ASN:OXT	1:A:519:ASN:ND2	0.50	2.44	12	2
1:A:479:LEU:CB	1:A:487:LEU:HD22	0.50	2.35	7	1
1:A:491:ILE:N	1:A:494:GLN:O	0.50	2.44	4	18
1:A:402:LEU:HG	1:A:403:GLY:N	0.50	2.22	19	7
1:A:385:ASN:O	1:A:496:CYS:SG	0.50	2.70	14	15
1:A:410:TYR:HB2	1:A:462:ALA:HB2	0.50	1.84	19	1
1:A:509:ASN:O	1:A:513:TYR:CB	0.50	2.60	17	7
1:A:515:LYS:CE	1:A:515:LYS:O	0.49	2.59	6	4
1:A:383:ILE:HG13	1:A:384:ILE:N	0.49	2.23	13	20
1:A:400:ARG:HD3	1:A:401:HIS:N	0.49	2.22	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:386:ILE:HG13	1:A:461:GLN:N	0.49	2.22	18	5
1:A:510:TYR:CE2	1:A:514:ILE:HD12	0.49	2.42	18	13
1:A:381:ILE:HG23	1:A:464:ILE:HG23	0.49	1.84	12	2
1:A:397:LEU:CD1	1:A:397:LEU:C	0.49	2.80	11	9
1:A:404:TYR:HD2	1:A:475:ALA:HB2	0.49	1.67	11	1
1:A:404:TYR:OH	1:A:474:LEU:CD2	0.49	2.57	5	5
1:A:472:GLN:OE1	1:A:472:GLN:O	0.49	2.30	17	2
1:A:376:LYS:HB2	1:A:379:CYS:SG	0.49	2.48	3	18
1:A:513:TYR:CE1	1:A:517:LYS:HD2	0.49	2.42	2	2
1:A:390:THR:HG23	1:A:394:GLU:CB	0.49	2.36	13	3
1:A:468:ASN:HB2	1:A:471:GLU:CG	0.48	2.38	5	3
1:A:464:ILE:CD1	1:A:464:ILE:C	0.48	2.82	4	9
1:A:387:PRO:CA	1:A:494:GLN:OE1	0.48	2.61	12	2
1:A:489:ILE:HG13	1:A:490:GLU:N	0.48	2.23	16	2
1:A:404:TYR:CD2	1:A:471:GLU:HB3	0.48	2.42	8	1
1:A:380:LEU:HD23	1:A:465:ARG:CG	0.48	2.38	4	1
1:A:378:ASN:O	1:A:472:GLN:OE1	0.48	2.32	8	1
1:A:465:ARG:NH2	1:A:511:TRP:NE1	0.48	2.62	13	1
1:A:518:LYS:O	1:A:519:ASN:OD1	0.48	2.31	3	6
1:A:476:ILE:HA	1:A:479:LEU:HD12	0.48	1.85	5	2
1:A:397:LEU:HD22	1:A:397:LEU:O	0.48	2.09	10	3
1:A:397:LEU:C	1:A:397:LEU:HD22	0.48	2.29	3	1
1:A:383:ILE:HD11	1:A:496:CYS:HB2	0.48	1.86	4	1
1:A:400:ARG:HD2	1:A:406:PHE:CZ	0.48	2.44	16	1
1:A:510:TYR:O	1:A:514:ILE:HG12	0.47	2.09	13	20
1:A:410:TYR:CD1	1:A:410:TYR:C	0.47	2.87	20	2
1:A:402:LEU:HD11	1:A:478:LYS:CB	0.47	2.39	16	1
1:A:491:ILE:HG23	1:A:496:CYS:SG	0.47	2.49	4	1
1:A:466:PHE:CD1	1:A:472:GLN:CG	0.47	2.97	12	7
1:A:380:LEU:C	1:A:381:ILE:CG2	0.47	2.82	8	12
1:A:399:VAL:HG23	1:A:400:ARG:N	0.47	2.24	13	16
1:A:473:ARG:HD3	1:A:474:LEU:N	0.47	2.24	2	6
1:A:400:ARG:CD	1:A:401:HIS:N	0.47	2.77	18	3
1:A:465:ARG:HB2	1:A:510:TYR:CE2	0.47	2.44	2	2
1:A:386:ILE:HD13	1:A:387:PRO:O	0.47	2.08	3	1
1:A:390:THR:CG2	1:A:492:ARG:CG	0.47	2.91	16	2
1:A:406:PHE:CE2	1:A:466:PHE:CE2	0.47	3.02	7	6
1:A:378:ASN:CB	1:A:472:GLN:OE1	0.47	2.63	20	1
1:A:511:TRP:O	1:A:514:ILE:HG12	0.47	2.09	19	20
1:A:378:ASN:O	1:A:472:GLN:CD	0.47	2.53	10	13
1:A:378:ASN:O	1:A:472:GLN:HG3	0.47	2.09	4	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:476:ILE:CD1	1:A:500:SER:HB2	0.47	2.37	3	9
1:A:400:ARG:HG2	1:A:404:TYR:O	0.47	2.09	6	8
1:A:394:GLU:OE1	1:A:394:GLU:CA	0.47	2.63	17	1
1:A:393:ALA:HB3	1:A:394:GLU:OE2	0.47	2.10	19	1
1:A:404:TYR:OH	1:A:474:LEU:CD1	0.47	2.60	20	1
1:A:487:LEU:HD23	1:A:487:LEU:N	0.47	2.25	20	1
1:A:386:ILE:O	1:A:386:ILE:CG2	0.47	2.63	1	2
1:A:515:LYS:HE3	1:A:515:LYS:O	0.47	2.10	16	5
1:A:515:LYS:O	1:A:515:LYS:HD2	0.47	2.09	17	1
1:A:406:PHE:O	1:A:408:CYS:SG	0.47	2.73	8	15
1:A:397:LEU:O	1:A:401:HIS:CB	0.47	2.62	3	3
1:A:387:PRO:CD	1:A:491:ILE:HD11	0.47	2.40	4	1
1:A:386:ILE:CG1	1:A:461:GLN:N	0.47	2.78	20	3
1:A:510:TYR:CD2	1:A:514:ILE:HD11	0.47	2.45	1	5
1:A:380:LEU:CD1	1:A:507:GLU:HG3	0.47	2.39	2	8
1:A:397:LEU:O	1:A:401:HIS:HB2	0.47	2.10	10	4
1:A:400:ARG:HG3	1:A:401:HIS:N	0.47	2.23	9	1
1:A:402:LEU:CD2	1:A:475:ALA:O	0.47	2.62	11	1
1:A:387:PRO:O	1:A:390:THR:OG1	0.47	2.32	15	1
1:A:392:LYS:CB	1:A:410:TYR:HB3	0.46	2.40	19	8
1:A:406:PHE:CD1	1:A:464:ILE:HG12	0.46	2.44	2	10
1:A:464:ILE:CG1	1:A:466:PHE:CE1	0.46	2.98	8	1
1:A:379:CYS:HA	1:A:472:GLN:HG2	0.46	1.86	1	5
1:A:391:LEU:N	1:A:391:LEU:HD22	0.46	2.25	10	2
1:A:381:ILE:HD12	1:A:498:VAL:CG2	0.46	2.40	8	1
1:A:384:ILE:CD1	1:A:497:ASP:HB2	0.46	2.40	11	1
1:A:505:ASP:O	1:A:508:LYS:HG3	0.46	2.11	9	20
1:A:386:ILE:O	1:A:386:ILE:HG23	0.46	2.11	11	4
1:A:390:THR:CG2	1:A:492:ARG:CB	0.46	2.94	16	1
1:A:383:ILE:HG23	1:A:462:ALA:O	0.46	2.11	20	3
1:A:383:ILE:HB	1:A:498:VAL:HG13	0.46	1.86	9	1
1:A:406:PHE:CE2	1:A:466:PHE:CZ	0.46	3.04	17	1
1:A:400:ARG:C	1:A:402:LEU:N	0.46	2.68	16	16
1:A:501:THR:CG2	1:A:501:THR:O	0.46	2.62	20	2
1:A:391:LEU:HD22	1:A:391:LEU:N	0.46	2.24	15	1
1:A:379:CYS:SG	1:A:468:ASN:C	0.46	2.93	20	1
1:A:380:LEU:HD13	1:A:507:GLU:CB	0.46	2.41	2	3
1:A:396:VAL:CG1	1:A:408:CYS:SG	0.46	2.98	9	7
1:A:383:ILE:HG13	1:A:497:ASP:O	0.46	2.11	3	19
1:A:514:ILE:HA	1:A:517:LYS:CG	0.46	2.41	13	13
1:A:376:LYS:HB3	1:A:379:CYS:SG	0.46	2.51	2	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:515:LYS:O	1:A:519:ASN:CA	0.46	2.64	2	3
1:A:519:ASN:ND2	1:A:519:ASN:C	0.46	2.69	2	3
1:A:396:VAL:O	1:A:399:VAL:HG23	0.46	2.10	16	1
1:A:393:ALA:O	1:A:397:LEU:CB	0.46	2.63	20	1
1:A:514:ILE:O	1:A:518:LYS:HG3	0.46	2.10	20	2
1:A:376:LYS:HE3	1:A:511:TRP:CE2	0.46	2.45	8	1
1:A:405:GLU:O	1:A:405:GLU:CG	0.46	2.63	11	1
1:A:379:CYS:O	1:A:465:ARG:HA	0.46	2.10	12	15
1:A:390:THR:OG1	1:A:492:ARG:HD2	0.46	2.11	7	6
1:A:478:LYS:N	1:A:478:LYS:HE3	0.46	2.25	18	3
1:A:409:ASP:O	1:A:463:MET:CB	0.46	2.64	8	1
1:A:494:GLN:OE1	1:A:496:CYS:SG	0.46	2.73	14	1
1:A:396:VAL:CG1	1:A:400:ARG:NH1	0.46	2.79	16	1
1:A:378:ASN:HB2	1:A:472:GLN:OE1	0.45	2.10	20	1
1:A:509:ASN:O	1:A:513:TYR:HB2	0.45	2.11	5	3
1:A:376:LYS:HD2	1:A:376:LYS:N	0.45	2.26	19	2
1:A:396:VAL:HA	1:A:399:VAL:CG2	0.45	2.41	4	3
1:A:404:TYR:CE1	1:A:471:GLU:HB3	0.45	2.46	19	1
1:A:376:LYS:HG2	1:A:379:CYS:SG	0.45	2.51	10	1
1:A:380:LEU:O	1:A:381:ILE:CG2	0.45	2.64	8	1
1:A:502:ILE:O	1:A:502:ILE:HG22	0.45	2.11	15	1
1:A:479:LEU:CB	1:A:487:LEU:HD23	0.45	2.41	17	1
1:A:513:TYR:O	1:A:517:LYS:CG	0.45	2.65	19	5
1:A:466:PHE:N	1:A:466:PHE:CD1	0.45	2.85	19	10
1:A:472:GLN:CD	1:A:476:ILE:HD13	0.45	2.31	13	10
1:A:399:VAL:CG2	1:A:406:PHE:CE1	0.45	3.00	8	10
1:A:407:TYR:CD1	1:A:407:TYR:N	0.45	2.83	13	2
1:A:394:GLU:OE1	1:A:394:GLU:N	0.45	2.49	14	3
1:A:410:TYR:HA	1:A:462:ALA:HA	0.45	1.89	17	11
1:A:404:TYR:OH	1:A:474:LEU:HB3	0.45	2.12	11	4
1:A:491:ILE:CG1	1:A:496:CYS:SG	0.45	3.05	1	3
1:A:407:TYR:O	1:A:465:ARG:N	0.45	2.43	11	6
1:A:406:PHE:HB2	1:A:466:PHE:HA	0.45	1.89	18	11
1:A:478:LYS:HE2	1:A:478:LYS:N	0.45	2.27	14	3
1:A:463:MET:SD	1:A:464:ILE:N	0.45	2.90	3	1
1:A:402:LEU:HD11	1:A:478:LYS:HB3	0.45	1.89	16	1
1:A:515:LYS:O	1:A:519:ASN:HB2	0.45	2.12	14	2
1:A:518:LYS:HG3	1:A:519:ASN:N	0.45	2.26	18	3
1:A:518:LYS:O	1:A:519:ASN:CG	0.45	2.56	17	3
1:A:380:LEU:CD1	1:A:507:GLU:HB2	0.44	2.42	13	1
1:A:392:LYS:HE2	1:A:410:TYR:CD1	0.44	2.47	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:TYR:CD1	1:A:514:ILE:HD13	0.44	2.47	2	7
1:A:386:ILE:HG23	1:A:386:ILE:O	0.44	2.12	16	4
1:A:378:ASN:O	1:A:380:LEU:N	0.44	2.50	16	6
1:A:466:PHE:CZ	1:A:472:GLN:HG2	0.44	2.46	12	3
1:A:403:GLY:C	1:A:404:TYR:CD1	0.44	2.91	7	1
1:A:389:GLY:O	1:A:390:THR:C	0.44	2.56	13	19
1:A:466:PHE:CE1	1:A:472:GLN:HG3	0.44	2.47	10	2
1:A:399:VAL:HG23	1:A:406:PHE:CE1	0.44	2.47	9	5
1:A:478:LYS:HE3	1:A:478:LYS:N	0.44	2.28	13	2
1:A:383:ILE:O	1:A:461:GLN:HB2	0.44	2.13	16	2
1:A:382:LYS:O	1:A:499:ILE:HD12	0.44	2.13	5	2
1:A:383:ILE:CG1	1:A:497:ASP:O	0.44	2.66	11	4
1:A:499:ILE:CG2	1:A:501:THR:HG22	0.44	2.42	6	2
1:A:479:LEU:CB	1:A:487:LEU:CD2	0.44	2.95	2	1
1:A:519:ASN:OD1	1:A:519:ASN:C	0.44	2.56	17	3
1:A:478:LYS:CA	1:A:478:LYS:HE2	0.44	2.43	15	1
1:A:515:LYS:O	1:A:515:LYS:CD	0.44	2.66	17	1
1:A:471:GLU:O	1:A:472:GLN:C	0.43	2.56	10	20
1:A:466:PHE:CD1	1:A:472:GLN:HG3	0.43	2.48	5	2
1:A:379:CYS:HA	1:A:472:GLN:CB	0.43	2.44	1	3
1:A:385:ASN:CB	1:A:496:CYS:HA	0.43	2.43	13	9
1:A:470:ASP:O	1:A:473:ARG:HB3	0.43	2.13	10	8
1:A:379:CYS:HA	1:A:472:GLN:HG3	0.43	1.90	20	5
1:A:406:PHE:HB2	1:A:465:ARG:O	0.43	2.13	15	7
1:A:390:THR:CG2	1:A:492:ARG:CD	0.43	2.96	15	1
1:A:387:PRO:HG3	1:A:494:GLN:OE1	0.43	2.13	12	2
1:A:400:ARG:HD2	1:A:401:HIS:N	0.43	2.29	2	1
1:A:381:ILE:HB	1:A:500:SER:HA	0.43	1.89	12	9
1:A:387:PRO:HG3	1:A:494:GLN:CG	0.43	2.43	4	1
1:A:478:LYS:N	1:A:478:LYS:HE2	0.43	2.29	11	5
1:A:515:LYS:O	1:A:515:LYS:HE3	0.43	2.13	9	4
1:A:400:ARG:HD2	1:A:406:PHE:CE1	0.43	2.48	16	1
1:A:406:PHE:CG	1:A:466:PHE:CD2	0.43	3.07	20	1
1:A:473:ARG:O	1:A:476:ILE:HB	0.43	2.13	3	6
1:A:379:CYS:HB2	1:A:466:PHE:HB2	0.43	1.90	10	8
1:A:517:LYS:HB2	1:A:517:LYS:NZ	0.43	2.28	7	1
1:A:466:PHE:CD2	1:A:472:GLN:HA	0.43	2.47	2	1
1:A:515:LYS:O	1:A:519:ASN:CG	0.43	2.57	9	1
1:A:387:PRO:HG2	1:A:390:THR:CB	0.43	2.44	16	1
1:A:390:THR:CG2	1:A:394:GLU:HB2	0.43	2.43	20	1
1:A:390:THR:C	1:A:391:LEU:HD13	0.43	2.34	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:381:ILE:HG21	1:A:472:GLN:NE2	0.43	2.29	7	1
1:A:385:ASN:HB2	1:A:496:CYS:HA	0.43	1.90	8	2
1:A:387:PRO:HB3	1:A:494:GLN:CG	0.43	2.43	17	1
1:A:383:ILE:O	1:A:461:GLN:HA	0.43	2.13	20	1
1:A:466:PHE:CD1	1:A:466:PHE:N	0.43	2.87	6	5
1:A:474:LEU:O	1:A:478:LYS:HE3	0.43	2.14	13	5
1:A:479:LEU:HB3	1:A:487:LEU:HD23	0.43	1.90	17	1
1:A:409:ASP:N	1:A:463:MET:O	0.43	2.52	3	10
1:A:519:ASN:C	1:A:519:ASN:OD1	0.43	2.57	11	3
1:A:492:ARG:O	1:A:492:ARG:HD3	0.43	2.14	16	3
1:A:399:VAL:HG23	1:A:406:PHE:CZ	0.43	2.49	17	4
1:A:477:GLN:HG2	1:A:478:LYS:CE	0.43	2.43	14	2
1:A:404:TYR:CE2	1:A:471:GLU:HB3	0.43	2.48	8	1
1:A:471:GLU:O	1:A:474:LEU:HB2	0.43	2.14	8	1
1:A:390:THR:HG23	1:A:492:ARG:CD	0.43	2.44	16	1
1:A:379:CYS:SG	1:A:469:SER:CA	0.43	3.07	20	1
1:A:387:PRO:HG2	1:A:491:ILE:HD11	0.43	1.91	12	1
1:A:518:LYS:O	1:A:519:ASN:HB3	0.42	2.14	14	3
1:A:380:LEU:CD1	1:A:507:GLU:CG	0.42	2.96	5	1
1:A:403:GLY:O	1:A:404:TYR:CG	0.42	2.72	7	2
1:A:384:ILE:O	1:A:385:ASN:HB2	0.42	2.14	8	1
1:A:387:PRO:HB2	1:A:390:THR:OG1	0.42	2.13	15	2
1:A:401:HIS:O	1:A:401:HIS:ND1	0.42	2.52	2	1
1:A:512:ASN:O	1:A:516:PHE:HB2	0.42	2.14	4	2
1:A:402:LEU:HD12	1:A:402:LEU:C	0.42	2.34	14	1
1:A:387:PRO:HG2	1:A:390:THR:OG1	0.42	2.14	16	1
1:A:383:ILE:O	1:A:461:GLN:HB3	0.42	2.14	3	1
1:A:492:ARG:HD3	1:A:492:ARG:O	0.42	2.14	14	2
1:A:379:CYS:CB	1:A:466:PHE:HB2	0.42	2.44	8	1
1:A:390:THR:HG22	1:A:492:ARG:HG3	0.42	1.90	15	1
1:A:395:VAL:HG22	1:A:491:ILE:HD13	0.42	1.92	17	1
1:A:387:PRO:N	1:A:494:GLN:NE2	0.42	2.68	10	1
1:A:380:LEU:HD13	1:A:507:GLU:HB2	0.42	1.91	2	1
1:A:408:CYS:C	1:A:409:ASP:OD1	0.42	2.57	5	1
1:A:378:ASN:HB3	1:A:472:GLN:NE2	0.42	2.30	8	2
1:A:384:ILE:HG13	1:A:497:ASP:CB	0.42	2.45	1	2
1:A:477:GLN:HG2	1:A:478:LYS:HE2	0.42	1.90	3	1
1:A:508:LYS:HD2	1:A:509:ASN:ND2	0.42	2.30	3	1
1:A:402:LEU:CD2	1:A:475:ALA:HB1	0.42	2.42	6	2
1:A:400:ARG:C	1:A:400:ARG:CD	0.42	2.87	7	2
1:A:465:ARG:CZ	1:A:511:TRP:NE1	0.42	2.82	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:379:CYS:SG	1:A:469:SER:HA	0.42	2.54	20	1
1:A:386:ILE:CD1	1:A:387:PRO:O	0.42	2.68	3	1
1:A:489:ILE:HD13	1:A:490:GLU:C	0.42	2.35	10	2
1:A:379:CYS:HB3	1:A:468:ASN:O	0.42	2.15	8	1
1:A:396:VAL:O	1:A:400:ARG:HB3	0.42	2.15	9	1
1:A:515:LYS:O	1:A:519:ASN:HA	0.41	2.15	1	3
1:A:387:PRO:HG2	1:A:390:THR:CG2	0.41	2.44	4	3
1:A:404:TYR:CD1	1:A:471:GLU:HB3	0.41	2.49	20	1
1:A:404:TYR:CE1	1:A:471:GLU:CD	0.41	2.93	4	1
1:A:395:VAL:HA	1:A:491:ILE:HD13	0.41	1.91	9	2
1:A:387:PRO:HB3	1:A:494:GLN:HG2	0.41	1.90	12	1
1:A:472:GLN:NE2	1:A:476:ILE:HD11	0.41	2.30	3	3
1:A:376:LYS:HD2	1:A:511:TRP:NE1	0.41	2.29	8	1
1:A:396:VAL:CG1	1:A:400:ARG:CZ	0.41	2.98	16	1
1:A:402:LEU:HD22	1:A:479:LEU:HG	0.41	1.90	18	1
1:A:514:ILE:HA	1:A:517:LYS:HG3	0.41	1.91	3	3
1:A:394:GLU:N	1:A:394:GLU:CD	0.41	2.73	16	1
1:A:396:VAL:O	1:A:399:VAL:HG22	0.41	2.15	16	1
1:A:386:ILE:HD13	1:A:386:ILE:C	0.41	2.35	3	1
1:A:404:TYR:CE1	1:A:471:GLU:OE1	0.41	2.73	3	2
1:A:472:GLN:CD	1:A:476:ILE:HD12	0.41	2.35	6	1
1:A:490:GLU:CA	1:A:494:GLN:O	0.41	2.68	16	1
1:A:392:LYS:O	1:A:396:VAL:CB	0.41	2.69	20	1
1:A:376:LYS:HE3	1:A:467:GLN:O	0.41	2.15	17	1
1:A:515:LYS:C	1:A:515:LYS:HE2	0.41	2.36	17	1
1:A:478:LYS:O	1:A:479:LEU:C	0.41	2.59	10	1
1:A:510:TYR:CE1	1:A:514:ILE:CD1	0.41	3.04	1	1
1:A:380:LEU:C	1:A:381:ILE:HG22	0.41	2.36	3	1
1:A:393:ALA:O	1:A:397:LEU:HB3	0.41	2.16	13	1
1:A:377:GLN:OE1	1:A:469:SER:HB3	0.41	2.16	20	1
1:A:402:LEU:HD22	1:A:479:LEU:CG	0.41	2.45	2	1
1:A:468:ASN:HB3	1:A:471:GLU:HG2	0.41	1.93	7	1
1:A:464:ILE:CD1	1:A:466:PHE:CZ	0.41	3.04	19	1
1:A:513:TYR:CE2	1:A:517:LYS:HD3	0.41	2.50	12	1
1:A:386:ILE:CG2	1:A:386:ILE:O	0.40	2.69	2	1
1:A:515:LYS:HE2	1:A:515:LYS:C	0.40	2.36	8	1
1:A:515:LYS:HG2	1:A:515:LYS:O	0.40	2.16	16	1
1:A:376:LYS:O	1:A:376:LYS:HG2	0.40	2.17	8	1
1:A:379:CYS:HB3	1:A:466:PHE:HB2	0.40	1.93	8	1
1:A:390:THR:HG23	1:A:492:ARG:HD2	0.40	1.93	16	1
1:A:404:TYR:OH	1:A:474:LEU:CG	0.40	2.69	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:TYR:O	1:A:514:ILE:HD13	0.40	2.16	2	1
1:A:515:LYS:O	1:A:515:LYS:HG2	0.40	2.17	6	1
1:A:410:TYR:CD1	1:A:410:TYR:O	0.40	2.74	8	1
1:A:396:VAL:O	1:A:400:ARG:HD3	0.40	2.16	16	1
1:A:387:PRO:HB3	1:A:494:GLN:NE2	0.40	2.31	4	1
1:A:510:TYR:O	1:A:514:ILE:CG1	0.40	2.70	2	1
1:A:401:HIS:CD2	1:A:401:HIS:O	0.40	2.74	3	1
1:A:387:PRO:HA	1:A:494:GLN:NE2	0.40	2.31	14	1
1:A:463:MET:SD	1:A:510:TYR:CD1	0.40	3.15	10	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	86/137 (63%)	72±1 (84±1%)	11±1 (12±1%)	3±0 (3±0%)	6	36
All	All	1720/2740 (63%)	1447 (84%)	215 (12%)	58 (3%)	6	36

All 3 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	379	CYS	20
1	A	402	LEU	20
1	A	401	HIS	18

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	80/129 (62%)	46±2 (57±3%)	34±2 (43±3%)	0 3
All	All	1600/2580 (62%)	919 (57%)	681 (43%)	0 3

All 64 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	408	CYS	20
1	A	464	ILE	20
1	A	383	ILE	20
1	A	508	LYS	20
1	A	463	MET	20
1	A	509	ASN	20
1	A	514	ILE	20
1	A	391	LEU	20
1	A	492	ARG	20
1	A	511	TRP	20
1	A	400	ARG	20
1	A	476	ILE	20
1	A	410	TYR	19
1	A	381	ILE	19
1	A	392	LYS	19
1	A	473	ARG	18
1	A	380	LEU	18
1	A	478	LYS	18
1	A	470	ASP	17
1	A	474	LEU	17
1	A	519	ASN	16
1	A	518	LYS	16
1	A	506	GLU	15
1	A	517	LYS	15
1	A	461	GLN	14
1	A	494	GLN	13
1	A	397	LEU	12
1	A	497	ASP	12
1	A	488	GLN	11
1	A	505	ASP	11
1	A	376	LYS	10
1	A	377	GLN	9
1	A	491	ILE	9
1	A	472	GLN	8
1	A	467	GLN	8
1	A	515	LYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	512	ASN	8
1	A	516	PHE	7
1	A	487	LEU	7
1	A	501	THR	7
1	A	394	GLU	7
1	A	468	ASN	7
1	A	489	ILE	6
1	A	382	LYS	6
1	A	490	GLU	6
1	A	405	GLU	6
1	A	388	GLN	6
1	A	495	ILE	5
1	A	386	ILE	4
1	A	384	ILE	3
1	A	401	HIS	3
1	A	469	SER	3
1	A	378	ASN	2
1	A	498	VAL	2
1	A	409	ASP	2
1	A	379	CYS	2
1	A	407	TYR	2
1	A	499	ILE	2
1	A	465	ARG	1
1	A	496	CYS	1
1	A	390	THR	1
1	A	466	PHE	1
1	A	402	LEU	1
1	A	477	GLN	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 carbohydrates 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1449
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	127	-0.13 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	0.12 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	126	0.18 ± 0.15	None needed (< 0.5 ppm)
^{15}N	120	-0.27 ± 0.30	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 942 atoms were assigned a chemical shift out of a possible 1163. 10 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	429/431 (100%)	171/172 (99%)	174/174 (100%)	84/85 (99%)
Sidechain	485/645 (75%)	300/378 (79%)	185/233 (79%)	0/34 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	28/87 (32%)	15/45 (33%)	12/39 (31%)	1/3 (33%)
Overall	942/1163 (81%)	486/595 (82%)	371/446 (83%)	85/122 (70%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1317 atoms were assigned a chemical shift out of a possible 1697. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	616/644 (96%)	243/257 (95%)	253/260 (97%)	120/127 (94%)
Sidechain	673/950 (71%)	407/554 (73%)	266/346 (77%)	0/50 (0%)
Aromatic	28/103 (27%)	15/53 (28%)	12/43 (28%)	1/7 (14%)
Overall	1317/1697 (78%)	665/864 (77%)	531/649 (82%)	121/184 (66%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	513	TYR	CD2	115.20	140.11 – 125.31	-11.8
1	A	510	TYR	CE1	130.70	124.14 – 111.74	10.3
1	A	510	TYR	CE2	130.70	124.68 – 111.18	9.5
1	A	486	LYS	CE	35.07	46.00 – 37.80	-8.3
1	A	392	LYS	HE2	1.83	3.87 – 1.97	-5.7
1	A	392	LYS	HE3	1.83	3.86 – 1.96	-5.7
1	A	487	LEU	CD2	14.86	32.60 – 15.60	-5.4
1	A	375	ILE	CG2	24.72	24.63 – 10.43	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

