



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:36 pm BST

PDB ID : 2K7L  
Title : NMR structure of a complex formed by the C-terminal domain of human RAP74 and a phosphorylated peptide from the central domain of the FCP1  
Authors : Yang, A.; Abbott, K.L.; Desjardins, A.; Di Lello, P.; Omichinski, J.G.; Legault, P.  
Deposited on : 2008-08-13

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

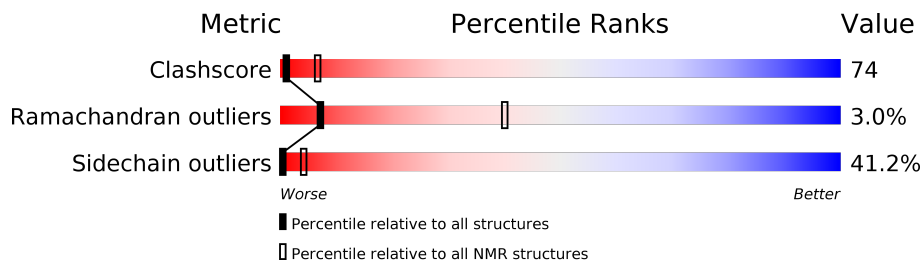
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 71%.

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  $\geq 3$ , 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	B	19	
2	A	67	

## 2 Ensemble composition and analysis i

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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	B:587-B:598, A:454-A:477, A:484-A:517 (70)	0.19	1

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 5 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 7, 8, 9, 15, 18, 19, 20
2	5, 6, 11
3	12, 17
4	10, 14
5	4, 16
Single-model clusters	2; 3; 13; 21

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1465 atoms, of which 746 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called centFCP1-T584PO4 peptide.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	P	
1	B	19	318	101	151	24	41	1	0

- Molecule 2 is a protein called General transcription factor IIF subunit 1.

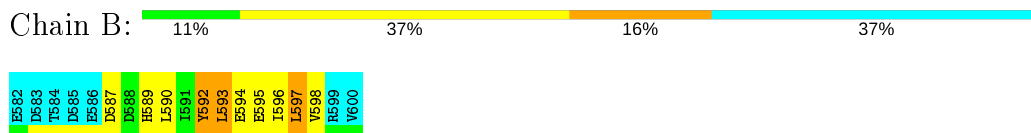
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	A	67	1147	346	595	101	102	3	0

## 4 Residue-property plots [i](#)

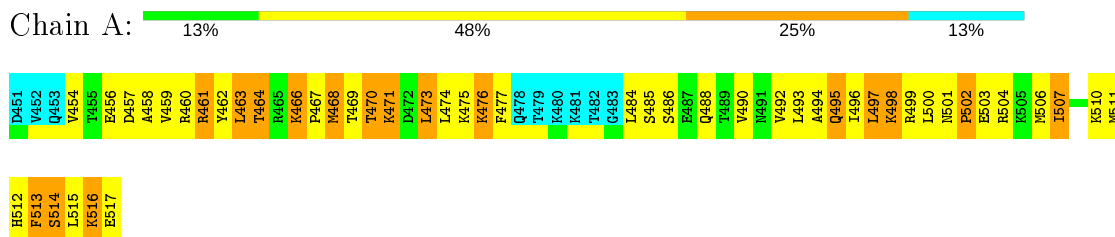
### 4.1 Average score per residue in the NMR ensemble

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: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

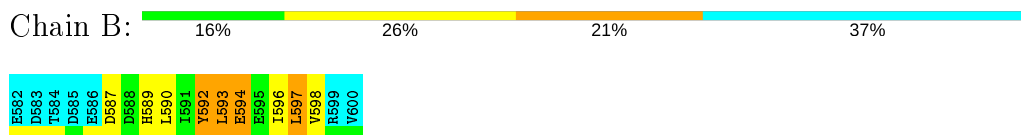


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

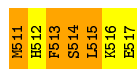
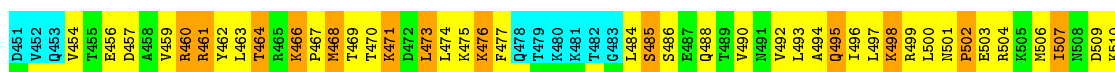
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1



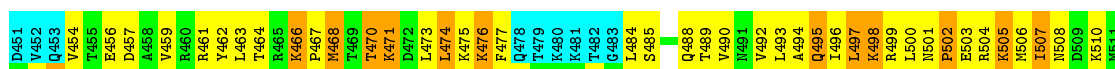
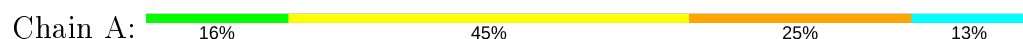


#### 4.2.2 Score per residue for model 2

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

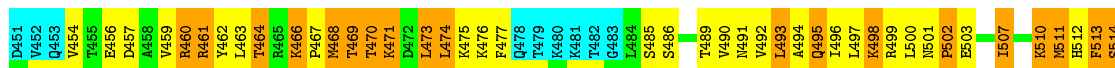
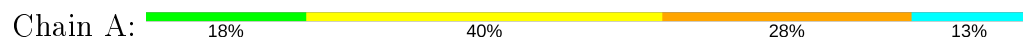


#### 4.2.3 Score per residue for model 3

- Molecule 1: centFCP1-T584PO4 peptide

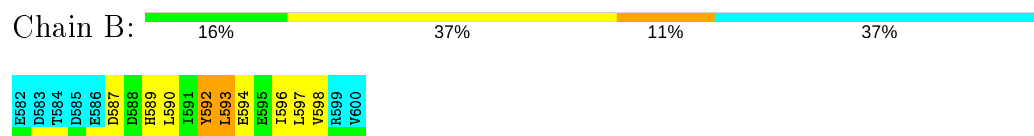


- Molecule 2: General transcription factor IIF subunit 1

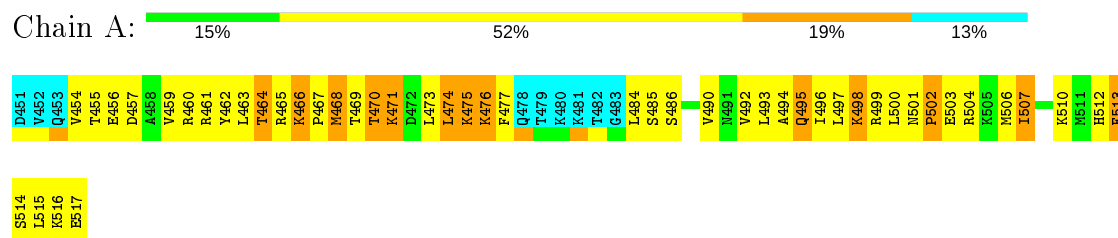


#### 4.2.4 Score per residue for model 4

- Molecule 1: centFCP1-T584PO4 peptide

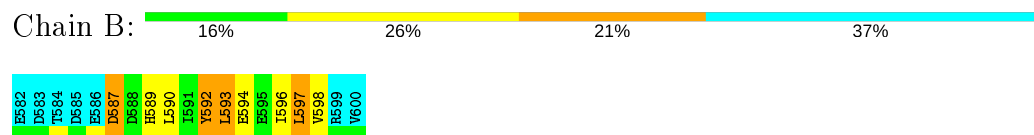


- Molecule 2: General transcription factor IIF subunit 1

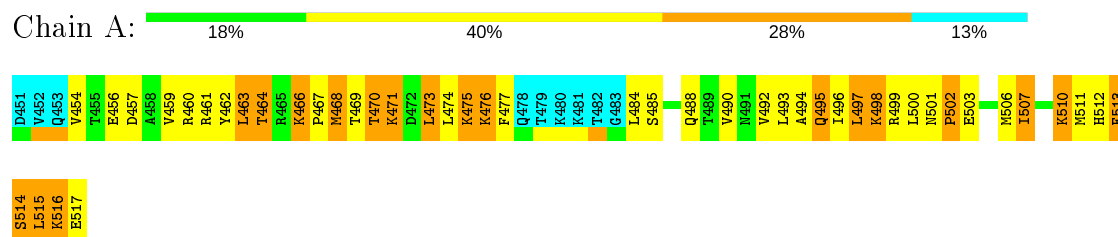


#### 4.2.5 Score per residue for model 5

- Molecule 1: centFCP1-T584PO4 peptide

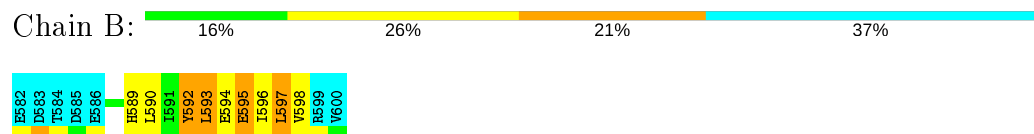


- Molecule 2: General transcription factor IIF subunit 1

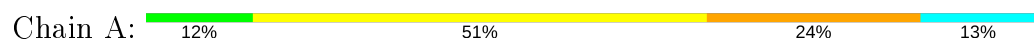


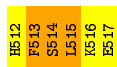
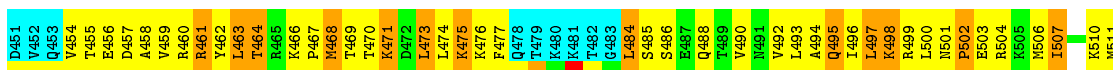
#### 4.2.6 Score per residue for model 6

- Molecule 1: centFCP1-T584PO4 peptide



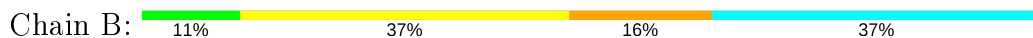
- Molecule 2: General transcription factor IIF subunit 1



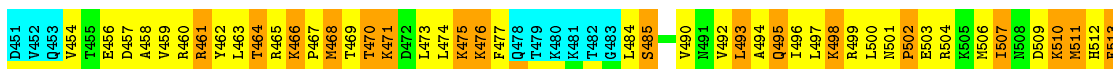


#### 4.2.7 Score per residue for model 7

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

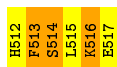


#### 4.2.8 Score per residue for model 8

- Molecule 1: centFCP1-T584PO4 peptide



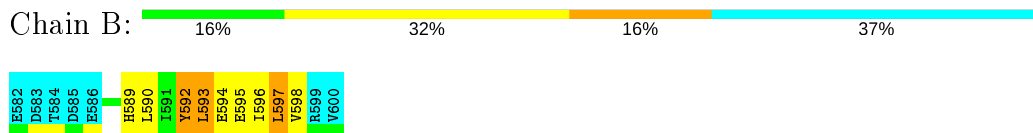
- Molecule 2: General transcription factor IIF subunit 1



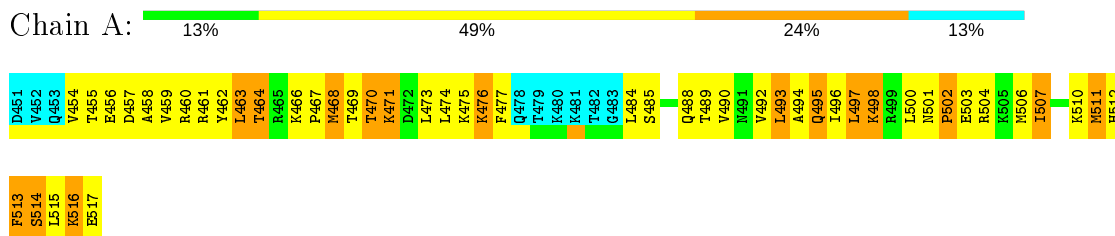
#### 4.2.9 Score per residue for model 9

- Molecule 1: centFCP1-T584PO4 peptide





- Molecule 2: General transcription factor IIF subunit 1

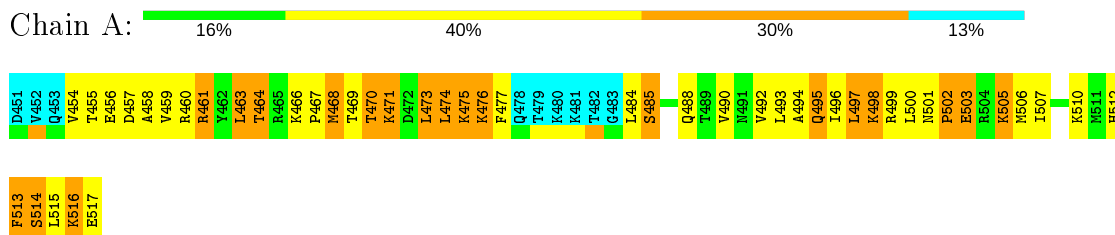


#### 4.2.10 Score per residue for model 10

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

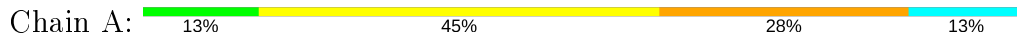


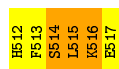
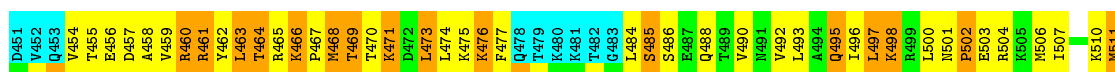
#### 4.2.11 Score per residue for model 11

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1



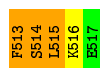
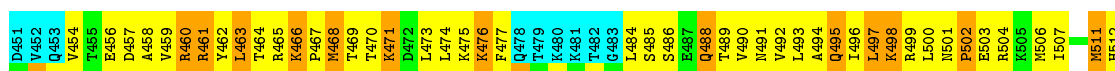
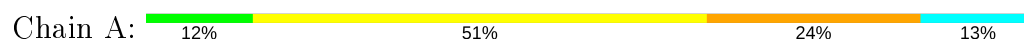


#### 4.2.12 Score per residue for model 12

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

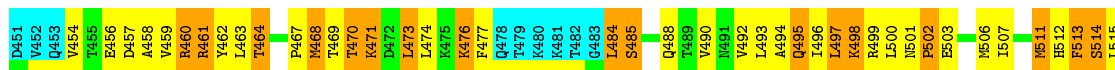
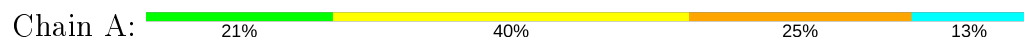


#### 4.2.13 Score per residue for model 13

- Molecule 1: centFCP1-T584PO4 peptide

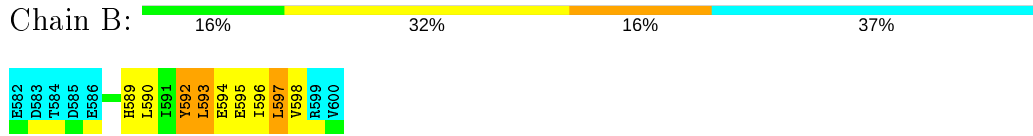


- Molecule 2: General transcription factor IIF subunit 1

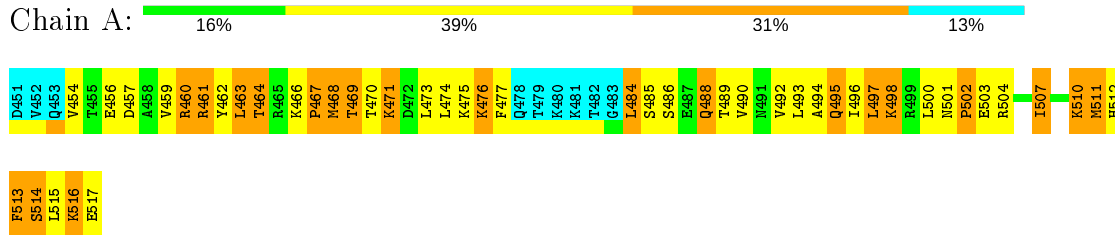


#### 4.2.14 Score per residue for model 14

- Molecule 1: centFCP1-T584PO4 peptide

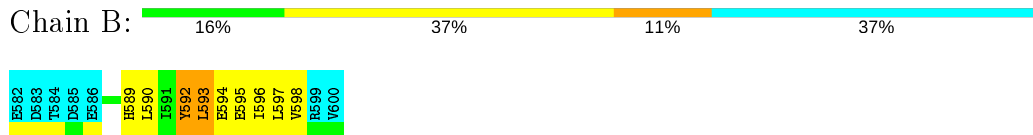


- Molecule 2: General transcription factor IIF subunit 1

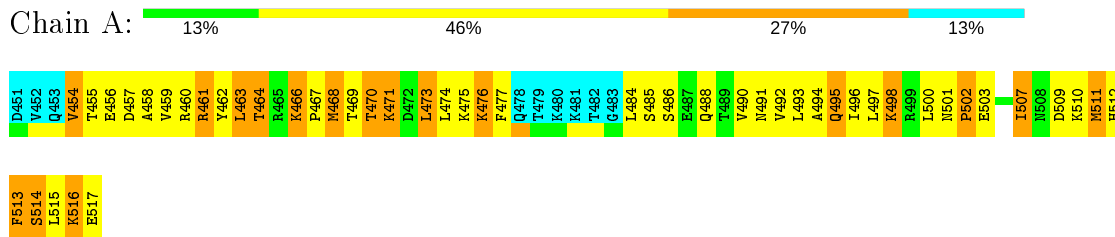


#### 4.2.15 Score per residue for model 15

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

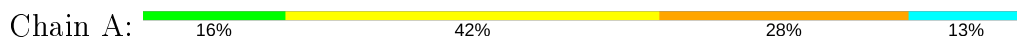


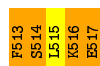
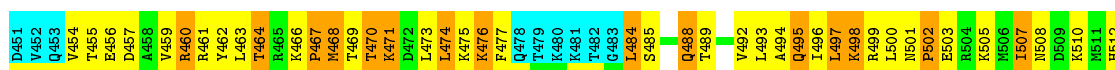
#### 4.2.16 Score per residue for model 16

- Molecule 1: centFCP1-T584PO4 peptide



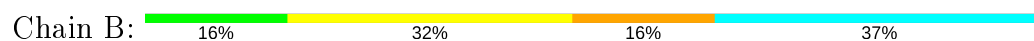
- Molecule 2: General transcription factor IIF subunit 1



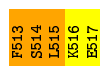
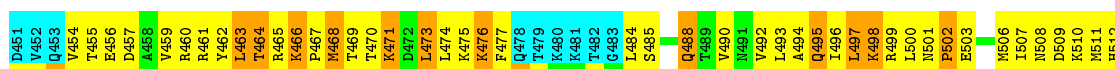


#### 4.2.17 Score per residue for model 17

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

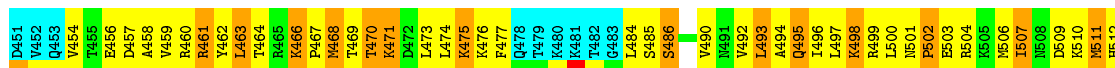


#### 4.2.18 Score per residue for model 18

- Molecule 1: centFCP1-T584PO4 peptide

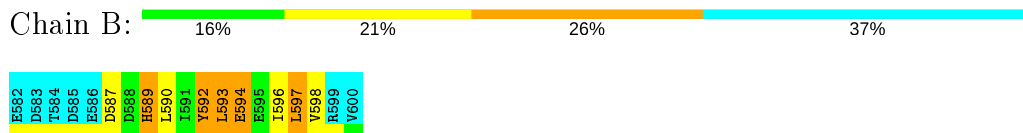


- Molecule 2: General transcription factor IIF subunit 1

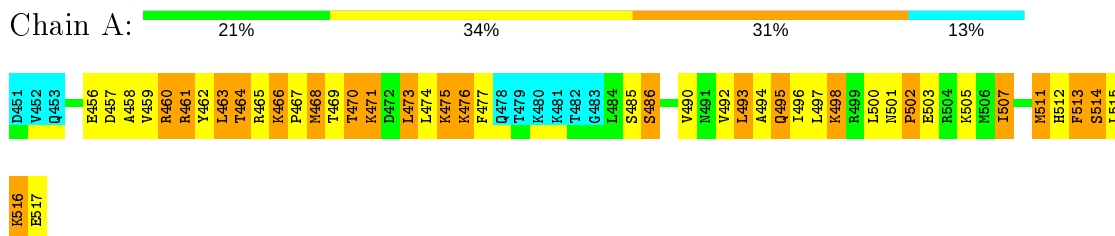


#### 4.2.19 Score per residue for model 19

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

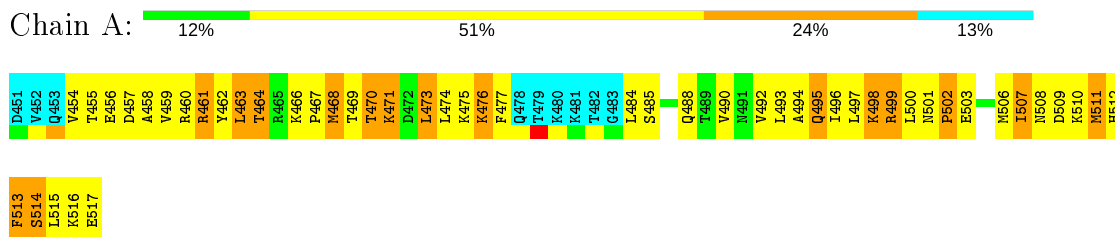


#### 4.2.20 Score per residue for model 20

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1

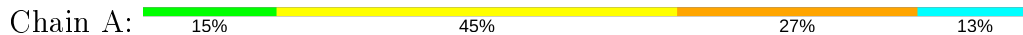


#### 4.2.21 Score per residue for model 21

- Molecule 1: centFCP1-T584PO4 peptide



- Molecule 2: General transcription factor IIF subunit 1



D451  
V452  
Q453  
Y454  
T455  
E456  
D457  
A458  
Y459  
R460  
R461  
Y462  
L463  
T464  
R465  
K466  
P467  
N468  
T469  
T470  
K471  
D472  
L473  
L474  
K475  
K476  
F477  
Q478  
T479  
K480  
K481  
T482  
G483  
L484  
S485  
S486  
K487  
Q488  
T489  
V490  
V491  
V492  
L493  
A494  
Q495  
T496  
L497  
K498  
R499  
L500  
R501  
P502  
E503  
R504  
K505  
R506  
I507  
K510  
M511

H512  
F513  
S514  
L515  
K516  
E517

## 5 Refinement protocol and experimental data overview

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

Of the 21 calculated structures, 21 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	1019
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	151
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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

## 6 Model quality i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TPO

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 i

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	B	103	101	100	33±3
2	A	483	521	520	76±9
All	All	12306	13062	13020	1871

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 74.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:463:LEU:HD11	2:A:500:LEU:HD22	1.06	1.23	17	16
2:A:474:LEU:HD22	2:A:490:VAL:HG22	1.06	1.27	5	11
1:B:593:LEU:HD21	2:A:470:THR:HG21	1.02	1.29	7	4
2:A:484:LEU:HD23	2:A:492:VAL:HG11	1.01	1.29	5	11
2:A:463:LEU:HD11	2:A:500:LEU:HD13	0.99	1.29	4	9
2:A:493:LEU:HD22	2:A:497:LEU:CD2	0.91	1.94	3	1
1:B:590:LEU:CD1	2:A:474:LEU:HD21	0.90	1.96	13	21
2:A:473:LEU:CD1	2:A:497:LEU:HD11	0.90	1.95	2	6
1:B:590:LEU:HD13	2:A:474:LEU:HD21	0.90	1.42	11	8
1:B:596:ILE:HD12	2:A:498:LYS:HE3	0.85	1.48	2	1
1:B:596:ILE:HD11	2:A:494:ALA:HB1	0.85	1.47	7	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:474:LEU:HB3	2:A:493:LEU:HD23	0.84	1.47	1	12
2:A:484:LEU:CD2	2:A:492:VAL:HG11	0.84	2.02	13	15
2:A:463:LEU:HD11	2:A:500:LEU:CD2	0.83	2.04	6	15
2:A:473:LEU:HD13	2:A:497:LEU:HD11	0.83	1.48	4	5
1:B:597:LEU:HD13	2:A:497:LEU:HB3	0.82	1.48	14	21
2:A:459:VAL:HG13	2:A:473:LEU:HD11	0.81	1.52	3	13
1:B:596:ILE:HD12	2:A:498:LYS:HE2	0.81	1.52	4	1
1:B:590:LEU:HD11	2:A:471:LYS:HA	0.81	1.53	21	21
2:A:459:VAL:CG1	2:A:473:LEU:HD11	0.81	2.04	3	11
2:A:468:MET:HG3	2:A:473:LEU:HD21	0.80	1.51	2	2
2:A:468:MET:HG2	2:A:473:LEU:HD21	0.80	1.54	16	1
2:A:463:LEU:CD1	2:A:500:LEU:HD22	0.79	2.08	9	13
1:B:590:LEU:HD12	2:A:474:LEU:HD21	0.78	1.54	9	10
2:A:469:THR:HG22	2:A:511:MET:O	0.78	1.78	9	13
1:B:596:ILE:HD12	2:A:498:LYS:NZ	0.78	1.94	7	3
2:A:459:VAL:HG12	2:A:500:LEU:HD21	0.77	1.55	6	5
1:B:593:LEU:HD22	1:B:593:LEU:C	0.77	2.00	20	7
2:A:470:THR:HG22	2:A:497:LEU:CD2	0.77	2.09	5	2
2:A:454:VAL:HG22	2:A:477:PHE:CD2	0.77	2.15	11	18
2:A:468:MET:CG	2:A:473:LEU:HD21	0.77	2.08	2	3
2:A:468:MET:SD	2:A:473:LEU:HD12	0.77	2.19	21	6
1:B:593:LEU:HD21	2:A:470:THR:CG2	0.76	2.10	7	8
2:A:474:LEU:HD22	2:A:490:VAL:HG13	0.76	1.57	20	7
1:B:593:LEU:O	1:B:593:LEU:HD22	0.76	1.81	18	13
1:B:593:LEU:C	1:B:593:LEU:HD22	0.75	2.01	6	14
1:B:593:LEU:HD23	2:A:494:ALA:CB	0.75	2.10	4	8
2:A:459:VAL:CG1	2:A:500:LEU:HD21	0.75	2.11	6	14
2:A:468:MET:CG	2:A:473:LEU:HD12	0.75	2.12	15	9
2:A:515:LEU:HD22	2:A:515:LEU:C	0.75	2.02	12	4
2:A:473:LEU:HD12	2:A:497:LEU:HD11	0.75	1.58	12	4
1:B:590:LEU:HD21	2:A:471:LYS:HG2	0.75	1.59	9	15
2:A:484:LEU:HD21	2:A:492:VAL:HG11	0.74	1.57	17	4
2:A:463:LEU:HD11	2:A:500:LEU:CD1	0.74	2.12	4	6
2:A:454:VAL:HG22	2:A:477:PHE:CE2	0.74	2.17	16	13
1:B:593:LEU:HD22	1:B:593:LEU:O	0.74	1.83	4	8
2:A:515:LEU:C	2:A:515:LEU:HD22	0.73	2.03	6	2
1:B:590:LEU:HD21	2:A:471:LYS:CG	0.73	2.13	19	14
1:B:593:LEU:CD2	2:A:470:THR:HG21	0.73	2.12	7	5
2:A:459:VAL:HB	2:A:500:LEU:HD21	0.73	1.61	8	18
2:A:469:THR:HG23	2:A:512:HIS:CD2	0.72	2.17	9	2
2:A:463:LEU:HD22	2:A:514:SER:OG	0.72	1.84	10	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:597:LEU:HD22	2:A:497:LEU:HG	0.72	1.60	11	7
2:A:469:THR:HG23	2:A:512:HIS:ND1	0.72	2.00	14	3
1:B:593:LEU:HD13	1:B:594:GLU:N	0.71	2.00	4	20
1:B:590:LEU:HD13	2:A:474:LEU:HD11	0.69	1.65	20	3
2:A:464:THR:HG22	2:A:517:GLU:HB2	0.69	1.63	19	5
2:A:459:VAL:HG11	2:A:500:LEU:HD11	0.69	1.62	8	16
2:A:473:LEU:HD22	2:A:493:LEU:CD1	0.69	2.18	5	1
1:B:590:LEU:HD21	2:A:471:LYS:HB3	0.68	1.63	6	6
1:B:592:TYR:CD1	1:B:593:LEU:N	0.68	2.61	8	21
2:A:493:LEU:CD1	2:A:497:LEU:HD22	0.68	2.18	14	9
2:A:460:ARG:O	2:A:464:THR:HG23	0.68	1.89	18	1
2:A:459:VAL:CG1	2:A:500:LEU:HD11	0.68	2.18	11	14
2:A:474:LEU:CB	2:A:493:LEU:HD23	0.67	2.19	9	9
2:A:473:LEU:HD22	2:A:493:LEU:HD11	0.67	1.65	5	2
2:A:493:LEU:HD12	2:A:493:LEU:O	0.67	1.89	9	4
2:A:493:LEU:HD11	2:A:497:LEU:HD22	0.67	1.66	14	6
2:A:463:LEU:HD12	2:A:515:LEU:CD2	0.67	2.19	10	9
2:A:469:THR:HG22	2:A:512:HIS:CD2	0.67	2.25	8	6
1:B:590:LEU:HD11	2:A:471:LYS:CA	0.67	2.21	7	17
2:A:484:LEU:HD23	2:A:492:VAL:CG1	0.66	2.17	5	6
2:A:468:MET:SD	2:A:473:LEU:HD21	0.66	2.31	11	3
1:B:596:ILE:HD12	2:A:498:LYS:CE	0.66	2.21	2	4
1:B:597:LEU:HD21	2:A:513:PHE:CD2	0.66	2.26	3	7
2:A:474:LEU:HD13	2:A:490:VAL:HG22	0.66	1.68	20	3
2:A:471:LYS:O	2:A:475:LYS:HG2	0.65	1.91	21	9
2:A:463:LEU:CD1	2:A:500:LEU:HD13	0.65	2.17	4	5
2:A:488:GLN:O	2:A:492:VAL:HG12	0.65	1.92	9	14
2:A:464:THR:HG22	2:A:517:GLU:CG	0.65	2.22	17	11
1:B:593:LEU:HD23	2:A:494:ALA:HA	0.64	1.69	18	13
2:A:468:MET:CE	2:A:473:LEU:HD11	0.64	2.22	16	2
1:B:590:LEU:O	1:B:593:LEU:CD1	0.64	2.45	7	21
2:A:454:VAL:HG22	2:A:477:PHE:CG	0.64	2.28	13	3
1:B:596:ILE:HD13	2:A:498:LYS:NZ	0.64	2.08	14	16
2:A:456:GLU:HA	2:A:496:ILE:HG23	0.64	1.70	14	21
1:B:597:LEU:HD21	2:A:513:PHE:CD1	0.64	2.28	11	12
2:A:470:THR:HG23	2:A:513:PHE:CZ	0.64	2.28	11	1
1:B:597:LEU:HD13	2:A:497:LEU:CB	0.64	2.23	16	9
2:A:468:MET:SD	2:A:473:LEU:HD11	0.63	2.33	11	3
2:A:493:LEU:HD22	2:A:497:LEU:HD22	0.63	1.69	3	1
1:B:597:LEU:HG	1:B:598:VAL:N	0.63	2.09	11	21
2:A:464:THR:HG22	2:A:517:GLU:HG2	0.62	1.71	5	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:469:THR:HG23	2:A:512:HIS:CE1	0.62	2.28	11	10
2:A:467:PRO:HA	2:A:514:SER:CB	0.62	2.24	17	20
1:B:589:HIS:HA	1:B:592:TYR:CD2	0.62	2.28	5	5
2:A:459:VAL:CG2	2:A:496:ILE:HG21	0.62	2.25	21	5
1:B:590:LEU:HD11	2:A:471:LYS:HB3	0.61	1.71	7	4
2:A:455:THR:O	2:A:459:VAL:HG23	0.61	1.95	10	9
1:B:597:LEU:HG	1:B:598:VAL:HG22	0.61	1.72	11	21
2:A:515:LEU:H	2:A:515:LEU:HD23	0.61	1.55	21	5
2:A:469:THR:O	2:A:473:LEU:HD12	0.61	1.96	17	2
1:B:593:LEU:O	1:B:596:ILE:HG13	0.60	1.96	18	19
2:A:470:THR:HG23	2:A:497:LEU:HG	0.60	1.73	18	3
2:A:470:THR:HA	2:A:473:LEU:HD12	0.60	1.73	4	2
2:A:470:THR:HG22	2:A:497:LEU:HD23	0.60	1.73	5	1
2:A:460:ARG:CD	2:A:500:LEU:HD23	0.60	2.25	9	4
2:A:493:LEU:O	2:A:497:LEU:HD23	0.60	1.97	19	5
1:B:597:LEU:HD13	2:A:497:LEU:C	0.60	2.16	1	19
1:B:597:LEU:HG	1:B:598:VAL:HG13	0.60	1.72	14	20
1:B:593:LEU:HD23	2:A:494:ALA:HB2	0.59	1.75	2	5
2:A:463:LEU:HD22	2:A:468:MET:SD	0.59	2.38	16	9
2:A:515:LEU:HD23	2:A:515:LEU:H	0.59	1.58	8	9
2:A:468:MET:CE	2:A:473:LEU:HD12	0.58	2.28	18	10
2:A:515:LEU:HD13	2:A:515:LEU:H	0.58	1.58	17	4
2:A:494:ALA:O	2:A:498:LYS:NZ	0.58	2.37	4	1
2:A:463:LEU:N	2:A:463:LEU:HD23	0.58	2.13	7	10
1:B:589:HIS:O	1:B:593:LEU:HD12	0.58	1.99	7	1
2:A:463:LEU:HD12	2:A:515:LEU:HD21	0.58	1.75	19	8
1:B:597:LEU:HD22	2:A:497:LEU:HB3	0.57	1.76	2	1
2:A:474:LEU:CD2	2:A:490:VAL:HG22	0.57	2.22	21	1
2:A:468:MET:HG3	2:A:473:LEU:CD2	0.57	2.29	4	1
2:A:501:ASN:N	2:A:502:PRO:HD3	0.57	2.14	17	21
2:A:463:LEU:HD23	2:A:463:LEU:N	0.57	2.15	20	10
2:A:486:SER:O	2:A:490:VAL:HG23	0.57	1.99	19	7
2:A:515:LEU:H	2:A:515:LEU:HD13	0.57	1.58	12	2
1:B:596:ILE:CD1	2:A:494:ALA:HB1	0.57	2.30	6	1
1:B:597:LEU:HD23	2:A:513:PHE:CZ	0.57	2.35	14	3
2:A:474:LEU:HD23	2:A:493:LEU:HD23	0.57	1.76	21	3
1:B:597:LEU:HD22	2:A:497:LEU:HD12	0.57	1.77	3	2
2:A:454:VAL:HG12	2:A:496:ILE:CD1	0.56	2.30	13	9
1:B:597:LEU:HD21	2:A:513:PHE:CE1	0.56	2.36	11	3
1:B:587:ASP:OD1	1:B:590:LEU:HD23	0.56	2.00	16	5
2:A:515:LEU:N	2:A:515:LEU:HD23	0.56	2.16	13	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:507:ILE:HG12	2:A:512:HIS:ND1	0.56	2.16	2	1
1:B:597:LEU:CD2	2:A:513:PHE:CD2	0.56	2.89	3	5
1:B:590:LEU:HD11	2:A:471:LYS:CB	0.56	2.30	7	4
2:A:467:PRO:HB2	2:A:512:HIS:CD2	0.56	2.36	2	1
1:B:594:GLU:HA	2:A:470:THR:HG21	0.55	1.77	11	1
2:A:515:LEU:CD2	2:A:515:LEU:C	0.55	2.74	12	4
2:A:462:TYR:CD2	2:A:473:LEU:HD21	0.55	2.37	3	3
1:B:593:LEU:HD23	2:A:494:ALA:CA	0.55	2.31	18	8
2:A:476:LYS:HE2	2:A:477:PHE:CD2	0.55	2.36	16	2
2:A:469:THR:CG2	2:A:512:HIS:CD2	0.55	2.90	4	8
1:B:597:LEU:CD2	2:A:513:PHE:CE2	0.55	2.90	21	7
2:A:492:VAL:O	2:A:495:GLN:NE2	0.55	2.40	3	21
1:B:597:LEU:CD2	2:A:513:PHE:CE1	0.55	2.90	9	14
2:A:473:LEU:HA	2:A:476:LYS:HZ1	0.55	1.62	21	1
2:A:473:LEU:HD13	2:A:493:LEU:HD11	0.54	1.77	13	2
1:B:598:VAL:HG21	2:A:513:PHE:CB	0.54	2.32	11	2
1:B:592:TYR:C	1:B:592:TYR:CD1	0.54	2.80	3	10
2:A:465:ARG:O	2:A:466:LYS:HD2	0.54	2.02	7	4
1:B:597:LEU:HD12	2:A:498:LYS:HA	0.54	1.79	9	20
2:A:515:LEU:C	2:A:515:LEU:CD2	0.54	2.75	6	2
2:A:464:THR:HG22	2:A:517:GLU:HB3	0.54	1.78	20	8
1:B:597:LEU:CD1	1:B:598:VAL:HG13	0.53	2.33	14	13
1:B:593:LEU:CD2	1:B:593:LEU:C	0.53	2.76	3	13
2:A:515:LEU:HD23	2:A:515:LEU:N	0.53	2.18	7	6
2:A:484:LEU:HD22	2:A:492:VAL:HG11	0.53	1.78	10	1
2:A:466:LYS:HD3	2:A:467:PRO:HD2	0.53	1.81	12	1
2:A:463:LEU:HB2	2:A:515:LEU:CD2	0.53	2.33	1	1
2:A:469:THR:CG2	2:A:512:HIS:CE1	0.53	2.92	17	9
2:A:459:VAL:CB	2:A:500:LEU:HD21	0.53	2.34	11	19
2:A:474:LEU:HD12	2:A:475:LYS:N	0.53	2.18	5	5
2:A:474:LEU:HA	2:A:493:LEU:HD23	0.53	1.79	7	1
2:A:473:LEU:HD13	2:A:497:LEU:CD1	0.52	2.33	2	1
2:A:459:VAL:HG21	2:A:496:ILE:CG2	0.52	2.34	10	10
1:B:592:TYR:CD1	1:B:592:TYR:C	0.52	2.83	11	6
1:B:598:VAL:HG21	2:A:513:PHE:HB3	0.52	1.80	7	8
1:B:596:ILE:HD12	2:A:498:LYS:HZ1	0.52	1.64	7	1
2:A:474:LEU:CA	2:A:493:LEU:HD23	0.52	2.34	7	7
1:B:597:LEU:CD1	2:A:498:LYS:HA	0.52	2.34	2	1
2:A:462:TYR:O	2:A:466:LYS:O	0.52	2.28	2	10
2:A:493:LEU:CD1	2:A:497:LEU:CD2	0.52	2.88	19	10
2:A:497:LEU:HD13	2:A:500:LEU:HD11	0.52	1.81	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:464:THR:HG22	2:A:517:GLU:CB	0.52	2.35	20	9
2:A:465:ARG:HG3	2:A:466:LYS:N	0.52	2.19	12	1
2:A:462:TYR:CE2	2:A:477:PHE:CE2	0.51	2.98	13	2
2:A:468:MET:HG2	2:A:473:LEU:HD11	0.51	1.82	2	1
2:A:474:LEU:HB3	2:A:493:LEU:HD12	0.51	1.80	3	1
2:A:465:ARG:O	2:A:466:LYS:HG2	0.51	2.04	12	2
2:A:476:LYS:CE	2:A:477:PHE:CE2	0.51	2.94	16	1
2:A:468:MET:HG3	2:A:473:LEU:HG	0.51	1.83	20	1
2:A:468:MET:N	2:A:468:MET:SD	0.51	2.84	4	2
2:A:476:LYS:HG2	2:A:477:PHE:N	0.51	2.20	21	3
2:A:466:LYS:HE2	2:A:467:PRO:HD3	0.51	1.83	17	1
2:A:459:VAL:HG21	2:A:496:ILE:HG21	0.51	1.83	21	3
2:A:462:TYR:HD2	2:A:473:LEU:HD21	0.51	1.65	3	2
1:B:593:LEU:C	1:B:593:LEU:CD2	0.51	2.77	15	6
2:A:466:LYS:HA	2:A:466:LYS:CE	0.51	2.36	12	2
2:A:467:PRO:CB	2:A:512:HIS:NE2	0.50	2.74	2	1
2:A:456:GLU:O	2:A:460:ARG:HG2	0.50	2.07	5	11
2:A:462:TYR:HH	2:A:477:PHE:HZ	0.50	1.50	18	1
2:A:454:VAL:CG2	2:A:477:PHE:CG	0.50	2.94	2	4
2:A:468:MET:CG	2:A:473:LEU:CD2	0.50	2.88	2	1
2:A:468:MET:SD	2:A:468:MET:N	0.50	2.85	16	3
2:A:493:LEU:HG	2:A:497:LEU:CD2	0.50	2.36	6	13
1:B:593:LEU:O	1:B:596:ILE:CG1	0.50	2.60	7	4
2:A:463:LEU:CD2	2:A:500:LEU:HD13	0.50	2.37	6	2
1:B:597:LEU:CG	1:B:598:VAL:HG13	0.49	2.37	14	5
2:A:468:MET:HG2	2:A:473:LEU:CG	0.49	2.38	2	2
2:A:473:LEU:CB	2:A:493:LEU:HD21	0.49	2.37	2	1
2:A:454:VAL:CG2	2:A:477:PHE:CD2	0.49	2.95	16	2
2:A:468:MET:HE3	2:A:513:PHE:O	0.49	2.07	21	1
2:A:474:LEU:HD22	2:A:490:VAL:CG2	0.49	2.28	17	1
2:A:484:LEU:HD13	2:A:492:VAL:HG11	0.49	1.83	8	1
2:A:471:LYS:H	2:A:471:LYS:CD	0.49	2.20	7	3
2:A:463:LEU:CB	2:A:515:LEU:CD2	0.49	2.91	1	1
1:B:597:LEU:CD2	2:A:513:PHE:CD1	0.49	2.96	1	7
2:A:507:ILE:CD1	2:A:512:HIS:CE1	0.49	2.95	2	1
2:A:466:LYS:CE	2:A:467:PRO:HD2	0.49	2.38	7	2
2:A:460:ARG:HD2	2:A:500:LEU:HD23	0.49	1.84	9	1
2:A:474:LEU:HD12	2:A:475:LYS:HD3	0.49	1.84	16	4
2:A:460:ARG:HD3	2:A:500:LEU:HD23	0.48	1.85	9	8
2:A:468:MET:CG	2:A:473:LEU:HG	0.48	2.39	4	1
1:B:593:LEU:HG	2:A:490:VAL:HG12	0.48	1.85	15	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:468:MET:HE3	2:A:513:PHE:CE1	0.48	2.44	11	1
2:A:505:LYS:HE3	2:A:512:HIS:CE1	0.48	2.44	2	1
1:B:597:LEU:HD13	2:A:498:LYS:N	0.48	2.23	2	3
2:A:463:LEU:HD11	2:A:500:LEU:HB3	0.48	1.85	2	3
1:B:589:HIS:CB	1:B:592:TYR:CE2	0.48	2.96	3	5
2:A:468:MET:SD	2:A:473:LEU:CD1	0.48	2.98	21	2
2:A:493:LEU:HG	2:A:497:LEU:HD23	0.48	1.83	6	3
1:B:597:LEU:CD2	2:A:513:PHE:CZ	0.48	2.97	11	2
2:A:468:MET:HE3	2:A:473:LEU:HD11	0.48	1.85	16	1
1:B:593:LEU:HA	1:B:596:ILE:HG12	0.48	1.86	2	1
2:A:468:MET:CE	2:A:513:PHE:CD1	0.47	2.97	11	1
2:A:474:LEU:HD13	2:A:490:VAL:CG2	0.47	2.37	20	1
2:A:473:LEU:CD1	2:A:497:LEU:CD1	0.47	2.92	12	2
2:A:473:LEU:HD11	2:A:497:LEU:HD11	0.47	1.78	2	1
2:A:463:LEU:HD21	2:A:500:LEU:HD13	0.47	1.85	6	2
2:A:463:LEU:HD22	2:A:514:SER:HG	0.47	1.69	1	2
1:B:598:VAL:CG2	2:A:513:PHE:CD2	0.47	2.97	17	7
2:A:476:LYS:HE3	2:A:477:PHE:CD2	0.47	2.44	7	6
2:A:489:THR:O	2:A:493:LEU:HB2	0.47	2.08	3	7
2:A:473:LEU:HB3	2:A:493:LEU:HD21	0.47	1.86	16	2
2:A:463:LEU:HD21	2:A:500:LEU:CD1	0.47	2.40	6	1
2:A:459:VAL:O	2:A:463:LEU:HG	0.47	2.09	13	3
1:B:598:VAL:CG2	2:A:513:PHE:CD1	0.47	2.98	7	1
2:A:463:LEU:HB3	2:A:514:SER:OG	0.47	2.10	13	1
1:B:597:LEU:CD2	2:A:497:LEU:HD12	0.46	2.40	3	1
2:A:459:VAL:HG12	2:A:500:LEU:HD11	0.46	1.86	11	1
2:A:470:THR:HG22	2:A:497:LEU:HG	0.46	1.87	13	2
2:A:467:PRO:HB2	2:A:512:HIS:NE2	0.46	2.25	2	1
2:A:474:LEU:HB3	2:A:493:LEU:HD22	0.46	1.87	5	1
2:A:474:LEU:HB3	2:A:493:LEU:CD2	0.46	2.41	6	2
2:A:492:VAL:HG22	2:A:492:VAL:O	0.46	2.11	21	6
1:B:593:LEU:HB2	2:A:494:ALA:HB2	0.46	1.88	13	6
2:A:468:MET:CE	2:A:513:PHE:CE1	0.46	2.98	11	1
2:A:459:VAL:HG11	2:A:473:LEU:HD11	0.46	1.88	13	2
2:A:470:THR:O	2:A:474:LEU:HD23	0.46	2.11	7	6
2:A:456:GLU:HA	2:A:496:ILE:CG2	0.46	2.40	2	11
2:A:456:GLU:HG2	2:A:499:ARG:HG3	0.46	1.86	2	1
2:A:476:LYS:HE2	2:A:477:PHE:CE2	0.46	2.45	12	9
2:A:515:LEU:HD13	2:A:515:LEU:N	0.46	2.25	12	2
2:A:492:VAL:O	2:A:492:VAL:HG22	0.46	2.11	16	2
1:B:590:LEU:HD21	2:A:471:LYS:CB	0.46	2.40	13	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:467:PRO:HA	2:A:514:SER:HB2	0.46	1.88	17	4
2:A:473:LEU:HA	2:A:476:LYS:NZ	0.46	2.26	21	1
2:A:463:LEU:CD1	2:A:500:LEU:HB3	0.46	2.40	2	5
2:A:469:THR:HG23	2:A:512:HIS:NE2	0.46	2.25	9	2
2:A:507:ILE:HB	2:A:512:HIS:CG	0.45	2.46	14	6
2:A:471:LYS:H	2:A:471:LYS:HD2	0.45	1.71	12	2
2:A:458:ALA:O	2:A:461:ARG:CG	0.45	2.64	21	9
1:B:590:LEU:HD11	2:A:471:LYS:HG3	0.45	1.88	9	1
2:A:468:MET:HG2	2:A:473:LEU:HD12	0.45	1.87	19	3
2:A:507:ILE:N	2:A:510:LYS:O	0.45	2.50	4	14
2:A:476:LYS:CE	2:A:477:PHE:CD2	0.45	3.00	5	2
2:A:468:MET:HE3	2:A:473:LEU:HD12	0.45	1.86	6	2
2:A:496:ILE:HA	2:A:499:ARG:HG2	0.45	1.88	10	8
2:A:502:PRO:HB2	2:A:514:SER:CA	0.45	2.42	17	8
2:A:473:LEU:O	2:A:476:LYS:CE	0.45	2.65	21	2
2:A:515:LEU:O	2:A:515:LEU:HD22	0.45	2.11	12	3
2:A:494:ALA:O	2:A:498:LYS:HD2	0.45	2.12	15	2
1:B:597:LEU:HD23	2:A:513:PHE:CE2	0.45	2.47	14	1
2:A:495:GLN:NE2	2:A:496:ILE:CD1	0.45	2.80	16	11
2:A:494:ALA:O	2:A:498:LYS:CE	0.44	2.65	4	1
2:A:473:LEU:O	2:A:476:LYS:HG3	0.44	2.12	4	3
1:B:596:ILE:HD13	2:A:498:LYS:HZ2	0.44	1.72	12	2
1:B:593:LEU:CG	2:A:494:ALA:HB2	0.44	2.42	7	3
2:A:459:VAL:HG12	2:A:463:LEU:HD21	0.44	1.89	4	2
2:A:468:MET:O	2:A:468:MET:HE3	0.44	2.12	17	1
1:B:597:LEU:CD1	2:A:497:LEU:C	0.44	2.86	11	3
1:B:593:LEU:HD13	1:B:593:LEU:C	0.44	2.33	14	2
2:A:463:LEU:HD11	2:A:500:LEU:CG	0.44	2.43	16	6
2:A:461:ARG:HG3	2:A:462:TYR:CD1	0.44	2.48	7	4
2:A:470:THR:HG23	2:A:513:PHE:CE2	0.44	2.46	11	1
1:B:593:LEU:CD2	2:A:470:THR:CG2	0.44	2.96	13	1
1:B:597:LEU:HD22	2:A:470:THR:HG23	0.44	1.89	16	1
2:A:454:VAL:HG12	2:A:454:VAL:O	0.44	2.13	17	1
2:A:462:TYR:CZ	2:A:477:PHE:CZ	0.44	3.06	13	1
2:A:462:TYR:N	2:A:462:TYR:CD1	0.43	2.85	5	2
1:B:591:ILE:HG23	1:B:594:GLU:OE1	0.43	2.13	13	1
2:A:468:MET:CG	2:A:473:LEU:CD1	0.43	2.96	20	2
2:A:463:LEU:HB3	2:A:515:LEU:HD13	0.43	1.90	2	2
2:A:499:ARG:N	2:A:499:ARG:HD2	0.43	2.29	2	1
2:A:512:HIS:CD2	2:A:513:PHE:N	0.43	2.86	2	1
2:A:458:ALA:O	2:A:462:TYR:CD1	0.43	2.72	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:468:MET:HE2	2:A:468:MET:O	0.43	2.12	12	1
1:B:590:LEU:HD11	2:A:474:LEU:HD21	0.43	1.88	19	2
2:A:468:MET:HE2	2:A:473:LEU:CD1	0.43	2.43	16	1
2:A:468:MET:CG	2:A:473:LEU:CG	0.43	2.96	4	1
2:A:516:LYS:N	2:A:516:LYS:CD	0.43	2.82	19	7
1:B:593:LEU:HB2	2:A:494:ALA:CB	0.43	2.44	10	3
2:A:473:LEU:HA	2:A:476:LYS:CE	0.43	2.44	10	1
2:A:471:LYS:O	2:A:475:LYS:CD	0.43	2.67	19	4
1:B:588:ASP:OD1	1:B:589:HIS:N	0.43	2.50	20	2
2:A:468:MET:HE2	2:A:513:PHE:O	0.43	2.13	9	1
2:A:493:LEU:HD12	2:A:497:LEU:CD2	0.43	2.44	7	2
2:A:467:PRO:HG2	2:A:507:ILE:HG13	0.43	1.89	4	3
2:A:459:VAL:HG12	2:A:500:LEU:CD2	0.43	2.37	6	1
2:A:459:VAL:HG21	2:A:496:ILE:HG22	0.42	1.90	16	2
2:A:468:MET:HG3	2:A:473:LEU:HD12	0.42	1.89	15	1
1:B:593:LEU:CD2	2:A:494:ALA:HB2	0.42	2.43	20	4
2:A:477:PHE:HB2	2:A:489:THR:HG21	0.42	1.90	3	1
2:A:458:ALA:O	2:A:461:ARG:HG2	0.42	2.14	13	3
2:A:516:LYS:CD	2:A:516:LYS:N	0.42	2.82	15	4
1:B:597:LEU:HD12	2:A:498:LYS:CA	0.42	2.45	14	1
2:A:468:MET:CE	2:A:473:LEU:CD1	0.42	2.95	16	1
1:B:596:ILE:HD13	2:A:498:LYS:HZ1	0.42	1.73	18	1
2:A:466:LYS:HD2	2:A:467:PRO:O	0.42	2.14	18	2
2:A:468:MET:HG2	2:A:473:LEU:CD1	0.42	2.43	2	1
2:A:459:VAL:HA	2:A:462:TYR:CD2	0.42	2.49	7	5
2:A:474:LEU:HA	2:A:493:LEU:CD2	0.42	2.44	7	1
2:A:468:MET:HE1	2:A:468:MET:O	0.42	2.14	16	1
2:A:466:LYS:N	2:A:466:LYS:HD3	0.42	2.29	2	1
2:A:473:LEU:O	2:A:476:LYS:HE3	0.42	2.14	13	1
2:A:462:TYR:OH	2:A:477:PHE:CE1	0.42	2.71	13	1
2:A:462:TYR:CE2	2:A:477:PHE:CZ	0.42	3.07	13	1
2:A:468:MET:HA	2:A:512:HIS:CD2	0.42	2.49	20	2
2:A:502:PRO:CB	2:A:514:SER:HA	0.42	2.44	2	1
1:B:593:LEU:C	1:B:593:LEU:HD13	0.42	2.35	10	2
2:A:498:LYS:H	2:A:498:LYS:HD2	0.42	1.75	4	1
2:A:495:GLN:O	2:A:498:LYS:CD	0.42	2.68	18	3
2:A:473:LEU:HB2	2:A:493:LEU:HD21	0.42	1.91	2	1
1:B:592:TYR:O	1:B:595:GLU:CG	0.42	2.68	3	2
2:A:468:MET:HE3	2:A:513:PHE:CD1	0.42	2.49	11	1
2:A:463:LEU:CB	2:A:515:LEU:CD1	0.41	2.98	12	3
2:A:473:LEU:HD22	2:A:476:LYS:HZ3	0.41	1.75	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:463:LEU:CD1	2:A:515:LEU:CD2	0.41	2.98	19	1
2:A:473:LEU:O	2:A:476:LYS:CG	0.41	2.67	9	3
2:A:458:ALA:O	2:A:462:TYR:CE1	0.41	2.73	20	3
2:A:470:THR:O	2:A:474:LEU:CD2	0.41	2.68	20	2
2:A:473:LEU:HD12	2:A:497:LEU:CD1	0.41	2.42	16	1
2:A:505:LYS:O	2:A:512:HIS:O	0.41	2.38	2	1
2:A:496:ILE:HA	2:A:499:ARG:CG	0.41	2.45	10	1
1:B:592:TYR:O	1:B:595:GLU:HG2	0.41	2.15	14	4
1:B:597:LEU:CG	1:B:598:VAL:N	0.41	2.79	12	1
2:A:459:VAL:O	2:A:462:TYR:HB2	0.41	2.15	13	1
2:A:493:LEU:HD22	2:A:497:LEU:HD21	0.41	1.82	3	1
2:A:463:LEU:HB3	2:A:514:SER:CB	0.41	2.46	21	1
2:A:497:LEU:HD13	2:A:500:LEU:CD1	0.41	2.45	15	1
2:A:470:THR:CG2	2:A:497:LEU:HG	0.41	2.45	20	1
2:A:496:ILE:O	2:A:499:ARG:HG2	0.41	2.16	2	1
2:A:474:LEU:CD2	2:A:490:VAL:HG13	0.41	2.43	3	1
2:A:468:MET:HE1	2:A:513:PHE:O	0.41	2.15	8	1
1:B:590:LEU:CD2	2:A:471:LYS:HG2	0.41	2.42	8	1
2:A:461:ARG:HG2	2:A:462:TYR:CD1	0.41	2.51	1	2
2:A:467:PRO:HB3	2:A:514:SER:CB	0.41	2.45	3	1
2:A:470:THR:HG22	2:A:497:LEU:HD21	0.41	1.90	5	1
2:A:471:LYS:CD	2:A:471:LYS:H	0.41	2.29	6	1
2:A:468:MET:CE	2:A:513:PHE:O	0.41	2.69	2	1
2:A:493:LEU:HG	2:A:497:LEU:HD21	0.41	1.93	7	1
2:A:503:GLU:O	2:A:505:LYS:CD	0.41	2.69	10	1
2:A:469:THR:CG2	2:A:511:MET:O	0.41	2.68	14	1
2:A:469:THR:C	2:A:473:LEU:HD12	0.41	2.36	17	1
2:A:462:TYR:OH	2:A:477:PHE:CZ	0.40	2.74	13	1
2:A:508:ASN:O	2:A:509:ASP:CB	0.40	2.69	17	1
1:B:596:ILE:HD12	2:A:498:LYS:HZ2	0.40	1.74	15	1
2:A:493:LEU:HG	2:A:497:LEU:HD22	0.40	1.92	5	1
1:B:598:VAL:HG21	2:A:513:PHE:CG	0.40	2.51	16	1
2:A:461:ARG:CG	2:A:462:TYR:CD1	0.40	3.04	14	1
1:B:596:ILE:HD12	1:B:597:LEU:N	0.40	2.31	14	1
2:A:468:MET:HA	2:A:512:HIS:ND1	0.40	2.32	16	1
1:B:589:HIS:HD2	1:B:590:LEU:N	0.40	2.15	19	1
2:A:467:PRO:CG	2:A:507:ILE:CG1	0.40	3.00	4	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	B	12/19 (63%)	10±0 (83±0%)	1±0 (11±4%)	1±0 (6±4%)	3	20
2	A	57/67 (85%)	51±2 (89±3%)	5±2 (8±3%)	1±0 (2±1%)	9	46
All	All	1449/1806 (80%)	1279 (88%)	126 (9%)	44 (3%)	7	40

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	502	PRO	21
1	B	597	LEU	15
2	A	485	SER	6
2	A	467	PRO	2

### 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	B	12/18 (67%)	8±1 (70±8%)	4±1 (30±8%)	1	16
2	A	56/64 (88%)	32±2 (56±3%)	24±2 (44±3%)	0	3
All	All	1428/1722 (83%)	839 (59%)	589 (41%)	0	4

All 47 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)
2	A	476	LYS	21
2	A	471	LYS	21
2	A	503	GLU	21

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Mol	Chain	Res	Type	Models (Total)
1	B	592	TYR	21
2	A	498	LYS	21
1	B	593	LEU	21
2	A	485	SER	21
2	A	457	ASP	21
2	A	495	GLN	21
2	A	461	ARG	21
2	A	468	MET	21
2	A	516	LYS	21
2	A	464	THR	20
2	A	466	LYS	20
2	A	513	PHE	20
2	A	514	SER	20
2	A	507	ILE	20
2	A	470	THR	20
2	A	506	MET	15
2	A	511	MET	14
1	B	587	ASP	14
2	A	463	LEU	13
2	A	497	LEU	12
2	A	473	LEU	12
2	A	475	LYS	11
2	A	504	ARG	11
2	A	460	ARG	11
2	A	510	LYS	9
2	A	484	LEU	8
1	B	595	GLU	8
2	A	499	ARG	7
2	A	486	SER	7
2	A	515	LEU	7
2	A	474	LEU	6
2	A	509	ASP	6
1	B	589	HIS	6
2	A	493	LEU	6
2	A	488	GLN	6
2	A	505	LYS	5
1	B	594	GLU	5
2	A	517	GLU	5
2	A	491	ASN	4
2	A	469	THR	3
2	A	508	ASN	3
2	A	454	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	B	596	ILE	1
2	A	512	HIS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

MODRES-GEOMETRY INFOmissingINFO

### 6.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.6 Other polymers [i](#)

There are no such molecules in this entry.

### 6.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 71% for the well-defined parts and 68% 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

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	1019
Number of shifts mapped to atoms	868
Number of unparsed shifts	0
Number of shifts with mapping errors	151
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 151 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	4	GLN	CG	33.94	0.05	1
A	11	THR	HA	4.61	0.02	1
A	9	LYS	HD2	1.668	0.02	2
A	9	LYS	HG3	1.396	0.02	2
A	3	PRO	HA	4.386	0.02	1
A	4	GLN	HG2	2.35	0.02	2
A	7	SER	C	175.235	0.05	1
A	12	PRO	HB2	1.903	0.02	2
A	5	PRO	HB2	1.96	0.02	2
A	9	LYS	CA	56.207	0.05	1
A	9	LYS	CG	24.905	0.05	1
A	12	PRO	C	176.657	0.05	1
A	9	LYS	C	176.811	0.05	1
A	7	SER	HB2	3.878	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	8	GLY	N	110.891	0.05	1
A	11	THR	HG23	1.26	0.02	1
A	13	ASN	HD22	6.934	0.02	2
A	10	THR	CG2	21.71	0.05	1
A	9	LYS	HE2	2.972	0.02	2
A	3	PRO	HG2	1.976	0.02	2
A	8	GLY	HA3	3.969	0.02	2
A	5	PRO	HD3	3.85	0.02	2
A	3	PRO	C	176.533	0.05	1
A	7	SER	N	115.996	0.05	1
A	15	GLY	CA	45.448	0.05	1
A	7	SER	CB	64.085	0.05	1
A	9	LYS	HD3	1.668	0.02	2
A	9	LYS	HG2	1.396	0.02	2
A	6	PRO	HD2	3.643	0.02	2
A	13	ASN	C	175.39	0.05	1
A	12	PRO	HB3	2.284	0.02	2
A	10	THR	HB	4.186	0.02	1
A	9	LYS	CB	33.344	0.05	1
A	8	GLY	H	8.407	0.02	1
A	9	LYS	N	120.757	0.05	1
A	13	ASN	HB2	2.768	0.02	2
A	7	SER	HA	4.422	0.02	1
A	5	PRO	CB	30.846	0.05	1
A	7	SER	HB3	3.878	0.02	2
A	8	GLY	CA	45.256	0.05	1
A	15	GLY	C	173.845	0.05	1
A	3	PRO	CG	27.349	0.05	1
A	12	PRO	CG	27.537	0.05	1
A	6	PRO	CG	27.349	0.05	1
A	12	PRO	CA	63.316	0.05	1
A	10	THR	HG21	1.16	0.02	1
A	2	THR	HG23	1.26	0.02	1
A	7	SER	H	8.398	0.02	1
A	6	PRO	HA	4.44	0.02	1
A	11	THR	H	8.243	0.02	1
A	5	PRO	HD2	3.677	0.02	2
A	9	LYS	H	8.189	0.02	1
A	12	PRO	HA	4.404	0.02	1
A	4	GLN	CA	53.517	0.05	1
A	6	PRO	HD3	3.806	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	SER	HA	4.404	0.02	1
A	1	SER	HB2	3.842	0.02	2
A	15	GLY	HA3	3.951	0.02	2
A	10	THR	N	115.64	0.05	1
A	3	PRO	HD3	3.842	0.02	2
A	13	ASN	HB3	2.851	0.02	2
A	5	PRO	HG2	2.076	0.02	2
A	13	ASN	CA	53.325	0.05	1
A	2	THR	CA	59.858	0.05	1
A	4	GLN	HB2	1.94	0.02	2
A	12	PRO	CD	51.034	0.05	1
A	1	SER	CB	63.892	0.05	1
A	11	THR	CB	69.656	0.05	1
A	1	SER	N	117.058	0.05	1
A	11	THR	N	118.913	0.05	1
A	2	THR	HG22	1.26	0.02	1
A	13	ASN	H	8.57	0.02	1
A	13	ASN	HA	4.712	0.02	1
A	8	GLY	C	173.968	0.05	1
A	5	PRO	HA	4.749	0.02	1
A	4	GLN	CB	29.117	0.05	1
A	1	SER	HB3	3.842	0.02	2
A	15	GLY	HA2	3.951	0.02	2
A	9	LYS	CD	29.041	0.05	1
A	3	PRO	HD2	3.679	0.02	2
A	1	SER	H	8.279	0.02	1
A	5	PRO	HG3	2.076	0.02	2
A	10	THR	H	8.236	0.02	1
A	13	ASN	CB	38.915	0.05	1
A	4	GLN	HB3	2.105	0.02	2
A	6	PRO	CB	31.999	0.05	1
A	9	LYS	HB2	1.831	0.02	2
A	13	ASN	HD21	7.66	0.02	2
A	6	PRO	HB2	1.94	0.02	2
A	3	PRO	HB2	1.87	0.02	2
A	1	SER	HA	4.483	0.02	1
A	10	THR	HG23	1.16	0.02	1
A	3	PRO	HB3	2.266	0.02	2
A	4	GLN	H	8.455	0.02	1
A	6	PRO	CA	63.065	0.05	1
A	13	ASN	ND2	113.375	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	2	THR	CG2	21.52	0.05	1
A	2	THR	HG21	1.26	0.02	1
A	6	PRO	HG3	2.03	0.02	2
A	12	PRO	HG2	2.012	0.02	2
A	10	THR	HA	4.386	0.02	1
A	10	THR	CB	70.04	0.05	1
A	9	LYS	CE	42.199	0.05	1
A	4	GLN	HE22	6.811	0.02	2
A	5	PRO	CA	60.84	0.05	1
A	6	PRO	HB3	2.302	0.02	2
A	14	SER	CB	63.7	0.05	1
A	14	SER	N	116.494	0.05	1
A	11	THR	HG21	1.26	0.02	1
A	9	LYS	HB3	1.831	0.02	2
A	3	PRO	CB	32.236	0.05	1
A	12	PRO	HD2	3.715	0.02	2
A	3	PRO	CD	51.034	0.05	1
A	12	PRO	CB	32.191	0.05	1
A	10	THR	HG22	1.16	0.02	1
A	14	SER	HB3	3.878	0.02	2
A	2	THR	H	8.152	0.02	1
A	4	GLN	NE2	112.912	0.05	1
A	4	GLN	HE21	7.541	0.02	2
A	2	THR	HA	4.66	0.02	1
A	14	SER	C	175.05	0.05	1
A	6	PRO	CD	50.47	0.05	1
A	2	THR	HB	4.18	0.02	1
A	11	THR	HB	4.13	0.02	1
A	10	THR	C	174.463	0.05	1
A	9	LYS	HA	4.404	0.02	1
A	11	THR	CG2	21.52	0.05	1
A	6	PRO	HG2	2.03	0.02	2
A	4	GLN	HG3	2.35	0.02	2
A	5	PRO	HB3	2.402	0.02	2
A	15	GLY	N	110.702	0.05	1
A	10	THR	CA	61.587	0.05	1
A	14	SER	H	8.33	0.02	1
A	4	GLN	HA	4.593	0.02	1
A	6	PRO	C	177.09	0.05	1
A	2	THR	N	118.415	0.05	1
A	13	ASN	N	119.127	0.05	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	14	SER	CA	58.705	0.05	1
A	2	THR	CB	69.849	0.05	1
A	11	THR	HG22	1.26	0.02	1
A	3	PRO	CA	63.065	0.05	1
A	12	PRO	HD3	3.86	0.02	2
A	1	SER	CA	58.128	0.05	1
A	11	THR	CA	59.858	0.05	1
A	14	SER	HB2	3.832	0.02	2
A	9	LYS	HE3	2.972	0.02	2
A	1	SER	C	174.184	0.05	1
A	8	GLY	HA2	3.969	0.02	2
A	15	GLY	H	8.399	0.02	1
A	4	GLN	N	122.187	0.05	1
A	7	SER	CA	58.321	0.05	1

### 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
$^{13}\text{C}_\alpha$	82	$-0.47 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	79	$-0.07 \pm 0.25$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	75	$-0.36 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	76	$0.51 \pm 0.33$	None needed (imprecise)

### 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 71%, i.e. 676 atoms were assigned a chemical shift out of a possible 951. 12 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	282/346 (82%)	113/138 (82%)	113/140 (81%)	56/68 (82%)
Sidechain	381/555 (69%)	239/324 (74%)	137/203 (67%)	5/28 (18%)
Aromatic	13/50 (26%)	13/26 (50%)	0/20 (0%)	0/4 (0%)
Overall	676/951 (71%)	365/488 (75%)	250/363 (69%)	61/100 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 68%, i.e. 776 atoms were assigned a chemical shift out of a possible 1136. 13 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	327/421 (78%)	131/168 (78%)	131/170 (77%)	65/83 (78%)
Sidechain	436/665 (66%)	274/387 (71%)	155/243 (64%)	7/35 (20%)
Aromatic	13/50 (26%)	13/26 (50%)	0/20 (0%)	0/4 (0%)
Overall	776/1136 (68%)	418/581 (72%)	286/433 (66%)	72/122 (59%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots [i](#)

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:

