



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:09 PM BST

PDB ID : 1ONV  
Title : NMR Structure of a Complex Containing the TFIIF Subunit RAP74 and the RNAP II CTD Phosphatase FCP1  
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Deposited on : 2003-03-02

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

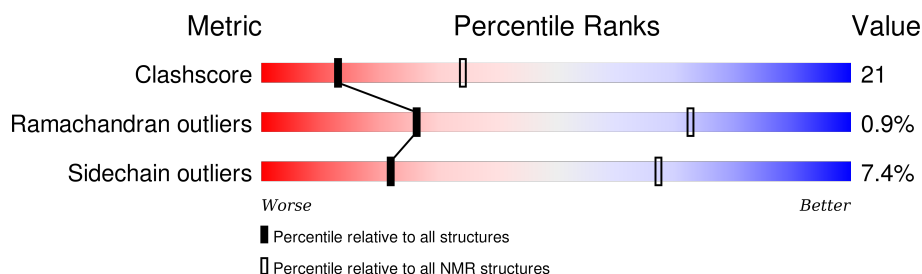
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	A	82	
2	B	83	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average, minimized average structure*.

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:453-A:517, B:945-B:961 (82)	0.54	12

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1437 atoms, of which 733 are hydrogens and 0 are deuteriums.

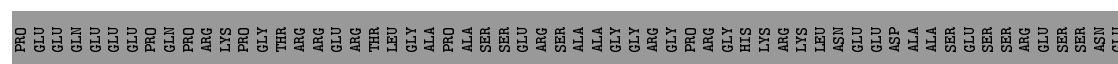
- Molecule 1 is a protein called Transcription initiation factor IIF, alpha subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	67	Total	C	H	N	O	S	0
			1145	346	593	101	102	3	

- Molecule 2 is a protein called serine phosphatase FCP1a.

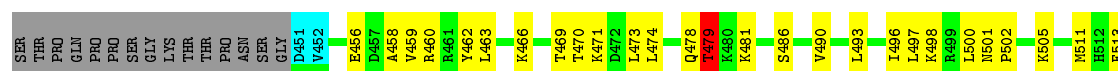
Mol	Chain	Residues	Atoms						Trace
2	B	21	Total	C	H	N	O	S	0
			292	89	140	23	38	2	





#### 4.2.2 Score per residue for model 2

- Molecule 1: Transcription initiation factor IIF, alpha subunit

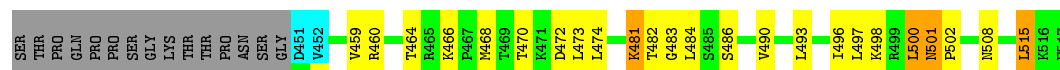


- Molecule 2: serine phosphatase FCP1a



#### 4.2.3 Score per residue for model 3

- Molecule 1: Transcription initiation factor IIF, alpha subunit

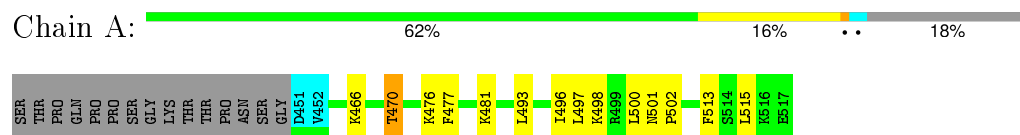


- Molecule 2: serine phosphatase FCP1a

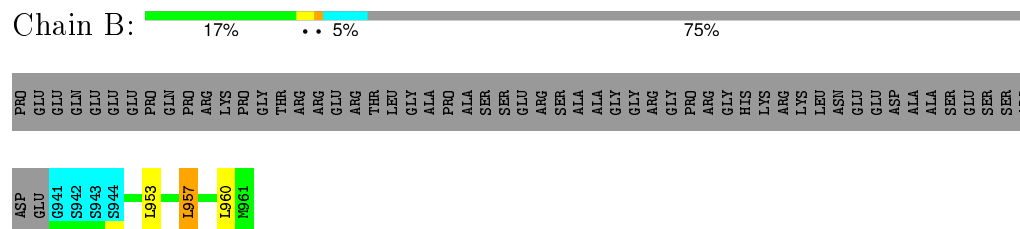


#### 4.2.4 Score per residue for model 4

- Molecule 1: Transcription initiation factor IIF, alpha subunit

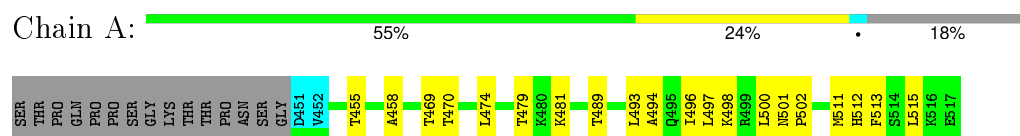


- Molecule 2: serine phosphatase FCP1a

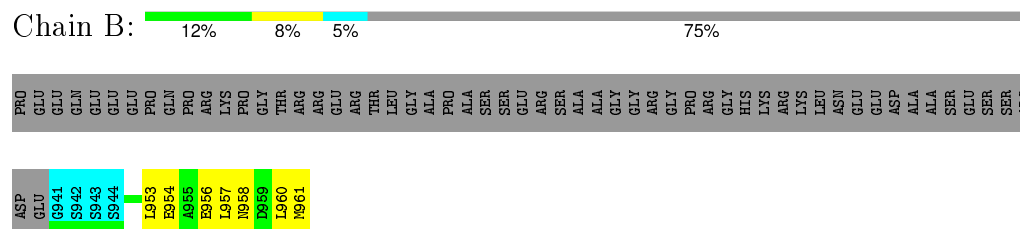


#### 4.2.5 Score per residue for model 5

- Molecule 1: Transcription initiation factor IIF, alpha subunit

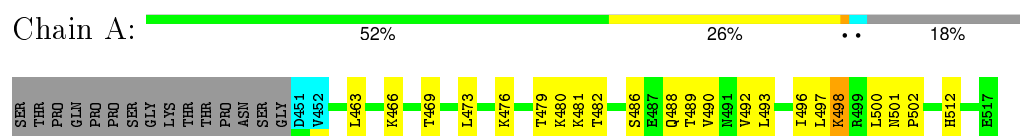


- Molecule 2: serine phosphatase FCP1a



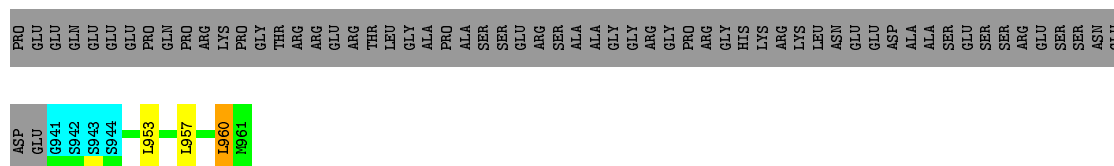
#### 4.2.6 Score per residue for model 6

- Molecule 1: Transcription initiation factor IIF, alpha subunit



- Molecule 2: serine phosphatase FCP1a

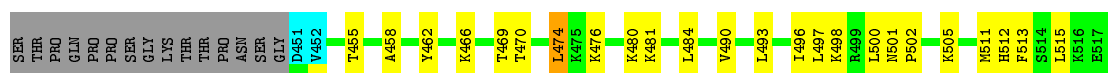
Chain B: 



#### 4.2.7 Score per residue for model 7

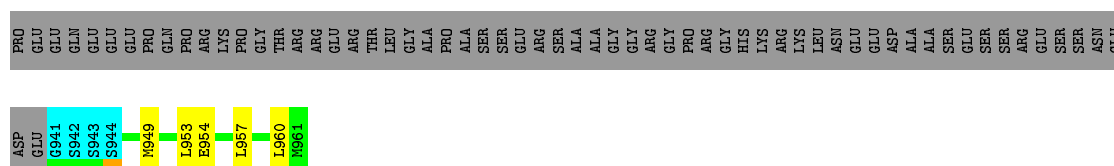
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



- Molecule 2: serine phosphatase FCP1a

Chain B: 



#### 4.2.8 Score per residue for model 8

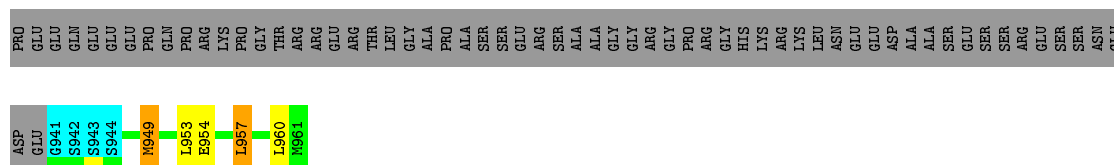
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



- Molecule 2: serine phosphatase FCP1a

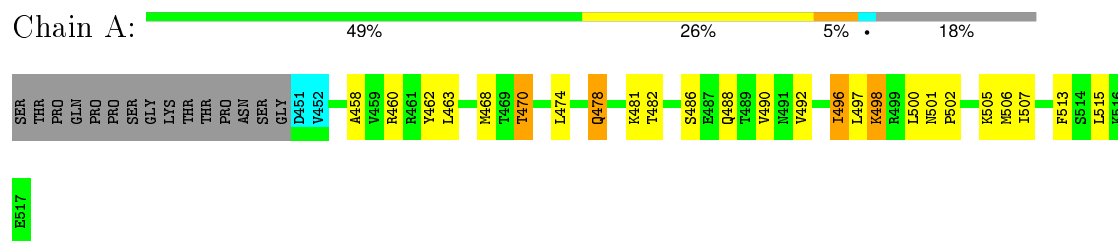
Chain B: 



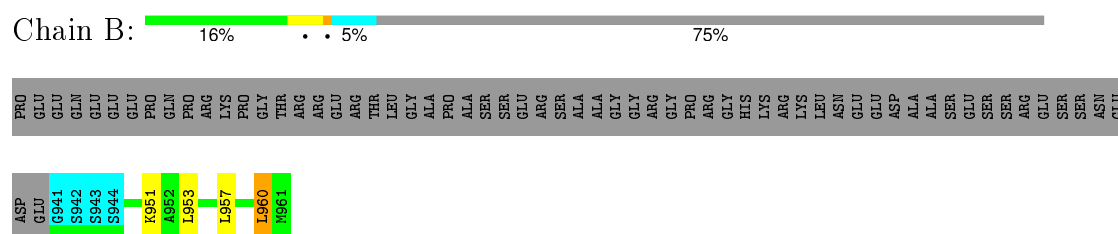


### 4.2.9 Score per residue for model 9

- Molecule 1: Transcription initiation factor IIF, alpha subunit

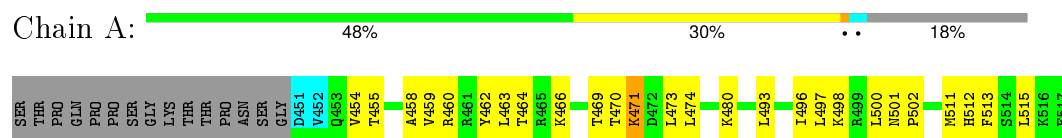


- Molecule 2: serine phosphatase FCP1a

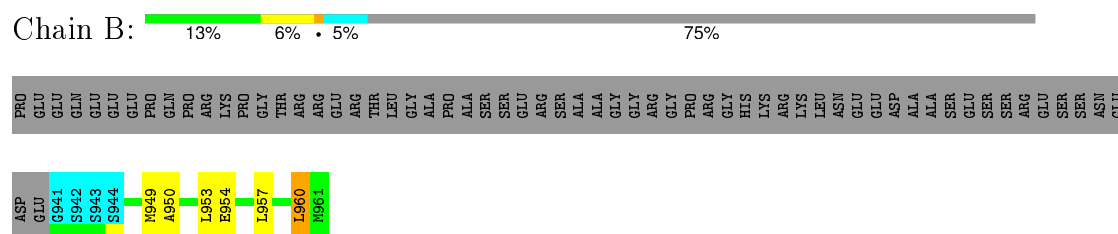


### 4.2.10 Score per residue for model 10

- Molecule 1: Transcription initiation factor IIF, alpha subunit



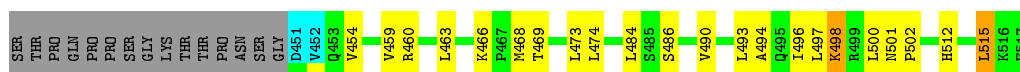
- Molecule 2: serine phosphatase FCP1a



### 4.2.11 Score per residue for model 11

- Molecule 1: Transcription initiation factor IIF, alpha subunit





- Molecule 2: serine phosphatase FCP1a



#### 4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Transcription initiation factor IIF, alpha subunit

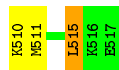
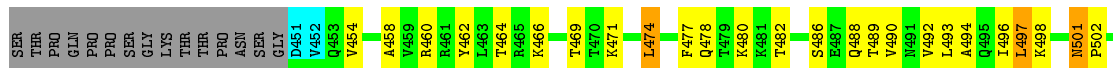


- Molecule 2: serine phosphatase FCP1a



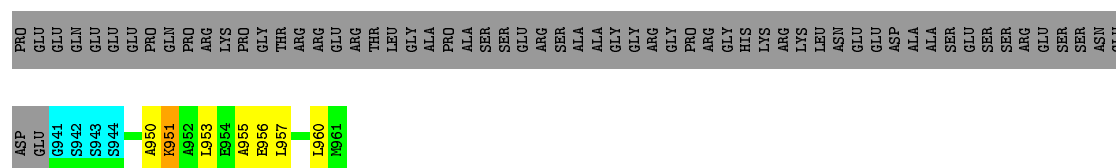
#### 4.2.13 Score per residue for model 13

- Molecule 1: Transcription initiation factor IIF, alpha subunit



- Molecule 2: serine phosphatase FCP1a

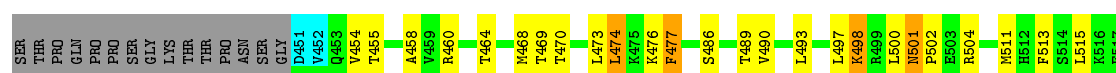
Chain B: 



#### 4.2.14 Score per residue for model 14

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



- Molecule 2: serine phosphatase FCP1a

Chain B: 



#### 4.2.15 Score per residue for model 15

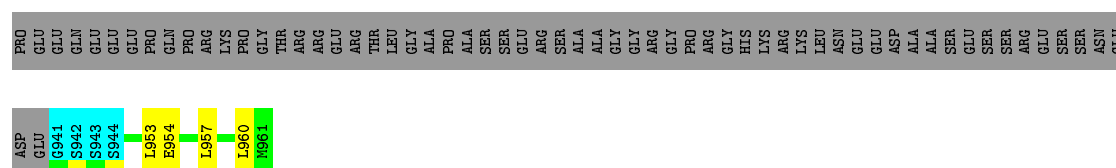
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



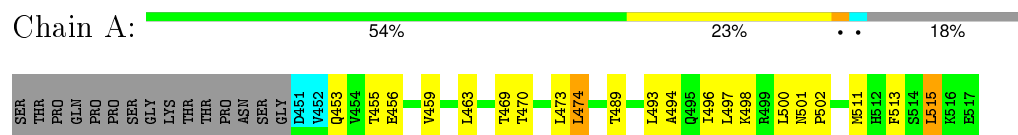
- Molecule 2: serine phosphatase FCP1a

Chain B: 

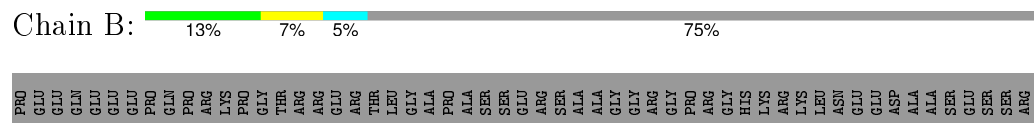


### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription initiation factor IIF, alpha subunit

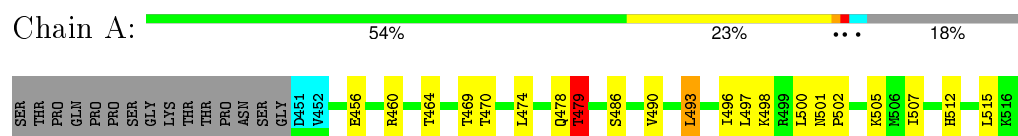


- Molecule 2: serine phosphatase FCP1a

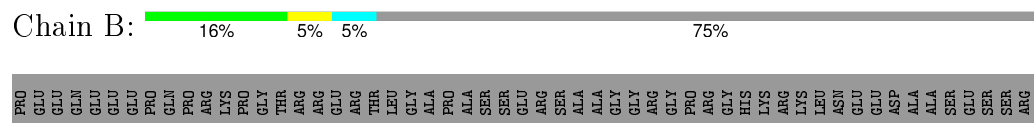


### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription initiation factor IIF, alpha subunit

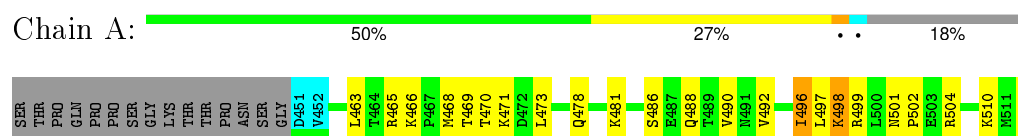


- Molecule 2: serine phosphatase FCP1a



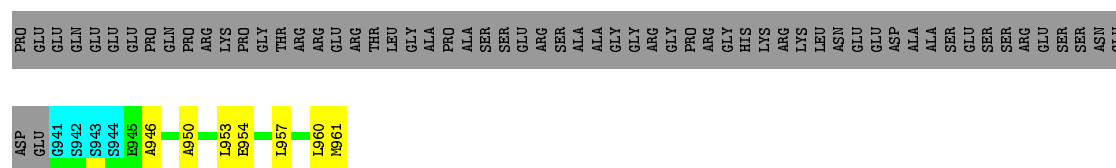
### 4.2.18 Score per residue for model 18

- Molecule 1: Transcription initiation factor IIF, alpha subunit



- Molecule 2: serine phosphatase FCP1a

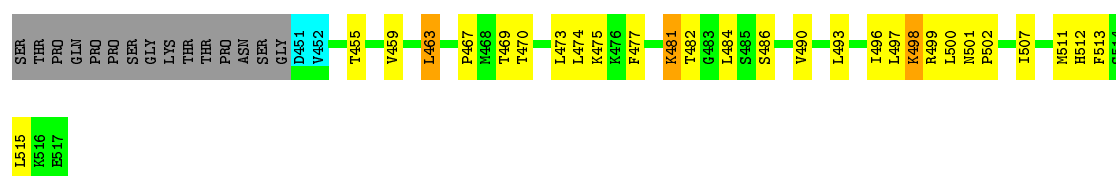
Chain B: 



#### 4.2.19 Score per residue for model 19

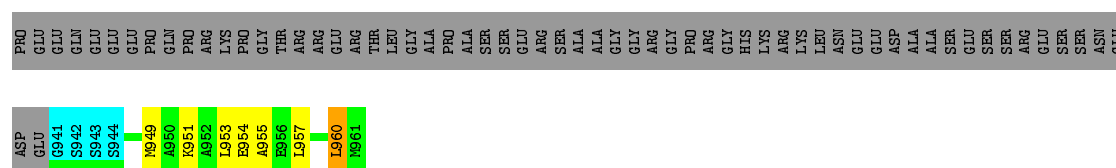
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



- Molecule 2: serine phosphatase FCP1a

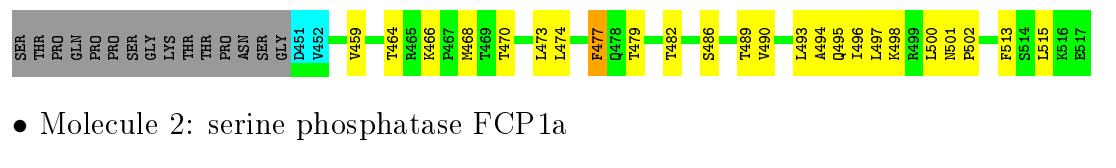
Chain B: 



#### 4.2.20 Score per residue for model 20

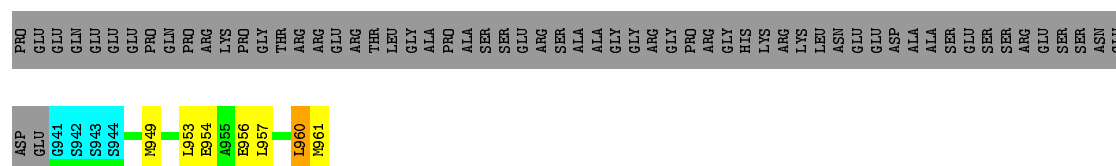
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 



- Molecule 2: serine phosphatase FCP1a

Chain B: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *Torsion Angle Dynamics*.

Of the 70 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	modified CNS with conformational database potential

No chemical shift data was provided. 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	537	580	579	27±5
2	B	130	122	122	15±5
All	All	13340	14040	14020	588

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 21.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:474:LEU:HD21	1:A:490:VAL:HG22	1.05	1.27	19	2
2:B:957:LEU:HD23	2:B:960:LEU:HD21	1.03	1.22	1	1
1:A:500:LEU:HD21	1:A:515:LEU:HD11	0.95	1.32	2	3
2:B:957:LEU:HD11	2:B:960:LEU:HD13	0.95	1.38	16	2
1:A:497:LEU:HD13	2:B:953:LEU:HD21	0.92	1.42	7	12
1:A:497:LEU:HD12	2:B:953:LEU:HD11	0.91	1.37	5	6
1:A:474:LEU:HD22	1:A:493:LEU:HD23	0.91	1.40	14	1
1:A:470:THR:HG22	2:B:953:LEU:HD23	0.89	1.40	4	3
1:A:498:LYS:O	2:B:960:LEU:HD11	0.89	1.68	5	9
2:B:957:LEU:CD2	2:B:960:LEU:HD21	0.89	1.98	1	1
1:A:470:THR:HG23	1:A:513:PHE:CE2	0.88	2.04	14	9
1:A:470:THR:HG23	1:A:513:PHE:CE1	0.82	2.10	5	3
1:A:497:LEU:O	2:B:957:LEU:HD21	0.82	1.73	1	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:500:LEU:HD11	1:A:515:LEU:HD11	0.81	1.52	16	2
1:A:497:LEU:CD1	2:B:953:LEU:HD21	0.81	2.05	3	8
1:A:498:LYS:O	2:B:960:LEU:HD13	0.80	1.75	6	7
1:A:477:PHE:CE2	1:A:482:THR:HG22	0.80	2.11	20	1
1:A:497:LEU:O	2:B:957:LEU:HD11	0.79	1.75	15	2
1:A:460:ARG:O	1:A:464:THR:HG23	0.79	1.78	3	5
1:A:502:PRO:HD2	2:B:957:LEU:HD11	0.77	1.57	12	3
1:A:497:LEU:O	2:B:957:LEU:HD13	0.77	1.79	3	4
1:A:501:ASN:HA	2:B:960:LEU:HD13	0.77	1.54	5	8
1:A:474:LEU:CD2	1:A:490:VAL:HG22	0.77	2.08	19	1
1:A:501:ASN:HA	2:B:960:LEU:HD21	0.76	1.56	19	8
1:A:469:THR:HG23	1:A:512:HIS:CD2	0.76	2.16	19	5
1:A:456:GLU:N	1:A:496:ILE:HD11	0.76	1.95	17	2
1:A:486:SER:O	1:A:490:VAL:HG23	0.75	1.81	12	14
1:A:497:LEU:HD13	1:A:500:LEU:HD12	0.75	1.57	19	1
1:A:513:PHE:CE1	2:B:957:LEU:HD23	0.75	2.17	14	1
1:A:502:PRO:HG3	2:B:957:LEU:HD21	0.74	1.58	3	4
2:B:957:LEU:CD1	2:B:960:LEU:HD13	0.74	2.13	17	2
1:A:471:LYS:HG2	2:B:950:ALA:HB2	0.74	1.58	13	2
1:A:502:PRO:CG	2:B:957:LEU:HD21	0.74	2.12	14	5
2:B:957:LEU:HD23	2:B:960:LEU:CD1	0.73	2.12	18	3
1:A:474:LEU:HD23	2:B:953:LEU:HD13	0.73	1.57	14	2
2:B:957:LEU:CD2	2:B:960:LEU:HD22	0.73	2.14	10	3
1:A:488:GLN:O	1:A:492:VAL:HG23	0.73	1.84	1	6
1:A:501:ASN:HA	2:B:960:LEU:HD11	0.73	1.61	16	2
1:A:501:ASN:OD1	2:B:960:LEU:HD22	0.72	1.83	5	2
1:A:501:ASN:OD1	2:B:960:LEU:HD11	0.72	1.85	19	1
1:A:497:LEU:HD13	2:B:953:LEU:HD11	0.71	1.62	11	2
2:B:957:LEU:HD13	2:B:960:LEU:CD1	0.71	2.15	13	2
1:A:455:THR:O	1:A:459:VAL:HG23	0.71	1.85	16	2
1:A:500:LEU:HD21	1:A:515:LEU:HD21	0.71	1.61	9	1
1:A:497:LEU:CD1	2:B:953:LEU:HD11	0.71	2.13	5	10
2:B:957:LEU:HD23	2:B:960:LEU:HD11	0.71	1.62	18	2
1:A:470:THR:CB	2:B:953:LEU:HD23	0.70	2.15	10	3
2:B:957:LEU:HG	2:B:960:LEU:HD22	0.69	1.61	17	1
1:A:498:LYS:O	2:B:960:LEU:HD23	0.69	1.88	1	1
1:A:493:LEU:HD12	2:B:953:LEU:HD11	0.69	1.65	17	1
1:A:477:PHE:O	1:A:489:THR:HG21	0.68	1.87	14	2
1:A:470:THR:HB	2:B:953:LEU:HD23	0.68	1.64	14	2
1:A:493:LEU:O	1:A:497:LEU:HD12	0.67	1.88	10	7
1:A:501:ASN:CG	2:B:960:LEU:HD11	0.67	2.09	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:493:LEU:O	1:A:497:LEU:HD23	0.67	1.89	19	2
1:A:469:THR:HG22	1:A:511:MET:O	0.67	1.90	13	8
1:A:477:PHE:O	1:A:482:THR:HG21	0.66	1.91	19	1
1:A:470:THR:CG2	2:B:953:LEU:HD23	0.66	2.19	4	3
1:A:498:LYS:O	2:B:960:LEU:HD22	0.66	1.91	11	4
1:A:502:PRO:HD2	2:B:957:LEU:HD22	0.66	1.66	5	4
1:A:477:PHE:O	1:A:482:THR:HG23	0.66	1.91	13	1
1:A:501:ASN:CB	2:B:960:LEU:HD22	0.65	2.21	2	2
1:A:498:LYS:O	2:B:960:LEU:HD21	0.65	1.90	14	7
1:A:470:THR:HG21	2:B:954:GLU:CA	0.65	2.21	10	5
1:A:471:LYS:CG	2:B:950:ALA:HB2	0.64	2.22	13	1
1:A:473:LEU:HD13	1:A:497:LEU:HD11	0.64	1.68	6	2
1:A:470:THR:HG22	2:B:953:LEU:CD2	0.64	2.20	4	1
1:A:494:ALA:HA	2:B:953:LEU:HD12	0.64	1.68	5	1
1:A:502:PRO:HD2	2:B:957:LEU:HD12	0.64	1.68	13	1
2:B:957:LEU:HD23	2:B:960:LEU:HD22	0.64	1.70	19	2
1:A:460:ARG:HG3	1:A:515:LEU:HD13	0.63	1.70	9	5
1:A:505:LYS:HD2	1:A:507:ILE:HD11	0.63	1.69	17	2
1:A:478:GLN:O	1:A:479:THR:HG23	0.63	1.94	1	3
1:A:505:LYS:CD	1:A:507:ILE:HD11	0.63	2.24	17	2
1:A:502:PRO:CD	2:B:957:LEU:HD22	0.63	2.24	5	1
1:A:474:LEU:O	1:A:474:LEU:HD23	0.63	1.93	1	1
1:A:497:LEU:HD23	1:A:500:LEU:HD22	0.61	1.71	11	8
1:A:469:THR:O	1:A:473:LEU:HD12	0.61	1.95	2	2
1:A:502:PRO:CD	2:B:957:LEU:HD21	0.61	2.25	14	2
1:A:474:LEU:HD21	1:A:490:VAL:CG2	0.61	2.14	19	1
1:A:500:LEU:HD23	1:A:502:PRO:HG3	0.61	1.72	16	6
1:A:501:ASN:HA	2:B:960:LEU:HD22	0.61	1.72	1	1
1:A:470:THR:HG21	2:B:954:GLU:HB3	0.60	1.73	19	3
1:A:500:LEU:HD11	1:A:515:LEU:CD1	0.60	2.25	16	2
1:A:460:ARG:HG3	1:A:515:LEU:HD22	0.60	1.70	11	2
1:A:490:VAL:HG21	2:B:949:MET:HA	0.60	1.72	2	1
1:A:474:LEU:HD22	2:B:949:MET:CE	0.60	2.26	20	3
1:A:501:ASN:N	1:A:502:PRO:HD3	0.60	2.12	5	4
2:B:957:LEU:HD12	2:B:960:LEU:HD11	0.60	1.74	14	1
1:A:468:MET:SD	1:A:473:LEU:HD23	0.60	2.37	18	3
2:B:957:LEU:CG	2:B:960:LEU:HD22	0.60	2.26	17	1
1:A:463:LEU:CD1	1:A:500:LEU:HD21	0.59	2.26	6	1
1:A:494:ALA:HB1	2:B:956:GLU:HG3	0.59	1.74	20	3
1:A:460:ARG:CG	1:A:515:LEU:HD22	0.59	2.27	11	2
1:A:474:LEU:HD22	2:B:949:MET:HE1	0.59	1.74	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:474:LEU:CD2	2:B:953:LEU:HD13	0.59	2.28	13	1
1:A:469:THR:HG22	1:A:512:HIS:CD2	0.58	2.33	18	2
1:A:470:THR:HG23	1:A:513:PHE:CD2	0.58	2.33	9	1
2:B:957:LEU:O	2:B:960:LEU:HD12	0.58	1.98	14	3
1:A:480:LYS:HG3	1:A:482:THR:HG23	0.58	1.75	6	1
1:A:484:LEU:HD22	1:A:484:LEU:N	0.58	2.14	11	5
1:A:494:ALA:HB1	2:B:956:GLU:OE1	0.58	1.98	13	1
1:A:470:THR:HG23	1:A:513:PHE:HE2	0.58	1.58	1	5
1:A:459:VAL:HG13	1:A:473:LEU:HD23	0.58	1.74	2	1
1:A:474:LEU:HD13	2:B:949:MET:HB3	0.58	1.76	10	2
1:A:501:ASN:CA	2:B:960:LEU:HD22	0.58	2.29	1	1
1:A:501:ASN:CA	2:B:960:LEU:HD11	0.58	2.29	16	2
1:A:459:VAL:HG12	1:A:463:LEU:CD1	0.58	2.29	12	1
1:A:493:LEU:HG	1:A:497:LEU:HD12	0.57	1.75	14	1
1:A:497:LEU:HB3	2:B:957:LEU:HD22	0.57	1.76	3	4
1:A:497:LEU:CD2	1:A:500:LEU:HD22	0.57	2.30	15	1
1:A:460:ARG:NE	1:A:515:LEU:HD22	0.56	2.15	13	1
1:A:459:VAL:O	1:A:463:LEU:HD12	0.56	2.00	15	4
1:A:477:PHE:CD2	1:A:482:THR:HG21	0.56	2.36	15	1
1:A:477:PHE:CD2	1:A:482:THR:HG22	0.56	2.35	20	1
1:A:474:LEU:HD13	1:A:474:LEU:O	0.56	2.00	7	1
1:A:502:PRO:HG2	2:B:957:LEU:HD21	0.56	1.77	14	1
1:A:500:LEU:CD1	1:A:515:LEU:HD11	0.56	2.30	16	2
1:A:501:ASN:CG	2:B:960:LEU:HD22	0.56	2.21	5	3
1:A:498:LYS:O	2:B:960:LEU:HD12	0.56	2.00	16	1
1:A:474:LEU:CD2	1:A:493:LEU:HD23	0.55	2.26	14	1
1:A:474:LEU:HD13	2:B:949:MET:CB	0.55	2.32	10	1
1:A:501:ASN:CA	2:B:960:LEU:HD13	0.55	2.30	5	2
2:B:960:LEU:HD12	2:B:961:MET:N	0.55	2.17	1	1
1:A:474:LEU:O	1:A:474:LEU:HD13	0.55	2.02	16	3
1:A:474:LEU:HD22	2:B:949:MET:HE2	0.54	1.79	20	1
1:A:497:LEU:O	2:B:957:LEU:CD1	0.54	2.55	14	1
1:A:502:PRO:CD	2:B:957:LEU:HD11	0.54	2.31	12	3
2:B:953:LEU:HD13	2:B:953:LEU:O	0.54	2.02	11	1
2:B:957:LEU:HD12	2:B:960:LEU:HD22	0.54	1.79	12	1
1:A:497:LEU:CD1	1:A:500:LEU:HD22	0.54	2.32	4	1
1:A:497:LEU:HB3	2:B:957:LEU:HD11	0.54	1.78	1	1
1:A:474:LEU:HD13	2:B:949:MET:HG2	0.54	1.79	3	1
1:A:478:GLN:HG3	1:A:479:THR:HG22	0.54	1.79	12	1
1:A:470:THR:HG21	2:B:954:GLU:HA	0.54	1.78	10	4
1:A:463:LEU:HD13	1:A:515:LEU:HD12	0.54	1.79	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:470:THR:HG21	2:B:954:GLU:CB	0.54	2.33	7	5
1:A:498:LYS:O	2:B:960:LEU:CD2	0.54	2.55	1	1
1:A:454:VAL:HG11	1:A:493:LEU:HD21	0.54	1.79	1	4
2:B:960:LEU:HD23	2:B:961:MET:N	0.54	2.18	12	1
1:A:468:MET:HE3	1:A:473:LEU:HD23	0.53	1.78	20	1
1:A:459:VAL:HG13	1:A:473:LEU:HD21	0.53	1.80	3	1
1:A:480:LYS:CG	1:A:482:THR:HG23	0.53	2.34	6	1
1:A:493:LEU:HB3	2:B:953:LEU:HD11	0.53	1.79	20	4
1:A:490:VAL:HG21	2:B:949:MET:HB2	0.53	1.78	7	1
1:A:502:PRO:HD2	2:B:957:LEU:HD21	0.53	1.79	14	1
1:A:471:LYS:HD2	2:B:950:ALA:HB2	0.53	1.78	10	1
1:A:489:THR:O	1:A:493:LEU:HD13	0.53	2.03	15	4
1:A:500:LEU:O	1:A:500:LEU:HD23	0.53	2.04	9	1
1:A:501:ASN:HB2	2:B:960:LEU:HD22	0.52	1.80	2	1
1:A:473:LEU:HD13	1:A:497:LEU:HD21	0.52	1.79	18	1
1:A:478:GLN:HA	1:A:489:THR:HG21	0.52	1.80	13	1
2:B:957:LEU:HD13	2:B:960:LEU:HD11	0.52	1.81	13	1
1:A:497:LEU:HG	2:B:953:LEU:HD21	0.52	1.80	19	1
1:A:459:VAL:HG11	1:A:497:LEU:HD21	0.52	1.81	12	4
1:A:470:THR:HG23	1:A:513:PHE:HE1	0.52	1.61	5	1
1:A:459:VAL:HG12	1:A:463:LEU:HD12	0.52	1.81	12	1
1:A:474:LEU:HD11	1:A:490:VAL:HG22	0.52	1.81	14	3
1:A:493:LEU:HD12	2:B:953:LEU:CD1	0.51	2.33	17	1
1:A:501:ASN:N	1:A:502:PRO:CD	0.51	2.73	19	18
1:A:497:LEU:HD13	2:B:953:LEU:CD2	0.51	2.32	16	2
1:A:489:THR:HG22	1:A:493:LEU:HD12	0.51	1.82	8	1
1:A:498:LYS:O	2:B:960:LEU:CD1	0.51	2.58	17	1
2:B:957:LEU:HD11	2:B:960:LEU:HD12	0.51	1.83	3	1
1:A:463:LEU:HD22	1:A:515:LEU:HD12	0.51	1.81	16	1
1:A:453:GLN:OE1	1:A:455:THR:HG23	0.51	2.06	16	1
1:A:455:THR:HG23	1:A:458:ALA:H	0.50	1.67	5	5
2:B:957:LEU:HD23	2:B:960:LEU:CD2	0.50	2.16	1	1
1:A:470:THR:CG2	2:B:953:LEU:HD22	0.50	2.36	3	1
1:A:474:LEU:HD12	1:A:478:GLN:OE1	0.50	2.07	13	1
1:A:501:ASN:CA	2:B:960:LEU:HD21	0.50	2.36	11	2
1:A:497:LEU:HD23	1:A:500:LEU:CD2	0.49	2.36	17	1
1:A:463:LEU:HB2	1:A:515:LEU:HD11	0.49	1.83	15	1
2:B:953:LEU:C	2:B:953:LEU:HD23	0.49	2.28	17	1
1:A:463:LEU:HD23	1:A:468:MET:HG2	0.49	1.82	12	1
1:A:477:PHE:HD2	1:A:482:THR:HG21	0.49	1.67	15	1
1:A:470:THR:HG21	2:B:954:GLU:HG2	0.49	1.84	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:957:LEU:HA	2:B:960:LEU:HD12	0.49	1.85	13	1
1:A:484:LEU:N	1:A:484:LEU:HD22	0.49	2.23	3	1
1:A:489:THR:HG22	1:A:493:LEU:CD1	0.48	2.38	20	1
1:A:474:LEU:HD21	2:B:949:MET:CE	0.48	2.38	8	1
1:A:463:LEU:HD13	1:A:500:LEU:HD21	0.48	1.85	6	1
2:B:951:LYS:O	2:B:955:ALA:HB2	0.48	2.07	13	2
1:A:463:LEU:HD23	1:A:468:MET:CG	0.48	2.39	9	1
1:A:493:LEU:CD1	2:B:953:LEU:HD11	0.48	2.36	17	1
2:B:957:LEU:CD2	2:B:960:LEU:HD12	0.48	2.39	7	2
1:A:474:LEU:HD23	2:B:949:MET:HB3	0.47	1.84	19	1
2:B:957:LEU:CD1	2:B:960:LEU:HD22	0.47	2.39	17	2
1:A:456:GLU:HB2	1:A:496:ILE:HD11	0.47	1.87	16	2
1:A:496:ILE:CG2	1:A:497:LEU:N	0.47	2.78	8	12
1:A:474:LEU:CD2	2:B:953:LEU:HD22	0.47	2.40	2	1
1:A:497:LEU:HD13	1:A:500:LEU:HD22	0.46	1.86	4	1
1:A:477:PHE:HB2	1:A:493:LEU:HD21	0.46	1.88	19	1
2:B:953:LEU:HD23	2:B:953:LEU:C	0.46	2.30	12	2
1:A:474:LEU:HD12	1:A:493:LEU:CD1	0.46	2.40	8	1
1:A:501:ASN:HA	2:B:960:LEU:CD1	0.46	2.40	3	3
1:A:463:LEU:HD12	1:A:515:LEU:HD12	0.46	1.88	10	2
1:A:471:LYS:HA	2:B:950:ALA:HB2	0.46	1.88	2	1
1:A:469:THR:CG2	1:A:512:HIS:CD2	0.45	3.00	5	7
1:A:460:ARG:CD	1:A:515:LEU:HD22	0.45	2.41	13	1
2:B:960:LEU:HD23	2:B:961:MET:OXT	0.45	2.10	16	1
1:A:474:LEU:HD22	1:A:493:LEU:CD2	0.45	2.27	14	1
1:A:513:PHE:CZ	2:B:961:MET:CE	0.45	3.00	1	1
1:A:501:ASN:HA	2:B:960:LEU:CD2	0.45	2.41	20	3
1:A:493:LEU:HD12	1:A:497:LEU:HD12	0.45	1.87	17	1
1:A:473:LEU:HD12	2:B:953:LEU:HD21	0.45	1.88	10	1
2:B:957:LEU:CD2	2:B:960:LEU:CD1	0.45	2.94	8	3
1:A:513:PHE:CE1	2:B:961:MET:CE	0.45	3.00	1	1
1:A:511:MET:CE	1:A:513:PHE:CE2	0.45	3.00	7	1
1:A:502:PRO:HD2	2:B:960:LEU:HD12	0.45	1.88	3	1
1:A:468:MET:HE3	1:A:472:ASP:OD2	0.45	2.12	3	1
1:A:498:LYS:HG3	1:A:499:ARG:N	0.44	2.25	19	2
1:A:493:LEU:HD13	1:A:493:LEU:O	0.44	2.11	17	1
1:A:500:LEU:C	1:A:500:LEU:HD23	0.44	2.32	9	1
1:A:497:LEU:C	2:B:957:LEU:HD11	0.44	2.32	15	1
1:A:497:LEU:HA	1:A:500:LEU:HD13	0.44	1.89	3	1
1:A:497:LEU:HD11	2:B:953:LEU:HD11	0.44	1.89	16	1
1:A:477:PHE:N	1:A:477:PHE:CD1	0.44	2.86	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:463:LEU:HD21	1:A:473:LEU:HD21	0.44	1.90	18	1
1:A:456:GLU:CA	1:A:496:ILE:HD11	0.43	2.43	16	1
2:B:957:LEU:CD1	2:B:960:LEU:HD11	0.43	2.41	14	1
1:A:454:VAL:HG22	1:A:477:PHE:CE1	0.43	2.48	14	1
1:A:463:LEU:HD21	1:A:473:LEU:HD11	0.43	1.90	2	1
2:B:957:LEU:CD1	2:B:960:LEU:HD12	0.43	2.42	3	1
1:A:494:ALA:HB1	2:B:956:GLU:CD	0.43	2.33	13	1
1:A:493:LEU:CB	2:B:953:LEU:HD11	0.43	2.43	3	1
2:B:958:ASN:O	2:B:961:MET:HE2	0.43	2.12	5	1
1:A:459:VAL:CG1	1:A:473:LEU:HD23	0.43	2.42	2	1
2:B:957:LEU:CD1	2:B:960:LEU:CD1	0.43	2.97	14	2
1:A:481:LYS:C	1:A:482:THR:HG23	0.43	2.33	3	1
2:B:957:LEU:HD12	2:B:957:LEU:O	0.43	2.14	20	1
1:A:470:THR:CA	2:B:953:LEU:HD23	0.43	2.43	10	1
1:A:474:LEU:HD13	1:A:474:LEU:C	0.43	2.35	9	1
1:A:474:LEU:C	1:A:474:LEU:HD23	0.42	2.35	1	1
1:A:470:THR:HG21	2:B:954:GLU:HB2	0.42	1.90	7	1
2:B:957:LEU:HD22	2:B:960:LEU:HD12	0.42	1.90	7	1
2:B:957:LEU:HD12	2:B:960:LEU:HG	0.42	1.91	3	1
1:A:470:THR:HG21	2:B:954:GLU:CG	0.42	2.45	18	1
1:A:497:LEU:HD23	1:A:500:LEU:HD23	0.42	1.92	17	1
1:A:484:LEU:CD2	1:A:484:LEU:N	0.42	2.83	12	3
1:A:463:LEU:CB	1:A:515:LEU:HD11	0.42	2.45	15	1
1:A:470:THR:HG21	2:B:953:LEU:CD2	0.42	2.45	3	1
1:A:474:LEU:HD11	2:B:949:MET:O	0.41	2.15	12	1
1:A:470:THR:HB	2:B:953:LEU:HD22	0.41	1.91	17	2
1:A:458:ALA:O	1:A:462:TYR:CD2	0.41	2.74	9	6
1:A:484:LEU:N	1:A:484:LEU:CD2	0.41	2.84	1	2
1:A:474:LEU:HD12	1:A:493:LEU:HD13	0.41	1.93	8	1
1:A:462:TYR:CZ	1:A:476:LYS:CE	0.41	3.04	7	1
1:A:483:GLY:C	1:A:484:LEU:HD22	0.41	2.36	3	1
1:A:496:ILE:HG22	1:A:497:LEU:N	0.41	2.31	1	3
1:A:497:LEU:O	2:B:957:LEU:CD2	0.41	2.61	5	1
1:A:489:THR:HG22	1:A:493:LEU:HD13	0.41	1.92	5	1
1:A:476:LYS:O	1:A:477:PHE:CG	0.40	2.74	4	1
1:A:470:THR:CG2	2:B:953:LEU:CD2	0.40	3.00	3	1
1:A:474:LEU:HD21	1:A:490:VAL:HA	0.40	1.94	14	1
1:A:467:PRO:CB	1:A:507:ILE:CD1	0.40	3.00	15	1
1:A:467:PRO:CG	1:A:507:ILE:CD1	0.40	3.00	19	1
1:A:482:THR:HB	1:A:484:LEU:HD23	0.40	1.93	1	1
2:B:958:ASN:OD1	2:B:959:ASP:N	0.40	2.55	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:957:LEU:HG	2:B:960:LEU:HD12	0.40	1.93	14	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	64/82 (78%)	60±2 (94±2%)	3±1 (5±2%)	1±1 (1±1%)	23	69
2	B	16/83 (19%)	16±1 (99±3%)	0±1 (1±3%)	0±0 (0±0%)	100	100
All	All	1600/3300 (48%)	1521 (95%)	65 (4%)	14 (1%)	26	73

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)
1	A	479	THR	7
1	A	481	LYS	4
1	A	478	GLN	2
1	A	508	ASN	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	62/77 (81%)	58±2 (93±3%)	4±2 (7±3%)	23	68
2	B	13/66 (20%)	12±1 (92±5%)	1±1 (8±5%)	18	63
All	All	1500/2860 (52%)	1389 (93%)	111 (7%)	22	67

All 39 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	466	LYS	11
1	A	515	LEU	9
2	B	960	LEU	8
1	A	498	LYS	8
1	A	496	ILE	7
1	A	481	LYS	6
1	A	474	LEU	5
1	A	480	LYS	4
1	A	479	THR	4
1	A	510	LYS	3
1	A	464	THR	3
1	A	501	ASN	3
2	B	961	MET	3
1	A	470	THR	3
1	A	505	LYS	2
2	B	951	LYS	2
2	B	954	GLU	2
1	A	475	LYS	2
1	A	476	LYS	2
2	B	949	MET	2
2	B	957	LEU	2
1	A	477	PHE	2
1	A	504	ARG	2
1	A	478	GLN	1
1	A	471	LYS	1
1	A	482	THR	1
1	A	500	LEU	1
2	B	953	LEU	1
2	B	958	ASN	1
1	A	497	LEU	1
1	A	495	GLN	1
1	A	506	MET	1
1	A	463	LEU	1
1	A	461	ARG	1
1	A	493	LEU	1
1	A	511	MET	1
1	A	465	ARG	1
2	B	956	GLU	1
1	A	455	THR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.



## 7 Chemical shift validation

No chemical shift data were provided