



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 01:19 AM UTC

PDB ID : 1ONV / pdb_00001onv
Title : NMR Structure of a Complex Containing the TFIIF Subunit RAP74 and the RNAP II CTD Phosphatase FCP1
Authors : Nguyen, B.D.; Abbott, K.L.; Potempa, K.; Kobor, M.S.; Archambault, J.; Greenblatt, J.; Legault, P.; Omichinski, J.G.
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

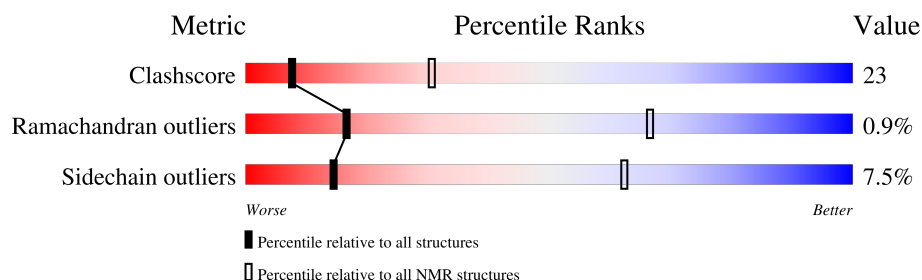
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	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)	0.94	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.

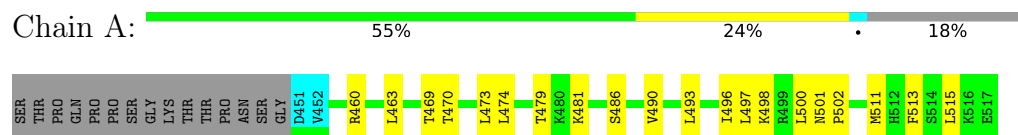
Mol	Chain	Residues	Atoms						Trace
2	B	21	Total	C	H	N	O	S	0
			292	89	140	23	38	2	

4 Residue-property plots [i](#)

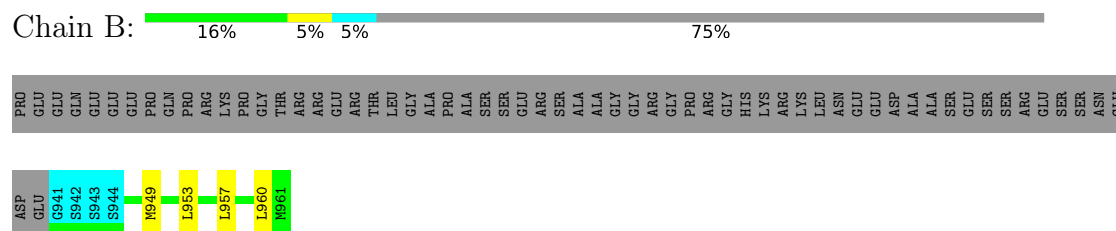
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Transcription initiation factor IIF', alpha subunit



- Molecule 2: serine phosphatase FCP1a

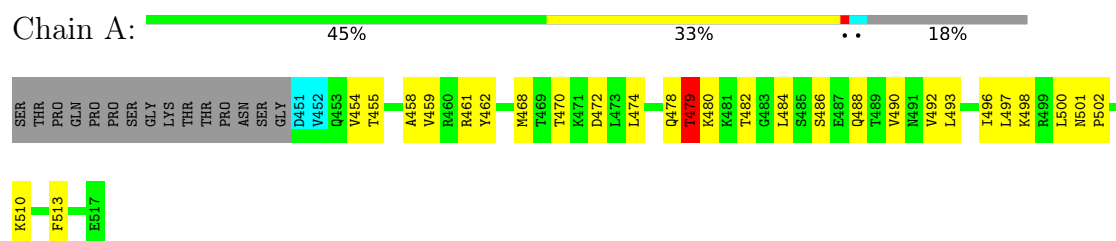


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Transcription initiation factor IIF', alpha subunit



- Molecule 2: serine phosphatase FCP1a

Chain B:  14% 6% 5% 75%

PRO GLU GLU GLN GLU GLU PRO GLN PRO ARG LYS PRO GLY THR ARG GLU ARG THR LEU GLY ALA PRO ALA SER SER ARG SER ALA ALA GLY GLY ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA SER GLU SER ARG GLU SER ASN GLU

ASP GLU G941 S942 S943 S944 M949 L953 L957 L960 M961

4.2.2 Score per residue for model 2

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A:  43% 34% ... 18%

SER THR PRO GLN PRO PRO SER GLY LYS THR THR PRO ASN SER GLY D451 V452 E456 D457 A458 V459 V460 R461 Y462 L463 K466 T469 T470 K471 D472 L473 L474 Q478 T479 R480 K481 S486 V490 L493 T496 L497 K498 R499 L500 N501 P502 K505 M506 D509 K510

M511 M512 F513 S514 L515 K516 E517

- Molecule 2: serine phosphatase FCP1a

Chain B:  14% 5% 5% 75%

PRO GLU GLU GLN GLU GLU PRO GLN PRO ARG LYS PRO GLY THR ARG ARG GLU ARG THR ARG LEU GLY ALA PRO ALA SER SER ARG SER ALA ALA GLY GLY ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA SER GLU SER ARG GLU SER ASN GLU

ASP GLU G941 S942 S943 S944 M949 A950 L953 L957 L960 M961

4.2.3 Score per residue for model 3

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A:  50% 24% 5% 18%

SER THR PRO GLN PRO PRO SER GLY LYS THR THR PRO ASN SER GLY D451 V452 V459 R460 T464 R465 R466 P467 M468 T469 T470 L473 L474 L475 K476 K481 T482 Q483 L484 S485 S486 V490 L493 T496 L497 K498 R499 L500 N501 P502 N508 L515 K516 E517

- Molecule 2: serine phosphatase FCP1a

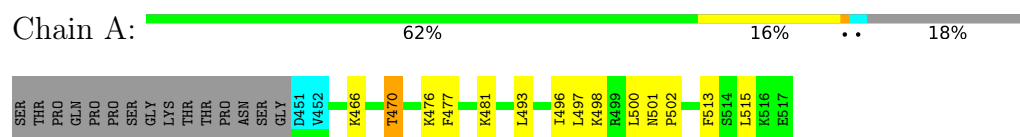
Chain B:  16% 5% 75%

PRO GLU GLU GLN GLU GLU PRO GLN PRO ARG LYS PRO GLY THR ARG ARG GLU ARG THR ARG LEU GLY ALA PRO ALA SER SER ARG SER ALA ALA GLY GLY ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA SER GLU SER ARG GLU SER ASN GLU

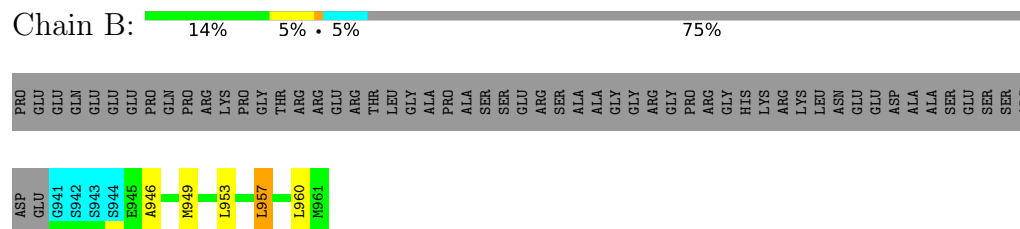
ASP GLU G941 S942 S943 S944 M949 L953 L957 L960 M961

4.2.4 Score per residue for model 4

- Molecule 1: Transcription initiation factor IIF, alpha subunit

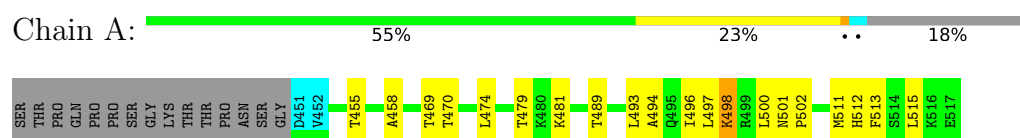


- Molecule 2: serine phosphatase FCP1a

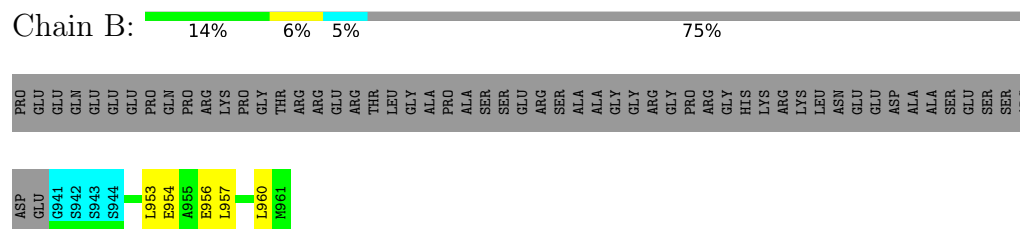


4.2.5 Score per residue for model 5

- Molecule 1: Transcription initiation factor IIF, alpha subunit

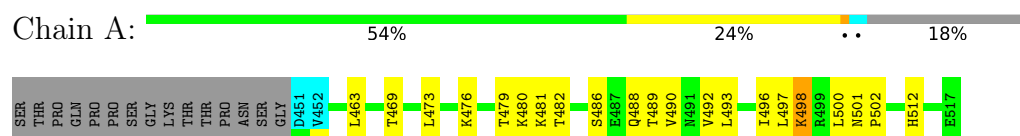


- Molecule 2: serine phosphatase FCP1a



4.2.6 Score per residue for model 6

- Molecule 1: Transcription initiation factor IIF, alpha subunit



- Molecule 2: serine phosphatase FCP1a

Chain B: 

PRO GLU GLU GLN GLU GLU PRO GLN ARG ARG LYS PRO GLY THR ARG ARG GLU ARG THR LEU GLY ALA ALA PRO ALA SER SER SER ARG ARG ALA ALA GLY ARG ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA ALA SER GLU SER ARG SER SER ASN GLU

ASP GLU G941 S942 S943 S944 L953 E956 L957 L960 M961

4.2.7 Score per residue for model 7

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 

SER THR PRO GLN PRO PRO SER GLY LYS THR THR PRO PRO ASN SER GLY D451 V452 T455 A458 Y462 K466 T469 T470 L474 K475 K476 K480 K481 L484 V490 L493 I496 L497 K498 R499 L500 N501 P502 K505 M511 H512 F513 S514 L515 K516 E517

- Molecule 2: serine phosphatase FCP1a

Chain B: 

PRO GLU GLU GLN GLU GLU PRO GLN ARG ARG LYS PRO GLY THR ARG ARG GLU ARG THR LEU GLY ALA ALA PRO ALA SER SER SER ARG ARG ALA ALA GLY ARG ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA ALA SER GLU SER ARG GLU SER SER ASN GLU

ASP GLU G941 S942 S943 S944 M949 L953 E954 L957 L960 M961

4.2.8 Score per residue for model 8

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 

SER THR PRO GLN PRO PRO SER GLY LYS THR THR PRO PRO ASN SER GLY D451 V452 R460 L463 M468 T469 T470 K471 D472 L473 L474 K475 K476 F477 Q478 T479 T489 L493 I496 L497 K498 R499 L500 N501 P502 M511 H512 F513 S514 L515 K516 E517

- Molecule 2: serine phosphatase FCP1a

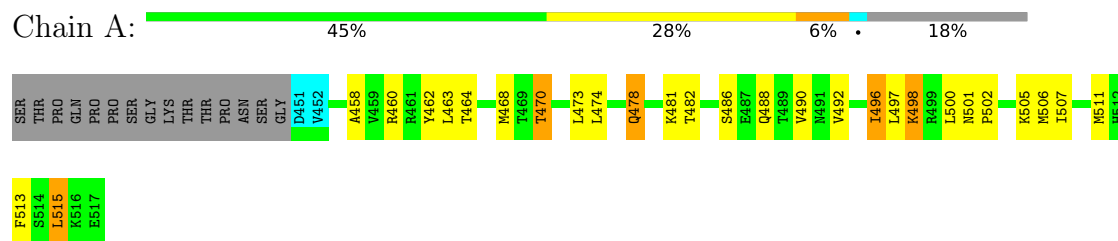
Chain B: 

PRO GLU GLU GLN GLU GLU PRO GLN ARG ARG LYS PRO GLY THR ARG ARG GLU ARG THR LEU GLY ALA ALA PRO ALA SER SER SER ARG ARG ALA ALA GLY ARG ARG GLY PRO ARG GLY HIS LYS ARG LYS LEU ASN GLU ASP ALA ALA SER GLU SER ARG GLU SER SER ASN GLU

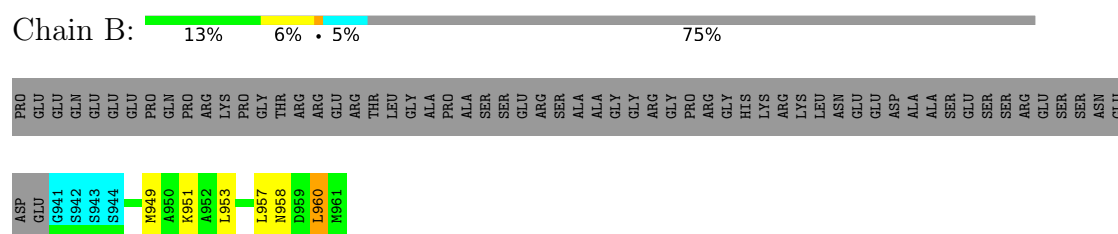
ASP GLU G941 S942 S943 S944 M949 L953 E954 L957 L960 M961

4.2.9 Score per residue for model 9

- Molecule 1: Transcription initiation factor IIF, alpha subunit

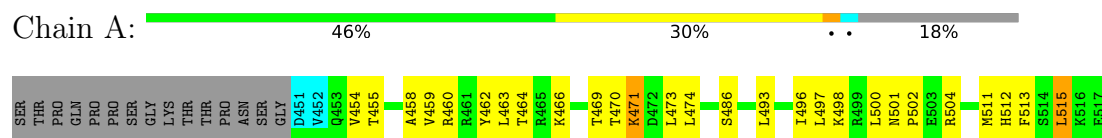


- Molecule 2: serine phosphatase FCP1a

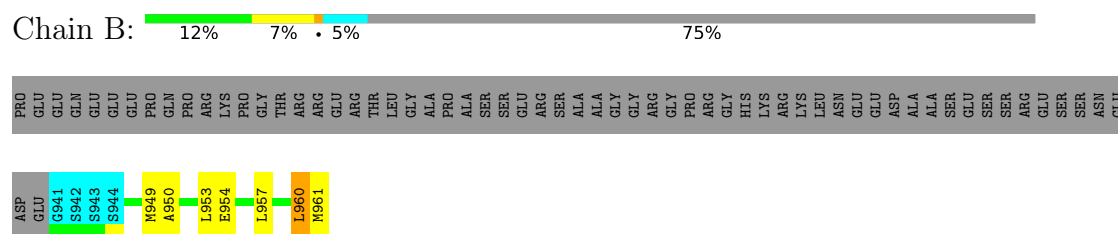


4.2.10 Score per residue for model 10

- Molecule 1: Transcription initiation factor IIF, alpha subunit



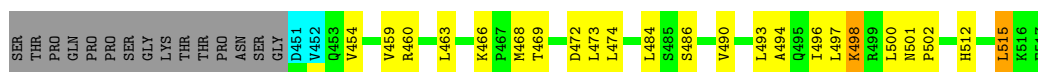
- Molecule 2: serine phosphatase FCP1a



4.2.11 Score per residue for model 11

- Molecule 1: Transcription initiation factor IIF, alpha subunit





- Molecule 2: serine phosphatase FCP1a

Chain B: 14% 5% 75%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 44% 34% 18%



- Molecule 2: serine phosphatase FCP1a

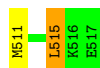
Chain B: 12% 6% 5% 75%



4.2.13 Score per residue for model 13

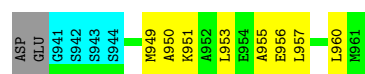
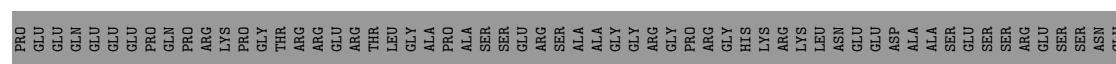
- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 46% 28% 5% 18%



- Molecule 2: serine phosphatase FCP1a

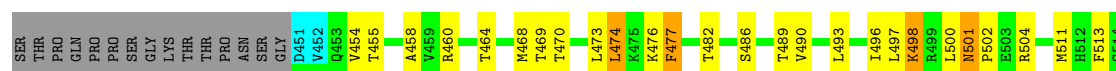
Chain B: 



4.2.14 Score per residue for model 14

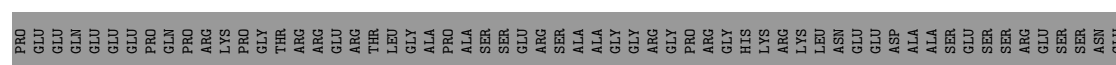
- Molecule 1: Transcription initiation factor IIF, alpha subunit

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

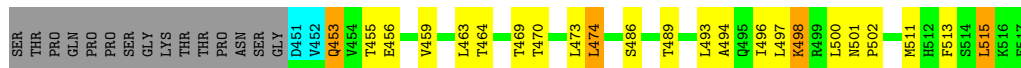
Chain B: 





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

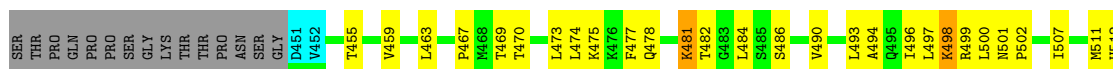
Chain B: 12% 8% 5% 75%



4.2.19 Score per residue for model 19

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 43% 34% 18%



- Molecule 2: serine phosphatase FCP1a

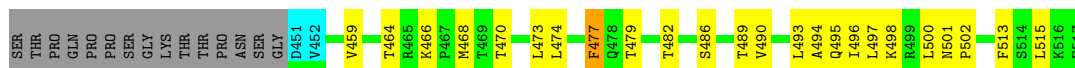
Chain B: 11% 8% 5% 75%



4.2.20 Score per residue for model 20

- Molecule 1: Transcription initiation factor IIF, alpha subunit

Chain A: 50% 28% 18%



- Molecule 2: serine phosphatase FCP1a

Chain B: 13% 6% 5% 75%

ASP	GLU	G941	G942	G943	G944	M949	L953	E954	A955	E956	L957	L960	M961	PRO	GLU	GLN	ARG	LYS	PRO	GLY	THR	ARG	ARG	GLU	ARG	THR	GLY	LEU	ALA	ALA	PRO	SER	SER	GLU	ARG	SER	ALA	ALA	GLY	GLY	ARG	GLY	PRO	ASN	GLU	GLY	ASP	ALA	ALA	SER	SER	GLU	SER	SER	ARG	GLU	SER	SER	ASN	GLU
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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.

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	28±5
2	B	130	122	122	16±5
All	All	13340	14040	14020	625

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 23.

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:474:LEU:HD22	2:B:949:MET:HE2	0.97	1.35	20	4
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
2:B:957:LEU:CD2	2:B:960:LEU:HD21	0.89	1.98	1	1
1:A:498:LYS:O	2:B:960:LEU:HD11	0.89	1.68	5	9
1:A:470:THR:HG23	1:A:513:PHE:CE2	0.88	2.04	14	9
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:470:THR:HG23	1:A:513:PHE:CE1	0.82	2.10	5	3
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:468:MET:HE2	1:A:473:LEU:HD23	0.78	1.55	9	2
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	1.58	12	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:474:LEU:HD21	2:B:949:MET:HE2	0.74	1.59	8	2
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
1:A:478:GLN:CD	2:B:949:MET:HE3	0.74	2.08	13	1
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:CG	2:B:960:LEU:HD11	0.72	2.09	19	1
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:486:SER:OG	2:B:949:MET:HE1	0.72	1.84	16	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
1:A:511:MET:HE1	2:B:958:ASN:ND2	0.70	2.02	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:478:GLN:OE1	2:B:949:MET:HE1	0.69	1.88	9	2
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:511:MET:HE1	1:A:513:PHE:CE2	0.69	2.22	7	1
1:A:477:PHE:O	1:A:489:THR:HG21	0.68	1.87	14	2
1:A:468:MET:HE2	1:A:473:LEU:CD2	0.68	2.19	9	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: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:468:MET:HE3	1:A:472:ASP:OD2	0.64	1.92	12	1
1:A:494:ALA:HA	2:B:953:LEU:HD12	0.64	1.68	5	1
2:B:957:LEU:HD23	2:B:960:LEU:HD22	0.64	1.70	19	2
1:A:502:PRO:HD2	2:B:957:LEU:HD12	0.64	1.68	13	1
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:474:LEU:CD2	2:B:949:MET:HE2	0.63	2.19	20	1
1:A:505:LYS:CD	1:A:507:ILE:HD11	0.63	2.24	17	2
1:A:474:LEU:HD23	1:A:474:LEU:O	0.63	1.93	1	1
1:A:502:PRO:CD	2:B:957:LEU:HD22	0.63	2.24	5	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:504:ARG:NH1	2:B:961:MET:HE1	0.61	2.09	10	1
1:A:470:THR:HG21	2:B:954:GLU:HB3	0.60	1.73	19	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:460:ARG:HG3	1:A:515:LEU:HD22	0.60	1.70	11	2
1:A:500:LEU:HD11	1:A:515:LEU:CD1	0.60	2.25	16	2
1:A:478:GLN:NE2	2:B:949:MET:HE3	0.60	2.11	13	1
1:A:490:VAL:HG21	2:B:949:MET:HA	0.60	1.72	2	1
1:A:501:ASN:CG	2:B:960:LEU:HD22	0.60	2.21	5	4
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:CD2	2:B:953:LEU:HD13	0.59	2.28	13	1
1:A:470:THR:HG23	1:A:513:PHE:CD2	0.58	2.33	9	1
1:A:469:THR:HG22	1:A:512:HIS:CD2	0.58	2.33	18	2
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	6
1:A:470:THR:HG23	1:A:513:PHE:HE2	0.58	1.58	1	5
1:A:494:ALA:HB1	2:B:956:GLU:OE1	0.58	1.98	13	1
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:459:VAL:HG12	1:A:463:LEU:CD1	0.58	2.29	12	1
1:A:501:ASN:CA	2:B:960:LEU:HD11	0.58	2.29	16	2
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:468:MET:HE2	1:A:472:ASP:HB3	0.57	1.76	15	2
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:486:SER:HA	2:B:949:MET:HE3	0.56	1.76	1	2
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:474:LEU:HD13	1:A:474:LEU:O	0.56	2.00	7	4
1:A:502:PRO:HG2	2:B:957:LEU:HD21	0.56	1.77	14	1
1:A:477:PHE:CD2	1:A:482:THR:HG22	0.56	2.35	20	1
1:A:500:LEU:CD1	1:A:515:LEU:HD11	0.56	2.30	16	2
1:A:498:LYS:O	2:B:960:LEU:HD12	0.56	2.00	16	1
1:A:468:MET:HE3	1:A:473:LEU:HD23	0.56	1.77	20	1
1:A:474:LEU:HD13	2:B:949:MET:CB	0.55	2.32	10	1
1:A:474:LEU:CD2	1:A:493:LEU:HD23	0.55	2.26	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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:O	2:B:953:LEU:HD13	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: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:497:LEU:CD1	1:A:500:LEU:HD22	0.54	2.32	4	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
2:B:953:LEU:C	2:B:953:LEU:HD23	0.54	2.28	17	3
1:A:463:LEU:HD13	1:A:515:LEU:HD12	0.54	1.79	9	2
1:A:498:LYS:O	2:B:960:LEU:CD2	0.54	2.55	1	1
1:A:470:THR:HG21	2:B:954:GLU:CB	0.54	2.33	7	5
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: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:471:LYS:HD2	2:B:950:ALA:HB2	0.53	1.78	10	1
1:A:502:PRO:HD2	2:B:957:LEU:HD21	0.53	1.79	14	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:468:MET:HE2	1:A:472:ASP:CG	0.52	2.30	8	2
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:489:THR:HG22	1:A:493:LEU:HD12	0.51	1.82	8	1
1:A:497:LEU:HD13	2:B:953:LEU:CD2	0.51	2.32	16	2
2:B:957:LEU:HD11	2:B:960:LEU:HD12	0.51	1.83	3	1
1:A:498:LYS:O	2:B:960:LEU:CD1	0.51	2.58	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:468:MET:HE1	1:A:476:LYS:HE2	0.50	1.83	8	1
1:A:501:ASN:CA	2:B:960:LEU:HD21	0.50	2.36	11	2
1:A:474:LEU:HD12	1:A:478:GLN:OE1	0.50	2.07	13	1
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
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
1:A:500:LEU:HD23	1:A:500:LEU:C	0.49	2.32	9	1
1:A:497:LEU:C	2:B:957:LEU:HD11	0.49	2.32	15	1
2:B:946:ALA:HA	2:B:949:MET:HE2	0.49	1.85	4	1
2:B:957:LEU:HA	2:B:960:LEU:HD12	0.49	1.85	13	1
1:A:474:LEU:HD22	2:B:949:MET:CE	0.48	2.37	17	2
1:A:489:THR:HG22	1:A:493:LEU:CD1	0.48	2.38	20	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:468:MET:HE1	1:A:476:LYS:CE	0.48	2.38	3	1
1:A:463:LEU:HD23	1:A:468:MET:CG	0.48	2.39	9	1
1:A:481:LYS:C	1:A:482:THR:HG23	0.48	2.33	3	1
2:B:957:LEU:CD2	2:B:960:LEU:HD12	0.48	2.39	7	2
1:A:494:ALA:HB1	2:B:956:GLU:CD	0.48	2.33	13	2
1:A:493:LEU:CD1	2:B:953:LEU:HD11	0.48	2.36	17	1
1:A:506:MET:HE2	1:A:509:ASP:HA	0.47	1.86	2	1
1:A:474:LEU:HD22	2:B:949:MET:HE3	0.47	1.85	3	1
1:A:474:LEU:C	1:A:474:LEU:HD13	0.47	2.35	9	1
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:474:LEU:HD23	1:A:474:LEU:C	0.47	2.35	1	1
1:A:456:GLU:HB2	1:A:496:ILE:HD11	0.47	1.87	16	2
1:A:511:MET:HE1	2:B:958:ASN:HD22	0.47	1.70	9	1
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:501:ASN:HA	2:B:960:LEU:CD1	0.46	2.40	3	3
1:A:474:LEU:HD12	1:A:493:LEU:CD1	0.46	2.40	8	1
1:A:477:PHE:HB2	1:A:493:LEU:HD21	0.46	1.88	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:483:GLY:C	1:A:484:LEU:HD22	0.46	2.36	3	1
1:A:463:LEU:HD12	1:A:515:LEU:HD12	0.46	1.88	10	2
2:B:961:MET:C	2:B:961:MET:HE3	0.46	2.36	12	1
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
1:A:474:LEU:HD22	1:A:493:LEU:CD2	0.45	2.27	14	1
2:B:960:LEU:HD23	2:B:961:MET:OXT	0.45	2.10	16	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:473:LEU:HD12	2:B:953:LEU:HD21	0.45	1.88	10	1
1:A:493:LEU:HD12	1:A:497:LEU:HD12	0.45	1.87	17	1
1:A:513:PHE:CE1	2:B:961:MET:CE	0.45	3.00	1	1
2:B:957:LEU:CD2	2:B:960:LEU:CD1	0.45	2.94	8	3
1:A:511:MET:HE1	1:A:513:PHE:CZ	0.45	2.47	7	1
1:A:502:PRO:HD2	2:B:960:LEU:HD12	0.45	1.88	3	1
1:A:497:LEU:C	2:B:957:LEU:HD13	0.45	2.37	17	1
1:A:493:LEU:HD13	1:A:493:LEU:O	0.44	2.11	17	1
1:A:498:LYS:HG3	1:A:499:ARG:N	0.44	2.25	19	2
1:A:511:MET:CE	1:A:513:PHE:CE2	0.44	3.00	7	1
1:A:497:LEU:HA	1:A:500:LEU:HD13	0.44	1.89	3	1
1:A:477:PHE:N	1:A:477:PHE:CD1	0.44	2.86	15	1
1:A:497:LEU:HD11	2:B:953:LEU:HD11	0.44	1.89	16	1
2:B:953:LEU:HD23	2:B:953:LEU:C	0.44	2.38	6	1
1:A:463:LEU:HD21	1:A:473:LEU:HD21	0.44	1.90	18	1
1:A:474:LEU:HD11	2:B:949:MET:HE3	0.43	1.89	9	1
1:A:454:VAL:HG22	1:A:477:PHE:CE1	0.43	2.48	14	1
2:B:957:LEU:CD1	2:B:960:LEU:HD11	0.43	2.41	14	1
1:A:456:GLU:CA	1:A:496:ILE:HD11	0.43	2.43	16	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:493:LEU:CB	2:B:953:LEU:HD11	0.43	2.43	3	1
2:B:960:LEU:HD23	2:B:960:LEU:C	0.43	2.38	16	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
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:493:LEU:C	1:A:497:LEU:HD12	0.43	2.39	10	1
1:A:470:THR:HG21	2:B:954:GLU:HB2	0.42	1.90	7	1
2:B:961:MET:HE3	2:B:961:MET:OXT	0.42	2.15	12	1
2:B:958:ASN:HA	2:B:961:MET:HE3	0.42	1.90	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:957:LEU:HD12	2:B:960:LEU:HG	0.42	1.91	3	1
1:A:497:LEU:C	2:B:957:LEU:HD21	0.42	2.40	4	1
2:B:957:LEU:HD22	2:B:960:LEU:HD12	0.42	1.90	7	1
1:A:497:LEU:HD23	1:A:500:LEU:HD23	0.42	1.92	17	1
1:A:470:THR:HG21	2:B:954:GLU:CG	0.42	2.45	18	1
1:A:484:LEU:N	1:A:484:LEU:CD2	0.42	2.83	12	5
1:A:470:THR:HG21	2:B:953:LEU:CD2	0.42	2.45	3	1
1:A:463:LEU:CB	1:A:515:LEU:HD11	0.42	2.45	15	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:462:TYR:CZ	1:A:476:LYS:CE	0.41	3.04	7	1
1:A:474:LEU:HD12	1:A:493:LEU:HD13	0.41	1.93	8	1
1:A:496:ILE:HG22	1:A:497:LEU:N	0.41	2.31	9	2
1:A:489:THR:HG22	1:A:493:LEU:HD13	0.41	1.92	5	1
1:A:497:LEU:O	2:B:957:LEU:CD2	0.41	2.61	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: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
2:B:957:LEU:HG	2:B:960:LEU:HD12	0.40	1.93	14	1
1:A:467:PRO:CG	1:A:507:ILE:CD1	0.40	3.00	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	64/82 (78%)	60±2 (94±2%)	3±1 (5±2%)	1±1 (1±1%)	14	63
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%)	16	66

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occur-

rence 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 ⓘ

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%)	57±2 (92±3%)	5±2 (7±3%)	15	63
2	B	13/66 (20%)	12±1 (92±6%)	1±1 (8±6%)	13	60
All	All	1493/2860 (52%)	1381 (92%)	112 (8%)	14	62

All 36 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	515	LEU	11
1	A	498	LYS	10
1	A	496	ILE	9
1	A	466	LYS	9
2	B	960	LEU	9
1	A	481	LYS	6
1	A	474	LEU	5
1	A	464	THR	5
1	A	479	THR	4
1	A	501	ASN	3
1	A	470	THR	3
1	A	480	LYS	2
1	A	510	LYS	2
1	A	505	LYS	2
2	B	949	MET	2
2	B	957	LEU	2
2	B	956	GLU	2
1	A	476	LYS	2
2	B	953	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	482	THR	2
2	B	961	MET	2
1	A	477	PHE	2
1	A	504	ARG	2
1	A	475	LYS	2
1	A	461	ARG	1
1	A	500	LEU	1
1	A	511	MET	1
1	A	506	MET	1
2	B	951	LYS	1
1	A	455	THR	1
1	A	471	LYS	1
1	A	497	LEU	1
2	B	958	ASN	1
1	A	453	GLN	1
1	A	493	LEU	1
1	A	495	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 oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided