Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 09:18 PM EST

PDB ID	:	2JNJ
Title	:	Solution structure of the p8 TFIIH subunit
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Deposited on	:	2007-01-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

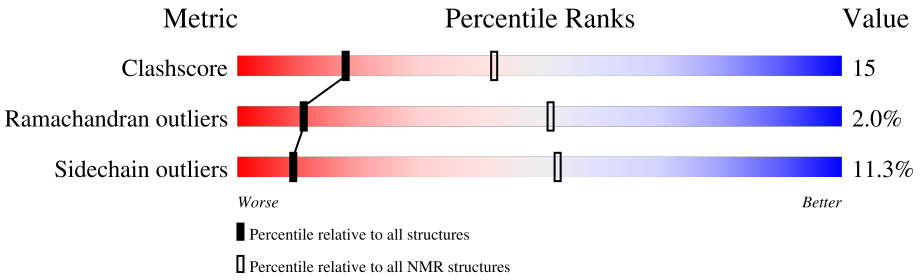
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	74	47% 23% • 28%
1	B	74	53% 22% • 23%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:5-A:57, B:5-B:61 (110)	1.02	3

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 2 clusters and 5 single-model clusters were found.

Cluster number	Models
1	2, 3, 6
2	1, 4
Single-model clusters	5; 7; 8; 9; 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2360 atoms, of which 1192 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TFIIH basal transcription factor complex TTD-A subunit.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	74	1180	373	596	95	112	4	0
1	B	74	1180	373	596	95	112	4	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q6ZYL4
A	2	SER	-	cloning artifact	UNP Q6ZYL4
A	3	HIS	-	cloning artifact	UNP Q6ZYL4
B	1	GLY	-	cloning artifact	UNP Q6ZYL4
B	2	SER	-	cloning artifact	UNP Q6ZYL4
B	3	HIS	-	cloning artifact	UNP Q6ZYL4

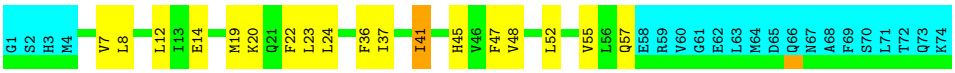
4 Residue-property plots (i)

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.

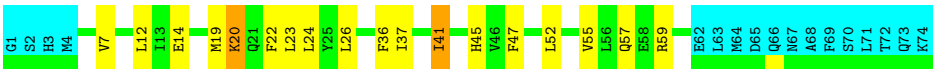
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 47% 23% • 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 53% 22% • 23%



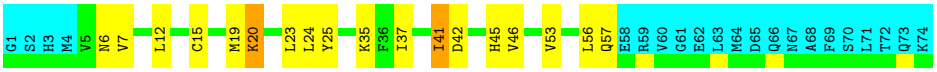
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

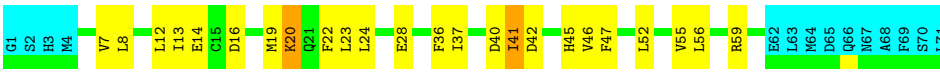
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 47% 22% • 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

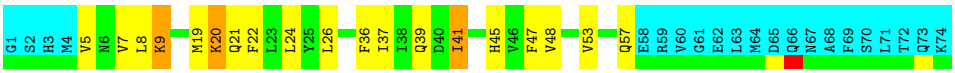
Chain B: 45% 30% • 23%



4.2.2 Score per residue for model 2

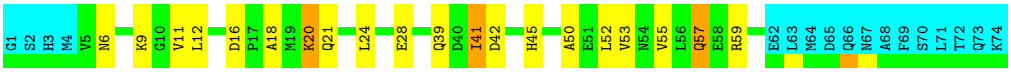
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 46% 22% • 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 50% 23% • 23%



4.2.3 Score per residue for model 3 (medoid)

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 43% 23% 5% 28%

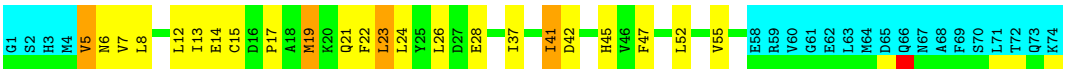
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 51% 22% • 23%

4.2.4 Score per residue for model 4

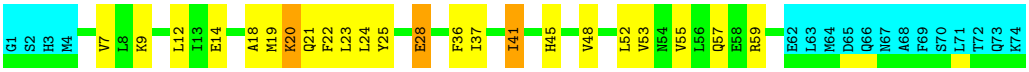
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 41% 26% 5% 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

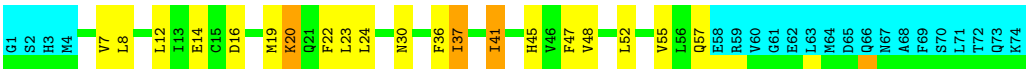
Chain B: 46% 27% • 23%



4.2.5 Score per residue for model 5

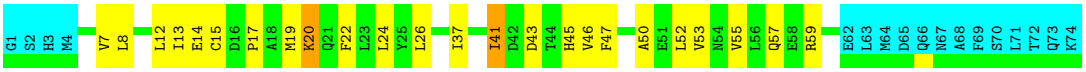
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 45% 23% • 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

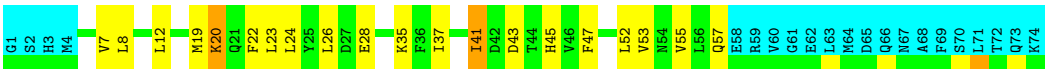
Chain B: 45% 30% • 23%



4.2.6 Score per residue for model 6

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 45% 24% • 28%



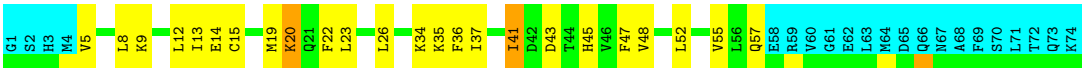
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 51% 22% • 23%

4.2.7 Score per residue for model 7

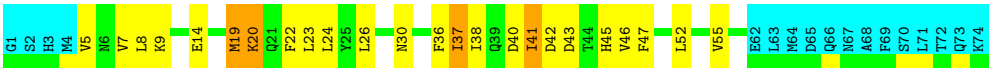
• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 39% 30% • 28%



• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 45% 27% 5% 23%



4.2.8 Score per residue for model 8

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 50% 18% • 28%

G1 S2 H3 M4 V5 L8 L12 I13 E14 M19 K20 Q21 F22 F36 I37 I41 D42 H45 V46 F47 V48 Q57 E58 R59 V60 G61 E62 L63 M64 D65 Q66 N67 A68 F69 S70 L71 T72 Q73 K74

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 43% 24% 9% 23%

G1 S2 H3 M4 V7 L8 K9 E14 C15 D16 P17 A18 M19 K20 Q21 F22 L23 L24 Y25 L26 K34 K35 F36 I37 I41 D42 D43 T44 H45 V46 F47 N54 V55 L56 Q57 E58 R59 E62 L63 M64 D65 Q66 N67 A68 F69 S70 L71 T72 Q73 K74

4.2.9 Score per residue for model 9

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain A: 41% 26% 5% 28%

G1 S2 H3 M4 L8 I13 E14 M19 K20 Q21 F22 L23 L24 D27 K35 F36 I37 I38 Q39 D40 I41 H45 V46 I49 L52 V53 N54 V55 L56 Q57 E58 R59 V60 G61 E62 L63 M64 D65 Q66 N67 A68 F69 S70 L71 T72 Q73 K74

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 51% 22% • 23%

G1 S2 H3 M4 V5 N6 M19 K20 Q21 F22 L23 L24 Y25 L26 K34 K35 F36 I37 D43 T44 H45 V48 L52 V53 N54 V55 L56 Q57 E62 L63 M64 D65 Q66 N67 A68 F69 S70 L71 T72 Q73 K74

4.2.10 Score per residue for model 10

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

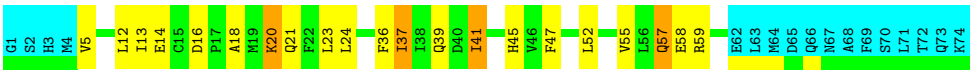
Chain A: 34% 34% • 28%

G1 S2 H3 M4 V5 N6 V7 L8 E14 C15 D16 P17 A18 M19 K20 Q21 F22 L23 L24 D27 N30 K34 K35 F36 I37 I41 H45 V46 F47 V48 I49 L52 V53 N54 V55 L56 Q57 E58 R59 V60 G61 E62 L63 M64 D65 Q66 N67 A68 F69 S70 L71 T72 Q73

K74

• Molecule 1: TFIIH basal transcription factor complex TTD-A subunit

Chain B: 49% 23% 5% 23%


G1
S2
H3
M4
V5
L12
I13
E14
C15
D16
P17
A18
M19
K20
Q21
F22
L23
L24
F36
I37
I38
Q39
D40
I41
H45
V46
F47
L52
V55
L56
Q57
E58
R59
E62
L63
M64
D65
Q66
N67
A68
F69
S70
L71
T72
Q73
K74

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 40 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure solution	
TALOS	geometry optimization	
X-PLOR NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	A	419	436	435	14±4
1	B	450	467	466	15±2
All	All	8690	9030	9010	263

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLU:HB2	1:A:45:HIS:CE1	0.74	2.17	4	5
1:B:37:ILE:HG13	1:B:46:VAL:HG13	0.70	1.61	1	1
1:B:14:GLU:HB2	1:B:45:HIS:NE2	0.68	2.04	5	2
1:B:14:GLU:HB2	1:B:45:HIS:CE1	0.66	2.26	4	4
1:B:15:CYS:HB2	1:B:19:MET:SD	0.65	2.32	5	2
1:B:12:LEU:HG	1:B:45:HIS:CD2	0.63	2.28	4	2
1:B:14:GLU:HB3	1:B:45:HIS:CE1	0.63	2.29	10	2
1:A:45:HIS:CE1	1:B:41:ILE:HG22	0.62	2.29	3	5
1:A:20:LYS:O	1:A:20:LYS:HE3	0.62	1.93	1	4
1:B:19:MET:HA	1:B:22:PHE:CE2	0.62	2.29	3	8
1:A:19:MET:HA	1:A:22:PHE:CE2	0.61	2.30	8	7
1:B:41:ILE:HD11	1:B:47:PHE:HB2	0.60	1.74	5	1
1:B:20:LYS:O	1:B:20:LYS:HE3	0.59	1.96	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:19:MET:O	1:B:23:LEU:HB2	0.58	1.98	7	3
1:A:15:CYS:HB3	1:A:19:MET:SD	0.57	2.39	10	5
1:A:41:ILE:HG22	1:B:45:HIS:CE1	0.57	2.35	9	3
1:A:12:LEU:O	1:B:7:VAL:HA	0.57	2.00	4	6
1:B:52:LEU:O	1:B:55:VAL:HG22	0.57	1.99	4	8
1:B:19:MET:O	1:B:23:LEU:HG	0.57	2.00	6	2
1:B:24:LEU:O	1:B:28:GLU:HG2	0.56	2.01	1	1
1:B:8:LEU:HG	1:B:47:PHE:CE2	0.55	2.35	3	4
1:A:8:LEU:HG	1:A:47:PHE:CE2	0.55	2.35	10	7
1:B:41:ILE:O	1:B:45:HIS:HB2	0.55	2.02	2	4
1:A:41:ILE:O	1:A:45:HIS:HB2	0.54	2.02	2	7
1:A:52:LEU:O	1:A:55:VAL:HG22	0.54	2.03	5	6
1:A:57:GLN:HE21	1:A:57:GLN:HA	0.54	1.63	8	3
1:B:57:GLN:HE21	1:B:57:GLN:N	0.53	2.01	6	3
1:B:36:PHE:O	1:B:48:VAL:HA	0.53	2.04	4	3
1:B:41:ILE:HG12	1:B:45:HIS:CB	0.53	2.34	1	2
1:B:17:PRO:HA	1:B:19:MET:SD	0.53	2.43	8	1
1:A:23:LEU:HB3	1:A:37:ILE:CD1	0.53	2.34	10	1
1:A:6:ASN:H	1:B:14:GLU:HB3	0.52	1.64	4	1
1:A:53:VAL:O	1:A:57:GLN:HG2	0.52	2.04	1	5
1:B:55:VAL:O	1:B:59:ARG:HG2	0.52	2.04	5	4
1:B:16:ASP:O	1:B:19:MET:HB3	0.52	2.04	1	1
1:A:36:PHE:O	1:A:48:VAL:HA	0.51	2.05	3	6
1:A:41:ILE:HB	1:B:43:ASP:OD2	0.51	2.05	9	1
1:B:57:GLN:HE21	1:B:57:GLN:HA	0.51	1.64	10	2
1:A:19:MET:O	1:A:23:LEU:HB2	0.51	2.05	10	1
1:A:41:ILE:HG12	1:A:45:HIS:CB	0.51	2.35	2	3
1:A:7:VAL:HG22	1:B:13:ILE:HG13	0.50	1.83	1	2
1:A:19:MET:O	1:A:23:LEU:HD22	0.50	2.07	7	2
1:B:14:GLU:HB2	1:B:45:HIS:ND1	0.50	2.22	3	1
1:A:17:PRO:O	1:A:20:LYS:HB3	0.50	2.06	10	1
1:A:41:ILE:HG12	1:A:45:HIS:HB2	0.49	1.83	10	2
1:A:23:LEU:HG	1:A:36:PHE:CZ	0.49	2.41	10	1
1:B:20:LYS:CE	1:B:24:LEU:HD23	0.49	2.37	8	5
1:A:20:LYS:O	1:A:24:LEU:HG	0.49	2.08	9	2
1:A:7:VAL:HA	1:B:12:LEU:O	0.48	2.08	4	5
1:B:19:MET:HA	1:B:22:PHE:CZ	0.48	2.42	8	1
1:A:14:GLU:HB2	1:A:45:HIS:ND1	0.48	2.23	5	2
1:B:26:LEU:O	1:B:30:ASN:HA	0.48	2.08	7	1
1:B:21:GLN:O	1:B:24:LEU:HG	0.48	2.09	2	3
1:A:6:ASN:H	1:B:14:GLU:HG2	0.48	1.68	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD13	1:A:46:VAL:HG21	0.47	1.86	9	1
1:B:52:LEU:O	1:B:55:VAL:HG12	0.47	2.09	9	1
1:B:16:ASP:OD2	1:B:18:ALA:HB3	0.47	2.09	10	2
1:A:37:ILE:HG12	1:A:46:VAL:HG13	0.47	1.84	3	1
1:A:57:GLN:HE21	1:A:57:GLN:CA	0.47	2.23	8	1
1:B:11:VAL:HG23	1:B:50:ALA:HA	0.46	1.86	2	1
1:A:19:MET:O	1:A:23:LEU:HG	0.46	2.10	6	1
1:B:57:GLN:HE21	1:B:57:GLN:CA	0.46	2.23	6	3
1:A:13:ILE:O	1:A:45:HIS:HA	0.46	2.10	7	1
1:B:20:LYS:O	1:B:24:LEU:HG	0.46	2.11	5	1
1:A:14:GLU:HB3	1:B:6:ASN:H	0.46	1.71	9	1
1:A:23:LEU:HB3	1:A:37:ILE:HD11	0.46	1.87	10	1
1:A:35:LYS:HA	1:A:35:LYS:HE2	0.46	1.88	6	3
1:B:57:GLN:CA	1:B:57:GLN:HE21	0.45	2.24	2	1
1:A:57:GLN:CA	1:A:57:GLN:HE21	0.45	2.24	3	1
1:B:25:TYR:O	1:B:28:GLU:HG3	0.45	2.11	4	1
1:B:8:LEU:HD11	1:B:38:ILE:HG21	0.45	1.88	7	1
1:B:18:ALA:HA	1:B:21:GLN:OE1	0.45	2.10	4	1
1:B:17:PRO:O	1:B:20:LYS:HB3	0.45	2.11	5	1
1:A:8:LEU:HG	1:A:47:PHE:CZ	0.45	2.45	7	1
1:B:53:VAL:O	1:B:57:GLN:HG2	0.45	2.12	9	3
1:B:41:ILE:HD12	1:B:41:ILE:N	0.45	2.25	5	1
1:B:13:ILE:O	1:B:45:HIS:HA	0.45	2.12	10	1
1:B:41:ILE:H	1:B:41:ILE:HD13	0.45	1.71	1	1
1:B:26:LEU:HB3	1:B:36:PHE:CZ	0.44	2.47	8	2
1:B:41:ILE:HG13	1:B:45:HIS:CB	0.44	2.42	2	1
1:A:20:LYS:O	1:A:20:LYS:HD2	0.44	2.12	8	1
1:A:14:GLU:O	1:B:5:VAL:HA	0.44	2.12	9	1
1:B:14:GLU:HB3	1:B:45:HIS:ND1	0.44	2.27	1	1
1:A:20:LYS:HG3	1:A:21:GLN:NE2	0.44	2.28	8	1
1:A:20:LYS:HE3	1:A:46:VAL:HG22	0.44	1.89	10	1
1:A:13:ILE:HG21	1:A:19:MET:SD	0.43	2.54	9	1
1:A:41:ILE:HG13	1:A:45:HIS:CB	0.43	2.43	1	5
1:A:9:LYS:HB3	1:B:11:VAL:HG22	0.43	1.90	2	1
1:A:27:ASP:OD1	1:A:35:LYS:HA	0.43	2.14	10	1
1:B:36:PHE:CG	1:B:56:LEU:HD21	0.43	2.49	1	1
1:B:23:LEU:HD12	1:B:36:PHE:CE1	0.43	2.49	1	1
1:A:14:GLU:HB3	1:A:45:HIS:ND1	0.43	2.28	10	1
1:B:37:ILE:HG12	1:B:46:VAL:HG13	0.43	1.90	3	2
1:A:23:LEU:HD21	1:A:37:ILE:HG13	0.42	1.90	9	1
1:A:21:GLN:HA	1:A:24:LEU:HD12	0.42	1.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:24:LEU:O	1:B:28:GLU:HG3	0.42	2.14	6	1
1:A:20:LYS:CE	1:A:24:LEU:HD23	0.42	2.45	5	1
1:B:54:ASN:O	1:B:58:GLU:HG3	0.42	2.15	8	1
1:A:57:GLN:HE21	1:A:57:GLN:N	0.42	2.12	3	1
1:B:20:LYS:HE3	1:B:24:LEU:HD23	0.42	1.90	7	2
1:B:39:GLN:NE2	1:B:41:ILE:HG23	0.42	2.30	3	2
1:B:26:LEU:HD12	1:B:36:PHE:CE1	0.42	2.50	3	1
1:A:5:VAL:HA	1:B:14:GLU:O	0.41	2.15	4	2
1:A:20:LYS:HG3	1:A:43:ASP:C	0.41	2.36	7	1
1:B:17:PRO:HG3	1:B:44:THR:HG23	0.41	1.90	8	1
1:A:8:LEU:HD21	1:A:38:ILE:HG21	0.41	1.91	9	1
1:A:23:LEU:HD11	1:A:37:ILE:HB	0.41	1.91	5	1
1:B:20:LYS:NZ	1:B:40:ASP:HB2	0.41	2.30	1	1
1:B:20:LYS:HE3	1:B:46:VAL:HG22	0.41	1.91	5	1
1:B:14:GLU:OE2	1:B:45:HIS:NE2	0.41	2.54	7	1
1:B:8:LEU:HD23	1:B:47:PHE:CD2	0.41	2.50	8	1
1:A:27:ASP:O	1:A:35:LYS:HE3	0.41	2.16	9	1
1:B:50:ALA:O	1:B:53:VAL:HG12	0.41	2.16	5	3
1:B:9:LYS:C	1:B:9:LYS:HD3	0.41	2.36	8	1
1:A:36:PHE:CD2	1:A:56:LEU:HG	0.41	2.51	9	1
1:A:41:ILE:HG13	1:A:45:HIS:C	0.41	2.36	3	1
1:A:42:ASP:HB2	1:B:42:ASP:HB3	0.41	1.92	8	1
1:A:23:LEU:CD2	1:A:46:VAL:HG11	0.40	2.46	1	1
1:A:21:GLN:O	1:A:24:LEU:HG	0.40	2.16	2	1
1:A:24:LEU:O	1:A:28:GLU:HG3	0.40	2.16	6	1
1:A:39:GLN:NE2	1:A:41:ILE:HG23	0.40	2.31	9	1
1:B:36:PHE:CE2	1:B:37:ILE:HG22	0.40	2.52	8	1
1:B:37:ILE:HA	1:B:47:PHE:O	0.40	2.16	10	1
1:A:20:LYS:HE3	1:A:20:LYS:C	0.40	2.36	1	1
1:B:12:LEU:CD1	1:B:41:ILE:HD12	0.40	2.47	10	1
1:B:39:GLN:HE21	1:B:41:ILE:HG23	0.40	1.76	10	1
1:A:16:ASP:O	1:A:19:MET:HG2	0.40	2.17	10	1
1:A:24:LEU:HD12	1:A:25:TYR:N	0.40	2.31	1	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	53/74 (72%)	48±1 (91±2%)	3±1 (6±2%)	1±1 (2±1%)	9 48
1	B	57/74 (77%)	53±1 (92±2%)	3±1 (6±2%)	1±1 (2±2%)	12 54
All	All	1100/1480 (74%)	1011 (92%)	67 (6%)	22 (2%)	11 52

All 10 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	42	ASP	4
1	B	42	ASP	4
1	A	5	VAL	3
1	A	43	ASP	2
1	A	30	ASN	2
1	B	43	ASP	2
1	B	5	VAL	2
1	A	17	PRO	1
1	B	17	PRO	1
1	B	44	THR	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	48/66 (73%)	42±2 (88±4%)	6±2 (12±4%)	8 51
1	B	51/66 (77%)	46±1 (89±3%)	5±1 (11±3%)	10 55
All	All	990/1320 (75%)	878 (89%)	112 (11%)	9 53

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	41	ILE	10
1	A	37	ILE	9
1	B	20	LYS	9
1	B	41	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	B	37	ILE	8
1	A	20	LYS	6
1	B	57	GLN	6
1	A	57	GLN	6
1	A	26	LEU	5
1	B	9	LYS	4
1	B	26	LEU	4
1	A	9	LYS	3
1	A	56	LEU	2
1	A	39	GLN	2
1	B	28	GLU	2
1	A	19	MET	2
1	A	22	PHE	2
1	A	34	LYS	2
1	B	19	MET	2
1	B	34	LYS	2
1	A	49	ILE	2
1	B	59	ARG	1
1	B	6	ASN	1
1	B	39	GLN	1
1	A	6	ASN	1
1	A	52	LEU	1
1	A	13	ILE	1
1	A	23	LEU	1
1	A	28	GLU	1
1	A	16	ASP	1
1	B	30	ASN	1
1	B	40	ASP	1
1	B	43	ASP	1
1	A	36	PHE	1
1	B	23	LEU	1
1	B	36	PHE	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 monosaccharides 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 (i)

No chemical shift data were provided