



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 12:11 PM UTC

PDB ID : 1C99 / pdb_00001c99
Title : ASP61 DEPROTONATED FORM OF SUBUNIT C OF THE F1FO ATP SYNTHASE OF ESCHERICHIA COLI
Authors : Rastogi, V.K.; Girvin, M.E.
Deposited on : 1999-04-30

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

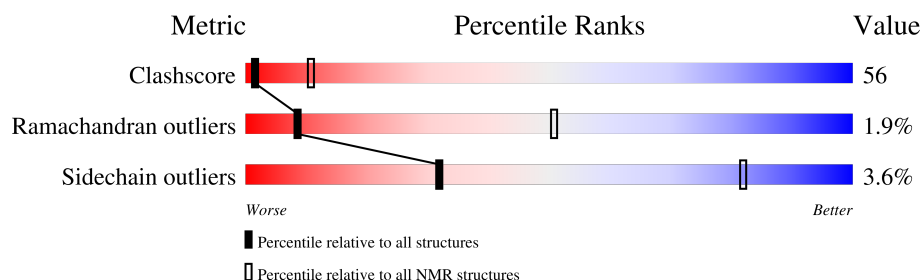
1 Overall quality at a glance

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	79	33% 66% .

2 Ensemble composition and analysis

This entry contains 9 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 9 as representative.

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:1-A:79 (79)	0.90	6

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 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1190 atoms, of which 616 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEOLIPID F1FO OF ATP SYNTHASE.

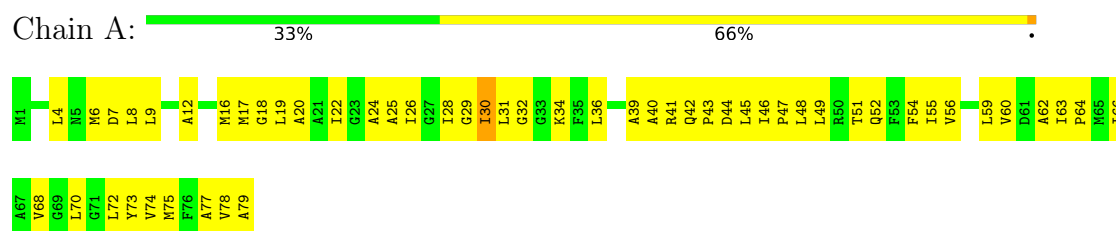
Mol	Chain	Residues	Atoms						Trace
1	A	79	Total	C	H	N	O	S	0
			1190	380	616	90	96	8	

4 Residue-property plots

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: PROTEOLIPID F1FO OF ATP SYNTHASE

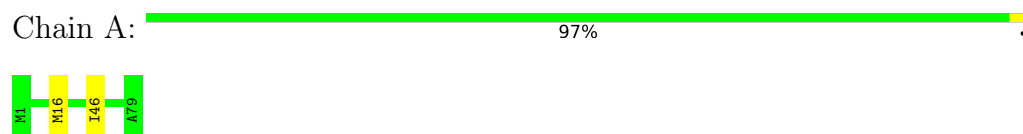


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

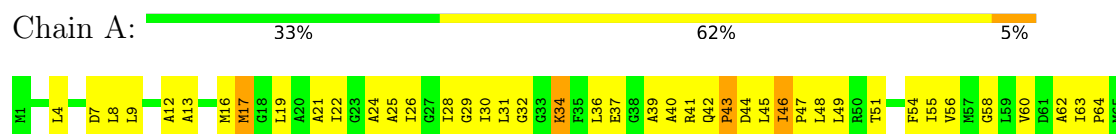
4.2.1 Score per residue for model 1

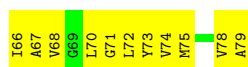
• Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE



4.2.2 Score per residue for model 2

• Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE





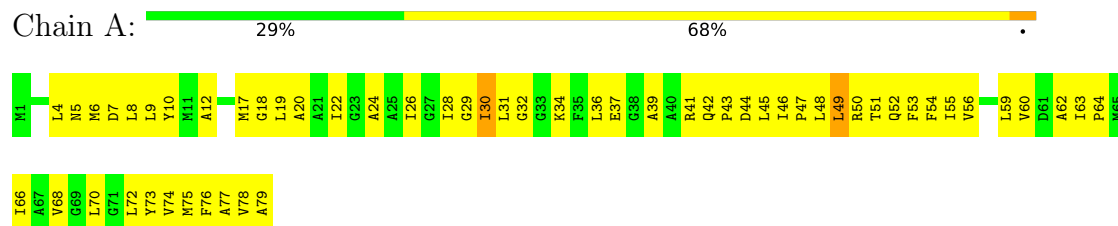
4.2.3 Score per residue for model 3

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE



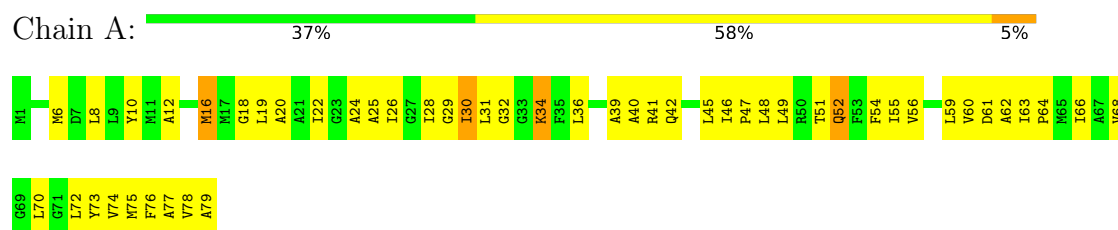
4.2.4 Score per residue for model 4

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE



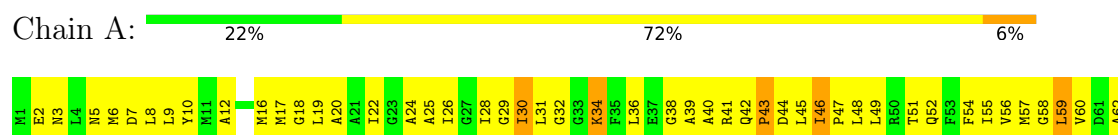
4.2.5 Score per residue for model 5

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE



4.2.6 Score per residue for model 6 (medoid)

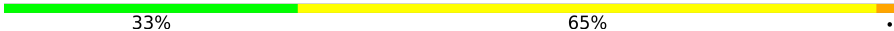
- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE



I63
P64
M65
I66
V67
V68
G69
L70
G71
L72
Y73
V74
M75
F76
A77
V78
A79

4.2.7 Score per residue for model 7

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE

Chain A:  33% 65%

M1
E2
N3
L4
N5
M6
D7
L8
L9
A12
M16
M17
G18
L19
A20
A21
I22
G23
A24
A25
I26
G27
I28
G29
I30
L31
G32
F35
L36
A39
A40
D44
L45
I46
P47
L48
L49
R50
T51
Q52
F53
F54
I55
V56
V60
D61
A62
I63
P64
M65
I66
A67
V68
G69

L72
Y73
V74
M75
F76
A77
V78
A79

4.2.8 Score per residue for model 8

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE

Chain A:  28% 66% 6%

M1
L4
N5
M6
D7
L8
L9
A12
V15
M16
M17
G18
L19
A20
A21
I22
G23
A24
A25
I26
G27
I28
G29
I30
L31
G32
G33
K34
F35
L36
E37
A40
R41
Q42
P43
D44
L45
I46
P47
L48
L49
R50
T51
Q52
F53
F54
I55
V56
M57
V60
D61
A62
I63
P64
M65

I66
A67
V68
G71
L72
Y73
V74
M75
F76
A77
V78
A79

4.2.9 Score per residue for model 9

- Molecule 1: PROTEOLIPID F1FO OF ATP SYNTHASE

Chain A:  30% 65% 5%

M1
E2
N3
L4
N5
M6
D7
L8
L9
A12
A13
M16
M17
G18
L19
A20
A21
I22
G23
A24
A25
I26
G27
I28
G29
I30
L31
G32
G33
K34
F35
L36
A39
A40
R41
Q42
P43
D44
L45
I46
P47
L48
L49
R50
T51
Q52
F53
F54
I55
V56
M57
G58
I59
V60
D61
A62
I63

P64
M65
I66
A67
V68
G69
L70
G71
L72
Y73
V74
M75
F76
A77
V78
A79

5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 9 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.854
CNS	refinement	0.3
DYANA	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.41±0.01	0±0/582 (0.0± 0.0%)	0.74±0.03	0±0/786 (0.1± 0.1%)
All	All	0.41	0/5238 (0.0%)	0.74	4/7074 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	46	ILE	CB-CA-C	-6.05	107.95	113.70	6	4

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	574	616	616	62±22
All	All	5166	5544	4928	562

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 56.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD13	1:A:49:LEU:N	0.92	1.79	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD22	1:A:49:LEU:HD22	0.86	1.43	5	1
1:A:42:GLN:HB3	1:A:43:PRO:HD3	0.85	1.48	9	1
1:A:73:TYR:O	1:A:77:ALA:HB3	0.84	1.72	8	7
1:A:48:LEU:HD22	1:A:48:LEU:O	0.84	1.72	8	1
1:A:40:ALA:HB2	1:A:49:LEU:HD21	0.84	1.50	3	3
1:A:42:GLN:CB	1:A:43:PRO:HD3	0.82	2.05	9	1
1:A:28:ILE:HD11	1:A:56:VAL:HG12	0.82	1.51	7	3
1:A:51:THR:HA	1:A:54:PHE:CE2	0.82	2.08	7	2
1:A:42:GLN:HB3	1:A:43:PRO:HD2	0.79	1.55	3	2
1:A:28:ILE:HD12	1:A:29:GLY:N	0.79	1.92	6	1
1:A:72:LEU:HD12	1:A:73:TYR:N	0.77	1.95	9	5
1:A:70:LEU:HD12	1:A:71:GLY:N	0.77	1.94	2	1
1:A:25:ALA:O	1:A:28:ILE:HG22	0.76	1.78	3	4
1:A:8:LEU:O	1:A:8:LEU:HD13	0.76	1.80	2	5
1:A:51:THR:O	1:A:55:ILE:HG13	0.76	1.81	5	2
1:A:28:ILE:HD13	1:A:57:MET:HE1	0.75	1.56	6	1
1:A:45:LEU:HD22	1:A:48:LEU:HB3	0.74	1.57	7	1
1:A:26:ILE:O	1:A:30:ILE:HG12	0.74	1.82	3	4
1:A:17:MET:HE2	1:A:68:VAL:HG21	0.74	1.59	7	3
1:A:48:LEU:HD22	1:A:48:LEU:C	0.74	2.07	8	1
1:A:45:LEU:HD13	1:A:45:LEU:O	0.73	1.83	7	1
1:A:19:LEU:HD12	1:A:20:ALA:N	0.72	1.99	8	7
1:A:75:MET:HA	1:A:79:ALA:HB3	0.72	1.59	2	2
1:A:36:LEU:HD22	1:A:49:LEU:CD2	0.72	2.14	5	1
1:A:39:ALA:O	1:A:45:LEU:HB2	0.72	1.85	3	6
1:A:54:PHE:CE1	1:A:55:ILE:HG12	0.71	2.20	6	3
1:A:42:GLN:HB3	1:A:43:PRO:CD	0.71	2.16	9	2
1:A:66:ILE:O	1:A:70:LEU:HD23	0.71	1.85	6	1
1:A:36:LEU:HD12	1:A:49:LEU:HD22	0.71	1.62	2	2
1:A:54:PHE:CE1	1:A:55:ILE:HG13	0.71	2.21	5	2
1:A:45:LEU:HD12	1:A:48:LEU:HD22	0.71	1.62	6	3
1:A:26:ILE:O	1:A:30:ILE:HG13	0.71	1.84	4	3
1:A:4:LEU:H	1:A:4:LEU:HD23	0.70	1.46	9	1
1:A:17:MET:CG	1:A:68:VAL:HG21	0.70	2.16	9	2
1:A:45:LEU:HD13	1:A:45:LEU:C	0.69	2.12	7	1
1:A:42:GLN:CG	1:A:43:PRO:HD3	0.68	2.17	9	1
1:A:9:LEU:HG	1:A:75:MET:HG2	0.68	1.65	7	1
1:A:74:VAL:HG13	1:A:75:MET:SD	0.68	2.28	7	2
1:A:40:ALA:HA	1:A:49:LEU:HD21	0.68	1.64	6	1
1:A:9:LEU:HD12	1:A:75:MET:HE3	0.66	1.67	8	1
1:A:17:MET:HG2	1:A:68:VAL:HG21	0.66	1.67	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD23	1:A:48:LEU:CD2	0.66	2.20	2	1
1:A:9:LEU:C	1:A:9:LEU:HD13	0.65	2.16	2	4
1:A:51:THR:O	1:A:55:ILE:HG12	0.65	1.90	9	5
1:A:56:VAL:O	1:A:60:VAL:HG23	0.65	1.92	5	6
1:A:68:VAL:HG12	1:A:72:LEU:HD22	0.65	1.69	6	1
1:A:16:MET:HE2	1:A:16:MET:O	0.64	1.92	3	2
1:A:49:LEU:C	1:A:49:LEU:HD12	0.64	2.17	4	2
1:A:26:ILE:O	1:A:30:ILE:HD13	0.64	1.93	5	1
1:A:48:LEU:HD23	1:A:52:GLN:NE2	0.64	2.08	8	1
1:A:36:LEU:CD2	1:A:49:LEU:HD22	0.64	2.20	5	1
1:A:36:LEU:C	1:A:36:LEU:HD23	0.64	2.16	4	1
1:A:36:LEU:HD13	1:A:36:LEU:O	0.64	1.93	5	1
1:A:16:MET:CE	1:A:19:LEU:HD11	0.64	2.23	3	2
1:A:59:LEU:HD22	1:A:59:LEU:C	0.63	2.17	6	1
1:A:42:GLN:CB	1:A:43:PRO:CD	0.63	2.76	9	2
1:A:45:LEU:HD23	1:A:45:LEU:C	0.63	2.18	8	1
1:A:46:ILE:H	1:A:46:ILE:HD12	0.63	1.54	7	2
1:A:62:ALA:O	1:A:66:ILE:HD13	0.62	1.94	5	1
1:A:39:ALA:HB2	1:A:48:LEU:HD23	0.62	1.71	5	1
1:A:24:ALA:HB1	1:A:60:VAL:CG1	0.62	2.25	6	1
1:A:1:MET:HA	1:A:4:LEU:HD21	0.61	1.71	9	1
1:A:31:LEU:C	1:A:31:LEU:HD13	0.61	2.21	2	4
1:A:59:LEU:HD13	1:A:60:VAL:N	0.60	2.11	6	1
1:A:30:ILE:O	1:A:34:LYS:HG2	0.60	1.95	9	1
1:A:42:GLN:CB	1:A:45:LEU:HD23	0.60	2.26	3	3
1:A:36:LEU:CD1	1:A:48:LEU:HD11	0.60	2.27	8	1
1:A:36:LEU:HD23	1:A:52:GLN:OE1	0.60	1.97	5	1
1:A:30:ILE:HG22	1:A:31:LEU:N	0.60	2.11	5	1
1:A:44:ASP:C	1:A:45:LEU:HD12	0.59	2.21	2	2
1:A:70:LEU:HD13	1:A:70:LEU:O	0.59	1.96	4	3
1:A:40:ALA:HA	1:A:45:LEU:HG	0.59	1.73	7	1
1:A:31:LEU:HD13	1:A:31:LEU:O	0.59	1.97	2	4
1:A:41:ARG:NE	1:A:41:ARG:HA	0.59	2.12	5	1
1:A:63:ILE:HB	1:A:64:PRO:HD3	0.59	1.73	2	8
1:A:55:ILE:O	1:A:59:LEU:HD12	0.59	1.98	6	1
1:A:39:ALA:CB	1:A:48:LEU:HD23	0.59	2.28	5	2
1:A:18:GLY:O	1:A:22:ILE:HG12	0.58	1.97	6	5
1:A:61:ASP:O	1:A:64:PRO:HD2	0.58	1.98	5	1
1:A:39:ALA:HB1	1:A:48:LEU:HD23	0.58	1.75	6	1
1:A:31:LEU:HD22	1:A:34:LYS:HD3	0.58	1.74	2	1
1:A:31:LEU:HD22	1:A:34:LYS:HD2	0.58	1.74	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:ASP:C	1:A:45:LEU:HD22	0.58	2.24	6	1
1:A:9:LEU:C	1:A:9:LEU:HD23	0.57	2.24	8	2
1:A:45:LEU:HD23	1:A:48:LEU:HD22	0.57	1.76	2	1
1:A:62:ALA:O	1:A:66:ILE:HG13	0.57	1.99	6	7
1:A:8:LEU:HD13	1:A:8:LEU:C	0.57	2.25	2	5
1:A:42:GLN:HB3	1:A:45:LEU:HB2	0.56	1.75	4	1
1:A:7:ASP:OD1	1:A:8:LEU:N	0.56	2.38	2	6
1:A:48:LEU:O	1:A:52:GLN:HG3	0.56	1.99	3	1
1:A:70:LEU:HD12	1:A:70:LEU:C	0.56	2.26	2	1
1:A:24:ALA:O	1:A:28:ILE:HB	0.56	2.01	7	6
1:A:72:LEU:HD22	1:A:76:PHE:CE2	0.56	2.36	7	1
1:A:72:LEU:HD12	1:A:72:LEU:C	0.56	2.25	9	4
1:A:31:LEU:HD12	1:A:34:LYS:HD3	0.55	1.77	6	1
1:A:28:ILE:CD1	1:A:56:VAL:HG12	0.55	2.31	4	3
1:A:36:LEU:HD23	1:A:36:LEU:O	0.55	2.01	4	1
1:A:39:ALA:O	1:A:45:LEU:HD23	0.55	2.01	7	1
1:A:70:LEU:HD23	1:A:70:LEU:O	0.55	2.01	3	1
1:A:19:LEU:HD12	1:A:19:LEU:C	0.55	2.26	3	7
1:A:59:LEU:HD12	1:A:60:VAL:N	0.55	2.17	4	2
1:A:40:ALA:N	1:A:49:LEU:HD21	0.55	2.16	5	2
1:A:16:MET:HE3	1:A:19:LEU:HD11	0.55	1.78	3	2
1:A:70:LEU:HD13	1:A:70:LEU:C	0.54	2.27	4	2
1:A:18:GLY:O	1:A:22:ILE:HG13	0.54	2.02	4	1
1:A:24:ALA:O	1:A:28:ILE:HG23	0.54	2.03	9	2
1:A:24:ALA:O	1:A:28:ILE:HG12	0.54	2.02	9	1
1:A:75:MET:O	1:A:79:ALA:N	0.54	2.39	2	5
1:A:56:VAL:HA	1:A:59:LEU:HD12	0.54	1.78	6	1
1:A:10:TYR:CD1	1:A:76:PHE:CZ	0.53	2.96	5	1
1:A:54:PHE:HA	1:A:57:MET:HE2	0.53	1.81	8	1
1:A:74:VAL:O	1:A:78:VAL:HG12	0.53	2.02	2	1
1:A:74:VAL:O	1:A:78:VAL:HB	0.53	2.03	6	7
1:A:24:ALA:CB	1:A:60:VAL:HG11	0.53	2.33	8	1
1:A:6:MET:HG2	1:A:10:TYR:CZ	0.53	2.39	5	1
1:A:70:LEU:C	1:A:70:LEU:HD13	0.53	2.28	5	1
1:A:45:LEU:HD23	1:A:45:LEU:O	0.53	2.03	8	1
1:A:28:ILE:O	1:A:32:GLY:N	0.53	2.41	2	8
1:A:41:ARG:O	1:A:43:PRO:HD3	0.53	2.03	6	2
1:A:41:ARG:HD2	1:A:41:ARG:O	0.53	2.03	3	1
1:A:9:LEU:C	1:A:9:LEU:CD1	0.53	2.81	2	3
1:A:36:LEU:HD21	1:A:49:LEU:HD13	0.53	1.80	4	1
1:A:45:LEU:HD12	1:A:45:LEU:N	0.53	2.19	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ALA:O	1:A:16:MET:HB2	0.53	2.03	5	7
1:A:54:PHE:CE1	1:A:55:ILE:CG1	0.53	2.92	5	2
1:A:70:LEU:HD23	1:A:70:LEU:C	0.53	2.29	3	1
1:A:46:ILE:N	1:A:47:PRO:HD2	0.52	2.20	3	4
1:A:51:THR:O	1:A:54:PHE:CE1	0.52	2.62	9	2
1:A:68:VAL:O	1:A:72:LEU:HG	0.52	2.04	5	4
1:A:63:ILE:HB	1:A:64:PRO:CD	0.52	2.34	3	3
1:A:65:MET:HE2	1:A:65:MET:HA	0.52	1.81	8	1
1:A:40:ALA:CA	1:A:49:LEU:HD21	0.52	2.34	6	2
1:A:42:GLN:HB3	1:A:45:LEU:HD23	0.52	1.81	3	2
1:A:9:LEU:HD21	1:A:75:MET:HG3	0.52	1.81	4	1
1:A:46:ILE:O	1:A:49:LEU:HB2	0.52	2.04	9	6
1:A:22:ILE:O	1:A:26:ILE:HG13	0.52	2.05	6	2
1:A:9:LEU:HD11	1:A:71:GLY:C	0.52	2.30	8	1
1:A:45:LEU:C	1:A:45:LEU:CD2	0.52	2.83	8	1
1:A:4:LEU:HA	1:A:7:ASP:OD1	0.52	2.05	4	3
1:A:46:ILE:N	1:A:47:PRO:CD	0.52	2.73	5	6
1:A:64:PRO:O	1:A:68:VAL:HG23	0.52	2.04	9	1
1:A:6:MET:HE1	1:A:79:ALA:HB1	0.51	1.83	7	1
1:A:36:LEU:C	1:A:36:LEU:CD2	0.51	2.83	4	1
1:A:36:LEU:HD11	1:A:49:LEU:HD13	0.51	1.82	4	1
1:A:39:ALA:C	1:A:45:LEU:HD23	0.51	2.31	7	1
1:A:56:VAL:O	1:A:59:LEU:CD1	0.51	2.58	6	1
1:A:45:LEU:HD22	1:A:45:LEU:N	0.51	2.21	5	3
1:A:48:LEU:HD13	1:A:48:LEU:C	0.51	2.31	8	1
1:A:28:ILE:HG21	1:A:57:MET:HA	0.51	1.83	9	1
1:A:36:LEU:HD13	1:A:36:LEU:C	0.51	2.31	5	1
1:A:28:ILE:O	1:A:28:ILE:HD13	0.51	2.06	3	1
1:A:9:LEU:HD11	1:A:71:GLY:CA	0.51	2.36	8	1
1:A:78:VAL:HG12	1:A:78:VAL:O	0.50	2.07	5	6
1:A:9:LEU:HD13	1:A:75:MET:HG3	0.50	1.84	6	1
1:A:32:GLY:O	1:A:36:LEU:HB2	0.50	2.06	3	2
1:A:9:LEU:CD2	1:A:75:MET:HG3	0.50	2.36	4	1
1:A:36:LEU:O	1:A:40:ALA:N	0.49	2.42	3	2
1:A:46:ILE:O	1:A:49:LEU:HB3	0.49	2.07	4	2
1:A:54:PHE:CD1	1:A:55:ILE:N	0.49	2.80	2	2
1:A:20:ALA:O	1:A:24:ALA:CB	0.49	2.60	9	5
1:A:49:LEU:HG	1:A:50:ARG:N	0.49	2.22	7	2
1:A:52:GLN:O	1:A:56:VAL:HG23	0.49	2.06	3	6
1:A:69:GLY:O	1:A:73:TYR:HB2	0.49	2.08	6	2
1:A:9:LEU:HG	1:A:75:MET:HG3	0.49	1.83	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:MET:HG3	1:A:68:VAL:HG21	0.49	1.83	3	1
1:A:28:ILE:CD1	1:A:29:GLY:N	0.49	2.73	6	1
1:A:32:GLY:O	1:A:36:LEU:CB	0.49	2.61	9	5
1:A:6:MET:HE1	1:A:75:MET:HB3	0.49	1.85	6	1
1:A:28:ILE:HG13	1:A:29:GLY:N	0.49	2.23	9	1
1:A:59:LEU:CD1	1:A:60:VAL:HG23	0.49	2.37	6	1
1:A:68:VAL:CG1	1:A:72:LEU:HD22	0.49	2.36	6	1
1:A:50:ARG:O	1:A:54:PHE:HD1	0.48	1.90	3	1
1:A:36:LEU:O	1:A:40:ALA:CB	0.48	2.61	6	3
1:A:48:LEU:HD13	1:A:49:LEU:CA	0.48	2.38	8	1
1:A:2:GLU:HA	1:A:5:ASN:OD1	0.48	2.09	6	1
1:A:17:MET:HE3	1:A:64:PRO:CB	0.48	2.39	2	1
1:A:28:ILE:CG2	1:A:29:GLY:N	0.48	2.77	8	6
1:A:36:LEU:HD11	1:A:49:LEU:CD1	0.48	2.39	4	1
1:A:45:LEU:C	1:A:45:LEU:CD1	0.48	2.82	7	1
1:A:39:ALA:HB1	1:A:45:LEU:HB3	0.48	1.85	4	1
1:A:42:GLN:HG3	1:A:43:PRO:HD3	0.48	1.86	9	1
1:A:13:ALA:O	1:A:17:MET:HG3	0.48	2.08	3	2
1:A:31:LEU:HD23	1:A:31:LEU:O	0.48	2.09	7	1
1:A:31:LEU:HD23	1:A:35:PHE:HB2	0.48	1.85	7	1
1:A:48:LEU:C	1:A:48:LEU:CD2	0.48	2.78	8	1
1:A:31:LEU:C	1:A:31:LEU:CD1	0.48	2.87	2	3
1:A:75:MET:HA	1:A:75:MET:HE3	0.48	1.85	2	1
1:A:19:LEU:CD1	1:A:20:ALA:N	0.48	2.76	3	5
1:A:2:GLU:O	1:A:6:MET:HG2	0.48	2.08	7	1
1:A:68:VAL:O	1:A:72:LEU:HD13	0.48	2.09	6	1
1:A:32:GLY:O	1:A:36:LEU:HD13	0.47	2.08	3	1
1:A:42:GLN:CB	1:A:45:LEU:HD13	0.47	2.39	2	1
1:A:34:LYS:O	1:A:37:GLU:HG2	0.47	2.09	4	1
1:A:4:LEU:O	1:A:8:LEU:CB	0.47	2.63	3	6
1:A:45:LEU:O	1:A:48:LEU:HB3	0.47	2.09	5	5
1:A:48:LEU:HD23	1:A:52:GLN:CD	0.47	2.34	8	1
1:A:28:ILE:HG22	1:A:60:VAL:HG21	0.47	1.86	9	1
1:A:48:LEU:O	1:A:52:GLN:HG2	0.47	2.09	7	3
1:A:2:GLU:O	1:A:6:MET:HG3	0.47	2.09	9	1
1:A:5:ASN:O	1:A:9:LEU:HB2	0.47	2.10	4	2
1:A:75:MET:O	1:A:79:ALA:HA	0.47	2.09	5	4
1:A:70:LEU:CD1	1:A:71:GLY:N	0.46	2.74	2	1
1:A:54:PHE:CD1	1:A:54:PHE:C	0.46	2.93	2	2
1:A:63:ILE:CB	1:A:64:PRO:HD3	0.46	2.39	6	1
1:A:68:VAL:HG12	1:A:72:LEU:CD1	0.46	2.41	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ALA:HA	1:A:28:ILE:CD1	0.46	2.41	9	1
1:A:17:MET:SD	1:A:68:VAL:HG21	0.46	2.51	4	2
1:A:45:LEU:O	1:A:48:LEU:N	0.46	2.49	7	1
1:A:24:ALA:HB1	1:A:60:VAL:HG12	0.46	1.88	9	1
1:A:33:GLY:O	1:A:37:GLU:HB2	0.45	2.12	3	1
1:A:8:LEU:O	1:A:12:ALA:HB2	0.45	2.11	2	3
1:A:40:ALA:HB2	1:A:49:LEU:CD2	0.45	2.33	3	2
1:A:49:LEU:CG	1:A:50:ARG:N	0.45	2.80	4	1
1:A:70:LEU:C	1:A:70:LEU:CD1	0.45	2.90	4	2
1:A:52:GLN:NE2	1:A:52:GLN:C	0.45	2.75	5	1
1:A:24:ALA:HB1	1:A:60:VAL:HG11	0.45	1.87	6	3
1:A:5:ASN:OD1	1:A:6:MET:N	0.45	2.50	8	1
1:A:44:ASP:O	1:A:44:ASP:OD1	0.45	2.35	7	1
1:A:17:MET:HE2	1:A:17:MET:HA	0.45	1.88	2	1
1:A:51:THR:O	1:A:54:PHE:CD1	0.45	2.70	9	4
1:A:72:LEU:HB2	1:A:76:PHE:CD2	0.45	2.47	4	1
1:A:56:VAL:CA	1:A:59:LEU:HD12	0.45	2.42	6	1
1:A:28:ILE:CG2	1:A:60:VAL:HG21	0.44	2.41	9	1
1:A:17:MET:HE2	1:A:68:VAL:CG2	0.44	2.41	6	1
1:A:59:LEU:HD12	1:A:59:LEU:C	0.44	2.38	9	1
1:A:9:LEU:HD13	1:A:9:LEU:O	0.44	2.11	3	1
1:A:38:GLY:HA2	1:A:41:ARG:HG2	0.44	1.88	6	1
1:A:45:LEU:O	1:A:46:ILE:C	0.44	2.60	7	1
1:A:62:ALA:O	1:A:66:ILE:HB	0.44	2.12	5	1
1:A:51:THR:O	1:A:55:ILE:CG1	0.44	2.66	8	1
1:A:68:VAL:HG12	1:A:72:LEU:HD23	0.44	1.89	8	1
1:A:17:MET:HA	1:A:17:MET:CE	0.44	2.43	2	1
1:A:48:LEU:HG	1:A:52:GLN:NE2	0.44	2.27	3	1
1:A:43:PRO:O	1:A:46:ILE:HG13	0.44	2.13	6	1
1:A:67:ALA:O	1:A:70:LEU:HG	0.44	2.12	2	1
1:A:12:ALA:O	1:A:16:MET:HE2	0.43	2.14	2	1
1:A:46:ILE:HB	1:A:47:PRO:HD3	0.43	1.90	7	1
1:A:45:LEU:C	1:A:47:PRO:HD2	0.43	2.38	9	1
1:A:46:ILE:HA	1:A:49:LEU:HG	0.43	1.90	9	1
1:A:39:ALA:HB3	1:A:52:GLN:HE22	0.43	1.73	6	1
1:A:6:MET:HG3	1:A:10:TYR:CZ	0.43	2.49	6	1
1:A:72:LEU:C	1:A:72:LEU:HD12	0.43	2.39	8	1
1:A:20:ALA:CB	1:A:64:PRO:HG3	0.43	2.44	9	1
1:A:8:LEU:C	1:A:8:LEU:CD1	0.43	2.92	2	2
1:A:31:LEU:O	1:A:34:LYS:HG2	0.43	2.14	6	3
1:A:38:GLY:O	1:A:42:GLN:HG3	0.43	2.13	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:GLU:O	1:A:5:ASN:OD1	0.43	2.37	6	1
1:A:38:GLY:O	1:A:41:ARG:HG2	0.43	2.14	6	1
1:A:24:ALA:CB	1:A:60:VAL:HG12	0.43	2.43	9	1
1:A:25:ALA:O	1:A:28:ILE:HG13	0.43	2.13	6	1
1:A:30:ILE:CG2	1:A:31:LEU:N	0.43	2.80	5	1
1:A:22:ILE:O	1:A:26:ILE:HG12	0.42	2.14	9	2
1:A:34:LYS:HB2	1:A:34:LYS:NZ	0.42	2.28	6	1
1:A:58:GLY:O	1:A:62:ALA:HB2	0.42	2.14	6	1
1:A:9:LEU:C	1:A:9:LEU:CD2	0.42	2.91	8	1
1:A:70:LEU:C	1:A:70:LEU:CD2	0.42	2.92	3	1
1:A:36:LEU:HD13	1:A:52:GLN:OE1	0.42	2.14	7	1
1:A:42:GLN:HB2	1:A:45:LEU:HD23	0.42	1.90	5	2
1:A:24:ALA:O	1:A:28:ILE:HG13	0.42	2.14	6	1
1:A:72:LEU:HG	1:A:76:PHE:CD2	0.42	2.49	6	1
1:A:6:MET:HG2	1:A:10:TYR:CE2	0.42	2.49	4	1
1:A:40:ALA:HA	1:A:45:LEU:HD12	0.42	1.90	8	1
1:A:31:LEU:CD2	1:A:34:LYS:HD2	0.42	2.45	5	1
1:A:53:PHE:CD1	1:A:53:PHE:C	0.42	2.98	4	2
1:A:10:TYR:CE1	1:A:76:PHE:CE1	0.42	3.08	6	1
1:A:4:LEU:O	1:A:7:ASP:OD1	0.42	2.38	2	1
1:A:3:ASN:O	1:A:7:ASP:OD2	0.42	2.38	6	1
1:A:21:ALA:O	1:A:25:ALA:CB	0.41	2.68	2	1
1:A:55:ILE:O	1:A:59:LEU:HG	0.41	2.15	5	1
1:A:15:VAL:HG12	1:A:19:LEU:HD23	0.41	1.93	8	1
1:A:28:ILE:O	1:A:32:GLY:CA	0.41	2.68	6	2
1:A:63:ILE:CB	1:A:64:PRO:CD	0.41	2.98	3	1
1:A:26:ILE:HD12	1:A:26:ILE:N	0.41	2.30	5	1
1:A:56:VAL:HA	1:A:59:LEU:CD1	0.41	2.44	6	1
1:A:44:ASP:O	1:A:47:PRO:HD2	0.41	2.16	7	1
1:A:37:GLU:O	1:A:41:ARG:N	0.41	2.53	2	1
1:A:17:MET:O	1:A:21:ALA:HB2	0.41	2.15	3	3
1:A:71:GLY:O	1:A:75:MET:HG2	0.41	2.16	6	1
1:A:49:LEU:O	1:A:52:GLN:HG2	0.41	2.15	7	1
1:A:28:ILE:HG23	1:A:29:GLY:N	0.41	2.30	2	2
1:A:37:GLU:O	1:A:41:ARG:HG3	0.41	2.16	4	1
1:A:45:LEU:N	1:A:45:LEU:CD2	0.41	2.84	5	1
1:A:25:ALA:HA	1:A:28:ILE:HD11	0.41	1.92	9	1
1:A:13:ALA:O	1:A:17:MET:CG	0.41	2.68	2	1
1:A:34:LYS:NZ	1:A:34:LYS:HB2	0.41	2.31	2	1
1:A:58:GLY:O	1:A:62:ALA:N	0.41	2.53	9	2
1:A:45:LEU:HG	1:A:48:LEU:HD22	0.41	1.93	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HD13	1:A:60:VAL:HG23	0.41	1.92	6	1
1:A:68:VAL:CG1	1:A:72:LEU:CD1	0.41	2.98	7	1
1:A:31:LEU:HA	1:A:34:LYS:HG2	0.41	1.93	8	1
1:A:50:ARG:O	1:A:54:PHE:CD2	0.41	2.74	7	1
1:A:40:ALA:HA	1:A:49:LEU:HD11	0.40	1.93	5	1
1:A:45:LEU:N	1:A:45:LEU:CD1	0.40	2.84	2	1
1:A:12:ALA:O	1:A:16:MET:CB	0.40	2.69	8	1
1:A:35:PHE:CD1	1:A:52:GLN:OE1	0.40	2.74	8	1
1:A:20:ALA:HB1	1:A:64:PRO:HG3	0.40	1.92	9	1
1:A:75:MET:O	1:A:79:ALA:C	0.40	2.65	2	1
1:A:49:LEU:O	1:A:52:GLN:HG3	0.40	2.16	5	1
1:A:36:LEU:O	1:A:40:ALA:HB2	0.40	2.17	8	1
1:A:36:LEU:C	1:A:36:LEU:CD1	0.40	2.95	5	1
1:A:16:MET:HA	1:A:19:LEU:CD2	0.40	2.47	2	1
1:A:25:ALA:HA	1:A:28:ILE:CG1	0.40	2.47	6	1
1:A:44:ASP:O	1:A:45:LEU:HB3	0.40	2.16	8	1
1:A:52:GLN:O	1:A:56:VAL:CG2	0.40	2.69	8	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	77/79 (97%)	69±2 (90±2%)	6±2 (8±2%)	1±1 (2±1%)	8	51
All	All	693/711 (97%)	625 (90%)	55 (8%)	13 (2%)	8	51

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	30	ILE	6
1	A	43	PRO	5
1	A	49	LEU	1
1	A	42	GLN	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	56/56 (100%)	54±1 (96±2%)	2±1 (4±2%)	32 82
All	All	504/504 (100%)	486 (96%)	18 (4%)	32 82

All 11 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	34	LYS	4
1	A	16	MET	3
1	A	28	ILE	2
1	A	49	LEU	2
1	A	17	MET	1
1	A	52	GLN	1
1	A	59	LEU	1
1	A	37	GLU	1
1	A	48	LEU	1
1	A	65	MET	1
1	A	4	LEU	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 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