



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 03:43 AM UTC

PDB ID : 1HXV / pdb_00001hxx
Title : PPIASE DOMAIN OF THE MYCOPLASMA GENITALIUM TRIGGER FACTOR
Authors : Vogtherr, M.; Parac, T.N.; Maurer, M.; Pahl, A.; Fiebig, K.
Deposited on : 2001-01-17

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

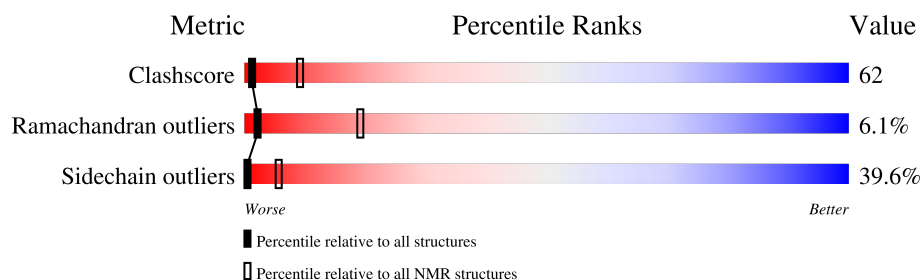
1 Overall quality at a glance

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	113	

2 Ensemble composition and analysis

This entry contains 12 models. Model 4 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:30-A:113 (84)	0.31	4

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 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 7, 10
2	5, 8, 11
3	1, 3, 9
Single-model clusters	6; 12

3 Entry composition

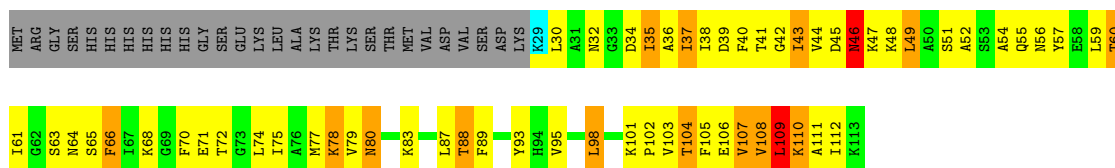
There is only 1 type of molecule in this entry. The entry contains 1342 atoms, of which 688 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TRIGGER FACTOR.

Mol	Chain	Residues	Atoms						Trace
1	A	85	Total	C	H	N	O	S	0
			1342	423	688	106	124	1	

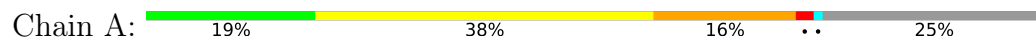
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P47480
A	2	ARG	-	expression tag	UNP P47480
A	3	GLY	-	expression tag	UNP P47480
A	4	SER	-	expression tag	UNP P47480
A	5	HIS	-	expression tag	UNP P47480
A	6	HIS	-	expression tag	UNP P47480
A	7	HIS	-	expression tag	UNP P47480
A	8	HIS	-	expression tag	UNP P47480
A	9	HIS	-	expression tag	UNP P47480
A	10	HIS	-	expression tag	UNP P47480
A	11	GLY	-	expression tag	UNP P47480
A	12	SER	-	expression tag	UNP P47480



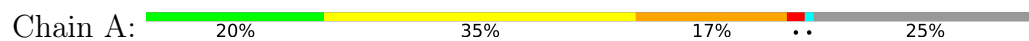
4.2.3 Score per residue for model 3

- Molecule 1: TRIGGER FACTOR



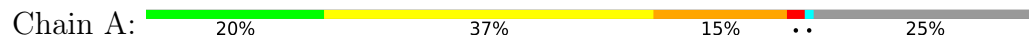
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: TRIGGER FACTOR



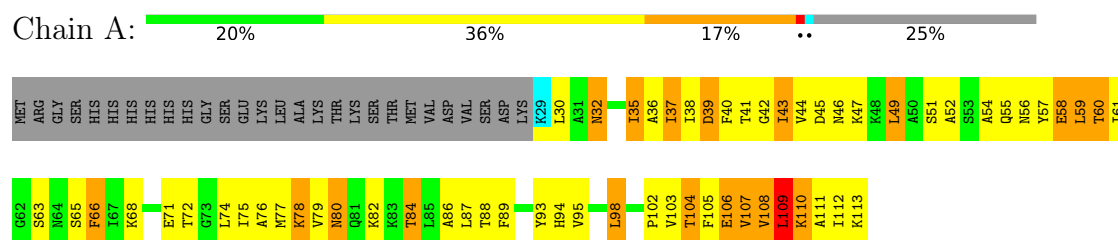
4.2.5 Score per residue for model 5

- Molecule 1: TRIGGER FACTOR



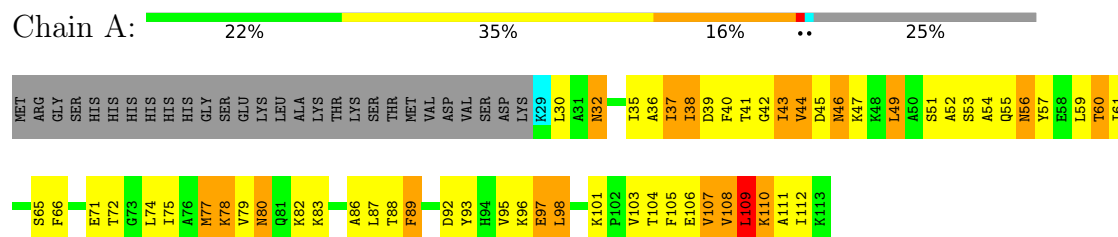
4.2.6 Score per residue for model 6

- Molecule 1: TRIGGER FACTOR



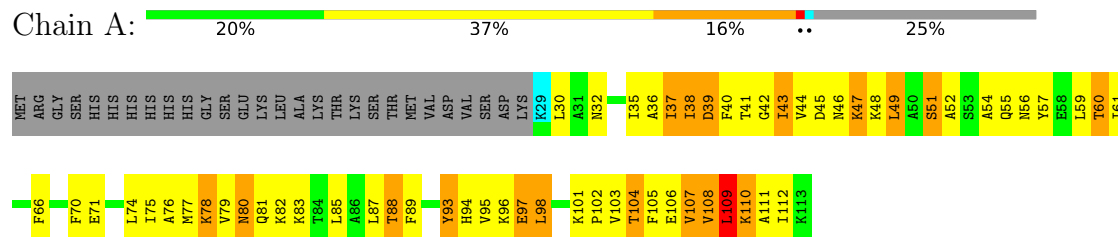
4.2.7 Score per residue for model 7

- Molecule 1: TRIGGER FACTOR



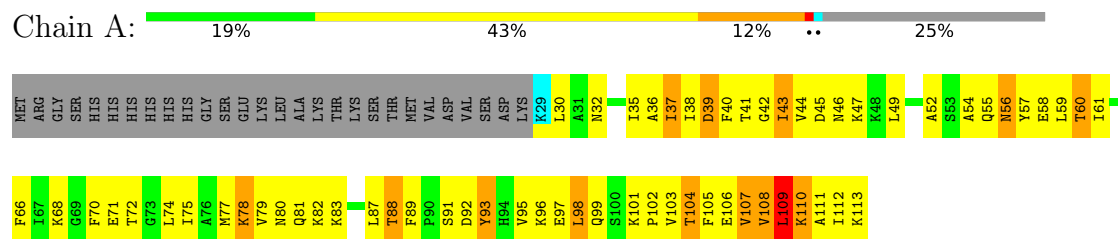
4.2.8 Score per residue for model 8

- Molecule 1: TRIGGER FACTOR



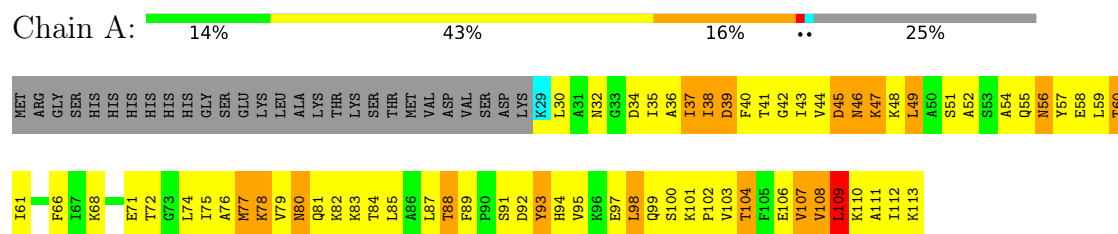
4.2.9 Score per residue for model 9

- Molecule 1: TRIGGER FACTOR



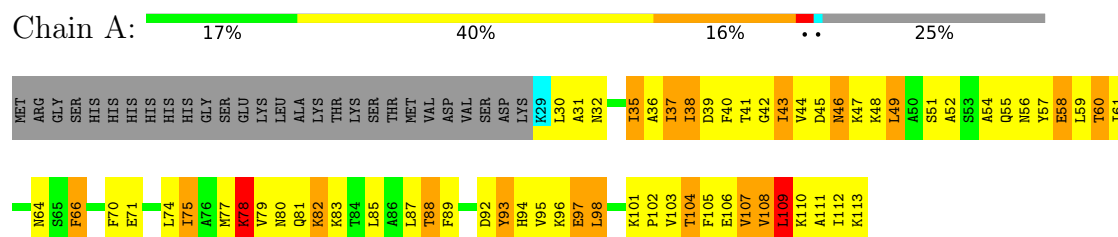
4.2.10 Score per residue for model 10

- Molecule 1: TRIGGER FACTOR



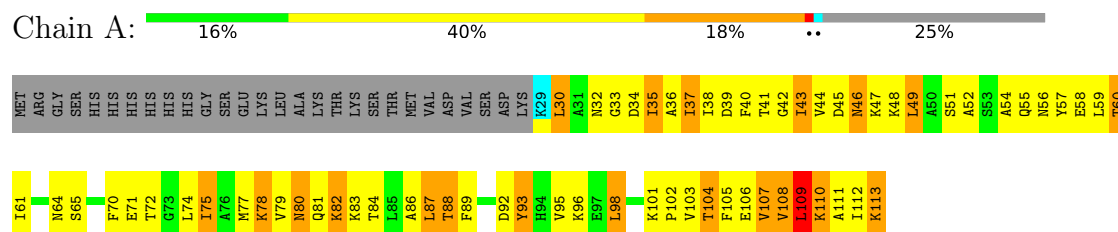
4.2.11 Score per residue for model 11

- Molecule 1: TRIGGER FACTOR



4.2.12 Score per residue for model 12

- Molecule 1: TRIGGER FACTOR



5 Refinement protocol and experimental data overview

Of the 160 calculated structures, 12 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
CNS	structure solution	1.0
DipoCoup	structure solution	1.0
DipoCoup	refinement	1.0

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	0.37±0.01	0±0/654 (0.0± 0.0%)	0.76±0.02	0±0/880 (0.0± 0.0%)
All	All	0.37	0/7848 (0.0%)	0.76	3/10560 (0.0%)

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	44	VAL	N-CA-C	5.15	111.72	106.21	7	3

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	645	675	674	82±6
All	All	7740	8100	8088	986

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 62.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:VAL:HG11	1:A:98:LEU:HD22	0.98	1.34	6	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:PHE:HB3	1:A:107:VAL:HG13	0.92	1.42	1	12
1:A:71:GLU:O	1:A:75:ILE:HG23	0.87	1.69	12	12
1:A:38:ILE:HD13	1:A:74:LEU:CD1	0.84	2.02	8	1
1:A:74:LEU:HD11	1:A:107:VAL:HB	0.82	1.49	9	9
1:A:38:ILE:HB	1:A:107:VAL:HG12	0.82	1.52	10	11
1:A:35:ILE:HB	1:A:112:ILE:O	0.81	1.75	6	12
1:A:38:ILE:HD12	1:A:38:ILE:O	0.81	1.76	3	2
1:A:36:ALA:HB3	1:A:59:LEU:HD12	0.80	1.51	6	2
1:A:78:LYS:O	1:A:109:LEU:HD13	0.79	1.77	7	9
1:A:52:ALA:HB1	1:A:105:PHE:CZ	0.79	2.13	6	1
1:A:59:LEU:HD22	1:A:60:THR:N	0.78	1.93	6	2
1:A:74:LEU:O	1:A:109:LEU:HD11	0.78	1.78	7	9
1:A:61:ILE:HG21	1:A:75:ILE:HG22	0.77	1.53	11	11
1:A:59:LEU:HD13	1:A:59:LEU:C	0.77	2.05	4	2
1:A:77:MET:HE2	1:A:81:GLN:OE1	0.77	1.78	8	1
1:A:42:GLY:HA3	1:A:52:ALA:HB3	0.76	1.56	6	12
1:A:61:ILE:CD1	1:A:75:ILE:HG22	0.76	2.10	5	11
1:A:59:LEU:HD11	1:A:61:ILE:HG23	0.76	1.55	6	2
1:A:40:PHE:CE1	1:A:54:ALA:HB3	0.76	2.16	3	2
1:A:89:PHE:CZ	1:A:103:VAL:HG11	0.75	2.17	12	1
1:A:40:PHE:CE2	1:A:54:ALA:HB3	0.75	2.16	7	10
1:A:74:LEU:O	1:A:109:LEU:HD21	0.74	1.83	2	5
1:A:59:LEU:HD22	1:A:60:THR:H	0.74	1.41	6	2
1:A:37:ILE:HD13	1:A:110:LYS:HB3	0.73	1.60	1	4
1:A:38:ILE:HG21	1:A:74:LEU:HG	0.73	1.58	12	8
1:A:87:LEU:HD11	1:A:105:PHE:CD2	0.72	2.19	12	1
1:A:38:ILE:HG21	1:A:74:LEU:HD13	0.71	1.61	8	2
1:A:70:PHE:CE1	1:A:74:LEU:HD11	0.70	2.21	3	1
1:A:59:LEU:HD12	1:A:60:THR:H	0.69	1.47	9	10
1:A:37:ILE:HD11	1:A:56:ASN:OD1	0.69	1.88	9	3
1:A:95:VAL:CG1	1:A:98:LEU:HD22	0.68	2.15	6	12
1:A:74:LEU:HD11	1:A:107:VAL:CB	0.68	2.18	6	10
1:A:35:ILE:HD12	1:A:35:ILE:N	0.68	2.04	5	6
1:A:40:PHE:CB	1:A:107:VAL:HG13	0.67	2.20	11	7
1:A:95:VAL:CG1	1:A:98:LEU:HB2	0.67	2.20	7	12
1:A:59:LEU:HD21	1:A:71:GLU:OE2	0.67	1.89	6	2
1:A:61:ILE:HD12	1:A:75:ILE:HG22	0.65	1.67	5	6
1:A:89:PHE:CE2	1:A:103:VAL:HG11	0.64	2.28	9	6
1:A:103:VAL:HG11	1:A:105:PHE:CE1	0.64	2.27	3	5
1:A:38:ILE:HG22	1:A:109:LEU:HA	0.64	1.70	10	7
1:A:108:VAL:HG12	1:A:108:VAL:O	0.63	1.93	4	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:VAL:HG11	1:A:98:LEU:CD2	0.62	2.23	7	7
1:A:93:TYR:CE1	1:A:98:LEU:HD23	0.61	2.30	12	1
1:A:70:PHE:O	1:A:74:LEU:HD22	0.61	1.94	4	2
1:A:45:ASP:O	1:A:46:ASN:HB2	0.60	1.96	8	3
1:A:37:ILE:HG22	1:A:58:GLU:HA	0.60	1.73	6	2
1:A:80:ASN:N	1:A:109:LEU:O	0.60	2.35	4	12
1:A:103:VAL:HG11	1:A:105:PHE:CZ	0.59	2.32	11	4
1:A:40:PHE:HA	1:A:106:GLU:O	0.59	1.98	10	11
1:A:30:LEU:HD22	1:A:111:ALA:CB	0.59	2.28	11	10
1:A:59:LEU:HD21	1:A:71:GLU:CG	0.59	2.27	12	6
1:A:55:GLN:O	1:A:57:TYR:N	0.58	2.36	7	12
1:A:39:ASP:HB3	1:A:108:VAL:HB	0.58	1.74	12	2
1:A:88:THR:HA	1:A:102:PRO:HA	0.58	1.75	12	10
1:A:61:ILE:HG21	1:A:75:ILE:CG2	0.58	2.27	12	9
1:A:38:ILE:HD13	1:A:74:LEU:HD13	0.58	1.76	8	1
1:A:38:ILE:HD12	1:A:40:PHE:CD2	0.57	2.33	9	2
1:A:40:PHE:CD2	1:A:54:ALA:HB3	0.57	2.34	12	6
1:A:44:VAL:HG13	1:A:44:VAL:O	0.57	1.99	3	12
1:A:36:ALA:N	1:A:59:LEU:O	0.57	2.37	9	12
1:A:38:ILE:H	1:A:38:ILE:HD13	0.57	1.60	7	1
1:A:39:ASP:HA	1:A:55:GLN:O	0.57	1.99	3	12
1:A:61:ILE:CG2	1:A:75:ILE:HG22	0.56	2.29	11	1
1:A:40:PHE:CD1	1:A:54:ALA:HB3	0.56	2.34	3	1
1:A:39:ASP:OD2	1:A:108:VAL:HG11	0.56	2.01	6	2
1:A:30:LEU:HD11	1:A:34:ASP:OD1	0.55	2.01	2	1
1:A:37:ILE:O	1:A:110:LYS:HB3	0.55	2.00	8	2
1:A:108:VAL:O	1:A:108:VAL:CG1	0.55	2.54	4	9
1:A:70:PHE:CD1	1:A:74:LEU:HD21	0.55	2.37	4	1
1:A:40:PHE:N	1:A:54:ALA:O	0.54	2.40	7	12
1:A:39:ASP:HB2	1:A:108:VAL:HB	0.54	1.79	7	8
1:A:61:ILE:HD13	1:A:75:ILE:HG22	0.54	1.79	10	8
1:A:35:ILE:HG12	1:A:60:THR:HG23	0.54	1.78	8	6
1:A:36:ALA:O	1:A:38:ILE:HD13	0.54	2.03	10	2
1:A:74:LEU:HD12	1:A:109:LEU:CD2	0.54	2.32	11	1
1:A:59:LEU:CD1	1:A:61:ILE:HG23	0.53	2.31	6	2
1:A:74:LEU:CD1	1:A:107:VAL:HG11	0.53	2.33	8	2
1:A:37:ILE:O	1:A:110:LYS:CB	0.53	2.56	7	10
1:A:38:ILE:HG21	1:A:74:LEU:CG	0.53	2.32	12	1
1:A:59:LEU:C	1:A:59:LEU:CD1	0.53	2.79	4	2
1:A:89:PHE:HB3	1:A:98:LEU:O	0.53	2.04	1	12
1:A:44:VAL:HG13	1:A:47:LYS:HB2	0.53	1.81	9	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD11	1:A:105:PHE:CE2	0.53	2.39	12	1
1:A:44:VAL:N	1:A:47:LYS:O	0.52	2.43	2	12
1:A:95:VAL:HG13	1:A:98:LEU:H	0.52	1.65	1	11
1:A:89:PHE:CE1	1:A:93:TYR:CE2	0.52	2.97	12	1
1:A:35:ILE:N	1:A:35:ILE:CD1	0.52	2.72	12	6
1:A:40:PHE:CZ	1:A:54:ALA:CB	0.52	2.92	6	5
1:A:66:PHE:CD2	1:A:70:PHE:CD1	0.52	2.98	11	3
1:A:37:ILE:HG22	1:A:58:GLU:CA	0.52	2.35	6	2
1:A:38:ILE:HD13	1:A:38:ILE:H	0.52	1.65	10	1
1:A:89:PHE:CD1	1:A:93:TYR:CE2	0.52	2.98	12	1
1:A:40:PHE:CD1	1:A:40:PHE:O	0.52	2.63	8	10
1:A:37:ILE:HA	1:A:57:TYR:O	0.51	2.04	7	7
1:A:30:LEU:O	1:A:75:ILE:HA	0.51	2.06	1	5
1:A:40:PHE:CE2	1:A:54:ALA:CB	0.51	2.94	12	7
1:A:37:ILE:HG13	1:A:110:LYS:C	0.51	2.31	3	2
1:A:79:VAL:HA	1:A:109:LEU:O	0.51	2.06	6	11
1:A:93:TYR:HD2	1:A:95:VAL:HG12	0.51	1.65	6	8
1:A:89:PHE:CE1	1:A:93:TYR:CE1	0.50	2.99	6	1
1:A:66:PHE:CE2	1:A:70:PHE:CE1	0.50	3.00	1	3
1:A:108:VAL:O	1:A:110:LYS:N	0.50	2.44	6	12
1:A:49:LEU:H	1:A:49:LEU:HD13	0.50	1.67	3	10
1:A:74:LEU:HD11	1:A:107:VAL:HG11	0.50	1.84	4	2
1:A:59:LEU:HD21	1:A:71:GLU:HG3	0.50	1.82	2	3
1:A:70:PHE:CE2	1:A:105:PHE:CD2	0.50	2.99	4	2
1:A:59:LEU:HD12	1:A:60:THR:N	0.50	2.19	10	7
1:A:87:LEU:HD21	1:A:105:PHE:HB2	0.49	1.84	12	1
1:A:85:LEU:C	1:A:85:LEU:HD23	0.49	2.32	10	4
1:A:43:ILE:HB	1:A:104:THR:HB	0.49	1.82	7	2
1:A:79:VAL:HG22	1:A:111:ALA:HB3	0.49	1.83	5	4
1:A:78:LYS:O	1:A:109:LEU:HD12	0.49	2.07	8	3
1:A:45:ASP:O	1:A:46:ASN:CB	0.49	2.61	11	10
1:A:66:PHE:CE2	1:A:70:PHE:CD1	0.49	3.01	11	3
1:A:40:PHE:CZ	1:A:54:ALA:HB3	0.49	2.43	2	4
1:A:82:LYS:HG2	1:A:108:VAL:HG23	0.49	1.84	12	1
1:A:43:ILE:O	1:A:104:THR:N	0.49	2.44	5	9
1:A:74:LEU:HD22	1:A:74:LEU:N	0.49	2.22	5	4
1:A:37:ILE:O	1:A:37:ILE:HG12	0.49	2.08	5	7
1:A:37:ILE:HG21	1:A:112:ILE:HD12	0.49	1.84	3	2
1:A:89:PHE:CE2	1:A:103:VAL:CG1	0.49	2.96	5	4
1:A:84:THR:HA	1:A:106:GLU:HA	0.48	1.83	6	1
1:A:95:VAL:HG22	1:A:97:GLU:CG	0.48	2.38	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ILE:HG22	1:A:71:GLU:HB2	0.48	1.83	9	1
1:A:78:LYS:O	1:A:109:LEU:HD22	0.48	2.07	1	3
1:A:37:ILE:N	1:A:110:LYS:O	0.48	2.46	7	12
1:A:74:LEU:HD11	1:A:107:VAL:CG1	0.48	2.39	11	5
1:A:87:LEU:O	1:A:103:VAL:O	0.48	2.31	12	10
1:A:30:LEU:HD11	1:A:34:ASP:OD2	0.48	2.08	12	1
1:A:43:ILE:HG22	1:A:47:LYS:O	0.48	2.09	3	6
1:A:74:LEU:HD21	1:A:107:VAL:HG21	0.48	1.85	8	2
1:A:74:LEU:CD2	1:A:107:VAL:HG11	0.48	2.39	8	2
1:A:95:VAL:HG22	1:A:97:GLU:HG2	0.48	1.84	5	3
1:A:89:PHE:CZ	1:A:105:PHE:CZ	0.48	3.01	12	1
1:A:79:VAL:HG12	1:A:80:ASN:N	0.47	2.24	9	8
1:A:74:LEU:HD12	1:A:109:LEU:HD22	0.47	1.86	11	1
1:A:49:LEU:C	1:A:49:LEU:CD1	0.47	2.87	1	1
1:A:79:VAL:CG2	1:A:111:ALA:HB3	0.47	2.38	5	3
1:A:103:VAL:HG22	1:A:104:THR:N	0.47	2.25	5	12
1:A:70:PHE:CE2	1:A:105:PHE:CE2	0.47	3.03	9	2
1:A:79:VAL:HG13	1:A:110:LYS:HA	0.47	1.85	6	6
1:A:37:ILE:CG2	1:A:58:GLU:HA	0.47	2.40	6	2
1:A:37:ILE:C	1:A:110:LYS:O	0.47	2.57	6	11
1:A:39:ASP:HA	1:A:55:GLN:C	0.46	2.34	3	8
1:A:38:ILE:CB	1:A:107:VAL:HG12	0.46	2.35	10	2
1:A:35:ILE:HG23	1:A:59:LEU:O	0.46	2.10	4	3
1:A:103:VAL:CG1	1:A:105:PHE:CE1	0.46	2.99	3	2
1:A:30:LEU:HD11	1:A:34:ASP:CG	0.46	2.34	2	1
1:A:59:LEU:HD21	1:A:71:GLU:HG2	0.46	1.88	7	3
1:A:89:PHE:CE2	1:A:103:VAL:HB	0.46	2.46	12	1
1:A:38:ILE:HB	1:A:107:VAL:CG1	0.46	2.40	4	4
1:A:59:LEU:HD11	1:A:71:GLU:OE2	0.46	2.11	2	1
1:A:75:ILE:HG13	1:A:76:ALA:N	0.46	2.25	8	4
1:A:87:LEU:HB3	1:A:105:PHE:CD2	0.46	2.46	2	6
1:A:74:LEU:CA	1:A:109:LEU:HD21	0.46	2.41	11	2
1:A:40:PHE:CE1	1:A:54:ALA:CB	0.46	2.93	3	2
1:A:40:PHE:HA	1:A:107:VAL:HA	0.45	1.88	9	7
1:A:70:PHE:O	1:A:74:LEU:CD2	0.45	2.64	5	2
1:A:38:ILE:O	1:A:55:GLN:O	0.45	2.35	9	1
1:A:37:ILE:O	1:A:110:LYS:O	0.45	2.35	11	8
1:A:81:GLN:O	1:A:109:LEU:N	0.45	2.49	3	4
1:A:86:ALA:HA	1:A:104:THR:HA	0.45	1.89	6	3
1:A:103:VAL:CG1	1:A:105:PHE:CZ	0.45	2.99	4	3
1:A:72:THR:O	1:A:75:ILE:HG12	0.45	2.11	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:PHE:CD1	1:A:93:TYR:CE1	0.45	3.05	6	1
1:A:35:ILE:HG21	1:A:58:GLU:HG2	0.45	1.88	10	1
1:A:79:VAL:CG1	1:A:80:ASN:N	0.45	2.80	5	11
1:A:49:LEU:C	1:A:49:LEU:HD12	0.45	2.37	1	1
1:A:52:ALA:HB1	1:A:105:PHE:CE1	0.45	2.47	6	2
1:A:41:THR:HG22	1:A:48:LYS:HG3	0.45	1.88	1	1
1:A:40:PHE:CE2	1:A:52:ALA:O	0.45	2.70	3	1
1:A:30:LEU:HD22	1:A:111:ALA:HB2	0.45	1.89	8	2
1:A:35:ILE:O	1:A:112:ILE:O	0.44	2.35	9	7
1:A:49:LEU:CD2	1:A:49:LEU:C	0.44	2.90	2	9
1:A:35:ILE:HD13	1:A:113:LYS:OXT	0.44	2.12	12	1
1:A:61:ILE:CG2	1:A:75:ILE:CG2	0.44	2.96	9	4
1:A:89:PHE:CE2	1:A:98:LEU:HG	0.44	2.48	11	1
1:A:38:ILE:HG12	1:A:74:LEU:HD13	0.44	1.89	3	1
1:A:95:VAL:HG13	1:A:98:LEU:HB2	0.44	1.90	11	3
1:A:89:PHE:CG	1:A:98:LEU:HG	0.44	2.48	12	2
1:A:37:ILE:HG13	1:A:110:LYS:O	0.44	2.13	3	1
1:A:30:LEU:O	1:A:75:ILE:CA	0.44	2.66	1	7
1:A:37:ILE:O	1:A:110:LYS:HB2	0.44	2.13	2	2
1:A:87:LEU:HD21	1:A:105:PHE:CD2	0.43	2.47	6	1
1:A:40:PHE:CD2	1:A:40:PHE:O	0.43	2.71	6	1
1:A:70:PHE:C	1:A:70:PHE:CD1	0.43	2.96	12	1
1:A:40:PHE:CE1	1:A:52:ALA:O	0.43	2.71	9	4
1:A:77:MET:CB	1:A:109:LEU:CD1	0.43	2.96	4	5
1:A:91:SER:HA	1:A:99:GLN:HA	0.43	1.90	4	5
1:A:77:MET:HB2	1:A:109:LEU:CD1	0.43	2.43	7	1
1:A:89:PHE:CD2	1:A:98:LEU:HG	0.43	2.48	7	2
1:A:37:ILE:HD13	1:A:110:LYS:CB	0.43	2.40	1	1
1:A:93:TYR:CE2	1:A:98:LEU:HD23	0.43	2.49	8	5
1:A:34:ASP:C	1:A:35:ILE:HD12	0.43	2.39	12	1
1:A:49:LEU:C	1:A:49:LEU:CD2	0.43	2.91	7	1
1:A:89:PHE:HB2	1:A:101:LYS:O	0.43	2.13	8	1
1:A:39:ASP:OD1	1:A:39:ASP:N	0.43	2.52	6	2
1:A:39:ASP:OD1	1:A:56:ASN:N	0.43	2.51	9	1
1:A:35:ILE:HG13	1:A:60:THR:HG23	0.43	1.90	11	5
1:A:40:PHE:O	1:A:40:PHE:CG	0.43	2.72	3	2
1:A:106:GLU:O	1:A:106:GLU:CG	0.42	2.67	6	1
1:A:77:MET:HE2	1:A:109:LEU:HD12	0.42	1.91	6	1
1:A:88:THR:HG23	1:A:102:PRO:CA	0.42	2.44	6	1
1:A:59:LEU:HD23	1:A:66:PHE:CD2	0.42	2.50	6	1
1:A:38:ILE:HD13	1:A:74:LEU:HD11	0.42	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:TYR:CD2	1:A:95:VAL:HG12	0.42	2.48	6	1
1:A:95:VAL:HG22	1:A:97:GLU:HG3	0.42	1.92	7	1
1:A:74:LEU:C	1:A:109:LEU:HD21	0.42	2.40	11	2
1:A:33:GLY:N	1:A:61:ILE:O	0.41	2.53	12	1
1:A:74:LEU:HD22	1:A:74:LEU:H	0.41	1.76	5	1
1:A:85:LEU:HD23	1:A:87:LEU:N	0.41	2.31	11	2
1:A:43:ILE:N	1:A:104:THR:O	0.41	2.54	11	2
1:A:42:GLY:O	1:A:49:LEU:HD22	0.41	2.16	11	4
1:A:87:LEU:O	1:A:103:VAL:HG12	0.41	2.15	6	1
1:A:95:VAL:HG13	1:A:95:VAL:O	0.41	2.15	6	1
1:A:42:GLY:O	1:A:49:LEU:CD1	0.41	2.67	1	1
1:A:38:ILE:HD12	1:A:40:PHE:HD2	0.41	1.76	8	1
1:A:78:LYS:O	1:A:109:LEU:CD1	0.41	2.69	2	1
1:A:37:ILE:CD1	1:A:110:LYS:HB3	0.41	2.46	6	1
1:A:74:LEU:CD1	1:A:107:VAL:HB	0.41	2.38	6	1
1:A:31:ALA:O	1:A:61:ILE:CD1	0.41	2.69	11	1
1:A:42:GLY:CA	1:A:52:ALA:HB3	0.41	2.41	12	2
1:A:37:ILE:O	1:A:37:ILE:CG1	0.40	2.69	7	1
1:A:30:LEU:HD23	1:A:61:ILE:CD1	0.40	2.46	1	1
1:A:57:TYR:CD1	1:A:57:TYR:C	0.40	3.00	4	1
1:A:37:ILE:HD12	1:A:110:LYS:HB3	0.40	1.94	6	1
1:A:42:GLY:O	1:A:49:LEU:CD2	0.40	2.70	11	1
1:A:95:VAL:CG2	1:A:97:GLU:CG	0.40	2.99	7	1
1:A:82:LYS:CD	1:A:108:VAL:HG23	0.40	2.47	11	1
1:A:103:VAL:CG2	1:A:104:THR:N	0.40	2.84	12	1
1:A:74:LEU:CG	1:A:107:VAL:HG11	0.40	2.47	2	1
1:A:39:ASP:CG	1:A:55:GLN:HA	0.40	2.41	12	1
1:A:61:ILE:HG22	1:A:71:GLU:HB3	0.40	1.93	12	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	83/113 (73%)	62±2 (75±2%)	16±2 (19±2%)	5±1 (6±1%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	996/1356 (73%)	749 (75%)	186 (19%)	61 (6%)	2 19

All 7 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	32	ASN	12
1	A	56	ASN	12
1	A	109	LEU	12
1	A	51	SER	10
1	A	46	ASN	7
1	A	58	GLU	5
1	A	78	LYS	3

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	71/97 (73%)	43±3 (60±4%)	28±3 (40±4%)	0 6
All	All	852/1164 (73%)	515 (60%)	337 (40%)	0 6

All 54 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	37	ILE	12
1	A	43	ILE	12
1	A	49	LEU	12
1	A	60	THR	12
1	A	98	LEU	12
1	A	107	VAL	12
1	A	108	VAL	12
1	A	109	LEU	12
1	A	66	PHE	11
1	A	88	THR	11
1	A	104	THR	11
1	A	41	THR	11

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Mol	Chain	Res	Type	Models (Total)
1	A	93	TYR	10
1	A	78	LYS	9
1	A	110	LYS	9
1	A	72	THR	8
1	A	83	LYS	8
1	A	101	LYS	8
1	A	82	LYS	8
1	A	96	LYS	8
1	A	68	LYS	7
1	A	94	HIS	7
1	A	113	LYS	7
1	A	48	LYS	7
1	A	77	MET	7
1	A	80	ASN	7
1	A	35	ILE	6
1	A	92	ASP	6
1	A	97	GLU	6
1	A	39	ASP	5
1	A	46	ASN	5
1	A	51	SER	5
1	A	65	SER	5
1	A	38	ILE	5
1	A	47	LYS	4
1	A	81	GLN	4
1	A	58	GLU	3
1	A	64	ASN	3
1	A	53	SER	3
1	A	75	ILE	3
1	A	32	ASN	3
1	A	84	THR	3
1	A	30	LEU	2
1	A	100	SER	2
1	A	63	SER	2
1	A	91	SER	2
1	A	59	LEU	2
1	A	74	LEU	2
1	A	55	GLN	1
1	A	106	GLU	1
1	A	89	PHE	1
1	A	34	ASP	1
1	A	45	ASP	1
1	A	87	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 [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