



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 07:39 PM UTC

PDB ID : 2PP4 / pdb_00002pp4
Title : Solution Structure of ETO-TAFH refined in explicit solvent
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Yokoyama, S.; Werner, M.H.
Deposited on : 2007-04-27

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

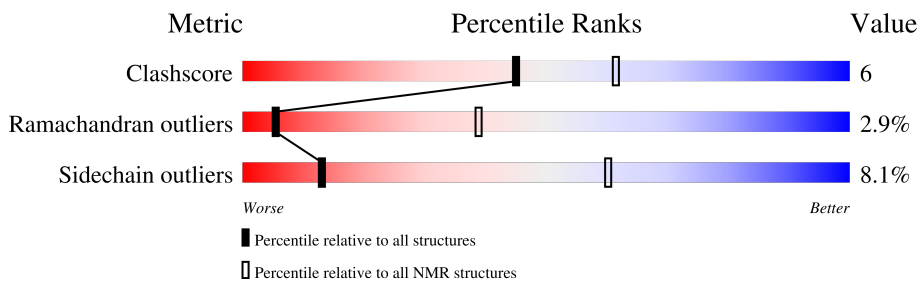
1 Overall quality at a glance

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	107	 68% 18% • 12%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:121-A:214 (94)	0.67	8

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 and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1739 atoms, of which 885 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein ETO.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1739	546	885	153	154	1	0

There is a discrepancy between the modelled and reference sequences:

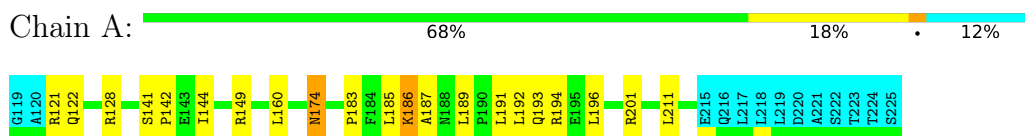
Chain	Residue	Modelled	Actual	Comment	Reference
A	136	TYR	PHE	engineered mutation	UNP Q06455

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: Protein ETO

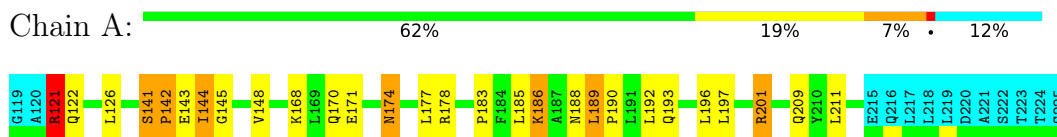


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

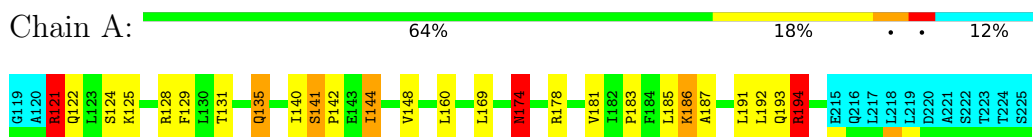
4.2.1 Score per residue for model 1

- Molecule 1: Protein ETO



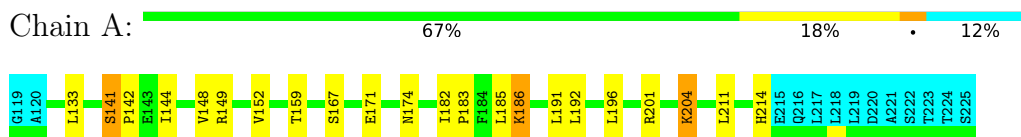
4.2.2 Score per residue for model 2

- Molecule 1: Protein ETO



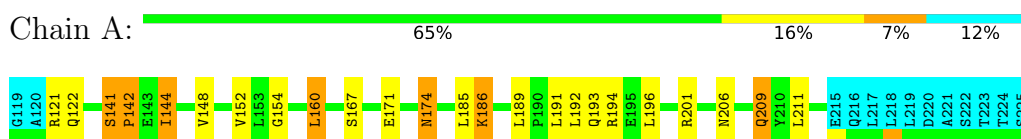
4.2.3 Score per residue for model 3

- Molecule 1: Protein ETO



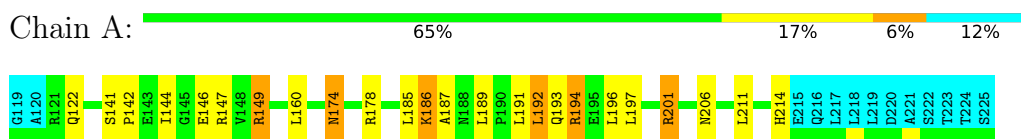
4.2.4 Score per residue for model 4

- Molecule 1: Protein ETO



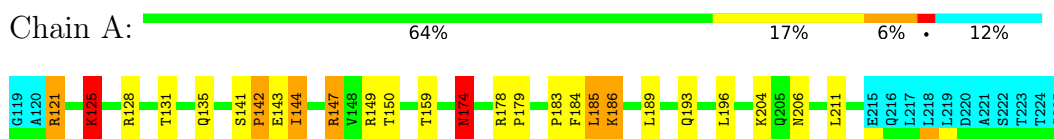
4.2.5 Score per residue for model 5

- Molecule 1: Protein ETO



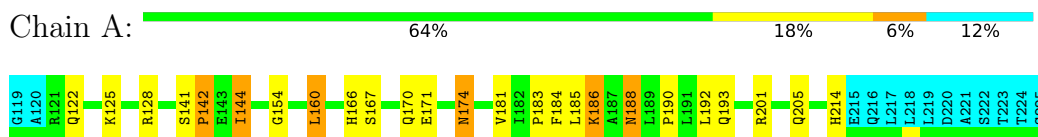
4.2.6 Score per residue for model 6

- Molecule 1: Protein ETO



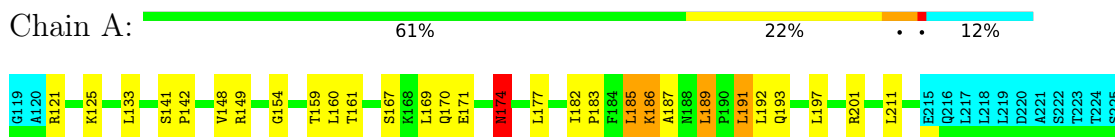
4.2.7 Score per residue for model 7

- Molecule 1: Protein ETO



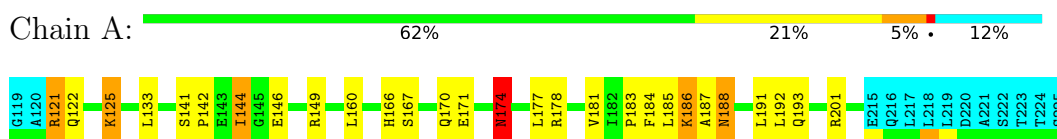
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Protein ETO



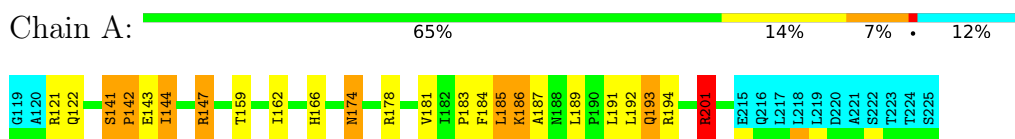
4.2.9 Score per residue for model 9

- Molecule 1: Protein ETO



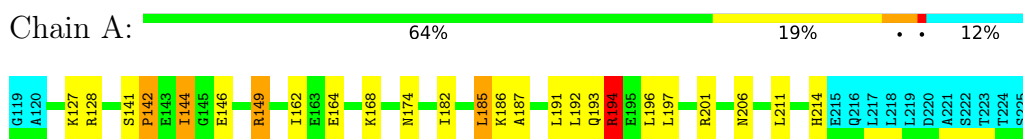
4.2.10 Score per residue for model 10

- Molecule 1: Protein ETO



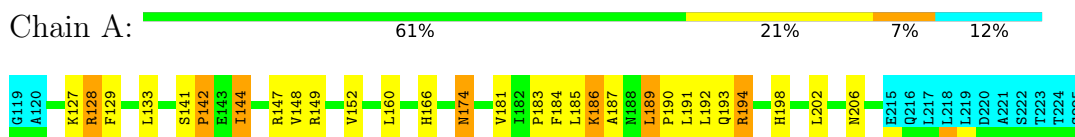
4.2.11 Score per residue for model 11

- Molecule 1: Protein ETO



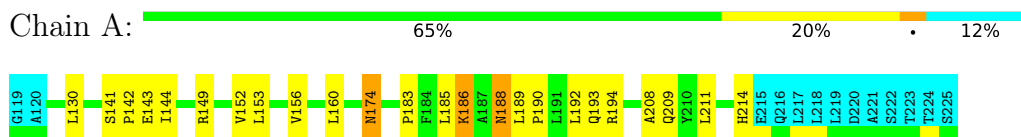
4.2.12 Score per residue for model 12

- Molecule 1: Protein ETO



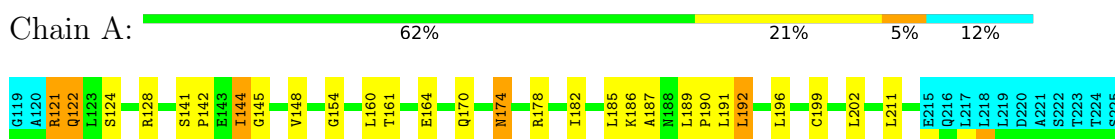
4.2.13 Score per residue for model 13

- Molecule 1: Protein ETO



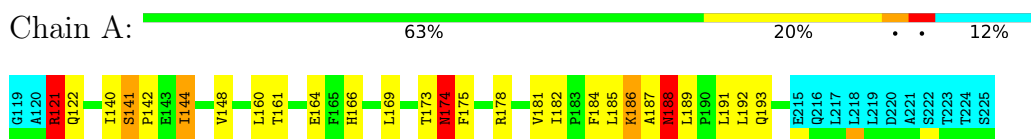
4.2.14 Score per residue for model 14

- Molecule 1: Protein ETO



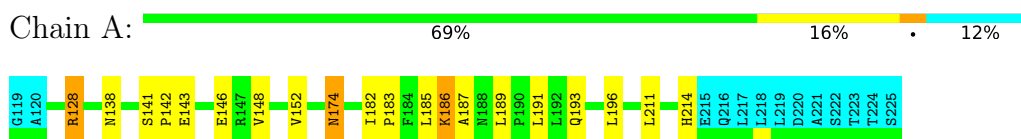
4.2.15 Score per residue for model 15

- Molecule 1: Protein ETO



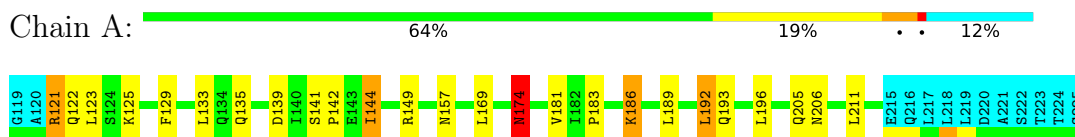
4.2.16 Score per residue for model 16

- Molecule 1: Protein ETO



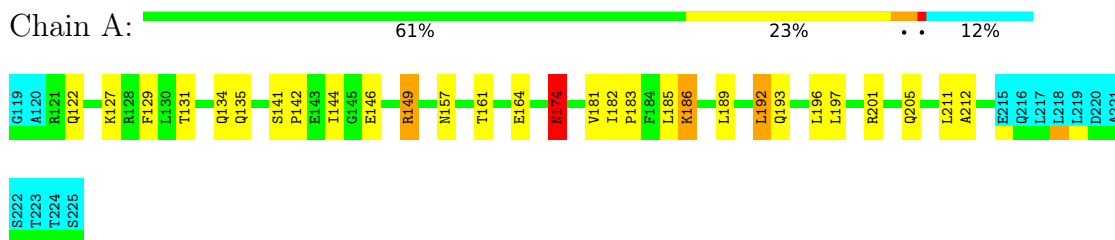
4.2.17 Score per residue for model 17

- Molecule 1: Protein ETO



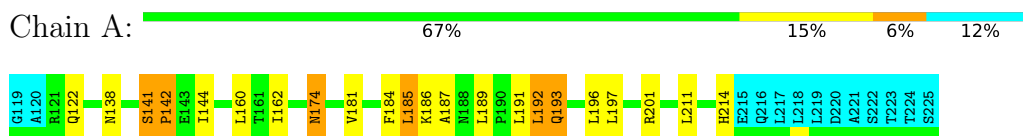
4.2.18 Score per residue for model 18

- Molecule 1: Protein ETO



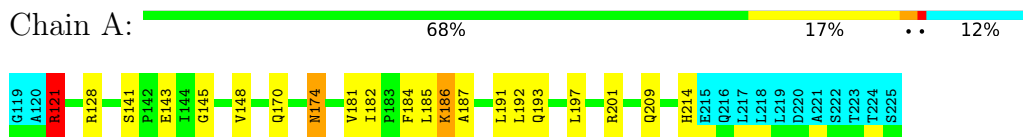
4.2.19 Score per residue for model 19

- Molecule 1: Protein ETO



4.2.20 Score per residue for model 20

- Molecule 1: Protein ETO



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
XPLOR-NIH	refinement	2.14

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	1.14±0.04	3±2/781 (0.4± 0.2%)	1.09±0.03	1±1/1059 (0.1± 0.1%)
All	All	1.14	61/15620 (0.4%)	1.09	25/21180 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±1.2
All	All	0	35

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	193	GLN	C-O	-7.55	1.15	1.24	2	8
1	A	174	ASN	N-CA	7.41	1.55	1.46	2	18
1	A	182	ILE	CA-CB	7.35	1.58	1.54	8	5
1	A	144	ILE	N-CA	-6.76	1.37	1.46	6	12
1	A	159	THR	C-O	6.59	1.30	1.24	8	1
1	A	159	THR	C-N	6.57	1.42	1.33	8	2
1	A	161	THR	CA-CB	6.20	1.63	1.53	8	1
1	A	209	GLN	C-N	6.14	1.41	1.33	20	1
1	A	121	ARG	NE-CZ	5.85	1.39	1.33	1	1
1	A	141	SER	N-CA	5.65	1.54	1.46	3	2
1	A	189	LEU	N-CA	-5.54	1.43	1.46	1	1
1	A	201	ARG	NE-CZ	5.41	1.39	1.33	10	1
1	A	194	ARG	NE-CZ	5.34	1.39	1.33	2	2
1	A	201	ARG	CD-NE	5.30	1.53	1.46	10	1
1	A	189	LEU	C-O	-5.12	1.20	1.24	12	1
1	A	189	LEU	C-N	5.09	1.39	1.34	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	162	ILE	CA-CB	5.04	1.59	1.54	10	1
1	A	125	LYS	CA-C	5.03	1.60	1.52	8	1
1	A	121	ARG	N-CA	-5.00	1.40	1.46	14	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	159	THR	N-CA-C	-8.17	105.31	114.62	8	1
1	A	209	GLN	CA-C-N	-7.19	111.10	120.44	20	1
1	A	209	GLN	C-N-CA	-7.19	111.10	120.44	20	1
1	A	201	ARG	CD-NE-CZ	6.12	132.97	124.40	10	1
1	A	188	ASN	CA-CB-CG	6.08	118.68	112.60	7	4
1	A	125	LYS	N-CA-C	-6.06	104.96	112.90	6	1
1	A	194	ARG	CD-NE-CZ	5.80	132.52	124.40	11	1
1	A	193	GLN	N-CA-C	5.65	118.16	111.33	6	4
1	A	182	ILE	N-CA-CB	5.63	114.84	110.45	8	3
1	A	138	ASN	CA-CB-CG	5.58	118.18	112.60	19	2
1	A	174	ASN	CA-CB-CG	5.57	118.17	112.60	15	3
1	A	214	HIS	CA-C-N	-5.45	110.95	121.58	7	1
1	A	214	HIS	C-N-CA	-5.45	110.95	121.58	7	1
1	A	211	LEU	N-CA-C	-5.07	106.79	113.12	8	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	121	ARG	Sidechain	9
1	A	178	ARG	Sidechain	6
1	A	201	ARG	Sidechain	6
1	A	149	ARG	Sidechain	5
1	A	147	ARG	Sidechain	3
1	A	128	ARG	Sidechain	3
1	A	194	ARG	Sidechain	3

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	765	797	800	10±2
All	All	15300	15940	16000	198

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:196:LEU:HD11	1:A:211:LEU:HB3	0.79	1.51	6	11
1:A:122:GLN:HE22	1:A:192:LEU:HG	0.74	1.39	17	1
1:A:187:ALA:O	1:A:191:LEU:HB2	0.64	1.92	5	10
1:A:189:LEU:O	1:A:193:GLN:HG3	0.63	1.93	15	5
1:A:147:ARG:HB2	1:A:147:ARG:HH11	0.63	1.52	10	1
1:A:161:THR:HB	1:A:164:GLU:OE1	0.63	1.94	15	2
1:A:121:ARG:HG2	1:A:121:ARG:HH11	0.63	1.54	17	1
1:A:197:LEU:O	1:A:201:ARG:HG2	0.62	1.93	1	3
1:A:121:ARG:H	1:A:121:ARG:HD3	0.59	1.56	15	1
1:A:121:ARG:HD2	1:A:121:ARG:H	0.57	1.59	20	3
1:A:201:ARG:HE	1:A:201:ARG:HA	0.57	1.60	11	1
1:A:131:THR:O	1:A:135:GLN:HG3	0.56	1.99	2	1
1:A:170:GLN:HE21	1:A:177:LEU:HD23	0.56	1.58	1	1
1:A:201:ARG:HA	1:A:201:ARG:NE	0.56	2.16	11	1
1:A:189:LEU:O	1:A:193:GLN:HG2	0.56	2.01	10	5
1:A:166:HIS:O	1:A:170:GLN:HG2	0.56	2.02	9	2
1:A:167:SER:O	1:A:171:GLU:HG2	0.55	2.01	3	4
1:A:187:ALA:O	1:A:191:LEU:HG	0.55	2.01	10	2
1:A:128:ARG:HH11	1:A:128:ARG:HG3	0.54	1.62	20	1
1:A:185:LEU:O	1:A:189:LEU:HG	0.54	2.02	8	2
1:A:128:ARG:HA	1:A:128:ARG:HE	0.54	1.62	16	1
1:A:154:GLY:HA3	1:A:160:LEU:HD23	0.53	1.79	7	4
1:A:182:ILE:HB	1:A:183:PRO:HD3	0.52	1.81	16	2
1:A:197:LEU:O	1:A:201:ARG:HG3	0.52	2.05	8	4
1:A:122:GLN:HG3	1:A:191:LEU:HD23	0.52	1.82	14	1
1:A:122:GLN:O	1:A:125:LYS:HG3	0.51	2.05	7	1
1:A:194:ARG:HH11	1:A:194:ARG:HG3	0.51	1.65	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:VAL:HG13	1:A:169:LEU:HD11	0.51	1.83	2	3
1:A:186:LYS:HA	1:A:186:LYS:HE2	0.50	1.84	10	9
1:A:198:HIS:O	1:A:202:LEU:HG	0.50	2.06	12	1
1:A:122:GLN:HG3	1:A:192:LEU:HG	0.50	1.84	18	1
1:A:189:LEU:HB2	1:A:190:PRO:HD3	0.49	1.84	13	4
1:A:124:SER:O	1:A:128:ARG:HB2	0.49	2.08	2	2
1:A:201:ARG:HH11	1:A:201:ARG:HB3	0.49	1.68	10	1
1:A:183:PRO:HA	1:A:186:LYS:HB2	0.49	1.84	9	12
1:A:122:GLN:HG3	1:A:191:LEU:HD13	0.49	1.84	10	1
1:A:204:LYS:O	1:A:204:LYS:HE2	0.48	2.08	3	1
1:A:146:GLU:HA	1:A:149:ARG:NH1	0.48	2.23	11	2
1:A:122:GLN:NE2	1:A:192:LEU:HG	0.48	2.24	19	1
1:A:122:GLN:NE2	1:A:188:ASN:HB3	0.48	2.24	1	1
1:A:170:GLN:NE2	1:A:177:LEU:HD22	0.47	2.23	8	2
1:A:142:PRO:C	1:A:144:ILE:H	0.47	2.16	7	17
1:A:157:ASN:HA	1:A:212:ALA:HB1	0.47	1.86	18	1
1:A:122:GLN:HG3	1:A:188:ASN:ND2	0.47	2.25	15	1
1:A:148:VAL:O	1:A:152:VAL:HG23	0.47	2.10	12	4
1:A:201:ARG:HB3	1:A:201:ARG:NH1	0.47	2.25	10	1
1:A:129:PHE:O	1:A:133:LEU:HD12	0.47	2.09	12	1
1:A:145:GLY:HA2	1:A:148:VAL:HG22	0.47	1.87	14	3
1:A:162:ILE:HD12	1:A:185:LEU:HD12	0.47	1.87	11	1
1:A:189:LEU:HB3	1:A:193:GLN:HE21	0.47	1.69	19	1
1:A:129:PHE:HE1	1:A:181:VAL:HG22	0.47	1.69	17	3
1:A:199:CYS:O	1:A:202:LEU:HG	0.47	2.10	14	1
1:A:166:HIS:CE1	1:A:182:ILE:HG12	0.47	2.44	15	1
1:A:194:ARG:HH11	1:A:194:ARG:CG	0.46	2.23	2	1
1:A:194:ARG:HB2	1:A:194:ARG:HH11	0.46	1.70	11	1
1:A:192:LEU:HD23	1:A:192:LEU:O	0.46	2.11	9	1
1:A:122:GLN:NE2	1:A:125:LYS:HD2	0.46	2.26	9	1
1:A:121:ARG:O	1:A:125:LYS:HG3	0.46	2.11	17	1
1:A:181:VAL:O	1:A:184:PHE:HB3	0.45	2.11	20	7
1:A:122:GLN:HE21	1:A:191:LEU:HD13	0.45	1.70	10	1
1:A:161:THR:HB	1:A:164:GLU:HG3	0.45	1.87	14	1
1:A:122:GLN:NE2	1:A:192:LEU:HD12	0.45	2.27	5	2
1:A:166:HIS:HE1	1:A:185:LEU:HD21	0.45	1.70	10	1
1:A:149:ARG:HH11	1:A:149:ARG:CG	0.45	2.24	11	1
1:A:206:ASN:O	1:A:209:GLN:HG2	0.44	2.11	4	1
1:A:149:ARG:O	1:A:153:LEU:HG	0.44	2.12	13	1
1:A:146:GLU:O	1:A:149:ARG:HG3	0.44	2.13	9	1
1:A:121:ARG:O	1:A:125:LYS:HB3	0.44	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:GLN:HA	1:A:125:LYS:HG2	0.43	1.90	9	1
1:A:164:GLU:O	1:A:168:LYS:HG3	0.43	2.12	11	1
1:A:131:THR:O	1:A:135:GLN:HG2	0.43	2.12	18	2
1:A:208:ALA:O	1:A:211:LEU:HG	0.43	2.12	13	1
1:A:186:LYS:O	1:A:190:PRO:HD2	0.43	2.14	7	2
1:A:194:ARG:H	1:A:194:ARG:HD3	0.42	1.74	5	1
1:A:146:GLU:HA	1:A:146:GLU:OE1	0.42	2.14	16	1
1:A:122:GLN:HE21	1:A:191:LEU:HD23	0.42	1.74	2	1
1:A:174:ASN:HD22	1:A:174:ASN:N	0.42	2.12	2	1
1:A:168:LYS:O	1:A:171:GLU:HB3	0.42	2.15	1	1
1:A:140:ILE:O	1:A:141:SER:HB2	0.42	2.15	15	2
1:A:162:ILE:HD12	1:A:185:LEU:CD1	0.42	2.45	19	2
1:A:161:THR:HB	1:A:164:GLU:CD	0.42	2.40	18	1
1:A:135:GLN:O	1:A:139:ASP:HB2	0.42	2.14	17	1
1:A:167:SER:O	1:A:171:GLU:HG3	0.41	2.14	9	1
1:A:146:GLU:OE2	1:A:149:ARG:HD2	0.41	2.15	18	1
1:A:179:PRO:O	1:A:183:PRO:HD2	0.41	2.15	6	1
1:A:147:ARG:O	1:A:150:THR:HB	0.41	2.16	6	1
1:A:130:LEU:HD21	1:A:156:VAL:HG21	0.41	1.92	13	1
1:A:173:THR:C	1:A:175:PHE:H	0.40	2.24	15	1
1:A:142:PRO:HG2	1:A:144:ILE:HB	0.40	1.93	18	1
1:A:177:LEU:HG	1:A:178:ARG:N	0.40	2.31	9	1
1:A:125:LYS:HD2	1:A:184:PHE:CE1	0.40	2.51	6	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	94/107 (88%)	82±1 (87±2%)	9±2 (10±2%)	3±1 (3±1%)	5	39
All	All	1880/2140 (88%)	1644 (87%)	182 (10%)	54 (3%)	5	39

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	141	SER	20
1	A	174	ASN	20
1	A	142	PRO	10
1	A	143	GLU	4

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	85/95 (89%)	78±1 (92±2%)	7±1 (8±2%)	13 60
All	All	1700/1900 (89%)	1562 (92%)	138 (8%)	13 60

All 33 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	186	LYS	20
1	A	185	LEU	19
1	A	192	LEU	17
1	A	160	LEU	9
1	A	174	ASN	7
1	A	121	ARG	6
1	A	206	ASN	5
1	A	133	LEU	4
1	A	188	ASN	4
1	A	141	SER	3
1	A	209	GLN	3
1	A	125	LYS	3
1	A	194	ARG	3
1	A	191	LEU	3
1	A	128	ARG	3
1	A	205	GLN	3
1	A	149	ARG	3
1	A	127	LYS	3
1	A	204	LYS	2
1	A	122	GLN	2
1	A	159	THR	2
1	A	143	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	170	GLN	2
1	A	126	LEU	1
1	A	135	GLN	1
1	A	178	ARG	1
1	A	147	ARG	1
1	A	201	ARG	1
1	A	166	HIS	1
1	A	152	VAL	1
1	A	123	LEU	1
1	A	169	LEU	1
1	A	134	GLN	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