



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:02 AM UTC

PDB ID : 1D1N / pdb_00001d1n
Title : SOLUTION STRUCTURE OF THE FMET-TRNA^{FMET} BINDING DOMAIN OF BECILLUS STEAROTHERMOPHILLUS TRANSLATION INITIATION FACTOR IF2
Authors : Meunier, S.; Spurio, S.; Czisch, M.; Wechselberger, R.; Gueunneugues, M.
Deposited on : 1999-09-20

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

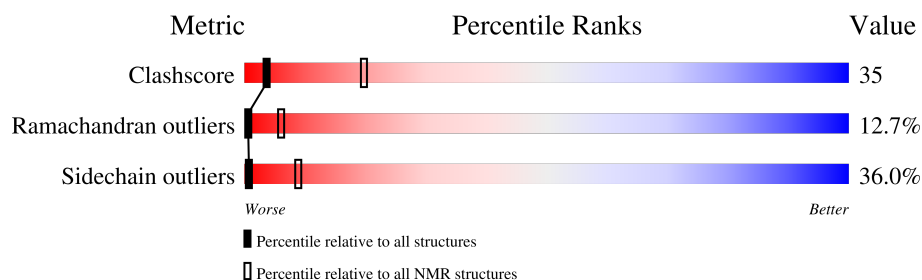
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

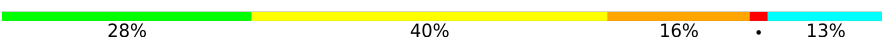
The overall completeness of chemical shifts assignment was not calculated.

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	99	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:146-A:200, A:204-A:234 (86)	0.38	1

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 5 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1581 atoms, of which 797 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INITIATION FACTOR 2.

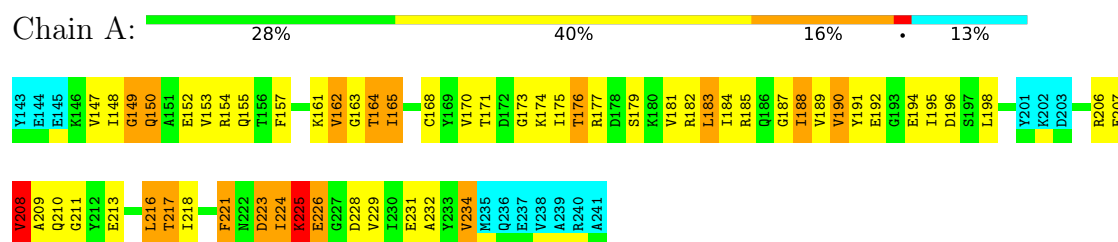
Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1581	492	797	136	153	3	

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: INITIATION FACTOR 2

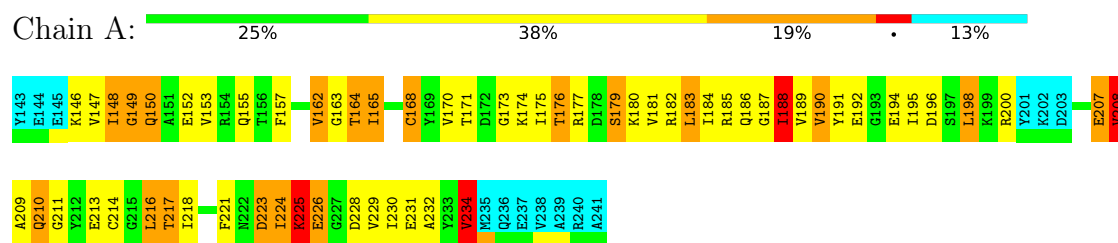


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: INITIATION FACTOR 2



4.2.2 Score per residue for model 2

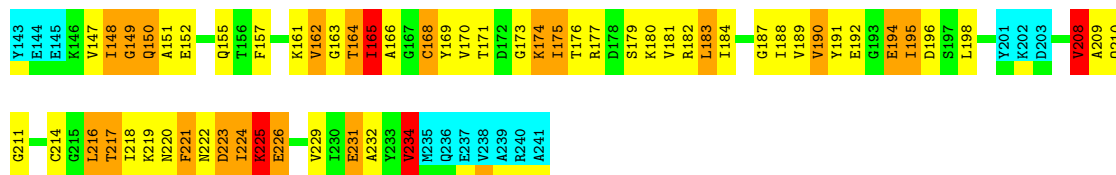
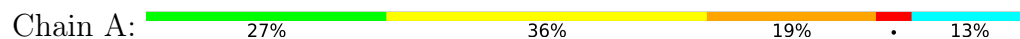
- Molecule 1: INITIATION FACTOR 2





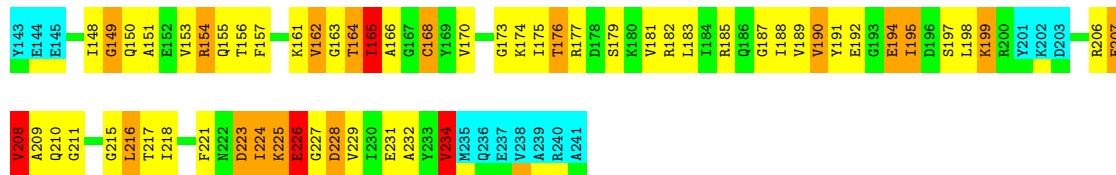
4.2.3 Score per residue for model 3

- Molecule 1: INITIATION FACTOR 2



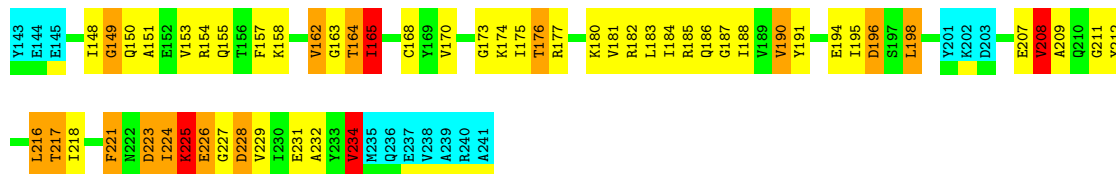
4.2.4 Score per residue for model 4

- Molecule 1: INITIATION FACTOR 2



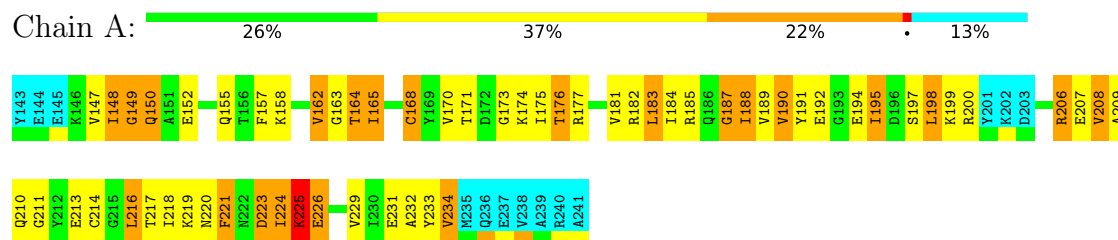
4.2.5 Score per residue for model 5

- Molecule 1: INITIATION FACTOR 2



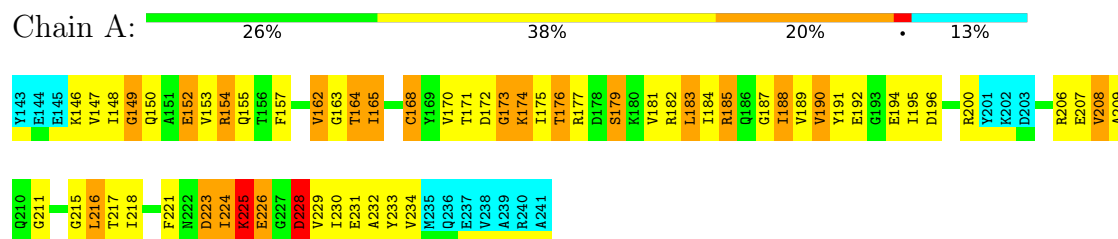
4.2.6 Score per residue for model 6

- Molecule 1: INITIATION FACTOR 2



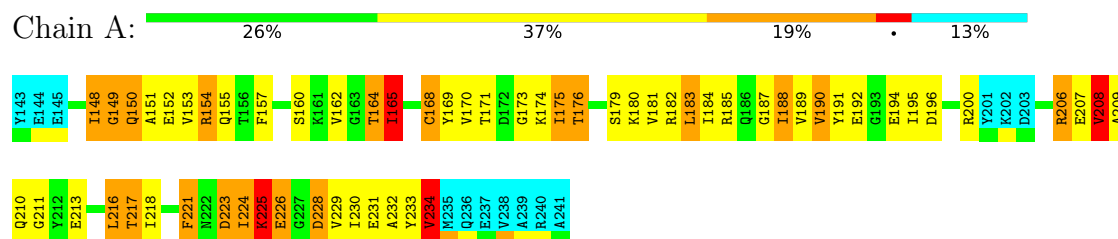
4.2.7 Score per residue for model 7

- Molecule 1: INITIATION FACTOR 2



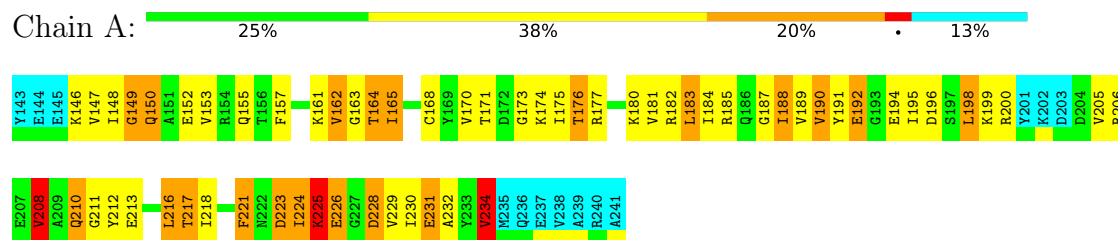
4.2.8 Score per residue for model 8

- Molecule 1: INITIATION FACTOR 2



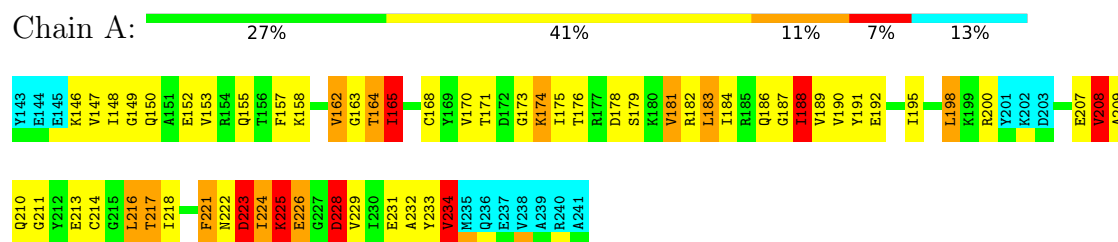
4.2.9 Score per residue for model 9

- Molecule 1: INITIATION FACTOR 2



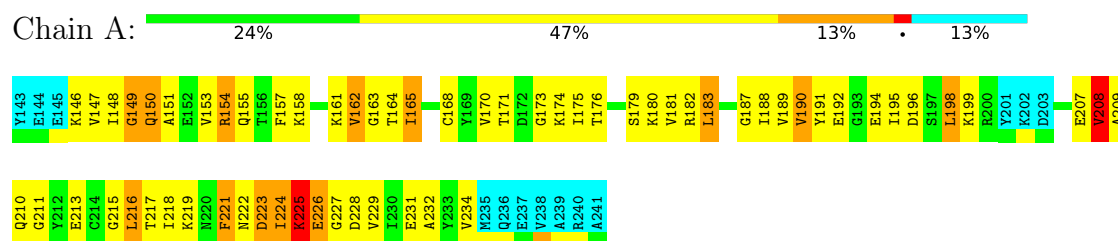
4.2.10 Score per residue for model 10

- Molecule 1: INITIATION FACTOR 2



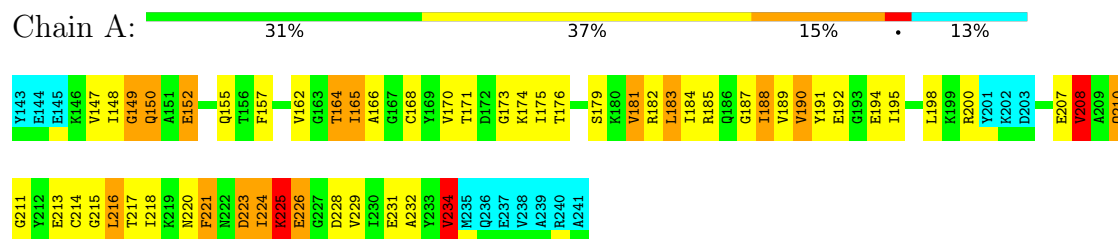
4.2.11 Score per residue for model 11

- Molecule 1: INITIATION FACTOR 2



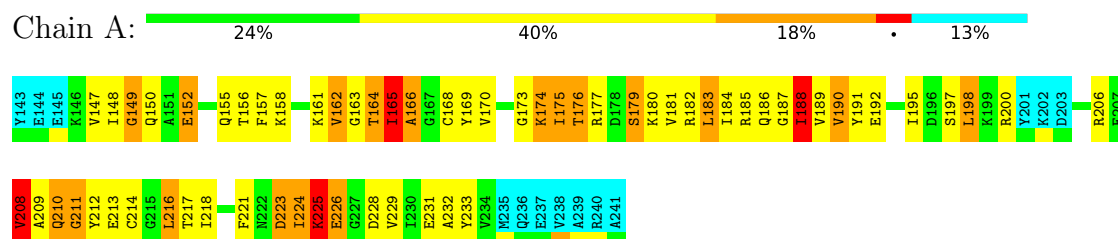
4.2.12 Score per residue for model 12

- Molecule 1: INITIATION FACTOR 2



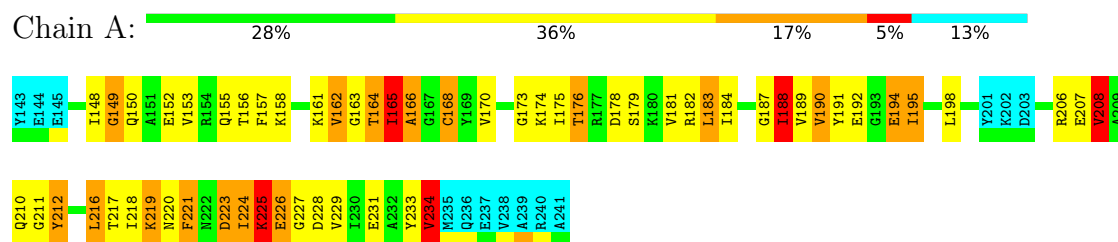
4.2.13 Score per residue for model 13

- Molecule 1: INITIATION FACTOR 2



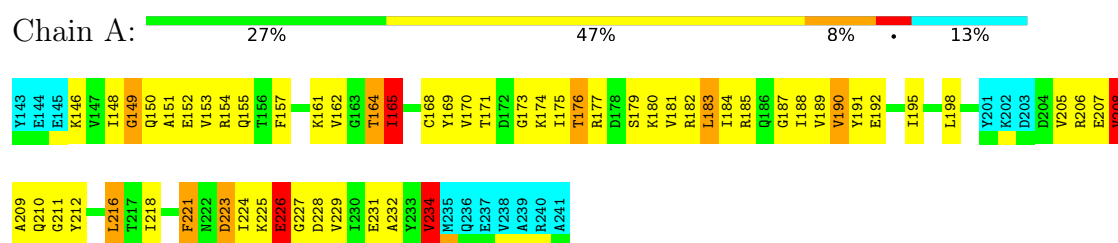
4.2.14 Score per residue for model 14

• Molecule 1: INITIATION FACTOR 2



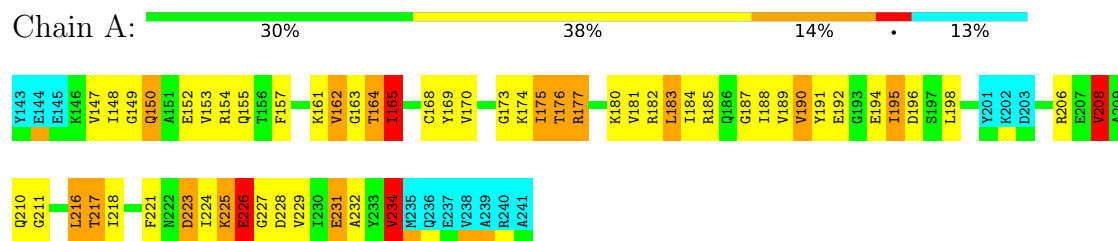
4.2.15 Score per residue for model 15

• Molecule 1: INITIATION FACTOR 2



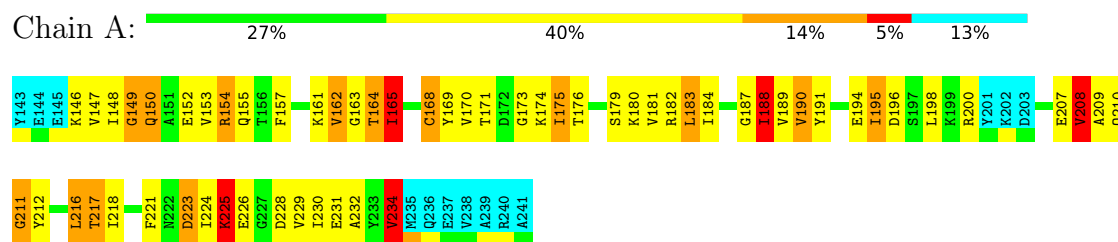
4.2.16 Score per residue for model 16

• Molecule 1: INITIATION FACTOR 2



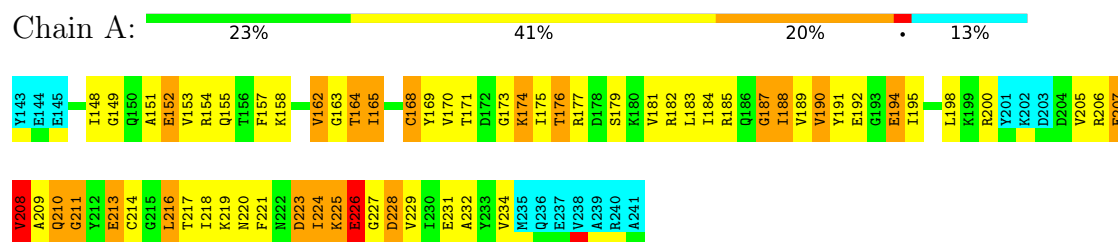
4.2.17 Score per residue for model 17

• Molecule 1: INITIATION FACTOR 2



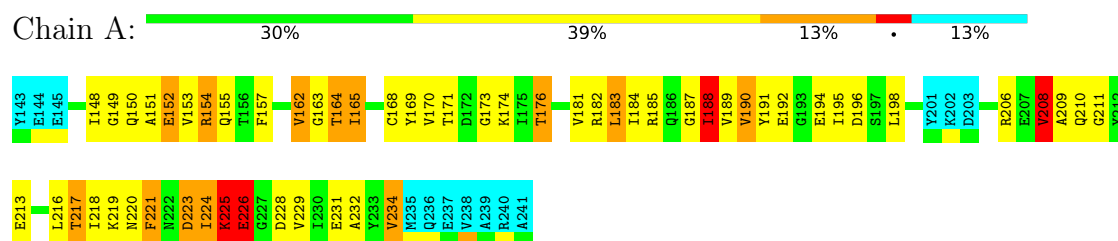
4.2.18 Score per residue for model 18

- Molecule 1: INITIATION FACTOR 2



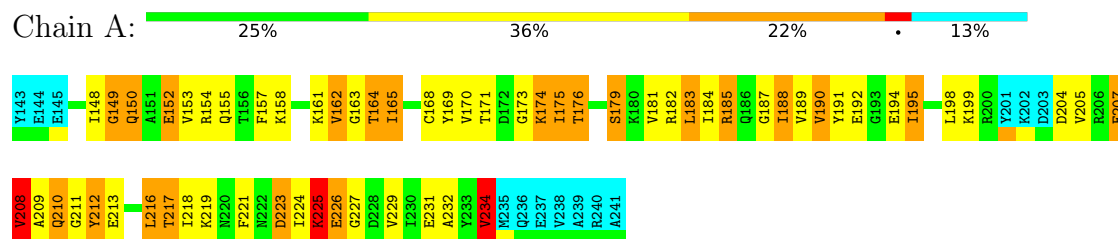
4.2.19 Score per residue for model 19

- Molecule 1: INITIATION FACTOR 2



4.2.20 Score per residue for model 20

- Molecule 1: INITIATION FACTOR 2



5 Refinement protocol and experimental data overview ⓘ

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH ACCEPTABLE COVALENT GEOMETRY, STRUCTURES WITH FAVORABLE NON-BOND ENERGY, STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS, STRUCTURES WITH THE LOWEST ENERGY.*

The authors did not provide any information on software used for structure solution, optimization or refinement.

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	0.54±0.01	0±0/678 (0.0± 0.0%)	0.81±0.02	1±1/911 (0.1± 0.1%)
All	All	0.54	0/13560 (0.0%)	0.81	12/18220 (0.1%)

There are no bond-length outliers.

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	228	ASP	N-CA-C	6.05	115.45	108.49	10	9
1	A	154	ARG	N-CA-C	-5.38	104.38	111.96	5	1
1	A	223	ASP	CA-CB-CG	5.29	117.89	112.60	10	1
1	A	221	PHE	N-CA-C	5.13	117.33	110.35	17	1

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	672	693	693	48±6
All	All	13440	13860	13860	956

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:ILE:HD11	1:A:216:LEU:HD13	1.10	1.10	6	3
1:A:148:ILE:HG21	1:A:234:VAL:HG12	1.01	1.29	6	10
1:A:164:THR:HG21	1:A:224:ILE:HG21	0.92	1.38	4	8
1:A:198:LEU:CD1	1:A:216:LEU:HD23	0.80	2.06	18	1
1:A:190:VAL:HG12	1:A:223:ASP:OD2	0.80	1.76	15	13
1:A:198:LEU:HD13	1:A:216:LEU:HD23	0.79	1.52	17	2
1:A:181:VAL:CG1	1:A:195:ILE:HD12	0.79	2.08	3	1
1:A:198:LEU:CD1	1:A:216:LEU:HD22	0.78	2.08	3	5
1:A:176:THR:O	1:A:195:ILE:HD13	0.77	1.80	8	3
1:A:166:ALA:O	1:A:216:LEU:HD12	0.77	1.80	4	1
1:A:152:GLU:CG	1:A:229:VAL:HG22	0.76	2.10	18	9
1:A:158:LYS:CB	1:A:224:ILE:HD13	0.76	2.11	5	1
1:A:184:ILE:HG23	1:A:188:ILE:O	0.75	1.81	17	12
1:A:195:ILE:HD12	1:A:216:LEU:HD13	0.75	1.57	18	1
1:A:195:ILE:CD1	1:A:216:LEU:HD13	0.74	2.03	6	2
1:A:179:SER:O	1:A:195:ILE:HD12	0.74	1.83	7	7
1:A:175:ILE:CG2	1:A:216:LEU:HD21	0.73	2.12	4	1
1:A:183:LEU:HD13	1:A:191:TYR:HB3	0.73	1.61	4	3
1:A:148:ILE:HD13	1:A:234:VAL:HG12	0.72	1.61	17	1
1:A:170:VAL:HG21	1:A:208:VAL:O	0.72	1.84	16	18
1:A:152:GLU:HG2	1:A:229:VAL:HG22	0.72	1.58	15	14
1:A:198:LEU:HD13	1:A:216:LEU:HD22	0.72	1.62	3	3
1:A:195:ILE:HD13	1:A:217:THR:O	0.71	1.84	16	2
1:A:168:CYS:SG	1:A:216:LEU:HD11	0.70	2.26	18	6
1:A:195:ILE:HG12	1:A:216:LEU:HD13	0.70	1.61	12	2
1:A:195:ILE:HD11	1:A:216:LEU:CD1	0.70	2.16	20	4
1:A:190:VAL:HG21	1:A:228:ASP:CB	0.70	2.17	13	5
1:A:148:ILE:HD13	1:A:234:VAL:CG1	0.70	2.16	17	1
1:A:189:VAL:HG11	1:A:192:GLU:CG	0.70	2.17	16	18
1:A:189:VAL:HG11	1:A:192:GLU:CD	0.70	2.10	12	6
1:A:185:ARG:NH2	1:A:190:VAL:HG13	0.69	2.01	6	1
1:A:198:LEU:HD12	1:A:216:LEU:HD23	0.69	1.62	18	1
1:A:183:LEU:HD22	1:A:221:PHE:CZ	0.69	2.22	5	3
1:A:174:LYS:CG	1:A:209:ALA:HB2	0.69	2.18	18	10
1:A:190:VAL:HG21	1:A:228:ASP:HB2	0.68	1.64	14	2
1:A:184:ILE:N	1:A:190:VAL:HG23	0.68	2.04	13	5
1:A:176:THR:O	1:A:195:ILE:HD12	0.68	1.88	5	1
1:A:164:THR:HG21	1:A:224:ILE:CG2	0.67	2.18	4	9
1:A:147:VAL:O	1:A:148:ILE:HD13	0.67	1.90	16	3
1:A:162:VAL:HG11	1:A:165:ILE:HD12	0.67	1.65	10	4
1:A:183:LEU:HD13	1:A:221:PHE:CZ	0.67	2.25	3	7
1:A:174:LYS:HG3	1:A:209:ALA:HB2	0.67	1.65	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:VAL:HG21	1:A:218:ILE:HD12	0.67	1.65	12	2
1:A:198:LEU:HG	1:A:216:LEU:HD23	0.66	1.68	4	1
1:A:162:VAL:CG1	1:A:165:ILE:HD12	0.65	2.21	5	4
1:A:174:LYS:HG2	1:A:209:ALA:HB2	0.65	1.69	19	11
1:A:233:TYR:O	1:A:234:VAL:HG23	0.64	1.93	8	2
1:A:158:LYS:HB2	1:A:224:ILE:HD13	0.64	1.69	5	1
1:A:195:ILE:CG1	1:A:216:LEU:HD13	0.63	2.22	12	2
1:A:194:GLU:O	1:A:218:ILE:HG23	0.63	1.93	12	3
1:A:190:VAL:HG21	1:A:228:ASP:CG	0.62	2.19	4	3
1:A:181:VAL:HG21	1:A:218:ILE:HG23	0.62	1.71	17	8
1:A:147:VAL:HG11	1:A:150:GLN:HB2	0.62	1.71	3	10
1:A:224:ILE:HD12	1:A:225:LYS:HG2	0.62	1.69	5	2
1:A:152:GLU:HG3	1:A:229:VAL:HG22	0.62	1.69	20	6
1:A:208:VAL:HG12	1:A:212:TYR:HB3	0.61	1.70	15	2
1:A:195:ILE:HD11	1:A:216:LEU:HD12	0.61	1.72	3	3
1:A:176:THR:HG22	1:A:207:GLU:HB3	0.61	1.73	20	7
1:A:183:LEU:C	1:A:184:ILE:HD12	0.60	2.20	1	6
1:A:175:ILE:O	1:A:175:ILE:HG23	0.60	1.96	17	8
1:A:175:ILE:O	1:A:198:LEU:HD11	0.60	1.96	5	1
1:A:188:ILE:HG23	1:A:189:VAL:N	0.60	2.12	13	6
1:A:217:THR:O	1:A:218:ILE:HD13	0.60	1.96	17	1
1:A:198:LEU:HD12	1:A:216:LEU:HD22	0.60	1.72	15	1
1:A:183:LEU:O	1:A:184:ILE:HD13	0.60	1.97	18	3
1:A:176:THR:C	1:A:198:LEU:HD11	0.60	2.22	19	1
1:A:189:VAL:HG11	1:A:192:GLU:HG3	0.59	1.74	6	7
1:A:224:ILE:HD13	1:A:224:ILE:N	0.59	2.13	7	14
1:A:195:ILE:HD11	1:A:216:LEU:HB2	0.59	1.75	16	1
1:A:148:ILE:HD13	1:A:179:SER:OG	0.58	1.98	14	2
1:A:165:ILE:HD12	1:A:215:GLY:O	0.58	1.98	4	3
1:A:153:VAL:HB	1:A:230:ILE:HD11	0.58	1.75	1	3
1:A:189:VAL:HG11	1:A:192:GLU:HG2	0.58	1.74	11	5
1:A:168:CYS:HB3	1:A:230:ILE:HD13	0.58	1.76	8	4
1:A:183:LEU:HD12	1:A:191:TYR:HB3	0.58	1.74	15	6
1:A:191:TYR:CE1	1:A:218:ILE:HG22	0.57	2.34	18	1
1:A:195:ILE:CD1	1:A:216:LEU:HD22	0.57	2.30	4	1
1:A:198:LEU:HD22	1:A:216:LEU:HB3	0.57	1.76	1	2
1:A:148:ILE:HD11	1:A:179:SER:HB3	0.57	1.75	12	5
1:A:148:ILE:HD12	1:A:233:TYR:C	0.56	2.24	2	2
1:A:189:VAL:HG11	1:A:192:GLU:OE2	0.56	1.99	10	1
1:A:149:GLY:HA3	1:A:232:ALA:HB3	0.56	1.77	9	1
1:A:195:ILE:HD11	1:A:216:LEU:HD22	0.56	1.76	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:GLY:C	1:A:188:ILE:HD13	0.56	2.26	6	2
1:A:181:VAL:HG22	1:A:194:GLU:CA	0.56	2.31	5	12
1:A:218:ILE:HG22	1:A:218:ILE:O	0.56	2.01	9	15
1:A:198:LEU:HD11	1:A:206:ARG:C	0.55	2.27	9	1
1:A:198:LEU:HD13	1:A:216:LEU:HB3	0.55	1.78	14	1
1:A:183:LEU:HD21	1:A:221:PHE:CZ	0.55	2.37	10	8
1:A:181:VAL:HG21	1:A:218:ILE:CD1	0.54	2.33	12	1
1:A:184:ILE:CA	1:A:190:VAL:HG23	0.54	2.33	20	9
1:A:200:ARG:NH1	1:A:205:VAL:HG11	0.54	2.17	9	1
1:A:164:THR:CG2	1:A:224:ILE:HG22	0.54	2.33	10	3
1:A:170:VAL:HG22	1:A:175:ILE:CG1	0.53	2.34	11	5
1:A:175:ILE:CG2	1:A:208:VAL:HG23	0.53	2.33	3	2
1:A:148:ILE:HG21	1:A:234:VAL:O	0.52	2.04	5	1
1:A:191:TYR:CB	1:A:221:PHE:CE1	0.52	2.92	10	1
1:A:166:ALA:HB3	1:A:218:ILE:HD13	0.52	1.82	3	1
1:A:216:LEU:HD12	1:A:218:ILE:HD11	0.52	1.80	5	5
1:A:157:PHE:HB2	1:A:165:ILE:HB	0.52	1.82	13	13
1:A:198:LEU:HD22	1:A:206:ARG:C	0.52	2.29	13	1
1:A:183:LEU:O	1:A:189:VAL:HG13	0.52	2.05	2	7
1:A:148:ILE:HD13	1:A:148:ILE:O	0.52	2.05	1	1
1:A:216:LEU:HD12	1:A:218:ILE:CD1	0.51	2.34	15	6
1:A:148:ILE:HG22	1:A:232:ALA:C	0.51	2.31	19	1
1:A:182:ARG:NH1	1:A:184:ILE:HD11	0.51	2.20	2	1
1:A:165:ILE:HG22	1:A:165:ILE:O	0.51	2.06	15	17
1:A:198:LEU:HD22	1:A:216:LEU:CB	0.51	2.35	1	1
1:A:148:ILE:HG13	1:A:234:VAL:HG12	0.51	1.81	2	1
1:A:175:ILE:O	1:A:198:LEU:HD21	0.51	2.06	11	1
1:A:175:ILE:HG22	1:A:175:ILE:O	0.51	2.06	7	4
1:A:170:VAL:HG22	1:A:175:ILE:HG13	0.51	1.83	1	5
1:A:157:PHE:CD1	1:A:165:ILE:HG22	0.51	2.41	13	1
1:A:198:LEU:HD21	1:A:205:VAL:O	0.51	2.06	20	2
1:A:157:PHE:CE2	1:A:165:ILE:HG21	0.51	2.41	14	1
1:A:198:LEU:CD2	1:A:205:VAL:HG23	0.51	2.35	15	1
1:A:225:LYS:O	1:A:227:GLY:N	0.50	2.45	20	8
1:A:181:VAL:HG13	1:A:195:ILE:HD12	0.50	1.79	3	1
1:A:198:LEU:HD11	1:A:205:VAL:O	0.50	2.07	20	1
1:A:181:VAL:HG11	1:A:195:ILE:HD12	0.50	1.82	3	1
1:A:198:LEU:HD11	1:A:216:LEU:HD22	0.50	1.83	10	2
1:A:195:ILE:HG23	1:A:216:LEU:HB2	0.50	1.84	12	1
1:A:217:THR:C	1:A:218:ILE:HD12	0.49	2.32	10	4
1:A:224:ILE:HD13	1:A:224:ILE:H	0.49	1.67	8	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:223:ASP:OD1	1:A:223:ASP:N	0.49	2.43	5	6
1:A:221:PHE:CZ	1:A:223:ASP:CG	0.49	2.90	10	1
1:A:175:ILE:HB	1:A:208:VAL:HG23	0.49	1.84	7	1
1:A:149:GLY:O	1:A:175:ILE:HD11	0.49	2.06	14	2
1:A:149:GLY:CA	1:A:232:ALA:HB3	0.49	2.38	9	8
1:A:185:ARG:N	1:A:190:VAL:HG22	0.49	2.23	2	10
1:A:152:GLU:CD	1:A:229:VAL:HG22	0.49	2.33	2	3
1:A:148:ILE:HG22	1:A:232:ALA:O	0.49	2.08	19	1
1:A:165:ILE:HG23	1:A:215:GLY:C	0.48	2.33	7	1
1:A:175:ILE:HG21	1:A:216:LEU:HD11	0.48	1.83	9	1
1:A:183:LEU:CD2	1:A:221:PHE:CZ	0.48	2.96	10	11
1:A:196:ASP:HB3	1:A:217:THR:HG23	0.48	1.85	5	3
1:A:164:THR:CG2	1:A:224:ILE:HG21	0.48	2.37	14	9
1:A:183:LEU:CD1	1:A:221:PHE:CZ	0.48	2.96	3	6
1:A:175:ILE:HG22	1:A:198:LEU:HD11	0.48	1.85	14	1
1:A:175:ILE:HD12	1:A:232:ALA:HB2	0.48	1.84	10	3
1:A:181:VAL:HG11	1:A:218:ILE:HG13	0.48	1.84	20	2
1:A:148:ILE:HD13	1:A:232:ALA:C	0.48	2.34	2	2
1:A:223:ASP:OD1	1:A:223:ASP:C	0.48	2.56	10	1
1:A:175:ILE:O	1:A:175:ILE:HG22	0.48	2.07	5	1
1:A:191:TYR:CZ	1:A:218:ILE:CG2	0.48	2.96	15	1
1:A:183:LEU:HA	1:A:229:VAL:O	0.48	2.09	6	10
1:A:191:TYR:CD2	1:A:218:ILE:CG2	0.47	2.97	2	6
1:A:148:ILE:O	1:A:148:ILE:HG22	0.47	2.08	11	4
1:A:194:GLU:CG	1:A:195:ILE:N	0.47	2.78	14	4
1:A:198:LEU:HD23	1:A:205:VAL:O	0.47	2.09	18	1
1:A:181:VAL:HG22	1:A:194:GLU:C	0.47	2.33	17	6
1:A:148:ILE:HG12	1:A:234:VAL:HG12	0.47	1.86	4	4
1:A:225:LYS:O	1:A:226:GLU:C	0.47	2.58	5	14
1:A:154:ARG:O	1:A:226:GLU:HB3	0.47	2.10	20	7
1:A:148:ILE:CD1	1:A:234:VAL:HG12	0.47	2.38	17	1
1:A:191:TYR:CD1	1:A:192:GLU:N	0.47	2.82	18	1
1:A:184:ILE:HA	1:A:190:VAL:HG23	0.47	1.86	17	7
1:A:224:ILE:HD12	1:A:225:LYS:CG	0.47	2.39	20	1
1:A:221:PHE:CE1	1:A:223:ASP:HB3	0.47	2.45	10	1
1:A:182:ARG:N	1:A:231:GLU:O	0.47	2.48	20	20
1:A:176:THR:HG22	1:A:207:GLU:CB	0.47	2.40	18	1
1:A:175:ILE:HG23	1:A:208:VAL:HG23	0.46	1.87	20	2
1:A:221:PHE:CZ	1:A:223:ASP:OD1	0.46	2.68	10	1
1:A:181:VAL:HG13	1:A:195:ILE:CD1	0.46	2.40	11	1
1:A:149:GLY:O	1:A:232:ALA:HB3	0.46	2.10	3	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:ARG:HB2	1:A:198:LEU:HD22	0.46	1.88	9	1
1:A:162:VAL:HG12	1:A:163:GLY:N	0.46	2.26	16	17
1:A:221:PHE:CD1	1:A:223:ASP:O	0.46	2.68	19	16
1:A:148:ILE:O	1:A:174:LYS:O	0.46	2.33	18	7
1:A:191:TYR:CD2	1:A:192:GLU:N	0.46	2.84	15	1
1:A:148:ILE:HG21	1:A:234:VAL:CG1	0.46	2.41	18	1
1:A:198:LEU:HD22	1:A:206:ARG:O	0.46	2.10	13	1
1:A:162:VAL:HG12	1:A:165:ILE:HD13	0.46	1.87	2	2
1:A:198:LEU:HD23	1:A:199:LYS:N	0.46	2.25	4	1
1:A:165:ILE:HD13	1:A:217:THR:OG1	0.46	2.11	6	1
1:A:223:ASP:OD1	1:A:224:ILE:N	0.45	2.49	17	1
1:A:191:TYR:CE2	1:A:220:ASN:O	0.45	2.70	6	3
1:A:208:VAL:HG21	1:A:214:CYS:HB3	0.45	1.87	12	2
1:A:148:ILE:HD13	1:A:179:SER:HB3	0.45	1.89	20	1
1:A:156:THR:HA	1:A:166:ALA:HA	0.45	1.89	14	2
1:A:157:PHE:CD1	1:A:165:ILE:CG2	0.45	3.00	13	1
1:A:170:VAL:HG12	1:A:212:TYR:N	0.45	2.27	14	3
1:A:148:ILE:HD13	1:A:148:ILE:C	0.45	2.37	8	1
1:A:148:ILE:C	1:A:148:ILE:HD12	0.45	2.37	20	2
1:A:147:VAL:HG11	1:A:150:GLN:HG3	0.45	1.88	7	1
1:A:224:ILE:C	1:A:224:ILE:HD12	0.45	2.37	15	1
1:A:153:VAL:HB	1:A:228:ASP:O	0.44	2.13	14	3
1:A:175:ILE:HD11	1:A:181:VAL:CG1	0.44	2.43	10	1
1:A:164:THR:HG22	1:A:224:ILE:CG2	0.44	2.42	8	4
1:A:177:ARG:CB	1:A:198:LEU:HD22	0.44	2.42	9	1
1:A:165:ILE:O	1:A:216:LEU:C	0.44	2.60	13	1
1:A:208:VAL:HG12	1:A:212:TYR:O	0.44	2.12	14	1
1:A:195:ILE:HG22	1:A:196:ASP:N	0.44	2.27	19	1
1:A:230:ILE:N	1:A:230:ILE:HD12	0.44	2.28	1	2
1:A:218:ILE:O	1:A:220:ASN:N	0.44	2.51	14	3
1:A:218:ILE:HD12	1:A:218:ILE:N	0.44	2.28	3	2
1:A:148:ILE:CG2	1:A:234:VAL:HG12	0.44	2.42	18	2
1:A:164:THR:CG2	1:A:224:ILE:CG2	0.44	2.96	1	13
1:A:176:THR:HB	1:A:206:ARG:O	0.44	2.13	13	5
1:A:191:TYR:HB2	1:A:221:PHE:CE1	0.44	2.48	4	10
1:A:151:ALA:O	1:A:229:VAL:HG13	0.44	2.12	15	6
1:A:188:ILE:CG2	1:A:189:VAL:N	0.43	2.81	10	2
1:A:147:VAL:HG22	1:A:231:GLU:OE2	0.43	2.12	11	1
1:A:181:VAL:HG13	1:A:195:ILE:HD11	0.43	1.90	12	1
1:A:177:ARG:O	1:A:195:ILE:HG22	0.43	2.13	16	1
1:A:200:ARG:NH1	1:A:212:TYR:CD1	0.43	2.87	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LEU:N	1:A:183:LEU:HD12	0.43	2.28	18	1
1:A:148:ILE:HD12	1:A:149:GLY:N	0.43	2.29	20	1
1:A:158:LYS:HG3	1:A:224:ILE:HD13	0.43	1.89	20	1
1:A:152:GLU:HG3	1:A:229:VAL:HG13	0.43	1.89	13	1
1:A:172:ASP:O	1:A:173:GLY:O	0.43	2.37	7	1
1:A:208:VAL:HG12	1:A:212:TYR:CB	0.43	2.43	15	1
1:A:191:TYR:CE2	1:A:218:ILE:CG2	0.43	3.01	14	2
1:A:152:GLU:N	1:A:169:TYR:O	0.43	2.52	15	5
1:A:153:VAL:HG12	1:A:228:ASP:O	0.42	2.13	11	11
1:A:208:VAL:HG21	1:A:214:CYS:CB	0.42	2.44	18	3
1:A:169:TYR:CD2	1:A:213:GLU:CG	0.42	3.02	18	1
1:A:184:ILE:HD12	1:A:184:ILE:N	0.42	2.28	15	1
1:A:233:TYR:CD1	1:A:233:TYR:O	0.42	2.72	13	2
1:A:156:THR:OG1	1:A:225:LYS:N	0.42	2.50	4	1
1:A:195:ILE:HD12	1:A:216:LEU:CD1	0.42	2.45	9	1
1:A:183:LEU:CD1	1:A:191:TYR:HB3	0.42	2.44	15	4
1:A:154:ARG:NE	1:A:154:ARG:CA	0.42	2.83	4	5
1:A:226:GLU:O	1:A:226:GLU:CG	0.42	2.68	18	4
1:A:218:ILE:O	1:A:218:ILE:CG2	0.42	2.67	9	7
1:A:165:ILE:HD12	1:A:217:THR:HG23	0.42	1.90	9	1
1:A:227:GLY:O	1:A:228:ASP:CG	0.42	2.62	14	1
1:A:181:VAL:HG21	1:A:218:ILE:HG13	0.42	1.91	7	1
1:A:183:LEU:HB2	1:A:229:VAL:O	0.42	2.13	10	1
1:A:175:ILE:HG21	1:A:216:LEU:HD21	0.42	1.92	12	1
1:A:181:VAL:HG11	1:A:195:ILE:CD1	0.42	2.45	18	1
1:A:191:TYR:CE2	1:A:218:ILE:HG22	0.42	2.50	13	3
1:A:218:ILE:N	1:A:218:ILE:CD1	0.42	2.83	3	2
1:A:183:LEU:CB	1:A:230:ILE:HA	0.42	2.45	8	2
1:A:157:PHE:CG	1:A:165:ILE:HB	0.42	2.50	15	2
1:A:165:ILE:O	1:A:166:ALA:C	0.42	2.63	14	1
1:A:150:GLN:CG	1:A:231:GLU:CG	0.41	2.99	20	3
1:A:185:ARG:N	1:A:190:VAL:CG2	0.41	2.84	5	3
1:A:198:LEU:HD13	1:A:216:LEU:CD2	0.41	2.34	17	1
1:A:151:ALA:HB1	1:A:169:TYR:O	0.41	2.16	19	3
1:A:224:ILE:N	1:A:224:ILE:CD1	0.41	2.83	13	4
1:A:181:VAL:CG1	1:A:195:ILE:CD1	0.41	2.99	19	1
1:A:183:LEU:HD21	1:A:191:TYR:CB	0.41	2.45	17	1
1:A:175:ILE:HG22	1:A:216:LEU:HD21	0.41	1.90	4	1
1:A:195:ILE:HD13	1:A:216:LEU:HD13	0.41	1.93	5	1
1:A:191:TYR:CD1	1:A:223:ASP:OD1	0.41	2.74	12	2
1:A:183:LEU:HB3	1:A:190:VAL:HG23	0.41	1.93	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:ILE:O	1:A:225:LYS:O	0.41	2.39	11	1
1:A:157:PHE:CD2	1:A:165:ILE:CG2	0.41	3.03	15	1
1:A:191:TYR:CE2	1:A:192:GLU:O	0.41	2.74	15	1
1:A:153:VAL:CG1	1:A:226:GLU:HA	0.41	2.46	4	2
1:A:233:TYR:O	1:A:234:VAL:CG2	0.41	2.69	7	1
1:A:157:PHE:CD2	1:A:165:ILE:HB	0.41	2.51	8	2
1:A:195:ILE:HD12	1:A:195:ILE:N	0.41	2.31	10	1
1:A:166:ALA:N	1:A:216:LEU:O	0.41	2.54	12	1
1:A:169:TYR:CE1	1:A:211:GLY:O	0.41	2.74	18	2
1:A:176:THR:HA	1:A:206:ARG:O	0.41	2.16	14	1
1:A:195:ILE:HD11	1:A:216:LEU:CD2	0.41	2.46	17	1
1:A:154:ARG:CA	1:A:154:ARG:NE	0.40	2.84	8	1
1:A:198:LEU:CD1	1:A:216:LEU:CD2	0.40	2.99	12	1
1:A:165:ILE:O	1:A:216:LEU:O	0.40	2.39	14	1
1:A:169:TYR:CE1	1:A:170:VAL:O	0.40	2.74	15	2
1:A:191:TYR:CE1	1:A:221:PHE:HA	0.40	2.52	3	1
1:A:164:THR:HG22	1:A:224:ILE:HG22	0.40	1.93	10	1
1:A:169:TYR:CE2	1:A:211:GLY:O	0.40	2.75	17	1
1:A:175:ILE:O	1:A:175:ILE:CG2	0.40	2.68	17	1
1:A:148:ILE:HD13	1:A:232:ALA:O	0.40	2.17	6	1
1:A:157:PHE:O	1:A:163:GLY:O	0.40	2.39	13	1
1:A:221:PHE:CG	1:A:223:ASP:O	0.40	2.74	14	1
1:A:169:TYR:CD2	1:A:213:GLU:HG2	0.40	2.51	18	1
1:A:153:VAL:O	1:A:153:VAL:CG1	0.40	2.70	11	2
1:A:146:LYS:HG3	1:A:147:VAL:HG23	0.40	1.92	10	1
1:A:181:VAL:HG22	1:A:194:GLU:HA	0.40	1.93	12	1
1:A:216:LEU:CD1	1:A:218:ILE:HD11	0.40	2.47	8	1
1:A:183:LEU:HD11	1:A:190:VAL:HB	0.40	1.92	9	1
1:A:195:ILE:CD1	1:A:218:ILE:CD1	0.40	3.00	18	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	86/99 (87%)	58±3 (67±3%)	17±2 (20±3%)	11±1 (13±2%)	0 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1720/1980 (87%)	1157 (67%)	344 (20%)	219 (13%)	0 6

All 15 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	162	VAL	20
1	A	165	ILE	20
1	A	173	GLY	20
1	A	187	GLY	20
1	A	211	GLY	20
1	A	225	LYS	19
1	A	226	GLU	19
1	A	149	GLY	18
1	A	208	VAL	18
1	A	210	GLN	16
1	A	234	VAL	16
1	A	188	ILE	6
1	A	219	LYS	3
1	A	146	LYS	2
1	A	166	ALA	2

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	73/84 (87%)	47±3 (64±4%)	26±3 (36±4%)	1 9
All	All	1460/1680 (87%)	934 (64%)	526 (36%)	1 9

All 57 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	155	GLN	20
1	A	164	THR	20
1	A	168	CYS	20
1	A	176	THR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	188	ILE	20
1	A	190	VAL	20
1	A	208	VAL	20
1	A	216	LEU	20
1	A	223	ASP	20
1	A	217	THR	18
1	A	150	GLN	17
1	A	183	LEU	17
1	A	224	ILE	16
1	A	171	THR	15
1	A	225	LYS	15
1	A	234	VAL	15
1	A	213	GLU	11
1	A	161	LYS	11
1	A	221	PHE	11
1	A	177	ARG	10
1	A	180	LYS	10
1	A	196	ASP	10
1	A	207	GLU	10
1	A	165	ILE	10
1	A	174	LYS	10
1	A	200	ARG	8
1	A	210	GLN	8
1	A	206	ARG	8
1	A	198	LEU	7
1	A	157	PHE	7
1	A	175	ILE	7
1	A	195	ILE	7
1	A	179	SER	6
1	A	154	ARG	6
1	A	158	LYS	6
1	A	152	GLU	6
1	A	148	ILE	5
1	A	186	GLN	5
1	A	199	LYS	5
1	A	226	GLU	5
1	A	219	LYS	5
1	A	197	SER	4
1	A	194	GLU	4
1	A	146	LYS	4
1	A	185	ARG	4
1	A	212	TYR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	222	ASN	3
1	A	231	GLU	3
1	A	181	VAL	3
1	A	214	CYS	2
1	A	228	ASP	2
1	A	178	ASP	1
1	A	220	ASN	1
1	A	160	SER	1
1	A	192	GLU	1
1	A	153	VAL	1
1	A	204	ASP	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