



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 07:24 PM UTC

PDB ID : 7Y8Q / pdb_00007y8q
BMRB ID : 36495
Title : Amyloid-beta assemblage on GM1-containing membranes
Authors : Yagi-Utsumi, M.; Itoh, S.G.; Okumura, H.; Yanagisawa, K.; Kato, K.;
Nishimura, K.
Deposited on : 2022-06-24

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

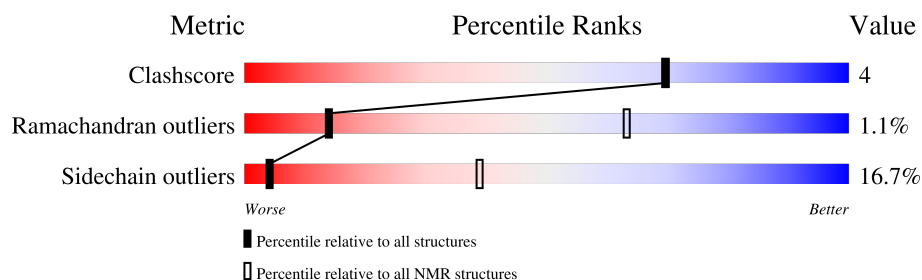
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 4%.

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	40	18% 42% 8% 5% 28%
1	B	40	22% 40% 10% 28%
1	C	40	32% 28% 12% 28%
1	D	40	25% 38% 10% 28%
1	E	40	30% 20% 12% • 8% 28%
1	F	40	28% 32% 12% 28%
1	G	40	30% 38% 5% 28%
1	H	40	20% 20% 10% • 20% 28%

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 6 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:14-A:40, B:12-B:40, C:12-C:40, D:12-D:40, E:15-E:40, F:12-F:40, G:12-G:40, H:18-H:38 (219)	1.00	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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 8, 9
2	2, 3, 4
3	1, 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3456 atoms, of which 1752 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Amyloid-beta protein 40.

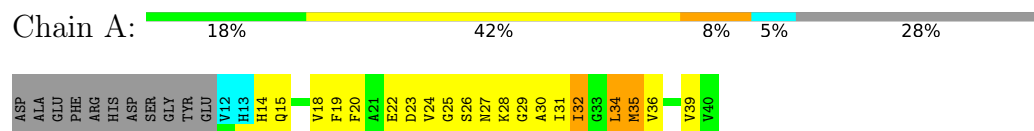
Mol	Chain	Residues	Atoms						Trace
1	A	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	B	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	C	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	D	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	E	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	F	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	G	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	
1	H	29	Total	C	H	N	O	S	0
			432	138	219	37	37	1	

4 Residue-property plots [i](#)

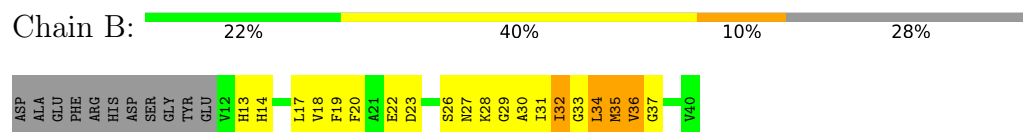
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

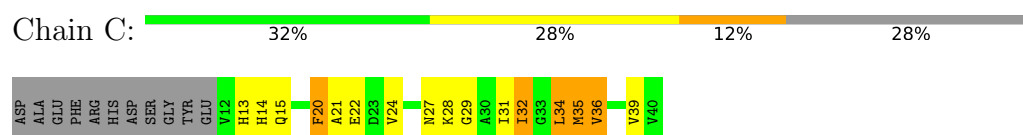
- Molecule 1: Amyloid-beta protein 40



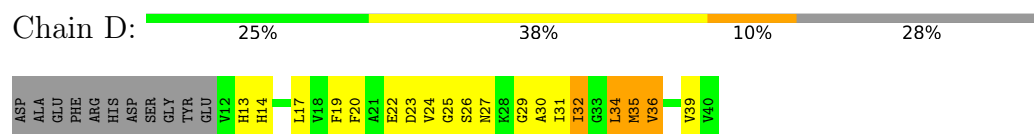
- Molecule 1: Amyloid-beta protein 40



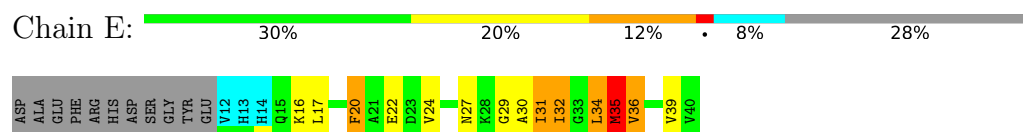
- Molecule 1: Amyloid-beta protein 40



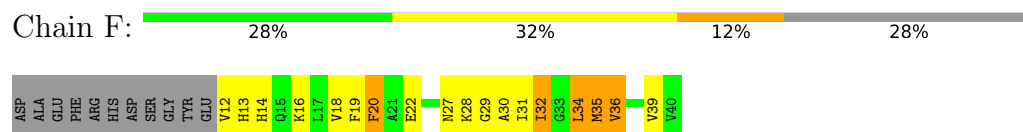
- Molecule 1: Amyloid-beta protein 40



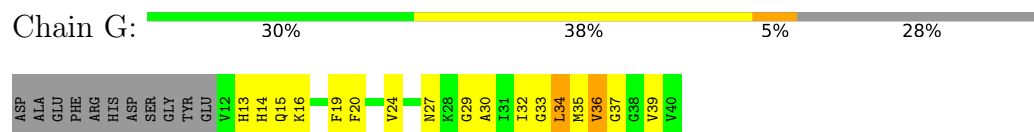
- Molecule 1: Amyloid-beta protein 40



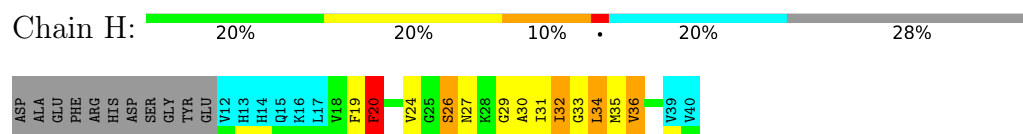
- Molecule 1: Amyloid-beta protein 40



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- Molecule 1: Amyloid-beta protein 40

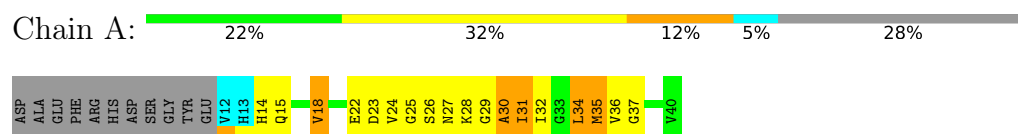


4.2 Scores per residue for each member of the ensemble

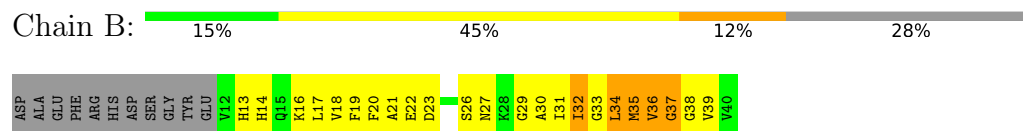
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

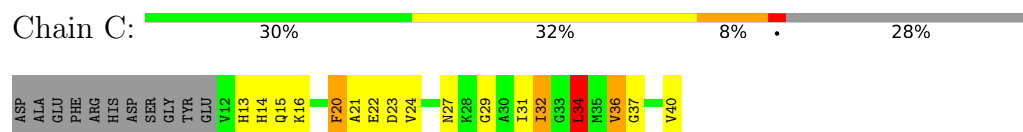
- Molecule 1: Amyloid-beta protein 40



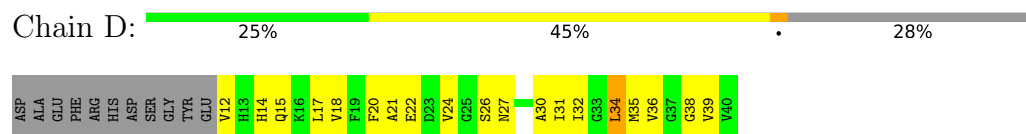
- Molecule 1: Amyloid-beta protein 40



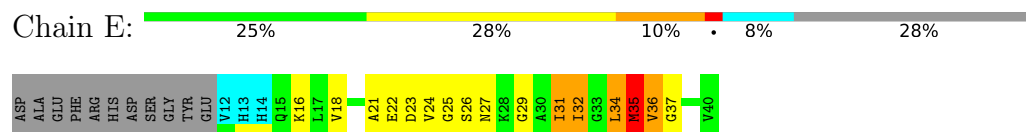
- Molecule 1: Amyloid-beta protein 40



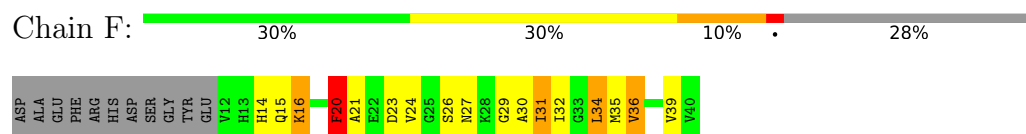
- Molecule 1: Amyloid-beta protein 40



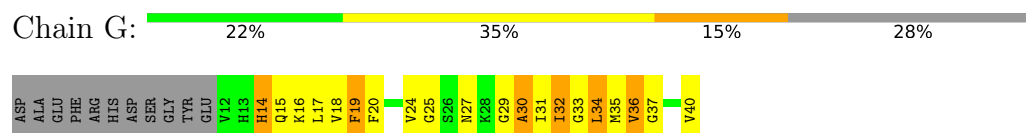
- Molecule 1: Amyloid-beta protein 40



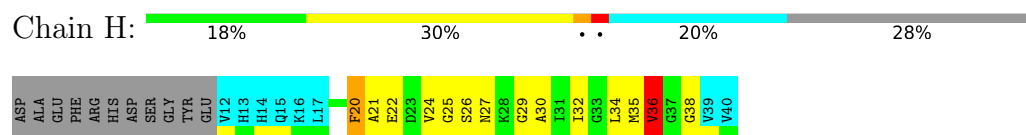
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

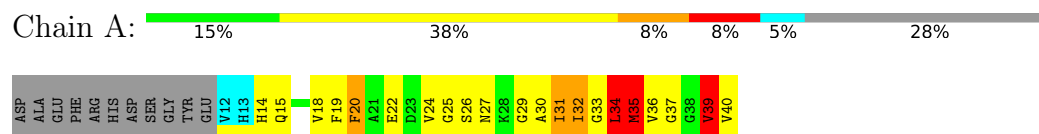


- Molecule 1: Amyloid-beta protein 40

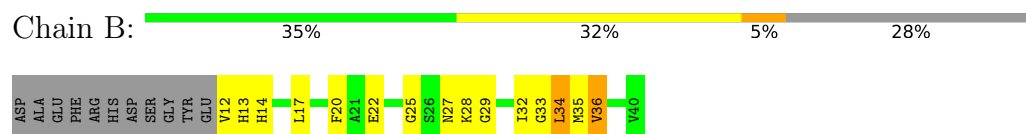


4.2.2 Score per residue for model 2

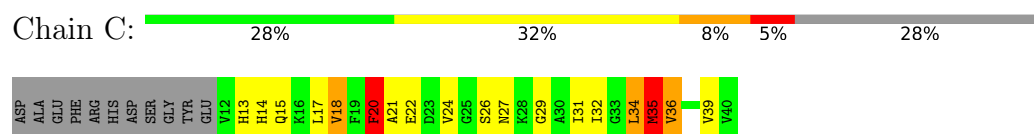
- Molecule 1: Amyloid-beta protein 40



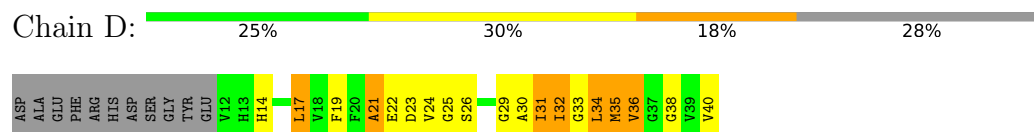
- Molecule 1: Amyloid-beta protein 40



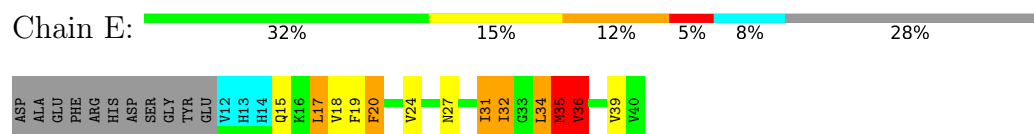
- Molecule 1: Amyloid-beta protein 40



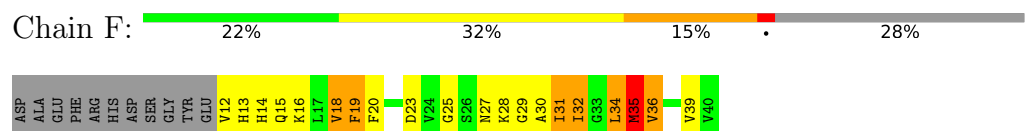
- Molecule 1: Amyloid-beta protein 40



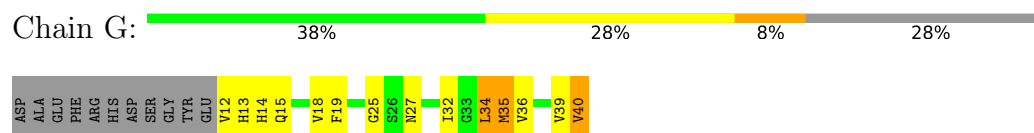
- Molecule 1: Amyloid-beta protein 40



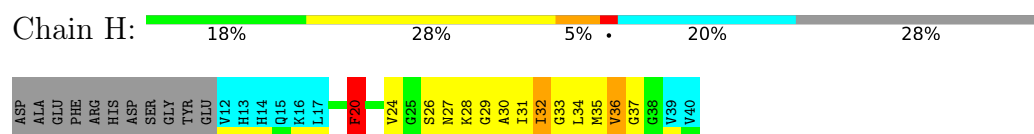
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

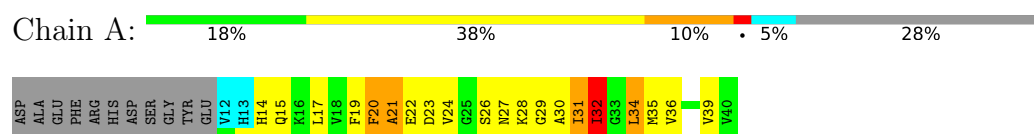


- Molecule 1: Amyloid-beta protein 40



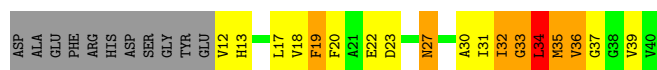
4.2.3 Score per residue for model 3

- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

Chain B: 

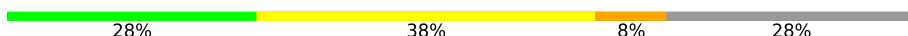


- Molecule 1: Amyloid-beta protein 40

Chain C: 



- Molecule 1: Amyloid-beta protein 40

Chain D: 



- Molecule 1: Amyloid-beta protein 40

Chain E: 



- Molecule 1: Amyloid-beta protein 40

Chain F: 

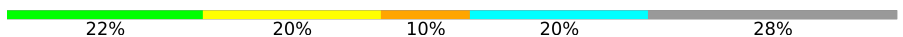


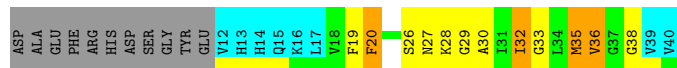
- Molecule 1: Amyloid-beta protein 40

Chain G: 



- Molecule 1: Amyloid-beta protein 40

Chain H: 



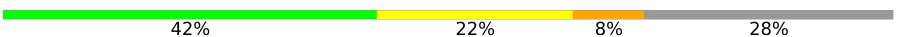
4.2.4 Score per residue for model 4

- Molecule 1: Amyloid-beta protein 40

Chain A: 

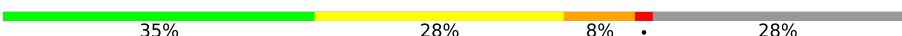


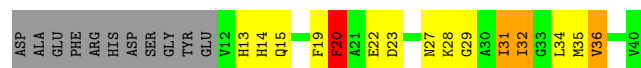
- Molecule 1: Amyloid-beta protein 40

Chain B: 



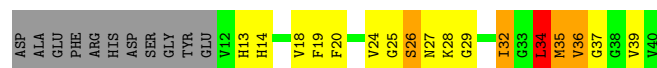
- Molecule 1: Amyloid-beta protein 40

Chain C: 



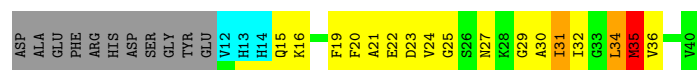
- Molecule 1: Amyloid-beta protein 40

Chain D: 



- Molecule 1: Amyloid-beta protein 40

Chain E: 

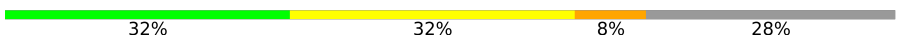


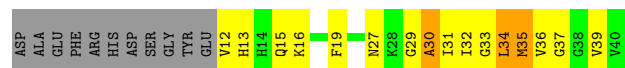
- Molecule 1: Amyloid-beta protein 40

Chain F: 

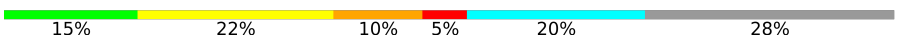


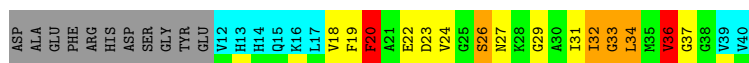
- Molecule 1: Amyloid-beta protein 40

Chain G: 



- Molecule 1: Amyloid-beta protein 40

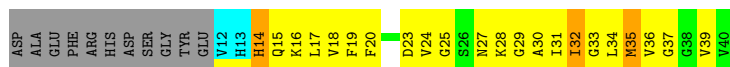
Chain H: 



4.2.5 Score per residue for model 5

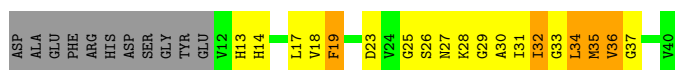
- Molecule 1: Amyloid-beta protein 40

Chain A: 12% 48% 8% 5% 28%



- Molecule 1: Amyloid-beta protein 40

Chain B: 25% 35% 12% 28%



- Molecule 1: Amyloid-beta protein 40

Chain C: 25% 35% 10% 28%



- Molecule 1: Amyloid-beta protein 40

Chain D: 32% 30% 10% 28%



- Molecule 1: Amyloid-beta protein 40

Chain E: 30% 22% 10% 8% 28%



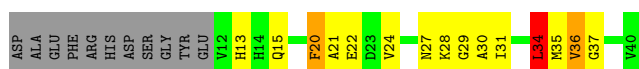
- Molecule 1: Amyloid-beta protein 40

Chain F: 25% 35% 12% 28%



- Molecule 1: Amyloid-beta protein 40

Chain G: 35% 30% 5% 28%

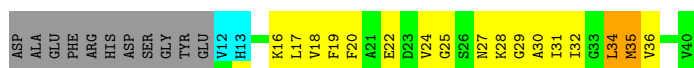
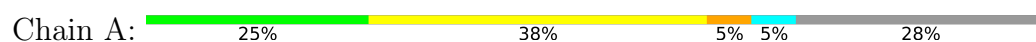


- Molecule 1: Amyloid-beta protein 40

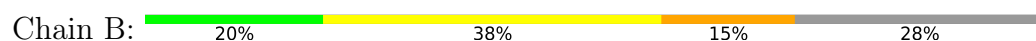


4.2.6 Score per residue for model 6 (medoid)

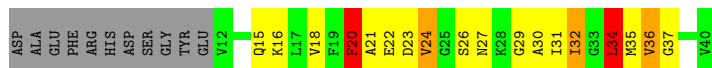
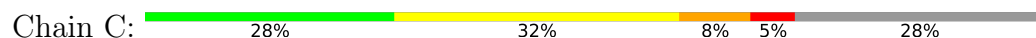
- Molecule 1: Amyloid-beta protein 40



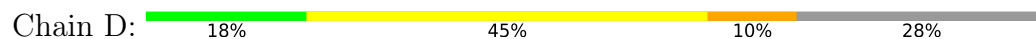
- Molecule 1: Amyloid-beta protein 40



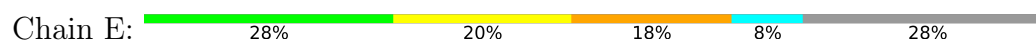
- Molecule 1: Amyloid-beta protein 40



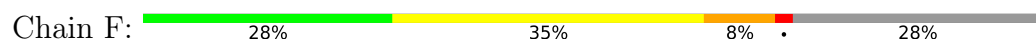
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

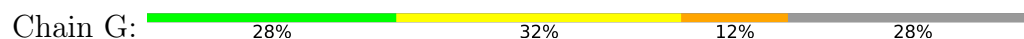


- Molecule 1: Amyloid-beta protein 40





- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

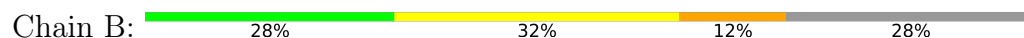


4.2.7 Score per residue for model 7

- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40



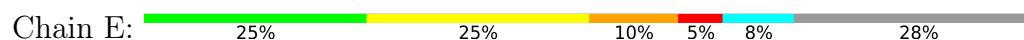
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

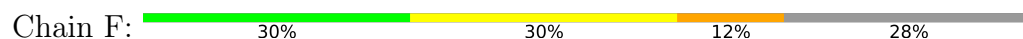


- Molecule 1: Amyloid-beta protein 40





- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

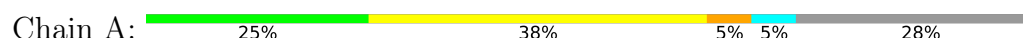


- Molecule 1: Amyloid-beta protein 40

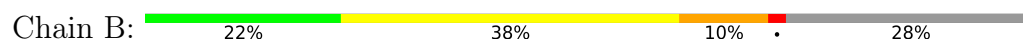


4.2.8 Score per residue for model 8

- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

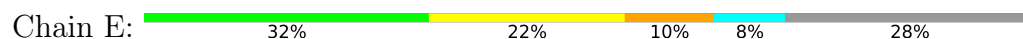


- Molecule 1: Amyloid-beta protein 40

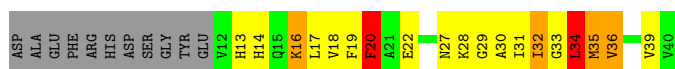
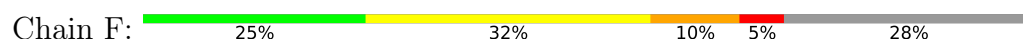




- Molecule 1: Amyloid-beta protein 40



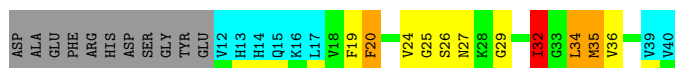
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

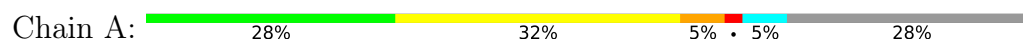


- Molecule 1: Amyloid-beta protein 40

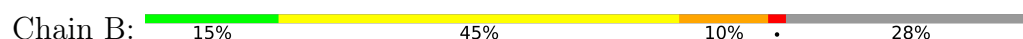


4.2.9 Score per residue for model 9

- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

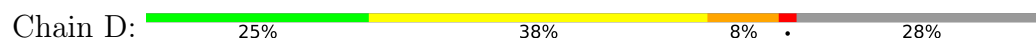


- Molecule 1: Amyloid-beta protein 40

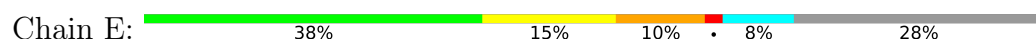




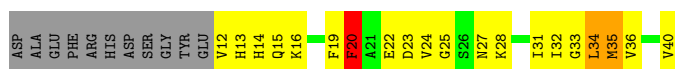
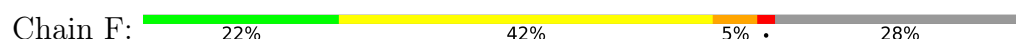
- Molecule 1: Amyloid-beta protein 40



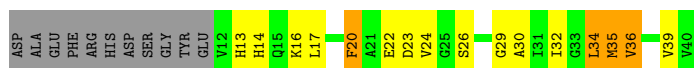
- Molecule 1: Amyloid-beta protein 40



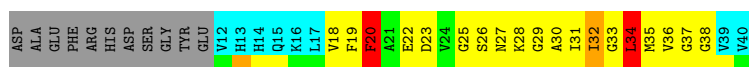
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

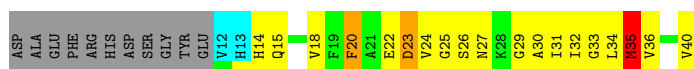
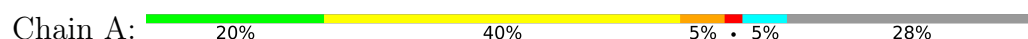


- Molecule 1: Amyloid-beta protein 40

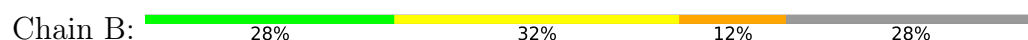


4.2.10 Score per residue for model 10

- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40

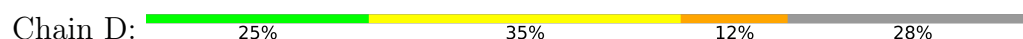




- Molecule 1: Amyloid-beta protein 40



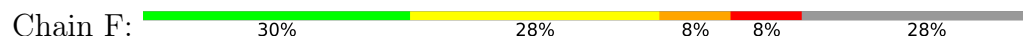
- Molecule 1: Amyloid-beta protein 40



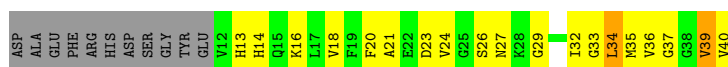
- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40



- Molecule 1: Amyloid-beta protein 40



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
Amber	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	135
Number of shifts mapped to atoms	135
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	4%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality

6.1 Standard geometry

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	2.16±0.10	6±3/198 (3.0± 1.3%)	2.87±0.07	24±3/263 (9.2± 1.0%)
1	B	2.15±0.11	8±2/216 (3.6± 0.9%)	2.80±0.16	23±5/288 (8.0± 1.9%)
1	C	2.12±0.08	6±2/216 (2.6± 0.9%)	2.76±0.18	21±5/288 (7.3± 1.6%)
1	D	2.11±0.09	6±1/216 (2.6± 0.5%)	2.71±0.15	20±5/288 (6.8± 1.6%)
1	E	2.05±0.12	4±2/187 (2.2± 1.1%)	3.03±0.12	22±5/248 (8.9± 2.0%)
1	F	2.19±0.07	8±2/216 (3.8± 0.9%)	2.99±0.15	26±4/288 (9.1± 1.3%)
1	G	2.06±0.10	5±3/216 (2.4± 1.2%)	2.70±0.13	21±4/288 (7.2± 1.3%)
1	H	2.18±0.19	5±3/147 (3.5± 1.8%)	2.81±0.18	17±4/197 (8.5± 2.3%)
All	All	2.13	480/16120 (3.0%)	2.84	1739/21480 (8.1%)

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	B	0.0±0.0	1.5±0.9
1	D	0.0±0.0	1.4±0.8
1	F	0.0±0.0	1.7±0.6
1	G	0.0±0.0	1.2±0.7
1	H	0.0±0.0	0.9±0.5
1	A	0.0±0.0	1.1±0.8
1	C	0.0±0.0	1.1±0.7
1	E	0.0±0.0	0.6±0.5
All	All	0	95

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	31	ILE	C-N	-10.16	1.24	1.33	4	3
1	B	30	ALA	CA-C	10.03	1.65	1.52	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	19	PHE	CA-C	9.94	1.64	1.52	9	2
1	D	31	ILE	C-N	-9.12	1.25	1.33	6	1
1	H	29	GLY	CA-C	-9.12	1.43	1.52	6	1
1	G	37	GLY	CA-C	8.96	1.59	1.51	4	3
1	C	32	ILE	N-CA	-8.94	1.36	1.46	10	3
1	F	31	ILE	C-O	-8.85	1.14	1.24	10	3
1	H	32	ILE	N-CA	-8.63	1.37	1.46	2	4
1	D	32	ILE	N-CA	-8.60	1.36	1.46	4	3
1	H	32	ILE	CA-C	8.49	1.63	1.52	3	1
1	F	14	HIS	CE1-NE2	8.48	1.41	1.32	3	2
1	B	35	MET	CA-C	8.42	1.61	1.52	2	1
1	C	37	GLY	CA-C	8.40	1.58	1.51	6	2
1	F	14	HIS	ND1-CE1	8.30	1.40	1.32	9	1
1	C	14	HIS	ND1-CE1	8.22	1.40	1.32	4	2
1	H	24	VAL	N-CA	8.20	1.56	1.46	8	2
1	F	23	ASP	CA-C	8.16	1.63	1.52	1	2
1	F	32	ILE	N-CA	-8.15	1.37	1.46	5	3
1	C	22	GLU	CA-C	8.13	1.62	1.52	2	2
1	H	31	ILE	CA-C	-8.12	1.42	1.52	2	1
1	B	29	GLY	N-CA	8.10	1.53	1.45	5	4
1	A	14	HIS	CE1-NE2	8.01	1.40	1.32	1	2
1	F	29	GLY	CA-C	8.01	1.59	1.52	7	2
1	F	31	ILE	CA-C	-8.00	1.42	1.52	6	2
1	H	36	VAL	C-O	-7.88	1.15	1.23	4	1
1	A	18	VAL	CA-C	7.88	1.62	1.52	6	2
1	E	24	VAL	CA-C	7.84	1.62	1.52	5	2
1	H	24	VAL	CA-CB	7.82	1.65	1.54	2	2
1	B	13	HIS	CE1-NE2	7.80	1.40	1.32	2	2
1	E	31	ILE	C-N	-7.76	1.26	1.33	1	2
1	A	25	GLY	CA-C	7.75	1.58	1.52	8	3
1	H	30	ALA	CA-C	7.74	1.62	1.52	6	1
1	F	32	ILE	CA-C	7.72	1.62	1.52	8	5
1	H	37	GLY	CA-C	7.72	1.60	1.51	10	1
1	B	37	GLY	CA-C	7.72	1.58	1.51	1	3
1	E	32	ILE	N-CA	-7.69	1.38	1.46	10	3
1	E	39	VAL	CA-C	7.67	1.59	1.52	5	3
1	A	37	GLY	CA-C	7.66	1.58	1.52	5	2
1	D	29	GLY	CA-C	7.66	1.59	1.52	7	3
1	A	25	GLY	N-CA	7.63	1.52	1.45	2	1
1	A	24	VAL	C-O	-7.62	1.16	1.24	4	1
1	C	27	ASN	CA-C	7.62	1.63	1.52	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	H	35	MET	CA-C	-7.60	1.44	1.52	3	1
1	B	32	ILE	N-CA	-7.57	1.38	1.46	4	2
1	C	37	GLY	N-CA	7.53	1.53	1.45	6	1
1	C	14	HIS	CD2-NE2	7.52	1.46	1.37	3	1
1	D	24	VAL	CA-CB	7.46	1.64	1.54	7	2
1	B	21	ALA	CA-C	7.46	1.61	1.52	1	1
1	H	19	PHE	N-CA	7.45	1.55	1.46	5	2
1	F	29	GLY	N-CA	7.44	1.52	1.45	8	1
1	G	27	ASN	N-CA	7.40	1.55	1.46	2	1
1	G	29	GLY	CA-C	7.36	1.59	1.51	10	1
1	C	20	PHE	C-N	-7.30	1.24	1.33	10	1
1	A	28	LYS	N-CA	7.28	1.55	1.46	1	1
1	F	21	ALA	CA-C	7.24	1.60	1.52	3	1
1	A	14	HIS	CD2-NE2	7.16	1.45	1.37	5	3
1	D	23	ASP	CA-CB	7.14	1.62	1.53	3	2
1	F	30	ALA	CA-C	-7.14	1.43	1.52	1	1
1	B	36	VAL	CA-C	-7.14	1.44	1.52	4	1
1	F	34	LEU	N-CA	-7.11	1.38	1.46	2	1
1	D	21	ALA	N-CA	-7.10	1.37	1.46	6	1
1	E	22	GLU	N-CA	-7.03	1.37	1.45	4	1
1	H	20	PHE	N-CA	7.02	1.54	1.45	10	2
1	F	13	HIS	CB-CG	7.00	1.59	1.50	9	1
1	C	17	LEU	N-CA	-6.98	1.37	1.46	9	2
1	H	36	VAL	N-CA	6.97	1.54	1.46	7	1
1	F	16	LYS	CA-C	6.96	1.61	1.52	8	2
1	F	28	LYS	N-CA	6.93	1.54	1.46	8	1
1	C	39	VAL	N-CA	6.92	1.54	1.46	7	1
1	C	35	MET	C-N	-6.90	1.24	1.33	8	2
1	A	14	HIS	N-CA	6.89	1.54	1.45	3	2
1	E	19	PHE	CA-C	6.89	1.61	1.52	10	1
1	A	35	MET	C-N	6.87	1.42	1.33	1	1
1	D	31	ILE	C-O	-6.87	1.16	1.24	6	1
1	D	26	SER	CA-C	6.87	1.61	1.52	8	1
1	H	31	ILE	CA-CB	6.86	1.62	1.53	6	1
1	E	34	LEU	C-N	-6.84	1.25	1.33	5	1
1	B	29	GLY	CA-C	6.83	1.58	1.52	2	3
1	A	14	HIS	CA-C	6.83	1.61	1.52	2	1
1	A	17	LEU	CA-C	6.78	1.60	1.52	5	2
1	B	13	HIS	CG-CD2	6.77	1.43	1.35	4	2
1	D	37	GLY	CA-C	6.75	1.58	1.51	6	3
1	F	25	GLY	C-O	-6.74	1.18	1.24	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	E	29	GLY	N-CA	6.73	1.52	1.45	5	1
1	F	28	LYS	CA-C	6.73	1.61	1.52	4	1
1	H	35	MET	C-N	6.72	1.41	1.33	10	1
1	C	13	HIS	ND1-CE1	6.71	1.39	1.32	10	1
1	G	14	HIS	CG-CD2	6.70	1.43	1.35	2	1
1	C	34	LEU	CA-C	6.68	1.59	1.52	7	3
1	F	39	VAL	N-CA	6.65	1.53	1.46	8	1
1	F	17	LEU	C-O	-6.65	1.16	1.24	3	1
1	F	14	HIS	N-CA	-6.63	1.37	1.45	1	2
1	F	22	GLU	CA-C	6.62	1.61	1.52	6	2
1	A	23	ASP	CA-C	6.62	1.61	1.52	1	1
1	E	24	VAL	N-CA	6.60	1.54	1.46	8	2
1	B	32	ILE	CA-CB	6.58	1.62	1.55	9	1
1	G	32	ILE	CA-CB	-6.57	1.45	1.55	4	3
1	E	36	VAL	CA-CB	-6.53	1.47	1.55	8	1
1	D	39	VAL	N-CA	6.52	1.54	1.46	3	2
1	G	32	ILE	N-CA	-6.50	1.39	1.46	3	1
1	B	27	ASN	CA-C	6.49	1.61	1.52	9	2
1	G	18	VAL	N-CA	6.49	1.54	1.46	7	2
1	A	15	GLN	CA-C	6.49	1.61	1.52	5	1
1	H	23	ASP	CA-C	6.46	1.61	1.52	5	1
1	H	28	LYS	C-O	-6.45	1.17	1.23	2	1
1	G	36	VAL	N-CA	6.45	1.53	1.46	9	1
1	G	20	PHE	N-CA	6.44	1.54	1.46	3	2
1	D	31	ILE	N-CA	6.43	1.54	1.46	3	2
1	F	37	GLY	N-CA	6.42	1.51	1.45	3	1
1	G	23	ASP	N-CA	6.42	1.54	1.46	8	1
1	H	30	ALA	N-CA	6.42	1.53	1.45	10	1
1	D	27	ASN	CA-C	6.41	1.61	1.52	3	1
1	C	16	LYS	CA-C	6.41	1.60	1.52	7	1
1	C	33	GLY	CA-C	-6.40	1.45	1.51	9	2
1	C	31	ILE	C-N	-6.38	1.26	1.33	9	1
1	E	34	LEU	N-CA	-6.38	1.38	1.46	10	1
1	A	14	HIS	ND1-CE1	6.37	1.39	1.32	9	2
1	A	18	VAL	C-N	6.34	1.42	1.33	10	1
1	C	13	HIS	CD2-NE2	6.33	1.44	1.37	1	1
1	E	21	ALA	CA-C	6.33	1.59	1.52	1	2
1	B	17	LEU	CA-C	6.31	1.60	1.52	2	3
1	H	28	LYS	CA-C	6.31	1.60	1.53	5	2
1	G	34	LEU	CA-C	-6.30	1.45	1.52	6	1
1	E	16	LYS	CA-C	-6.29	1.44	1.52	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	F	33	GLY	N-CA	-6.28	1.39	1.45	4	1
1	A	14	HIS	CA-CB	6.27	1.63	1.53	3	1
1	B	23	ASP	N-CA	6.26	1.54	1.46	7	2
1	B	33	GLY	N-CA	-6.26	1.38	1.45	6	2
1	A	17	LEU	N-CA	6.25	1.53	1.45	6	1
1	F	18	VAL	CA-C	6.25	1.60	1.52	2	1
1	B	16	LYS	CA-C	6.22	1.60	1.52	1	1
1	A	33	GLY	CA-C	6.22	1.57	1.51	4	1
1	G	16	LYS	C-N	-6.21	1.25	1.33	4	1
1	H	26	SER	N-CA	6.19	1.54	1.46	5	2
1	C	21	ALA	CA-C	6.18	1.59	1.52	5	2
1	G	28	LYS	CA-C	6.18	1.60	1.52	7	2
1	A	24	VAL	CA-C	6.18	1.60	1.52	10	1
1	H	21	ALA	CA-C	6.16	1.59	1.52	10	1
1	B	19	PHE	N-CA	6.14	1.53	1.46	1	1
1	B	34	LEU	CA-C	6.14	1.59	1.52	2	2
1	H	31	ILE	C-N	-6.14	1.28	1.33	2	1
1	F	19	PHE	N-CA	6.13	1.54	1.46	2	2
1	E	18	VAL	N-CA	6.13	1.52	1.46	10	1
1	G	31	ILE	C-N	-6.12	1.26	1.33	3	1
1	H	29	GLY	C-O	-6.12	1.17	1.23	9	1
1	G	36	VAL	CA-CB	-6.12	1.46	1.54	1	1
1	F	17	LEU	CA-CB	6.11	1.62	1.53	10	1
1	F	28	LYS	C-O	6.10	1.30	1.23	2	1
1	A	20	PHE	N-CA	6.09	1.53	1.45	10	1
1	D	14	HIS	CD2-NE2	6.09	1.44	1.37	2	2
1	C	28	LYS	CA-C	6.09	1.60	1.53	9	1
1	A	34	LEU	CA-C	-6.09	1.45	1.52	1	1
1	B	28	LYS	CA-C	6.09	1.60	1.52	5	1
1	D	38	GLY	CA-C	6.08	1.60	1.51	1	1
1	E	24	VAL	C-N	6.08	1.41	1.32	1	1
1	F	36	VAL	C-O	-6.08	1.18	1.24	4	1
1	B	38	GLY	N-CA	6.06	1.51	1.45	1	1
1	C	23	ASP	CA-CB	6.04	1.60	1.52	1	1
1	B	13	HIS	CD2-NE2	6.03	1.44	1.37	5	2
1	H	19	PHE	CA-C	6.03	1.60	1.52	7	2
1	H	33	GLY	N-CA	6.01	1.51	1.45	3	1
1	B	31	ILE	C-O	-6.00	1.17	1.24	8	1
1	G	12	VAL	N-CA	5.99	1.57	1.46	4	1
1	F	30	ALA	N-CA	5.97	1.53	1.46	10	3
1	F	18	VAL	N-CA	-5.95	1.39	1.46	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	35	MET	CA-C	5.94	1.59	1.52	6	2
1	E	31	ILE	CA-C	5.93	1.60	1.52	10	1
1	A	28	LYS	CA-CB	5.92	1.62	1.53	3	1
1	A	31	ILE	N-CA	5.90	1.53	1.46	8	2
1	B	36	VAL	N-CA	-5.90	1.39	1.46	3	1
1	H	27	ASN	CA-C	5.89	1.60	1.52	4	1
1	D	30	ALA	CA-C	5.89	1.59	1.52	9	2
1	D	13	HIS	CD2-NE2	5.89	1.44	1.37	10	2
1	D	39	VAL	CA-C	5.88	1.59	1.52	4	1
1	D	28	LYS	CA-C	5.87	1.60	1.52	5	1
1	B	37	GLY	C-N	5.87	1.40	1.33	6	1
1	A	30	ALA	CA-C	5.87	1.59	1.52	1	1
1	C	16	LYS	N-CA	5.86	1.53	1.46	6	1
1	D	33	GLY	N-CA	-5.86	1.39	1.45	2	1
1	D	39	VAL	CA-CB	5.86	1.63	1.55	9	1
1	B	14	HIS	CE1-NE2	5.82	1.38	1.32	10	3
1	E	32	ILE	CA-CB	-5.82	1.49	1.55	10	1
1	E	35	MET	CA-C	5.81	1.59	1.52	6	1
1	C	23	ASP	CA-C	5.81	1.60	1.52	5	1
1	F	34	LEU	CA-C	-5.81	1.45	1.52	8	2
1	C	13	HIS	CE1-NE2	5.80	1.38	1.32	7	1
1	D	23	ASP	CA-C	5.79	1.60	1.52	7	1
1	H	33	GLY	CA-C	5.79	1.56	1.51	10	2
1	D	14	HIS	CG-ND1	5.78	1.44	1.38	9	1
1	E	16	LYS	CA-CB	5.77	1.61	1.53	6	2
1	H	34	LEU	C-N	-5.76	1.26	1.33	2	1
1	H	38	GLY	N-CA	5.76	1.50	1.44	3	3
1	A	24	VAL	CA-CB	5.76	1.61	1.54	3	1
1	B	37	GLY	N-CA	5.75	1.50	1.44	3	1
1	A	32	ILE	N-CA	-5.75	1.39	1.46	3	1
1	G	39	VAL	N-CA	5.75	1.53	1.46	7	2
1	B	24	VAL	N-CA	5.74	1.52	1.46	6	3
1	A	26	SER	CA-CB	5.74	1.62	1.53	1	1
1	F	21	ALA	N-CA	-5.74	1.39	1.46	6	1
1	G	13	HIS	N-CA	5.74	1.53	1.46	7	1
1	B	13	HIS	ND1-CE1	5.74	1.38	1.32	9	1
1	F	25	GLY	N-CA	-5.73	1.40	1.45	9	1
1	E	30	ALA	N-CA	5.73	1.53	1.45	8	1
1	C	24	VAL	CA-C	5.72	1.59	1.52	8	2
1	D	24	VAL	C-O	-5.70	1.18	1.24	7	1
1	F	19	PHE	CA-C	5.70	1.59	1.52	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	13	HIS	CG-ND1	5.70	1.44	1.38	3	1
1	H	22	GLU	CA-CB	5.69	1.62	1.53	4	1
1	G	25	GLY	N-CA	5.68	1.53	1.45	1	2
1	E	35	MET	N-CA	-5.68	1.38	1.45	7	2
1	C	34	LEU	N-CA	-5.67	1.39	1.46	2	2
1	G	36	VAL	CA-C	-5.67	1.45	1.52	9	1
1	E	30	ALA	C-N	5.67	1.40	1.33	10	1
1	F	13	HIS	ND1-CE1	5.67	1.38	1.32	8	2
1	G	17	LEU	N-CA	5.66	1.52	1.46	1	1
1	D	33	GLY	CA-C	-5.65	1.45	1.51	6	1
1	B	25	GLY	N-CA	5.64	1.53	1.45	6	1
1	C	20	PHE	N-CA	5.64	1.53	1.45	8	2
1	D	18	VAL	C-O	-5.63	1.18	1.24	7	1
1	E	25	GLY	N-CA	5.63	1.49	1.44	8	2
1	B	33	GLY	C-N	-5.63	1.26	1.33	5	1
1	A	32	ILE	CB-CG1	5.62	1.64	1.53	4	1
1	H	31	ILE	N-CA	5.62	1.52	1.46	9	2
1	B	17	LEU	C-O	5.61	1.30	1.24	5	1
1	C	21	ALA	N-CA	-5.61	1.39	1.46	8	2
1	G	35	MET	CA-C	5.61	1.58	1.52	7	1
1	C	24	VAL	CA-CB	5.60	1.61	1.54	2	1
1	H	29	GLY	N-CA	5.60	1.50	1.45	6	1
1	G	15	GLN	CA-C	5.60	1.59	1.52	7	2
1	G	13	HIS	CA-C	5.59	1.60	1.52	9	1
1	F	23	ASP	C-N	5.59	1.41	1.33	9	1
1	A	32	ILE	CA-C	5.58	1.58	1.52	4	1
1	D	25	GLY	N-CA	5.57	1.51	1.45	6	1
1	C	29	GLY	CA-C	5.56	1.57	1.52	8	2
1	G	39	VAL	CA-C	-5.56	1.46	1.52	6	2
1	A	19	PHE	CA-C	5.56	1.59	1.52	3	1
1	B	28	LYS	N-CA	5.55	1.53	1.46	6	1
1	F	39	VAL	CA-C	-5.55	1.45	1.52	7	4
1	D	24	VAL	CA-C	5.54	1.59	1.52	3	2
1	A	26	SER	N-CA	5.53	1.53	1.46	2	1
1	A	15	GLN	CA-CB	5.53	1.61	1.53	9	1
1	D	32	ILE	CB-CG1	5.52	1.64	1.53	7	1
1	A	14	HIS	CG-ND1	-5.51	1.32	1.38	2	1
1	D	13	HIS	C-N	5.51	1.40	1.33	9	1
1	F	36	VAL	N-CA	5.50	1.52	1.46	2	2
1	B	33	GLY	C-O	-5.49	1.18	1.24	7	1
1	B	23	ASP	CA-CB	5.49	1.60	1.53	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	F	26	SER	CA-CB	-5.49	1.44	1.53	5	1
1	G	19	PHE	CA-C	5.48	1.59	1.52	3	1
1	F	20	PHE	C-N	-5.47	1.26	1.33	1	1
1	H	38	GLY	CA-C	5.47	1.56	1.51	9	1
1	A	27	ASN	C-O	-5.47	1.17	1.24	2	1
1	G	32	ILE	CA-C	5.46	1.59	1.52	2	1
1	E	37	GLY	C-O	-5.46	1.17	1.23	5	1
1	G	21	ALA	CA-C	-5.46	1.46	1.52	5	2
1	E	34	LEU	CA-C	5.46	1.59	1.52	7	1
1	E	21	ALA	N-CA	-5.45	1.39	1.46	1	1
1	E	16	LYS	N-CA	5.45	1.52	1.46	3	1
1	D	27	ASN	N-CA	5.45	1.52	1.46	1	1
1	A	21	ALA	CA-CB	-5.44	1.43	1.53	3	1
1	D	32	ILE	CA-C	5.44	1.59	1.52	5	1
1	B	22	GLU	CA-C	5.43	1.59	1.52	4	1
1	G	17	LEU	CA-C	5.43	1.59	1.52	7	1
1	G	13	HIS	CE1-NE2	5.42	1.38	1.32	10	1
1	D	30	ALA	N-CA	5.41	1.52	1.45	10	1
1	F	13	HIS	CD2-NE2	5.40	1.43	1.37	8	1
1	F	33	GLY	C-O	-5.39	1.18	1.24	9	1
1	B	35	MET	N-CA	-5.39	1.40	1.46	10	1
1	G	16	LYS	CA-CB	5.39	1.60	1.53	10	1
1	A	26	SER	CA-C	5.39	1.60	1.52	1	1
1	B	20	PHE	CA-C	5.37	1.59	1.52	7	2
1	D	22	GLU	C-O	-5.36	1.17	1.24	3	1
1	D	25	GLY	CA-C	5.35	1.59	1.51	8	1
1	B	20	PHE	CA-CB	5.33	1.66	1.53	3	1
1	F	35	MET	N-CA	-5.33	1.40	1.46	3	1
1	D	19	PHE	CA-C	5.33	1.59	1.52	4	1
1	H	26	SER	CA-C	5.33	1.59	1.52	10	1
1	G	13	HIS	CG-CD2	5.32	1.41	1.35	9	1
1	H	34	LEU	C-O	-5.32	1.17	1.23	10	1
1	A	33	GLY	N-CA	5.31	1.50	1.45	2	1
1	F	14	HIS	CA-CB	5.30	1.62	1.53	6	1
1	D	25	GLY	C-N	5.27	1.41	1.33	4	1
1	D	22	GLU	N-CA	5.27	1.52	1.46	3	1
1	A	35	MET	CA-C	-5.26	1.47	1.52	10	2
1	B	19	PHE	C-O	5.25	1.30	1.24	6	2
1	C	39	VAL	CA-C	5.25	1.58	1.52	3	1
1	F	15	GLN	N-CA	5.25	1.52	1.45	2	1
1	H	25	GLY	N-CA	5.24	1.52	1.45	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	F	15	GLN	C-O	-5.24	1.17	1.23	5	1
1	A	40	VAL	N-CA	5.23	1.56	1.46	10	1
1	F	35	MET	C-N	-5.23	1.26	1.33	10	1
1	G	24	VAL	C-O	-5.22	1.18	1.24	1	1
1	B	23	ASP	CG-OD2	5.21	1.35	1.25	7	1
1	F	37	GLY	CA-C	5.21	1.56	1.51	3	1
1	G	14	HIS	CA-C	5.21	1.59	1.52	7	2
1	D	35	MET	N-CA	-5.20	1.40	1.46	8	1
1	C	14	HIS	CA-C	5.20	1.59	1.52	7	1
1	B	18	VAL	C-O	5.19	1.29	1.24	3	1
1	F	23	ASP	CA-CB	5.19	1.59	1.53	6	2
1	C	36	VAL	N-CA	5.19	1.52	1.46	5	1
1	D	37	GLY	N-CA	5.19	1.50	1.45	9	1
1	F	20	PHE	N-CA	5.18	1.52	1.46	2	1
1	D	38	GLY	C-O	5.18	1.30	1.23	2	1
1	B	21	ALA	CA-CB	5.18	1.62	1.53	7	1
1	B	14	HIS	CG-CD2	5.18	1.41	1.35	8	2
1	G	20	PHE	CA-C	5.17	1.58	1.52	9	1
1	E	39	VAL	C-O	-5.17	1.18	1.23	6	1
1	C	26	SER	N-CA	5.17	1.52	1.46	6	1
1	E	25	GLY	CA-C	5.17	1.57	1.51	1	1
1	C	24	VAL	N-CA	5.17	1.52	1.46	3	1
1	B	39	VAL	C-N	5.16	1.40	1.33	10	1
1	F	21	ALA	CA-CB	5.16	1.62	1.53	1	1
1	A	30	ALA	C-N	5.15	1.40	1.33	4	1
1	A	23	ASP	CA-CB	5.15	1.59	1.53	5	1
1	F	24	VAL	N-CA	5.15	1.52	1.46	6	1
1	C	26	SER	CA-C	5.14	1.59	1.52	6	1
1	C	32	ILE	CA-CB	-5.14	1.50	1.55	10	1
1	A	22	GLU	CA-C	5.14	1.59	1.52	10	1
1	F	31	ILE	C-N	-5.13	1.27	1.33	9	2
1	B	13	HIS	CA-C	5.13	1.59	1.52	2	1
1	G	37	GLY	C-O	5.13	1.29	1.23	10	1
1	C	29	GLY	N-CA	-5.12	1.40	1.45	9	1
1	G	33	GLY	C-O	-5.11	1.18	1.24	6	1
1	H	26	SER	C-O	-5.11	1.17	1.24	6	1
1	B	34	LEU	C-N	-5.11	1.27	1.33	6	1
1	E	28	LYS	N-CA	5.09	1.52	1.46	10	1
1	B	14	HIS	CD2-NE2	5.09	1.43	1.37	10	1
1	B	18	VAL	CA-CB	5.09	1.62	1.54	4	1
1	F	31	ILE	CA-CB	-5.08	1.48	1.54	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	F	38	GLY	CA-C	5.07	1.59	1.51	7	1
1	A	14	HIS	CG-CD2	5.07	1.41	1.35	3	1
1	E	31	ILE	N-CA	5.07	1.52	1.46	2	1
1	H	20	PHE	CA-C	5.07	1.58	1.52	9	1
1	C	17	LEU	C-O	-5.05	1.18	1.24	8	1
1	B	29	GLY	C-N	5.05	1.40	1.33	8	1
1	C	30	ALA	N-CA	5.04	1.51	1.46	8	1
1	F	13	HIS	CE1-NE2	5.04	1.37	1.32	9	1
1	G	35	MET	N-CA	-5.04	1.39	1.46	10	1
1	D	34	LEU	N-CA	5.04	1.52	1.46	10	1
1	B	23	ASP	CA-C	5.03	1.59	1.53	1	1
1	D	12	VAL	C-N	-5.03	1.27	1.33	1	1
1	A	18	VAL	N-CA	5.02	1.52	1.46	5	1
1	G	29	GLY	N-CA	5.01	1.50	1.45	7	1
1	D	14	HIS	ND1-CE1	-5.00	1.27	1.32	1	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	F	31	ILE	CA-C-N	19.37	147.88	122.51	9	9
1	F	31	ILE	C-N-CA	19.37	147.88	122.51	9	9
1	E	34	LEU	CA-C-N	15.81	147.83	122.21	1	10
1	E	34	LEU	C-N-CA	15.81	147.83	122.21	1	10
1	D	24	VAL	CA-C-N	13.94	134.70	121.46	6	3
1	D	24	VAL	C-N-CA	13.94	134.70	121.46	6	3
1	C	27	ASN	CA-C-N	12.72	142.34	122.11	5	9
1	C	27	ASN	C-N-CA	12.72	142.34	122.11	5	9
1	C	36	VAL	CA-C-N	12.65	130.25	121.65	6	3
1	C	36	VAL	C-N-CA	12.65	130.25	121.65	6	3
1	B	36	VAL	CA-C-N	12.29	130.66	122.18	9	4
1	B	36	VAL	C-N-CA	12.29	130.66	122.18	9	4
1	A	29	GLY	CA-C-N	11.61	140.91	121.87	1	8
1	A	29	GLY	C-N-CA	11.61	140.91	121.87	1	8
1	E	27	ASN	CA-C-N	11.42	140.27	122.11	7	10
1	E	27	ASN	C-N-CA	11.42	140.27	122.11	7	10
1	F	27	ASN	CA-C-N	11.41	140.25	122.11	1	9
1	F	27	ASN	C-N-CA	11.41	140.25	122.11	1	9
1	B	27	ASN	CA-C-N	11.23	141.51	122.20	1	10
1	B	27	ASN	C-N-CA	11.23	141.51	122.20	1	10
1	F	31	ILE	O-C-N	11.15	136.14	123.10	9	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	G	19	PHE	CA-CB-CG	10.97	124.77	113.80	7	3
1	C	31	ILE	CA-C-O	10.87	132.16	120.53	5	6
1	G	27	ASN	CA-C-N	10.82	139.32	122.11	7	9
1	G	27	ASN	C-N-CA	10.82	139.32	122.11	7	9
1	G	37	GLY	O-C-N	-10.79	113.88	123.37	5	4
1	E	15	GLN	OE1-CD-NE2	-10.72	111.88	122.60	9	3
1	G	14	HIS	CA-CB-CG	10.72	124.52	113.80	10	2
1	E	29	GLY	CA-C-N	10.34	138.83	121.87	10	5
1	E	29	GLY	C-N-CA	10.34	138.83	121.87	10	5
1	C	28	LYS	CA-C-O	-10.33	110.41	121.36	4	4
1	E	34	LEU	CA-C-O	10.20	134.08	120.11	10	4
1	A	15	GLN	OE1-CD-NE2	-10.19	112.41	122.60	8	5
1	D	23	ASP	N-CA-C	10.03	124.56	108.41	3	4
1	E	31	ILE	CA-C-O	9.81	131.29	120.59	4	9
1	G	24	VAL	CA-C-N	9.76	133.45	122.42	5	1
1	G	24	VAL	C-N-CA	9.76	133.45	122.42	5	1
1	F	35	MET	O-C-N	-9.74	111.67	123.36	7	5
1	F	20	PHE	CA-CB-CG	9.68	123.48	113.80	7	4
1	A	29	GLY	O-C-N	9.66	132.43	123.54	6	3
1	D	25	GLY	CA-C-O	-9.52	112.53	121.19	5	3
1	G	32	ILE	CA-C-N	9.35	132.79	121.38	10	3
1	G	32	ILE	C-N-CA	9.35	132.79	121.38	10	3
1	H	27	ASN	OD1-CG-ND2	-9.29	113.31	122.60	1	2
1	E	34	LEU	N-CA-C	9.19	123.08	107.93	6	7
1	D	23	ASP	CA-CB-CG	-9.15	103.45	112.60	2	3
1	H	30	ALA	CA-C-N	-9.12	110.98	122.93	1	4
1	H	30	ALA	C-N-CA	-9.12	110.98	122.93	1	4
1	H	35	MET	CA-C-N	-9.08	107.99	122.25	9	5
1	H	35	MET	C-N-CA	-9.08	107.99	122.25	9	5
1	C	33	GLY	O-C-N	-9.07	116.38	123.27	5	1
1	G	31	ILE	CA-C-O	9.06	130.46	120.59	1	3
1	B	29	GLY	CA-C-N	9.03	136.68	121.87	8	2
1	B	29	GLY	C-N-CA	9.03	136.68	121.87	8	2
1	E	32	ILE	CB-CA-C	9.01	124.10	111.40	5	9
1	C	37	GLY	O-C-N	-9.00	115.15	123.25	3	2
1	F	32	ILE	N-CA-C	-9.00	95.36	108.23	10	4
1	D	15	GLN	OE1-CD-NE2	-8.98	113.62	122.60	10	3
1	D	22	GLU	CB-CA-C	8.96	124.49	109.80	6	6
1	A	34	LEU	CB-CA-C	8.93	123.20	110.79	3	1
1	F	27	ASN	CA-CB-CG	8.91	121.52	112.60	3	3
1	B	39	VAL	CA-C-O	-8.88	111.86	121.28	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	36	VAL	CA-C-N	8.88	129.28	121.82	8	1
1	A	36	VAL	C-N-CA	8.88	129.28	121.82	8	1
1	B	31	ILE	CA-C-O	8.87	131.04	120.66	1	4
1	C	15	GLN	OE1-CD-NE2	-8.84	113.76	122.60	4	4
1	C	24	VAL	CA-C-N	8.83	132.40	122.42	1	2
1	C	24	VAL	C-N-CA	8.83	132.40	122.42	1	2
1	A	31	ILE	CA-C-O	8.81	131.45	120.97	3	7
1	E	23	ASP	CA-CB-CG	8.77	121.37	112.60	4	2
1	B	35	MET	N-CA-CB	-8.75	97.60	110.37	5	4
1	G	29	GLY	N-CA-C	8.72	123.95	110.96	9	2
1	C	13	HIS	CB-CG-CD2	-8.71	119.87	131.20	1	3
1	A	32	ILE	CB-CA-C	8.69	123.66	111.40	9	2
1	E	35	MET	N-CA-C	-8.67	96.04	108.96	6	9
1	G	35	MET	O-C-N	-8.67	112.96	123.36	2	6
1	C	34	LEU	CA-C-N	8.63	134.80	121.76	5	5
1	C	34	LEU	C-N-CA	8.63	134.80	121.76	5	5
1	E	27	ASN	OD1-CG-ND2	-8.60	114.00	122.60	2	5
1	E	39	VAL	N-CA-C	8.57	118.98	108.53	5	3
1	A	27	ASN	CA-C-N	8.53	136.26	122.10	7	9
1	A	27	ASN	C-N-CA	8.53	136.26	122.10	7	9
1	A	19	PHE	CA-CB-CG	8.50	122.30	113.80	2	2
1	A	20	PHE	CA-CB-CG	8.49	122.29	113.80	4	3
1	E	29	GLY	CA-C-O	8.47	130.69	121.63	1	2
1	E	35	MET	O-C-N	-8.46	113.37	123.10	10	6
1	A	35	MET	O-C-N	-8.42	113.26	123.36	10	4
1	G	32	ILE	CA-CB-CG2	8.40	124.79	110.50	6	8
1	G	16	LYS	N-CA-C	8.40	122.60	109.07	3	3
1	E	36	VAL	CA-C-N	8.40	127.98	122.18	3	3
1	E	36	VAL	C-N-CA	8.40	127.98	122.18	3	3
1	E	30	ALA	CA-C-N	-8.38	112.17	122.90	4	5
1	E	30	ALA	C-N-CA	-8.38	112.17	122.90	4	5
1	A	36	VAL	CA-C-O	-8.38	111.54	120.76	2	1
1	D	31	ILE	CA-C-O	8.33	129.45	120.53	6	6
1	E	27	ASN	CA-CB-CG	-8.33	104.27	112.60	7	2
1	A	26	SER	CA-C-O	-8.30	111.83	120.80	3	3
1	H	36	VAL	CA-CB-CG1	8.30	124.51	110.40	4	2
1	A	28	LYS	CA-C-O	-8.30	112.43	121.31	4	3
1	B	35	MET	O-C-N	-8.29	112.98	123.26	8	5
1	B	30	ALA	CA-C-N	-8.28	112.35	123.12	7	2
1	B	30	ALA	C-N-CA	-8.28	112.35	123.12	7	2
1	G	22	GLU	N-CA-C	8.27	123.19	109.46	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	32	ILE	CB-CA-C	8.26	126.04	111.18	7	5
1	H	37	GLY	O-C-N	8.24	132.03	123.29	4	3
1	E	24	VAL	N-CA-C	8.22	120.17	108.17	1	1
1	G	27	ASN	OD1-CG-ND2	-8.20	114.40	122.60	3	3
1	G	35	MET	N-CA-CB	-8.12	98.52	110.37	4	3
1	G	39	VAL	CA-C-N	8.11	136.29	121.70	8	3
1	G	39	VAL	C-N-CA	8.11	136.29	121.70	8	3
1	B	23	ASP	N-CA-C	8.09	121.44	108.41	6	4
1	E	16	LYS	CB-CA-C	8.09	123.55	110.29	3	1
1	E	33	GLY	CA-C-O	8.07	128.53	121.19	3	1
1	H	19	PHE	CA-CB-CG	-8.06	105.73	113.80	4	2
1	F	14	HIS	CE1-NE2-CD2	-8.06	100.94	109.00	3	2
1	G	29	GLY	CA-C-N	8.05	135.07	121.87	5	3
1	G	29	GLY	C-N-CA	8.05	135.07	121.87	5	3
1	F	34	LEU	CA-C-N	8.01	133.57	121.40	7	7
1	F	34	LEU	C-N-CA	8.01	133.57	121.40	7	7
1	C	29	GLY	CA-C-N	8.00	134.99	121.87	4	4
1	C	29	GLY	C-N-CA	8.00	134.99	121.87	4	4
1	B	32	ILE	CA-C-N	7.99	131.13	121.38	10	5
1	B	32	ILE	C-N-CA	7.99	131.13	121.38	10	5
1	D	34	LEU	CA-C-N	7.98	134.00	121.72	3	4
1	D	34	LEU	C-N-CA	7.98	134.00	121.72	3	4
1	B	27	ASN	N-CA-C	7.96	121.90	109.96	3	4
1	A	30	ALA	CA-C-N	-7.95	112.52	122.93	5	6
1	A	30	ALA	C-N-CA	-7.95	112.52	122.93	5	6
1	F	13	HIS	ND1-CE1-NE2	7.95	116.34	108.40	2	1
1	F	27	ASN	CA-C-O	7.93	129.69	120.49	1	1
1	H	27	ASN	CA-C-N	7.92	136.26	122.32	5	9
1	H	27	ASN	C-N-CA	7.92	136.26	122.32	5	9
1	A	30	ALA	CA-C-O	-7.90	112.85	121.31	5	2
1	F	22	GLU	O-C-N	-7.90	114.05	123.13	3	2
1	D	35	MET	O-C-N	-7.90	113.88	123.36	10	2
1	F	27	ASN	OD1-CG-ND2	-7.89	114.70	122.60	1	2
1	H	38	GLY	O-C-N	-7.89	117.27	123.27	1	3
1	A	31	ILE	N-CA-C	7.87	119.23	107.51	5	5
1	B	17	LEU	CB-CA-C	7.87	123.09	110.19	2	2
1	E	29	GLY	N-CA-C	7.86	122.67	110.96	10	2
1	B	32	ILE	CA-C-O	7.85	127.53	121.09	5	1
1	D	19	PHE	CA-CB-CG	7.83	121.64	113.80	3	5
1	F	29	GLY	N-CA-C	7.83	122.54	111.10	8	3
1	C	27	ASN	CA-C-O	7.83	129.57	120.49	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	F	28	LYS	N-CA-C	-7.83	98.59	108.45	4	2
1	A	33	GLY	CA-C-O	-7.82	114.02	121.06	9	2
1	H	36	VAL	O-C-N	7.81	131.72	123.05	7	3
1	F	15	GLN	OE1-CD-NE2	-7.79	114.81	122.60	2	4
1	H	33	GLY	CA-C-O	-7.77	114.06	121.06	3	1
1	D	36	VAL	N-CA-C	7.76	119.65	108.48	6	4
1	F	21	ALA	CA-C-N	7.75	133.56	122.09	1	1
1	F	21	ALA	C-N-CA	7.75	133.56	122.09	1	1
1	C	35	MET	N-CA-CB	-7.72	97.58	110.32	9	4
1	D	35	MET	CA-C-N	-7.71	111.61	122.71	4	2
1	D	35	MET	C-N-CA	-7.71	111.61	122.71	4	2
1	B	27	ASN	CA-C-O	7.69	129.41	120.49	1	3
1	H	34	LEU	CA-C-O	7.69	130.64	120.11	4	2
1	B	34	LEU	CA-C-N	7.66	133.05	121.40	5	7
1	B	34	LEU	C-N-CA	7.66	133.05	121.40	5	7
1	D	36	VAL	CA-CB-CG2	7.66	123.42	110.40	4	2
1	C	35	MET	CB-CA-C	7.62	121.38	110.79	7	3
1	F	14	HIS	N-CA-C	7.62	121.88	109.76	10	2
1	C	31	ILE	N-CA-CB	7.62	120.13	111.21	1	7
1	H	24	VAL	CA-C-N	7.62	126.83	121.65	10	1
1	H	24	VAL	C-N-CA	7.62	126.83	121.65	10	1
1	D	27	ASN	CA-C-N	7.60	135.27	122.20	4	7
1	D	27	ASN	C-N-CA	7.60	135.27	122.20	4	7
1	G	33	GLY	O-C-N	-7.60	117.08	123.23	10	3
1	G	34	LEU	N-CA-C	7.58	120.44	107.93	2	5
1	D	35	MET	N-CA-CB	-7.57	99.13	110.71	8	6
1	C	20	PHE	CA-CB-CG	-7.56	106.24	113.80	4	2
1	G	30	ALA	N-CA-CB	-7.54	99.32	111.24	3	1
1	D	35	MET	CA-C-O	-7.54	109.83	120.15	2	2
1	H	24	VAL	N-CA-C	7.53	119.59	108.45	5	2
1	D	35	MET	CB-CA-C	7.51	121.23	110.79	2	5
1	F	29	GLY	CA-C-N	7.51	134.74	121.75	7	6
1	F	29	GLY	C-N-CA	7.51	134.74	121.75	7	6
1	A	22	GLU	CB-CA-C	7.48	122.30	109.51	9	6
1	F	35	MET	CB-CA-C	7.47	121.17	110.79	4	5
1	H	29	GLY	N-CA-C	7.46	122.08	110.96	5	6
1	H	27	ASN	CA-CB-CG	7.45	120.05	112.60	1	2
1	F	31	ILE	N-CA-CB	7.43	121.03	111.67	6	6
1	H	29	GLY	CA-C-N	7.42	134.60	121.75	9	3
1	H	29	GLY	C-N-CA	7.42	134.60	121.75	9	3
1	D	36	VAL	N-CA-CB	-7.42	99.28	111.45	10	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	29	GLY	N-CA-C	7.41	124.89	111.03	10	4
1	A	29	GLY	N-CA-C	7.40	124.88	111.03	8	6
1	B	28	LYS	CA-C-O	-7.40	113.52	121.36	6	2
1	H	22	GLU	CB-CA-C	7.39	121.72	109.53	7	2
1	A	25	GLY	CA-C-N	7.38	131.87	121.24	7	3
1	A	25	GLY	C-N-CA	7.38	131.87	121.24	7	3
1	C	18	VAL	CB-CA-C	7.37	121.09	110.33	6	1
1	H	29	GLY	O-C-N	7.36	130.42	123.57	2	3
1	F	28	LYS	O-C-N	-7.36	115.11	122.99	9	2
1	C	14	HIS	CE1-NE2-CD2	-7.35	101.65	109.00	2	4
1	B	18	VAL	CB-CA-C	7.34	123.42	110.71	6	1
1	G	34	LEU	CA-C-O	7.34	130.17	120.11	3	2
1	F	24	VAL	CA-CB-CG1	7.34	122.88	110.40	9	1
1	F	13	HIS	CE1-NE2-CD2	-7.32	101.68	109.00	2	2
1	G	23	ASP	N-CA-C	7.31	120.71	108.20	10	3
1	B	22	GLU	CB-CA-C	7.31	121.59	109.53	1	6
1	B	19	PHE	CB-CA-C	7.29	122.27	110.16	7	1
1	D	17	LEU	CA-C-O	-7.29	112.83	120.70	8	2
1	A	14	HIS	CE1-NE2-CD2	-7.29	101.71	109.00	5	3
1	C	21	ALA	CA-C-N	7.28	132.86	122.09	1	1
1	C	21	ALA	C-N-CA	7.28	132.86	122.09	1	1
1	E	19	PHE	CA-CB-CG	7.27	121.07	113.80	7	2
1	B	32	ILE	CB-CG1-CD1	7.27	129.07	113.80	1	1
1	F	17	LEU	CA-C-O	-7.26	112.53	120.30	7	1
1	E	24	VAL	CA-CB-CG2	7.26	122.75	110.40	10	1
1	D	13	HIS	CA-CB-CG	-7.24	106.56	113.80	4	2
1	C	27	ASN	OD1-CG-ND2	-7.24	115.36	122.60	3	1
1	A	33	GLY	N-CA-C	-7.24	99.73	110.87	4	2
1	F	18	VAL	O-C-N	-7.24	115.25	123.07	5	1
1	A	35	MET	CA-C-N	-7.23	112.30	122.71	10	4
1	A	35	MET	C-N-CA	-7.23	112.30	122.71	10	4
1	D	13	HIS	CA-C-N	7.22	131.13	120.87	7	1
1	D	13	HIS	C-N-CA	7.22	131.13	120.87	7	1
1	E	24	VAL	CA-C-N	7.22	131.27	122.03	9	1
1	E	24	VAL	C-N-CA	7.22	131.27	122.03	9	1
1	C	36	VAL	N-CA-CB	-7.21	98.43	111.92	1	2
1	A	27	ASN	OD1-CG-ND2	-7.19	115.41	122.60	1	4
1	G	29	GLY	CA-C-O	7.17	129.31	121.63	3	3
1	B	27	ASN	OD1-CG-ND2	-7.17	115.43	122.60	10	3
1	E	27	ASN	N-CA-C	7.17	119.47	109.15	5	2
1	F	34	LEU	N-CA-C	7.14	119.72	107.93	4	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	14	HIS	CA-C-N	7.14	131.63	121.42	3	1
1	D	14	HIS	C-N-CA	7.14	131.63	121.42	3	1
1	C	21	ALA	CA-C-O	-7.12	112.67	120.36	5	2
1	G	17	LEU	N-CA-CB	-7.12	99.59	110.77	9	1
1	C	36	VAL	CA-CB-CG2	7.09	122.46	110.40	8	3
1	B	12	VAL	CA-C-N	7.08	130.86	120.95	3	2
1	B	12	VAL	C-N-CA	7.08	130.86	120.95	3	2
1	F	14	HIS	CB-CG-CD2	-7.06	122.02	131.20	6	7
1	G	12	VAL	CA-CB-CG1	7.06	122.40	110.40	2	1
1	B	33	GLY	CA-C-O	-7.05	114.77	121.19	10	2
1	G	25	GLY	CA-C-N	7.05	131.81	121.31	2	2
1	G	25	GLY	C-N-CA	7.05	131.81	121.31	2	2
1	A	35	MET	N-CA-C	-7.04	95.24	107.49	1	6
1	C	34	LEU	O-C-N	7.03	132.97	123.34	8	1
1	C	30	ALA	O-C-N	-7.02	115.03	123.10	7	1
1	E	30	ALA	CA-C-O	-7.01	113.95	121.45	5	3
1	A	29	GLY	CA-C-O	7.00	129.11	121.48	8	3
1	C	37	GLY	CA-C-O	7.00	126.40	120.94	6	1
1	D	14	HIS	CB-CG-CD2	-6.98	122.13	131.20	2	4
1	A	37	GLY	O-C-N	-6.97	115.49	123.51	1	1
1	G	31	ILE	CA-C-N	6.96	129.91	122.11	1	1
1	G	31	ILE	C-N-CA	6.96	129.91	122.11	1	1
1	G	35	MET	CB-CA-C	6.96	119.84	110.94	2	1
1	A	27	ASN	CA-C-O	6.95	128.65	120.58	2	2
1	H	31	ILE	CA-C-O	6.95	128.80	120.74	9	3
1	E	36	VAL	N-CA-C	6.94	117.45	107.88	1	1
1	F	36	VAL	CA-C-N	6.94	130.43	121.27	2	1
1	F	36	VAL	C-N-CA	6.94	130.43	121.27	2	1
1	H	23	ASP	CA-C-O	-6.93	113.55	121.66	6	2
1	A	23	ASP	N-CA-C	6.92	119.11	109.15	10	4
1	F	13	HIS	CA-CB-CG	6.92	120.72	113.80	7	1
1	H	33	GLY	N-CA-C	-6.92	100.22	110.87	9	3
1	G	39	VAL	CA-CB-CG2	6.91	122.15	110.40	2	2
1	B	29	GLY	CA-C-O	6.91	129.83	121.61	1	3
1	A	24	VAL	CA-C-N	6.90	128.79	121.48	2	2
1	A	24	VAL	C-N-CA	6.90	128.79	121.48	2	2
1	C	32	ILE	CB-CA-C	6.89	121.12	111.40	8	6
1	B	19	PHE	CA-CB-CG	6.89	120.69	113.80	9	5
1	C	17	LEU	CA-C-O	-6.89	113.41	120.71	2	1
1	C	36	VAL	N-CA-C	6.89	118.72	108.46	7	2
1	G	30	ALA	CA-C-N	-6.88	113.76	122.43	5	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	G	30	ALA	C-N-CA	-6.88	113.76	122.43	5	7
1	A	27	ASN	CA-CB-CG	6.87	119.47	112.60	3	1
1	E	16	LYS	O-C-N	-6.87	115.19	123.16	4	1
1	F	35	MET	N-CA-CB	-6.86	99.00	110.32	5	6
1	D	29	GLY	CA-C-O	6.85	128.96	121.63	6	1
1	D	22	GLU	CA-C-O	-6.85	112.80	120.54	6	2
1	F	25	GLY	CA-C-N	6.85	131.16	121.02	4	3
1	F	25	GLY	C-N-CA	6.85	131.16	121.02	4	3
1	F	24	VAL	O-C-N	-6.83	115.69	123.07	3	1
1	D	34	LEU	CA-C-O	6.83	128.47	120.14	10	2
1	E	37	GLY	O-C-N	-6.83	117.11	123.25	10	1
1	H	34	LEU	CA-C-N	6.79	132.59	121.86	2	4
1	H	34	LEU	C-N-CA	6.79	132.59	121.86	2	4
1	G	13	HIS	CB-CG-CD2	-6.79	122.37	131.20	8	3
1	B	15	GLN	OE1-CD-NE2	-6.79	115.81	122.60	7	2
1	C	23	ASP	CA-CB-CG	-6.79	105.81	112.60	10	2
1	D	24	VAL	CA-CB-CG1	6.78	121.93	110.40	4	1
1	F	14	HIS	O-C-N	-6.78	114.86	122.86	8	1
1	E	26	SER	N-CA-C	-6.78	99.86	109.96	10	2
1	B	29	GLY	O-C-N	6.77	129.77	123.54	10	2
1	F	30	ALA	CA-C-N	-6.75	114.35	123.12	2	4
1	F	30	ALA	C-N-CA	-6.75	114.35	123.12	2	4
1	B	36	VAL	CA-CB-CG2	6.75	121.87	110.40	6	3
1	B	21	ALA	N-CA-C	-6.75	97.28	108.34	8	2
1	F	24	VAL	N-CA-CB	6.74	122.50	111.58	3	1
1	C	22	GLU	CB-CG-CD	-6.74	101.13	112.60	9	2
1	H	21	ALA	N-CA-CB	-6.74	100.18	110.77	10	1
1	B	35	MET	CB-CA-C	6.74	119.57	110.94	1	3
1	F	39	VAL	O-C-N	-6.73	115.41	123.02	3	1
1	H	32	ILE	CB-CG1-CD1	6.72	127.92	113.80	4	1
1	G	24	VAL	O-C-N	-6.72	115.59	123.05	9	2
1	E	27	ASN	N-CA-CB	-6.71	99.38	109.71	7	1
1	H	35	MET	O-C-N	-6.71	114.95	123.26	8	1
1	D	23	ASP	CA-C-N	-6.69	113.05	122.75	10	1
1	D	23	ASP	C-N-CA	-6.69	113.05	122.75	10	1
1	A	18	VAL	CB-CA-C	6.69	120.10	110.33	2	2
1	F	36	VAL	CA-CB-CG2	6.69	121.77	110.40	6	3
1	H	35	MET	N-CA-C	-6.69	96.90	107.93	8	4
1	A	19	PHE	O-C-N	6.69	131.70	123.21	7	2
1	C	35	MET	CA-C-O	6.68	128.13	119.98	9	2
1	E	25	GLY	CA-C-N	6.68	130.30	120.95	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	E	25	GLY	C-N-CA	6.68	130.30	120.95	8	3
1	D	36	VAL	CA-C-N	6.68	126.79	122.18	4	1
1	D	36	VAL	C-N-CA	6.68	126.79	122.18	4	1
1	G	34	LEU	CA-C-N	6.67	131.84	121.76	5	4
1	G	34	LEU	C-N-CA	6.67	131.84	121.76	5	4
1	F	20	PHE	N-CA-C	6.67	120.03	108.76	8	2
1	F	14	HIS	CA-CB-CG	6.67	120.47	113.80	3	2
1	B	13	HIS	ND1-CE1-NE2	-6.65	101.75	108.40	8	4
1	C	35	MET	O-C-N	-6.64	114.47	123.24	5	5
1	A	31	ILE	CB-CA-C	-6.63	102.03	111.31	9	1
1	B	13	HIS	CB-CA-C	6.63	120.50	109.89	3	1
1	G	39	VAL	O-C-N	-6.63	115.53	123.02	6	1
1	A	34	LEU	CA-C-N	6.62	131.47	121.40	3	4
1	A	34	LEU	C-N-CA	6.62	131.47	121.40	3	4
1	G	28	LYS	CA-C-N	-6.62	114.46	121.48	8	2
1	G	28	LYS	C-N-CA	-6.62	114.46	121.48	8	2
1	B	38	GLY	N-CA-C	6.62	120.41	110.75	8	1
1	F	26	SER	O-C-N	-6.61	114.01	123.07	1	1
1	B	30	ALA	CA-C-O	-6.61	114.37	121.38	3	2
1	B	13	HIS	CB-CG-CD2	-6.61	122.61	131.20	1	3
1	D	17	LEU	CB-CA-C	6.60	121.98	109.37	8	3
1	H	36	VAL	CB-CA-C	6.59	120.70	110.28	3	6
1	F	12	VAL	CA-CB-CG1	6.59	121.60	110.40	6	2
1	H	33	GLY	O-C-N	-6.59	118.26	123.27	2	3
1	G	26	SER	CB-CA-C	6.59	119.64	110.16	10	2
1	A	27	ASN	N-CA-C	6.58	119.32	109.25	5	3
1	D	14	HIS	CA-CB-CG	6.58	120.38	113.80	10	3
1	F	36	VAL	CB-CA-C	6.56	120.92	110.82	7	1
1	B	34	LEU	N-CA-C	6.55	119.40	108.13	3	3
1	A	16	LYS	O-C-N	-6.55	115.75	123.22	6	3
1	B	31	ILE	CB-CG1-CD1	-6.54	100.07	113.80	9	1
1	D	32	ILE	CA-C-O	6.53	126.45	121.09	6	2
1	D	18	VAL	CA-C-N	6.52	132.00	123.00	6	1
1	D	18	VAL	C-N-CA	6.52	132.00	123.00	6	1
1	E	37	GLY	CA-C-O	6.52	126.98	121.11	10	1
1	D	24	VAL	CA-C-O	6.51	127.53	120.43	5	1
1	D	18	VAL	O-C-N	-6.51	116.17	123.20	10	2
1	G	39	VAL	CA-C-O	-6.51	115.19	121.63	3	1
1	A	39	VAL	CA-C-N	6.50	133.40	121.70	7	1
1	A	39	VAL	C-N-CA	6.50	133.40	121.70	7	1
1	F	27	ASN	N-CA-C	6.49	119.13	109.59	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	25	GLY	N-CA-C	6.48	123.14	111.03	7	4
1	F	21	ALA	O-C-N	-6.47	115.48	123.44	5	1
1	D	13	HIS	CE1-NE2-CD2	-6.47	102.53	109.00	4	2
1	G	18	VAL	N-CA-C	6.46	118.02	108.45	2	1
1	H	28	LYS	CA-C-N	-6.46	114.69	121.35	5	2
1	H	28	LYS	C-N-CA	-6.46	114.69	121.35	5	2
1	E	20	PHE	CA-C-N	6.46	132.62	121.64	4	1
1	E	20	PHE	C-N-CA	6.46	132.62	121.64	4	1
1	B	13	HIS	CE1-NE2-CD2	-6.45	102.55	109.00	2	2
1	F	22	GLU	CB-CG-CD	-6.45	101.63	112.60	9	1
1	H	32	ILE	CA-CB-CG2	6.45	121.47	110.50	10	1
1	A	35	MET	CB-CA-C	6.45	119.19	110.94	4	3
1	E	28	LYS	CA-C-O	-6.44	114.42	121.31	10	1
1	F	14	HIS	CG-CD2-NE2	6.44	113.64	107.20	9	2
1	F	13	HIS	CG-CD2-NE2	6.43	113.63	107.20	9	1
1	A	32	ILE	N-CA-C	6.43	116.75	107.88	4	1
1	A	36	VAL	CB-CA-C	6.42	121.82	110.71	6	5
1	G	35	MET	N-CA-C	-6.42	96.32	107.49	2	1
1	F	31	ILE	CA-C-O	-6.42	113.59	120.59	7	1
1	C	15	GLN	CG-CD-NE2	6.41	126.02	116.40	2	1
1	G	30	ALA	CA-C-O	-6.40	114.58	121.36	4	2
1	E	36	VAL	O-C-N	-6.39	117.05	123.19	8	3
1	B	32	ILE	O-C-N	-6.38	117.42	122.97	1	1
1	D	30	ALA	N-CA-C	6.38	118.46	108.96	6	1
1	E	22	GLU	O-C-N	-6.36	115.97	123.22	6	1
1	G	36	VAL	CA-CB-CG2	6.36	121.20	110.40	3	4
1	H	20	PHE	CA-CB-CG	-6.36	107.44	113.80	4	3
1	A	31	ILE	CA-C-N	-6.34	114.20	122.51	2	2
1	A	31	ILE	C-N-CA	-6.34	114.20	122.51	2	2
1	A	37	GLY	CA-C-N	6.34	132.77	121.05	8	1
1	A	37	GLY	C-N-CA	6.34	132.77	121.05	8	1
1	B	13	HIS	ND1-CG-CD2	6.33	112.43	106.10	2	1
1	F	18	VAL	N-CA-C	6.33	117.41	108.17	5	1
1	E	20	PHE	N-CA-C	6.33	118.79	109.24	4	1
1	C	13	HIS	CA-C-O	-6.33	114.67	121.56	10	1
1	D	24	VAL	N-CA-C	6.32	117.40	108.17	6	3
1	H	36	VAL	CA-C-O	6.32	127.32	120.43	3	1
1	C	14	HIS	CB-CG-CD2	-6.32	122.99	131.20	7	2
1	B	20	PHE	CA-CB-CG	6.31	120.11	113.80	6	2
1	F	18	VAL	N-CA-CB	-6.31	101.11	111.45	6	1
1	F	13	HIS	N-CA-C	6.30	119.49	110.10	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	40	VAL	CA-CB-CG2	6.29	121.10	110.40	1	1
1	C	30	ALA	CA-C-N	-6.29	114.94	123.12	6	2
1	C	30	ALA	C-N-CA	-6.29	114.94	123.12	6	2
1	F	28	LYS	CA-C-O	-6.29	114.58	121.31	9	2
1	H	22	GLU	CA-C-O	-6.28	113.83	120.80	9	2
1	F	36	VAL	N-CA-C	6.28	117.82	108.46	6	2
1	D	39	VAL	CA-C-O	-6.28	114.72	121.19	1	2
1	F	40	VAL	CA-CB-CG2	6.28	121.07	110.40	9	1
1	C	14	HIS	ND1-CE1-NE2	6.28	114.68	108.40	2	1
1	B	36	VAL	CG1-CB-CG2	-6.27	97.01	110.80	10	1
1	D	30	ALA	CA-C-O	-6.25	114.75	121.38	1	1
1	D	15	GLN	N-CA-CB	6.24	119.78	110.29	6	1
1	E	31	ILE	N-CA-CB	6.24	118.51	111.21	1	3
1	C	22	GLU	CB-CA-C	6.24	119.82	109.53	9	2
1	C	31	ILE	CA-CB-CG2	6.24	121.10	110.50	9	1
1	C	15	GLN	N-CA-C	6.23	119.50	110.28	7	1
1	G	14	HIS	CE1-NE2-CD2	-6.23	102.77	109.00	7	2
1	H	25	GLY	N-CA-C	-6.23	98.42	113.18	1	2
1	G	27	ASN	CA-CB-CG	6.22	118.82	112.60	7	1
1	C	12	VAL	CA-CB-CG1	6.20	120.94	110.40	7	1
1	E	32	ILE	CB-CG1-CD1	6.20	126.81	113.80	7	1
1	E	26	SER	CB-CA-C	6.18	119.06	110.16	10	1
1	C	24	VAL	CA-CB-CG2	6.18	120.90	110.40	1	1
1	A	36	VAL	CG1-CB-CG2	-6.18	97.21	110.80	3	2
1	B	29	GLY	N-CA-C	6.18	120.16	110.96	9	6
1	D	33	GLY	O-C-N	6.18	129.30	123.56	10	1
1	G	23	ASP	CA-CB-CG	6.17	118.77	112.60	3	1
1	B	33	GLY	N-CA-C	-6.17	99.50	111.03	1	2
1	C	24	VAL	N-CA-C	6.17	117.65	108.46	8	1
1	E	27	ASN	CB-CG-ND2	6.17	125.65	116.40	2	2
1	A	22	GLU	CA-CB-CG	-6.16	101.78	114.10	10	2
1	H	18	VAL	CA-CB-CG1	6.16	120.88	110.40	5	2
1	G	15	GLN	OE1-CD-NE2	-6.15	116.45	122.60	4	2
1	F	24	VAL	CB-CA-C	6.15	119.31	110.33	9	2
1	B	36	VAL	N-CA-C	6.13	117.31	108.48	2	2
1	E	16	LYS	CA-C-O	-6.13	113.38	120.49	3	1
1	F	37	GLY	CA-C-N	6.12	133.41	121.41	6	1
1	F	37	GLY	C-N-CA	6.12	133.41	121.41	6	1
1	C	32	ILE	CB-CG1-CD1	6.12	126.65	113.80	5	2
1	C	13	HIS	CA-CB-CG	-6.11	107.69	113.80	4	1
1	B	25	GLY	CA-C-N	6.10	129.43	120.82	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	25	GLY	C-N-CA	6.10	129.43	120.82	2	2
1	E	18	VAL	O-C-N	-6.10	116.48	123.07	2	1
1	C	15	GLN	N-CA-CB	-6.09	101.02	109.97	7	1
1	F	30	ALA	N-CA-C	6.08	118.02	108.96	4	1
1	H	21	ALA	CA-C-N	6.07	131.10	122.72	6	1
1	H	21	ALA	C-N-CA	6.07	131.10	122.72	6	1
1	B	18	VAL	N-CA-C	6.07	117.43	108.45	5	4
1	H	27	ASN	CB-CG-ND2	6.05	125.47	116.40	1	1
1	F	19	PHE	CA-CB-CG	6.05	119.85	113.80	9	1
1	G	14	HIS	CB-CG-CD2	-6.05	123.34	131.20	10	1
1	C	15	GLN	CA-C-O	6.04	127.76	120.81	6	1
1	E	22	GLU	CA-C-N	6.04	130.45	122.42	10	1
1	E	22	GLU	C-N-CA	6.04	130.45	122.42	10	1
1	B	31	ILE	N-CA-C	6.03	116.79	107.99	9	1
1	E	37	GLY	CA-C-N	6.02	133.21	121.41	1	2
1	E	37	GLY	C-N-CA	6.02	133.21	121.41	1	2
1	H	32	ILE	CB-CA-C	6.01	120.16	111.80	9	3
1	C	34	LEU	CB-CA-C	6.01	119.02	110.24	10	2
1	F	33	GLY	O-C-N	-6.01	118.36	123.23	7	2
1	A	25	GLY	CA-C-O	6.00	128.05	121.63	5	1
1	C	27	ASN	CA-CB-CG	6.00	118.60	112.60	4	2
1	D	38	GLY	O-C-N	5.99	130.48	122.70	8	1
1	A	22	GLU	N-CA-C	5.99	119.66	110.20	2	1
1	H	23	ASP	N-CA-C	5.99	118.52	107.99	5	1
1	C	13	HIS	ND1-CG-CD2	5.99	112.09	106.10	7	1
1	D	37	GLY	O-C-N	-5.98	117.86	123.25	3	1
1	F	22	GLU	CB-CA-C	5.98	120.21	110.22	3	1
1	C	18	VAL	N-CA-C	5.97	116.71	108.12	2	1
1	F	13	HIS	CB-CG-CD2	-5.96	123.45	131.20	3	3
1	F	36	VAL	O-C-N	-5.96	116.72	123.10	2	2
1	A	35	MET	N-CA-CB	-5.96	101.67	110.37	4	2
1	C	31	ILE	CB-CA-C	5.95	119.14	110.98	2	1
1	A	14	HIS	CB-CG-CD2	-5.95	123.46	131.20	5	2
1	C	13	HIS	O-C-N	-5.95	115.84	122.86	1	1
1	D	13	HIS	CB-CG-CD2	-5.95	123.47	131.20	7	2
1	G	32	ILE	CA-CB-CG1	5.95	120.51	110.40	10	1
1	A	37	GLY	CA-C-O	-5.94	115.21	121.57	8	1
1	A	16	LYS	CA-C-O	5.94	127.25	120.54	6	1
1	G	13	HIS	CA-C-O	-5.94	113.69	120.58	2	1
1	G	12	VAL	CA-C-N	5.93	129.18	120.82	7	1
1	G	12	VAL	C-N-CA	5.93	129.18	120.82	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	E	18	VAL	N-CA-C	5.92	117.28	108.46	1	1
1	B	33	GLY	O-C-N	-5.92	118.10	123.54	6	1
1	B	24	VAL	O-C-N	-5.92	116.97	123.18	9	2
1	C	13	HIS	ND1-CE1-NE2	5.92	114.32	108.40	2	1
1	G	18	VAL	CA-CB-CG1	5.91	120.44	110.40	1	1
1	H	32	ILE	O-C-N	5.90	128.10	122.97	9	1
1	D	36	VAL	CB-CA-C	5.89	119.40	110.62	6	1
1	E	32	ILE	CA-C-O	5.89	125.91	120.96	6	1
1	A	14	HIS	N-CA-CB	-5.87	101.41	110.04	9	1
1	H	32	ILE	CA-C-O	5.87	125.89	120.96	6	3
1	C	16	LYS	CA-C-N	5.87	131.09	123.00	1	1
1	C	16	LYS	C-N-CA	5.87	131.09	123.00	1	1
1	E	20	PHE	CA-C-O	5.86	127.85	121.06	7	1
1	H	38	GLY	N-CA-C	5.86	119.15	110.42	10	1
1	H	30	ALA	CA-C-O	-5.85	115.18	121.38	7	2
1	D	36	VAL	CG1-CB-CG2	-5.85	97.94	110.80	4	2
1	C	38	GLY	CA-C-N	5.85	131.23	122.58	5	1
1	C	38	GLY	C-N-CA	5.85	131.23	122.58	5	1
1	B	36	VAL	CB-CA-C	5.84	119.50	110.50	1	2
1	H	32	ILE	CA-CB-CG1	5.84	120.33	110.40	8	2
1	H	34	LEU	CD1-CG-CD2	-5.84	97.95	110.80	7	1
1	G	39	VAL	CG1-CB-CG2	-5.84	97.95	110.80	10	1
1	C	13	HIS	CB-CG-ND1	5.83	131.45	122.70	1	2
1	D	34	LEU	N-CA-C	5.83	118.15	108.13	7	2
1	C	14	HIS	CA-C-O	-5.82	114.64	121.16	9	3
1	D	33	GLY	CA-C-N	5.81	131.00	121.58	3	1
1	D	33	GLY	C-N-CA	5.81	131.00	121.58	3	1
1	A	34	LEU	O-C-N	5.81	130.47	123.26	6	2
1	F	35	MET	CA-C-N	-5.81	114.87	122.94	6	2
1	F	35	MET	C-N-CA	-5.81	114.87	122.94	6	2
1	A	28	LYS	N-CA-C	-5.80	100.54	108.38	8	2
1	B	20	PHE	N-CA-C	5.80	118.86	109.40	7	2
1	G	16	LYS	CA-C-O	5.79	126.55	120.36	10	2
1	E	22	GLU	CB-CA-C	5.79	119.29	109.80	6	3
1	E	23	ASP	N-CA-C	5.78	118.79	107.57	1	1
1	E	39	VAL	CA-CB-CG1	5.77	120.22	110.40	8	1
1	B	24	VAL	N-CA-C	5.77	116.43	108.12	10	1
1	G	26	SER	N-CA-C	-5.77	101.37	109.96	10	1
1	F	14	HIS	N-CA-CB	5.76	118.44	109.97	9	1
1	D	29	GLY	O-C-N	-5.76	118.22	123.57	9	2
1	H	29	GLY	CA-C-O	5.75	127.75	121.48	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	26	SER	CB-CA-C	-5.75	98.97	110.42	7	1
1	C	19	PHE	CA-CB-CG	-5.75	108.05	113.80	4	1
1	D	15	GLN	CA-C-N	5.75	130.06	121.72	6	2
1	D	15	GLN	C-N-CA	5.75	130.06	121.72	6	2
1	C	14	HIS	O-C-N	-5.75	116.67	123.22	4	1
1	G	35	MET	CA-CB-CG	-5.75	102.61	114.10	2	2
1	G	35	MET	CA-C-N	-5.75	114.95	122.94	3	1
1	G	35	MET	C-N-CA	-5.75	114.95	122.94	3	1
1	H	37	GLY	CA-C-O	-5.74	114.85	121.46	4	1
1	F	36	VAL	CG1-CB-CG2	-5.74	98.17	110.80	8	2
1	F	37	GLY	O-C-N	-5.74	118.58	123.23	6	1
1	D	13	HIS	ND1-CE1-NE2	5.74	114.14	108.40	7	3
1	E	20	PHE	CA-CB-CG	-5.73	108.07	113.80	9	1
1	D	35	MET	N-CA-C	-5.73	97.67	107.23	3	1
1	G	24	VAL	CA-C-O	5.72	126.67	120.43	5	2
1	D	28	LYS	CA-C-O	-5.72	115.19	121.31	5	2
1	E	15	GLN	CA-C-O	-5.72	114.97	121.72	9	1
1	F	36	VAL	N-CA-CB	-5.70	102.10	111.44	4	1
1	B	28	LYS	N-CA-C	-5.69	100.89	108.74	4	3
1	B	26	SER	O-C-N	-5.69	115.89	122.95	5	2
1	E	24	VAL	CA-C-O	5.68	126.39	120.36	2	1
1	D	21	ALA	CA-C-N	5.68	130.56	122.72	2	2
1	D	21	ALA	C-N-CA	5.68	130.56	122.72	2	2
1	B	26	SER	N-CA-CB	5.68	117.94	109.19	6	2
1	A	36	VAL	N-CA-CB	-5.68	102.14	111.45	5	1
1	C	18	VAL	CA-C-N	5.68	131.49	122.74	6	1
1	C	18	VAL	C-N-CA	5.68	131.49	122.74	6	1
1	C	14	HIS	ND1-CG-CD2	5.68	111.78	106.10	7	1
1	G	36	VAL	CB-CA-C	5.67	118.62	110.33	1	1
1	G	19	PHE	CA-C-N	5.67	132.13	122.37	2	1
1	G	19	PHE	C-N-CA	5.67	132.13	122.37	2	1
1	B	14	HIS	CA-CB-CG	5.67	119.47	113.80	6	3
1	E	20	PHE	O-C-N	-5.67	116.70	123.27	5	2
1	D	32	ILE	CA-CB-CG2	5.66	120.13	110.50	7	1
1	C	13	HIS	N-CA-C	5.66	118.48	110.50	1	1
1	F	39	VAL	N-CA-C	5.66	117.98	108.81	1	1
1	E	36	VAL	CA-C-O	-5.66	116.20	120.96	2	1
1	F	27	ASN	CB-CG-ND2	5.66	124.89	116.40	10	1
1	H	27	ASN	N-CA-C	5.66	117.91	109.25	1	2
1	E	15	GLN	CA-C-N	5.65	129.91	121.72	3	2
1	E	15	GLN	C-N-CA	5.65	129.91	121.72	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	E	30	ALA	N-CA-CB	-5.65	102.63	111.56	4	1
1	D	29	GLY	CA-C-N	5.64	131.45	121.80	5	1
1	D	29	GLY	C-N-CA	5.64	131.45	121.80	5	1
1	A	39	VAL	CA-CB-CG2	5.64	119.99	110.40	5	1
1	F	30	ALA	CA-C-O	-5.64	115.20	121.51	1	1
1	G	28	LYS	O-C-N	-5.64	116.96	122.99	5	1
1	B	19	PHE	O-C-N	-5.63	116.81	123.22	3	1
1	D	29	GLY	N-CA-C	5.62	119.34	110.96	2	1
1	C	26	SER	O-C-N	-5.62	115.97	122.95	10	1
1	D	18	VAL	CG1-CB-CG2	-5.62	98.44	110.80	1	1
1	H	35	MET	CB-CA-C	5.62	118.44	110.24	3	2
1	C	39	VAL	CA-C-O	-5.61	114.78	121.28	2	2
1	H	31	ILE	CB-CA-C	5.61	119.16	111.31	4	1
1	A	40	VAL	CG1-CB-CG2	-5.60	98.47	110.80	2	1
1	G	22	GLU	O-C-N	-5.60	116.66	123.16	8	1
1	A	18	VAL	N-CA-CB	-5.57	103.08	112.44	1	1
1	A	26	SER	CA-C-N	-5.57	113.21	121.24	8	1
1	A	26	SER	C-N-CA	-5.57	113.21	121.24	8	1
1	F	29	GLY	O-C-N	-5.57	118.53	123.65	2	1
1	B	14	HIS	O-C-N	-5.57	116.67	122.96	9	1
1	C	39	VAL	CA-CB-CG1	5.56	119.86	110.40	5	1
1	B	16	LYS	CA-C-N	5.56	130.84	123.00	10	1
1	B	16	LYS	C-N-CA	5.56	130.84	123.00	10	1
1	E	36	VAL	CA-CB-CG2	5.56	119.85	110.40	9	2
1	D	17	LEU	O-C-N	5.55	129.91	123.30	1	1
1	A	39	VAL	N-CA-C	5.55	117.40	108.85	3	1
1	B	39	VAL	CA-C-N	5.55	131.69	121.70	1	2
1	B	39	VAL	C-N-CA	5.55	131.69	121.70	1	2
1	F	14	HIS	ND1-CE1-NE2	5.55	113.95	108.40	2	1
1	G	13	HIS	CA-CB-CG	5.55	119.35	113.80	10	1
1	A	22	GLU	CA-C-N	5.54	130.56	122.41	9	1
1	A	22	GLU	C-N-CA	5.54	130.56	122.41	9	1
1	D	30	ALA	CA-C-N	-5.54	115.58	123.11	2	1
1	D	30	ALA	C-N-CA	-5.54	115.58	123.11	2	1
1	D	32	ILE	CB-CA-C	5.54	119.20	111.40	6	2
1	G	21	ALA	CA-C-O	5.53	127.69	120.11	10	1
1	B	26	SER	CA-C-O	-5.53	114.93	120.96	1	2
1	F	24	VAL	CA-C-O	5.53	126.22	120.36	9	1
1	A	22	GLU	CG-CD-OE2	5.52	131.10	118.40	7	1
1	E	35	MET	CA-C-N	-5.52	115.28	122.51	4	1
1	E	35	MET	C-N-CA	-5.52	115.28	122.51	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	F	13	HIS	CA-C-N	5.52	128.71	120.87	9	1
1	F	13	HIS	C-N-CA	5.52	128.71	120.87	9	1
1	H	28	LYS	CA-C-O	-5.52	115.26	121.05	3	1
1	B	38	GLY	CA-C-O	-5.52	115.66	121.56	9	1
1	H	23	ASP	CA-CB-CG	5.52	118.12	112.60	9	1
1	C	34	LEU	N-CA-C	5.51	117.20	107.61	2	3
1	B	32	ILE	CA-CB-CG2	5.51	119.86	110.50	9	1
1	E	17	LEU	CB-CA-C	5.50	119.28	109.65	10	1
1	B	37	GLY	N-CA-C	-5.50	102.71	111.18	3	1
1	D	37	GLY	N-CA-C	5.49	120.80	111.19	4	1
1	C	35	MET	CA-C-N	-5.49	115.31	122.94	2	1
1	C	35	MET	C-N-CA	-5.49	115.31	122.94	2	1
1	G	30	ALA	N-CA-C	5.49	116.31	108.74	4	2
1	F	24	VAL	CA-C-N	5.48	132.16	121.41	1	1
1	F	24	VAL	C-N-CA	5.48	132.16	121.41	1	1
1	G	26	SER	CA-C-O	5.48	126.43	120.95	3	1
1	F	35	MET	CA-C-O	5.47	126.39	119.98	2	2
1	D	31	ILE	O-C-N	-5.47	116.69	123.10	3	1
1	G	28	LYS	CA-C-O	-5.47	115.45	121.31	6	1
1	G	16	LYS	CA-C-N	5.47	130.49	122.77	9	2
1	G	16	LYS	C-N-CA	5.47	130.49	122.77	9	2
1	H	37	GLY	CA-C-N	5.47	126.28	121.58	6	1
1	H	37	GLY	C-N-CA	5.47	126.28	121.58	6	1
1	A	16	LYS	N-CA-C	5.47	118.54	109.46	8	1
1	H	25	GLY	CA-C-O	-5.47	116.21	121.19	6	1
1	F	17	LEU	N-CA-CB	-5.47	101.34	110.80	8	1
1	H	36	VAL	N-CA-CB	-5.46	102.40	111.36	4	1
1	F	27	ASN	O-C-N	5.46	129.73	123.02	3	1
1	E	21	ALA	N-CA-CB	-5.46	101.35	110.57	4	1
1	H	34	LEU	O-C-N	-5.46	115.87	123.34	4	1
1	E	39	VAL	CA-C-N	5.46	131.52	121.70	10	2
1	E	39	VAL	C-N-CA	5.46	131.52	121.70	10	2
1	D	12	VAL	CA-C-N	5.45	130.08	120.87	1	1
1	D	12	VAL	C-N-CA	5.45	130.08	120.87	1	1
1	F	15	GLN	O-C-N	-5.45	116.29	123.21	1	1
1	A	15	GLN	O-C-N	-5.44	116.59	123.01	8	1
1	A	14	HIS	CA-CB-CG	5.44	119.24	113.80	2	1
1	B	33	GLY	CA-C-N	-5.43	113.55	121.76	7	1
1	B	33	GLY	C-N-CA	-5.43	113.55	121.76	7	1
1	G	19	PHE	CA-C-O	-5.42	114.50	120.36	6	1
1	A	15	GLN	CA-C-N	5.42	130.72	122.65	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	GLN	C-N-CA	5.42	130.72	122.65	1	1
1	C	29	GLY	O-C-N	5.42	128.53	123.54	10	1
1	D	22	GLU	O-C-N	-5.42	117.05	123.22	1	1
1	A	26	SER	N-CA-C	-5.42	100.97	109.25	10	1
1	E	22	GLU	N-CA-CB	-5.41	101.59	110.41	3	1
1	F	17	LEU	CB-CA-C	5.41	119.06	110.19	3	1
1	A	18	VAL	O-C-N	-5.40	117.36	123.20	8	1
1	C	32	ILE	CA-CB-CG2	5.40	119.68	110.50	9	1
1	D	16	LYS	N-CA-C	-5.40	102.29	110.28	3	1
1	A	27	ASN	O-C-N	5.40	129.76	122.96	9	2
1	C	28	LYS	CG-CD-CE	5.40	123.71	111.30	9	1
1	F	39	VAL	CA-CB-CG1	5.39	119.57	110.40	10	2
1	G	34	LEU	O-C-N	5.39	129.83	123.36	7	1
1	G	15	GLN	N-CA-CB	5.39	120.29	111.08	3	1
1	E	27	ASN	O-C-N	5.39	129.56	122.93	8	2
1	F	31	ILE	CB-CA-C	-5.39	103.10	110.96	10	1
1	B	36	VAL	N-CA-CB	-5.38	103.40	112.44	10	1
1	B	19	PHE	CA-C-O	-5.38	115.01	120.71	8	1
1	D	26	SER	O-C-N	-5.37	115.45	122.59	4	1
1	E	24	VAL	O-C-N	-5.37	117.36	123.10	5	1
1	D	14	HIS	CG-CD2-NE2	-5.37	101.83	107.20	9	1
1	E	24	VAL	CA-CB-CG1	5.36	119.52	110.40	8	1
1	C	39	VAL	O-C-N	5.36	128.74	123.00	10	1
1	C	24	VAL	CB-CA-C	-5.36	102.50	110.33	2	1
1	D	14	HIS	CB-CG-ND1	5.36	130.74	122.70	5	2
1	H	20	PHE	N-CA-C	5.36	117.33	109.24	10	1
1	F	12	VAL	CA-CB-CG2	5.36	119.51	110.40	9	2
1	B	27	ASN	CA-CB-CG	5.35	117.95	112.60	3	1
1	G	36	VAL	N-CA-C	5.35	116.44	108.46	9	1
1	G	13	HIS	N-CA-C	5.35	117.93	109.96	4	1
1	D	27	ASN	OD1-CG-ND2	-5.35	117.25	122.60	9	1
1	G	36	VAL	N-CA-CB	-5.35	103.72	111.52	7	1
1	A	21	ALA	CA-C-O	5.34	126.13	120.36	3	1
1	B	20	PHE	CA-C-N	5.34	131.18	121.89	1	1
1	B	20	PHE	C-N-CA	5.34	131.18	121.89	1	1
1	G	27	ASN	O-C-N	5.34	129.31	123.01	10	1
1	B	28	LYS	CB-CG-CD	5.32	123.53	111.30	7	1
1	G	15	GLN	O-C-N	-5.31	117.10	123.31	5	1
1	D	36	VAL	CA-C-O	5.31	126.60	120.76	4	1
1	B	37	GLY	CA-C-O	5.31	126.25	121.47	5	1
1	F	32	ILE	CB-CA-C	5.31	119.56	110.38	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	F	30	ALA	CB-CA-C	-5.31	99.04	111.09	4	1
1	B	14	HIS	CB-CG-CD2	-5.31	124.30	131.20	8	1
1	C	14	HIS	N-CA-CB	-5.30	102.17	109.97	9	1
1	H	36	VAL	CA-C-N	5.30	131.84	121.93	10	1
1	H	36	VAL	C-N-CA	5.30	131.84	121.93	10	1
1	H	30	ALA	O-C-N	-5.29	117.21	123.25	3	1
1	G	31	ILE	N-CA-CB	5.29	117.82	111.31	5	1
1	G	22	GLU	CB-CA-C	5.29	118.48	109.80	9	1
1	D	30	ALA	O-C-N	5.29	129.18	123.10	2	1
1	H	20	PHE	CA-C-O	-5.29	114.04	120.54	2	1
1	G	31	ILE	CA-CB-CG2	5.28	119.48	110.50	5	1
1	D	39	VAL	CA-CB-CG1	5.28	119.38	110.40	10	1
1	H	21	ALA	CA-C-O	-5.28	114.65	120.24	1	1
1	A	32	ILE	CA-CB-CG2	5.28	119.47	110.50	3	1
1	E	39	VAL	CA-CB-CG2	5.28	119.37	110.40	5	1
1	C	23	ASP	CA-C-O	5.27	126.40	120.92	4	1
1	D	28	LYS	CA-C-N	-5.27	113.78	121.26	8	1
1	D	28	LYS	C-N-CA	-5.27	113.78	121.26	8	1
1	B	14	HIS	CE1-NE2-CD2	-5.26	103.73	109.00	8	1
1	H	26	SER	O-C-N	-5.26	115.59	122.59	5	1
1	D	31	ILE	CB-CG1-CD1	5.26	124.85	113.80	2	1
1	E	38	GLY	CA-C-O	-5.26	111.42	120.57	6	1
1	E	34	LEU	N-CA-CB	5.26	119.27	110.59	10	1
1	A	24	VAL	O-C-N	-5.26	117.39	123.07	1	1
1	B	28	LYS	CA-C-N	-5.26	115.94	121.35	8	1
1	B	28	LYS	C-N-CA	-5.26	115.94	121.35	8	1
1	A	23	ASP	CA-C-N	5.26	130.30	122.99	9	1
1	A	23	ASP	C-N-CA	5.26	130.30	122.99	9	1
1	D	28	LYS	O-C-N	5.25	128.61	122.99	8	2
1	D	20	PHE	CG-CD1-CE1	-5.25	111.78	120.70	3	1
1	A	24	VAL	N-CA-C	-5.25	100.51	108.17	1	1
1	H	31	ILE	N-CA-C	5.24	115.32	107.51	2	1
1	G	37	GLY	CA-C-O	5.24	125.03	120.94	7	1
1	A	34	LEU	N-CA-C	-5.24	99.29	107.93	6	1
1	C	23	ASP	CA-C-N	5.24	130.22	122.94	1	1
1	C	23	ASP	C-N-CA	5.24	130.22	122.94	1	1
1	F	34	LEU	N-CA-CB	-5.24	101.72	110.57	1	1
1	B	37	GLY	O-C-N	-5.23	118.71	123.36	5	1
1	G	29	GLY	O-C-N	5.23	128.35	123.54	4	1
1	B	39	VAL	CA-CB-CG2	5.23	119.28	110.40	7	1
1	B	34	LEU	O-C-N	5.22	129.63	123.36	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	F	14	HIS	CA-C-O	-5.22	115.31	121.16	5	1
1	F	12	VAL	CG1-CB-CG2	-5.22	99.32	110.80	2	1
1	C	16	LYS	CA-C-O	5.21	126.16	120.58	1	1
1	A	39	VAL	CB-CA-C	5.21	119.03	110.69	9	1
1	F	20	PHE	CA-C-O	5.21	126.69	120.28	7	1
1	F	29	GLY	CA-C-O	5.20	127.47	121.49	2	1
1	F	30	ALA	N-CA-CB	-5.20	103.34	111.56	6	2
1	G	26	SER	O-C-N	-5.20	117.29	123.11	3	1
1	E	40	VAL	N-CA-CB	-5.20	102.67	111.50	7	1
1	F	19	PHE	N-CA-C	-5.20	101.24	109.76	10	1
1	C	17	LEU	O-C-N	-5.19	116.93	123.27	3	1
1	B	16	LYS	O-C-N	-5.19	117.09	122.96	9	1
1	C	18	VAL	N-CA-CB	-5.19	103.17	111.58	5	1
1	D	38	GLY	CA-C-O	-5.19	116.51	121.49	9	1
1	F	19	PHE	O-C-N	-5.19	117.14	123.16	3	1
1	C	19	PHE	CB-CG-CD2	-5.18	111.90	120.70	9	1
1	C	22	GLU	O-C-N	-5.17	117.32	123.22	6	2
1	C	17	LEU	CA-C-N	5.17	129.92	123.14	8	1
1	C	17	LEU	C-N-CA	5.17	129.92	123.14	8	1
1	A	36	VAL	N-CA-C	5.17	116.10	108.45	1	1
1	A	17	LEU	CA-C-N	5.16	129.66	122.23	9	1
1	A	17	LEU	C-N-CA	5.16	129.66	122.23	9	1
1	E	32	ILE	CA-CB-CG2	5.16	119.27	110.50	7	1
1	C	16	LYS	CB-CA-C	5.16	118.14	109.48	7	2
1	H	30	ALA	N-CA-CB	-5.15	103.05	111.66	1	1
1	B	35	MET	N-CA-C	-5.15	98.52	107.49	6	1
1	F	32	ILE	CA-CB-CG1	5.15	119.16	110.40	5	1
1	D	16	LYS	O-C-N	-5.15	117.01	123.04	9	1
1	F	32	ILE	CA-C-O	5.15	126.60	121.45	8	1
1	G	24	VAL	N-CA-C	5.14	115.53	108.12	7	1
1	A	24	VAL	CA-C-O	-5.14	114.82	120.43	6	1
1	G	15	GLN	CA-C-N	5.14	129.43	122.19	5	1
1	G	15	GLN	C-N-CA	5.14	129.43	122.19	5	1
1	H	27	ASN	O-C-N	5.14	129.43	122.96	7	1
1	G	14	HIS	CB-CA-C	5.13	118.10	109.89	10	1
1	A	18	VAL	CA-C-N	5.13	129.22	122.30	6	1
1	A	18	VAL	C-N-CA	5.13	129.22	122.30	6	1
1	C	20	PHE	N-CA-CB	5.13	120.41	111.13	10	1
1	E	18	VAL	CA-C-N	5.12	130.35	122.93	5	1
1	E	18	VAL	C-N-CA	5.12	130.35	122.93	5	1
1	D	39	VAL	O-C-N	5.12	128.73	123.05	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	20	PHE	CA-C-N	5.12	129.97	122.39	8	1
1	C	20	PHE	C-N-CA	5.12	129.97	122.39	8	1
1	C	33	GLY	N-CA-C	-5.12	101.93	111.14	10	1
1	G	40	VAL	CA-CB-CG1	5.12	119.10	110.40	10	1
1	G	26	SER	N-CA-CB	5.12	117.07	109.19	9	1
1	B	17	LEU	N-CA-CB	-5.12	102.67	110.65	9	2
1	F	39	VAL	CA-C-O	-5.11	115.43	120.90	10	1
1	B	34	LEU	CA-C-O	5.11	125.96	119.98	2	1
1	G	40	VAL	CB-CA-C	5.11	121.11	111.40	2	1
1	F	23	ASP	CA-CB-CG	-5.11	107.49	112.60	9	1
1	D	25	GLY	O-C-N	-5.11	116.06	122.70	2	1
1	B	18	VAL	N-CA-CB	-5.11	103.08	111.45	6	1
1	C	28	LYS	N-CA-C	5.10	114.97	108.24	3	1
1	D	32	ILE	CB-CG1-CD1	5.10	124.51	113.80	6	1
1	F	39	VAL	CA-C-N	5.10	130.88	121.70	2	1
1	F	39	VAL	C-N-CA	5.10	130.88	121.70	2	1
1	D	31	ILE	N-CA-C	5.10	114.92	107.37	2	1
1	H	24	VAL	CA-CB-CG1	5.08	119.04	110.40	4	1
1	F	13	HIS	CB-CG-ND1	5.08	130.32	122.70	9	1
1	C	25	GLY	CA-C-N	5.08	128.31	121.05	5	1
1	C	25	GLY	C-N-CA	5.08	128.31	121.05	5	1
1	B	12	VAL	CB-CA-C	5.08	121.05	111.40	8	1
1	H	22	GLU	O-C-N	-5.07	117.54	123.27	5	1
1	B	30	ALA	N-CA-CB	-5.07	103.66	111.46	3	1
1	A	34	LEU	CD1-CG-CD2	-5.06	99.66	110.80	4	1
1	F	14	HIS	CB-CA-C	5.06	118.77	109.46	1	1
1	E	15	GLN	CB-CG-CD	-5.06	103.99	112.60	4	1
1	F	19	PHE	CB-CA-C	5.06	117.88	109.53	5	1
1	A	39	VAL	N-CA-CB	-5.05	103.15	111.44	2	1
1	F	12	VAL	CA-C-N	5.05	128.03	120.95	10	1
1	F	12	VAL	C-N-CA	5.05	128.03	120.95	10	1
1	G	33	GLY	CA-C-O	-5.04	116.52	121.06	4	1
1	F	15	GLN	CB-CA-C	5.04	118.59	109.37	9	1
1	C	22	GLU	CA-C-O	-5.04	115.13	120.92	3	1
1	A	14	HIS	CB-CG-ND1	5.04	130.25	122.70	10	1
1	F	32	ILE	CA-C-N	-5.03	116.68	121.46	2	1
1	F	32	ILE	C-N-CA	-5.03	116.68	121.46	2	1
1	C	13	HIS	CE1-NE2-CD2	-5.01	103.99	109.00	3	1
1	A	20	PHE	CA-C-N	-5.01	116.03	123.05	7	1
1	A	20	PHE	C-N-CA	-5.01	116.03	123.05	7	1
1	A	23	ASP	CA-C-O	-5.01	115.80	121.66	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	23	ASP	O-C-N	-5.01	116.31	122.82	6	1
1	E	22	GLU	CB-CG-CD	-5.00	104.09	112.60	1	1
1	C	22	GLU	N-CA-C	5.00	118.37	109.96	1	1
1	F	26	SER	CA-C-N	-5.00	114.04	121.24	4	1
1	F	26	SER	C-N-CA	-5.00	114.04	121.24	4	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	H	20	PHE	Sidechain	8
1	F	20	PHE	Sidechain	7
1	B	20	PHE	Sidechain	7
1	D	35	MET	Mainchain	7
1	F	35	MET	Mainchain	7
1	D	20	PHE	Sidechain	6
1	C	20	PHE	Sidechain	6
1	E	20	PHE	Sidechain	6
1	G	35	MET	Mainchain	5
1	A	35	MET	Mainchain	4
1	C	35	MET	Mainchain	4
1	B	35	MET	Mainchain	4
1	G	20	PHE	Sidechain	4
1	B	14	HIS	Sidechain,Mainchain	2
1	G	19	PHE	Sidechain	2
1	F	19	PHE	Sidechain	2
1	A	19	PHE	Sidechain	2
1	G	14	HIS	Sidechain	1
1	A	39	VAL	Mainchain	1
1	A	20	PHE	Sidechain	1
1	A	32	ILE	Peptide	1
1	F	13	HIS	Sidechain	1
1	H	33	GLY	Peptide	1
1	A	14	HIS	Sidechain	1
1	B	30	ALA	Mainchain	1
1	B	13	HIS	Sidechain	1
1	C	19	PHE	Sidechain	1
1	A	23	ASP	Mainchain	1
1	D	30	ALA	Mainchain	1

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	196	203	203	1±1
1	B	213	219	218	3±1
1	C	213	219	218	2±1
1	D	213	219	218	3±1
1	E	186	196	196	4±2
1	F	213	219	218	3±1
1	G	213	219	218	3±1
1	H	145	146	146	1±1
All	All	15920	16400	16349	117

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:36:VAL:H	1:G:36:VAL:H	0.82	1.17	3	10
1:B:36:VAL:H	1:C:36:VAL:H	0.77	1.22	9	10
1:D:36:VAL:H	1:E:36:VAL:H	0.72	1.26	3	10
1:H:20:PHE:CZ	1:H:34:LEU:HD22	0.68	2.24	5	3
1:B:36:VAL:N	1:C:36:VAL:H	0.63	1.92	9	6
1:F:36:VAL:N	1:G:36:VAL:H	0.62	1.91	6	7
1:D:36:VAL:N	1:E:36:VAL:H	0.58	1.97	8	9
1:E:31:ILE:HG22	1:F:35:MET:CG	0.54	2.32	2	1
1:G:30:ALA:CB	1:H:36:VAL:HG23	0.54	2.33	6	3
1:H:20:PHE:CE1	1:H:34:LEU:HD22	0.54	2.38	5	2
1:B:23:ASP:H	1:B:32:ILE:CD1	0.52	2.17	8	1
1:E:17:LEU:HD13	1:E:18:VAL:N	0.52	2.20	6	1
1:C:20:PHE:CE1	1:C:34:LEU:HD11	0.51	2.40	5	2
1:A:30:ALA:HB1	1:B:37:GLY:H	0.50	1.66	1	2
1:A:32:ILE:HD12	1:B:34:LEU:HD21	0.50	1.82	9	1
1:B:36:VAL:H	1:C:36:VAL:N	0.50	2.01	4	1
1:A:31:ILE:HB	1:B:35:MET:HG3	0.50	1.83	1	1
1:G:33:GLY:O	1:H:32:ILE:HA	0.49	2.07	8	1
1:E:35:MET:O	1:E:36:VAL:HB	0.49	2.06	3	4
1:D:36:VAL:H	1:E:36:VAL:N	0.49	2.04	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ALA:HB3	1:B:19:PHE:O	0.49	2.07	3	1
1:G:20:PHE:CD1	1:G:34:LEU:HD11	0.48	2.44	5	1
1:D:20:PHE:O	1:E:16:LYS:HE3	0.47	2.07	10	2
1:B:15:GLN:HA	1:B:40:VAL:HG12	0.46	1.87	9	1
1:F:22:GLU:H	1:G:39:VAL:CG1	0.46	2.22	10	1
1:C:35:MET:CG	1:D:31:ILE:HG22	0.46	2.40	9	1
1:E:35:MET:C	1:F:31:ILE:O	0.45	2.60	2	4
1:A:31:ILE:C	1:A:32:ILE:HG22	0.45	2.37	2	3
1:B:33:GLY:O	1:B:34:LEU:HD22	0.45	2.12	3	1
1:F:36:VAL:H	1:G:36:VAL:N	0.45	2.07	7	2
1:C:20:PHE:CZ	1:C:34:LEU:HD21	0.45	2.47	1	1
1:E:31:ILE:HG22	1:F:35:MET:HG2	0.44	1.89	2	1
1:E:37:GLY:H	1:F:30:ALA:HB1	0.44	1.72	6	1
1:E:31:ILE:CG2	1:F:35:MET:CG	0.44	2.95	2	1
1:G:32:ILE:HB	1:H:34:LEU:HG	0.44	1.90	6	1
1:C:35:MET:HG3	1:D:31:ILE:HB	0.43	1.88	2	1
1:A:30:ALA:CB	1:B:37:GLY:H	0.43	2.26	1	2
1:C:31:ILE:HG22	1:D:35:MET:CG	0.42	2.43	9	1
1:C:20:PHE:CE1	1:D:21:ALA:O	0.42	2.73	2	1
1:F:36:VAL:N	1:G:36:VAL:N	0.42	2.65	6	1
1:C:28:LYS:HE2	1:D:39:VAL:O	0.42	2.15	8	1
1:F:20:PHE:CE1	1:F:34:LEU:HD11	0.42	2.50	10	2
1:E:35:MET:CG	1:F:31:ILE:HG22	0.41	2.45	4	1
1:E:17:LEU:HD11	1:E:19:PHE:CE2	0.41	2.50	2	1
1:E:31:ILE:HB	1:F:35:MET:HG3	0.41	1.92	1	1
1:D:20:PHE:CE2	1:D:34:LEU:HD21	0.41	2.51	4	1
1:A:20:PHE:CE1	1:A:34:LEU:HD22	0.41	2.51	2	1
1:E:31:ILE:O	1:F:35:MET:C	0.41	2.64	6	1
1:G:21:ALA:O	1:H:20:PHE:CE1	0.40	2.75	6	1
1:A:31:ILE:HB	1:B:35:MET:CG	0.40	2.46	3	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	26/40 (65%)	26±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	27/40 (68%)	27±0 (99±1%)	0±0 (1±1%)	0±0 (0±0%)	100	100
1	C	27/40 (68%)	26±1 (96±2%)	1±1 (4±2%)	0±0 (0±1%)	31	76
1	D	27/40 (68%)	26±1 (95±2%)	0±1 (1±2%)	1±0 (4±0%)	4	32
1	E	25/40 (62%)	25±0 (98±2%)	0±0 (1±2%)	0±0 (0±1%)	31	76
1	F	27/40 (68%)	26±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
1	G	27/40 (68%)	26±0 (98±2%)	1±0 (2±2%)	0±0 (0±0%)	100	100
1	H	21/40 (52%)	20±0 (93±2%)	0±0 (2±2%)	1±0 (5±0%)	3	25
All	All	2070/3200 (65%)	2013 (97%)	35 (2%)	22 (1%)	14	63

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	D	26	SER	10
1	H	26	SER	10
1	E	26	SER	1
1	C	26	SER	1

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	20/31 (65%)	16±1 (80±3%)	4±1 (20±3%)	3	33
1	B	22/31 (71%)	19±1 (88±3%)	3±1 (12±3%)	7	49
1	C	22/31 (71%)	19±1 (85±4%)	3±1 (15±4%)	5	41
1	D	22/31 (71%)	19±1 (87±3%)	3±1 (13±3%)	6	47
1	E	19/31 (61%)	14±1 (75±6%)	5±1 (25±6%)	2	25
1	F	22/31 (71%)	18±1 (82±5%)	4±1 (18±5%)	3	36
1	G	22/31 (71%)	20±1 (92±4%)	2±1 (8±4%)	14	61
1	H	14/31 (45%)	10±1 (71±6%)	4±1 (29±6%)	1	18
All	All	1630/2480 (66%)	1357 (83%)	273 (17%)	4	39

All 61 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	32	ILE	10
1	A	35	MET	10
1	B	32	ILE	10
1	B	34	LEU	10
1	C	32	ILE	10
1	C	34	LEU	10
1	D	32	ILE	10
1	D	34	LEU	10
1	E	32	ILE	10
1	E	34	LEU	10
1	E	35	MET	10
1	F	32	ILE	10
1	F	34	LEU	10
1	G	34	LEU	10
1	H	32	ILE	10
1	H	36	VAL	10
1	A	34	LEU	9
1	H	20	PHE	9
1	C	20	PHE	8
1	F	16	LYS	8
1	H	34	LEU	7
1	A	20	PHE	5
1	F	20	PHE	4
1	E	20	PHE	4
1	A	36	VAL	4
1	E	16	LYS	3
1	E	17	LEU	3
1	E	31	ILE	3
1	B	19	PHE	3
1	G	32	ILE	2
1	G	40	VAL	2
1	D	17	LEU	2
1	D	40	VAL	2
1	E	36	VAL	2
1	F	18	VAL	2
1	B	27	ASN	2
1	H	35	MET	2
1	C	31	ILE	2
1	F	12	VAL	2
1	F	35	MET	2
1	A	18	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	H	24	VAL	1
1	A	39	VAL	1
1	C	18	VAL	1
1	C	39	VAL	1
1	F	36	VAL	1
1	D	18	VAL	1
1	E	19	PHE	1
1	C	24	VAL	1
1	D	36	VAL	1
1	E	39	VAL	1
1	H	26	SER	1
1	F	22	GLU	1
1	G	13	HIS	1
1	B	22	GLU	1
1	D	20	PHE	1
1	G	20	PHE	1
1	G	39	VAL	1
1	H	18	VAL	1
1	C	17	LEU	1
1	D	12	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 4% for the well-defined parts and 4% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Chemical_shifts_Abeta.txt*

7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	135
Number of shifts mapped to atoms	135
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	29	2.00 ± 0.45	Should be checked
$^{13}\text{C}_\beta$	23	—	None (insufficient data)
$^{13}\text{C}'$	27	2.70 ± 0.29	Should be applied
^{15}N	28	1.66 ± 0.70	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 4%, i.e. 123 atoms were assigned a chemical shift out of a possible 2863. 0 out of 58 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	80/1135 (7%)	0/478 (0%)	53/438 (12%)	27/219 (12%)
Sidechain	39/1491 (3%)	0/996 (0%)	39/465 (8%)	0/30 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	4/237 (2%)	0/124 (0%)	4/102 (4%)	0/11 (0%)
Overall	123/2863 (4%)	0/1598 (0%)	96/1005 (10%)	27/260 (10%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 4%, i.e. 131 atoms were assigned a chemical shift out of a possible 3064. 0 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	84/1200 (7%)	0/504 (0%)	56/464 (12%)	28/232 (12%)
Sidechain	42/1592 (3%)	0/1064 (0%)	42/496 (8%)	0/32 (0%)
Aromatic	5/272 (2%)	0/144 (0%)	5/112 (4%)	0/16 (0%)
Overall	131/3064 (4%)	0/1712 (0%)	103/1072 (10%)	28/280 (10%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	15	GLN	CD	173.25	173.59 – 185.85	-5.3

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

