



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 12:53 PM UTC

PDB ID : 2NNT / pdb_00002nnt
Title : General structural motifs of amyloid protofilaments
Authors : Ferguson, N.; Becker, J.; Tidow, H.; Tremmel, S.; Sharpe, T.D.; Krause, G.;
Flinders, J.; Petrovich, M.; Berriman, J.; Oschkinat, H.; Fersht, A.R.
Deposited on : 2006-10-24

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

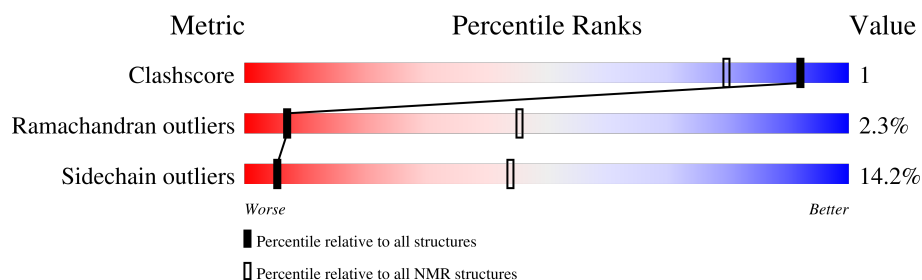
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment 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	40	 45% 30% • 22%
1	B	40	 45% 25% 8% 22%
1	C	40	 58% 18% • 22%
1	D	40	 52% 22% • 22%

2 Ensemble composition and analysis

This entry contains 10 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:201-A:230, B:300-B:330, C:400-C:430, D:500-D:530 (123)	0.46	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 3 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1944 atoms, of which 924 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription elongation regulator 1.

Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			486	162	231	40	52	1	
1	B	31	Total	C	H	N	O	S	0
			486	162	231	40	52	1	
1	C	31	Total	C	H	N	O	S	0
			486	162	231	40	52	1	
1	D	31	Total	C	H	N	O	S	0
			486	162	231	40	52	1	

There are 16 discrepancies between the modelled and reference sequences:

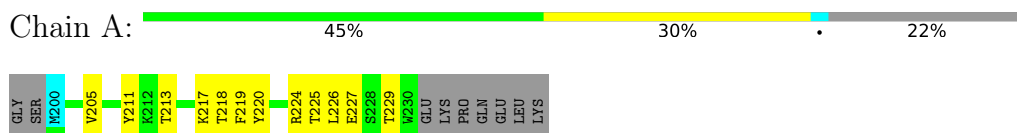
Chain	Residue	Modelled	Actual	Comment	Reference
A	198	GLY	-	cloning artifact	UNP O14776
A	199	SER	-	cloning artifact	UNP O14776
A	200	MET	-	cloning artifact	UNP O14776
A	219	PHE	TYR	engineered mutation	UNP O14776
B	298	GLY	-	cloning artifact	UNP O14776
B	299	SER	-	cloning artifact	UNP O14776
B	300	MET	-	cloning artifact	UNP O14776
B	319	PHE	TYR	engineered mutation	UNP O14776
C	398	GLY	-	cloning artifact	UNP O14776
C	399	SER	-	cloning artifact	UNP O14776
C	400	MET	-	cloning artifact	UNP O14776
C	419	PHE	TYR	engineered mutation	UNP O14776
D	498	GLY	-	cloning artifact	UNP O14776
D	499	SER	-	cloning artifact	UNP O14776
D	500	MET	-	cloning artifact	UNP O14776
D	519	PHE	TYR	engineered mutation	UNP O14776

4 Residue-property plots [i](#)

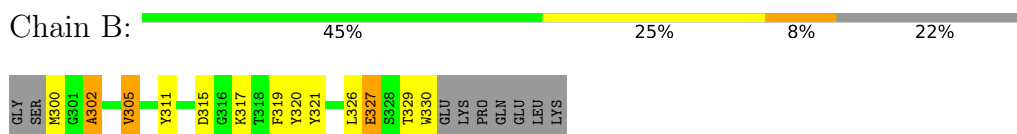
4.1 Average score per residue in the NMR ensemble

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.

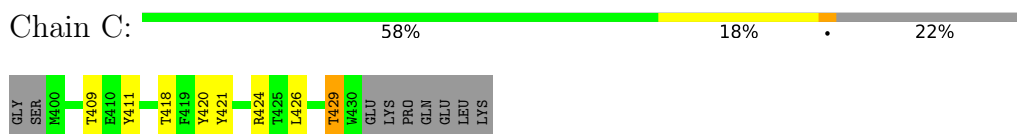
- Molecule 1: Transcription elongation regulator 1



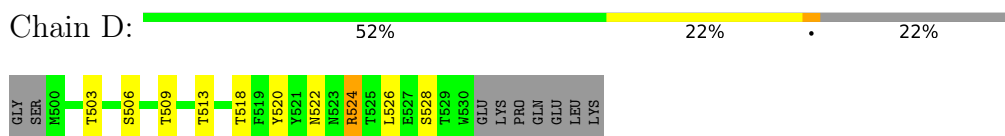
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

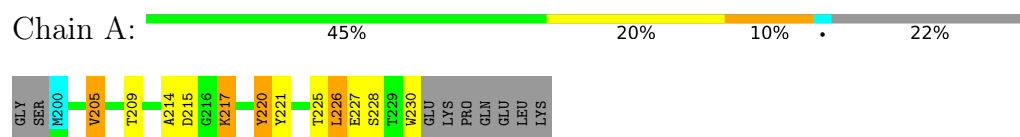


4.2 Scores per residue for each member of the ensemble

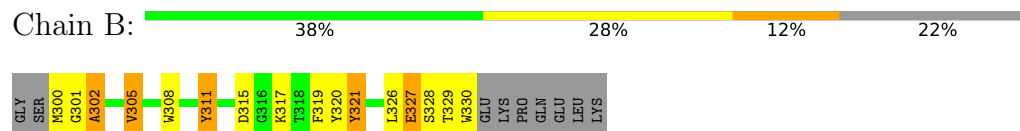
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

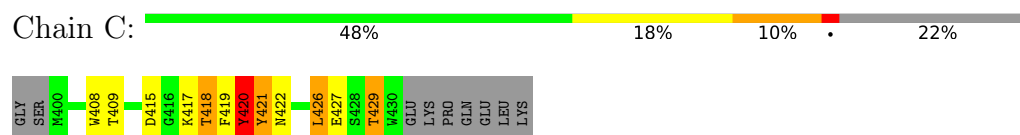
- Molecule 1: Transcription elongation regulator 1



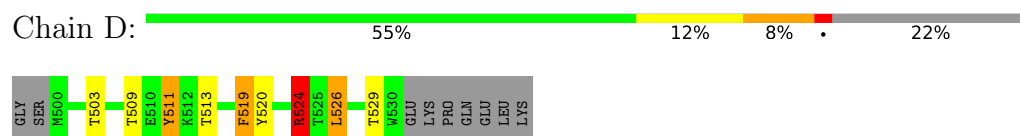
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

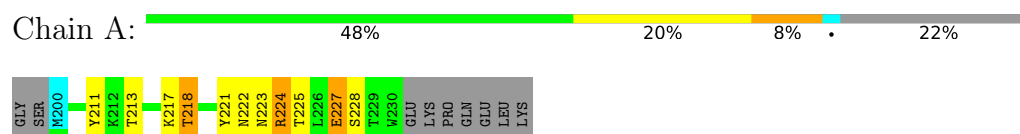


- Molecule 1: Transcription elongation regulator 1

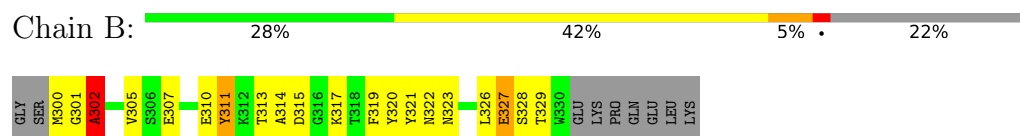


4.2.2 Score per residue for model 2

- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1





- Molecule 1: Transcription elongation regulator 1



4.2.3 Score per residue for model 3

- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

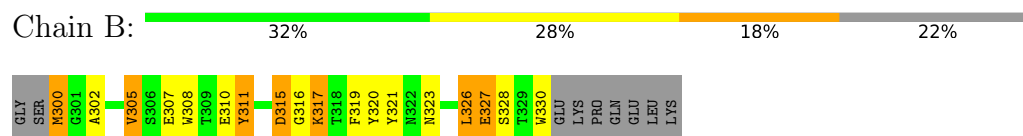


4.2.4 Score per residue for model 4

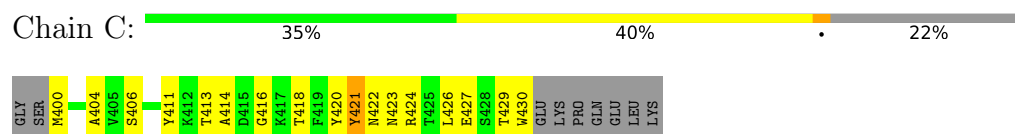
- Molecule 1: Transcription elongation regulator 1



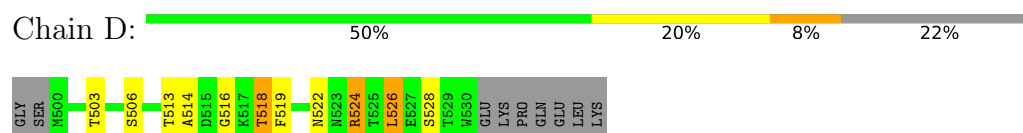
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

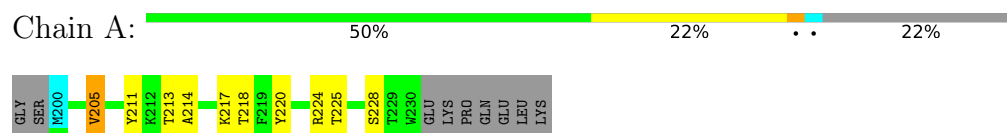


- Molecule 1: Transcription elongation regulator 1

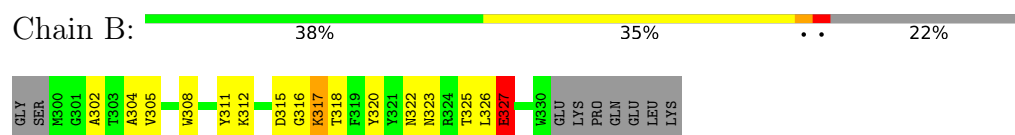


4.2.5 Score per residue for model 5

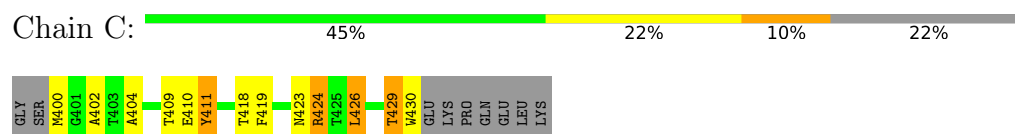
- Molecule 1: Transcription elongation regulator 1



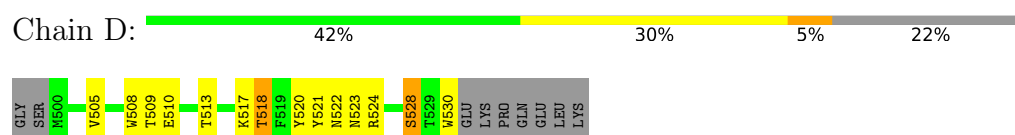
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

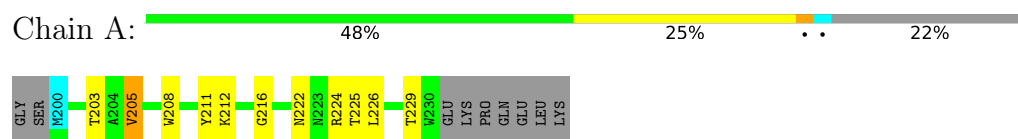


- Molecule 1: Transcription elongation regulator 1

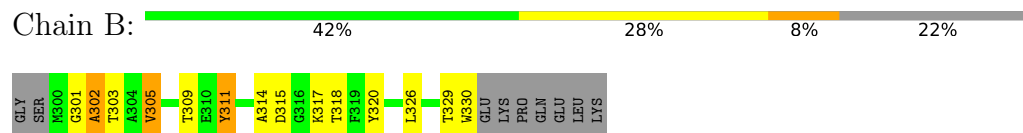


4.2.6 Score per residue for model 6

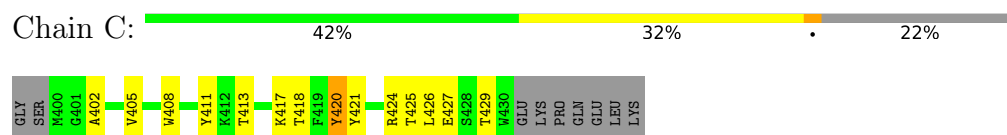
- Molecule 1: Transcription elongation regulator 1



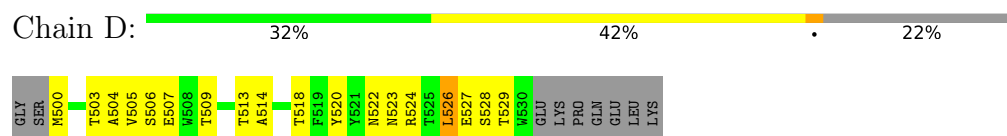
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

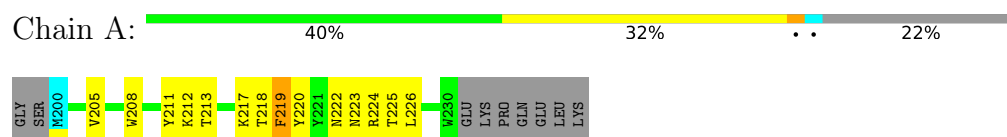


- Molecule 1: Transcription elongation regulator 1

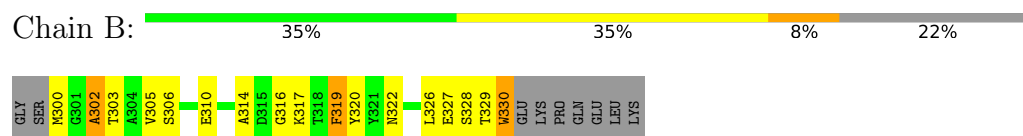


4.2.7 Score per residue for model 7

- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1





- Molecule 1: Transcription elongation regulator 1



4.2.8 Score per residue for model 8

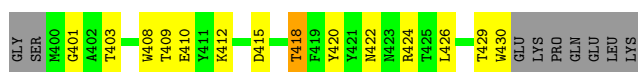
- Molecule 1: Transcription elongation regulator 1



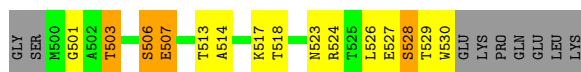
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

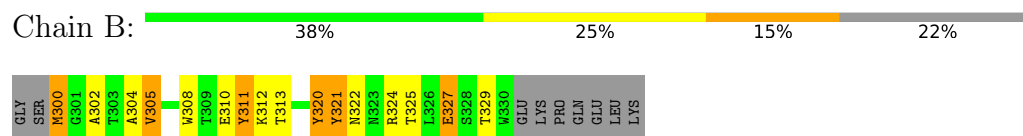


4.2.9 Score per residue for model 9

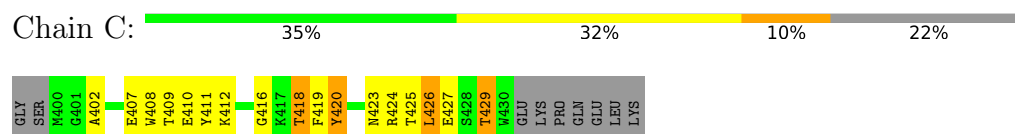
- Molecule 1: Transcription elongation regulator 1



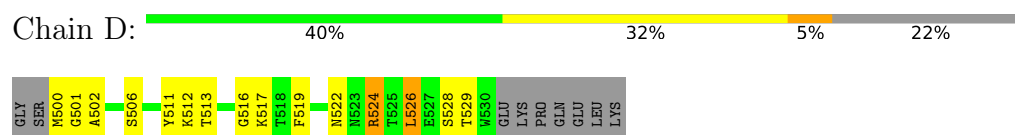
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1

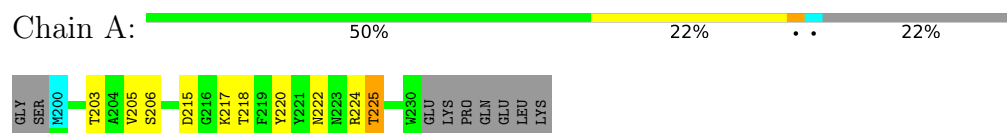


- Molecule 1: Transcription elongation regulator 1

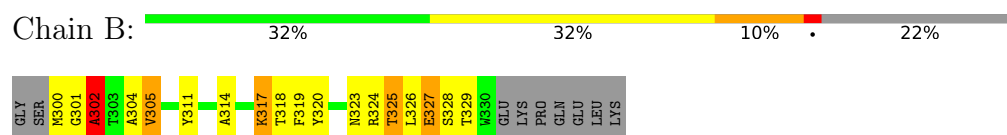


4.2.10 Score per residue for model 10

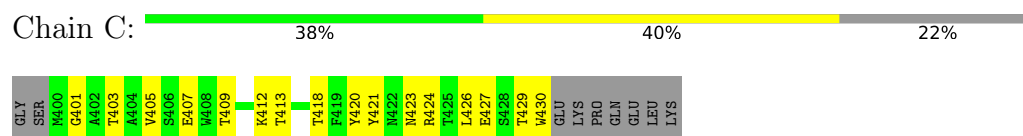
- Molecule 1: Transcription elongation regulator 1



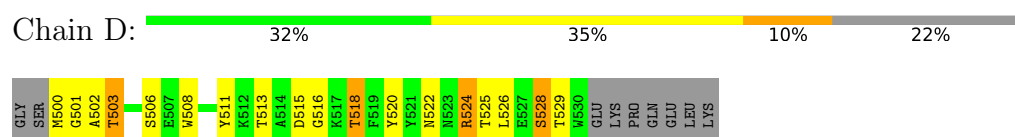
- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



- Molecule 1: Transcription elongation regulator 1



5 Refinement protocol and experimental data overview ⓘ

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

Of the 30 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 solution	7.0
Amber	refinement	7.0

No chemical shift data was provided. 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	1.89±0.09	4±2/254 (1.7± 1.0%)	2.17±0.12	8±2/346 (2.2± 0.7%)
1	B	1.83±0.11	3±2/262 (1.3± 0.7%)	2.20±0.11	10±4/356 (2.9± 1.1%)
1	C	1.88±0.10	5±2/262 (1.8± 0.6%)	2.17±0.10	11±3/356 (3.2± 0.9%)
1	D	1.93±0.08	4±2/262 (1.7± 0.8%)	2.24±0.10	10±3/356 (2.9± 1.0%)
All	All	1.88	169/10400 (1.6%)	2.20	394/14140 (2.8%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.8±1.0
1	B	0.0±0.0	3.0±1.0
1	C	0.0±0.0	1.6±0.8
1	D	0.0±0.0	1.6±0.8
All	All	0	90

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	B	307	GLU	CA-C	8.22	1.62	1.52	4	1
1	C	407	GLU	N-CA	8.21	1.55	1.46	9	1
1	D	514	ALA	N-CA	8.12	1.56	1.46	8	1
1	D	519	PHE	CA-C	8.09	1.63	1.52	1	1
1	C	421	TYR	CA-C	7.96	1.62	1.52	3	1
1	D	529	THR	CA-C	7.87	1.61	1.53	1	2
1	A	213	THR	CA-C	7.84	1.62	1.52	7	1
1	D	504	ALA	N-CA	7.81	1.55	1.46	7	2
1	C	418	THR	CA-C	7.40	1.61	1.52	3	2
1	C	423	ASN	N-CA	7.27	1.56	1.46	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	228	SER	CA-CB	7.25	1.65	1.53	5	1
1	A	229	THR	CA-C	7.12	1.59	1.52	6	2
1	B	328	SER	CA-C	7.06	1.61	1.52	10	3
1	A	204	ALA	CA-C	6.96	1.60	1.52	8	2
1	D	509	THR	CA-CB	6.94	1.64	1.53	6	2
1	B	312	LYS	N-CA	-6.89	1.36	1.46	5	2
1	B	321	TYR	CA-C	6.84	1.60	1.52	1	2
1	A	227	GLU	CA-C	-6.82	1.45	1.53	4	1
1	C	409	THR	CA-C	6.80	1.59	1.52	1	4
1	C	427	GLU	CA-C	6.73	1.60	1.52	9	1
1	C	410	GLU	CA-C	6.71	1.60	1.52	8	1
1	D	513	THR	CA-C	6.70	1.61	1.52	2	1
1	D	527	GLU	CA-C	6.70	1.60	1.52	2	2
1	D	528	SER	CA-C	6.66	1.61	1.52	10	1
1	C	403	THR	N-CA	6.60	1.53	1.45	8	1
1	C	422	ASN	CA-CB	6.60	1.61	1.52	3	1
1	B	311	TYR	N-CA	6.58	1.54	1.46	4	1
1	C	424	ARG	CA-C	6.58	1.60	1.52	7	1
1	A	211	TYR	N-CA	-6.56	1.38	1.46	9	1
1	B	319	PHE	CA-C	6.56	1.60	1.52	1	1
1	A	205	VAL	N-CA	6.56	1.53	1.46	7	2
1	C	413	THR	N-CA	6.54	1.54	1.46	10	1
1	B	313	THR	CA-C	6.44	1.61	1.52	2	1
1	B	305	VAL	CA-C	6.43	1.60	1.52	6	2
1	B	310	GLU	CA-C	-6.42	1.46	1.53	2	1
1	B	325	THR	N-CA	6.37	1.54	1.46	9	1
1	D	502	ALA	CA-C	6.36	1.61	1.53	9	1
1	A	201	GLY	C-N	6.36	1.41	1.33	9	1
1	C	408	TRP	CA-C	6.29	1.59	1.53	6	2
1	A	222	ASN	CA-CB	6.29	1.60	1.52	7	2
1	B	329	THR	CB-OG1	-6.29	1.33	1.43	6	2
1	A	215	ASP	CA-C	6.28	1.60	1.52	10	1
1	A	205	VAL	CA-CB	6.26	1.62	1.54	6	1
1	A	212	LYS	CA-C	6.25	1.59	1.52	7	2
1	A	220	TYR	N-CA	-6.22	1.38	1.47	1	1
1	C	425	THR	N-CA	-6.17	1.38	1.46	6	1
1	D	522	ASN	N-CA	6.15	1.53	1.46	2	2
1	D	506	SER	CA-CB	6.14	1.61	1.52	10	1
1	D	506	SER	CA-C	6.12	1.59	1.53	4	1
1	B	302	ALA	C-N	6.05	1.41	1.33	2	1
1	B	322	ASN	C-O	-6.02	1.17	1.23	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	202	ALA	N-CA	-6.00	1.38	1.45	9	2
1	B	304	ALA	CA-CB	5.98	1.64	1.53	10	1
1	A	209	THR	CA-C	5.91	1.59	1.52	1	1
1	B	311	TYR	C-N	5.88	1.40	1.33	9	1
1	D	506	SER	C-O	5.86	1.30	1.23	10	1
1	D	528	SER	N-CA	5.82	1.53	1.46	7	1
1	C	415	ASP	CA-C	-5.78	1.45	1.52	2	1
1	A	227	GLU	C-O	-5.78	1.17	1.23	2	1
1	B	314	ALA	C-O	5.78	1.30	1.24	7	1
1	D	522	ASN	CA-C	5.76	1.59	1.52	3	2
1	B	325	THR	CA-CB	5.75	1.61	1.52	3	1
1	A	203	THR	CA-C	5.74	1.59	1.52	4	1
1	C	402	ALA	CA-C	5.73	1.59	1.52	9	1
1	C	407	GLU	C-O	-5.72	1.17	1.24	10	1
1	D	509	THR	CA-C	5.70	1.59	1.52	6	1
1	C	410	GLU	C-O	5.70	1.30	1.24	5	1
1	D	509	THR	N-CA	-5.68	1.39	1.46	5	2
1	C	401	GLY	CA-C	5.68	1.59	1.51	8	1
1	D	505	VAL	CA-C	-5.66	1.45	1.52	6	2
1	A	214	ALA	CA-C	-5.66	1.45	1.52	1	1
1	D	506	SER	N-CA	-5.66	1.39	1.46	8	1
1	C	419	PHE	N-CA	5.63	1.53	1.46	7	1
1	B	317	LYS	C-O	5.63	1.31	1.24	10	1
1	C	409	THR	CB-OG1	-5.62	1.34	1.43	3	1
1	D	529	THR	CB-OG1	-5.62	1.34	1.43	1	1
1	B	319	PHE	N-CA	5.61	1.52	1.46	2	1
1	C	429	THR	CA-CB	5.61	1.62	1.53	1	1
1	C	403	THR	C-O	5.60	1.30	1.23	10	1
1	B	301	GLY	N-CA	-5.58	1.37	1.45	1	1
1	C	420	TYR	N-CA	5.54	1.52	1.46	1	1
1	D	503	THR	CA-C	5.52	1.59	1.52	8	1
1	A	224	ARG	CD-NE	5.51	1.53	1.46	2	1
1	D	523	ASN	N-CA	5.50	1.52	1.46	7	1
1	D	507	GLU	CA-CB	5.50	1.60	1.53	6	1
1	D	511	TYR	N-CA	-5.50	1.39	1.46	10	1
1	D	511	TYR	CA-C	-5.47	1.46	1.52	9	1
1	A	211	TYR	CA-C	5.46	1.59	1.52	2	1
1	A	213	THR	CB-OG1	-5.45	1.35	1.43	3	1
1	C	421	TYR	CA-CB	5.45	1.61	1.53	10	1
1	A	223	ASN	CA-C	5.45	1.59	1.52	7	1
1	C	414	ALA	N-CA	-5.44	1.40	1.47	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	217	LYS	CA-C	5.44	1.60	1.52	2	1
1	D	524	ARG	CD-NE	5.42	1.53	1.46	1	1
1	A	225	THR	CB-OG1	-5.41	1.35	1.43	10	1
1	B	302	ALA	CA-C	5.40	1.60	1.52	10	1
1	B	303	THR	CA-C	5.39	1.58	1.52	8	1
1	C	404	ALA	N-CA	-5.38	1.40	1.46	4	1
1	C	417	LYS	CA-C	5.38	1.60	1.52	6	1
1	D	518	THR	CA-C	5.36	1.59	1.52	7	1
1	A	205	VAL	CA-C	5.34	1.58	1.52	10	1
1	B	322	ASN	N-CA	-5.33	1.39	1.46	9	1
1	D	507	GLU	CA-C	5.31	1.59	1.52	2	1
1	D	520	TYR	N-CA	5.31	1.52	1.46	5	1
1	A	207	GLU	CA-C	5.31	1.59	1.52	8	1
1	C	417	LYS	C-O	5.30	1.31	1.24	2	1
1	A	216	GLY	N-CA	5.29	1.53	1.45	6	1
1	A	210	GLU	CA-C	-5.29	1.47	1.53	4	1
1	A	224	ARG	CA-C	-5.28	1.46	1.52	6	1
1	C	429	THR	CA-C	5.26	1.58	1.52	9	1
1	D	514	ALA	C-O	5.24	1.30	1.24	6	1
1	C	401	GLY	C-N	5.24	1.40	1.33	10	1
1	A	219	PHE	CA-C	5.21	1.58	1.52	9	1
1	A	218	THR	CA-CB	5.21	1.59	1.53	2	1
1	A	218	THR	C-N	-5.21	1.26	1.33	10	2
1	C	420	TYR	CA-C	5.20	1.58	1.52	6	1
1	C	430	TRP	NE1-CE2	5.19	1.43	1.37	3	1
1	A	228	SER	C-O	-5.18	1.17	1.24	2	1
1	B	324	ARG	CD-NE	5.18	1.53	1.46	10	1
1	D	523	ASN	CA-C	5.17	1.58	1.52	8	1
1	B	326	LEU	CA-C	5.17	1.58	1.52	8	1
1	C	426	LEU	CA-C	5.15	1.58	1.52	1	1
1	B	327	GLU	CA-C	5.15	1.58	1.52	7	1
1	D	522	ASN	CA-CB	5.13	1.64	1.53	9	1
1	C	424	ARG	NE-CZ	5.12	1.38	1.33	7	2
1	C	427	GLU	N-CA	5.11	1.52	1.46	4	1
1	D	511	TYR	CG-CD2	5.11	1.50	1.39	9	1
1	A	227	GLU	N-CA	-5.10	1.40	1.47	9	1
1	C	426	LEU	C-N	5.09	1.40	1.33	5	1
1	D	512	LYS	N-CA	5.08	1.52	1.46	7	1
1	C	406	SER	CB-OG	5.07	1.52	1.42	4	1
1	B	317	LYS	CA-C	5.06	1.59	1.52	4	1
1	C	414	ALA	CA-C	5.06	1.57	1.53	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	228	SER	N-CA	5.05	1.52	1.46	9	1
1	C	424	ARG	C-O	-5.04	1.18	1.24	5	1
1	D	509	THR	C-N	5.04	1.40	1.33	2	1
1	B	318	THR	CB-OG1	-5.03	1.35	1.43	6	1
1	D	526	LEU	CB-CG	5.03	1.63	1.53	6	1
1	D	503	THR	C-N	-5.02	1.27	1.33	10	1
1	A	202	ALA	C-N	5.01	1.40	1.33	8	1
1	A	223	ASN	N-CA	5.00	1.52	1.46	2	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	B	319	PHE	CA-CB-CG	10.50	124.30	113.80	4	3
1	A	222	ASN	OD1-CG-ND2	-9.82	112.78	122.60	6	3
1	D	512	LYS	CA-C-N	8.80	135.76	122.65	3	2
1	D	512	LYS	C-N-CA	8.80	135.76	122.65	3	2
1	D	501	GLY	O-C-N	-8.69	116.08	123.73	8	2
1	B	315	ASP	CA-CB-CG	-8.63	103.97	112.60	4	1
1	D	526	LEU	CB-CA-C	8.59	122.67	111.42	4	2
1	D	506	SER	N-CA-CB	-8.43	97.88	110.86	10	5
1	C	429	THR	O-C-N	-8.31	113.27	123.33	2	1
1	B	323	ASN	OD1-CG-ND2	-8.18	114.42	122.60	4	3
1	C	411	TYR	N-CA-C	-8.15	95.61	108.90	9	1
1	C	422	ASN	CA-CB-CG	8.10	120.70	112.60	4	1
1	C	417	LYS	CA-C-N	8.03	132.53	121.05	7	2
1	C	417	LYS	C-N-CA	8.03	132.53	121.05	7	2
1	A	219	PHE	CA-CB-CG	8.00	121.80	113.80	8	2
1	C	413	THR	CA-CB-CG2	7.96	124.04	110.50	6	1
1	B	321	TYR	CB-CA-C	7.82	122.65	110.14	1	4
1	A	220	TYR	CA-C-N	7.72	133.66	123.00	7	1
1	A	220	TYR	C-N-CA	7.72	133.66	123.00	7	1
1	B	317	LYS	CA-C-N	7.71	133.59	121.56	10	3
1	B	317	LYS	C-N-CA	7.71	133.59	121.56	10	3
1	B	325	THR	CA-CB-CG2	7.67	123.54	110.50	5	1
1	A	218	THR	CA-C-O	7.62	128.04	120.88	5	1
1	C	407	GLU	CA-C-O	7.48	128.64	120.71	9	1
1	C	423	ASN	OD1-CG-ND2	-7.47	115.13	122.60	9	1
1	B	329	THR	CA-CB-OG1	7.38	120.67	109.60	8	1
1	B	324	ARG	NE-CZ-NH2	7.35	125.81	119.20	10	2
1	B	313	THR	CA-CB-OG1	-7.28	98.68	109.60	9	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	215	ASP	CA-CB-CG	7.27	119.87	112.60	4	1
1	D	517	LYS	CA-C-N	7.23	131.10	120.90	8	5
1	D	517	LYS	C-N-CA	7.23	131.10	120.90	8	5
1	A	211	TYR	CA-C-N	7.16	132.57	121.76	7	1
1	A	211	TYR	C-N-CA	7.16	132.57	121.76	7	1
1	C	421	TYR	CA-C-O	-7.09	112.72	120.24	2	1
1	C	418	THR	CA-CB-OG1	-7.08	98.97	109.60	8	2
1	C	425	THR	CA-CB-OG1	7.07	120.20	109.60	2	1
1	C	419	PHE	CA-CB-CG	7.04	120.84	113.80	7	2
1	A	224	ARG	NE-CZ-NH2	-7.03	112.88	119.20	9	2
1	C	420	TYR	CA-C-O	6.98	129.63	120.21	2	1
1	B	301	GLY	CA-C-N	6.95	134.82	121.54	2	3
1	B	301	GLY	C-N-CA	6.95	134.82	121.54	2	3
1	D	509	THR	O-C-N	-6.95	114.70	122.55	1	1
1	B	305	VAL	O-C-N	6.94	130.43	123.00	10	1
1	C	427	GLU	CA-C-O	6.92	128.64	120.20	1	1
1	C	410	GLU	CA-CB-CG	-6.88	100.33	114.10	9	1
1	C	403	THR	CA-CB-OG1	6.88	119.92	109.60	2	1
1	A	222	ASN	CA-CB-CG	-6.85	105.75	112.60	6	2
1	B	318	THR	O-C-N	-6.84	115.45	123.11	10	1
1	B	323	ASN	CA-CB-CG	-6.78	105.82	112.60	10	2
1	B	329	THR	CB-CA-C	6.77	121.89	109.71	7	1
1	C	424	ARG	CD-NE-CZ	6.73	133.82	124.40	6	1
1	A	205	VAL	CA-CB-CG1	6.73	121.83	110.40	9	1
1	B	324	ARG	NE-CZ-NH1	-6.72	114.78	121.50	8	1
1	B	330	TRP	CD2-CE3-CZ3	6.71	127.33	118.60	6	2
1	A	230	TRP	CZ3-CH2-CZ2	-6.71	112.78	121.50	9	1
1	A	224	ARG	NE-CZ-NH1	6.67	128.16	121.50	9	1
1	C	409	THR	CB-CA-C	6.60	119.96	110.79	1	2
1	D	514	ALA	CA-C-O	-6.59	114.08	121.00	4	1
1	A	217	LYS	O-C-N	6.58	131.34	122.59	5	1
1	D	523	ASN	OD1-CG-ND2	-6.55	116.05	122.60	5	1
1	C	404	ALA	CB-CA-C	6.55	120.22	110.14	5	1
1	D	503	THR	N-CA-CB	-6.54	100.32	111.69	6	1
1	D	525	THR	CA-C-N	6.52	132.98	123.13	7	1
1	D	525	THR	C-N-CA	6.52	132.98	123.13	7	1
1	D	524	ARG	NH1-CZ-NH2	-6.50	110.85	119.30	9	1
1	C	418	THR	CA-CB-CG2	6.48	121.52	110.50	8	2
1	C	400	MET	CB-CA-C	6.47	122.39	110.10	4	1
1	B	330	TRP	CE2-CD2-CE3	-6.47	112.33	118.80	6	2
1	B	308	TRP	CE2-CD2-CE3	-6.47	112.33	118.80	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	503	THR	N-CA-C	6.45	120.03	109.06	7	1
1	A	209	THR	CB-CA-C	6.43	120.44	110.14	1	1
1	D	508	TRP	CB-CA-C	6.42	122.21	111.30	7	1
1	C	403	THR	CB-CA-C	6.42	121.31	109.70	3	1
1	C	415	ASP	CA-CB-CG	6.41	119.01	112.60	1	2
1	B	313	THR	CA-CB-CG2	6.41	121.39	110.50	2	1
1	C	422	ASN	CA-C-N	6.41	132.02	123.05	3	1
1	C	422	ASN	C-N-CA	6.41	132.02	123.05	3	1
1	A	213	THR	CA-CB-CG2	6.41	121.39	110.50	9	1
1	D	508	TRP	CB-CG-CD2	6.39	135.75	126.80	5	1
1	A	205	VAL	CB-CA-C	6.36	119.62	110.33	5	1
1	C	418	THR	CA-C-N	6.36	131.49	122.72	4	1
1	C	418	THR	C-N-CA	6.36	131.49	122.72	4	1
1	C	427	GLU	CB-CA-C	6.34	119.88	110.62	9	1
1	D	528	SER	N-CA-CB	-6.30	101.33	110.47	8	2
1	D	519	PHE	CA-C-O	-6.29	113.99	120.54	9	1
1	A	208	TRP	CG-CD2-CE3	-6.28	127.62	133.90	7	1
1	C	418	THR	CB-CA-C	6.27	119.25	109.84	7	3
1	C	425	THR	CA-C-O	-6.26	112.58	120.28	9	1
1	B	314	ALA	O-C-N	6.22	128.75	122.03	10	3
1	A	220	TYR	CA-C-O	6.21	128.07	120.25	10	1
1	B	305	VAL	N-CA-C	6.19	117.40	108.48	6	1
1	A	221	TYR	CA-C-O	-6.19	113.55	120.54	1	2
1	D	515	ASP	CA-CB-CG	-6.18	106.42	112.60	10	1
1	D	520	TYR	CB-CA-C	-6.18	100.62	110.14	10	1
1	D	527	GLU	N-CA-C	6.17	119.18	108.76	7	3
1	B	328	SER	O-C-N	-6.15	116.07	123.27	2	1
1	A	214	ALA	N-CA-CB	-6.15	101.03	110.07	5	1
1	B	326	LEU	O-C-N	-6.15	115.01	123.12	4	1
1	A	225	THR	CA-C-N	-6.14	112.15	122.29	3	2
1	A	225	THR	C-N-CA	-6.14	112.15	122.29	3	2
1	D	503	THR	CA-CB-CG2	6.13	120.92	110.50	3	3
1	D	520	TYR	CA-C-N	6.12	131.63	123.00	2	2
1	D	520	TYR	C-N-CA	6.12	131.63	123.00	2	2
1	D	519	PHE	CA-C-N	6.12	131.31	122.44	4	1
1	D	519	PHE	C-N-CA	6.12	131.31	122.44	4	1
1	C	422	ASN	N-CA-C	6.11	118.36	108.34	1	1
1	D	500	MET	N-CA-CB	6.11	120.88	110.50	6	1
1	A	214	ALA	CA-C-O	-6.08	114.41	120.80	5	1
1	C	430	TRP	NE1-CE2-CD2	-6.08	99.50	107.40	8	1
1	D	507	GLU	CB-CA-C	6.06	120.21	109.72	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	423	ASN	CA-C-O	6.04	126.76	120.30	5	2
1	C	408	TRP	CD2-CE3-CZ3	6.03	126.44	118.60	9	1
1	D	524	ARG	NE-CZ-NH2	6.03	124.62	119.20	9	2
1	C	423	ASN	O-C-N	6.03	130.08	123.27	7	1
1	D	516	GLY	O-C-N	-6.02	114.88	122.70	4	1
1	A	221	TYR	CG-CD2-CE2	-5.98	112.22	121.20	8	1
1	A	219	PHE	CA-C-O	-5.96	114.14	120.40	7	1
1	A	226	LEU	O-C-N	5.96	130.05	123.25	7	1
1	C	414	ALA	CA-C-O	-5.95	112.74	120.00	4	1
1	C	412	LYS	CA-C-O	5.95	126.92	120.32	10	1
1	D	508	TRP	CA-C-N	5.95	133.12	123.37	7	2
1	D	508	TRP	C-N-CA	5.95	133.12	123.37	7	2
1	C	405	VAL	O-C-N	-5.95	115.68	122.94	7	1
1	C	416	GLY	CA-C-N	5.94	130.11	120.60	9	2
1	C	416	GLY	C-N-CA	5.94	130.11	120.60	9	2
1	C	413	THR	CA-CB-OG1	5.94	118.51	109.60	2	1
1	B	308	TRP	CB-CG-CD2	5.93	135.10	126.80	4	2
1	D	526	LEU	O-C-N	-5.92	116.71	123.40	1	1
1	C	406	SER	CA-C-N	5.92	129.76	121.24	4	1
1	C	406	SER	C-N-CA	5.92	129.76	121.24	4	1
1	B	330	TRP	CB-CG-CD2	5.90	135.06	126.80	7	3
1	A	229	THR	CA-CB-OG1	5.90	118.45	109.60	8	2
1	B	304	ALA	N-CA-C	5.90	118.05	108.26	5	1
1	C	415	ASP	O-C-N	-5.89	116.36	123.13	3	1
1	D	522	ASN	CA-CB-CG	5.89	118.49	112.60	3	2
1	D	522	ASN	CB-CG-ND2	5.88	125.22	116.40	9	2
1	B	308	TRP	CG-CD2-CE3	5.88	139.78	133.90	5	1
1	B	319	PHE	O-C-N	-5.87	116.46	123.27	7	1
1	C	430	TRP	CE2-CD2-CE3	-5.87	112.93	118.80	4	1
1	C	402	ALA	N-CA-C	5.87	117.77	108.79	5	1
1	A	203	THR	CA-C-N	5.87	131.78	122.74	6	1
1	A	203	THR	C-N-CA	5.87	131.78	122.74	6	1
1	C	424	ARG	NE-CZ-NH2	-5.86	113.93	119.20	6	1
1	A	229	THR	N-CA-C	-5.85	104.28	112.12	4	1
1	A	218	THR	CA-CB-OG1	-5.84	100.83	109.60	4	1
1	D	530	TRP	CE2-CD2-CE3	-5.84	112.96	118.80	5	2
1	D	506	SER	CB-CA-C	5.84	118.67	111.43	4	2
1	C	424	ARG	O-C-N	-5.80	116.54	123.27	2	1
1	B	306	SER	O-C-N	5.79	129.98	123.27	7	1
1	B	324	ARG	CB-CA-C	5.78	120.28	109.71	9	1
1	B	322	ASN	OD1-CG-ND2	-5.77	116.83	122.60	7	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	329	THR	CA-C-O	5.77	128.19	121.44	9	1
1	D	529	THR	N-CA-C	5.77	117.66	110.91	1	1
1	D	508	TRP	CE2-CD2-CE3	-5.76	113.04	118.80	5	1
1	B	305	VAL	CA-C-O	-5.76	114.60	121.28	10	1
1	D	511	TYR	O-C-N	-5.75	116.60	123.27	1	1
1	A	203	THR	O-C-N	-5.75	116.49	123.10	10	1
1	A	207	GLU	CA-C-N	5.73	131.57	122.74	3	1
1	A	207	GLU	C-N-CA	5.73	131.57	122.74	3	1
1	B	304	ALA	CB-CA-C	5.73	120.07	109.70	9	1
1	C	430	TRP	CG-CD2-CE3	5.71	139.61	133.90	4	2
1	A	205	VAL	CG1-CB-CG2	-5.70	98.27	110.80	1	1
1	D	530	TRP	CD2-CE3-CZ3	5.69	125.99	118.60	8	2
1	C	408	TRP	CD2-CE2-CZ2	-5.69	116.71	122.40	9	1
1	C	429	THR	CA-CB-OG1	5.68	118.13	109.60	5	2
1	A	228	SER	N-CA-C	-5.68	105.23	111.82	2	1
1	C	414	ALA	O-C-N	5.68	128.51	122.38	7	1
1	D	502	ALA	N-CA-CB	5.67	118.46	110.36	9	1
1	C	422	ASN	CA-C-O	-5.66	114.24	120.24	1	1
1	C	412	LYS	CA-C-N	5.66	131.83	122.33	8	3
1	C	412	LYS	C-N-CA	5.66	131.83	122.33	8	3
1	B	302	ALA	CA-C-N	-5.66	111.98	121.94	10	1
1	B	302	ALA	C-N-CA	-5.66	111.98	121.94	10	1
1	D	518	THR	CA-C-O	-5.65	114.80	120.96	5	1
1	D	501	GLY	CA-C-O	-5.64	115.44	121.88	10	1
1	D	518	THR	CA-CB-OG1	5.64	118.06	109.60	5	1
1	B	329	THR	CA-C-N	5.64	131.85	121.70	10	1
1	B	329	THR	C-N-CA	5.64	131.85	121.70	10	1
1	B	300	MET	CB-CA-C	5.63	120.81	110.10	9	2
1	C	402	ALA	O-C-N	-5.63	117.17	123.48	6	2
1	B	321	TYR	CA-C-O	-5.62	113.34	120.20	3	1
1	C	409	THR	CA-CB-CG2	5.61	120.03	110.50	3	1
1	A	213	THR	N-CA-C	5.60	117.64	108.52	4	1
1	A	230	TRP	CE2-CD2-CE3	-5.58	113.22	118.80	8	1
1	D	508	TRP	CD2-CE2-CZ2	5.55	127.95	122.40	7	1
1	C	430	TRP	NE1-CE2-CZ2	5.55	138.43	130.10	8	1
1	D	506	SER	CA-CB-OG	5.55	122.19	111.10	10	1
1	D	505	VAL	CA-CB-CG1	5.54	119.83	110.40	5	1
1	B	322	ASN	CA-C-N	-5.52	115.01	123.07	2	1
1	B	322	ASN	C-N-CA	-5.52	115.01	123.07	2	1
1	D	510	GLU	CB-CA-C	5.51	118.67	110.62	5	1
1	B	300	MET	CA-CB-CG	5.50	125.11	114.10	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	209	THR	CA-CB-CG2	5.50	119.85	110.50	4	1
1	B	315	ASP	CB-CA-C	5.50	116.56	109.80	5	1
1	D	510	GLU	O-C-N	-5.49	115.87	123.12	3	1
1	C	408	TRP	CG-CD2-CE3	-5.48	128.42	133.90	8	1
1	B	330	TRP	CA-CB-CG	5.48	124.01	113.60	4	1
1	C	407	GLU	N-CA-C	-5.46	100.80	109.59	9	1
1	C	405	VAL	CA-CB-CG2	5.45	119.67	110.40	2	2
1	A	228	SER	CA-CB-OG	-5.45	100.20	111.10	1	1
1	B	311	TYR	CA-CB-CG	5.45	123.71	113.90	4	1
1	A	208	TRP	NE1-CE2-CZ2	5.45	138.27	130.10	7	1
1	A	217	LYS	CA-C-N	5.45	128.84	121.05	1	1
1	A	217	LYS	C-N-CA	5.45	128.84	121.05	1	1
1	A	221	TYR	CD1-CG-CD2	5.45	126.27	118.10	8	1
1	B	325	THR	N-CA-C	5.45	118.33	109.24	10	1
1	B	310	GLU	CA-C-O	-5.44	114.34	120.32	4	2
1	B	328	SER	CB-CA-C	5.43	118.95	111.23	7	2
1	C	409	THR	CA-C-N	5.43	130.82	123.11	5	1
1	C	409	THR	C-N-CA	5.43	130.82	123.11	5	1
1	B	311	TYR	CB-CG-CD1	-5.42	112.67	120.80	6	1
1	D	502	ALA	N-CA-C	-5.41	102.03	110.42	10	1
1	C	427	GLU	N-CA-C	5.40	117.20	108.34	6	1
1	D	510	GLU	CA-C-N	5.40	130.39	122.77	2	1
1	D	510	GLU	C-N-CA	5.40	130.39	122.77	2	1
1	C	430	TRP	CZ3-CH2-CZ2	-5.40	114.48	121.50	4	1
1	C	422	ASN	OD1-CG-ND2	-5.40	117.20	122.60	8	1
1	B	310	GLU	CB-CG-CD	5.39	121.77	112.60	9	1
1	B	314	ALA	N-CA-C	-5.37	105.51	111.36	2	1
1	B	330	TRP	CG-CD2-CE3	5.37	139.27	133.90	4	1
1	D	530	TRP	CA-CB-CG	5.37	123.80	113.60	8	1
1	C	417	LYS	N-CA-C	-5.36	106.58	113.01	6	1
1	C	412	LYS	N-CA-CB	-5.35	101.83	110.81	3	1
1	C	427	GLU	CA-C-N	5.35	129.79	122.84	10	1
1	C	427	GLU	C-N-CA	5.35	129.79	122.84	10	1
1	C	418	THR	N-CA-CB	-5.32	102.75	110.36	1	1
1	D	523	ASN	CA-CB-CG	-5.32	107.28	112.60	6	1
1	A	223	ASN	N-CA-C	5.31	117.30	107.73	3	1
1	B	311	TYR	CB-CA-C	5.31	119.45	110.79	1	1
1	A	213	THR	CA-C-O	5.31	125.87	120.24	8	1
1	D	516	GLY	CA-C-N	5.30	131.45	122.65	9	1
1	D	516	GLY	C-N-CA	5.30	131.45	122.65	9	1
1	B	308	TRP	NE1-CE2-CD2	-5.29	100.52	107.40	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	509	THR	CA-CB-CG2	-5.29	101.50	110.50	3	1
1	A	217	LYS	CA-C-O	-5.29	112.95	120.51	5	1
1	C	418	THR	CA-C-O	-5.29	115.37	121.19	6	1
1	C	421	TYR	CA-C-N	5.28	130.22	122.77	1	1
1	C	421	TYR	C-N-CA	5.28	130.22	122.77	1	1
1	C	411	TYR	CB-CA-C	5.28	119.26	109.70	5	1
1	A	205	VAL	CA-CB-CG2	5.28	119.37	110.40	1	1
1	C	413	THR	CA-C-O	5.27	127.06	121.11	7	1
1	B	309	THR	N-CA-C	5.25	118.05	109.59	6	1
1	A	203	THR	CA-CB-OG1	5.25	117.47	109.60	4	1
1	C	426	LEU	N-CA-C	5.25	117.98	108.69	7	1
1	C	413	THR	OG1-CB-CG2	-5.24	98.81	109.30	4	1
1	A	211	TYR	O-C-N	-5.22	117.08	123.30	7	1
1	B	313	THR	CA-C-N	5.22	127.54	120.44	8	1
1	B	313	THR	C-N-CA	5.22	127.54	120.44	8	1
1	B	314	ALA	CA-C-O	-5.21	115.53	120.90	10	1
1	C	408	TRP	NE1-CE2-CZ2	5.21	137.92	130.10	8	1
1	D	517	LYS	N-CA-CB	-5.21	103.25	110.65	8	1
1	C	412	LYS	CA-CB-CG	-5.21	103.69	114.10	9	1
1	A	214	ALA	CB-CA-C	5.20	119.43	110.86	5	1
1	C	423	ASN	CA-CB-CG	-5.19	107.41	112.60	4	1
1	B	326	LEU	N-CA-C	5.19	116.88	108.41	7	1
1	C	413	THR	N-CA-C	-5.19	101.42	109.72	7	1
1	A	218	THR	CA-C-N	5.19	131.05	122.33	9	1
1	A	218	THR	C-N-CA	5.19	131.05	122.33	9	1
1	C	429	THR	CA-C-O	5.19	126.83	120.60	2	1
1	C	419	PHE	N-CA-C	5.18	117.42	109.07	5	1
1	D	527	GLU	CA-C-N	5.17	130.36	122.29	6	2
1	D	527	GLU	C-N-CA	5.17	130.36	122.29	6	2
1	D	500	MET	CB-CA-C	5.16	119.91	110.10	10	1
1	D	517	LYS	O-C-N	5.16	130.02	122.39	7	1
1	B	310	GLU	CA-C-N	5.16	130.27	123.05	2	1
1	B	310	GLU	C-N-CA	5.16	130.27	123.05	2	1
1	B	310	GLU	CA-CB-CG	-5.15	103.79	114.10	7	1
1	A	202	ALA	CA-C-N	5.15	130.79	122.29	4	1
1	A	202	ALA	C-N-CA	5.15	130.79	122.29	4	1
1	A	208	TRP	CB-CG-CD1	-5.15	119.17	126.90	6	1
1	A	221	TYR	CB-CA-C	5.15	118.23	109.84	2	1
1	D	530	TRP	CE3-CZ3-CH2	-5.13	114.43	121.10	8	1
1	A	205	VAL	CA-C-O	5.12	126.67	120.67	10	1
1	A	221	TYR	N-CA-C	-5.12	101.62	109.76	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	D	500	MET	CA-C-N	5.12	128.30	122.67	10	1
1	D	500	MET	C-N-CA	5.12	128.30	122.67	10	1
1	B	327	GLU	CA-CB-CG	5.12	124.34	114.10	5	1
1	D	518	THR	CA-CB-CG2	5.12	119.20	110.50	10	1
1	D	508	TRP	O-C-N	5.12	129.16	122.87	10	1
1	B	326	LEU	N-CA-CB	5.09	118.59	110.65	8	1
1	B	307	GLU	CA-C-O	-5.08	114.68	120.32	2	1
1	A	211	TYR	CB-CA-C	5.08	118.91	110.78	6	1
1	A	213	THR	CA-C-N	5.08	129.11	120.88	5	1
1	A	213	THR	C-N-CA	5.08	129.11	120.88	5	1
1	C	400	MET	N-CA-CB	-5.07	101.88	110.50	5	1
1	C	430	TRP	CG-CD1-NE1	-5.06	103.62	110.20	10	1
1	C	411	TYR	CG-CD1-CE1	-5.05	113.62	121.20	3	1
1	D	521	TYR	CA-C-O	-5.05	114.91	120.36	7	1
1	A	230	TRP	NE1-CE2-CD2	-5.05	100.84	107.40	1	1
1	C	403	THR	N-CA-C	5.05	117.72	109.59	7	1
1	C	428	SER	CA-C-N	5.04	129.37	121.76	3	1
1	C	428	SER	C-N-CA	5.04	129.37	121.76	3	1
1	B	329	THR	CA-CB-CG2	5.02	119.03	110.50	6	1
1	A	215	ASP	N-CA-C	-5.01	100.56	108.73	1	1
1	A	219	PHE	O-C-N	-5.01	117.41	123.27	8	1
1	B	318	THR	CA-C-N	5.01	130.06	123.05	10	1
1	B	318	THR	C-N-CA	5.01	130.06	123.05	10	1
1	C	408	TRP	CA-C-N	5.01	129.32	121.76	1	1
1	C	408	TRP	C-N-CA	5.01	129.32	121.76	1	1
1	C	408	TRP	NE1-CE2-CD2	-5.00	100.90	107.40	1	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	225	THR	Peptide	10
1	B	302	ALA	Peptide,Mainchain	10
1	B	327	GLU	Peptide	8
1	B	320	TYR	Sidechain	5
1	C	420	TYR	Sidechain	5
1	A	224	ARG	Sidechain,Peptide	5
1	C	411	TYR	Sidechain	4
1	A	220	TYR	Sidechain	3
1	D	524	ARG	Sidechain,Peptide	3

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Mol	Chain	Res	Type	Group	Models (Total)
1	D	520	TYR	Sidechain	3
1	D	521	TYR	Sidechain	3
1	A	226	LEU	Peptide	3
1	C	424	ARG	Sidechain	3
1	A	206	SER	Peptide	3
1	B	321	TYR	Sidechain	2
1	D	511	TYR	Sidechain	2
1	B	311	TYR	Sidechain	2
1	C	421	TYR	Sidechain	2
1	A	211	TYR	Sidechain	2
1	B	329	THR	Mainchain	1
1	A	218	THR	Peptide	1
1	C	410	GLU	Peptide	1
1	C	429	THR	Mainchain	1
1	D	518	THR	Peptide	1
1	D	528	SER	Peptide	1
1	A	217	LYS	Peptide	1
1	B	319	PHE	Sidechain	1
1	D	519	PHE	Sidechain	1
1	D	500	MET	Peptide	1
1	D	525	THR	Peptide	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	247	222	222	0±0
1	B	255	231	230	2±2
1	C	255	231	230	1±1
1	D	255	231	230	0±1
All	All	10120	9150	9120	28

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:305:VAL:HB	1:B:326:LEU:HD11	0.53	1.78	4	1
1:B:320:TYR:CE1	1:C:420:TYR:CE1	0.52	2.97	4	2
1:C:420:TYR:CD1	1:D:520:TYR:CD1	0.51	2.98	1	1
1:B:302:ALA:HB3	1:C:402:ALA:H	0.51	1.66	2	1
1:B:326:LEU:HD12	1:B:326:LEU:N	0.50	2.21	5	2
1:B:305:VAL:CG1	1:B:326:LEU:HD11	0.50	2.37	4	2
1:C:424:ARG:HH22	1:D:507:GLU:CD	0.49	2.15	8	1
1:B:320:TYR:CD2	1:C:420:TYR:CD2	0.49	3.01	6	1
1:C:426:LEU:N	1:C:426:LEU:HD13	0.49	2.23	9	1
1:B:305:VAL:CB	1:B:326:LEU:HD11	0.48	2.39	4	1
1:B:325:THR:C	1:B:326:LEU:HD12	0.48	2.33	10	1
1:A:205:VAL:HB	1:A:226:LEU:HD22	0.45	1.89	1	1
1:C:426:LEU:N	1:C:426:LEU:CD1	0.45	2.79	9	1
1:B:321:TYR:CE1	1:C:421:TYR:CD1	0.45	3.05	4	1
1:B:320:TYR:CE2	1:C:420:TYR:CE2	0.44	3.06	6	1
1:C:421:TYR:C	1:C:421:TYR:CD1	0.44	2.96	1	1
1:A:205:VAL:N	1:A:226:LEU:HD13	0.43	2.28	6	1
1:C:420:TYR:CD1	1:C:420:TYR:C	0.42	2.98	3	1
1:B:326:LEU:N	1:B:326:LEU:HD12	0.41	2.31	8	1
1:D:524:ARG:HD2	1:D:524:ARG:H	0.41	1.76	4	1
1:A:205:VAL:HB	1:B:305:VAL:HG23	0.41	1.93	4	1
1:A:219:PHE:CD1	1:A:219:PHE:C	0.40	2.98	7	1
1:C:419:PHE:CE1	1:D:519:PHE:CD2	0.40	3.10	1	1
1:B:320:TYR:CD1	1:B:320:TYR:C	0.40	2.99	8	1
1:B:320:TYR:CD1	1:C:420:TYR:CE2	0.40	3.09	10	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	29/40 (72%)	25±1 (88±5%)	3±2 (11±5%)	0±0 (1±2%)	15	65
1	B	29/40 (72%)	24±1 (81±4%)	4±1 (13±5%)	2±1 (6±3%)	2	21
1	C	29/40 (72%)	27±1 (93±3%)	2±1 (6±3%)	0±0 (1±1%)	20	70
1	D	29/40 (72%)	25±1 (86±4%)	4±1 (12±4%)	1±1 (2±2%)	8	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1160/1600 (72%)	1008 (87%)	125 (11%)	27 (2%)	7 45

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	302	ALA	6
1	B	317	LYS	5
1	B	316	GLY	3
1	D	529	THR	3
1	A	217	LYS	2
1	D	516	GLY	2
1	C	417	LYS	1
1	C	416	GLY	1
1	A	214	ALA	1
1	B	318	THR	1
1	D	518	THR	1
1	B	301	GLY	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	25/34 (74%)	24±1 (94±3%)	2±1 (6±3%)	19 68
1	B	26/34 (76%)	21±1 (82±5%)	5±1 (18±5%)	3 35
1	C	26/34 (76%)	23±1 (90±3%)	3±1 (10±3%)	9 53
1	D	26/34 (76%)	20±1 (78±5%)	6±1 (22±5%)	3 30
All	All	1030/1360 (76%)	884 (86%)	146 (14%)	5 44

All 35 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	B	305	VAL	10
1	C	426	LEU	10
1	C	429	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	D	513	THR	10
1	D	524	ARG	10
1	B	311	TYR	8
1	B	327	GLU	8
1	D	528	SER	8
1	D	526	LEU	7
1	D	518	THR	7
1	B	300	MET	6
1	B	315	ASP	6
1	D	503	THR	6
1	C	418	THR	5
1	A	227	GLU	3
1	B	326	LEU	3
1	A	205	VAL	3
1	B	303	THR	3
1	D	506	SER	3
1	A	213	THR	2
1	A	212	LYS	2
1	A	218	THR	2
1	B	330	TRP	2
1	A	226	LEU	1
1	B	317	LYS	1
1	D	500	MET	1
1	A	229	THR	1
1	B	306	SER	1
1	D	509	THR	1
1	D	525	THR	1
1	D	530	TRP	1
1	A	219	PHE	1
1	C	409	THR	1
1	D	512	LYS	1
1	C	405	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 [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