Full wwPDB NMR Structure Validation Report (i)

Oct 11, 2021 – 05:17 PM EDT

PDB ID	:	2NNT
Title	:	General structural motifs of amyloid protofilaments
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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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

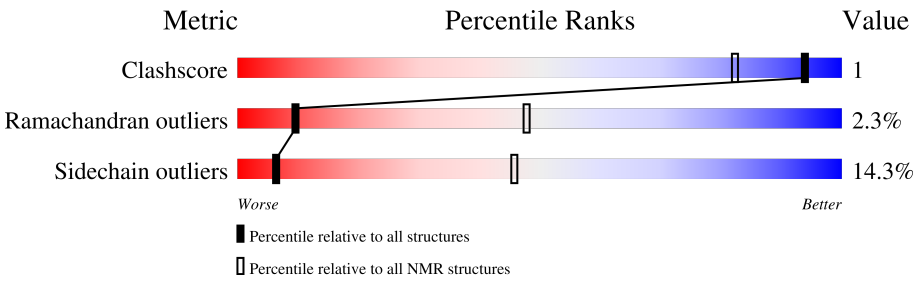
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	40	55% 18% • • 22%
1	B	40	45% 22% 10% 22%
1	C	40	55% 20% • 22%
1	D	40	42% 32% • 22%

2 Ensemble composition and analysis (i)

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)	0.27	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 (i)

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
			Total	C	H	N	O	S	
1	A	31	486	162	231	40	52	1	0
1	B	31	486	162	231	40	52	1	0
1	C	31	486	162	231	40	52	1	0
1	D	31	486	162	231	40	52	1	0

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

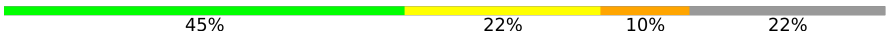
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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.

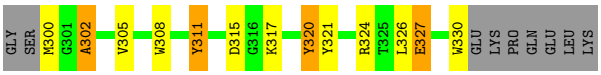
• Molecule 1: Transcription elongation regulator 1

Chain A:

• Molecule 1: Transcription elongation regulator 1

Chain B:



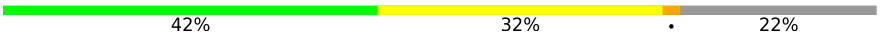


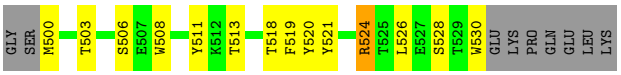
• Molecule 1: Transcription elongation regulator 1

Chain C:

• Molecule 1: Transcription elongation regulator 1

Chain D:





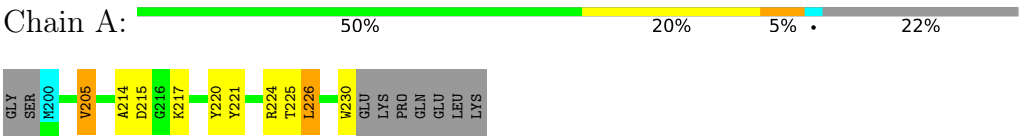
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

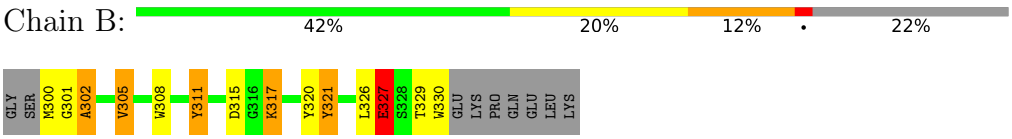
- Molecule 1: Transcription elongation regulator 1

Chain A:



- Molecule 1: Transcription elongation regulator 1

Chain B:



- Molecule 1: Transcription elongation regulator 1

Chain C:

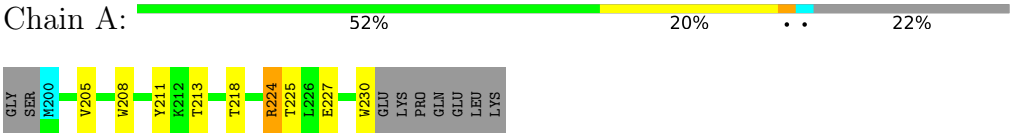
- Molecule 1: Transcription elongation regulator 1

Chain D:

4.2.2 Score per residue for model 2

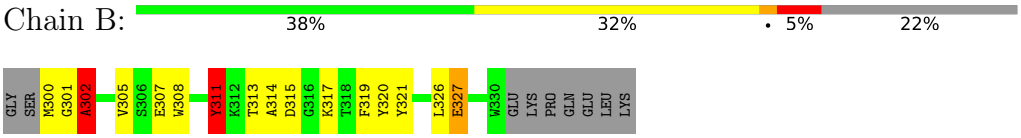
- Molecule 1: Transcription elongation regulator 1

Chain A:



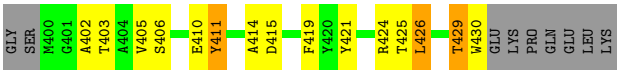
- Molecule 1: Transcription elongation regulator 1

Chain B:



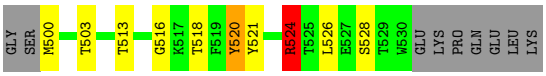
- Molecule 1: Transcription elongation regulator 1

Chain C:



• Molecule 1: Transcription elongation regulator 1

Chain D:



4.2.3 Score per residue for model 3

• Molecule 1: Transcription elongation regulator 1

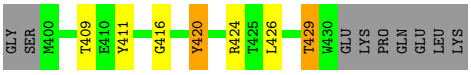
Chain A:

• Molecule 1: Transcription elongation regulator 1

Chain B:

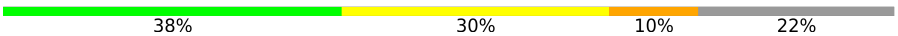
• Molecule 1: Transcription elongation regulator 1

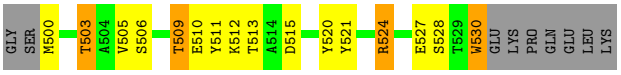
Chain C:



• Molecule 1: Transcription elongation regulator 1

Chain D:

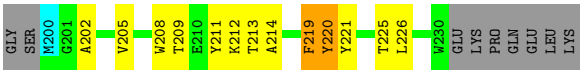




4.2.4 Score per residue for model 4

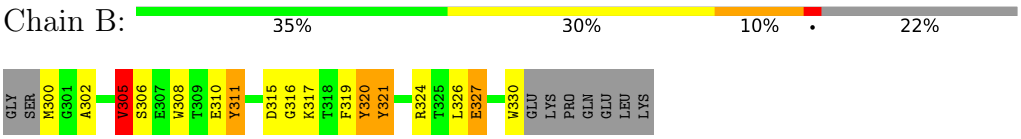
• Molecule 1: Transcription elongation regulator 1

Chain A:



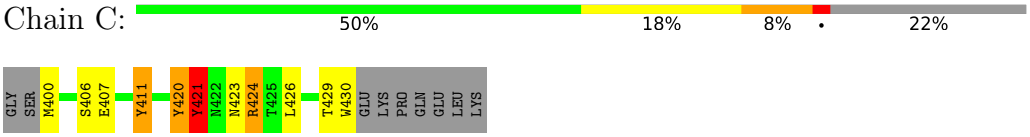
• Molecule 1: Transcription elongation regulator 1

Chain B:



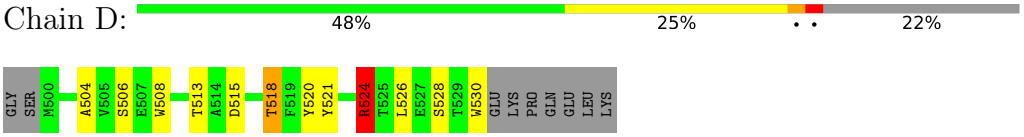
• Molecule 1: Transcription elongation regulator 1

Chain C:



• Molecule 1: Transcription elongation regulator 1

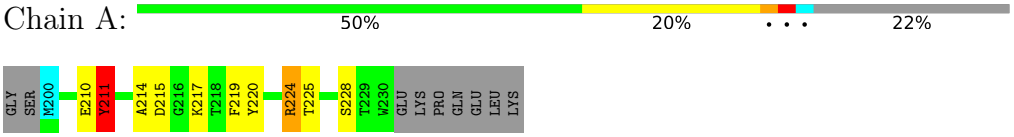
Chain D:



4.2.5 Score per residue for model 5

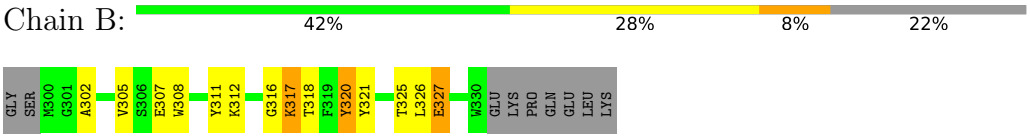
• Molecule 1: Transcription elongation regulator 1

Chain A:



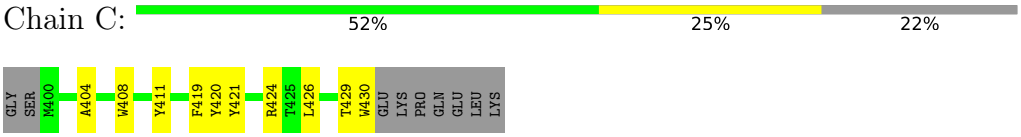
• Molecule 1: Transcription elongation regulator 1

Chain B:



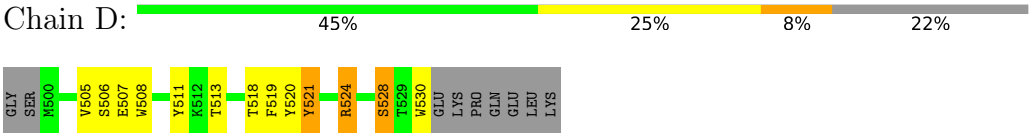
• Molecule 1: Transcription elongation regulator 1

Chain C:



• Molecule 1: Transcription elongation regulator 1

Chain D:



4.2.6 Score per residue for model 6

- Molecule 1: Transcription elongation regulator 1

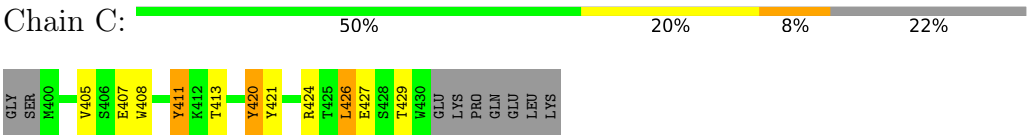
Chain A:

- Molecule 1: Transcription elongation regulator 1

Chain B:

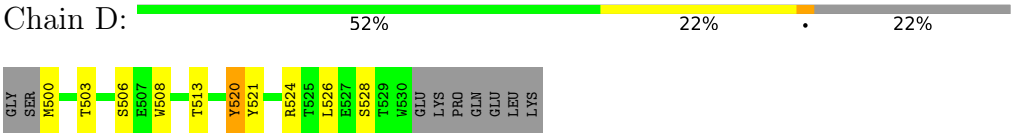
- Molecule 1: Transcription elongation regulator 1

Chain C:



- Molecule 1: Transcription elongation regulator 1

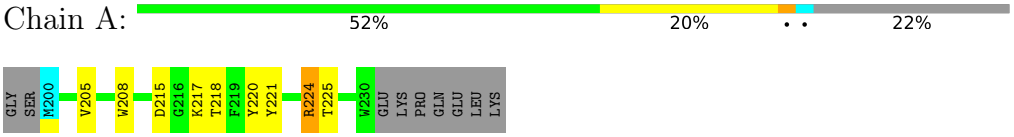
Chain D:



4.2.7 Score per residue for model 7

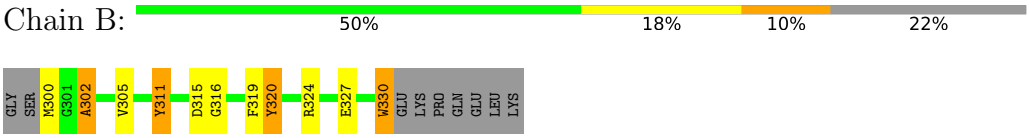
- Molecule 1: Transcription elongation regulator 1

Chain A:



- Molecule 1: Transcription elongation regulator 1

Chain B:

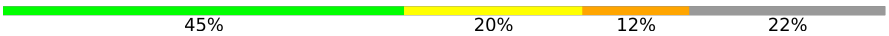


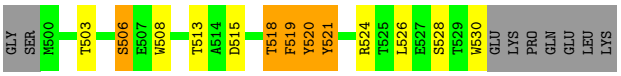
- Molecule 1: Transcription elongation regulator 1

Chain C:

• Molecule 1: Transcription elongation regulator 1

Chain D:

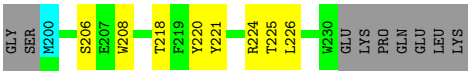




4.2.8 Score per residue for model 8

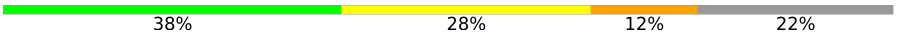
• Molecule 1: Transcription elongation regulator 1

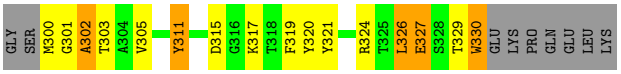
Chain A:



• Molecule 1: Transcription elongation regulator 1

Chain B:



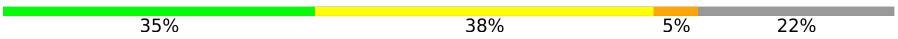


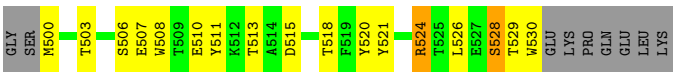
• Molecule 1: Transcription elongation regulator 1

Chain C:

• Molecule 1: Transcription elongation regulator 1

Chain D:





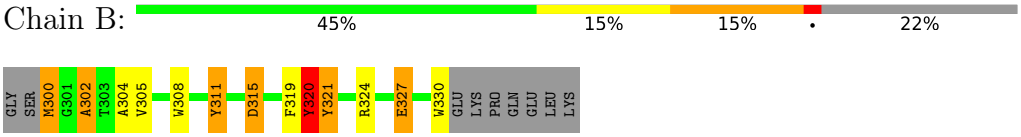
4.2.9 Score per residue for model 9

• Molecule 1: Transcription elongation regulator 1

Chain A:

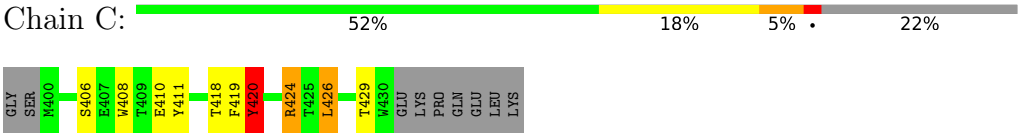
• Molecule 1: Transcription elongation regulator 1

Chain B:



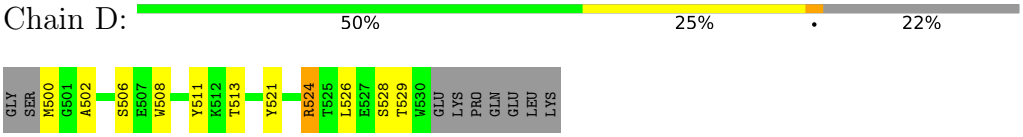
• Molecule 1: Transcription elongation regulator 1

Chain C:



• Molecule 1: Transcription elongation regulator 1

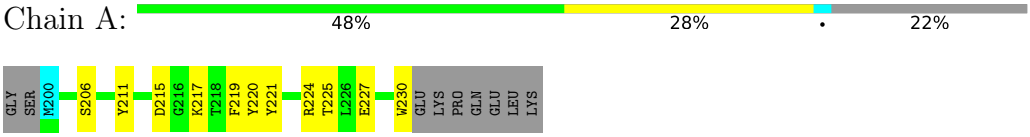
Chain D:



4.2.10 Score per residue for model 10

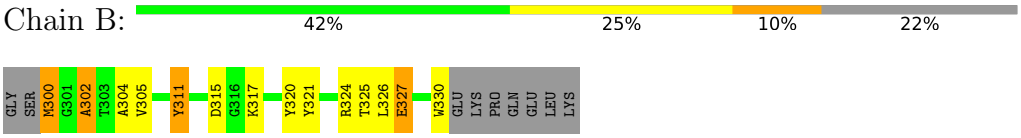
• Molecule 1: Transcription elongation regulator 1

Chain A:



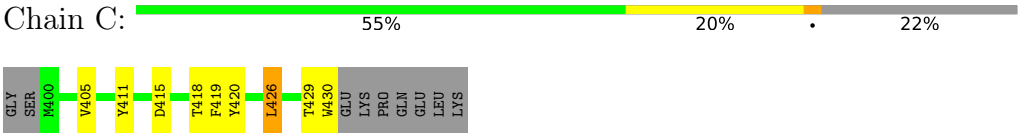
• Molecule 1: Transcription elongation regulator 1

Chain B:



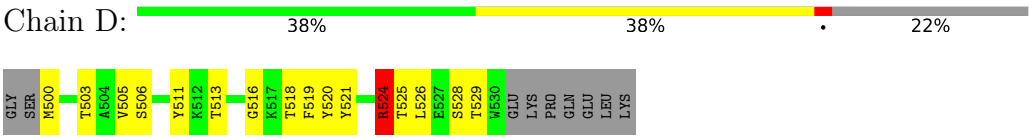
• Molecule 1: Transcription elongation regulator 1

Chain C:



• Molecule 1: Transcription elongation regulator 1

Chain D:



5 Refinement protocol and experimental data overview (i)

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 (i)

6.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.62±0.10	1±1/254 (0.5± 0.5%)	2.06±0.15	9±2/346 (2.5± 0.6%)
1	B	1.57±0.06	2±1/262 (0.7± 0.4%)	2.05±0.11	9±4/356 (2.5± 1.0%)
1	C	1.54±0.06	1±1/262 (0.4± 0.3%)	2.05±0.11	10±4/356 (2.7± 1.0%)
1	D	1.61±0.09	2±1/262 (0.6± 0.5%)	2.05±0.14	10±4/356 (2.8± 1.2%)
All	All	1.59	57/10400 (0.5%)	2.06	371/14140 (2.6%)

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	D	511	TYR	CG-CD2	8.40	1.50	1.39	9	2
1	A	228	SER	CA-CB	8.25	1.65	1.52	5	1
1	C	406	SER	CB-OG	7.72	1.52	1.42	4	2
1	A	220	TYR	CD2-CE2	7.25	1.50	1.39	4	1
1	B	307	GLU	CG-CD	6.75	1.62	1.51	2	2
1	D	530	TRP	CD2-CE2	6.73	1.49	1.41	1	1
1	A	220	TYR	CG-CD2	6.60	1.47	1.39	6	1
1	D	520	TYR	CE2-CZ	6.59	1.47	1.38	3	2
1	D	511	TYR	CB-CG	6.49	1.61	1.51	8	1
1	A	221	TYR	CE2-CZ	6.45	1.47	1.38	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	D	521	TYR	CG-CD2	6.43	1.47	1.39	7	2
1	D	508	TRP	CD2-CE2	6.21	1.48	1.41	8	1
1	D	511	TYR	CE1-CZ	6.08	1.46	1.38	8	1
1	B	311	TYR	CE1-CZ	5.99	1.46	1.38	3	1
1	B	319	PHE	CG-CD1	5.91	1.47	1.38	8	1
1	A	221	TYR	CG-CD1	5.90	1.46	1.39	6	2
1	B	301	GLY	N-CA	-5.84	1.37	1.46	1	1
1	D	506	SER	CA-CB	5.77	1.61	1.52	10	1
1	A	211	TYR	CG-CD2	5.75	1.46	1.39	4	1
1	B	321	TYR	CE2-CZ	5.74	1.46	1.38	9	2
1	A	206	SER	CB-OG	5.71	1.49	1.42	3	1
1	D	519	PHE	CG-CD2	5.63	1.47	1.38	7	1
1	B	320	TYR	CG-CD2	5.60	1.46	1.39	5	1
1	B	304	ALA	CA-CB	5.55	1.64	1.52	10	1
1	A	210	GLU	CG-CD	5.53	1.60	1.51	5	1
1	C	421	TYR	CE1-CZ	5.47	1.45	1.38	5	1
1	A	211	TYR	CE2-CZ	5.44	1.45	1.38	10	1
1	B	321	TYR	CG-CD2	5.42	1.46	1.39	10	1
1	A	227	GLU	CB-CG	5.40	1.62	1.52	10	1
1	C	420	TYR	CE2-CZ	5.39	1.45	1.38	6	1
1	C	421	TYR	CG-CD1	5.38	1.46	1.39	2	1
1	B	311	TYR	CD2-CE2	5.38	1.47	1.39	9	1
1	A	221	TYR	CZ-OH	-5.23	1.28	1.37	10	1
1	D	521	TYR	CE2-CZ	5.22	1.45	1.38	1	2
1	B	311	TYR	CB-CG	5.20	1.59	1.51	10	1
1	A	211	TYR	CD2-CE2	5.19	1.47	1.39	4	1
1	D	527	GLU	CG-CD	5.16	1.59	1.51	3	1
1	C	427	GLU	CD-OE2	5.15	1.31	1.25	6	1
1	C	420	TYR	CE1-CZ	5.14	1.45	1.38	3	1
1	B	320	TYR	CB-CG	5.14	1.59	1.51	7	1
1	C	423	ASN	N-CA	5.12	1.56	1.46	4	1
1	B	312	LYS	N-CA	-5.10	1.36	1.46	5	1
1	B	311	TYR	CE2-CZ	5.08	1.45	1.38	7	1
1	C	419	PHE	CB-CG	5.06	1.59	1.51	10	1
1	D	510	GLU	CD-OE1	5.05	1.31	1.25	3	1
1	B	320	TYR	CG-CD1	5.03	1.45	1.39	4	1
1	C	401	GLY	CA-C	5.03	1.59	1.51	8	1
1	B	319	PHE	CE2-CZ	5.02	1.46	1.37	9	1
1	B	306	SER	CB-OG	-5.01	1.35	1.42	4	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	224	ARG	NE-CZ-NH1	15.73	128.16	120.30	9	4
1	A	224	ARG	NE-CZ-NH2	-14.85	112.88	120.30	9	6
1	B	311	TYR	CB-CG-CD1	-13.88	112.67	121.00	6	6
1	C	424	ARG	NE-CZ-NH2	-12.74	113.93	120.30	6	4
1	C	424	ARG	NE-CZ-NH1	12.28	126.44	120.30	6	3
1	B	324	ARG	NE-CZ-NH2	-11.87	114.36	120.30	3	4
1	C	411	TYR	CB-CG-CD1	-11.51	114.10	121.00	3	7
1	A	221	TYR	CG-CD2-CE2	-11.35	112.22	121.30	8	2
1	B	324	ARG	NE-CZ-NH1	11.30	125.95	120.30	4	3
1	A	221	TYR	CB-CG-CD2	-10.99	114.41	121.00	8	4
1	A	219	PHE	CB-CG-CD1	-10.46	113.47	120.80	4	3
1	B	321	TYR	CB-CG-CD1	10.30	127.18	121.00	5	1
1	A	220	TYR	CB-CG-CD1	9.65	126.79	121.00	8	4
1	C	411	TYR	CG-CD1-CE1	-9.60	113.62	121.30	3	3
1	D	524	ARG	NE-CZ-NH2	-9.45	115.58	120.30	5	6
1	B	319	PHE	CB-CG-CD2	-9.35	114.25	120.80	2	2
1	D	511	TYR	CB-CG-CD2	-9.15	115.51	121.00	8	1
1	B	311	TYR	CB-CG-CD2	9.01	126.40	121.00	6	3
1	D	524	ARG	NE-CZ-NH1	8.99	124.80	120.30	3	5
1	C	420	TYR	CB-CG-CD1	-8.81	115.72	121.00	5	2
1	A	215	ASP	CB-CG-OD1	8.71	126.14	118.30	10	3
1	B	330	TRP	CD1-NE1-CE2	8.50	116.65	109.00	3	3
1	A	219	PHE	CB-CG-CD2	-8.48	114.86	120.80	10	3
1	C	420	TYR	CG-CD1-CE1	-8.45	114.54	121.30	1	1
1	D	506	SER	N-CA-CB	-8.41	97.88	110.50	10	6
1	D	520	TYR	CB-CG-CD1	-8.37	115.98	121.00	8	4
1	D	511	TYR	CG-CD1-CE1	-8.36	114.62	121.30	5	2
1	C	413	THR	CA-CB-CG2	8.31	124.04	112.40	6	1
1	B	315	ASP	CB-CG-OD2	8.23	125.71	118.30	9	2
1	A	220	TYR	CB-CG-CD2	-8.13	116.12	121.00	8	2
1	B	325	THR	CA-CB-CG2	7.96	123.54	112.40	5	1
1	A	221	TYR	CB-CG-CD1	-7.90	116.26	121.00	4	4
1	A	205	VAL	CG1-CB-CG2	-7.90	98.27	110.90	1	4
1	C	430	TRP	NE1-CE2-CD2	-7.80	99.50	107.30	8	1
1	D	509	THR	CA-CB-CG2	-7.79	101.50	112.40	3	1
1	D	524	ARG	NH1-CZ-NH2	-7.77	110.85	119.40	9	1
1	C	411	TYR	CD1-CE1-CZ	7.72	126.75	119.80	3	2
1	D	508	TRP	CD1-NE1-CE2	7.65	115.88	109.00	5	2
1	C	420	TYR	CG-CD2-CE2	-7.64	115.19	121.30	6	3
1	A	221	TYR	CD1-CG-CD2	7.61	126.27	117.90	8	1
1	B	310	GLU	OE1-CD-OE2	-7.59	114.20	123.30	4	1
1	D	515	ASP	CB-CG-OD1	7.58	125.12	118.30	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	B	315	ASP	CB-CG-OD1	7.55	125.09	118.30	10	1
1	C	421	TYR	CB-CG-CD2	-7.54	116.48	121.00	7	4
1	D	521	TYR	CG-CD1-CE1	-7.46	115.33	121.30	5	3
1	D	520	TYR	CG-CD1-CE1	-7.41	115.37	121.30	10	3
1	B	321	TYR	CB-CG-CD2	-7.41	116.56	121.00	9	4
1	D	519	PHE	CB-CG-CD1	-7.35	115.65	120.80	5	3
1	A	230	TRP	CZ3-CH2-CZ2	-7.35	112.78	121.60	9	2
1	C	424	ARG	CD-NE-CZ	7.30	133.82	123.60	6	4
1	C	430	TRP	NE1-CE2-CZ2	7.30	138.43	130.40	8	2
1	D	530	TRP	CD1-CG-CD2	-7.30	100.46	106.30	3	2
1	A	205	VAL	CA-CB-CG1	7.29	121.83	110.90	9	1
1	D	521	TYR	CB-CG-CD1	-7.24	116.65	121.00	1	2
1	A	208	TRP	CD1-NE1-CE2	7.22	115.50	109.00	7	3
1	C	411	TYR	CB-CG-CD2	7.19	125.31	121.00	6	4
1	C	419	PHE	CB-CG-CD1	-7.18	115.78	120.80	9	3
1	A	208	TRP	NE1-CE2-CZ2	7.16	138.27	130.40	7	1
1	C	415	ASP	CB-CG-OD1	7.08	124.67	118.30	2	1
1	D	508	TRP	CB-CG-CD2	7.04	135.75	126.60	5	1
1	B	321	TYR	CG-CD2-CE2	-7.00	115.70	121.30	9	1
1	A	208	TRP	CG-CD2-CE3	-6.98	127.62	133.90	7	3
1	B	308	TRP	CD1-NE1-CE2	6.96	115.27	109.00	1	1
1	B	300	MET	CA-CB-CG	6.95	125.11	113.30	10	2
1	C	408	TRP	NE1-CE2-CZ2	6.83	137.92	130.40	8	2
1	B	308	TRP	NE1-CE2-CD2	-6.78	100.52	107.30	1	2
1	C	404	ALA	CB-CA-C	6.75	120.22	110.10	5	1
1	B	319	PHE	CB-CG-CD1	6.72	125.50	120.80	2	3
1	B	320	TYR	CB-CG-CD1	-6.68	116.99	121.00	3	4
1	B	330	TRP	CE2-CD2-CG	6.66	112.62	107.30	7	2
1	B	304	ALA	CB-CA-C	6.64	120.07	110.10	9	1
1	A	230	TRP	CE2-CD2-CG	6.61	112.59	107.30	1	1
1	A	221	TYR	CG-CD1-CE1	-6.61	116.02	121.30	7	2
1	D	520	TYR	CB-CG-CD2	-6.59	117.04	121.00	6	4
1	D	515	ASP	CB-CG-OD2	-6.59	112.37	118.30	7	3
1	D	519	PHE	CB-CG-CD2	6.58	125.41	120.80	10	3
1	D	526	LEU	CB-CA-C	6.56	122.67	110.20	4	2
1	B	330	TRP	CD2-CE3-CZ3	6.56	127.33	118.80	6	2
1	A	230	TRP	CD1-NE1-CE2	6.55	114.90	109.00	2	1
1	C	421	TYR	CG-CD2-CE2	-6.55	116.06	121.30	2	1
1	B	308	TRP	CB-CG-CD2	6.54	135.10	126.60	4	2
1	B	308	TRP	CG-CD2-CE3	6.53	139.78	133.90	5	1
1	D	526	LEU	CB-CG-CD1	6.53	122.09	111.00	2	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	407	GLU	OE1-CD-OE2	-6.52	115.48	123.30	4	2
1	C	418	THR	CA-CB-CG2	6.51	121.52	112.40	8	1
1	B	330	TRP	CB-CG-CD2	6.51	135.06	126.60	7	3
1	C	430	TRP	CG-CD1-NE1	-6.48	103.62	110.10	10	1
1	A	214	ALA	N-CA-CB	-6.48	101.03	110.10	5	1
1	A	230	TRP	NE1-CE2-CD2	-6.46	100.84	107.30	1	1
1	A	215	ASP	CB-CG-OD2	-6.45	112.49	118.30	10	3
1	B	313	THR	CA-CB-CG2	6.42	121.39	112.40	2	1
1	A	213	THR	CA-CB-CG2	6.42	121.39	112.40	9	1
1	A	211	TYR	CB-CG-CD1	6.41	124.85	121.00	3	2
1	C	408	TRP	NE1-CE2-CD2	-6.40	100.90	107.30	1	2
1	A	208	TRP	NE1-CE2-CD2	-6.38	100.92	107.30	7	1
1	D	508	TRP	NE1-CE2-CZ2	6.37	137.41	130.40	8	1
1	A	230	TRP	CH2-CZ2-CE2	6.36	123.76	117.40	10	1
1	C	430	TRP	CG-CD2-CE3	6.35	139.61	133.90	4	2
1	C	430	TRP	CD1-NE1-CE2	6.30	114.67	109.00	8	2
1	B	311	TYR	CG-CD2-CE2	-6.30	116.26	121.30	2	2
1	A	220	TYR	CG-CD1-CE1	-6.28	116.28	121.30	10	1
1	A	214	ALA	CB-CA-C	6.22	119.43	110.10	5	2
1	C	408	TRP	CD1-CG-CD2	-6.17	101.36	106.30	5	2
1	A	219	PHE	CG-CD2-CE2	6.16	127.58	120.80	5	1
1	D	530	TRP	CE3-CZ3-CH2	-6.16	114.43	121.20	8	1
1	B	321	TYR	CB-CA-C	6.12	122.65	110.40	1	1
1	B	327	GLU	OE1-CD-OE2	-6.12	115.96	123.30	1	1
1	A	221	TYR	CZ-CE2-CD2	6.12	125.31	119.80	8	1
1	C	404	ALA	N-CA-CB	6.11	118.66	110.10	8	1
1	D	528	SER	N-CA-CB	-6.11	101.33	110.50	8	2
1	C	408	TRP	CG-CD2-CE3	-6.09	128.42	133.90	8	2
1	D	503	THR	CA-CB-CG2	6.08	120.92	112.40	3	1
1	C	419	PHE	CG-CD2-CE2	-6.08	114.11	120.80	9	1
1	A	208	TRP	CB-CG-CD1	-6.02	119.17	127.00	6	1
1	B	330	TRP	NE1-CE2-CD2	-6.01	101.29	107.30	7	1
1	C	400	MET	CB-CA-C	6.00	122.39	110.40	4	1
1	D	502	ALA	N-CA-CB	5.97	118.46	110.10	9	1
1	B	330	TRP	CG-CD2-CE3	5.96	139.27	133.90	4	1
1	C	419	PHE	CZ-CE2-CD2	5.96	127.25	120.10	9	1
1	C	420	TYR	CZ-CE2-CD2	5.95	125.16	119.80	4	1
1	D	505	VAL	CA-CB-CG1	5.95	119.83	110.90	5	1
1	C	410	GLU	CA-CB-CG	-5.94	100.33	113.40	9	1
1	C	430	TRP	CZ3-CH2-CZ2	-5.93	114.48	121.60	4	1
1	C	408	TRP	CH2-CZ2-CE2	5.92	123.32	117.40	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	408	TRP	CD1-NE1-CE2	5.91	114.32	109.00	1	1
1	C	419	PHE	CB-CG-CD2	-5.91	116.66	120.80	5	2
1	D	508	TRP	CB-CA-C	5.91	122.21	110.40	7	1
1	C	429	THR	O-C-N	-5.89	113.27	122.70	2	1
1	B	305	VAL	CG1-CB-CG2	-5.89	101.48	110.90	4	2
1	C	408	TRP	CD2-CE3-CZ3	5.88	126.44	118.80	9	1
1	A	230	TRP	CG-CD1-NE1	5.85	115.95	110.10	6	1
1	C	405	VAL	CA-CB-CG2	5.84	119.67	110.90	2	2
1	D	508	TRP	NE1-CE2-CD2	-5.82	101.48	107.30	4	5
1	D	508	TRP	CB-CG-CD1	-5.80	119.46	127.00	8	2
1	A	230	TRP	CB-CG-CD1	-5.80	119.47	127.00	2	1
1	D	507	GLU	OE1-CD-OE2	-5.73	116.42	123.30	5	1
1	C	408	TRP	CE2-CD2-CG	5.72	111.88	107.30	8	1
1	B	330	TRP	CE3-CZ3-CH2	-5.72	114.91	121.20	6	1
1	D	500	MET	N-CA-CB	5.71	120.88	110.60	6	1
1	C	411	TYR	N-CA-C	-5.70	95.61	111.00	9	1
1	C	421	TYR	CB-CG-CD1	5.67	124.40	121.00	8	2
1	D	521	TYR	CB-CG-CD2	-5.66	117.60	121.00	10	1
1	D	530	TRP	CE2-CD2-CG	5.65	111.82	107.30	3	3
1	A	205	VAL	CA-CB-CG2	5.65	119.37	110.90	1	1
1	A	202	ALA	CB-CA-C	5.63	118.55	110.10	4	1
1	B	330	TRP	CD1-CG-CD2	-5.63	101.80	106.30	6	1
1	D	504	ALA	CB-CA-C	5.63	118.54	110.10	4	1
1	D	512	LYS	C-N-CA	5.63	135.76	121.70	3	1
1	D	520	TYR	CZ-CE2-CD2	5.61	124.85	119.80	6	2
1	B	330	TRP	NE1-CE2-CZ2	5.60	136.56	130.40	1	2
1	D	530	TRP	NE1-CE2-CD2	-5.59	101.71	107.30	5	3
1	A	220	TYR	CD1-CG-CD2	5.57	124.03	117.90	10	1
1	C	426	LEU	CA-CB-CG	5.57	128.10	115.30	2	2
1	D	500	MET	CG-SD-CE	5.56	109.09	100.20	3	1
1	C	415	ASP	CB-CG-OD2	-5.56	113.30	118.30	10	1
1	B	329	THR	CA-CB-OG1	5.55	120.67	109.00	8	1
1	B	330	TRP	CB-CG-CD1	-5.54	119.80	127.00	8	2
1	D	530	TRP	CD2-CE3-CZ3	5.53	125.99	118.80	8	2
1	A	210	GLU	OE1-CD-OE2	-5.52	116.68	123.30	9	1
1	A	211	TYR	CZ-CE2-CD2	5.51	124.76	119.80	2	1
1	D	519	PHE	CG-CD2-CE2	-5.48	114.77	120.80	7	1
1	C	409	THR	CA-CB-CG2	5.45	120.03	112.40	3	1
1	B	311	TYR	CA-CB-CG	5.43	123.71	113.40	4	1
1	B	330	TRP	CA-CB-CG	5.42	124.01	113.70	4	1
1	B	302	ALA	CB-CA-C	5.42	118.23	110.10	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	217	LYS	O-C-N	5.40	131.34	122.70	5	1
1	A	230	TRP	NE1-CE2-CZ2	5.38	136.32	130.40	1	1
1	A	221	TYR	CD1-CE1-CZ	5.36	124.62	119.80	7	1
1	C	425	THR	CA-CB-OG1	5.33	120.20	109.00	2	1
1	A	219	PHE	CZ-CE2-CD2	-5.33	113.70	120.10	5	1
1	B	317	LYS	C-N-CA	5.33	135.02	121.70	5	1
1	A	209	THR	CA-CB-CG2	5.32	119.85	112.40	4	1
1	D	530	TRP	CA-CB-CG	5.32	123.80	113.70	8	1
1	B	330	TRP	CE2-CD2-CE3	-5.31	112.33	118.70	6	1
1	B	308	TRP	CE2-CD2-CE3	-5.30	112.33	118.70	9	1
1	C	414	ALA	CB-CA-C	5.30	118.05	110.10	2	1
1	A	211	TYR	CB-CG-CD2	-5.28	117.83	121.00	3	2
1	C	430	TRP	CB-CG-CD2	5.28	133.46	126.60	7	1
1	D	503	THR	N-CA-CB	-5.25	100.32	110.30	6	1
1	B	301	GLY	C-N-CA	5.25	134.82	121.70	2	1
1	C	406	SER	N-CA-CB	-5.23	102.65	110.50	9	1
1	B	300	MET	CB-CA-C	5.20	120.81	110.40	9	1
1	C	403	THR	CA-CB-OG1	5.20	119.92	109.00	2	1
1	D	520	TYR	CD1-CG-CD2	5.19	123.61	117.90	10	2
1	A	230	TRP	CD1-CG-CD2	-5.18	102.16	106.30	6	2
1	C	420	TYR	CB-CG-CD2	-5.16	117.91	121.00	9	1
1	B	311	TYR	CD1-CE1-CZ	5.16	124.44	119.80	9	2
1	B	308	TRP	CD1-CG-CD2	-5.15	102.18	106.30	3	1
1	B	314	ALA	CB-CA-C	5.14	117.82	110.10	2	1
1	D	511	TYR	CG-CD2-CE2	-5.14	117.18	121.30	9	1
1	A	211	TYR	CG-CD1-CE1	5.14	125.41	121.30	2	1
1	B	326	LEU	CB-CG-CD1	5.13	119.72	111.00	3	1
1	B	305	VAL	CA-CB-CG2	5.12	118.58	110.90	3	1
1	D	505	VAL	CG1-CB-CG2	-5.08	102.76	110.90	10	1
1	C	408	TRP	CG-CD1-NE1	5.06	115.16	110.10	5	1
1	B	321	TYR	CD1-CE1-CZ	5.06	124.35	119.80	3	1
1	B	330	TRP	CH2-CZ2-CE2	5.05	122.45	117.40	8	1
1	D	510	GLU	OE1-CD-OE2	-5.03	117.26	123.30	8	1
1	B	308	TRP	CB-CG-CD1	-5.03	120.46	127.00	2	1
1	C	430	TRP	CD1-CG-CD2	-5.03	102.28	106.30	7	1
1	D	530	TRP	CZ3-CH2-CZ2	-5.02	115.58	121.60	5	1
1	C	426	LEU	CB-CG-CD2	5.02	119.53	111.00	10	1
1	A	208	TRP	CE3-CZ3-CH2	-5.01	115.69	121.20	4	1
1	D	505	VAL	CA-CB-CG2	5.00	118.41	110.90	3	1
1	D	509	THR	O-C-N	-5.00	114.70	122.70	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
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	247	222	222	0±0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
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	24

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: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: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:C:424:ARG:HH22	1:D:507:GLU:CD	0.45	2.15	8	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:A:205:VAL:N	1:A:226:LEU:HD13	0.43	2.28	6	1
1:B:325:THR:C	1:B:326:LEU:HD12	0.43	2.33	10	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:C:419:PHE:CE1	1:D:519:PHE:CD2	0.40	3.10	1	1
1:B:320:TYR:CD1	1:C:420:TYR:CE2	0.40	3.09	10	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	29/40 (72%)	25±1 (88±5%)	3±2 (11±5%)	0±0 (1±2%)	20 68
1	B	29/40 (72%)	24±1 (81±4%)	4±1 (13±5%)	2±1 (6±3%)	3 23
1	C	29/40 (72%)	27±1 (93±3%)	2±1 (6±3%)	0±0 (1±1%)	26 73
1	D	29/40 (72%)	25±1 (86±4%)	4±1 (12±4%)	1±1 (2±2%)	10 50
All	All	1160/1600 (72%)	1008 (87%)	125 (11%)	27 (2%)	9 48

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±4%)	2±1 (6±4%)	23 72
1	B	26/34 (76%)	20±2 (78±6%)	6±2 (22±6%)	3 31
1	C	26/34 (76%)	24±1 (91±3%)	2±1 (9±3%)	13 59
1	D	26/34 (76%)	21±2 (80±6%)	5±2 (20±6%)	4 34
All	All	1030/1360 (76%)	883 (86%)	147 (14%)	6 46

All 36 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	B	311	TYR	10
1	C	426	LEU	10
1	C	429	THR	10
1	D	513	THR	10
1	D	524	ARG	10
1	B	327	GLU	9
1	B	315	ASP	8
1	D	528	SER	8
1	B	300	MET	7
1	D	503	THR	6
1	D	518	THR	6
1	B	317	LYS	4
1	D	500	MET	3
1	A	224	ARG	3
1	D	526	LEU	3
1	D	506	SER	3
1	A	213	THR	2
1	A	227	GLU	2
1	B	326	LEU	2
1	A	212	LYS	2
1	B	303	THR	2
1	A	218	THR	2
1	B	330	TRP	2
1	C	418	THR	2
1	A	226	LEU	1
1	A	229	THR	1
1	B	306	SER	1
1	D	509	THR	1
1	D	530	TRP	1
1	A	219	PHE	1
1	A	211	TYR	1
1	B	324	ARG	1
1	C	409	THR	1
1	D	508	TRP	1
1	C	405	VAL	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

No chemical shift data were provided