



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:52 pm GMT

PDB ID : 1SFW  
Title : PORCINE PANCREAS PHOSPHOLIPASE A2, NMR, 18 STRUCTURES  
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Deposited on : 1996-02-23

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

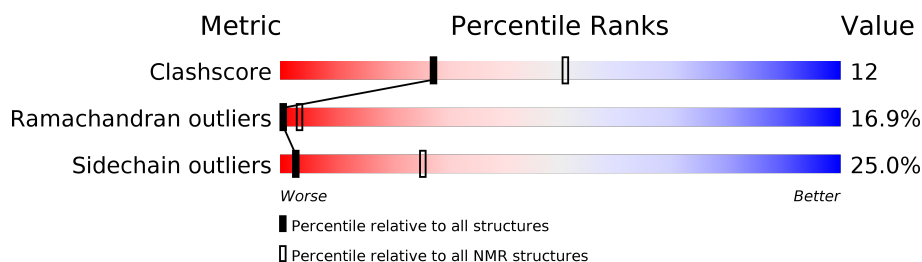
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

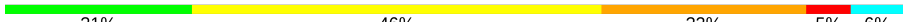
The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	124	 <div>21% 46% 23% 5% 6%</div>

## 2 Ensemble composition and analysis

This entry contains 18 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:1-A:61, A:69-A:124 (117)	0.54	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, 2, 3, 4, 5, 6, 7, 8, 12, 14, 15, 16
2	13, 17, 18
3	9, 10, 11

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 972 atoms, of which 0 are hydrogens and 0 are deuteriums.

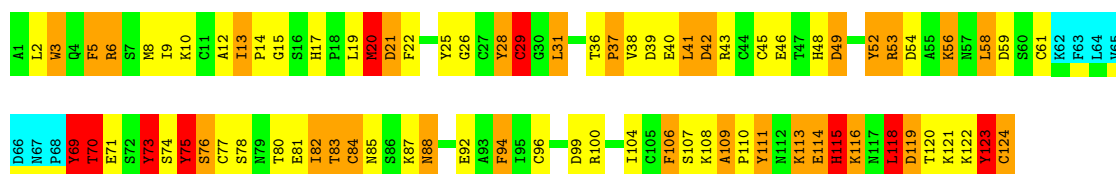
- Molecule 1 is a protein called PHOSPHOLIPASE A2.

Mol	Chain	Residues	Atoms					Trace
1	A	124	Total	C	N	O	S	0
			971	596	166	193	16	

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

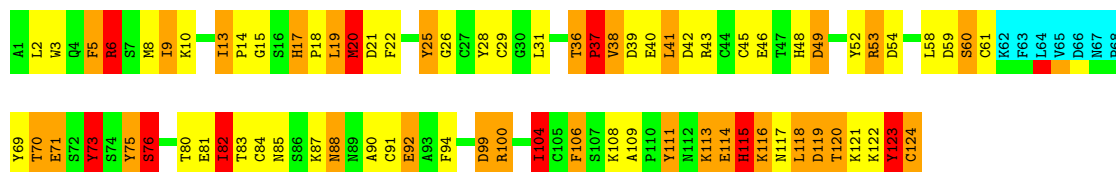




### 4.2.3 Score per residue for model 3

- Molecule 1: PHOSPHOLIPASE A2

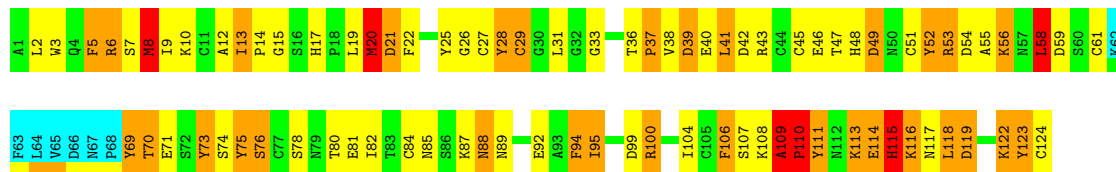
Chain A: 32% 32% 23% 7% 6%



### 4.2.4 Score per residue for model 4

- Molecule 1: PHOSPHOLIPASE A2

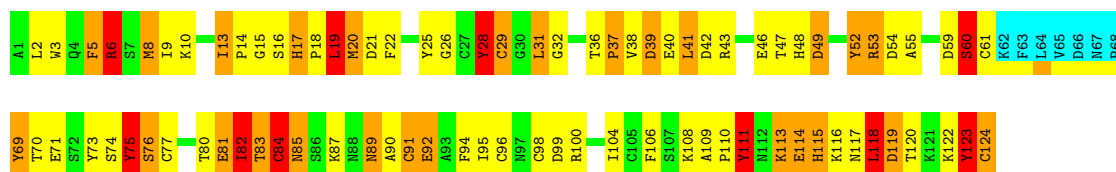
Chain A: 27% 38% 25% 5% 6%



### 4.2.5 Score per residue for model 5

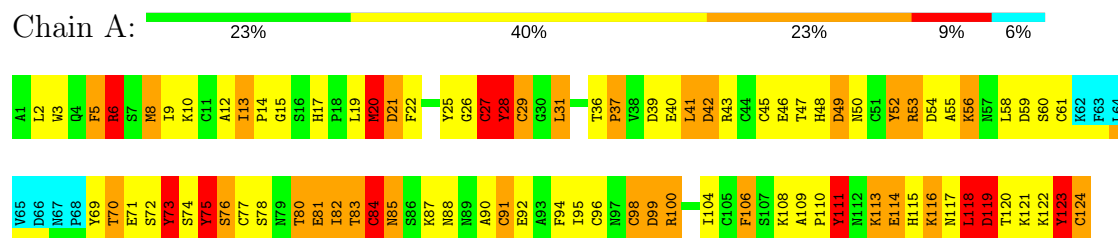
- Molecule 1: PHOSPHOLIPASE A2

Chain A: 27% 39% 21% 8% 6%



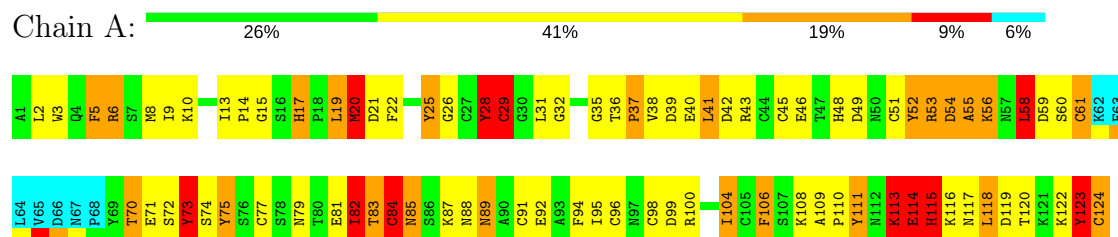
### 4.2.6 Score per residue for model 6

- Molecule 1: PHOSPHOLIPASE A2



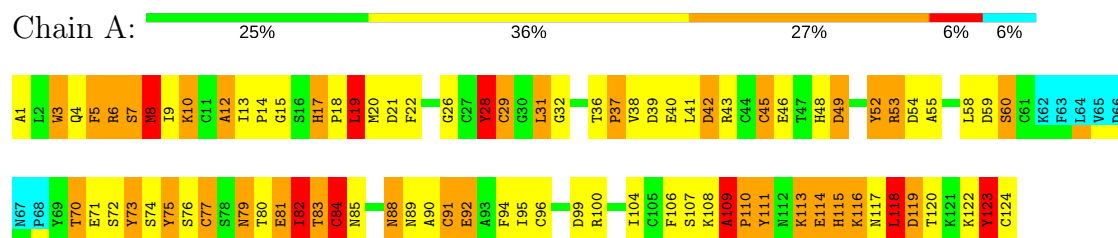
#### 4.2.7 Score per residue for model 7

- Molecule 1: PHOSPHOLIPASE A2



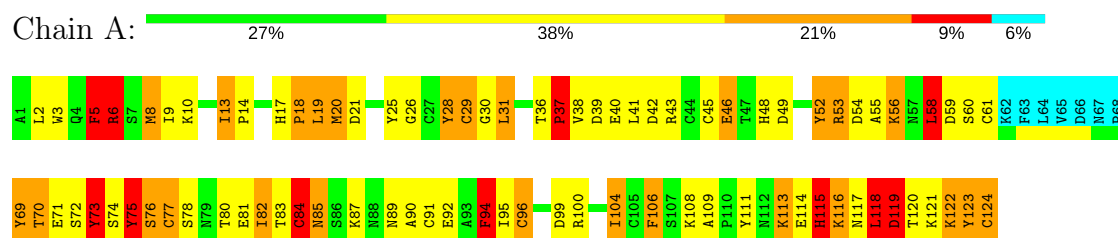
#### 4.2.8 Score per residue for model 8

- Molecule 1: PHOSPHOLIPASE A2



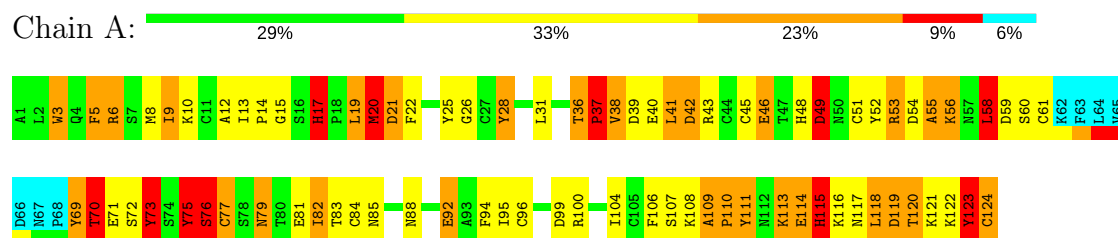
#### 4.2.9 Score per residue for model 9

- Molecule 1: PHOSPHOLIPASE A2



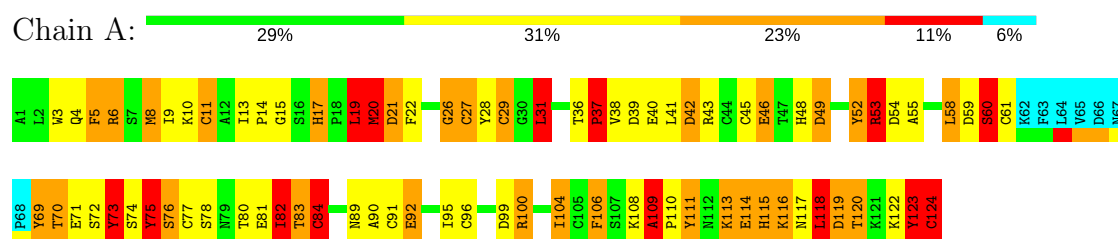
#### 4.2.10 Score per residue for model 10

- Molecule 1: PHOSPHOLIPASE A2



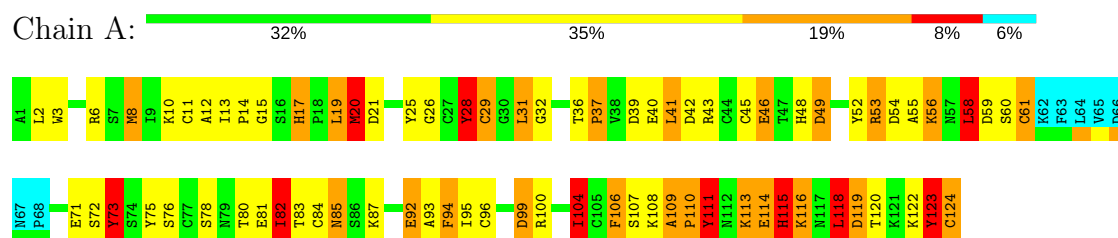
#### 4.2.11 Score per residue for model 11

- Molecule 1: PHOSPHOLIPASE A2



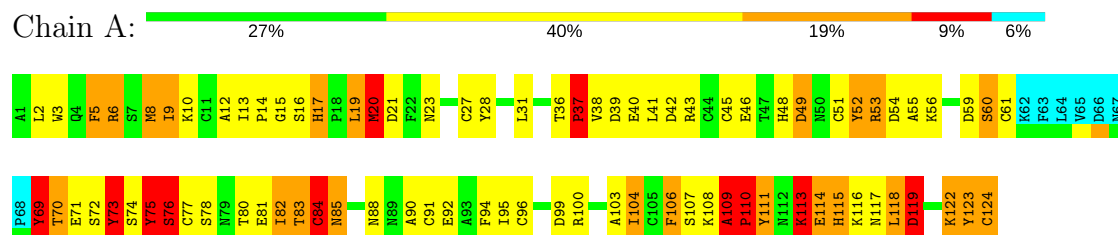
#### 4.2.12 Score per residue for model 12

- Molecule 1: PHOSPHOLIPASE A2



#### 4.2.13 Score per residue for model 13

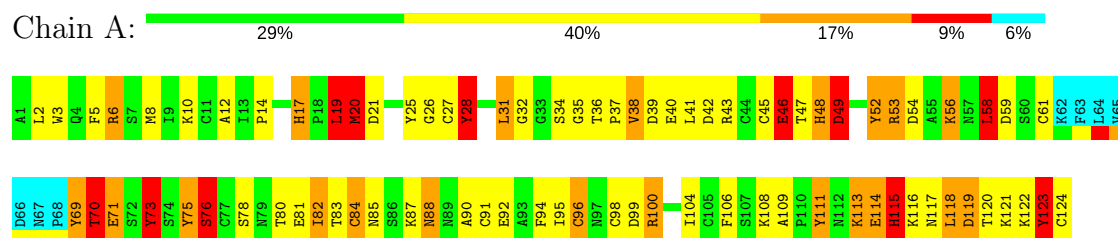
- Molecule 1: PHOSPHOLIPASE A2





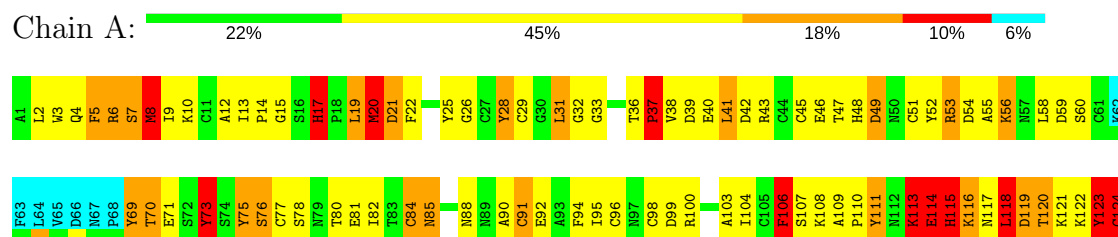
#### 4.2.14 Score per residue for model 14

- Molecule 1: PHOSPHOLIPASE A2



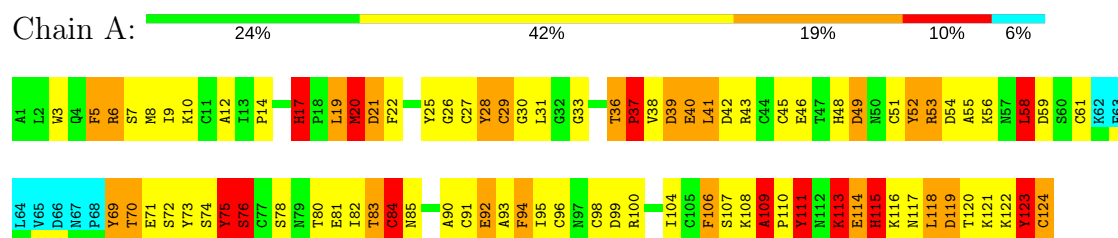
#### 4.2.15 Score per residue for model 15

- Molecule 1: PHOSPHOLIPASE A2



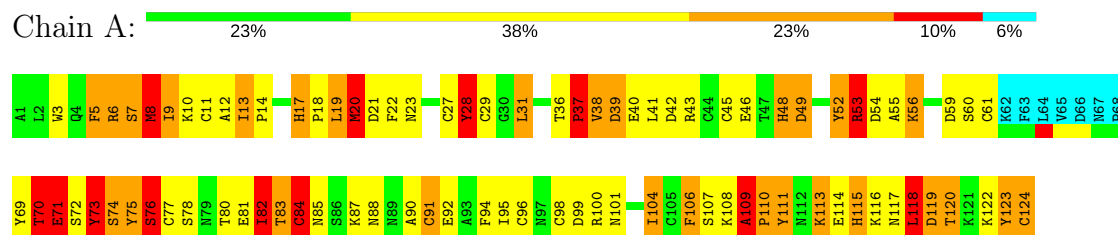
#### 4.2.16 Score per residue for model 16

- Molecule 1: PHOSPHOLIPASE A2



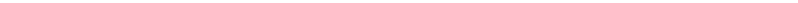
#### 4.2.17 Score per residue for model 17

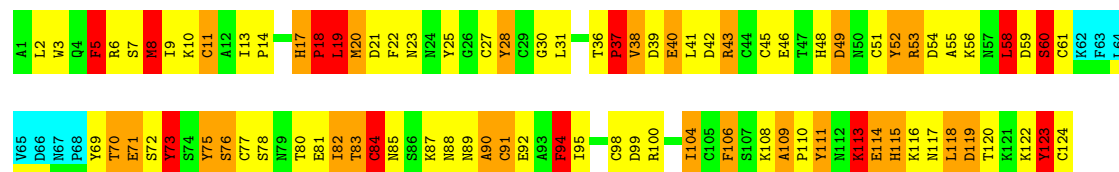
- Molecule 1: PHOSPHOLIPASE A2



#### 4.2.18 Score per residue for model 18

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 18 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DISCOVER	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality (i)

### 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:  
CA

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	1.48±0.02	15±1/933 (1.6±0.1%)	2.27±0.03	59±4/1258 (4.7±0.3%)
All	All	1.48	274/16794 (1.6%)	2.27	1063/22644 (4.7%)

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	15.4±2.2
All	All	0	277

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	92	GLU	CD-OE1	11.12	1.37	1.25	7	2
1	A	71	GLU	CD-OE1	11.09	1.37	1.25	2	9
1	A	71	GLU	CD-OE2	11.02	1.37	1.25	5	9
1	A	40	GLU	CD-OE2	10.98	1.37	1.25	16	15
1	A	81	GLU	CD-OE2	10.97	1.37	1.25	1	2
1	A	46	GLU	CD-OE1	10.96	1.37	1.25	11	7
1	A	81	GLU	CD-OE1	10.95	1.37	1.25	15	16
1	A	114	GLU	CD-OE2	10.94	1.37	1.25	5	11
1	A	40	GLU	CD-OE1	10.94	1.37	1.25	12	3
1	A	46	GLU	CD-OE2	10.90	1.37	1.25	9	11
1	A	92	GLU	CD-OE2	10.89	1.37	1.25	9	16
1	A	114	GLU	CD-OE1	10.89	1.37	1.25	10	7
1	A	124	CYS	C-OXT	7.70	1.38	1.23	4	18
1	A	123	TYR	CB-CG	5.87	1.60	1.51	2	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	39	ASP	CG-OD1	5.42	1.37	1.25	15	9
1	A	119	ASP	CG-OD1	5.42	1.37	1.25	16	7
1	A	49	ASP	CG-OD1	5.41	1.37	1.25	4	5
1	A	54	ASP	CG-OD2	5.40	1.37	1.25	9	11
1	A	21	ASP	CG-OD1	5.39	1.37	1.25	16	9
1	A	54	ASP	CG-OD1	5.39	1.37	1.25	18	7
1	A	21	ASP	CG-OD2	5.38	1.37	1.25	2	9
1	A	49	ASP	CG-OD2	5.37	1.37	1.25	11	13
1	A	59	ASP	CG-OD2	5.36	1.37	1.25	11	8
1	A	119	ASP	CG-OD2	5.35	1.37	1.25	12	11
1	A	59	ASP	CG-OD1	5.35	1.37	1.25	6	10
1	A	69	TYR	CB-CG	5.31	1.59	1.51	5	2
1	A	39	ASP	CG-OD2	5.30	1.37	1.25	4	9
1	A	42	ASP	CG-OD1	5.30	1.37	1.25	13	9
1	A	42	ASP	CG-OD2	5.24	1.37	1.25	5	8
1	A	99	ASP	CG-OD2	5.19	1.37	1.25	9	6
1	A	99	ASP	CG-OD1	5.17	1.37	1.25	3	5
1	A	110	PRO	CA-C	5.13	1.63	1.52	10	3
1	A	111	TYR	CA-CB	5.11	1.65	1.53	12	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	111	TYR	CB-CG-CD2	-15.18	111.89	121.00	11	18
1	A	73	TYR	CB-CG-CD2	-14.30	112.42	121.00	3	7
1	A	111	TYR	CB-CG-CD1	-13.24	113.05	121.00	4	18
1	A	106	PHE	CB-CG-CD2	-13.17	111.58	120.80	3	17
1	A	123	TYR	N-CA-CB	-11.84	89.28	110.60	12	18
1	A	73	TYR	CB-CG-CD1	11.71	128.03	121.00	12	8
1	A	106	PHE	CB-CG-CD1	11.52	128.86	120.80	3	17
1	A	19	LEU	CB-CG-CD1	11.25	130.13	111.00	18	1
1	A	28	TYR	CB-CG-CD1	10.96	127.58	121.00	1	9
1	A	75	TYR	CB-CG-CD2	-10.69	114.58	121.00	8	16
1	A	28	TYR	CB-CG-CD2	-10.59	114.65	121.00	1	9
1	A	118	LEU	CB-CG-CD1	10.55	128.94	111.00	1	2
1	A	56	LYS	N-CA-CB	-10.46	91.77	110.60	7	3
1	A	6	ARG	NE-CZ-NH1	10.29	125.44	120.30	7	18
1	A	100	ARG	NE-CZ-NH1	10.13	125.36	120.30	17	18
1	A	118	LEU	CB-CA-C	10.01	129.22	110.20	9	9
1	A	109	ALA	CB-CA-C	10.01	125.12	110.10	16	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	TYR	CB-CG-CD1	9.42	126.65	121.00	8	14
1	A	10	LYS	N-CA-CB	-9.25	93.95	110.60	8	4
1	A	69	TYR	CB-CG-CD1	9.05	126.43	121.00	11	9
1	A	123	TYR	CB-CG-CD2	-9.01	115.60	121.00	6	14
1	A	53	ARG	NE-CZ-NH1	8.93	124.76	120.30	16	18
1	A	76	SER	N-CA-CB	-8.88	97.18	110.50	14	16
1	A	122	LYS	N-CA-CB	-8.82	94.72	110.60	5	18
1	A	84	CYS	CB-CA-C	8.60	127.60	110.40	9	1
1	A	94	PHE	CB-CG-CD1	-8.50	114.85	120.80	9	3
1	A	114	GLU	CB-CA-C	8.49	127.38	110.40	12	18
1	A	39	ASP	CB-CG-OD2	-8.36	110.78	118.30	9	16
1	A	31	LEU	CB-CA-C	8.33	126.03	110.20	14	14
1	A	42	ASP	CB-CG-OD1	-8.22	110.90	118.30	6	14
1	A	39	ASP	CB-CG-OD1	8.13	125.61	118.30	9	15
1	A	123	TYR	CB-CG-CD1	8.12	125.87	121.00	6	11
1	A	89	ASN	N-CA-CB	7.98	124.97	110.60	7	2
1	A	43	ARG	NE-CZ-NH1	7.92	124.26	120.30	16	18
1	A	119	ASP	CB-CA-C	7.90	126.21	110.40	9	1
1	A	119	ASP	N-CA-CB	-7.90	96.38	110.60	4	2
1	A	8	MET	N-CA-CB	-7.80	96.56	110.60	18	7
1	A	42	ASP	CB-CG-OD2	-7.63	111.43	118.30	14	12
1	A	82	ILE	CA-CB-CG1	7.62	125.47	111.00	17	6
1	A	99	ASP	CB-CG-OD2	-7.61	111.45	118.30	8	18
1	A	20	MET	N-CA-CB	-7.60	96.93	110.60	3	17
1	A	117	ASN	N-CA-CB	-7.58	96.96	110.60	7	3
1	A	49	ASP	CB-CG-OD2	-7.56	111.49	118.30	1	15
1	A	21	ASP	CB-CG-OD2	-7.56	111.50	118.30	9	18
1	A	123	TYR	CA-CB-CG	7.51	127.67	113.40	4	2
1	A	119	ASP	CB-CG-OD2	-7.51	111.54	118.30	14	16
1	A	41	LEU	CB-CA-C	7.48	124.41	110.20	6	10
1	A	116	LYS	N-CA-CB	-7.25	97.55	110.60	6	12
1	A	111	TYR	N-CA-CB	-7.25	97.55	110.60	4	4
1	A	70	THR	N-CA-CB	7.24	124.06	110.30	11	9
1	A	37	PRO	N-CA-CB	-7.17	94.70	103.30	9	9
1	A	72	SER	N-CA-CB	-7.11	99.84	110.50	17	10
1	A	84	CYS	N-CA-CB	7.05	123.29	110.60	9	11
1	A	54	ASP	CB-CG-OD2	-7.03	111.97	118.30	14	18
1	A	38	VAL	CG1-CB-CG2	-7.00	99.69	110.90	13	13
1	A	119	ASP	CB-CG-OD1	-6.95	112.05	118.30	10	18
1	A	54	ASP	CB-CG-OD1	-6.89	112.10	118.30	18	18
1	A	49	ASP	CB-CG-OD1	6.87	124.48	118.30	14	17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	99	ASP	CB-CG-OD1	-6.85	112.13	118.30	13	15
1	A	59	ASP	CB-CG-OD1	-6.81	112.17	118.30	6	18
1	A	59	ASP	CB-CG-OD2	-6.79	112.19	118.30	11	18
1	A	31	LEU	CA-C-N	-6.76	102.68	116.20	2	2
1	A	21	ASP	CB-CG-OD1	-6.73	112.25	118.30	18	18
1	A	17	HIS	CG-ND1-CE1	-6.72	96.97	105.70	17	18
1	A	8	MET	CG-SD-CE	-6.71	89.47	100.20	17	5
1	A	58	LEU	CB-CA-C	6.67	122.87	110.20	10	6
1	A	122	LYS	C-N-CA	6.66	138.36	121.70	13	3
1	A	9	ILE	CB-CA-C	6.64	124.88	111.60	3	1
1	A	71	GLU	N-CA-CB	6.62	122.51	110.60	5	2
1	A	115	HIS	CG-ND1-CE1	-6.58	97.15	105.70	18	17
1	A	3	TRP	CG-CD2-CE3	-6.55	128.00	133.90	10	2
1	A	60	SER	N-CA-CB	-6.50	100.76	110.50	11	8
1	A	118	LEU	CB-CG-CD2	6.47	122.00	111.00	17	6
1	A	114	GLU	N-CA-CB	-6.40	99.07	110.60	7	13
1	A	13	ILE	N-CA-C	-6.34	93.89	111.00	1	8
1	A	111	TYR	CB-CA-C	-6.24	97.93	110.40	12	4
1	A	78	SER	CB-CA-C	6.23	121.93	110.10	6	13
1	A	70	THR	N-CA-C	6.17	127.66	111.00	4	2
1	A	19	LEU	CB-CA-C	-6.15	98.52	110.20	9	3
1	A	69	TYR	CA-CB-CG	6.13	125.04	113.40	13	8
1	A	5	PHE	CA-CB-CG	6.11	128.55	113.90	18	1
1	A	58	LEU	CA-CB-CG	6.09	129.32	115.30	11	2
1	A	82	ILE	CB-CA-C	6.04	123.69	111.60	1	5
1	A	19	LEU	CA-CB-CG	6.04	129.19	115.30	18	1
1	A	93	ALA	CB-CA-C	-5.97	101.15	110.10	12	2
1	A	56	LYS	CB-CA-C	5.96	122.33	110.40	4	8
1	A	6	ARG	NE-CZ-NH2	-5.94	117.33	120.30	3	4
1	A	123	TYR	CB-CA-C	5.92	122.25	110.40	17	4
1	A	75	TYR	N-CA-CB	-5.92	99.95	110.60	1	5
1	A	41	LEU	CB-CG-CD2	-5.90	100.98	111.00	8	6
1	A	29	CYS	CB-CA-C	5.88	122.16	110.40	5	2
1	A	7	SER	CB-CA-C	5.87	121.24	110.10	8	4
1	A	8	MET	N-CA-C	5.85	126.80	111.00	8	2
1	A	109	ALA	N-CA-CB	-5.84	101.92	110.10	16	1
1	A	19	LEU	C-N-CA	5.83	136.29	121.70	11	11
1	A	100	ARG	NE-CZ-NH2	-5.83	117.39	120.30	7	10
1	A	3	TRP	CD1-NE1-CE2	-5.82	103.76	109.00	1	18
1	A	12	ALA	N-CA-CB	-5.81	101.97	110.10	6	1
1	A	118	LEU	CA-C-N	-5.80	104.44	117.20	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	89	ASN	CB-CA-C	5.78	121.97	110.40	4	1
1	A	69	TYR	CB-CG-CD2	-5.78	117.53	121.00	11	4
1	A	53	ARG	NE-CZ-NH2	-5.75	117.43	120.30	16	4
1	A	122	LYS	CA-C-N	-5.74	104.58	117.20	9	2
1	A	40	GLU	N-CA-CB	5.73	120.92	110.60	3	2
1	A	48	HIS	CG-ND1-CE1	-5.73	98.25	105.70	13	15
1	A	100	ARG	CG-CD-NE	5.68	123.73	111.80	3	1
1	A	6	ARG	CB-CG-CD	5.67	126.35	111.60	17	3
1	A	17	HIS	N-CA-CB	5.67	120.80	110.60	9	2
1	A	38	VAL	CA-CB-CG2	5.67	119.40	110.90	15	5
1	A	90	ALA	N-CA-C	5.64	126.22	111.00	9	2
1	A	53	ARG	N-CA-CB	-5.60	100.53	110.60	9	3
1	A	55	ALA	N-CA-CB	-5.57	102.30	110.10	7	2
1	A	19	LEU	CB-CG-CD2	-5.57	101.53	111.00	18	1
1	A	77	CYS	N-CA-CB	5.57	120.63	110.60	10	2
1	A	110	PRO	CA-C-N	-5.55	105.00	117.20	15	5
1	A	115	HIS	CA-CB-CG	5.55	123.03	113.60	15	1
1	A	29	CYS	N-CA-C	5.52	125.91	111.00	7	1
1	A	12	ALA	CB-CA-C	5.51	118.37	110.10	8	1
1	A	100	ARG	N-CA-CB	-5.47	100.76	110.60	12	2
1	A	9	ILE	CA-CB-CG2	5.45	121.81	110.90	13	3
1	A	20	MET	CB-CA-C	5.44	121.28	110.40	9	2
1	A	25	TYR	CB-CG-CD1	-5.43	117.74	121.00	18	1
1	A	76	SER	CB-CA-C	-5.42	99.79	110.10	16	1
1	A	13	ILE	N-CA-CB	-5.41	98.36	110.80	3	1
1	A	29	CYS	CA-CB-SG	-5.40	104.28	114.00	2	1
1	A	124	CYS	N-CA-CB	5.38	120.28	110.60	10	2
1	A	98	CYS	CA-CB-SG	-5.38	104.32	114.00	6	4
1	A	56	LYS	N-CA-C	5.37	125.50	111.00	7	1
1	A	95	ILE	CA-CB-CG1	5.33	121.14	111.00	4	1
1	A	20	MET	N-CA-C	5.33	125.38	111.00	13	6
1	A	27	CYS	N-CA-CB	5.32	120.17	110.60	11	2
1	A	79	ASN	CA-C-N	-5.31	105.53	117.20	8	1
1	A	28	TYR	N-CA-CB	5.29	120.13	110.60	17	2
1	A	91	CYS	N-CA-CB	-5.26	101.12	110.60	18	1
1	A	87	LYS	CB-CG-CD	5.26	125.28	111.60	17	1
1	A	116	LYS	CA-C-N	-5.26	105.63	117.20	3	2
1	A	94	PHE	CB-CA-C	5.23	120.86	110.40	9	3
1	A	6	ARG	CG-CD-NE	5.22	122.77	111.80	17	1
1	A	73	TYR	N-CA-CB	5.21	119.97	110.60	8	2
1	A	116	LYS	N-CA-C	5.20	125.05	111.00	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	LEU	N-CA-C	5.19	125.01	111.00	7	1
1	A	28	TYR	CA-CB-CG	5.18	123.25	113.40	8	1
1	A	17	HIS	CB-CG-CD2	-5.18	114.74	130.80	17	1
1	A	96	CYS	N-CA-CB	-5.18	101.28	110.60	9	1
1	A	75	TYR	CB-CA-C	5.17	120.74	110.40	3	1
1	A	110	PRO	N-CA-CB	-5.17	96.92	102.60	13	1
1	A	42	ASP	CB-CA-C	5.15	120.69	110.40	16	2
1	A	79	ASN	CB-CA-C	-5.14	100.11	110.40	10	1
1	A	38	VAL	CA-CB-CG1	5.13	118.60	110.90	13	1
1	A	22	PHE	CB-CG-CD1	5.13	124.39	120.80	18	1
1	A	48	HIS	N-CA-CB	5.12	119.81	110.60	7	3
1	A	104	ILE	CA-CB-CG2	5.11	121.13	110.90	12	2
1	A	49	ASP	N-CA-C	-5.10	97.22	111.00	14	1
1	A	77	CYS	CB-CA-C	5.07	120.54	110.40	9	1
1	A	115	HIS	CB-CA-C	5.07	120.53	110.40	16	1
1	A	80	THR	N-CA-CB	5.03	119.85	110.30	6	1
1	A	26	GLY	CA-C-N	-5.02	106.15	117.20	11	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	14	PRO	Peptide	18
1	A	113	LYS	Peptide	18
1	A	115	HIS	Sidechain	17
1	A	20	MET	Peptide	17
1	A	75	TYR	Sidechain,Peptide	17
1	A	52	TYR	Sidechain	15
1	A	69	TYR	Sidechain,Peptide	14
1	A	73	TYR	Sidechain	14
1	A	123	TYR	Sidechain	14
1	A	111	TYR	Sidechain	13
1	A	25	TYR	Sidechain	12
1	A	88	ASN	Peptide	12
1	A	28	TYR	Sidechain,Peptide	10
1	A	22	PHE	Sidechain	10
1	A	76	SER	Peptide	10
1	A	31	LEU	Peptide	9
1	A	118	LEU	Peptide	6
1	A	7	SER	Peptide	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	70	THR	Peptide	4
1	A	19	LEU	Mainchain,Peptide	4
1	A	94	PHE	Sidechain	4
1	A	89	ASN	Peptide	3
1	A	53	ARG	Peptide	3
1	A	26	GLY	Peptide	3
1	A	6	ARG	Sidechain,Peptide	2
1	A	55	ALA	Peptide	2
1	A	74	SER	Peptide	2
1	A	36	THR	Peptide	2
1	A	18	PRO	Peptide	2
1	A	116	LYS	Peptide	1
1	A	5	PHE	Sidechain	1
1	A	29	CYS	Peptide	1
1	A	10	LYS	Peptide	1
1	A	110	PRO	Peptide	1
1	A	72	SER	Peptide	1
1	A	106	PHE	Peptide	1
1	A	47	THR	Peptide	1
1	A	50	ASN	Peptide	1
1	A	46	GLU	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	913	0	827	21±5
All	All	16452	0	14886	385

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:MET:SD	1:A:82:ILE:HG21	1.10	1.86	12	5
1:A:9:ILE:HG22	1:A:18:PRO:HB2	0.77	1.54	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ALA:HB2	1:A:95:ILE:HD11	0.76	1.58	18	8
1:A:58:LEU:HD23	1:A:61:CYS:HB2	0.73	1.59	10	6
1:A:8:MET:SD	1:A:82:ILE:CG2	0.71	2.75	12	4
1:A:55:ALA:HB3	1:A:95:ILE:CD1	0.71	2.14	9	1
1:A:12:ALA:HB1	1:A:107:SER:HB2	0.71	1.60	15	4
1:A:118:LEU:HD23	1:A:123:TYR:CG	0.71	2.20	12	10
1:A:55:ALA:HB2	1:A:94:PHE:CE1	0.70	2.22	9	1
1:A:26:GLY:HA2	1:A:118:LEU:HD22	0.69	1.63	8	4
1:A:109:ALA:HB1	1:A:110:PRO:HD2	0.68	1.63	17	9
1:A:9:ILE:HG22	1:A:18:PRO:CB	0.67	2.20	9	1
1:A:55:ALA:HB1	1:A:58:LEU:HD22	0.67	1.66	9	1
1:A:5:PHE:O	1:A:8:MET:SD	0.67	2.53	18	5
1:A:5:PHE:CE2	1:A:9:ILE:HD11	0.66	2.26	13	14
1:A:8:MET:SD	1:A:75:TYR:CD2	0.63	2.91	5	9
1:A:12:ALA:HB1	1:A:107:SER:HB3	0.62	1.71	10	5
1:A:83:THR:HG23	1:A:84:CYS:H	0.62	1.54	17	12
1:A:119:ASP:HB3	1:A:123:TYR:CD2	0.61	2.30	9	3
1:A:55:ALA:CB	1:A:95:ILE:HD11	0.61	2.25	18	7
1:A:45:CYS:SG	1:A:106:PHE:CZ	0.61	2.94	18	7
1:A:122:LYS:HB2	1:A:123:TYR:CD2	0.61	2.31	4	3
1:A:26:GLY:H	1:A:118:LEU:HD13	0.61	1.55	4	3
1:A:45:CYS:SG	1:A:106:PHE:CE1	0.60	2.94	17	11
1:A:109:ALA:HB1	1:A:110:PRO:CD	0.60	2.26	13	6
1:A:91:CYS:O	1:A:95:ILE:HD13	0.60	1.97	16	9
1:A:6:ARG:HH11	1:A:9:ILE:HG21	0.60	1.57	7	2
1:A:115:HIS:HB2	1:A:118:LEU:HD21	0.59	1.74	14	6
1:A:8:MET:SD	1:A:75:TYR:CG	0.59	2.95	16	5
1:A:9:ILE:O	1:A:12:ALA:HB3	0.59	1.97	15	3
1:A:120:THR:HB	1:A:124:CYS:SG	0.58	2.39	6	6
1:A:60:SER:HB3	1:A:90:ALA:HB3	0.56	1.77	11	3
1:A:60:SER:CB	1:A:90:ALA:HB3	0.56	2.30	13	10
1:A:84:CYS:SG	1:A:85:ASN:N	0.56	2.79	5	8
1:A:9:ILE:O	1:A:13:ILE:HD13	0.55	2.01	3	2
1:A:13:ILE:HG22	1:A:15:GLY:CA	0.54	2.31	7	6
1:A:55:ALA:HB2	1:A:94:PHE:CD1	0.54	2.37	9	1
1:A:58:LEU:HB3	1:A:61:CYS:H	0.54	1.62	7	1
1:A:109:ALA:CB	1:A:110:PRO:HD2	0.54	2.32	11	4
1:A:118:LEU:HD23	1:A:123:TYR:CB	0.54	2.32	4	3
1:A:73:TYR:CZ	1:A:84:CYS:SG	0.53	3.01	11	3
1:A:8:MET:CE	1:A:73:TYR:CE2	0.53	2.91	12	2
1:A:76:SER:HB2	1:A:83:THR:HG22	0.53	1.81	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:LEU:CD2	1:A:31:LEU:H	0.53	2.15	11	1
1:A:118:LEU:HD22	1:A:123:TYR:CG	0.53	2.39	6	2
1:A:8:MET:SD	1:A:82:ILE:HD13	0.53	2.44	3	1
1:A:26:GLY:CA	1:A:118:LEU:HD22	0.52	2.35	8	3
1:A:13:ILE:HG22	1:A:15:GLY:HA2	0.52	1.80	3	5
1:A:82:ILE:HG22	1:A:83:THR:H	0.52	1.65	14	6
1:A:119:ASP:HB3	1:A:123:TYR:CE2	0.52	2.39	4	3
1:A:13:ILE:HG22	1:A:15:GLY:HA3	0.52	1.82	8	6
1:A:118:LEU:HD12	1:A:118:LEU:H	0.52	1.64	12	1
1:A:42:ASP:HA	1:A:45:CYS:SG	0.51	2.45	8	3
1:A:29:CYS:O	1:A:45:CYS:SG	0.51	2.68	9	2
1:A:27:CYS:SG	1:A:28:TYR:CD2	0.51	3.03	6	1
1:A:118:LEU:HD23	1:A:123:TYR:CD1	0.51	2.41	12	2
1:A:5:PHE:CE1	1:A:9:ILE:HD11	0.51	2.41	18	1
1:A:58:LEU:HD23	1:A:61:CYS:CB	0.51	2.35	10	4
1:A:51:CYS:O	1:A:98:CYS:SG	0.51	2.69	16	2
1:A:118:LEU:HD23	1:A:123:TYR:HB3	0.51	1.83	1	2
1:A:76:SER:O	1:A:77:CYS:SG	0.50	2.69	5	4
1:A:55:ALA:HB3	1:A:95:ILE:HD11	0.50	1.83	9	1
1:A:58:LEU:HD11	1:A:90:ALA:HB1	0.50	1.82	14	2
1:A:1:ALA:HB2	1:A:70:THR:HG21	0.50	1.83	8	1
1:A:8:MET:SD	1:A:73:TYR:HE2	0.50	2.29	9	1
1:A:11:CYS:SG	1:A:82:ILE:HD11	0.50	2.46	18	2
1:A:113:LYS:H	1:A:113:LYS:CD	0.49	2.21	16	3
1:A:55:ALA:HB2	1:A:95:ILE:CD1	0.49	2.37	11	7
1:A:8:MET:SD	1:A:73:TYR:CE2	0.49	3.05	9	4
1:A:118:LEU:CD2	1:A:123:TYR:CG	0.49	2.95	3	11
1:A:115:HIS:HB2	1:A:118:LEU:HD11	0.49	1.84	12	3
1:A:84:CYS:SG	1:A:100:ARG:HG3	0.49	2.48	11	1
1:A:29:CYS:SG	1:A:42:ASP:OD1	0.48	2.71	11	1
1:A:8:MET:HB3	1:A:82:ILE:HD13	0.48	1.85	3	2
1:A:122:LYS:HB2	1:A:123:TYR:CE2	0.48	2.43	4	3
1:A:109:ALA:CB	1:A:110:PRO:CD	0.48	2.92	11	6
1:A:3:TRP:CZ3	1:A:70:THR:HG22	0.47	2.44	2	1
1:A:115:HIS:O	1:A:118:LEU:HD13	0.47	2.08	9	1
1:A:84:CYS:SG	1:A:100:ARG:HG2	0.47	2.50	3	1
1:A:26:GLY:H	1:A:118:LEU:CD1	0.47	2.22	14	2
1:A:1:ALA:CB	1:A:70:THR:HG21	0.47	2.39	8	1
1:A:6:ARG:NH1	1:A:9:ILE:HG21	0.47	2.25	7	2
1:A:8:MET:CB	1:A:82:ILE:HD13	0.47	2.40	14	1
1:A:123:TYR:O	1:A:124:CYS:SG	0.47	2.73	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:MET:HE1	1:A:73:TYR:CE1	0.47	2.45	7	1
1:A:17:HIS:CD2	1:A:21:ASP:H	0.46	2.29	1	4
1:A:60:SER:C	1:A:61:CYS:SG	0.46	2.94	3	1
1:A:118:LEU:HG	1:A:123:TYR:CD2	0.46	2.46	8	3
1:A:73:TYR:CE1	1:A:84:CYS:SG	0.46	3.08	18	1
1:A:5:PHE:HA	1:A:8:MET:SD	0.46	2.50	15	1
1:A:47:THR:O	1:A:51:CYS:SG	0.46	2.74	15	2
1:A:113:LYS:CD	1:A:113:LYS:H	0.45	2.24	7	2
1:A:6:ARG:HH21	1:A:19:LEU:H	0.45	1.54	14	1
1:A:8:MET:SD	1:A:75:TYR:CE2	0.45	3.09	11	1
1:A:27:CYS:SG	1:A:123:TYR:O	0.45	2.74	17	1
1:A:41:LEU:HD13	1:A:111:TYR:CE2	0.45	2.45	16	1
1:A:77:CYS:SG	1:A:82:ILE:HG12	0.45	2.51	11	1
1:A:120:THR:HA	1:A:124:CYS:H	0.45	1.71	17	1
1:A:23:ASN:HA	1:A:30:GLY:HA2	0.45	1.89	18	1
1:A:51:CYS:SG	1:A:51:CYS:O	0.44	2.75	7	1
1:A:55:ALA:HA	1:A:58:LEU:HB2	0.44	1.88	11	1
1:A:9:ILE:HD13	1:A:103:ALA:HA	0.44	1.89	15	2
1:A:27:CYS:SG	1:A:36:THR:O	0.44	2.76	16	1
1:A:8:MET:SD	1:A:82:ILE:CB	0.44	3.06	3	1
1:A:55:ALA:HA	1:A:58:LEU:HD22	0.43	1.89	12	1
1:A:40:GLU:HA	1:A:43:ARG:HG2	0.43	1.91	18	1
1:A:82:ILE:HG22	1:A:83:THR:N	0.43	2.29	6	1
1:A:84:CYS:SG	1:A:100:ARG:CG	0.43	3.07	3	1
1:A:37:PRO:HB2	1:A:42:ASP:HB3	0.42	1.91	6	1
1:A:84:CYS:SG	1:A:96:CYS:C	0.42	2.97	14	1
1:A:3:TRP:CH2	1:A:70:THR:HG22	0.42	2.49	8	1
1:A:6:ARG:HH21	1:A:9:ILE:HG21	0.42	1.73	5	2
1:A:51:CYS:O	1:A:51:CYS:SG	0.42	2.77	13	2
1:A:116:LYS:C	1:A:118:LEU:HD12	0.42	2.35	4	1
1:A:2:LEU:HD22	1:A:5:PHE:CD2	0.42	2.49	18	1
1:A:19:LEU:O	1:A:22:PHE:N	0.42	2.52	8	2
1:A:2:LEU:HG	1:A:69:TYR:CG	0.42	2.50	13	1
1:A:29:CYS:SG	1:A:106:PHE:CE1	0.41	3.13	2	1
1:A:29:CYS:HA	1:A:45:CYS:CB	0.41	2.45	9	1
1:A:9:ILE:HG22	1:A:18:PRO:C	0.41	2.36	3	1
1:A:81:GLU:C	1:A:82:ILE:HD13	0.41	2.36	8	1
1:A:4:GLN:O	1:A:8:MET:SD	0.41	2.79	11	1
1:A:9:ILE:HG22	1:A:18:PRO:HA	0.41	1.92	17	1
1:A:118:LEU:HD12	1:A:118:LEU:N	0.41	2.30	12	1
1:A:118:LEU:HD23	1:A:123:TYR:CA	0.41	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:LEU:CD1	1:A:94:PHE:CD2	0.41	3.04	18	1
1:A:3:TRP:HZ3	1:A:70:THR:HG22	0.41	1.75	10	1
1:A:75:TYR:CE1	1:A:96:CYS:SG	0.41	3.14	9	1
1:A:19:LEU:HD21	1:A:31:LEU:H	0.40	1.75	11	1
1:A:8:MET:CE	1:A:73:TYR:CE1	0.40	3.04	6	1
1:A:5:PHE:CD2	1:A:9:ILE:CD1	0.40	3.05	3	1
1:A:8:MET:HE3	1:A:73:TYR:CE1	0.40	2.52	15	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	115/124 (93%)	67±3 (58±3%)	29±3 (25±2%)	19±3 (17±2%)	0	3
All	All	2070/2232 (93%)	1204 (58%)	516 (25%)	350 (17%)	0	3

All 52 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	109	ALA	18
1	A	37	PRO	17
1	A	49	ASP	16
1	A	119	ASP	15
1	A	80	THR	15
1	A	20	MET	15
1	A	19	LEU	14
1	A	58	LEU	13
1	A	120	THR	13
1	A	84	CYS	13
1	A	70	THR	13
1	A	82	ILE	12
1	A	73	TYR	11
1	A	117	ASN	11
1	A	74	SER	11

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Mol	Chain	Res	Type	Models (Total)
1	A	83	THR	11
1	A	91	CYS	10
1	A	29	CYS	9
1	A	118	LEU	8
1	A	104	ILE	8
1	A	32	GLY	7
1	A	77	CYS	7
1	A	88	ASN	6
1	A	8	MET	5
1	A	121	LYS	5
1	A	28	TYR	5
1	A	27	CYS	4
1	A	71	GLU	4
1	A	25	TYR	4
1	A	16	SER	3
1	A	18	PRO	3
1	A	21	ASP	3
1	A	89	ASN	3
1	A	33	GLY	3
1	A	79	ASN	3
1	A	111	TYR	3
1	A	116	LYS	3
1	A	26	GLY	3
1	A	76	SER	2
1	A	81	GLU	2
1	A	56	LYS	2
1	A	23	ASN	2
1	A	35	GLY	2
1	A	47	THR	2
1	A	30	GLY	2
1	A	48	HIS	2
1	A	114	GLU	2
1	A	31	LEU	1
1	A	34	SER	1
1	A	12	ALA	1
1	A	6	ARG	1
1	A	110	PRO	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	103/110 (94%)	77±3 (75±3%)	26±3 (25±3%)	3	25
All	All	1854/1980 (94%)	1391 (75%)	463 (25%)	3	25

All 66 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	53	ARG	18
1	A	36	THR	18
1	A	113	LYS	18
1	A	108	LYS	18
1	A	104	ILE	18
1	A	85	ASN	17
1	A	37	PRO	17
1	A	52	TYR	17
1	A	5	PHE	17
1	A	94	PHE	16
1	A	114	GLU	16
1	A	28	TYR	15
1	A	17	HIS	14
1	A	10	LYS	14
1	A	96	CYS	13
1	A	41	LEU	12
1	A	6	ARG	12
1	A	56	LYS	11
1	A	87	LYS	11
1	A	2	LEU	10
1	A	61	CYS	10
1	A	84	CYS	8
1	A	29	CYS	8
1	A	82	ILE	8
1	A	70	THR	8
1	A	8	MET	7
1	A	124	CYS	7
1	A	92	GLU	7
1	A	116	LYS	7
1	A	60	SER	6
1	A	38	VAL	6
1	A	73	TYR	5
1	A	39	ASP	5

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Mol	Chain	Res	Type	Models (Total)
1	A	46	GLU	5
1	A	11	CYS	4
1	A	31	LEU	4
1	A	119	ASP	4
1	A	110	PRO	4
1	A	121	LYS	3
1	A	98	CYS	3
1	A	118	LEU	3
1	A	111	TYR	3
1	A	99	ASP	3
1	A	100	ARG	3
1	A	45	CYS	2
1	A	27	CYS	2
1	A	49	ASP	2
1	A	117	ASN	2
1	A	4	GLN	2
1	A	13	ILE	2
1	A	95	ILE	2
1	A	77	CYS	2
1	A	72	SER	1
1	A	18	PRO	1
1	A	40	GLU	1
1	A	21	ASP	1
1	A	101	ASN	1
1	A	54	ASP	1
1	A	19	LEU	1
1	A	106	PHE	1
1	A	69	TYR	1
1	A	48	HIS	1
1	A	80	THR	1
1	A	115	HIS	1
1	A	83	THR	1
1	A	71	GLU	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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 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