



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 10:42 AM UTC

PDB ID : 1SFW / pdb_00001sfw
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

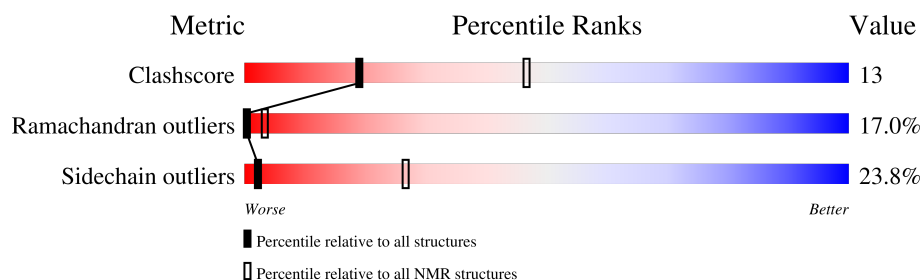
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	124	19% 40% 28% 6% 6%

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)	0.93	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

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 (CCD ID: CA) (formula: Ca).

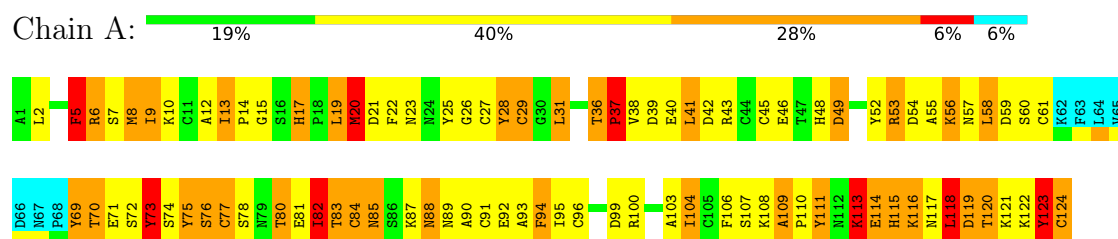
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: PHOSPHOLIPASE A2

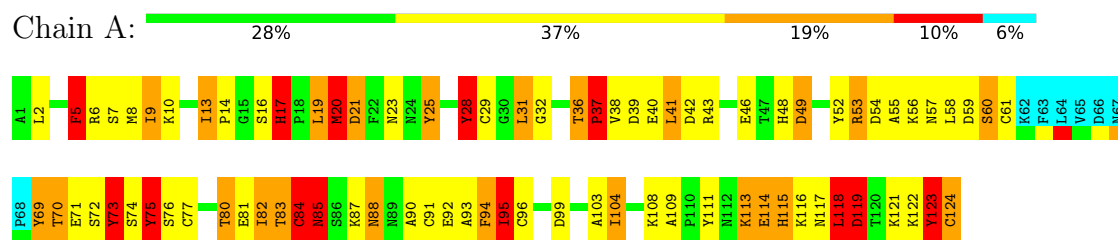


4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

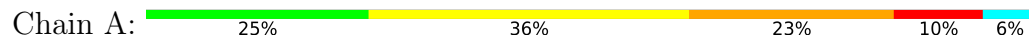
4.2.1 Score per residue for model 1 (medoid)

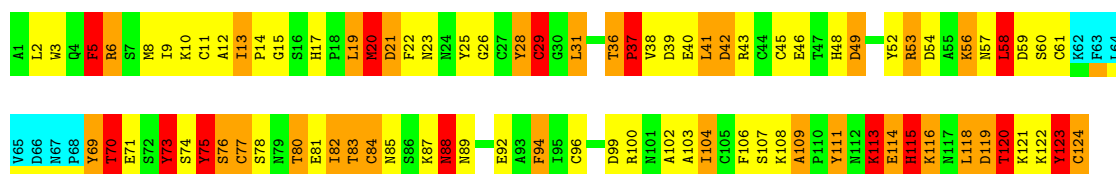
- Molecule 1: PHOSPHOLIPASE A2



4.2.2 Score per residue for model 2

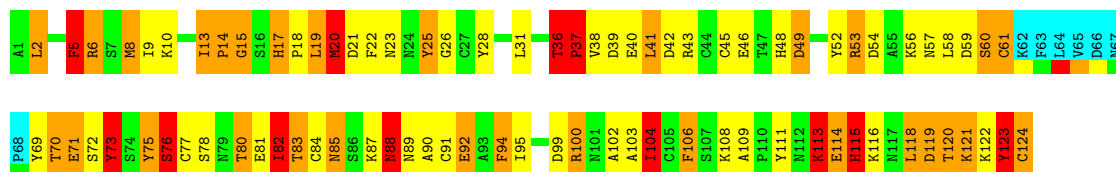
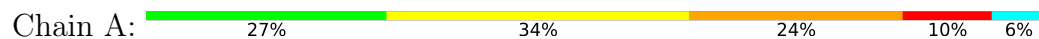
- Molecule 1: PHOSPHOLIPASE A2





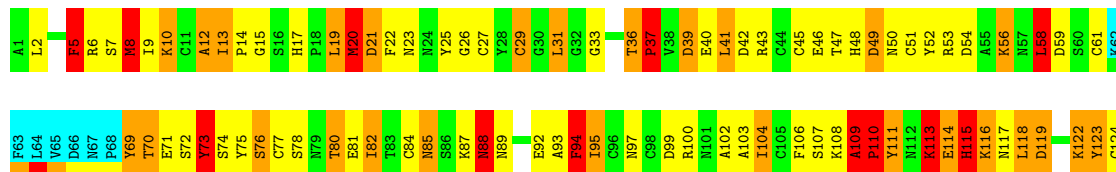
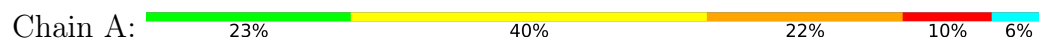
4.2.3 Score per residue for model 3

- Molecule 1: PHOSPHOLIPASE A2



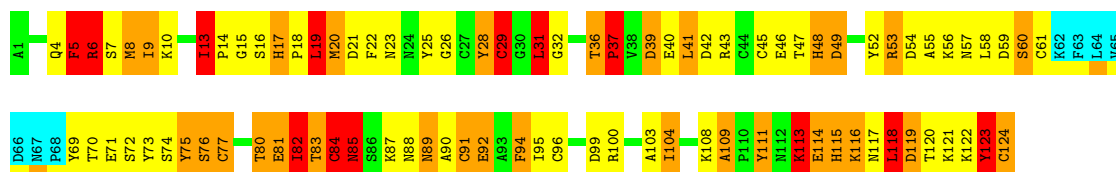
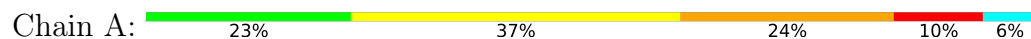
4.2.4 Score per residue for model 4

- Molecule 1: PHOSPHOLIPASE A2



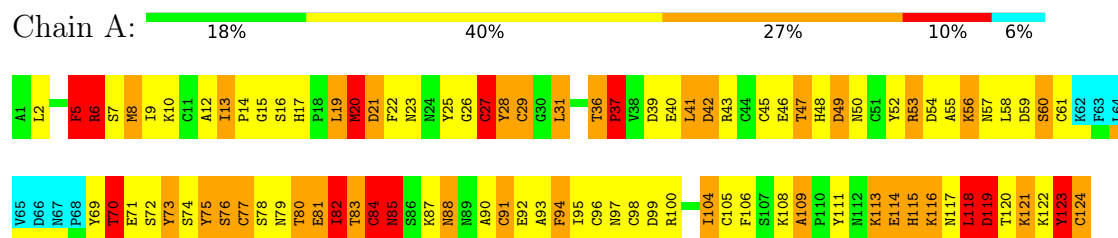
4.2.5 Score per residue for model 5

- Molecule 1: PHOSPHOLIPASE A2



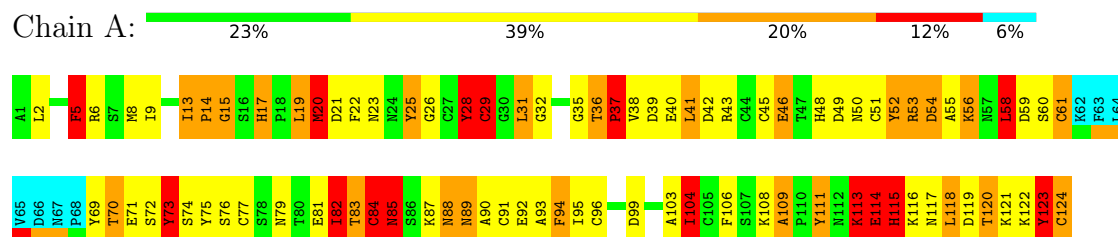
4.2.6 Score per residue for model 6

- Molecule 1: PHOSPHOLIPASE A2



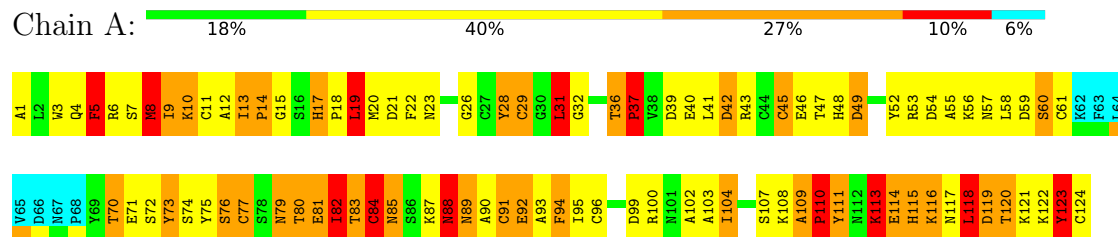
4.2.7 Score per residue for model 7

- Molecule 1: PHOSPHOLIPASE A2



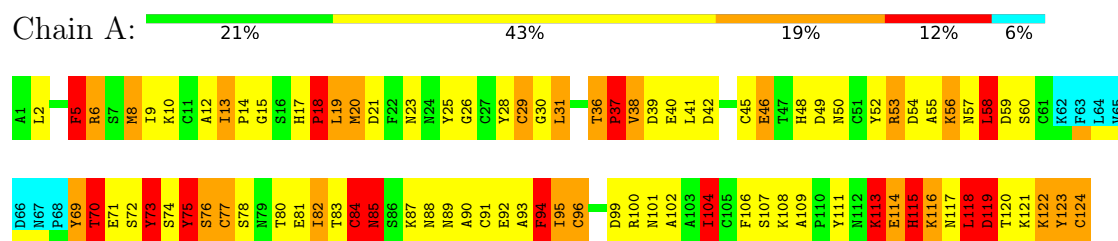
4.2.8 Score per residue for model 8

- Molecule 1: PHOSPHOLIPASE A2



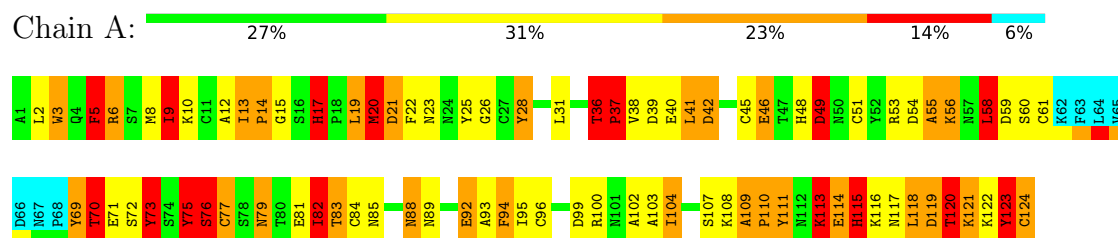
4.2.9 Score per residue for model 9

- Molecule 1: PHOSPHOLIPASE A2



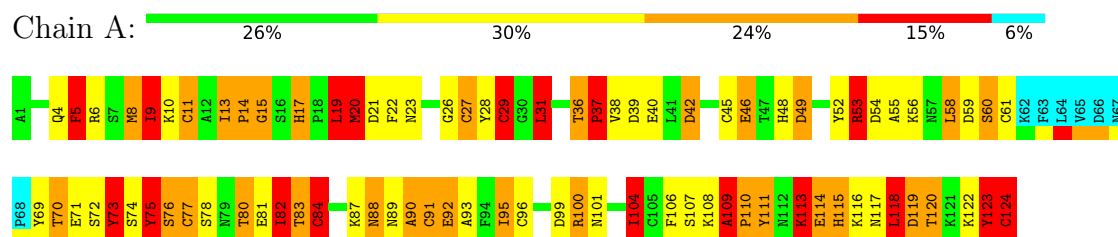
4.2.10 Score per residue for model 10

- Molecule 1: PHOSPHOLIPASE A2



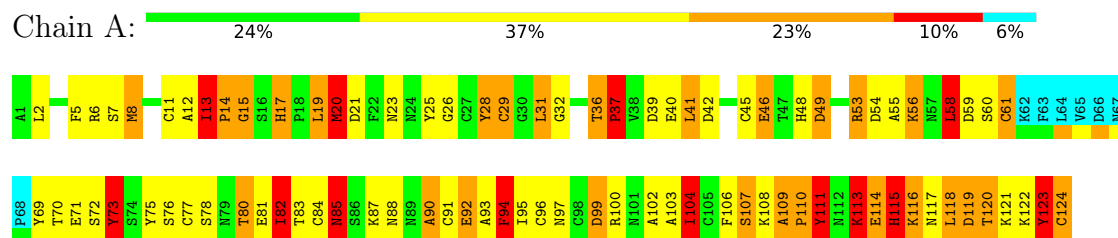
4.2.11 Score per residue for model 11

- Molecule 1: PHOSPHOLIPASE A2



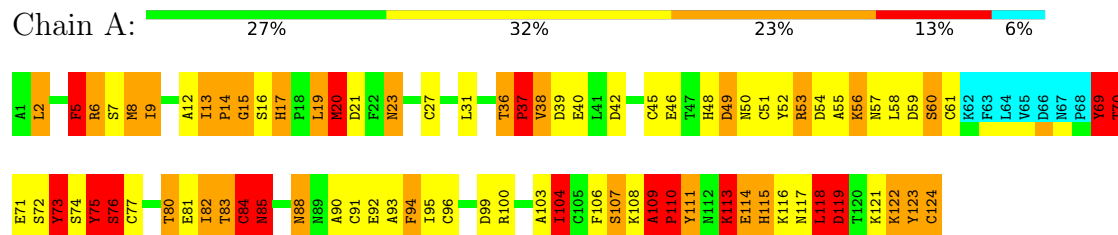
4.2.12 Score per residue for model 12

- Molecule 1: PHOSPHOLIPASE A2



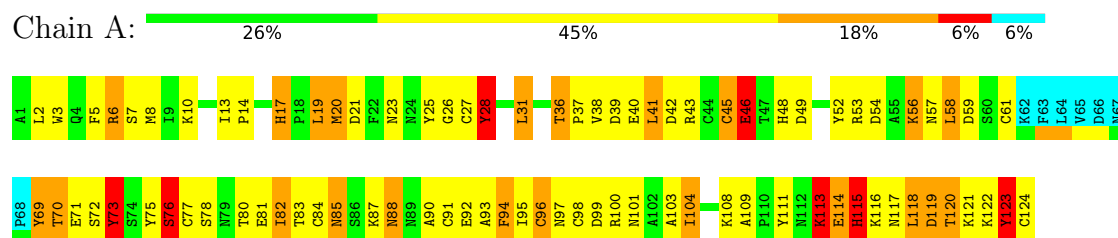
4.2.13 Score per residue for model 13

- Molecule 1: PHOSPHOLIPASE A2



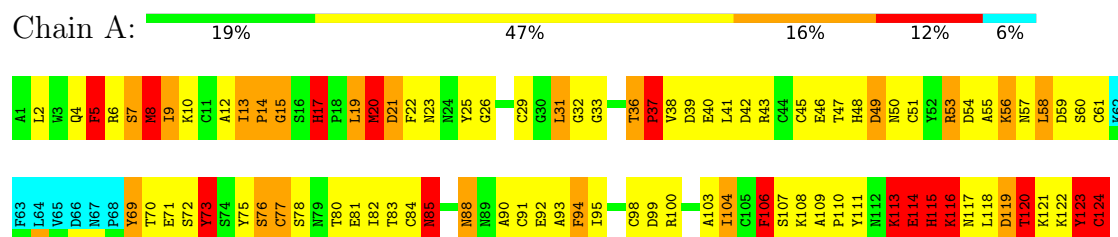
4.2.14 Score per residue for model 14

- Molecule 1: PHOSPHOLIPASE A2



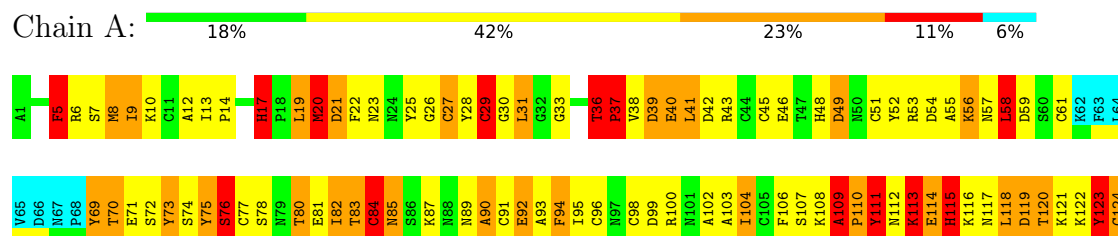
4.2.15 Score per residue for model 15

- Molecule 1: PHOSPHOLIPASE A2



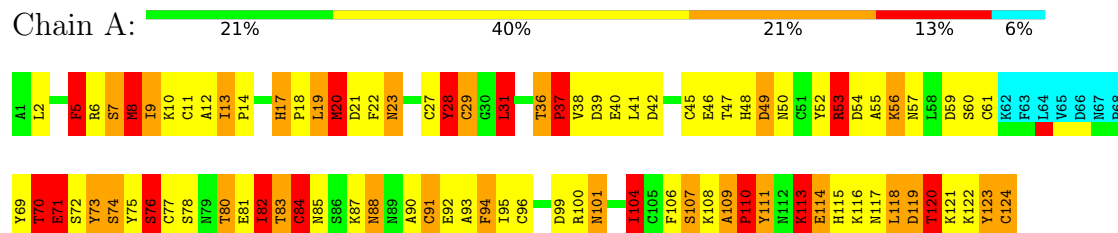
4.2.16 Score per residue for model 16

- Molecule 1: PHOSPHOLIPASE A2



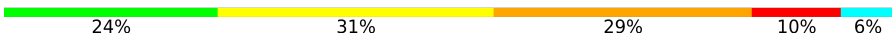
4.2.17 Score per residue for model 17

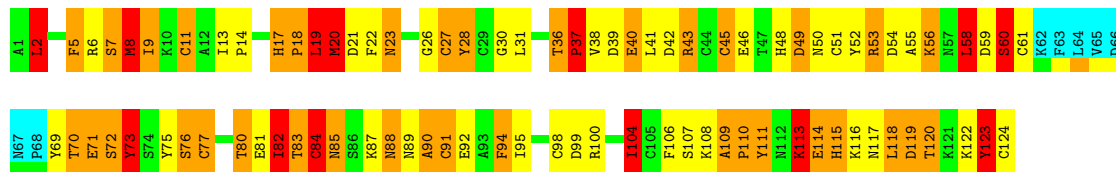
- Molecule 1: PHOSPHOLIPASE A2



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.

6 Model quality

6.1 Standard geometry

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	1.80±0.03	28±3/933 (3.0± 0.3%)	2.59±0.02	76±4/1258 (6.1± 0.3%)
All	All	1.80	502/16794 (3.0%)	2.59	1374/22644 (6.1%)

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

Mol	Chain	Chirality	Planarity
1	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	73	TYR	CA-C	10.71	1.65	1.52	3	6
1	A	122	LYS	CA-C	8.76	1.64	1.52	9	15
1	A	82	ILE	CA-C	7.91	1.62	1.52	6	7
1	A	119	ASP	CA-C	7.67	1.63	1.52	1	3
1	A	110	PRO	CA-C	7.54	1.63	1.52	10	9
1	A	77	CYS	CA-C	7.45	1.61	1.52	2	5
1	A	13	ILE	CA-C	7.30	1.59	1.52	14	7
1	A	124	CYS	C-OXT	7.22	1.38	1.23	4	18
1	A	36	THR	CA-C	7.18	1.59	1.52	8	18
1	A	23	ASN	N-CA	7.17	1.55	1.46	18	7
1	A	11	CYS	CA-C	7.01	1.61	1.52	8	2
1	A	49	ASP	CA-C	6.97	1.62	1.52	14	10
1	A	111	TYR	CA-CB	6.94	1.65	1.53	12	4
1	A	80	THR	CA-C	6.68	1.61	1.52	18	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	GLU	CD-OE1	6.60	1.37	1.25	7	2
1	A	71	GLU	CD-OE1	6.58	1.37	1.25	2	9
1	A	39	ASP	CG-OD1	6.57	1.37	1.25	15	9
1	A	119	ASP	CG-OD1	6.56	1.37	1.25	16	7
1	A	49	ASP	CG-OD1	6.55	1.37	1.25	4	5
1	A	116	LYS	N-CA	6.55	1.52	1.46	15	2
1	A	71	GLU	CD-OE2	6.54	1.37	1.25	5	9
1	A	54	ASP	CG-OD2	6.53	1.37	1.25	9	11
1	A	21	ASP	CG-OD1	6.53	1.37	1.25	16	9
1	A	54	ASP	CG-OD1	6.53	1.37	1.25	18	7
1	A	40	GLU	CD-OE2	6.52	1.37	1.25	16	15
1	A	21	ASP	CG-OD2	6.51	1.37	1.25	2	9
1	A	81	GLU	CD-OE2	6.51	1.37	1.25	1	2
1	A	46	GLU	CD-OE1	6.50	1.37	1.25	11	7
1	A	81	GLU	CD-OE1	6.50	1.37	1.25	15	16
1	A	49	ASP	CG-OD2	6.49	1.37	1.25	11	13
1	A	114	GLU	CD-OE2	6.49	1.37	1.25	5	11
1	A	59	ASP	CG-OD2	6.49	1.37	1.25	11	8
1	A	40	GLU	CD-OE1	6.49	1.37	1.25	12	3
1	A	69	TYR	CA-C	6.48	1.60	1.52	10	6
1	A	119	ASP	CG-OD2	6.48	1.37	1.25	12	11
1	A	59	ASP	CG-OD1	6.47	1.37	1.25	6	10
1	A	46	GLU	CD-OE2	6.47	1.37	1.25	9	11
1	A	92	GLU	CD-OE2	6.46	1.37	1.25	9	16
1	A	114	GLU	CD-OE1	6.46	1.37	1.25	10	7
1	A	122	LYS	CA-CB	6.45	1.63	1.53	4	8
1	A	39	ASP	CG-OD2	6.41	1.37	1.25	4	9
1	A	42	ASP	CG-OD1	6.41	1.37	1.25	13	10
1	A	21	ASP	CA-C	6.40	1.61	1.52	2	3
1	A	70	THR	CA-CB	6.35	1.64	1.53	7	2
1	A	42	ASP	CG-OD2	6.35	1.37	1.25	5	8
1	A	76	SER	CA-C	6.31	1.59	1.53	5	2
1	A	99	ASP	CG-OD2	6.28	1.37	1.25	9	10
1	A	48	HIS	CG-CD2	6.27	1.42	1.35	16	12
1	A	99	ASP	CG-OD1	6.25	1.37	1.25	3	8
1	A	83	THR	CA-C	6.21	1.61	1.52	10	2
1	A	14	PRO	N-CA	6.15	1.55	1.47	12	8
1	A	9	ILE	N-CA	6.04	1.53	1.46	18	2
1	A	115	HIS	ND1-CE1	6.04	1.38	1.32	16	11
1	A	71	GLU	CA-C	5.94	1.61	1.52	8	2
1	A	17	HIS	ND1-CE1	5.93	1.38	1.32	4	18

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	48	HIS	CA-C	5.89	1.60	1.52	14	2
1	A	48	HIS	CB-CG	5.83	1.58	1.50	6	3
1	A	103	ALA	N-CA	5.67	1.53	1.46	7	6
1	A	105	CYS	CA-C	5.61	1.60	1.52	6	1
1	A	109	ALA	CA-C	5.52	1.59	1.52	2	5
1	A	70	THR	CA-C	5.44	1.60	1.52	12	1
1	A	17	HIS	CE1-NE2	5.43	1.38	1.32	6	12
1	A	115	HIS	CA-C	5.38	1.59	1.52	4	1
1	A	7	SER	N-CA	5.36	1.53	1.46	13	1
1	A	31	LEU	CA-C	-5.27	1.49	1.52	10	1
1	A	17	HIS	CG-CD2	5.25	1.41	1.35	9	1
1	A	17	HIS	CA-C	5.23	1.59	1.52	9	1
1	A	48	HIS	N-CA	5.21	1.52	1.46	5	2
1	A	115	HIS	CE1-NE2	5.18	1.37	1.32	13	2
1	A	110	PRO	N-CA	5.18	1.53	1.47	15	1
1	A	47	THR	CA-C	5.17	1.60	1.53	6	1
1	A	16	SER	CA-C	5.14	1.56	1.53	6	1
1	A	38	VAL	CA-C	5.09	1.59	1.52	9	1
1	A	115	HIS	CB-CG	5.08	1.57	1.50	17	1
1	A	101	ASN	CA-C	5.05	1.59	1.52	14	1
1	A	103	ALA	CA-C	5.05	1.59	1.52	1	1
1	A	115	HIS	C-N	5.02	1.40	1.33	9	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	5	PHE	CA-CB-CG	14.75	128.55	113.80	18	18
1	A	13	ILE	N-CA-C	-14.40	93.89	108.15	1	14
1	A	123	TYR	N-CA-CB	-13.99	89.34	110.33	5	18
1	A	17	HIS	CB-CG-CD2	-12.66	114.74	131.20	17	18
1	A	115	HIS	ND1-CE1-NE2	12.17	120.57	108.40	17	18
1	A	115	HIS	CB-CG-CD2	-12.16	115.39	131.20	16	17
1	A	17	HIS	ND1-CE1-NE2	12.01	120.41	108.40	18	18
1	A	48	HIS	ND1-CE1-NE2	11.89	120.29	108.40	18	18
1	A	115	HIS	CE1-NE2-CD2	-11.70	97.31	109.00	11	18
1	A	71	GLU	N-CA-C	11.26	123.24	110.97	13	5
1	A	56	LYS	N-CA-CB	-11.08	91.77	110.49	7	4
1	A	106	PHE	CA-CB-CG	10.79	124.59	113.80	15	1
1	A	10	LYS	N-CA-CB	-10.78	93.95	110.44	8	4
1	A	19	LEU	N-CA-C	10.59	122.82	111.28	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	122	LYS	N-CA-CB	-10.54	94.72	110.01	5	18
1	A	122	LYS	CA-C-N	10.47	137.84	120.88	9	15
1	A	122	LYS	C-N-CA	10.47	137.84	120.88	9	15
1	A	70	THR	N-CA-C	10.43	124.63	110.55	7	5
1	A	94	PHE	CA-CB-CG	10.30	124.10	113.80	2	16
1	A	85	ASN	CA-CB-CG	10.14	122.75	112.60	7	15
1	A	17	HIS	CE1-NE2-CD2	-10.01	98.99	109.00	17	18
1	A	76	SER	N-CA-CB	-9.93	97.18	110.88	14	17
1	A	88	ASN	N-CA-C	9.81	122.39	110.91	15	14
1	A	90	ALA	N-CA-C	9.64	124.87	112.34	18	6
1	A	118	LEU	CB-CA-C	9.45	129.22	110.42	9	6
1	A	115	HIS	CA-CB-CG	9.23	123.03	113.80	15	10
1	A	77	CYS	N-CA-C	9.20	122.86	110.35	15	6
1	A	13	ILE	N-CA-CB	-9.18	98.36	111.21	3	11
1	A	48	HIS	CE1-NE2-CD2	-9.15	99.85	109.00	13	18
1	A	54	ASP	CA-CB-CG	9.10	121.70	112.60	9	4
1	A	82	ILE	CA-CB-CG1	8.87	125.47	110.40	17	7
1	A	117	ASN	N-CA-CB	-8.83	96.96	110.91	7	3
1	A	84	CYS	CB-CA-C	8.63	127.60	110.42	9	1
1	A	41	LEU	CB-CA-C	8.62	124.41	110.88	6	10
1	A	15	GLY	N-CA-C	8.60	121.92	112.29	11	7
1	A	89	ASN	N-CA-CB	8.57	124.97	110.49	7	2
1	A	49	ASP	CA-CB-CG	8.54	121.14	112.60	4	13
1	A	23	ASN	CA-CB-CG	8.53	121.13	112.60	11	18
1	A	114	GLU	CB-CA-C	8.52	127.38	110.42	12	18
1	A	101	ASN	CA-CB-CG	8.44	121.04	112.60	17	3
1	A	119	ASP	N-CA-CB	-8.35	96.38	110.49	4	2
1	A	99	ASP	CA-CB-CG	8.30	120.90	112.60	12	5
1	A	8	MET	N-CA-CB	-8.24	96.56	110.49	18	8
1	A	37	PRO	N-CA-CB	-8.15	94.70	103.25	9	17
1	A	89	ASN	CA-CB-CG	8.12	120.72	112.60	7	3
1	A	70	THR	N-CA-CB	8.03	124.06	110.49	11	10
1	A	20	MET	N-CA-CB	-8.03	96.93	110.49	3	17
1	A	119	ASP	CA-CB-CG	8.02	120.62	112.60	11	9
1	A	54	ASP	N-CA-C	8.01	122.75	112.34	16	15
1	A	79	ASN	CA-CB-CG	7.95	120.55	112.60	10	2
1	A	76	SER	N-CA-C	7.95	123.68	114.62	15	6
1	A	116	LYS	N-CA-CB	-7.80	98.39	110.56	10	13
1	A	13	ILE	CB-CA-C	7.79	118.48	111.08	1	5
1	A	39	ASP	CA-CB-CG	7.77	120.37	112.60	6	6
1	A	72	SER	N-CA-C	7.75	121.74	109.65	8	14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LEU	CA-C-N	7.72	136.29	121.54	11	14
1	A	19	LEU	C-N-CA	7.72	136.29	121.54	11	14
1	A	111	TYR	N-CA-CB	-7.66	97.55	110.49	4	7
1	A	123	TYR	CA-CB-CG	7.65	127.67	113.90	4	2
1	A	40	GLU	CB-CG-CD	7.62	125.55	112.60	3	3
1	A	109	ALA	CB-CA-C	7.59	125.12	110.17	16	3
1	A	75	TYR	N-CA-C	7.58	120.08	109.31	9	2
1	A	84	CYS	N-CA-CB	7.58	123.29	110.49	9	11
1	A	82	ILE	CB-CA-C	7.56	123.69	111.29	1	8
1	A	6	ARG	N-CA-C	7.54	120.38	111.71	10	6
1	A	8	MET	N-CA-C	7.51	126.80	110.80	8	5
1	A	31	LEU	CB-CA-C	7.48	122.42	111.65	10	15
1	A	19	LEU	CB-CA-C	-7.40	99.26	110.88	8	3
1	A	40	GLU	N-CA-CB	7.37	120.92	109.94	3	8
1	A	13	ILE	CA-C-O	-7.30	115.92	120.88	5	2
1	A	56	LYS	CB-CA-C	7.29	122.33	110.88	4	11
1	A	17	HIS	CG-ND1-CE1	-7.25	96.97	109.30	17	18
1	A	116	LYS	N-CA-C	7.22	123.44	112.54	15	8
1	A	57	ASN	CA-CB-CG	7.19	119.79	112.60	9	8
1	A	116	LYS	CA-C-O	7.16	126.71	118.55	3	4
1	A	115	HIS	CG-ND1-CE1	-7.15	97.15	109.30	18	18
1	A	71	GLU	N-CA-CB	7.11	122.51	110.49	5	2
1	A	42	ASP	CA-CB-CG	7.10	119.70	112.60	4	4
1	A	29	CYS	N-CA-C	7.09	125.91	110.80	7	5
1	A	58	LEU	N-CA-C	7.06	120.24	110.35	11	9
1	A	89	ASN	N-CA-C	-7.02	98.01	108.34	8	6
1	A	93	ALA	N-CA-C	7.00	119.76	111.71	17	14
1	A	26	GLY	O-C-N	6.97	127.57	122.62	18	1
1	A	80	THR	CB-CA-C	6.94	122.52	111.48	8	1
1	A	111	TYR	CB-CA-C	-6.91	100.10	109.71	18	5
1	A	75	TYR	N-CA-CB	-6.91	100.46	108.96	13	6
1	A	56	LYS	N-CA-C	6.90	125.50	110.80	7	10
1	A	7	SER	CA-C-N	6.89	131.72	120.63	16	2
1	A	7	SER	C-N-CA	6.89	131.72	120.63	16	2
1	A	20	MET	N-CA-C	6.84	125.38	110.80	13	15
1	A	122	LYS	O-C-N	6.83	129.37	122.12	9	4
1	A	113	LYS	N-CA-CB	-6.81	102.72	110.35	15	2
1	A	121	LYS	CA-C-N	6.80	129.28	120.44	3	10
1	A	121	LYS	C-N-CA	6.80	129.28	120.44	3	10
1	A	12	ALA	N-CA-C	6.79	119.54	111.33	4	2
1	A	113	LYS	N-CA-C	6.77	119.18	110.65	12	11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	114	GLU	N-CA-CB	-6.76	99.07	110.49	7	14
1	A	102	ALA	CA-C-O	-6.75	112.75	120.24	2	8
1	A	9	ILE	CA-CB-CG2	6.65	121.81	110.50	13	7
1	A	123	TYR	CB-CA-C	6.64	121.95	110.79	2	6
1	A	17	HIS	N-CA-CB	6.64	120.80	110.12	9	9
1	A	72	SER	N-CA-CB	-6.63	99.84	110.39	17	7
1	A	120	THR	CB-CA-C	6.60	123.55	110.42	17	9
1	A	103	ALA	CA-C-N	6.60	132.03	121.34	10	8
1	A	103	ALA	C-N-CA	6.60	132.03	121.34	10	8
1	A	56	LYS	CG-CD-CE	6.58	126.44	111.30	10	1
1	A	17	HIS	CB-CG-ND1	6.58	132.56	122.70	17	3
1	A	6	ARG	CB-CG-CD	6.54	126.35	111.30	17	5
1	A	118	LEU	N-CA-C	6.53	118.24	108.31	6	2
1	A	48	HIS	CG-ND1-CE1	-6.50	98.25	109.30	13	18
1	A	19	LEU	CB-CG-CD1	6.48	130.13	110.70	18	1
1	A	100	ARG	N-CA-C	6.47	119.16	111.33	11	7
1	A	43	ARG	CB-CA-C	-6.45	100.71	110.90	8	12
1	A	17	HIS	ND1-CG-CD2	6.43	112.53	106.10	17	17
1	A	88	ASN	CA-CB-CG	6.42	119.02	112.60	3	14
1	A	2	LEU	CA-C-O	-6.38	114.10	120.80	3	1
1	A	49	ASP	N-CA-C	-6.37	97.22	110.80	14	2
1	A	21	ASP	CA-CB-CG	6.36	118.96	112.60	11	3
1	A	100	ARG	N-CA-CB	-6.34	100.76	110.20	12	3
1	A	53	ARG	N-CA-CB	-6.32	100.53	109.94	9	6
1	A	104	ILE	N-CA-CB	-6.32	100.20	110.31	14	18
1	A	95	ILE	CA-CB-CG1	6.31	121.14	110.40	4	2
1	A	41	LEU	N-CA-CB	-6.29	100.88	110.12	12	7
1	A	58	LEU	CB-CA-C	6.26	122.87	110.42	10	9
1	A	104	ILE	CA-CB-CG2	6.25	121.13	110.50	12	13
1	A	19	LEU	CA-C-O	-6.24	114.27	120.82	8	4
1	A	60	SER	N-CA-CB	-6.21	100.76	110.44	11	10
1	A	69	TYR	CA-CB-CG	6.19	125.04	113.90	13	8
1	A	117	ASN	CA-CB-CG	6.17	118.77	112.60	7	2
1	A	40	GLU	CB-CA-C	-6.09	101.06	110.81	9	7
1	A	118	LEU	CB-CG-CD1	6.08	128.94	110.70	1	1
1	A	87	LYS	CB-CG-CD	6.08	125.28	111.30	17	1
1	A	7	SER	N-CA-C	6.06	118.68	111.71	6	5
1	A	79	ASN	N-CA-C	6.06	119.50	111.75	6	1
1	A	9	ILE	CB-CA-C	6.05	119.38	111.81	11	1
1	A	119	ASP	CB-CA-C	6.05	126.21	113.80	9	1
1	A	111	TYR	N-CA-C	6.04	119.25	110.42	11	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	PRO	N-CA-CB	-6.03	96.92	103.25	13	4
1	A	17	HIS	CA-CB-CG	-6.01	107.79	113.80	9	2
1	A	31	LEU	CA-C-O	6.00	130.56	122.51	2	2
1	A	118	LEU	CA-C-N	6.00	133.01	121.54	4	1
1	A	118	LEU	C-N-CA	6.00	133.01	121.54	4	1
1	A	106	PHE	N-CA-C	6.00	120.42	112.25	15	1
1	A	77	CYS	N-CA-CB	6.00	120.63	110.49	10	4
1	A	94	PHE	CB-CA-C	5.99	120.86	110.79	9	4
1	A	41	LEU	N-CA-C	5.99	118.60	111.71	3	5
1	A	18	PRO	N-CA-C	5.99	121.38	114.20	9	1
1	A	115	HIS	CA-C-O	-5.95	112.76	119.79	9	3
1	A	31	LEU	N-CA-C	5.94	123.46	110.80	17	1
1	A	111	TYR	CB-CG-CD2	-5.94	111.89	120.80	11	5
1	A	29	CYS	CB-CA-C	5.90	122.16	110.42	5	2
1	A	3	TRP	CG-CD2-CE3	-5.90	128.00	133.90	10	1
1	A	48	HIS	N-CA-C	-5.89	98.25	110.80	6	1
1	A	60	SER	N-CA-C	-5.89	107.91	114.62	10	1
1	A	79	ASN	CA-C-O	5.88	128.92	120.51	8	1
1	A	115	HIS	CB-CA-C	5.87	120.16	111.88	11	5
1	A	78	SER	CA-C-O	5.84	121.33	117.94	3	2
1	A	96	CYS	N-CA-CB	-5.82	101.28	109.94	9	2
1	A	89	ASN	CB-CA-C	5.80	121.97	110.42	4	1
1	A	78	SER	CB-CA-C	5.79	121.93	110.42	6	9
1	A	124	CYS	N-CA-CB	5.75	120.28	110.50	10	3
1	A	2	LEU	N-CA-CB	-5.75	101.27	110.19	18	1
1	A	13	ILE	O-C-N	-5.74	114.56	121.10	3	2
1	A	76	SER	CB-CA-C	-5.74	101.65	109.28	15	2
1	A	27	CYS	N-CA-CB	5.73	120.17	110.49	11	2
1	A	118	LEU	CD1-CG-CD2	-5.71	98.23	110.80	13	3
1	A	93	ALA	CB-CA-C	-5.71	101.67	110.81	16	2
1	A	28	TYR	N-CA-CB	5.70	120.13	110.49	17	2
1	A	53	ARG	CB-CA-C	5.68	120.26	110.84	3	8
1	A	53	ARG	N-CA-C	5.66	117.91	111.11	13	2
1	A	10	LYS	CB-CA-C	5.65	120.19	110.01	8	2
1	A	107	SER	N-CA-C	5.65	118.20	111.71	12	6
1	A	41	LEU	CD1-CG-CD2	5.64	123.21	110.80	8	4
1	A	47	THR	N-CA-CB	-5.63	101.66	110.44	17	2
1	A	52	TYR	N-CA-CB	5.63	118.91	110.19	7	1
1	A	72	SER	CA-C-N	5.63	131.42	121.80	3	1
1	A	72	SER	C-N-CA	5.63	131.42	121.80	3	1
1	A	73	TYR	N-CA-CB	5.61	119.97	110.49	8	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	TYR	CB-CG-CD2	-5.59	112.42	120.80	3	2
1	A	13	ILE	CA-CB-CG1	5.58	119.88	110.40	11	3
1	A	112	ASN	CA-C-N	5.57	130.52	122.16	16	1
1	A	112	ASN	C-N-CA	5.57	130.52	122.16	16	1
1	A	50	ASN	N-CA-CB	5.56	118.86	110.30	9	2
1	A	17	HIS	N-CA-C	-5.56	97.50	109.01	9	1
1	A	91	CYS	N-CA-CB	-5.54	101.12	110.49	18	2
1	A	80	THR	N-CA-CB	5.54	119.85	110.49	6	1
1	A	115	HIS	CG-CD2-NE2	5.53	112.73	107.20	17	5
1	A	48	HIS	N-CA-CB	5.51	119.81	110.49	7	3
1	A	82	ILE	CA-C-N	5.49	132.02	121.54	3	1
1	A	82	ILE	C-N-CA	5.49	132.02	121.54	3	1
1	A	5	PHE	CB-CA-C	5.48	119.58	110.81	12	2
1	A	7	SER	CB-CA-C	5.48	119.54	111.65	18	2
1	A	92	GLU	N-CA-CB	5.47	118.67	110.19	9	1
1	A	82	ILE	CA-CB-CG2	5.47	119.80	110.50	11	2
1	A	100	ARG	CA-C-O	-5.47	115.07	120.70	18	6
1	A	50	ASN	N-CA-C	5.46	119.11	112.23	4	5
1	A	20	MET	CB-CA-C	5.45	121.28	110.17	9	2
1	A	5	PHE	N-CA-CB	5.44	118.21	110.16	6	1
1	A	13	ILE	CA-CB-CG2	5.43	119.73	110.50	17	4
1	A	19	LEU	O-C-N	5.41	129.78	122.59	10	8
1	A	31	LEU	O-C-N	5.41	126.69	120.58	14	1
1	A	116	LYS	O-C-N	5.40	127.65	121.93	12	2
1	A	3	TRP	N-CA-C	5.38	117.84	111.33	14	1
1	A	119	ASP	N-CA-C	-5.38	99.34	110.80	6	1
1	A	106	PHE	CB-CA-C	5.37	118.61	111.14	15	1
1	A	27	CYS	N-CA-C	5.37	122.23	110.80	18	1
1	A	106	PHE	CB-CG-CD2	-5.36	111.58	120.70	3	1
1	A	81	GLU	N-CA-CB	5.36	119.55	110.49	5	1
1	A	19	LEU	CD1-CG-CD2	-5.36	99.02	110.80	18	1
1	A	95	ILE	CB-CG1-CD1	5.33	125.00	113.80	4	1
1	A	57	ASN	N-CA-CB	-5.33	102.69	110.53	1	5
1	A	100	ARG	CG-CD-NE	5.33	123.73	112.00	3	1
1	A	56	LYS	CA-C-N	5.33	129.12	121.71	16	1
1	A	56	LYS	C-N-CA	5.33	129.12	121.71	16	1
1	A	97	ASN	CA-CB-CG	5.31	117.91	112.60	12	3
1	A	113	LYS	CB-CG-CD	5.30	123.49	111.30	2	1
1	A	38	VAL	CA-CB-CG2	5.29	119.40	110.40	15	1
1	A	61	CYS	N-CA-CB	-5.27	103.04	111.58	3	1
1	A	59	ASP	N-CA-CB	-5.26	102.12	110.28	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	97	ASN	N-CA-C	5.25	117.09	111.36	14	1
1	A	54	ASP	CA-C-N	5.24	127.56	120.38	15	4
1	A	54	ASP	C-N-CA	5.24	127.56	120.38	15	4
1	A	48	HIS	CB-CG-CD2	-5.23	124.40	131.20	13	3
1	A	82	ILE	N-CA-CB	-5.23	102.60	111.23	2	1
1	A	8	MET	CG-SD-CE	-5.20	89.47	100.90	17	3
1	A	28	TYR	CA-CB-CG	5.19	123.25	113.90	8	1
1	A	122	LYS	CA-C-O	5.19	126.05	120.55	9	1
1	A	75	TYR	CB-CA-C	5.18	120.74	110.42	3	1
1	A	79	ASN	CB-CA-C	-5.18	100.11	110.42	10	1
1	A	111	TYR	CB-CG-CD1	5.17	128.55	120.80	11	5
1	A	42	ASP	CB-CA-C	5.17	120.49	110.46	8	1
1	A	83	THR	CA-CB-CG2	5.17	119.28	110.50	15	1
1	A	110	PRO	CB-CA-C	-5.16	103.05	111.56	18	1
1	A	76	SER	CA-C-N	5.16	131.39	121.54	8	1
1	A	76	SER	C-N-CA	5.16	131.39	121.54	8	1
1	A	120	THR	N-CA-CB	5.12	119.15	110.49	15	1
1	A	80	THR	CA-CB-CG2	5.12	119.20	110.50	18	3
1	A	28	TYR	N-CA-C	5.11	121.69	110.80	1	1
1	A	45	CYS	CA-C-O	-5.09	113.64	119.60	18	1
1	A	77	CYS	CB-CA-C	5.08	120.54	110.42	9	1
1	A	91	CYS	N-CA-C	5.08	121.62	110.80	11	1
1	A	7	SER	CA-C-O	5.08	122.65	119.55	15	1
1	A	80	THR	N-CA-C	5.06	118.75	112.47	8	1
1	A	38	VAL	CG1-CB-CG2	-5.05	99.69	110.80	13	1
1	A	12	ALA	N-CA-CB	-5.04	101.97	110.49	6	1
1	A	45	CYS	N-CA-CB	-5.03	102.21	110.40	14	1
1	A	36	THR	O-C-N	-5.02	118.50	121.71	5	1
1	A	73	TYR	CA-C-O	5.01	126.61	121.10	14	1
1	A	22	PHE	CA-CB-CG	5.01	118.81	113.80	18	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	20	MET	Peptide	17
1	A	75	TYR	Sidechain,Peptide	17
1	A	115	HIS	Sidechain	17

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Mol	Chain	Res	Type	Group	Models (Total)
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	22	PHE	Sidechain	10
1	A	28	TYR	Peptide,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
1	A	70	THR	Peptide	4
1	A	94	PHE	Sidechain	4
1	A	19	LEU	Mainchain,Peptide	4
1	A	53	ARG	Peptide	3
1	A	26	GLY	Peptide	3
1	A	89	ASN	Peptide	3
1	A	6	ARG	Peptide,Sidechain	2
1	A	36	THR	Peptide	2
1	A	74	SER	Peptide	2
1	A	55	ALA	Peptide	2
1	A	18	PRO	Peptide	2
1	A	47	THR	Peptide	1
1	A	50	ASN	Peptide	1
1	A	10	LYS	Peptide	1
1	A	5	PHE	Sidechain	1
1	A	72	SER	Peptide	1
1	A	110	PRO	Peptide	1
1	A	46	GLU	Peptide	1
1	A	106	PHE	Peptide	1
1	A	116	LYS	Peptide	1
1	A	29	CYS	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	22±5
All	All	16452	0	14886	402

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 13.

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:8:MET:HE1	1:A:73:TYR:CE1	0.79	2.12	5	4
1:A:9:ILE:HG22	1:A:18:PRO:HB2	0.77	1.54	9	1
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:8:MET:HE3	1:A:73:TYR:CE2	0.69	2.21	14	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:45:CYS:SG	1:A:106:PHE:CZ	0.61	2.94	18	7
1:A:55:ALA:CB	1:A:95:ILE:HD11	0.61	2.25	18	7
1:A:26:GLY:H	1:A:118:LEU:HD13	0.61	1.55	4	3
1:A:122:LYS:HB2	1:A:123:TYR:CD2	0.61	2.31	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:8:MET:HE3	1:A:73:TYR:CZ	0.56	2.35	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:5:PHE:HA	1:A:8:MET:HE2	0.55	1.78	13	4
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
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:60:SER:C	1:A:61:CYS:SG	0.51	2.94	3	2
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:8:MET:SD	1:A:73:TYR:OH	0.50	2.69	14	1
1:A:11:CYS:SG	1:A:82:ILE:HD11	0.50	2.46	18	2
1:A:113:LYS:CD	1:A:113:LYS:H	0.49	2.21	16	5
1:A:8:MET:SD	1:A:73:TYR:CE2	0.49	3.05	9	4
1:A:55:ALA:HB2	1:A:95:ILE:CD1	0.49	2.37	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:84:CYS:SG	1:A:96:CYS:C	0.48	2.97	14	1
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:116:LYS:C	1:A:118:LEU:HD12	0.47	2.35	4	1
1:A:123:TYR:O	1:A:124:CYS:SG	0.47	2.73	13	1
1:A:17:HIS:CD2	1:A:21:ASP:H	0.46	2.29	1	4
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:9:ILE:HG22	1:A:18:PRO:C	0.46	2.36	3	1
1:A:47:THR:O	1:A:51:CYS:SG	0.46	2.74	15	2
1:A:8:MET:SD	1:A:75:TYR:CE2	0.45	3.09	11	1
1:A:6:ARG:HH21	1:A:19:LEU:H	0.45	1.54	14	1
1:A:81:GLU:C	1:A:82:ILE:HD13	0.45	2.36	8	1
1:A:27:CYS:SG	1:A:123:TYR:O	0.45	2.74	17	1
1:A:77:CYS:SG	1:A:82:ILE:HG12	0.45	2.51	11	1
1:A:41:LEU:HD13	1:A:111:TYR:CE2	0.45	2.45	16	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:4:GLN:O	1:A:8:MET:HE2	0.44	2.12	5	1
1:A:29:CYS:C	1:A:45:CYS:SG	0.44	3.01	5	1
1:A:51:CYS:SG	1:A:51:CYS:O	0.44	2.75	7	2
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:3:TRP:CH2	1:A:70:THR:HG22	0.42	2.49	8	1
1:A:8:MET:HE2	1:A:82:ILE:HG21	0.42	1.91	14	1
1:A:6:ARG:HH21	1:A:9:ILE:HG21	0.42	1.73	5	2
1:A:115:HIS:C	1:A:118:LEU:HD13	0.42	2.40	9	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:58:LEU:HD21	1:A:90:ALA:C	0.41	2.41	16	2
1:A:29:CYS:HA	1:A:45:CYS:CB	0.41	2.45	9	1
1:A:4:GLN:O	1:A:8:MET:SD	0.41	2.79	11	1
1:A:118:LEU:HD12	1:A:118:LEU:N	0.41	2.30	12	1
1:A:9:ILE:HG22	1:A:18:PRO:HA	0.41	1.92	17	1
1:A:118:LEU:HD23	1:A:123:TYR:CA	0.41	2.46	4	1
1:A:51:CYS:O	1:A:51:CYS:SG	0.41	2.79	10	1
1:A:58:LEU:CD1	1:A:94:PHE:CD2	0.41	3.04	18	1
1:A:75:TYR:CE1	1:A:96:CYS:SG	0.41	3.14	9	1
1:A:3:TRP:HZ3	1:A:70:THR:HG22	0.41	1.75	10	1
1:A:8:MET:HE1	1:A:73:TYR:CE2	0.41	2.50	11	1
1:A:8:MET:HE3	1:A:73:TYR:CE1	0.41	2.51	15	1
1:A:19:LEU:HD21	1:A:31:LEU:H	0.40	1.75	11	1
1:A:5:PHE:CD2	1:A:9:ILE:CD1	0.40	3.05	3	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	115/124 (93%)	64±11 (55±10%)	26±6 (23±5%)	18±4 (16±4%)	0	4
All	All	1955/2232 (88%)	1146 (59%)	477 (24%)	332 (17%)	0	3

All 50 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	15
1	A	119	ASP	15
1	A	20	MET	14
1	A	19	LEU	13
1	A	80	THR	13
1	A	120	THR	13
1	A	82	ILE	12
1	A	84	CYS	12
1	A	58	LEU	12
1	A	70	THR	11
1	A	73	TYR	11
1	A	74	SER	11
1	A	83	THR	11
1	A	117	ASN	11
1	A	91	CYS	9
1	A	29	CYS	9
1	A	118	LEU	8
1	A	104	ILE	8
1	A	77	CYS	7
1	A	32	GLY	6
1	A	28	TYR	5
1	A	88	ASN	5
1	A	121	LYS	5
1	A	8	MET	5
1	A	25	TYR	4
1	A	27	CYS	4
1	A	16	SER	3
1	A	21	ASP	3
1	A	71	GLU	3
1	A	33	GLY	3
1	A	111	TYR	3
1	A	18	PRO	3
1	A	89	ASN	3
1	A	26	GLY	3
1	A	116	LYS	3
1	A	79	ASN	3
1	A	76	SER	2
1	A	81	GLU	2
1	A	56	LYS	2
1	A	114	GLU	2
1	A	30	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ASN	2
1	A	110	PRO	1
1	A	47	THR	1
1	A	48	HIS	1
1	A	35	GLY	1
1	A	6	ARG	1
1	A	31	LEU	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%)	78±2 (76±2%)	24±2 (24±2%)	2	27
All	All	1854/1980 (94%)	1413 (76%)	441 (24%)	2	27

All 64 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	36	THR	18
1	A	53	ARG	18
1	A	104	ILE	18
1	A	108	LYS	18
1	A	113	LYS	18
1	A	114	GLU	18
1	A	37	PRO	17
1	A	85	ASN	16
1	A	94	PHE	16
1	A	2	LEU	14
1	A	5	PHE	14
1	A	17	HIS	14
1	A	87	LYS	14
1	A	38	VAL	12
1	A	41	LEU	12
1	A	96	CYS	12
1	A	28	TYR	11
1	A	56	LYS	11

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Mol	Chain	Res	Type	Models (Total)
1	A	10	LYS	10
1	A	61	CYS	10
1	A	6	ARG	10
1	A	31	LEU	9
1	A	70	THR	8
1	A	124	CYS	8
1	A	82	ILE	8
1	A	29	CYS	7
1	A	92	GLU	7
1	A	46	GLU	6
1	A	13	ILE	5
1	A	95	ILE	5
1	A	116	LYS	5
1	A	84	CYS	4
1	A	119	ASP	4
1	A	110	PRO	4
1	A	8	MET	4
1	A	11	CYS	4
1	A	73	TYR	3
1	A	27	CYS	3
1	A	39	ASP	3
1	A	100	ARG	3
1	A	19	LEU	3
1	A	98	CYS	3
1	A	9	ILE	3
1	A	60	SER	3
1	A	121	LYS	3
1	A	77	CYS	2
1	A	120	THR	2
1	A	117	ASN	2
1	A	4	GLN	2
1	A	45	CYS	2
1	A	118	LEU	2
1	A	69	TYR	1
1	A	54	ASP	1
1	A	80	THR	1
1	A	83	THR	1
1	A	49	ASP	1
1	A	88	ASN	1
1	A	99	ASP	1
1	A	106	PHE	1
1	A	111	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	40	GLU	1
1	A	71	GLU	1
1	A	101	ASN	1
1	A	72	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

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