



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:13 PM UTC

PDB ID : 1PIS / pdb_00001pis
Title : SOLUTION STRUCTURE OF PORCINE PANCREATIC PHOSPHOLIPASE A2
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Deposited on : 1994-12-22

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

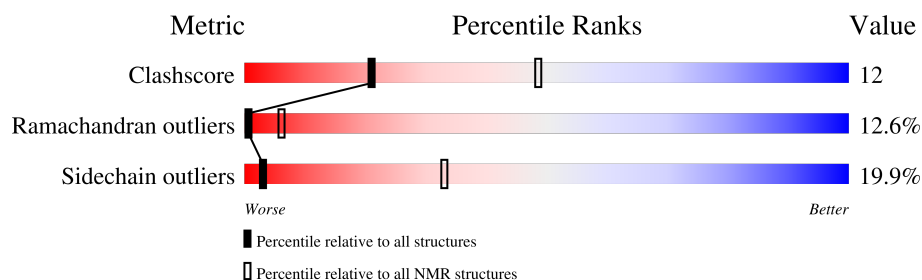
1 Overall quality at a glance

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	27% 35% 21% 7% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:2-A:58, A:70-A:124 (112)	0.52	7

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20

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).

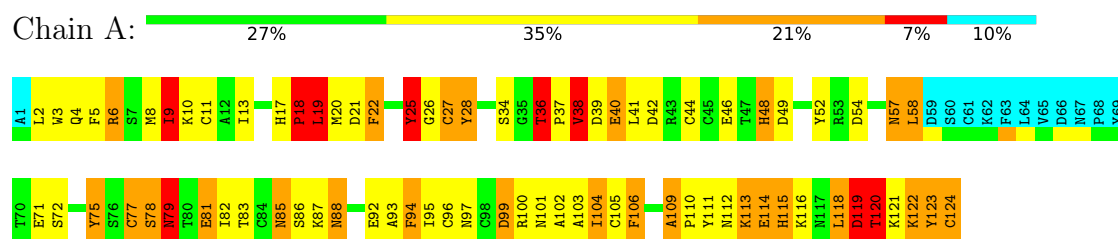
Mol	Chain	Residues	Atoms	
2	A	1	Total	Ca
			1	1

4 Residue-property plots

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

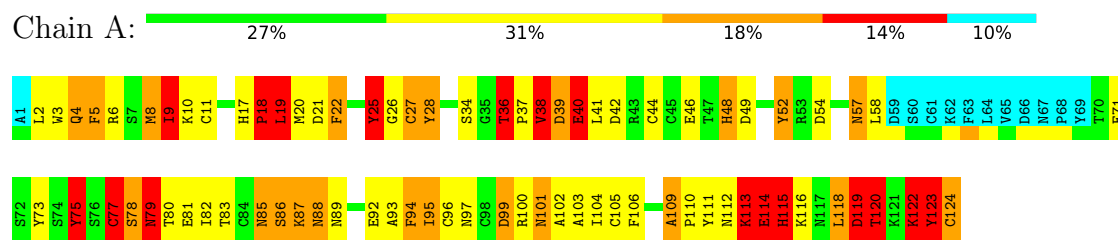


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

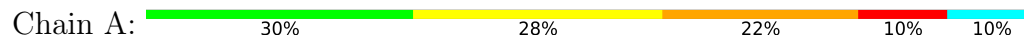
4.2.1 Score per residue for model 1

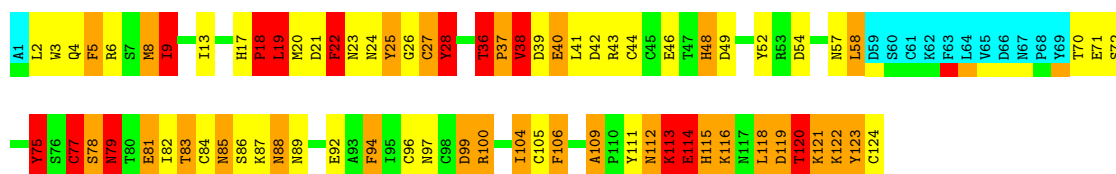
• Molecule 1: PHOSPHOLIPASE A2



4.2.2 Score per residue for model 2

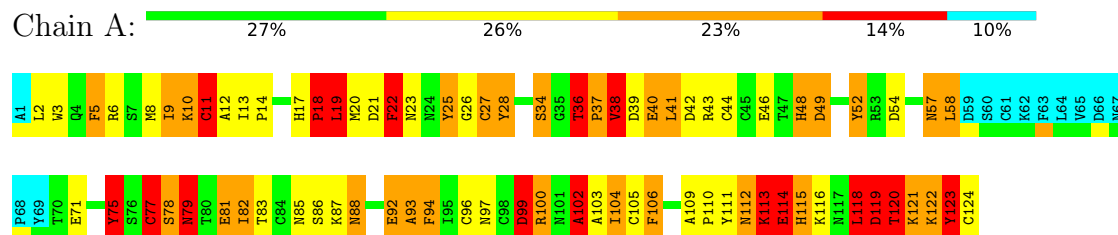
• Molecule 1: PHOSPHOLIPASE A2





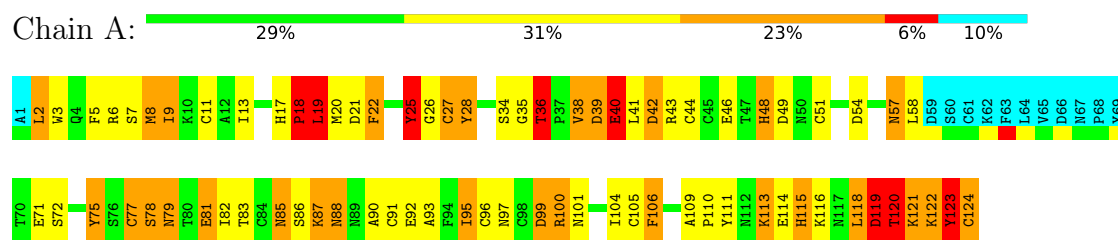
4.2.3 Score per residue for model 3

- Molecule 1: PHOSPHOLIPASE A2



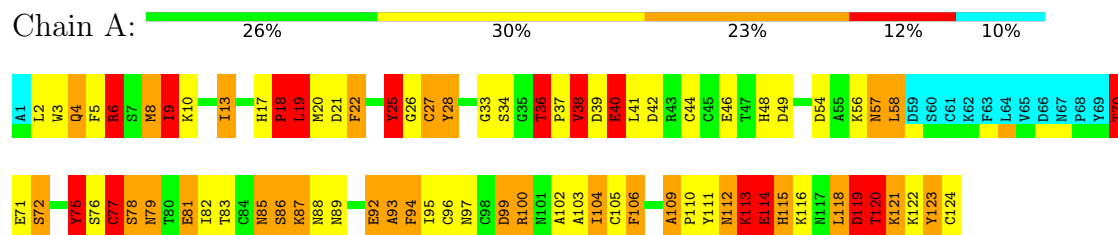
4.2.4 Score per residue for model 4

- Molecule 1: PHOSPHOLIPASE A2



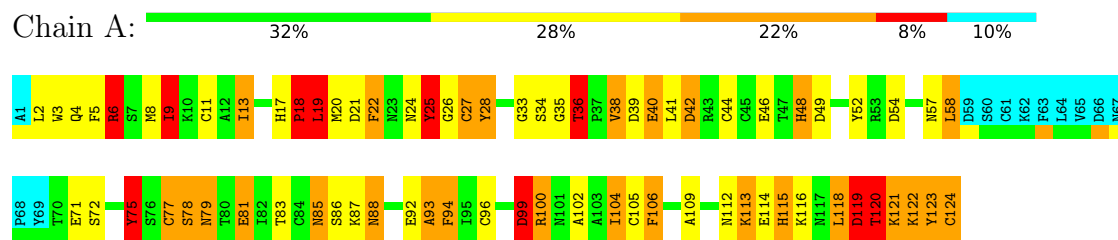
4.2.5 Score per residue for model 5

- Molecule 1: PHOSPHOLIPASE A2



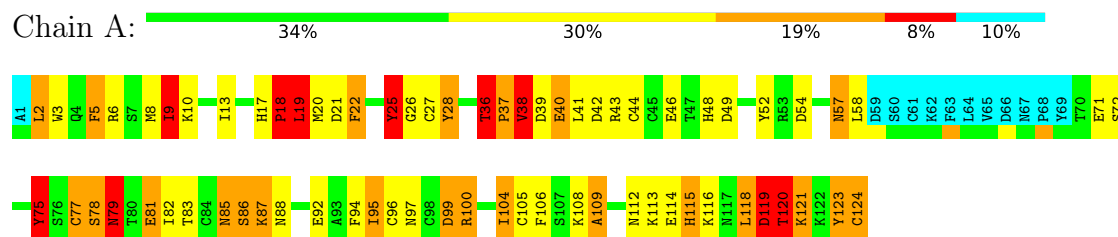
4.2.6 Score per residue for model 6

- Molecule 1: PHOSPHOLIPASE A2



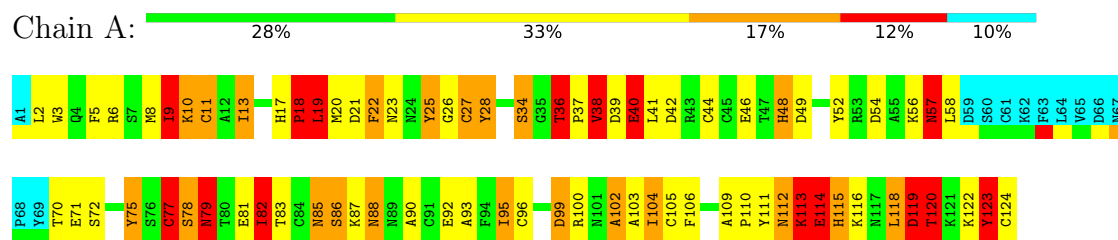
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PHOSPHOLIPASE A2



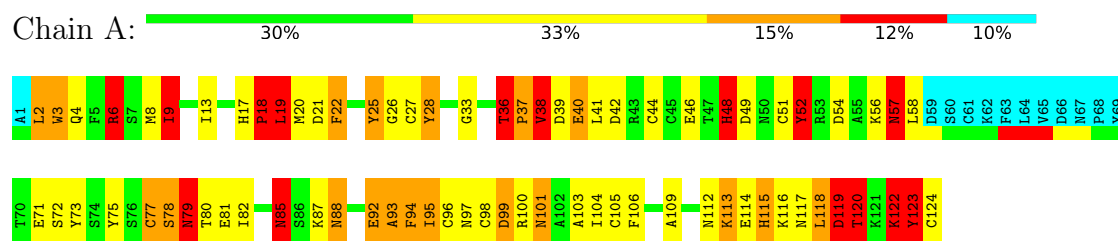
4.2.8 Score per residue for model 8

- Molecule 1: PHOSPHOLIPASE A2



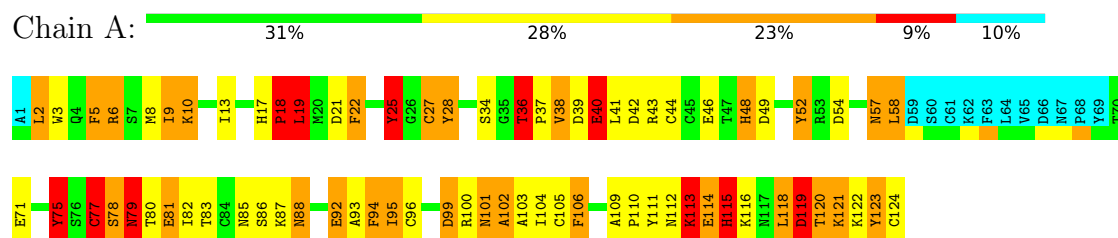
4.2.9 Score per residue for model 9

- Molecule 1: PHOSPHOLIPASE A2



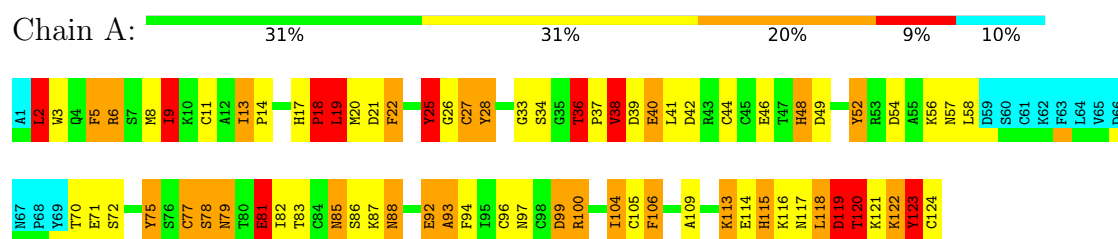
4.2.10 Score per residue for model 10

- Molecule 1: PHOSPHOLIPASE A2



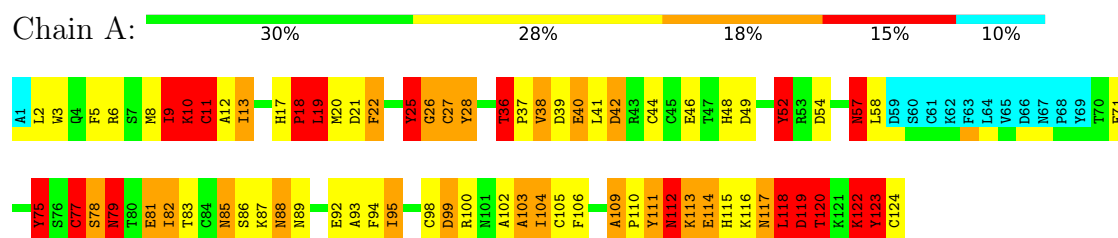
4.2.11 Score per residue for model 11

- Molecule 1: PHOSPHOLIPASE A2



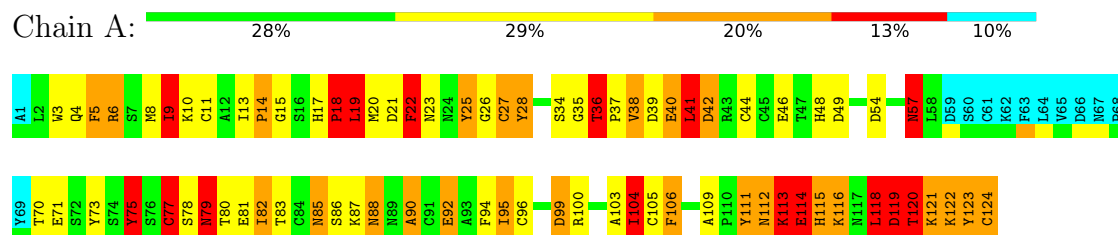
4.2.12 Score per residue for model 12

- Molecule 1: PHOSPHOLIPASE A2



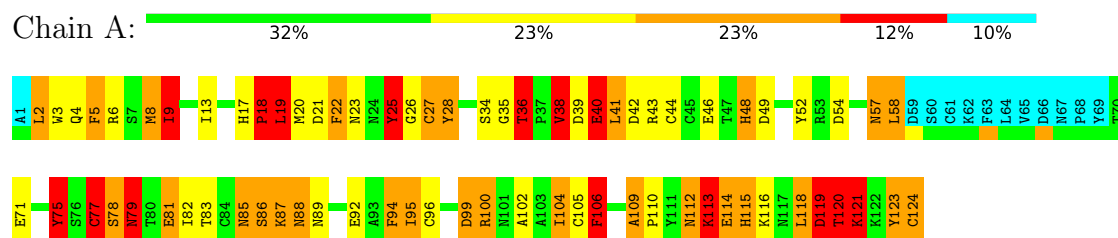
4.2.13 Score per residue for model 13

- Molecule 1: PHOSPHOLIPASE A2



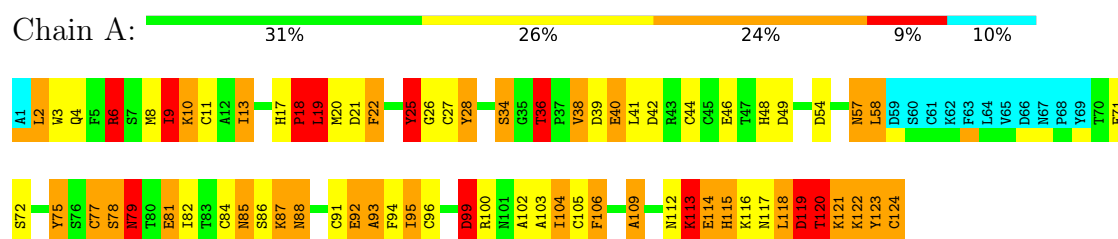
4.2.14 Score per residue for model 14

- Molecule 1: PHOSPHOLIPASE A2



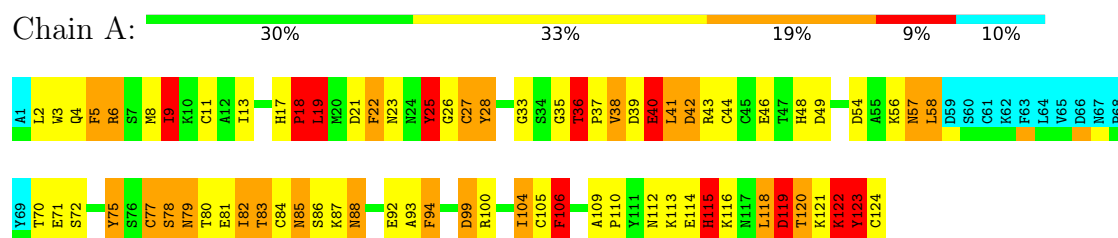
4.2.15 Score per residue for model 15

- Molecule 1: PHOSPHOLIPASE A2



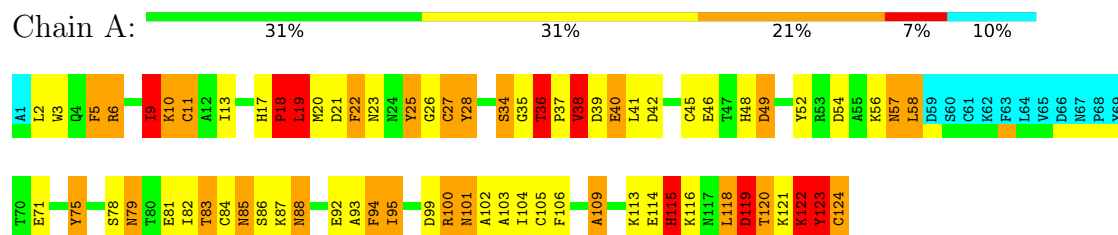
4.2.16 Score per residue for model 16

- Molecule 1: PHOSPHOLIPASE A2



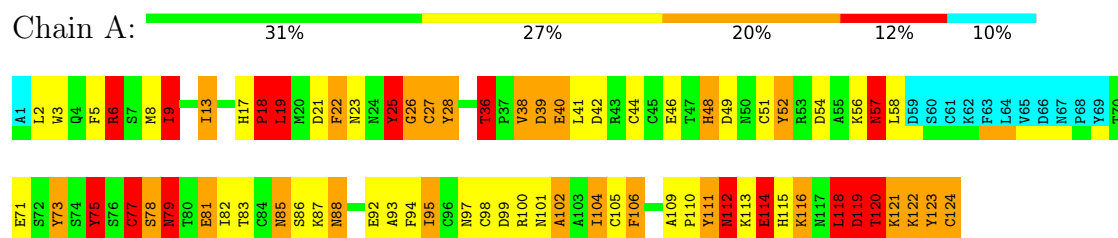
4.2.17 Score per residue for model 17

- Molecule 1: PHOSPHOLIPASE A2



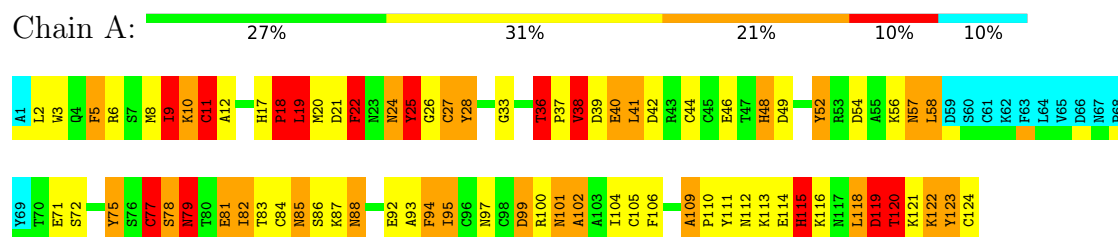
4.2.18 Score per residue for model 18

- Molecule 1: PHOSPHOLIPASE A2



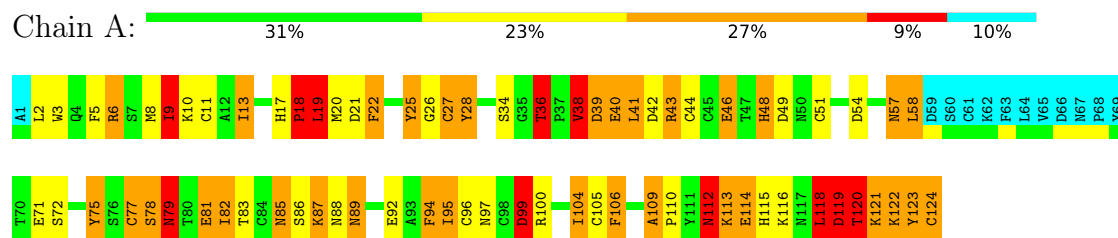
4.2.19 Score per residue for model 19

- Molecule 1: PHOSPHOLIPASE A2



4.2.20 Score per residue for model 20

- Molecule 1: PHOSPHOLIPASE A2



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or 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	1.87±0.01	19±1/895 (2.1± 0.2%)	2.51±0.03	67±5/1206 (5.5± 0.5%)
All	All	1.87	377/17900 (2.1%)	2.51	1334/24120 (5.5%)

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	17.3±1.9
All	All	0	346

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	89	ASN	CA-C	7.41	1.57	1.53	12	2
1	A	124	CYS	C-OXT	7.31	1.38	1.23	17	20
1	A	39	ASP	CG-OD1	6.56	1.37	1.25	13	6
1	A	21	ASP	CG-OD1	6.56	1.37	1.25	1	7
1	A	81	GLU	CD-OE2	6.56	1.37	1.25	12	8
1	A	46	GLU	CD-OE1	6.52	1.37	1.25	9	10
1	A	40	GLU	CD-OE2	6.52	1.37	1.25	13	5
1	A	92	GLU	CD-OE1	6.51	1.37	1.25	3	10
1	A	71	GLU	CD-OE1	6.50	1.37	1.25	15	15
1	A	81	GLU	CD-OE1	6.50	1.37	1.25	15	12
1	A	92	GLU	CD-OE2	6.50	1.37	1.25	6	10
1	A	54	ASP	CG-OD1	6.50	1.37	1.25	3	7
1	A	114	GLU	CD-OE1	6.50	1.37	1.25	19	7
1	A	114	GLU	CD-OE2	6.49	1.37	1.25	14	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	71	GLU	CD-OE2	6.49	1.37	1.25	11	5
1	A	54	ASP	CG-OD2	6.49	1.37	1.25	12	13
1	A	119	ASP	CG-OD1	6.49	1.37	1.25	17	9
1	A	119	ASP	CG-OD2	6.48	1.37	1.25	14	11
1	A	21	ASP	CG-OD2	6.48	1.37	1.25	14	13
1	A	40	GLU	CD-OE1	6.47	1.37	1.25	16	15
1	A	46	GLU	CD-OE2	6.47	1.37	1.25	8	10
1	A	39	ASP	CG-OD2	6.46	1.37	1.25	20	14
1	A	99	ASP	CG-OD2	6.41	1.37	1.25	15	12
1	A	99	ASP	CG-OD1	6.41	1.37	1.25	9	8
1	A	49	ASP	CG-OD2	6.41	1.37	1.25	9	15
1	A	42	ASP	CG-OD1	6.35	1.37	1.25	7	12
1	A	42	ASP	CG-OD2	6.34	1.37	1.25	14	8
1	A	49	ASP	CG-OD1	6.30	1.37	1.25	1	5
1	A	57	ASN	CA-C	6.08	1.58	1.52	1	1
1	A	9	ILE	CA-C	6.04	1.59	1.52	13	6
1	A	5	PHE	CA-C	5.85	1.59	1.52	6	8
1	A	20	MET	CA-C	5.83	1.60	1.52	15	17
1	A	113	LYS	CA-C	5.67	1.60	1.52	6	7
1	A	101	ASN	CA-C	5.56	1.60	1.52	10	5
1	A	48	HIS	ND1-CE1	5.55	1.38	1.32	5	16
1	A	48	HIS	CG-CD2	5.42	1.41	1.35	13	1
1	A	89	ASN	N-CA	5.40	1.49	1.46	12	2
1	A	17	HIS	ND1-CE1	5.30	1.37	1.32	18	20
1	A	109	ALA	CA-C	5.21	1.59	1.53	20	3
1	A	10	LYS	CA-C	5.20	1.57	1.53	17	1
1	A	113	LYS	N-CA	5.20	1.52	1.46	20	1
1	A	6	ARG	N-CA	5.16	1.52	1.46	13	4
1	A	114	GLU	N-CA	5.05	1.52	1.46	7	3

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	115	HIS	ND1-CE1-NE2	15.10	123.50	108.40	11	20
1	A	22	PHE	CA-CB-CG	14.19	127.99	113.80	9	20
1	A	115	HIS	CE1-NE2-CD2	-14.00	95.00	109.00	9	20
1	A	119	ASP	N-CA-CB	-12.37	91.77	110.20	20	20
1	A	17	HIS	ND1-CE1-NE2	12.00	120.40	108.40	3	20
1	A	48	HIS	ND1-CE1-NE2	11.92	120.32	108.40	1	20
1	A	115	HIS	CB-CG-CD2	-11.28	116.54	131.20	18	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	113	LYS	N-CA-CB	-10.56	95.99	110.56	8	12
1	A	88	ASN	CA-CB-CG	9.68	122.28	112.60	14	14
1	A	48	HIS	CE1-NE2-CD2	-9.45	99.55	109.00	5	20
1	A	28	TYR	CA-CB-CG	9.26	130.57	113.90	2	19
1	A	17	HIS	CE1-NE2-CD2	-9.19	99.81	109.00	6	20
1	A	99	ASP	CA-CB-CG	8.99	121.59	112.60	10	7
1	A	78	SER	N-CA-C	8.96	123.12	109.23	16	17
1	A	106	PHE	CA-CB-CG	8.88	122.68	113.80	20	20
1	A	3	TRP	N-CA-C	8.87	123.11	111.75	8	6
1	A	112	ASN	CA-CB-CG	8.71	121.31	112.60	18	6
1	A	9	ILE	CA-CB-CG1	8.53	124.91	110.40	5	20
1	A	25	TYR	CA-CB-CG	8.45	129.12	113.90	10	20
1	A	118	LEU	CA-C-N	8.38	134.91	120.58	20	20
1	A	118	LEU	C-N-CA	8.38	134.91	120.58	20	20
1	A	82	ILE	CA-CB-CG2	8.31	124.63	110.50	19	18
1	A	49	ASP	CA-CB-CG	8.24	120.84	112.60	14	14
1	A	3	TRP	CB-CG-CD1	-8.19	114.61	126.90	6	20
1	A	121	LYS	CA-C-N	8.07	131.61	120.63	5	2
1	A	121	LYS	C-N-CA	8.07	131.61	120.63	5	2
1	A	88	ASN	N-CA-C	7.94	122.54	113.01	20	1
1	A	97	ASN	CA-CB-CG	7.87	120.47	112.60	20	6
1	A	48	HIS	CA-CB-CG	7.84	121.64	113.80	11	20
1	A	9	ILE	N-CA-CB	-7.82	98.33	111.23	9	1
1	A	85	ASN	CA-CB-CG	7.76	120.36	112.60	5	19
1	A	105	CYS	N-CA-CB	-7.76	97.14	110.32	17	1
1	A	104	ILE	N-CA-CB	-7.73	101.93	110.51	3	14
1	A	38	VAL	CB-CA-C	7.67	123.87	111.29	2	20
1	A	3	TRP	CB-CG-CD2	7.67	137.54	126.80	13	18
1	A	83	THR	CB-CA-C	7.65	125.64	110.42	13	18
1	A	58	LEU	N-CA-C	7.63	120.49	108.67	4	14
1	A	36	THR	CA-CB-CG2	7.54	123.32	110.50	9	2
1	A	115	HIS	CG-ND1-CE1	-7.51	96.53	109.30	16	20
1	A	28	TYR	CB-CG-CD2	-7.50	109.56	120.80	2	1
1	A	21	ASP	CA-CB-CG	7.49	120.09	112.60	1	12
1	A	3	TRP	N-CA-CB	7.46	121.21	110.40	20	6
1	A	6	ARG	CA-CB-CG	7.44	128.99	114.10	18	1
1	A	88	ASN	N-CA-CB	-7.38	98.01	110.49	17	13
1	A	84	CYS	N-CA-CB	-7.38	98.02	110.49	15	1
1	A	119	ASP	CA-CB-CG	7.36	119.96	112.60	11	14
1	A	48	HIS	CB-CG-CD2	-7.32	121.69	131.20	9	16
1	A	93	ALA	N-CA-C	7.25	118.82	111.07	11	12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	ASP	CA-CB-CG	7.19	119.79	112.60	13	3
1	A	123	TYR	CB-CA-C	7.18	122.69	110.56	3	20
1	A	40	GLU	CA-CB-CG	7.14	128.37	114.10	3	1
1	A	38	VAL	N-CA-CB	-6.99	99.70	111.23	4	14
1	A	80	THR	N-CA-C	6.98	120.28	111.69	10	1
1	A	95	ILE	CA-CB-CG1	6.96	122.22	110.40	14	14
1	A	75	TYR	N-CA-C	6.95	118.33	108.74	17	15
1	A	122	LYS	N-CA-CB	-6.90	99.97	109.98	5	4
1	A	113	LYS	CA-C-N	6.89	130.37	120.79	20	1
1	A	113	LYS	C-N-CA	6.89	130.37	120.79	20	1
1	A	120	THR	N-CA-C	6.87	125.43	110.80	11	20
1	A	2	LEU	N-CA-CB	6.85	120.33	109.51	11	1
1	A	118	LEU	N-CA-C	6.81	119.61	110.35	2	18
1	A	52	TYR	CB-CG-CD2	-6.79	110.62	120.80	3	13
1	A	41	LEU	N-CA-C	6.76	125.21	110.80	13	1
1	A	27	CYS	N-CA-C	6.76	118.53	111.03	10	18
1	A	18	PRO	N-CA-C	6.71	126.29	112.47	9	20
1	A	88	ASN	CB-CA-C	6.68	120.58	109.89	15	6
1	A	103	ALA	N-CA-C	6.66	118.62	111.36	9	5
1	A	115	HIS	CA-CB-CG	6.64	120.44	113.80	2	10
1	A	83	THR	CA-CB-CG2	6.61	121.74	110.50	1	18
1	A	117	ASN	CB-CA-C	6.61	120.94	111.82	12	1
1	A	6	ARG	N-CA-CB	6.60	121.65	110.49	6	3
1	A	82	ILE	CA-CB-CG1	6.59	121.61	110.40	8	1
1	A	115	HIS	CG-CD2-NE2	6.58	113.78	107.20	9	18
1	A	28	TYR	CB-CG-CD1	6.57	130.66	120.80	2	1
1	A	86	SER	N-CA-CB	-6.55	99.52	110.39	20	19
1	A	48	HIS	CG-ND1-CE1	-6.49	98.26	109.30	9	20
1	A	11	CYS	N-CA-CB	-6.46	99.58	110.49	12	4
1	A	6	ARG	CG-CD-NE	6.44	126.17	112.00	18	1
1	A	57	ASN	N-CA-CB	-6.44	99.99	110.42	19	11
1	A	116	LYS	CB-CA-C	6.43	123.75	110.31	18	16
1	A	57	ASN	CA-CB-CG	6.38	118.98	112.60	9	9
1	A	17	HIS	CB-CG-CD2	-6.38	122.91	131.20	11	20
1	A	116	LYS	N-CA-CB	-6.36	98.74	110.32	15	13
1	A	112	ASN	N-CA-CB	6.34	119.80	110.35	2	6
1	A	117	ASN	CA-CB-CG	6.33	118.93	112.60	12	1
1	A	18	PRO	N-CA-CB	-6.31	96.63	103.25	9	20
1	A	48	HIS	CB-CA-C	6.30	119.03	111.22	15	3
1	A	13	ILE	CB-CA-C	6.30	122.82	111.36	10	9
1	A	17	HIS	CG-ND1-CE1	-6.23	98.72	109.30	1	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	89	ASN	N-CA-C	6.17	113.83	108.78	12	1
1	A	102	ALA	N-CA-CB	-6.14	100.56	110.14	19	7
1	A	24	ASN	N-CA-CB	6.13	120.86	110.49	2	2
1	A	109	ALA	CA-C-N	6.12	127.50	119.84	3	12
1	A	109	ALA	C-N-CA	6.12	127.50	119.84	3	12
1	A	17	HIS	CA-CB-CG	6.08	119.88	113.80	11	1
1	A	105	CYS	N-CA-C	6.08	119.79	112.38	17	1
1	A	79	ASN	N-CA-C	-6.00	98.02	110.80	10	1
1	A	28	TYR	CB-CA-C	6.00	120.64	111.95	6	8
1	A	34	SER	N-CA-C	5.94	123.46	110.80	17	5
1	A	100	ARG	N-CA-CB	5.93	118.58	109.98	3	3
1	A	5	PHE	CB-CA-C	5.92	120.74	110.68	14	2
1	A	90	ALA	N-CA-C	5.91	123.39	110.80	13	3
1	A	103	ALA	CB-CA-C	5.91	122.18	110.42	12	2
1	A	25	TYR	N-CA-C	5.91	117.67	110.41	1	6
1	A	104	ILE	N-CA-C	5.90	116.56	110.36	5	10
1	A	109	ALA	N-CA-C	5.90	117.25	109.93	2	3
1	A	87	LYS	N-CA-C	5.90	120.01	112.34	16	12
1	A	9	ILE	N-CA-C	5.88	121.57	109.34	9	1
1	A	96	CYS	N-CA-C	5.85	117.66	111.28	20	3
1	A	118	LEU	CA-C-O	5.84	128.66	121.94	20	19
1	A	87	LYS	CA-C-N	5.83	132.69	121.54	8	12
1	A	87	LYS	C-N-CA	5.83	132.69	121.54	8	12
1	A	115	HIS	CB-CG-ND1	5.83	131.44	122.70	18	3
1	A	23	ASN	N-CA-C	5.80	117.61	111.28	16	3
1	A	33	GLY	N-CA-C	5.80	123.06	115.40	9	5
1	A	42	ASP	CA-CB-CG	-5.75	106.84	112.60	2	3
1	A	99	ASP	N-CA-CB	-5.75	99.83	110.18	9	5
1	A	52	TYR	CB-CG-CD1	5.72	129.38	120.80	3	3
1	A	109	ALA	N-CA-CB	5.72	118.21	110.14	17	4
1	A	70	THR	N-CA-C	5.71	117.30	111.14	8	2
1	A	22	PHE	N-CA-C	5.68	118.25	111.71	10	10
1	A	111	TYR	CA-CB-CG	5.67	124.10	113.90	12	3
1	A	48	HIS	ND1-CG-CD2	5.63	111.73	106.10	9	11
1	A	25	TYR	N-CA-CB	5.58	119.92	110.49	2	1
1	A	19	LEU	N-CA-C	5.57	122.66	110.80	17	9
1	A	120	THR	CB-CA-C	5.57	119.50	109.64	17	2
1	A	115	HIS	ND1-CG-CD2	5.55	111.65	106.10	2	14
1	A	5	PHE	N-CA-CB	-5.54	101.69	109.94	17	3
1	A	10	LYS	CB-CG-CD	5.52	124.00	111.30	10	8
1	A	5	PHE	N-CA-C	5.52	117.74	111.11	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	119	ASP	N-CA-C	5.46	117.68	111.02	2	5
1	A	78	SER	N-CA-CB	-5.46	101.37	111.53	16	7
1	A	72	SER	N-CA-CB	5.43	119.67	110.49	5	1
1	A	4	GLN	CB-CA-C	5.42	120.41	110.11	1	1
1	A	118	LEU	CD1-CG-CD2	-5.37	98.98	110.80	2	1
1	A	38	VAL	CG1-CB-CG2	-5.33	99.08	110.80	2	4
1	A	37	PRO	N-CA-CB	-5.31	97.67	103.25	7	1
1	A	41	LEU	CB-CA-C	5.31	119.57	110.01	20	3
1	A	46	GLU	CB-CG-CD	5.29	121.60	112.60	9	2
1	A	89	ASN	CA-CB-CG	5.26	117.86	112.60	20	1
1	A	113	LYS	O-C-N	-5.24	115.66	122.37	3	4
1	A	38	VAL	CA-CB-CG1	5.24	119.30	110.40	13	1
1	A	70	THR	CA-CB-CG2	5.20	119.34	110.50	11	2
1	A	57	ASN	N-CA-C	5.20	119.37	113.19	7	3
1	A	2	LEU	CB-CA-C	-5.19	102.68	110.16	11	1
1	A	18	PRO	CA-C-N	5.19	131.45	121.54	18	1
1	A	18	PRO	C-N-CA	5.19	131.45	121.54	18	1
1	A	85	ASN	CB-CA-C	5.19	120.74	110.42	9	1
1	A	106	PHE	CB-CA-C	5.17	121.22	110.32	11	3
1	A	38	VAL	CA-CB-CG2	5.16	119.18	110.40	10	3
1	A	11	CYS	N-CA-C	5.16	119.84	111.37	20	3
1	A	43	ARG	N-CA-C	5.12	117.60	111.71	20	1
1	A	96	CYS	N-CA-CB	-5.11	102.35	110.22	14	1
1	A	76	SER	N-CA-CB	-5.11	103.39	111.05	5	1
1	A	101	ASN	CA-C-N	5.09	130.31	122.42	17	1
1	A	101	ASN	C-N-CA	5.09	130.31	122.42	17	1
1	A	118	LEU	CB-CA-C	5.07	120.10	110.51	11	1
1	A	89	ASN	N-CA-CB	-5.06	101.94	110.49	2	1
1	A	14	PRO	N-CA-C	5.01	122.78	112.47	13	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	28	TYR	Sidechain	20
1	A	41	LEU	Peptide	20
1	A	57	ASN	Peptide	20
1	A	75	TYR	Sidechain	20
1	A	79	ASN	Peptide	20
1	A	120	THR	Peptide	20

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	77	CYS	Peptide	19
1	A	119	ASP	Peptide	19
1	A	85	ASN	Peptide	17
1	A	113	LYS	Peptide	17
1	A	94	PHE	Sidechain	15
1	A	109	ALA	Peptide	15
1	A	123	TYR	Sidechain	15
1	A	25	TYR	Sidechain	13
1	A	38	VAL	Peptide	13
1	A	111	TYR	Sidechain	10
1	A	52	TYR	Sidechain	7
1	A	87	LYS	Peptide	7
1	A	4	GLN	Peptide	6
1	A	35	GLY	Peptide	6
1	A	86	SER	Peptide	5
1	A	2	LEU	Peptide	5
1	A	10	LYS	Peptide	5
1	A	73	TYR	Sidechain	4
1	A	122	LYS	Peptide	4
1	A	6	ARG	Peptide	4
1	A	117	ASN	Peptide	4
1	A	116	LYS	Peptide	3
1	A	112	ASN	Peptide	3
1	A	121	LYS	Peptide	2
1	A	37	PRO	Peptide	1
1	A	36	THR	Peptide	1
1	A	115	HIS	Sidechain	1
1	A	48	HIS	Sidechain	1
1	A	56	LYS	Peptide	1
1	A	78	SER	Peptide	1
1	A	45	CYS	Peptide	1
1	A	101	ASN	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	876	0	798	20±3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	17540	0	15960	400

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:118:LEU:HD12	1:A:119:ASP:HB2	0.77	1.55	13	19
1:A:9:ILE:HG23	1:A:103:ALA:HA	0.74	1.58	8	4
1:A:6:ARG:HG2	1:A:19:LEU:HD21	0.67	1.63	9	3
1:A:8:MET:HE2	1:A:82:ILE:CG2	0.67	2.19	8	8
1:A:118:LEU:HD12	1:A:119:ASP:H	0.66	1.51	10	17
1:A:93:ALA:HA	1:A:96:CYS:SG	0.64	2.32	8	9
1:A:6:ARG:HG3	1:A:19:LEU:HD21	0.61	1.73	11	15
1:A:75:TYR:CE2	1:A:77:CYS:SG	0.61	2.94	12	12
1:A:8:MET:SD	1:A:99:ASP:OD1	0.61	2.59	10	6
1:A:27:CYS:SG	1:A:36:THR:O	0.58	2.61	1	19
1:A:9:ILE:HG22	1:A:13:ILE:CG1	0.58	2.28	12	4
1:A:19:LEU:HD13	1:A:19:LEU:H	0.58	1.59	18	8
1:A:18:PRO:HA	1:A:22:PHE:CD2	0.57	2.35	4	20
1:A:6:ARG:CB	1:A:19:LEU:HD21	0.56	2.30	18	1
1:A:119:ASP:HB3	1:A:122:LYS:CE	0.55	2.32	13	15
1:A:38:VAL:HG11	1:A:118:LEU:HD11	0.54	1.79	2	1
1:A:36:THR:CG2	1:A:37:PRO:HD2	0.54	2.32	9	2
1:A:12:ALA:HB2	1:A:82:ILE:CG1	0.54	2.32	12	3
1:A:48:HIS:HA	1:A:51:CYS:SG	0.53	2.43	9	4
1:A:36:THR:HG22	1:A:37:PRO:HD2	0.53	1.80	9	1
1:A:100:ARG:O	1:A:104:ILE:HD12	0.53	2.04	9	20
1:A:8:MET:SD	1:A:99:ASP:O	0.52	2.68	11	3
1:A:9:ILE:HB	1:A:18:PRO:HG3	0.52	1.82	9	1
1:A:92:GLU:O	1:A:96:CYS:SG	0.51	2.67	9	7
1:A:36:THR:HG22	1:A:37:PRO:CD	0.51	2.36	9	1
1:A:5:PHE:CZ	1:A:9:ILE:HD11	0.51	2.40	16	10
1:A:52:TYR:CD1	1:A:98:CYS:SG	0.51	3.04	12	2
1:A:19:LEU:H	1:A:19:LEU:HD13	0.51	1.66	5	10
1:A:11:CYS:SG	1:A:75:TYR:OH	0.51	2.66	19	3
1:A:36:THR:CB	1:A:37:PRO:HD2	0.51	2.35	7	1
1:A:26:GLY:HA2	1:A:38:VAL:HG21	0.51	1.83	15	18
1:A:58:LEU:HD13	1:A:94:PHE:CE2	0.50	2.41	5	15
1:A:44:CYS:SG	1:A:105:CYS:O	0.50	2.70	11	19
1:A:6:ARG:CG	1:A:19:LEU:HD21	0.48	2.37	20	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:MET:SD	1:A:99:ASP:OD2	0.48	2.72	8	9
1:A:118:LEU:CD1	1:A:123:TYR:HD2	0.48	2.22	19	14
1:A:18:PRO:HB3	1:A:19:LEU:HD22	0.47	1.85	9	9
1:A:26:GLY:C	1:A:118:LEU:HD12	0.46	2.34	2	1
1:A:8:MET:HE3	1:A:75:TYR:CB	0.46	2.40	6	3
1:A:2:LEU:HD11	1:A:52:TYR:OH	0.46	2.10	11	1
1:A:6:ARG:HG3	1:A:19:LEU:CD2	0.46	2.41	18	2
1:A:12:ALA:N	1:A:82:ILE:HD11	0.46	2.26	3	1
1:A:38:VAL:HG12	1:A:123:TYR:CB	0.46	2.41	14	3
1:A:121:LYS:H	1:A:121:LYS:HE2	0.45	1.72	14	1
1:A:5:PHE:CE1	1:A:102:ALA:HB1	0.44	2.47	3	4
1:A:6:ARG:HG2	1:A:19:LEU:HD11	0.44	1.89	15	2
1:A:75:TYR:CD2	1:A:82:ILE:HG23	0.44	2.48	3	2
1:A:8:MET:SD	1:A:99:ASP:C	0.44	3.01	10	1
1:A:38:VAL:HG23	1:A:39:ASP:H	0.44	1.73	4	3
1:A:5:PHE:HE1	1:A:102:ALA:HB1	0.44	1.72	5	2
1:A:100:ARG:C	1:A:104:ILE:HD12	0.43	2.38	10	3
1:A:52:TYR:HD1	1:A:98:CYS:SG	0.43	2.36	18	1
1:A:4:GLN:H	1:A:70:THR:HG21	0.43	1.73	5	1
1:A:121:LYS:CE	1:A:122:LYS:HD2	0.43	2.44	4	8
1:A:8:MET:HE2	1:A:82:ILE:HG23	0.43	1.89	8	1
1:A:9:ILE:HG22	1:A:13:ILE:HG13	0.42	1.90	5	2
1:A:18:PRO:CB	1:A:19:LEU:HD22	0.42	2.44	11	3
1:A:83:THR:C	1:A:84:CYS:SG	0.42	3.02	16	3
1:A:118:LEU:CD1	1:A:119:ASP:H	0.42	2.27	5	1
1:A:12:ALA:HB2	1:A:82:ILE:HG13	0.42	1.91	3	1
1:A:36:THR:CB	1:A:37:PRO:CD	0.42	2.97	7	2
1:A:36:THR:OG1	1:A:37:PRO:HD2	0.42	2.14	7	1
1:A:6:ARG:HE	1:A:19:LEU:HG	0.41	1.75	9	1
1:A:5:PHE:CE2	1:A:9:ILE:HD11	0.41	2.50	1	2
1:A:41:LEU:CD1	1:A:106:PHE:HA	0.41	2.45	14	2
1:A:38:VAL:HG23	1:A:115:HIS:ND1	0.41	2.31	19	3
1:A:38:VAL:HG11	1:A:118:LEU:HD22	0.41	1.93	7	1
1:A:115:HIS:HB3	1:A:118:LEU:HD13	0.41	1.92	1	1
1:A:40:GLU:HA	1:A:43:ARG:HB2	0.41	1.93	16	2
1:A:113:LYS:C	1:A:114:GLU:HG2	0.41	2.41	15	1
1:A:36:THR:O	1:A:124:CYS:SG	0.40	2.79	1	1
1:A:9:ILE:CG2	1:A:13:ILE:HD12	0.40	2.46	11	1
1:A:9:ILE:HG22	1:A:13:ILE:HD12	0.40	1.92	6	3

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	111/124 (90%)	76±3 (69±3%)	21±3 (19±3%)	14±2 (13±2%)	1	6
All	All	2220/2480 (90%)	1528 (69%)	412 (19%)	280 (13%)	1	6

All 38 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	18	PRO	20
1	A	19	LEU	20
1	A	78	SER	19
1	A	79	ASN	19
1	A	36	THR	18
1	A	120	THR	17
1	A	81	GLU	14
1	A	37	PRO	13
1	A	88	ASN	13
1	A	34	SER	12
1	A	110	PRO	12
1	A	72	SER	12
1	A	2	LEU	11
1	A	11	CYS	9
1	A	87	LYS	8
1	A	114	GLU	7
1	A	40	GLU	6
1	A	23	ASN	5
1	A	102	ALA	5
1	A	57	ASN	5
1	A	38	VAL	4
1	A	89	ASN	4
1	A	22	PHE	4
1	A	6	ARG	4
1	A	14	PRO	3
1	A	24	ASN	2
1	A	26	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	121	LYS	2
1	A	7	SER	1
1	A	3	TRP	1
1	A	9	ILE	1
1	A	85	ASN	1
1	A	25	TYR	1
1	A	33	GLY	1
1	A	58	LEU	1
1	A	15	GLY	1
1	A	41	LEU	1
1	A	90	ALA	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	99/110 (90%)	79±3 (80±3%)	20±3 (20±3%)	3	33
All	All	1980/2200 (90%)	1586 (80%)	394 (20%)	3	33

All 49 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	18	PRO	20
1	A	19	LEU	20
1	A	25	TYR	20
1	A	36	THR	20
1	A	40	GLU	20
1	A	9	ILE	19
1	A	77	CYS	18
1	A	112	ASN	17
1	A	115	HIS	17
1	A	79	ASN	15
1	A	95	ILE	15
1	A	122	LYS	15
1	A	121	LYS	14
1	A	106	PHE	13

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Mol	Chain	Res	Type	Models (Total)
1	A	113	LYS	11
1	A	114	GLU	11
1	A	48	HIS	9
1	A	2	LEU	9
1	A	124	CYS	9
1	A	13	ILE	9
1	A	56	LYS	7
1	A	101	ASN	6
1	A	43	ARG	6
1	A	100	ARG	6
1	A	10	LYS	6
1	A	99	ASP	6
1	A	8	MET	5
1	A	118	LEU	5
1	A	42	ASP	5
1	A	97	ASN	5
1	A	6	ARG	5
1	A	80	THR	4
1	A	88	ASN	4
1	A	4	GLN	3
1	A	70	THR	3
1	A	49	ASP	2
1	A	11	CYS	2
1	A	91	CYS	2
1	A	39	ASP	1
1	A	28	TYR	1
1	A	108	LYS	1
1	A	82	ILE	1
1	A	85	ASN	1
1	A	81	GLU	1
1	A	104	ILE	1
1	A	111	TYR	1
1	A	73	TYR	1
1	A	84	CYS	1
1	A	46	GLU	1

6.3.3 RNA ⓘ

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