Full wwPDB NMR Structure Validation Report (i)

Feb 17, 2022 – 12:19 PM EST

PDB ID	:	1PIS
Title	:	SOLUTION STRUCTURE OF PORCINE PANCREATIC PHOSPHOLIPASE A2
Authors	:	Van Den Berg, B.D.; Tessari, M.; De Haas, G.H.; Verheij, H.M.; Boelens, R.; Kaptein, R.
Deposited on	:	1994-12-22

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

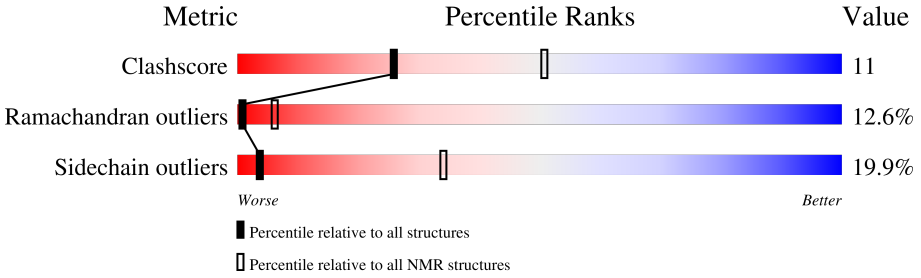
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	124	29% 33% 21% 7% 10%

2 Ensemble composition and analysis (i)

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)	0.30	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 (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
			Total	C	N	O	S	
1	A	124	971	596	166	193	16	0

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

Mol	Chain	Residues	Atoms	
			Total	Ca
2	A	1	1	1

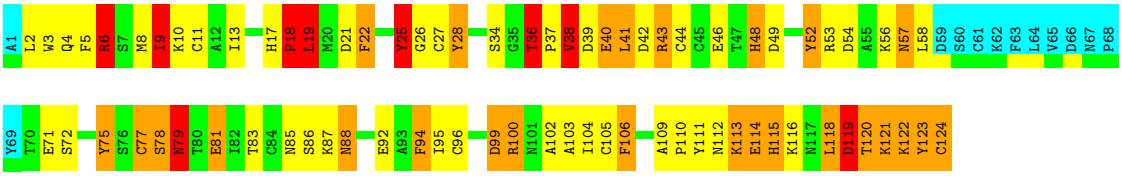
4 Residue-property plots (i)

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

Chain A: 29% 33% 21% 7% 10%



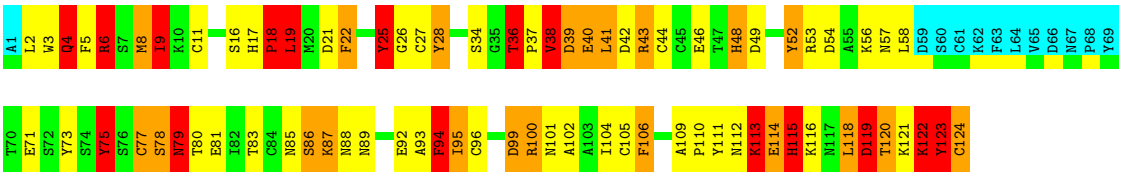
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PHOSPHOLIPASE A2

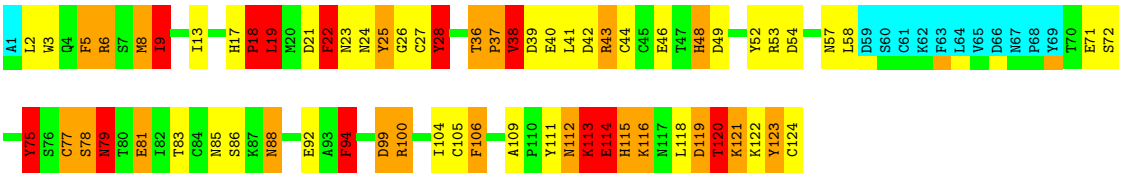
Chain A: 27% 33% 17% 13% 10%



4.2.2 Score per residue for model 2

• Molecule 1: PHOSPHOLIPASE A2

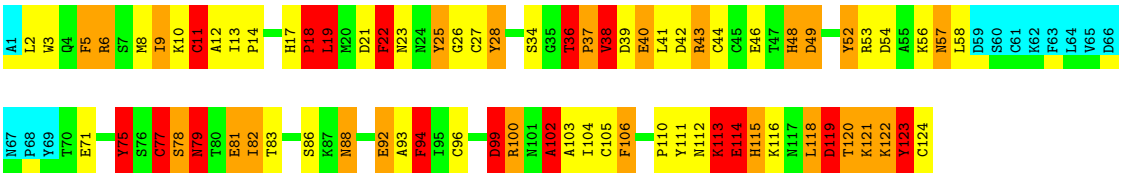
Chain A: 36% 27% 17% 10% 10%



4.2.3 Score per residue for model 3

- Molecule 1: PHOSPHOLIPASE A2

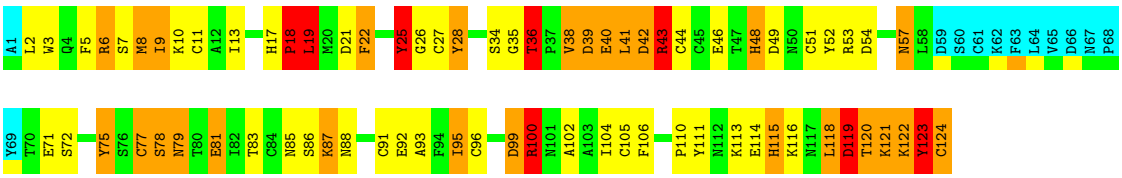
Chain A: 30% 28% 19% 13% 10%



4.2.4 Score per residue for model 4

- Molecule 1: PHOSPHOLIPASE A2

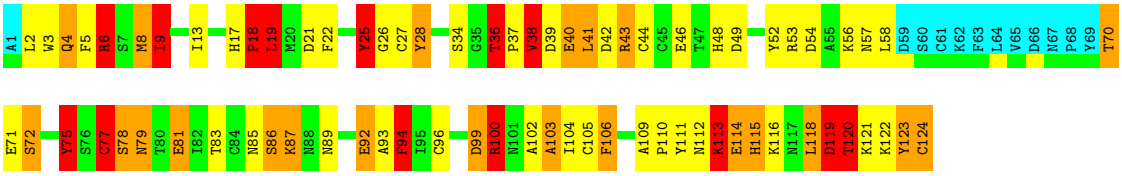
Chain A: 31% 31% 21% 6% 10%



4.2.5 Score per residue for model 5

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 30% 31% 18% 11% 10%



4.2.6 Score per residue for model 6

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 31% 31% 20% 7% 10%

A1 L2 W3 Q4 F5 R6 S7 M8 I9 K10 C11 A12 I13 H17 P18 L19 M20 D21 F22 N23 N24 Y25 G26 C27 Y28 S34 G35 T36 P37 V38 D39 E40 L41 D42 R43 C44 C45 E46 T47 H48 D49 Y52 R53 D54 A55 K56 N57 L58 D59 S60 C61 K62 F63 L64 V65 D66 N67

P68 Y69 T70 E71 S72 Y75 S76 C77 S78 N79 T80 E81 I82 T83 C84 N85 S86 K87 N88 E92 A93 F94 I95 C96 D99 R100 N101 A102 A103 I104 C105 F106 A109 N112 K113 E114 H115 K116 N117 L118 D119 T120 K121 K122 Y123 C124

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 40% 24% 19% 6% 10%

A1 L2 W3 Q4 F5 R6 I9 H17 P18 L19 M20 D21 F22 Y25 G26 C27 Y28 T36 P37 V38 D39 E40 L41 D42 R43 C44 C45 E46 T47 H48 D49 Y52 R53 D54 N57 L58 D59 S60 C61 K62 F63 L64 V65 D66 N67 P68 Y69 T70 E71 S72 Y75 S76 C77

S78 N79 T80 E81 I82 T83 C84 N85 S86 K87 E92 A93 F94 I95 C96 N97 C98 D99 R100 I104 C105 F106 A109 N112 K113 E114 H115 K116 N117 L118 D119 T120 K121 K122 Y123 C124

4.2.8 Score per residue for model 8

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 30% 32% 18% 10% 10%

A1 L2 W3 Q4 F5 R6 S7 M8 I9 K10 C11 A12 I13 H17 P18 L19 M20 D21 F22 N23 N24 Y25 G26 C27 Y28 S34 G35 T36 P37 V38 D39 E40 L41 D42 R43 C44 C45 E46 T47 H48 D49 Y52 R53 D54 A55 K56 N57 L58 D59 S60 C61 K62 F63 L64 V65 D66 N67

P68 Y69 T70 E71 S72 Y73 S74 Y75 S76 C77 S78 N79 T80 E81 I82 T83 C84 N85 S86 K87 N88 E92 A93 F94 I95 C96 D99 R100 N101 A102 A103 I104 C105 F106 P110 Y111 N112 K113 E114 H115 K116 N117 L118 D119 T120 K121 K122 Y123 C124

4.2.9 Score per residue for model 9

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 31% 31% 19% 10% 10%

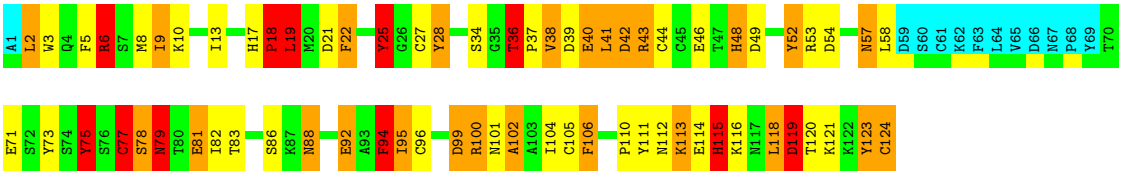
A1 L2 W3 Q4 F5 R6 S7 M8 I9 K10 I13 H17 P18 L19 M20 D21 F22 Y25 G26 C27 Y28 T36 P37 V38 D39 E40 L41 D42 R43 C44 C45 E46 T47 H48 D49 N50 C51 Y52 R53 D54 A55 K56 N57 L58 D59 S60 C61 K62 F63 L64 V65 D66 N67 P68 Y69 T70

E71 S72 Y73 S74 Y75 S76 C77 S78 N79 T80 E81 N85 S86 K87 N88 E92 A93 F94 I95 C96 N97 C98 D99 R100 N101 A102 A103 I104 C105 F106 A109 N112 K113 E114 H115 K116 N117 L118 D119 T120 K121 K122 Y123 C124

4.2.10 Score per residue for model 10

- Molecule 1: PHOSPHOLIPASE A2

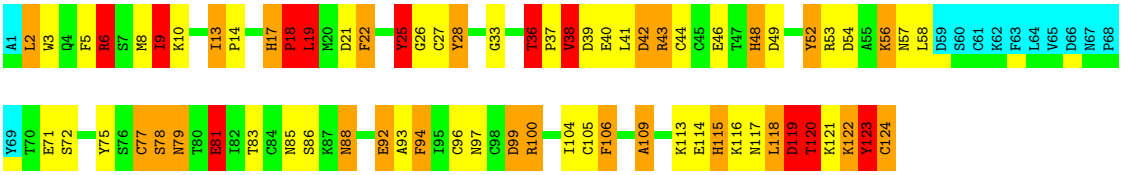
Chain A: 35% 27% 20% 9% 10%



4.2.11 Score per residue for model 11

- Molecule 1: PHOSPHOLIPASE A2

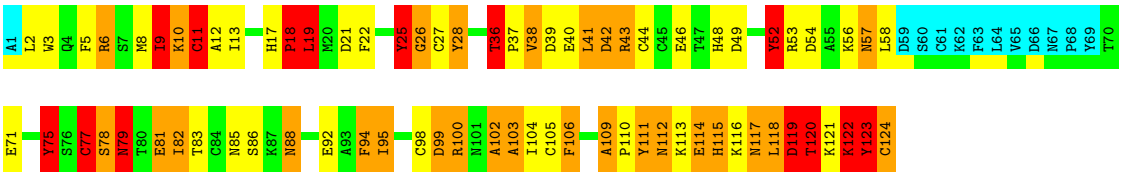
Chain A: 33% 29% 19% 9% 10%



4.2.12 Score per residue for model 12

- Molecule 1: PHOSPHOLIPASE A2

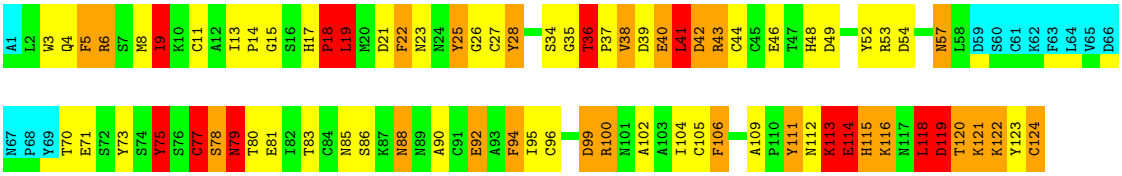
Chain A: 30% 27% 23% 11% 10%



4.2.13 Score per residue for model 13

- Molecule 1: PHOSPHOLIPASE A2

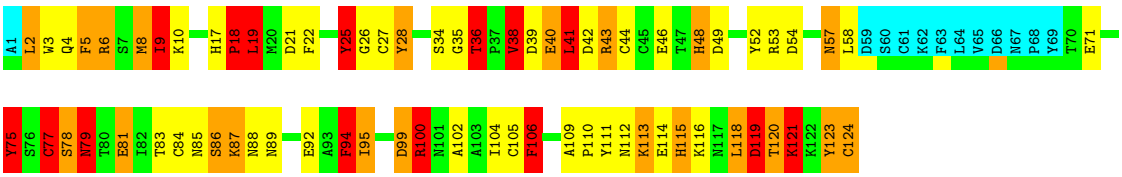
Chain A: 29% 32% 19% 10% 10%



4.2.14 Score per residue for model 14

- Molecule 1: PHOSPHOLIPASE A2

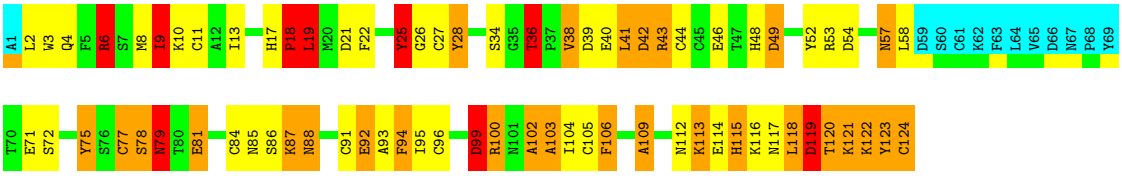
Chain A: 33% 28% 17% 12% 10%



4.2.15 Score per residue for model 15

- Molecule 1: PHOSPHOLIPASE A2

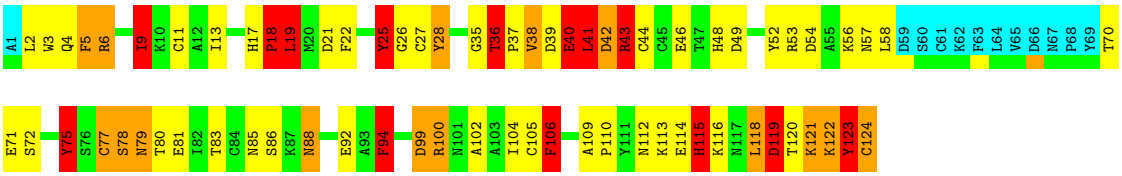
Chain A: 31% 30% 23% 7% 10%



4.2.16 Score per residue for model 16

- Molecule 1: PHOSPHOLIPASE A2

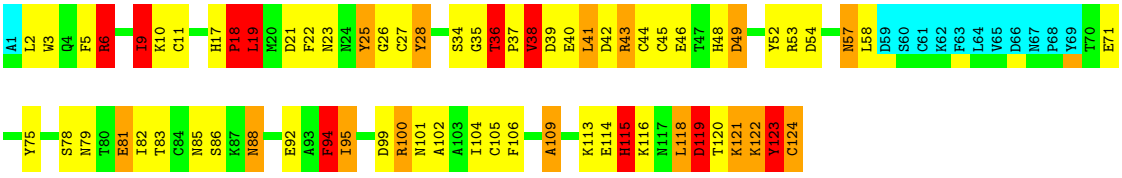
Chain A: 33% 34% 12% 11% 10%



4.2.17 Score per residue for model 17

- Molecule 1: PHOSPHOLIPASE A2

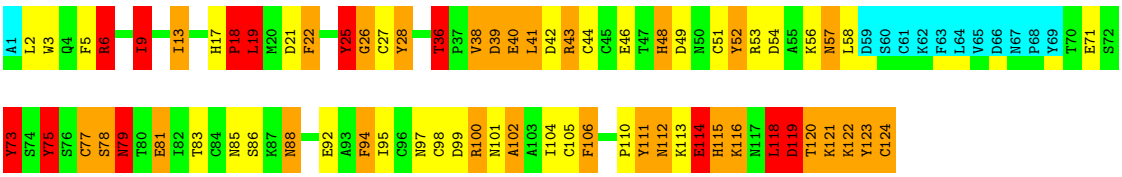
Chain A: 35% 35% 12% 8% 10%



4.2.18 Score per residue for model 18

- Molecule 1: PHOSPHOLIPASE A2

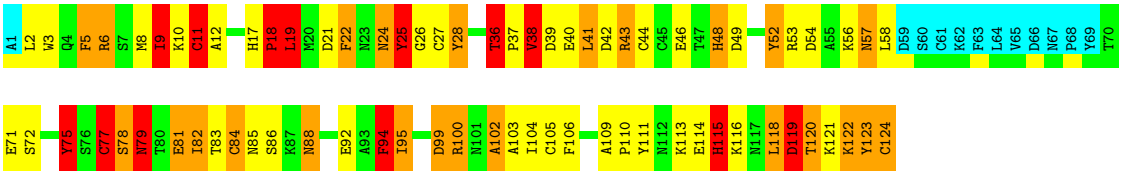
Chain A: 34% 23% 23% 10% 10%



4.2.19 Score per residue for model 19

- Molecule 1: PHOSPHOLIPASE A2

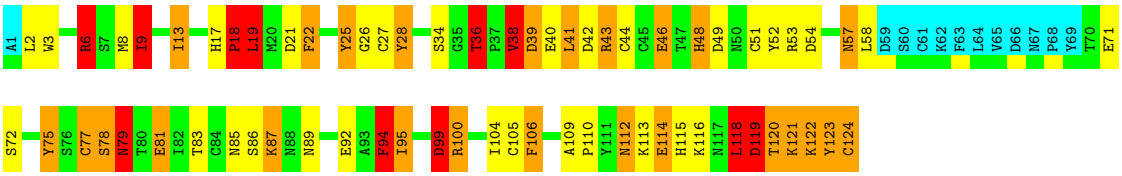
Chain A: 31% 30% 19% 10% 10%



4.2.20 Score per residue for model 20

- Molecule 1: PHOSPHOLIPASE A2

Chain A: 36% 25% 20% 9% 10%



5 Refinement protocol and experimental data overview (i)

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 (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	1.52±0.01	13±1/895 (1.5± 0.1%)	2.17±0.04	55±3/1206 (4.6± 0.2%)
All	All	1.52	266/17900 (1.5%)	2.17	1103/24120 (4.6%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	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	81	GLU	CD-OE2	11.05	1.37	1.25	12	8
1	A	46	GLU	CD-OE1	10.98	1.37	1.25	9	10
1	A	40	GLU	CD-OE2	10.98	1.37	1.25	13	5
1	A	92	GLU	CD-OE1	10.97	1.37	1.25	3	10
1	A	71	GLU	CD-OE1	10.96	1.37	1.25	15	15
1	A	81	GLU	CD-OE1	10.95	1.37	1.25	15	12
1	A	92	GLU	CD-OE2	10.95	1.37	1.25	6	10
1	A	114	GLU	CD-OE1	10.95	1.37	1.25	19	7
1	A	114	GLU	CD-OE2	10.94	1.37	1.25	14	13
1	A	71	GLU	CD-OE2	10.93	1.37	1.25	11	5
1	A	40	GLU	CD-OE1	10.91	1.37	1.25	16	15
1	A	46	GLU	CD-OE2	10.91	1.37	1.25	8	10
1	A	124	CYS	C-OXT	7.80	1.38	1.23	17	20
1	A	39	ASP	CG-OD1	5.42	1.37	1.25	13	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	21	ASP	CG-OD1	5.42	1.37	1.25	1	7
1	A	54	ASP	CG-OD1	5.37	1.37	1.25	3	7
1	A	54	ASP	CG-OD2	5.36	1.37	1.25	12	13
1	A	119	ASP	CG-OD1	5.36	1.37	1.25	17	9
1	A	119	ASP	CG-OD2	5.35	1.37	1.25	14	11
1	A	21	ASP	CG-OD2	5.35	1.37	1.25	14	13
1	A	39	ASP	CG-OD2	5.33	1.37	1.25	14	14
1	A	99	ASP	CG-OD2	5.30	1.37	1.25	15	12
1	A	99	ASP	CG-OD1	5.30	1.37	1.25	9	6
1	A	49	ASP	CG-OD2	5.29	1.37	1.25	9	10
1	A	42	ASP	CG-OD1	5.25	1.37	1.25	7	8
1	A	42	ASP	CG-OD2	5.24	1.37	1.25	14	7
1	A	49	ASP	CG-OD1	5.21	1.37	1.25	1	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	28	TYR	CB-CG-CD2	-19.07	109.56	121.00	2	20
1	A	52	TYR	CB-CG-CD2	-17.30	110.62	121.00	3	19
1	A	28	TYR	CB-CG-CD1	16.10	130.66	121.00	2	15
1	A	52	TYR	CB-CG-CD1	13.98	129.38	121.00	3	19
1	A	119	ASP	N-CA-CB	-10.46	91.77	110.60	20	20
1	A	75	TYR	CB-CG-CD1	-9.69	115.19	121.00	18	18
1	A	3	TRP	CB-CG-CD1	-9.53	114.61	127.00	6	20
1	A	28	TYR	CA-CB-CG	9.04	130.57	113.40	2	19
1	A	99	ASP	CB-CG-OD1	-8.92	110.27	118.30	11	12
1	A	42	ASP	CB-CG-OD2	-8.47	110.68	118.30	6	18
1	A	3	TRP	CB-CG-CD2	8.41	137.54	126.60	13	18
1	A	42	ASP	CB-CG-OD1	-8.30	110.83	118.30	2	13
1	A	43	ARG	NE-CZ-NH1	8.29	124.44	120.30	7	20
1	A	25	TYR	CA-CB-CG	8.27	129.12	113.40	10	20
1	A	113	LYS	N-CA-CB	-8.12	95.99	110.60	8	8
1	A	6	ARG	NE-CZ-NH1	8.11	124.35	120.30	18	20
1	A	103	ALA	CB-CA-C	8.05	122.18	110.10	12	7
1	A	100	ARG	NE-CZ-NH1	7.89	124.25	120.30	1	20
1	A	25	TYR	CB-CG-CD2	-7.88	116.27	121.00	6	7
1	A	39	ASP	CB-CG-OD2	-7.82	111.27	118.30	5	15
1	A	36	THR	CA-CB-CG2	7.80	123.32	112.40	9	1
1	A	53	ARG	NE-CZ-NH1	7.59	124.10	120.30	4	20
1	A	54	ASP	CB-CG-OD2	-7.56	111.50	118.30	10	20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	73	TYR	CB-CG-CD1	-7.56	116.47	121.00	18	1
1	A	21	ASP	CB-CG-OD2	-7.50	111.55	118.30	15	19
1	A	105	CYS	N-CA-CB	-7.48	97.14	110.60	17	1
1	A	38	VAL	CG1-CB-CG2	-7.38	99.08	110.90	2	20
1	A	86	SER	N-CA-CB	-7.32	99.52	110.50	20	19
1	A	9	ILE	CA-CB-CG1	7.32	124.91	111.00	5	20
1	A	49	ASP	CB-CG-OD2	-7.27	111.75	118.30	13	20
1	A	25	TYR	CB-CG-CD1	-7.26	116.65	121.00	4	5
1	A	39	ASP	CB-CG-OD1	7.09	124.68	118.30	5	19
1	A	6	ARG	CA-CB-CG	7.08	128.99	113.40	18	1
1	A	115	HIS	CG-ND1-CE1	-7.05	96.53	105.70	16	20
1	A	119	ASP	CB-CG-OD2	-7.00	112.00	118.30	2	20
1	A	88	ASN	N-CA-CB	-7.00	98.01	110.60	17	13
1	A	84	CYS	N-CA-CB	-6.99	98.02	110.60	15	1
1	A	54	ASP	CB-CG-OD1	6.98	124.58	118.30	10	20
1	A	49	ASP	CB-CG-OD1	6.92	124.53	118.30	13	16
1	A	75	TYR	CB-CG-CD2	6.92	125.15	121.00	18	1
1	A	21	ASP	CB-CG-OD1	6.89	124.50	118.30	15	20
1	A	82	ILE	CA-CB-CG2	6.87	124.63	110.90	19	5
1	A	6	ARG	CG-CD-NE	6.84	126.17	111.80	18	1
1	A	22	PHE	CB-CG-CD1	6.82	125.57	120.80	4	6
1	A	102	ALA	N-CA-CB	-6.81	100.56	110.10	19	14
1	A	40	GLU	CA-CB-CG	6.80	128.37	113.40	3	1
1	A	94	PHE	CB-CG-CD2	-6.78	116.05	120.80	18	19
1	A	106	PHE	CB-CG-CD2	-6.76	116.07	120.80	8	11
1	A	99	ASP	CB-CG-OD2	-6.69	112.28	118.30	2	20
1	A	116	LYS	CB-CA-C	6.68	123.75	110.40	18	16
1	A	83	THR	CA-CB-CG2	6.67	121.74	112.40	1	18
1	A	119	ASP	CB-CG-OD1	-6.66	112.31	118.30	10	20
1	A	5	PHE	CB-CG-CD1	-6.61	116.17	120.80	8	9
1	A	116	LYS	N-CA-CB	-6.59	98.74	110.60	15	9
1	A	38	VAL	CB-CA-C	6.56	123.87	111.40	2	20
1	A	3	TRP	CD1-NE1-CE2	-6.54	103.12	109.00	17	20
1	A	118	LEU	CA-C-N	-6.44	103.03	117.20	20	19
1	A	78	SER	N-CA-C	6.26	127.91	111.00	2	11
1	A	22	PHE	CB-CG-CD2	-6.22	116.45	120.80	4	5
1	A	115	HIS	ND1-CE1-NE2	6.18	123.50	109.90	11	20
1	A	44	CYS	CA-CB-SG	-6.16	102.91	114.00	17	1
1	A	123	TYR	CB-CA-C	6.14	122.69	110.40	3	19
1	A	6	ARG	N-CA-CB	6.14	121.65	110.60	6	2
1	A	11	CYS	N-CA-CB	-6.12	99.58	110.60	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	72	SER	N-CA-CB	6.12	119.67	110.50	5	1
1	A	106	PHE	CB-CG-CD1	6.11	125.08	120.80	13	9
1	A	78	SER	N-CA-CB	-6.09	101.37	110.50	16	19
1	A	57	ASN	N-CA-CB	-6.00	99.79	110.60	7	9
1	A	99	ASP	N-CA-CB	-5.98	99.83	110.60	9	4
1	A	73	TYR	CB-CG-CD2	-5.96	117.43	121.00	10	2
1	A	109	ALA	N-CA-CB	5.93	118.40	110.10	15	7
1	A	95	ILE	CA-CB-CG1	5.91	122.22	111.00	14	11
1	A	122	LYS	N-CA-CB	-5.91	99.97	110.60	5	1
1	A	3	TRP	N-CA-CB	5.89	121.21	110.60	20	5
1	A	22	PHE	CA-CB-CG	5.87	127.99	113.90	9	5
1	A	41	LEU	CB-CG-CD1	5.76	120.80	111.00	19	7
1	A	48	HIS	CG-ND1-CE1	-5.72	98.26	105.70	9	20
1	A	24	ASN	N-CA-CB	5.70	120.86	110.60	2	2
1	A	111	TYR	CA-CB-CG	5.63	124.10	113.40	12	3
1	A	13	ILE	CB-CA-C	5.61	122.82	111.60	10	9
1	A	38	VAL	CA-CB-CG1	5.60	119.30	110.90	13	3
1	A	82	ILE	CA-CB-CG1	5.58	121.61	111.00	8	1
1	A	38	VAL	CA-CB-CG2	5.52	119.18	110.90	10	5
1	A	3	TRP	N-CA-C	5.48	125.80	111.00	9	1
1	A	18	PRO	N-CA-C	5.46	126.29	112.10	9	8
1	A	18	PRO	N-CA-CB	-5.43	96.63	102.60	9	5
1	A	9	ILE	N-CA-CB	-5.42	98.33	110.80	9	1
1	A	106	PHE	CB-CA-C	5.41	121.22	110.40	11	8
1	A	17	HIS	CG-ND1-CE1	-5.37	98.72	105.70	1	20
1	A	3	TRP	NE1-CE2-CZ2	-5.37	124.50	130.40	10	2
1	A	38	VAL	N-CA-CB	-5.36	99.70	111.50	4	4
1	A	118	LEU	C-N-CA	5.36	135.10	121.70	18	11
1	A	120	THR	N-CA-C	5.34	125.43	111.00	11	5
1	A	118	LEU	CB-CA-C	5.34	120.34	110.20	18	11
1	A	41	LEU	CB-CG-CD2	5.34	120.07	111.00	20	1
1	A	41	LEU	CB-CA-C	5.29	120.25	110.20	19	11
1	A	117	ASN	CB-CA-C	5.27	120.94	110.40	12	1
1	A	41	LEU	N-CA-C	5.26	125.21	111.00	13	1
1	A	83	THR	CB-CA-C	5.20	125.64	111.60	13	1
1	A	25	TYR	N-CA-CB	5.18	119.92	110.60	2	1
1	A	85	ASN	CB-CA-C	5.17	120.74	110.40	9	1
1	A	5	PHE	CB-CA-C	5.17	120.74	110.40	14	1
1	A	28	TYR	CB-CA-C	5.17	120.73	110.40	15	3
1	A	84	CYS	CA-CB-SG	-5.12	104.79	114.00	19	2
1	A	112	ASN	N-CA-CB	5.11	119.80	110.60	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	88	ASN	CB-CA-C	5.09	120.58	110.40	15	1
1	A	48	HIS	CB-CA-C	5.08	120.56	110.40	12	1
1	A	6	ARG	NE-CZ-NH2	-5.01	117.80	120.30	15	2
1	A	4	GLN	CB-CA-C	5.00	120.41	110.40	1	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	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
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

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Mol	Chain	Res	Type	Group	Models (Total)
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	876	0	798	19±3
All	All	17540	0	15960	380

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 11.

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: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	11
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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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	7
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
1:A:11:CYS:SG	1:A:75:TYR:OH	0.48	2.66	3	3
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: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: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: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: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:118:LEU:CD1	1:A:119:ASP:H	0.42	2.27	5	1
1:A:26:GLY:C	1:A:118:LEU:HD12	0.42	2.34	2	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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: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 (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	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

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Mol	Chain	Res	Type	Models (Total)
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
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±2 (80±2%)	20±2 (20±2%)	4 34
All	All	1980/2200 (90%)	1586 (80%)	394 (20%)	4 34

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	43	ARG	20
1	A	9	ILE	19
1	A	115	HIS	19
1	A	121	LYS	19
1	A	106	PHE	18
1	A	112	ASN	16
1	A	77	CYS	15
1	A	124	CYS	15
1	A	79	ASN	14
1	A	95	ILE	14
1	A	122	LYS	14
1	A	56	LYS	11
1	A	113	LYS	11
1	A	48	HIS	9
1	A	42	ASP	9
1	A	10	LYS	8
1	A	6	ARG	7
1	A	114	GLU	7
1	A	2	LEU	6
1	A	99	ASP	6
1	A	8	MET	5
1	A	80	THR	4
1	A	88	ASN	4
1	A	101	ASN	4
1	A	4	GLN	3
1	A	40	GLU	3
1	A	49	ASP	3
1	A	100	ARG	3
1	A	70	THR	3
1	A	97	ASN	3
1	A	118	LEU	3
1	A	11	CYS	2
1	A	91	CYS	2
1	A	13	ILE	2
1	A	81	GLU	2
1	A	111	TYR	2
1	A	16	SER	1
1	A	39	ASP	1
1	A	28	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	ARG	1
1	A	82	ILE	1
1	A	17	HIS	1
1	A	73	TYR	1
1	A	84	CYS	1
1	A	46	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

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 (i)

No chemical shift data were provided