WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 04:42 PM BST

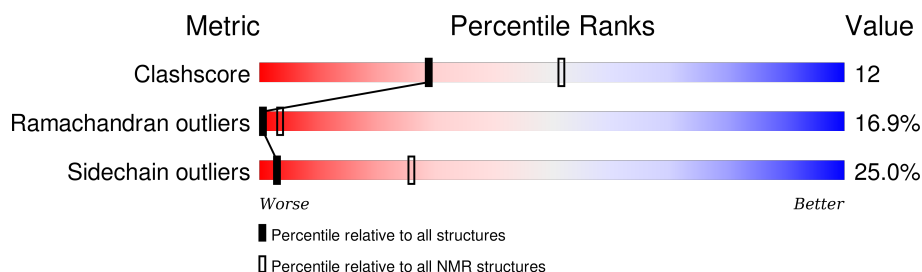|		
PDB ID	:	1SFW
Title	:	PORCINE PANCREAS PHOSPHOLIPASE A2, NMR, 18 STRUCTURES
Authors	:	Van Den Berg, B.; Tessari, M.; Boelens, R.; Dijkman, R.; Kaptein, R.; De Haas, G.H.; Verheij, H.M.
Deposited on	:	1996-02-23

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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		16.9%
Sidechain outliers		25.0%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	21%　46%　23%　5%　6%

Full wwPDB NMR Structure Validation Report

2 Ensemble composition and analysis ⓘ

This entry contains 18 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:61, A:69-A:124 (117)	0.54	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

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

- Molecule 1 is a protein called PHOSPHOLIPASE A2.

Mol	Chain	Residues	Atoms					Trace
			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 and DNA 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
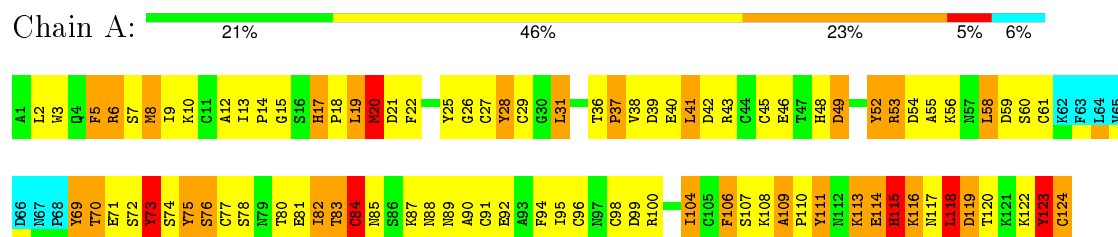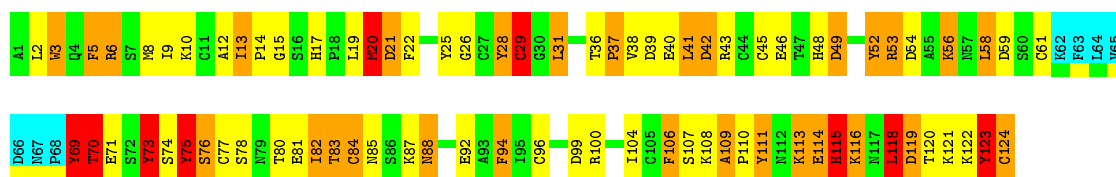
4.2.3 Score per residue for model 3

• Molecule 1: PHOSPHOLIPASE A2

4.2.4 Score per residue for model 4

• Molecule 1: PHOSPHOLIPASE A2
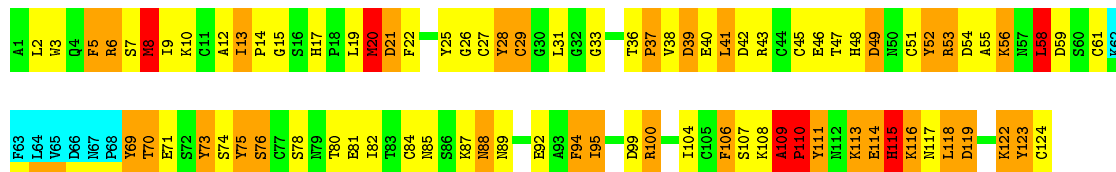
4.2.5 Score per residue for model 5

• Molecule 1: PHOSPHOLIPASE A2
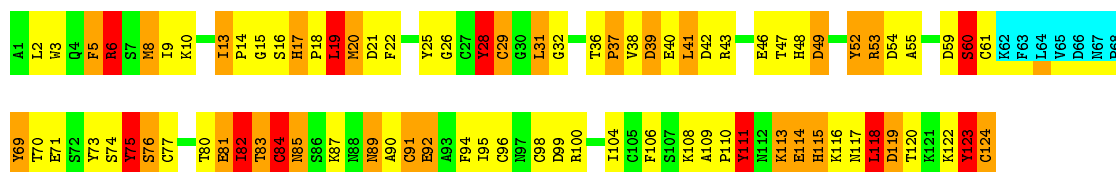
4.2.6 Score per residue for model 6

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
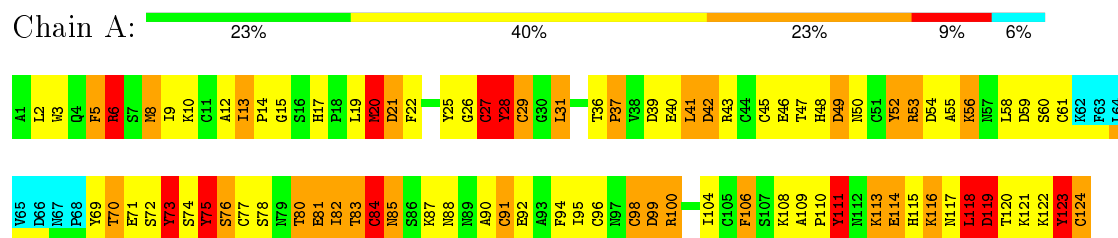
4.2.7 Score per residue for model 7

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
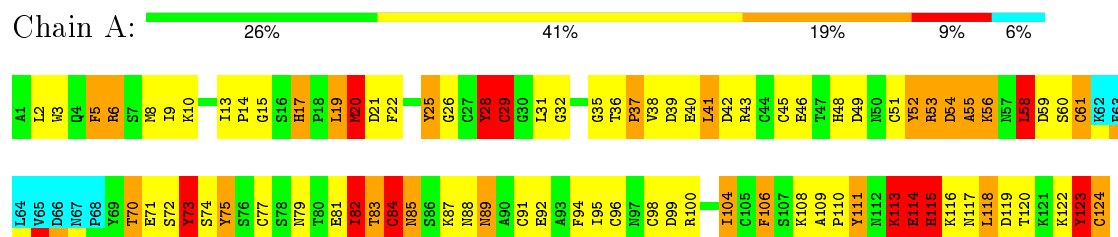
4.2.8 Score per residue for model 8

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
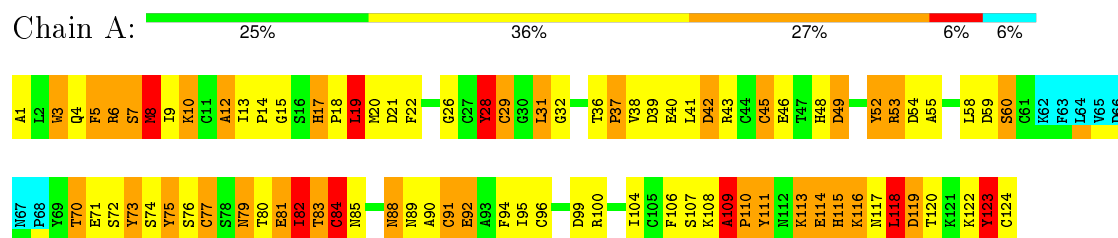
4.2.9 Score per residue for model 9

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
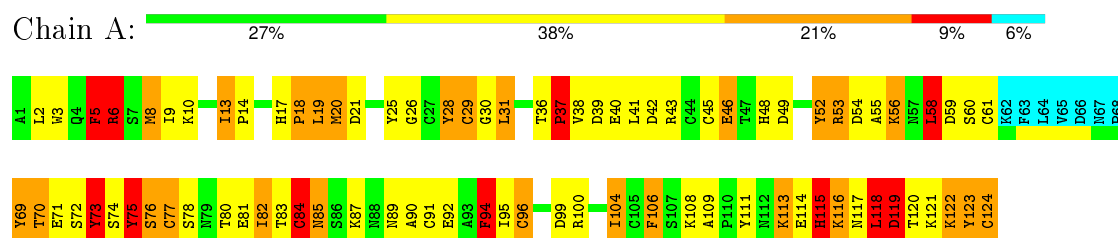
4.2.10 Score per residue for model 10

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
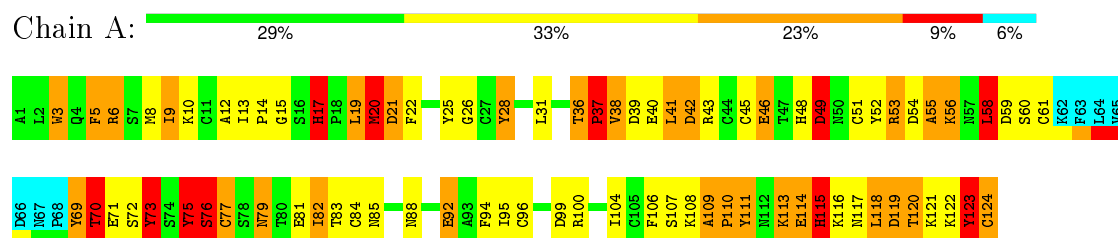
4.2.11 Score per residue for model 11

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
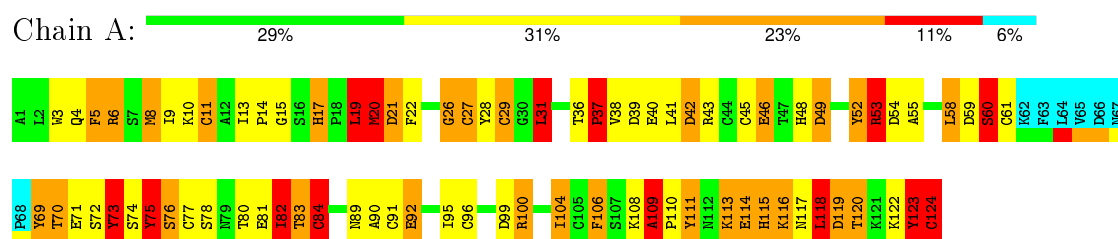
4.2.12 Score per residue for model 12

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
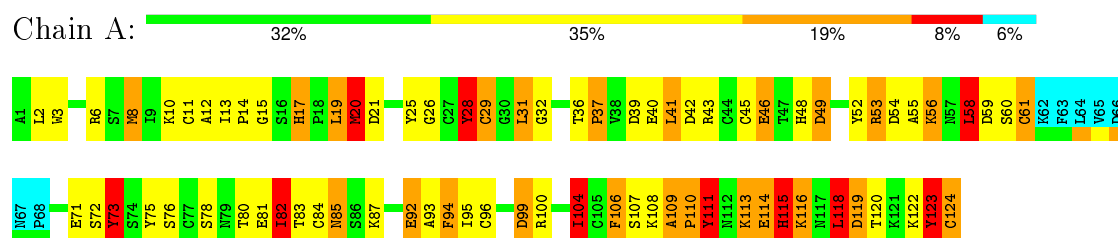
4.2.13 Score per residue for model 13

• Molecule 1: PHOSPHOLIPASE A2

Chain A:
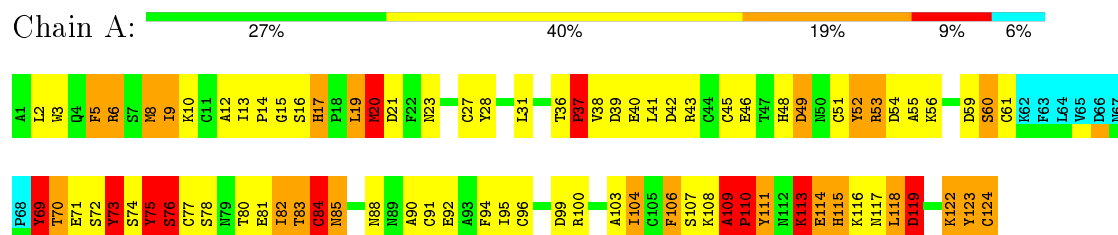
4.2.14 Score per residue for model 14

● Molecule 1: PHOSPHOLIPASE A2

Chain A:
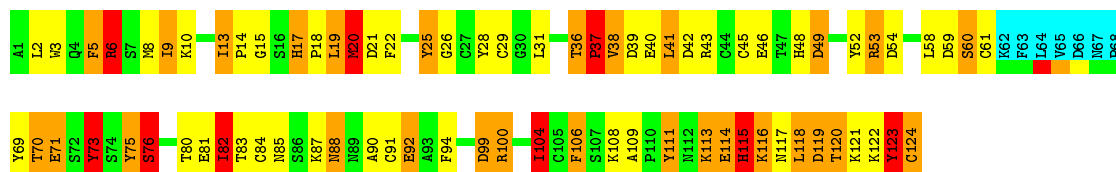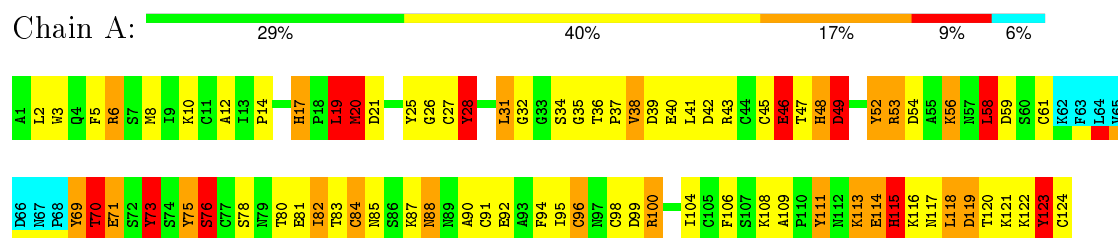

4.2.15 Score per residue for model 15

● Molecule 1: PHOSPHOLIPASE A2

Chain A:
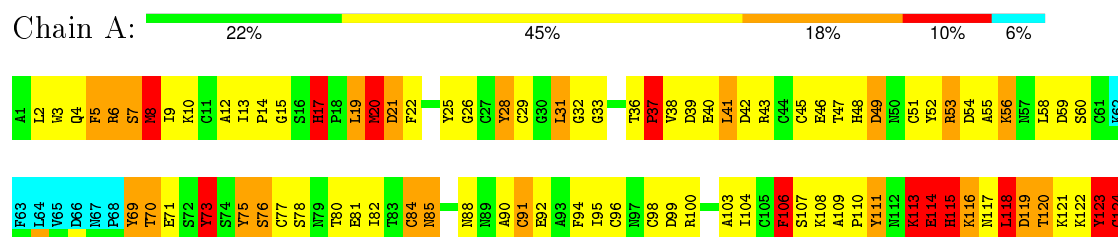
4.2.16 Score per residue for model 16

● Molecule 1: PHOSPHOLIPASE A2

Chain A:
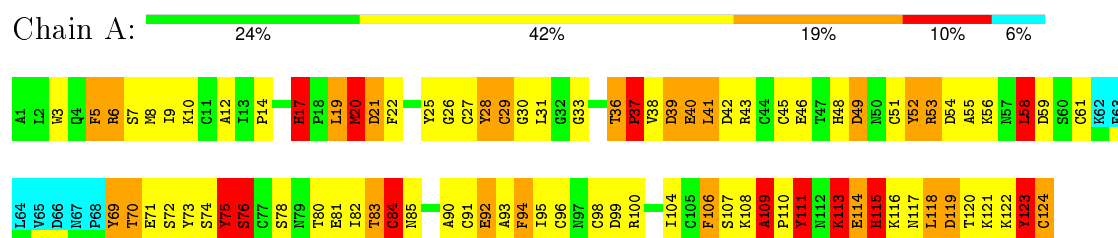
4.2.17 Score per residue for model 17

● Molecule 1: PHOSPHOLIPASE A2

Chain A:
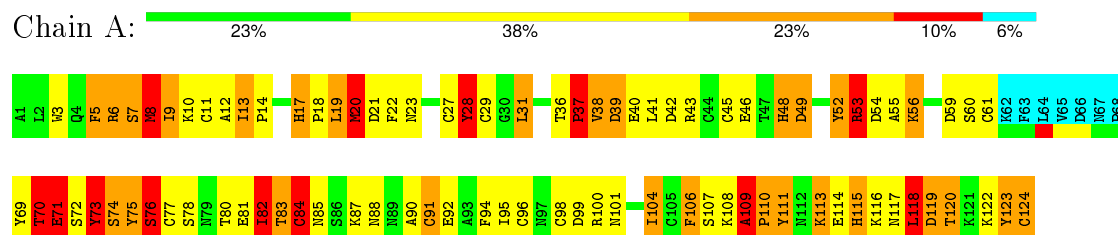
4.2.18 Score per residue for model 18

● Molecule 1: PHOSPHOLIPASE A2

Chain A:
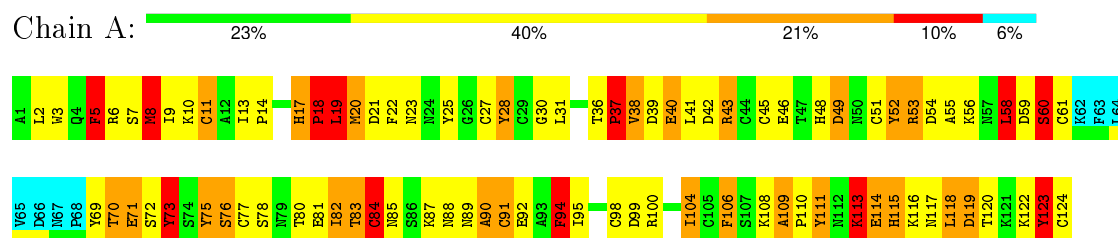
5 Refinement protocol and experimental data overview (i)

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

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

Software name	Classification	Version
DISCOVER	refinement	

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

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.48±0.02	15±1/933 (1.6±0.1%)	2.27±0.03	59±4/1258 (4.7±0.3%)
All	All	1.48	274/16794 (1.6%)	2.27	1063/22644 (4.7%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	15.4±2.2
All	All	0	277

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	GLU	CD-OE1	11.12	1.37	1.25	7	2
1	A	71	GLU	CD-OE1	11.09	1.37	1.25	2	9
1	A	71	GLU	CD-OE2	11.02	1.37	1.25	5	9
1	A	40	GLU	CD-OE2	10.98	1.37	1.25	16	15
1	A	81	GLU	CD-OE2	10.97	1.37	1.25	1	2
1	A	46	GLU	CD-OE1	10.96	1.37	1.25	11	7
1	A	81	GLU	CD-OE1	10.95	1.37	1.25	15	16
1	A	114	GLU	CD-OE2	10.94	1.37	1.25	5	11
1	A	40	GLU	CD-OE1	10.94	1.37	1.25	12	3
1	A	46	GLU	CD-OE2	10.90	1.37	1.25	9	11
1	A	92	GLU	CD-OE2	10.89	1.37	1.25	9	16
1	A	114	GLU	CD-OE1	10.89	1.37	1.25	10	7
1	A	124	CYS	C-OXT	7.70	1.38	1.23	4	18
1	A	123	TYR	CB-CG	5.87	1.60	1.51	2	6

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

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

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

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

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

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

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

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	14	PRO	Peptide	18
1	A	113	LYS	Peptide	18
1	A	75	TYR	Sidechain,Peptide	17
1	A	20	MET	Peptide	17
1	A	115	HIS	Sidechain	17
1	A	52	TYR	Sidechain	15
1	A	73	TYR	Sidechain	14
1	A	69	TYR	Sidechain,Peptide	14
1	A	123	TYR	Sidechain	14
1	A	111	TYR	Sidechain	13
1	A	88	ASN	Peptide	12
1	A	25	TYR	Sidechain	12
1	A	76	SER	Peptide	10
1	A	22	PHE	Sidechain	10
1	A	28	TYR	Sidechain,Peptide	10
1	A	31	LEU	Peptide	9
1	A	118	LEU	Peptide	6
1	A	7	SER	Peptide	5

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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

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

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

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

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

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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
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:19:LEU:HD21	1:A:31:LEU:H	0.40	1.75	11	1
1:A:8:MET:CE	1:A:73:TYR:CE1	0.40	3.04	6	1
1:A:5:PHE:CD2	1:A:9:ILE:CD1	0.40	3.05	3	1
1:A:8:MET:HE3	1:A:73:TYR:CE1	0.40	2.52	15	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	115/124 (93%)	67±3 (58±3%)	29±3 (25±2%)	19±3 (17±2%)	0	3
All	All	2070/2232 (93%)	1204 (58%)	516 (25%)	350 (17%)	0	3

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

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

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

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR

entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/110 (94%)	77±3 (75±3%)	26±3 (25±3%)	3	26
All	All	1854/1980 (94%)	1391 (75%)	463 (25%)	3	26

All 66 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

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

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

6.3.3   RNA (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 carbohydrates in this entry.

6.6 Ligand geometry (i)

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

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided