Full wwPDB NMR Structure Validation Report (i)

Jun 11, 2024 – 11:41 PM EDT

PDB ID	:	2ABD
Title	:	THE THREE-DIMENSIONAL STRUCTURE OF ACYL-COENZYME A BINDING PROTEIN FROM BOVINE LIVER. STRUCTURAL REFINEMENT USING HETERONUCLEAR MULTIDIMENSIONAL NMR SPECTROSCOPY
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Deposited on	:	1993-03-05

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

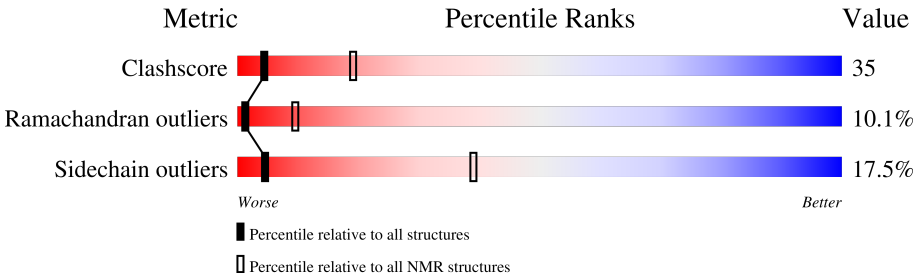
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	86	20% 55% 13% 13%

2 Ensemble composition and analysis (i)

This entry contains 29 models. Model 10 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:4-A:43, A:52-A:86 (75)	0.61	10

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	2, 4, 8, 10, 16, 17, 18, 20, 23, 25, 26, 27
2	1, 3, 5, 6, 7, 11, 12, 15, 21, 28, 29
3	9, 13, 14, 19, 22, 24

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1391 atoms, of which 693 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ACYL-COENZYME A BINDING PROTEIN.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1391	445	693	114	136	3	0

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: ACYL-COENZYME A BINDING PROTEIN

Chain A: 20% 55% 13% 13%

S1 Q2 A3 E4 F5 D6 K7 V12 K13 H14 L15 K16 T17 K18 P19 A20 D21 E22 E23 M24 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 D38 I39 N40 T41 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 W58 N59 E60 L61 K62 G63 T64 S65

K66 E67 D68 A69 M70 K71 A72 Y73 I74 D75 K76 V77 E78 E79 L80 K81 K82 K83 Y84 G85 I86

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: ACYL-COENZYME A BINDING PROTEIN

Chain A: 27% 36% 22% • 13%

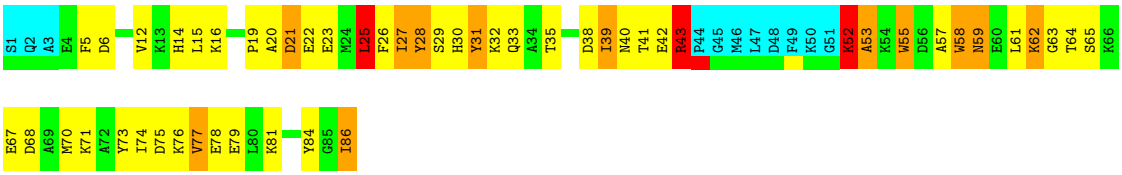
S1 Q2 A3 E4 F5 D6 K7 E10 E11 V12 K13 H14 L15 K16 D21 E22 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 D38 I39 N40 T41 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 D56 A57 W58 N59 E60 L61 K62 G63 T64 S65 K66

E67 M70 Y73 I74 D75 K76 V77 E78 E79 L80 K81 K82 K83 Y84 G85 I86

4.2.2 Score per residue for model 2

• Molecule 1: ACYL-COENZYME A BINDING PROTEIN

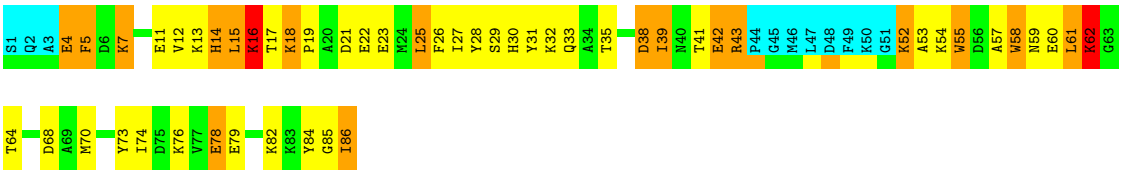
Chain A: 27% 43% 14% • 13%



4.2.3 Score per residue for model 3

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

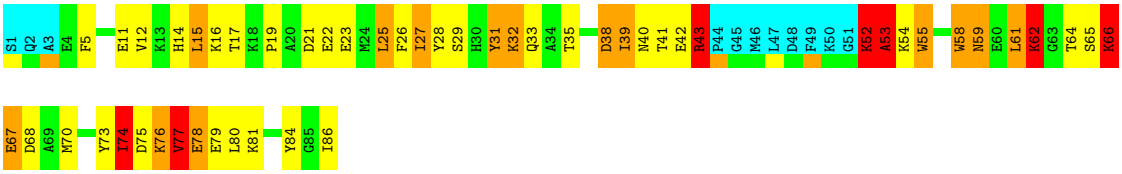
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

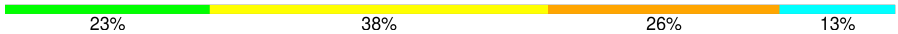
Chain A:

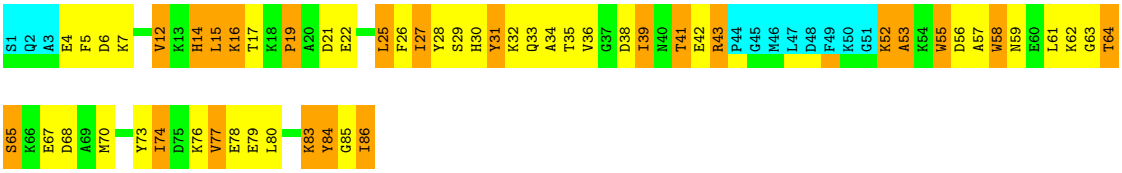


4.2.5 Score per residue for model 5

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A:





4.2.6 Score per residue for model 6

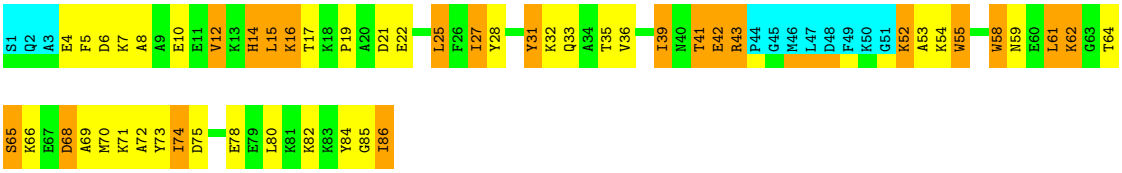
- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 24% 37% 21% 5% 13%

4.2.7 Score per residue for model 7

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

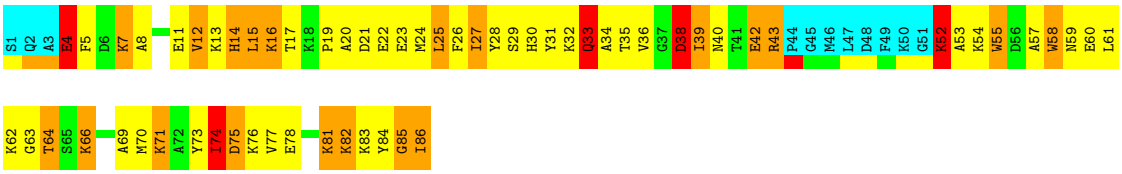
Chain A: 28% 36% 23% 13%



4.2.8 Score per residue for model 8

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

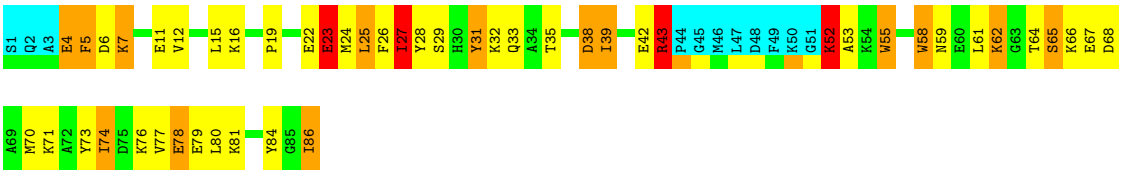
Chain A: 15% 43% 23% 6% 13%



4.2.9 Score per residue for model 9

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 30% 36% 16% 5% 13%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 31% 35% 19% • 13%

S1 Q2 A3 E4 F5 D6 K7 A8 A9 V12 K13 H14 L15 K16 P19 A20 D21 M24 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 D38 I39 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 W58 N59 E60 L61 K62 G63 T64 D68

A69 M70 K71 A72 Y73 I74 D75 K76 L80 K81 K82 K83 Y84 G85 I86

4.2.11 Score per residue for model 11

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 16% 45% 22% • 13%

S1 Q2 A3 E4 F5 D6 K7 A8 A9 E10 E11 V12 K13 H14 L15 K16 P19 A20 D21 E22 E23 M24 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 V36 G37 D38 I39 M40 T41 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 W58 L61 K62 G63

T64 S65 K66 E67 D68 A69 M70 K71 A72 Y73 I74 D75 K76 V77 E78 E79 L80 K81 Y84 G85 I86

4.2.12 Score per residue for model 12

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 33% 31% 20% • 13%

S1 Q2 A3 E4 F5 D6 K7 A8 V12 K13 H14 L15 K16 P19 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 V36 G37 D38 I39 M40 T41 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 W58 N59 E60 L61 K62 G63 T64 E67 D68 A69

M70 K71 A72 Y73 I74 D75 K76 V77 E78 E79 L80 K81 K82 K83 Y84 G85 I86

4.2.13 Score per residue for model 13

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 31% 40% 15% • 13%

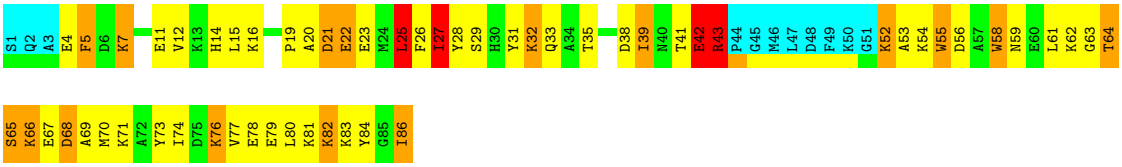
S1 Q2 A3 E4 F5 D6 K7 E11 V12 K13 H14 L15 K16 P19 A20 D21 L25 F26 I27 Y28 S29 H30 Y31 K32 Q33 A34 T35 V36 I39 M40 T41 E42 R43 P44 G45 M46 L47 D48 F49 K50 G51 K52 A53 K54 W55 W58 N59 E60 L61 K62 G63 T64 E67

M70 K71 A72 Y73 I74 D75 K76 V77 E78 K81 K82 K83 Y84 G85 I86

4.2.14 Score per residue for model 14

• Molecule 1: ACYL-COENZYME A BINDING PROTEIN

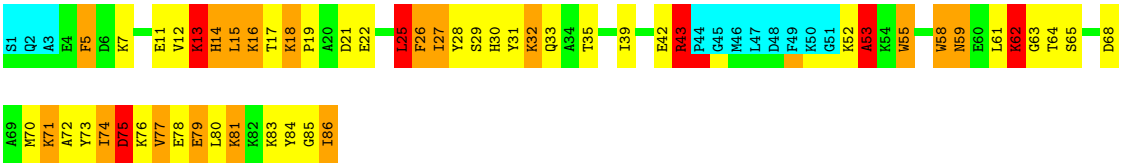
Chain A: 21% 43% 19% 5% 13%



4.2.15 Score per residue for model 15

• Molecule 1: ACYL-COENZYME A BINDING PROTEIN

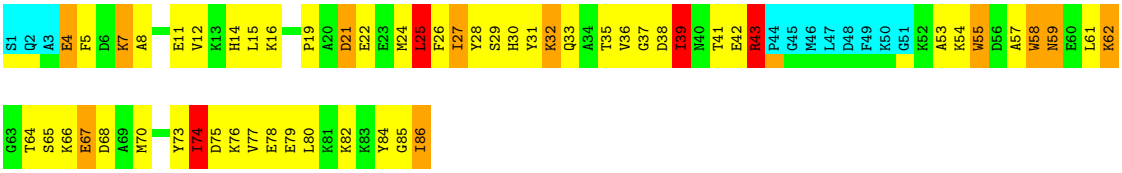
Chain A: 26% 35% 20% 7% 13%



4.2.16 Score per residue for model 16

• Molecule 1: ACYL-COENZYME A BINDING PROTEIN

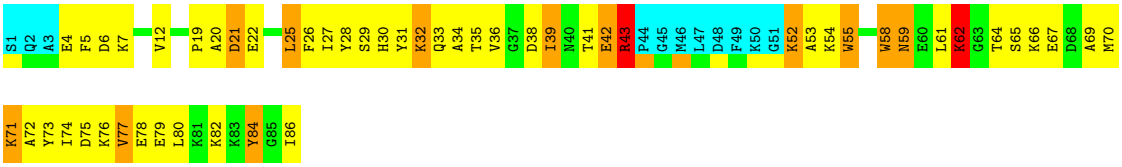
Chain A: 22% 48% 13% 5% 13%



4.2.17 Score per residue for model 17

• Molecule 1: ACYL-COENZYME A BINDING PROTEIN

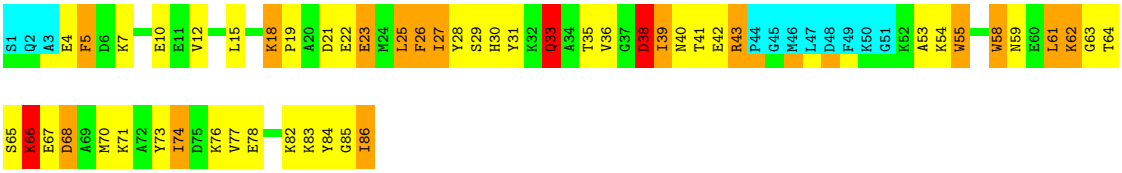
Chain A: 26% 45% 14% • 13%



4.2.18 Score per residue for model 18

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

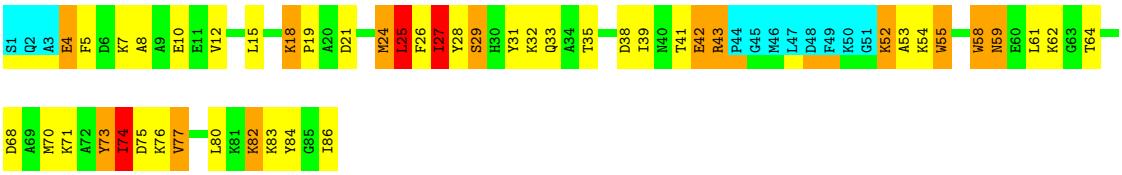
Chain A: 27% 40% 17% • 13%



4.2.19 Score per residue for model 19

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

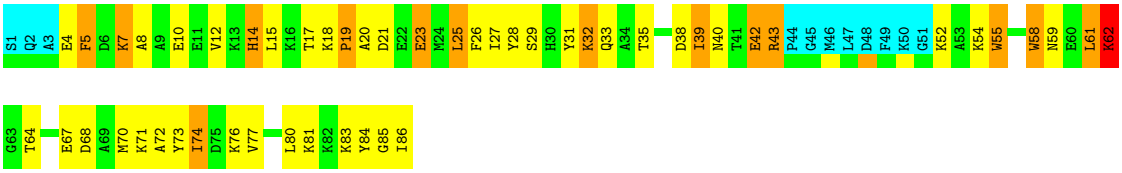
Chain A: 33% 36% 15% • 13%



4.2.20 Score per residue for model 20

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 28% 42% 16% • 13%



4.2.21 Score per residue for model 21

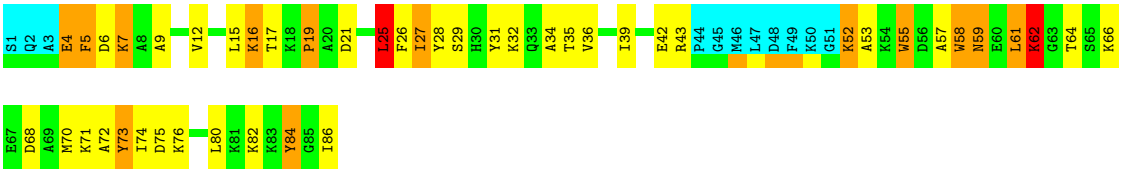
- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 24% 40% 20% • 13%

4.2.22 Score per residue for model 22

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

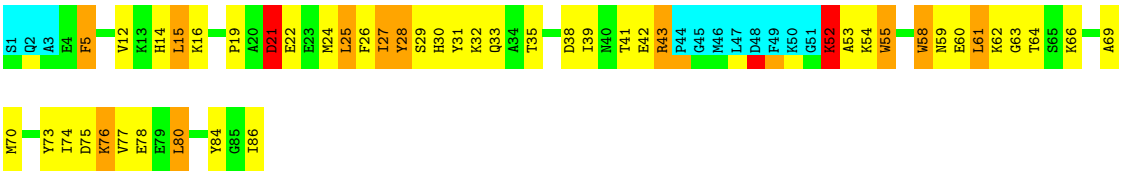
Chain A: 34% 36% 15% • 13%



4.2.23 Score per residue for model 23

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

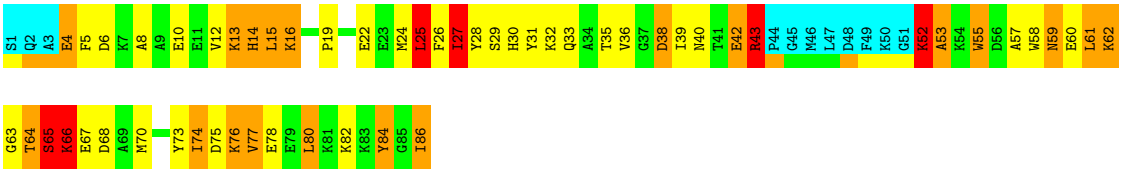
Chain A: 33% 40% 13% • 13%



4.2.24 Score per residue for model 24

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

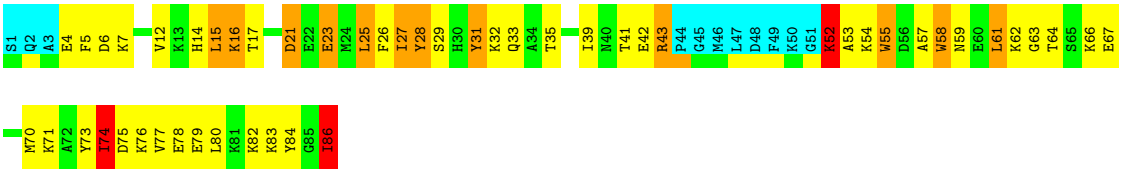
Chain A: 23% 35% 22% 7% 13%



4.2.25 Score per residue for model 25

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

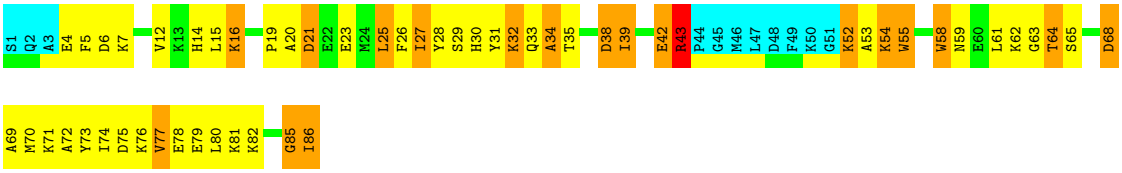
Chain A: 28% 42% 14% • 13%



4.2.26 Score per residue for model 26

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

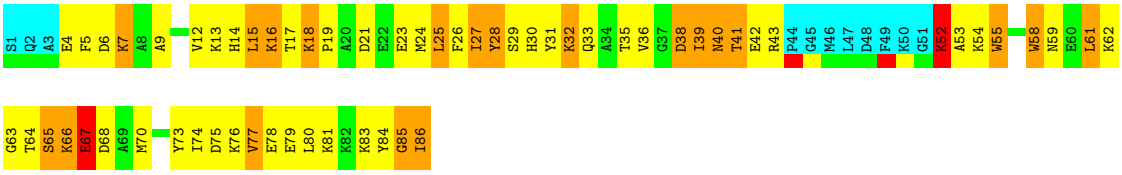
Chain A: 23% 42% 21% • 13%



4.2.27 Score per residue for model 27

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 16% 45% 23% • 13%



4.2.28 Score per residue for model 28

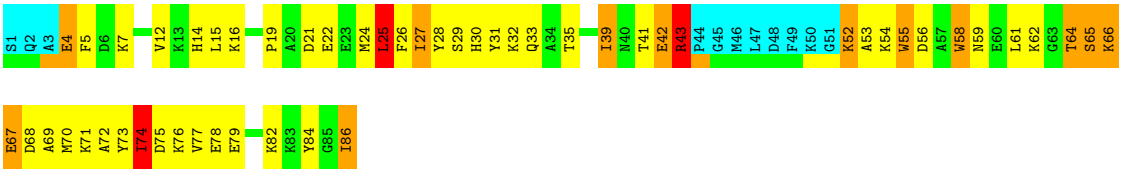
- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 24% 38% 20% 5% 13%

4.2.29 Score per residue for model 29

- Molecule 1: ACYL-COENZYME A BINDING PROTEIN

Chain A: 26% 44% 14% • 13%



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 29 were deposited, based on the following criterion: *?*.

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

Software name	Classification	Version
DIANA	refinement	2.0
X-PLOR	refinement	3.0

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	1.51±0.02	3±1/631 (0.4± 0.1%)	2.02±0.05	21±3/843 (2.4± 0.3%)
All	All	1.51	78/18299 (0.4%)	2.03	595/24447 (2.4%)

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	0.9±0.3
All	All	0	27

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	55	TRP	CG-CD2	-6.89	1.31	1.43	14	12
1	A	4	GLU	CB-CG	6.70	1.64	1.52	27	2
1	A	43	ARG	CZ-NH2	-6.39	1.24	1.33	17	5
1	A	55	TRP	NE1-CE2	-6.29	1.29	1.37	10	24
1	A	58	TRP	CG-CD2	-5.97	1.33	1.43	15	27
1	A	23	GLU	CB-CG	5.58	1.62	1.52	28	3
1	A	14	HIS	CG-ND1	-5.42	1.26	1.38	12	1
1	A	43	ARG	CZ-NH1	-5.21	1.26	1.33	15	1
1	A	58	TRP	NE1-CE2	-5.13	1.30	1.37	21	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	43	ARG	NE-CZ-NH2	-19.35	110.63	120.30	24	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	53	ALA	N-CA-CB	-12.04	93.25	110.10	6	10
1	A	58	TRP	CD1-NE1-CE2	10.73	118.66	109.00	29	29
1	A	55	TRP	CD1-NE1-CE2	10.65	118.58	109.00	12	29
1	A	55	TRP	CA-CB-CG	-9.64	95.38	113.70	14	28
1	A	58	TRP	NE1-CE2-CZ2	9.59	140.94	130.40	27	27
1	A	58	TRP	CG-CD1-NE1	-9.22	100.88	110.10	4	29
1	A	55	TRP	NE1-CE2-CZ2	9.14	140.45	130.40	14	3
1	A	68	ASP	CB-CG-OD2	-8.79	110.39	118.30	21	13
1	A	55	TRP	CG-CD1-NE1	-8.68	101.42	110.10	12	29
1	A	21	ASP	CB-CG-OD2	-8.48	110.67	118.30	23	5
1	A	38	ASP	CB-CG-OD2	-8.08	111.02	118.30	27	15
1	A	56	ASP	CB-CG-OD2	-8.00	111.10	118.30	14	1
1	A	67	GLU	OE1-CD-OE2	7.94	132.83	123.30	2	1
1	A	84	TYR	CB-CG-CD1	-7.93	116.24	121.00	6	5
1	A	33	GLN	N-CA-CB	-7.93	96.33	110.60	8	4
1	A	82	LYS	N-CA-CB	-7.78	96.60	110.60	1	2
1	A	58	TRP	CG-CD2-CE3	-7.72	126.96	133.90	11	23
1	A	52	LYS	N-CA-CB	-7.56	96.99	110.60	29	6
1	A	43	ARG	NH1-CZ-NH2	7.49	127.64	119.40	23	10
1	A	43	ARG	NE-CZ-NH1	7.45	124.03	120.30	17	3
1	A	6	ASP	CB-CA-C	7.42	125.24	110.40	5	11
1	A	14	HIS	N-CA-CB	-7.38	97.31	110.60	12	1
1	A	14	HIS	CB-CA-C	-7.32	95.75	110.40	23	16
1	A	58	TRP	NE1-CE2-CD2	-7.20	100.10	107.30	11	25
1	A	74	ILE	CB-CA-C	-7.20	97.20	111.60	11	23
1	A	61	LEU	CB-CG-CD1	-7.02	99.06	111.00	27	15
1	A	75	ASP	CB-CG-OD2	-6.88	112.11	118.30	7	7
1	A	28	TYR	CB-CG-CD1	-6.87	116.88	121.00	2	5
1	A	58	TRP	CE2-CD2-CG	6.69	112.65	107.30	11	8
1	A	25	LEU	CB-CG-CD1	-6.55	99.87	111.00	11	9
1	A	4	GLU	OE1-CD-OE2	6.55	131.16	123.30	21	3
1	A	21	ASP	CB-CG-OD1	-6.51	112.44	118.30	28	1
1	A	55	TRP	CD1-CG-CD2	6.43	111.44	106.30	14	8
1	A	32	LYS	CB-CA-C	6.40	123.20	110.40	20	11
1	A	55	TRP	NE1-CE2-CD2	-6.39	100.91	107.30	17	9
1	A	38	ASP	N-CA-CB	-6.33	99.21	110.60	27	10
1	A	5	PHE	N-CA-CB	-6.33	99.21	110.60	22	10
1	A	59	ASN	N-CA-CB	-6.27	99.31	110.60	19	4
1	A	10	GLU	OE1-CD-OE2	6.26	130.81	123.30	21	1
1	A	42	GLU	N-CA-C	6.25	127.87	111.00	14	1
1	A	84	TYR	CB-CG-CD2	6.23	124.74	121.00	22	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	ALA	N-CA-CB	-6.22	101.39	110.10	17	3
1	A	80	LEU	CB-CG-CD1	-6.17	100.50	111.00	12	15
1	A	73	TYR	CB-CG-CD1	-6.14	117.32	121.00	19	2
1	A	68	ASP	CB-CA-C	6.05	122.51	110.40	10	3
1	A	4	GLU	CB-CA-C	5.97	122.33	110.40	19	2
1	A	31	TYR	CB-CG-CD2	-5.95	117.43	121.00	25	7
1	A	41	THR	OG1-CB-CG2	-5.92	96.38	110.00	14	7
1	A	31	TYR	CB-CG-CD1	-5.91	117.45	121.00	7	3
1	A	68	ASP	CB-CG-OD1	-5.89	112.99	118.30	14	4
1	A	81	LYS	N-CA-CB	-5.88	100.03	110.60	10	3
1	A	43	ARG	N-CA-CB	-5.86	100.06	110.60	10	1
1	A	52	LYS	CB-CA-C	5.78	121.95	110.40	4	1
1	A	25	LEU	CB-CG-CD2	5.75	120.78	111.00	9	5
1	A	67	GLU	N-CA-CB	-5.74	100.27	110.60	29	2
1	A	23	GLU	OE1-CD-OE2	5.72	130.17	123.30	9	4
1	A	39	ILE	CA-CB-CG1	-5.71	100.16	111.00	16	1
1	A	17	THR	OG1-CB-CG2	-5.66	96.97	110.00	20	1
1	A	62	LYS	CB-CA-C	5.66	121.71	110.40	15	2
1	A	42	GLU	OE1-CD-OE2	5.63	130.06	123.30	6	2
1	A	60	GLU	N-CA-CB	-5.63	100.46	110.60	23	1
1	A	6	ASP	CB-CG-OD2	-5.63	113.23	118.30	2	2
1	A	26	PHE	CB-CG-CD2	-5.60	116.88	120.80	15	2
1	A	23	GLU	CB-CA-C	5.58	121.57	110.40	28	2
1	A	20	ALA	CB-CA-C	-5.57	101.75	110.10	2	1
1	A	41	THR	N-CA-C	-5.56	95.99	111.00	11	2
1	A	5	PHE	N-CA-C	-5.55	96.02	111.00	28	1
1	A	75	ASP	CB-CA-C	5.55	121.50	110.40	11	1
1	A	11	GLU	OE1-CD-OE2	5.54	129.95	123.30	3	2
1	A	18	LYS	N-CA-CB	-5.54	100.63	110.60	28	1
1	A	55	TRP	CG-CD2-CE3	-5.53	128.92	133.90	14	1
1	A	66	LYS	N-CA-CB	-5.51	100.68	110.60	27	1
1	A	83	LYS	N-CA-CB	-5.46	100.77	110.60	1	3
1	A	42	GLU	CB-CA-C	-5.38	99.63	110.40	24	1
1	A	61	LEU	CB-CA-C	-5.34	100.06	110.20	23	1
1	A	55	TRP	CB-CG-CD1	-5.33	120.06	127.00	9	5
1	A	68	ASP	CA-CB-CG	-5.31	101.73	113.40	10	2
1	A	72	ALA	N-CA-CB	-5.30	102.68	110.10	11	1
1	A	26	PHE	CA-CB-CG	-5.29	101.21	113.90	18	1
1	A	62	LYS	CA-C-N	-5.23	105.75	116.20	17	2
1	A	86	ILE	CA-CB-CG1	-5.19	101.13	111.00	18	1
1	A	33	GLN	CB-CA-C	5.16	120.73	110.40	18	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	43	ARG	CG-CD-NE	-5.16	100.95	111.80	24	1
1	A	79	GLU	OE1-CD-OE2	5.14	129.47	123.30	26	1
1	A	39	ILE	CB-CA-C	5.14	121.88	111.60	6	2
1	A	15	LEU	CB-CG-CD1	-5.12	102.29	111.00	21	1
1	A	84	TYR	N-CA-CB	-5.11	101.41	110.60	11	2
1	A	32	LYS	N-CA-CB	-5.10	101.42	110.60	16	1
1	A	29	SER	N-CA-CB	-5.10	102.86	110.50	19	1
1	A	86	ILE	N-CA-C	-5.10	97.24	111.00	25	1
1	A	84	TYR	CA-CB-CG	-5.08	103.75	113.40	5	1
1	A	7	LYS	CA-CB-CG	-5.06	102.26	113.40	16	1
1	A	74	ILE	CA-CB-CG1	5.05	120.59	111.00	21	1
1	A	24	MET	CB-CA-C	5.03	120.45	110.40	24	1
1	A	53	ALA	N-CA-C	-5.02	97.44	111.00	5	1
1	A	65	SER	CA-CB-OG	-5.01	97.67	111.20	5	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	43	ARG	Sidechain	27

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	619	614	614	43±7
All	All	17951	17806	17806	1252

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 35.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:N	1:A:74:ILE:HD13	0.77	1.94	13	5
1:A:42:GLU:O	1:A:55:TRP:CD1	0.71	2.43	8	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:TYR:CE2	1:A:35:THR:HG21	0.71	2.20	13	23
1:A:5:PHE:CD1	1:A:70:MET:HA	0.71	2.21	28	21
1:A:5:PHE:HA	1:A:74:ILE:CD1	0.69	2.18	13	5
1:A:31:TYR:HB2	1:A:73:TYR:CE1	0.69	2.22	12	23
1:A:5:PHE:CZ	1:A:31:TYR:CD1	0.68	2.82	10	28
1:A:66:LYS:NZ	1:A:70:MET:SD	0.67	2.68	8	3
1:A:42:GLU:C	1:A:55:TRP:CD1	0.66	2.69	10	21
1:A:5:PHE:CZ	1:A:31:TYR:CD2	0.64	2.85	26	1
1:A:15:LEU:O	1:A:17:THR:N	0.63	2.31	8	11
1:A:19:PRO:HA	1:A:84:TYR:CE2	0.63	2.29	13	20
1:A:68:ASP:CG	1:A:71:LYS:HZ3	0.63	1.97	14	1
1:A:25:LEU:HD11	1:A:53:ALA:HB1	0.62	1.71	23	11
1:A:40:ASN:C	1:A:40:ASN:HD22	0.62	1.98	27	1
1:A:19:PRO:HB2	1:A:24:MET:SD	0.62	2.35	11	5
1:A:31:TYR:CZ	1:A:35:THR:HG21	0.61	2.30	13	21
1:A:19:PRO:HA	1:A:84:TYR:CZ	0.61	2.30	28	22
1:A:52:LYS:HD3	1:A:53:ALA:N	0.61	2.10	3	6
1:A:5:PHE:CE1	1:A:73:TYR:CD2	0.61	2.89	11	6
1:A:32:LYS:HE2	1:A:58:TRP:CZ3	0.61	2.31	14	1
1:A:8:ALA:HB1	1:A:77:VAL:HG21	0.61	1.72	28	5
1:A:16:LYS:HZ2	1:A:16:LYS:CB	0.61	2.09	27	6
1:A:33:GLN:HG3	1:A:61:LEU:HB3	0.60	1.72	23	8
1:A:7:LYS:HA	1:A:7:LYS:HE2	0.60	1.72	27	1
1:A:26:PHE:CE2	1:A:76:LYS:CB	0.60	2.85	29	21
1:A:4:GLU:H	1:A:4:GLU:CD	0.60	2.00	16	1
1:A:23:GLU:CD	1:A:83:LYS:NZ	0.59	2.56	14	3
1:A:7:LYS:HZ1	1:A:7:LYS:HA	0.59	1.58	20	1
1:A:52:LYS:CG	1:A:53:ALA:N	0.58	2.66	11	4
1:A:76:LYS:HZ3	1:A:79:GLU:CD	0.58	2.02	5	5
1:A:28:TYR:CZ	1:A:32:LYS:HG3	0.58	2.34	22	1
1:A:28:TYR:CE1	1:A:32:LYS:HG3	0.58	2.33	28	13
1:A:5:PHE:CD2	1:A:70:MET:HA	0.57	2.35	10	4
1:A:66:LYS:N	1:A:66:LYS:HD2	0.57	2.15	23	1
1:A:27:ILE:HG22	1:A:28:TYR:N	0.57	2.14	19	26
1:A:65:SER:O	1:A:67:GLU:N	0.57	2.38	27	7
1:A:13:LYS:NZ	1:A:13:LYS:HB2	0.57	2.14	11	1
1:A:39:ILE:HD11	1:A:55:TRP:CD1	0.57	2.35	10	15
1:A:32:LYS:HB3	1:A:58:TRP:CE2	0.57	2.34	23	12
1:A:71:LYS:CG	1:A:72:ALA:N	0.56	2.68	15	5
1:A:5:PHE:CE2	1:A:73:TYR:CD2	0.56	2.93	9	3
1:A:55:TRP:CZ3	1:A:59:ASN:ND2	0.56	2.73	29	24

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:MET:SD	1:A:54:LYS:NZ	0.56	2.74	8	1
1:A:16:LYS:HZ1	1:A:86:ILE:C	0.56	2.04	26	2
1:A:4:GLU:O	1:A:7:LYS:N	0.56	2.39	9	14
1:A:52:LYS:O	1:A:55:TRP:N	0.56	2.39	15	4
1:A:16:LYS:HZ2	1:A:16:LYS:HB3	0.56	1.61	6	2
1:A:13:LYS:NZ	1:A:14:HIS:CG	0.55	2.74	1	1
1:A:16:LYS:HB3	1:A:16:LYS:HZ3	0.55	1.61	28	2
1:A:76:LYS:CE	1:A:76:LYS:HA	0.55	2.31	10	1
1:A:5:PHE:CD1	1:A:73:TYR:CD2	0.55	2.94	6	18
1:A:33:GLN:HG3	1:A:61:LEU:CB	0.55	2.32	2	16
1:A:62:LYS:HB3	1:A:62:LYS:NZ	0.55	2.17	4	3
1:A:26:PHE:CE2	1:A:76:LYS:HB2	0.55	2.37	15	3
1:A:28:TYR:CE2	1:A:54:LYS:HB3	0.55	2.36	26	9
1:A:39:ILE:CD1	1:A:55:TRP:CE2	0.55	2.90	14	3
1:A:25:LEU:HD13	1:A:57:ALA:HB2	0.55	1.79	28	8
1:A:26:PHE:CE2	1:A:76:LYS:HB3	0.54	2.37	26	6
1:A:16:LYS:HB3	1:A:16:LYS:NZ	0.54	2.17	6	3
1:A:13:LYS:HZ1	1:A:14:HIS:CE1	0.54	2.19	1	1
1:A:13:LYS:NZ	1:A:14:HIS:CE1	0.54	2.74	11	2
1:A:16:LYS:NZ	1:A:16:LYS:HB3	0.54	2.17	5	5
1:A:43:ARG:HG3	1:A:55:TRP:CE3	0.54	2.37	21	6
1:A:83:LYS:HG2	1:A:84:TYR:CE2	0.54	2.38	5	1
1:A:16:LYS:CB	1:A:16:LYS:NZ	0.54	2.70	27	3
1:A:16:LYS:NZ	1:A:86:ILE:C	0.54	2.60	29	10
1:A:7:LYS:HA	1:A:7:LYS:NZ	0.54	2.17	20	1
1:A:33:GLN:HG2	1:A:58:TRP:CD1	0.53	2.38	14	12
1:A:61:LEU:O	1:A:63:GLY:N	0.53	2.41	23	13
1:A:16:LYS:HB3	1:A:16:LYS:HZ2	0.53	1.63	15	1
1:A:38:ASP:CB	1:A:62:LYS:HG2	0.53	2.34	12	2
1:A:32:LYS:HE3	1:A:58:TRP:CH2	0.53	2.39	9	4
1:A:67:GLU:HB3	1:A:71:LYS:NZ	0.53	2.19	9	1
1:A:25:LEU:HD13	1:A:57:ALA:CB	0.53	2.33	24	2
1:A:14:HIS:NE2	1:A:86:ILE:HG12	0.53	2.19	3	3
1:A:70:MET:O	1:A:73:TYR:HB3	0.52	2.04	28	19
1:A:5:PHE:HA	1:A:74:ILE:HD11	0.52	1.79	13	3
1:A:28:TYR:O	1:A:32:LYS:HG2	0.52	2.05	14	9
1:A:43:ARG:HB2	1:A:55:TRP:CZ2	0.52	2.39	9	3
1:A:5:PHE:HA	1:A:74:ILE:HD12	0.52	1.82	13	4
1:A:41:THR:OG1	1:A:42:GLU:N	0.52	2.42	13	8
1:A:5:PHE:CD2	1:A:73:TYR:CD2	0.52	2.98	7	4
1:A:64:THR:O	1:A:66:LYS:N	0.52	2.42	24	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:O	1:A:8:ALA:HB2	0.52	2.03	19	3
1:A:15:LEU:O	1:A:18:LYS:NZ	0.52	2.42	27	1
1:A:74:ILE:HD13	1:A:74:ILE:H	0.52	1.62	1	1
1:A:67:GLU:CD	1:A:71:LYS:NZ	0.52	2.63	20	2
1:A:27:ILE:HD11	1:A:77:VAL:HG23	0.52	1.82	20	6
1:A:23:GLU:CD	1:A:83:LYS:HZ3	0.52	2.08	25	1
1:A:25:LEU:CD2	1:A:54:LYS:HD2	0.52	2.34	28	1
1:A:43:ARG:HG3	1:A:55:TRP:CZ3	0.51	2.40	14	2
1:A:28:TYR:CG	1:A:54:LYS:HD2	0.51	2.40	14	1
1:A:7:LYS:HA	1:A:7:LYS:CE	0.51	2.35	20	2
1:A:43:ARG:NH2	1:A:52:LYS:HB2	0.51	2.20	4	1
1:A:26:PHE:CE1	1:A:76:LYS:CB	0.51	2.93	6	4
1:A:52:LYS:HG2	1:A:53:ALA:N	0.51	2.19	11	2
1:A:42:GLU:C	1:A:55:TRP:NE1	0.51	2.64	26	21
1:A:54:LYS:H	1:A:54:LYS:HD2	0.51	1.65	1	2
1:A:77:VAL:O	1:A:80:LEU:N	0.51	2.44	28	10
1:A:52:LYS:HD3	1:A:52:LYS:C	0.51	2.25	3	3
1:A:52:LYS:CD	1:A:53:ALA:H	0.51	2.19	11	3
1:A:74:ILE:N	1:A:74:ILE:CD1	0.51	2.70	13	5
1:A:14:HIS:CG	1:A:15:LEU:N	0.51	2.79	15	2
1:A:42:GLU:HG2	1:A:55:TRP:CD1	0.51	2.41	14	1
1:A:16:LYS:HZ2	1:A:86:ILE:C	0.51	2.09	6	2
1:A:55:TRP:CZ3	1:A:59:ASN:HB2	0.51	2.41	9	2
1:A:22:GLU:O	1:A:25:LEU:HB2	0.51	2.05	28	17
1:A:16:LYS:HD3	1:A:17:THR:N	0.51	2.21	3	1
1:A:78:GLU:CD	1:A:82:LYS:NZ	0.51	2.63	17	2
1:A:18:LYS:NZ	1:A:19:PRO:O	0.51	2.35	15	1
1:A:30:HIS:ND1	1:A:69:ALA:HA	0.51	2.21	17	1
1:A:39:ILE:HD11	1:A:55:TRP:CE2	0.51	2.41	14	2
1:A:23:GLU:OE1	1:A:83:LYS:NZ	0.51	2.44	27	1
1:A:83:LYS:HG2	1:A:84:TYR:CZ	0.50	2.41	18	1
1:A:26:PHE:CD2	1:A:76:LYS:HG2	0.50	2.42	9	1
1:A:52:LYS:CG	1:A:53:ALA:H	0.50	2.19	24	1
1:A:71:LYS:NZ	1:A:75:ASP:OD2	0.50	2.45	21	2
1:A:17:THR:HG22	1:A:18:LYS:H	0.50	1.67	28	2
1:A:39:ILE:HG21	1:A:59:ASN:HA	0.50	1.83	14	5
1:A:25:LEU:HD22	1:A:54:LYS:HA	0.50	1.84	12	9
1:A:11:GLU:CD	1:A:81:LYS:HZ2	0.50	2.09	11	1
1:A:52:LYS:HD3	1:A:53:ALA:H	0.49	1.65	6	3
1:A:52:LYS:O	1:A:53:ALA:C	0.49	2.50	15	7
1:A:13:LYS:NZ	1:A:14:HIS:ND1	0.49	2.60	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LYS:HD2	1:A:54:LYS:N	0.49	2.23	1	3
1:A:21:ASP:O	1:A:25:LEU:HG	0.49	2.07	16	15
1:A:16:LYS:NZ	1:A:86:ILE:OXT	0.49	2.46	14	6
1:A:32:LYS:NZ	1:A:58:TRP:CZ3	0.49	2.80	2	2
1:A:43:ARG:HB2	1:A:55:TRP:CH2	0.49	2.43	9	2
1:A:7:LYS:NZ	1:A:7:LYS:HA	0.49	2.23	14	1
1:A:29:SER:OG	1:A:30:HIS:N	0.49	2.46	23	17
1:A:39:ILE:O	1:A:62:LYS:NZ	0.49	2.45	17	2
1:A:14:HIS:O	1:A:15:LEU:C	0.48	2.52	5	7
1:A:39:ILE:HA	1:A:58:TRP:CZ2	0.48	2.43	29	10
1:A:29:SER:HB2	1:A:58:TRP:HA	0.48	1.85	8	4
1:A:16:LYS:NZ	1:A:16:LYS:CB	0.48	2.76	11	1
1:A:66:LYS:N	1:A:66:LYS:CD	0.48	2.75	23	1
1:A:4:GLU:O	1:A:7:LYS:CB	0.48	2.62	5	3
1:A:15:LEU:O	1:A:16:LYS:C	0.48	2.51	6	2
1:A:70:MET:O	1:A:71:LYS:C	0.48	2.52	25	8
1:A:52:LYS:C	1:A:52:LYS:CD	0.48	2.82	3	1
1:A:4:GLU:CG	1:A:74:ILE:HG21	0.48	2.38	1	2
1:A:5:PHE:CE1	1:A:73:TYR:CG	0.48	3.02	26	15
1:A:4:GLU:O	1:A:7:LYS:HB3	0.48	2.07	17	2
1:A:67:GLU:OE1	1:A:71:LYS:NZ	0.48	2.46	20	1
1:A:32:LYS:HB3	1:A:58:TRP:CZ2	0.48	2.44	29	16
1:A:71:LYS:HG2	1:A:72:ALA:H	0.48	1.68	26	1
1:A:36:VAL:HG12	1:A:40:ASN:HD22	0.48	1.68	8	2
1:A:61:LEU:O	1:A:62:LYS:C	0.47	2.52	20	6
1:A:32:LYS:NZ	1:A:36:VAL:HG21	0.47	2.24	11	7
1:A:22:GLU:H	1:A:22:GLU:CD	0.47	2.12	17	1
1:A:5:PHE:CA	1:A:74:ILE:HD11	0.47	2.40	13	3
1:A:76:LYS:NZ	1:A:79:GLU:OE1	0.47	2.48	2	2
1:A:18:LYS:O	1:A:18:LYS:HG3	0.47	2.09	18	1
1:A:78:GLU:OE2	1:A:82:LYS:NZ	0.47	2.47	18	4
1:A:16:LYS:NZ	1:A:86:ILE:O	0.47	2.48	22	7
1:A:27:ILE:CG2	1:A:28:TYR:N	0.47	2.78	5	10
1:A:17:THR:HG22	1:A:18:LYS:N	0.47	2.25	28	2
1:A:21:ASP:OD1	1:A:54:LYS:NZ	0.47	2.47	6	2
1:A:22:GLU:OE1	1:A:22:GLU:N	0.47	2.48	9	1
1:A:20:ALA:O	1:A:21:ASP:C	0.47	2.53	26	9
1:A:38:ASP:O	1:A:40:ASN:N	0.47	2.48	18	4
1:A:78:GLU:O	1:A:82:LYS:HE2	0.47	2.10	7	1
1:A:5:PHE:CD2	1:A:70:MET:HE3	0.46	2.45	1	1
1:A:21:ASP:OD2	1:A:54:LYS:NZ	0.46	2.48	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LYS:CD	1:A:53:ALA:N	0.46	2.78	3	2
1:A:82:LYS:CG	1:A:83:LYS:N	0.46	2.78	10	3
1:A:11:GLU:OE1	1:A:81:LYS:NZ	0.46	2.49	9	3
1:A:41:THR:OG1	1:A:58:TRP:CZ3	0.46	2.67	5	1
1:A:78:GLU:O	1:A:82:LYS:CE	0.46	2.63	7	1
1:A:14:HIS:O	1:A:18:LYS:NZ	0.46	2.48	20	1
1:A:33:GLN:OE1	1:A:66:LYS:NZ	0.46	2.48	23	1
1:A:39:ILE:HD12	1:A:58:TRP:HB3	0.46	1.88	29	11
1:A:76:LYS:NZ	1:A:79:GLU:CD	0.46	2.69	3	2
1:A:39:ILE:HA	1:A:58:TRP:CE2	0.46	2.44	21	2
1:A:13:LYS:HZ2	1:A:14:HIS:CE1	0.46	2.28	11	1
1:A:52:LYS:O	1:A:55:TRP:HB3	0.46	2.11	9	6
1:A:18:LYS:N	1:A:18:LYS:CD	0.46	2.79	6	1
1:A:7:LYS:HZ3	1:A:11:GLU:CD	0.46	2.14	8	1
1:A:55:TRP:CZ3	1:A:59:ASN:CG	0.46	2.89	28	7
1:A:13:LYS:NZ	1:A:73:TYR:OH	0.46	2.48	27	1
1:A:59:ASN:OD1	1:A:62:LYS:NZ	0.46	2.49	4	1
1:A:23:GLU:CD	1:A:83:LYS:HZ2	0.46	2.14	14	1
1:A:4:GLU:HB2	1:A:74:ILE:HG21	0.46	1.88	19	1
1:A:41:THR:O	1:A:42:GLU:HB3	0.46	2.11	28	2
1:A:42:GLU:CG	1:A:55:TRP:CD1	0.46	2.99	14	1
1:A:7:LYS:NZ	1:A:10:GLU:OE1	0.45	2.49	19	2
1:A:65:SER:O	1:A:68:ASP:N	0.45	2.49	14	4
1:A:52:LYS:HZ2	1:A:52:LYS:HB3	0.45	1.71	22	1
1:A:25:LEU:HD21	1:A:54:LYS:HD3	0.45	1.88	25	1
1:A:12:VAL:HG21	1:A:27:ILE:HG12	0.45	1.88	7	1
1:A:81:LYS:O	1:A:85:GLY:CA	0.45	2.64	8	3
1:A:71:LYS:O	1:A:72:ALA:C	0.45	2.55	22	1
1:A:80:LEU:HD23	1:A:80:LEU:N	0.45	2.27	4	1
1:A:8:ALA:HB1	1:A:77:VAL:HG11	0.45	1.88	8	2
1:A:7:LYS:HA	1:A:7:LYS:HZ1	0.45	1.70	14	1
1:A:34:ALA:HA	1:A:66:LYS:HA	0.45	1.88	22	1
1:A:22:GLU:O	1:A:23:GLU:C	0.45	2.55	18	2
1:A:78:GLU:OE1	1:A:82:LYS:NZ	0.45	2.50	3	5
1:A:29:SER:HA	1:A:58:TRP:HB2	0.45	1.87	19	10
1:A:38:ASP:O	1:A:39:ILE:C	0.45	2.54	16	8
1:A:67:GLU:N	1:A:67:GLU:CD	0.45	2.70	14	2
1:A:33:GLN:OE1	1:A:64:THR:N	0.45	2.50	8	1
1:A:40:ASN:C	1:A:40:ASN:ND2	0.45	2.69	27	1
1:A:43:ARG:NH2	1:A:56:ASP:OD1	0.45	2.50	29	1
1:A:4:GLU:O	1:A:5:PHE:C	0.45	2.55	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:HIS:CE1	1:A:15:LEU:HD23	0.44	2.47	28	2
1:A:5:PHE:O	1:A:8:ALA:HB3	0.44	2.12	11	2
1:A:43:ARG:CG	1:A:55:TRP:CZ3	0.44	3.01	9	1
1:A:28:TYR:CD2	1:A:54:LYS:HB3	0.44	2.46	19	2
1:A:10:GLU:O	1:A:14:HIS:ND1	0.44	2.50	1	3
1:A:13:LYS:HZ1	1:A:14:HIS:CD2	0.44	2.31	1	1
1:A:77:VAL:O	1:A:78:GLU:C	0.44	2.56	13	10
1:A:17:THR:CG2	1:A:18:LYS:H	0.44	2.25	28	2
1:A:52:LYS:NZ	1:A:56:ASP:OD2	0.44	2.48	5	1
1:A:78:GLU:CD	1:A:82:LYS:HZ1	0.44	2.15	24	1
1:A:64:THR:O	1:A:65:SER:C	0.44	2.56	26	1
1:A:34:ALA:HB1	1:A:70:MET:CG	0.44	2.42	26	3
1:A:22:GLU:CD	1:A:22:GLU:N	0.44	2.71	14	1
1:A:69:ALA:O	1:A:73:TYR:HB2	0.44	2.12	21	7
1:A:35:THR:OG1	1:A:36:VAL:N	0.44	2.50	28	5
1:A:81:LYS:O	1:A:85:GLY:HA2	0.44	2.13	26	1
1:A:15:LEU:HD13	1:A:84:TYR:HB2	0.44	1.89	23	1
1:A:76:LYS:HA	1:A:76:LYS:NZ	0.44	2.28	6	1
1:A:78:GLU:O	1:A:79:GLU:C	0.44	2.56	14	1
1:A:76:LYS:O	1:A:79:GLU:HB2	0.43	2.13	9	1
1:A:29:SER:HA	1:A:58:TRP:HA	0.43	1.89	14	1
1:A:39:ILE:HG13	1:A:41:THR:OG1	0.43	2.13	5	1
1:A:4:GLU:HB2	1:A:74:ILE:HG12	0.43	1.91	8	1
1:A:7:LYS:NZ	1:A:11:GLU:CG	0.43	2.81	11	1
1:A:15:LEU:C	1:A:17:THR:N	0.43	2.72	6	1
1:A:83:LYS:HG3	1:A:84:TYR:CZ	0.43	2.48	13	1
1:A:39:ILE:CG2	1:A:59:ASN:HA	0.43	2.43	24	2
1:A:71:LYS:HG3	1:A:72:ALA:H	0.43	1.74	17	1
1:A:52:LYS:O	1:A:56:ASP:HB2	0.43	2.14	21	1
1:A:43:ARG:NH2	1:A:56:ASP:OD2	0.43	2.52	1	1
1:A:76:LYS:NZ	1:A:79:GLU:OE2	0.43	2.52	3	4
1:A:52:LYS:O	1:A:55:TRP:CB	0.43	2.66	9	1
1:A:19:PRO:HG3	1:A:84:TYR:CD2	0.43	2.49	19	2
1:A:54:LYS:H	1:A:54:LYS:CD	0.43	2.27	1	1
1:A:5:PHE:CD1	1:A:73:TYR:CG	0.43	3.07	16	4
1:A:74:ILE:O	1:A:77:VAL:N	0.43	2.52	9	1
1:A:31:TYR:O	1:A:32:LYS:C	0.43	2.57	26	3
1:A:18:LYS:N	1:A:18:LYS:HD2	0.43	2.29	19	1
1:A:25:LEU:N	1:A:25:LEU:HD23	0.43	2.29	27	1
1:A:8:ALA:O	1:A:12:VAL:HB	0.43	2.14	7	1
1:A:26:PHE:CE2	1:A:76:LYS:HG2	0.43	2.49	22	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:THR:O	1:A:19:PRO:HD3	0.43	2.14	21	3
1:A:83:LYS:CG	1:A:84:TYR:CE2	0.42	3.02	5	1
1:A:7:LYS:O	1:A:8:ALA:C	0.42	2.57	7	2
1:A:71:LYS:NZ	1:A:75:ASP:OD1	0.42	2.52	8	2
1:A:23:GLU:CG	1:A:80:LEU:HD21	0.42	2.44	9	1
1:A:4:GLU:CD	1:A:4:GLU:N	0.42	2.72	11	2
1:A:33:GLN:HG2	1:A:58:TRP:NE1	0.42	2.28	11	1
1:A:22:GLU:HA	1:A:25:LEU:HB2	0.42	1.91	21	1
1:A:9:ALA:HA	1:A:73:TYR:OH	0.42	2.13	22	1
1:A:33:GLN:HE21	1:A:58:TRP:HE1	0.42	1.58	15	1
1:A:39:ILE:CD1	1:A:55:TRP:O	0.42	2.67	21	1
1:A:10:GLU:OE2	1:A:13:LYS:NZ	0.42	2.52	24	1
1:A:21:ASP:CG	1:A:54:LYS:HZ3	0.42	2.18	25	1
1:A:57:ALA:O	1:A:60:GLU:HB3	0.42	2.12	3	1
1:A:43:ARG:NH2	1:A:52:LYS:HG3	0.42	2.29	17	1
1:A:29:SER:O	1:A:33:GLN:HB3	0.42	2.15	8	2
1:A:5:PHE:CE2	1:A:73:TYR:CG	0.42	3.08	10	1
1:A:21:ASP:C	1:A:25:LEU:HG	0.42	2.35	14	2
1:A:82:LYS:HG3	1:A:83:LYS:N	0.42	2.30	19	1
1:A:55:TRP:CH2	1:A:59:ASN:CG	0.42	2.93	18	3
1:A:12:VAL:HA	1:A:15:LEU:HG	0.42	1.92	8	1
1:A:38:ASP:CG	1:A:62:LYS:HG2	0.42	2.35	12	1
1:A:5:PHE:CD1	1:A:70:MET:HG2	0.42	2.50	13	1
1:A:79:GLU:CD	1:A:83:LYS:NZ	0.42	2.73	15	1
1:A:39:ILE:CG1	1:A:41:THR:OG1	0.42	2.67	6	1
1:A:28:TYR:CE1	1:A:32:LYS:CG	0.42	3.03	22	1
1:A:76:LYS:NZ	1:A:79:GLU:HG3	0.42	2.30	29	1
1:A:74:ILE:C	1:A:76:LYS:N	0.42	2.73	10	1
1:A:4:GLU:HG2	1:A:74:ILE:CD1	0.42	2.45	16	1
1:A:78:GLU:CD	1:A:82:LYS:HZ2	0.42	2.17	17	1
1:A:9:ALA:C	1:A:13:LYS:HZ3	0.42	2.18	27	1
1:A:5:PHE:CB	1:A:74:ILE:HD11	0.42	2.45	1	1
1:A:66:LYS:HB3	1:A:66:LYS:NZ	0.42	2.30	6	1
1:A:5:PHE:CE2	1:A:31:TYR:CE1	0.42	3.08	8	3
1:A:43:ARG:NH2	1:A:52:LYS:HG2	0.42	2.30	26	1
1:A:15:LEU:HD23	1:A:15:LEU:N	0.42	2.28	28	1
1:A:34:ALA:HB1	1:A:70:MET:HG3	0.42	1.92	8	3
1:A:77:VAL:O	1:A:79:GLU:N	0.42	2.53	5	1
1:A:38:ASP:HB3	1:A:62:LYS:CG	0.42	2.44	9	1
1:A:23:GLU:HG2	1:A:84:TYR:CE2	0.42	2.50	20	1
1:A:31:TYR:O	1:A:34:ALA:HB3	0.42	2.15	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:THR:HB	1:A:84:TYR:CD1	0.42	2.50	25	1
1:A:25:LEU:HD11	1:A:53:ALA:CB	0.42	2.45	27	1
1:A:11:GLU:OE2	1:A:81:LYS:NZ	0.41	2.53	13	3
1:A:33:GLN:HE21	1:A:37:GLY:C	0.41	2.19	12	2
1:A:34:ALA:HB1	1:A:70:MET:HG2	0.41	1.91	13	1
1:A:33:GLN:HG3	1:A:61:LEU:CD1	0.41	2.44	29	2
1:A:29:SER:HA	1:A:58:TRP:CB	0.41	2.46	17	3
1:A:31:TYR:CE1	1:A:35:THR:HG21	0.41	2.50	11	1
1:A:43:ARG:HD2	1:A:55:TRP:CZ3	0.41	2.50	16	1
1:A:66:LYS:NZ	1:A:67:GLU:OE2	0.41	2.54	17	1
1:A:5:PHE:CD2	1:A:6:ASP:N	0.41	2.88	26	1
1:A:16:LYS:HZ3	1:A:86:ILE:C	0.41	2.18	28	1
1:A:7:LYS:HZ2	1:A:11:GLU:CD	0.41	2.18	16	1
1:A:78:GLU:HG3	1:A:82:LYS:NZ	0.41	2.30	28	1
1:A:4:GLU:O	1:A:7:LYS:HB2	0.41	2.16	1	1
1:A:33:GLN:NE2	1:A:62:LYS:HA	0.41	2.30	12	1
1:A:81:LYS:O	1:A:85:GLY:HA3	0.41	2.15	27	1
1:A:21:ASP:CG	1:A:54:LYS:NZ	0.41	2.74	3	1
1:A:61:LEU:O	1:A:64:THR:N	0.41	2.53	24	2
1:A:39:ILE:O	1:A:39:ILE:HG23	0.41	2.16	14	1
1:A:19:PRO:HB2	1:A:24:MET:CG	0.41	2.45	23	2
1:A:82:LYS:HG2	1:A:83:LYS:N	0.41	2.31	8	1
1:A:13:LYS:NZ	1:A:13:LYS:CB	0.41	2.83	11	1
1:A:32:LYS:HB3	1:A:58:TRP:CH2	0.41	2.51	20	1
1:A:4:GLU:O	1:A:8:ALA:CB	0.41	2.68	28	1
1:A:12:VAL:HG21	1:A:77:VAL:HG22	0.41	1.93	5	1
1:A:12:VAL:HG21	1:A:27:ILE:CG1	0.41	2.46	7	1
1:A:68:ASP:OD1	1:A:71:LYS:NZ	0.41	2.51	26	2
1:A:9:ALA:O	1:A:13:LYS:NZ	0.41	2.52	10	1
1:A:9:ALA:CB	1:A:31:TYR:CE1	0.41	3.03	11	1
1:A:55:TRP:CZ3	1:A:59:ASN:CB	0.40	3.05	6	1
1:A:13:LYS:HZ2	1:A:27:ILE:CG2	0.40	2.29	8	1
1:A:67:GLU:CD	1:A:67:GLU:N	0.40	2.74	1	1
1:A:24:MET:HB3	1:A:54:LYS:NZ	0.40	2.30	10	1
1:A:62:LYS:NZ	1:A:62:LYS:HB3	0.40	2.32	20	1
1:A:26:PHE:O	1:A:29:SER:OG	0.40	2.38	22	1
1:A:30:HIS:O	1:A:31:TYR:C	0.40	2.59	5	1
1:A:11:GLU:OE1	1:A:81:LYS:CE	0.40	2.69	15	1
1:A:72:ALA:O	1:A:73:TYR:C	0.40	2.59	20	1
1:A:16:LYS:NZ	1:A:85:GLY:O	0.40	2.54	11	1
1:A:29:SER:HA	1:A:58:TRP:CA	0.40	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LYS:HD2	1:A:13:LYS:C	0.40	2.36	15	1
1:A:40:ASN:OD1	1:A:40:ASN:N	0.40	2.54	20	1
1:A:4:GLU:C	1:A:74:ILE:HG12	0.40	2.37	28	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	74/86 (86%)	50±3 (68±4%)	16±3 (22±4%)	7±2 (10±2%)	1 9
All	All	2146/2494 (86%)	1464 (68%)	466 (22%)	216 (10%)	1 9

All 23 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	15	LEU	28
1	A	62	LYS	28
1	A	39	ILE	24
1	A	16	LYS	17
1	A	75	ASP	15
1	A	85	GLY	15
1	A	42	GLU	14
1	A	66	LYS	14
1	A	52	LYS	13
1	A	65	SER	10
1	A	13	LYS	6
1	A	27	ILE	5
1	A	53	ALA	5
1	A	19	PRO	5
1	A	21	ASP	3
1	A	38	ASP	3
1	A	18	LYS	2
1	A	77	VAL	2
1	A	43	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	71	LYS	2
1	A	78	GLU	1
1	A	60	GLU	1
1	A	5	PHE	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	64/72 (89%)	53±3 (83±4%)	11±3 (17±4%)	4 39
All	All	1856/2088 (89%)	1532 (83%)	324 (17%)	4 39

All 42 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	12	VAL	29
1	A	25	LEU	29
1	A	64	THR	28
1	A	86	ILE	28
1	A	27	ILE	27
1	A	74	ILE	16
1	A	52	LYS	16
1	A	62	LYS	13
1	A	77	VAL	13
1	A	7	LYS	12
1	A	76	LYS	8
1	A	65	SER	8
1	A	59	ASN	7
1	A	14	HIS	7
1	A	78	GLU	7
1	A	82	LYS	7
1	A	4	GLU	6
1	A	41	THR	6
1	A	67	GLU	6
1	A	33	GLN	5
1	A	23	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	66	LYS	4
1	A	71	LYS	4
1	A	21	ASP	4
1	A	18	LYS	4
1	A	54	LYS	3
1	A	81	LYS	3
1	A	13	LYS	2
1	A	16	LYS	2
1	A	40	ASN	2
1	A	60	GLU	2
1	A	10	GLU	2
1	A	75	ASP	1
1	A	22	GLU	1
1	A	42	GLU	1
1	A	79	GLU	1
1	A	24	MET	1
1	A	19	PRO	1
1	A	56	ASP	1
1	A	68	ASP	1
1	A	6	ASP	1
1	A	83	LYS	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)

There are no ligands in this entry.

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