



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:09 PM UTC

PDB ID : 1YUS / pdb_00001yus
Title : Solution structure of apo-S100A13
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Structural Proteomics in Europe (SPINE)
Deposited on : 2005-02-14

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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 ⓘ symbol.

The types of validation reports are described at

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

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

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

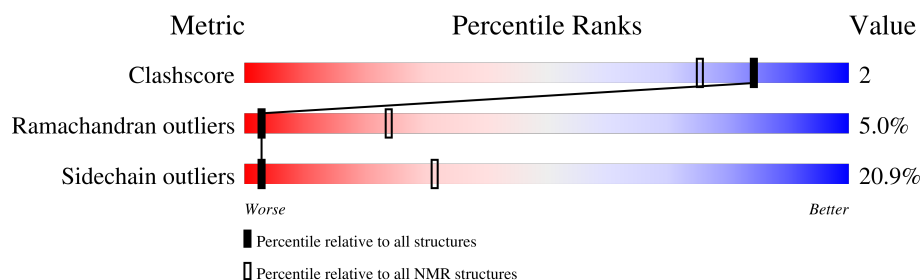
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	98	 65% 21% 13%
1	B	98	 63% 24% 12%

2 Ensemble composition and analysis

This entry contains 25 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 18 as representative, based on the following criterion: *fewest violations*.

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:22, A:31-A:96, B:4-B:22, B:30-B:96 (171)	1.07	20

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 and 5 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 7, 9, 10, 11, 13, 15, 19, 20, 21, 23, 24, 25
2	6, 8
3	14, 16
Single-model clusters	5; 12; 17; 18; 22

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3280 atoms, of which 1666 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called S100 calcium binding protein A13.

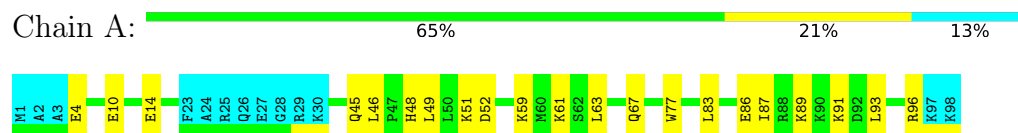
Mol	Chain	Residues	Atoms						Trace
1	A	98	Total	C	H	N	O	S	0
			1640	512	833	136	157	2	
1	B	98	Total	C	H	N	O	S	0
			1640	512	833	136	157	2	

4 Residue-property plots

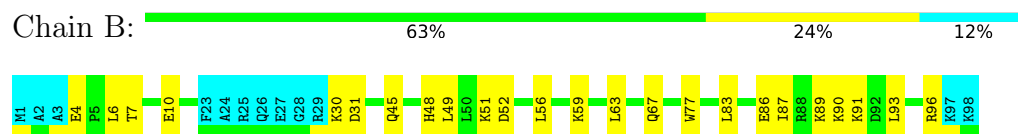
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: S100 calcium binding protein A13



- Molecule 1: S100 calcium binding protein A13

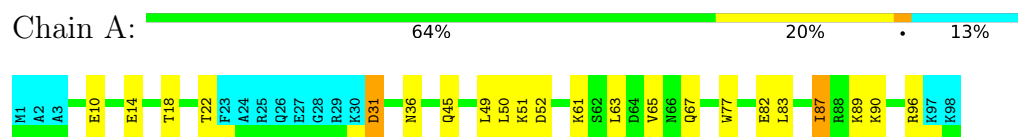


4.2 Scores per residue for each member of the ensemble

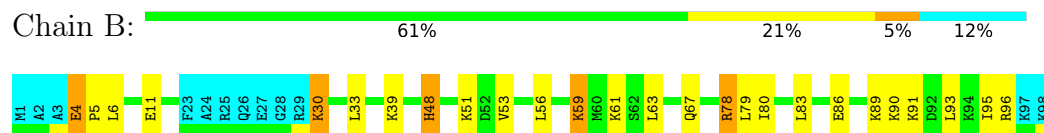
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: S100 calcium binding protein A13

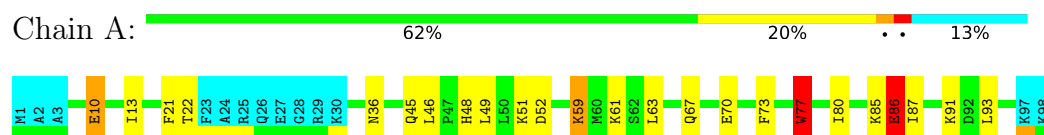


- Molecule 1: S100 calcium binding protein A13

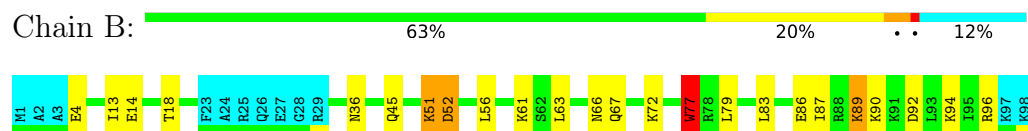


4.2.2 Score per residue for model 2

- Molecule 1: S100 calcium binding protein A13

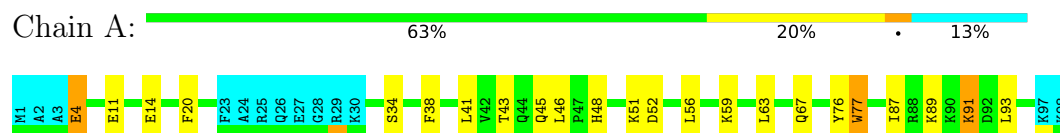


- Molecule 1: S100 calcium binding protein A13

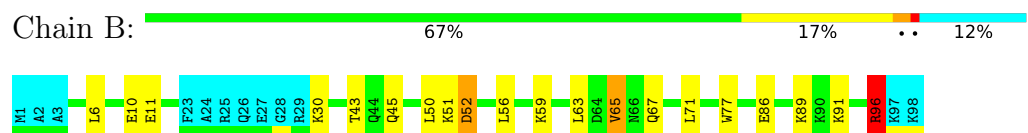


4.2.3 Score per residue for model 3

- Molecule 1: S100 calcium binding protein A13

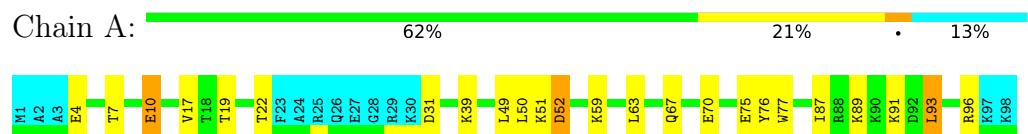


- Molecule 1: S100 calcium binding protein A13

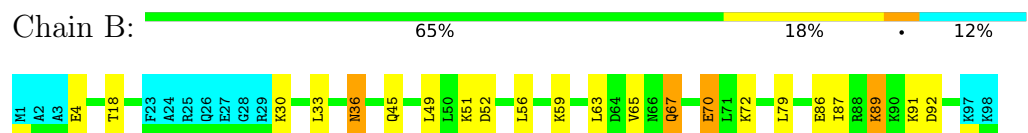


4.2.4 Score per residue for model 4

- Molecule 1: S100 calcium binding protein A13

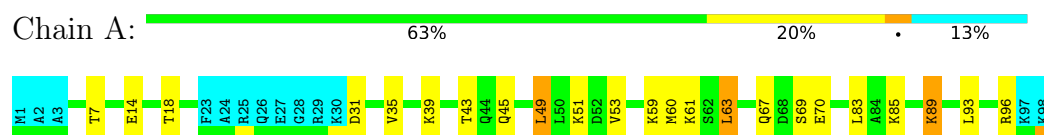


- Molecule 1: S100 calcium binding protein A13

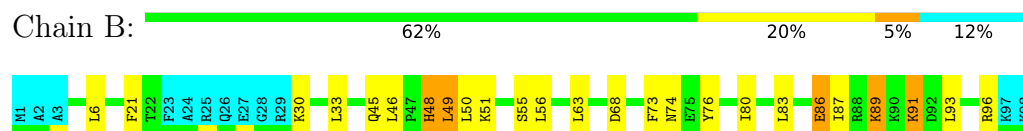


4.2.5 Score per residue for model 5

- Molecule 1: S100 calcium binding protein A13

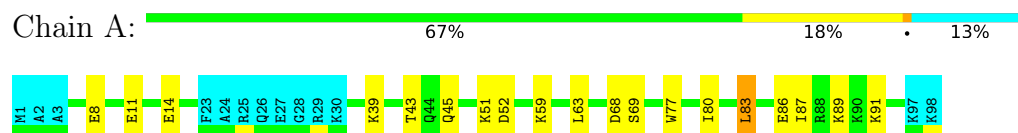


- Molecule 1: S100 calcium binding protein A13

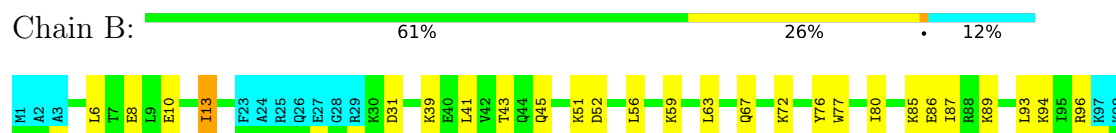


4.2.6 Score per residue for model 6

- Molecule 1: S100 calcium binding protein A13

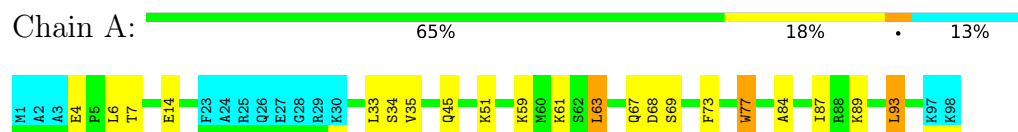


- Molecule 1: S100 calcium binding protein A13

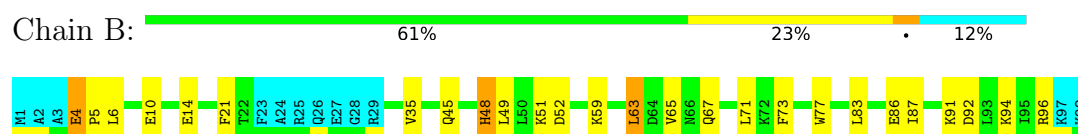


4.2.7 Score per residue for model 7

- Molecule 1: S100 calcium binding protein A13

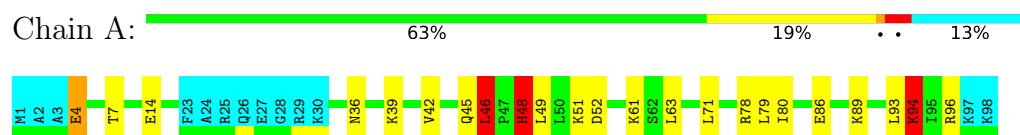


- Molecule 1: S100 calcium binding protein A13

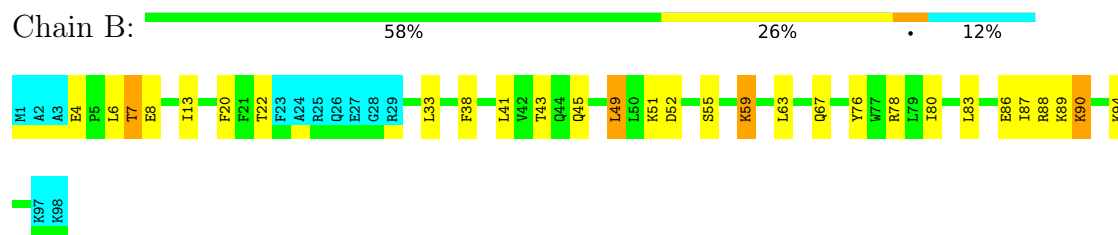


4.2.8 Score per residue for model 8

- Molecule 1: S100 calcium binding protein A13

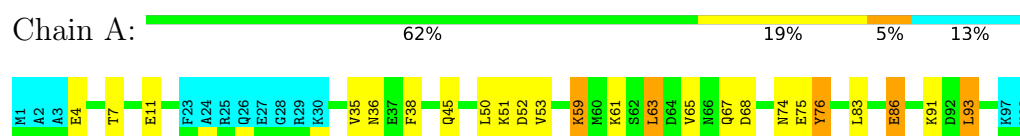


- Molecule 1: S100 calcium binding protein A13

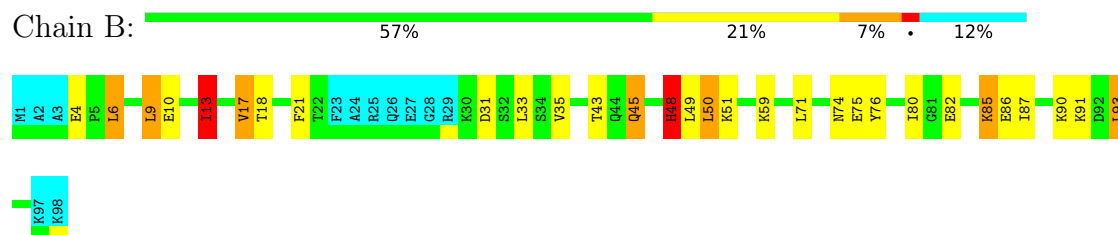


4.2.9 Score per residue for model 9

- Molecule 1: S100 calcium binding protein A13

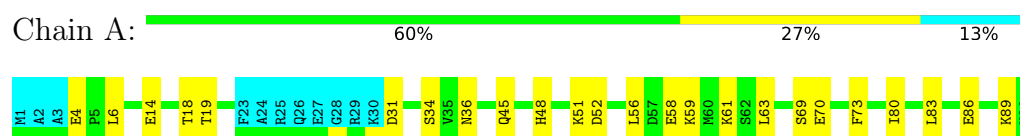


- Molecule 1: S100 calcium binding protein A13

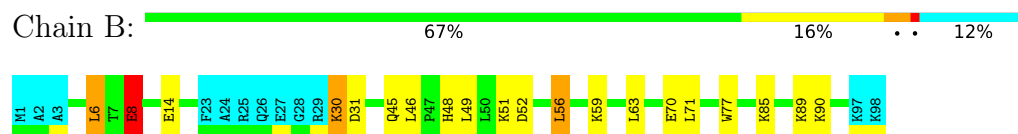


4.2.10 Score per residue for model 10

- Molecule 1: S100 calcium binding protein A13

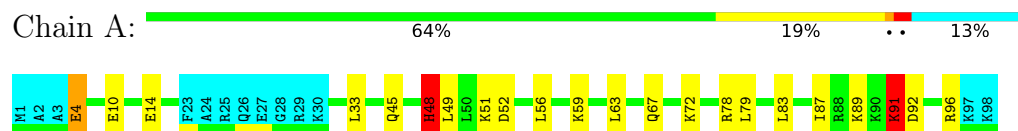


- Molecule 1: S100 calcium binding protein A13

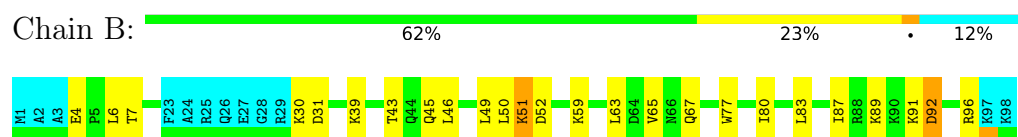


4.2.11 Score per residue for model 11

- Molecule 1: S100 calcium binding protein A13

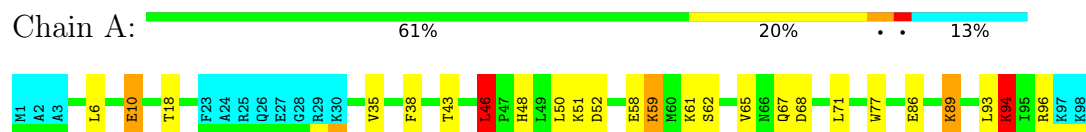


- Molecule 1: S100 calcium binding protein A13

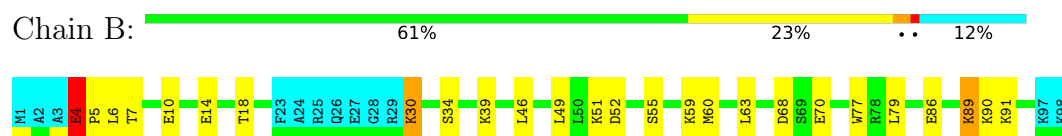


4.2.12 Score per residue for model 12

- Molecule 1: S100 calcium binding protein A13

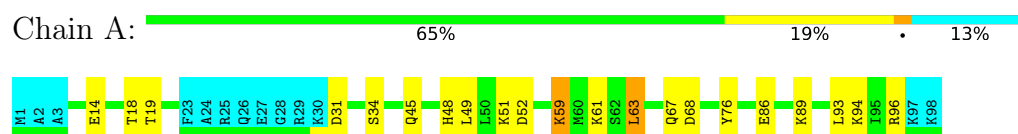


- Molecule 1: S100 calcium binding protein A13

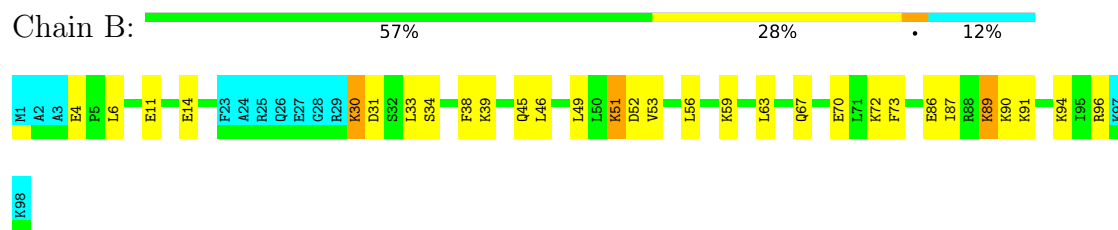


4.2.13 Score per residue for model 13

- Molecule 1: S100 calcium binding protein A13

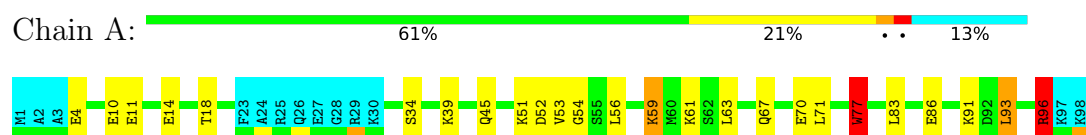


- Molecule 1: S100 calcium binding protein A13

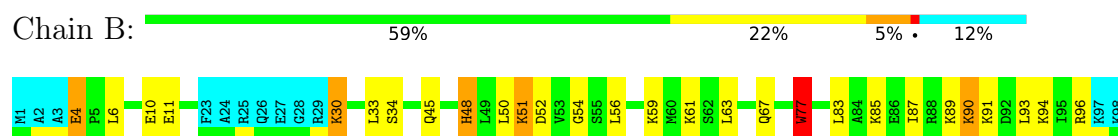


4.2.14 Score per residue for model 14

- Molecule 1: S100 calcium binding protein A13

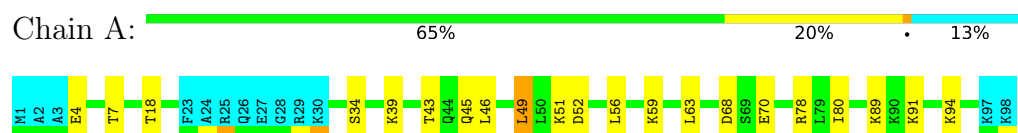


- Molecule 1: S100 calcium binding protein A13

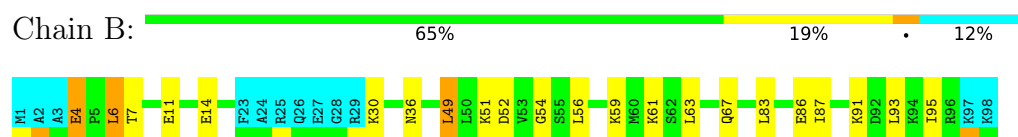


4.2.15 Score per residue for model 15

- Molecule 1: S100 calcium binding protein A13



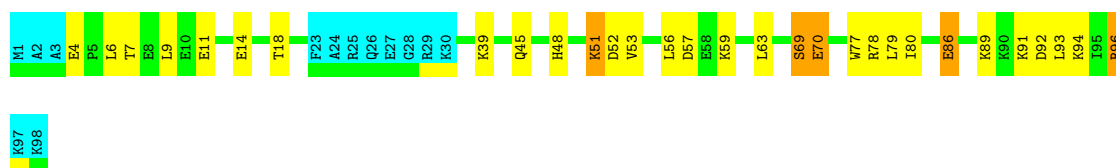
- Molecule 1: S100 calcium binding protein A13



4.2.16 Score per residue for model 16

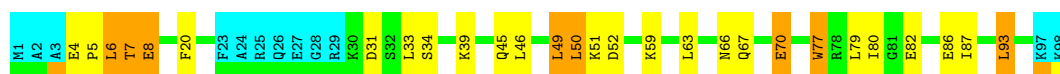
- Molecule 1: S100 calcium binding protein A13





- Molecule 1: S100 calcium binding protein A13

Chain B: 59% 20% 8% 12%



4.2.17 Score per residue for model 17

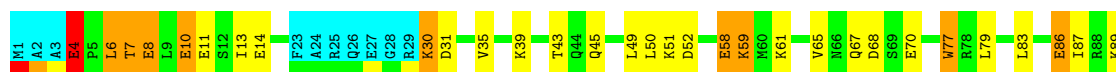
- Molecule 1: S100 calcium binding protein A13

Chain A: 58% 24% • • 13%



- Molecule 1: S100 calcium binding protein A13

Chain B: 53% 24% 9% • 12%



4.2.18 Score per residue for model 18

- Molecule 1: S100 calcium binding protein A13

Chain A: 59% 22% • • 13%



- Molecule 1: S100 calcium binding protein A13

Chain B: 59% 27% • • 12%





4.2.19 Score per residue for model 19

- Molecule 1: S100 calcium binding protein A13

Chain A: 69% 16% 13%



- Molecule 1: S100 calcium binding protein A13

Chain B: 61% 22% 12%



4.2.20 Score per residue for model 20 (medoid)

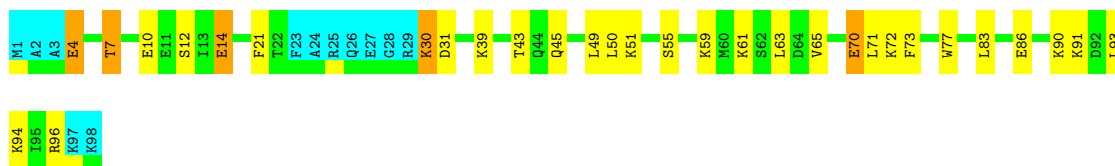
- Molecule 1: S100 calcium binding protein A13

Chain A: 63% 19% 13%



- Molecule 1: S100 calcium binding protein A13

Chain B: 56% 27% 5% 12%



4.2.21 Score per residue for model 21

- Molecule 1: S100 calcium binding protein A13

Chain A: 62% 19% 5% 13%



- Molecule 1: S100 calcium binding protein A13

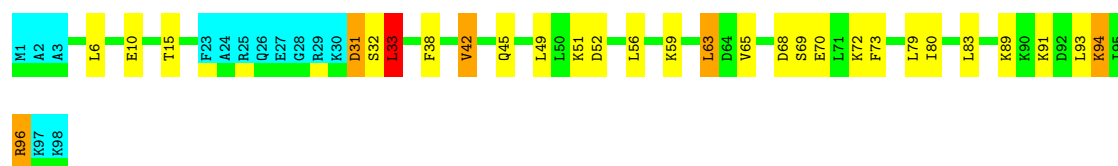
Chain B: 



4.2.22 Score per residue for model 22

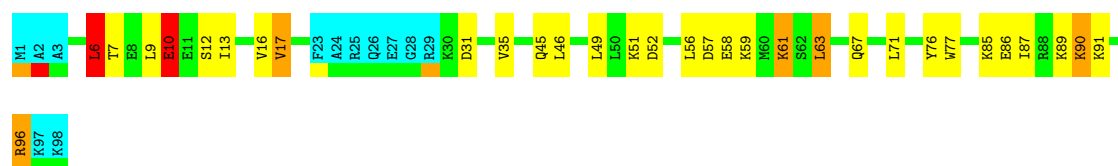
- Molecule 1: S100 calcium binding protein A13

Chain A: 



- Molecule 1: S100 calcium binding protein A13

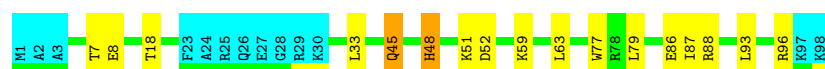
Chain B: 



4.2.23 Score per residue for model 23

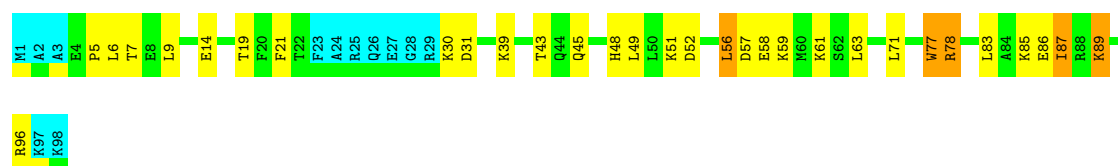
- Molecule 1: S100 calcium binding protein A13

Chain A: 



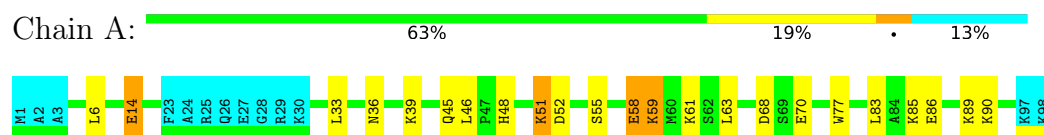
- Molecule 1: S100 calcium binding protein A13

Chain B: 

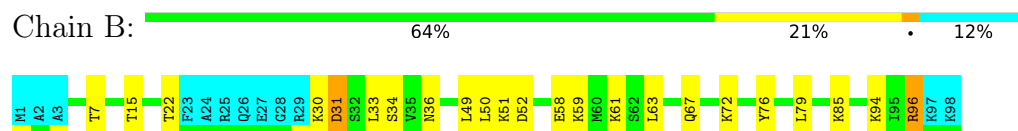


4.2.24 Score per residue for model 24

- Molecule 1: S100 calcium binding protein A13

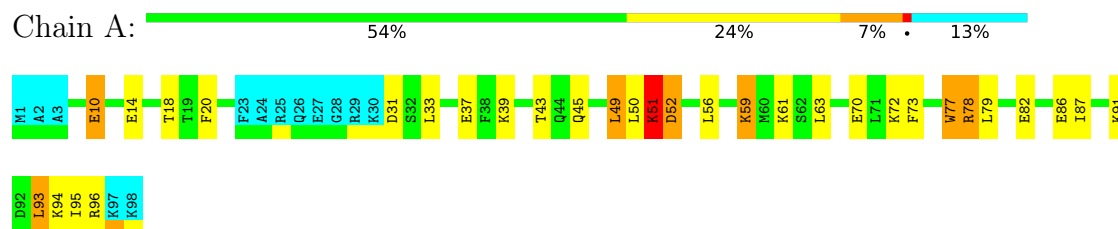


- Molecule 1: S100 calcium binding protein A13

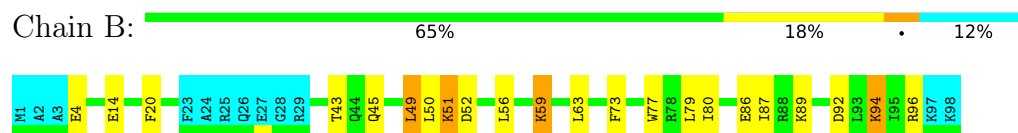


4.2.25 Score per residue for model 25

- Molecule 1: S100 calcium binding protein A13



- Molecule 1: S100 calcium binding protein A13



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *Restrained energy minimization*.

Of the 300 calculated structures, 25 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
DYANA	structure solution	5.1
Amber	refinement	6

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	0.61±0.02	0±0/711 (0.0± 0.0%)	1.35±0.17	2±2/957 (0.2± 0.2%)
1	B	0.61±0.02	0±0/720 (0.0± 0.0%)	1.33±0.06	2±2/968 (0.2± 0.2%)
All	All	0.61	1/35775 (0.0%)	1.35	103/48125 (0.2%)

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	0.7±1.1	1.4±1.1
1	B	0.7±1.0	1.2±1.1
All	All	35	66

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	THR	CA-C	5.79	1.60	1.52	13	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	19	THR	O-C-N	40.48	171.18	122.20	13	1
1	A	19	THR	CA-C-O	-31.05	84.69	121.02	13	1
1	B	8	GLU	CA-CB-CG	13.82	141.74	114.10	10	1
1	B	10	GLU	CB-CA-C	11.78	133.31	110.46	22	1
1	B	17	VAL	CB-CA-C	9.23	126.43	111.29	22	1
1	A	88	ARG	CB-CG-CD	9.15	132.34	111.30	21	1
1	B	48	HIS	CA-CB-CG	9.08	122.88	113.80	19	1
1	A	52	ASP	CA-CB-CG	8.67	121.27	112.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	87	ILE	CB-CA-C	8.50	120.81	111.80	21	1
1	B	86	GLU	CA-CB-CG	8.45	131.00	114.10	9	1
1	B	52	ASP	CA-CB-CG	7.95	120.55	112.60	10	1
1	A	87	ILE	N-CA-C	7.86	118.53	107.37	21	1
1	A	48	HIS	CB-CG-CD2	-7.44	121.53	131.20	8	5
1	A	22	THR	CA-C-N	7.39	135.01	121.70	17	1
1	A	22	THR	C-N-CA	7.39	135.01	121.70	17	1
1	B	4	GLU	CB-CA-C	7.17	124.29	110.17	12	5
1	A	89	LYS	CB-CG-CD	7.07	127.56	111.30	12	1
1	B	7	THR	CA-C-N	7.07	135.04	121.54	17	2
1	B	7	THR	C-N-CA	7.07	135.04	121.54	17	2
1	A	21	PHE	N-CA-C	6.90	119.82	111.40	17	1
1	B	21	PHE	CA-CB-CG	6.72	120.52	113.80	19	2
1	B	7	THR	N-CA-CB	-6.65	100.92	110.44	22	1
1	B	13	ILE	CA-CB-CG1	6.43	121.33	110.40	6	1
1	B	36	ASN	CA-CB-CG	6.40	119.00	112.60	4	1
1	A	33	LEU	N-CA-CB	6.37	119.54	110.44	22	1
1	B	32	SER	N-CA-CB	-6.26	105.77	111.59	21	1
1	A	46	LEU	N-CA-C	6.18	123.47	109.81	12	1
1	B	14	GLU	CB-CA-C	6.03	120.85	110.84	20	1
1	A	67	GLN	CA-C-N	6.02	130.23	120.60	9	2
1	A	67	GLN	C-N-CA	6.02	130.23	120.60	9	2
1	A	31	ASP	CA-C-N	5.99	132.49	121.70	1	1
1	A	31	ASP	C-N-CA	5.99	132.49	121.70	1	1
1	B	6	LEU	CA-C-N	5.97	134.23	121.45	22	1
1	B	6	LEU	C-N-CA	5.97	134.23	121.45	22	1
1	A	48	HIS	CA-CB-CG	5.92	119.72	113.80	11	2
1	A	51	LYS	N-CA-CB	5.87	118.82	110.13	21	1
1	B	85	LYS	CA-C-N	5.84	128.43	120.54	14	1
1	B	85	LYS	C-N-CA	5.84	128.43	120.54	14	1
1	B	67	GLN	CA-C-N	5.78	129.85	120.60	4	2
1	B	67	GLN	C-N-CA	5.78	129.85	120.60	4	2
1	B	48	HIS	CB-CG-CD2	-5.77	123.70	131.20	23	5
1	B	13	ILE	N-CA-CB	5.71	116.85	110.62	6	1
1	A	94	LYS	N-CA-CB	5.70	120.11	110.49	12	2
1	A	17	VAL	CA-C-N	5.66	127.80	120.44	4	1
1	A	17	VAL	C-N-CA	5.66	127.80	120.44	4	1
1	B	13	ILE	CB-CA-C	5.65	120.55	111.29	9	1
1	B	88	ARG	CA-C-N	5.63	129.60	120.60	21	1
1	B	88	ARG	C-N-CA	5.63	129.60	120.60	21	1
1	B	87	ILE	CB-CA-C	5.59	117.73	111.80	23	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	51	LYS	CA-C-N	5.57	132.18	121.54	25	3
1	B	51	LYS	C-N-CA	5.57	132.18	121.54	25	3
1	A	96	ARG	CA-CB-CG	5.53	125.16	114.10	14	1
1	A	69	SER	CA-C-N	5.50	132.04	121.54	16	1
1	A	69	SER	C-N-CA	5.50	132.04	121.54	16	1
1	B	31	ASP	CA-CB-CG	5.47	118.08	112.60	24	2
1	A	94	LYS	CB-CA-C	5.47	121.42	109.99	22	1
1	B	7	THR	CA-CB-CG2	5.46	119.77	110.50	17	1
1	B	6	LEU	N-CA-C	5.44	115.31	108.45	22	1
1	A	84	ALA	CA-C-N	5.42	127.81	120.44	7	1
1	A	84	ALA	C-N-CA	5.42	127.81	120.44	7	1
1	B	13	ILE	N-CA-C	5.42	120.61	109.34	9	1
1	B	7	THR	CB-CA-C	5.33	118.61	109.51	24	1
1	A	32	SER	CA-C-N	5.31	132.82	121.45	22	1
1	A	32	SER	C-N-CA	5.31	132.82	121.45	22	1
1	B	36	ASN	CA-C-N	5.28	127.66	120.54	2	1
1	B	36	ASN	C-N-CA	5.28	127.66	120.54	2	1
1	A	51	LYS	CA-C-N	5.24	131.55	121.54	24	1
1	A	51	LYS	C-N-CA	5.24	131.55	121.54	24	1
1	B	16	VAL	N-CA-C	-5.22	105.29	110.62	22	1
1	A	63	LEU	N-CA-CB	5.18	117.80	110.13	13	1
1	A	85	LYS	CA-C-N	5.17	127.97	120.79	21	1
1	A	85	LYS	C-N-CA	5.17	127.97	120.79	21	1
1	A	87	ILE	N-CA-CB	5.14	117.46	111.90	21	1
1	B	12	SER	N-CA-CB	5.12	119.14	110.49	20	1
1	A	36	ASN	CA-C-N	5.08	127.86	120.79	18	1
1	A	36	ASN	C-N-CA	5.08	127.86	120.79	18	1
1	A	93	LEU	N-CA-C	5.01	117.12	111.11	17	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	19	THR	CB,CA	3
1	B	7	THR	CB,CA	3
1	A	22	THR	CB	2
1	A	11	GLU	CA	2
1	B	10	GLU	CA	2
1	A	46	LEU	CA	2
1	A	94	LYS	CA	2
1	B	11	GLU	CA	2
1	A	31	ASP	CA	1

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Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	6	LEU	CA	1
1	B	13	ILE	CA	1
1	B	9	LEU	CA	1
1	B	4	GLU	CA	1
1	B	5	PRO	CA	1
1	A	6	LEU	CA	1
1	A	95	ILE	CB	1
1	A	96	ARG	CA	1
1	A	18	THR	CA	1
1	B	15	THR	CB	1
1	B	12	SER	CA	1
1	B	14	GLU	CA	1
1	A	33	LEU	CA	1
1	B	17	VAL	CA	1
1	A	92	ASP	CA	1

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	73	PHE	Sidechain	8
1	A	96	ARG	Sidechain	6
1	B	96	ARG	Sidechain	5
1	B	73	PHE	Sidechain	5
1	B	76	TYR	Sidechain	5
1	A	76	TYR	Sidechain	4
1	B	78	ARG	Sidechain	3
1	B	4	GLU	Peptide	3
1	B	20	PHE	Sidechain	3
1	A	78	ARG	Sidechain	3
1	B	21	PHE	Sidechain	3
1	A	22	THR	Peptide	2
1	A	20	PHE	Sidechain	2
1	A	70	GLU	Peptide	2
1	A	48	HIS	Sidechain	2
1	A	38	PHE	Sidechain	2
1	B	48	HIS	Sidechain	1
1	B	88	ARG	Sidechain	1
1	B	38	PHE	Sidechain	1
1	A	21	PHE	Peptide	1
1	A	91	LYS	Peptide	1
1	A	34	SER	Peptide	1
1	A	33	LEU	Peptide	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	51	LYS	Peptide	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	701	716	716	4±2
1	B	710	729	729	4±2
All	All	35275	36125	36125	164

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:THR:HG23	1:B:8:GLU:HB2	0.68	1.64	10	1
1:A:93:LEU:H	1:A:93:LEU:HD23	0.66	1.51	17	4
1:B:6:LEU:HD23	1:B:6:LEU:O	0.63	1.93	16	1
1:A:93:LEU:HD13	1:A:93:LEU:H	0.61	1.56	9	3
1:A:7:THR:HG21	1:B:45:GLN:HG3	0.57	1.76	9	1
1:A:19:THR:CG2	1:B:8:GLU:HB2	0.56	2.31	10	1
1:B:56:LEU:HD13	1:B:57:ASP:N	0.55	2.15	23	1
1:B:30:LYS:NZ	1:B:70:GLU:OE2	0.54	2.40	20	4
1:A:94:LYS:HB3	1:B:4:GLU:HB3	0.54	1.79	12	1
1:B:6:LEU:HD12	1:B:10:GLU:HG3	0.54	1.80	9	1
1:B:10:GLU:HA	1:B:13:ILE:HD12	0.52	1.80	17	1
1:B:93:LEU:H	1:B:93:LEU:HD13	0.52	1.65	9	1
1:A:94:LYS:HG2	1:B:6:LEU:HD22	0.51	1.82	16	1
1:A:45:GLN:HG3	1:B:7:THR:HG22	0.50	1.84	20	2
1:A:51:LYS:HD3	1:A:52:ASP:N	0.50	2.22	16	1
1:A:39:LYS:CB	1:A:63:LEU:HD21	0.49	2.36	8	3
1:B:7:THR:HG23	1:B:8:GLU:H	0.49	1.67	8	1
1:A:83:LEU:C	1:A:83:LEU:HD12	0.48	2.33	6	1
1:A:35:VAL:CG1	1:A:63:LEU:HD12	0.48	2.39	7	3
1:A:51:LYS:HD3	1:A:52:ASP:H	0.48	1.68	25	1
1:B:4:GLU:CG	1:B:6:LEU:HD22	0.48	2.39	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:GLU:N	1:A:4:GLU:CD	0.48	2.72	11	4
1:B:4:GLU:HG2	1:B:6:LEU:HD22	0.48	1.85	17	1
1:B:83:LEU:O	1:B:87:ILE:HG22	0.48	2.09	19	1
1:B:35:VAL:CG1	1:B:63:LEU:HD12	0.47	2.39	7	1
1:A:7:THR:HG21	1:B:45:GLN:CG	0.47	2.39	9	1
1:A:33:LEU:HD22	1:A:33:LEU:N	0.47	2.23	17	1
1:B:39:LYS:CB	1:B:63:LEU:HD21	0.47	2.40	21	1
1:B:56:LEU:C	1:B:56:LEU:HD13	0.47	2.35	3	10
1:B:6:LEU:HD22	1:B:10:GLU:OE1	0.46	2.11	6	1
1:A:59:LYS:NZ	1:A:86:GLU:OE1	0.46	2.48	12	6
1:B:49:LEU:C	1:B:50:LEU:HD13	0.46	2.36	16	2
1:B:7:THR:H	1:B:10:GLU:CD	0.46	2.18	17	1
1:A:33:LEU:HD23	1:A:38:PHE:CD1	0.46	2.45	17	1
1:A:48:HIS:NE2	1:A:93:LEU:HD12	0.46	2.26	3	1
1:A:49:LEU:C	1:A:50:LEU:HD13	0.45	2.36	18	1
1:B:13:ILE:O	1:B:17:VAL:HG13	0.45	2.11	9	1
1:A:59:LYS:HZ1	1:A:86:GLU:CD	0.45	2.20	18	1
1:A:10:GLU:OE2	1:B:89:LYS:NZ	0.45	2.48	12	3
1:A:93:LEU:HD21	1:B:14:GLU:OE1	0.45	2.11	7	1
1:B:7:THR:C	1:B:10:GLU:OE1	0.45	2.59	17	1
1:A:45:GLN:CG	1:B:9:LEU:HD13	0.45	2.42	23	1
1:B:30:LYS:HZ1	1:B:70:GLU:CD	0.44	2.19	10	1
1:A:63:LEU:HD11	1:A:79:LEU:HD21	0.44	1.89	22	1
1:A:89:LYS:HG2	1:A:93:LEU:HD22	0.44	1.88	7	3
1:B:6:LEU:C	1:B:6:LEU:HD23	0.44	2.37	10	1
1:B:4:GLU:HG3	1:B:6:LEU:HD22	0.44	1.89	15	1
1:A:35:VAL:HG23	1:A:69:SER:O	0.44	2.11	7	1
1:A:89:LYS:CG	1:A:93:LEU:HD13	0.44	2.41	3	1
1:A:89:LYS:HG2	1:A:93:LEU:HD13	0.44	1.89	17	3
1:B:82:GLU:OE1	1:B:85:LYS:NZ	0.44	2.50	9	1
1:A:80:ILE:CD1	1:B:77:TRP:HE1	0.43	2.26	16	1
1:B:51:LYS:HD3	1:B:52:ASP:N	0.43	2.28	13	2
1:A:56:LEU:HD13	1:A:56:LEU:C	0.43	2.39	22	5
1:B:58:GLU:OE1	1:B:85:LYS:NZ	0.43	2.51	22	1
1:B:89:LYS:HG3	1:B:93:LEU:HD13	0.43	1.91	1	1
1:B:33:LEU:HD22	1:B:33:LEU:N	0.43	2.29	13	2
1:A:76:TYR:CD1	1:A:76:TYR:C	0.43	2.97	9	1
1:A:56:LEU:HD23	1:A:57:ASP:H	0.43	1.74	20	1
1:A:77:TRP:HE1	1:B:80:ILE:CD1	0.43	2.27	25	1
1:A:94:LYS:NZ	1:B:14:GLU:CD	0.42	2.78	13	2
1:A:14:GLU:CB	1:B:93:LEU:HD11	0.42	2.44	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:59:LYS:NZ	1:B:86:GLU:OE1	0.42	2.52	8	2
1:B:59:LYS:NZ	1:B:86:GLU:OE2	0.42	2.52	17	2
1:A:91:LYS:NZ	1:A:92:ASP:OD2	0.42	2.49	16	2
1:A:45:GLN:CG	1:B:7:THR:HG22	0.42	2.44	8	1
1:A:42:VAL:O	1:A:46:LEU:HD12	0.42	2.15	8	1
1:A:48:HIS:NE2	1:A:93:LEU:C	0.42	2.78	8	1
1:A:77:TRP:CD1	1:B:77:TRP:CD1	0.42	3.07	14	1
1:A:93:LEU:HD22	1:A:93:LEU:H	0.42	1.75	4	1
1:B:38:PHE:CE1	1:B:76:TYR:CD1	0.42	3.07	18	1
1:B:38:PHE:CZ	1:B:76:TYR:CD2	0.42	3.07	8	1
1:B:70:GLU:OE1	1:B:72:LYS:NZ	0.42	2.52	19	1
1:B:58:GLU:OE2	1:B:61:LYS:NZ	0.42	2.52	24	1
1:B:56:LEU:HD13	1:B:56:LEU:C	0.41	2.40	10	1
1:A:14:GLU:OE2	1:B:94:LYS:NZ	0.41	2.52	24	1
1:A:59:LYS:NZ	1:A:86:GLU:OE2	0.41	2.53	13	3
1:B:58:GLU:OE1	1:B:61:LYS:NZ	0.41	2.52	17	1
1:A:10:GLU:OE1	1:B:89:LYS:NZ	0.41	2.51	25	3
1:B:92:ASP:O	1:B:95:ILE:CG1	0.41	2.68	17	1
1:B:6:LEU:CD1	1:B:10:GLU:HB2	0.41	2.45	22	1
1:B:48:HIS:NE2	1:B:89:LYS:NZ	0.41	2.68	5	1
1:B:8:GLU:H	1:B:8:GLU:CD	0.41	2.23	16	1
1:A:57:ASP:OD2	1:A:61:LYS:NZ	0.41	2.53	18	1
1:A:38:PHE:CD1	1:A:76:TYR:CE2	0.41	3.09	3	1
1:A:67:GLN:H	1:A:67:GLN:NE2	0.41	2.13	21	1
1:A:87:ILE:O	1:A:87:ILE:HG23	0.41	2.16	1	1
1:A:31:ASP:CG	1:B:90:LYS:NZ	0.41	2.79	22	1
1:B:35:VAL:HG12	1:B:63:LEU:HG	0.41	1.93	22	1
1:A:13:ILE:HG23	1:A:77:TRP:CH2	0.41	2.51	2	1
1:B:13:ILE:HG23	1:B:77:TRP:CH2	0.41	2.50	2	1
1:A:39:LYS:HB3	1:A:63:LEU:HD21	0.41	1.92	8	1
1:B:9:LEU:H	1:B:9:LEU:HD22	0.41	1.75	9	1
1:A:93:LEU:H	1:A:93:LEU:CD2	0.41	2.23	17	1
1:A:38:PHE:O	1:A:42:VAL:HG13	0.41	2.16	22	1
1:A:14:GLU:OE2	1:B:89:LYS:NZ	0.41	2.53	11	2
1:A:61:LYS:CG	1:A:62:SER:N	0.41	2.83	12	1
1:A:96:ARG:HB3	1:B:4:GLU:CB	0.41	2.46	14	1
1:B:7:THR:HG23	1:B:8:GLU:N	0.40	2.31	8	1
1:A:6:LEU:C	1:A:6:LEU:HD12	0.40	2.41	12	1
1:B:58:GLU:OE2	1:B:85:LYS:NZ	0.40	2.54	23	1
1:A:58:GLU:OE2	1:A:61:LYS:NZ	0.40	2.52	24	1
1:A:14:GLU:OE1	1:B:94:LYS:NZ	0.40	2.53	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:HIS:CE1	1:B:93:LEU:HD11	0.40	2.51	1	1
1:B:91:LYS:NZ	1:B:92:ASP:OD2	0.40	2.55	11	1
1:B:32:SER:OG	1:B:71:LEU:HD11	0.40	2.15	18	1
1:B:57:ASP:OD1	1:B:61:LYS:NZ	0.40	2.54	22	1
1:A:78:ARG:HH21	1:B:82:GLU:CD	0.40	2.25	16	1
1:B:95:ILE:C	1:B:96:ARG:HG3	0.40	2.42	19	1
1:A:89:LYS:NZ	1:B:10:GLU:OE2	0.40	2.55	21	1
1:B:4:GLU:CD	1:B:4:GLU:N	0.40	2.80	25	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/98 (87%)	66±2 (78±3%)	15±2 (18±3%)	4±1 (5±1%)	3	26
1	B	86/98 (88%)	64±3 (74±3%)	18±3 (20±4%)	5±2 (5±2%)	2	22
All	All	4275/4900 (87%)	3246 (76%)	815 (19%)	214 (5%)	3	24

All 40 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	52	ASP	22
1	B	52	ASP	18
1	B	91	LYS	12
1	A	77	TRP	11
1	B	86	GLU	10
1	A	91	LYS	9
1	B	31	ASP	9
1	B	30	LYS	8
1	B	90	LYS	8
1	B	77	TRP	8
1	A	46	LEU	7
1	B	65	VAL	7
1	A	31	ASP	7

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Mol	Chain	Res	Type	Models (Total)
1	B	5	PRO	6
1	A	49	LEU	6
1	B	49	LEU	6
1	A	48	HIS	6
1	A	86	GLU	5
1	B	96	ARG	5
1	A	69	SER	5
1	A	70	GLU	5
1	B	46	LEU	4
1	A	96	ARG	4
1	A	65	VAL	3
1	B	70	GLU	3
1	A	50	LEU	2
1	B	4	GLU	2
1	B	48	HIS	2
1	A	89	LYS	2
1	B	54	GLY	2
1	A	94	LYS	1
1	A	53	VAL	1
1	B	13	ILE	1
1	B	50	LEU	1
1	A	54	GLY	1
1	B	93	LEU	1
1	B	8	GLU	1
1	B	69	SER	1
1	B	89	LYS	1
1	A	90	LYS	1

6.3.2 Protein sidechains ⓘ

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	82/91 (90%)	66±2 (80±3%)	16±2 (20±3%)	3	33
1	B	83/91 (91%)	65±3 (78±3%)	18±3 (22±3%)	2	30
All	All	4125/4550 (91%)	3262 (79%)	863 (21%)	3	31

All 132 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	51	LYS	25
1	B	51	LYS	25
1	B	59	LYS	23
1	A	45	GLN	22
1	B	63	LEU	22
1	A	59	LYS	22
1	B	45	GLN	21
1	A	63	LEU	19
1	B	6	LEU	18
1	B	87	ILE	18
1	B	67	GLN	16
1	B	49	LEU	15
1	A	67	GLN	13
1	B	89	LYS	13
1	A	61	LYS	12
1	A	83	LEU	12
1	A	89	LYS	12
1	B	83	LEU	12
1	A	93	LEU	12
1	B	77	TRP	12
1	A	18	THR	11
1	A	49	LEU	11
1	A	87	ILE	11
1	A	4	GLU	11
1	A	14	GLU	10
1	A	96	ARG	10
1	B	4	GLU	10
1	B	30	LYS	10
1	B	39	LYS	10
1	B	96	ARG	10
1	A	77	TRP	10
1	A	43	THR	10
1	B	43	THR	10
1	B	79	LEU	9
1	B	50	LEU	9
1	A	68	ASP	9
1	B	93	LEU	9
1	A	33	LEU	9
1	A	10	GLU	8
1	B	61	LYS	8
1	A	80	ILE	8
1	B	14	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	B	94	LYS	8
1	A	39	LYS	8
1	A	79	LEU	8
1	A	36	ASN	7
1	B	11	GLU	7
1	B	33	LEU	7
1	B	80	ILE	7
1	B	72	LYS	7
1	A	46	LEU	7
1	B	10	GLU	7
1	B	71	LEU	7
1	A	7	THR	7
1	A	86	GLU	6
1	B	18	THR	6
1	B	56	LEU	6
1	A	34	SER	6
1	A	91	LYS	6
1	B	86	GLU	6
1	A	6	LEU	6
1	B	7	THR	6
1	B	34	SER	6
1	A	70	GLU	5
1	B	92	ASP	5
1	A	11	GLU	5
1	A	56	LEU	5
1	B	48	HIS	5
1	A	72	LYS	5
1	A	50	LEU	4
1	A	85	LYS	4
1	B	36	ASN	4
1	B	55	SER	4
1	B	68	ASP	4
1	B	91	LYS	4
1	B	85	LYS	4
1	A	71	LEU	4
1	A	94	LYS	4
1	A	82	GLU	3
1	B	95	ILE	3
1	B	52	ASP	3
1	A	75	GLU	3
1	A	53	VAL	3
1	B	46	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	74	ASN	3
1	B	8	GLU	3
1	B	13	ILE	3
1	B	21	PHE	3
1	A	48	HIS	3
1	B	90	LYS	3
1	B	31	ASP	3
1	A	58	GLU	3
1	A	35	VAL	3
1	B	70	GLU	3
1	A	31	ASP	2
1	B	53	VAL	2
1	B	78	ARG	2
1	B	66	ASN	2
1	A	60	MET	2
1	A	8	GLU	2
1	B	41	LEU	2
1	B	76	TYR	2
1	A	78	ARG	2
1	B	22	THR	2
1	B	9	LEU	2
1	B	17	VAL	2
1	B	35	VAL	2
1	B	75	GLU	2
1	A	88	ARG	2
1	A	90	LYS	1
1	A	21	PHE	1
1	A	41	LEU	1
1	B	65	VAL	1
1	A	19	THR	1
1	A	22	THR	1
1	A	74	ASN	1
1	A	76	TYR	1
1	B	60	MET	1
1	A	9	LEU	1
1	A	57	ASP	1
1	A	44	GLN	1
1	A	66	ASN	1
1	B	58	GLU	1
1	A	69	SER	1
1	A	15	THR	1
1	A	42	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	65	VAL	1
1	B	12	SER	1
1	B	19	THR	1
1	A	55	SER	1
1	B	15	THR	1
1	A	37	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 oligosaccharides 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

No chemical shift data were provided