



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:20 PM BST

PDB ID : 2BDS
Title : DETERMINATION OF THE THREE-DIMENSIONAL SOLUTION STRUCTURE OF THE ANTIHYPERTENSIVE AND ANTIVIRAL PROTEIN BDS-I FROM THE SEA ANEMONE ANEMONIA SULCATA. A STUDY USING NUCLEAR MAGNETIC RESONANCE AND HYBRID DISTANCE GEOMETRY-DYNAMICAL SIMULATED ANNEALING
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Deposited on : 1988-11-14

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
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

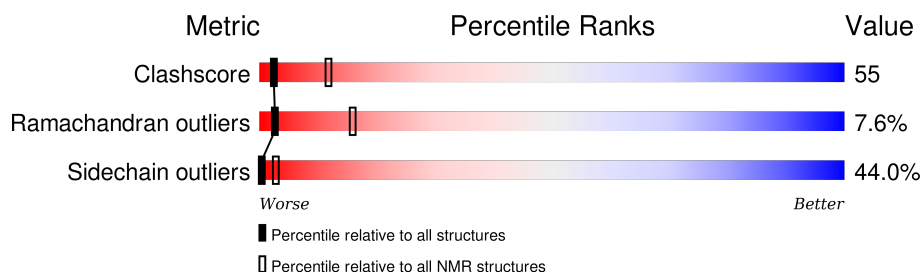
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	43	<div> <div></div> <div>28%</div> <div>44%</div> <div>21%</div> <div>5% •</div> </div>

2 Ensemble composition and analysis

This entry contains 42 models. Model 3 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:43 (42)	0.39	3

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 7 clusters. No single-model clusters were found.

Cluster number	Models
1	6, 7, 11, 18, 19, 20, 27, 28, 30, 33, 34, 35, 38, 42
2	2, 3, 5, 12, 14, 16, 22, 24, 25, 31, 32, 36, 39
3	1, 8, 9, 15, 21, 40
4	4, 17, 26
5	10, 29
6	23, 37
7	13, 41

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 629 atoms, of which 300 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BDS-I.

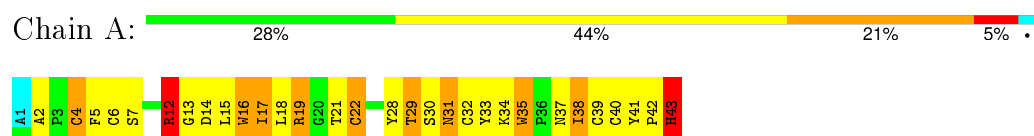
Mol	Chain	Residues	Atoms						Trace
1	A	43	Total	C	H	N	O	S	0
			629	210	300	57	56	6	

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: BDS-I

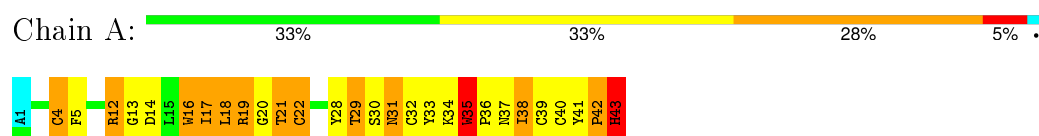


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

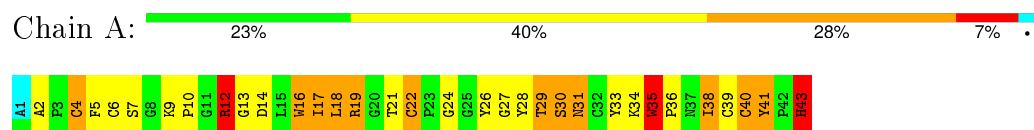
4.2.1 Score per residue for model 1

- Molecule 1: BDS-I



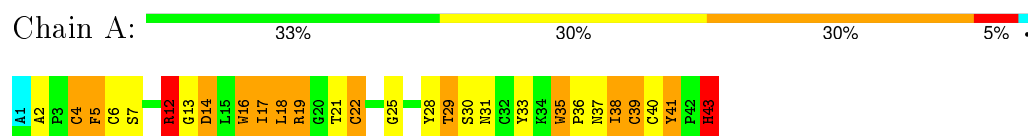
4.2.2 Score per residue for model 2

- Molecule 1: BDS-I



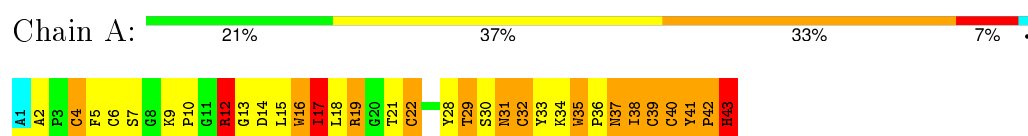
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: BDS-I



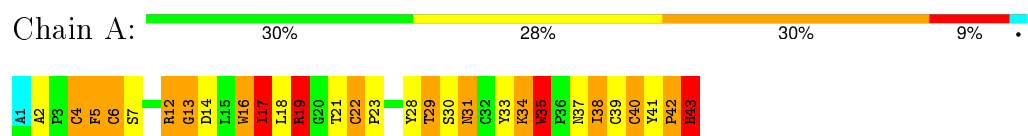
4.2.4 Score per residue for model 4

- Molecule 1: BDS-I



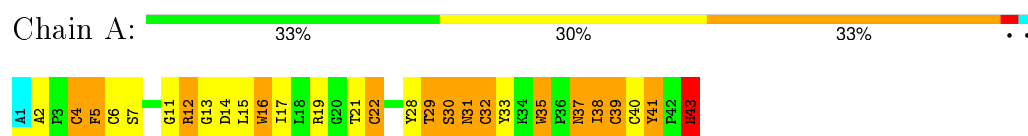
4.2.5 Score per residue for model 5

- Molecule 1: BDS-I



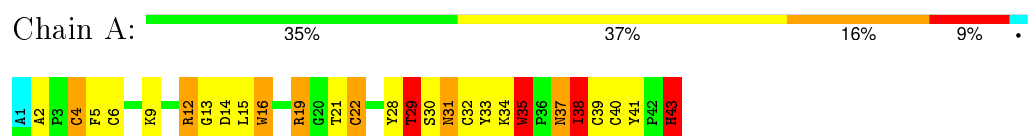
4.2.6 Score per residue for model 6

- Molecule 1: BDS-I



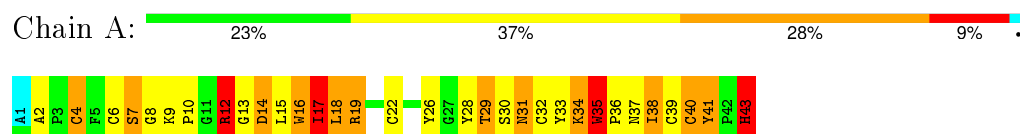
4.2.7 Score per residue for model 7

- Molecule 1: BDS-I



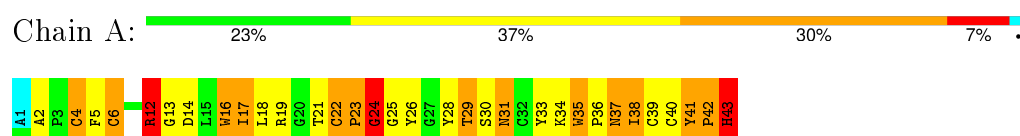
4.2.8 Score per residue for model 8

- Molecule 1: BDS-I



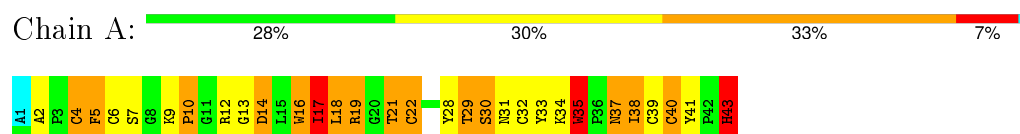
4.2.9 Score per residue for model 9

- Molecule 1: BDS-I



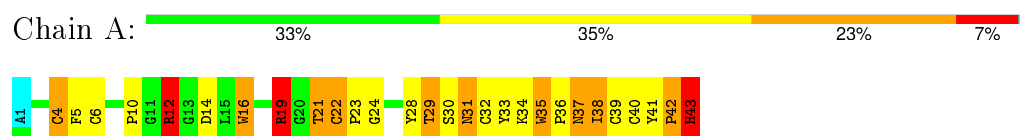
4.2.10 Score per residue for model 10

- Molecule 1: BDS-I



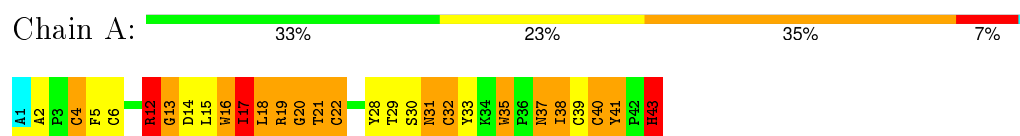
4.2.11 Score per residue for model 11

- Molecule 1: BDS-I



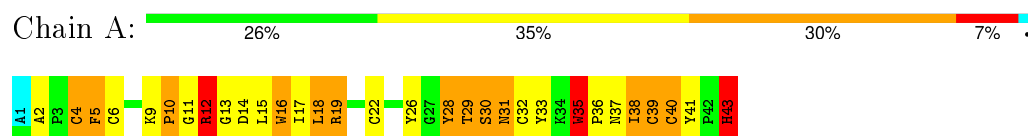
4.2.12 Score per residue for model 12

- Molecule 1: BDS-I



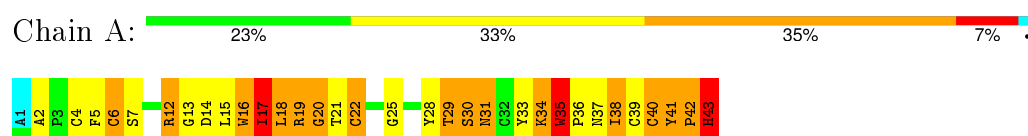
4.2.13 Score per residue for model 13

- Molecule 1: BDS-I



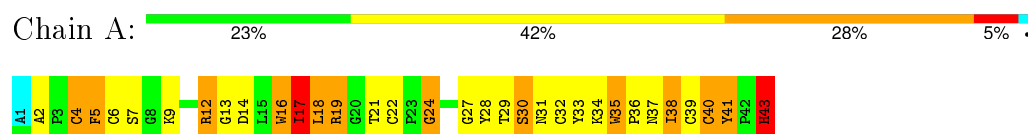
4.2.14 Score per residue for model 14

- Molecule 1: BDS-I



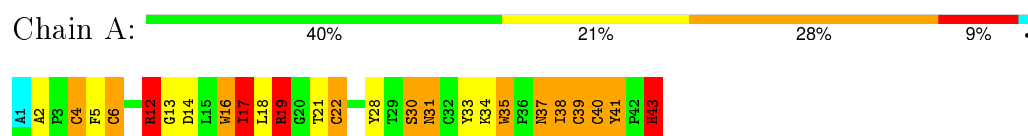
4.2.15 Score per residue for model 15

- Molecule 1: BDS-I



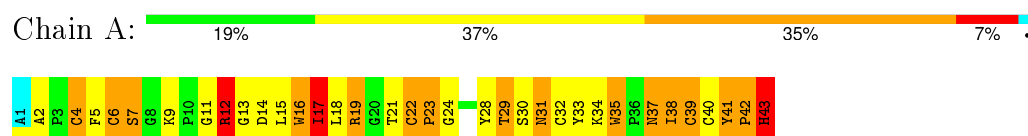
4.2.16 Score per residue for model 16

- Molecule 1: BDS-I



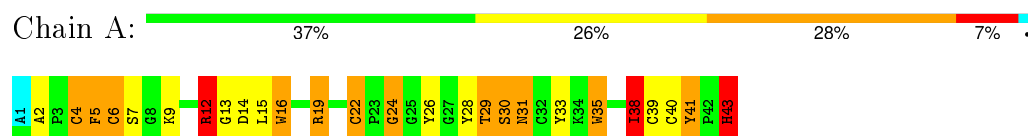
4.2.17 Score per residue for model 17

- Molecule 1: BDS-I



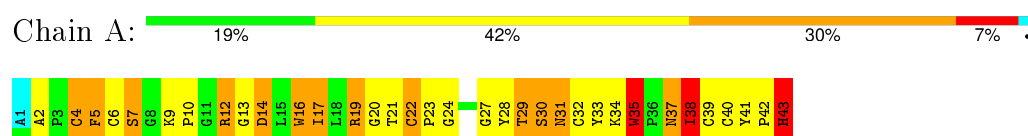
4.2.18 Score per residue for model 18

- Molecule 1: BDS-I



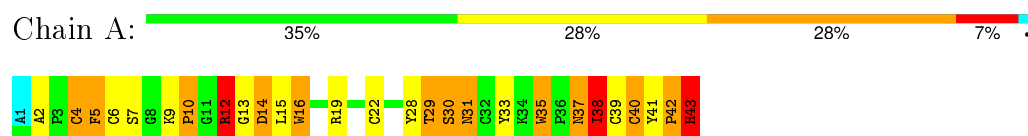
4.2.19 Score per residue for model 19

- Molecule 1: BDS-I



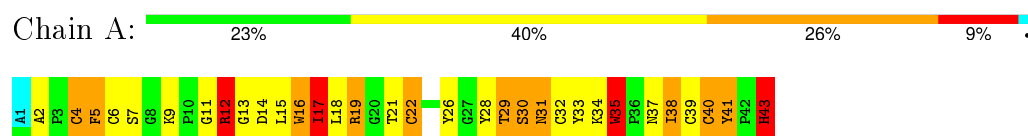
4.2.20 Score per residue for model 20

- Molecule 1: BDS-I



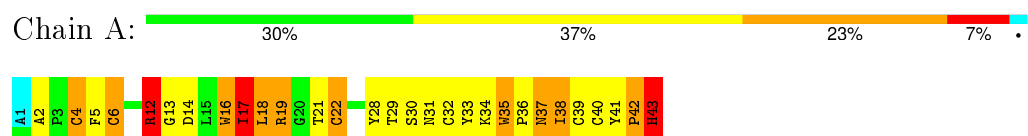
4.2.21 Score per residue for model 21

- Molecule 1: BDS-I



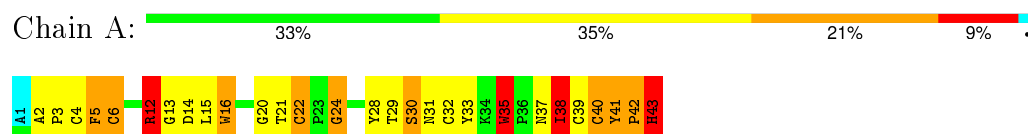
4.2.22 Score per residue for model 22

- Molecule 1: BDS-I



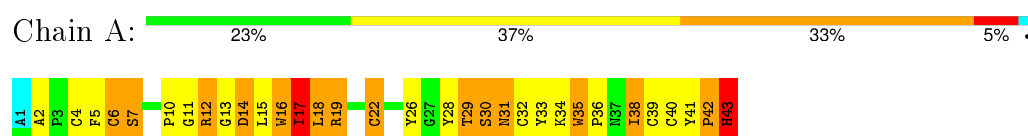
4.2.23 Score per residue for model 23

- Molecule 1: BDS-I



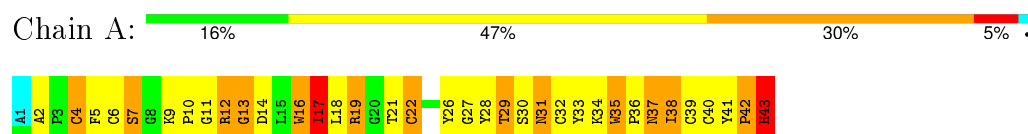
4.2.24 Score per residue for model 24

- Molecule 1: BDS-I



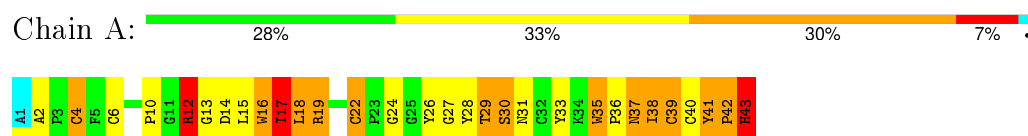
4.2.25 Score per residue for model 25

- Molecule 1: BDS-I



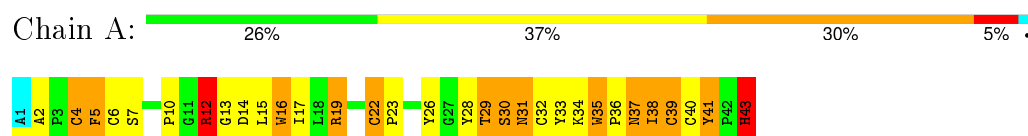
4.2.26 Score per residue for model 26

- Molecule 1: BDS-I



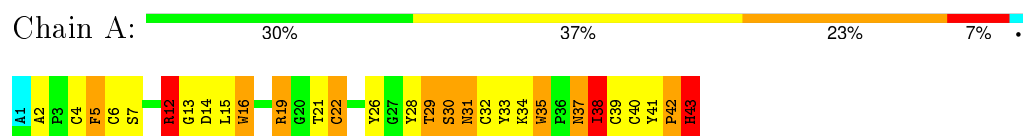
4.2.27 Score per residue for model 27

- Molecule 1: BDS-I



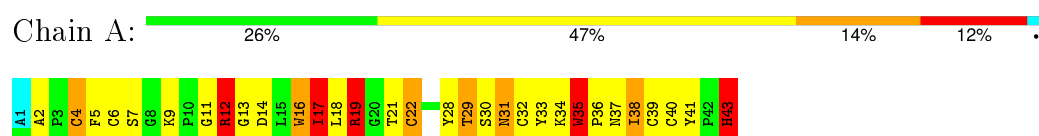
4.2.28 Score per residue for model 28

- Molecule 1: BDS-I



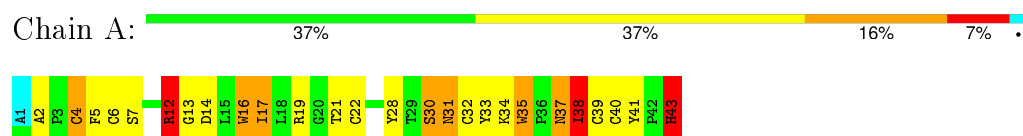
4.2.29 Score per residue for model 29

- Molecule 1: BDS-I



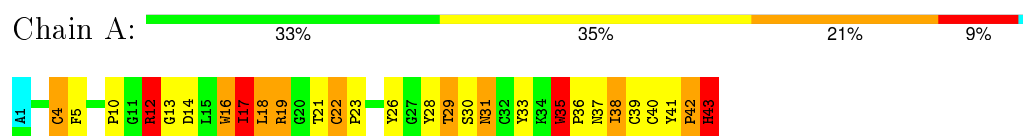
4.2.30 Score per residue for model 30

- Molecule 1: BDS-I



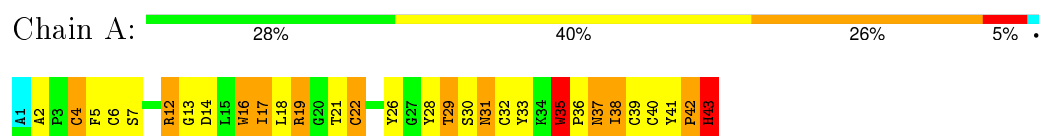
4.2.31 Score per residue for model 31

- Molecule 1: BDS-I



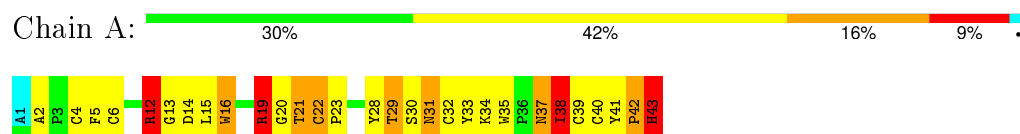
4.2.32 Score per residue for model 32

- Molecule 1: BDS-I



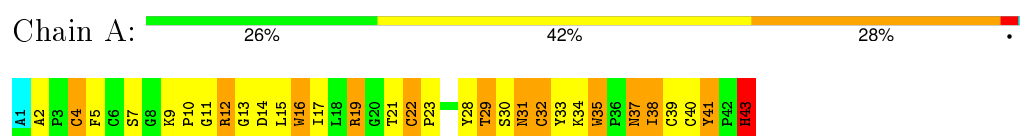
4.2.33 Score per residue for model 33

- Molecule 1: BDS-I



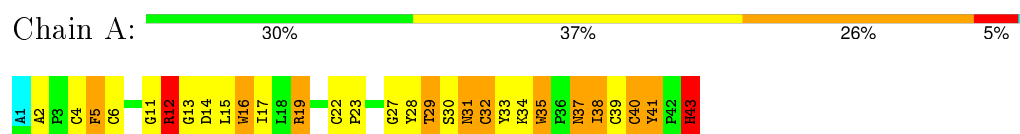
4.2.34 Score per residue for model 34

- Molecule 1: BDS-I



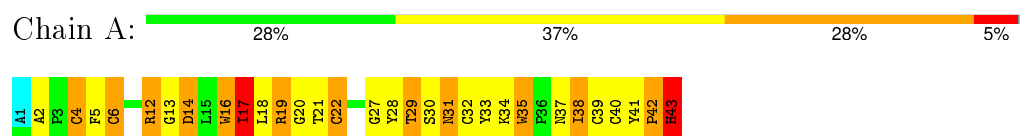
4.2.35 Score per residue for model 35

- Molecule 1: BDS-I



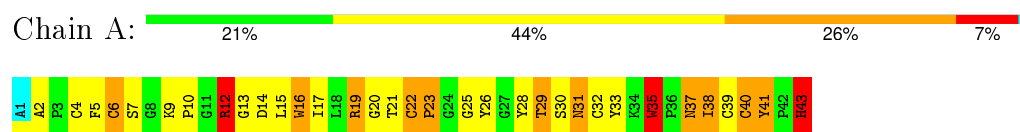
4.2.36 Score per residue for model 36

- Molecule 1: BDS-I



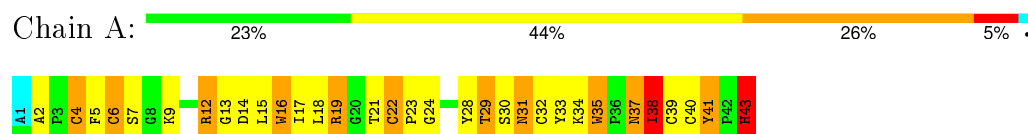
4.2.37 Score per residue for model 37

- Molecule 1: BDS-I



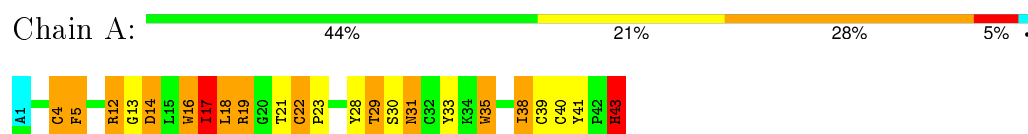
4.2.38 Score per residue for model 38

- Molecule 1: BDS-I



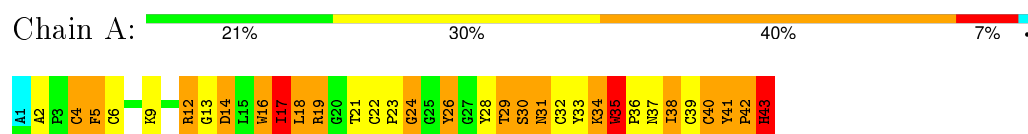
4.2.39 Score per residue for model 39

- Molecule 1: BDS-I



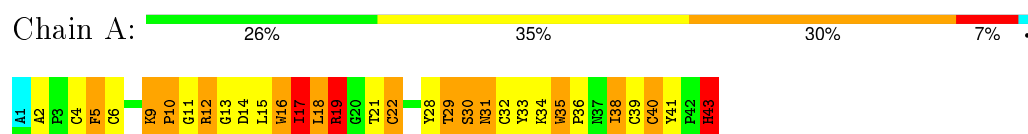
4.2.40 Score per residue for model 40

- Molecule 1: BDS-I



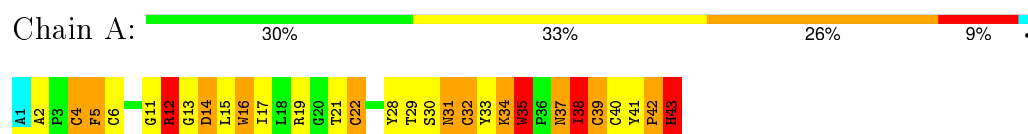
4.2.41 Score per residue for model 41

- Molecule 1: BDS-I



4.2.42 Score per residue for model 42

- Molecule 1: BDS-I



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 42 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	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

6.1 Standard geometry

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	1.31±0.02	3±0/338 (1.0±0.1%)	1.67±0.03	14±1/459 (3.0±0.2%)
All	All	1.31	136/14196 (1.0%)	1.67	569/19278 (3.0%)

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	1.9±0.3
All	All	0	78

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	16	TRP	CG-CD2	-8.08	1.29	1.43	18	42
1	A	35	TRP	CG-CD2	-7.72	1.30	1.43	9	42
1	A	43	HIS	CG-ND1	-6.47	1.24	1.38	5	42
1	A	35	TRP	CG-CD1	-6.15	1.28	1.36	36	10

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	35	TRP	NE1-CE2-CZ2	10.27	141.69	130.40	9	42
1	A	16	TRP	NE1-CE2-CZ2	9.69	141.06	130.40	14	42
1	A	35	TRP	NE1-CE2-CD2	-8.47	98.83	107.30	9	42
1	A	24	GLY	N-CA-C	7.88	132.80	113.10	9	8
1	A	16	TRP	CG-CD2-CE3	-7.71	126.96	133.90	18	42
1	A	16	TRP	NE1-CE2-CD2	-7.64	99.66	107.30	14	42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	35	TRP	CG-CD2-CE3	-7.45	127.20	133.90	9	38
1	A	25	GLY	N-CA-C	7.03	130.68	113.10	3	2
1	A	16	TRP	CG-CD1-NE1	-7.01	103.09	110.10	17	42
1	A	11	GLY	N-CA-C	6.98	130.54	113.10	35	5
1	A	35	TRP	CD1-CG-CD2	6.82	111.76	106.30	9	37
1	A	35	TRP	CG-CD1-NE1	-6.57	103.53	110.10	10	42
1	A	35	TRP	CD1-NE1-CE2	6.17	114.55	109.00	13	42
1	A	16	TRP	CD1-NE1-CE2	6.09	114.48	109.00	13	42
1	A	16	TRP	CD1-CG-CD2	5.99	111.09	106.30	25	42
1	A	16	TRP	CE2-CD2-CG	5.89	112.01	107.30	14	42
1	A	13	GLY	N-CA-C	5.59	127.07	113.10	12	3
1	A	35	TRP	CE2-CD2-CG	5.46	111.67	107.30	9	12
1	A	20	GLY	N-CA-C	5.43	126.67	113.10	12	2

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	12	ARG	Sidechain	40
1	A	19	ARG	Sidechain	38

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	324	293	293	34±5
All	All	13608	12306	12306	1433

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 55.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASN:N	1:A:37:ASN:HD22	0.83	1.71	35	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:ASN:HD22	1:A:37:ASN:N	0.79	1.76	34	4
1:A:33:TYR:CE2	1:A:38:ILE:HD12	0.77	2.14	12	41
1:A:33:TYR:CD2	1:A:38:ILE:HD12	0.76	2.15	40	40
1:A:33:TYR:CD1	1:A:38:ILE:HD12	0.75	2.16	27	1
1:A:16:TRP:HB2	1:A:38:ILE:HG23	0.73	1.60	42	41
1:A:17:ILE:HD12	1:A:17:ILE:H	0.73	1.43	12	5
1:A:17:ILE:N	1:A:17:ILE:HD13	0.70	2.01	8	2
1:A:37:ASN:HD22	1:A:37:ASN:H	0.69	1.29	30	4
1:A:5:PHE:N	1:A:5:PHE:CD1	0.69	2.59	20	9
1:A:28:TYR:CD2	1:A:40:CYS:SG	0.68	2.87	12	42
1:A:31:ASN:ND2	1:A:31:ASN:N	0.68	2.40	38	10
1:A:36:PRO:C	1:A:37:ASN:HD22	0.68	1.92	27	2
1:A:31:ASN:N	1:A:31:ASN:ND2	0.68	2.41	31	5
1:A:16:TRP:CB	1:A:38:ILE:HG23	0.67	2.20	33	42
1:A:17:ILE:O	1:A:38:ILE:HG22	0.67	1.90	16	26
1:A:37:ASN:N	1:A:37:ASN:ND2	0.66	2.43	20	11
1:A:37:ASN:ND2	1:A:37:ASN:N	0.66	2.43	27	14
1:A:28:TYR:CG	1:A:40:CYS:SG	0.66	2.89	30	35
1:A:5:PHE:CD1	1:A:5:PHE:N	0.66	2.62	41	10
1:A:2:ALA:HB3	1:A:13:GLY:O	0.66	1.90	12	10
1:A:4:CYS:O	1:A:13:GLY:N	0.66	2.29	5	39
1:A:19:ARG:HH11	1:A:19:ARG:CG	0.65	2.04	7	1
1:A:33:TYR:CE1	1:A:38:ILE:HD12	0.63	2.28	27	1
1:A:43:HIS:C	1:A:43:HIS:CD2	0.62	2.73	20	21
1:A:37:ASN:ND2	1:A:37:ASN:H	0.62	1.92	12	3
1:A:22:CYS:SG	1:A:28:TYR:CD2	0.62	2.93	29	33
1:A:12:ARG:O	1:A:43:HIS:ND1	0.62	2.33	5	21
1:A:17:ILE:H	1:A:17:ILE:HD12	0.62	1.55	29	1
1:A:31:ASN:H	1:A:31:ASN:ND2	0.61	1.92	29	3
1:A:18:LEU:H	1:A:18:LEU:HD12	0.61	1.55	1	2
1:A:43:HIS:CD2	1:A:43:HIS:C	0.61	2.73	1	21
1:A:6:CYS:SG	1:A:41:TYR:CD1	0.61	2.93	9	12
1:A:18:LEU:N	1:A:18:LEU:HD12	0.61	2.11	1	5
1:A:26:TYR:CD1	1:A:26:TYR:N	0.61	2.68	40	1
1:A:18:LEU:HD22	1:A:18:LEU:H	0.60	1.55	10	1
1:A:17:ILE:HG22	1:A:18:LEU:HD13	0.60	1.73	13	1
1:A:22:CYS:SG	1:A:28:TYR:CE2	0.60	2.95	17	22
1:A:31:ASN:OD1	1:A:31:ASN:N	0.60	2.35	28	10
1:A:7:SER:O	1:A:9:LYS:N	0.59	2.35	8	3
1:A:17:ILE:HG22	1:A:18:LEU:H	0.59	1.56	13	1
1:A:19:ARG:NH2	1:A:23:PRO:N	0.59	2.51	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:CD1	1:A:18:LEU:H	0.59	2.11	1	4
1:A:17:ILE:H	1:A:17:ILE:CD1	0.59	2.11	12	2
1:A:41:TYR:CE2	1:A:43:HIS:ND1	0.58	2.71	20	16
1:A:2:ALA:HB2	1:A:15:LEU:CB	0.58	2.27	35	11
1:A:12:ARG:O	1:A:41:TYR:CE1	0.58	2.57	24	14
1:A:23:PRO:O	1:A:26:TYR:CD2	0.58	2.56	40	1
1:A:12:ARG:H	1:A:43:HIS:CE1	0.58	2.16	25	16
1:A:16:TRP:N	1:A:38:ILE:O	0.58	2.37	4	26
1:A:18:LEU:H	1:A:18:LEU:HD13	0.58	1.59	13	1
1:A:41:TYR:CD2	1:A:42:PRO:O	0.57	2.57	40	19
1:A:18:LEU:HD12	1:A:18:LEU:N	0.57	2.14	2	6
1:A:41:TYR:CZ	1:A:43:HIS:ND1	0.57	2.72	5	17
1:A:2:ALA:HB3	1:A:15:LEU:HB2	0.57	1.77	4	6
1:A:12:ARG:O	1:A:43:HIS:CG	0.57	2.57	24	18
1:A:12:ARG:HE	1:A:13:GLY:N	0.57	1.96	37	5
1:A:2:ALA:O	1:A:13:GLY:O	0.57	2.23	42	28
1:A:30:SER:O	1:A:41:TYR:O	0.56	2.23	10	37
1:A:31:ASN:ND2	1:A:31:ASN:H	0.56	1.99	21	5
1:A:31:ASN:N	1:A:31:ASN:OD1	0.56	2.38	42	8
1:A:12:ARG:NH1	1:A:14:ASP:OD1	0.56	2.37	33	4
1:A:18:LEU:HD12	1:A:18:LEU:H	0.56	1.59	2	4
1:A:28:TYR:O	1:A:29:THR:HG23	0.56	2.01	11	33
1:A:37:ASN:C	1:A:38:ILE:HG22	0.56	2.21	7	8
1:A:37:ASN:H	1:A:37:ASN:HD22	0.55	1.44	19	5
1:A:19:ARG:O	1:A:21:THR:N	0.55	2.39	12	5
1:A:14:ASP:O	1:A:39:CYS:HA	0.55	2.01	9	41
1:A:17:ILE:O	1:A:19:ARG:N	0.55	2.39	21	26
1:A:12:ARG:O	1:A:43:HIS:CE1	0.55	2.60	32	4
1:A:5:PHE:CD2	1:A:11:GLY:O	0.54	2.61	34	4
1:A:4:CYS:SG	1:A:34:LYS:NZ	0.54	2.81	9	1
1:A:2:ALA:HB2	1:A:15:LEU:HB3	0.54	1.78	35	14
1:A:32:CYS:SG	1:A:39:CYS:O	0.53	2.66	35	11
1:A:19:ARG:NH1	1:A:19:ARG:CG	0.53	2.67	7	2
1:A:19:ARG:NE	1:A:21:THR:O	0.53	2.41	7	3
1:A:12:ARG:HH11	1:A:43:HIS:HB2	0.53	1.63	33	1
1:A:12:ARG:O	1:A:41:TYR:CZ	0.53	2.62	39	15
1:A:18:LEU:N	1:A:18:LEU:HD13	0.53	2.18	10	1
1:A:12:ARG:HH22	1:A:14:ASP:CG	0.53	2.07	4	2
1:A:31:ASN:ND2	1:A:33:TYR:OH	0.53	2.42	40	3
1:A:31:ASN:HD22	1:A:31:ASN:H	0.53	1.47	38	2
1:A:12:ARG:CG	1:A:13:GLY:N	0.53	2.72	31	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:HIS:CG	1:A:43:HIS:O	0.53	2.62	33	7
1:A:12:ARG:O	1:A:41:TYR:CE2	0.52	2.62	11	1
1:A:12:ARG:NH2	1:A:14:ASP:OD1	0.52	2.43	8	5
1:A:2:ALA:HB3	1:A:15:LEU:H	0.52	1.64	7	2
1:A:33:TYR:CD1	1:A:33:TYR:N	0.52	2.77	40	4
1:A:43:HIS:O	1:A:43:HIS:CG	0.52	2.62	16	3
1:A:17:ILE:O	1:A:17:ILE:HG22	0.52	2.04	37	4
1:A:17:ILE:HD13	1:A:17:ILE:N	0.52	2.19	40	1
1:A:4:CYS:SG	1:A:5:PHE:O	0.52	2.68	42	4
1:A:33:TYR:CE2	1:A:38:ILE:CD1	0.51	2.93	31	38
1:A:36:PRO:C	1:A:37:ASN:ND2	0.51	2.64	26	15
1:A:2:ALA:O	1:A:12:ARG:NH2	0.51	2.42	15	1
1:A:4:CYS:SG	1:A:13:GLY:O	0.51	2.68	28	2
1:A:4:CYS:O	1:A:4:CYS:SG	0.51	2.69	28	7
1:A:9:LYS:O	1:A:10:PRO:O	0.51	2.29	20	4
1:A:30:SER:O	1:A:41:TYR:CB	0.51	2.59	15	19
1:A:19:ARG:C	1:A:21:THR:N	0.50	2.65	1	3
1:A:33:TYR:CZ	1:A:38:ILE:CD1	0.50	2.94	3	2
1:A:43:HIS:CG	1:A:43:HIS:OXT	0.50	2.65	37	2
1:A:5:PHE:CE2	1:A:11:GLY:O	0.50	2.65	17	3
1:A:19:ARG:C	1:A:21:THR:H	0.50	2.10	1	2
1:A:33:TYR:N	1:A:33:TYR:CD1	0.50	2.80	37	10
1:A:17:ILE:CD1	1:A:17:ILE:N	0.50	2.67	8	1
1:A:6:CYS:SG	1:A:34:LYS:NZ	0.49	2.86	22	2
1:A:18:LEU:H	1:A:18:LEU:CD1	0.49	2.18	40	4
1:A:35:TRP:CD1	1:A:35:TRP:C	0.49	2.86	22	3
1:A:17:ILE:N	1:A:17:ILE:CD1	0.49	2.75	4	2
1:A:33:TYR:CE1	1:A:38:ILE:CD1	0.49	2.95	27	1
1:A:4:CYS:SG	1:A:4:CYS:O	0.49	2.71	24	5
1:A:12:ARG:O	1:A:43:HIS:CB	0.49	2.61	34	9
1:A:14:ASP:O	1:A:40:CYS:N	0.49	2.46	41	4
1:A:17:ILE:HG22	1:A:18:LEU:CD1	0.48	2.38	13	1
1:A:12:ARG:HE	1:A:12:ARG:C	0.48	2.12	27	5
1:A:12:ARG:C	1:A:12:ARG:HE	0.48	2.12	16	2
1:A:42:PRO:O	1:A:43:HIS:ND1	0.48	2.47	23	4
1:A:23:PRO:O	1:A:24:GLY:C	0.48	2.51	40	1
1:A:18:LEU:CA	1:A:36:PRO:O	0.48	2.62	24	8
1:A:17:ILE:CD1	1:A:17:ILE:H	0.48	2.12	41	1
1:A:35:TRP:C	1:A:35:TRP:CD1	0.48	2.87	26	2
1:A:30:SER:O	1:A:41:TYR:C	0.48	2.52	17	27
1:A:20:GLY:CA	1:A:35:TRP:HE1	0.48	2.22	37	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:TYR:HH	1:A:43:HIS:HD1	0.48	1.51	12	1
1:A:10:PRO:O	1:A:41:TYR:OH	0.47	2.32	4	2
1:A:18:LEU:CD1	1:A:18:LEU:N	0.47	2.78	2	2
1:A:38:ILE:HG13	1:A:39:CYS:N	0.47	2.25	2	3
1:A:28:TYR:CD1	1:A:41:TYR:O	0.47	2.68	12	2
1:A:12:ARG:HG3	1:A:13:GLY:N	0.47	2.25	28	5
1:A:16:TRP:O	1:A:38:ILE:N	0.47	2.48	18	13
1:A:17:ILE:HG22	1:A:17:ILE:O	0.47	2.10	35	1
1:A:17:ILE:HG22	1:A:18:LEU:HD22	0.47	1.87	10	1
1:A:17:ILE:HG22	1:A:18:LEU:CD2	0.47	2.40	10	1
1:A:7:SER:C	1:A:9:LYS:N	0.47	2.69	4	1
1:A:12:ARG:CZ	1:A:14:ASP:OD1	0.46	2.63	8	2
1:A:18:LEU:N	1:A:18:LEU:HD22	0.46	2.26	13	1
1:A:15:LEU:HD23	1:A:15:LEU:C	0.46	2.30	7	1
1:A:2:ALA:HB3	1:A:15:LEU:N	0.46	2.26	20	2
1:A:42:PRO:O	1:A:43:HIS:CB	0.46	2.64	14	14
1:A:32:CYS:SG	1:A:34:LYS:NZ	0.46	2.89	28	1
1:A:3:PRO:O	1:A:5:PHE:CE1	0.46	2.69	23	1
1:A:22:CYS:O	1:A:24:GLY:N	0.45	2.49	9	1
1:A:35:TRP:HA	1:A:37:ASN:N	0.45	2.27	21	6
1:A:43:HIS:OXT	1:A:43:HIS:CG	0.45	2.69	8	1
1:A:43:HIS:CD2	1:A:43:HIS:OXT	0.45	2.69	37	2
1:A:41:TYR:CZ	1:A:43:HIS:CE1	0.45	3.04	22	6
1:A:32:CYS:C	1:A:33:TYR:CD1	0.45	2.90	35	3
1:A:34:LYS:O	1:A:35:TRP:C	0.45	2.54	30	17
1:A:12:ARG:HH21	1:A:43:HIS:HB2	0.45	1.72	21	1
1:A:43:HIS:OXT	1:A:43:HIS:CD2	0.45	2.70	28	1
1:A:7:SER:C	1:A:9:LYS:H	0.45	2.15	4	4
1:A:7:SER:OG	1:A:7:SER:O	0.45	2.34	20	2
1:A:14:ASP:O	1:A:39:CYS:CA	0.45	2.65	13	2
1:A:41:TYR:CE2	1:A:43:HIS:CE1	0.45	3.04	20	4
1:A:14:ASP:OD1	1:A:14:ASP:N	0.45	2.48	41	2
1:A:38:ILE:CG1	1:A:39:CYS:N	0.45	2.80	10	2
1:A:18:LEU:CB	1:A:36:PRO:O	0.45	2.65	31	6
1:A:35:TRP:CD1	1:A:36:PRO:N	0.45	2.85	22	3
1:A:22:CYS:O	1:A:23:PRO:O	0.44	2.34	37	2
1:A:22:CYS:N	1:A:33:TYR:OH	0.44	2.50	3	1
1:A:12:ARG:HG3	1:A:43:HIS:CD2	0.44	2.48	1	3
1:A:23:PRO:O	1:A:25:GLY:N	0.44	2.50	9	1
1:A:28:TYR:CE2	1:A:40:CYS:SG	0.44	3.11	12	4
1:A:31:ASN:HD22	1:A:31:ASN:N	0.44	2.07	38	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:ASN:OD1	1:A:33:TYR:OH	0.44	2.34	27	1
1:A:20:GLY:O	1:A:33:TYR:CE2	0.44	2.70	19	3
1:A:10:PRO:O	1:A:12:ARG:N	0.44	2.50	41	2
1:A:43:HIS:O	1:A:43:HIS:CD2	0.44	2.71	16	3
1:A:19:ARG:HH11	1:A:19:ARG:HG3	0.44	1.69	7	1
1:A:19:ARG:O	1:A:21:THR:OG1	0.44	2.36	1	1
1:A:33:TYR:CZ	1:A:38:ILE:HD12	0.43	2.47	3	3
1:A:42:PRO:O	1:A:43:HIS:OXT	0.43	2.36	25	1
1:A:12:ARG:CG	1:A:43:HIS:CD2	0.43	3.01	5	4
1:A:43:HIS:CD2	1:A:43:HIS:O	0.43	2.71	35	2
1:A:2:ALA:C	1:A:4:CYS:H	0.43	2.17	41	7
1:A:17:ILE:CG2	1:A:18:LEU:HD22	0.43	2.43	10	1
1:A:42:PRO:O	1:A:43:HIS:O	0.43	2.36	32	4
1:A:17:ILE:O	1:A:17:ILE:CG2	0.43	2.66	37	1
1:A:18:LEU:N	1:A:18:LEU:CD1	0.43	2.82	40	1
1:A:37:ASN:H	1:A:37:ASN:ND2	0.43	2.10	38	2
1:A:30:SER:O	1:A:41:TYR:N	0.43	2.52	5	2
1:A:12:ARG:O	1:A:41:TYR:OH	0.43	2.37	39	1
1:A:28:TYR:CD1	1:A:40:CYS:SG	0.43	3.12	36	1
1:A:17:ILE:HD12	1:A:17:ILE:N	0.42	2.22	12	1
1:A:19:ARG:CG	1:A:19:ARG:HH11	0.42	2.27	32	1
1:A:13:GLY:CA	1:A:41:TYR:CZ	0.42	3.02	13	1
1:A:14:ASP:OD2	1:A:28:TYR:OH	0.42	2.36	35	2
1:A:6:CYS:SG	1:A:39:CYS:O	0.42	2.77	2	1
1:A:19:ARG:NH2	1:A:22:CYS:C	0.42	2.73	33	1
1:A:42:PRO:O	1:A:43:HIS:CG	0.42	2.73	23	1
1:A:12:ARG:NH1	1:A:14:ASP:CG	0.41	2.73	26	1
1:A:2:ALA:HB1	1:A:4:CYS:HB3	0.41	1.92	12	6
1:A:17:ILE:N	1:A:17:ILE:HD12	0.41	2.29	29	1
1:A:28:TYR:O	1:A:29:THR:CG2	0.41	2.69	36	2
1:A:31:ASN:CG	1:A:33:TYR:OH	0.41	2.59	42	4
1:A:2:ALA:HB3	1:A:15:LEU:CB	0.41	2.45	6	2
1:A:14:ASP:CB	1:A:28:TYR:OH	0.41	2.68	37	1
1:A:32:CYS:O	1:A:39:CYS:O	0.41	2.39	12	1
1:A:15:LEU:C	1:A:15:LEU:HD23	0.41	2.36	20	1
1:A:37:ASN:C	1:A:38:ILE:CG2	0.41	2.88	7	1
1:A:16:TRP:CH2	1:A:23:PRO:CG	0.41	3.04	39	1
1:A:24:GLY:O	1:A:27:GLY:N	0.41	2.54	26	1
1:A:6:CYS:SG	1:A:41:TYR:CE1	0.41	3.14	5	1
1:A:2:ALA:CB	1:A:15:LEU:H	0.41	2.29	7	1
1:A:34:LYS:O	1:A:37:ASN:N	0.41	2.54	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:TYR:O	1:A:28:TYR:N	0.40	2.54	31	1
1:A:12:ARG:HH12	1:A:14:ASP:CG	0.40	2.19	17	1
1:A:24:GLY:O	1:A:26:TYR:N	0.40	2.54	2	1
1:A:14:ASP:CG	1:A:28:TYR:OH	0.40	2.60	33	1
1:A:12:ARG:NH2	1:A:14:ASP:CG	0.40	2.75	11	1
1:A:24:GLY:C	1:A:26:TYR:N	0.40	2.74	2	1
1:A:18:LEU:CD2	1:A:18:LEU:H	0.40	2.23	10	1
1:A:16:TRP:HE1	1:A:28:TYR:HH	0.40	1.58	13	1
1:A:34:LYS:O	1:A:35:TRP:O	0.40	2.39	8	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	41/43 (95%)	29±2 (71±5%)	9±2 (21±4%)	3±1 (8±3%)	2	16
All	All	1722/1806 (95%)	1222 (71%)	369 (21%)	131 (8%)	2	16

All 15 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	29	THR	39
1	A	42	PRO	21
1	A	17	ILE	20
1	A	38	ILE	10
1	A	23	PRO	10
1	A	10	PRO	10
1	A	27	GLY	6
1	A	24	GLY	5
1	A	20	GLY	3
1	A	11	GLY	2
1	A	28	TYR	1
1	A	25	GLY	1
1	A	26	TYR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	35	TRP	1
1	A	8	GLY	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	34/34 (100%)	19±2 (56±6%)	15±2 (44±6%)	0	3
All	All	1428/1428 (100%)	799 (56%)	629 (44%)	0	3

All 27 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	43	HIS	42
1	A	38	ILE	42
1	A	22	CYS	42
1	A	31	ASN	42
1	A	5	PHE	36
1	A	6	CYS	35
1	A	4	CYS	34
1	A	35	TRP	31
1	A	21	THR	30
1	A	17	ILE	29
1	A	12	ARG	28
1	A	18	LEU	27
1	A	37	ASN	25
1	A	32	CYS	25
1	A	7	SER	22
1	A	41	TYR	21
1	A	30	SER	19
1	A	40	CYS	17
1	A	19	ARG	16
1	A	34	LYS	15
1	A	26	TYR	12
1	A	9	LYS	11
1	A	14	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	39	CYS	9
1	A	29	THR	4
1	A	10	PRO	4
1	A	23	PRO	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](#)

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