Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2020 – 03:58 am BST

PDB ID	:	1BRZ
Title	:	SOLUTION STRUCTURE OF THE SWEET PROTEIN BRAZZEIN, NMR, 43 STRUCTURES
Authors	:	Caldwell, J.E.; Abildgaard, F.; Dzakula, Z.; Ming, D.; Hellekant, G.; Markley, J.L.
Deposited on	:	1998-03-12

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

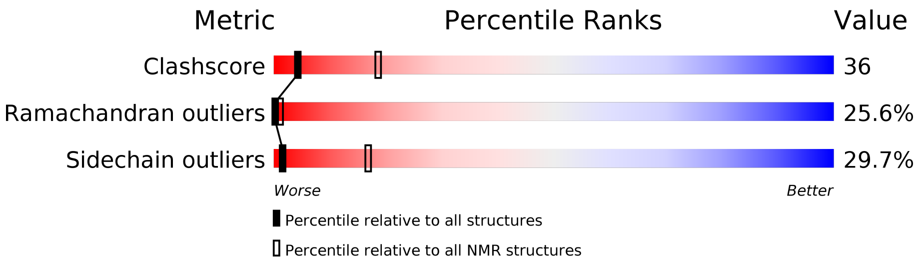
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	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	54	

2 Ensemble composition and analysis ⓘ

This entry contains 43 models. Model 14 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:52 (49)	0.69	14

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 3 single-model clusters were found.

Cluster number	**Models**
1	1, 2, 3, 4, 7, 8, 9, 11, 13, 14, 15, 17, 18, 19, 21, 22, 23, 24, 25, 29, 30, 32, 33, 34, 38, 39, 41, 42, 43
2	5, 6, 12, 16, 20, 26, 27, 28, 36
3	10, 31
Single-model clusters	35; 37; 40

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 859 atoms, of which 410 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BRAZZEIN.

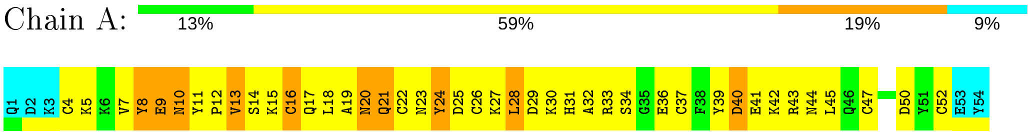
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	54	859	276	410	76	89	8	0

4 Residue-property plots ⓘ

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: BRAZZEIN

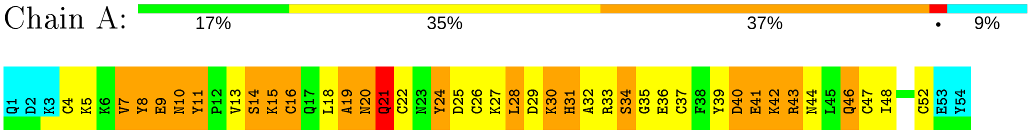


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

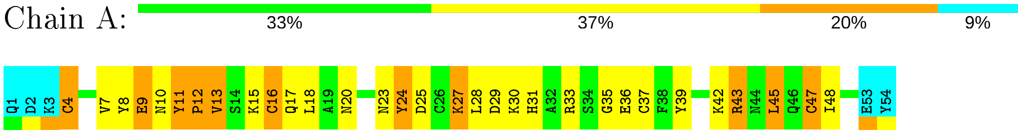
4.2.1 Score per residue for model 1

- Molecule 1: BRAZZEIN



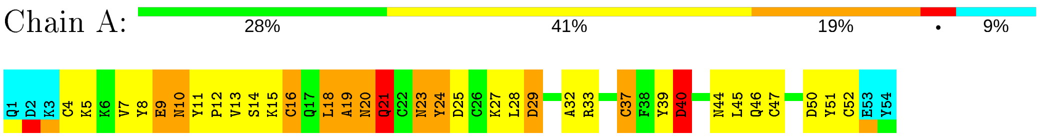
4.2.2 Score per residue for model 2

- Molecule 1: BRAZZEIN



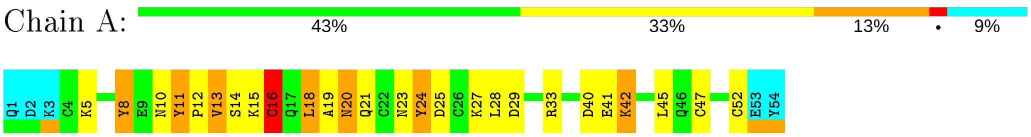
4.2.3 Score per residue for model 3

- Molecule 1: BRAZZEIN



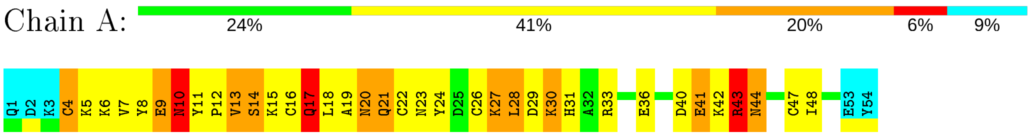
4.2.4 Score per residue for model 4

- Molecule 1: BRAZZEIN



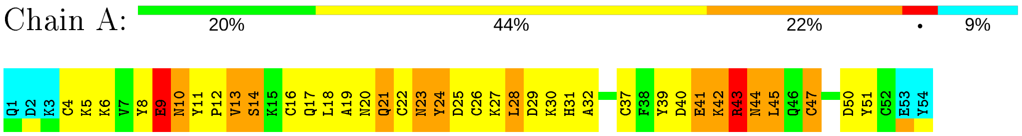
4.2.5 Score per residue for model 5

- Molecule 1: BRAZZEIN



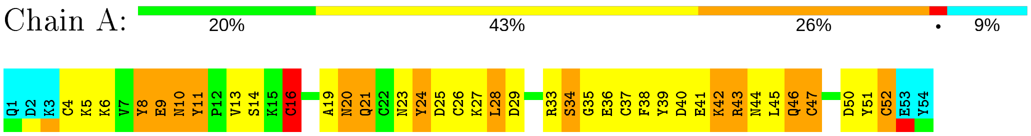
4.2.6 Score per residue for model 6

- Molecule 1: BRAZZEIN



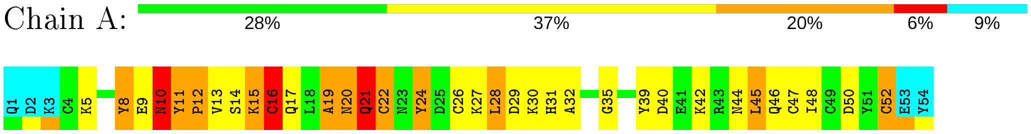
4.2.7 Score per residue for model 7

- Molecule 1: BRAZZEIN



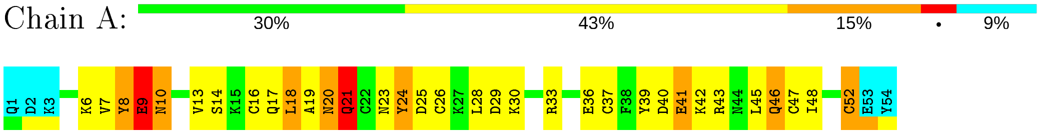
4.2.8 Score per residue for model 8

- Molecule 1: BRAZZEIN



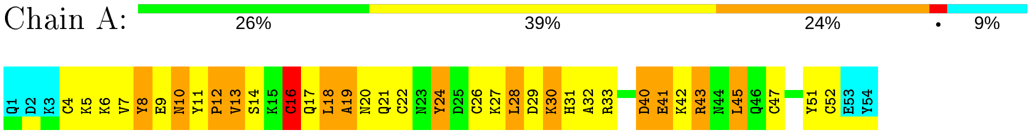
4.2.9 Score per residue for model 9

- Molecule 1: BRAZZEIN



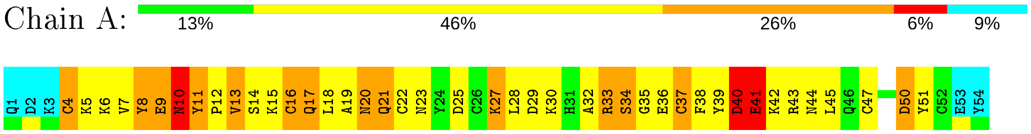
4.2.10 Score per residue for model 10

- Molecule 1: BRAZZEIN



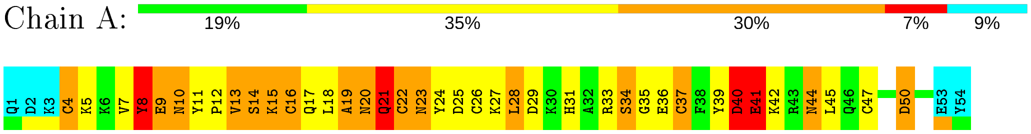
4.2.11 Score per residue for model 11

- Molecule 1: BRAZZEIN



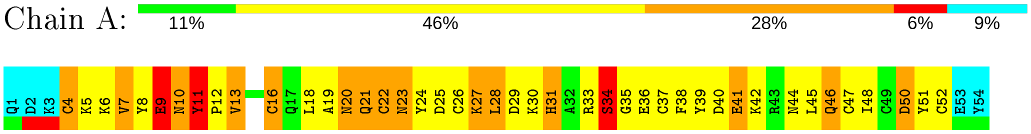
4.2.12 Score per residue for model 12

- Molecule 1: BRAZZEIN



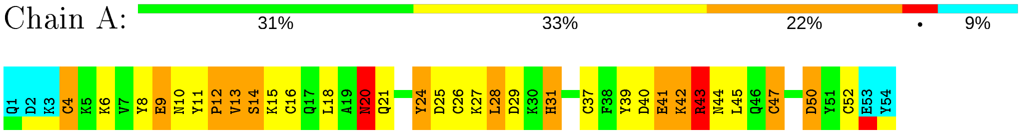
4.2.13 Score per residue for model 13

- Molecule 1: BRAZZEIN



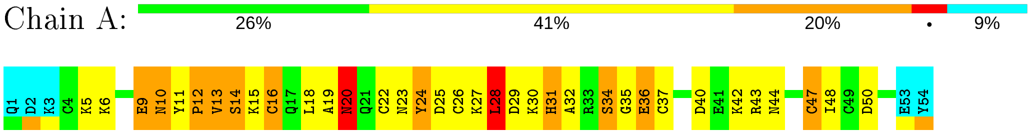
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: BRAZZEIN



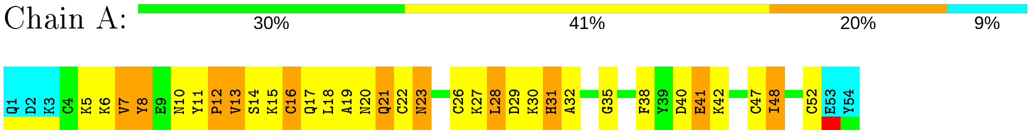
4.2.15 Score per residue for model 15

- Molecule 1: BRAZZEIN



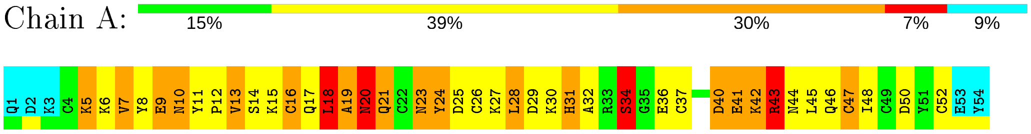
4.2.16 Score per residue for model 16

- Molecule 1: BRAZZEIN



4.2.17 Score per residue for model 17

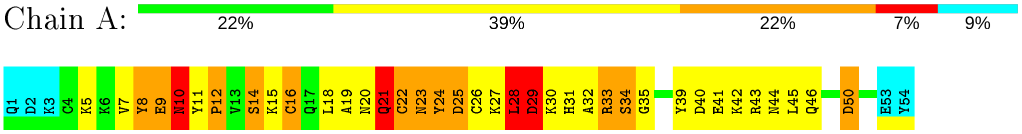
- Molecule 1: BRAZZEIN



4.2.18 Score per residue for model 18

- Molecule 1: BRAZZEIN

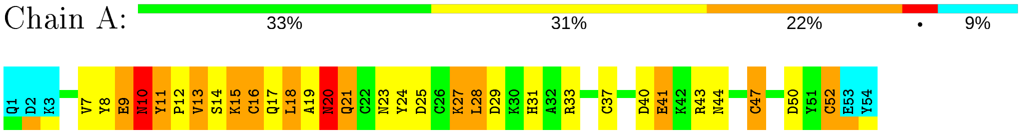
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: BRAZZEIN

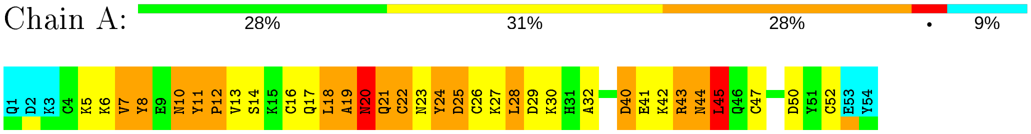
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: BRAZZEIN

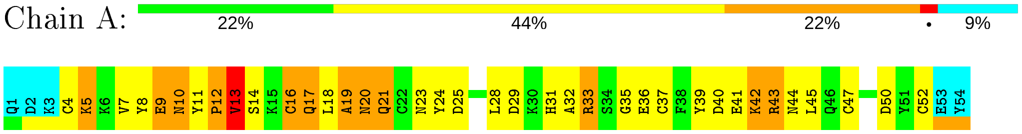
Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: BRAZZEIN

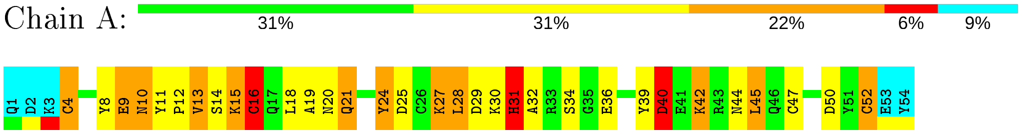
Chain A:



4.2.22 Score per residue for model 22

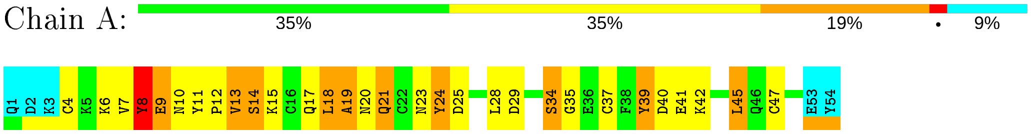
- Molecule 1: BRAZZEIN

Chain A:



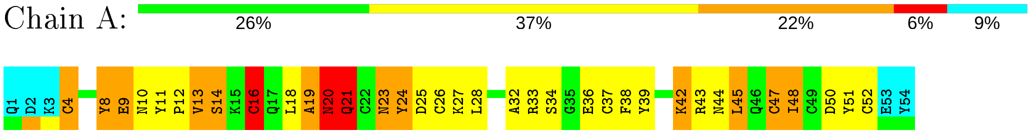
4.2.23 Score per residue for model 23

- Molecule 1: BRAZZEIN



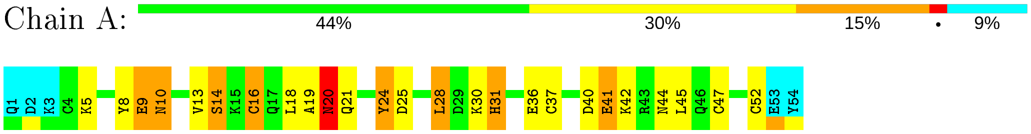
4.2.24 Score per residue for model 24

- Molecule 1: BRAZZEIN



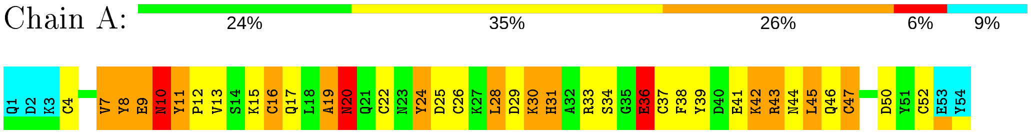
4.2.25 Score per residue for model 25

- Molecule 1: BRAZZEIN



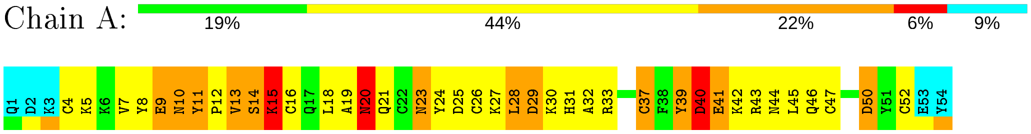
4.2.26 Score per residue for model 26

- Molecule 1: BRAZZEIN



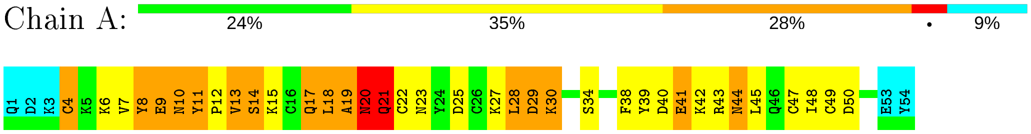
4.2.27 Score per residue for model 27

- Molecule 1: BRAZZEIN



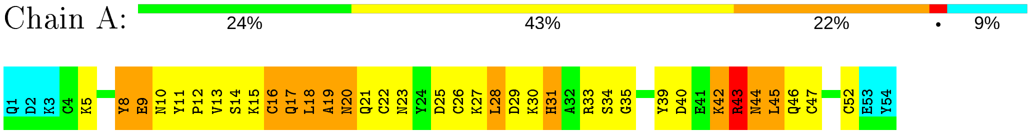
4.2.28 Score per residue for model 28

- Molecule 1: BRAZZEIN



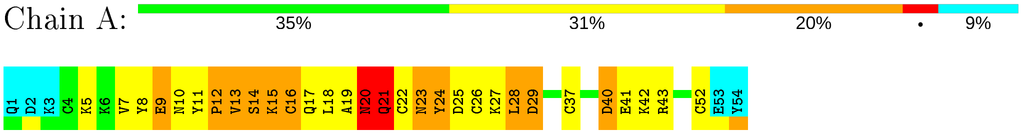
4.2.29 Score per residue for model 29

- Molecule 1: BRAZZEIN



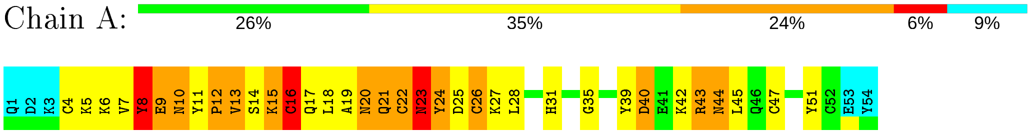
4.2.30 Score per residue for model 30

- Molecule 1: BRAZZEIN



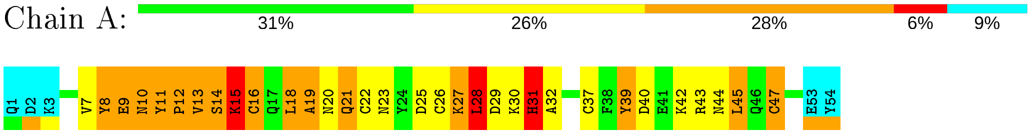
4.2.31 Score per residue for model 31

- Molecule 1: BRAZZEIN



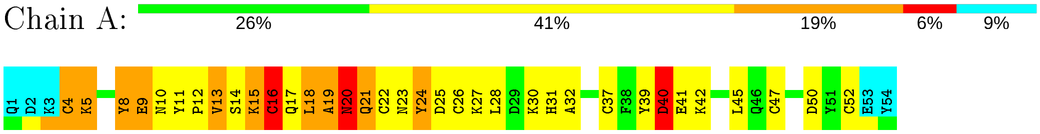
4.2.32 Score per residue for model 32

- Molecule 1: BRAZZEIN



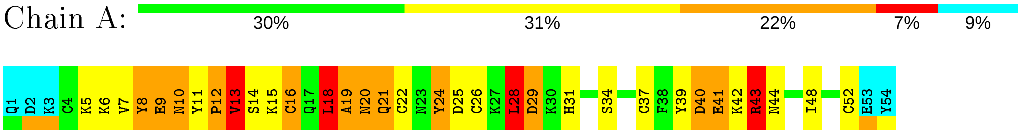
4.2.33 Score per residue for model 33

- Molecule 1: BRAZZEIN



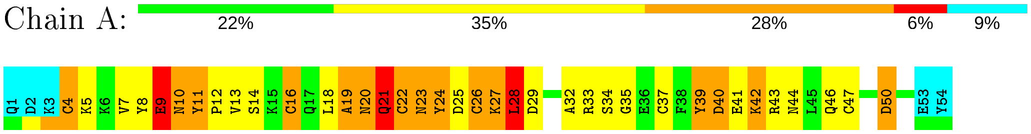
4.2.34 Score per residue for model 34

- Molecule 1: BRAZZEIN



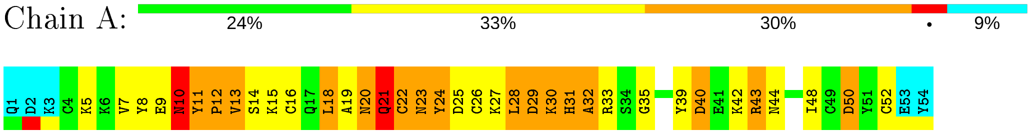
4.2.35 Score per residue for model 35

- Molecule 1: BRAZZEIN



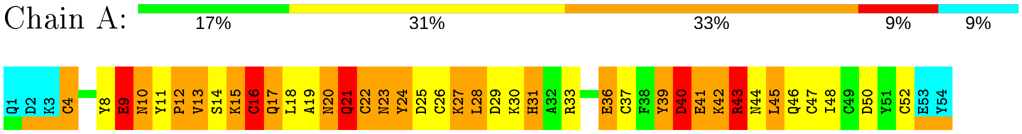
4.2.36 Score per residue for model 36

- Molecule 1: BRAZZEIN



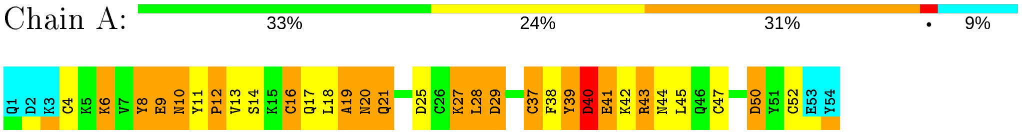
4.2.37 Score per residue for model 37

- Molecule 1: BRAZZEIN



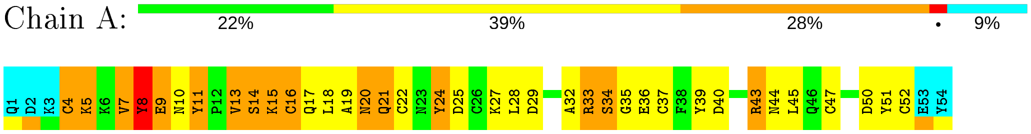
4.2.38 Score per residue for model 38

- Molecule 1: BRAZZEIN



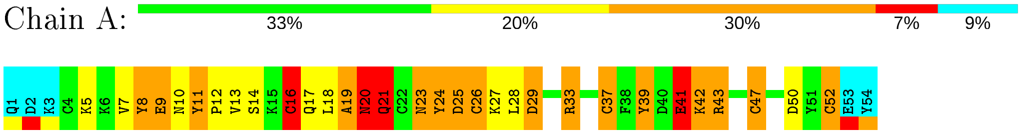
4.2.39 Score per residue for model 39

- Molecule 1: BRAZZEIN



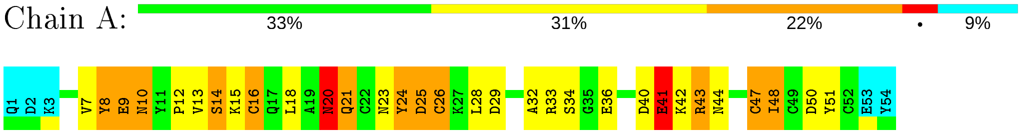
4.2.40 Score per residue for model 40

- Molecule 1: BRAZZEIN



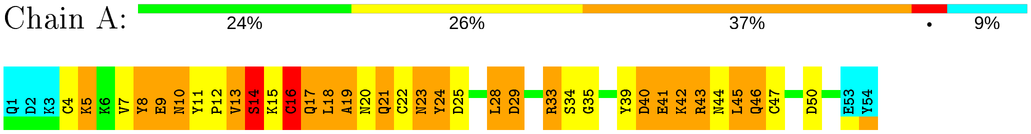
4.2.41 Score per residue for model 41

- Molecule 1: BRAZZEIN



4.2.42 Score per residue for model 42

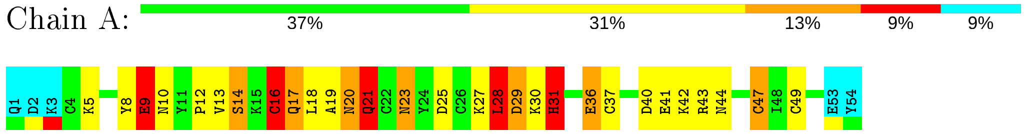
- Molecule 1: BRAZZEIN



4.2.43 Score per residue for model 43

- Molecule 1: BRAZZEIN

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DYNAMICAL SIMULATED ANNEALING*.

Of the 80 calculated structures, 43 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION*.

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

Software name	**Classification**	**Version**
X-PLOR	refinement	3.843
X-PLOR	structure solution	

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

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	402	372	371	28±7
All	All	17286	15996	15953	1188

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:CYS:O	1:A:32:ALA:HB3	0.84	1.73	8	7
1:A:18:LEU:HD12	1:A:18:LEU:N	0.83	1.88	17	3
1:A:12:PRO:O	1:A:13:VAL:HG23	0.83	1.73	37	3
1:A:44:ASN:O	1:A:45:LEU:HD23	0.81	1.75	29	1
1:A:18:LEU:N	1:A:18:LEU:HD12	0.80	1.90	9	3
1:A:45:LEU:HD23	1:A:45:LEU:H	0.80	1.34	8	2
1:A:44:ASN:C	1:A:45:LEU:HD23	0.80	1.96	6	3
1:A:28:LEU:O	1:A:30:LYS:N	0.79	2.15	10	7
1:A:32:ALA:HB2	1:A:51:TYR:CZ	0.79	2.13	39	1
1:A:39:TYR:CG	1:A:40:ASP:N	0.76	2.52	37	1
1:A:48:ILE:HD12	1:A:48:ILE:N	0.76	1.96	41	3
1:A:11:TYR:O	1:A:13:VAL:N	0.73	2.21	16	15

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:10:ASN:O	1:A:11:TYR:O	0.72	2.08	19	4
1:A:8:TYR:CE2	1:A:11:TYR:CZ	0.71	2.79	13	1
1:A:45:LEU:HD13	1:A:45:LEU:N	0.71	2.00	10	1
1:A:13:VAL:O	1:A:13:VAL:HG12	0.71	1.85	2	5
1:A:20:ASN:HD22	1:A:21:GLN:N	0.70	1.84	35	2
1:A:13:VAL:HG22	1:A:14:SER:N	0.70	2.01	11	1
1:A:22:CYS:SG	1:A:37:CYS:SG	0.70	2.90	37	7
1:A:16:CYS:O	1:A:18:LEU:N	0.70	2.22	37	3
1:A:15:LYS:O	1:A:17:GLN:N	0.70	2.24	37	2
1:A:20:ASN:ND2	1:A:21:GLN:N	0.69	2.40	35	2
1:A:11:TYR:CE1	1:A:22:CYS:SG	0.69	2.86	10	1
1:A:11:TYR:CE2	1:A:47:CYS:SG	0.68	2.86	11	10
1:A:45:LEU:N	1:A:45:LEU:HD23	0.68	2.03	8	1
1:A:8:TYR:CD1	1:A:10:ASN:ND2	0.68	2.61	18	1
1:A:40:ASP:O	1:A:42:LYS:N	0.68	2.27	13	20
1:A:38:PHE:CD2	1:A:48:ILE:HD12	0.68	2.24	13	1
1:A:8:TYR:CD2	1:A:26:CYS:SG	0.67	2.87	31	2
1:A:21:GLN:N	1:A:21:GLN:HE21	0.67	1.86	36	3
1:A:11:TYR:CD2	1:A:47:CYS:SG	0.67	2.88	19	6
1:A:12:PRO:O	1:A:13:VAL:HG12	0.67	1.89	13	1
1:A:28:LEU:HD13	1:A:28:LEU:C	0.67	2.10	38	5
1:A:21:GLN:N	1:A:21:GLN:NE2	0.67	2.43	36	2
1:A:11:TYR:CE2	1:A:22:CYS:SG	0.66	2.88	39	6
1:A:16:CYS:SG	1:A:47:CYS:SG	0.66	2.94	32	16
1:A:18:LEU:O	1:A:19:ALA:HB3	0.65	1.92	34	5
1:A:16:CYS:SG	1:A:22:CYS:SG	0.65	2.95	11	1
1:A:25:ASP:O	1:A:29:ASP:N	0.64	2.30	22	31
1:A:10:ASN:HD22	1:A:11:TYR:N	0.64	1.89	18	2
1:A:9:GLU:O	1:A:11:TYR:N	0.64	2.30	6	12
1:A:12:PRO:O	1:A:14:SER:N	0.64	2.31	16	10
1:A:45:LEU:HD12	1:A:45:LEU:N	0.64	2.06	9	1
1:A:37:CYS:SG	1:A:47:CYS:SG	0.64	2.95	40	5
1:A:13:VAL:HG22	1:A:14:SER:H	0.64	1.53	11	1
1:A:13:VAL:O	1:A:15:LYS:N	0.64	2.30	27	5
1:A:11:TYR:CE1	1:A:47:CYS:SG	0.64	2.90	15	3
1:A:32:ALA:HB2	1:A:51:TYR:CE2	0.64	2.27	39	3
1:A:39:TYR:CD2	1:A:44:ASN:O	0.64	2.51	21	11
1:A:45:LEU:HD23	1:A:45:LEU:N	0.63	2.08	24	3
1:A:32:ALA:HB1	1:A:50:ASP:O	0.63	1.93	39	12
1:A:8:TYR:CD1	1:A:10:ASN:O	0.63	2.51	16	3
1:A:39:TYR:CE1	1:A:45:LEU:HD13	0.62	2.29	11	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:11:TYR:O	1:A:12:PRO:O	0.62	2.17	37	3
1:A:9:GLU:O	1:A:10:ASN:ND2	0.62	2.33	9	2
1:A:39:TYR:CD1	1:A:44:ASN:O	0.62	2.53	36	2
1:A:20:ASN:O	1:A:22:CYS:N	0.61	2.33	8	8
1:A:8:TYR:CG	1:A:8:TYR:O	0.61	2.53	17	2
1:A:45:LEU:N	1:A:45:LEU:HD12	0.61	2.10	39	1
1:A:20:ASN:OD1	1:A:21:GLN:N	0.61	2.34	33	2
1:A:20:ASN:O	1:A:23:ASN:N	0.61	2.34	9	10
1:A:8:TYR:CD1	1:A:8:TYR:O	0.61	2.54	17	3
1:A:21:GLN:O	1:A:22:CYS:SG	0.61	2.58	37	3
1:A:8:TYR:O	1:A:8:TYR:CD1	0.61	2.54	5	3
1:A:21:GLN:HE21	1:A:21:GLN:CA	0.61	2.08	36	1
1:A:42:LYS:N	1:A:44:ASN:OD1	0.60	2.34	12	1
1:A:18:LEU:O	1:A:20:ASN:N	0.60	2.33	6	9
1:A:48:ILE:N	1:A:48:ILE:CD1	0.60	2.63	41	1
1:A:44:ASN:C	1:A:45:LEU:HD12	0.60	2.17	28	1
1:A:15:LYS:O	1:A:16:CYS:SG	0.60	2.59	19	5
1:A:23:ASN:ND2	1:A:35:GLY:O	0.60	2.35	35	3
1:A:31:HIS:N	1:A:31:HIS:CD2	0.60	2.69	22	3
1:A:33:ARG:NE	1:A:33:ARG:O	0.60	2.35	11	2
1:A:39:TYR:CG	1:A:44:ASN:O	0.60	2.55	26	3
1:A:17:GLN:O	1:A:19:ALA:N	0.60	2.35	28	1
1:A:25:ASP:N	1:A:25:ASP:OD1	0.59	2.35	18	2
1:A:17:GLN:C	1:A:18:LEU:HD12	0.59	2.18	42	3
1:A:13:VAL:HG22	1:A:45:LEU:O	0.59	1.97	13	1
1:A:42:LYS:O	1:A:44:ASN:ND2	0.59	2.36	25	1
1:A:20:ASN:ND2	1:A:21:GLN:H	0.59	1.94	35	1
1:A:43:ARG:O	1:A:43:ARG:NE	0.59	2.33	5	1
1:A:44:ASN:N	1:A:44:ASN:OD1	0.59	2.34	31	2
1:A:9:GLU:O	1:A:10:ASN:CB	0.58	2.51	21	9
1:A:11:TYR:CD2	1:A:22:CYS:SG	0.58	2.96	42	3
1:A:20:ASN:O	1:A:24:TYR:N	0.58	2.37	3	8
1:A:34:SER:O	1:A:50:ASP:N	0.58	2.35	11	3
1:A:8:TYR:CE1	1:A:10:ASN:O	0.58	2.56	20	2
1:A:18:LEU:O	1:A:19:ALA:CB	0.58	2.52	20	6
1:A:12:PRO:O	1:A:13:VAL:CG2	0.58	2.51	31	3
1:A:47:CYS:C	1:A:48:ILE:HD12	0.58	2.19	2	1
1:A:28:LEU:O	1:A:31:HIS:N	0.58	2.34	8	6
1:A:7:VAL:O	1:A:9:GLU:N	0.58	2.36	12	5
1:A:34:SER:OG	1:A:35:GLY:N	0.58	2.36	7	5
1:A:21:GLN:O	1:A:22:CYS:CB	0.58	2.52	18	2

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:26:CYS:C	1:A:28:LEU:H	0.58	2.02	5	23
1:A:39:TYR:O	1:A:41:GLU:N	0.58	2.35	42	1
1:A:9:GLU:O	1:A:10:ASN:O	0.58	2.22	37	7
1:A:14:SER:O	1:A:16:CYS:N	0.58	2.36	16	1
1:A:33:ARG:NE	1:A:51:TYR:O	0.58	2.37	10	2
1:A:30:LYS:O	1:A:31:HIS:CD2	0.58	2.57	26	1
1:A:20:ASN:CG	1:A:21:GLN:N	0.58	2.57	33	8
1:A:41:GLU:O	1:A:44:ASN:ND2	0.58	2.37	41	1
1:A:22:CYS:SG	1:A:36:GLU:O	0.57	2.62	15	2
1:A:21:GLN:O	1:A:47:CYS:SG	0.57	2.62	37	1
1:A:24:TYR:CD1	1:A:24:TYR:C	0.57	2.78	34	17
1:A:18:LEU:O	1:A:19:ALA:HB2	0.57	1.98	10	5
1:A:40:ASP:O	1:A:43:ARG:N	0.57	2.38	6	1
1:A:21:GLN:H	1:A:21:GLN:HE21	0.57	1.43	12	1
1:A:39:TYR:CE1	1:A:45:LEU:HD21	0.57	2.34	27	3
1:A:50:ASP:OD1	1:A:51:TYR:N	0.57	2.36	7	2
1:A:10:ASN:O	1:A:11:TYR:CB	0.57	2.52	7	3
1:A:7:VAL:HG23	1:A:9:GLU:H	0.57	1.60	40	3
1:A:4:CYS:O	1:A:51:TYR:N	0.57	2.37	39	2
1:A:18:LEU:N	1:A:18:LEU:CD2	0.57	2.68	32	1
1:A:22:CYS:O	1:A:26:CYS:SG	0.56	2.62	36	6
1:A:14:SER:OG	1:A:15:LYS:N	0.56	2.38	30	8
1:A:20:ASN:O	1:A:21:GLN:C	0.56	2.43	16	24
1:A:8:TYR:O	1:A:9:GLU:O	0.56	2.23	3	17
1:A:40:ASP:N	1:A:40:ASP:OD1	0.56	2.38	28	7
1:A:9:GLU:O	1:A:10:ASN:C	0.56	2.43	27	11
1:A:39:TYR:CE2	1:A:45:LEU:CD2	0.56	2.88	23	2
1:A:10:ASN:OD1	1:A:11:TYR:N	0.56	2.38	2	1
1:A:5:LYS:H	1:A:5:LYS:CD	0.56	2.12	39	1
1:A:10:ASN:HD22	1:A:10:ASN:N	0.56	1.97	39	1
1:A:10:ASN:O	1:A:11:TYR:C	0.56	2.44	11	5
1:A:19:ALA:O	1:A:20:ASN:CB	0.56	2.53	26	5
1:A:28:LEU:HD23	1:A:28:LEU:O	0.56	2.00	1	1
1:A:13:VAL:HG13	1:A:14:SER:N	0.56	2.15	11	1
1:A:14:SER:O	1:A:15:LYS:CB	0.56	2.54	23	5
1:A:8:TYR:O	1:A:10:ASN:N	0.56	2.39	41	4
1:A:13:VAL:O	1:A:14:SER:CB	0.56	2.53	28	2
1:A:10:ASN:CG	1:A:11:TYR:N	0.56	2.59	2	2
1:A:24:TYR:C	1:A:24:TYR:CD1	0.55	2.80	25	10
1:A:42:LYS:O	1:A:43:ARG:CG	0.55	2.54	10	1
1:A:8:TYR:CD2	1:A:11:TYR:CE2	0.55	2.94	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:TYR:O	1:A:9:GLU:CG	0.55	2.55	25	2
1:A:45:LEU:HD12	1:A:46:GLN:N	0.55	2.17	37	1
1:A:10:ASN:OD1	1:A:10:ASN:O	0.55	2.23	9	1
1:A:40:ASP:O	1:A:41:GLU:CB	0.55	2.54	23	4
1:A:30:LYS:C	1:A:31:HIS:CG	0.55	2.79	37	9
1:A:21:GLN:HE21	1:A:22:CYS:N	0.55	1.99	36	1
1:A:19:ALA:O	1:A:21:GLN:N	0.55	2.40	17	3
1:A:36:GLU:CG	1:A:38:PHE:CZ	0.55	2.90	11	1
1:A:18:LEU:O	1:A:19:ALA:C	0.54	2.45	21	1
1:A:45:LEU:N	1:A:45:LEU:CD1	0.54	2.70	10	2
1:A:13:VAL:CG2	1:A:45:LEU:O	0.54	2.55	26	1
1:A:12:PRO:O	1:A:13:VAL:CG1	0.54	2.56	13	1
1:A:28:LEU:HD13	1:A:28:LEU:O	0.54	2.01	19	5
1:A:12:PRO:O	1:A:13:VAL:C	0.54	2.45	28	8
1:A:28:LEU:C	1:A:30:LYS:H	0.54	2.06	26	1
1:A:42:LYS:O	1:A:43:ARG:CB	0.54	2.54	1	8
1:A:8:TYR:C	1:A:8:TYR:CD1	0.54	2.80	35	2
1:A:12:PRO:O	1:A:13:VAL:CB	0.54	2.55	31	5
1:A:38:PHE:CD2	1:A:48:ILE:CD1	0.54	2.90	24	1
1:A:13:VAL:HG13	1:A:14:SER:H	0.54	1.62	11	1
1:A:8:TYR:O	1:A:9:GLU:C	0.54	2.45	1	19
1:A:19:ALA:O	1:A:20:ASN:O	0.54	2.25	38	2
1:A:39:TYR:CD1	1:A:40:ASP:N	0.54	2.75	37	1
1:A:39:TYR:CZ	1:A:43:ARG:O	0.54	2.61	32	1
1:A:11:TYR:CZ	1:A:47:CYS:SG	0.54	3.01	1	3
1:A:34:SER:O	1:A:50:ASP:CB	0.53	2.56	11	7
1:A:26:CYS:SG	1:A:48:ILE:O	0.53	2.66	16	1
1:A:42:LYS:O	1:A:44:ASN:N	0.53	2.41	35	4
1:A:40:ASP:OD2	1:A:44:ASN:ND2	0.53	2.40	14	1
1:A:13:VAL:O	1:A:13:VAL:CG1	0.53	2.57	2	3
1:A:39:TYR:O	1:A:40:ASP:O	0.53	2.26	22	5
1:A:42:LYS:O	1:A:43:ARG:CD	0.53	2.56	29	1
1:A:39:TYR:CZ	1:A:45:LEU:CD2	0.53	2.91	29	1
1:A:42:LYS:C	1:A:44:ASN:H	0.53	2.06	37	5
1:A:9:GLU:CG	1:A:9:GLU:O	0.53	2.56	25	1
1:A:19:ALA:HB1	1:A:23:ASN:HD22	0.53	1.64	19	1
1:A:43:ARG:C	1:A:45:LEU:H	0.53	2.05	37	1
1:A:8:TYR:O	1:A:9:GLU:CB	0.53	2.57	25	4
1:A:26:CYS:C	1:A:28:LEU:N	0.52	2.63	26	10
1:A:9:GLU:CD	1:A:9:GLU:N	0.52	2.61	43	1
1:A:21:GLN:NE2	1:A:22:CYS:N	0.52	2.57	36	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:N	1:A:18:LEU:HD22	0.52	2.20	32	1
1:A:10:ASN:CG	1:A:11:TYR:H	0.52	2.07	2	2
1:A:40:ASP:OD1	1:A:40:ASP:N	0.52	2.43	29	2
1:A:28:LEU:C	1:A:30:LYS:N	0.52	2.63	26	1
1:A:43:ARG:HE	1:A:43:ARG:N	0.52	2.02	41	1
1:A:8:TYR:O	1:A:10:ASN:OD1	0.52	2.28	18	1
1:A:39:TYR:CZ	1:A:45:LEU:HD11	0.52	2.40	39	2
1:A:16:CYS:C	1:A:18:LEU:H	0.52	2.07	40	2
1:A:19:ALA:O	1:A:20:ASN:OD1	0.52	2.28	33	1
1:A:8:TYR:CE2	1:A:11:TYR:CE1	0.51	2.99	13	1
1:A:11:TYR:OH	1:A:14:SER:OG	0.51	2.28	16	1
1:A:45:LEU:CD1	1:A:45:LEU:N	0.51	2.73	9	1
1:A:17:GLN:CD	1:A:17:GLN:N	0.51	2.64	31	1
1:A:21:GLN:NE2	1:A:22:CYS:H	0.51	2.03	36	1
1:A:13:VAL:O	1:A:15:LYS:O	0.51	2.27	30	1
1:A:7:VAL:O	1:A:7:VAL:CG2	0.51	2.59	12	2
1:A:30:LYS:O	1:A:31:HIS:CG	0.51	2.63	32	2
1:A:39:TYR:CE1	1:A:45:LEU:HD22	0.51	2.40	6	1
1:A:7:VAL:O	1:A:9:GLU:OE1	0.51	2.29	35	1
1:A:12:PRO:C	1:A:13:VAL:HG22	0.51	2.26	21	1
1:A:8:TYR:O	1:A:8:TYR:CG	0.51	2.64	7	2
1:A:13:VAL:O	1:A:14:SER:C	0.51	2.49	25	6
1:A:39:TYR:CE2	1:A:45:LEU:HD21	0.51	2.41	23	2
1:A:23:ASN:OD1	1:A:35:GLY:O	0.50	2.30	21	5
1:A:13:VAL:C	1:A:15:LYS:H	0.50	2.09	31	2
1:A:38:PHE:CD1	1:A:48:ILE:HD12	0.50	2.40	28	1
1:A:28:LEU:O	1:A:28:LEU:HD13	0.50	2.06	14	3
1:A:42:LYS:O	1:A:43:ARG:HB2	0.50	2.06	29	1
1:A:43:ARG:O	1:A:44:ASN:OD1	0.50	2.29	26	2
1:A:35:GLY:O	1:A:36:GLU:CG	0.50	2.60	13	2
1:A:39:TYR:O	1:A:44:ASN:O	0.50	2.29	38	1
1:A:6:LYS:C	1:A:7:VAL:HG12	0.50	2.27	16	2
1:A:12:PRO:C	1:A:14:SER:H	0.50	2.09	19	5
1:A:10:ASN:N	1:A:10:ASN:OD1	0.50	2.44	42	1
1:A:31:HIS:CD2	1:A:31:HIS:N	0.50	2.77	17	2
1:A:22:CYS:N	1:A:25:ASP:OD1	0.50	2.44	13	2
1:A:15:LYS:O	1:A:16:CYS:C	0.50	2.50	33	4
1:A:42:LYS:C	1:A:44:ASN:N	0.50	2.65	35	4
1:A:48:ILE:N	1:A:48:ILE:HD13	0.50	2.22	17	1
1:A:42:LYS:O	1:A:43:ARG:C	0.50	2.50	6	5
1:A:11:TYR:CE2	1:A:16:CYS:SG	0.50	3.05	7	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:40:ASP:C	1:A:42:LYS:H	0.50	2.11	43	12
1:A:9:GLU:O	1:A:10:ASN:CG	0.50	2.50	17	4
1:A:9:GLU:C	1:A:10:ASN:ND2	0.49	2.65	26	1
1:A:34:SER:O	1:A:50:ASP:CA	0.49	2.60	11	1
1:A:17:GLN:O	1:A:18:LEU:O	0.49	2.30	20	1
1:A:21:GLN:O	1:A:25:ASP:OD2	0.49	2.30	14	4
1:A:30:LYS:C	1:A:31:HIS:CD2	0.49	2.85	26	3
1:A:21:GLN:H	1:A:21:GLN:NE2	0.49	2.04	12	1
1:A:33:ARG:O	1:A:34:SER:CB	0.49	2.59	18	1
1:A:40:ASP:OD1	1:A:42:LYS:N	0.49	2.45	18	2
1:A:28:LEU:HD23	1:A:28:LEU:C	0.49	2.27	1	1
1:A:16:CYS:O	1:A:17:GLN:CB	0.49	2.61	21	2
1:A:11:TYR:O	1:A:11:TYR:CD2	0.49	2.65	35	1
1:A:36:GLU:CG	1:A:37:CYS:H	0.49	2.20	37	1
1:A:8:TYR:CD1	1:A:9:GLU:N	0.49	2.81	35	1
1:A:40:ASP:O	1:A:41:GLU:C	0.49	2.50	10	13
1:A:11:TYR:OH	1:A:21:GLN:OE1	0.49	2.30	23	3
1:A:10:ASN:HD22	1:A:11:TYR:H	0.49	1.49	18	1
1:A:20:ASN:C	1:A:22:CYS:H	0.49	2.10	37	2
1:A:28:LEU:CD1	1:A:28:LEU:C	0.49	2.80	38	2
1:A:41:GLU:O	1:A:41:GLU:OE1	0.49	2.30	40	1
1:A:18:LEU:O	1:A:20:ASN:OD1	0.49	2.30	36	1
1:A:20:ASN:OD1	1:A:21:GLN:OE1	0.48	2.31	38	2
1:A:8:TYR:O	1:A:9:GLU:OE2	0.48	2.31	35	1
1:A:32:ALA:CB	1:A:51:TYR:CE2	0.48	2.96	39	1
1:A:45:LEU:O	1:A:46:GLN:OE1	0.48	2.30	7	3
1:A:7:VAL:O	1:A:8:TYR:O	0.48	2.31	23	1
1:A:40:ASP:OD1	1:A:40:ASP:C	0.48	2.52	17	2
1:A:40:ASP:OD1	1:A:44:ASN:O	0.48	2.30	3	2
1:A:38:PHE:CD2	1:A:48:ILE:HD13	0.48	2.44	24	1
1:A:16:CYS:O	1:A:17:GLN:CG	0.48	2.62	11	3
1:A:5:LYS:CD	1:A:5:LYS:N	0.48	2.76	33	2
1:A:20:ASN:OD1	1:A:21:GLN:NE2	0.48	2.46	18	2
1:A:21:GLN:CA	1:A:21:GLN:HE21	0.48	2.22	12	2
1:A:18:LEU:HD21	1:A:37:CYS:O	0.48	2.09	38	1
1:A:30:LYS:O	1:A:31:HIS:CB	0.48	2.62	32	3
1:A:36:GLU:CG	1:A:38:PHE:CE2	0.48	2.97	11	1
1:A:39:TYR:CD1	1:A:39:TYR:C	0.48	2.86	40	1
1:A:18:LEU:CD2	1:A:18:LEU:N	0.48	2.77	43	1
1:A:7:VAL:O	1:A:9:GLU:OE2	0.48	2.31	26	1
1:A:42:LYS:O	1:A:44:ASN:OD1	0.48	2.30	13	3

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:39:TYR:O	1:A:40:ASP:OD2	0.48	2.31	12	1
1:A:11:TYR:CE2	1:A:25:ASP:OD2	0.48	2.67	18	1
1:A:10:ASN:ND2	1:A:10:ASN:N	0.48	2.61	39	1
1:A:45:LEU:HD13	1:A:46:GLN:N	0.48	2.23	17	1
1:A:50:ASP:OD2	1:A:52:CYS:SG	0.48	2.72	38	1
1:A:15:LYS:O	1:A:16:CYS:O	0.48	2.32	22	2
1:A:41:GLU:N	1:A:41:GLU:OE1	0.48	2.43	14	1
1:A:16:CYS:O	1:A:17:GLN:C	0.48	2.52	29	1
1:A:8:TYR:N	1:A:47:CYS:O	0.48	2.47	24	1
1:A:20:ASN:CG	1:A:21:GLN:H	0.48	2.11	5	4
1:A:40:ASP:C	1:A:42:LYS:N	0.48	2.68	9	6
1:A:26:CYS:O	1:A:32:ALA:CB	0.48	2.55	8	3
1:A:34:SER:O	1:A:50:ASP:OD2	0.48	2.32	12	2
1:A:11:TYR:OH	1:A:25:ASP:OD2	0.48	2.30	28	3
1:A:9:GLU:CD	1:A:10:ASN:H	0.47	2.12	43	1
1:A:19:ALA:O	1:A:20:ASN:C	0.47	2.53	38	1
1:A:8:TYR:OH	1:A:29:ASP:OD2	0.47	2.32	26	1
1:A:19:ALA:C	1:A:20:ASN:OD1	0.47	2.53	36	1
1:A:44:ASN:C	1:A:46:GLN:OE1	0.47	2.52	42	2
1:A:17:GLN:O	1:A:18:LEU:C	0.47	2.53	12	5
1:A:41:GLU:O	1:A:41:GLU:CG	0.47	2.62	35	1
1:A:8:TYR:C	1:A:10:ASN:H	0.47	2.13	42	2
1:A:33:ARG:N	1:A:50:ASP:O	0.47	2.47	40	1
1:A:39:TYR:O	1:A:40:ASP:CB	0.47	2.63	12	1
1:A:41:GLU:CG	1:A:42:LYS:N	0.47	2.78	11	1
1:A:44:ASN:O	1:A:45:LEU:O	0.47	2.31	20	3
1:A:21:GLN:O	1:A:25:ASP:CG	0.47	2.53	7	19
1:A:9:GLU:OE1	1:A:10:ASN:OD1	0.47	2.32	40	1
1:A:43:ARG:CD	1:A:43:ARG:N	0.47	2.76	26	1
1:A:43:ARG:O	1:A:43:ARG:CG	0.47	2.63	14	1
1:A:21:GLN:O	1:A:25:ASP:OD1	0.47	2.33	23	3
1:A:18:LEU:C	1:A:20:ASN:H	0.47	2.10	43	1
1:A:8:TYR:CD2	1:A:11:TYR:CZ	0.47	3.03	13	1
1:A:13:VAL:CG2	1:A:14:SER:H	0.47	2.17	11	1
1:A:13:VAL:HG13	1:A:45:LEU:O	0.47	2.10	4	1
1:A:7:VAL:HG23	1:A:7:VAL:O	0.47	2.10	12	1
1:A:12:PRO:O	1:A:13:VAL:HB	0.47	2.09	32	2
1:A:39:TYR:C	1:A:39:TYR:CD1	0.46	2.87	35	2
1:A:39:TYR:O	1:A:40:ASP:CG	0.46	2.54	38	3
1:A:40:ASP:OD1	1:A:43:ARG:N	0.46	2.48	5	2
1:A:28:LEU:CD1	1:A:29:ASP:N	0.46	2.78	18	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:39:TYR:CE2	1:A:45:LEU:HD23	0.46	2.44	33	1
1:A:15:LYS:C	1:A:17:GLN:H	0.46	2.14	8	2
1:A:14:SER:C	1:A:16:CYS:H	0.46	2.14	41	2
1:A:39:TYR:CE2	1:A:43:ARG:O	0.46	2.68	32	1
1:A:35:GLY:C	1:A:36:GLU:OE1	0.46	2.53	2	1
1:A:20:ASN:C	1:A:20:ASN:HD22	0.46	2.11	27	4
1:A:45:LEU:CD2	1:A:45:LEU:N	0.46	2.79	24	1
1:A:37:CYS:SG	1:A:46:GLN:O	0.46	2.74	27	1
1:A:39:TYR:CZ	1:A:45:LEU:HD22	0.46	2.46	8	2
1:A:28:LEU:HD12	1:A:29:ASP:H	0.46	1.71	18	1
1:A:9:GLU:CD	1:A:9:GLU:H	0.46	2.13	43	1
1:A:43:ARG:HE	1:A:43:ARG:H	0.46	1.50	41	1
1:A:48:ILE:CD1	1:A:48:ILE:N	0.46	2.79	5	1
1:A:8:TYR:C	1:A:9:GLU:OE2	0.46	2.54	35	1
1:A:8:TYR:CE1	1:A:10:ASN:ND2	0.46	2.84	18	1
1:A:5:LYS:N	1:A:5:LYS:CD	0.46	2.79	21	1
1:A:8:TYR:CD2	1:A:11:TYR:CD1	0.46	3.04	39	1
1:A:45:LEU:N	1:A:45:LEU:CD2	0.46	2.74	8	1
1:A:40:ASP:N	1:A:44:ASN:O	0.46	2.49	32	1
1:A:9:GLU:C	1:A:10:ASN:OD1	0.46	2.54	42	1
1:A:40:ASP:CG	1:A:46:GLN:NE2	0.46	2.69	29	2
1:A:27:LYS:O	1:A:27:LYS:CG	0.46	2.64	37	1
1:A:24:TYR:CD1	1:A:24:TYR:O	0.46	2.69	4	1
1:A:9:GLU:O	1:A:9:GLU:CD	0.46	2.55	25	1
1:A:11:TYR:CZ	1:A:22:CYS:SG	0.45	3.09	10	1
1:A:45:LEU:O	1:A:45:LEU:HD22	0.45	2.11	10	1
1:A:25:ASP:O	1:A:28:LEU:C	0.45	2.55	26	1
1:A:30:LYS:CG	1:A:51:TYR:OH	0.45	2.65	6	1
1:A:18:LEU:CD1	1:A:18:LEU:N	0.45	2.63	9	2
1:A:30:LYS:O	1:A:31:HIS:C	0.45	2.55	1	7
1:A:12:PRO:C	1:A:13:VAL:HG23	0.45	2.32	2	1
1:A:7:VAL:HG12	1:A:46:GLN:OE1	0.45	2.11	13	1
1:A:40:ASP:CG	1:A:44:ASN:HD22	0.45	2.14	14	1
1:A:18:LEU:N	1:A:18:LEU:CD1	0.45	2.61	17	1
1:A:35:GLY:CA	1:A:48:ILE:O	0.45	2.64	16	3
1:A:7:VAL:C	1:A:9:GLU:H	0.45	2.15	10	1
1:A:35:GLY:O	1:A:36:GLU:CD	0.45	2.55	39	1
1:A:40:ASP:OD1	1:A:44:ASN:N	0.45	2.50	14	3
1:A:38:PHE:O	1:A:46:GLN:N	0.45	2.50	26	1
1:A:9:GLU:C	1:A:11:TYR:N	0.45	2.68	11	1
1:A:13:VAL:HG12	1:A:13:VAL:O	0.45	2.11	19	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:11:TYR:O	1:A:12:PRO:C	0.45	2.55	38	3
1:A:45:LEU:C	1:A:46:GLN:OE1	0.45	2.54	42	2
1:A:40:ASP:CG	1:A:46:GLN:HE22	0.45	2.14	29	1
1:A:34:SER:O	1:A:50:ASP:OD1	0.45	2.35	35	1
1:A:50:ASP:N	1:A:50:ASP:OD1	0.45	2.48	14	1
1:A:10:ASN:ND2	1:A:11:TYR:N	0.45	2.62	19	2
1:A:8:TYR:CD1	1:A:8:TYR:C	0.45	2.90	4	1
1:A:46:GLN:O	1:A:48:ILE:HD12	0.45	2.12	1	1
1:A:17:GLN:H	1:A:18:LEU:HD12	0.44	1.72	9	2
1:A:34:SER:O	1:A:50:ASP:CG	0.44	2.55	12	1
1:A:11:TYR:C	1:A:11:TYR:CD1	0.44	2.90	20	1
1:A:9:GLU:C	1:A:11:TYR:H	0.44	2.13	38	1
1:A:39:TYR:CZ	1:A:45:LEU:HD13	0.44	2.48	42	1
1:A:39:TYR:CZ	1:A:45:LEU:HD21	0.44	2.47	23	1
1:A:16:CYS:O	1:A:45:LEU:HD21	0.44	2.12	22	1
1:A:7:VAL:C	1:A:9:GLU:N	0.44	2.70	10	1
1:A:40:ASP:OD2	1:A:40:ASP:O	0.44	2.36	23	1
1:A:8:TYR:CE1	1:A:30:LYS:NZ	0.44	2.82	32	1
1:A:8:TYR:CE2	1:A:11:TYR:CD1	0.44	3.06	39	1
1:A:23:ASN:OD1	1:A:23:ASN:C	0.44	2.56	20	1
1:A:18:LEU:HD23	1:A:37:CYS:H	0.44	1.72	38	1
1:A:11:TYR:C	1:A:13:VAL:H	0.44	2.16	32	2
1:A:28:LEU:HD12	1:A:29:ASP:N	0.44	2.27	18	1
1:A:26:CYS:O	1:A:28:LEU:N	0.44	2.50	5	7
1:A:38:PHE:CE1	1:A:48:ILE:CG1	0.44	3.00	16	1
1:A:14:SER:C	1:A:15:LYS:CG	0.44	2.86	11	1
1:A:12:PRO:C	1:A:14:SER:N	0.43	2.71	18	4
1:A:17:GLN:O	1:A:18:LEU:HD12	0.43	2.13	10	2
1:A:18:LEU:O	1:A:19:ALA:O	0.43	2.36	23	2
1:A:20:ASN:C	1:A:20:ASN:ND2	0.43	2.71	27	1
1:A:46:GLN:O	1:A:48:ILE:CD1	0.43	2.65	9	2
1:A:43:ARG:C	1:A:44:ASN:OD1	0.43	2.55	7	1
1:A:39:TYR:CE1	1:A:45:LEU:CD1	0.43	3.00	11	1
1:A:21:GLN:NE2	1:A:21:GLN:CA	0.43	2.80	36	1
1:A:17:GLN:HE21	1:A:17:GLN:CA	0.43	2.26	43	1
1:A:11:TYR:CD1	1:A:22:CYS:SG	0.43	3.11	10	1
1:A:29:ASP:N	1:A:29:ASP:OD1	0.43	2.50	34	1
1:A:6:LYS:NZ	1:A:51:TYR:OH	0.43	2.44	13	2
1:A:6:LYS:C	1:A:7:VAL:CG1	0.43	2.86	16	2
1:A:23:ASN:O	1:A:27:LYS:CB	0.43	2.66	37	1
1:A:9:GLU:OE2	1:A:9:GLU:N	0.43	2.52	43	1

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Atom-1	**Atom-2**	**Clash(Å)**	**Distance(Å)**	**Models**	
				Worst	Total
1:A:12:PRO:C	1:A:13:VAL:CG2	0.43	2.86	21	1
1:A:21:GLN:O	1:A:25:ASP:CB	0.43	2.66	21	2
1:A:18:LEU:C	1:A:20:ASN:OD1	0.43	2.57	36	1
1:A:39:TYR:CE2	1:A:44:ASN:O	0.43	2.71	26	1
1:A:10:ASN:OD1	1:A:10:ASN:N	0.43	2.51	11	2
1:A:26:CYS:C	1:A:32:ALA:HB3	0.43	2.33	32	2
1:A:7:VAL:O	1:A:30:LYS:NZ	0.43	2.52	20	1
1:A:23:ASN:HD22	1:A:23:ASN:C	0.43	2.17	13	1
1:A:10:ASN:ND2	1:A:11:TYR:H	0.43	2.11	18	1
1:A:14:SER:O	1:A:15:LYS:CG	0.43	2.66	32	1
1:A:17:GLN:C	1:A:19:ALA:N	0.43	2.72	28	1
1:A:5:LYS:CD	1:A:5:LYS:C	0.43	2.87	34	1
1:A:44:ASN:OD1	1:A:44:ASN:N	0.43	2.52	29	1
1:A:38:PHE:CE2	1:A:48:ILE:HD13	0.43	2.49	24	1
1:A:20:ASN:ND2	1:A:20:ASN:C	0.43	2.72	15	1
1:A:35:GLY:C	1:A:36:GLU:OE2	0.42	2.57	39	1
1:A:11:TYR:CD1	1:A:11:TYR:C	0.42	2.92	36	1
1:A:20:ASN:HD22	1:A:20:ASN:C	0.42	2.17	25	1
1:A:13:VAL:O	1:A:14:SER:OG	0.42	2.32	28	1
1:A:40:ASP:OD2	1:A:46:GLN:OE1	0.42	2.36	3	2
1:A:48:ILE:N	1:A:48:ILE:HD12	0.42	2.30	5	1
1:A:36:GLU:N	1:A:48:ILE:O	0.42	2.52	37	1
1:A:10:ASN:O	1:A:10:ASN:OD1	0.42	2.37	38	1
1:A:39:TYR:C	1:A:40:ASP:OD1	0.42	2.57	22	1
1:A:39:TYR:C	1:A:40:ASP:CG	0.42	2.77	11	5
1:A:8:TYR:C	1:A:10:ASN:N	0.42	2.73	42	1
1:A:40:ASP:CG	1:A:40:ASP:O	0.42	2.57	9	1
1:A:23:ASN:HD22	1:A:35:GLY:N	0.42	2.13	36	1
1:A:12:PRO:O	1:A:13:VAL:O	0.42	2.38	11	1
1:A:23:ASN:C	1:A:23:ASN:HD22	0.42	2.18	27	1
1:A:9:GLU:OE1	1:A:10:ASN:N	0.42	2.37	43	1
1:A:18:LEU:HD12	1:A:18:LEU:H	0.42	1.74	12	1
1:A:43:ARG:C	1:A:45:LEU:N	0.42	2.72	37	1
1:A:13:VAL:CG1	1:A:14:SER:N	0.42	2.79	11	1
1:A:12:PRO:O	1:A:13:VAL:HG22	0.42	2.14	21	1
1:A:11:TYR:CZ	1:A:25:ASP:OD2	0.42	2.73	28	1
1:A:40:ASP:OD1	1:A:40:ASP:O	0.42	2.38	17	1
1:A:44:ASN:N	1:A:44:ASN:ND2	0.42	2.67	25	1
1:A:10:ASN:O	1:A:10:ASN:CG	0.42	2.58	15	1
1:A:16:CYS:C	1:A:18:LEU:N	0.41	2.73	40	1
1:A:18:LEU:C	1:A:20:ASN:N	0.41	2.73	43	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:TYR:O	1:A:24:TYR:CD1	0.41	2.72	42	1
1:A:8:TYR:O	1:A:11:TYR:CB	0.41	2.68	31	1
1:A:10:ASN:O	1:A:10:ASN:ND2	0.41	2.52	15	1
1:A:37:CYS:O	1:A:38:PHE:CD1	0.41	2.73	38	1
1:A:5:LYS:O	1:A:5:LYS:CE	0.41	2.68	42	1
1:A:45:LEU:C	1:A:45:LEU:HD22	0.41	2.35	10	1
1:A:23:ASN:CG	1:A:35:GLY:O	0.41	2.59	31	1
1:A:30:LYS:O	1:A:32:ALA:N	0.41	2.53	1	2
1:A:10:ASN:C	1:A:11:TYR:O	0.41	2.59	13	1
1:A:30:LYS:NZ	1:A:49:CYS:SG	0.41	2.88	28	1
1:A:27:LYS:CG	1:A:33:ARG:O	0.41	2.69	35	1
1:A:7:VAL:O	1:A:7:VAL:HG23	0.41	2.15	30	1
1:A:33:ARG:CB	1:A:50:ASP:O	0.41	2.69	24	2
1:A:11:TYR:OH	1:A:21:GLN:CG	0.41	2.69	19	1
1:A:43:ARG:HE	1:A:43:ARG:C	0.41	2.17	5	1
1:A:42:LYS:CG	1:A:42:LYS:O	0.41	2.68	6	1
1:A:36:GLU:CD	1:A:38:PHE:CZ	0.41	2.94	11	1
1:A:9:GLU:N	1:A:9:GLU:CD	0.41	2.75	39	1
1:A:20:ASN:C	1:A:22:CYS:N	0.41	2.75	20	1
1:A:40:ASP:C	1:A:40:ASP:OD1	0.41	2.59	43	1
1:A:27:LYS:CG	1:A:27:LYS:O	0.41	2.69	40	1
1:A:42:LYS:C	1:A:44:ASN:OD1	0.41	2.59	12	1
1:A:43:ARG:O	1:A:45:LEU:N	0.41	2.54	37	1
1:A:39:TYR:OH	1:A:45:LEU:HD11	0.41	2.14	31	1
1:A:21:GLN:OE1	1:A:25:ASP:OD2	0.40	2.39	7	1
1:A:39:TYR:CZ	1:A:45:LEU:CD1	0.40	3.05	3	2
1:A:11:TYR:CG	1:A:47:CYS:SG	0.40	3.14	19	1
1:A:44:ASN:HD22	1:A:44:ASN:N	0.40	2.14	39	1
1:A:6:LYS:O	1:A:7:VAL:HG12	0.40	2.16	16	1
1:A:38:PHE:O	1:A:45:LEU:HD12	0.40	2.17	7	1
1:A:8:TYR:CE2	1:A:29:ASP:OD2	0.40	2.74	26	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	49/54 (91%)	26±2 (53±5%)	11±3 (22±5%)	13±2 (26±5%)	0	1
All	All	2107/2322 (91%)	1110 (53%)	458 (22%)	539 (26%)	0	1

All 30 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	28	LEU	42
1	A	10	ASN	38
1	A	19	ALA	37
1	A	13	VAL	35
1	A	9	GLU	34
1	A	27	LYS	33
1	A	21	GLN	33
1	A	20	ASN	31
1	A	14	SER	28
1	A	41	GLU	27
1	A	16	CYS	27
1	A	12	PRO	26
1	A	43	ARG	20
1	A	18	LEU	15
1	A	23	ASN	12
1	A	4	CYS	12
1	A	11	TYR	11
1	A	15	LYS	10
1	A	40	ASP	9
1	A	8	TYR	8
1	A	17	GLN	8
1	A	31	HIS	8
1	A	34	SER	7
1	A	22	CYS	6
1	A	29	ASP	6
1	A	45	LEU	5
1	A	39	TYR	4
1	A	36	GLU	4
1	A	25	ASP	2
1	A	32	ALA	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	46/50 (92%)	32±3 (70±7%)	14±3 (30±7%)	1	17
All	All	1978/2150 (92%)	1390 (70%)	588 (30%)	1	17

All 43 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	24	TYR	36
1	A	16	CYS	33
1	A	8	TYR	27
1	A	5	LYS	27
1	A	7	VAL	22
1	A	47	CYS	22
1	A	37	CYS	21
1	A	33	ARG	21
1	A	20	ASN	21
1	A	43	ARG	20
1	A	42	LYS	20
1	A	4	CYS	18
1	A	40	ASP	18
1	A	21	GLN	18
1	A	23	ASN	17
1	A	31	HIS	16
1	A	52	CYS	13
1	A	6	LYS	13
1	A	15	LYS	13
1	A	36	GLU	12
1	A	45	LEU	12
1	A	18	LEU	12
1	A	29	ASP	12
1	A	9	GLU	11
1	A	50	ASP	11
1	A	44	ASN	11
1	A	10	ASN	9
1	A	27	LYS	9
1	A	28	LEU	9
1	A	30	LYS	9
1	A	41	GLU	9
1	A	11	TYR	8
1	A	34	SER	8

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Mol	Chain	Res	Type	Models (Total)
1	A	17	GLN	8
1	A	46	GLN	7
1	A	26	CYS	6
1	A	22	CYS	6
1	A	39	TYR	5
1	A	13	VAL	5
1	A	14	SER	5
1	A	48	ILE	4
1	A	25	ASP	3
1	A	49	CYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	PCA	A	1	1	7,8,9	0.81±0.02	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	PCA	A	1	1	9,10,12	0.89±0.02	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0±0,0,11,13	0±0,1,1,1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation ⓘ

No chemical shift data were provided