



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 05:11 PM BST

PDB ID : 1TEY
Title : NMR structure of human histone chaperone, ASF1A
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Deposited on : 2004-05-26

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

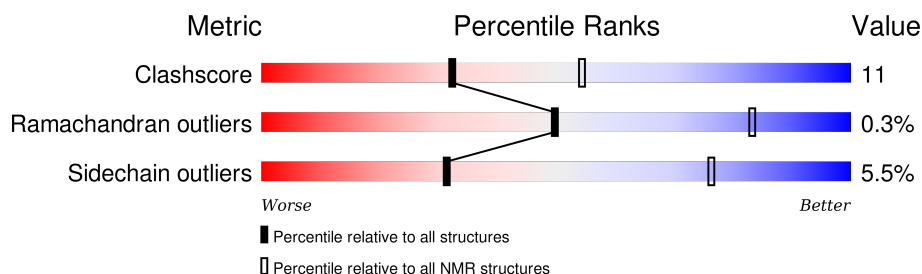
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 89%.

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	158	 74% 24% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:156 (155)	0.38	19

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 2 single-model clusters were found.

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

3 Entry composition

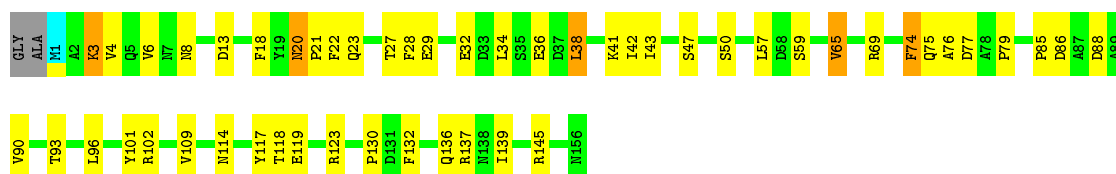
There is only 1 type of molecule in this entry. The entry contains 2461 atoms, of which 1204 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ASF1 anti-silencing function 1 homolog A.

Mol	Chain	Residues	Atoms						Trace
1	A	156	Total	C	H	N	O	S	0
			2461	804	1204	205	244	4	

There are 2 discrepancies between the modelled and reference sequences:

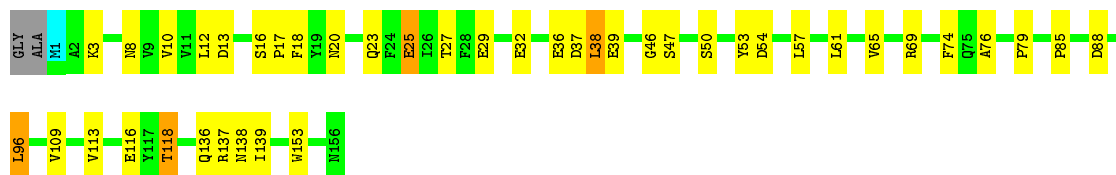
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9Y294
A	0	ALA	-	CLONING ARTIFACT	UNP Q9Y294



4.2.3 Score per residue for model 3

- Molecule 1: ASF1 anti-silencing function 1 homolog A

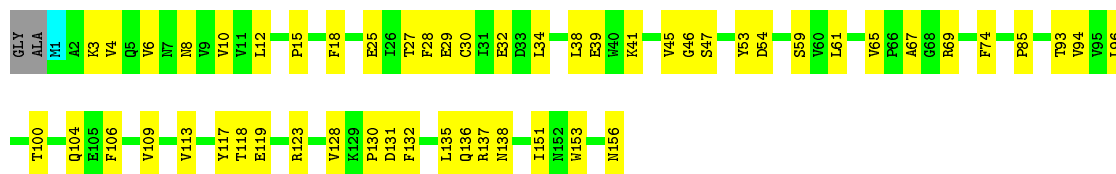
Chain A: 72% 24% ..



4.2.4 Score per residue for model 4

- Molecule 1: ASF1 anti-silencing function 1 homolog A

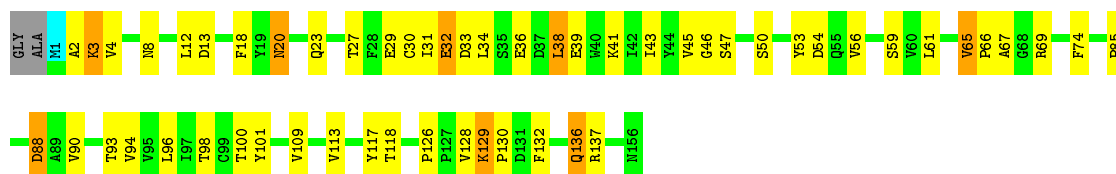
Chain A: 65% 34% ..



4.2.5 Score per residue for model 5

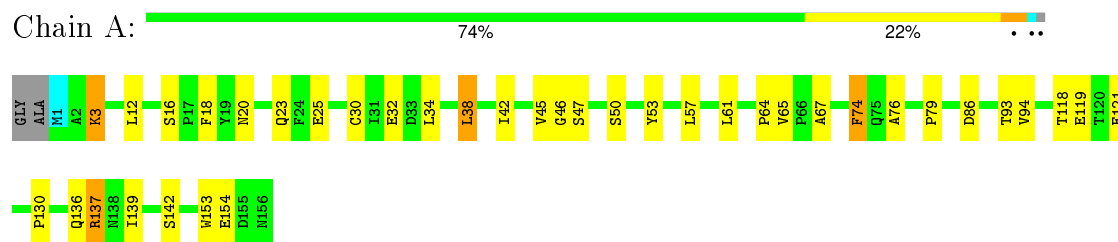
- Molecule 1: ASF1 anti-silencing function 1 homolog A

Chain A: 63% 30% 5% ..



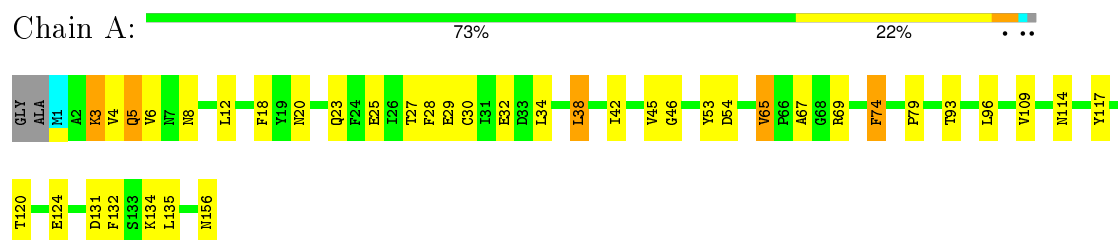
4.2.6 Score per residue for model 6

- Molecule 1: ASF1 anti-silencing function 1 homolog A



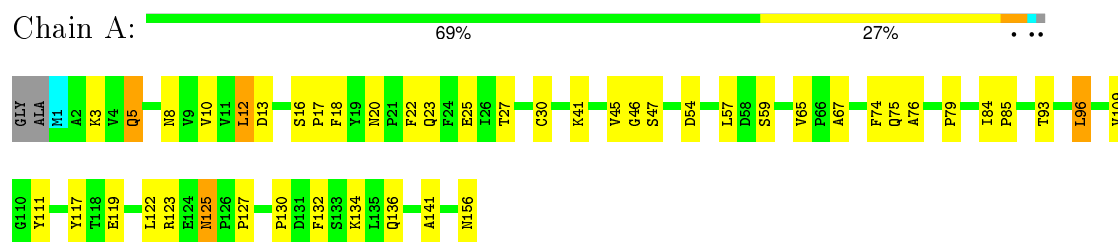
4.2.7 Score per residue for model 7

- Molecule 1: ASF1 anti-silencing function 1 homolog A



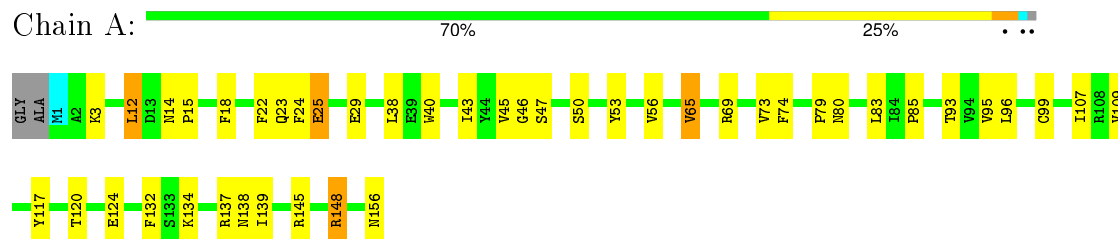
4.2.8 Score per residue for model 8

- Molecule 1: ASF1 anti-silencing function 1 homolog A



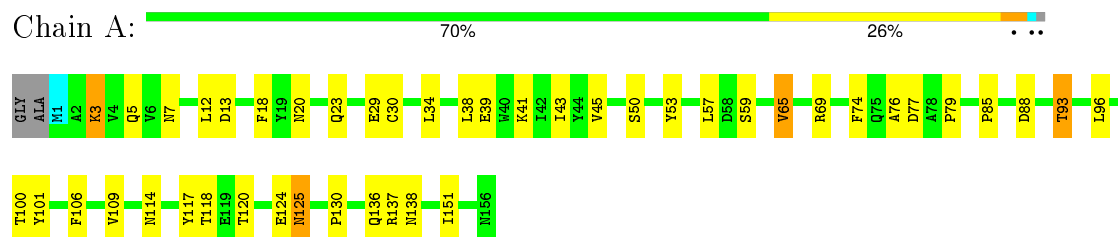
4.2.9 Score per residue for model 9

- Molecule 1: ASF1 anti-silencing function 1 homolog A



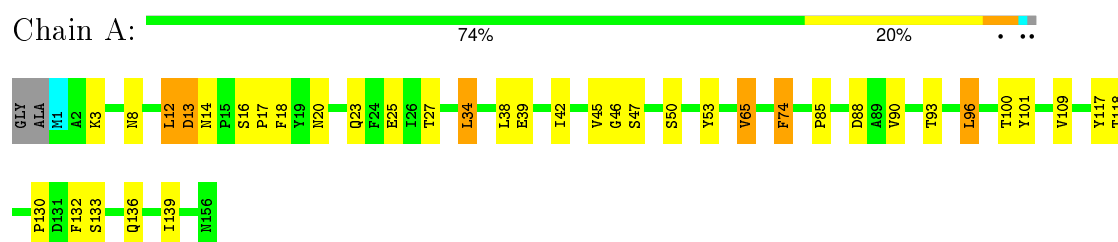
4.2.10 Score per residue for model 10

- Molecule 1: ASF1 anti-silencing function 1 homolog A



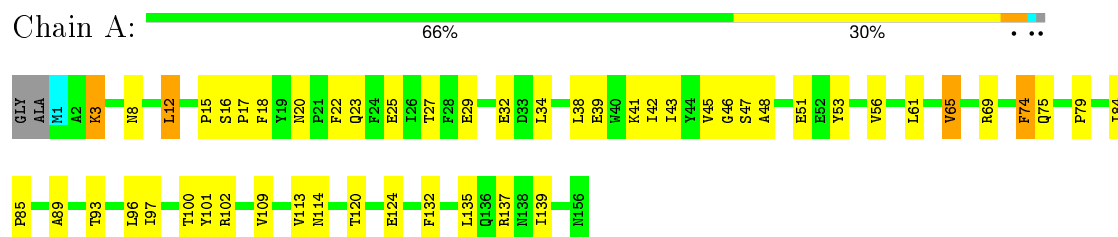
4.2.11 Score per residue for model 11

- Molecule 1: ASF1 anti-silencing function 1 homolog A



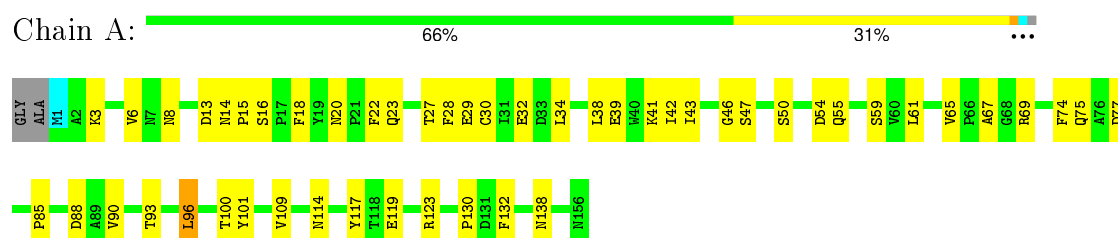
4.2.12 Score per residue for model 12

- Molecule 1: ASF1 anti-silencing function 1 homolog A



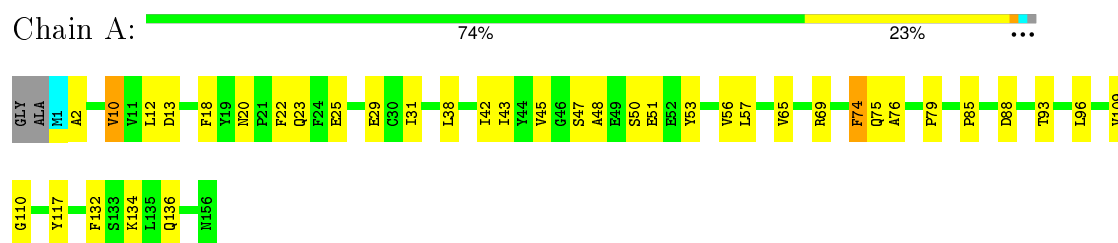
4.2.13 Score per residue for model 13

- Molecule 1: ASF1 anti-silencing function 1 homolog A



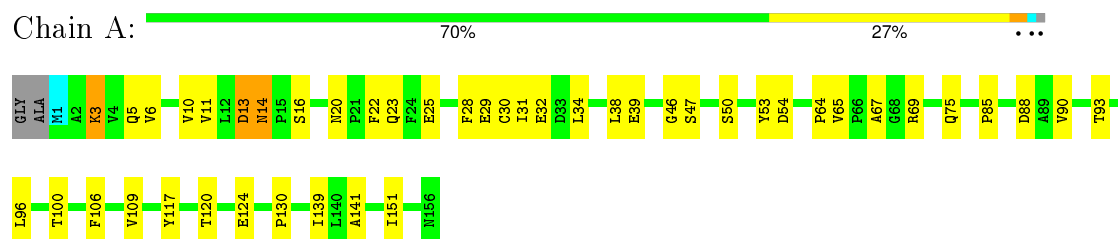
4.2.14 Score per residue for model 14

- Molecule 1: ASF1 anti-silencing function 1 homolog A



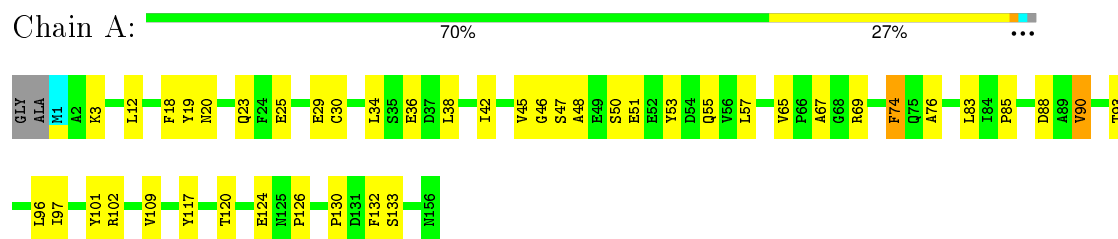
4.2.15 Score per residue for model 15

- Molecule 1: ASF1 anti-silencing function 1 homolog A



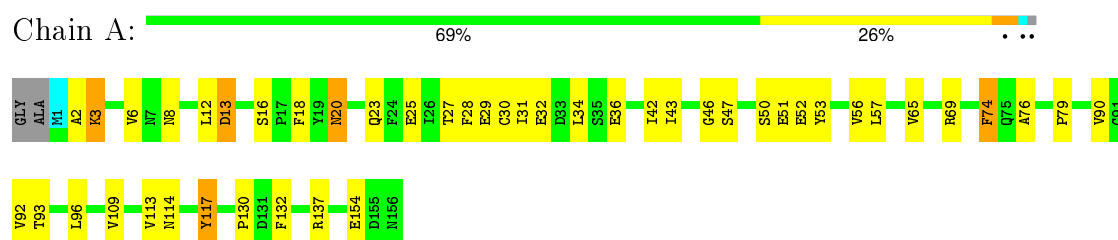
4.2.16 Score per residue for model 16

- Molecule 1: ASF1 anti-silencing function 1 homolog A



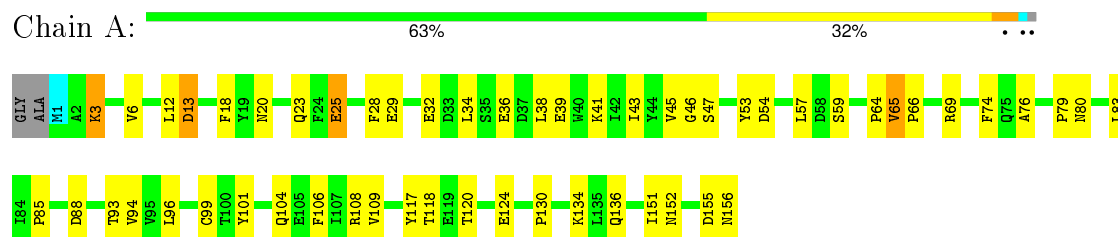
4.2.17 Score per residue for model 17

- Molecule 1: ASF1 anti-silencing function 1 homolog A



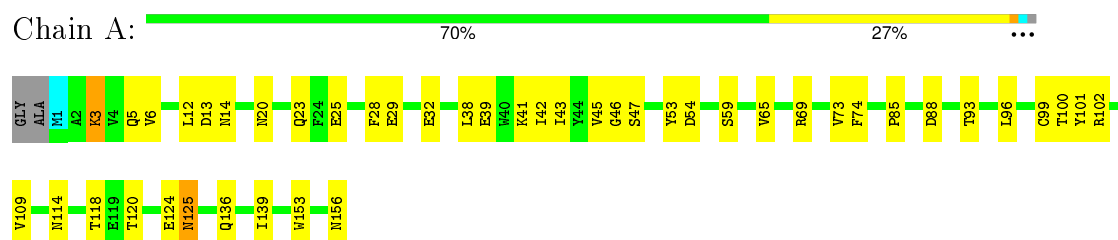
4.2.18 Score per residue for model 18

- Molecule 1: ASF1 anti-silencing function 1 homolog A



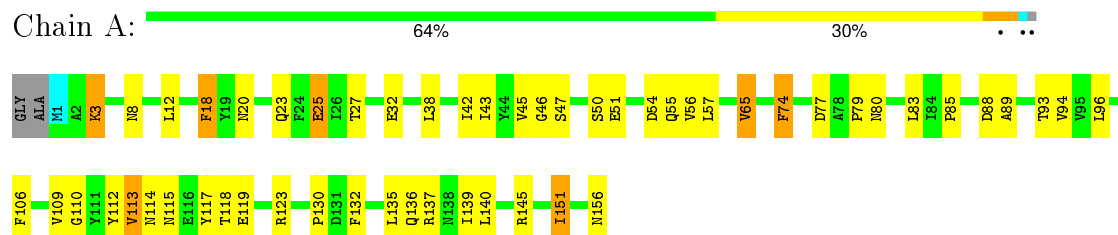
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: ASF1 anti-silencing function 1 homolog A



4.2.20 Score per residue for model 20

- Molecule 1: ASF1 anti-silencing function 1 homolog A



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics followed by cartesian dynamics*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
ARIA	refinement	1.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 6298
Number of chemical shift lists	1
Total number of shifts	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	0.42±0.04	0±1/1282 (0.0±0.1%)	0.45±0.01	0±0/1753 (0.0±0.0%)
All	All	0.43	6/25640 (0.0%)	0.45	0/35060 (0.0%)

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	0.1±0.2
All	All	0	1

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	53	TYR	CE2-CZ	-7.33	1.29	1.38	4	1
1	A	53	TYR	CE1-CZ	7.01	1.47	1.38	4	1
1	A	101	TYR	CE2-CZ	-6.36	1.30	1.38	10	1
1	A	101	TYR	CE1-CZ	5.51	1.45	1.38	10	1
1	A	44	TYR	CE1-CZ	-5.42	1.31	1.38	1	1
1	A	44	TYR	CE2-CZ	5.14	1.45	1.38	1	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	117	TYR	Sidechain	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	1249	1195	1193	27±5
All	All	24980	23900	23860	548

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:PRO:HG2	1:A:88:ASP:HB3	0.93	1.38	16	5
1:A:34:LEU:HD21	1:A:65:VAL:HB	0.89	1.42	17	2
1:A:12:LEU:HD11	1:A:25:GLU:HG3	0.79	1.55	11	2
1:A:118:THR:HG23	1:A:136:GLN:HB2	0.78	1.55	6	8
1:A:13:ASP:HB2	1:A:23:GLN:HE21	0.78	1.37	13	4
1:A:3:LYS:HG3	1:A:32:GLU:HB3	0.77	1.54	5	2
1:A:12:LEU:HD21	1:A:25:GLU:HG3	0.77	1.57	12	1
1:A:137:ARG:HH11	1:A:139:ILE:HG13	0.76	1.40	2	2
1:A:14:ASN:OD1	1:A:139:ILE:HB	0.75	1.81	9	1
1:A:12:LEU:HG	1:A:23:GLN:HG2	0.75	1.58	8	1
1:A:3:LYS:HG3	1:A:32:GLU:HB2	0.74	1.58	12	8
1:A:47:SER:HA	1:A:85:PRO:HD3	0.71	1.61	12	1
1:A:34:LEU:HD11	1:A:65:VAL:HG23	0.69	1.64	17	2
1:A:5:GLN:HE21	1:A:5:GLN:HA	0.69	1.48	7	1
1:A:43:ILE:HG12	1:A:56:VAL:HG22	0.68	1.65	12	4
1:A:38:LEU:HB2	1:A:65:VAL:HG21	0.68	1.65	7	6
1:A:39:GLU:HA	1:A:61:LEU:HG	0.68	1.64	12	4
1:A:12:LEU:HB2	1:A:23:GLN:HE21	0.67	1.48	9	3
1:A:25:GLU:HG2	1:A:73:VAL:HG22	0.67	1.65	19	1
1:A:47:SER:HB3	1:A:50:SER:O	0.67	1.90	13	9
1:A:29:GLU:HA	1:A:69:ARG:HA	0.67	1.65	10	16
1:A:38:LEU:O	1:A:61:LEU:HA	0.67	1.90	12	6
1:A:85:PRO:HD2	1:A:88:ASP:HB3	0.66	1.67	11	2
1:A:20:ASN:ND2	1:A:137:ARG:HH21	0.65	1.89	20	2
1:A:96:LEU:HA	1:A:109:VAL:O	0.65	1.92	4	19
1:A:152:ASN:HD21	1:A:155:ASP:HA	0.65	1.52	18	1
1:A:42:ILE:HG13	1:A:74:PHE:CE2	0.64	2.27	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HB2	1:A:65:VAL:HG23	0.64	1.67	18	1
1:A:18:PHE:CD2	1:A:132:PHE:HB3	0.64	2.27	11	13
1:A:43:ILE:HB	1:A:96:LEU:HD11	0.63	1.70	5	2
1:A:13:ASP:O	1:A:16:SER:HB2	0.63	1.93	17	2
1:A:5:GLN:HA	1:A:5:GLN:HE21	0.63	1.53	8	1
1:A:3:LYS:HG2	1:A:32:GLU:HB2	0.63	1.71	3	2
1:A:117:TYR:OH	1:A:130:PRO:HA	0.62	1.94	20	13
1:A:85:PRO:HD2	1:A:88:ASP:HB2	0.62	1.71	5	4
1:A:90:VAL:HG11	1:A:126:PRO:HB3	0.61	1.72	5	2
1:A:8:ASN:HB3	1:A:27:THR:HB	0.61	1.72	5	12
1:A:10:VAL:HG12	1:A:25:GLU:HB3	0.61	1.71	14	1
1:A:38:LEU:HG	1:A:65:VAL:HG21	0.60	1.73	12	1
1:A:34:LEU:HD21	1:A:101:TYR:CE1	0.60	2.31	11	1
1:A:4:VAL:HG23	1:A:34:LEU:HD21	0.60	1.74	2	3
1:A:45:VAL:HB	1:A:93:THR:HG22	0.60	1.73	10	13
1:A:137:ARG:HD2	1:A:137:ARG:O	0.59	1.97	3	1
1:A:48:ALA:H	1:A:85:PRO:HG3	0.59	1.57	12	1
1:A:10:VAL:HB	1:A:25:GLU:HB2	0.59	1.75	4	1
1:A:16:SER:HB3	1:A:17:PRO:HD2	0.58	1.75	11	4
1:A:3:LYS:O	1:A:30:CYS:HA	0.58	1.98	5	3
1:A:36:GLU:HB2	1:A:101:TYR:CE1	0.58	2.33	5	1
1:A:30:CYS:HB2	1:A:67:ALA:HA	0.58	1.76	15	9
1:A:6:VAL:HA	1:A:28:PHE:HA	0.57	1.76	2	8
1:A:36:GLU:HB3	1:A:101:TYR:CE1	0.57	2.35	2	3
1:A:85:PRO:CG	1:A:88:ASP:HB3	0.57	2.30	20	2
1:A:113:VAL:HG21	1:A:137:ARG:HG2	0.57	1.77	4	1
1:A:18:PHE:CE1	1:A:79:PRO:HD2	0.57	2.35	2	11
1:A:80:ASN:CB	1:A:83:LEU:HD13	0.56	2.30	18	2
1:A:34:LEU:CD2	1:A:65:VAL:HB	0.56	2.25	17	2
1:A:22:PHE:O	1:A:75:GLN:HA	0.56	2.00	15	6
1:A:120:THR:O	1:A:124:GLU:HG3	0.56	2.01	16	1
1:A:101:TYR:HD1	1:A:102:ARG:HG2	0.56	1.61	12	1
1:A:10:VAL:HB	1:A:25:GLU:HB3	0.56	1.78	8	2
1:A:3:LYS:HE3	1:A:154:GLU:OE2	0.55	2.01	17	1
1:A:47:SER:HB3	1:A:85:PRO:HG3	0.54	1.78	1	1
1:A:12:LEU:HB2	1:A:23:GLN:HG2	0.54	1.78	20	8
1:A:47:SER:OG	1:A:85:PRO:HG3	0.54	2.03	9	5
1:A:12:LEU:N	1:A:12:LEU:HD23	0.54	2.17	8	1
1:A:57:LEU:HB3	1:A:76:ALA:HB1	0.54	1.80	6	9
1:A:46:GLY:HA3	1:A:53:TYR:O	0.54	2.03	19	10
1:A:137:ARG:NH1	1:A:139:ILE:HG13	0.54	2.14	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:118:THR:CG2	1:A:136:GLN:HB2	0.54	2.32	11	4
1:A:18:PHE:HA	1:A:137:ARG:HG3	0.54	1.78	1	2
1:A:39:GLU:HB3	1:A:100:THR:HB	0.54	1.80	15	9
1:A:86:ASP:HA	1:A:130:PRO:HG3	0.54	1.80	2	1
1:A:46:GLY:O	1:A:85:PRO:HD3	0.54	2.02	19	2
1:A:113:VAL:HG21	1:A:137:ARG:CG	0.54	2.33	4	1
1:A:113:VAL:HB	1:A:139:ILE:HG12	0.53	1.79	12	1
1:A:12:LEU:HD11	1:A:25:GLU:HB2	0.53	1.81	7	4
1:A:112:TYR:HE1	1:A:145:ARG:HG3	0.53	1.64	20	1
1:A:14:ASN:HD21	1:A:139:ILE:HD12	0.53	1.64	9	1
1:A:85:PRO:HD2	1:A:88:ASP:CB	0.52	2.34	5	1
1:A:38:LEU:HD12	1:A:40:TRP:NE1	0.52	2.18	9	1
1:A:120:THR:O	1:A:124:GLU:HG2	0.52	2.04	15	7
1:A:41:LYS:CD	1:A:59:SER:HB3	0.52	2.35	19	1
1:A:34:LEU:O	1:A:64:PRO:HB2	0.52	2.05	15	2
1:A:101:TYR:CD1	1:A:102:ARG:HG2	0.52	2.39	12	1
1:A:16:SER:HB3	1:A:20:ASN:ND2	0.51	2.20	17	1
1:A:50:SER:HB3	1:A:53:TYR:CE2	0.51	2.40	6	4
1:A:47:SER:CB	1:A:85:PRO:HG3	0.51	2.36	18	4
1:A:34:LEU:HD21	1:A:65:VAL:CB	0.51	2.27	17	1
1:A:38:LEU:HD11	1:A:99:CYS:SG	0.51	2.46	9	1
1:A:113:VAL:HG13	1:A:137:ARG:HG3	0.51	1.83	5	1
1:A:80:ASN:HB3	1:A:83:LEU:HB2	0.50	1.83	9	1
1:A:137:ARG:HD3	1:A:139:ILE:CG1	0.50	2.36	3	1
1:A:48:ALA:HB3	1:A:88:ASP:OD1	0.50	2.06	14	2
1:A:3:LYS:HG3	1:A:32:GLU:CB	0.50	2.35	12	1
1:A:46:GLY:H	1:A:54:ASP:HA	0.50	1.67	7	10
1:A:119:GLU:O	1:A:123:ARG:HG3	0.49	2.06	20	5
1:A:46:GLY:N	1:A:54:ASP:HA	0.49	2.22	4	1
1:A:50:SER:HB2	1:A:53:TYR:CE2	0.49	2.42	14	3
1:A:107:ILE:HA	1:A:148:ARG:HA	0.49	1.83	9	1
1:A:128:VAL:HG13	1:A:129:LYS:HD2	0.49	1.82	5	1
1:A:43:ILE:O	1:A:96:LEU:HG	0.49	2.08	5	5
1:A:47:SER:HA	1:A:85:PRO:CD	0.49	2.34	12	1
1:A:33:ASP:OD1	1:A:66:PRO:HA	0.48	2.08	5	1
1:A:42:ILE:HG13	1:A:74:PHE:CZ	0.48	2.44	14	11
1:A:34:LEU:HD13	1:A:65:VAL:O	0.48	2.07	10	1
1:A:117:TYR:HA	1:A:134:LYS:O	0.48	2.08	14	5
1:A:13:ASP:HB2	1:A:23:GLN:H	0.48	1.69	5	1
1:A:47:SER:O	1:A:51:GLU:HA	0.48	2.09	17	2
1:A:110:GLY:O	1:A:145:ARG:HB2	0.48	2.08	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LYS:HE3	1:A:153:TRP:HB2	0.48	1.85	3	1
1:A:80:ASN:HB2	1:A:83:LEU:HD13	0.48	1.85	18	1
1:A:13:ASP:HB3	1:A:23:GLN:HB3	0.48	1.86	2	1
1:A:3:LYS:HD2	1:A:3:LYS:N	0.48	2.24	19	2
1:A:115:ASN:HD22	1:A:135:LEU:HD11	0.47	1.67	20	1
1:A:113:VAL:HA	1:A:138:ASN:O	0.47	2.09	3	1
1:A:11:VAL:HG13	1:A:14:ASN:OD1	0.47	2.09	15	1
1:A:39:GLU:O	1:A:99:CYS:HA	0.47	2.08	19	2
1:A:5:GLN:HB2	1:A:31:ILE:HD11	0.47	1.86	15	1
1:A:34:LEU:HD23	1:A:65:VAL:HB	0.47	1.86	2	1
1:A:15:PRO:HB3	1:A:138:ASN:HA	0.47	1.84	13	4
1:A:50:SER:O	1:A:53:TYR:HD2	0.47	1.93	5	1
1:A:41:LYS:HG2	1:A:59:SER:HB3	0.47	1.86	5	1
1:A:47:SER:HB2	1:A:85:PRO:HD3	0.47	1.87	20	2
1:A:4:VAL:HG23	1:A:34:LEU:HD11	0.47	1.85	4	1
1:A:41:LYS:HG3	1:A:59:SER:HB2	0.47	1.86	4	2
1:A:3:LYS:CG	1:A:32:GLU:HB2	0.47	2.40	3	1
1:A:16:SER:HB2	1:A:20:ASN:ND2	0.46	2.25	15	2
1:A:79:PRO:HB2	1:A:84:ILE:HD11	0.46	1.86	8	1
1:A:43:ILE:HA	1:A:56:VAL:HA	0.46	1.88	5	1
1:A:47:SER:CB	1:A:85:PRO:HG2	0.46	2.41	13	1
1:A:148:ARG:C	1:A:148:ARG:HD2	0.46	2.31	9	1
1:A:125:ASN:N	1:A:125:ASN:HD22	0.46	2.09	10	2
1:A:22:PHE:CE1	1:A:95:VAL:HG11	0.46	2.45	9	1
1:A:11:VAL:HG12	1:A:141:ALA:HB2	0.46	1.87	15	1
1:A:85:PRO:HG2	1:A:88:ASP:HB2	0.46	1.86	18	1
1:A:85:PRO:HG2	1:A:88:ASP:CB	0.46	2.41	18	2
1:A:125:ASN:HD22	1:A:125:ASN:N	0.46	2.08	8	1
1:A:47:SER:OG	1:A:85:PRO:HG2	0.46	2.09	2	2
1:A:47:SER:HB2	1:A:85:PRO:CG	0.46	2.41	13	3
1:A:2:ALA:O	1:A:31:ILE:HD12	0.46	2.10	5	2
1:A:41:LYS:HG3	1:A:59:SER:HB3	0.46	1.88	18	4
1:A:64:PRO:O	1:A:66:PRO:HD3	0.46	2.11	18	1
1:A:13:ASP:HB2	1:A:23:GLN:NE2	0.46	2.17	13	1
1:A:12:LEU:HD21	1:A:25:GLU:HB2	0.46	1.87	9	1
1:A:43:ILE:HB	1:A:96:LEU:CD1	0.45	2.39	5	1
1:A:57:LEU:HD23	1:A:77:ASP:O	0.45	2.11	20	2
1:A:3:LYS:HZ3	1:A:32:GLU:CD	0.45	2.15	4	1
1:A:36:GLU:HG2	1:A:37:ASP:N	0.45	2.26	3	1
1:A:101:TYR:CD2	1:A:102:ARG:HG2	0.45	2.47	16	3
1:A:3:LYS:HG2	1:A:153:TRP:CE3	0.45	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ASN:HB2	1:A:138:ASN:HB3	0.45	1.87	10	1
1:A:86:ASP:O	1:A:130:PRO:HG3	0.45	2.12	6	1
1:A:96:LEU:HD13	1:A:98:THR:HG23	0.45	1.86	5	1
1:A:57:LEU:HD21	1:A:79:PRO:HG3	0.45	1.88	8	5
1:A:113:VAL:CG2	1:A:137:ARG:HG3	0.45	2.42	20	1
1:A:119:GLU:HG2	1:A:121:GLU:HB3	0.45	1.89	6	1
1:A:34:LEU:HD23	1:A:101:TYR:HE2	0.45	1.71	12	1
1:A:14:ASN:ND2	1:A:139:ILE:HD12	0.45	2.27	9	2
1:A:40:TRP:O	1:A:59:SER:HA	0.45	2.12	1	1
1:A:11:VAL:HG11	1:A:139:ILE:HG21	0.45	1.89	1	1
1:A:137:ARG:HD3	1:A:139:ILE:HG13	0.44	1.88	6	1
1:A:45:VAL:HB	1:A:93:THR:CG2	0.44	2.43	7	1
1:A:114:ASN:HB2	1:A:140:LEU:HD11	0.44	1.89	20	1
1:A:12:LEU:O	1:A:13:ASP:HB3	0.44	2.12	10	1
1:A:14:ASN:CG	1:A:139:ILE:HB	0.44	2.32	19	2
1:A:106:PHE:HB3	1:A:151:ILE:CD1	0.44	2.43	15	5
1:A:50:SER:C	1:A:52:GLU:H	0.44	2.15	17	1
1:A:45:VAL:HG21	1:A:94:VAL:HB	0.44	1.88	5	1
1:A:39:GLU:HA	1:A:61:LEU:HD13	0.44	1.88	5	1
1:A:131:ASP:O	1:A:135:LEU:HB2	0.44	2.12	4	2
1:A:41:LYS:HD3	1:A:59:SER:HB3	0.44	1.89	19	1
1:A:19:TYR:CE2	1:A:133:SER:HA	0.44	2.48	16	1
1:A:45:VAL:CG2	1:A:94:VAL:HB	0.44	2.43	20	4
1:A:22:PHE:CE2	1:A:79:PRO:HD3	0.44	2.48	1	1
1:A:3:LYS:HB3	1:A:34:LEU:CD1	0.43	2.43	10	1
1:A:85:PRO:O	1:A:89:ALA:HB2	0.43	2.13	20	1
1:A:113:VAL:CG2	1:A:137:ARG:HB3	0.43	2.43	17	1
1:A:41:LYS:CG	1:A:59:SER:HB3	0.43	2.44	19	1
1:A:22:PHE:HB3	1:A:24:PHE:CE2	0.43	2.48	9	1
1:A:14:ASN:ND2	1:A:139:ILE:HB	0.43	2.29	15	1
1:A:20:ASN:OD1	1:A:137:ARG:HD3	0.43	2.13	1	1
1:A:13:ASP:OD2	1:A:20:ASN:HB2	0.43	2.14	13	1
1:A:145:ARG:HA	1:A:145:ARG:HE	0.43	1.73	2	1
1:A:43:ILE:HG13	1:A:56:VAL:HG22	0.43	1.90	17	1
1:A:99:CYS:O	1:A:105:GLU:HA	0.43	2.14	1	1
1:A:38:LEU:CD1	1:A:99:CYS:SG	0.42	3.07	9	1
1:A:34:LEU:HD12	1:A:101:TYR:CE1	0.42	2.50	5	1
1:A:20:ASN:ND2	1:A:137:ARG:NH2	0.42	2.65	20	1
1:A:118:THR:HG22	1:A:136:GLN:HB2	0.42	1.92	18	2
1:A:12:LEU:HD23	1:A:23:GLN:HB3	0.42	1.91	12	1
1:A:79:PRO:HG2	1:A:84:ILE:HD11	0.42	1.92	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD22	1:A:65:VAL:HG11	0.42	1.90	14	1
1:A:92:VAL:HB	1:A:114:ASN:ND2	0.42	2.29	17	1
1:A:47:SER:HB2	1:A:85:PRO:HG3	0.42	1.91	18	1
1:A:2:ALA:O	1:A:31:ILE:HB	0.42	2.14	17	1
1:A:41:LYS:HD2	1:A:43:ILE:HD11	0.42	1.90	18	2
1:A:18:PHE:CZ	1:A:79:PRO:HD2	0.42	2.50	2	1
1:A:21:PRO:HA	1:A:77:ASP:HA	0.42	1.89	2	1
1:A:13:ASP:CG	1:A:137:ARG:HH21	0.42	2.17	10	1
1:A:113:VAL:HG21	1:A:137:ARG:CZ	0.42	2.44	1	1
1:A:34:LEU:HD12	1:A:36:GLU:O	0.42	2.15	17	1
1:A:55:GLN:HB3	1:A:83:LEU:HD13	0.42	1.91	16	1
1:A:8:ASN:HB3	1:A:27:THR:CB	0.42	2.44	11	2
1:A:3:LYS:HB2	1:A:153:TRP:CE3	0.41	2.50	6	1
1:A:10:VAL:HG13	1:A:25:GLU:HB3	0.41	1.91	15	1
1:A:90:VAL:HG22	1:A:130:PRO:HB3	0.41	1.91	11	1
1:A:13:ASP:OD1	1:A:20:ASN:ND2	0.41	2.48	5	1
1:A:20:ASN:HD21	1:A:137:ARG:NH2	0.41	2.13	20	1
1:A:12:LEU:HD12	1:A:12:LEU:N	0.41	2.29	19	1
1:A:38:LEU:HB2	1:A:65:VAL:CG2	0.41	2.45	9	1
1:A:18:PHE:HB3	1:A:132:PHE:O	0.41	2.15	12	1
1:A:111:TYR:CE1	1:A:141:ALA:HA	0.41	2.50	8	1
1:A:18:PHE:HE1	1:A:79:PRO:HG2	0.41	1.75	12	1
1:A:15:PRO:HA	1:A:137:ARG:O	0.41	2.16	12	1
1:A:46:GLY:O	1:A:84:ILE:HA	0.41	2.14	12	1
1:A:122:LEU:HD22	1:A:127:PRO:HG3	0.41	1.93	8	1
1:A:12:LEU:HB2	1:A:23:GLN:HB2	0.41	1.93	3	1
1:A:47:SER:HB2	1:A:50:SER:O	0.41	2.15	6	1
1:A:89:ALA:O	1:A:135:LEU:HD21	0.41	2.16	12	1
1:A:38:LEU:HD23	1:A:65:VAL:HG21	0.41	1.91	11	1
1:A:34:LEU:HD22	1:A:65:VAL:CG1	0.41	2.46	16	1
1:A:14:ASN:N	1:A:14:ASN:HD22	0.41	2.14	9	1
1:A:12:LEU:H	1:A:12:LEU:HD22	0.41	1.74	9	1
1:A:25:GLU:HG2	1:A:73:VAL:HG12	0.41	1.92	9	1
1:A:34:LEU:HD21	1:A:101:TYR:HE1	0.41	1.68	11	1
1:A:96:LEU:HD23	1:A:110:GLY:HA2	0.41	1.92	14	1
1:A:3:LYS:HD3	1:A:153:TRP:HB3	0.40	1.93	19	1
1:A:17:PRO:HA	1:A:135:LEU:O	0.40	2.16	12	1
1:A:42:ILE:HG12	1:A:97:ILE:HG12	0.40	1.93	16	1
1:A:41:LYS:O	1:A:97:ILE:HA	0.40	2.16	12	1
1:A:39:GLU:OE2	1:A:41:LYS:HE2	0.40	2.16	1	1
1:A:16:SER:HB2	1:A:20:ASN:CG	0.40	2.36	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD23	1:A:101:TYR:CE1	0.40	2.52	13	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	154/158 (97%)	145±2 (94±1%)	8±2 (5±1%)	0±1 (0±0%)	50	83
All	All	3080/3160 (97%)	2904 (94%)	168 (5%)	8 (0%)	50	83

All 3 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	90	VAL	6
1	A	77	ASP	1
1	A	128	VAL	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/141 (99%)	132±2 (94±1%)	8±2 (6±1%)	31	76
All	All	2800/2820 (99%)	2645 (94%)	155 (6%)	31	76

All 38 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	74	PHE	17

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Mol	Chain	Res	Type	Models (Total)
1	A	65	VAL	16
1	A	3	LYS	15
1	A	20	ASN	13
1	A	38	LEU	10
1	A	13	ASP	8
1	A	93	THR	7
1	A	156	ASN	7
1	A	25	GLU	6
1	A	5	GLN	5
1	A	114	ASN	5
1	A	96	LEU	4
1	A	12	LEU	4
1	A	51	GLU	3
1	A	55	GLN	3
1	A	125	ASN	3
1	A	136	GLN	3
1	A	145	ARG	2
1	A	14	ASN	2
1	A	154	GLU	2
1	A	118	THR	2
1	A	104	GLN	2
1	A	133	SER	1
1	A	7	ASN	1
1	A	23	GLN	1
1	A	108	ARG	1
1	A	34	LEU	1
1	A	137	ARG	1
1	A	113	VAL	1
1	A	18	PHE	1
1	A	142	SER	1
1	A	148	ARG	1
1	A	129	LYS	1
1	A	116	GLU	1
1	A	10	VAL	1
1	A	151	ILE	1
1	A	32	GLU	1
1	A	88	ASP	1

6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6298

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1925
Number of shifts mapped to atoms	1925
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	0.21 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	-0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	146	0.31 ± 0.19	None needed (< 0.5 ppm)
^{15}N	143	-0.32 ± 0.36	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1701 atoms were assigned a chemical shift out of a possible 1920. 29 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	739/751 (98%)	297/298 (100%)	300/310 (97%)	142/143 (99%)
Sidechain	863/992 (87%)	533/578 (92%)	309/371 (83%)	21/43 (49%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	99/177 (56%)	55/93 (59%)	42/78 (54%)	2/6 (33%)
Overall	1701/1920 (89%)	885/969 (91%)	651/759 (86%)	165/192 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1713 atoms were assigned a chemical shift out of a possible 1933. 29 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	744/756 (98%)	299/300 (100%)	302/312 (97%)	143/144 (99%)
Sidechain	870/1000 (87%)	537/583 (92%)	312/374 (83%)	21/43 (49%)
Aromatic	99/177 (56%)	55/93 (59%)	42/78 (54%)	2/6 (33%)
Overall	1713/1933 (89%)	891/976 (91%)	656/764 (86%)	166/193 (86%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	102	ARG	NE	124.89	92.63 – 76.73	25.3
1	A	108	ARG	NE	123.85	92.63 – 76.73	24.6
1	A	137	ARG	NE	121.72	92.63 – 76.73	23.3
1	A	3	LYS	H	3.63	11.24 – 5.14	-7.5
1	A	70	HIS	HB2	1.13	4.91 – 1.31	-5.5
1	A	40	TRP	HE1	7.20	12.85 – 7.35	-5.3
1	A	153	TRP	HH2	5.02	8.94 – 5.04	-5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

