



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 07:04 PM BST

PDB ID : 2B3W
Title : NMR structure of the E.coli protein YbiA, Northeast Structural Genomics target ET24.
Authors : Ramelot, T.A.; Cort, J.R.; Xiao, R.; Shih, L.Y.; Acton, T.B.; Montelione, G.T.; Kennedy, M.A.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2005-09-21

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

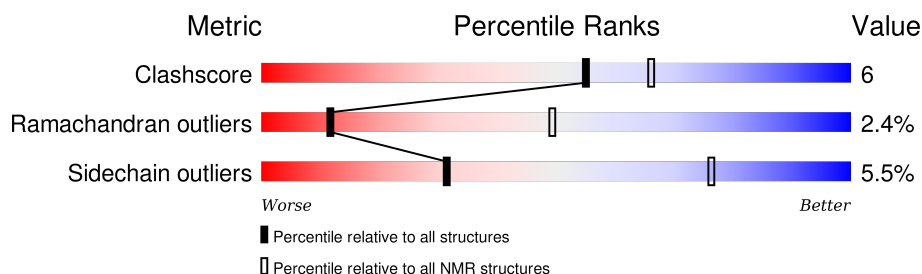
1 Overall quality at a glance

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	168	<div> <div></div> <div>82%</div> <div>12%</div> <div>7%</div> </div>

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 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:3-A:6, A:10-A:162 (157)	0.69	18

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2768 atoms, of which 1375 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hypothetical protein ybiA.

Mol	Chain	Residues	Atoms						Trace
1	A	168	Total	C	H	N	O	S	0
			2768	877	1375	262	248	6	

There are 8 discrepancies between the modelled and reference sequences:

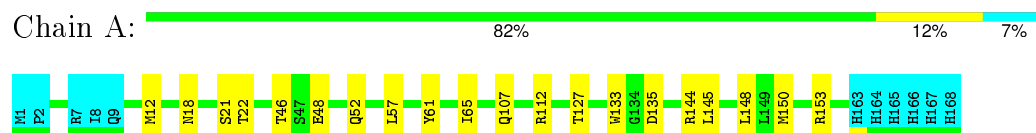
Chain	Residue	Modelled	Actual	Comment	Reference
A	161	LEU	-	CLONING ARTIFACT	UNP P30176
A	162	GLU	-	CLONING ARTIFACT	UNP P30176
A	163	HIS	-	EXPRESSION TAG	UNP P30176
A	164	HIS	-	EXPRESSION TAG	UNP P30176
A	165	HIS	-	EXPRESSION TAG	UNP P30176
A	166	HIS	-	EXPRESSION TAG	UNP P30176
A	167	HIS	-	EXPRESSION TAG	UNP P30176
A	168	HIS	-	EXPRESSION TAG	UNP P30176

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: Hypothetical protein ybiA

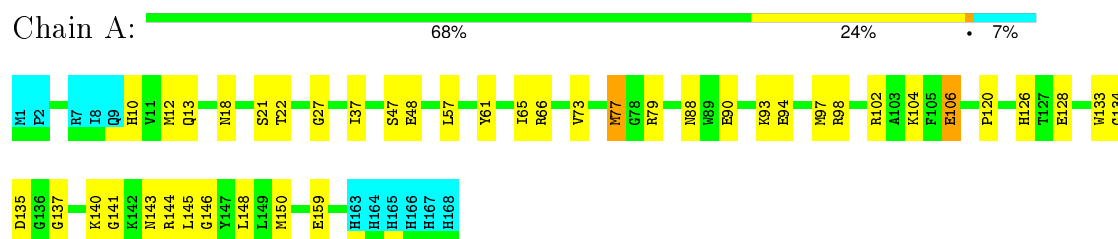


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

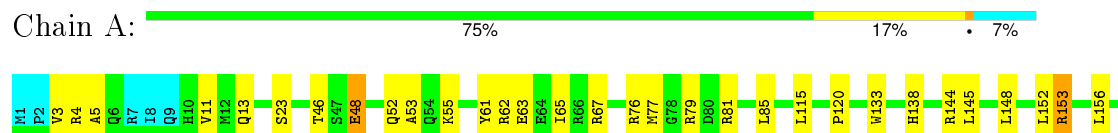
4.2.1 Score per residue for model 1

- Molecule 1: Hypothetical protein ybiA



4.2.2 Score per residue for model 2

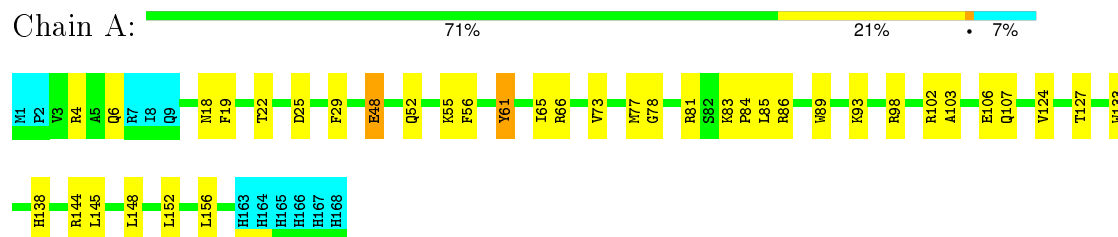
- Molecule 1: Hypothetical protein ybiA



H163
H164
H165
H166
H167
H168

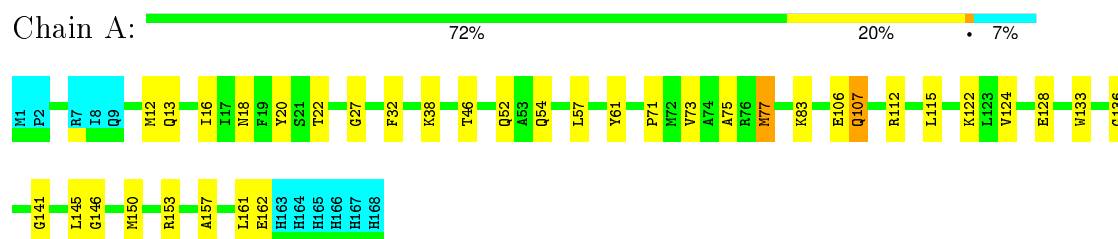
4.2.3 Score per residue for model 3

- Molecule 1: Hypothetical protein ybiA



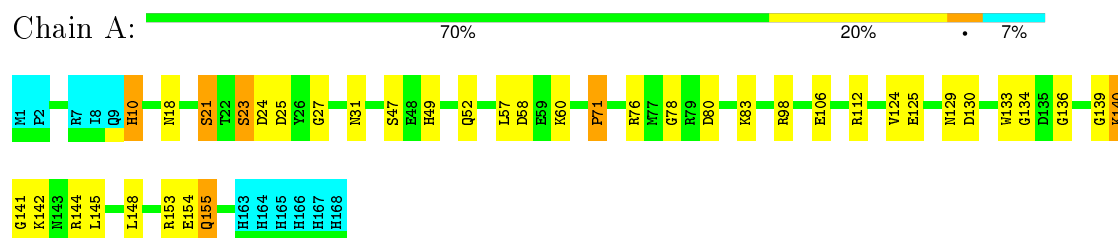
4.2.4 Score per residue for model 4

- Molecule 1: Hypothetical protein ybiA



4.2.5 Score per residue for model 5

- Molecule 1: Hypothetical protein ybiA



4.2.6 Score per residue for model 6

- Molecule 1: Hypothetical protein ybiA

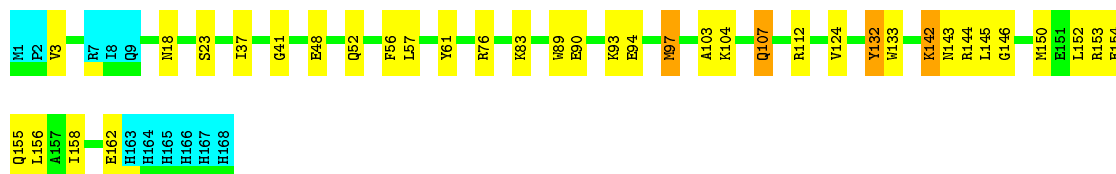




4.2.7 Score per residue for model 7

- Molecule 1: Hypothetical protein ybiA

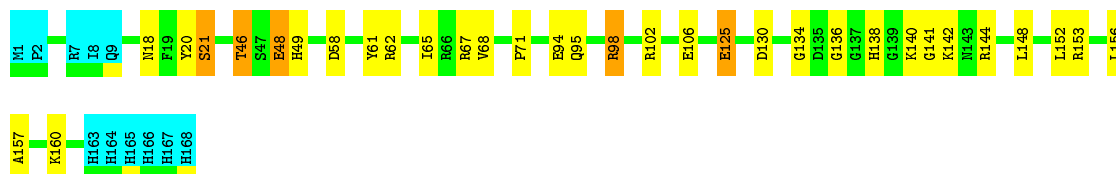
Chain A: 71% 20% 7%



4.2.8 Score per residue for model 8

- Molecule 1: Hypothetical protein ybiA

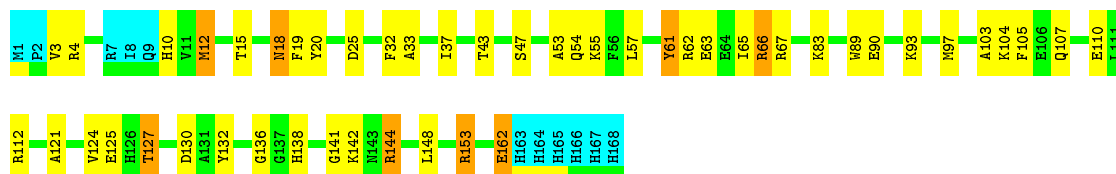
Chain A: 74% 17% 7%



4.2.9 Score per residue for model 9

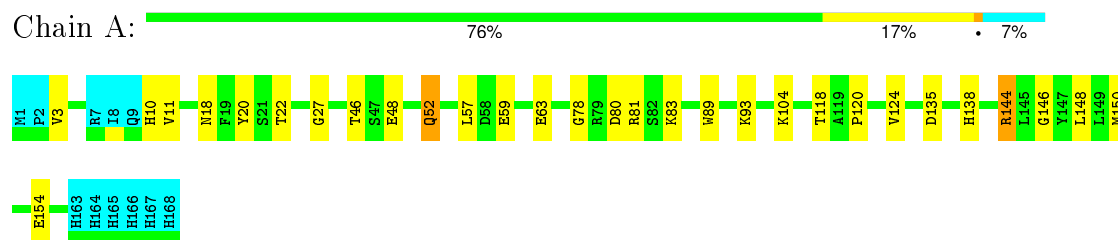
- Molecule 1: Hypothetical protein ybiA

Chain A: 64% 24% 5% 7%



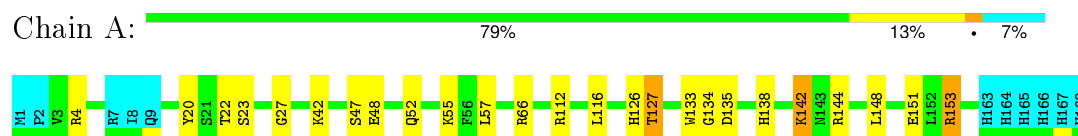
4.2.10 Score per residue for model 10

- Molecule 1: Hypothetical protein ybiA



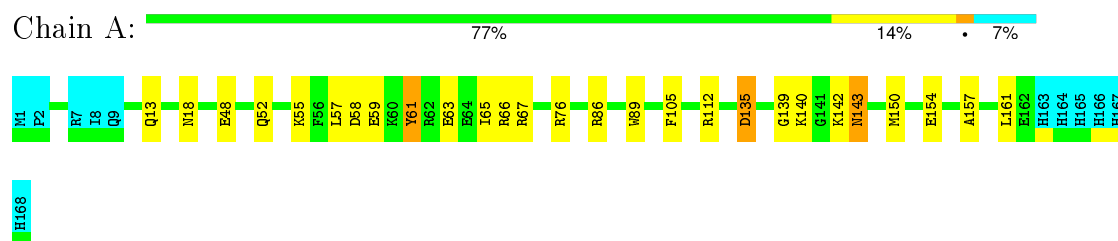
4.2.11 Score per residue for model 11

- Molecule 1: Hypothetical protein ybiA



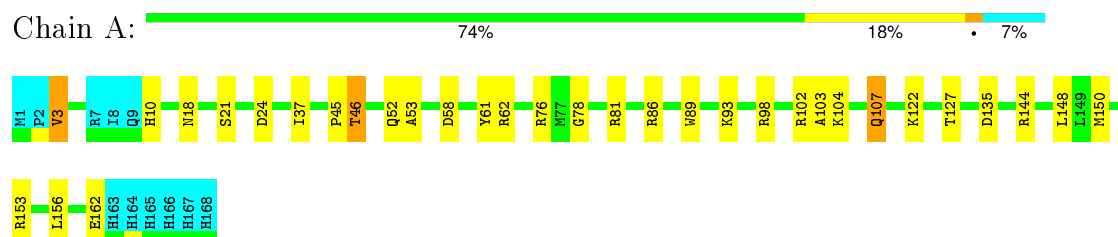
4.2.12 Score per residue for model 12

- Molecule 1: Hypothetical protein ybiA



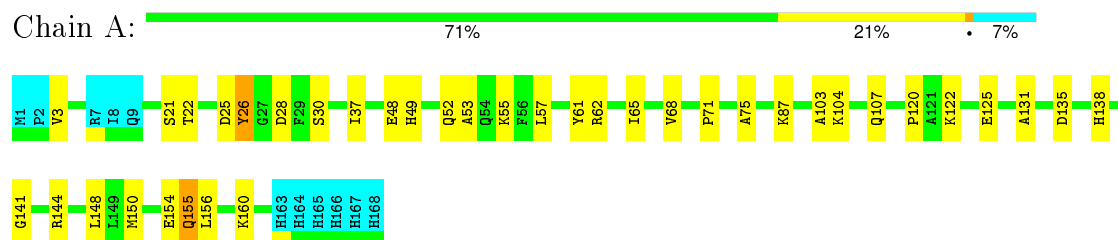
4.2.13 Score per residue for model 13

- Molecule 1: Hypothetical protein ybiA



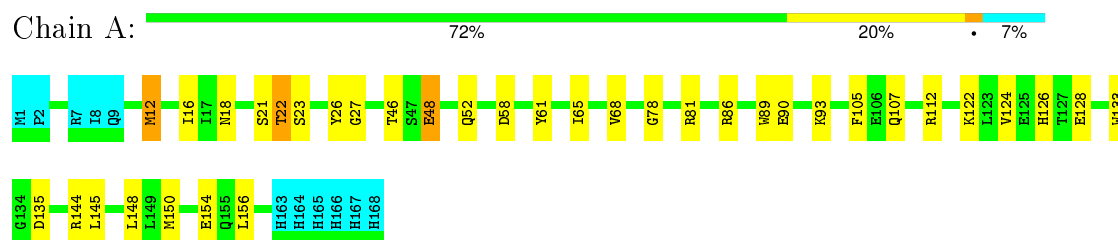
4.2.14 Score per residue for model 14

- Molecule 1: Hypothetical protein ybiA



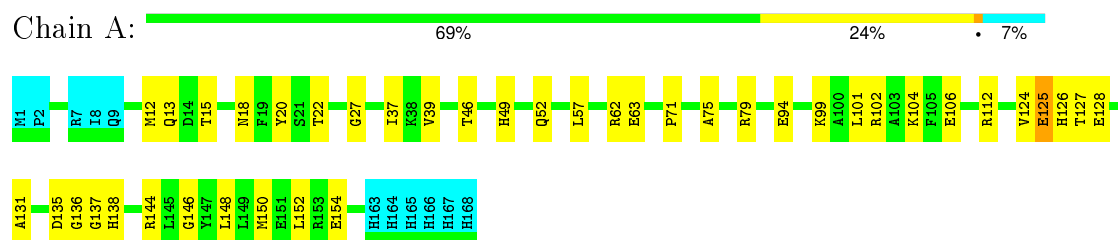
4.2.15 Score per residue for model 15

- Molecule 1: Hypothetical protein ybiA



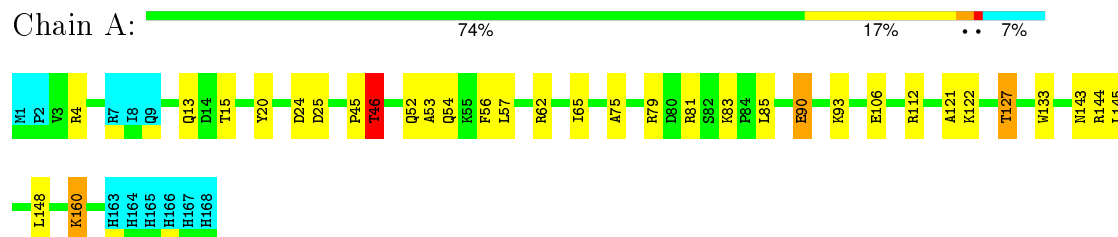
4.2.16 Score per residue for model 16

- Molecule 1: Hypothetical protein ybiA



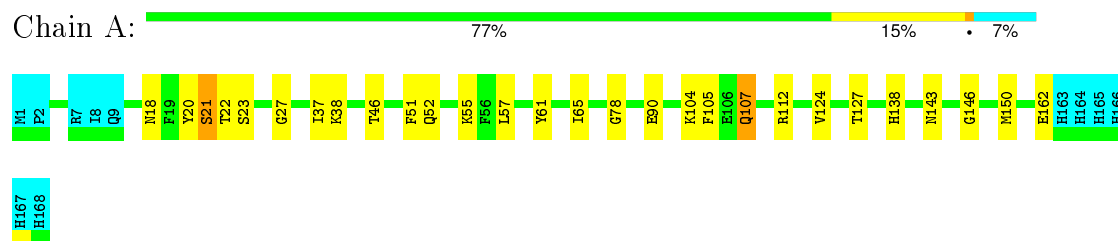
4.2.17 Score per residue for model 17

- Molecule 1: Hypothetical protein ybiA



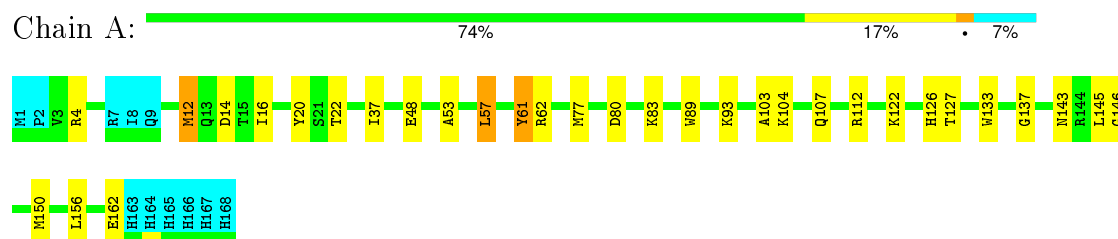
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Hypothetical protein ybiA



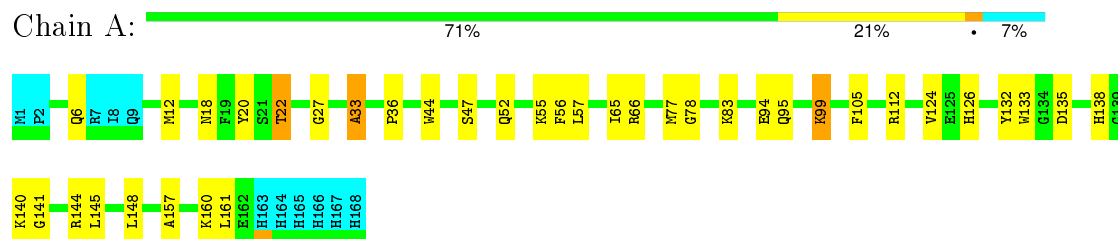
4.2.19 Score per residue for model 19

- Molecule 1: Hypothetical protein ybiA



4.2.20 Score per residue for model 20

- Molecule 1: Hypothetical protein ybiA



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *distance geometry simulated annealing cns water refinement*.

Of the ? calculated structures, 20 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	structure solution	xplor-nih-2.10
CNS	refinement	1.1

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 ⓘ

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	1289	1277	1272	17±3
All	All	25780	25540	25440	331

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:LYS:HA	1:A:160:LYS:HE3	0.80	1.54	17	1
1:A:135:ASP:HA	1:A:141:GLY:HA3	0.79	1.52	14	1
1:A:53:ALA:HB1	1:A:62:ARG:HG3	0.75	1.58	14	5
1:A:90:GLU:HA	1:A:93:LYS:HE3	0.73	1.60	17	1
1:A:153:ARG:HB3	1:A:153:ARG:HH11	0.71	1.43	9	2
1:A:46:THR:HB	1:A:48:GLU:OE1	0.69	1.85	8	1
1:A:130:ASP:O	1:A:136:GLY:HA2	0.68	1.89	8	2
1:A:48:GLU:O	1:A:52:GLN:HB2	0.68	1.89	12	1
1:A:155:GLN:HA	1:A:155:GLN:HE21	0.67	1.49	5	2
1:A:106:GLU:HA	1:A:112:ARG:HH21	0.67	1.49	16	3
1:A:95:GLN:HA	1:A:98:ARG:HD2	0.66	1.67	8	1
1:A:97:MET:HG3	1:A:133:TRP:CH2	0.65	2.27	7	1
1:A:116:LEU:HD23	1:A:153:ARG:HG2	0.63	1.68	11	1
1:A:153:ARG:HH11	1:A:153:ARG:HB3	0.63	1.53	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:THR:HG23	1:A:48:GLU:OE1	0.63	1.93	2	1
1:A:4:ARG:HB2	1:A:25:ASP:HB3	0.63	1.68	17	1
1:A:57:LEU:HD23	1:A:57:LEU:H	0.62	1.55	18	5
1:A:22:THR:HA	1:A:27:GLY:HA3	0.62	1.71	15	5
1:A:57:LEU:H	1:A:57:LEU:HD23	0.62	1.55	4	7
1:A:22:THR:O	1:A:27:GLY:HA3	0.60	1.96	20	4
1:A:144:ARG:O	1:A:148:LEU:HG	0.60	1.96	3	13
1:A:11:VAL:HG21	1:A:120:PRO:HD2	0.60	1.72	10	2
1:A:106:GLU:HA	1:A:112:ARG:NH2	0.60	2.12	16	3
1:A:58:ASP:HB2	1:A:61:TYR:HB2	0.60	1.74	12	2
1:A:128:GLU:OE2	1:A:137:GLY:HA3	0.59	1.97	1	1
1:A:83:LYS:HE3	1:A:84:PRO:HD2	0.59	1.75	3	1
1:A:20:TYR:O	1:A:21:SER:HB2	0.59	1.97	18	2
1:A:112:ARG:HG3	1:A:156:LEU:HD13	0.58	1.76	15	3
1:A:133:TRP:HB3	1:A:145:LEU:HD22	0.57	1.76	7	8
1:A:132:TYR:HA	1:A:141:GLY:O	0.57	1.99	20	1
1:A:107:GLN:HE21	1:A:107:GLN:N	0.57	1.98	18	1
1:A:37:ILE:HG22	1:A:104:LYS:HA	0.57	1.75	1	7
1:A:156:LEU:O	1:A:160:LYS:HG2	0.57	1.99	14	1
1:A:126:HIS:HA	1:A:135:ASP:HB3	0.57	1.77	20	2
1:A:77:MET:HA	1:A:80:ASP:HB2	0.56	1.76	19	1
1:A:52:GLN:HB3	1:A:65:ILE:HD13	0.56	1.75	17	1
1:A:52:GLN:HE21	1:A:78:GLY:HA3	0.56	1.60	13	1
1:A:133:TRP:O	1:A:145:LEU:HB3	0.56	2.01	20	3
1:A:20:TYR:CE1	1:A:127:THR:HA	0.55	2.37	9	2
1:A:94:GLU:OE2	1:A:144:ARG:HD3	0.55	2.02	7	1
1:A:103:ALA:O	1:A:107:GLN:HB2	0.55	2.00	7	6
1:A:48:GLU:O	1:A:52:GLN:HG2	0.55	2.02	11	5
1:A:45:PRO:O	1:A:46:THR:HB	0.55	2.02	13	1
1:A:62:ARG:HH11	1:A:62:ARG:HG2	0.55	1.60	13	1
1:A:90:GLU:HA	1:A:93:LYS:NZ	0.54	2.18	1	3
1:A:61:TYR:O	1:A:65:ILE:HG12	0.54	2.02	6	4
1:A:146:GLY:O	1:A:150:MET:HG3	0.54	2.02	1	8
1:A:73:VAL:O	1:A:77:MET:HG2	0.54	2.03	3	2
1:A:135:ASP:CA	1:A:141:GLY:HA3	0.54	2.30	14	1
1:A:18:ASN:HA	1:A:124:VAL:O	0.53	2.03	16	10
1:A:102:ARG:HG2	1:A:106:GLU:HG3	0.53	1.79	8	2
1:A:115:LEU:HG	1:A:153:ARG:HB2	0.53	1.79	2	1
1:A:55:LYS:HZ2	1:A:55:LYS:HB2	0.53	1.63	14	2
1:A:19:PHE:CE2	1:A:125:GLU:HB2	0.53	2.39	9	1
1:A:153:ARG:HB3	1:A:153:ARG:NH1	0.53	2.19	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:GLN:NE2	1:A:75:ALA:HA	0.53	2.19	4	2
1:A:89:TRP:O	1:A:93:LYS:HG3	0.52	2.04	15	3
1:A:12:MET:HB2	1:A:15:THR:HB	0.52	1.82	16	1
1:A:56:PHE:CE1	1:A:83:LYS:HB2	0.52	2.40	7	2
1:A:126:HIS:CE1	1:A:137:GLY:HA2	0.52	2.40	1	2
1:A:3:VAL:HG22	1:A:5:ALA:H	0.51	1.66	2	1
1:A:133:TRP:HB3	1:A:145:LEU:HB2	0.51	1.82	5	3
1:A:101:LEU:HB3	1:A:152:LEU:HD22	0.51	1.81	16	1
1:A:32:PHE:CE1	1:A:71:PRO:HB2	0.51	2.41	4	1
1:A:55:LYS:HG3	1:A:89:TRP:CZ2	0.51	2.40	12	1
1:A:52:GLN:OE1	1:A:78:GLY:HA3	0.51	2.06	18	3
1:A:52:GLN:HG3	1:A:78:GLY:HA3	0.51	1.82	10	1
1:A:94:GLU:HG2	1:A:133:TRP:CZ3	0.51	2.41	7	1
1:A:49:HIS:CE1	1:A:71:PRO:HA	0.51	2.41	14	4
1:A:3:VAL:HG13	1:A:4:ARG:H	0.50	1.66	2	1
1:A:150:MET:O	1:A:154:GLU:HG2	0.50	2.05	10	4
1:A:16:ILE:HG13	1:A:122:LYS:HD3	0.50	1.81	15	1
1:A:55:LYS:HB2	1:A:89:TRP:CZ2	0.50	2.41	3	1
1:A:80:ASP:OD1	1:A:83:LYS:HG2	0.50	2.06	10	1
1:A:42:LYS:HD2	1:A:66:ARG:HD3	0.50	1.83	11	1
1:A:53:ALA:HA	1:A:62:ARG:HG2	0.50	1.84	17	1
1:A:127:THR:OG1	1:A:134:GLY:HA3	0.50	2.07	11	1
1:A:138:HIS:CE1	1:A:140:LYS:HB2	0.50	2.42	20	1
1:A:55:LYS:HB2	1:A:55:LYS:HZ2	0.50	1.67	11	2
1:A:45:PRO:O	1:A:46:THR:HG22	0.50	2.06	17	1
1:A:141:GLY:O	1:A:142:LYS:HG3	0.50	2.06	8	1
1:A:56:PHE:HE1	1:A:83:LYS:HG3	0.49	1.67	3	1
1:A:4:ARG:HD2	1:A:25:ASP:HB2	0.49	1.82	17	1
1:A:81:ARG:HG3	1:A:85:LEU:HD11	0.49	1.83	17	1
1:A:86:ARG:HB2	1:A:89:TRP:HB2	0.49	1.83	15	3
1:A:105:PHE:O	1:A:112:ARG:HB2	0.49	2.08	18	6
1:A:153:ARG:HH11	1:A:153:ARG:HG2	0.49	1.67	8	2
1:A:81:ARG:O	1:A:81:ARG:HD3	0.49	2.06	10	1
1:A:86:ARG:HH21	1:A:88:ASN:ND2	0.49	2.06	6	1
1:A:112:ARG:O	1:A:116:LEU:HG	0.49	2.08	11	1
1:A:160:LYS:CA	1:A:160:LYS:HE3	0.49	2.34	17	1
1:A:136:GLY:HA3	1:A:141:GLY:HA3	0.48	1.85	9	2
1:A:98:ARG:HH21	1:A:148:LEU:HD23	0.48	1.68	5	2
1:A:75:ALA:O	1:A:79:ARG:HG2	0.48	2.08	16	1
1:A:59:GLU:O	1:A:63:GLU:HG2	0.48	2.08	10	1
1:A:51:PHE:CD2	1:A:55:LYS:HE3	0.48	2.43	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LYS:HE2	1:A:87:LYS:HA	0.47	1.86	6	1
1:A:22:THR:HG21	1:A:33:ALA:HA	0.47	1.86	20	1
1:A:90:GLU:HA	1:A:93:LYS:HZ2	0.47	1.69	1	1
1:A:132:TYR:O	1:A:142:LYS:HB3	0.47	2.09	7	1
1:A:153:ARG:CB	1:A:153:ARG:HH11	0.47	2.19	9	1
1:A:48:GLU:CD	1:A:48:GLU:H	0.47	2.13	1	1
1:A:20:TYR:HE1	1:A:126:HIS:O	0.47	1.92	16	1
1:A:3:VAL:HG23	1:A:25:ASP:HB2	0.47	1.86	14	1
1:A:134:GLY:O	1:A:141:GLY:HA3	0.46	2.09	1	1
1:A:52:GLN:HG3	1:A:65:ILE:HD13	0.46	1.86	20	1
1:A:89:TRP:O	1:A:93:LYS:HB2	0.46	2.09	19	2
1:A:43:THR:HB	1:A:66:ARG:HH21	0.46	1.69	9	1
1:A:157:ALA:O	1:A:161:LEU:HD13	0.46	2.11	20	1
1:A:65:ILE:O	1:A:68:VAL:HG12	0.46	2.11	14	2
1:A:51:PHE:O	1:A:55:LYS:HG3	0.46	2.11	18	1
1:A:98:ARG:HA	1:A:148:LEU:HD11	0.46	1.87	13	1
1:A:126:HIS:HA	1:A:135:ASP:OD1	0.46	2.10	11	2
1:A:52:GLN:NE2	1:A:78:GLY:HA3	0.46	2.24	13	3
1:A:125:GLU:CD	1:A:127:THR:HG22	0.46	2.31	16	1
1:A:52:GLN:HB3	1:A:65:ILE:HG21	0.46	1.88	12	1
1:A:52:GLN:HE21	1:A:75:ALA:HA	0.46	1.70	4	1
1:A:55:LYS:HE3	1:A:85:LEU:HD21	0.45	1.88	3	1
1:A:125:GLU:OE1	1:A:134:GLY:HA3	0.45	2.12	8	1
1:A:115:LEU:HG	1:A:153:ARG:HG3	0.45	1.88	4	1
1:A:124:VAL:HG23	1:A:143:ASN:OD1	0.45	2.12	18	1
1:A:94:GLU:H	1:A:94:GLU:CD	0.45	2.15	16	2
1:A:63:GLU:O	1:A:67:ARG:HG3	0.45	2.12	12	2
1:A:133:TRP:HB3	1:A:145:LEU:CB	0.45	2.42	5	1
1:A:45:PRO:O	1:A:46:THR:CB	0.45	2.65	13	1
1:A:131:ALA:HB1	1:A:141:GLY:HA2	0.44	1.89	14	1
1:A:37:ILE:CG2	1:A:104:LYS:HA	0.44	2.42	19	1
1:A:75:ALA:O	1:A:79:ARG:HG3	0.44	2.12	17	2
1:A:30:SER:HA	1:A:125:GLU:OE2	0.44	2.12	14	1
1:A:58:ASP:O	1:A:62:ARG:HG3	0.44	2.12	8	1
1:A:58:ASP:OD2	1:A:61:TYR:HB2	0.44	2.12	13	1
1:A:152:LEU:O	1:A:156:LEU:HG	0.44	2.11	3	4
1:A:62:ARG:NE	1:A:63:GLU:HG3	0.44	2.28	16	1
1:A:95:GLN:O	1:A:99:LYS:HD3	0.44	2.13	20	1
1:A:133:TRP:H	1:A:142:LYS:HB3	0.44	1.72	11	1
1:A:16:ILE:HG12	1:A:122:LYS:HE3	0.44	1.89	4	1
1:A:135:ASP:HB2	1:A:143:ASN:HB2	0.44	1.90	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:HB3	1:A:107:GLN:OE1	0.44	2.13	18	1
1:A:56:PHE:CE1	1:A:83:LYS:HG3	0.43	2.48	20	1
1:A:127:THR:HB	1:A:130:ASP:O	0.43	2.12	9	1
1:A:158:ILE:O	1:A:162:GLU:HG3	0.43	2.13	7	1
1:A:65:ILE:HA	1:A:68:VAL:HG12	0.43	1.90	15	1
1:A:54:GLN:HG2	1:A:96:VAL:HG22	0.43	1.90	6	1
1:A:131:ALA:HB2	1:A:136:GLY:HA3	0.43	1.90	16	1
1:A:63:GLU:HG2	1:A:67:ARG:NH1	0.43	2.29	2	1
1:A:86:ARG:HG2	1:A:89:TRP:HB2	0.43	1.90	3	1
1:A:16:ILE:HG13	1:A:122:LYS:HD2	0.43	1.90	19	1
1:A:31:ASN:HB2	1:A:47:SER:HB2	0.43	1.89	5	1
1:A:12:MET:SD	1:A:12:MET:N	0.43	2.92	15	2
1:A:102:ARG:HG3	1:A:156:LEU:HD21	0.43	1.89	13	1
1:A:81:ARG:HG3	1:A:85:LEU:CD1	0.43	2.44	17	1
1:A:15:THR:O	1:A:121:ALA:HB1	0.43	2.14	9	1
1:A:12:MET:N	1:A:12:MET:SD	0.43	2.90	9	1
1:A:86:ARG:CG	1:A:89:TRP:HB2	0.43	2.43	3	1
1:A:55:LYS:HA	1:A:89:TRP:CZ3	0.43	2.49	9	1
1:A:61:TYR:O	1:A:65:ILE:HG13	0.43	2.13	1	1
1:A:157:ALA:O	1:A:161:LEU:HB2	0.43	2.13	4	2
1:A:61:TYR:CZ	1:A:83:LYS:HE3	0.42	2.49	4	1
1:A:21:SER:O	1:A:27:GLY:HA3	0.42	2.13	5	1
1:A:55:LYS:HB2	1:A:55:LYS:NZ	0.42	2.29	14	1
1:A:15:THR:HB	1:A:121:ALA:HB2	0.42	1.91	17	1
1:A:94:GLU:O	1:A:98:ARG:HB2	0.42	2.14	1	1
1:A:22:THR:CG2	1:A:33:ALA:HA	0.42	2.44	20	1
1:A:132:TYR:CE2	1:A:142:LYS:HD3	0.42	2.49	9	1
1:A:139:GLY:O	1:A:140:LYS:HB2	0.42	2.13	5	1
1:A:122:LYS:HA	1:A:150:MET:SD	0.42	2.54	13	1
1:A:6:GLN:HA	1:A:6:GLN:OE1	0.42	2.14	3	1
1:A:4:ARG:HB3	1:A:25:ASP:CG	0.42	2.36	9	1
1:A:57:LEU:HD23	1:A:57:LEU:N	0.42	2.28	4	1
1:A:36:PRO:HA	1:A:44:TRP:O	0.41	2.15	20	1
1:A:61:TYR:OH	1:A:83:LYS:HE3	0.41	2.15	19	1
1:A:135:ASP:CG	1:A:143:ASN:HB2	0.41	2.36	6	1
1:A:39:VAL:HG13	1:A:99:LYS:HD3	0.41	1.92	16	1
1:A:38:LYS:HB2	1:A:107:GLN:NE2	0.41	2.29	4	1
1:A:58:ASP:OD2	1:A:60:LYS:HB2	0.41	2.15	5	1
1:A:19:PHE:CD1	1:A:29:PHE:HB2	0.41	2.51	3	1
1:A:73:VAL:O	1:A:77:MET:HG3	0.41	2.16	4	2
1:A:22:THR:HA	1:A:27:GLY:CA	0.41	2.44	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:THR:HB	1:A:121:ALA:CB	0.41	2.46	17	1
1:A:135:ASP:HA	1:A:141:GLY:CA	0.41	2.35	14	2
1:A:157:ALA:O	1:A:160:LYS:HB3	0.41	2.16	8	1
1:A:65:ILE:HG12	1:A:77:MET:SD	0.41	2.56	20	2
1:A:66:ARG:HD3	1:A:66:ARG:O	0.41	2.16	9	1
1:A:102:ARG:O	1:A:106:GLU:HG3	0.41	2.16	3	1
1:A:97:MET:SD	1:A:145:LEU:HD13	0.41	2.55	1	1
1:A:102:ARG:O	1:A:106:GLU:HB2	0.41	2.15	1	1
1:A:80:ASP:OD2	1:A:83:LYS:HG2	0.41	2.16	5	1
1:A:55:LYS:HG3	1:A:89:TRP:CE2	0.41	2.51	12	1
1:A:81:ARG:HB2	1:A:85:LEU:HD11	0.40	1.93	2	1
1:A:128:GLU:HG2	1:A:137:GLY:CA	0.40	2.47	16	1
1:A:127:THR:HG23	1:A:127:THR:O	0.40	2.16	19	1
1:A:116:LEU:HA	1:A:153:ARG:NE	0.40	2.31	11	1
1:A:133:TRP:CE3	1:A:145:LEU:HB2	0.40	2.51	19	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/168 (93%)	140±3 (89±2%)	13±3 (9±2%)	4±2 (2±1%)	12	49
All	All	3140/3360 (93%)	2797 (89%)	267 (9%)	76 (2%)	12	49

All 25 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	138	HIS	9
1	A	21	SER	8
1	A	23	SER	7
1	A	13	GLN	6
1	A	10	HIS	5
1	A	142	LYS	4
1	A	3	VAL	4

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Mol	Chain	Res	Type	Models (Total)
1	A	140	LYS	4
1	A	24	ASP	3
1	A	46	THR	3
1	A	120	PRO	2
1	A	143	ASN	2
1	A	25	ASP	2
1	A	12	MET	2
1	A	144	ARG	2
1	A	4	ARG	2
1	A	33	ALA	2
1	A	141	GLY	2
1	A	41	GLY	1
1	A	134	GLY	1
1	A	139	GLY	1
1	A	132	TYR	1
1	A	14	ASP	1
1	A	71	PRO	1
1	A	129	ASN	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	133/144 (92%)	126±2 (94±1%)	7±2 (6±1%)	31	76
All	All	2660/2880 (92%)	2513 (94%)	147 (6%)	31	76

All 56 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	61	TYR	8
1	A	46	THR	8
1	A	48	GLU	7
1	A	127	THR	6
1	A	12	MET	6
1	A	18	ASN	5
1	A	107	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	66	ARG	5
1	A	22	THR	5
1	A	76	ARG	5
1	A	20	TYR	5
1	A	47	SER	4
1	A	57	LEU	4
1	A	125	GLU	3
1	A	153	ARG	3
1	A	155	GLN	3
1	A	81	ARG	3
1	A	143	ASN	3
1	A	154	GLU	3
1	A	54	GLN	3
1	A	162	GLU	3
1	A	90	GLU	3
1	A	135	ASP	3
1	A	128	GLU	2
1	A	87	LYS	2
1	A	79	ARG	2
1	A	26	TYR	2
1	A	77	MET	2
1	A	97	MET	2
1	A	122	LYS	2
1	A	67	ARG	2
1	A	144	ARG	2
1	A	4	ARG	2
1	A	52	GLN	2
1	A	83	LYS	1
1	A	106	GLU	1
1	A	6	GLN	1
1	A	31	ASN	1
1	A	148	LEU	1
1	A	23	SER	1
1	A	24	ASP	1
1	A	151	GLU	1
1	A	98	ARG	1
1	A	88	ASN	1
1	A	104	LYS	1
1	A	110	GLU	1
1	A	94	GLU	1
1	A	159	GLU	1
1	A	160	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	28	ASP	1
1	A	93	LYS	1
1	A	99	LYS	1
1	A	59	GLU	1
1	A	32	PHE	1
1	A	10	HIS	1
1	A	64	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no 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