Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 03:47 PM EST

PDB ID	:	2CSF
Title	:	Solution structure of the second CUT domain of human SATB2
Authors	:	Inoue, K.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-21

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

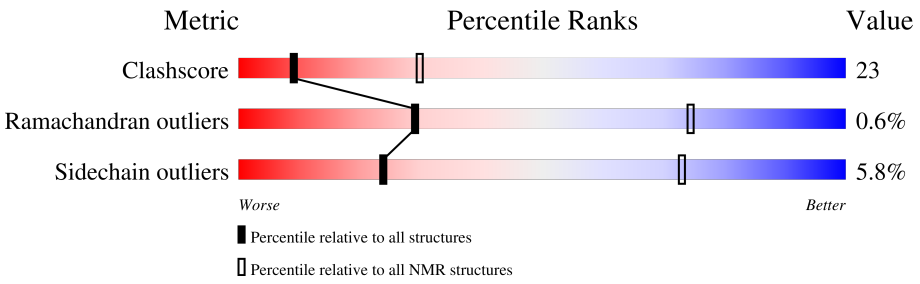
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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	101	41% 36% • 22%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:16-A:94 (79)	0.08	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1567 atoms, of which 776 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding protein SATB2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1567	491	776	142	155	3	0

There are 13 discrepancies between the modelled and reference sequences:

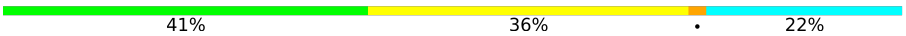
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q9UPW6
A	2	SER	-	cloning artifact	UNP Q9UPW6
A	3	SER	-	cloning artifact	UNP Q9UPW6
A	4	GLY	-	cloning artifact	UNP Q9UPW6
A	5	SER	-	cloning artifact	UNP Q9UPW6
A	6	SER	-	cloning artifact	UNP Q9UPW6
A	7	GLY	-	cloning artifact	UNP Q9UPW6
A	96	SER	-	cloning artifact	UNP Q9UPW6
A	97	GLY	-	cloning artifact	UNP Q9UPW6
A	98	PRO	-	cloning artifact	UNP Q9UPW6
A	99	SER	-	cloning artifact	UNP Q9UPW6
A	100	SER	-	cloning artifact	UNP Q9UPW6
A	101	GLY	-	cloning artifact	UNP Q9UPW6

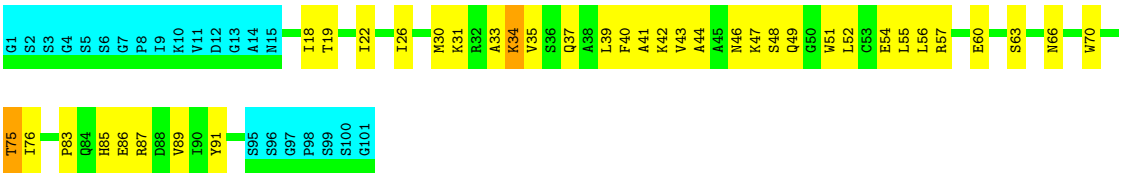
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: DNA-binding protein SATB2

Chain A: 



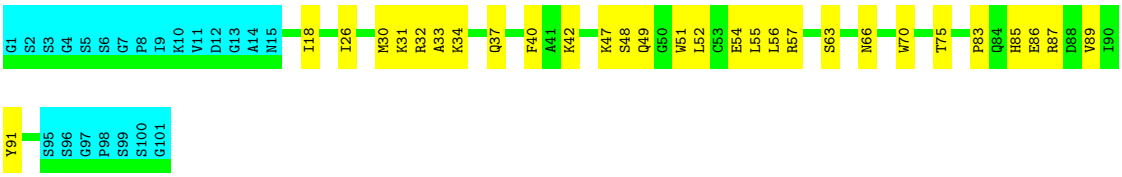
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

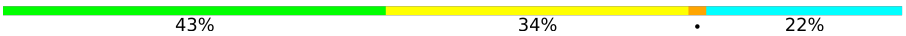
• Molecule 1: DNA-binding protein SATB2

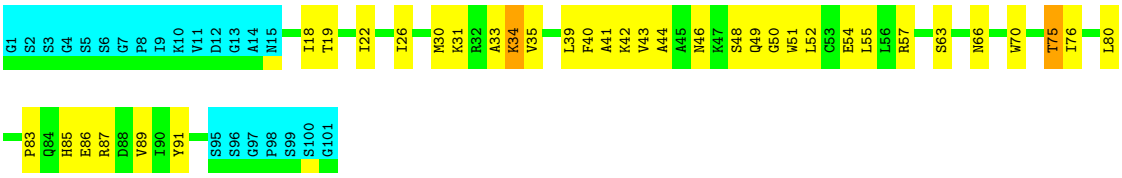
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: DNA-binding protein SATB2

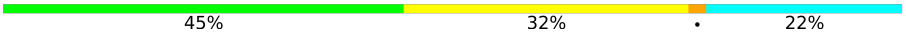
Chain A: 

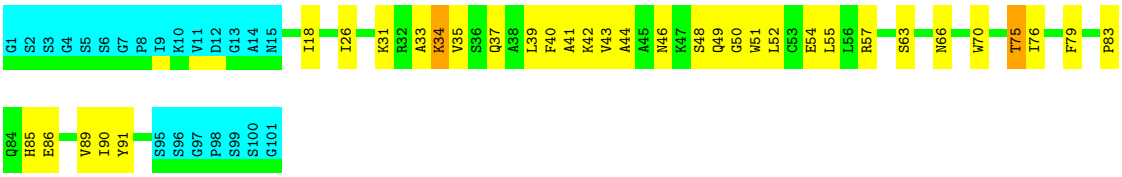


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: DNA-binding protein SATB2

Chain A:

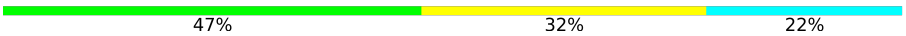


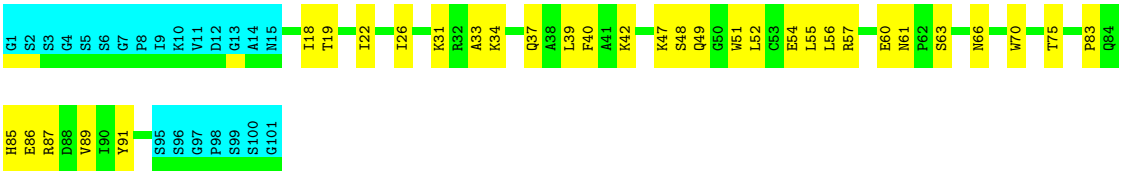


4.2.4 Score per residue for model 4

- Molecule 1: DNA-binding protein SATB2

Chain A:

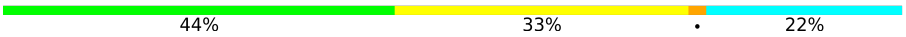


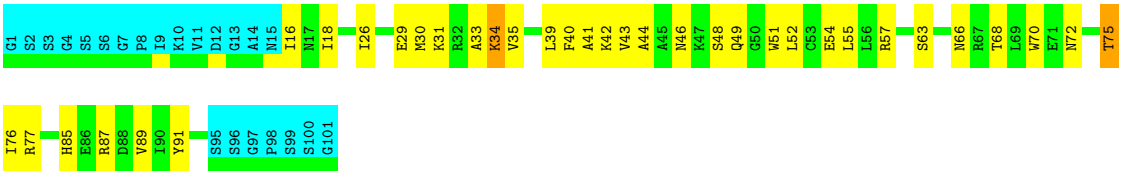


4.2.5 Score per residue for model 5

- Molecule 1: DNA-binding protein SATB2

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: DNA-binding protein SATB2

Chain A: 40% 38% • 22%

G1 S2 S3 G4 S5 S6 G7 P8 I9 K10 V11 D12 G13 A14 N15 I18 E25 I26 K31 R32 A33 K34 V35 S36 Q37 A38 L39 F40 A41 K42 V43 A44 A45 N46 K47 S48 Q49 G50 W51 L52 C53 E54 L55 L56 R57 E60 S63 N66 W70 T75 I76 R77

R78 F79 P83 Q84 H85 E86 R87 D88 V89 I90 Y91 E94 S95 S96 G97 P98 S99 S100 G101

4.2.7 Score per residue for model 7

- Molecule 1: DNA-binding protein SATB2

Chain A: 46% 31% • 22%

G1 S2 S3 G4 S5 S6 G7 P8 I9 K10 V11 D12 G13 A14 N15 I18 T19 I22 I26 M30 K31 R32 A33 K34 Q37 A38 L39 F40 A41 K42 K47 S48 Q49 G50 W51 L52 C53 E54 L55 L56 R57 S63 N66 W70 T75 I76 P83 Q84 H85

E86 R87 D88 V89 I90 Y91 S95 S96 G97 P98 S99 S100 G101

4.2.8 Score per residue for model 8

- Molecule 1: DNA-binding protein SATB2

Chain A: 35% 40% • 22%

G1 S2 S3 G4 S5 S6 G7 P8 I9 K10 V11 D12 G13 A14 N15 I16 N17 I18 T19 I22 Y23 I26 M30 K31 R32 A33 K34 V35 S36 Q37 A38 L39 F40 A41 K42 V43 A44 A45 N46 K47 S48 Q49 G50 W51 L52 C53 E54 L55 L56 R57 W58 K59 E60 S63 N66

R67 T68 L69 W70 E71 N72 T75 I76 R77 R78 F79 L80 H85 E86 R87 D88 V89 I90 Y91 E94 S95 S96 G97 P98 S99 S100 G101

4.2.9 Score per residue for model 9

- Molecule 1: DNA-binding protein SATB2

Chain A: 44% 33% • 22%

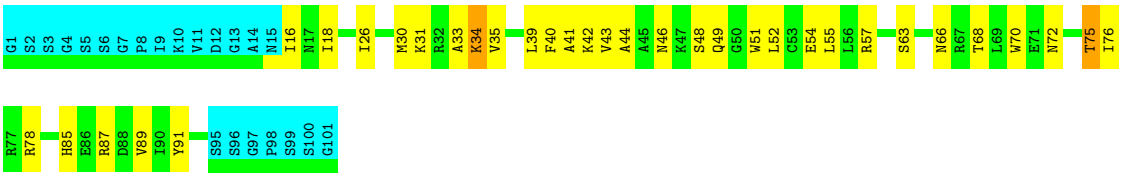
G1 S2 S3 G4 S5 S6 G7 P8 I9 K10 V11 D12 G13 A14 N15 I18 I26 M30 K31 R32 A33 K34 V35 S36 Q37 A38 L39 F40 A41 K42 N46 K47 S48 Q49 G50 W51 L52 C53 E54 L55 L56 R57 W58 K59 E60 N61 P62 S63 N66 W70 T75 I76

P83 Q84 H85 E86 R87 D88 V89 I90 Y91 S95 S96 G97 P98 S99 S100 G101

4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding protein SATB2

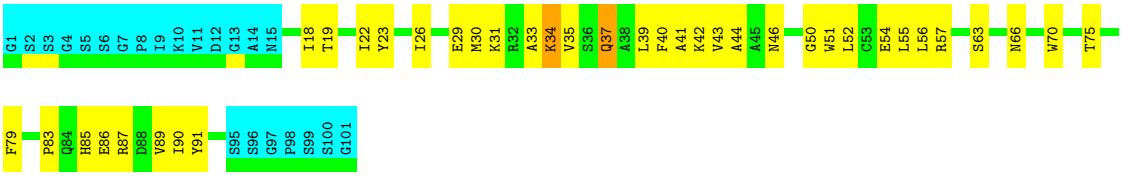
Chain A: 45% 32% • 22%



4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding protein SATB2

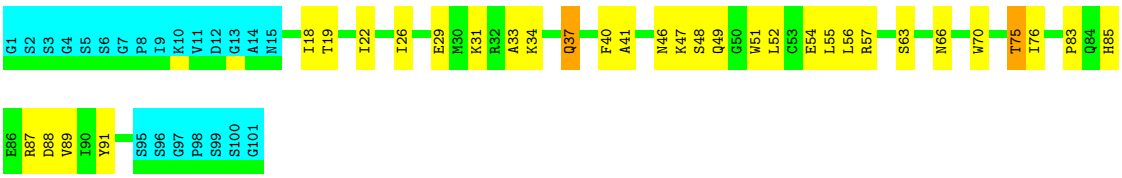
Chain A: 41% 36% • 22%



4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding protein SATB2

Chain A: 47% 30% • 22%



4.2.13 Score per residue for model 13

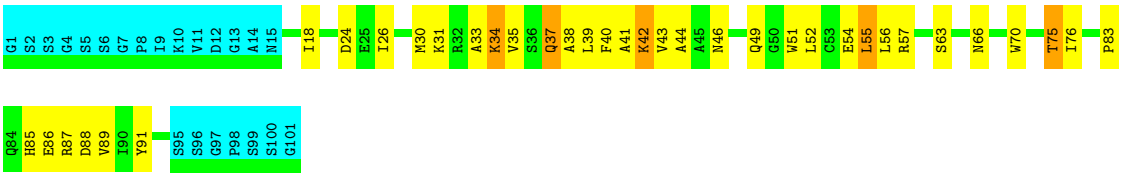
- Molecule 1: DNA-binding protein SATB2

Chain A: 42% 36% • 22%

4.2.14 Score per residue for model 14

- Molecule 1: DNA-binding protein SATB2

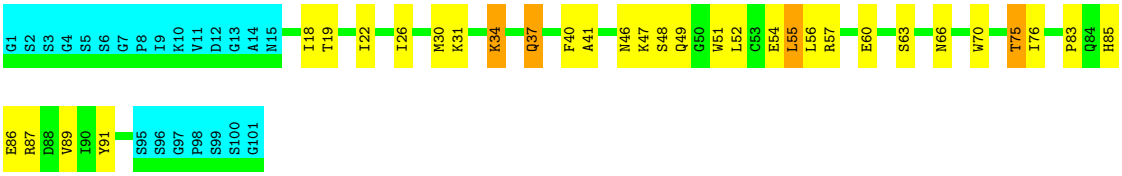
Chain A: 43% 31% 5% 22%



4.2.15 Score per residue for model 15

- Molecule 1: DNA-binding protein SATB2

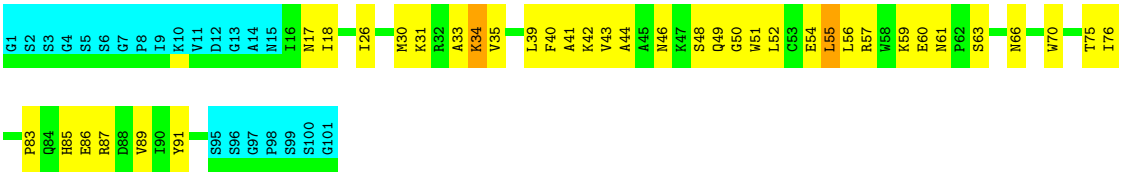
Chain A: 47% 28% • 22%



4.2.16 Score per residue for model 16

- Molecule 1: DNA-binding protein SATB2

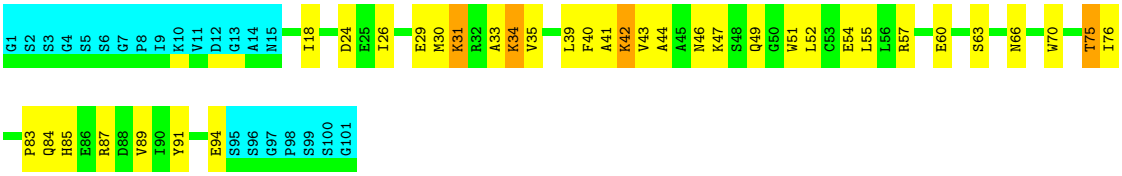
Chain A: 41% 36% • 22%



4.2.17 Score per residue for model 17

- Molecule 1: DNA-binding protein SATB2

Chain A: 43% 32% • 22%



4.2.18 Score per residue for model 18

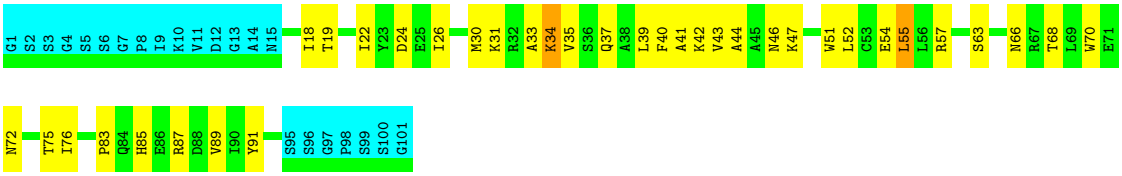
- Molecule 1: DNA-binding protein SATB2

Chain A: 43% 34% • 22%

4.2.19 Score per residue for model 19

- Molecule 1: DNA-binding protein SATB2

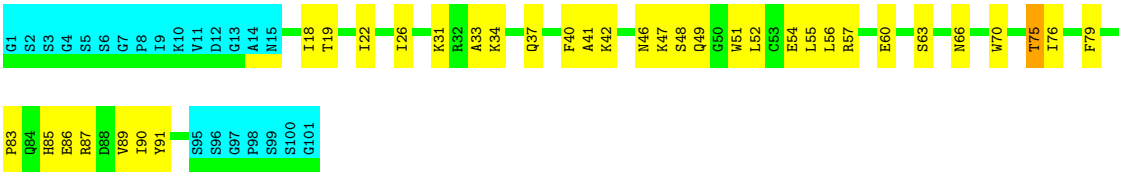
Chain A: 43% 34% • 22%



4.2.20 Score per residue for model 20

- Molecule 1: DNA-binding protein SATB2

Chain A: 44% 34% • 22%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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	660	656	655	30±4
All	All	13200	13120	13100	604

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 23.

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:HIS:O	1:A:89:VAL:HG23	0.81	1.76	18	20
1:A:37:GLN:HB3	1:A:52:LEU:HD12	0.70	1.62	9	9
1:A:33:ALA:HB1	1:A:91:TYR:CD2	0.69	2.23	17	19
1:A:51:TRP:CH2	1:A:55:LEU:HD21	0.69	2.22	19	20
1:A:52:LEU:C	1:A:52:LEU:HD13	0.65	2.12	14	20
1:A:35:VAL:HB	1:A:39:LEU:HD23	0.62	1.71	6	8
1:A:26:ILE:O	1:A:30:MET:HE2	0.61	1.96	9	6
1:A:37:GLN:NE2	1:A:56:LEU:HD12	0.59	2.12	8	5
1:A:63:SER:C	1:A:70:TRP:CE3	0.59	2.75	4	20
1:A:87:ARG:O	1:A:91:TYR:CD2	0.59	2.55	6	15
1:A:30:MET:HG2	1:A:35:VAL:HG23	0.59	1.74	13	7
1:A:35:VAL:HG11	1:A:91:TYR:CD1	0.58	2.33	2	12
1:A:51:TRP:CZ3	1:A:55:LEU:CD2	0.57	2.86	19	17
1:A:19:THR:O	1:A:22:ILE:HG22	0.57	2.00	12	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ALA:CB	1:A:91:TYR:CE2	0.56	2.89	17	4
1:A:39:LEU:O	1:A:43:VAL:HG22	0.56	2.01	19	12
1:A:26:ILE:HG23	1:A:40:PHE:CE1	0.56	2.36	17	6
1:A:79:PHE:CZ	1:A:90:ILE:HD13	0.56	2.36	3	4
1:A:79:PHE:CZ	1:A:90:ILE:CD1	0.55	2.89	3	1
1:A:51:TRP:CH2	1:A:55:LEU:CD2	0.55	2.89	19	15
1:A:51:TRP:O	1:A:55:LEU:HD13	0.54	2.01	2	10
1:A:35:VAL:HG11	1:A:91:TYR:CG	0.54	2.38	2	9
1:A:40:PHE:C	1:A:40:PHE:CD1	0.54	2.80	7	15
1:A:31:LYS:O	1:A:34:LYS:CE	0.53	2.56	17	1
1:A:75:THR:CG2	1:A:76:ILE:N	0.52	2.72	10	16
1:A:52:LEU:C	1:A:52:LEU:CD1	0.51	2.78	4	16
1:A:40:PHE:O	1:A:44:ALA:CB	0.51	2.59	19	12
1:A:79:PHE:CE2	1:A:90:ILE:HD13	0.50	2.41	3	1
1:A:41:ALA:O	1:A:46:ASN:N	0.50	2.44	8	16
1:A:66:ASN:O	1:A:70:TRP:CB	0.50	2.60	19	20
1:A:68:THR:O	1:A:72:ASN:ND2	0.50	2.45	8	4
1:A:35:VAL:CG1	1:A:39:LEU:HD23	0.50	2.37	16	2
1:A:54:GLU:O	1:A:57:ARG:N	0.49	2.45	8	20
1:A:29:GLU:OE2	1:A:87:ARG:NE	0.49	2.45	17	4
1:A:18:ILE:HB	1:A:70:TRP:CZ3	0.49	2.43	18	20
1:A:37:GLN:OE1	1:A:56:LEU:HD12	0.49	2.07	1	5
1:A:52:LEU:HD13	1:A:52:LEU:O	0.49	2.07	4	12
1:A:29:GLU:OE1	1:A:87:ARG:CZ	0.48	2.61	17	3
1:A:37:GLN:HE22	1:A:56:LEU:HD12	0.48	1.68	12	2
1:A:40:PHE:O	1:A:44:ALA:HB3	0.48	2.08	19	12
1:A:43:VAL:HG21	1:A:91:TYR:CE1	0.48	2.43	2	4
1:A:16:ILE:HD11	1:A:78:ARG:HE	0.48	1.67	8	2
1:A:26:ILE:HG12	1:A:40:PHE:CZ	0.48	2.44	18	18
1:A:39:LEU:O	1:A:42:LYS:N	0.48	2.47	3	15
1:A:23:TYR:HA	1:A:26:ILE:HD12	0.47	1.87	8	3
1:A:47:LYS:HE3	1:A:51:TRP:CD1	0.47	2.45	1	11
1:A:49:GLN:O	1:A:52:LEU:N	0.46	2.49	1	12
1:A:41:ALA:HB2	1:A:52:LEU:HB2	0.46	1.86	14	9
1:A:56:LEU:O	1:A:59:LYS:CG	0.46	2.63	16	1
1:A:29:GLU:CD	1:A:87:ARG:CZ	0.46	2.84	17	2
1:A:26:ILE:HG12	1:A:40:PHE:CE1	0.46	2.46	16	1
1:A:50:GLY:O	1:A:54:GLU:CD	0.45	2.55	3	4
1:A:51:TRP:CZ2	1:A:55:LEU:HD21	0.45	2.47	19	1
1:A:48:SER:O	1:A:49:GLN:C	0.45	2.55	12	15
1:A:84:GLN:OE1	1:A:87:ARG:NH1	0.45	2.50	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:ARG:HB3	1:A:91:TYR:CE2	0.45	2.47	18	3
1:A:29:GLU:OE1	1:A:87:ARG:NH1	0.44	2.50	5	1
1:A:17:ASN:O	1:A:77:ARG:NH1	0.44	2.50	13	1
1:A:35:VAL:CB	1:A:39:LEU:HD23	0.44	2.42	16	3
1:A:61:ASN:OD1	1:A:61:ASN:C	0.44	2.56	16	1
1:A:33:ALA:CB	1:A:91:TYR:CD2	0.44	3.00	19	2
1:A:39:LEU:C	1:A:39:LEU:HD13	0.44	2.33	4	1
1:A:30:MET:O	1:A:34:LYS:N	0.43	2.51	16	8
1:A:40:PHE:CZ	1:A:80:LEU:HD21	0.43	2.49	2	2
1:A:36:SER:O	1:A:39:LEU:N	0.43	2.52	9	2
1:A:38:ALA:HB2	1:A:49:GLN:HB2	0.43	1.91	14	1
1:A:83:PRO:CG	1:A:85:HIS:CE1	0.43	3.02	13	4
1:A:25:GLU:OE2	1:A:77:ARG:NH1	0.42	2.52	6	1
1:A:40:PHE:CD1	1:A:40:PHE:C	0.42	2.93	17	4
1:A:48:SER:O	1:A:51:TRP:N	0.42	2.53	15	5
1:A:39:LEU:HD11	1:A:94:GLU:HG2	0.42	1.90	17	3
1:A:29:GLU:OE2	1:A:87:ARG:CZ	0.41	2.68	12	1
1:A:86:GLU:O	1:A:89:VAL:N	0.41	2.53	7	5
1:A:83:PRO:HG2	1:A:86:GLU:CG	0.41	2.46	4	13
1:A:34:LYS:CA	1:A:34:LYS:CE	0.41	2.99	5	3
1:A:16:ILE:CG2	1:A:77:ARG:HG2	0.40	2.46	5	1
1:A:34:LYS:HA	1:A:34:LYS:CE	0.40	2.45	18	3
1:A:26:ILE:HG22	1:A:30:MET:CE	0.40	2.46	8	1
1:A:34:LYS:CE	1:A:34:LYS:HA	0.40	2.46	8	1
1:A:16:ILE:HD11	1:A:78:ARG:NE	0.40	2.31	18	1
1:A:59:LYS:O	1:A:60:GLU:O	0.40	2.40	8	2
1:A:52:LEU:O	1:A:53:CYS:C	0.40	2.59	8	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	79/101 (78%)	66±2 (84±2%)	12±1 (15±2%)	0±0 (1±1%)	29	74
All	All	1580/2020 (78%)	1330 (84%)	240 (15%)	10 (1%)	29	74

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	60	GLU	10

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	71/86 (83%)	67±1 (94±2%)	4±1 (6±2%)	24	73
All	All	1420/1720 (83%)	1337 (94%)	83 (6%)	24	73

All 11 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	31	LYS	20
1	A	34	LYS	19
1	A	75	THR	17
1	A	42	LYS	6
1	A	55	LEU	6
1	A	37	GLN	4
1	A	61	ASN	3
1	A	88	ASP	3
1	A	24	ASP	3
1	A	32	ARG	1
1	A	17	ASN	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 monosaccharides 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 (i)

No chemical shift data were provided