Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 02:51 PM EST

PDB ID	:	2CSH
Title	:	Solution structure of tandem repeat of the zf-C2H2 domains of human zinc finger protein 297B
Authors	:	Inoue, K.; Saitoh, K.; Hayashi, F.; Kigawa, T.; 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:

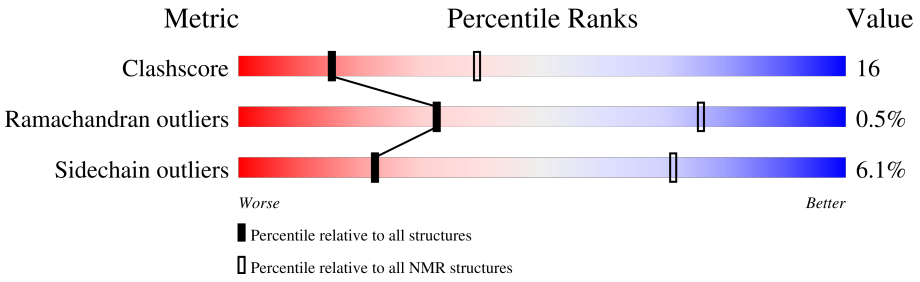
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	110	46% 17% • 35%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 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:11-A:32 (22)	0.16	4
2	A:40-A:60 (21)	0.08	4
3	A:66-A:93 (28)	0.15	12

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1680 atoms, of which 824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein 297B.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	110	1677	525	824	164	152	12	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP O43298
A	2	SER	-	cloning artifact	UNP O43298
A	3	SER	-	cloning artifact	UNP O43298
A	4	GLY	-	cloning artifact	UNP O43298
A	5	SER	-	cloning artifact	UNP O43298
A	6	SER	-	cloning artifact	UNP O43298
A	7	GLY	-	cloning artifact	UNP O43298
A	105	SER	-	cloning artifact	UNP O43298
A	106	GLY	-	cloning artifact	UNP O43298
A	107	PRO	-	cloning artifact	UNP O43298
A	108	SER	-	cloning artifact	UNP O43298
A	109	SER	-	cloning artifact	UNP O43298
A	110	GLY	-	cloning artifact	UNP O43298

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

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: Zinc finger protein 297B

Chain A: 46% 17% • 35%

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

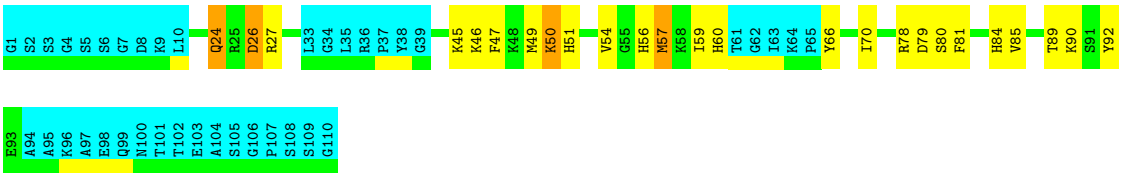
• Molecule 1: Zinc finger protein 297B

Chain A: 42% 20% • 35%

4.2.2 Score per residue for model 2

• Molecule 1: Zinc finger protein 297B

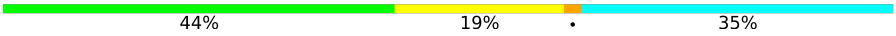
Chain A: 42% 19% • 35%



4.2.3 Score per residue for model 3

- Molecule 1: Zinc finger protein 297B

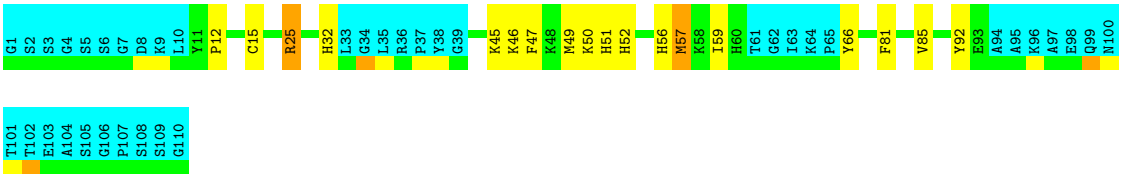
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger protein 297B

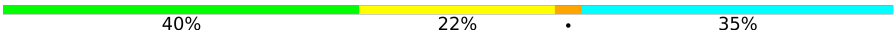
Chain A:

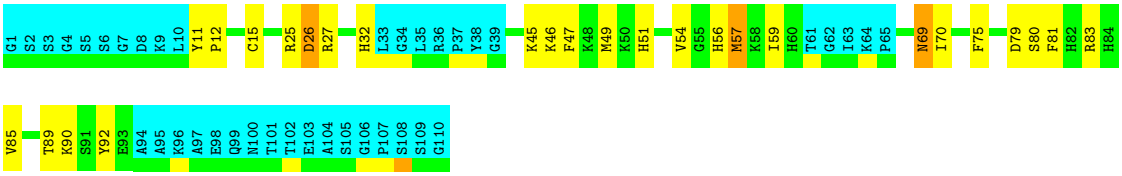


4.2.5 Score per residue for model 5

- Molecule 1: Zinc finger protein 297B

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Zinc finger protein 297B

Chain A: 42% 22% • 35%

G1 S2 S3 G4 S5 S6 G7 D8 K9 L10 Y11 P12 R25 H28 M31 H32 L33 G34 L35 R36 P37 Y38 G39 V42 K45 K46 F47 K50 V54 G55 H56 M57 K58 I59 H60 T61 G62 I63 K64 P65 Y66 R74 F75 M76 W77 F81 H84 V85 T89

K90 A94 A95 K96 A97 E98 Q99 N100 T101 T102 E103 A104 S105 G106 P107 S108 S109 G110

4.2.7 Score per residue for model 7

- Molecule 1: Zinc finger protein 297B

Chain A: 43% 20% • 35%

G1 S2 S3 G4 S5 S6 G7 D8 K9 L10 Y11 C15 K22 H32 L33 G34 L35 R36 P37 Y38 G39 V42 K45 K46 F47 K50 H51 H56 M57 K58 I59 H60 T61 G62 I63 K64 P65 Y66 N69 I70 C71 A72 R78 F81 V85 T89 K90 S91

Y92 E93 A94 A95 K96 A97 E98 Q99 N100 T101 T102 E103 A104 S105 G106 P107 S108 S109 G110

4.2.8 Score per residue for model 8

- Molecule 1: Zinc finger protein 297B

Chain A: 43% 20% • 35%

G1 S2 S3 G4 S5 S6 G7 D8 K9 L10 Y11 C15 G16 K17 S18 F19 K22 S30 M31 H32 L33 G34 L35 R36 P37 Y38 G39 K45 K46 F47 K50 V54 G55 H56 M57 K58 I59 H60 T61 G62 I63 K64 P65 Y66 N69 I70 R78 F81 H84 V85

T89 K90 A94 A95 K96 A97 E98 Q99 N100 T101 T102 E103 A104 S105 G106 P107 S108 S109 G110

4.2.9 Score per residue for model 9

- Molecule 1: Zinc finger protein 297B

Chain A: 45% 17% •• 35%

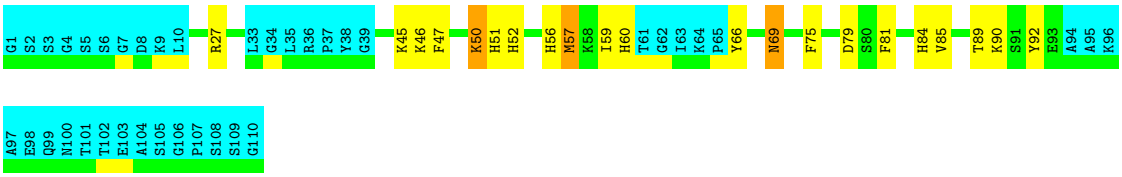
G1 S2 S3 G4 S5 S6 G7 D8 K9 L10 M31 H32 L33 G34 L35 R36 P37 Y38 G39 C43 K46 F47 K50 H51 H52 L53 H56 M57 K58 I59 H60 T61 G62 I63 K64 P65 C68 N69 F81 H84 V85 T89 K90 S91 Y92 E93 A94 A95 K96 A97 E98

Q99 N100 T101 T102 E103 A104 S105 G106 P107 S108 S109 G110

4.2.10 Score per residue for model 10

- Molecule 1: Zinc finger protein 297B

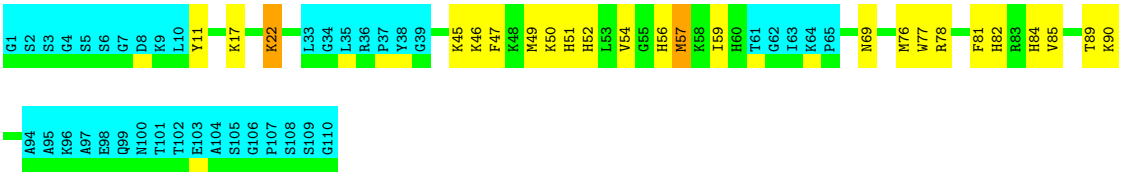
Chain A: 45% 16% • 35%



4.2.11 Score per residue for model 11

- Molecule 1: Zinc finger protein 297B

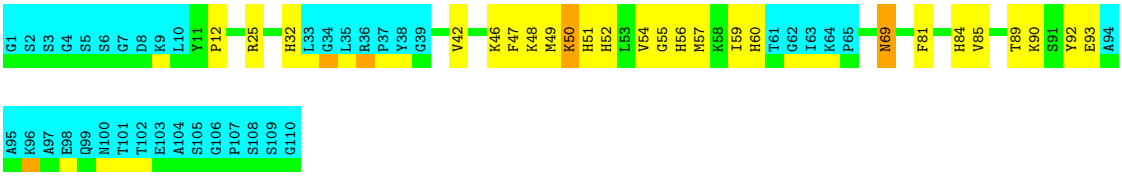
Chain A: 43% 20% • 35%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: Zinc finger protein 297B

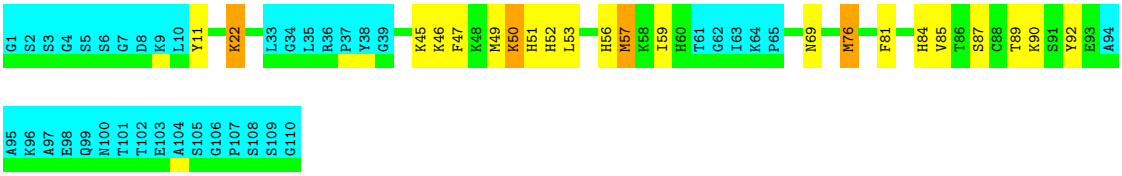
Chain A: 42% 21% • 35%



4.2.13 Score per residue for model 13

- Molecule 1: Zinc finger protein 297B

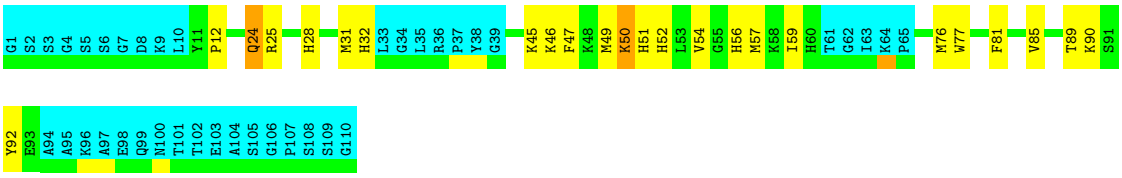
Chain A: 45% 16% • 35%



4.2.14 Score per residue for model 14

- Molecule 1: Zinc finger protein 297B

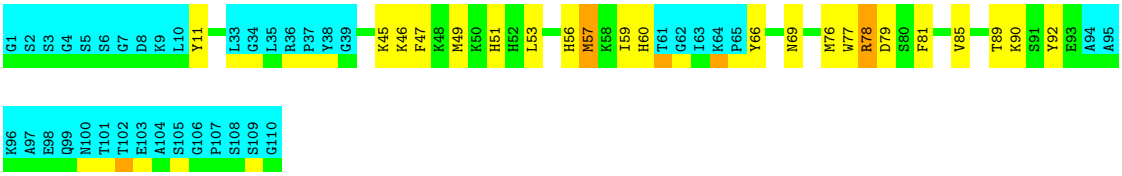
Chain A: 43% 20% • 35%



4.2.15 Score per residue for model 15

- Molecule 1: Zinc finger protein 297B

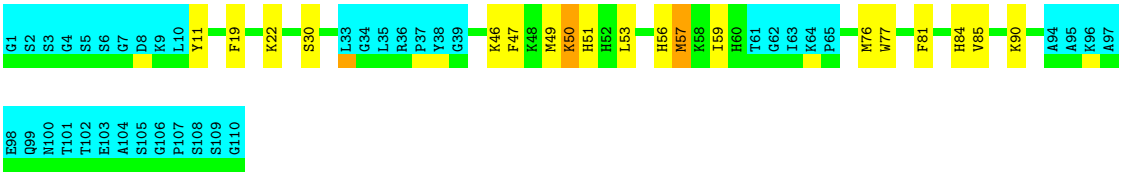
Chain A: 45% 18% • 35%



4.2.16 Score per residue for model 16

- Molecule 1: Zinc finger protein 297B

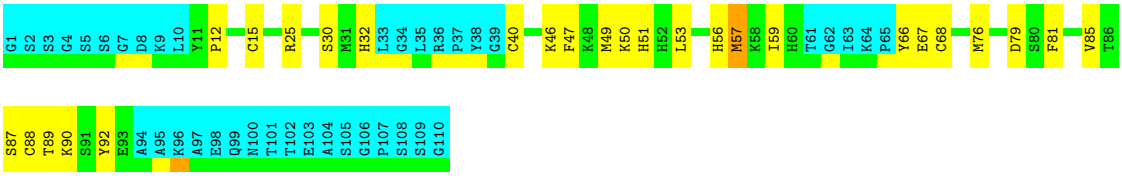
Chain A: 47% 15% • 35%



4.2.17 Score per residue for model 17

- Molecule 1: Zinc finger protein 297B

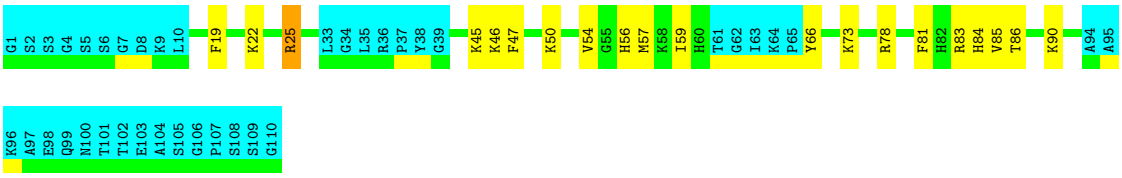
Chain A: 40% 24% • 35%



4.2.18 Score per residue for model 18

- Molecule 1: Zinc finger protein 297B

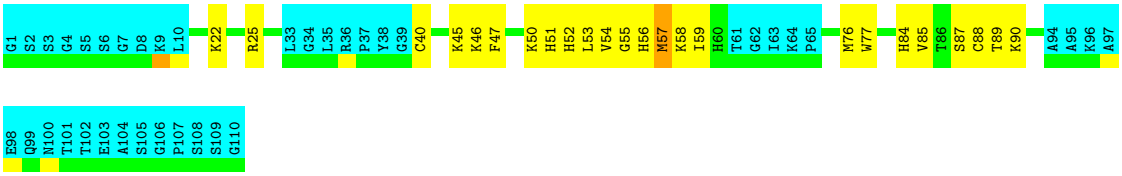
Chain A: 46% 17% • 35%



4.2.19 Score per residue for model 19

- Molecule 1: Zinc finger protein 297B

Chain A: 43% 21% • 35%



4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger protein 297B

Chain A: 33% 31% • 35%

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)

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

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	592	568	568	19±4
All	All	11900	11360	11360	383

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:PHE:O	1:A:85:VAL:HG23	0.84	1.72	7	18
1:A:81:PHE:CE1	1:A:85:VAL:HG21	0.83	2.08	5	14
1:A:56:HIS:O	1:A:59:ILE:HG23	0.78	1.76	19	20
1:A:69:ASN:OD1	1:A:70:ILE:HD12	0.76	1.80	8	1
1:A:46:LYS:C	1:A:47:PHE:CD1	0.66	2.69	18	20
1:A:47:PHE:CE1	1:A:53:LEU:CD1	0.62	2.81	9	7
1:A:49:MET:SD	1:A:52:HIS:CE1	0.59	2.95	11	2
1:A:47:PHE:CD2	1:A:52:HIS:O	0.59	2.56	3	10
1:A:47:PHE:CE1	1:A:53:LEU:HD13	0.59	2.32	9	3
1:A:76:MET:SD	1:A:77:TRP:CD1	0.57	2.98	19	2
1:A:47:PHE:CD1	1:A:53:LEU:HD13	0.54	2.37	9	6
1:A:26:ASP:CG	1:A:27:ARG:N	0.53	2.61	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:TYR:CE1	1:A:78:ARG:CD	0.53	2.92	7	1
1:A:56:HIS:CE1	1:A:59:ILE:CD1	0.53	2.92	2	10
1:A:66:TYR:CE1	1:A:78:ARG:HD3	0.53	2.38	7	1
1:A:76:MET:SD	1:A:77:TRP:CG	0.53	3.02	19	2
1:A:11:TYR:CE2	1:A:22:LYS:HD3	0.52	2.39	1	5
1:A:76:MET:HG3	1:A:77:TRP:CD1	0.52	2.40	15	7
1:A:19:PHE:N	1:A:19:PHE:CD1	0.52	2.77	16	1
1:A:70:ILE:H	1:A:70:ILE:HD12	0.52	1.64	2	1
1:A:66:TYR:CE2	1:A:78:ARG:HA	0.52	2.39	20	1
1:A:47:PHE:CD1	1:A:47:PHE:N	0.52	2.78	20	14
1:A:69:ASN:ND2	1:A:69:ASN:N	0.52	2.57	10	1
1:A:76:MET:SD	1:A:77:TRP:CE2	0.52	3.03	19	2
1:A:84:HIS:CD2	1:A:85:VAL:N	0.51	2.79	19	11
1:A:26:ASP:OD1	1:A:27:ARG:N	0.51	2.44	2	2
1:A:49:MET:HG3	1:A:52:HIS:CE1	0.51	2.41	12	2
1:A:92:TYR:CD1	1:A:92:TYR:C	0.50	2.84	3	12
1:A:76:MET:SD	1:A:77:TRP:CD2	0.50	3.04	19	2
1:A:49:MET:HB3	1:A:51:HIS:CE1	0.50	2.42	13	5
1:A:66:TYR:CE2	1:A:78:ARG:CA	0.50	2.95	20	1
1:A:11:TYR:CZ	1:A:22:LYS:HD3	0.49	2.42	20	6
1:A:47:PHE:CE1	1:A:53:LEU:HD12	0.49	2.41	16	5
1:A:11:TYR:CE2	1:A:22:LYS:CD	0.49	2.95	7	3
1:A:69:ASN:OD1	1:A:69:ASN:N	0.49	2.45	3	5
1:A:84:HIS:CD2	1:A:84:HIS:C	0.49	2.86	6	5
1:A:22:LYS:NZ	1:A:25:ARG:NH2	0.49	2.60	18	1
1:A:78:ARG:O	1:A:81:PHE:N	0.49	2.46	15	2
1:A:49:MET:CB	1:A:51:HIS:CE1	0.49	2.96	17	1
1:A:66:TYR:CE1	1:A:78:ARG:HD2	0.48	2.43	18	1
1:A:45:LYS:HD2	1:A:56:HIS:CE1	0.48	2.44	19	9
1:A:66:TYR:CE2	1:A:78:ARG:HB2	0.48	2.43	20	2
1:A:54:VAL:O	1:A:56:HIS:N	0.48	2.47	19	9
1:A:70:ILE:HD12	1:A:70:ILE:N	0.48	2.23	2	2
1:A:45:LYS:HD3	1:A:56:HIS:CE1	0.48	2.43	18	1
1:A:46:LYS:O	1:A:47:PHE:CG	0.47	2.67	9	3
1:A:49:MET:SD	1:A:51:HIS:NE2	0.47	2.87	4	2
1:A:45:LYS:O	1:A:46:LYS:CG	0.47	2.62	13	5
1:A:56:HIS:CE1	1:A:59:ILE:HD11	0.47	2.45	13	3
1:A:28:HIS:O	1:A:32:HIS:CD2	0.47	2.67	6	3
1:A:71:CYS:O	1:A:72:ALA:HB3	0.47	2.10	7	1
1:A:50:LYS:HG3	1:A:51:HIS:N	0.47	2.25	4	2
1:A:73:LYS:HE3	1:A:84:HIS:CE1	0.46	2.45	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LYS:HD3	1:A:51:HIS:N	0.46	2.26	3	3
1:A:79:ASP:O	1:A:83:ARG:CB	0.46	2.64	5	3
1:A:55:GLY:O	1:A:58:LYS:CD	0.46	2.64	20	1
1:A:66:TYR:HB3	1:A:81:PHE:CD1	0.46	2.46	4	1
1:A:31:MET:SD	1:A:32:HIS:N	0.46	2.89	14	2
1:A:67:GLU:CD	1:A:68:CYS:O	0.46	2.54	20	2
1:A:24:GLN:N	1:A:24:GLN:CD	0.45	2.70	14	2
1:A:15:CYS:HB3	1:A:32:HIS:CE1	0.45	2.46	7	5
1:A:87:SER:O	1:A:90:LYS:N	0.45	2.49	17	1
1:A:89:THR:O	1:A:90:LYS:C	0.45	2.55	3	17
1:A:89:THR:O	1:A:92:TYR:N	0.45	2.50	10	4
1:A:89:THR:O	1:A:91:SER:N	0.45	2.50	9	1
1:A:46:LYS:O	1:A:47:PHE:CD1	0.45	2.70	17	1
1:A:11:TYR:CD1	1:A:11:TYR:N	0.45	2.84	15	3
1:A:12:PRO:O	1:A:25:ARG:NH1	0.45	2.50	4	6
1:A:50:LYS:CD	1:A:51:HIS:N	0.45	2.80	3	3
1:A:31:MET:O	1:A:32:HIS:C	0.45	2.55	9	1
1:A:49:MET:CB	1:A:51:HIS:NE2	0.45	2.80	2	2
1:A:46:LYS:C	1:A:47:PHE:CG	0.45	2.91	9	2
1:A:76:MET:C	1:A:76:MET:SD	0.44	2.95	13	1
1:A:66:TYR:CZ	1:A:78:ARG:HD3	0.44	2.47	20	2
1:A:84:HIS:O	1:A:85:VAL:C	0.44	2.56	13	2
1:A:66:TYR:HB3	1:A:81:PHE:CG	0.44	2.48	2	4
1:A:81:PHE:CE1	1:A:85:VAL:CG2	0.44	3.00	13	2
1:A:56:HIS:CE1	1:A:59:ILE:HD13	0.44	2.48	2	1
1:A:76:MET:CG	1:A:77:TRP:CD1	0.44	3.01	20	3
1:A:31:MET:SD	1:A:32:HIS:ND1	0.44	2.91	20	1
1:A:78:ARG:O	1:A:79:ASP:C	0.43	2.56	15	2
1:A:50:LYS:HD2	1:A:51:HIS:N	0.43	2.27	13	1
1:A:40:CYS:SG	1:A:57:MET:CE	0.43	3.07	19	2
1:A:75:PHE:CD1	1:A:75:PHE:N	0.43	2.87	10	2
1:A:19:PHE:CD1	1:A:25:ARG:HA	0.43	2.49	18	1
1:A:22:LYS:O	1:A:25:ARG:N	0.43	2.52	19	1
1:A:87:SER:O	1:A:89:THR:N	0.42	2.52	19	1
1:A:11:TYR:CE2	1:A:22:LYS:HB3	0.42	2.50	11	1
1:A:40:CYS:SG	1:A:57:MET:HE1	0.42	2.54	17	2
1:A:78:ARG:NH1	1:A:82:HIS:CE1	0.42	2.88	11	1
1:A:83:ARG:O	1:A:86:THR:HG22	0.42	2.14	18	2
1:A:24:GLN:OE1	1:A:24:GLN:N	0.42	2.52	2	1
1:A:49:MET:SD	1:A:51:HIS:CE1	0.42	3.13	4	1
1:A:54:VAL:C	1:A:56:HIS:N	0.42	2.73	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:MET:CE	1:A:57:MET:HA	0.42	2.45	11	9
1:A:42:VAL:HG11	1:A:60:HIS:CG	0.42	2.50	7	3
1:A:59:ILE:HG13	1:A:60:HIS:N	0.42	2.29	15	1
1:A:19:PHE:CD1	1:A:19:PHE:N	0.41	2.88	3	2
1:A:69:ASN:ND2	1:A:69:ASN:H	0.41	2.11	10	1
1:A:84:HIS:O	1:A:87:SER:N	0.41	2.52	13	1
1:A:11:TYR:N	1:A:11:TYR:CD1	0.41	2.86	16	2
1:A:74:ARG:C	1:A:75:PHE:CD1	0.41	2.94	6	1
1:A:57:MET:HA	1:A:57:MET:CE	0.41	2.45	6	2
1:A:26:ASP:OD1	1:A:26:ASP:C	0.41	2.59	2	1
1:A:81:PHE:CD1	1:A:85:VAL:HG21	0.41	2.49	5	1
1:A:47:PHE:CD1	1:A:53:LEU:HB2	0.40	2.51	9	1
1:A:87:SER:O	1:A:88:CYS:C	0.40	2.59	17	1
1:A:87:SER:C	1:A:89:THR:N	0.40	2.73	19	1
1:A:43:CYS:HB3	1:A:60:HIS:CE1	0.40	2.52	9	1
1:A:47:PHE:CE2	1:A:52:HIS:O	0.40	2.75	3	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	71/110 (65%)	62±2 (88±3%)	8±2 (11±3%)	0±1 (0±1%)	32	76
All	All	1420/2200 (65%)	1250 (88%)	163 (11%)	7 (0%)	32	76

All 5 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	17	LYS	2
1	A	55	GLY	2
1	A	68	CYS	1
1	A	90	LYS	1
1	A	88	CYS	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	66/93 (71%)	62±1 (94±2%)	4±1 (6±2%)	22	71
All	All	1320/1860 (71%)	1239 (94%)	81 (6%)	22	71

All 18 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	57	MET	20
1	A	50	LYS	15
1	A	69	ASN	8
1	A	22	LYS	7
1	A	51	HIS	4
1	A	24	GLN	3
1	A	80	SER	3
1	A	90	LYS	3
1	A	31	MET	2
1	A	58	LYS	2
1	A	26	ASP	2
1	A	48	LYS	2
1	A	25	ARG	2
1	A	27	ARG	2
1	A	79	ASP	2
1	A	76	MET	2
1	A	78	ARG	1
1	A	73	LYS	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)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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