Full wwPDB NMR Structure Validation Report (i)

Feb 28, 2022 – 07:18 PM EST

PDB ID	:	2EJ4
Title	:	Functional and structural basis of nuclear localization signal in ZIC3 zinc finger domain: a role of conserved tryptophan residue in the zinc finger domain
Authors	:	Tomizawa, T.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-03-14

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:

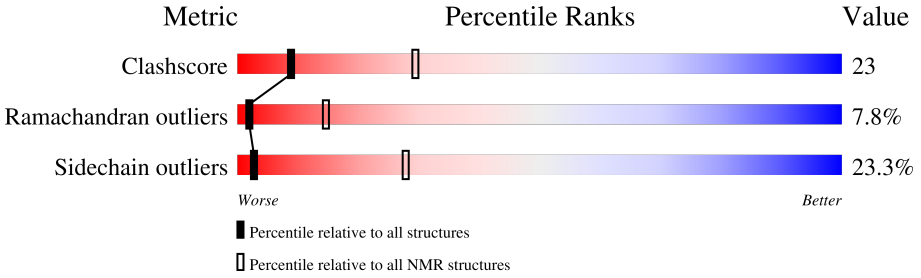
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	95	23% 45% 6% 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 13 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:13-A:21, A:27-A:88 (71)	0.33	13

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 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1455 atoms, of which 711 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein ZIC 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	95	1453	456	711	137	143	6	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP O60481
A	2	SER	-	expression tag	UNP O60481
A	3	SER	-	expression tag	UNP O60481
A	4	GLY	-	expression tag	UNP O60481
A	5	SER	-	expression tag	UNP O60481
A	6	SER	-	expression tag	UNP O60481
A	7	GLY	-	expression tag	UNP O60481
A	90	SER	-	expression tag	UNP O60481
A	91	GLY	-	expression tag	UNP O60481
A	92	PRO	-	expression tag	UNP O60481
A	93	SER	-	expression tag	UNP O60481
A	94	SER	-	expression tag	UNP O60481
A	95	GLY	-	expression tag	UNP O60481

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

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 ZIC 3

Chain A: 23% 45% 6% 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 C16 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 E40 T43 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 V59 W62 E63 E64 C65 P66 R67 E68 G69

K70 S71 F72 K73 A74 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 E88 K89 S90 G91 P92 S93 S94 G95

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 ZIC 3

Chain A: 21% 41% 12% • 25%

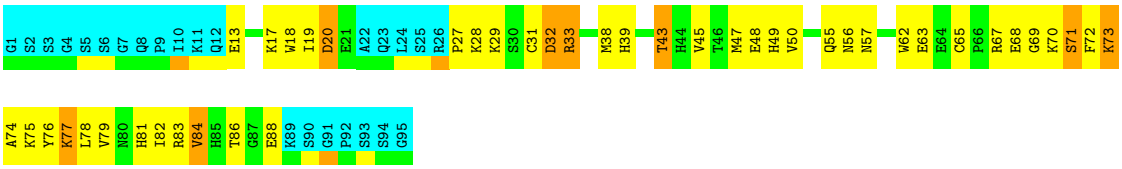
G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 C16 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 T34 F35 S36 T37 M38 H39 E40 L41 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 V59 C60 Y61 W62 E63

E64 C65 P66 R67 E68 G69 K70 S71 F72 K73 Y76 K77 L78 V79 N80 H81 I82 R83 V84 H85 T86 G87 E88 K89 S90 G91 P92 S93 S94 G95

4.2.2 Score per residue for model 2

• Molecule 1: Zinc finger protein ZIC 3

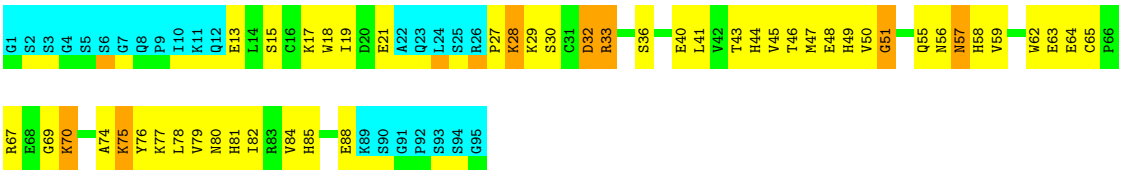
Chain A: 28% 38% 8% 25%



4.2.3 Score per residue for model 3

- Molecule 1: Zinc finger protein ZIC 3

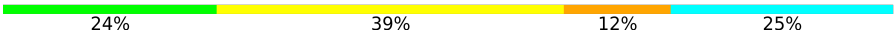
Chain A:

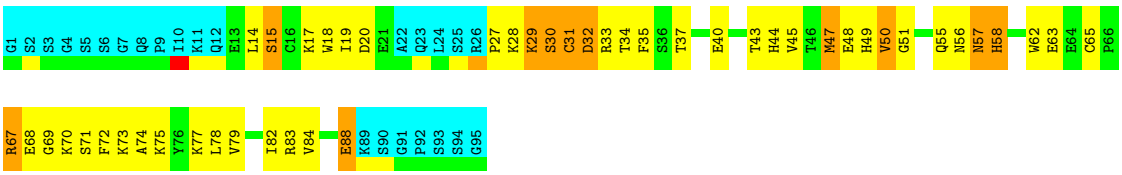


4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger protein ZIC 3

Chain A:

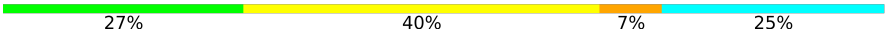


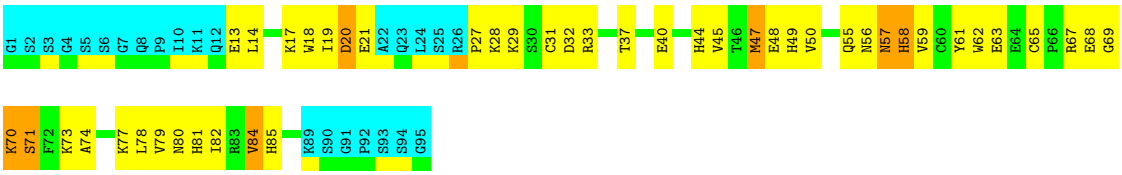


4.2.5 Score per residue for model 5

- Molecule 1: Zinc finger protein ZIC 3

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 27% 42% • • 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 T34 F35 S36 T37 M38 H39 E40 L41 V42 T43 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 V59 W62 E63 E64 C65

P66 R67 E68 G69 K70 K73 A74 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 E88 K89 S90 G91 P92 S93 S94 G95

4.2.7 Score per residue for model 7

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 31% 33% 12% 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 C16 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 E40 T43 H44 M47 E48 H49 V50 G51 Q55 N56 N57 H58 V59 C60 Y61 W62 E63 E64 C65 P66 R67 E68 G69

K70 S71 F72 K75 Y76 K77 N80 H81 V84 H85 E88 K89 S90 G91 P92 S93 S94 G95

4.2.8 Score per residue for model 8

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 28% 35% 9% • 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 S36 E40 T43 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 V59 C60 Y61 W62 E63 E64 C65 P66 R67

E68 G69 K70 S71 F72 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 E88 K89 S90 G91 P92 S93 S94 G95

4.2.9 Score per residue for model 9

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 29% 36% 8% • 25%

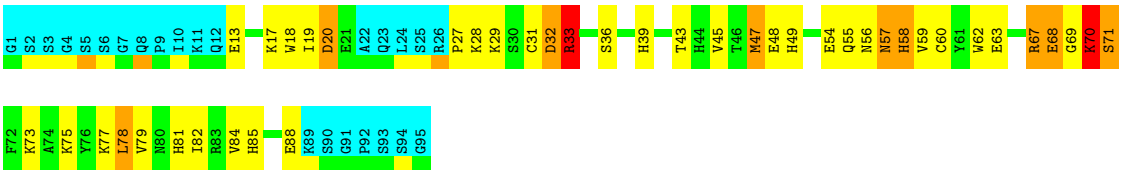
G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 C16 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 D32 R33 T34 F35 M38 H39 E40 T43 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 W62 E63 R67 E68 G69

K70 S71 F72 K73 A74 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 H85 T86 K89 S90 G91 P92 S93 S94 G95

4.2.10 Score per residue for model 10

- Molecule 1: Zinc finger protein ZIC 3

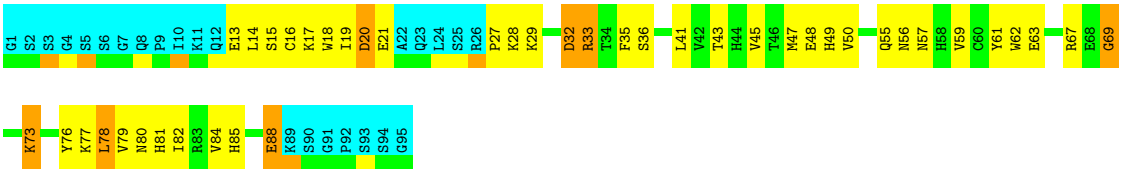
Chain A: 31% 33% 9% • 25%



4.2.11 Score per residue for model 11

- Molecule 1: Zinc finger protein ZIC 3

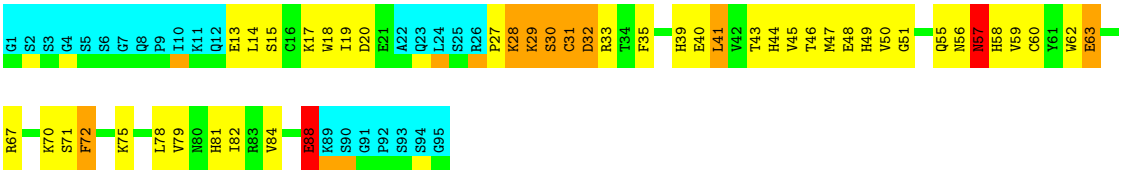
Chain A: 29% 38% 7% 25%



4.2.12 Score per residue for model 12

- Molecule 1: Zinc finger protein ZIC 3

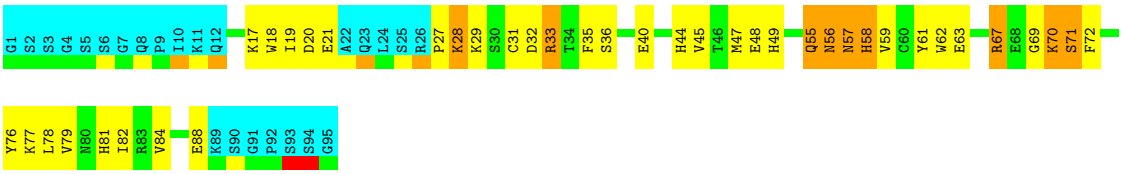
Chain A: 26% 38% 8% • 25%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 33% 33% 9% 25%



4.2.14 Score per residue for model 14

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 36% 26% 12% • 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 S15 W18 I19 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 Y61 W62 E63 E64 C65 P66 R67 E68 G69 K70 S71 F72 K73 Y76 K77 L78

V79 N80 H81 I82 R83 V84 E88 K89 S90 G91 P92 S93 S94 G95

4.2.15 Score per residue for model 15

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 28% 36% 11% 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 K17 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 S36 T37 M38 H39 E40 T43 H44 V45 T46 M47 E48 G51 E54 Q55 N56 N57 H58 V59 W62 E63 E64 C65 P66 R67

K70 S71 F72 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 H85 T86 G87 E88 K89 S90 G91 P92 S93 S94 G95

4.2.16 Score per residue for model 16

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 29% 38% 7% 25%

G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 C16 K17 W18 I19 A22 Q23 L24 S25 R26 P27 K28 K29 R33 E40 L41 V42 T43 H44 V45 T46 M47 E48 H49 V50 G51 Q55 N56 N57 H58 W62 E63 E64 C65 P66 R67 E68 G69 K70 S71 F72

K73 A74 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 H85 T86 G87 E88 K89 S90 G91 P92 S93 S94 G95

4.2.17 Score per residue for model 17

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 25% 38% 11% • 25%

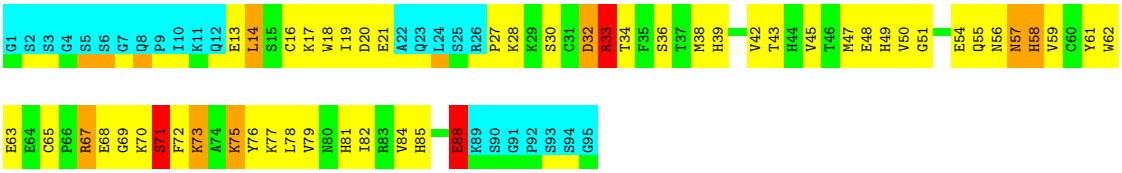
G1 S2 S3 G4 S5 S6 G7 Q8 P9 I10 K11 Q12 E13 L14 S15 W18 I19 D20 E21 A22 Q23 L24 S25 R26 P27 K28 K29 S30 C31 D32 R33 T34 F35 H39 E40 T43 H44 V45 T46 M47 E48 H49 V50 G51 G52 Q55 N56 N57 H58 V59 C60 Y61 W62 E63 E64 C65

P66 R67 E68 G69 K70 S71 F72 K73 A74 K75 Y76 K77 L78 V79 N80 H81 I82 R83 V84 E88 K89 S90 G91 P92 S93 S94 G95

4.2.18 Score per residue for model 18

- Molecule 1: Zinc finger protein ZIC 3

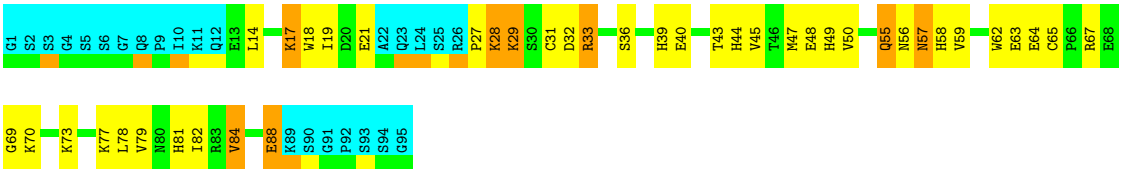
Chain A: 20% 44% 7% • 25%



4.2.19 Score per residue for model 19

- Molecule 1: Zinc finger protein ZIC 3

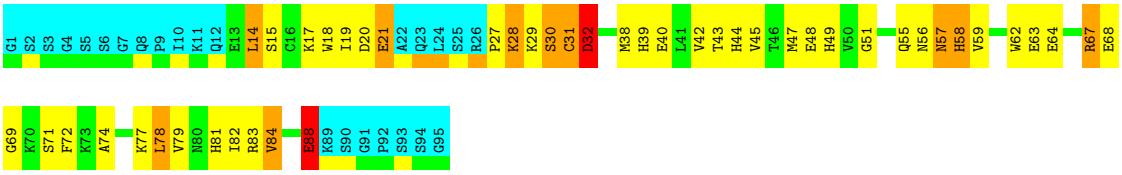
Chain A: 32% 35% 8% 25%



4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger protein ZIC 3

Chain A: 26% 36% 11% • 25%



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	583	552	552	27±4
All	All	11700	11040	11040	532

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:59:VAL:HG22	1:A:71:SER:HB2	0.79	1.52	10	3
1:A:50:VAL:HG22	1:A:78:LEU:HD23	0.75	1.56	5	8
1:A:79:VAL:HA	1:A:82:ILE:HD12	0.70	1.63	8	19
1:A:18:TRP:CZ3	1:A:45:VAL:CG1	0.69	2.75	17	17
1:A:74:ALA:HB3	1:A:77:LYS:HG3	0.69	1.63	20	3
1:A:18:TRP:CE3	1:A:45:VAL:CG1	0.68	2.77	13	17
1:A:18:TRP:CG	1:A:49:HIS:CD2	0.67	2.82	18	19
1:A:59:VAL:HG22	1:A:71:SER:CB	0.67	2.20	10	3
1:A:81:HIS:O	1:A:84:VAL:HG12	0.66	1.89	10	17
1:A:58:HIS:CD2	1:A:58:HIS:N	0.65	2.65	9	4
1:A:58:HIS:HB2	1:A:78:LEU:HD23	0.65	1.67	10	1
1:A:76:TYR:CD1	1:A:77:LYS:N	0.65	2.64	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:TRP:CE3	1:A:45:VAL:HG13	0.64	2.27	17	18
1:A:67:ARG:NH1	1:A:72:PHE:CE2	0.64	2.65	8	4
1:A:55:GLN:NE2	1:A:56:ASN:H	0.62	1.92	8	1
1:A:59:VAL:HG13	1:A:69:GLY:O	0.62	1.94	1	6
1:A:18:TRP:CD1	1:A:49:HIS:CE1	0.61	2.88	4	9
1:A:74:ALA:HB3	1:A:77:LYS:HB2	0.60	1.74	2	2
1:A:67:ARG:CZ	1:A:72:PHE:CE2	0.60	2.84	8	1
1:A:76:TYR:CG	1:A:77:LYS:N	0.60	2.70	18	8
1:A:33:ARG:O	1:A:34:THR:HG23	0.59	1.97	4	2
1:A:19:ILE:HD11	1:A:63:GLU:HB2	0.58	1.76	17	19
1:A:67:ARG:CZ	1:A:72:PHE:CZ	0.58	2.86	8	3
1:A:17:LYS:O	1:A:62:TRP:CE3	0.57	2.58	4	13
1:A:50:VAL:HG22	1:A:78:LEU:CD2	0.56	2.30	6	7
1:A:76:TYR:C	1:A:76:TYR:CD1	0.55	2.80	7	1
1:A:18:TRP:CD2	1:A:49:HIS:CD2	0.54	2.96	17	5
1:A:19:ILE:HG23	1:A:29:LYS:O	0.54	2.02	12	1
1:A:58:HIS:CE1	1:A:74:ALA:C	0.53	2.82	4	1
1:A:50:VAL:HG21	1:A:79:VAL:HG23	0.53	1.79	17	1
1:A:55:GLN:NE2	1:A:56:ASN:N	0.53	2.56	8	2
1:A:14:LEU:HD22	1:A:38:MET:CE	0.53	2.32	18	1
1:A:59:VAL:HG12	1:A:60:CYS:N	0.52	2.18	10	1
1:A:18:TRP:CZ3	1:A:45:VAL:HG13	0.52	2.39	15	4
1:A:75:LYS:CD	1:A:75:LYS:C	0.52	2.78	7	4
1:A:67:ARG:HD3	1:A:72:PHE:CZ	0.51	2.39	17	2
1:A:17:LYS:N	1:A:62:TRP:CH2	0.51	2.79	3	15
1:A:67:ARG:CD	1:A:72:PHE:CZ	0.51	2.94	17	1
1:A:32:ASP:CG	1:A:33:ARG:N	0.50	2.63	15	1
1:A:27:PRO:O	1:A:29:LYS:N	0.50	2.45	15	17
1:A:47:MET:CG	1:A:48:GLU:N	0.50	2.75	6	20
1:A:70:LYS:O	1:A:71:SER:CB	0.50	2.60	17	9
1:A:58:HIS:CE1	1:A:75:LYS:N	0.50	2.80	4	1
1:A:59:VAL:CG1	1:A:69:GLY:CA	0.50	2.90	6	2
1:A:30:SER:O	1:A:32:ASP:N	0.50	2.45	20	4
1:A:59:VAL:CG1	1:A:69:GLY:C	0.50	2.80	3	1
1:A:76:TYR:CE1	1:A:77:LYS:HG3	0.50	2.42	6	1
1:A:40:GLU:O	1:A:44:HIS:N	0.49	2.45	16	14
1:A:84:VAL:HG13	1:A:85:HIS:ND1	0.49	2.22	18	9
1:A:58:HIS:C	1:A:78:LEU:CD2	0.49	2.81	10	1
1:A:31:CYS:O	1:A:32:ASP:CB	0.49	2.60	1	1
1:A:33:ARG:CD	1:A:35:PHE:CE1	0.49	2.95	17	1
1:A:56:ASN:O	1:A:57:ASN:CB	0.49	2.61	14	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ALA:HB1	1:A:76:TYR:CE1	0.49	2.43	2	1
1:A:72:PHE:O	1:A:73:LYS:CB	0.49	2.60	2	3
1:A:59:VAL:CG1	1:A:60:CYS:N	0.49	2.76	10	2
1:A:20:ASP:OD1	1:A:61:TYR:CD2	0.49	2.66	17	1
1:A:67:ARG:O	1:A:69:GLY:N	0.48	2.46	1	10
1:A:59:VAL:CG1	1:A:69:GLY:O	0.48	2.60	10	2
1:A:43:THR:O	1:A:43:THR:CG2	0.48	2.62	2	12
1:A:67:ARG:NH1	1:A:72:PHE:CE1	0.48	2.82	7	1
1:A:18:TRP:CZ3	1:A:45:VAL:HG11	0.48	2.44	20	2
1:A:46:THR:O	1:A:51:GLY:N	0.47	2.46	8	8
1:A:67:ARG:NH2	1:A:71:SER:C	0.47	2.68	13	1
1:A:33:ARG:CD	1:A:35:PHE:CZ	0.47	2.98	17	1
1:A:32:ASP:OD1	1:A:33:ARG:N	0.47	2.48	2	1
1:A:39:HIS:CD2	1:A:39:HIS:C	0.47	2.86	2	1
1:A:33:ARG:HB3	1:A:35:PHE:CE2	0.47	2.45	13	2
1:A:59:VAL:HG22	1:A:71:SER:HA	0.47	1.87	18	2
1:A:71:SER:O	1:A:73:LYS:N	0.46	2.48	17	1
1:A:70:LYS:CD	1:A:72:PHE:CE1	0.46	2.99	12	1
1:A:33:ARG:HG3	1:A:44:HIS:CE1	0.46	2.45	15	1
1:A:16:CYS:N	1:A:32:ASP:O	0.46	2.48	18	2
1:A:59:VAL:HG22	1:A:71:SER:CA	0.46	2.41	18	2
1:A:35:PHE:CD1	1:A:35:PHE:N	0.46	2.84	4	1
1:A:59:VAL:C	1:A:78:LEU:HD21	0.45	2.31	10	1
1:A:43:THR:CG2	1:A:43:THR:O	0.45	2.63	12	1
1:A:21:GLU:HB2	1:A:61:TYR:CE2	0.45	2.45	18	1
1:A:70:LYS:O	1:A:70:LYS:CG	0.45	2.64	3	1
1:A:33:ARG:O	1:A:34:THR:CG2	0.45	2.64	4	1
1:A:30:SER:O	1:A:31:CYS:C	0.45	2.55	20	5
1:A:58:HIS:HB3	1:A:78:LEU:HD23	0.45	1.89	13	1
1:A:69:GLY:O	1:A:70:LYS:C	0.45	2.55	5	4
1:A:67:ARG:O	1:A:70:LYS:N	0.45	2.50	2	2
1:A:70:LYS:HD2	1:A:72:PHE:CZ	0.45	2.47	12	1
1:A:18:TRP:CG	1:A:49:HIS:NE2	0.45	2.84	18	3
1:A:38:MET:CE	1:A:86:THR:O	0.45	2.64	9	4
1:A:67:ARG:O	1:A:68:GLU:C	0.45	2.55	1	3
1:A:17:LYS:HB2	1:A:62:TRP:CZ2	0.45	2.46	3	1
1:A:67:ARG:NH2	1:A:71:SER:O	0.45	2.50	13	1
1:A:27:PRO:O	1:A:28:LYS:C	0.45	2.55	20	8
1:A:35:PHE:CE2	1:A:41:LEU:HD13	0.45	2.46	12	1
1:A:17:LYS:O	1:A:62:TRP:CD2	0.45	2.70	6	3
1:A:67:ARG:HD2	1:A:72:PHE:CE1	0.45	2.46	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:PHE:CD1	1:A:40:GLU:HB3	0.44	2.48	6	1
1:A:32:ASP:O	1:A:33:ARG:CB	0.44	2.65	10	2
1:A:19:ILE:O	1:A:61:TYR:CD1	0.44	2.70	14	2
1:A:18:TRP:CD1	1:A:49:HIS:ND1	0.44	2.85	4	1
1:A:80:ASN:OD1	1:A:80:ASN:C	0.44	2.56	14	1
1:A:14:LEU:CD2	1:A:38:MET:SD	0.44	3.06	20	1
1:A:47:MET:CG	1:A:48:GLU:OE1	0.43	2.66	20	2
1:A:72:PHE:CZ	1:A:81:HIS:CB	0.43	3.01	13	1
1:A:18:TRP:CD1	1:A:49:HIS:CG	0.43	3.06	5	1
1:A:55:GLN:NE2	1:A:57:ASN:O	0.43	2.51	19	3
1:A:67:ARG:NH1	1:A:72:PHE:CZ	0.43	2.87	7	2
1:A:67:ARG:C	1:A:69:GLY:N	0.43	2.72	2	6
1:A:21:GLU:HB2	1:A:61:TYR:CE1	0.43	2.49	11	2
1:A:67:ARG:HD2	1:A:72:PHE:CZ	0.43	2.49	4	2
1:A:59:VAL:CA	1:A:78:LEU:HD21	0.43	2.44	10	1
1:A:56:ASN:CG	1:A:56:ASN:O	0.43	2.57	11	1
1:A:42:VAL:HG11	1:A:83:ARG:CZ	0.42	2.44	20	1
1:A:14:LEU:HB3	1:A:41:LEU:HD22	0.42	1.91	1	1
1:A:84:VAL:CG1	1:A:85:HIS:ND1	0.42	2.82	5	2
1:A:72:PHE:CE1	1:A:78:LEU:HD13	0.42	2.49	20	1
1:A:35:PHE:CE1	1:A:41:LEU:HD13	0.42	2.49	11	1
1:A:49:HIS:O	1:A:51:GLY:N	0.42	2.52	4	4
1:A:47:MET:HG2	1:A:48:GLU:N	0.42	2.30	5	5
1:A:19:ILE:CD1	1:A:63:GLU:HA	0.42	2.45	14	6
1:A:33:ARG:HD3	1:A:35:PHE:CE1	0.42	2.50	17	2
1:A:59:VAL:HG22	1:A:71:SER:OG	0.42	2.15	5	1
1:A:41:LEU:HG	1:A:86:THR:HG22	0.42	1.91	16	1
1:A:18:TRP:CE2	1:A:61:TYR:HB2	0.41	2.50	13	4
1:A:33:ARG:HB3	1:A:35:PHE:CE1	0.41	2.51	1	1
1:A:49:HIS:C	1:A:51:GLY:N	0.41	2.74	20	3
1:A:58:HIS:HB2	1:A:78:LEU:HD22	0.41	1.92	5	1
1:A:19:ILE:CG2	1:A:28:LYS:HB3	0.41	2.46	19	2
1:A:42:VAL:HG21	1:A:88:GLU:OE2	0.41	2.16	18	1
1:A:39:HIS:CE1	1:A:43:THR:OG1	0.41	2.73	19	1
1:A:38:MET:O	1:A:42:VAL:HG23	0.41	2.15	6	1
1:A:59:VAL:HG22	1:A:69:GLY:O	0.41	2.16	8	1
1:A:30:SER:C	1:A:32:ASP:N	0.41	2.74	20	2
1:A:77:LYS:O	1:A:80:ASN:ND2	0.41	2.54	15	1
1:A:14:LEU:O	1:A:15:SER:CB	0.41	2.68	4	1
1:A:21:GLU:HB2	1:A:61:TYR:CZ	0.41	2.51	5	2
1:A:58:HIS:HB2	1:A:78:LEU:CD2	0.41	2.45	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ASP:O	1:A:33:ARG:CG	0.41	2.68	10	1
1:A:37:THR:OG1	1:A:40:GLU:CG	0.41	2.69	4	1
1:A:78:LEU:HG	1:A:82:ILE:HD11	0.41	1.93	8	1
1:A:19:ILE:CD1	1:A:63:GLU:CA	0.40	2.99	17	1
1:A:18:TRP:CE2	1:A:49:HIS:HB3	0.40	2.52	4	1
1:A:18:TRP:CE3	1:A:45:VAL:HG11	0.40	2.47	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	71/95 (75%)	51±2 (71±3%)	15±2 (21±3%)	6±2 (8±2%)	2 14
All	All	1420/1900 (75%)	1011 (71%)	298 (21%)	111 (8%)	2 14

All 18 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	28	LYS	20
1	A	32	ASP	17
1	A	20	ASP	10
1	A	68	GLU	10
1	A	88	GLU	10
1	A	57	ASN	8
1	A	33	ARG	6
1	A	73	LYS	5
1	A	71	SER	4
1	A	51	GLY	4
1	A	15	SER	3
1	A	31	CYS	3
1	A	70	LYS	3
1	A	50	VAL	2
1	A	69	GLY	2
1	A	72	PHE	2

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Mol	Chain	Res	Type	Models (Total)
1	A	52	GLY	1
1	A	14	LEU	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	66/84 (79%)	51±2 (77±3%)	15±2 (23±3%)	3 28
All	All	1320/1680 (79%)	1012 (77%)	308 (23%)	3 28

All 39 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	55	GLN	20
1	A	67	ARG	18
1	A	88	GLU	18
1	A	33	ARG	17
1	A	58	HIS	14
1	A	65	CYS	14
1	A	57	ASN	12
1	A	13	GLU	12
1	A	31	CYS	11
1	A	70	LYS	11
1	A	73	LYS	11
1	A	71	SER	11
1	A	75	LYS	11
1	A	20	ASP	10
1	A	36	SER	10
1	A	84	VAL	10
1	A	15	SER	9
1	A	80	ASN	9
1	A	29	LYS	9
1	A	14	LEU	8
1	A	43	THR	7
1	A	77	LYS	7
1	A	30	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	47	MET	7
1	A	39	HIS	6
1	A	64	GLU	4
1	A	32	ASP	3
1	A	76	TYR	3
1	A	54	GLU	3
1	A	78	LEU	3
1	A	63	GLU	2
1	A	83	ARG	2
1	A	41	LEU	2
1	A	56	ASN	2
1	A	38	MET	1
1	A	37	THR	1
1	A	16	CYS	1
1	A	17	LYS	1
1	A	21	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 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