Full wwPDB NMR Structure Validation Report (i)

Feb 26, 2022 – 06:13 PM EST

PDB ID	:	2CS2
Title	:	Solution structure of the second Zn-finger domain of poly(ADP-ribose) polymerase-1
Authors	:	Nagashima, T.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-05-20

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:

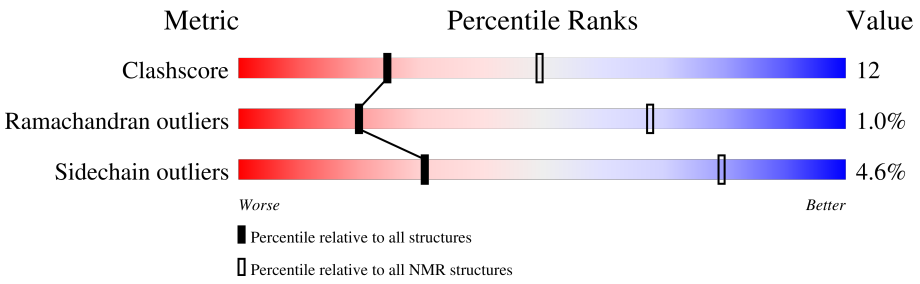
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	134	57% 13% 30%

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:106 (94)	0.41	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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2036 atoms, of which 1020 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	134	2035	627	1020	181	201	6	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P09874
A	2	SER	-	cloning artifact	UNP P09874
A	3	SER	-	cloning artifact	UNP P09874
A	4	GLY	-	cloning artifact	UNP P09874
A	5	SER	-	cloning artifact	UNP P09874
A	6	SER	-	cloning artifact	UNP P09874
A	7	GLY	-	cloning artifact	UNP P09874
A	129	SER	-	cloning artifact	UNP P09874
A	130	GLY	-	cloning artifact	UNP P09874
A	131	PRO	-	cloning artifact	UNP P09874
A	132	SER	-	cloning artifact	UNP P09874
A	133	SER	-	cloning artifact	UNP P09874
A	134	GLY	-	cloning artifact	UNP P09874

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

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	1	1	1

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: Poly [ADP-ribose] polymerase-1

Chain A: 57% 13% 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 D17 A23 C30 K36 R43 L44 S45 M58 W62 Y63 H64 Y81 G88 F89 L92 A93 T94 E95 D96 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120 V121 D122 E123 V124

A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

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: Poly [ADP-ribose] polymerase-1

Chain A: 54% 15% • 30%

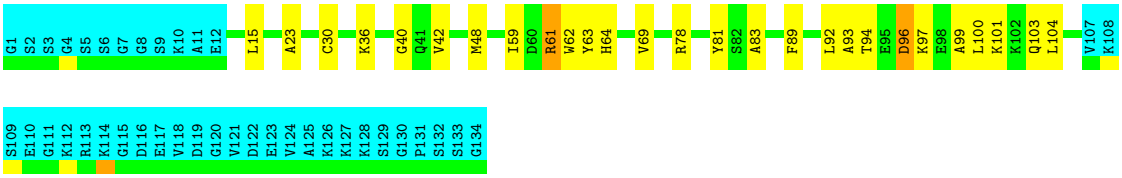
G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 G16 D17 F18 C30 K36 L44 V49 G57 M58 W62 Y63 H64 E80 Y81 S84 Q85 L86 K87 G88 F89 S90 L91 L92 D96 A99 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117

V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.2 Score per residue for model 2

• Molecule 1: Poly [ADP-ribose] polymerase-1

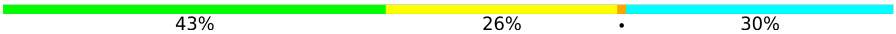
Chain A: 50% 19% • 30%

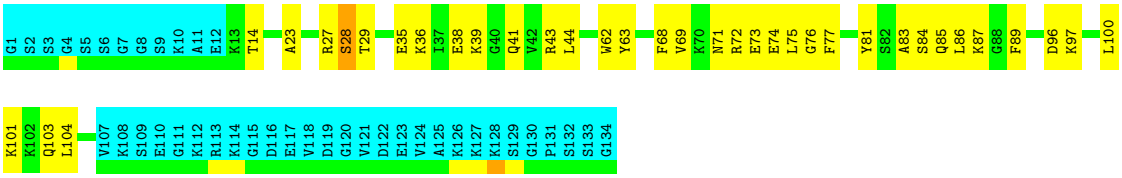


4.2.3 Score per residue for model 3

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:





4.2.4 Score per residue for model 4

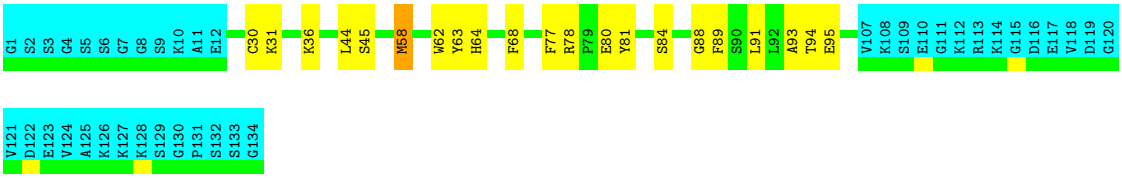
- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 54% 13% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 C30 K36 R43 K46 M58 I59 D60 R61 W62 Y63 H64 E80 Y81 S82 A83 S84 Q85 F89 L92 A93 T94 E95 D96 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120

V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.7 Score per residue for model 7

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 47% 22% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 L15 G16 D17 A23 R27 S28 T29 C30 K36 G40 R43 L44 S45 M48 M58 I59 D60 R61 W62 Y63 H64 F77 R78 P79 E80 Y81 S82 A83 S84 Q85 L86 K87 G88 F89 S90 L91 L92

L100 Q103 G106 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.8 Score per residue for model 8

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 42% 27% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 L15 A20 A23 R27 S28 T29 C30 K31 K36 G40 R43 L44 S45 M48 V49 G57 M58 I59 D60 R61 W62 Y63 H64 Y81 S84 Q85 G88 F89 S90 L91 L92 A93 T94 E95 D96

K97 L100 K101 K102 Q103 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.9 Score per residue for model 9

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 55% 14% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 A23 K24 S25 N26 C30 K36 I37 E38 V42 S45 K46 K47 Q55 M58 I59 D60 R61 W62 Y63 H64 K87 G88 L92 G106 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120

V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.10 Score per residue for model 10

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 53% 16% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 L15 F18 A19 A20 A23 N26 T29 C30 E35 K36 I37 E38 R43 L44 S45 K46 W62 Y63 A83 K87 G88 F89 A93 T94 E95 D96 L104 V107 K108 S109 E110 G111 K112 R113

K114 G115 D116 E117 V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.11 Score per residue for model 11

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 46% 23% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 L15 G16 D17 F18 A19 A20 E21 S28 T29 C33 M34 E35 K36 I37 R43 L44 S45 K46 M58 W62 Y63 F68 R72 E73 E74 L75 Y81 S84 G88 F89 S90 L91 L92 D96 K97

G106 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116 E117 V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.12 Score per residue for model 12

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A: 54% 13% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 K13 T14 L15 G16 D17 R27 S28 T29 C30 K36 I37 Q41 V42 R43 L44 S45 M58 W62 Y63 H64 V69 R78 Y81 A93 D96 Q103 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116

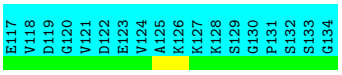
E117 V118 D119 G120 V121 D122 E123 V124 A125 K126 K127 K128 S129 G130 P131 S132 S133 G134

4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Poly [ADP-ribose] polymerase-1

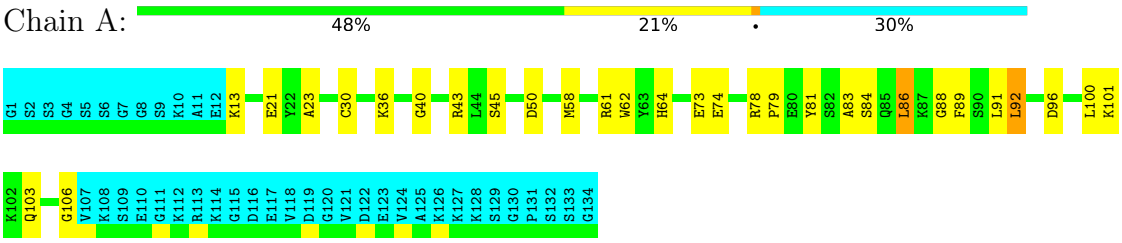
Chain A: 54% 14% • 30%

G1 S2 S3 G4 S5 S6 G7 G8 S9 K10 A11 E12 F18 A19 A20 A23 C30 K36 R43 L44 S45 K46 M58 W62 Y63 H64 E74 F77 Y81 G88 F89 S90 L91 L92 D96 A99 V107 K108 S109 E110 G111 K112 R113 K114 G115 D116



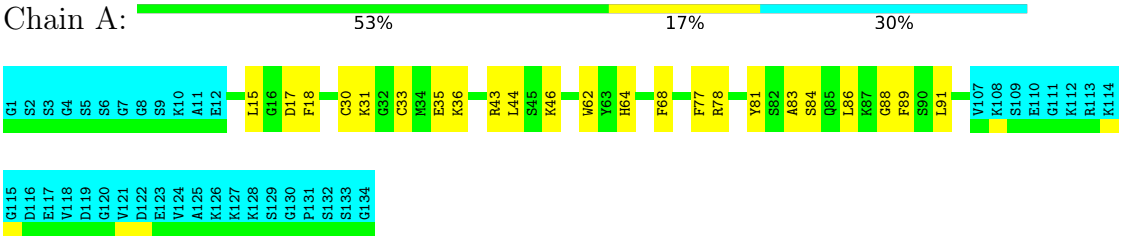
4.2.14 Score per residue for model 14

• Molecule 1: Poly [ADP-ribose] polymerase-1



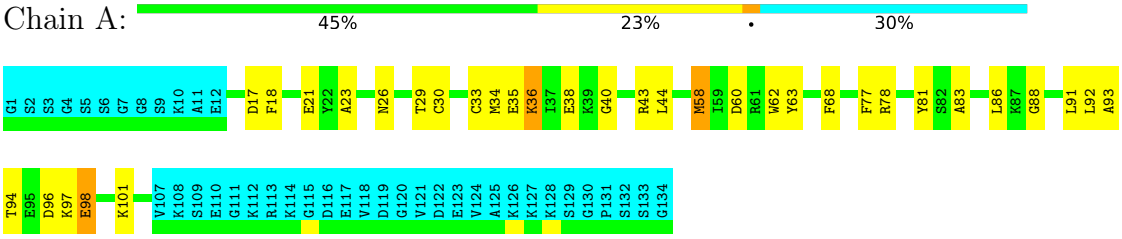
4.2.15 Score per residue for model 15

• Molecule 1: Poly [ADP-ribose] polymerase-1



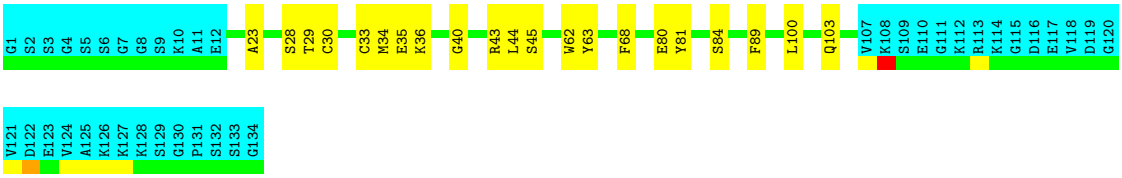
4.2.16 Score per residue for model 16

• Molecule 1: Poly [ADP-ribose] polymerase-1



4.2.17 Score per residue for model 17

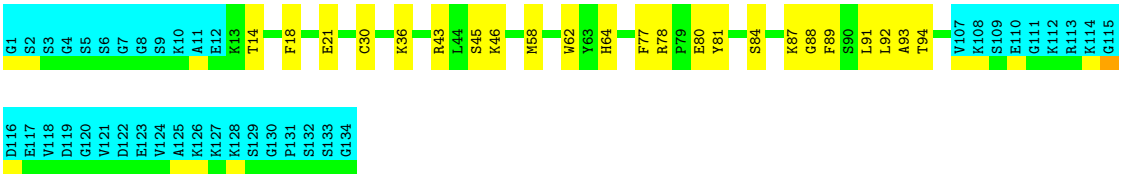
• Molecule 1: Poly [ADP-ribose] polymerase-1



4.2.18 Score per residue for model 18

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:



4.2.19 Score per residue for model 19

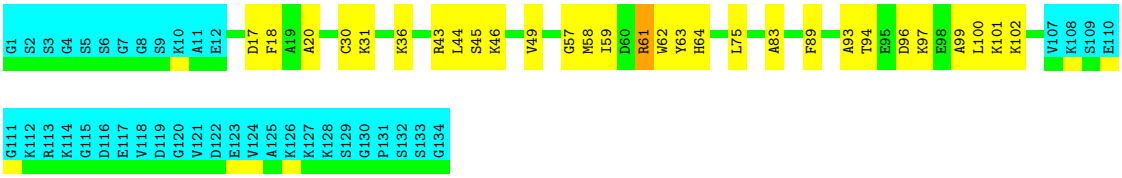
- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:

4.2.20 Score per residue for model 20

- Molecule 1: Poly [ADP-ribose] polymerase-1

Chain A:



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*.

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	746	755	755	18±5
All	All	14940	15100	15100	353

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:ALA:HB2	1:A:44:LEU:HD23	0.80	1.52	11	5
1:A:20:ALA:HB2	1:A:44:LEU:CD2	0.74	2.10	11	2
1:A:15:LEU:HD13	1:A:81:TYR:CE2	0.72	2.19	4	1
1:A:29:THR:HG23	1:A:35:GLU:O	0.72	1.85	11	6
1:A:21:GLU:HA	1:A:92:LEU:HD21	0.69	1.64	14	3
1:A:15:LEU:HD21	1:A:81:TYR:CD1	0.68	2.22	8	2
1:A:89:PHE:HA	1:A:92:LEU:HD12	0.68	1.66	13	2
1:A:43:ARG:NE	1:A:62:TRP:CZ3	0.68	2.62	12	6
1:A:15:LEU:HD11	1:A:81:TYR:CD1	0.66	2.25	11	3
1:A:80:GLU:CG	1:A:81:TYR:CE1	0.66	2.77	5	1
1:A:83:ALA:HB2	1:A:104:LEU:HD12	0.65	1.66	10	1
1:A:14:THR:HG21	1:A:87:LYS:HA	0.64	1.68	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:TRP:C	1:A:63:TYR:CD1	0.64	2.71	3	15
1:A:43:ARG:NE	1:A:62:TRP:CE3	0.64	2.66	11	5
1:A:71:ASN:O	1:A:75:LEU:HD12	0.62	1.94	3	1
1:A:43:ARG:CD	1:A:62:TRP:CE3	0.62	2.83	11	5
1:A:23:ALA:HB3	1:A:40:GLY:H	0.60	1.55	7	6
1:A:17:ASP:OD2	1:A:18:PHE:CE2	0.59	2.55	16	4
1:A:23:ALA:HB2	1:A:43:ARG:HD3	0.59	1.73	19	1
1:A:63:TYR:CD1	1:A:63:TYR:N	0.58	2.72	12	5
1:A:83:ALA:O	1:A:89:PHE:CD2	0.57	2.58	2	4
1:A:14:THR:HG23	1:A:85:GLN:O	0.57	1.98	8	4
1:A:43:ARG:NH2	1:A:62:TRP:CH2	0.57	2.73	12	1
1:A:44:LEU:HD21	1:A:86:LEU:HD13	0.55	1.75	19	1
1:A:14:THR:HG21	1:A:87:LYS:HG2	0.55	1.78	7	1
1:A:69:VAL:HG22	1:A:104:LEU:HG	0.54	1.79	2	1
1:A:42:VAL:HG22	1:A:92:LEU:HD22	0.54	1.77	9	1
1:A:46:LYS:HD3	1:A:75:LEU:HD22	0.54	1.79	20	1
1:A:69:VAL:HG21	1:A:103:GLN:HB3	0.53	1.78	19	1
1:A:42:VAL:HG21	1:A:96:ASP:OD2	0.53	2.02	2	1
1:A:80:GLU:CG	1:A:81:TYR:CD1	0.53	2.92	5	1
1:A:77:PHE:CZ	1:A:81:TYR:HB2	0.53	2.38	15	5
1:A:44:LEU:CD2	1:A:86:LEU:HD13	0.53	2.33	19	1
1:A:17:ASP:OD2	1:A:18:PHE:CD2	0.53	2.61	1	2
1:A:30:CYS:HB2	1:A:64:HIS:CE1	0.53	2.40	18	14
1:A:43:ARG:CZ	1:A:62:TRP:CZ2	0.52	2.92	19	1
1:A:17:ASP:OD1	1:A:18:PHE:CD2	0.52	2.63	1	1
1:A:77:PHE:CE2	1:A:81:TYR:HB3	0.51	2.40	7	1
1:A:59:ILE:HD12	1:A:61:ARG:HD3	0.51	1.83	6	2
1:A:61:ARG:HB3	1:A:63:TYR:CE1	0.51	2.40	9	2
1:A:74:GLU:OE1	1:A:74:GLU:N	0.51	2.44	13	1
1:A:62:TRP:O	1:A:63:TYR:CD1	0.51	2.64	19	2
1:A:49:VAL:HG12	1:A:57:GLY:C	0.51	2.26	4	1
1:A:83:ALA:HA	1:A:86:LEU:HD12	0.50	1.83	14	5
1:A:43:ARG:HD2	1:A:62:TRP:CE3	0.50	2.41	11	11
1:A:77:PHE:CZ	1:A:81:TYR:HB3	0.50	2.42	18	3
1:A:93:ALA:O	1:A:95:GLU:N	0.50	2.45	6	1
1:A:83:ALA:O	1:A:89:PHE:CG	0.50	2.65	19	2
1:A:29:THR:CG2	1:A:35:GLU:O	0.50	2.60	17	6
1:A:37:ILE:HG23	1:A:41:GLN:OE1	0.50	2.06	12	1
1:A:83:ALA:HB1	1:A:89:PHE:CE1	0.50	2.42	20	1
1:A:96:ASP:O	1:A:99:ALA:HB3	0.49	2.07	13	4
1:A:92:LEU:HD13	1:A:96:ASP:OD2	0.49	2.07	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:LEU:O	1:A:103:GLN:N	0.49	2.45	14	5
1:A:28:SER:HB3	1:A:37:ILE:HD12	0.49	1.85	11	1
1:A:59:ILE:HD12	1:A:61:ARG:CD	0.49	2.37	8	2
1:A:88:GLY:O	1:A:91:LEU:N	0.49	2.46	11	9
1:A:93:ALA:O	1:A:96:ASP:N	0.49	2.46	6	4
1:A:89:PHE:CD1	1:A:89:PHE:C	0.49	2.85	4	1
1:A:14:THR:HG21	1:A:87:LYS:CG	0.49	2.38	7	1
1:A:17:ASP:N	1:A:17:ASP:OD1	0.48	2.45	4	2
1:A:23:ALA:CB	1:A:38:GLU:O	0.48	2.61	10	1
1:A:77:PHE:CZ	1:A:81:TYR:O	0.48	2.66	13	1
1:A:69:VAL:HG22	1:A:104:LEU:CG	0.47	2.39	2	1
1:A:43:ARG:NH2	1:A:62:TRP:CZ2	0.47	2.81	19	2
1:A:84:SER:HA	1:A:89:PHE:CD2	0.47	2.44	14	9
1:A:93:ALA:O	1:A:94:THR:C	0.47	2.53	2	10
1:A:96:ASP:OD1	1:A:97:LYS:N	0.47	2.47	3	1
1:A:44:LEU:HD13	1:A:68:PHE:CD2	0.47	2.45	17	1
1:A:49:VAL:HG22	1:A:57:GLY:C	0.47	2.30	1	2
1:A:18:PHE:CE2	1:A:46:LYS:HG3	0.47	2.44	4	2
1:A:31:LYS:HB2	1:A:63:TYR:CE2	0.47	2.45	19	2
1:A:78:ARG:HB2	1:A:81:TYR:CD2	0.46	2.45	14	1
1:A:78:ARG:HB2	1:A:81:TYR:CE2	0.46	2.46	15	4
1:A:80:GLU:HG3	1:A:81:TYR:CD1	0.46	2.46	6	3
1:A:69:VAL:HG22	1:A:104:LEU:HD21	0.46	1.88	3	1
1:A:98:GLU:N	1:A:98:GLU:CD	0.46	2.68	16	1
1:A:43:ARG:CZ	1:A:62:TRP:CH2	0.46	2.98	19	3
1:A:80:GLU:HG3	1:A:81:TYR:CE1	0.46	2.46	1	3
1:A:84:SER:HA	1:A:89:PHE:CD1	0.46	2.46	18	1
1:A:78:ARG:HB2	1:A:81:TYR:CD1	0.46	2.45	18	1
1:A:38:GLU:CG	1:A:41:GLN:HG3	0.46	2.41	3	1
1:A:45:SER:HB3	1:A:62:TRP:CZ3	0.46	2.46	7	6
1:A:18:PHE:CE1	1:A:46:LYS:HG3	0.46	2.46	10	3
1:A:100:LEU:O	1:A:101:LYS:C	0.45	2.55	20	5
1:A:74:GLU:CG	1:A:75:LEU:N	0.45	2.79	3	1
1:A:23:ALA:O	1:A:24:LYS:C	0.45	2.55	9	1
1:A:49:VAL:HG22	1:A:57:GLY:O	0.45	2.10	20	1
1:A:27:ARG:O	1:A:28:SER:C	0.45	2.54	12	4
1:A:45:SER:HB3	1:A:62:TRP:CE3	0.45	2.46	8	5
1:A:50:ASP:OD2	1:A:61:ARG:NH2	0.45	2.50	14	1
1:A:16:GLY:O	1:A:17:ASP:C	0.45	2.55	7	2
1:A:79:PRO:O	1:A:106:GLY:C	0.45	2.55	14	2
1:A:43:ARG:HD2	1:A:62:TRP:CZ3	0.45	2.46	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:HD22	1:A:68:PHE:CD2	0.45	2.47	15	4
1:A:80:GLU:HG2	1:A:81:TYR:CE1	0.45	2.47	5	1
1:A:36:LYS:NZ	1:A:38:GLU:OE2	0.45	2.50	16	1
1:A:88:GLY:O	1:A:89:PHE:C	0.45	2.56	11	7
1:A:30:CYS:N	1:A:35:GLU:O	0.45	2.49	10	3
1:A:78:ARG:HB2	1:A:81:TYR:CE1	0.45	2.47	18	1
1:A:17:ASP:OD1	1:A:18:PHE:N	0.45	2.50	20	1
1:A:17:ASP:OD2	1:A:18:PHE:CZ	0.44	2.69	1	1
1:A:83:ALA:HB1	1:A:89:PHE:CE2	0.44	2.46	19	1
1:A:15:LEU:CD1	1:A:81:TYR:CE2	0.44	2.99	4	1
1:A:96:ASP:O	1:A:97:LYS:C	0.44	2.56	2	5
1:A:89:PHE:CE2	1:A:97:LYS:HD3	0.44	2.47	11	1
1:A:89:PHE:CE1	1:A:97:LYS:HE2	0.44	2.48	2	1
1:A:94:THR:O	1:A:95:GLU:C	0.43	2.57	8	2
1:A:33:CYS:SG	1:A:35:GLU:CD	0.43	2.96	15	1
1:A:96:ASP:O	1:A:99:ALA:N	0.43	2.52	2	1
1:A:48:MET:SD	1:A:48:MET:C	0.43	2.96	7	1
1:A:33:CYS:O	1:A:34:MET:C	0.43	2.57	17	3
1:A:72:ARG:CG	1:A:73:GLU:N	0.43	2.82	3	2
1:A:88:GLY:HA2	1:A:91:LEU:HD12	0.43	1.90	16	1
1:A:77:PHE:CZ	1:A:81:TYR:CB	0.43	3.02	15	1
1:A:80:GLU:HG2	1:A:81:TYR:CD1	0.43	2.48	5	1
1:A:73:GLU:O	1:A:76:GLY:N	0.43	2.52	4	2
1:A:30:CYS:CB	1:A:64:HIS:CE1	0.42	3.02	2	7
1:A:17:ASP:CG	1:A:18:PHE:CD2	0.42	2.93	1	1
1:A:89:PHE:CE1	1:A:97:LYS:HG2	0.42	2.49	3	1
1:A:43:ARG:NE	1:A:62:TRP:CH2	0.42	2.87	17	1
1:A:18:PHE:CE2	1:A:46:LYS:HG2	0.42	2.49	18	1
1:A:62:TRP:O	1:A:63:TYR:CG	0.42	2.72	13	2
1:A:87:LYS:O	1:A:88:GLY:C	0.42	2.57	9	1
1:A:68:PHE:CE1	1:A:75:LEU:HD13	0.42	2.49	11	1
1:A:38:GLU:CG	1:A:41:GLN:CG	0.41	2.98	3	1
1:A:14:THR:HG21	1:A:87:LYS:CA	0.41	2.42	18	1
1:A:23:ALA:HB3	1:A:39:LYS:HA	0.41	1.89	3	1
1:A:59:ILE:HD12	1:A:61:ARG:NE	0.41	2.30	8	1
1:A:73:GLU:HG3	1:A:74:GLU:N	0.41	2.31	14	1
1:A:98:GLU:O	1:A:101:LYS:N	0.41	2.53	16	1
1:A:58:MET:CE	1:A:58:MET:HA	0.41	2.45	9	4
1:A:43:ARG:NH1	1:A:62:TRP:CE2	0.41	2.89	19	1
1:A:38:GLU:HG3	1:A:41:GLN:CG	0.41	2.46	3	1
1:A:58:MET:HA	1:A:58:MET:CE	0.41	2.46	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LYS:HG2	1:A:75:LEU:HD22	0.41	1.92	11	1
1:A:69:VAL:HG21	1:A:103:GLN:OE1	0.41	2.16	12	1
1:A:26:ASN:CG	1:A:26:ASN:O	0.41	2.59	16	1
1:A:72:ARG:HG3	1:A:73:GLU:N	0.41	2.31	3	1
1:A:18:PHE:HB3	1:A:86:LEU:CD2	0.41	2.46	16	1
1:A:44:LEU:HD23	1:A:86:LEU:HD13	0.41	1.92	1	1
1:A:93:ALA:C	1:A:95:GLU:N	0.40	2.75	6	1
1:A:93:ALA:O	1:A:96:ASP:OD1	0.40	2.39	12	1
1:A:99:ALA:O	1:A:103:GLN:OE1	0.40	2.40	2	1
1:A:77:PHE:CE2	1:A:81:TYR:HB2	0.40	2.52	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	94/134 (70%)	84±2 (89±2%)	10±2 (10±2%)	1±1 (1±1%)	20	68
All	All	1880/2680 (70%)	1670 (89%)	191 (10%)	19 (1%)	20	68

All 8 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	92	LEU	8
1	A	28	SER	4
1	A	23	ALA	2
1	A	94	THR	1
1	A	38	GLU	1
1	A	15	LEU	1
1	A	36	LYS	1
1	A	86	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	80/109 (73%)	76±1 (95±2%)	4±1 (5±2%)	31	79
All	All	1600/2180 (73%)	1527 (95%)	73 (5%)	31	79

All 21 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	36	LYS	19
1	A	58	MET	14
1	A	13	LYS	5
1	A	17	ASP	4
1	A	61	ARG	4
1	A	96	ASP	4
1	A	31	LYS	4
1	A	60	ASP	3
1	A	48	MET	2
1	A	26	ASN	2
1	A	21	GLU	2
1	A	85	GLN	1
1	A	46	LYS	1
1	A	47	LYS	1
1	A	55	GLN	1
1	A	63	TYR	1
1	A	78	ARG	1
1	A	74	GLU	1
1	A	98	GLU	1
1	A	80	GLU	1
1	A	102	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 1 ligands modelled in this entry, 1 is 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