



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 2EBW / pdb_00002ebw
Title : Solution structure of the BRCT domain from human DNA repair protein REV1
Authors : Nagashima, T.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-09

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

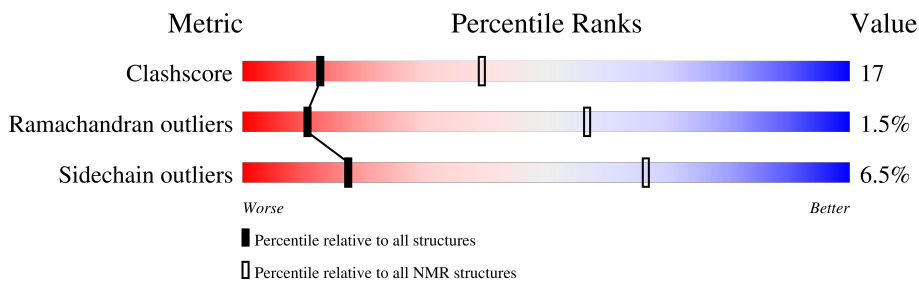
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	97	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:47-A:132 (86)	0.49	5

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 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1527 atoms, of which 768 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA repair protein REV1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	97	1527	486	768	128	143	2	0

There are 7 discrepancies between the modelled and reference sequences:

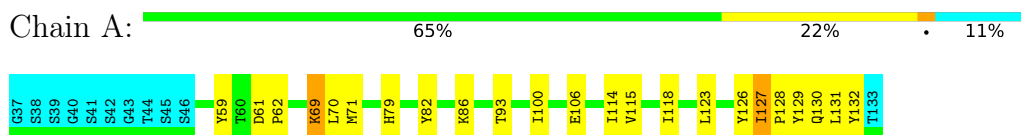
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	cloning artifact	UNP Q9UBZ9
A	38	SER	-	cloning artifact	UNP Q9UBZ9
A	39	SER	-	cloning artifact	UNP Q9UBZ9
A	40	GLY	-	cloning artifact	UNP Q9UBZ9
A	41	SER	-	cloning artifact	UNP Q9UBZ9
A	42	SER	-	cloning artifact	UNP Q9UBZ9
A	43	GLY	-	cloning artifact	UNP Q9UBZ9

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 repair protein REV1

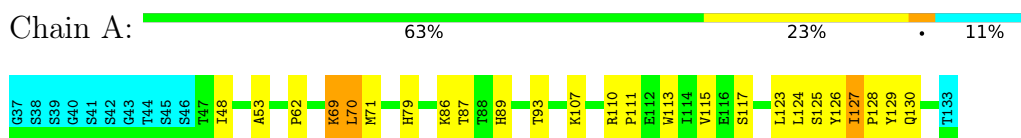


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

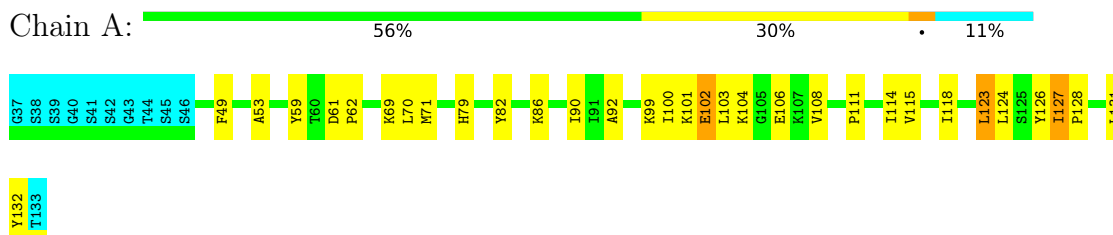
4.2.1 Score per residue for model 1

- Molecule 1: DNA repair protein REV1



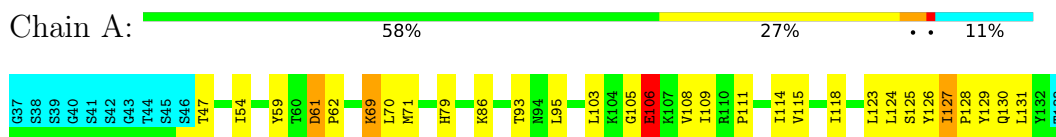
4.2.2 Score per residue for model 2

- Molecule 1: DNA repair protein REV1



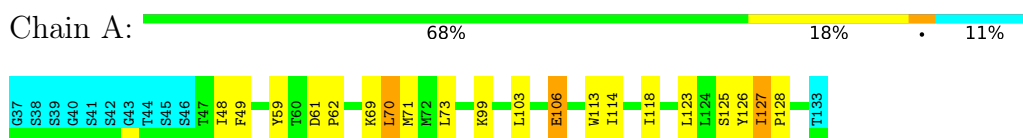
4.2.3 Score per residue for model 3

- Molecule 1: DNA repair protein REV1



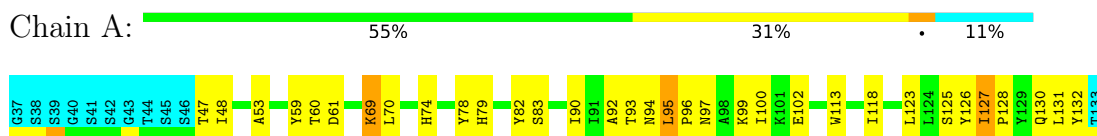
4.2.4 Score per residue for model 4

- Molecule 1: DNA repair protein REV1



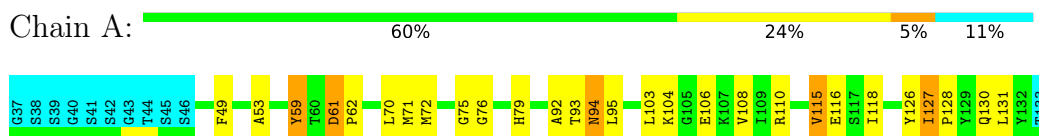
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: DNA repair protein REV1



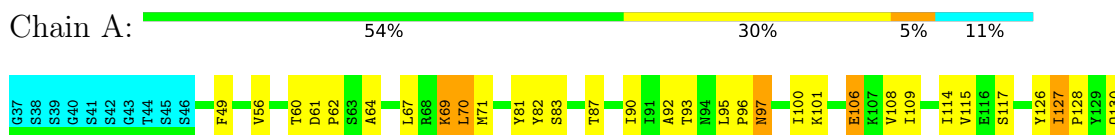
4.2.6 Score per residue for model 6

- Molecule 1: DNA repair protein REV1



4.2.7 Score per residue for model 7

- Molecule 1: DNA repair protein REV1



L131
Y132
T133

4.2.8 Score per residue for model 8

- Molecule 1: DNA repair protein REV1

Chain A:  56% 30% 11%

G37 S38 S39 G40 S41 S42 G43 T44 S45 S46 S50 G51 V52 D61 P62 L67 R68 K69 L70 H74 H79 Y80 Y81 Y82 K86 T90 T93 P96 N97 A98 K99 I100 V108 W113 I114 V115 I118 L123 L124 S125 Y126 I127 P128 Y129 Q130 T133

4.2.9 Score per residue for model 9

- Molecule 1: DNA repair protein REV1

Chain A:  63% 23% 11%

G37 S38 S39 G40 S41 S42 G43 T44 S45 S46 F49 Y55 Y59 D61 K69 L70 M71 Y82 I90 T93 N94 L95 K99 I100 E106 P111 I114 V115 L123 L124 S125 Y126 P128 Y129 Q130 L131 Y132 T133

4.2.10 Score per residue for model 10

- Molecule 1: DNA repair protein REV1

Chain A:  56% 28% 11%

G37 S38 S39 G40 S41 S42 G43 T44 S45 S46 A53 Y59 T60 P62 K69 L70 M71 G75 H79 Y82 K86 T87 I90 I91 A92 T93 N94 L95 P96 N97 A98 K99 I100 K101 K104 G105 E106 W113 S125 Y126 I127 P128 Y129 T133

4.2.11 Score per residue for model 11

- Molecule 1: DNA repair protein REV1

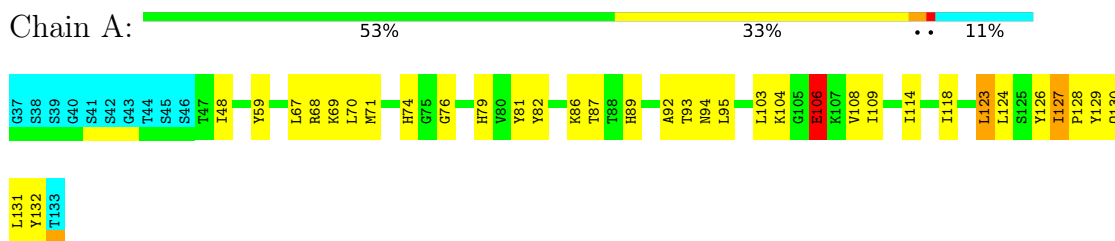
Chain A:  54% 32% 11%

G37 S38 S39 G40 S41 S42 G43 T44 S45 S46 F49 A53 I54 Y55 Y59 T60 D61 P62 L67 R68 K69 L70 M71 L73 H79 Y80 Y81 Y82 K86 T87 T88 H89 A92 T93 N94 I95 I96 P96 N97 A98 K99 I100 K104 G105 E106 I114 V115 E116 S117 Y126

I127 P128 Q130 L131 Y132 T133

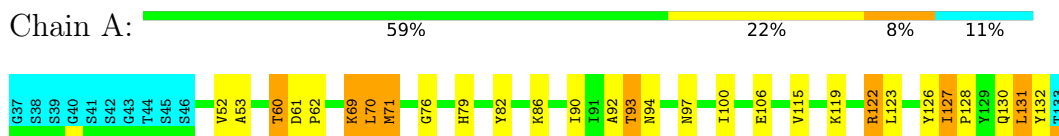
4.2.12 Score per residue for model 12

- Molecule 1: DNA repair protein REV1



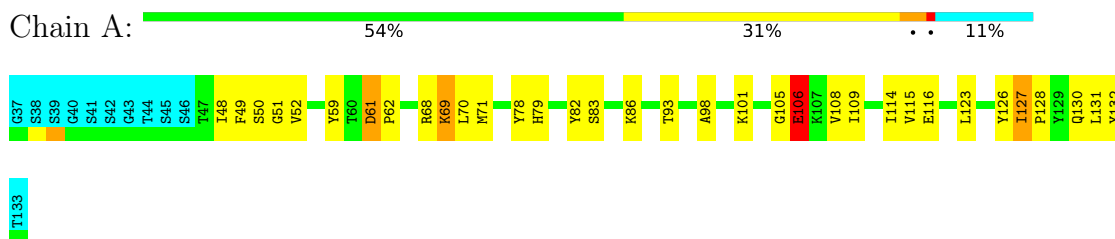
4.2.13 Score per residue for model 13

- Molecule 1: DNA repair protein REV1



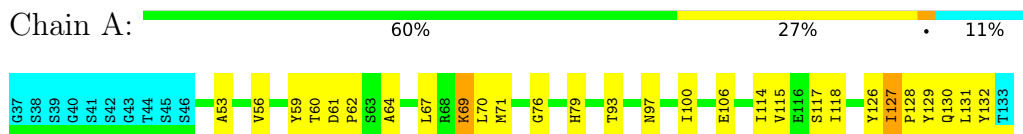
4.2.14 Score per residue for model 14

- Molecule 1: DNA repair protein REV1



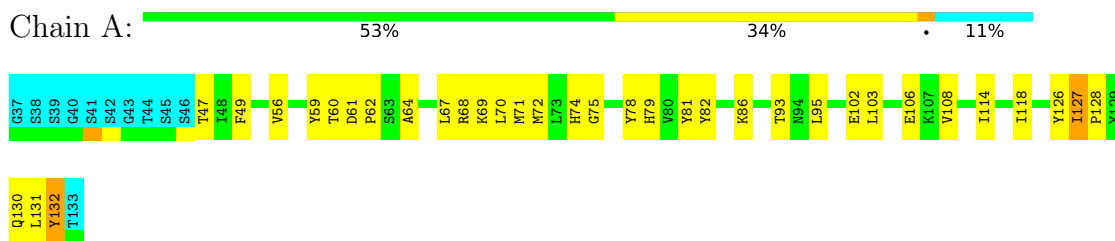
4.2.15 Score per residue for model 15

- Molecule 1: DNA repair protein REV1



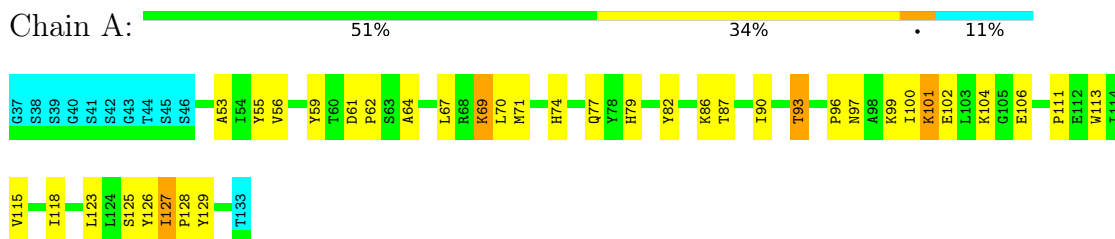
4.2.16 Score per residue for model 16

- Molecule 1: DNA repair protein REV1



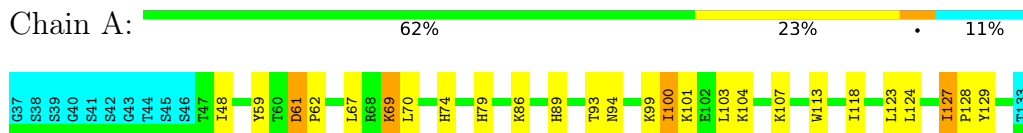
4.2.17 Score per residue for model 17

- Molecule 1: DNA repair protein REV1



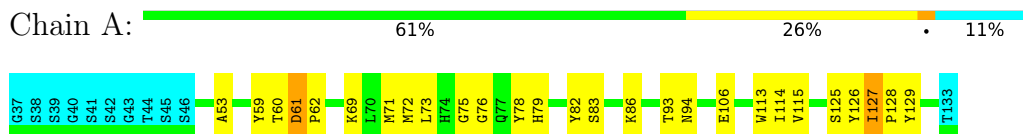
4.2.18 Score per residue for model 18

- Molecule 1: DNA repair protein REV1



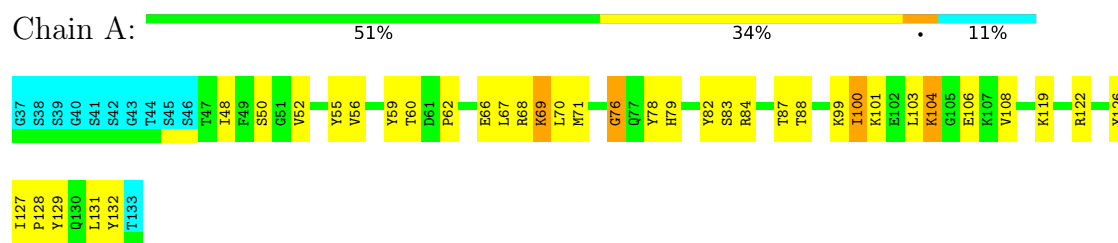
4.2.19 Score per residue for model 19

- Molecule 1: DNA repair protein REV1



4.2.20 Score per residue for model 20

- Molecule 1: DNA repair protein REV1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *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	2.0.17
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	697	715	715	23±4
All	All	13940	14300	14300	469

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:CZ	1:A:114:ILE:HG23	0.80	2.11	7	7
1:A:67:LEU:HA	1:A:70:LEU:HD12	0.76	1.56	12	8
1:A:70:LEU:HD22	1:A:118:ILE:HD13	0.75	1.56	16	7
1:A:60:THR:HG22	1:A:93:THR:HG23	0.70	1.63	19	1
1:A:82:TYR:CE1	1:A:90:ILE:HD11	0.69	2.23	10	6
1:A:111:PRO:O	1:A:115:VAL:HG23	0.69	1.87	9	4
1:A:53:ALA:HB1	1:A:79:HIS:CE1	0.67	2.24	2	10
1:A:48:ILE:O	1:A:123:LEU:HD12	0.66	1.90	18	2
1:A:95:LEU:O	1:A:100:ILE:HD11	0.65	1.91	10	3
1:A:114:ILE:HG22	1:A:118:ILE:HD11	0.63	1.69	4	3
1:A:53:ALA:CB	1:A:79:HIS:CE1	0.61	2.84	10	4
1:A:95:LEU:N	1:A:95:LEU:CD2	0.60	2.65	10	1
1:A:95:LEU:N	1:A:95:LEU:HD22	0.60	2.12	10	1
1:A:126:TYR:C	1:A:126:TYR:CD1	0.59	2.80	6	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:LEU:HD13	1:A:124:LEU:N	0.59	2.13	12	2
1:A:71:MET:HA	1:A:71:MET:HE2	0.58	1.72	1	7
1:A:92:ALA:HB1	1:A:95:LEU:HD11	0.58	1.75	5	1
1:A:113:TRP:CD1	1:A:125:SER:O	0.57	2.58	8	3
1:A:110:ARG:HG2	1:A:131:LEU:HD11	0.57	1.76	6	1
1:A:81:TYR:CD1	1:A:81:TYR:N	0.57	2.72	8	2
1:A:94:ASN:C	1:A:95:LEU:HD22	0.57	2.23	10	1
1:A:92:ALA:CB	1:A:95:LEU:HD11	0.56	2.30	5	1
1:A:108:VAL:O	1:A:109:ILE:HD13	0.56	2.00	7	3
1:A:56:VAL:HG11	1:A:64:ALA:HB2	0.56	1.77	16	1
1:A:62:PRO:HD3	1:A:115:VAL:HG21	0.56	1.78	17	6
1:A:70:LEU:HD13	1:A:118:ILE:CD1	0.56	2.30	3	1
1:A:90:ILE:O	1:A:108:VAL:HG13	0.56	2.01	8	1
1:A:59:TYR:CD1	1:A:59:TYR:C	0.55	2.84	20	12
1:A:108:VAL:C	1:A:109:ILE:HD13	0.55	2.27	7	2
1:A:56:VAL:HG21	1:A:67:LEU:HD12	0.55	1.79	20	1
1:A:95:LEU:HD22	1:A:95:LEU:N	0.55	2.17	5	1
1:A:56:VAL:HG21	1:A:64:ALA:HA	0.55	1.79	7	4
1:A:82:TYR:CG	1:A:82:TYR:O	0.54	2.60	20	1
1:A:59:TYR:C	1:A:59:TYR:CD1	0.54	2.84	6	4
1:A:115:VAL:HG12	1:A:119:LYS:HD2	0.54	1.79	13	1
1:A:62:PRO:CD	1:A:115:VAL:HG21	0.54	2.33	1	6
1:A:131:LEU:O	1:A:132:TYR:C	0.53	2.51	9	9
1:A:50:SER:O	1:A:52:VAL:HG23	0.53	2.04	8	3
1:A:69:LYS:O	1:A:73:LEU:HD12	0.52	2.04	11	2
1:A:125:SER:O	1:A:129:TYR:CD1	0.52	2.62	3	4
1:A:127:ILE:N	1:A:128:PRO:HD2	0.52	2.20	19	20
1:A:71:MET:HE2	1:A:71:MET:HA	0.52	1.80	13	2
1:A:74:HIS:NE2	1:A:118:ILE:HG23	0.51	2.21	18	4
1:A:79:HIS:CE1	1:A:86:LYS:HB3	0.51	2.41	1	12
1:A:101:LYS:O	1:A:104:LYS:N	0.50	2.45	17	5
1:A:78:TYR:CD1	1:A:79:HIS:N	0.50	2.79	19	3
1:A:96:PRO:O	1:A:97:ASN:C	0.50	2.55	10	6
1:A:99:LYS:O	1:A:100:ILE:C	0.50	2.54	18	7
1:A:54:ILE:HG21	1:A:114:ILE:HD11	0.50	1.83	3	1
1:A:67:LEU:O	1:A:68:ARG:C	0.50	2.55	8	2
1:A:87:THR:CG2	1:A:89:HIS:O	0.50	2.60	12	3
1:A:71:MET:O	1:A:76:GLY:N	0.50	2.45	12	5
1:A:123:LEU:CD1	1:A:124:LEU:O	0.50	2.60	2	2
1:A:48:ILE:O	1:A:123:LEU:HD13	0.50	2.06	14	3
1:A:126:TYR:O	1:A:127:ILE:C	0.50	2.53	15	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:ASN:HA	1:A:100:ILE:HD12	0.49	1.84	11	4
1:A:69:LYS:O	1:A:70:LEU:C	0.49	2.55	12	16
1:A:90:ILE:CD1	1:A:106:GLU:OE1	0.49	2.60	17	1
1:A:89:HIS:CD2	1:A:107:LYS:HE3	0.49	2.43	18	1
1:A:83:SER:O	1:A:84:ARG:C	0.49	2.55	20	1
1:A:60:THR:C	1:A:62:PRO:O	0.49	2.55	20	3
1:A:82:TYR:CZ	1:A:106:GLU:OE1	0.49	2.65	17	1
1:A:95:LEU:HD13	1:A:103:LEU:CD1	0.49	2.38	16	3
1:A:95:LEU:O	1:A:100:ILE:CD1	0.49	2.60	10	1
1:A:113:TRP:HB2	1:A:129:TYR:CD2	0.49	2.43	19	6
1:A:69:LYS:O	1:A:71:MET:N	0.49	2.45	4	4
1:A:108:VAL:O	1:A:131:LEU:N	0.49	2.46	3	4
1:A:55:TYR:HB3	1:A:87:THR:HG21	0.49	1.84	17	1
1:A:114:ILE:HG22	1:A:118:ILE:CD1	0.49	2.37	4	2
1:A:126:TYR:O	1:A:130:GLN:N	0.49	2.45	7	5
1:A:87:THR:HG22	1:A:89:HIS:O	0.49	2.08	11	1
1:A:48:ILE:O	1:A:123:LEU:CD1	0.49	2.61	18	1
1:A:101:LYS:O	1:A:103:LEU:N	0.48	2.46	2	1
1:A:61:ASP:C	1:A:61:ASP:OD1	0.48	2.56	9	1
1:A:72:MET:O	1:A:75:GLY:N	0.48	2.47	10	4
1:A:123:LEU:HD23	1:A:124:LEU:N	0.48	2.23	18	5
1:A:114:ILE:O	1:A:115:VAL:C	0.48	2.55	11	4
1:A:113:TRP:CZ2	1:A:123:LEU:HD11	0.48	2.43	17	1
1:A:126:TYR:O	1:A:129:TYR:N	0.47	2.46	19	5
1:A:48:ILE:O	1:A:123:LEU:HD23	0.47	2.09	12	1
1:A:81:TYR:O	1:A:82:TYR:C	0.47	2.57	8	4
1:A:71:MET:SD	1:A:71:MET:N	0.47	2.87	12	1
1:A:115:VAL:CG1	1:A:116:GLU:N	0.47	2.78	14	2
1:A:71:MET:O	1:A:75:GLY:N	0.47	2.47	16	1
1:A:109:ILE:HD12	1:A:126:TYR:HB2	0.47	1.86	14	1
1:A:127:ILE:HG22	1:A:128:PRO:N	0.47	2.25	1	18
1:A:70:LEU:HD13	1:A:118:ILE:HD13	0.47	1.85	3	1
1:A:99:LYS:O	1:A:102:GLU:N	0.47	2.48	5	1
1:A:49:PHE:CE1	1:A:123:LEU:CD1	0.47	2.98	14	1
1:A:101:LYS:O	1:A:102:GLU:C	0.47	2.57	17	2
1:A:87:THR:HG22	1:A:88:THR:N	0.47	2.25	20	1
1:A:90:ILE:HD11	1:A:106:GLU:OE1	0.46	2.09	17	1
1:A:68:ARG:HD2	1:A:78:TYR:CD2	0.46	2.45	20	1
1:A:92:ALA:O	1:A:131:LEU:HD11	0.46	2.10	13	1
1:A:89:HIS:CD2	1:A:107:LYS:NZ	0.46	2.84	1	1
1:A:92:ALA:O	1:A:131:LEU:CD1	0.46	2.64	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ASP:O	1:A:61:ASP:CG	0.46	2.58	13	3
1:A:98:ALA:O	1:A:101:LYS:CG	0.46	2.63	14	1
1:A:95:LEU:HD13	1:A:103:LEU:HD12	0.46	1.85	6	2
1:A:127:ILE:HD13	1:A:130:GLN:NE2	0.46	2.25	6	3
1:A:78:TYR:CD1	1:A:78:TYR:C	0.46	2.94	16	3
1:A:94:ASN:OD1	1:A:94:ASN:C	0.45	2.58	6	1
1:A:55:TYR:CE2	1:A:82:TYR:HB2	0.45	2.46	17	3
1:A:82:TYR:CZ	1:A:90:ILE:HD11	0.45	2.47	9	1
1:A:78:TYR:O	1:A:79:HIS:CD2	0.45	2.69	5	1
1:A:72:MET:C	1:A:74:HIS:N	0.45	2.73	16	1
1:A:101:LYS:C	1:A:103:LEU:N	0.45	2.75	18	3
1:A:105:GLY:O	1:A:106:GLU:C	0.44	2.60	10	3
1:A:62:PRO:CD	1:A:115:VAL:CG2	0.44	2.95	1	6
1:A:69:LYS:C	1:A:71:MET:N	0.44	2.74	4	4
1:A:82:TYR:CD1	1:A:83:SER:N	0.44	2.86	19	3
1:A:68:ARG:HA	1:A:78:TYR:CD2	0.44	2.48	16	1
1:A:93:THR:HG23	1:A:111:PRO:HG3	0.44	1.90	17	1
1:A:55:TYR:CD2	1:A:82:TYR:HB2	0.44	2.47	9	1
1:A:61:ASP:HA	1:A:62:PRO:C	0.43	2.38	3	13
1:A:83:SER:O	1:A:87:THR:N	0.43	2.52	7	1
1:A:55:TYR:CD2	1:A:55:TYR:O	0.43	2.71	9	1
1:A:114:ILE:O	1:A:117:SER:N	0.43	2.52	15	3
1:A:55:TYR:CB	1:A:87:THR:HG21	0.43	2.44	17	1
1:A:49:PHE:CG	1:A:71:MET:HE1	0.43	2.48	6	1
1:A:122:ARG:NH1	1:A:123:LEU:O	0.43	2.52	13	1
1:A:110:ARG:CD	1:A:129:TYR:O	0.43	2.67	1	1
1:A:50:SER:O	1:A:51:GLY:C	0.42	2.61	14	2
1:A:61:ASP:OD1	1:A:61:ASP:C	0.42	2.60	19	1
1:A:117:SER:N	1:A:124:LEU:CD1	0.42	2.83	1	1
1:A:55:TYR:CZ	1:A:82:TYR:HB2	0.42	2.49	11	1
1:A:69:LYS:HA	1:A:72:MET:HE3	0.42	1.90	11	1
1:A:70:LEU:O	1:A:71:MET:C	0.42	2.62	10	1
1:A:56:VAL:CG2	1:A:67:LEU:HD12	0.42	2.43	20	1
1:A:127:ILE:CB	1:A:128:PRO:CD	0.42	2.98	1	16
1:A:97:ASN:C	1:A:97:ASN:OD1	0.42	2.62	5	1
1:A:109:ILE:HD13	1:A:130:GLN:HA	0.42	1.91	3	1
1:A:54:ILE:HD13	1:A:114:ILE:CD1	0.42	2.44	3	1
1:A:52:VAL:O	1:A:52:VAL:HG12	0.42	2.15	13	1
1:A:69:LYS:C	1:A:73:LEU:HD12	0.42	2.39	19	1
1:A:100:ILE:HD11	1:A:132:TYR:CE1	0.42	2.49	2	1
1:A:71:MET:N	1:A:71:MET:SD	0.42	2.93	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:ILE:HG21	1:A:122:ARG:HA	0.42	1.91	20	1
1:A:101:LYS:N	1:A:101:LYS:HD2	0.41	2.29	17	1
1:A:127:ILE:N	1:A:128:PRO:CD	0.41	2.83	15	2
1:A:55:TYR:CE1	1:A:82:TYR:HB2	0.41	2.50	20	1
1:A:103:LEU:C	1:A:106:GLU:OE2	0.41	2.63	4	1
1:A:68:ARG:HD2	1:A:78:TYR:CG	0.41	2.51	20	1
1:A:113:TRP:HA	1:A:129:TYR:CE2	0.41	2.50	18	2
1:A:78:TYR:CE1	1:A:79:HIS:O	0.41	2.74	20	1
1:A:106:GLU:N	1:A:106:GLU:CD	0.40	2.79	12	2
1:A:60:THR:HG22	1:A:93:THR:H	0.40	1.76	15	1
1:A:102:GLU:CD	1:A:102:GLU:N	0.40	2.78	16	1
1:A:92:ALA:HB3	1:A:95:LEU:HD21	0.40	1.92	10	1
1:A:106:GLU:N	1:A:106:GLU:OE1	0.40	2.54	10	1
1:A:72:MET:O	1:A:74:HIS:N	0.40	2.54	16	1
1:A:106:GLU:H	1:A:106:GLU:CD	0.40	2.25	14	1
1:A:82:TYR:OH	1:A:106:GLU:CD	0.40	2.64	17	1
1:A:93:THR:OG1	1:A:94:ASN:N	0.40	2.53	13	1
1:A:105:GLY:O	1:A:106:GLU:O	0.40	2.40	14	1
1:A:106:GLU:CD	1:A:106:GLU:N	0.40	2.79	14	1
1:A:71:MET:O	1:A:74:HIS:N	0.40	2.54	17	1
1:A:56:VAL:CG1	1:A:60:THR:OG1	0.40	2.69	7	1
1:A:68:ARG:HG3	1:A:78:TYR:CG	0.40	2.52	14	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	86/97 (89%)	75±3 (87±4%)	10±3 (12±4%)	1±1 (1±1%)	11	57
All	All	1720/1940 (89%)	1491 (87%)	204 (12%)	25 (1%)	11	57

All 7 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	106	GLU	12
1	A	70	LEU	4
1	A	100	ILE	3
1	A	132	TYR	2
1	A	76	GLY	2
1	A	102	GLU	1
1	A	131	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	75/83 (90%)	70±2 (93±2%)	5±2 (7±2%)	17	66
All	All	1500/1660 (90%)	1402 (93%)	98 (7%)	17	66

All 27 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	127	ILE	19
1	A	69	LYS	15
1	A	93	THR	14
1	A	106	GLU	8
1	A	94	ASN	6
1	A	61	ASP	5
1	A	104	LYS	4
1	A	99	LYS	3
1	A	123	LEU	2
1	A	60	THR	2
1	A	95	LEU	2
1	A	59	TYR	2
1	A	101	LYS	2
1	A	47	THR	1
1	A	115	VAL	1
1	A	97	ASN	1
1	A	81	TYR	1
1	A	132	TYR	1
1	A	87	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	125	SER	1
1	A	71	MET	1
1	A	86	LYS	1
1	A	122	ARG	1
1	A	108	VAL	1
1	A	77	GLN	1
1	A	66	GLU	1
1	A	119	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided