



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 11:04 PM UTC

PDB ID : 2RQB / pdb_00002rqb
Title : Solution structure of MDA5 CTD
Authors : Takahasi, K.; Kumeta, H.; Tsuduki, N.; Narita, R.; Shigemoto, T.; Hirai, R.; Yoneyama, M.; Horiuchi, M.; Ogura, K.; Fujita, T.; Fuyuhiko, I.
Deposited on : 2009-03-17

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

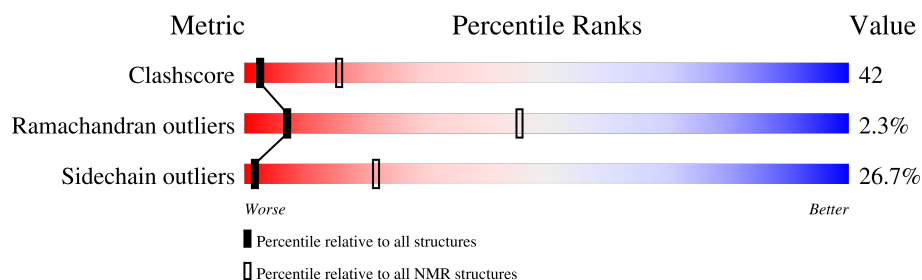
1 Overall quality at a glance

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	135	27% 33% 13% 27%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 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:898-A:922, A:929-A:948, A:955-A:992, A:997-A:1011 (98)	0.26	18

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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2159 atoms, of which 1078 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Interferon-induced helicase C domain-containing protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	135	Total	C	H	N	O	S	0
			2158	691	1078	180	196	13	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	891	GLY	-	expression tag	UNP Q9BYX4
A	892	PRO	-	expression tag	UNP Q9BYX4
A	893	LEU	-	expression tag	UNP Q9BYX4
A	894	GLY	-	expression tag	UNP Q9BYX4
A	895	SER	-	expression tag	UNP Q9BYX4

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

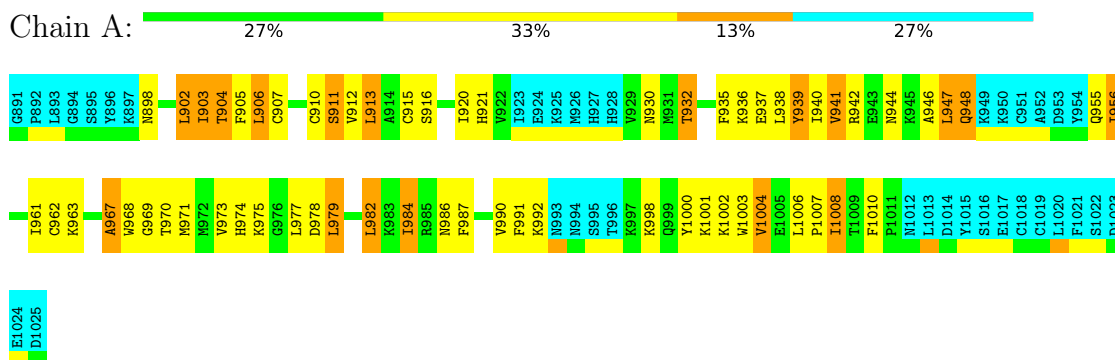
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

4 Residue-property plots

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: Interferon-induced helicase C domain-containing protein 1

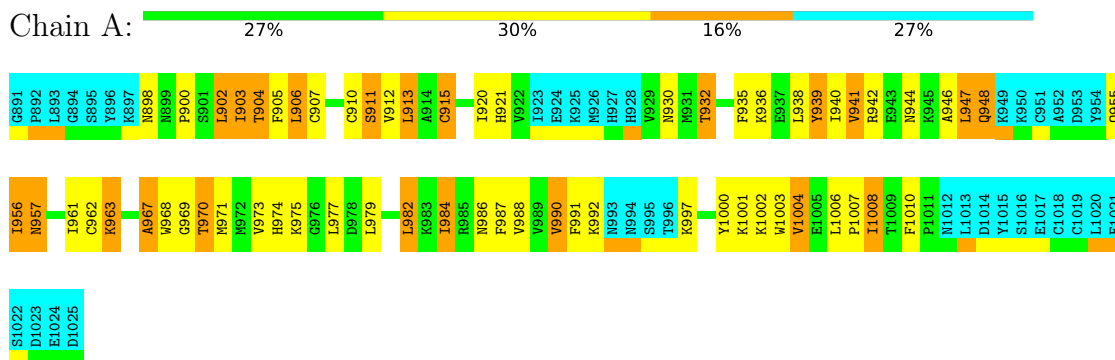


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

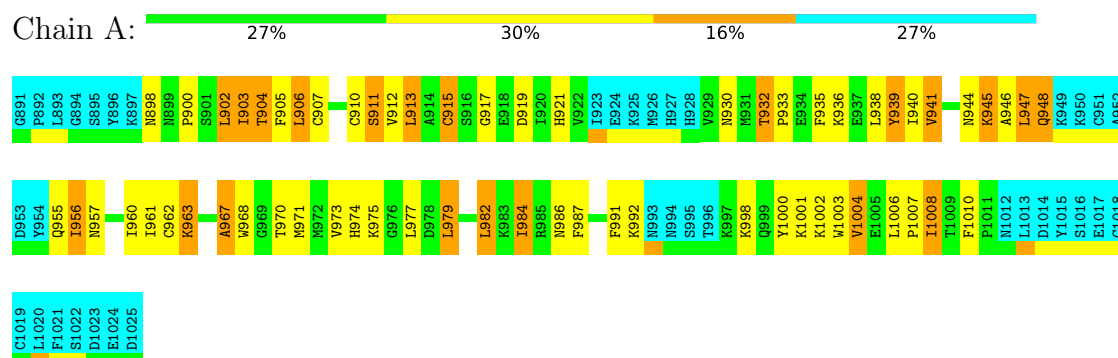
4.2.1 Score per residue for model 1

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



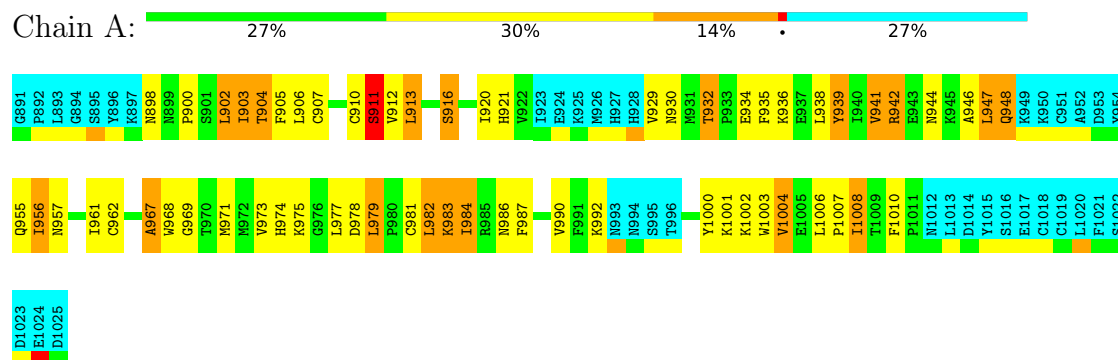
4.2.2 Score per residue for model 2

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



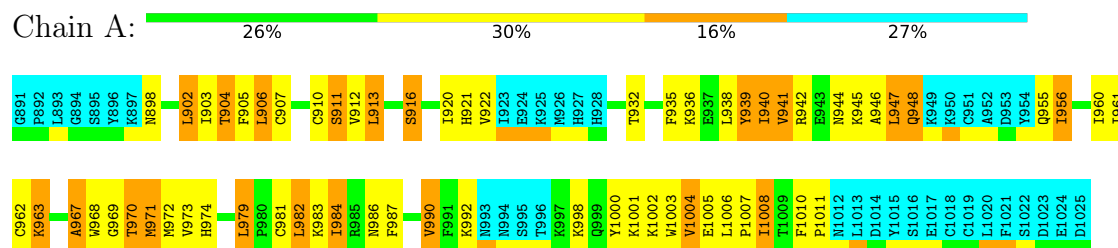
4.2.3 Score per residue for model 3

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



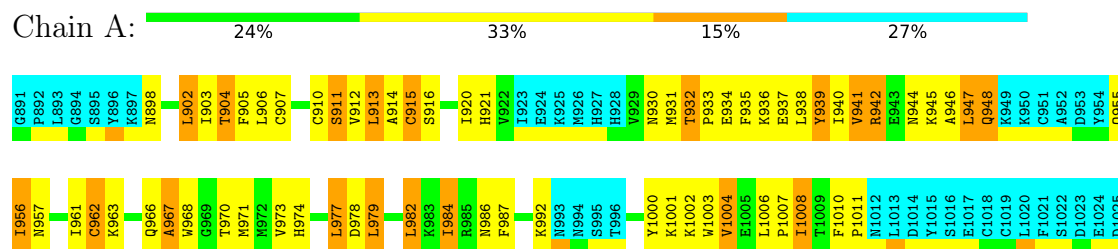
4.2.4 Score per residue for model 4

- Molecule 1: Interferon-induced helicase C domain-containing protein 1

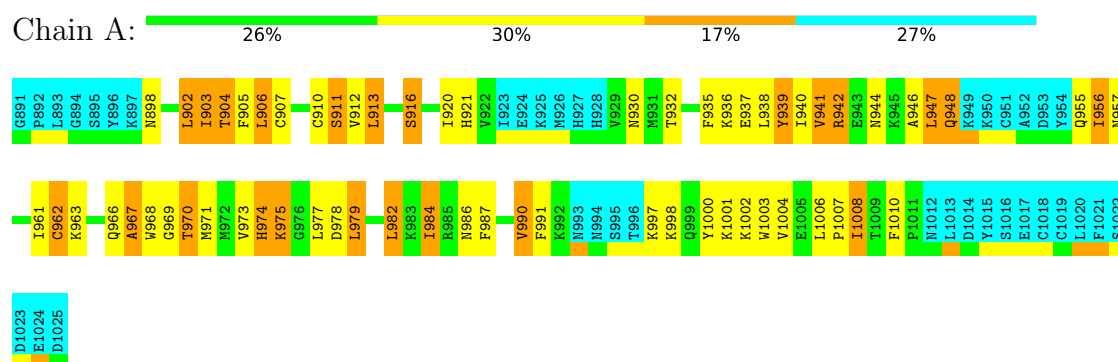


4.2.5 Score per residue for model 5

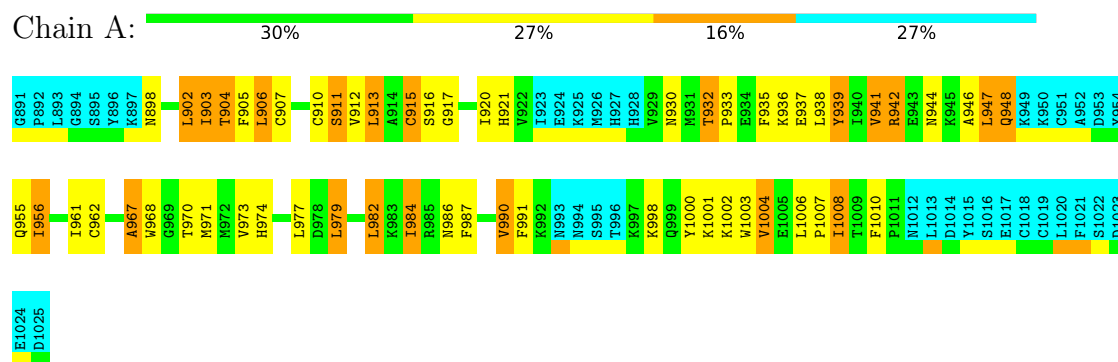
- Molecule 1: Interferon-induced helicase C domain-containing protein 1



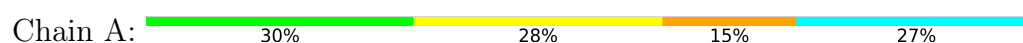
- Molecule 1: Interferon-induced helicase C domain-containing protein 1

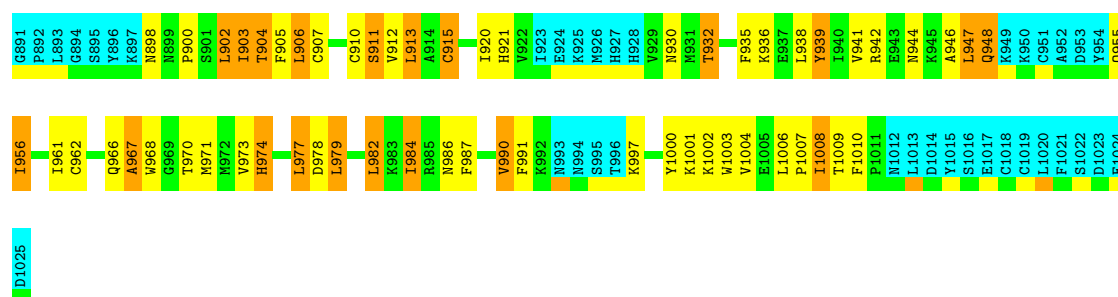


- Molecule 1: Interferon-induced helicase C domain-containing protein 1



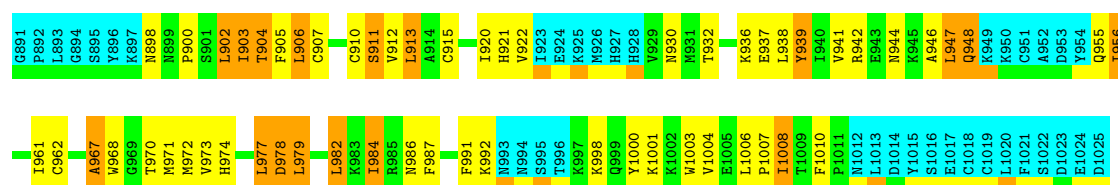
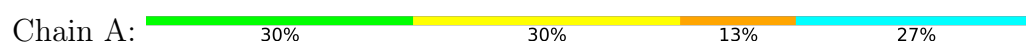
- Molecule 1: Interferon-induced helicase C domain-containing protein 1





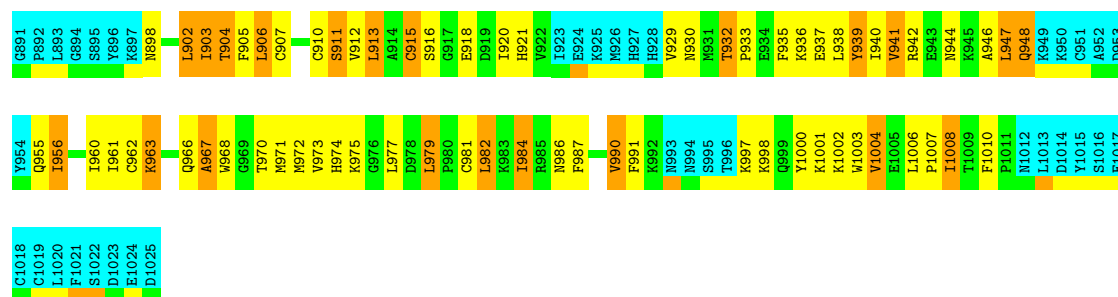
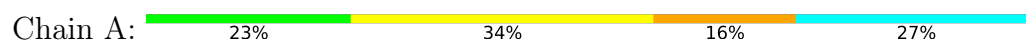
4.2.9 Score per residue for model 9

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



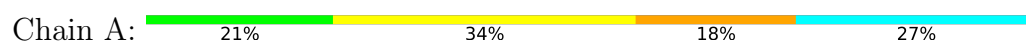
4.2.10 Score per residue for model 10

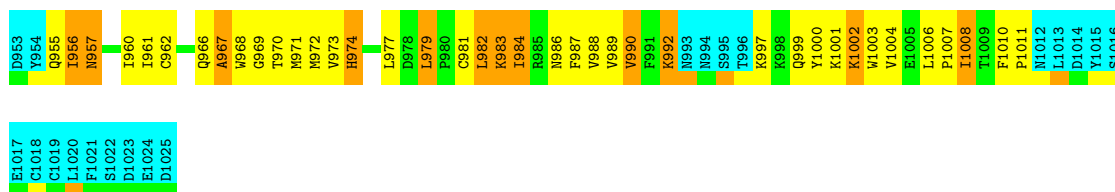
- Molecule 1: Interferon-induced helicase C domain-containing protein 1



4.2.11 Score per residue for model 11

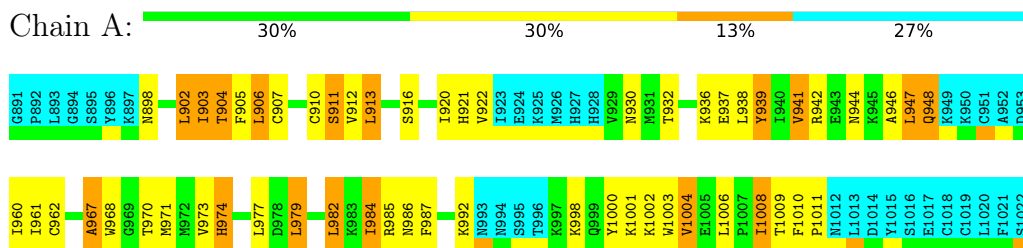
- Molecule 1: Interferon-induced helicase C domain-containing protein 1





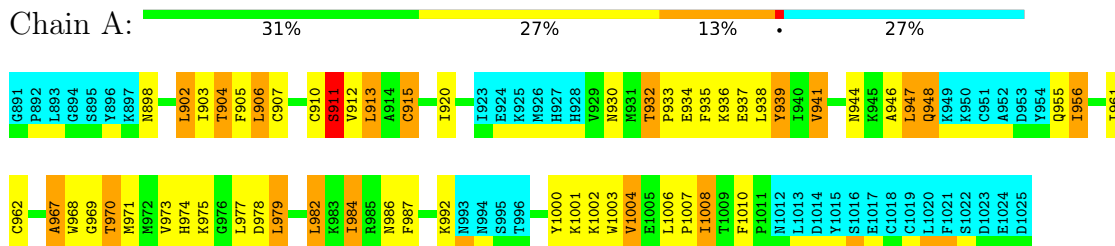
4.2.12 Score per residue for model 12

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



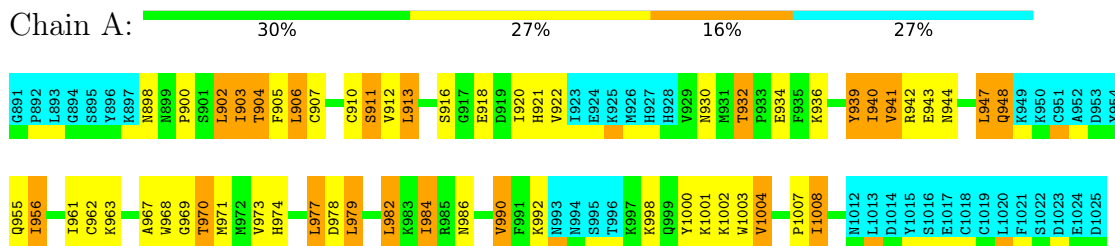
4.2.13 Score per residue for model 13

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



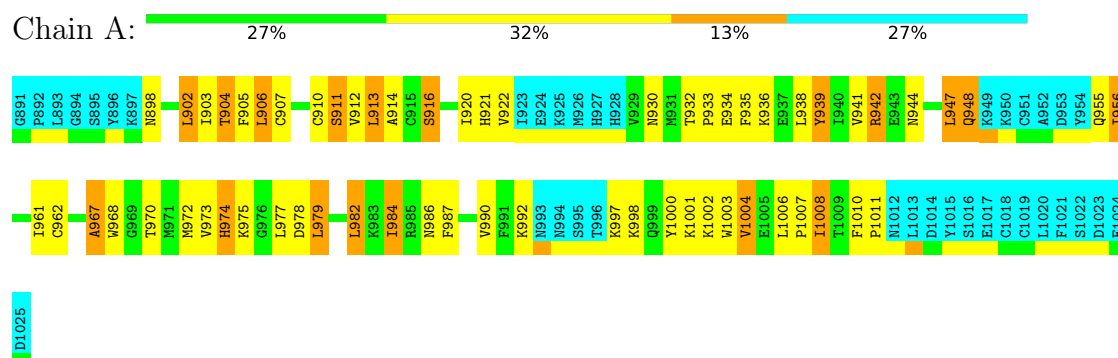
4.2.14 Score per residue for model 14

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



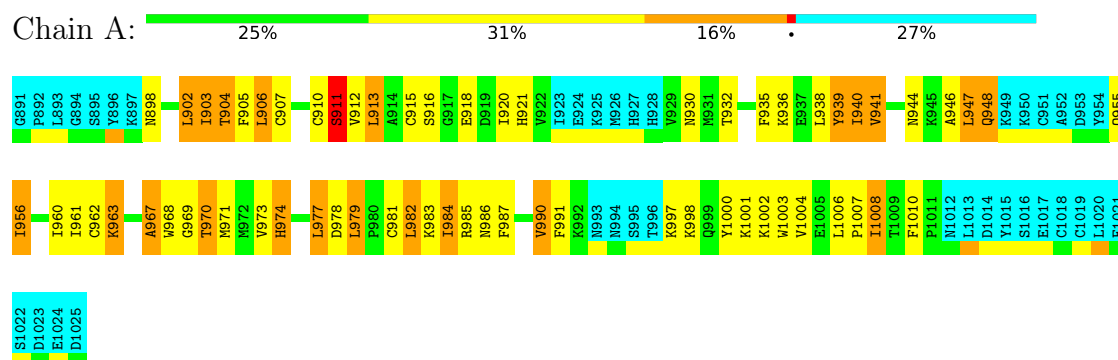
4.2.15 Score per residue for model 15

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



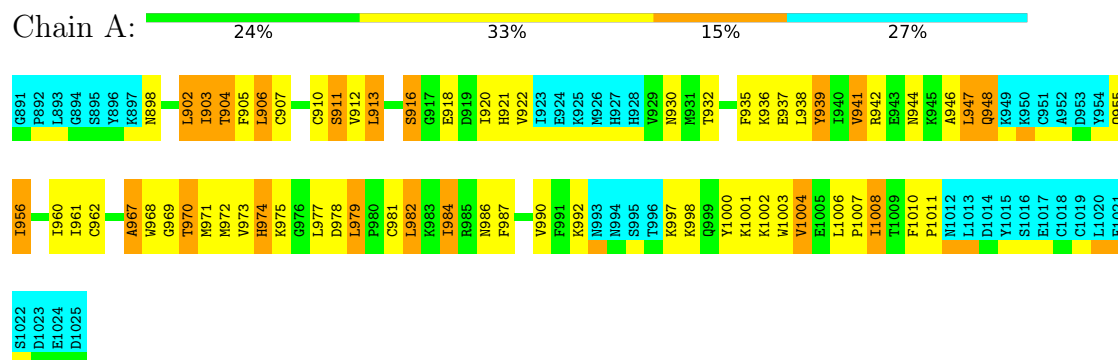
4.2.16 Score per residue for model 16

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



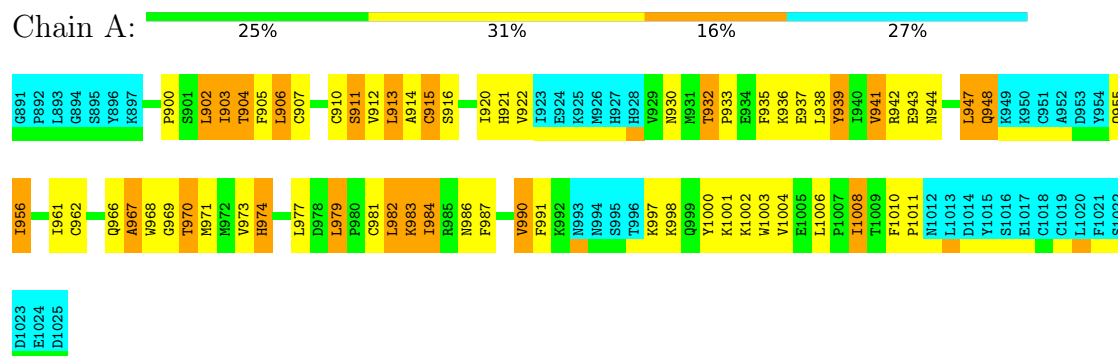
4.2.17 Score per residue for model 17

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



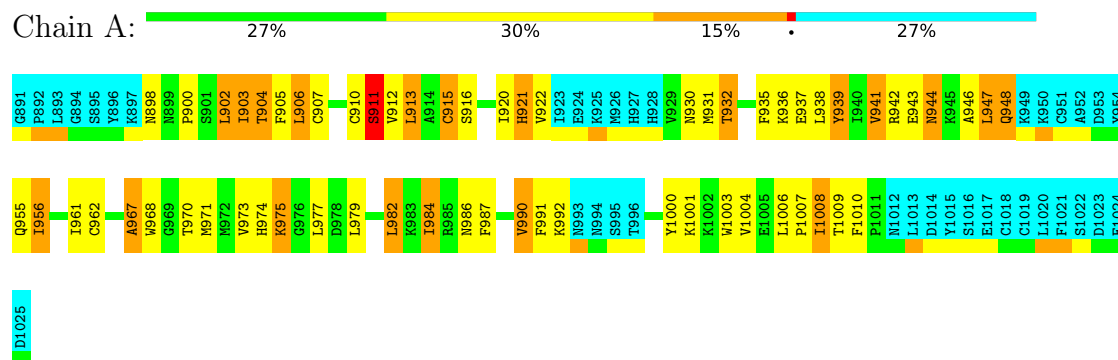
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



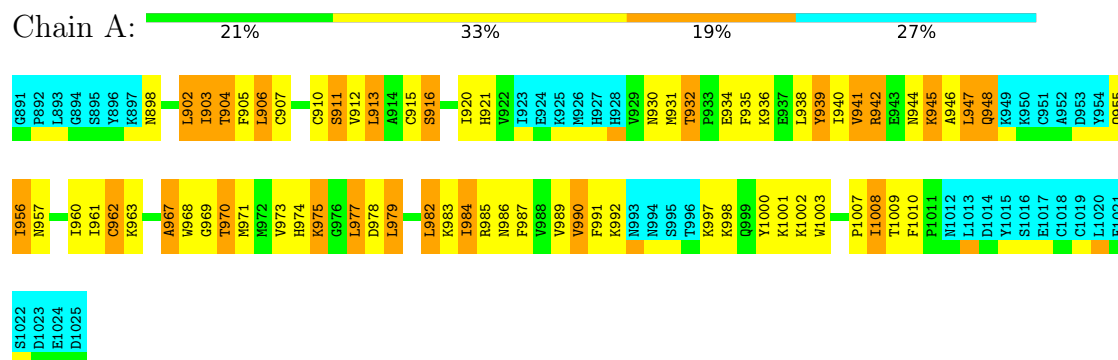
4.2.19 Score per residue for model 19

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Interferon-induced helicase C domain-containing protein 1



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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	785	808	813	67±6
All	All	15720	16160	16260	1349

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 42.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:978:ASP:C	1:A:979:LEU:HD23	0.92	1.88	13	1
1:A:915:CYS:SG	1:A:932:THR:HG21	0.89	2.08	5	9
1:A:935:PHE:CZ	1:A:982:LEU:HD21	0.81	2.09	18	16
1:A:973:VAL:HG13	1:A:977:LEU:O	0.81	1.75	2	17
1:A:1006:LEU:HD23	1:A:1010:PHE:CE1	0.80	2.12	2	18
1:A:974:HIS:HB3	1:A:979:LEU:HD11	0.80	1.53	17	10
1:A:974:HIS:CB	1:A:979:LEU:HD11	0.78	2.09	17	2
1:A:920:ILE:HD13	1:A:930:ASN:OD1	0.76	1.80	8	8
1:A:904:THR:HG22	1:A:913:LEU:HD21	0.75	1.57	12	20
1:A:968:TRP:CG	1:A:987:PHE:CZ	0.74	2.75	9	19
1:A:942:ARG:HD3	1:A:961:ILE:HD11	0.73	1.57	15	14
1:A:940:ILE:HD11	1:A:963:LYS:HZ2	0.72	1.42	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:979:LEU:HD23	1:A:979:LEU:N	0.72	1.97	13	1
1:A:904:THR:HG22	1:A:913:LEU:CD2	0.72	2.14	12	20
1:A:940:ILE:HD11	1:A:963:LYS:NZ	0.72	2.00	6	7
1:A:1006:LEU:HD23	1:A:1010:PHE:CZ	0.71	2.21	4	15
1:A:972:MET:HE2	1:A:981:CYS:SG	0.71	2.26	4	2
1:A:977:LEU:HD13	1:A:978:ASP:N	0.70	2.02	8	5
1:A:961:ILE:HG22	1:A:967:ALA:HA	0.70	1.64	14	20
1:A:939:TYR:C	1:A:939:TYR:CD1	0.69	2.70	10	20
1:A:977:LEU:HD13	1:A:978:ASP:H	0.67	1.49	5	5
1:A:990:VAL:CG2	1:A:997:LYS:HZ3	0.66	2.04	17	1
1:A:981:CYS:HB3	1:A:983:LYS:HZ1	0.66	1.50	11	1
1:A:940:ILE:CD1	1:A:963:LYS:HZ2	0.64	2.06	5	2
1:A:977:LEU:HD23	1:A:978:ASP:N	0.64	2.07	17	4
1:A:948:GLN:CD	1:A:948:GLN:C	0.63	2.67	15	9
1:A:982:LEU:N	1:A:982:LEU:HD12	0.62	2.10	3	17
1:A:942:ARG:CD	1:A:961:ILE:HD11	0.62	2.25	19	8
1:A:905:PHE:O	1:A:906:LEU:HD23	0.61	1.95	9	5
1:A:955:GLN:O	1:A:973:VAL:HG23	0.61	1.94	17	15
1:A:984:ILE:HD12	1:A:1003:TRP:HA	0.61	1.71	4	18
1:A:938:LEU:O	1:A:968:TRP:CH2	0.60	2.54	5	18
1:A:935:PHE:CE1	1:A:982:LEU:HD21	0.60	2.32	17	6
1:A:982:LEU:N	1:A:982:LEU:CD1	0.59	2.65	11	5
1:A:982:LEU:HD23	1:A:987:PHE:CZ	0.59	2.33	17	12
1:A:904:THR:HG23	1:A:916:SER:CB	0.59	2.27	17	14
1:A:910:CYS:O	1:A:911:SER:CB	0.59	2.51	5	20
1:A:1002:LYS:HB3	1:A:1004:VAL:HG12	0.58	1.75	8	15
1:A:903:ILE:HG22	1:A:991:PHE:CD1	0.58	2.34	20	11
1:A:977:LEU:HD23	1:A:978:ASP:H	0.58	1.58	16	4
1:A:903:ILE:CD1	1:A:1008:ILE:HG21	0.58	2.29	18	5
1:A:982:LEU:CD1	1:A:982:LEU:N	0.57	2.66	13	12
1:A:940:ILE:CD1	1:A:963:LYS:NZ	0.56	2.69	6	2
1:A:990:VAL:HG22	1:A:997:LYS:HB2	0.55	1.77	6	7
1:A:983:LYS:N	1:A:983:LYS:CD	0.55	2.70	3	1
1:A:969:GLY:C	1:A:983:LYS:HZ1	0.55	2.10	20	1
1:A:961:ILE:HG22	1:A:967:ALA:CA	0.55	2.31	9	19
1:A:906:LEU:HD11	1:A:990:VAL:CG2	0.55	2.32	20	11
1:A:938:LEU:O	1:A:968:TRP:CZ3	0.55	2.60	6	14
1:A:941:VAL:HG23	1:A:960:ILE:HG22	0.54	1.78	17	5
1:A:939:TYR:HE1	1:A:941:VAL:HG23	0.54	1.63	19	18
1:A:940:ILE:CG1	1:A:963:LYS:HZ2	0.53	2.16	5	2
1:A:969:GLY:O	1:A:970:THR:HG23	0.53	2.04	6	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:968:TRP:CG	1:A:987:PHE:CE1	0.53	2.97	18	16
1:A:979:LEU:N	1:A:979:LEU:CD2	0.53	2.68	13	1
1:A:904:THR:CG2	1:A:913:LEU:CD2	0.52	2.87	20	19
1:A:1008:ILE:N	1:A:1008:ILE:CD1	0.52	2.72	1	20
1:A:968:TRP:CD1	1:A:987:PHE:CE1	0.52	2.97	17	15
1:A:984:ILE:CG2	1:A:1000:TYR:C	0.52	2.83	20	11
1:A:1006:LEU:CD2	1:A:1010:PHE:CZ	0.52	2.92	13	4
1:A:968:TRP:CD1	1:A:987:PHE:CZ	0.52	2.97	18	16
1:A:984:ILE:HG13	1:A:1003:TRP:CE3	0.52	2.40	6	20
1:A:956:ILE:HG23	1:A:971:MET:O	0.52	2.05	16	19
1:A:962:CYS:HB2	1:A:968:TRP:CZ2	0.52	2.40	4	20
1:A:968:TRP:CD2	1:A:987:PHE:CZ	0.52	2.98	9	1
1:A:979:LEU:HD12	1:A:979:LEU:N	0.51	2.19	20	5
1:A:967:ALA:O	1:A:986:ASN:CB	0.51	2.59	12	4
1:A:963:LYS:HZ3	1:A:963:LYS:HA	0.51	1.65	4	5
1:A:939:TYR:CE1	1:A:941:VAL:HG23	0.51	2.40	14	19
1:A:904:THR:CG2	1:A:913:LEU:HD21	0.51	2.33	10	20
1:A:974:HIS:ND1	1:A:974:HIS:C	0.50	2.69	11	8
1:A:974:HIS:CE1	1:A:975:LYS:CG	0.50	2.95	6	1
1:A:955:GLN:O	1:A:973:VAL:CG2	0.50	2.59	17	2
1:A:974:HIS:CE1	1:A:975:LYS:HG3	0.50	2.41	15	8
1:A:906:LEU:HD23	1:A:913:LEU:HA	0.49	1.83	16	4
1:A:981:CYS:C	1:A:982:LEU:HD12	0.49	2.33	3	5
1:A:905:PHE:CE2	1:A:920:ILE:HG13	0.49	2.43	16	18
1:A:933:PRO:O	1:A:936:LYS:CE	0.49	2.60	7	8
1:A:936:LYS:HA	1:A:939:TYR:CE2	0.49	2.43	17	20
1:A:940:ILE:CG1	1:A:963:LYS:NZ	0.49	2.76	5	2
1:A:898:ASN:ND2	1:A:1007:PRO:O	0.49	2.46	20	18
1:A:967:ALA:O	1:A:986:ASN:ND2	0.48	2.46	20	20
1:A:967:ALA:O	1:A:986:ASN:CG	0.48	2.57	1	20
1:A:906:LEU:O	1:A:987:PHE:CD2	0.48	2.67	13	11
1:A:956:ILE:CG2	1:A:971:MET:O	0.48	2.61	6	16
1:A:905:PHE:N	1:A:905:PHE:CD1	0.48	2.80	17	19
1:A:962:CYS:HB3	1:A:968:TRP:CE2	0.48	2.44	15	20
1:A:962:CYS:CB	1:A:968:TRP:CE2	0.48	2.97	20	20
1:A:960:ILE:CD1	1:A:982:LEU:CD1	0.47	2.93	20	2
1:A:935:PHE:CZ	1:A:982:LEU:HD11	0.47	2.44	20	1
1:A:898:ASN:O	1:A:898:ASN:CG	0.47	2.57	7	5
1:A:942:ARG:NE	1:A:961:ILE:CD1	0.47	2.76	17	1
1:A:944:ASN:OD1	1:A:946:ALA:HB3	0.47	2.09	2	16
1:A:905:PHE:CZ	1:A:917:GLY:HA2	0.47	2.44	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:948:GLN:NE2	1:A:955:GLN:HE22	0.47	2.08	17	4
1:A:973:VAL:CG1	1:A:977:LEU:O	0.47	2.59	6	2
1:A:984:ILE:HG22	1:A:1001:LYS:C	0.47	2.35	17	19
1:A:984:ILE:HG22	1:A:1001:LYS:CA	0.47	2.40	2	20
1:A:955:GLN:O	1:A:973:VAL:N	0.47	2.47	17	19
1:A:989:VAL:HG21	1:A:1000:TYR:CD1	0.47	2.45	20	2
1:A:1002:LYS:CB	1:A:1004:VAL:HG12	0.47	2.40	12	2
1:A:977:LEU:HD22	1:A:979:LEU:HD21	0.47	1.87	17	1
1:A:935:PHE:HA	1:A:938:LEU:HD12	0.46	1.87	5	4
1:A:970:THR:HG23	1:A:983:LYS:NZ	0.46	2.25	20	1
1:A:920:ILE:CD1	1:A:930:ASN:OD1	0.46	2.63	20	4
1:A:939:TYR:OH	1:A:971:MET:HE1	0.46	2.10	4	1
1:A:905:PHE:CE2	1:A:1003:TRP:CZ3	0.46	3.04	18	2
1:A:932:THR:HG22	1:A:934:GLU:HG2	0.46	1.88	20	3
1:A:907:CYS:SG	1:A:962:CYS:SG	0.46	3.14	15	20
1:A:930:ASN:OD1	1:A:930:ASN:C	0.46	2.59	14	11
1:A:955:GLN:NE2	1:A:956:ILE:O	0.46	2.49	9	9
1:A:966:GLN:O	1:A:968:TRP:N	0.46	2.49	10	6
1:A:988:VAL:HG22	1:A:999:GLN:NE2	0.45	2.25	11	1
1:A:974:HIS:HB2	1:A:979:LEU:HD11	0.45	1.87	17	1
1:A:940:ILE:HD11	1:A:963:LYS:HE2	0.45	1.89	20	1
1:A:974:HIS:O	1:A:974:HIS:ND1	0.45	2.50	19	7
1:A:955:GLN:OE1	1:A:955:GLN:C	0.45	2.60	3	6
1:A:970:THR:HG23	1:A:983:LYS:HZ1	0.45	1.70	20	2
1:A:963:LYS:HZ2	1:A:963:LYS:HB3	0.45	1.72	2	3
1:A:944:ASN:ND2	1:A:947:LEU:N	0.45	2.65	19	17
1:A:929:VAL:HG12	1:A:981:CYS:SG	0.45	2.52	3	1
1:A:974:HIS:CG	1:A:974:HIS:O	0.45	2.70	16	1
1:A:930:ASN:ND2	1:A:935:PHE:CG	0.45	2.84	17	1
1:A:900:PRO:HA	1:A:903:ILE:CD1	0.45	2.42	1	9
1:A:1006:LEU:HD23	1:A:1010:PHE:HE1	0.45	1.67	15	1
1:A:948:GLN:NE2	1:A:955:GLN:NE2	0.45	2.64	6	3
1:A:906:LEU:HD11	1:A:990:VAL:HB	0.44	1.90	14	1
1:A:984:ILE:HG13	1:A:1003:TRP:CD2	0.44	2.47	12	20
1:A:918:GLU:OE1	1:A:918:GLU:C	0.44	2.60	14	1
1:A:948:GLN:CB	1:A:956:ILE:HB	0.44	2.43	10	13
1:A:948:GLN:NE2	1:A:955:GLN:OE1	0.44	2.50	17	3
1:A:1001:LYS:CG	1:A:1002:LYS:N	0.44	2.79	8	1
1:A:903:ILE:HD13	1:A:1008:ILE:HG12	0.44	1.90	17	1
1:A:974:HIS:O	1:A:974:HIS:CG	0.44	2.71	17	1
1:A:984:ILE:HG22	1:A:1001:LYS:N	0.44	2.28	2	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:941:VAL:CG2	1:A:960:ILE:HG22	0.44	2.41	4	3
1:A:903:ILE:HD11	1:A:1008:ILE:HG21	0.44	1.90	10	2
1:A:984:ILE:HG21	1:A:1000:TYR:CB	0.44	2.43	20	9
1:A:988:VAL:HG11	1:A:997:LYS:NZ	0.44	2.28	1	1
1:A:940:ILE:HD11	1:A:963:LYS:HZ3	0.44	1.71	16	4
1:A:944:ASN:ND2	1:A:944:ASN:C	0.43	2.76	19	4
1:A:944:ASN:ND2	1:A:947:LEU:CD2	0.43	2.82	10	11
1:A:944:ASN:HD21	1:A:947:LEU:N	0.43	2.11	8	14
1:A:982:LEU:HD13	1:A:982:LEU:N	0.43	2.29	14	1
1:A:918:GLU:CD	1:A:918:GLU:C	0.43	2.86	10	2
1:A:984:ILE:CG2	1:A:1000:TYR:HB2	0.43	2.44	15	17
1:A:977:LEU:HD22	1:A:979:LEU:CD2	0.43	2.43	17	1
1:A:990:VAL:CG2	1:A:997:LYS:NZ	0.43	2.78	17	1
1:A:969:GLY:CA	1:A:983:LYS:CE	0.42	2.97	3	1
1:A:992:LYS:CB	1:A:992:LYS:NZ	0.42	2.82	11	1
1:A:955:GLN:O	1:A:973:VAL:CB	0.42	2.68	17	1
1:A:1003:TRP:C	1:A:1005:GLU:N	0.42	2.76	4	1
1:A:940:ILE:HD11	1:A:963:LYS:HD2	0.42	1.90	14	1
1:A:955:GLN:CD	1:A:956:ILE:O	0.42	2.63	4	1
1:A:929:VAL:CG1	1:A:981:CYS:SG	0.42	3.07	10	1
1:A:977:LEU:HD23	1:A:979:LEU:HD21	0.42	1.91	10	1
1:A:915:CYS:SG	1:A:930:ASN:ND2	0.42	2.93	11	1
1:A:936:LYS:HA	1:A:939:TYR:CD2	0.42	2.50	17	1
1:A:905:PHE:C	1:A:906:LEU:HD23	0.42	2.39	9	1
1:A:922:VAL:HG21	1:A:1010:PHE:HB3	0.42	1.92	19	1
1:A:957:ASN:ND2	1:A:973:VAL:HG21	0.42	2.29	1	2
1:A:989:VAL:CG2	1:A:1000:TYR:CD1	0.42	3.03	20	1
1:A:974:HIS:NE2	1:A:975:LYS:NZ	0.42	2.60	1	1
1:A:902:LEU:O	1:A:992:LYS:N	0.42	2.53	15	3
1:A:910:CYS:O	1:A:911:SER:OG	0.41	2.38	4	2
1:A:981:CYS:HB3	1:A:983:LYS:HZ3	0.41	1.74	18	1
1:A:910:CYS:O	1:A:911:SER:HB2	0.41	2.15	2	3
1:A:969:GLY:HA2	1:A:983:LYS:CD	0.41	2.46	11	1
1:A:930:ASN:HB2	1:A:982:LEU:CD2	0.41	2.45	12	1
1:A:914:ALA:HA	1:A:938:LEU:HD13	0.41	1.92	15	1
1:A:918:GLU:C	1:A:918:GLU:OE1	0.41	2.64	16	1
1:A:1003:TRP:O	1:A:1006:LEU:N	0.41	2.53	4	1
1:A:945:LYS:NZ	1:A:945:LYS:CB	0.41	2.83	20	1
1:A:930:ASN:OD1	1:A:930:ASN:O	0.41	2.39	9	3
1:A:911:SER:O	1:A:911:SER:OG	0.41	2.33	7	3
1:A:930:ASN:OD1	1:A:932:THR:OG1	0.41	2.39	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:969:GLY:CA	1:A:983:LYS:HD3	0.41	2.46	3	1
1:A:969:GLY:CA	1:A:983:LYS:HE3	0.41	2.46	3	1
1:A:984:ILE:HG21	1:A:1000:TYR:HB2	0.41	1.93	17	5
1:A:914:ALA:O	1:A:915:CYS:SG	0.41	2.79	5	2
1:A:939:TYR:CD1	1:A:960:ILE:HG22	0.40	2.51	2	1
1:A:898:ASN:CG	1:A:898:ASN:O	0.40	2.64	19	1
1:A:975:LYS:CB	1:A:975:LYS:NZ	0.40	2.84	20	1
1:A:904:THR:HG23	1:A:916:SER:HB3	0.40	1.94	3	1
1:A:984:ILE:HG13	1:A:1003:TRP:CZ3	0.40	2.50	20	1
1:A:945:LYS:O	1:A:948:GLN:O	0.40	2.40	2	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	98/135 (73%)	83±2 (85±2%)	13±2 (13±2%)	2±0 (2±0%)	7	45
All	All	1960/2700 (73%)	1662 (85%)	253 (13%)	45 (2%)	7	45

All 4 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	911	SER	20
1	A	967	ALA	19
1	A	962	CYS	3
1	A	943	GLU	3

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	90/124 (73%)	66±2 (73±3%)	24±2 (27±3%)	2	22
All	All	1800/2480 (73%)	1319 (73%)	481 (27%)	2	22

All 47 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	902	LEU	20
1	A	903	ILE	20
1	A	904	THR	20
1	A	906	LEU	20
1	A	912	VAL	20
1	A	913	LEU	20
1	A	932	THR	20
1	A	939	TYR	20
1	A	947	LEU	20
1	A	948	GLN	20
1	A	956	ILE	20
1	A	979	LEU	20
1	A	982	LEU	20
1	A	984	ILE	20
1	A	1008	ILE	20
1	A	970	THR	19
1	A	941	VAL	18
1	A	1004	VAL	15
1	A	990	VAL	13
1	A	915	CYS	12
1	A	937	GLU	11
1	A	957	ASN	8
1	A	974	HIS	8
1	A	998	LYS	7
1	A	916	SER	7
1	A	942	ARG	7
1	A	977	LEU	6
1	A	963	LYS	5
1	A	945	LYS	4
1	A	911	SER	4
1	A	983	LYS	4
1	A	975	LYS	4
1	A	1009	THR	4
1	A	940	ILE	3
1	A	934	GLU	3
1	A	1002	LYS	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	985	ARG	3
1	A	978	ASP	2
1	A	920	ILE	2
1	A	918	GLU	2
1	A	919	ASP	1
1	A	971	MET	1
1	A	992	LYS	1
1	A	921	HIS	1
1	A	944	ASN	1
1	A	931	MET	1
1	A	997	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](#)

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

No chemical shift data were provided