



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 09:46 AM UTC

PDB ID : 1U5M / pdb_00001u5m
Title : Structure of a Chordin-like Cysteine-rich Repeat (VWC module) from Collagen IIA
Authors : O'Leary, J.M.; Hamilton, J.m.; Deane, C.M.; Valeyev, N.V.; Sandell, L.J.; Downing, A.K.
Deposited on : 2004-07-28

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

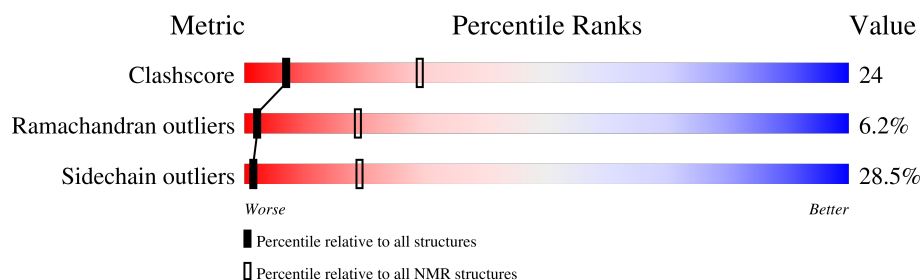
1 Overall quality at a glance

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	73	23% 41% . 33%

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1,2 as representative, based on the following criterion: *closest to the average*.

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:9-A:43 (35)	0.54	11
2	A:53-A:66 (14)	0.31	2

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1063 atoms, of which 513 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called alpha 1 type II collagen isoform 1.

Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1063	340	513	87	113	10	

There are 7 discrepancies between the modelled and reference sequences:

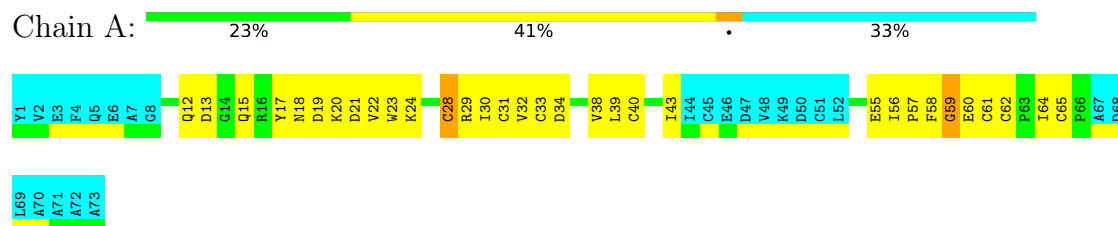
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	TYR	GLY	cloning artifact	UNP P02458
A	2	VAL	GLN	cloning artifact	UNP P02458
A	3	GLU	ASP	cloning artifact	UNP P02458
A	4	PHE	VAL	cloning artifact	UNP P02458
A	67	ALA	THR	engineered mutation	UNP P02458
A	71	ALA	THR	engineered mutation	UNP P02458
A	73	ALA	SER	engineered mutation	UNP P02458

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: alpha 1 type II collagen isoform 1

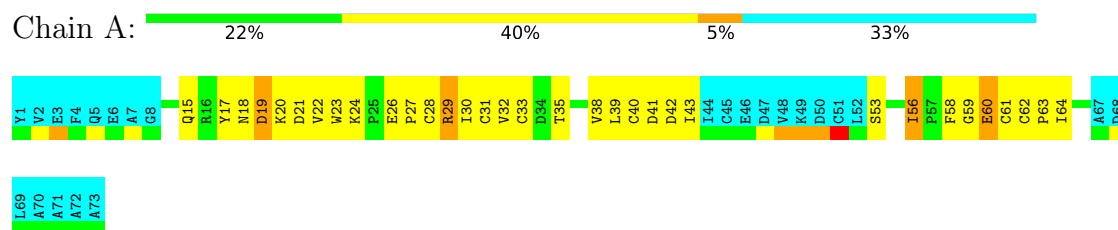


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

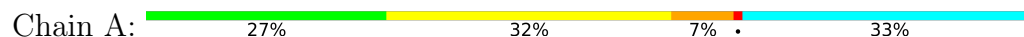
4.2.1 Score per residue for model 1

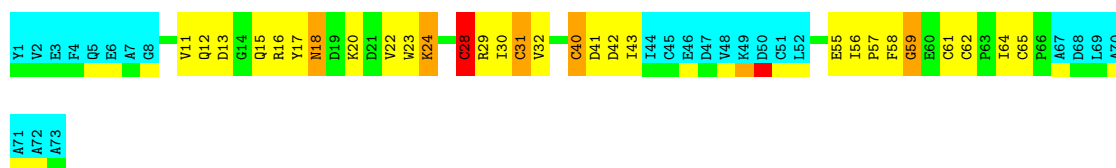
- Molecule 1: alpha 1 type II collagen isoform 1



4.2.2 Score per residue for model 2

- Molecule 1: alpha 1 type II collagen isoform 1

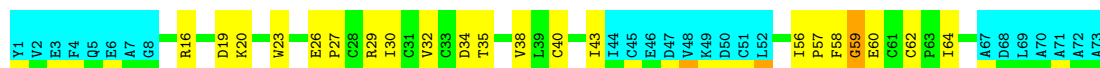




4.2.3 Score per residue for model 3

- Molecule 1: alpha 1 type II collagen isoform 1

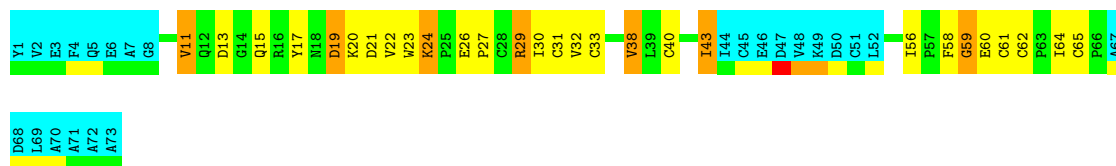
Chain A: 38% 27% 33%



4.2.4 Score per residue for model 4

- Molecule 1: alpha 1 type II collagen isoform 1

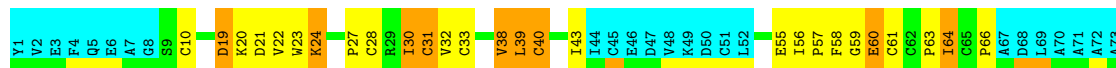
Chain A: 29% 29% 10% 33%



4.2.5 Score per residue for model 5

- Molecule 1: alpha 1 type II collagen isoform 1

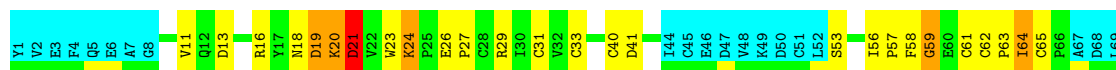
Chain A: 30% 25% 12% 33%



4.2.6 Score per residue for model 6

- Molecule 1: alpha 1 type II collagen isoform 1

Chain A: 32% 27% 7% 33%



A70
A71
A72
A73

4.2.7 Score per residue for model 7

- Molecule 1: alpha 1 type II collagen isoform 1

Chain A: 21% 32% 14% • 33%

Y1 Y2 E3 E4 Q5 E6 E7 A7 A8 S9 C10 V11 V12 D13 R16 Y17 N18 D19 K20 K21 D22 V23 W24 K25 P26 E27 P28 C29 R30 T31 C32 V33 C34 D35 T36 G37 V38 L39 C40 I43 I44 Q45 E46 D47 V48 K49 D50 C51 L52 I56 P57 F58 G59 C61 C62 P63 I64

G65 P66 A67 D68 A70 A71 A72 A73

4.2.8 Score per residue for model 8

- Molecule 1: alpha 1 type II collagen isoform 1

Chain A: 33% 22% 12% 33%

Y1 V2 E3 F4 Q5 E6 E7 A8 S9 D19 K20 V21 D22 W23 K24 C28 R29 T30 C31 V32 C33 G36 T37 V38 L39 C40 D41 V42 I43 I44 C45 E46 D47 V48 K49 D50 C51 L52 S53 P54 E55 I56 P57 F58 G59 P63 I64 C65 A67 D68 L69 A70 A71 A72 A73

4.2.9 Score per residue for model 9

- Molecule 1: alpha 1 type II collagen isoform 1

Chain A: 25% 27% 15% 33%

Y1 V2 E3 F4 Q5 E6 E7 A8 S9 C10 V11 V12 D13 Q15 R16 Y17 N18 D19 K20 K21 D22 V23 W24 K25 P26 E27 P28 C29 R30 T31 C32 V33 C34 D35 T36 L39 C40 I43 I44 C45 E46 D47 V48 K49 D50 C51 L52 E55 I56 P57 F58 G59 E60 C61 C62 P63 I64 A67

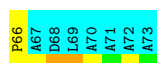
D68 L69 A70 A71 A72 A73

4.2.10 Score per residue for model 10

- Molecule 1: alpha 1 type II collagen isoform 1

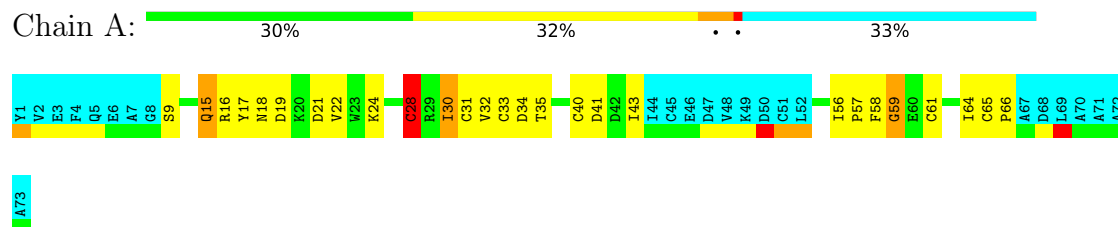
Chain A: 22% 32% 14% 33%

Y1 V2 E3 F4 Q5 E6 E7 A8 S9 C10 V11 V12 D13 G14 Q15 R16 Y17 N18 D19 K20 D21 V22 W23 W24 K25 C28 R29 T30 C31 V32 C33 D34 T35 G36 T37 V38 L39 C40 D41 D42 I43 I44 C45 E46 D47 V48 K49 D50 C51 L52 S53 I56 P57 F58 G59 E60 I64 C65



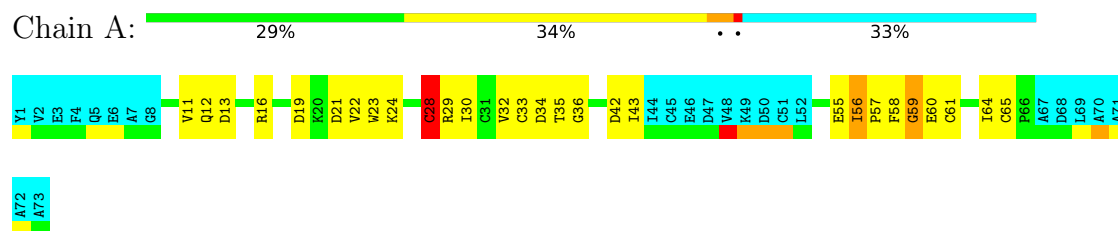
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: alpha 1 type II collagen isoform 1



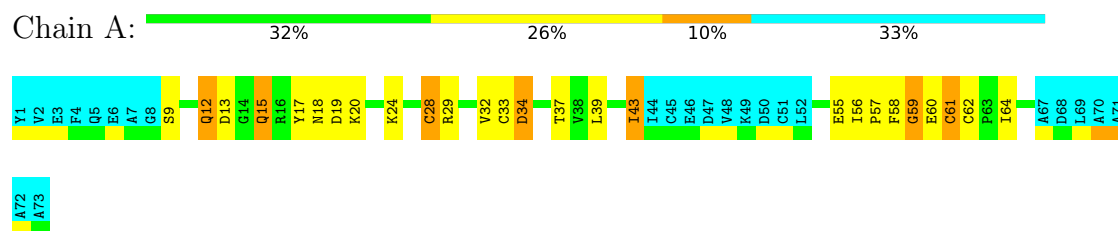
4.2.12 Score per residue for model 12

- Molecule 1: alpha 1 type II collagen isoform 1



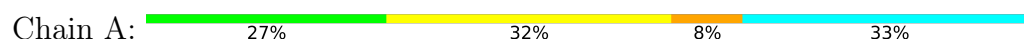
4.2.13 Score per residue for model 13

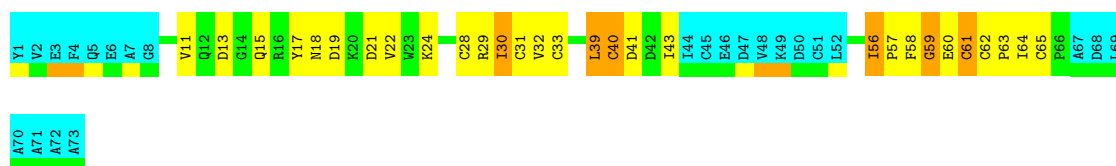
- Molecule 1: alpha 1 type II collagen isoform 1



4.2.14 Score per residue for model 14

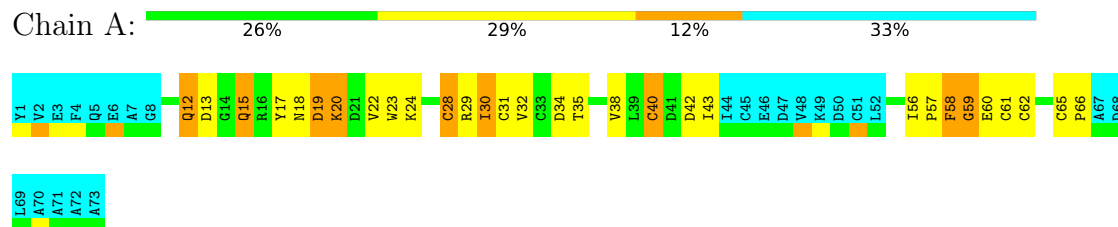
- Molecule 1: alpha 1 type II collagen isoform 1





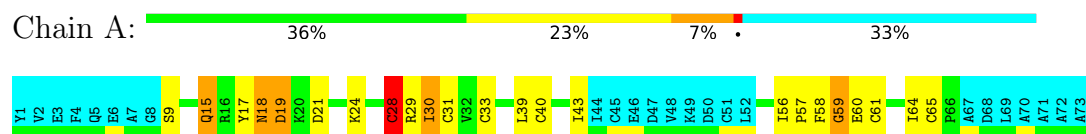
4.2.15 Score per residue for model 15

- Molecule 1: alpha 1 type II collagen isoform 1



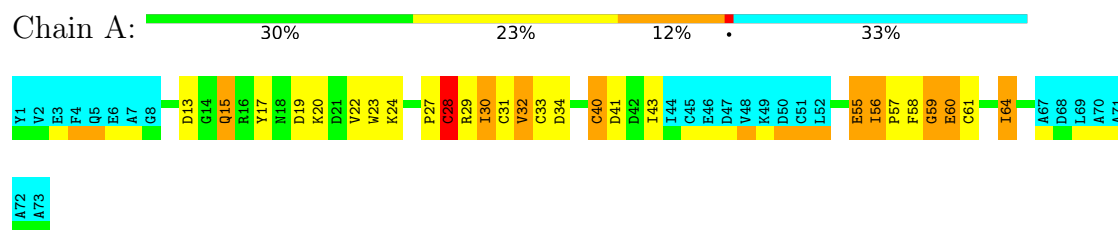
4.2.16 Score per residue for model 16

- Molecule 1: alpha 1 type II collagen isoform 1



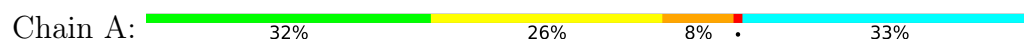
4.2.17 Score per residue for model 17

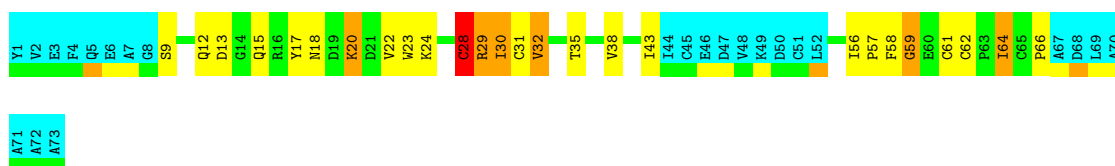
- Molecule 1: alpha 1 type II collagen isoform 1



4.2.18 Score per residue for model 18

- Molecule 1: alpha 1 type II collagen isoform 1





4.2.19 Score per residue for model 19

- Molecule 1: alpha 1 type II collagen isoform 1

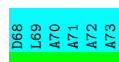
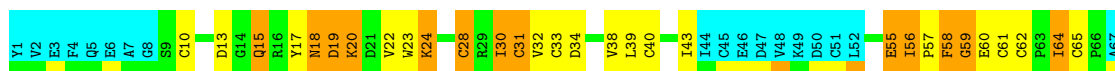
Chain A: 30% 27% 8% 33%



4.2.20 Score per residue for model 20

- Molecule 1: alpha 1 type II collagen isoform 1

Chain A: 26% 23% 18% 33%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *semi-automated assignment and torsion angle dynamics*.

Of the 600 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	1.0.6
CYANA	refinement	1.0.6

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	374	347	342	17±5
All	All	7480	6940	6840	348

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HD22	1:A:40:CYS:N	0.89	1.82	14	1
1:A:28:CYS:C	1:A:43:ILE:HD12	0.84	1.97	20	12
1:A:22:VAL:HG22	1:A:32:VAL:HG23	0.83	1.48	4	5
1:A:22:VAL:CG2	1:A:30:ILE:HD11	0.83	2.03	19	2
1:A:30:ILE:HG23	1:A:43:ILE:HD11	0.79	1.52	15	6
1:A:39:LEU:HD12	1:A:40:CYS:N	0.79	1.93	19	5
1:A:56:ILE:HD12	1:A:63:PRO:HB3	0.78	1.54	9	4
1:A:22:VAL:HG22	1:A:30:ILE:HD11	0.77	1.56	19	2
1:A:24:LYS:HD2	1:A:30:ILE:HG22	0.76	1.57	10	4
1:A:30:ILE:HD13	1:A:31:CYS:N	0.76	1.95	5	4
1:A:39:LEU:HD12	1:A:39:LEU:C	0.73	2.08	19	1
1:A:39:LEU:HD22	1:A:39:LEU:C	0.73	2.08	14	1
1:A:28:CYS:CA	1:A:43:ILE:HD12	0.71	2.15	17	11
1:A:22:VAL:HG22	1:A:32:VAL:CG2	0.69	2.17	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:C	1:A:30:ILE:HD13	0.69	2.12	8	1
1:A:30:ILE:HG23	1:A:43:ILE:CD1	0.68	2.18	15	4
1:A:23:TRP:CZ2	1:A:38:VAL:HG21	0.66	2.24	10	4
1:A:20:LYS:O	1:A:22:VAL:HG23	0.66	1.90	18	3
1:A:56:ILE:HD12	1:A:63:PRO:CB	0.66	2.20	9	4
1:A:27:PRO:C	1:A:43:ILE:HD12	0.65	2.16	3	1
1:A:30:ILE:HD13	1:A:30:ILE:C	0.64	2.18	7	3
1:A:22:VAL:HG12	1:A:32:VAL:HG23	0.62	1.70	5	3
1:A:39:LEU:O	1:A:39:LEU:HD13	0.61	1.94	14	1
1:A:23:TRP:HH2	1:A:38:VAL:HG22	0.58	1.58	8	2
1:A:30:ILE:HG23	1:A:43:ILE:CG1	0.57	2.29	12	1
1:A:20:LYS:O	1:A:22:VAL:HG13	0.57	2.00	15	1
1:A:58:PHE:CG	1:A:59:GLY:N	0.57	2.72	1	1
1:A:56:ILE:HD12	1:A:63:PRO:CA	0.57	2.30	14	2
1:A:30:ILE:HG23	1:A:43:ILE:HG12	0.56	1.77	12	1
1:A:21:ASP:O	1:A:32:VAL:HG23	0.55	2.01	11	1
1:A:56:ILE:HD11	1:A:63:PRO:CA	0.55	2.31	6	1
1:A:28:CYS:C	1:A:43:ILE:CD1	0.55	2.80	2	9
1:A:18:ASN:CG	1:A:19:ASP:N	0.54	2.66	1	1
1:A:56:ILE:HD11	1:A:63:PRO:HA	0.54	1.80	6	1
1:A:35:THR:O	1:A:35:THR:HG22	0.53	2.04	18	8
1:A:56:ILE:CD1	1:A:63:PRO:HA	0.53	2.34	6	1
1:A:58:PHE:O	1:A:59:GLY:C	0.53	2.52	9	3
1:A:28:CYS:N	1:A:43:ILE:HD12	0.52	2.19	17	6
1:A:22:VAL:HG23	1:A:32:VAL:HB	0.52	1.82	7	3
1:A:23:TRP:CH2	1:A:38:VAL:HG22	0.51	2.40	1	2
1:A:56:ILE:HD12	1:A:63:PRO:N	0.51	2.20	14	1
1:A:15:GLN:HB3	1:A:17:TYR:CE2	0.51	2.41	2	12
1:A:43:ILE:CG2	1:A:43:ILE:O	0.50	2.59	7	4
1:A:24:LYS:O	1:A:24:LYS:CD	0.50	2.59	6	1
1:A:20:LYS:O	1:A:21:ASP:C	0.50	2.54	9	3
1:A:11:VAL:CG1	1:A:11:VAL:O	0.50	2.59	10	1
1:A:11:VAL:HG23	1:A:11:VAL:O	0.50	2.07	7	3
1:A:30:ILE:C	1:A:30:ILE:CD1	0.50	2.85	8	3
1:A:43:ILE:CG2	1:A:61:CYS:CB	0.50	2.90	14	2
1:A:57:PRO:O	1:A:58:PHE:C	0.49	2.55	15	15
1:A:11:VAL:HG13	1:A:11:VAL:O	0.49	2.07	6	1
1:A:11:VAL:O	1:A:11:VAL:CG1	0.49	2.61	2	2
1:A:11:VAL:O	1:A:11:VAL:HG13	0.49	2.08	2	2
1:A:57:PRO:O	1:A:60:GLU:CG	0.49	2.61	3	2
1:A:24:LYS:CD	1:A:30:ILE:HG22	0.49	2.38	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:PHE:O	1:A:58:PHE:CG	0.49	2.65	7	2
1:A:11:VAL:O	1:A:11:VAL:CG2	0.48	2.61	4	4
1:A:56:ILE:O	1:A:56:ILE:CG2	0.48	2.62	8	7
1:A:23:TRP:CZ2	1:A:38:VAL:HG13	0.48	2.42	7	3
1:A:11:VAL:O	1:A:11:VAL:HG23	0.47	2.07	4	1
1:A:58:PHE:O	1:A:59:GLY:O	0.47	2.33	4	16
1:A:30:ILE:CG2	1:A:43:ILE:HD11	0.47	2.40	11	2
1:A:19:ASP:CA	1:A:33:CYS:O	0.47	2.63	14	4
1:A:63:PRO:C	1:A:64:ILE:CG2	0.47	2.87	6	2
1:A:27:PRO:C	1:A:60:GLU:O	0.46	2.59	19	1
1:A:41:ASP:CG	1:A:42:ASP:N	0.46	2.74	19	2
1:A:12:GLN:HG3	1:A:23:TRP:CZ2	0.46	2.46	9	3
1:A:28:CYS:O	1:A:43:ILE:CG1	0.46	2.64	20	2
1:A:29:ARG:HH21	1:A:43:ILE:H	0.46	1.52	18	1
1:A:32:VAL:O	1:A:34:ASP:N	0.45	2.50	11	2
1:A:39:LEU:C	1:A:39:LEU:HD13	0.45	2.36	14	1
1:A:34:ASP:O	1:A:37:THR:N	0.45	2.49	10	2
1:A:58:PHE:O	1:A:58:PHE:CD2	0.45	2.69	7	1
1:A:12:GLN:OE1	1:A:12:GLN:C	0.45	2.60	13	2
1:A:19:ASP:OD1	1:A:19:ASP:N	0.45	2.50	16	1
1:A:53:SER:O	1:A:65:CYS:CB	0.45	2.65	6	1
1:A:12:GLN:OE1	1:A:12:GLN:CA	0.45	2.64	13	1
1:A:19:ASP:C	1:A:21:ASP:N	0.45	2.74	4	6
1:A:27:PRO:C	1:A:61:CYS:SG	0.45	3.00	6	1
1:A:33:CYS:SG	1:A:36:GLY:C	0.45	3.00	12	1
1:A:32:VAL:HG22	1:A:33:CYS:H	0.45	1.72	13	1
1:A:19:ASP:O	1:A:33:CYS:O	0.45	2.35	6	13
1:A:30:ILE:C	1:A:30:ILE:HD12	0.45	2.37	12	1
1:A:56:ILE:HG23	1:A:59:GLY:HA2	0.44	1.88	6	1
1:A:34:ASP:O	1:A:35:THR:C	0.44	2.59	10	1
1:A:22:VAL:HG22	1:A:32:VAL:HB	0.44	1.89	17	1
1:A:26:GLU:O	1:A:29:ARG:O	0.44	2.36	1	6
1:A:22:VAL:CG2	1:A:30:ILE:CD1	0.44	2.89	19	1
1:A:23:TRP:CE2	1:A:31:CYS:HB3	0.44	2.48	17	3
1:A:22:VAL:HG12	1:A:32:VAL:CG2	0.44	2.43	15	1
1:A:15:GLN:HG2	1:A:17:TYR:CE2	0.44	2.48	4	1
1:A:43:ILE:CG2	1:A:61:CYS:HB3	0.43	2.43	14	1
1:A:22:VAL:HG22	1:A:32:VAL:HG21	0.43	1.90	20	1
1:A:32:VAL:HG22	1:A:33:CYS:N	0.43	2.28	13	1
1:A:18:ASN:CB	1:A:21:ASP:CG	0.43	2.91	7	1
1:A:23:TRP:NE1	1:A:31:CYS:CB	0.43	2.82	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TRP:CZ2	1:A:31:CYS:HB3	0.43	2.49	20	2
1:A:56:ILE:CG1	1:A:63:PRO:HA	0.43	2.43	6	1
1:A:22:VAL:HG22	1:A:32:VAL:CB	0.43	2.43	17	1
1:A:34:ASP:OD1	1:A:34:ASP:C	0.42	2.62	9	1
1:A:32:VAL:HG13	1:A:39:LEU:CD1	0.42	2.44	14	1
1:A:28:CYS:HA	1:A:43:ILE:HD12	0.42	1.91	8	1
1:A:62:CYS:O	1:A:62:CYS:SG	0.42	2.77	20	1
1:A:39:LEU:CD2	1:A:40:CYS:N	0.42	2.71	14	1
1:A:39:LEU:C	1:A:39:LEU:CD2	0.42	2.80	14	1
1:A:10:CYS:SG	1:A:38:VAL:CG2	0.42	3.08	20	1
1:A:9:SER:OG	1:A:16:ARG:CG	0.42	2.67	10	1
1:A:23:TRP:HZ2	1:A:38:VAL:HG21	0.42	1.65	10	1
1:A:24:LYS:CE	1:A:27:PRO:HA	0.42	2.45	5	1
1:A:59:GLY:O	1:A:60:GLU:OE1	0.42	2.38	4	1
1:A:39:LEU:HD22	1:A:40:CYS:C	0.42	2.39	14	1
1:A:39:LEU:HD22	1:A:40:CYS:CA	0.42	2.44	14	1
1:A:23:TRP:O	1:A:31:CYS:O	0.42	2.38	6	1
1:A:27:PRO:O	1:A:61:CYS:SG	0.41	2.79	4	3
1:A:12:GLN:HG3	1:A:23:TRP:CE2	0.41	2.50	12	3
1:A:56:ILE:HD11	1:A:63:PRO:C	0.41	2.40	6	1
1:A:56:ILE:O	1:A:56:ILE:HG22	0.41	2.15	6	1
1:A:39:LEU:C	1:A:39:LEU:CD1	0.41	2.80	19	1
1:A:43:ILE:HG22	1:A:61:CYS:HB3	0.41	1.91	9	1
1:A:35:THR:C	1:A:37:THR:N	0.41	2.78	10	1
1:A:16:ARG:O	1:A:16:ARG:CG	0.41	2.69	3	2
1:A:19:ASP:OD2	1:A:20:LYS:N	0.41	2.53	1	1
1:A:23:TRP:CZ2	1:A:38:VAL:CG2	0.41	3.03	18	2
1:A:55:GLU:O	1:A:64:ILE:O	0.41	2.39	8	4
1:A:30:ILE:C	1:A:40:CYS:SG	0.41	3.03	14	1
1:A:15:GLN:CB	1:A:17:TYR:CE2	0.41	3.04	2	1
1:A:43:ILE:O	1:A:43:ILE:HG22	0.41	2.16	13	1
1:A:39:LEU:HD12	1:A:40:CYS:C	0.41	2.41	19	1
1:A:33:CYS:SG	1:A:36:GLY:CA	0.41	3.09	7	1
1:A:19:ASP:OD1	1:A:19:ASP:C	0.41	2.64	15	1
1:A:27:PRO:O	1:A:60:GLU:O	0.41	2.39	17	1
1:A:28:CYS:SG	1:A:60:GLU:O	0.40	2.79	1	2
1:A:24:LYS:HD2	1:A:30:ILE:CG2	0.40	2.47	4	1
1:A:30:ILE:O	1:A:40:CYS:SG	0.40	2.79	2	3
1:A:19:ASP:OD1	1:A:33:CYS:O	0.40	2.40	17	1
1:A:41:ASP:OD1	1:A:42:ASP:O	0.40	2.40	2	1
1:A:59:GLY:C	1:A:60:GLU:HG2	0.40	2.41	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:LYS:O	1:A:21:ASP:O	0.40	2.40	6	1
1:A:17:TYR:C	1:A:18:ASN:O	0.40	2.64	7	1
1:A:43:ILE:O	1:A:61:CYS:O	0.40	2.40	5	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	49/73 (67%)	40±2 (83±4%)	6±1 (11±3%)	3±2 (6±3%)	2	19
All	All	980/1460 (67%)	809 (83%)	110 (11%)	61 (6%)	2	19

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	59	GLY	19
1	A	18	ASN	11
1	A	28	CYS	11
1	A	61	CYS	11
1	A	58	PHE	5
1	A	21	ASP	2
1	A	9	SER	2

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	46/63 (73%)	33±2 (72±4%)	13±2 (28±4%)	1	19
All	All	920/1260 (73%)	658 (72%)	262 (28%)	1	19

All 31 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	24	LYS	19
1	A	56	ILE	19
1	A	64	ILE	18
1	A	40	CYS	16
1	A	29	ARG	14
1	A	30	ILE	14
1	A	13	ASP	13
1	A	20	LYS	12
1	A	19	ASP	11
1	A	31	CYS	10
1	A	60	GLU	10
1	A	62	CYS	10
1	A	39	LEU	9
1	A	28	CYS	9
1	A	55	GLU	8
1	A	16	ARG	7
1	A	65	CYS	7
1	A	15	GLN	7
1	A	34	ASP	6
1	A	21	ASP	5
1	A	41	ASP	5
1	A	42	ASP	5
1	A	18	ASN	4
1	A	32	VAL	4
1	A	10	CYS	4
1	A	12	GLN	4
1	A	53	SER	3
1	A	43	ILE	3
1	A	9	SER	3
1	A	38	VAL	2
1	A	11	VAL	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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