



Full wwPDB NMR Structure Validation Report ⓘ

May 7, 2024 – 12:56 pm BST

PDB ID : 2W0N
Title : Plasticity of PAS domain and potential role for signal transduction in the histidine-kinase DcuS
Authors : Etzkorn, M.; Kneuper, H.; Duennwald, P.; Vijayan, V.; Kraemer, J.; Griesinger, C.; Becker, S.; Unden, G.; Baldus, M.
Deposited on : 2008-08-19

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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.36.2

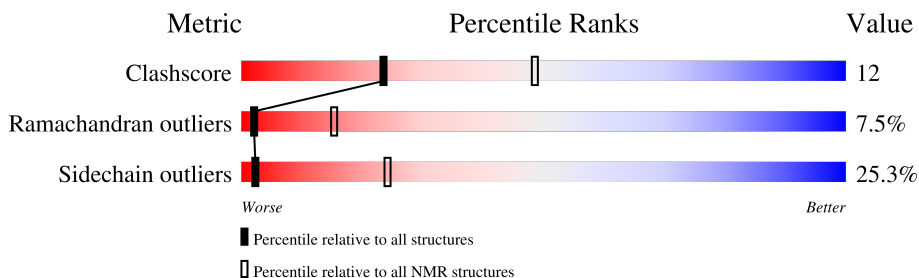
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	118	

2 Ensemble composition and analysis

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 8 is the overall representative, medoid model (most similar to other models).

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:25-A:116 (92)	2.70	8

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. No single-model clusters were found.

Cluster number	Models
1	4, 5, 6, 7, 8, 9, 10
2	1, 2, 3

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1868 atoms, of which 937 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SENSOR PROTEIN DCUS.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	118	1868	576	937	165	188	2	0

There are 3 discrepancies between the modelled and reference sequences:

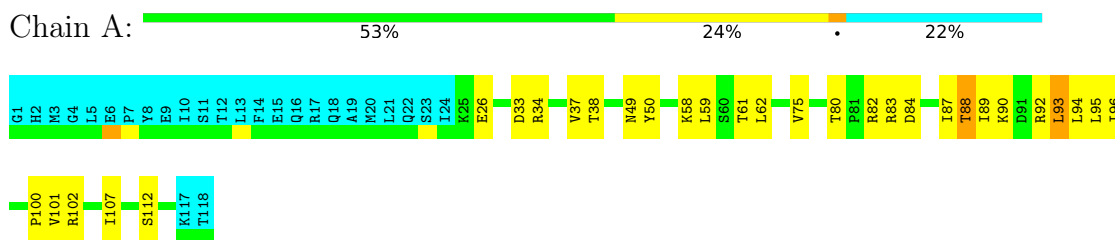
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P0AEC8
A	2	HIS	-	expression tag	UNP P0AEC8
A	3	MET	-	expression tag	UNP P0AEC8

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: SENSOR PROTEIN DCUS

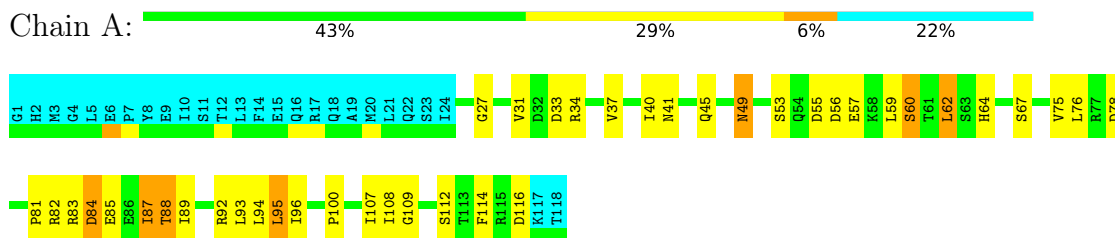


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: SENSOR PROTEIN DCUS



4.2.2 Score per residue for model 2

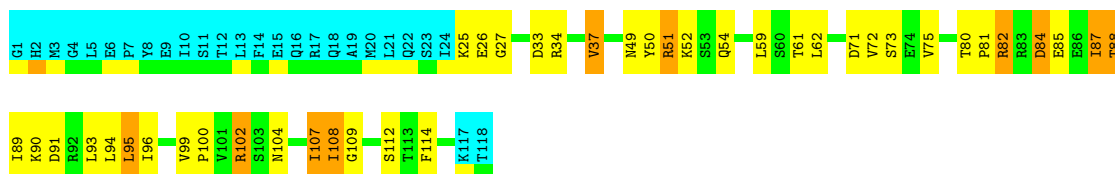
- Molecule 1: SENSOR PROTEIN DCUS





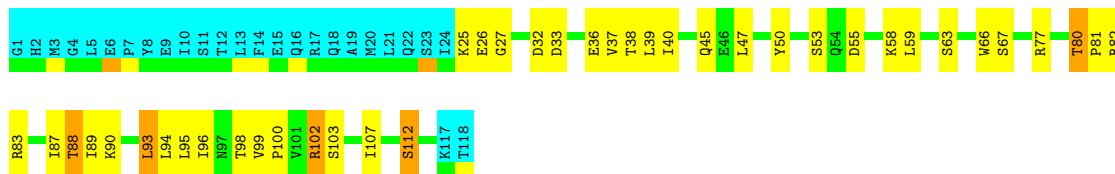
4.2.3 Score per residue for model 3

- Molecule 1: SENSOR PROTEIN DCUS



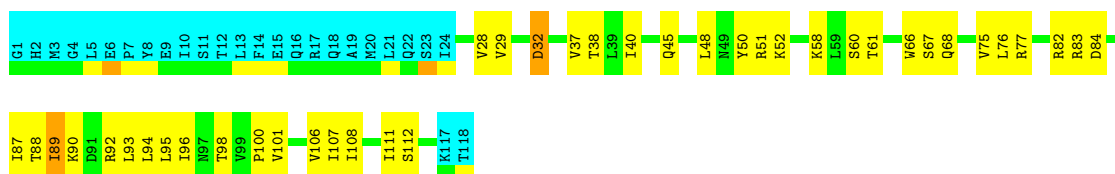
4.2.4 Score per residue for model 4

- Molecule 1: SENSOR PROTEIN DCUS



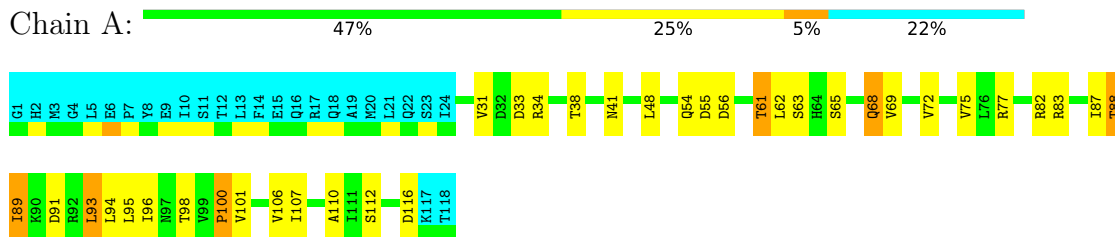
4.2.5 Score per residue for model 5

- Molecule 1: SENSOR PROTEIN DCUS



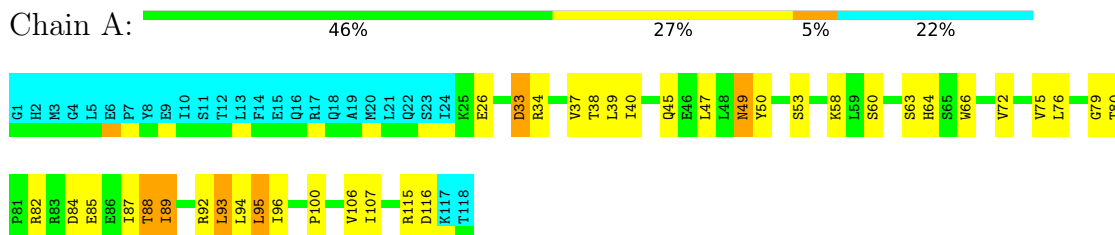
4.2.6 Score per residue for model 6

- Molecule 1: SENSOR PROTEIN DCUS



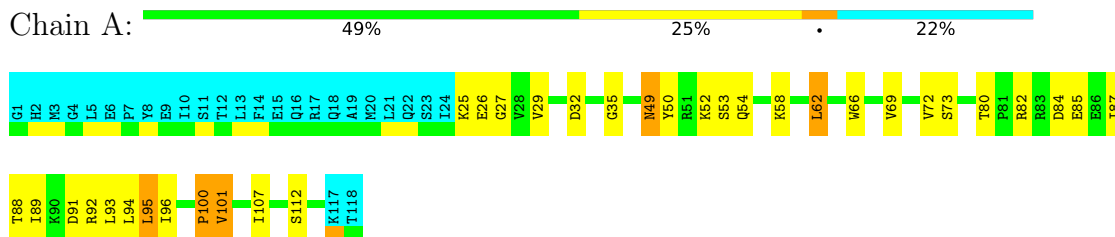
4.2.7 Score per residue for model 7

- Molecule 1: SENSOR PROTEIN DCUS



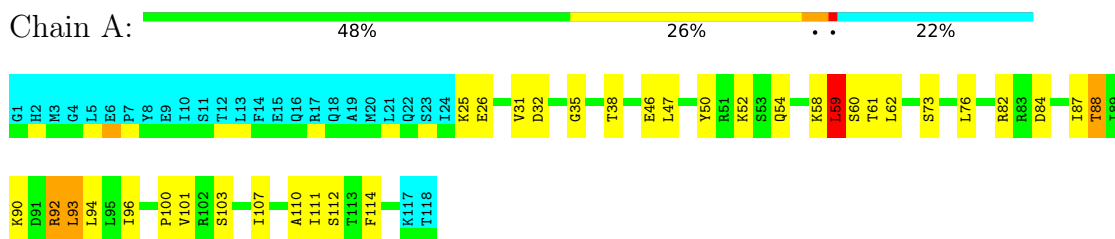
4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: SENSOR PROTEIN DCUS



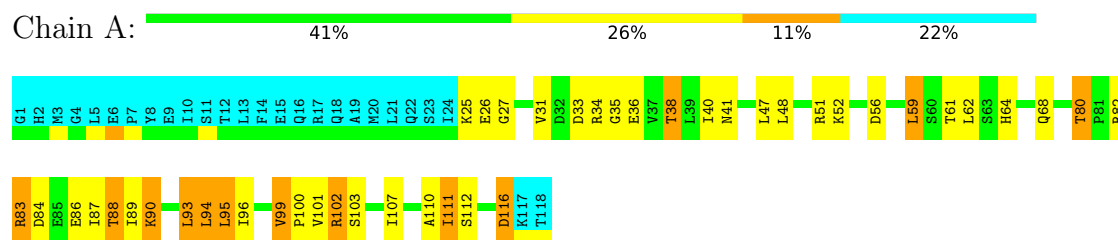
4.2.9 Score per residue for model 9

- Molecule 1: SENSOR PROTEIN DCUS



4.2.10 Score per residue for model 10

- Molecule 1: SENSOR PROTEIN DCUS



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 10 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided. Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	722	727	727	18±2
All	All	7220	7270	7270	177

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:36:GLU:O	1:A:38:THR:HG22	0.78	1.78	10	1
1:A:87:ILE:HG22	1:A:94:LEU:HD12	0.76	1.57	6	10
1:A:95:LEU:HD13	1:A:95:LEU:N	0.71	2.00	7	1
1:A:100:PRO:HB2	1:A:107:ILE:HD11	0.71	1.60	7	4
1:A:38:THR:HG23	1:A:39:LEU:HD12	0.71	1.61	7	1
1:A:100:PRO:HB2	1:A:107:ILE:HD13	0.70	1.63	8	2
1:A:72:VAL:O	1:A:75:VAL:HG12	0.68	1.87	6	3
1:A:111:ILE:HD13	1:A:112:SER:N	0.68	2.04	10	1
1:A:82:ARG:HB2	1:A:99:VAL:HG12	0.67	1.65	2	2
1:A:62:LEU:HD11	1:A:87:ILE:HG21	0.65	1.67	1	2
1:A:103:SER:HB3	1:A:107:ILE:HG22	0.65	1.69	2	1
1:A:82:ARG:CB	1:A:99:VAL:HG12	0.64	2.22	2	1
1:A:89:ILE:HG23	1:A:94:LEU:HD11	0.64	1.70	4	9
1:A:84:ASP:CB	1:A:95:LEU:HD13	0.63	2.24	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:ILE:O	1:A:108:ILE:HD13	0.63	1.93	5	1
1:A:98:THR:HG23	1:A:111:ILE:O	0.61	1.94	2	1
1:A:84:ASP:HB3	1:A:95:LEU:HD13	0.60	1.73	1	1
1:A:92:ARG:O	1:A:93:LEU:HD23	0.60	1.96	2	1
1:A:96:ILE:N	1:A:96:ILE:HD12	0.60	2.11	5	10
1:A:87:ILE:O	1:A:94:LEU:HD12	0.60	1.96	10	10
1:A:40:ILE:HD13	1:A:45:GLN:CG	0.59	2.28	7	3
1:A:95:LEU:O	1:A:95:LEU:HD12	0.59	1.97	2	2
1:A:101:VAL:HG22	1:A:111:ILE:HD13	0.59	1.74	9	1
1:A:107:ILE:O	1:A:107:ILE:HG23	0.59	1.98	10	3
1:A:75:VAL:HG11	1:A:82:ARG:HD3	0.59	1.74	1	1
1:A:87:ILE:HG22	1:A:87:ILE:O	0.56	1.99	3	5
1:A:40:ILE:HD13	1:A:45:GLN:HG2	0.56	1.77	7	1
1:A:72:VAL:O	1:A:75:VAL:HG22	0.56	2.00	2	1
1:A:94:LEU:C	1:A:95:LEU:HD13	0.56	2.22	7	1
1:A:101:VAL:O	1:A:101:VAL:HG22	0.55	2.01	6	1
1:A:107:ILE:HG23	1:A:107:ILE:O	0.54	2.02	3	1
1:A:29:VAL:O	1:A:111:ILE:HG23	0.54	2.02	5	1
1:A:49:ASN:ND2	1:A:49:ASN:N	0.54	2.55	8	1
1:A:88:THR:HB	1:A:93:LEU:N	0.54	2.18	7	5
1:A:100:PRO:HB2	1:A:107:ILE:HG21	0.54	1.79	4	1
1:A:86:GLU:C	1:A:87:ILE:HD12	0.53	2.23	10	1
1:A:29:VAL:HG13	1:A:29:VAL:O	0.53	2.04	8	1
1:A:100:PRO:CB	1:A:107:ILE:HD11	0.53	2.32	6	4
1:A:49:ASN:N	1:A:49:ASN:HD22	0.52	2.01	8	1
1:A:111:ILE:HD12	1:A:111:ILE:N	0.52	2.20	9	1
1:A:31:VAL:HG23	1:A:110:ALA:HB3	0.52	1.81	10	1
1:A:88:THR:O	1:A:88:THR:HG22	0.52	2.04	10	1
1:A:37:VAL:HG12	1:A:37:VAL:O	0.52	2.05	7	3
1:A:31:VAL:HG23	1:A:31:VAL:O	0.51	2.06	1	1
1:A:87:ILE:HD12	1:A:87:ILE:N	0.51	2.21	10	1
1:A:89:ILE:HD12	1:A:94:LEU:HD11	0.51	1.83	5	1
1:A:37:VAL:HG12	1:A:39:LEU:O	0.51	2.05	4	1
1:A:95:LEU:N	1:A:95:LEU:CD1	0.50	2.73	7	1
1:A:80:THR:HG22	1:A:81:PRO:HD2	0.50	1.84	4	1
1:A:31:VAL:HG22	1:A:110:ALA:O	0.50	2.07	9	2
1:A:69:VAL:O	1:A:72:VAL:HG12	0.49	2.08	6	1
1:A:100:PRO:O	1:A:101:VAL:HG22	0.49	2.08	8	1
1:A:111:ILE:HD13	1:A:111:ILE:C	0.49	2.28	10	1
1:A:89:ILE:N	1:A:89:ILE:HD13	0.49	2.22	5	1
1:A:100:PRO:CG	1:A:107:ILE:HD11	0.48	2.38	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ARG:HB2	1:A:99:VAL:HG13	0.48	1.83	10	1
1:A:88:THR:HB	1:A:93:LEU:HA	0.48	1.86	9	2
1:A:94:LEU:C	1:A:95:LEU:HD23	0.48	2.29	10	1
1:A:96:ILE:N	1:A:96:ILE:CD1	0.48	2.77	7	8
1:A:87:ILE:O	1:A:94:LEU:CG	0.47	2.62	9	8
1:A:86:GLU:CG	1:A:88:THR:HG22	0.47	2.39	2	1
1:A:93:LEU:N	1:A:93:LEU:HD23	0.46	2.26	1	1
1:A:40:ILE:HG23	1:A:45:GLN:HE21	0.46	1.71	4	1
1:A:40:ILE:HG23	1:A:40:ILE:O	0.46	2.11	10	1
1:A:92:ARG:O	1:A:93:LEU:CB	0.45	2.64	2	1
1:A:48:LEU:HD22	1:A:55:ASP:CG	0.45	2.31	6	1
1:A:84:ASP:HB2	1:A:95:LEU:HD13	0.45	1.87	3	1
1:A:87:ILE:O	1:A:94:LEU:CB	0.44	2.64	10	2
1:A:37:VAL:HG23	1:A:37:VAL:O	0.44	2.11	1	1
1:A:100:PRO:O	1:A:101:VAL:CG2	0.44	2.65	8	1
1:A:94:LEU:O	1:A:95:LEU:HD23	0.44	2.13	10	1
1:A:62:LEU:CD1	1:A:87:ILE:HG21	0.44	2.42	6	3
1:A:93:LEU:HD21	1:A:95:LEU:HD21	0.44	1.90	10	1
1:A:101:VAL:HG22	1:A:102:ARG:N	0.44	2.28	10	1
1:A:59:LEU:O	1:A:61:THR:N	0.44	2.51	9	1
1:A:106:VAL:HG22	1:A:107:ILE:N	0.43	2.28	5	1
1:A:48:LEU:HD22	1:A:55:ASP:OD1	0.43	2.12	6	1
1:A:86:GLU:HG2	1:A:88:THR:HG22	0.43	1.90	2	1
1:A:62:LEU:HD13	1:A:87:ILE:HG21	0.43	1.90	9	1
1:A:108:ILE:HG22	1:A:109:GLY:N	0.43	2.29	1	1
1:A:87:ILE:O	1:A:94:LEU:CD1	0.43	2.67	5	3
1:A:98:THR:HG22	1:A:112:SER:HA	0.43	1.90	4	2
1:A:40:ILE:HD13	1:A:45:GLN:HG3	0.43	1.91	1	1
1:A:108:ILE:HG23	1:A:109:GLY:N	0.43	2.29	3	1
1:A:38:THR:OG1	1:A:39:LEU:N	0.42	2.52	4	1
1:A:95:LEU:HD23	1:A:95:LEU:N	0.42	2.29	8	1
1:A:100:PRO:HG2	1:A:107:ILE:HD11	0.42	1.91	5	1
1:A:100:PRO:HB2	1:A:107:ILE:HD12	0.42	1.91	1	1
1:A:99:VAL:HG12	1:A:100:PRO:HD2	0.41	1.90	4	1
1:A:87:ILE:O	1:A:87:ILE:CG2	0.41	2.69	3	1
1:A:50:TYR:O	1:A:50:TYR:CD2	0.41	2.74	5	1
1:A:75:VAL:HG13	1:A:82:ARG:HG2	0.41	1.93	5	1
1:A:69:VAL:O	1:A:72:VAL:HG22	0.41	2.15	8	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	92/118 (78%)	68±4 (73±5%)	18±4 (19±4%)	7±3 (8±3%)	2	15
All	All	920/1180 (78%)	675 (73%)	176 (19%)	69 (8%)	2	15

All 35 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	33	ASP	6
1	A	27	GLY	5
1	A	100	PRO	5
1	A	35	GLY	4
1	A	50	TYR	3
1	A	32	ASP	3
1	A	38	THR	3
1	A	49	ASN	2
1	A	60	SER	2
1	A	81	PRO	2
1	A	58	LYS	2
1	A	93	LEU	2
1	A	91	ASP	2
1	A	102	ARG	2
1	A	101	VAL	2
1	A	61	THR	2
1	A	68	GLN	2
1	A	106	VAL	2
1	A	59	LEU	2
1	A	64	HIS	1
1	A	34	ARG	1
1	A	63	SER	1
1	A	67	SER	1
1	A	37	VAL	1
1	A	51	ARG	1
1	A	104	ASN	1
1	A	36	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	103	SER	1
1	A	53	SER	1
1	A	79	GLY	1
1	A	92	ARG	1
1	A	26	GLU	1
1	A	56	ASP	1
1	A	80	THR	1
1	A	90	LYS	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	83/106 (78%)	62±2 (75±3%)	21±2 (25±3%)	2 24
All	All	830/1060 (78%)	620 (75%)	210 (25%)	2 24

All 64 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	88	THR	10
1	A	84	ASP	8
1	A	95	LEU	7
1	A	93	LEU	7
1	A	82	ARG	7
1	A	34	ARG	6
1	A	83	ARG	6
1	A	112	SER	6
1	A	80	THR	6
1	A	59	LEU	5
1	A	85	GLU	5
1	A	92	ARG	5
1	A	25	LYS	5
1	A	52	LYS	5
1	A	90	LYS	5
1	A	41	ASN	4
1	A	49	ASN	4

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Mol	Chain	Res	Type	Models (Total)
1	A	76	LEU	4
1	A	116	ASP	4
1	A	51	ARG	4
1	A	61	THR	4
1	A	63	SER	4
1	A	54	GLN	4
1	A	26	GLU	4
1	A	47	LEU	4
1	A	58	LYS	4
1	A	66	TRP	4
1	A	53	SER	3
1	A	60	SER	3
1	A	62	LEU	3
1	A	67	SER	3
1	A	87	ILE	3
1	A	114	PHE	3
1	A	48	LEU	3
1	A	68	GLN	3
1	A	73	SER	3
1	A	102	ARG	3
1	A	77	ARG	3
1	A	89	ILE	3
1	A	55	ASP	2
1	A	56	ASP	2
1	A	65	SER	2
1	A	33	ASP	2
1	A	50	TYR	2
1	A	32	ASP	2
1	A	64	HIS	2
1	A	103	SER	2
1	A	57	GLU	1
1	A	78	ASP	1
1	A	36	GLU	1
1	A	42	ASP	1
1	A	113	THR	1
1	A	71	ASP	1
1	A	107	ILE	1
1	A	108	ILE	1
1	A	28	VAL	1
1	A	38	THR	1
1	A	98	THR	1
1	A	91	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	115	ARG	1
1	A	46	GLU	1
1	A	94	LEU	1
1	A	99	VAL	1
1	A	111	ILE	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](#)

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