



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:55 pm BST

PDB ID : 2L21
Title : chicken IGF2R domain 11
Authors : Williams, C.; Hoppe, H.; Strickland, M.; Frago, S.; Ellis, R.Z.; Wattana-Amorn, P.; Prince, S.N.; Zaccheo, O.J.; Forbes, B.; Jones, E.Y.; Rezgui, D.Z.; Crump, M.P.; Hassan, A.B.
Deposited on : 2010-08-10

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

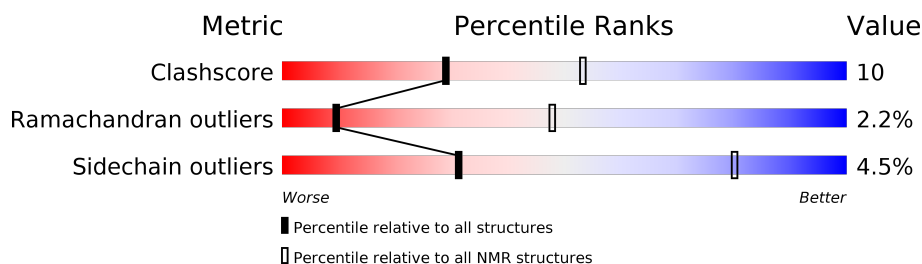
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	154	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 15 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:1887-A:2026 (140)	0.74	15

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2241 atoms, of which 1097 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cation-independent mannose-6-phosphate receptor.

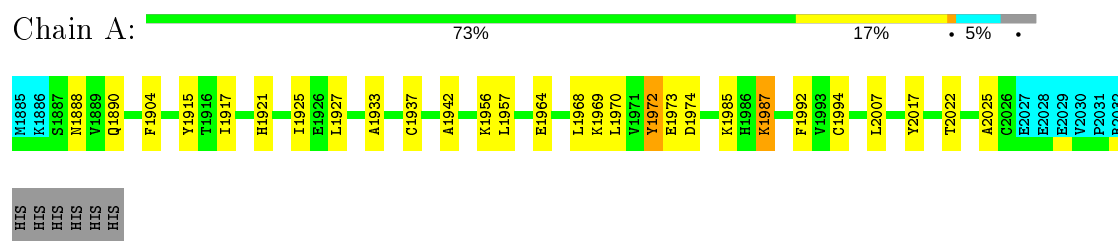
Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2241	708	1097	192	234	10	

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1885	MET	LEU	engineered mutation	UNP Q90681
A	1896	THR	MET	engineered mutation	UNP Q90681
A	1984	MET	THR	engineered mutation	UNP Q90681
A	2031	PRO	-	expression tag	UNP Q90681
A	2032	ARG	-	expression tag	UNP Q90681
A	2033	HIS	-	expression tag	UNP Q90681
A	2034	HIS	-	expression tag	UNP Q90681
A	2035	HIS	-	expression tag	UNP Q90681
A	2036	HIS	-	expression tag	UNP Q90681
A	2037	HIS	-	expression tag	UNP Q90681
A	2038	HIS	-	expression tag	UNP Q90681

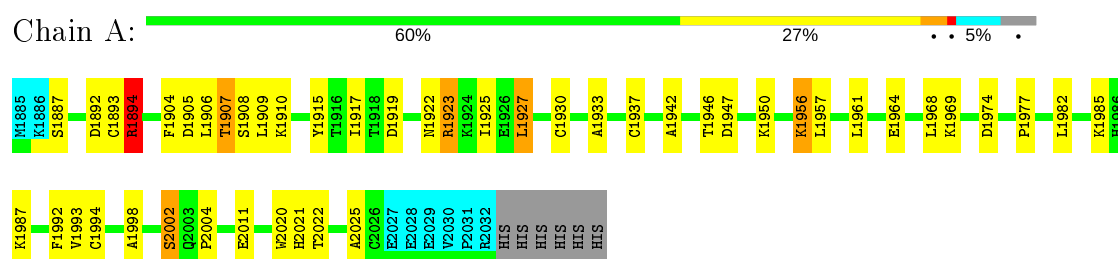
4.2.6 Score per residue for model 6

- Molecule 1: Cation-independent mannose-6-phosphate receptor



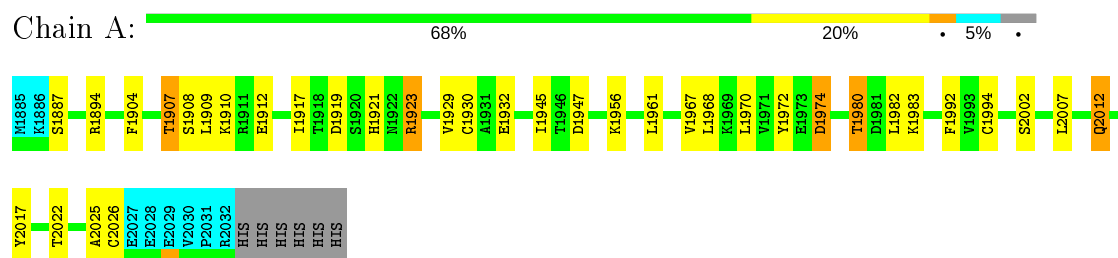
4.2.7 Score per residue for model 7

- Molecule 1: Cation-independent mannose-6-phosphate receptor



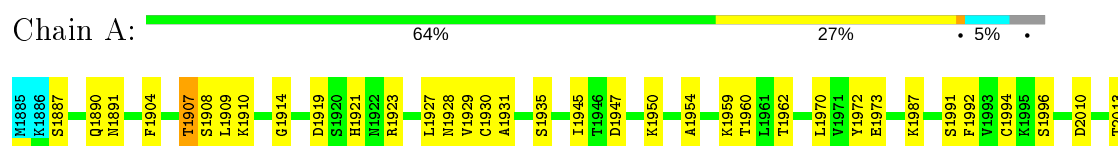
4.2.8 Score per residue for model 8

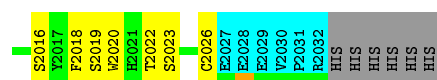
- Molecule 1: Cation-independent mannose-6-phosphate receptor



4.2.9 Score per residue for model 9

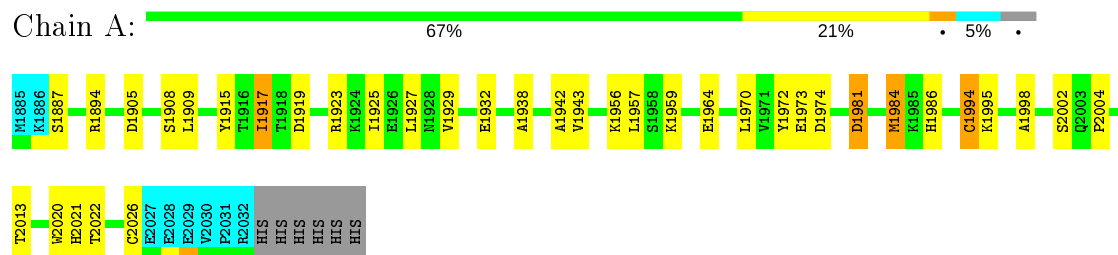
- Molecule 1: Cation-independent mannose-6-phosphate receptor





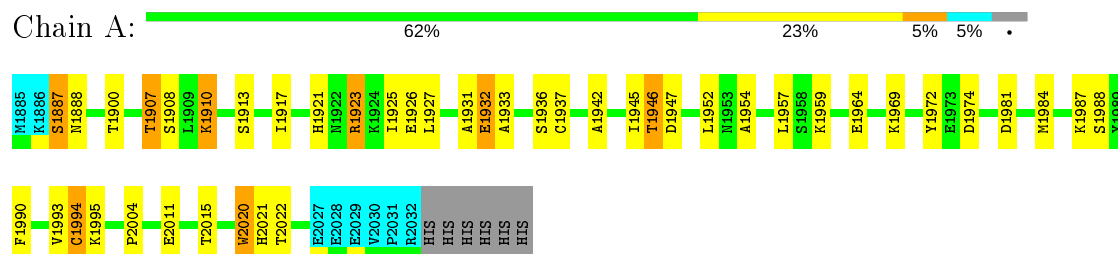
4.2.10 Score per residue for model 10

- Molecule 1: Cation-independent mannose-6-phosphate receptor



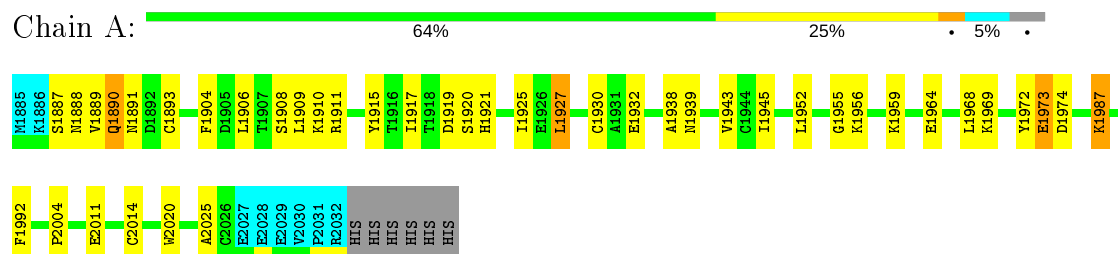
4.2.11 Score per residue for model 11

- Molecule 1: Cation-independent mannose-6-phosphate receptor



4.2.12 Score per residue for model 12

- Molecule 1: Cation-independent mannose-6-phosphate receptor

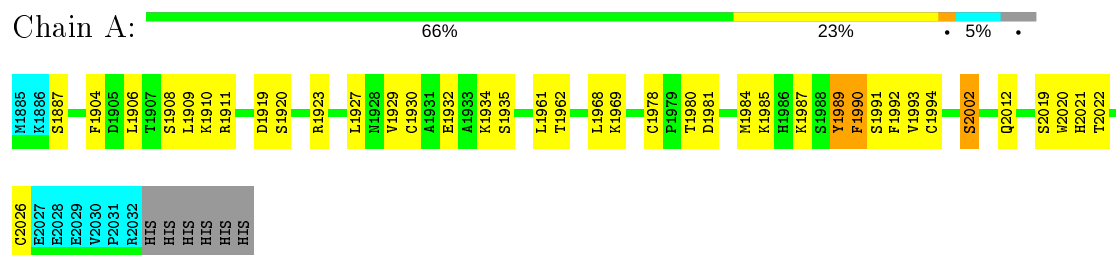


4.2.13 Score per residue for model 13

- Molecule 1: Cation-independent mannose-6-phosphate receptor

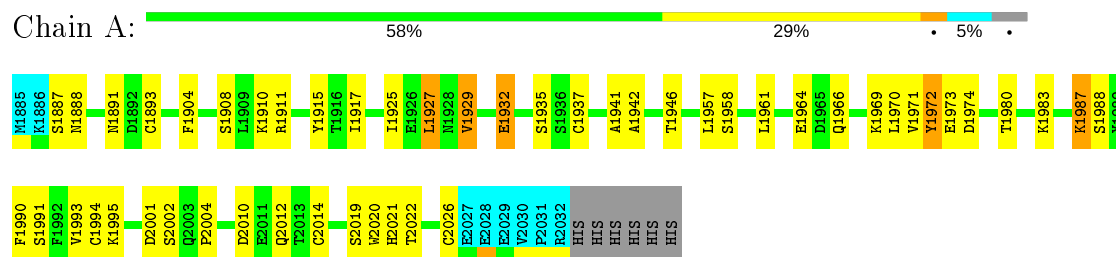
4.2.17 Score per residue for model 17

- Molecule 1: Cation-independent mannose-6-phosphate receptor



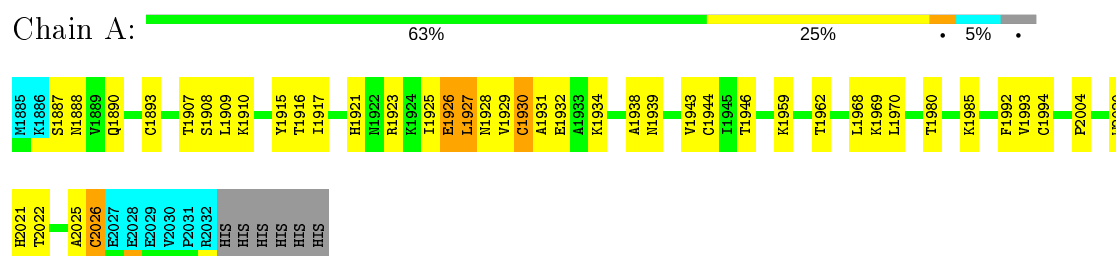
4.2.18 Score per residue for model 18

- Molecule 1: Cation-independent mannose-6-phosphate receptor



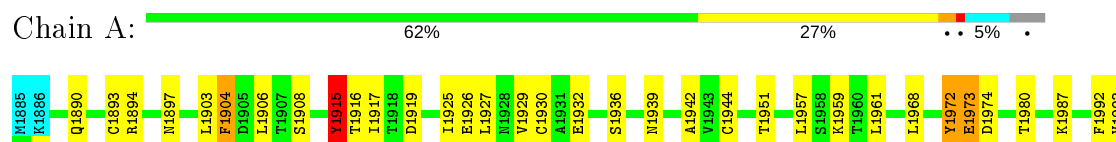
4.2.19 Score per residue for model 19

- Molecule 1: Cation-independent mannose-6-phosphate receptor



4.2.20 Score per residue for model 20

- Molecule 1: Cation-independent mannose-6-phosphate receptor



C1994	K1995	S1996	D1997	F2009	Q2012	T2015	S2016	W2020	HE2021	C2026	E2027	E2028	E2029	V2030	P2031	R2032	HIS	HIS	HIS	HIS	HIS	HIS

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.2
CNS	refinement	1.2
TALOS	geometry optimization	
ARIA	structure solution	1.2
ARIA	refinement	1.2
iCing	refinement	r765

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1705
Number of shifts mapped to atoms	1705
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1075	1026	1022	22±5
All	All	21500	20520	20440	434

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1923:ARG:HG2	1:A:1947:ASP:HB3	0.90	1.41	9	1
1:A:1887:SER:HA	1:A:1908:SER:HA	0.89	1.40	4	2
1:A:1968:LEU:HB3	1:A:1992:PHE:HB2	0.84	1.50	5	15
1:A:1964:GLU:HB3	1:A:1969:LYS:HG3	0.81	1.52	12	3
1:A:1915:TYR:HB3	1:A:1927:LEU:HB2	0.81	1.53	10	1
1:A:1923:ARG:HB3	1:A:1947:ASP:HB3	0.81	1.49	16	1
1:A:1894:ARG:HD3	1:A:1905:ASP:HB3	0.80	1.52	10	1
1:A:1907:THR:HA	1:A:1910:LYS:HE3	0.79	1.53	4	1
1:A:1916:THR:HG22	1:A:1926:GLU:HA	0.78	1.54	20	1
1:A:1890:GLN:HG2	1:A:1910:LYS:HD2	0.77	1.56	13	2
1:A:1964:GLU:HB3	1:A:1969:LYS:HD2	0.77	1.57	18	1
1:A:1973:GLU:HA	1:A:1987:LYS:HB3	0.76	1.56	12	2
1:A:1916:THR:HB	1:A:1926:GLU:HG2	0.76	1.56	19	1
1:A:1909:LEU:HG	1:A:1929:VAL:HG21	0.76	1.58	17	1
1:A:1964:GLU:HB2	1:A:1969:LYS:HD2	0.75	1.58	6	1
1:A:1893:CYS:HB2	1:A:1959:LYS:HB2	0.75	1.57	12	2
1:A:1923:ARG:HD2	1:A:1945:ILE:HG22	0.74	1.58	8	2
1:A:1956:LYS:HD2	1:A:1974:ASP:HB3	0.73	1.57	1	5
1:A:1994:CYS:HA	1:A:2022:THR:O	0.73	1.84	11	13
1:A:1995:LYS:HB2	1:A:2021:HIS:HB3	0.72	1.59	18	5
1:A:1990:PHE:HE1	1:A:2020:TRP:HB2	0.72	1.45	18	6
1:A:1998:ALA:HB1	1:A:2002:SER:HA	0.71	1.59	10	3
1:A:1919:ASP:HB2	1:A:1925:ILE:HG13	0.71	1.60	10	3
1:A:1994:CYS:HB2	1:A:2026:CYS:HA	0.70	1.62	14	2
1:A:1917:ILE:HG13	1:A:1925:ILE:HB	0.70	1.63	1	11
1:A:1964:GLU:HB2	1:A:1969:LYS:HG3	0.69	1.64	4	1
1:A:1919:ASP:HB3	1:A:1923:ARG:HB2	0.68	1.64	1	1
1:A:1910:LYS:HE3	1:A:1930:CYS:HB3	0.68	1.66	8	4
1:A:1964:GLU:HB3	1:A:1969:LYS:HD3	0.67	1.64	7	1
1:A:1891:ASN:HD21	1:A:1959:LYS:HG3	0.66	1.51	4	1
1:A:1907:THR:HA	1:A:1910:LYS:HG2	0.65	1.67	11	3
1:A:1932:GLU:HB3	1:A:1957:LEU:HD22	0.64	1.69	11	1
1:A:1887:SER:H	1:A:1908:SER:HA	0.64	1.53	3	2
1:A:1978:CYS:HB2	1:A:1981:ASP:OD2	0.64	1.93	2	1
1:A:1887:SER:CA	1:A:1908:SER:HA	0.64	2.22	4	2
1:A:1926:GLU:HB3	1:A:1936:SER:HB3	0.63	1.70	1	1
1:A:1974:ASP:HA	1:A:1985:LYS:HD3	0.63	1.70	1	1
1:A:1987:LYS:O	1:A:2015:THR:HA	0.63	1.92	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2022:THR:HG23	1:A:2025:ALA:HB2	0.62	1.70	1	6
1:A:1995:LYS:HB2	1:A:2021:HIS:HB2	0.62	1.69	15	1
1:A:1961:LEU:HG	1:A:1970:LEU:HD11	0.62	1.70	1	1
1:A:1921:HIS:HB2	1:A:1923:ARG:HG2	0.62	1.71	19	2
1:A:1981:ASP:HA	1:A:1984:MET:HG3	0.62	1.71	11	1
1:A:1925:ILE:HG22	1:A:1927:LEU:HD11	0.61	1.70	18	1
1:A:1930:CYS:HB2	1:A:1959:LYS:HA	0.61	1.70	3	1
1:A:1960:THR:O	1:A:1970:LEU:HG	0.60	1.96	9	2
1:A:1926:GLU:HG3	1:A:1936:SER:HB2	0.60	1.73	14	2
1:A:1915:TYR:OH	1:A:1929:VAL:HB	0.60	1.96	20	1
1:A:1983:LYS:HG3	1:A:1984:MET:HG2	0.60	1.72	3	1
1:A:1887:SER:HB2	1:A:1908:SER:HA	0.59	1.74	17	2
1:A:1961:LEU:HA	1:A:1970:LEU:HD21	0.59	1.73	8	1
1:A:1937:CYS:SG	1:A:1951:THR:HB	0.59	2.38	4	1
1:A:1929:VAL:HA	1:A:1972:TYR:OH	0.59	1.97	15	1
1:A:1917:ILE:HG23	1:A:2004:PRO:HG2	0.58	1.75	10	1
1:A:1924:LYS:HE3	1:A:1926:GLU:HB2	0.58	1.75	2	1
1:A:2012:GLN:HA	1:A:2012:GLN:HE21	0.58	1.58	8	1
1:A:1945:ILE:HB	1:A:1952:LEU:HB3	0.58	1.75	3	4
1:A:1887:SER:HB3	1:A:1908:SER:HA	0.58	1.75	2	8
1:A:1932:GLU:HB2	1:A:1939:ASN:O	0.58	1.99	12	3
1:A:1933:ALA:HB1	1:A:1936:SER:HB2	0.57	1.76	1	1
1:A:1893:CYS:SG	1:A:1961:LEU:HG	0.57	2.39	7	2
1:A:1888:ASN:HB3	1:A:1910:LYS:HG3	0.57	1.74	19	2
1:A:1962:THR:OG1	1:A:1969:LYS:HB2	0.57	2.00	1	3
1:A:1924:LYS:HG2	1:A:1946:THR:HB	0.57	1.77	2	1
1:A:1919:ASP:HB2	1:A:1925:ILE:CG1	0.57	2.28	7	2
1:A:1954:ALA:HA	1:A:1986:HIS:HE1	0.57	1.60	15	1
1:A:1942:ALA:HB2	1:A:1957:LEU:HA	0.56	1.77	1	7
1:A:1981:ASP:HB3	1:A:2013:THR:HA	0.56	1.76	2	1
1:A:1926:GLU:HG2	1:A:1936:SER:HB2	0.56	1.77	11	1
1:A:2010:ASP:O	1:A:2014:CYS:HA	0.56	2.00	18	1
1:A:1987:LYS:HB2	1:A:2015:THR:HG22	0.56	1.78	1	1
1:A:1925:ILE:HG22	1:A:1927:LEU:HD12	0.56	1.76	16	2
1:A:1995:LYS:HD3	1:A:2021:HIS:HB3	0.56	1.77	11	2
1:A:1890:GLN:HG2	1:A:1910:LYS:HD3	0.56	1.76	9	1
1:A:1930:CYS:HA	1:A:1972:TYR:OH	0.56	2.01	16	1
1:A:2020:TRP:CD1	1:A:2022:THR:HB	0.56	2.36	7	5
1:A:1917:ILE:HD13	1:A:2004:PRO:HB2	0.55	1.77	11	2
1:A:1890:GLN:CG	1:A:1910:LYS:HD2	0.55	2.30	13	1
1:A:2009:PHE:HD1	1:A:2016:SER:HB2	0.55	1.61	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1973:GLU:HB3	1:A:1987:LYS:HB3	0.55	1.78	2	2
1:A:2016:SER:HB3	1:A:2018:PHE:CE2	0.55	2.35	9	2
1:A:1990:PHE:CE1	1:A:2020:TRP:HB2	0.55	2.36	3	6
1:A:1993:VAL:O	1:A:2021:HIS:HA	0.55	2.01	2	8
1:A:1927:LEU:HA	1:A:1942:ALA:O	0.55	2.02	2	5
1:A:1980:THR:HB	1:A:2012:GLN:O	0.55	2.02	8	4
1:A:1974:ASP:HA	1:A:1985:LYS:HD2	0.55	1.79	6	2
1:A:1982:LEU:HG	1:A:1983:LYS:HG2	0.54	1.78	8	1
1:A:2004:PRO:HG3	1:A:2020:TRP:CZ2	0.54	2.38	19	1
1:A:1954:ALA:HA	1:A:1986:HIS:CE1	0.53	2.37	15	1
1:A:1922:ASN:HB3	1:A:1947:ASP:HB2	0.53	1.79	7	1
1:A:1919:ASP:HB3	1:A:1923:ARG:HG3	0.53	1.81	17	1
1:A:1944:CYS:SG	1:A:1951:THR:HB	0.53	2.43	1	1
1:A:2020:TRP:CE3	1:A:2022:THR:HG21	0.53	2.38	9	1
1:A:1915:TYR:CE1	1:A:1927:LEU:HG	0.52	2.39	20	1
1:A:1915:TYR:CE2	1:A:1927:LEU:HB2	0.52	2.39	15	1
1:A:1996:SER:HA	1:A:2023:SER:HB3	0.52	1.79	9	1
1:A:1890:GLN:HG3	1:A:1910:LYS:HD3	0.52	1.80	12	1
1:A:1910:LYS:HD3	1:A:1930:CYS:HB3	0.52	1.79	19	1
1:A:1910:LYS:HD3	1:A:1930:CYS:SG	0.52	2.44	15	1
1:A:1893:CYS:SG	1:A:1961:LEU:HB2	0.52	2.44	20	2
1:A:1933:ALA:O	1:A:1937:CYS:HB2	0.52	2.05	6	3
1:A:2009:PHE:CD1	1:A:2016:SER:HB2	0.52	2.40	15	1
1:A:1978:CYS:HB3	1:A:1979:PRO:HD2	0.52	1.80	14	1
1:A:1910:LYS:HG2	1:A:1930:CYS:HB2	0.52	1.82	7	1
1:A:1906:LEU:HD13	1:A:1909:LEU:HD23	0.52	1.82	12	2
1:A:1925:ILE:HG21	1:A:2018:PHE:CZ	0.52	2.40	16	1
1:A:1887:SER:CB	1:A:1908:SER:HA	0.51	2.35	2	5
1:A:1980:THR:HB	1:A:2014:CYS:SG	0.51	2.44	3	1
1:A:1919:ASP:OD2	1:A:1923:ARG:HD2	0.51	2.06	1	1
1:A:1956:LYS:HD2	1:A:1974:ASP:CB	0.51	2.35	1	1
1:A:1894:ARG:HG3	1:A:1903:LEU:HD21	0.51	1.79	2	1
1:A:1957:LEU:HD11	1:A:1959:LYS:HE3	0.51	1.81	10	3
1:A:1906:LEU:HB3	1:A:1909:LEU:HB2	0.51	1.80	13	1
1:A:1925:ILE:HG21	1:A:2018:PHE:HZ	0.51	1.66	16	1
1:A:1955:GLY:HA3	1:A:1972:TYR:HB3	0.51	1.82	12	2
1:A:1907:THR:HA	1:A:1910:LYS:HD2	0.51	1.81	16	1
1:A:1953:ASN:ND2	1:A:1975:GLY:HA2	0.50	2.20	14	1
1:A:1894:ARG:HA	1:A:1904:PHE:O	0.50	2.05	13	2
1:A:1919:ASP:O	1:A:1923:ARG:HA	0.50	2.07	10	1
1:A:1990:PHE:HZ	1:A:2004:PRO:HB3	0.50	1.66	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1941:ALA:HA	1:A:1956:LYS:HA	0.49	1.84	13	1
1:A:1893:CYS:SG	1:A:1906:LEU:HB2	0.49	2.46	2	1
1:A:1957:LEU:HD12	1:A:1959:LYS:HE3	0.49	1.84	4	1
1:A:1930:CYS:O	1:A:1959:LYS:HE2	0.49	2.08	2	1
1:A:2009:PHE:HD1	1:A:2016:SER:HB3	0.49	1.67	20	1
1:A:1888:ASN:HB3	1:A:1910:LYS:HB2	0.49	1.84	18	1
1:A:2007:LEU:HB2	1:A:2017:TYR:HB2	0.49	1.84	8	2
1:A:1977:PRO:HB2	1:A:1982:LEU:HA	0.48	1.83	7	1
1:A:2004:PRO:HG3	1:A:2020:TRP:CZ3	0.48	2.43	7	1
1:A:1929:VAL:HG13	1:A:1970:LEU:HD22	0.48	1.84	10	1
1:A:1910:LYS:HB2	1:A:1931:ALA:HB2	0.48	1.84	15	1
1:A:1994:CYS:N	1:A:2026:CYS:SG	0.48	2.86	20	2
1:A:1991:SER:O	1:A:2019:SER:HA	0.48	2.09	4	4
1:A:1994:CYS:HB2	1:A:2026:CYS:CA	0.48	2.36	14	1
1:A:1996:SER:H	1:A:2021:HIS:HB3	0.48	1.68	20	1
1:A:1995:LYS:HE2	1:A:1997:ASP:HB3	0.48	1.84	3	2
1:A:1992:PHE:HB3	1:A:2025:ALA:HB1	0.48	1.85	12	1
1:A:1977:PRO:HA	1:A:1986:HIS:CE1	0.48	2.43	2	1
1:A:1932:GLU:O	1:A:1934:LYS:HE2	0.48	2.09	19	1
1:A:1932:GLU:HG3	1:A:1934:LYS:HE2	0.48	1.86	17	1
1:A:1910:LYS:HE2	1:A:1930:CYS:HB2	0.48	1.85	4	1
1:A:1946:THR:HA	1:A:1950:LYS:O	0.48	2.07	7	1
1:A:1906:LEU:O	1:A:1910:LYS:HG3	0.48	2.09	17	1
1:A:1994:CYS:HB3	1:A:2026:CYS:H	0.48	1.69	4	1
1:A:1925:ILE:HG22	1:A:1927:LEU:HD22	0.48	1.85	11	2
1:A:1913:SER:HA	1:A:1934:LYS:HB3	0.47	1.86	16	2
1:A:1909:LEU:HA	1:A:1915:TYR:OH	0.47	2.09	2	1
1:A:1910:LYS:HB3	1:A:1930:CYS:HB2	0.47	1.84	9	5
1:A:2004:PRO:HB3	1:A:2020:TRP:CE3	0.47	2.44	14	2
1:A:1910:LYS:HE2	1:A:1930:CYS:SG	0.47	2.50	17	1
1:A:1995:LYS:CB	1:A:2021:HIS:HB3	0.47	2.39	14	3
1:A:1981:ASP:OD2	1:A:1984:MET:HB2	0.47	2.09	10	1
1:A:1981:ASP:HA	1:A:1984:MET:CG	0.47	2.39	11	1
1:A:2020:TRP:CE3	1:A:2022:THR:HB	0.47	2.45	2	1
1:A:1927:LEU:HB3	1:A:1943:VAL:HG23	0.47	1.86	14	1
1:A:1995:LYS:HE2	1:A:1997:ASP:O	0.47	2.10	20	1
1:A:2002:SER:HA	1:A:2020:TRP:CZ2	0.47	2.45	2	1
1:A:2011:GLU:HA	1:A:2014:CYS:HA	0.47	1.85	12	1
1:A:1927:LEU:HB3	1:A:1943:VAL:HA	0.47	1.85	19	1
1:A:1972:TYR:HE1	1:A:1990:PHE:HB2	0.47	1.69	4	1
1:A:1890:GLN:HG3	1:A:1931:ALA:HB2	0.46	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1909:LEU:HD11	1:A:2020:TRP:CZ2	0.46	2.46	19	2
1:A:1970:LEU:HD21	1:A:1972:TYR:OH	0.46	2.10	18	2
1:A:1961:LEU:HB3	1:A:1968:LEU:HD11	0.46	1.88	17	1
1:A:1990:PHE:CZ	1:A:2004:PRO:HB3	0.46	2.45	13	1
1:A:1932:GLU:HA	1:A:1957:LEU:HG	0.46	1.86	10	2
1:A:1975:GLY:HA3	1:A:1986:HIS:CE1	0.46	2.46	4	1
1:A:1927:LEU:HG	1:A:1943:VAL:HA	0.46	1.88	10	1
1:A:1888:ASN:O	1:A:1910:LYS:HD3	0.46	2.11	11	1
1:A:1945:ILE:HG12	1:A:1954:ALA:HB2	0.46	1.87	11	1
1:A:1961:LEU:HD13	1:A:1970:LEU:HD21	0.46	1.87	13	1
1:A:1890:GLN:NE2	1:A:1930:CYS:HB2	0.46	2.25	20	1
1:A:1932:GLU:HB3	1:A:1939:ASN:O	0.45	2.11	2	2
1:A:1980:THR:HG21	1:A:2012:GLN:O	0.45	2.12	20	2
1:A:1973:GLU:OE2	1:A:1987:LYS:HE3	0.45	2.12	16	1
1:A:1937:CYS:HB3	1:A:1941:ALA:HB3	0.45	1.87	18	1
1:A:1990:PHE:CZ	1:A:2020:TRP:HE3	0.45	2.29	17	1
1:A:1915:TYR:CE1	1:A:1927:LEU:HD13	0.45	2.47	7	1
1:A:1915:TYR:CE1	1:A:1929:VAL:HG13	0.45	2.45	18	1
1:A:1947:ASP:HB3	1:A:1950:LYS:HE2	0.45	1.87	1	1
1:A:1956:LYS:HG2	1:A:1973:GLU:O	0.45	2.11	6	1
1:A:1919:ASP:CG	1:A:1920:SER:H	0.45	2.15	12	3
1:A:1894:ARG:HB2	1:A:1903:LEU:HD21	0.45	1.88	20	2
1:A:1926:GLU:CD	1:A:1935:SER:HB3	0.45	2.32	2	1
1:A:1915:TYR:CE1	1:A:1929:VAL:HG23	0.45	2.47	15	1
1:A:1906:LEU:HD13	1:A:1909:LEU:HD22	0.45	1.87	14	1
1:A:1897:ASN:HB2	1:A:1904:PHE:CE2	0.45	2.47	20	1
1:A:1904:PHE:CD2	1:A:1968:LEU:HD13	0.44	2.46	3	1
1:A:1888:ASN:HB3	1:A:1910:LYS:O	0.44	2.11	14	1
1:A:1937:CYS:HA	1:A:1951:THR:HB	0.44	1.89	4	1
1:A:1957:LEU:CD1	1:A:1959:LYS:HE3	0.44	2.43	4	1
1:A:1973:GLU:HB3	1:A:1987:LYS:HA	0.44	1.88	6	1
1:A:1926:GLU:O	1:A:1944:CYS:HB2	0.44	2.11	19	1
1:A:1909:LEU:HD12	1:A:1929:VAL:HB	0.44	1.90	8	1
1:A:1981:ASP:OD1	1:A:2013:THR:HA	0.44	2.13	10	2
1:A:1932:GLU:HG3	1:A:1957:LEU:HG	0.44	1.88	15	1
1:A:1947:ASP:OD2	1:A:1950:LYS:HD3	0.44	2.13	9	1
1:A:1944:CYS:HB2	1:A:1951:THR:HG23	0.44	1.89	20	1
1:A:1954:ALA:O	1:A:1987:LYS:HG3	0.44	2.13	9	1
1:A:1923:ARG:HD3	1:A:1945:ILE:CG2	0.43	2.43	16	2
1:A:1922:ASN:O	1:A:1923:ARG:HG3	0.43	2.13	7	1
1:A:1909:LEU:HB2	1:A:2020:TRP:CH2	0.43	2.48	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1917:ILE:HD11	1:A:1927:LEU:HD21	0.43	1.90	14	1
1:A:1923:ARG:CD	1:A:1945:ILE:HG22	0.43	2.41	9	1
1:A:1995:LYS:HB3	1:A:2021:HIS:HB3	0.43	1.90	10	2
1:A:1972:TYR:HE1	1:A:1990:PHE:HD2	0.43	1.57	3	1
1:A:1906:LEU:O	1:A:1910:LYS:HG2	0.43	2.13	15	1
1:A:1924:LYS:HB3	1:A:1924:LYS:NZ	0.43	2.28	16	1
1:A:1928:ASN:OD1	1:A:1931:ALA:HB3	0.43	2.14	19	1
1:A:1934:LYS:HB2	1:A:1934:LYS:HZ2	0.43	1.73	5	1
1:A:1932:GLU:CD	1:A:1932:GLU:H	0.42	2.17	11	3
1:A:1906:LEU:HB2	1:A:1930:CYS:SG	0.42	2.54	12	1
1:A:1973:GLU:HB3	1:A:1987:LYS:CA	0.42	2.45	6	1
1:A:1994:CYS:CB	1:A:2026:CYS:HA	0.42	2.42	13	1
1:A:2004:PRO:HG3	1:A:2020:TRP:CE2	0.42	2.49	19	1
1:A:1909:LEU:HD23	1:A:1929:VAL:HB	0.42	1.90	9	1
1:A:1978:CYS:SG	1:A:1981:ASP:HB3	0.42	2.54	17	1
1:A:1971:VAL:HA	1:A:1988:SER:O	0.42	2.14	18	1
1:A:1891:ASN:ND2	1:A:1959:LYS:HG3	0.42	2.27	4	1
1:A:2010:ASP:OD1	1:A:2013:THR:HG22	0.42	2.13	9	1
1:A:1936:SER:HB3	1:A:1946:THR:HG21	0.42	1.92	11	1
1:A:1962:THR:HG1	1:A:1969:LYS:HB2	0.42	1.74	1	1
1:A:1931:ALA:HA	1:A:1959:LYS:HE2	0.42	1.89	11	1
1:A:1932:GLU:HB3	1:A:1939:ASN:HA	0.42	1.91	20	1
1:A:1972:TYR:HB2	1:A:1988:SER:HB3	0.42	1.92	11	1
1:A:1992:PHE:HB3	1:A:2025:ALA:CB	0.42	2.44	12	1
1:A:1890:GLN:HE22	1:A:1906:LEU:HB2	0.42	1.73	20	1
1:A:1914:GLY:HA2	1:A:1928:ASN:HB2	0.42	1.90	9	1
1:A:1888:ASN:OD1	1:A:1890:GLN:HG2	0.41	2.14	3	1
1:A:1929:VAL:HG13	1:A:1970:LEU:HD13	0.41	1.90	9	1
1:A:1918:THR:HA	1:A:1924:LYS:HA	0.41	1.91	16	1
1:A:1893:CYS:HB3	1:A:1959:LYS:HG3	0.41	1.91	19	1
1:A:1909:LEU:CD2	1:A:1929:VAL:HB	0.41	2.44	9	1
1:A:1923:ARG:HD3	1:A:1947:ASP:HB2	0.41	1.91	11	1
1:A:1993:VAL:HG13	1:A:2021:HIS:HD2	0.41	1.75	7	3
1:A:1909:LEU:HA	1:A:1915:TYR:CE1	0.41	2.50	14	1
1:A:1909:LEU:HA	1:A:1915:TYR:HE1	0.41	1.73	14	1
1:A:1929:VAL:HG12	1:A:1930:CYS:SG	0.41	2.55	15	1
1:A:1929:VAL:HG13	1:A:1992:PHE:CZ	0.41	2.50	4	1
1:A:1913:SER:HA	1:A:1934:LYS:CB	0.41	2.45	1	1
1:A:1926:GLU:CB	1:A:1936:SER:HB3	0.41	2.42	1	1
1:A:1995:LYS:HB3	1:A:2021:HIS:O	0.41	2.16	2	1
1:A:1930:CYS:HB3	1:A:1970:LEU:HD11	0.41	1.92	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1888:ASN:ND2	1:A:1890:GLN:HE22	0.41	2.12	6	1
1:A:2020:TRP:HA	1:A:2020:TRP:CE3	0.41	2.50	11	1
1:A:1981:ASP:OD1	1:A:1984:MET:HG3	0.41	2.15	17	1
1:A:1890:GLN:HB2	1:A:1910:LYS:HE2	0.41	1.90	2	1
1:A:1894:ARG:HB3	1:A:1905:ASP:HB3	0.41	1.91	7	1
1:A:1923:ARG:HD3	1:A:1947:ASP:HB3	0.41	1.92	8	1
1:A:2020:TRP:CE3	1:A:2021:HIS:N	0.41	2.89	11	1
1:A:2002:SER:HA	1:A:2021:HIS:O	0.41	2.16	17	1
1:A:1993:VAL:HG13	1:A:2021:HIS:CD2	0.41	2.50	17	1
1:A:1919:ASP:HB3	1:A:1923:ARG:O	0.41	2.16	8	1
1:A:1915:TYR:HE1	1:A:1927:LEU:HG	0.41	1.74	20	1
1:A:1923:ARG:HD3	1:A:1945:ILE:HG22	0.40	1.93	1	1
1:A:1927:LEU:HB3	1:A:1943:VAL:HG13	0.40	1.93	12	1
1:A:1923:ARG:HG3	1:A:1945:ILE:HG22	0.40	1.92	2	1
1:A:1929:VAL:HG13	1:A:1970:LEU:CD2	0.40	2.46	19	1
1:A:1995:LYS:HG3	1:A:1997:ASP:HB3	0.40	1.93	13	1
1:A:1904:PHE:CE1	1:A:2026:CYS:HA	0.40	2.51	17	1
1:A:1978:CYS:HB3	1:A:1981:ASP:HB2	0.40	1.94	4	1
1:A:1888:ASN:O	1:A:1907:THR:HA	0.40	2.16	5	1
1:A:1994:CYS:HB3	1:A:2026:CYS:HB2	0.40	1.74	10	1

5.2 Torsion angles ⓘ

5.2.1 Protein backbone ⓘ

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	140/154 (91%)	119±3 (85±2%)	18±3 (13±2%)	3±2 (2±1%)	9	48
All	All	2800/3080 (91%)	2376 (85%)	361 (13%)	63 (2%)	9	48

All 25 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	1921	HIS	9
1	A	2002	SER	9

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Mol	Chain	Res	Type	Models (Total)
1	A	1974	ASP	7
1	A	1938	ALA	6
1	A	1891	ASN	4
1	A	1930	CYS	3
1	A	1887	SER	3
1	A	1892	ASP	2
1	A	2001	ASP	2
1	A	1935	SER	2
1	A	1932	GLU	2
1	A	1984	MET	1
1	A	2008	SER	1
1	A	1929	VAL	1
1	A	1987	LYS	1
1	A	1997	ASP	1
1	A	1998	ALA	1
1	A	1889	VAL	1
1	A	1923	ARG	1
1	A	1986	HIS	1
1	A	1937	CYS	1
1	A	1890	GLN	1
1	A	2025	ALA	1
1	A	1913	SER	1
1	A	1965	ASP	1

5.2.2 Protein sidechains ⓘ

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	124/138 (90%)	118±2 (96±2%)	6±2 (4±2%)	31	80
All	All	2480/2760 (90%)	2369 (96%)	111 (4%)	31	80

All 40 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	1927	LEU	13
1	A	1990	PHE	8

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Mol	Chain	Res	Type	Models (Total)
1	A	1907	THR	8
1	A	1987	LYS	6
1	A	1932	GLU	5
1	A	1973	GLU	5
1	A	1917	ILE	5
1	A	1946	THR	4
1	A	1919	ASP	4
1	A	1956	LYS	3
1	A	1980	THR	3
1	A	2020	TRP	3
1	A	1994	CYS	3
1	A	2011	GLU	3
1	A	1985	LYS	3
1	A	2026	CYS	3
1	A	1993	VAL	2
1	A	1910	LYS	2
1	A	1923	ARG	2
1	A	1894	ARG	2
1	A	1959	LYS	2
1	A	1962	THR	2
1	A	1964	GLU	2
1	A	1926	GLU	2
1	A	1929	VAL	1
1	A	2004	PRO	1
1	A	1909	LEU	1
1	A	1983	LYS	1
1	A	1935	SER	1
1	A	1981	ASP	1
1	A	1915	TYR	1
1	A	2002	SER	1
1	A	1912	GLU	1
1	A	2012	GLN	1
1	A	1930	CYS	1
1	A	1890	GLN	1
1	A	1887	SER	1
1	A	1958	SER	1
1	A	2003	GLN	1
1	A	2015	THR	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 88% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

6.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1705
Number of shifts mapped to atoms	1705
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	0.06 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	139	0.08 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	0.34 ± 0.07	None needed (< 0.5 ppm)
^{15}N	138	0.10 ± 0.39	None needed (< 0.5 ppm)

6.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1441 atoms were assigned a chemical shift out of a possible 1627. 2 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	679/690 (98%)	275/275 (100%)	271/280 (97%)	133/135 (99%)
Sidechain	671/799 (84%)	418/468 (89%)	239/300 (80%)	14/31 (45%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	91/138 (66%)	52/72 (72%)	38/57 (67%)	1/9 (11%)
Overall	1441/1627 (89%)	745/815 (91%)	548/637 (86%)	148/175 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 1528 atoms were assigned a chemical shift out of a possible 1740. 2 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	708/728 (97%)	287/290 (99%)	283/296 (96%)	138/142 (97%)
Sidechain	729/874 (83%)	455/513 (89%)	259/326 (79%)	15/35 (43%)
Aromatic	91/138 (66%)	52/72 (72%)	38/57 (67%)	1/9 (11%)
Overall	1528/1740 (88%)	794/875 (91%)	580/679 (85%)	154/186 (83%)

6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

