



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 1NMW / pdb_00001nmw
Title : Solution structure of the PPIase domain of human Pin1
Authors : Bayer, E.; Goettsch, S.; Mueller, J.W.; Griewel, B.; Guiberman, E.; Mayr, L.;
Bayer, P.
Deposited on : 2003-01-12

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
Mogul	:	2022.3.0, CSD as543be (2022)
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

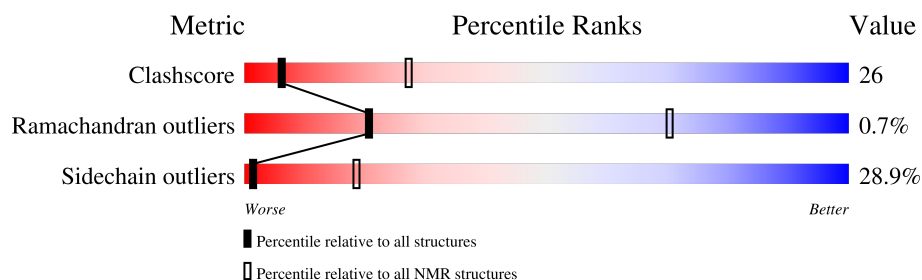
1 Overall quality at a glance

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	114	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 7 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:53-A:163 (111)	0.84	3

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 and 1 single-model cluster was found.

Cluster number	Models
1	5, 6, 7, 8, 10
2	1, 3
3	2, 9
Single-model clusters	4

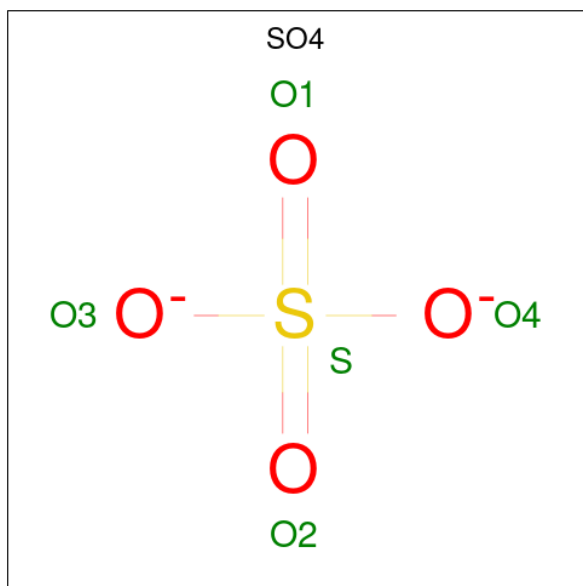
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1785 atoms, of which 885 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1.

Mol	Chain	Residues	Atoms						Trace
1	A	114	Total	C	H	N	O	S	0
			1780	551	885	165	175	4	

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



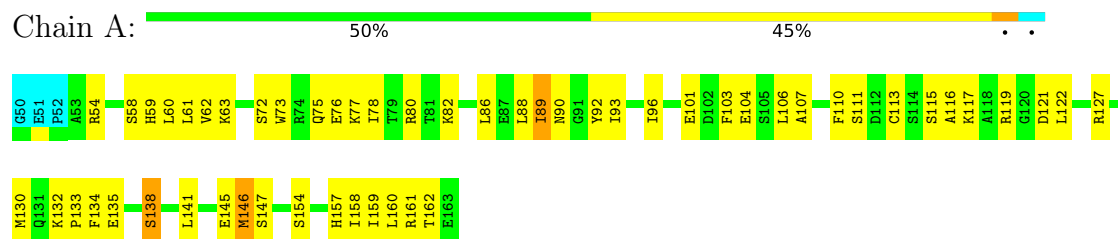
Mol	Chain	Residues	Atoms		
2	A	1	Total	O	S
			5	4	1

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: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

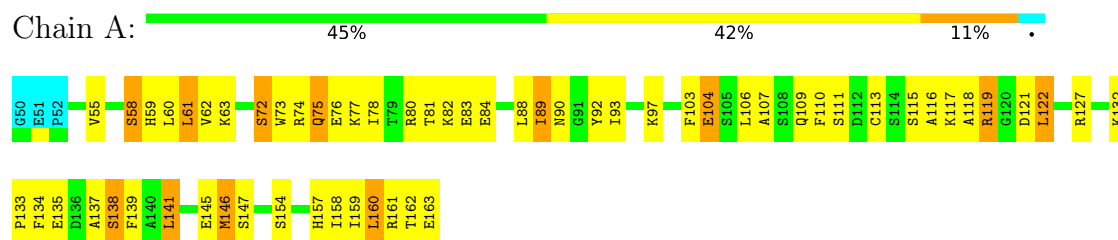


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

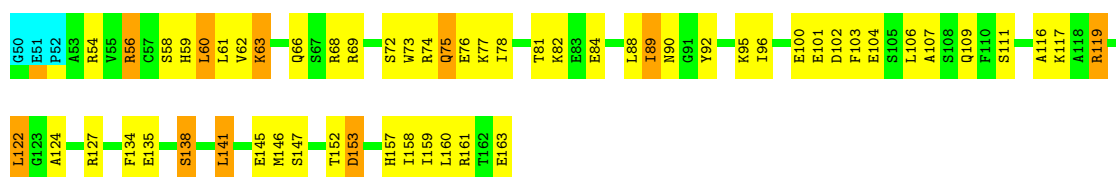
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



4.2.2 Score per residue for model 2

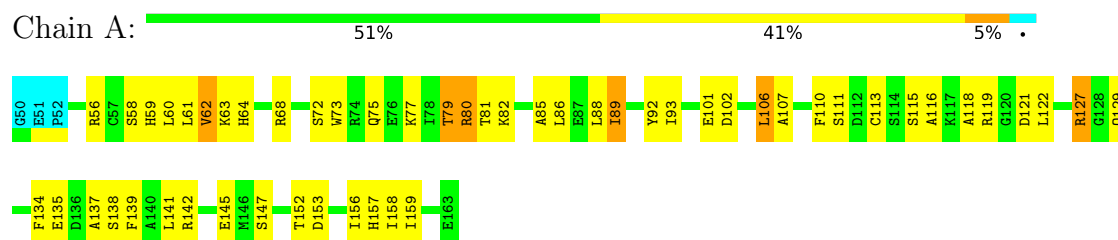
- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1





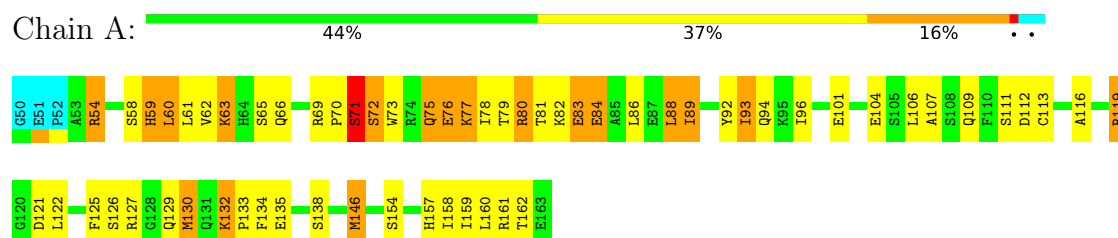
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



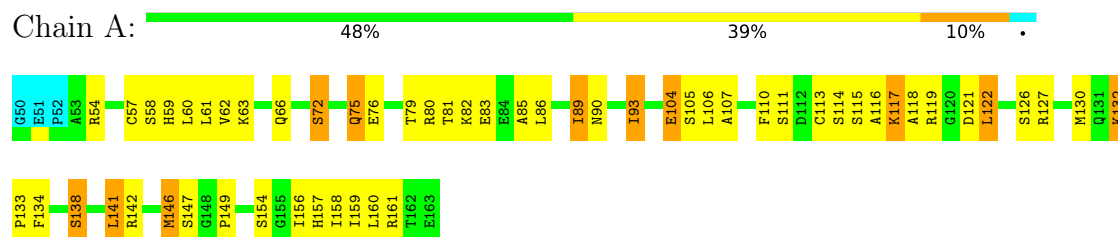
4.2.4 Score per residue for model 4

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



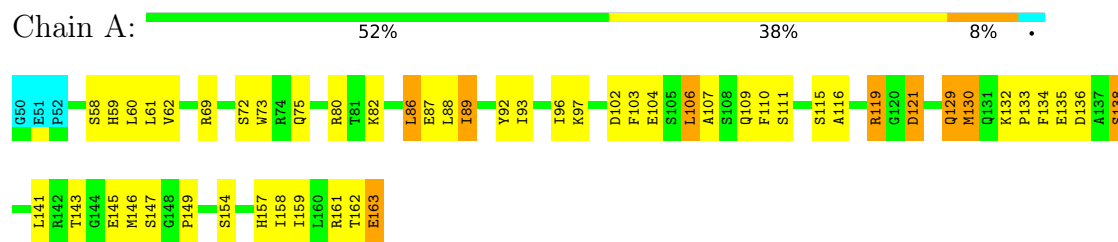
4.2.5 Score per residue for model 5

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



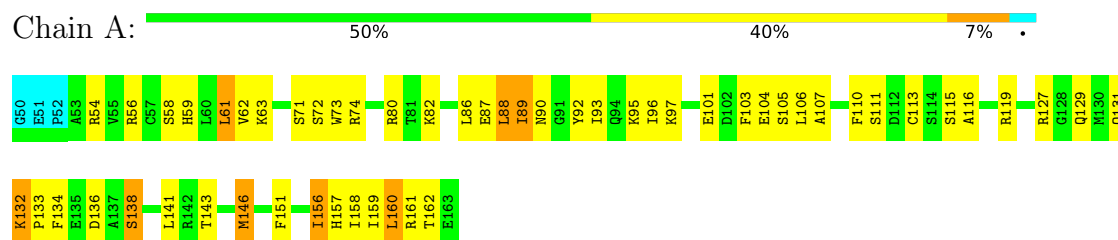
4.2.6 Score per residue for model 6

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



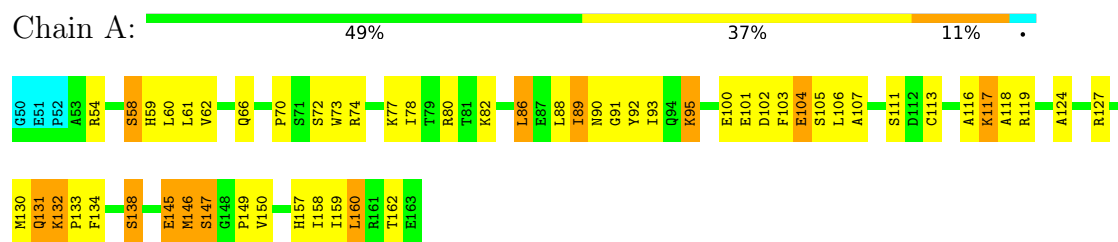
4.2.7 Score per residue for model 7

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



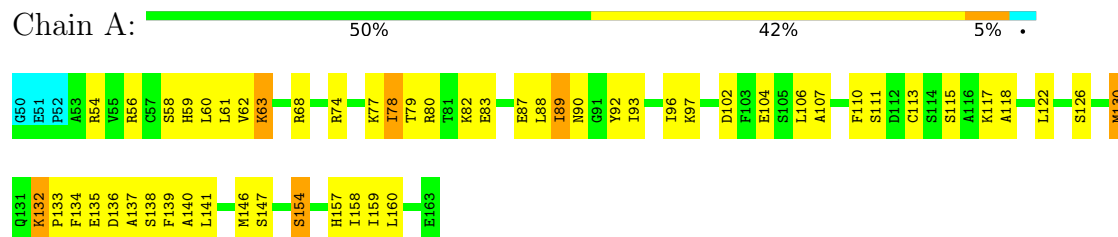
4.2.8 Score per residue for model 8

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



4.2.9 Score per residue for model 9

- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1



- Molecule 1: Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1

G50	E51	P52	A53	R54	S55	H56	L60	V62	K63	H64	S65	Q66	S67	R68	R69	S72	W73	R74	Q75	E76	R80	T81	K82	P83	E84	A85	L88	I89	N90	G91	Y92	I93	I96	E101	D102	F103	E104	S105	L106	A107	F110	S111	A116	K117	A118	R119	L122	P127
K131	Q132	P133	F134	E135	D136	A137	S138	L141	E145	M146	S147	D153	I156	H157	I158	I159	L160	R161	T162	E163																												

5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	875	867	864	45±5
All	All	8800	8670	8640	454

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:ILE:HG23	1:A:146:MET:HE1	1.01	1.33	1	1
1:A:62:VAL:HG11	1:A:88:LEU:HD11	0.90	1.41	10	1
1:A:146:MET:HE2	1:A:160:LEU:HD23	0.88	1.46	8	1
1:A:61:LEU:HD13	1:A:157:HIS:NE2	0.87	1.85	2	10
1:A:92:TYR:CD1	1:A:106:LEU:HD21	0.85	2.06	4	2
1:A:103:PHE:CD2	1:A:160:LEU:HD21	0.85	2.05	8	1
1:A:61:LEU:HD12	1:A:62:VAL:N	0.84	1.87	5	9
1:A:146:MET:HE2	1:A:160:LEU:HD13	0.84	1.46	9	2
1:A:107:ALA:O	1:A:111:SER:N	0.83	2.11	9	10
1:A:103:PHE:CD1	1:A:160:LEU:HD11	0.83	2.08	1	1
1:A:146:MET:HE2	1:A:160:LEU:CD1	0.82	2.05	7	1
1:A:93:ILE:HD11	1:A:158:ILE:CD1	0.80	2.05	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:HIS:CD2	1:A:122:LEU:HD21	0.80	2.10	2	3
1:A:96:ILE:HD13	1:A:103:PHE:CD2	0.80	2.10	7	3
1:A:89:ILE:HG23	1:A:158:ILE:HD11	0.80	1.51	3	9
1:A:146:MET:CE	1:A:160:LEU:HD13	0.76	2.11	9	1
1:A:103:PHE:CZ	1:A:160:LEU:HD11	0.76	2.15	8	1
1:A:73:TRP:CZ2	1:A:116:ALA:HB2	0.76	2.14	7	6
1:A:61:LEU:HD13	1:A:157:HIS:CE1	0.76	2.15	4	5
1:A:60:LEU:HD23	1:A:60:LEU:O	0.75	1.81	2	1
1:A:106:LEU:HD13	1:A:107:ALA:N	0.74	1.98	6	1
1:A:86:LEU:HD21	1:A:149:PRO:CG	0.72	2.14	8	1
1:A:96:ILE:HD12	1:A:146:MET:HE1	0.71	1.60	2	1
1:A:88:LEU:HD12	1:A:89:ILE:N	0.70	2.01	10	1
1:A:58:SER:O	1:A:160:LEU:HD12	0.70	1.87	8	1
1:A:62:VAL:CG1	1:A:62:VAL:O	0.69	2.40	3	1
1:A:146:MET:HE2	1:A:160:LEU:HD12	0.69	1.62	10	2
1:A:106:LEU:HD22	1:A:110:PHE:CD2	0.67	2.24	6	1
1:A:102:ASP:O	1:A:106:LEU:HD12	0.67	1.90	2	1
1:A:96:ILE:CG1	1:A:106:LEU:HD12	0.67	2.20	10	2
1:A:101:GLU:HB3	1:A:106:LEU:HD11	0.66	1.65	2	3
1:A:60:LEU:HD12	1:A:106:LEU:CD1	0.66	2.20	6	1
1:A:103:PHE:CE1	1:A:160:LEU:HD11	0.66	2.26	8	1
1:A:61:LEU:HD23	1:A:113:CYS:HB2	0.65	1.68	1	6
1:A:160:LEU:HD23	1:A:160:LEU:O	0.65	1.90	4	2
1:A:103:PHE:CG	1:A:160:LEU:HD11	0.65	2.26	1	1
1:A:137:ALA:HB1	1:A:147:SER:HB2	0.65	1.67	10	1
1:A:122:LEU:HD22	1:A:130:MET:SD	0.64	2.31	5	1
1:A:60:LEU:HD12	1:A:106:LEU:HD11	0.64	1.68	6	1
1:A:138:SER:OG	1:A:159:ILE:HG21	0.64	1.92	2	7
1:A:141:LEU:HD11	1:A:147:SER:HB3	0.64	1.70	9	3
1:A:134:PHE:CE1	1:A:159:ILE:HG12	0.63	2.28	10	3
1:A:134:PHE:CD1	1:A:159:ILE:HD11	0.63	2.28	3	1
1:A:88:LEU:N	1:A:88:LEU:HD13	0.63	2.08	4	1
1:A:60:LEU:HD11	1:A:92:TYR:CD2	0.63	2.29	2	1
1:A:141:LEU:HD12	1:A:142:ARG:O	0.63	1.93	5	1
1:A:93:ILE:HD11	1:A:158:ILE:HD13	0.62	1.71	8	2
1:A:62:VAL:HG11	1:A:88:LEU:CD1	0.62	2.21	10	2
1:A:141:LEU:HD21	1:A:146:MET:C	0.62	2.19	7	1
1:A:101:GLU:HG2	1:A:106:LEU:HD21	0.62	1.72	8	1
1:A:61:LEU:HD23	1:A:113:CYS:SG	0.61	2.34	7	1
1:A:103:PHE:CG	1:A:160:LEU:HD21	0.61	2.29	8	1
1:A:60:LEU:HD22	1:A:60:LEU:O	0.61	1.95	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD11	1:A:92:TYR:CE2	0.61	2.30	2	1
1:A:102:ASP:C	1:A:106:LEU:HD12	0.61	2.19	2	1
1:A:59:HIS:CD2	1:A:122:LEU:HD11	0.61	2.30	10	2
1:A:61:LEU:HD13	1:A:157:HIS:CD2	0.60	2.30	9	5
1:A:71:SER:HB2	1:A:76:GLU:O	0.60	1.95	4	1
1:A:134:PHE:CE2	1:A:159:ILE:HG12	0.60	2.32	8	7
1:A:59:HIS:HA	1:A:158:ILE:O	0.60	1.97	6	10
1:A:96:ILE:HG12	1:A:106:LEU:HD12	0.60	1.73	7	1
1:A:93:ILE:CG2	1:A:146:MET:HE1	0.59	2.19	1	1
1:A:106:LEU:HD13	1:A:110:PHE:CE2	0.59	2.33	3	1
1:A:141:LEU:HD12	1:A:145:GLU:HB3	0.59	1.75	10	1
1:A:60:LEU:HD11	1:A:106:LEU:HD22	0.58	1.74	4	1
1:A:61:LEU:HD12	1:A:62:VAL:H	0.58	1.56	8	5
1:A:60:LEU:HD12	1:A:106:LEU:HD23	0.58	1.72	5	1
1:A:96:ILE:HG13	1:A:106:LEU:HD13	0.58	1.76	4	1
1:A:103:PHE:CE2	1:A:160:LEU:HD21	0.58	2.34	1	1
1:A:104:GLU:O	1:A:119:ARG:HB3	0.57	1.98	4	7
1:A:93:ILE:HD12	1:A:158:ILE:HD13	0.57	1.76	4	1
1:A:160:LEU:HD12	1:A:160:LEU:N	0.57	2.14	8	1
1:A:159:ILE:C	1:A:160:LEU:HD23	0.57	2.24	1	1
1:A:92:TYR:CG	1:A:106:LEU:HD21	0.57	2.35	4	1
1:A:61:LEU:HD22	1:A:157:HIS:CE1	0.56	2.34	5	2
1:A:55:VAL:HG22	1:A:139:PHE:CE1	0.56	2.35	1	1
1:A:55:VAL:HG22	1:A:139:PHE:CZ	0.56	2.35	1	1
1:A:60:LEU:HD11	1:A:106:LEU:CD2	0.56	2.30	4	1
1:A:93:ILE:HG13	1:A:158:ILE:HD13	0.56	1.77	5	3
1:A:61:LEU:HD23	1:A:113:CYS:CB	0.55	2.31	1	4
1:A:117:LYS:HE3	1:A:118:ALA:HB2	0.55	1.78	8	1
1:A:106:LEU:HD13	1:A:110:PHE:HE2	0.55	1.62	3	1
1:A:147:SER:OG	1:A:159:ILE:HD12	0.55	2.01	5	1
1:A:137:ALA:O	1:A:141:LEU:HD22	0.55	2.01	1	1
1:A:96:ILE:CG1	1:A:106:LEU:HD13	0.55	2.32	2	2
1:A:62:VAL:O	1:A:62:VAL:HG13	0.55	2.02	3	1
1:A:106:LEU:HD22	1:A:110:PHE:HD2	0.54	1.58	6	1
1:A:89:ILE:HG23	1:A:158:ILE:CD1	0.54	2.30	3	2
1:A:60:LEU:CD1	1:A:103:PHE:CE1	0.53	2.91	10	1
1:A:61:LEU:HD12	1:A:61:LEU:C	0.53	2.29	1	4
1:A:118:ALA:HB3	1:A:121:ASP:O	0.53	2.03	3	2
1:A:92:TYR:CE1	1:A:110:PHE:CD2	0.53	2.97	9	2
1:A:60:LEU:HD11	1:A:110:PHE:HB2	0.53	1.80	5	2
1:A:60:LEU:HD12	1:A:106:LEU:CD2	0.53	2.34	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:HD12	1:A:145:GLU:OE1	0.53	2.03	10	1
1:A:114:SER:O	1:A:117:LYS:HG3	0.53	2.03	5	1
1:A:103:PHE:CE2	1:A:160:LEU:HD11	0.52	2.39	8	1
1:A:62:VAL:HG12	1:A:156:ILE:HB	0.52	1.81	3	1
1:A:122:LEU:HD13	1:A:130:MET:SD	0.52	2.44	9	1
1:A:73:TRP:CZ2	1:A:116:ALA:CB	0.52	2.92	10	6
1:A:159:ILE:O	1:A:160:LEU:HD23	0.52	2.04	1	1
1:A:60:LEU:HD13	1:A:60:LEU:N	0.52	2.20	10	1
1:A:92:TYR:CE1	1:A:110:PHE:CG	0.51	2.98	6	1
1:A:107:ALA:O	1:A:111:SER:CB	0.51	2.58	3	9
1:A:63:LYS:CB	1:A:78:ILE:HD12	0.51	2.35	4	1
1:A:101:GLU:CG	1:A:106:LEU:HD21	0.51	2.35	8	1
1:A:60:LEU:HD23	1:A:61:LEU:N	0.51	2.21	6	3
1:A:71:SER:HA	1:A:76:GLU:O	0.50	2.05	4	1
1:A:58:SER:HB2	1:A:160:LEU:HD13	0.50	1.83	8	1
1:A:62:VAL:CG2	1:A:89:ILE:HD13	0.50	2.36	1	1
1:A:152:THR:O	1:A:153:ASP:C	0.50	2.53	2	2
1:A:57:CYS:O	1:A:122:LEU:HD12	0.50	2.07	5	1
1:A:86:LEU:HD21	1:A:149:PRO:HB3	0.50	1.83	6	1
1:A:60:LEU:O	1:A:60:LEU:CD2	0.50	2.60	10	1
1:A:62:VAL:HG12	1:A:62:VAL:O	0.50	2.07	5	1
1:A:85:ALA:CB	1:A:156:ILE:HD12	0.50	2.37	10	2
1:A:84:GLU:O	1:A:88:LEU:HD13	0.49	2.07	2	1
1:A:73:TRP:HZ2	1:A:116:ALA:HB3	0.49	1.68	1	2
1:A:62:VAL:HB	1:A:89:ILE:HD13	0.49	1.84	3	1
1:A:62:VAL:HG13	1:A:85:ALA:HB1	0.49	1.83	3	1
1:A:111:SER:OG	1:A:116:ALA:HB2	0.49	2.07	5	1
1:A:106:LEU:HD13	1:A:106:LEU:C	0.49	2.31	6	1
1:A:101:GLU:CB	1:A:106:LEU:HD11	0.49	2.38	7	1
1:A:92:TYR:CZ	1:A:110:PHE:CG	0.49	3.01	1	4
1:A:60:LEU:HD23	1:A:60:LEU:C	0.49	2.33	2	2
1:A:93:ILE:CD1	1:A:158:ILE:HD13	0.49	2.36	8	1
1:A:71:SER:CB	1:A:76:GLU:O	0.48	2.60	4	1
1:A:88:LEU:HD22	1:A:92:TYR:OH	0.48	2.08	3	1
1:A:71:SER:OG	1:A:72:SER:N	0.48	2.46	4	1
1:A:96:ILE:CG2	1:A:146:MET:HE1	0.48	2.39	9	1
1:A:129:GLN:HB3	1:A:130:MET:HE3	0.48	1.85	6	1
1:A:62:VAL:CG1	1:A:88:LEU:HD11	0.48	2.28	10	1
1:A:62:VAL:HG21	1:A:89:ILE:HD13	0.47	1.85	1	1
1:A:60:LEU:HD13	1:A:92:TYR:CD2	0.47	2.44	9	1
1:A:72:SER:O	1:A:75:GLN:O	0.47	2.32	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:C	1:A:60:LEU:HD23	0.47	2.34	3	4
1:A:85:ALA:HB3	1:A:156:ILE:CD1	0.47	2.39	5	1
1:A:96:ILE:HD13	1:A:103:PHE:HD2	0.47	1.59	7	1
1:A:61:LEU:HD13	1:A:157:HIS:HE2	0.47	1.65	2	2
1:A:62:VAL:HG21	1:A:89:ILE:HD12	0.47	1.86	7	2
1:A:141:LEU:HD11	1:A:147:SER:CB	0.47	2.37	3	2
1:A:88:LEU:N	1:A:88:LEU:CD1	0.47	2.77	4	1
1:A:96:ILE:HG13	1:A:106:LEU:HD12	0.47	1.84	10	1
1:A:61:LEU:HD21	1:A:154:SER:HB3	0.47	1.85	5	2
1:A:59:HIS:HB2	1:A:158:ILE:O	0.47	2.09	10	2
1:A:137:ALA:O	1:A:141:LEU:HD12	0.47	2.10	9	2
1:A:134:PHE:CZ	1:A:159:ILE:HG12	0.47	2.44	8	3
1:A:132:LYS:N	1:A:133:PRO:HD2	0.46	2.25	6	4
1:A:63:LYS:HB2	1:A:78:ILE:HD12	0.46	1.84	4	2
1:A:54:ARG:HD3	1:A:124:ALA:HB1	0.46	1.87	8	1
1:A:141:LEU:HD21	1:A:147:SER:HB3	0.46	1.88	1	1
1:A:92:TYR:O	1:A:96:ILE:HD12	0.46	2.11	7	1
1:A:96:ILE:HD12	1:A:146:MET:CE	0.46	2.37	2	1
1:A:93:ILE:HA	1:A:146:MET:HE2	0.46	1.86	4	1
1:A:141:LEU:HD21	1:A:147:SER:N	0.46	2.26	2	1
1:A:141:LEU:HD12	1:A:142:ARG:N	0.46	2.25	5	1
1:A:89:ILE:HG22	1:A:90:ASN:N	0.46	2.26	5	5
1:A:86:LEU:HD21	1:A:156:ILE:HD11	0.46	1.87	7	1
1:A:151:PHE:CE2	1:A:156:ILE:HD11	0.46	2.46	7	1
1:A:106:LEU:O	1:A:107:ALA:C	0.46	2.58	9	6
1:A:138:SER:OG	1:A:139:PHE:N	0.46	2.49	9	1
1:A:60:LEU:C	1:A:60:LEU:CD2	0.45	2.89	6	3
1:A:106:LEU:CD2	1:A:110:PHE:CD2	0.45	2.98	6	1
1:A:71:SER:CA	1:A:76:GLU:O	0.45	2.63	4	1
1:A:88:LEU:O	1:A:92:TYR:CG	0.45	2.69	9	5
1:A:60:LEU:HD21	1:A:89:ILE:CD1	0.45	2.41	2	1
1:A:60:LEU:CD1	1:A:106:LEU:HD22	0.45	2.41	4	1
1:A:55:VAL:CG2	1:A:139:PHE:CE1	0.45	2.99	1	1
1:A:60:LEU:CD1	1:A:103:PHE:CZ	0.45	2.99	10	1
1:A:101:GLU:HB3	1:A:106:LEU:HD12	0.45	1.88	4	1
1:A:141:LEU:CD1	1:A:142:ARG:O	0.45	2.65	5	1
1:A:86:LEU:HD21	1:A:149:PRO:HG3	0.45	1.89	8	1
1:A:72:SER:OG	1:A:112:ASP:C	0.44	2.59	4	1
1:A:73:TRP:CZ2	1:A:111:SER:O	0.44	2.70	7	3
1:A:135:GLU:OE2	1:A:139:PHE:CZ	0.44	2.70	1	1
1:A:159:ILE:HG22	1:A:160:LEU:N	0.44	2.27	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:ILE:HG22	1:A:79:THR:N	0.44	2.27	4	1
1:A:96:ILE:CG1	1:A:106:LEU:CD1	0.44	2.95	7	2
1:A:82:LYS:HG2	1:A:83:GLU:N	0.44	2.28	4	1
1:A:151:PHE:CZ	1:A:156:ILE:HD11	0.44	2.48	7	1
1:A:89:ILE:CG2	1:A:90:ASN:N	0.44	2.81	5	5
1:A:60:LEU:HD21	1:A:110:PHE:O	0.44	2.13	3	1
1:A:85:ALA:HB3	1:A:156:ILE:HD12	0.44	1.90	5	2
1:A:106:LEU:CD1	1:A:107:ALA:N	0.44	2.77	6	1
1:A:145:GLU:O	1:A:160:LEU:HA	0.44	2.13	8	1
1:A:79:THR:O	1:A:79:THR:HG23	0.44	2.12	3	1
1:A:63:LYS:HB2	1:A:78:ILE:HG21	0.44	1.90	9	1
1:A:122:LEU:HD22	1:A:130:MET:HE2	0.43	1.88	4	1
1:A:162:THR:O	1:A:163:GLU:CB	0.43	2.66	6	1
1:A:115:SER:O	1:A:118:ALA:N	0.43	2.50	9	1
1:A:62:VAL:CG2	1:A:89:ILE:CD1	0.43	2.96	2	5
1:A:141:LEU:HD21	1:A:147:SER:CA	0.43	2.43	2	1
1:A:141:LEU:HD12	1:A:145:GLU:CB	0.43	2.42	10	1
1:A:88:LEU:O	1:A:92:TYR:CD2	0.43	2.72	6	4
1:A:60:LEU:HB2	1:A:103:PHE:CZ	0.43	2.48	1	1
1:A:59:HIS:CD2	1:A:59:HIS:C	0.43	2.97	4	1
1:A:96:ILE:HD11	1:A:106:LEU:CD1	0.43	2.44	6	1
1:A:96:ILE:HG13	1:A:106:LEU:CD1	0.43	2.44	10	1
1:A:73:TRP:CD1	1:A:73:TRP:H	0.43	2.32	3	1
1:A:61:LEU:HD21	1:A:154:SER:CB	0.43	2.42	5	1
1:A:86:LEU:HD21	1:A:156:ILE:CD1	0.43	2.44	7	1
1:A:141:LEU:HD21	1:A:147:SER:CB	0.43	2.44	1	1
1:A:86:LEU:HD13	1:A:149:PRO:HG2	0.43	1.91	5	1
1:A:89:ILE:CG1	1:A:158:ILE:HG13	0.42	2.44	10	2
1:A:70:PRO:HB2	1:A:78:ILE:O	0.42	2.14	4	1
1:A:58:SER:O	1:A:159:ILE:HA	0.42	2.14	8	1
1:A:132:LYS:CB	1:A:133:PRO:CD	0.42	2.97	10	2
1:A:137:ALA:C	1:A:141:LEU:HD12	0.42	2.39	9	1
1:A:84:GLU:O	1:A:88:LEU:HD22	0.42	2.14	4	1
1:A:61:LEU:HD22	1:A:157:HIS:HE1	0.42	1.71	5	1
1:A:147:SER:OG	1:A:159:ILE:N	0.42	2.52	8	1
1:A:80:ARG:HD2	1:A:88:LEU:HD21	0.42	1.92	4	1
1:A:62:VAL:CG2	1:A:89:ILE:HD12	0.42	2.45	9	2
1:A:60:LEU:HD22	1:A:62:VAL:HG23	0.42	1.91	6	1
1:A:91:GLY:O	1:A:95:LYS:HG3	0.42	2.15	8	1
1:A:75:GLN:O	1:A:76:GLU:O	0.42	2.38	4	1
1:A:61:LEU:HB2	1:A:157:HIS:CE1	0.42	2.50	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:CD1	1:A:92:TYR:CD2	0.42	3.02	2	2
1:A:70:PRO:HA	1:A:78:ILE:HD12	0.42	1.92	8	1
1:A:107:ALA:HB3	1:A:119:ARG:O	0.42	2.14	10	1
1:A:61:LEU:CD1	1:A:157:HIS:CE1	0.42	2.99	6	1
1:A:92:TYR:OH	1:A:110:PHE:CD1	0.42	2.69	6	1
1:A:93:ILE:CG2	1:A:94:GLN:N	0.42	2.83	4	1
1:A:58:SER:O	1:A:160:LEU:N	0.42	2.53	1	1
1:A:118:ALA:HB1	1:A:121:ASP:OD1	0.41	2.15	5	1
1:A:102:ASP:OD1	1:A:102:ASP:N	0.41	2.52	8	1
1:A:133:PRO:HB2	1:A:150:VAL:HG13	0.41	1.91	8	1
1:A:96:ILE:HA	1:A:101:GLU:O	0.41	2.15	10	1
1:A:70:PRO:O	1:A:77:LYS:HA	0.41	2.14	4	1
1:A:131:GLN:HG2	1:A:134:PHE:HB2	0.41	1.92	8	1
1:A:103:PHE:CD2	1:A:160:LEU:CB	0.41	3.03	10	1
1:A:54:ARG:CB	1:A:125:PHE:O	0.41	2.67	4	1
1:A:103:PHE:CD2	1:A:160:LEU:HB3	0.41	2.51	10	1
1:A:132:LYS:HB3	1:A:133:PRO:CD	0.41	2.46	8	1
1:A:160:LEU:N	1:A:160:LEU:CD1	0.41	2.83	8	1
1:A:69:ARG:CG	1:A:69:ARG:O	0.41	2.67	10	1
1:A:135:GLU:CD	1:A:139:PHE:CE1	0.41	2.99	1	1
1:A:92:TYR:OH	1:A:110:PHE:CG	0.41	2.73	7	1
1:A:65:SER:N	1:A:80:ARG:O	0.41	2.54	10	1
1:A:56:ARG:HD2	1:A:124:ALA:HB2	0.41	1.93	2	1
1:A:86:LEU:HD21	1:A:149:PRO:CB	0.41	2.46	6	1
1:A:134:PHE:CE2	1:A:159:ILE:CG1	0.41	3.02	8	1
1:A:60:LEU:HB3	1:A:107:ALA:HA	0.41	1.92	10	1
1:A:141:LEU:HD13	1:A:141:LEU:HA	0.41	1.81	10	1
1:A:103:PHE:CE2	1:A:158:ILE:HG22	0.41	2.51	6	1
1:A:58:SER:CB	1:A:160:LEU:HD13	0.41	2.45	8	1
1:A:136:ASP:O	1:A:140:ALA:CB	0.41	2.68	9	1
1:A:141:LEU:HD21	1:A:147:SER:HA	0.41	1.93	10	1
1:A:160:LEU:HD23	1:A:160:LEU:C	0.40	2.41	4	1
1:A:159:ILE:CG2	1:A:160:LEU:N	0.40	2.83	9	1
1:A:60:LEU:HD22	1:A:89:ILE:HD11	0.40	1.92	3	1
1:A:127:ARG:HB3	1:A:139:PHE:CZ	0.40	2.52	3	1
1:A:134:PHE:CE1	1:A:159:ILE:CG1	0.40	3.05	3	1
1:A:86:LEU:HD23	1:A:89:ILE:HG22	0.40	1.92	8	1
1:A:135:GLU:OE1	1:A:139:PHE:CD1	0.40	2.74	9	1
1:A:64:HIS:HA	1:A:80:ARG:O	0.40	2.17	3	1
1:A:78:ILE:CG2	1:A:80:ARG:HG3	0.40	2.46	4	1
1:A:132:LYS:HB2	1:A:133:PRO:CD	0.40	2.46	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ASP:O	1:A:106:LEU:CB	0.40	2.70	6	1
1:A:107:ALA:O	1:A:111:SER:HB2	0.40	2.15	7	1
1:A:104:GLU:O	1:A:119:ARG:HB2	0.40	2.15	8	1
1:A:61:LEU:HB3	1:A:113:CYS:HB3	0.40	1.92	9	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	110/114 (96%)	96±3 (87±3%)	14±3 (12±2%)	1±1 (1±1%)	20	70
All	All	1100/1140 (96%)	955 (87%)	137 (12%)	8 (1%)	20	70

All 8 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	153	ASP	1
1	A	80	ARG	1
1	A	71	SER	1
1	A	75	GLN	1
1	A	76	GLU	1
1	A	121	ASP	1
1	A	63	LYS	1
1	A	127	ARG	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	95/97 (98%)	68±3 (71±4%)	28±3 (29±4%)	1	18
All	All	950/970 (98%)	675 (71%)	275 (29%)	1	18

All 68 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	58	SER	10
1	A	89	ILE	10
1	A	82	LYS	9
1	A	138	SER	9
1	A	63	LYS	8
1	A	72	SER	7
1	A	80	ARG	7
1	A	127	ARG	7
1	A	146	MET	7
1	A	161	ARG	7
1	A	77	LYS	6
1	A	117	LYS	6
1	A	119	ARG	6
1	A	54	ARG	6
1	A	93	ILE	6
1	A	132	LYS	6
1	A	74	ARG	5
1	A	75	GLN	5
1	A	81	THR	5
1	A	115	SER	5
1	A	145	GLU	5
1	A	160	LEU	5
1	A	162	THR	5
1	A	66	GLN	5
1	A	135	GLU	5
1	A	76	GLU	4
1	A	83	GLU	4
1	A	97	LYS	4
1	A	104	GLU	4
1	A	109	GLN	4
1	A	141	LEU	4
1	A	154	SER	4
1	A	163	GLU	4
1	A	56	ARG	4
1	A	69	ARG	4
1	A	86	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	129	GLN	4
1	A	130	MET	4
1	A	84	GLU	3
1	A	122	LEU	3
1	A	60	LEU	3
1	A	68	ARG	3
1	A	95	LYS	3
1	A	79	THR	3
1	A	126	SER	3
1	A	105	SER	3
1	A	87	GLU	3
1	A	136	ASP	3
1	A	131	GLN	3
1	A	61	LEU	2
1	A	78	ILE	2
1	A	100	GLU	2
1	A	102	ASP	2
1	A	106	LEU	2
1	A	71	SER	2
1	A	88	LEU	2
1	A	121	ASP	2
1	A	143	THR	2
1	A	90	ASN	1
1	A	62	VAL	1
1	A	101	GLU	1
1	A	142	ARG	1
1	A	59	HIS	1
1	A	65	SER	1
1	A	156	ILE	1
1	A	147	SER	1
1	A	67	SER	1
1	A	153	ASP	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SO4	A	200	-	4,4,4	0.36±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SO4	A	200	-	6,6,6	0.07±0.00	0±0 (0±0%)

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided