

Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	6TT8
Title	:	Haddock model of NDM-1/morin complex
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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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

2019)
;

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $SOLUTION \ NMR$

The overall completeness of chemical shifts assignment is 39%.

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.



Motrio	Whole archive	NMR archive
Metric	$(\# { m Entries})$	$(\# { m Entries})$
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 <=5%

Mol	Chain	Length	Quality of chain		
1	А	227	85%	8%	7%



2 Ensemble composition and analysis (i)

This entry contains 56 models. Model 11 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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 ran	ge (total)	Backbone RMSD (Å)	Medoid model	
1	A:49-A:65,	A:73-A:267	0.18	11	
	(212)				

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 6 clusters and 3 single-model clusters were found.

Cluster number	Models
1	10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23,
1	24, 25, 26, 27, 28, 29, 30, 31, 32, 33
2	34,35,36,37,38,39,40,41
3	2, 3, 4, 6, 7, 8, 9
4	1,42,43,44,45,46,48
5	$49,\ 50,\ 51,\ 53,\ 56$
6	52, 55
Single-model clusters	5; 47; 54



3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3352 atoms, of which 1641 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called Metallo beta lactamase NDM-1.

Mol	Chain	Residues	Atoms				Trace		
1	Λ	207	Total	С	Η	Ν	Ο	S	0
	A	221	3323	1061	1636	298	320	8	U

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms
2	А	2	Total Zn

• Molecule 3 is 2-[2,4-bis(oxidanyl)phenyl]-3,5,7-tris(oxidanyl)chromen-4-one (three-letter code: MRI) (formula: C₁₅H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			
2	Δ	1	Total	С	Η	Ο
3	A	1	27	15	5	7



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: Metallo beta lactamase NDM-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: Metallo beta lactamase NDM-1



4.2.2 Score per residue for model 2





4.2.3 Score per residue for model 3

• Molecule 1: Metallo beta lactamase NDM-1



4.2.4 Score per residue for model 4

• Molecule 1: Metallo beta lactamase NDM-1



4.2.5 Score per residue for model 5

• Molecule 1: Metallo beta lactamase NDM-1



4.2.6 Score per residue for model 6

• Molecule 1: Metallo beta lactamase NDM-1



4.2.7 Score per residue for model 7

~			
Chain A:	81%	12%	7%



4.2.8 Score per residue for model 8

 \bullet Molecule 1: Metallo beta lactamase NDM-1



4.2.9 Score per residue for model 9

 \bullet Molecule 1: Metallo beta lactamase NDM-1



4.2.10 Score per residue for model 10

• Molecule 1: Metallo beta lactamase NDM-1



4.2.11 Score per residue for model 11 (medoid)



S246 D43 1255 1255 1256 144 1256 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1266 145 1267 145 1268 145 1269 145 1260 145 127 145 127 145 123 145 124 141 123 145 123 145 123 123 124 123 123 123 123 123 123 123 123 123 123 123 123 123 <tr/td>

4.2.12 Score per residue for model 12

• Molecule 1: Metallo beta lactamase NDM-1



4.2.13 Score per residue for model 13

• Molecule 1: Metallo beta lactamase NDM-1



4.2.14 Score per residue for model 14

• Molecule 1: Metallo beta lactamase NDM-1



4.2.15 Score per residue for model 15





4.2.16 Score per residue for model 16

• Molecule 1: Metallo beta lactamase NDM-1



4.2.17 Score per residue for model 17

• Molecule 1: Metallo beta lactamase NDM-1



4.2.18 Score per residue for model 18

 \bullet Molecule 1: Metallo beta lactamase NDM-1



84%

4.2.19 Score per residue for model 19

 \bullet Molecule 1: Metallo beta lactamase NDM-1

Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Metallo beta lactamase NDM-1



4.2.21 Score per residue for model 21

 \bullet Molecule 1: Metallo beta lactamase NDM-1



4.2.22 Score per residue for model 22

• Molecule 1: Metallo beta lactamase NDM-1



4.2.23 Score per residue for model 23





4.2.24 Score per residue for model 24

• Molecule 1: Metallo beta lactamase NDM-1



4.2.25 Score per residue for model 25

• Molecule 1: Metallo beta lactamase NDM-1



4.2.26 Score per residue for model 26

• Molecule 1: Metallo beta lactamase NDM-1



4.2.27 Score per residue for model 27





4.2.28 Score per residue for model 28

• Molecule 1: Metallo beta lactamase NDM-1



4.2.29 Score per residue for model 29

• Molecule 1: Metallo beta lactamase NDM-1



4.2.30 Score per residue for model 30

 \bullet Molecule 1: Metallo beta lactamase NDM-1



4.2.31 Score per residue for model 31





4.2.32 Score per residue for model 32

• Molecule 1: Metallo beta lactamase NDM-1



4.2.33 Score per residue for model 33

• Molecule 1: Metallo beta lactamase NDM-1



4.2.34 Score per residue for model 34

• Molecule 1: Metallo beta lactamase NDM-1



4.2.35 Score per residue for model 35





4.2.36 Score per residue for model 36

• Molecule 1: Metallo beta lactamase NDM-1



4.2.37 Score per residue for model 37

• Molecule 1: Metallo beta lactamase NDM-1



4.2.38 Score per residue for model 38

• Molecule 1: Metallo beta lactamase NDM-1



4.2.39 Score per residue for model 39





4.2.40 Score per residue for model 40

• Molecule 1: Metallo beta lactamase NDM-1



4.2.41 Score per residue for model 41

• Molecule 1: Metallo beta lactamase NDM-1



4.2.42 Score per residue for model 42

• Molecule 1: Metallo beta lactamase NDM-1



4.2.43 Score per residue for model 43





4.2.44 Score per residue for model 44

• Molecule 1: Metallo beta lactamase NDM-1



4.2.45 Score per residue for model 45

• Molecule 1: Metallo beta lactamase NDM-1



4.2.46 Score per residue for model 46

• Molecule 1: Metallo beta lactamase NDM-1



4.2.47 Score per residue for model 47

• Molecule 1: Metallo beta lactamase NDM-1



4.2.48 Score per residue for model 48





4.2.49 Score per residue for model 49

• Molecule 1: Metallo beta lactamase NDM-1



4.2.50 Score per residue for model 50

• Molecule 1: Metallo beta lactamase NDM-1



4.2.51 Score per residue for model 51

• Molecule 1: Metallo beta lactamase NDM-1



4.2.52 Score per residue for model 52

 \bullet Molecule 1: Metallo beta lactamase NDM-1

Chain A:



A255

4.2.53 Score per residue for model 53

• Molecule 1: Metallo beta lactamase NDM-1



4.2.54 Score per residue for model 54

• Molecule 1: Metallo beta lactamase NDM-1



4.2.55 Score per residue for model 55

• Molecule 1: Metallo beta lactamase NDM-1



4.2.56 Score per residue for model 56









5 Refinement protocol and experimental data overview (i)

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

Of the 2800 calculated structures, 56 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
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	993
Number of shifts mapped to atoms	993
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%



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: MRI, ZN $\,$

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (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	А	1571	1531	1530	9 ± 2
2	А	2	0	0	0 ± 0
3	А	22	5	5	3 ± 1
All	All	89320	86016	85997	616

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 4.

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

Atom 1	Atom 2	$Clash(\lambda)$	Distance(Å)	Models	
Atom-1	Atom-2		Distance(A)	Worst	Total
1:A:122:HIS:CG	3:A:303:MRI:H3	0.71	2.21	29	11
1:A:121:ALA:HA	1:A:126:MET:SD	0.70	2.25	35	42
1:A:220:ASN:H	3:A:303:MRI:H5	0.70	1.43	5	1
1:A:122:HIS:CE1	3:A:303:MRI:H3	0.66	2.25	30	3
2:A:302:ZN:ZN	3:A:303:MRI:OAD	0.66	1.45	5	8
2:A:301:ZN:ZN	3:A:303:MRI:OAD	0.64	1.47	15	6
1:A:248:MET:SD	1:A:251:SER:HB2	0.63	2.34	19	51
1:A:124:ASP:OD1	3:A:303:MRI:H9	0.63	1.94	23	3
1:A:122:HIS:HB3	1:A:124:ASP:OD1	0.62	1.93	4	23
1:A:120:HIS:CE1	1:A:125:LYS:HG3	0.62	2.30	19	47

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	lious page	0	0	Models	
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	Distance(A)	Worst	Total
3:A:303:MRI:OAB	3:A:303:MRI:OAE	0.62	2.17	36	56
1:A:55:ALA:HB3	1:A:58:VAL:HB	0.60	1.73	49	25
1:A:122:HIS:CD2	3:A:303:MRI:H3	0.56	2.36	28	2
1:A:149:ALA:HB3	1:A:150:PRO:HD3	0.55	1.77	35	16
1:A:75:SER:HA	1:A:249:SER:O	0.53	2.04	48	19
1:A:225:ASP:O	1:A:229:TYR:HB2	0.52	2.04	1	24
3:A:303:MRI:OAE	3:A:303:MRI:CAM	0.51	2.59	20	56
1:A:260:THR:O	1:A:264:ARG:HG3	0.50	2.07	31	3
1:A:82:ASP:O	1:A:85:ARG:HG2	0.50	2.06	4	20
1:A:61:HIS:O	1:A:76:ASN:HA	0.49	2.07	34	21
1:A:93:TRP:CH2	1:A:124:ASP:HB3	0.49	2.42	31	7
1:A:93:TRP:CZ3	1:A:124:ASP:HB3	0.49	2.42	8	4
1:A:65:LEU:HB2	1:A:93:TRP:CD2	0.49	2.42	31	2
1:A:211:LYS:O	1:A:258:ALA:HB1	0.49	2.08	41	26
1:A:124:ASP:O	1:A:125:LYS:HE2	0.49	2.07	5	2
1:A:119:THR:O	1:A:194:ILE:HG12	0.49	2.07	44	13
1:A:98:THR:OG1	1:A:128:GLY:HA3	0.49	2.08	35	17
1:A:123:GLN:HA	1:A:154:MET:SD	0.48	2.49	26	6
1:A:218:LEU:HG	1:A:265:MET:SD	0.48	2.49	34	1
1:A:142:ASN:HB3	1:A:145:SER:OG	0.47	2.08	28	36
1:A:138:ALA:HA	1:A:158:GLN:OE1	0.47	2.10	9	4
1:A:63:SER:O	1:A:74:ALA:HA	0.46	2.10	23	2
1:A:64:TYR:HA	1:A:73:VAL:O	0.46	2.10	10	6
1:A:208:CYS:HB3	3:A:303:MRI:H5	0.46	1.88	48	1
1:A:61:HIS:NE2	1:A:77:GLY:HA3	0.45	2.27	12	9
1:A:123:GLN:OE1	3:A:303:MRI:H9	0.45	2.11	39	1
1:A:120:HIS:CD2	1:A:122:HIS:HB2	0.45	2.47	47	4
1:A:173:THR:O	1:A:175:PRO:HD3	0.44	2.13	26	1
1:A:88:VAL:O	1:A:116:ALA:HA	0.44	2.13	28	4
1:A:49:LEU:HD11	1:A:97:GLN:HB3	0.44	1.90	17	1
1:A:75:SER:HB2	1:A:93:TRP:NE1	0.43	2.28	46	1
1:A:90:ASP:OD2	1:A:125:LYS:HD3	0.43	2.13	29	5
1:A:65:LEU:HD13	1:A:93:TRP:CE3	0.43	2.47	35	1
1:A:219:GLY:HA2	3:A:303:MRI:H6	0.43	1.91	25	1
1:A:208:CYS:SG	1:A:249:SER:HB2	0.43	2.54	46	1
1:A:122:HIS:CE1	3:A:303:MRI:H9	0.43	2.49	24	1
1:A:104:TRP:CE2	1:A:108:GLU:HG3	0.42	2.49	50	2
1:A:123:GLN:HB3	3:A:303:MRI:H9	0.42	1.91	39	2
1:A:96:ASP:O	1:A:100:GLN:HG3	0.42	2.15	35	4
1:A:125:LYS:HD2	1:A:208:CYS:SG	0.41	2.55	44	3
1:A:128:GLY:O	1:A:132:LEU:HG	0.41	2.16	41	1

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Atom 1	Atom 2	$Clack(\lambda)$	Distance (Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:65:LEU:HD22	1:A:93:TRP:CE3	0.41	2.51	6	1
1:A:57:ASN:OD1	1:A:81:ARG:HD2	0.41	2.16	8	1
1:A:173:THR:C	1:A:175:PRO:HD3	0.41	2.36	16	1
1:A:149:ALA:N	1:A:150:PRO:HD2	0.41	2.30	42	4
1:A:126:MET:HG2	1:A:129:MET:CG	0.41	2.46	56	1
1:A:121:ALA:O	1:A:152:GLU:HG3	0.40	2.16	9	1
1:A:89:VAL:O	1:A:90:ASP:HB2	0.40	2.16	43	1

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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	А	212/227~(93%)	203 ± 2 (96 $\pm1\%$)	$9\pm2~(4\pm1\%)$	0±0 (0±0%)	54 85
All	All	11872/12712 (93%)	$11381 \ (96\%)$	478 (4%)	13~(0%)	54 85

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	А	90	ASP	10
1	А	188	GLY	2
1	А	83	GLY	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	А	159/170~(94%)	$149\pm2 (93\pm1\%)$	$10\pm2~(7\pm1\%)$	21 69	
All	All	8904/9520~(94%)	8323 (93%)	581 (7%)	21 69	



Mol	Chain	Res	Type	Models (Total)
1	А	193	ASN	56
1	А	260	THR	52
1	А	122	HIS	50
1	А	244	SER	41
1	А	201	THR	35
1	А	191	SER	34
1	А	226	THR	33
1	А	173	THR	31
1	А	229	TYR	27
1	А	130	ASP	18
1	А	60	GLN	18
1	А	267	ASP	17
1	А	162	THR	17
1	А	125	LYS	15
1	А	94	THR	14
1	А	63	SER	13
1	А	255	SER	12
1	А	190	THR	11
1	А	217	SER	9
1	А	90	ASP	9
1	А	75	SER	8
1	А	177	PHE	8
1	А	223	ASP	6
1	А	202	ASP	6
1	А	115	LEU	5
1	А	212	ASP	4
1	А	126	MET	4
1	А	211	LYS	3
1	А	124	ASP	3
1	А	96	ASP	2
1	А	81	ARG	2
1	А	195	THR	2
1	А	56	PRO	2
1	А	106	LYS	1
1	A	216	LYS	1
1	A	154	MET	1
1	А	139	THR	1
1	A	232	SER	1
1	A	248	MET	1
1	A	62	THR	1
1	A	251	SER	1

All 47 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

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Mol	Chain	\mathbf{Res}	Type	Models (Total)
1	А	176	ASN	1
1	А	123	GLN	1
1	А	199	ASP	1
1	А	213	SER	1
1	А	227	GLU	1
1	А	214	LYS	1

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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)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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.

Mal	Tune	Chain	Dog	Tink		Bond leng	ths
	туре	Cham	nes		Counts	RMSZ	#Z>2
3	MRI	А	303	2	20,24,24	$0.66 {\pm} 0.00$	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.

Mal	Tuno	Chain	Res	Tink	Bond angles		
	туре				Counts	RMSZ	$\#Z{>}2$
3	MRI	А	303	2	$28,\!36,\!36$	$1.17 {\pm} 0.00$	4 ± 0 (14 $\pm0\%$)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MRI	А	303	2	-	$0 \pm 0,3,4,4$	$0{\pm}0{,}3{,}3{,}3$

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Chain	Dog	Tuno	Atoms	7	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$	Models	
	Chain	nes	туре	Atoms				Worst	Total
3	А	303	MRI	CAP-CAJ-CAI	3.23	119.48	123.05	1	56
3	А	303	MRI	OAA-CAJ-CAP	2.67	119.23	116.11	1	56
3	А	303	MRI	CAM-CAN-CAI	2.60	117.74	121.38	1	56
3	А	303	MRI	CAO-CAI-CAJ	2.16	120.32	117.82	1	56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 (i)

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

7.1.1 Bookkeeping (i)

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	993
Number of shifts mapped to atoms	993
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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\bf Correction}\pm{\bf precision},ppm$	Suggested action
$^{13}C_{\alpha}$	220	0.12 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	160	0.21 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	201	-0.06 ± 0.08	None needed (< 0.5 ppm)
¹⁵ N	206	0.65 ± 0.35	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 39%, i.e. 926 atoms were assigned a chemical shift out of a possible 2397. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	778/1040~(75%)	193/414~(47%)	392/424 ($92%$)	193/202~(96%)
Sidechain	148/1151~(13%)	0/667~(0%)	148/440~(34%)	0/44~(0%)

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	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$			
Aromatic	0/206~(0%)	0/111~(0%)	0/82~(0%)	0/13~(0%)			
Overall	926/2397 (39%)	193/1192~(16%)	540/946~(57%)	193/259~(75%)			

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 39%, i.e. 993 atoms were assigned a chemical shift out of a possible 2575. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	833/1113 (75%)	206/443~(47%)	421/454~(93%)	206/216 (95%)
Sidechain	160/1238~(13%)	0/719~(0%)	160/470~(34%)	0/49~(0%)
Aromatic	0/224~(0%)	0/121~(0%)	0/90~(0%)	0/13~(0%)
Overall	993/2575~(39%)	206/1283~(16%)	581/1014~(57%)	206/278~(74%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (1)

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:



