



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 27, 2016 – 08:48 AM BST

PDB ID : 2V93  
Title : EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR  
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
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A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

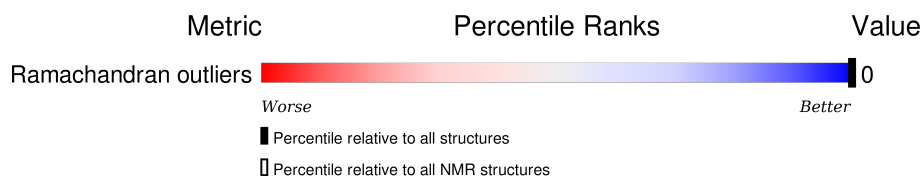
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

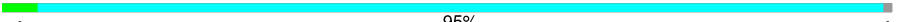
The overall completeness of chemical shifts assignment was not calculated.

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)
Ramachandran outliers	111179	9975

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  $\geq 3$ , 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	370	 95%

## 2 Ensemble composition and analysis ⓘ

This entry contains 50 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 39 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:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16)	-0.00	39

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

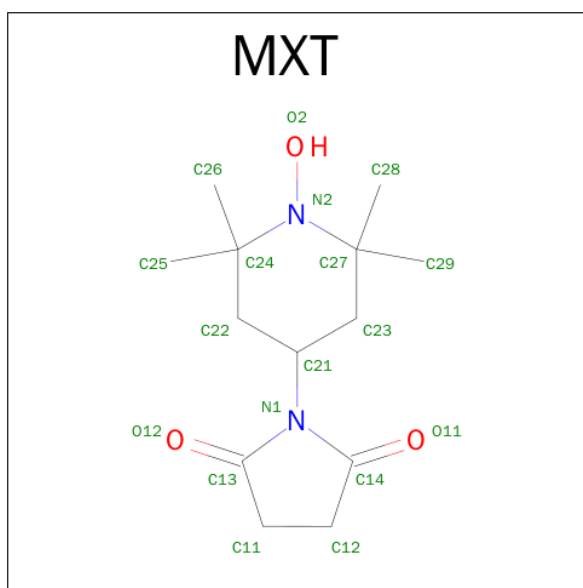
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	366	Total	C	H	N	O	S	0
			2904	1169	547	583	581	24	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	ASP	ENGINEERED MUTATION	UNP P0AEY0
A	211	CYS	SER	ENGINEERED MUTATION	UNP P0AEY0

- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPYRROLIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (three-letter code: MXT) (formula:  $C_{13}H_{22}N_2O_3$ ).



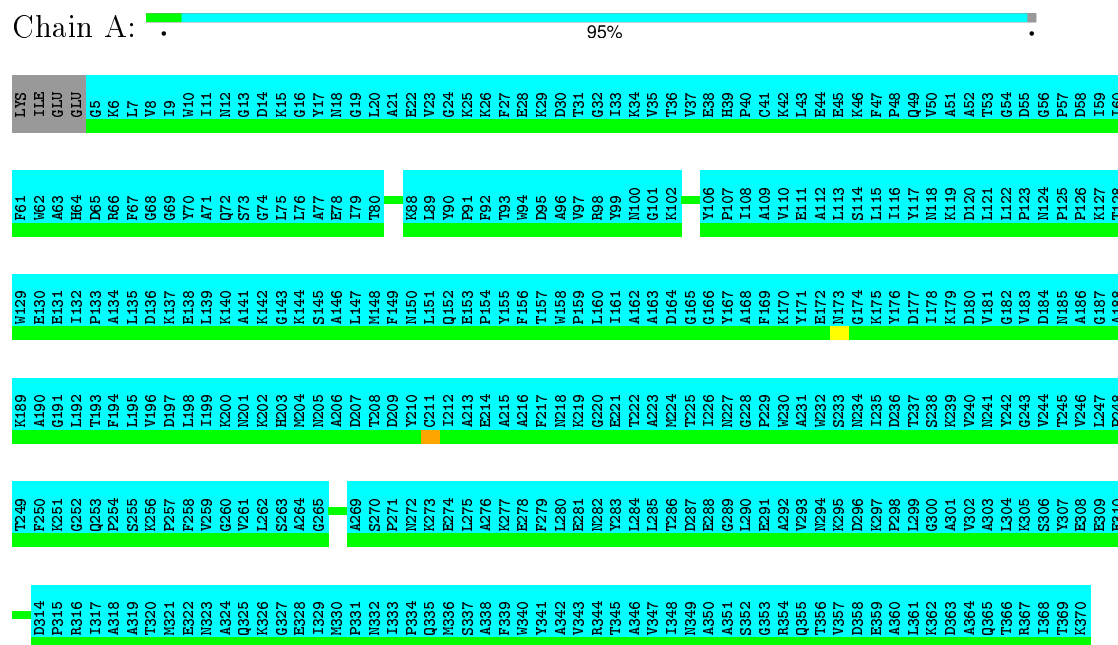
Mol	Chain	Residues	Atoms				
2	A	1	Total	C	H	N	O
			444	156	228	24	36
2	A	1	Total	C	H	N	O
			444	156	228	24	36

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

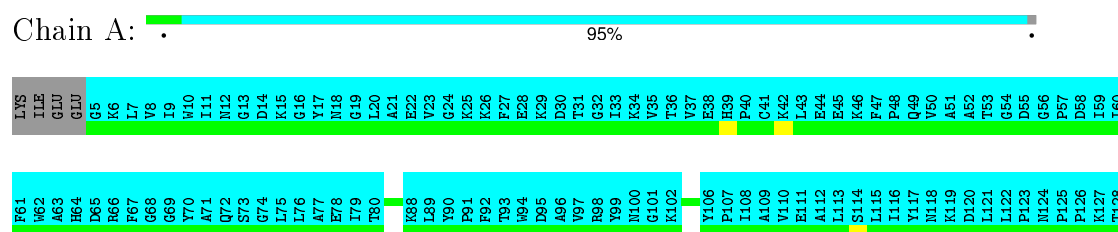
- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 39. Colouring as in section 4.1 above.

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN



D314	T249	K189	H129
F315	F250	A190	E130
R316	K251	G191	E131
I317	G252	L192	I132
A318	I317	T193	P133
A319	P254	F194	A134
T320	S255	L195	L135
M321	K256	V196	D136
E322	P257	D197	K137
N323	F258	L198	E138
A324	V259	I199	L139
Q325	G260	K200	K140
K326	V261	N201	A141
G327	L262	K202	K142
E328	S263	H203	G143
I329	A264	M204	K144
M330	G265	N205	S145
P331		A206	A146
N332	A269	D207	L147
I333	S270	T208	M148
P334	F271	D209	F149
Q335	N272	Y210	N150
M336	K273	C211	L151
S337	E274	I212	Q152
A338	L275	A213	E153
F339	A276	E214	P154
W340	K277	A215	Y155
Y341	E278	A216	F156
A342	F279	F217	T157
V343	L280	N218	W158
R344	E281	K219	P159
T345	N282	G220	L160
A346	Y283	E221	I161
V347	L284	T222	A162
I348	L285	A223	A163
M349	T286	M224	D164
A350	D287	T225	G165
A351	E288	I226	G166
S352	G289	N227	Y167
G353	L290	G228	A168
R354	E291	P229	F169
Q355	A292	W230	K170
T356	V293	A231	Y171
V357	N294	W232	E172
D358	K295	S233	N173
E359	D296	M234	G174
A360	K297	I235	K175
L361	P298	D236	Y176
K362	L299	T237	D177
D363	G300	S238	I178
A364	A301	K239	K179
Q365	V302	V240	D180
T366	A303	N241	V181
R367	L304	Y242	G182
I368	K305	G243	V183
T369	S306	V244	D184
K370	T307	T245	M185
	E308	V246	A186
	E309	L247	G187
	E310	P248	A188

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE SIMULATED ANNEALING DYNAMICS*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

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

Software name
A PRE PEUDOPOTENTIAL, A QUARTIC VAN DER WAALS REPULSION TERM TO PREVENT AT
XPLOR-NIH

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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: MXT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.00±0.01	0±0/64 (0.0±0.0%)	1.17±0.04	0±0/80 (0.1±0.2%)
All	All	1.00	0/3200 (0.0%)	1.17	2/4000 (0.1%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	313	LYS	O-C-N	-5.74	113.51	122.70	48	2

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	-2113	-424	14	0±0
2	A	432	456	500	14±4
All	All	-84050	1600	25660	695

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 0.

5 of 168 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:600[A]:MXT:O11	2:A:600[A]:MXT:H231	0.83	1.73	29	3
2:A:600[B]:MXT:O11	2:A:600[B]:MXT:H231	0.83	1.73	46	4
2:A:500[F]:MXT:H231	2:A:500[F]:MXT:O11	0.83	1.73	24	10
2:A:500[D]:MXT:H231	2:A:500[D]:MXT:O11	0.83	1.73	10	4
2:A:500[A]:MXT:H231	2:A:500[A]:MXT:O11	0.82	1.75	24	3

## 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	16/370 (4%)	15±0 (94±0%)	1±0 (6±0%)	0±0 (0±0%)	100	100
All	All	800/18500 (4%)	750 (94%)	50 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

### 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	0	-	-	-
All	All	0	-	-	-

There are no protein residues with a non-rotameric sidechain to report.

### 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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

24 ligands are 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	MXT	A	500[A]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[B]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[C]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[D]	1	19,19,19	1.88±0.00	0±0 (0±0%)
2	MXT	A	500[E]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[F]	1	19,19,19	1.91±0.00	0±0 (0±0%)
2	MXT	A	500[U]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[V]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	500[W]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[X]	1	19,19,19	1.88±0.00	0±0 (0±0%)
2	MXT	A	500[Y]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	500[Z]	1	19,19,19	1.91±0.00	0±0 (0±0%)
2	MXT	A	600[A]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[B]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[C]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[D]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[E]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[F]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[U]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[V]	1	19,19,19	1.89±0.00	0±0 (0±0%)
2	MXT	A	600[W]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[X]	1	19,19,19	1.89±0.00	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	600[Y]	1	19,19,19	1.90±0.00	0±0 (0±0%)
2	MXT	A	600[Z]	1	19,19,19	1.89±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	MXT	A	500[A]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[B]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[C]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[D]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[E]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[F]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	500[U]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[V]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[W]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	500[X]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[Y]	1	21,31,31	1.37±0.01	0±0 (0±0%)
2	MXT	A	500[Z]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[A]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	600[B]	1	21,31,31	1.36±0.01	0±0 (0±0%)
2	MXT	A	600[C]	1	21,31,31	1.39±0.01	0±0 (0±0%)
2	MXT	A	600[D]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[E]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[F]	1	21,31,31	1.35±0.01	0±0 (0±0%)
2	MXT	A	600[U]	1	21,31,31	1.38±0.01	0±0 (0±0%)
2	MXT	A	600[V]	1	21,31,31	1.36±0.01	0±0 (0±0%)
2	MXT	A	600[W]	1	21,31,31	1.39±0.01	0±0 (0±0%)
2	MXT	A	600[X]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[Y]	1	21,31,31	1.40±0.01	0±0 (0±0%)
2	MXT	A	600[Z]	1	21,31,31	1.35±0.01	0±0 (0±0%)

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
2	MXT	A	500[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	500[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	600[Z]	1	-	0±0,4,39,39	0±0,2,2,2

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 [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided