



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:34 PM BST

PDB ID : 1SHC
Title : SHC PTB DOMAIN COMPLEXED WITH A TRKA RECEPTOR PHOSPHOPEPTIDE, NMR, MINIMIZED AVERAGE STRUCTURE
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Deposited on : 1996-03-27

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
<http://wwpdb.org/validation/2016/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
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

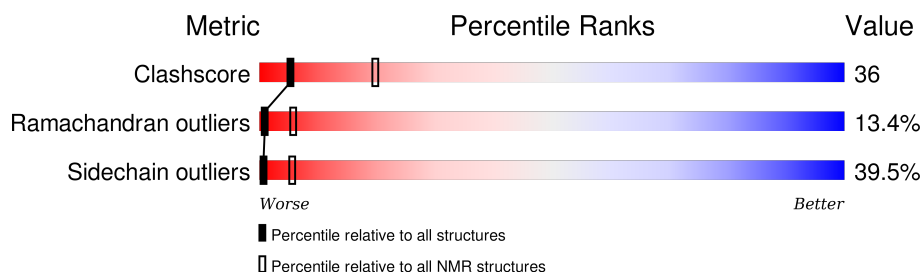
1 Overall quality at a glance

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)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	195	
2	B	12	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3189 atoms, of which 1587 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SHC.

Mol	Chain	Residues	Atoms						Trace
1	A	195	Total	C	H	N	O	S	0
			2993	932	1497	275	276	13	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	GLY	CONFLICT	UNP P29353

- Molecule 2 is a protein called TRKA RECEPTOR PHOSPHOPEPTIDE.

Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	0
			196	65	90	16	24	1	

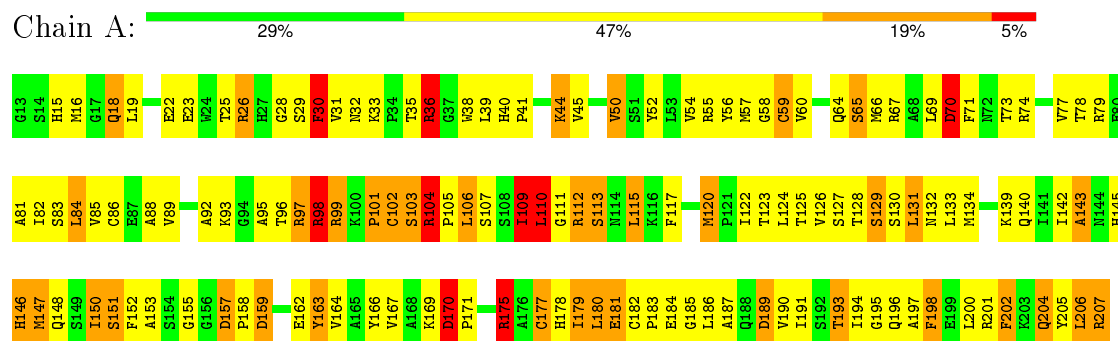
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	490	PTR	TYR	MODIFIED RESIDUE	UNP P04629

4 Residue-property plots

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: SHC



• Molecule 2: TRKA RECEPTOR PHOSHOPEPTIDE



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: ?.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

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

6.1 Standard geometry

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0	14
All	All	0	14

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	97	ARG	Sidechain
1	A	104	ARG	Sidechain
1	A	175	ARG	Sidechain
1	A	98	ARG	Sidechain
1	A	207	ARG	Sidechain
1	A	67	ARG	Sidechain
1	A	74	ARG	Sidechain
1	A	99	ARG	Sidechain
1	A	55	ARG	Sidechain
1	A	79	ARG	Sidechain
1	A	112	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	201	ARG	Sidechain
1	A	26	ARG	Sidechain

6.2 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	1496	1497	1494	115
2	B	106	90	85	12
All	All	1602	1587	1579	116

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:50:VAL:HG21	1:A:193:THR:HG21	1.01	1.29
1:A:45:VAL:O	1:A:128:THR:HG23	0.78	1.78
1:A:198:PHE:CD2	2:B:485:ILE:HG22	0.75	2.17
1:A:52:TYR:CD2	1:A:186:LEU:HD21	0.74	2.17
1:A:52:TYR:HB3	1:A:186:LEU:HD11	0.73	1.58
1:A:194:ILE:HG22	2:B:485:ILE:HG21	0.71	1.59
1:A:39:LEU:HD13	1:A:189:ASP:OD1	0.70	1.86
1:A:126:VAL:HG13	1:A:131:LEU:HG	0.70	1.61
1:A:106:LEU:HD22	1:A:110:LEU:HD12	0.69	1.64
1:A:177:CYS:SG	1:A:179:ILE:CD1	0.65	2.84
1:A:66:MET:SD	1:A:175:ARG:CD	0.65	2.85
1:A:131:LEU:HD12	1:A:147:MET:CE	0.65	2.21
1:A:44:LYS:HB3	1:A:50:VAL:HG13	0.64	1.69
1:A:44:LYS:CB	1:A:50:VAL:HG13	0.64	2.22
1:A:50:VAL:O	1:A:125:THR:HG23	0.64	1.93
1:A:50:VAL:HG21	1:A:193:THR:CG2	0.63	2.18
1:A:78:THR:HG22	1:A:82:ILE:HD12	0.63	1.70
1:A:177:CYS:SG	1:A:179:ILE:HD12	0.62	2.33
1:A:69:LEU:HD13	1:A:70:ASP:N	0.62	2.10
1:A:52:TYR:CB	1:A:186:LEU:HD11	0.61	2.24
1:A:131:LEU:HD12	1:A:147:MET:HE1	0.61	1.72
1:A:60:VAL:HG22	1:A:177:CYS:SG	0.61	2.35
1:A:56:TYR:HE2	1:A:59:CYS:HG	0.61	1.37
1:A:185:GLY:C	1:A:186:LEU:HD12	0.61	2.16
1:A:60:VAL:CG2	1:A:177:CYS:SG	0.60	2.89
1:A:185:GLY:O	1:A:186:LEU:HD12	0.60	1.96
1:A:195:GLY:HA2	2:B:485:ILE:HG23	0.59	1.74
1:A:41:PRO:CB	1:A:193:THR:HG23	0.59	2.27
1:A:41:PRO:HA	1:A:50:VAL:HG11	0.59	1.72
1:A:40:HIS:N	1:A:41:PRO:CD	0.59	2.66
1:A:177:CYS:SG	1:A:177:CYS:O	0.58	2.62

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:106:LEU:HD23	1:A:109:ILE:HG13	0.57	1.77
1:A:183:PRO:HB2	1:A:186:LEU:HD13	0.56	1.77
1:A:81:ALA:O	1:A:85:VAL:HG23	0.56	2.00
1:A:84:LEU:O	1:A:88:ALA:HB3	0.55	2.01
1:A:186:LEU:HD23	1:A:190:VAL:CG2	0.55	2.31
1:A:66:MET:SD	1:A:175:ARG:HD2	0.54	2.41
1:A:101:PRO:C	1:A:102:CYS:SG	0.54	2.85
1:A:147:MET:SD	1:A:197:ALA:HB1	0.54	2.43
1:A:19:LEU:HD23	1:A:22:GLU:OE1	0.54	2.02
1:A:120:MET:O	1:A:122:ILE:HG23	0.53	2.03
1:A:66:MET:SD	1:A:175:ARG:HD3	0.53	2.43
1:A:196:GLN:O	1:A:200:LEU:HD23	0.53	2.04
1:A:115:LEU:HD22	1:A:115:LEU:N	0.52	2.19
1:A:41:PRO:HB3	1:A:193:THR:HG23	0.52	1.82
1:A:152:PHE:CE1	2:B:491:PHE:CE2	0.50	2.99
1:A:69:LEU:C	1:A:69:LEU:HD13	0.50	2.27
1:A:186:LEU:HD23	1:A:190:VAL:HB	0.50	1.84
1:A:198:PHE:CE2	2:B:485:ILE:HG22	0.50	2.41
1:A:41:PRO:CA	1:A:193:THR:HG23	0.49	2.37
1:A:152:PHE:CD1	2:B:491:PHE:CZ	0.49	3.01
1:A:86:CYS:SG	1:A:92:ALA:HB2	0.49	2.48
1:A:184:GLU:O	1:A:186:LEU:HD12	0.48	2.08
1:A:177:CYS:HG	1:A:179:ILE:HD12	0.48	1.68
1:A:191:ILE:HG23	2:B:485:ILE:HD11	0.48	1.86
2:B:485:ILE:N	2:B:485:ILE:HD13	0.47	2.23
1:A:60:VAL:HG12	1:A:113:SER:HA	0.47	1.86
1:A:180:LEU:N	1:A:180:LEU:HD12	0.47	2.24
1:A:205:TYR:CD1	1:A:206:LEU:N	0.46	2.84
1:A:25:THR:O	1:A:25:THR:HG23	0.46	2.09
1:A:39:LEU:HD13	1:A:189:ASP:CG	0.46	2.30
1:A:166:TYR:CE1	1:A:180:LEU:HD11	0.46	2.46
1:A:177:CYS:SG	1:A:179:ILE:HD11	0.46	2.51
1:A:115:LEU:H	1:A:115:LEU:HD22	0.46	1.71
1:A:166:TYR:O	1:A:166:TYR:CG	0.46	2.69
1:A:19:LEU:HD23	1:A:22:GLU:CD	0.46	2.31
1:A:143:ALA:CB	1:A:146:HIS:CD2	0.46	2.99
1:A:23:GLU:O	1:A:25:THR:HG22	0.45	2.11
1:A:30:PHE:CD1	1:A:30:PHE:N	0.45	2.84
1:A:198:PHE:CE2	2:B:487:ASN:ND2	0.45	2.84
1:A:186:LEU:HD23	1:A:190:VAL:CB	0.45	2.42
1:A:164:VAL:O	1:A:180:LEU:HD12	0.45	2.11
1:A:202:PHE:CE1	2:B:489:GLN:CB	0.44	3.00

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:148:GLN:O	1:A:202:PHE:CE1	0.44	2.71
1:A:104:ARG:N	1:A:104:ARG:CD	0.44	2.80
1:A:167:VAL:HG12	1:A:177:CYS:HA	0.44	1.89
1:A:39:LEU:CB	1:A:41:PRO:HD2	0.43	2.43
1:A:202:PHE:CE2	2:B:487:ASN:CB	0.43	3.01
1:A:29:SER:O	1:A:31:VAL:N	0.43	2.52
1:A:106:LEU:HD23	1:A:109:ILE:CG1	0.43	2.43
1:A:64:GLN:HB2	1:A:109:ILE:HG22	0.43	1.89
1:A:64:GLN:CB	1:A:109:ILE:HG22	0.43	2.44
1:A:50:VAL:CG2	1:A:193:THR:HG21	0.42	2.21
1:A:153:ALA:HB3	2:B:485:ILE:HB	0.42	1.89
1:A:163:TYR:CD1	1:A:163:TYR:N	0.42	2.87
1:A:194:ILE:O	1:A:198:PHE:CD1	0.42	2.72
1:A:166:TYR:CE1	1:A:178:HIS:CB	0.42	3.03
1:A:40:HIS:CD2	1:A:41:PRO:CD	0.42	3.02
1:A:170:ASP:CB	1:A:171:PRO:CD	0.42	2.97
1:A:182:CYS:N	1:A:183:PRO:CD	0.42	2.82
1:A:157:ASP:CB	1:A:158:PRO:CD	0.41	2.98
1:A:157:ASP:N	1:A:158:PRO:HD2	0.41	2.30
1:A:182:CYS:N	1:A:183:PRO:HD3	0.41	2.31
1:A:56:TYR:CZ	1:A:58:GLY:O	0.41	2.74
1:A:85:VAL:O	1:A:89:VAL:HG13	0.41	2.16
1:A:190:VAL:HG13	1:A:191:ILE:N	0.41	2.31
1:A:183:PRO:O	1:A:184:GLU:CB	0.41	2.68
1:A:56:TYR:HH	1:A:59:CYS:CB	0.41	2.29
1:A:180:LEU:H	1:A:180:LEU:HD12	0.41	1.76
1:A:30:PHE:O	1:A:31:VAL:CB	0.41	2.68
1:A:104:ARG:CG	1:A:104:ARG:O	0.41	2.68
1:A:104:ARG:NE	1:A:104:ARG:N	0.41	2.69
1:A:77:VAL:CG1	1:A:78:THR:N	0.41	2.83
1:A:45:VAL:HG23	1:A:193:THR:HG22	0.40	1.92
1:A:166:TYR:CE1	1:A:178:HIS:HB3	0.40	2.51
1:A:40:HIS:CD2	1:A:41:PRO:N	0.40	2.89
1:A:170:ASP:N	1:A:171:PRO:HD2	0.40	2.31
1:A:57:MET:SD	1:A:181:GLU:CD	0.40	2.99
1:A:133:LEU:CD1	1:A:133:LEU:N	0.40	2.85
1:A:128:THR:O	1:A:129:SER:CB	0.40	2.70
1:A:115:LEU:N	1:A:115:LEU:HD13	0.40	2.29
1:A:183:PRO:C	1:A:186:LEU:HD13	0.40	2.37
1:A:40:HIS:N	1:A:41:PRO:HD3	0.40	2.32
1:A:39:LEU:HB3	1:A:41:PRO:HD2	0.40	1.93
1:A:77:VAL:HG13	1:A:78:THR:N	0.40	2.31

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:56:TYR:OH	1:A:178:HIS:CG	0.40	2.74

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	193/195 (99%)	107 (55%)	59 (31%)	27 (14%)	1	5
2	B	9/12 (75%)	7 (78%)	2 (22%)	0 (0%)	100	100
All	All	202/207 (98%)	114 (56%)	61 (30%)	27 (13%)	1	6

All 27 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	16	MET
1	A	95	ALA
1	A	151	SER
1	A	109	ILE
1	A	143	ALA
1	A	159	ASP
1	A	28	GLY
1	A	111	GLY
1	A	103	SER
1	A	150	ILE
1	A	204	GLN
1	A	35	THR
1	A	110	LEU
1	A	206	LEU
1	A	170	ASP
1	A	36	ARG
1	A	70	ASP
1	A	15	HIS
1	A	187	ALA
1	A	101	PRO
1	A	162	GLU

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Mol	Chain	Res	Type
1	A	65	SER
1	A	18	GLN
1	A	98	ARG
1	A	30	PHE
1	A	105	PRO
1	A	155	GLY

6.3.2 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	162/162 (100%)	96 (59%)	66 (41%)	0	4
2	B	10/10 (100%)	8 (80%)	2 (20%)	5	36
All	All	172/172 (100%)	104 (60%)	68 (40%)	1	5

All 68 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	97	ARG
1	A	123	THR
1	A	107	SER
1	A	193	THR
1	A	59	CYS
1	A	177	CYS
1	A	50	VAL
1	A	202	PHE
1	A	104	ARG
1	A	151	SER
1	A	120	MET
1	A	109	ILE
1	A	159	ASP
1	A	115	LEU
1	A	139	LYS
1	A	157	ASP
1	A	146	HIS
1	A	99	ARG

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Mol	Chain	Res	Type
1	A	32	ASN
1	A	106	LEU
1	A	175	ARG
1	A	96	THR
1	A	103	SER
1	A	127	SER
1	A	147	MET
1	A	54	VAL
1	A	117	PHE
1	A	163	TYR
1	A	132	ASN
1	A	134	MET
2	B	489	GLN
1	A	110	LEU
1	A	179	ILE
1	A	180	LEU
1	A	131	LEU
1	A	145	HIS
1	A	140	GLN
1	A	44	LYS
1	A	38	TRP
1	A	112	ARG
1	A	124	LEU
1	A	71	PHE
1	A	170	ASP
1	A	73	THR
1	A	36	ARG
1	A	84	LEU
1	A	70	ASP
1	A	93	LYS
1	A	33	LYS
1	A	204	GLN
1	A	207	ARG
1	A	130	SER
1	A	26	ARG
1	A	142	ILE
2	B	493	ASP
1	A	83	SER
1	A	189	ASP
1	A	102	CYS
1	A	113	SER
1	A	65	SER

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Mol	Chain	Res	Type
1	A	18	GLN
1	A	98	ARG
1	A	181	GLU
1	A	30	PHE
1	A	150	ILE
1	A	129	SER
1	A	198	PHE
1	A	169	LYS

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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	PTR	B	490	2	13,16,17	0.84	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	PTR	B	490	2	19,22,24	1.11	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	PTR	B	490	2	-	0,9,11,13	0,1,1,1

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.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided