



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 16, 2020 – 06:59 PM BST

PDB ID : 6KOI
Title : Crystal structure of SNX11-PXe domain in dimer form.
Authors : Xu, T.; Xu, J.; Liu, J.
Deposited on : 2019-08-11
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

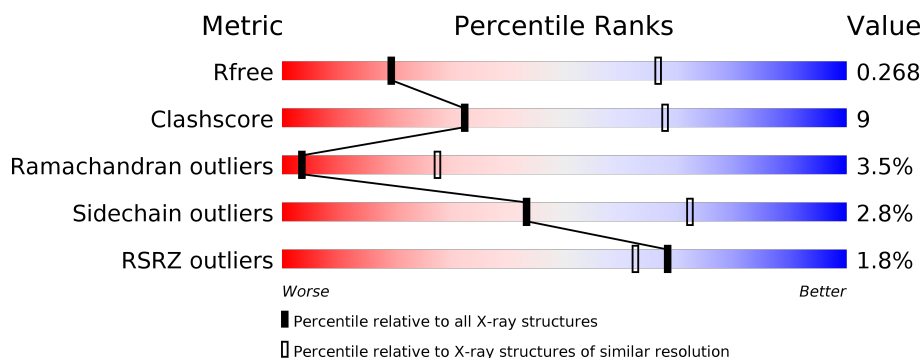
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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.



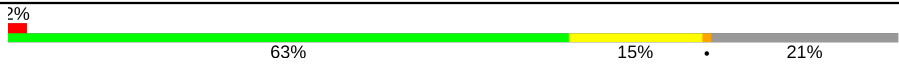



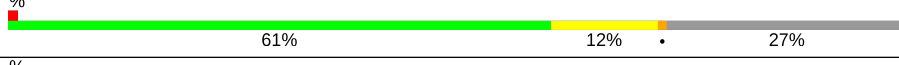
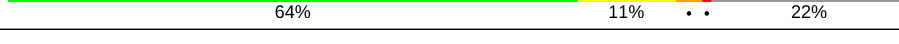


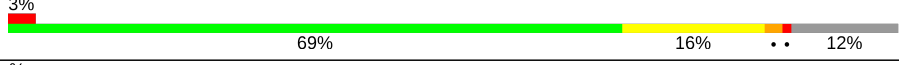


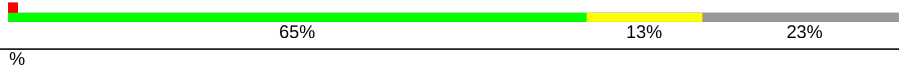




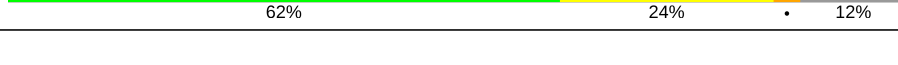
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	160	<div> <div>2%</div> <div>61% 14% • • 23%</div> </div>
1	B	160	<div> <div>2%</div> <div>66% 16% • • 13%</div> </div>
1	C	160	<div> <div>2%</div> <div>62% 16% • 21%</div> </div>
1	D	160	<div> <div>0%</div> <div>70% 17% 5% 8%</div> </div>
1	E	160	<div> <div>3%</div> <div>63% 14% • 22%</div> </div>
1	F	160	<div> <div>2%</div> <div>64% 19% • 14%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	160	
1	H	160	
1	I	160	
1	J	160	
1	K	160	
1	L	160	
1	M	160	
1	N	160	
1	O	160	
1	P	160	
1	Q	160	
1	R	160	
1	S	160	
1	T	160	
1	U	160	
1	V	160	
1	W	160	
1	X	160	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 25878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Sorting nexin-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	0	0	0
			1018	651	183	182	2			
1	B	140	Total	C	N	O	S	0	0	0
			1142	722	207	209	2			
1	C	126	Total	C	N	O	S	0	0	0
			1036	661	186	187	2			
1	D	147	Total	C	N	O	S	0	0	0
			1197	758	214	221	2			
1	E	125	Total	C	N	O	S	0	0	0
			1027	656	185	184	2			
1	F	138	Total	C	N	O	S	0	0	0
			1126	712	205	205	2			
1	G	126	Total	C	N	O	S	0	0	0
			1036	661	186	187	2			
1	H	144	Total	C	N	O	S	0	0	0
			1170	740	211	215	2			
1	I	125	Total	C	N	O	S	0	0	0
			1027	656	184	185	2			
1	J	141	Total	C	N	O	S	0	0	0
			1151	727	208	212	2			
1	K	117	Total	C	N	O	S	0	0	0
			971	621	176	172	2			
1	L	143	Total	C	N	O	S	0	0	0
			1164	737	210	213	2			
1	M	125	Total	C	N	O	S	0	0	0
			1027	656	185	184	2			
1	N	141	Total	C	N	O	S	0	0	0
			1148	725	208	211	2			
1	O	118	Total	C	N	O	S	0	0	0
			973	622	176	173	2			
1	P	141	Total	C	N	O	S	0	0	0
			1146	724	208	210	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	122	Total	C	N	O	S	0	0	0
			1005	644	181	178	2			
1	R	139	Total	C	N	O	S	Se	0	0
			1130	715	206	205	2	2		
1	S	124	Total	C	N	O	S		0	0
			1018	651	183	182	2			
1	T	143	Total	C	N	O	S	Se	0	0
			1164	737	210	213	2	2		
1	U	121	Total	C	N	O	S		0	0
			999	637	181	179	2			
1	V	130	Total	C	N	O	S	Se	0	0
			1065	673	195	193	2	2		
1	W	121	Total	C	N	O	S		0	0
			992	630	180	180	2			
1	X	141	Total	C	N	O	S	Se	0	0
			1146	724	208	210	2	2		

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	LEU	-	expression tag	UNP Q9Y5W9
A	160	GLU	-	expression tag	UNP Q9Y5W9
A	161	HIS	-	expression tag	UNP Q9Y5W9
A	162	HIS	-	expression tag	UNP Q9Y5W9
A	163	HIS	-	expression tag	UNP Q9Y5W9
A	164	HIS	-	expression tag	UNP Q9Y5W9
A	165	HIS	-	expression tag	UNP Q9Y5W9
A	166	HIS	-	expression tag	UNP Q9Y5W9
B	159	LEU	-	expression tag	UNP Q9Y5W9
B	160	GLU	-	expression tag	UNP Q9Y5W9
B	161	HIS	-	expression tag	UNP Q9Y5W9
B	162	HIS	-	expression tag	UNP Q9Y5W9
B	163	HIS	-	expression tag	UNP Q9Y5W9
B	164	HIS	-	expression tag	UNP Q9Y5W9
B	165	HIS	-	expression tag	UNP Q9Y5W9
B	166	HIS	-	expression tag	UNP Q9Y5W9
C	159	LEU	-	expression tag	UNP Q9Y5W9
C	160	GLU	-	expression tag	UNP Q9Y5W9
C	161	HIS	-	expression tag	UNP Q9Y5W9
C	162	HIS	-	expression tag	UNP Q9Y5W9
C	163	HIS	-	expression tag	UNP Q9Y5W9
C	164	HIS	-	expression tag	UNP Q9Y5W9
C	165	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	166	HIS	-	expression tag	UNP Q9Y5W9
D	159	LEU	-	expression tag	UNP Q9Y5W9
D	160	GLU	-	expression tag	UNP Q9Y5W9
D	161	HIS	-	expression tag	UNP Q9Y5W9
D	162	HIS	-	expression tag	UNP Q9Y5W9
D	163	HIS	-	expression tag	UNP Q9Y5W9
D	164	HIS	-	expression tag	UNP Q9Y5W9
D	165	HIS	-	expression tag	UNP Q9Y5W9
D	166	HIS	-	expression tag	UNP Q9Y5W9
E	159	LEU	-	expression tag	UNP Q9Y5W9
E	160	GLU	-	expression tag	UNP Q9Y5W9
E	161	HIS	-	expression tag	UNP Q9Y5W9
E	162	HIS	-	expression tag	UNP Q9Y5W9
E	163	HIS	-	expression tag	UNP Q9Y5W9
E	164	HIS	-	expression tag	UNP Q9Y5W9
E	165	HIS	-	expression tag	UNP Q9Y5W9
E	166	HIS	-	expression tag	UNP Q9Y5W9
F	159	LEU	-	expression tag	UNP Q9Y5W9
F	160	GLU	-	expression tag	UNP Q9Y5W9
F	161	HIS	-	expression tag	UNP Q9Y5W9
F	162	HIS	-	expression tag	UNP Q9Y5W9
F	163	HIS	-	expression tag	UNP Q9Y5W9
F	164	HIS	-	expression tag	UNP Q9Y5W9
F	165	HIS	-	expression tag	UNP Q9Y5W9
F	166	HIS	-	expression tag	UNP Q9Y5W9
G	159	LEU	-	expression tag	UNP Q9Y5W9
G	160	GLU	-	expression tag	UNP Q9Y5W9
G	161	HIS	-	expression tag	UNP Q9Y5W9
G	162	HIS	-	expression tag	UNP Q9Y5W9
G	163	HIS	-	expression tag	UNP Q9Y5W9
G	164	HIS	-	expression tag	UNP Q9Y5W9
G	165	HIS	-	expression tag	UNP Q9Y5W9
G	166	HIS	-	expression tag	UNP Q9Y5W9
H	159	LEU	-	expression tag	UNP Q9Y5W9
H	160	GLU	-	expression tag	UNP Q9Y5W9
H	161	HIS	-	expression tag	UNP Q9Y5W9
H	162	HIS	-	expression tag	UNP Q9Y5W9
H	163	HIS	-	expression tag	UNP Q9Y5W9
H	164	HIS	-	expression tag	UNP Q9Y5W9
H	165	HIS	-	expression tag	UNP Q9Y5W9
H	166	HIS	-	expression tag	UNP Q9Y5W9
I	159	LEU	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	160	GLU	-	expression tag	UNP Q9Y5W9
I	161	HIS	-	expression tag	UNP Q9Y5W9
I	162	HIS	-	expression tag	UNP Q9Y5W9
I	163	HIS	-	expression tag	UNP Q9Y5W9
I	164	HIS	-	expression tag	UNP Q9Y5W9
I	165	HIS	-	expression tag	UNP Q9Y5W9
I	166	HIS	-	expression tag	UNP Q9Y5W9
J	159	LEU	-	expression tag	UNP Q9Y5W9
J	160	GLU	-	expression tag	UNP Q9Y5W9
J	161	HIS	-	expression tag	UNP Q9Y5W9
J	162	HIS	-	expression tag	UNP Q9Y5W9
J	163	HIS	-	expression tag	UNP Q9Y5W9
J	164	HIS	-	expression tag	UNP Q9Y5W9
J	165	HIS	-	expression tag	UNP Q9Y5W9
J	166	HIS	-	expression tag	UNP Q9Y5W9
K	159	LEU	-	expression tag	UNP Q9Y5W9
K	160	GLU	-	expression tag	UNP Q9Y5W9
K	161	HIS	-	expression tag	UNP Q9Y5W9
K	162	HIS	-	expression tag	UNP Q9Y5W9
K	163	HIS	-	expression tag	UNP Q9Y5W9
K	164	HIS	-	expression tag	UNP Q9Y5W9
K	165	HIS	-	expression tag	UNP Q9Y5W9
K	166	HIS	-	expression tag	UNP Q9Y5W9
L	159	LEU	-	expression tag	UNP Q9Y5W9
L	160	GLU	-	expression tag	UNP Q9Y5W9
L	161	HIS	-	expression tag	UNP Q9Y5W9
L	162	HIS	-	expression tag	UNP Q9Y5W9
L	163	HIS	-	expression tag	UNP Q9Y5W9
L	164	HIS	-	expression tag	UNP Q9Y5W9
L	165	HIS	-	expression tag	UNP Q9Y5W9
L	166	HIS	-	expression tag	UNP Q9Y5W9
M	159	LEU	-	expression tag	UNP Q9Y5W9
M	160	GLU	-	expression tag	UNP Q9Y5W9
M	161	HIS	-	expression tag	UNP Q9Y5W9
M	162	HIS	-	expression tag	UNP Q9Y5W9
M	163	HIS	-	expression tag	UNP Q9Y5W9
M	164	HIS	-	expression tag	UNP Q9Y5W9
M	165	HIS	-	expression tag	UNP Q9Y5W9
M	166	HIS	-	expression tag	UNP Q9Y5W9
N	159	LEU	-	expression tag	UNP Q9Y5W9
N	160	GLU	-	expression tag	UNP Q9Y5W9
N	161	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	162	HIS	-	expression tag	UNP Q9Y5W9
N	163	HIS	-	expression tag	UNP Q9Y5W9
N	164	HIS	-	expression tag	UNP Q9Y5W9
N	165	HIS	-	expression tag	UNP Q9Y5W9
N	166	HIS	-	expression tag	UNP Q9Y5W9
O	159	LEU	-	expression tag	UNP Q9Y5W9
O	160	GLU	-	expression tag	UNP Q9Y5W9
O	161	HIS	-	expression tag	UNP Q9Y5W9
O	162	HIS	-	expression tag	UNP Q9Y5W9
O	163	HIS	-	expression tag	UNP Q9Y5W9
O	164	HIS	-	expression tag	UNP Q9Y5W9
O	165	HIS	-	expression tag	UNP Q9Y5W9
O	166	HIS	-	expression tag	UNP Q9Y5W9
P	159	LEU	-	expression tag	UNP Q9Y5W9
P	160	GLU	-	expression tag	UNP Q9Y5W9
P	161	HIS	-	expression tag	UNP Q9Y5W9
P	162	HIS	-	expression tag	UNP Q9Y5W9
P	163	HIS	-	expression tag	UNP Q9Y5W9
P	164	HIS	-	expression tag	UNP Q9Y5W9
P	165	HIS	-	expression tag	UNP Q9Y5W9
P	166	HIS	-	expression tag	UNP Q9Y5W9
Q	159	LEU	-	expression tag	UNP Q9Y5W9
Q	160	GLU	-	expression tag	UNP Q9Y5W9
Q	161	HIS	-	expression tag	UNP Q9Y5W9
Q	162	HIS	-	expression tag	UNP Q9Y5W9
Q	163	HIS	-	expression tag	UNP Q9Y5W9
Q	164	HIS	-	expression tag	UNP Q9Y5W9
Q	165	HIS	-	expression tag	UNP Q9Y5W9
Q	166	HIS	-	expression tag	UNP Q9Y5W9
R	159	LEU	-	expression tag	UNP Q9Y5W9
R	160	GLU	-	expression tag	UNP Q9Y5W9
R	161	HIS	-	expression tag	UNP Q9Y5W9
R	162	HIS	-	expression tag	UNP Q9Y5W9
R	163	HIS	-	expression tag	UNP Q9Y5W9
R	164	HIS	-	expression tag	UNP Q9Y5W9
R	165	HIS	-	expression tag	UNP Q9Y5W9
R	166	HIS	-	expression tag	UNP Q9Y5W9
S	159	LEU	-	expression tag	UNP Q9Y5W9
S	160	GLU	-	expression tag	UNP Q9Y5W9
S	161	HIS	-	expression tag	UNP Q9Y5W9
S	162	HIS	-	expression tag	UNP Q9Y5W9
S	163	HIS	-	expression tag	UNP Q9Y5W9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	164	HIS	-	expression tag	UNP Q9Y5W9
S	165	HIS	-	expression tag	UNP Q9Y5W9
S	166	HIS	-	expression tag	UNP Q9Y5W9
T	159	LEU	-	expression tag	UNP Q9Y5W9
T	160	GLU	-	expression tag	UNP Q9Y5W9
T	161	HIS	-	expression tag	UNP Q9Y5W9
T	162	HIS	-	expression tag	UNP Q9Y5W9
T	163	HIS	-	expression tag	UNP Q9Y5W9
T	164	HIS	-	expression tag	UNP Q9Y5W9
T	165	HIS	-	expression tag	UNP Q9Y5W9
T	166	HIS	-	expression tag	UNP Q9Y5W9
U	159	LEU	-	expression tag	UNP Q9Y5W9
U	160	GLU	-	expression tag	UNP Q9Y5W9
U	161	HIS	-	expression tag	UNP Q9Y5W9
U	162	HIS	-	expression tag	UNP Q9Y5W9
U	163	HIS	-	expression tag	UNP Q9Y5W9
U	164	HIS	-	expression tag	UNP Q9Y5W9
U	165	HIS	-	expression tag	UNP Q9Y5W9
U	166	HIS	-	expression tag	UNP Q9Y5W9
V	159	LEU	-	expression tag	UNP Q9Y5W9
V	160	GLU	-	expression tag	UNP Q9Y5W9
V	161	HIS	-	expression tag	UNP Q9Y5W9
V	162	HIS	-	expression tag	UNP Q9Y5W9
V	163	HIS	-	expression tag	UNP Q9Y5W9
V	164	HIS	-	expression tag	UNP Q9Y5W9
V	165	HIS	-	expression tag	UNP Q9Y5W9
V	166	HIS	-	expression tag	UNP Q9Y5W9
W	159	LEU	-	expression tag	UNP Q9Y5W9
W	160	GLU	-	expression tag	UNP Q9Y5W9
W	161	HIS	-	expression tag	UNP Q9Y5W9
W	162	HIS	-	expression tag	UNP Q9Y5W9
W	163	HIS	-	expression tag	UNP Q9Y5W9
W	164	HIS	-	expression tag	UNP Q9Y5W9
W	165	HIS	-	expression tag	UNP Q9Y5W9
W	166	HIS	-	expression tag	UNP Q9Y5W9
X	159	LEU	-	expression tag	UNP Q9Y5W9
X	160	GLU	-	expression tag	UNP Q9Y5W9
X	161	HIS	-	expression tag	UNP Q9Y5W9
X	162	HIS	-	expression tag	UNP Q9Y5W9
X	163	HIS	-	expression tag	UNP Q9Y5W9
X	164	HIS	-	expression tag	UNP Q9Y5W9
X	165	HIS	-	expression tag	UNP Q9Y5W9

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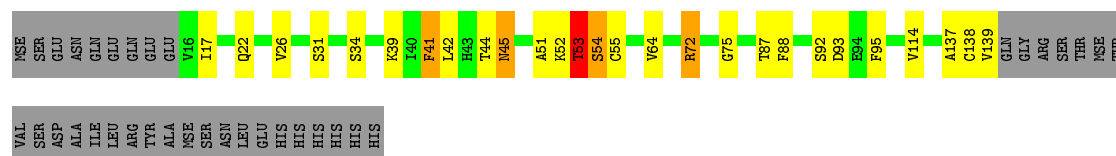
Chain	Residue	Modelled	Actual	Comment	Reference
X	166	HIS	-	expression tag	UNP Q9Y5W9

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

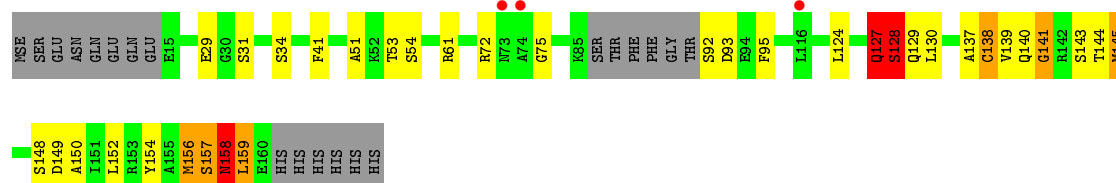
• Molecule 1: Sorting nexin-11

Chain A: 



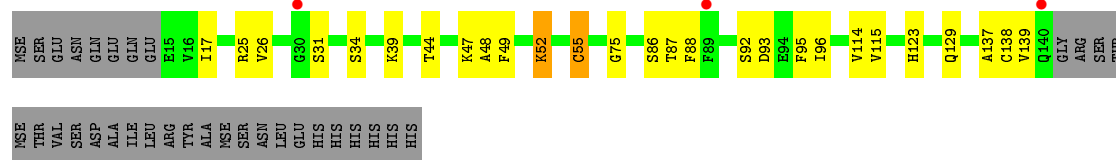
• Molecule 1: Sorting nexin-11

Chain B: 



• Molecule 1: Sorting nexin-11

Chain C: 



• Molecule 1: Sorting nexin-11

Chain D: 



GLU
HIS
HIS
HIS
HIS
HIS
HIS

• Molecule 1: Sorting nexin-11



MSE SER GLU THR VAL ASN GLN GLU GLN GLU GLU V16 V17 I17 T18 R25 V26 S31 S34 F41 N45 SER LYS ALA PHE THR A51 S54 G75 S86 T91 S92 D93 E94 F95 L111 V114 V115 H123 Q129 A137 C138 V139 GLN GLY ARG SER

THR MSE THR VAL SER ASP ALA LEU ARG TYR NSE SER ASN LEU LEU HIS HIS HIS HIS HIS

• Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLU GLN GLU E15 E29 G30 S31 W32 W33 S34 F41 F49 T50 T53 S54 R61 G75 L76 S86 THR PHE GLY T91 S92 D93 E94 F95 H123 L124 Q127 S128 A137 C138 V139 Q140 G141 R142 S143 T144 M145 T146 V147 D149

A150 S157 N158 L159 GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLU GLN GLU V16 R25 V26 Q27 S31 S34 N45 S46 A48 F49 T50 A51 A52 T53 S54 C55 V64 R72 G75 L76 R85 SER THR F88 D93 E94 F95 V114 V115 A137 C138 V139 GLN GLY ARG SER MSE THR

VAL SER ASP ALA ILE LEU ARG THR MSE ASN LEU GLU HIS HIS HIS HIS HIS

• Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLN GLU V16 S31 S32 S33 S34 F41 R47 A48 F49 T50 A51 K52 S54 C55 R61 G75 P83 G84 R85 S86 THR PHE PHE GLY THR S92 D93 E94 F95 Q127 L130 I135 E136 A137 C138 V139 Y139 Q140 G141 A142 S143 T144

H145 T146 V147 S148 D149 A150 I151 M156 S157 N158 L159 GLU HIS HIS HIS HIS HIS

• Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLN GLU V16 I17 R25 V26 Q27 S31 S34 T44 A48 C55 G75 S86 T87 S92 D93 E94 F95 I96 V114 V115 A137 C138 V139 GLY ARG SER THR MSE THR VAL SER ASP ALA ILE LEU ARG TYR ALA MSE

SER
ASN
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GLU
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- Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLN GLU GLU V16 S31 S34 F41 F49 T83 S54 R61 G75 S86 T87 F88 PHE GLY T91 S92 D93 E94 F95 L116 L117 H123 Q127 L130 A137 C138 V139 Q140 G141 R142 S143 T144 M145 T146 V147 S148 D149 A150

Y154 A155 M156 S157 E160
HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLN GLU GLU V16 V17 R25 V26 G30 S31 S34 K39 L40 F41 T44 M45 S46 K47 ALA PHE THR ALA F52 T53 R72 G75 E81 T87 S92 D93 E94 F95 I96 V114 V115 L116 L117 A137 C138 V139 Q140 ARG

SER THR MSE THR VAL SER ASP ALA ILE LEU ARG TYR ALA MSE SER ASN LEU GLU HIS HIS HIS HIS HIS

- Molecule 1: Sorting nexin-11



MSE SER GLU ASN GLN GLN GLU GLU VAL I17 T18 V19 Q22 E29 G30 S31 S34 L42 H43 T44 M45 A48 PHE THR ALA LYS T54 S54 C55 V56 R61 R72 G75 F83 GLY LYS SER PHE THR GLY THR S92 D93 L111 L116 Q129

I135 E136 A137 V139 Q140 Q141 R142 S143 T144 S148 D149 A150 R153 Y154 A155 M156 S157 M158 L159 GLU HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Sorting nexin-11

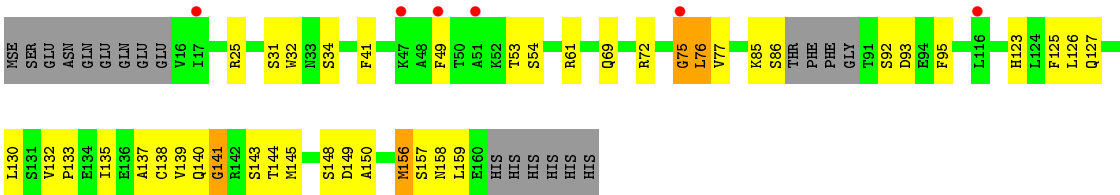


MSE SER GLU ASN GLN GLN GLU GLU E15 V16 I17 Q22 V26 S31 S34 F41 T44 M45 S46 F49 T50 A51 K52 T53 S54 C55 V64 G75 G84 LYS SER THR PHE G90 T91 S92 D93 E94 F95 I96 L103 V114 V115 A137 C138 V139

Q140 GLY ARG SER THR MSE THR VAL ASP ALA ILE LEU ARG TYR ALA MSE SER ASN LEU GLU HIS HIS HIS HIS HIS HIS

- Molecule 1: Sorting nexin-11





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	142.04Å 190.43Å 237.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.87 – 3.50 65.79 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.87-3.50) 99.1 (65.79-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.234 , 0.265 0.238 , 0.268	Depositor DCC
R_{free} test set	3921 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25878	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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	0.95	4/1040 (0.4%)	1.22	6/1406 (0.4%)
1	B	0.67	0/1160	0.94	5/1562 (0.3%)
1	C	0.69	0/1058	0.89	2/1430 (0.1%)
1	D	0.68	0/1218	0.90	5/1642 (0.3%)
1	E	0.69	0/1049	0.84	0/1418
1	F	0.68	0/1144	0.84	2/1540 (0.1%)
1	G	0.66	0/1058	0.82	0/1430
1	H	0.72	1/1189 (0.1%)	0.92	4/1601 (0.2%)
1	I	0.69	1/1049 (0.1%)	0.89	3/1418 (0.2%)
1	J	0.71	1/1169 (0.1%)	0.86	5/1574 (0.3%)
1	K	0.67	0/990	0.78	0/1335
1	L	0.69	1/1183 (0.1%)	0.86	3/1593 (0.2%)
1	M	0.72	2/1049 (0.2%)	0.85	1/1418 (0.1%)
1	N	0.68	0/1166	0.80	1/1570 (0.1%)
1	O	0.65	0/992	0.79	1/1338 (0.1%)
1	P	0.70	1/1164 (0.1%)	0.83	1/1568 (0.1%)
1	Q	0.70	1/1026 (0.1%)	0.82	1/1385 (0.1%)
1	R	0.69	0/1148	0.84	1/1546 (0.1%)
1	S	0.67	0/1040	0.80	0/1406
1	T	0.67	0/1183	0.88	4/1594 (0.3%)
1	U	0.69	0/1019	0.87	3/1375 (0.2%)
1	V	0.66	0/1081	0.92	4/1455 (0.3%)
1	W	0.68	0/1011	0.83	0/1366
1	X	0.70	0/1164	0.80	2/1568 (0.1%)
All	All	0.70	12/26350 (0.0%)	0.87	54/35538 (0.2%)

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 outliers	#Planarity outliers
1	A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	G	0	2
1	H	0	1
1	I	0	1
1	J	0	1
1	R	0	3
1	W	0	2
All	All	0	17

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	ARG	CZ-NH2	10.74	1.47	1.33
1	A	72	ARG	CZ-NH1	9.97	1.46	1.33
1	A	72	ARG	NE-CZ	8.87	1.44	1.33
1	A	72	ARG	CG-CD	7.93	1.71	1.51
1	H	75	GLY	C-O	-5.99	1.14	1.23

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH1	-26.54	107.03	120.30
1	A	72	ARG	NE-CZ-NH2	12.23	126.42	120.30
1	B	128	SER	N-CA-CB	11.80	128.19	110.50
1	V	72	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	72	ARG	CD-NE-CZ	-9.26	110.64	123.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	GLN	Sidechain
1	A	45	ASN	Mainchain,Peptide
1	A	53	THR	Mainchain
1	A	72	ARG	Sidechain
1	B	127	GLN	Mainchain

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1018	0	1028	20	0
1	B	1142	0	1154	24	0
1	C	1036	0	1042	33	0
1	D	1197	0	1201	42	0
1	E	1027	0	1036	27	0
1	F	1126	0	1139	37	0
1	G	1036	0	1042	25	0
1	H	1170	0	1178	36	0
1	I	1027	0	1034	19	0
1	J	1151	0	1160	31	1
1	K	971	0	978	27	0
1	L	1164	0	1173	32	0
1	M	1027	0	1036	19	0
1	N	1148	0	1159	21	1
1	O	973	0	980	12	0
1	P	1146	0	1160	21	1
1	Q	1005	0	1015	23	1
1	R	1130	0	1147	40	0
1	S	1018	0	1028	25	0
1	T	1164	0	1176	38	0
1	U	999	0	1009	23	0
1	V	1065	0	1075	27	0
1	W	992	0	998	20	0
1	X	1146	0	1160	38	0
All	All	25878	0	26108	457	2

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 9.

The worst 5 of 457 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:129:GLN:HE22	1:L:137:ALA:CB	1.62	1.12
1:I:39:LYS:HD2	1:J:138:CYS:SG	1.95	1.05
1:K:39:LYS:HD2	1:L:138:CYS:SG	1.99	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:O	1:B:156:MSE:HG3	1.64	0.97
1:Q:95:PHE:HD2	1:R:156:MSE:HE3	1.30	0.94

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:GLN:NE2	1:Q:94:GLU:OE2[4_555]	1.20	1.00
1:N:150:ALA:CB	1:P:75:GLY:O[3_444]	1.64	0.56

5.3 Torsion angles ⓘ

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	122/160 (76%)	103 (84%)	15 (12%)	4 (3%)	4	28
1	B	136/160 (85%)	116 (85%)	13 (10%)	7 (5%)	2	19
1	C	124/160 (78%)	102 (82%)	17 (14%)	5 (4%)	3	24
1	D	145/160 (91%)	128 (88%)	12 (8%)	5 (3%)	3	28
1	E	123/160 (77%)	104 (85%)	16 (13%)	3 (2%)	6	35
1	F	134/160 (84%)	119 (89%)	11 (8%)	4 (3%)	4	30
1	G	124/160 (78%)	106 (86%)	14 (11%)	4 (3%)	4	29
1	H	140/160 (88%)	120 (86%)	15 (11%)	5 (4%)	3	26
1	I	123/160 (77%)	104 (85%)	14 (11%)	5 (4%)	3	23
1	J	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	21
1	K	111/160 (69%)	99 (89%)	10 (9%)	2 (2%)	8	41
1	L	139/160 (87%)	119 (86%)	15 (11%)	5 (4%)	3	26
1	M	123/160 (77%)	106 (86%)	12 (10%)	5 (4%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	137/160 (86%)	119 (87%)	13 (10%)	5 (4%)	3	26
1	O	112/160 (70%)	101 (90%)	9 (8%)	2 (2%)	8	41
1	P	137/160 (86%)	120 (88%)	11 (8%)	6 (4%)	2	21
1	Q	118/160 (74%)	101 (86%)	14 (12%)	3 (2%)	5	34
1	R	135/160 (84%)	116 (86%)	15 (11%)	4 (3%)	4	30
1	S	122/160 (76%)	106 (87%)	12 (10%)	4 (3%)	4	28
1	T	139/160 (87%)	120 (86%)	12 (9%)	7 (5%)	2	19
1	U	117/160 (73%)	100 (86%)	14 (12%)	3 (3%)	5	33
1	V	124/160 (78%)	105 (85%)	13 (10%)	6 (5%)	2	20
1	W	117/160 (73%)	101 (86%)	13 (11%)	3 (3%)	5	33
1	X	137/160 (86%)	118 (86%)	13 (10%)	6 (4%)	2	21
All	All	3076/3840 (80%)	2651 (86%)	316 (10%)	109 (4%)	3	27

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	SER
1	A	87	THR
1	B	128	SER
1	B	141	GLY
1	B	158	ASN

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	115/145 (79%)	113 (98%)	2 (2%)	60	82
1	B	129/145 (89%)	123 (95%)	6 (5%)	26	60
1	C	117/145 (81%)	115 (98%)	2 (2%)	60	82
1	D	135/145 (93%)	131 (97%)	4 (3%)	41	71
1	E	116/145 (80%)	111 (96%)	5 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	127/145 (88%)	124 (98%)	3 (2%)	49	76
1	G	117/145 (81%)	114 (97%)	3 (3%)	46	74
1	H	132/145 (91%)	127 (96%)	5 (4%)	33	65
1	I	116/145 (80%)	112 (97%)	4 (3%)	37	68
1	J	130/145 (90%)	126 (97%)	4 (3%)	40	70
1	K	110/145 (76%)	108 (98%)	2 (2%)	59	81
1	L	131/145 (90%)	124 (95%)	7 (5%)	22	55
1	M	116/145 (80%)	114 (98%)	2 (2%)	60	82
1	N	130/145 (90%)	126 (97%)	4 (3%)	40	70
1	O	110/145 (76%)	106 (96%)	4 (4%)	35	66
1	P	130/145 (90%)	127 (98%)	3 (2%)	50	77
1	Q	113/145 (78%)	112 (99%)	1 (1%)	78	90
1	R	128/145 (88%)	125 (98%)	3 (2%)	50	77
1	S	115/145 (79%)	114 (99%)	1 (1%)	78	90
1	T	132/145 (91%)	127 (96%)	5 (4%)	33	65
1	U	114/145 (79%)	111 (97%)	3 (3%)	46	74
1	V	121/145 (83%)	117 (97%)	4 (3%)	38	68
1	W	112/145 (77%)	110 (98%)	2 (2%)	59	81
1	X	130/145 (90%)	128 (98%)	2 (2%)	65	84
All	All	2926/3480 (84%)	2845 (97%)	81 (3%)	43	72

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	140	GLN
1	L	145	MSE
1	V	93	ASP
1	J	145	MSE
1	L	54	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 109 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	129	GLN

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Mol	Chain	Res	Type
1	N	121	GLN
1	V	158	ASN
1	L	28	ASN
1	M	45	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	124/160 (77%)	0.22	0 100 100	63, 95, 159, 217	0
1	B	138/160 (86%)	0.39	3 (2%) 62 56	68, 120, 173, 184	0
1	C	126/160 (78%)	0.36	3 (2%) 59 53	68, 104, 170, 206	0
1	D	145/160 (90%)	0.17	2 (1%) 75 69	66, 110, 165, 201	0
1	E	125/160 (78%)	0.33	4 (3%) 47 42	71, 105, 177, 217	0
1	F	136/160 (85%)	0.22	3 (2%) 62 56	78, 131, 170, 180	0
1	G	126/160 (78%)	0.29	3 (2%) 59 53	60, 97, 173, 212	0
1	H	142/160 (88%)	0.19	2 (1%) 75 69	64, 102, 154, 215	0
1	I	125/160 (78%)	0.28	0 100 100	60, 94, 159, 204	0
1	J	139/160 (86%)	0.07	0 100 100	64, 105, 154, 186	0
1	K	117/160 (73%)	0.27	1 (0%) 84 79	72, 103, 155, 194	0
1	L	141/160 (88%)	0.14	2 (1%) 75 69	69, 121, 167, 188	0
1	M	125/160 (78%)	0.19	0 100 100	74, 105, 169, 220	0
1	N	139/160 (86%)	0.11	0 100 100	79, 135, 177, 195	0
1	O	118/160 (73%)	0.39	2 (1%) 70 64	77, 108, 165, 182	0
1	P	139/160 (86%)	0.35	5 (3%) 42 38	65, 122, 164, 200	0
1	Q	122/160 (76%)	0.30	1 (0%) 86 81	66, 100, 167, 205	0
1	R	137/160 (85%)	0.30	3 (2%) 62 56	70, 119, 166, 199	0
1	S	124/160 (77%)	0.16	1 (0%) 86 81	90, 123, 191, 211	0
1	T	141/160 (88%)	0.31	1 (0%) 87 83	92, 147, 184, 200	0
1	U	121/160 (75%)	0.36	2 (1%) 70 64	86, 120, 169, 193	0
1	V	128/160 (80%)	0.43	10 (7%) 13 13	92, 148, 185, 204	0
1	W	121/160 (75%)	0.34	4 (3%) 46 41	87, 122, 173, 199	0
1	X	139/160 (86%)	0.41	6 (4%) 35 31	86, 131, 187, 206	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	3138/3840 (81%)	0.27	58 (1%) 68 62	60, 116, 176, 220	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	GLN	7.1
1	V	111	LEU	4.1
1	P	49	PHE	3.8
1	R	51	ALA	3.7
1	G	49	PHE	3.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.