



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:14 am BST

PDB ID : 5X9Z
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 7.31 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
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

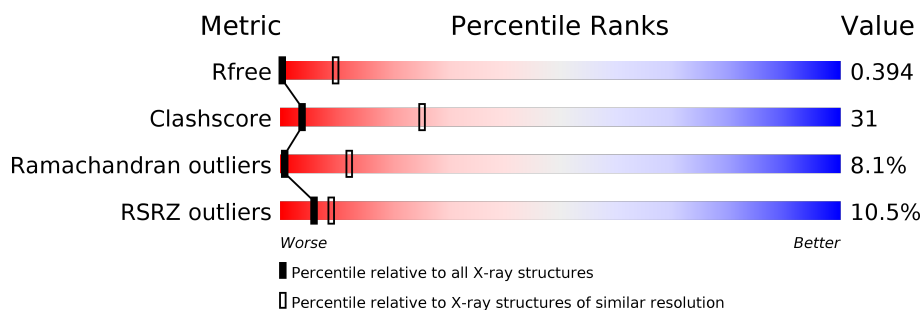
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.31 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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	2217	<div> <div>8%</div> <div>50%</div> <div>24%</div> <div>•</div> <div>23%</div> </div>
1	B	2217	<div> <div>8%</div> <div>52%</div> <div>22%</div> <div>•</div> <div>23%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16948 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.

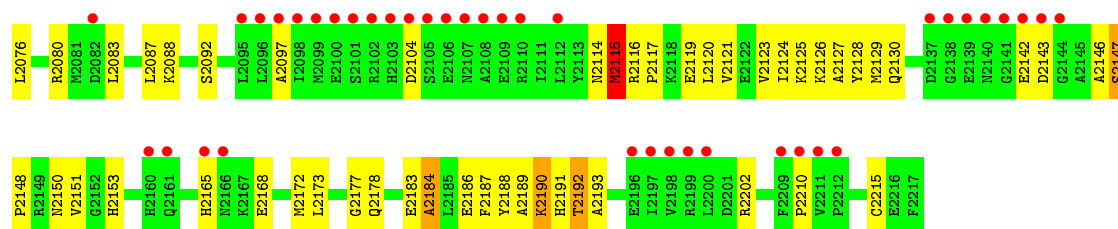
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	1710	Total	C	N	O	0	0	0
			8479	5059	1710	1710			
1	B	1708	Total	C	N	O	0	0	0
			8469	5053	1708	1708			

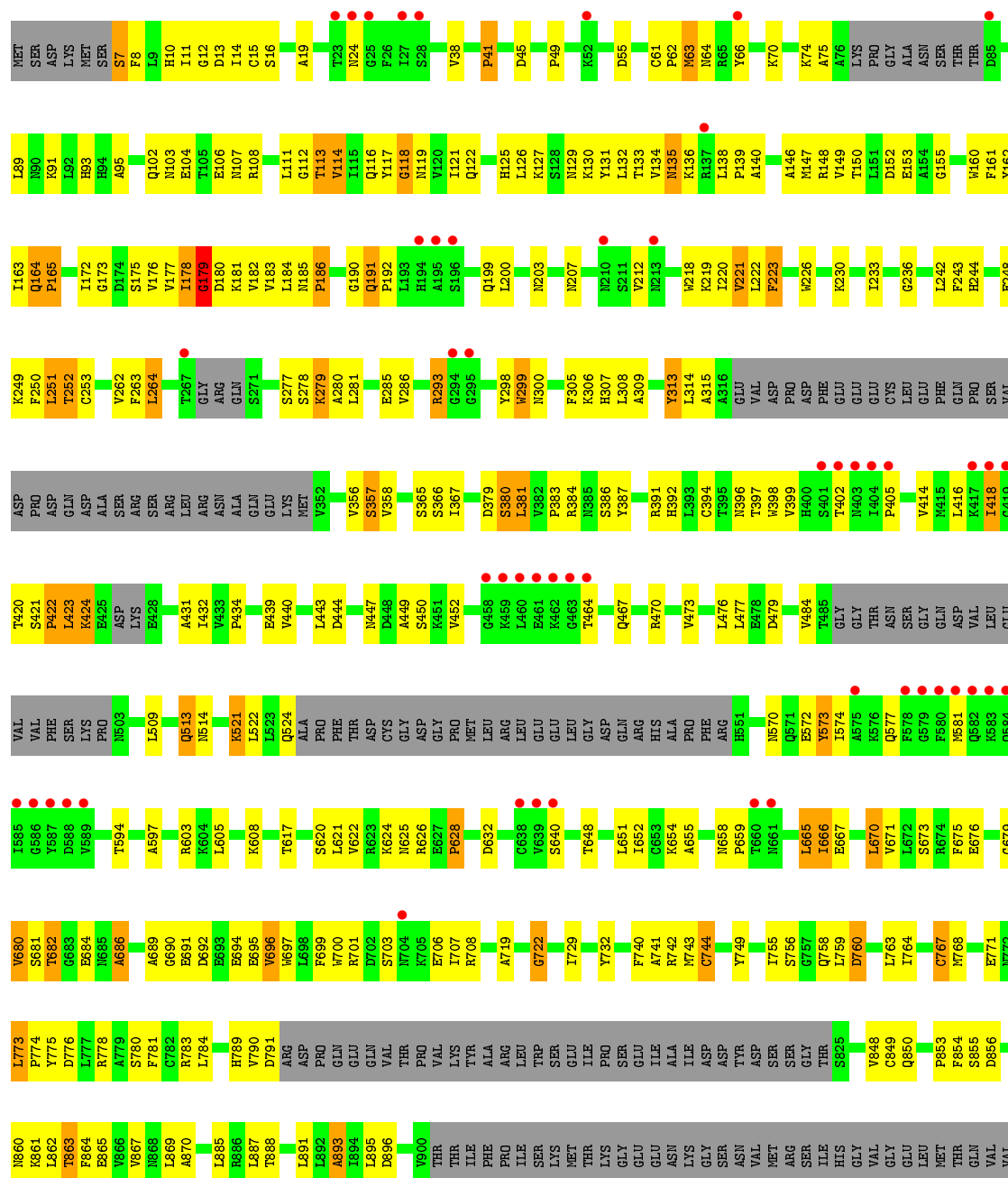
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

- [illegible]





• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



L2085	L2091	L2095	Y2113	P2117	L2120	V2123	M2129	Q2130	G2131	G2138	E2139	A2146	S2147	V2151	G2152	Y2156	I2157	L2158	A2159	H2160	Q2161	L2162	A2163	H2165	H2166	G2181	E2182	A2184	L2185	E2186	F2187	A2189	T2192	A2193	Q2194	I2197	D2201	R2202	T2203	M2204	E2205											
R1988	C1989	Q1990	N1991	Y1996	H1997	L1998	E2001	T2002	D2007	G2011	G2015	L2016	L2017	G2018	L2019	G2020	G2021	G2022	Y2023	L2024	V2029	A2030	L2036	T2040	Q2044	G2045	P2046	N2050	L2054	N2060	G2061	L2062	D2063	L2064	T2065	L2066	A2067	L2070	L2073	N2074	P2075	R2079	L2080	L1987								
GLN	ILE	THR	GLU	VAL	ARG	ASP	GLN	LEU	GLU	ALA	THR	ARG	LYS	ALA	PHE	THR	PHE	PHE	THR	ARG	GLU	ALA	ASP	PRO	GLY	SER	SER	GLY	GLY	THR	THR	THR	ALA	ALA	ASP	K1951	Q1966	P1967	R1970	C1976	H1979	Q1984	M1985	L1986								
R1818	Y1819	F1820	H1821	E1822	S1823	I1824	A1827	I1828	A1829	L1830	L1831	E1832	G1833	G1834	M1835	Q1839	H1840	S1841	F1842	F1843	L1846	T1847	E1848	D1849	K1850	K1851	S1852	E1853	K1854	Q1867	K1871	D1880	L1881	G1882	N1883	E1889	VAL	ASP	ARG	ALA	PRO	SER	ARG	LYS	ALA	GLU	PRO	THR				
ASN	ILE	ARG	PRO	SER	GLY	ARG	ARG	GLU	SER	LEU	THR	SER	PHE	GLY	ASN	GLY	PRO	LEU	SER	GLY	PRO	SER	LYS	PRO	GLY	GLY	GLY	GLY	PRO	PRO	GLY	SER	SER	SER	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
D1685	R1686	G1687	GLY	GLY	LYS	GLN	ILE	SER	ILE	ASP	GLU	SER	GLU	GLU	ALA	S1593	R1594	D1595	Y1596	R1597	N1598	I1599	I1600	E1601	D1605	N1609	S1608	A1609	D1612	R1613	P1631	E1632	L1634	L1635	F1636	P1637	E1638	M1639	T1640	G1649	G1650	F1651	K1657	K1660	L1678	R1679	E1680	M1681	M1682	TYR		
TRP	ARG	LEU	SER	ALA	ASN	ALA	ALA	ARG	ARG	ASP	VAL	LEU	ALA	ALA	ALA	S1593	R1594	D1595	Y1596	R1597	N1598	I1599	I1600	E1601	D1605	N1609	S1608	A1609	D1612	R1613	P1631	E1632	L1634	L1635	F1636	P1637	E1638	M1639	T1640	G1649	G1650	F1651	K1657	K1660	L1678	R1679	E1680	M1681	M1682	TYR		
PHE	ARG	VAL	THR	HIS	CYS	ASN	THR	LEU	MET	PRO	SER	GLN	LYS	ALA	VAL	GLU	SER	CYS	ILE	ARG	VAL	LEU	ASP	VAL	VAL	N1462	N1463	T1464	S1465	D1466	R1467	S1492	P1493	PHE	SER	ASP	GLN	SER	VAL	ASN	ASN	LEU	THR	GLN	THR	LEU	GLN	VAL	VAL	VAL	VAL	VAL
C1429	Y1430	V1431	D1432	T1433	E1434	V1435	E1436	M1437	E1438	E1439	Y1441	T1442	S1443	N1444	H1445	M1446	W1447	D1456	C1457	T1458	R1459	A1460	C1461	N1462	N1463	T1464	S1465	D1466	R1467	S1492	P1493	PHE	SER	ASP	GLN	SER	VAL	ASN	ASN	LEU	THR	GLN	THR	LEU	GLN	VAL	VAL	VAL	VAL	VAL		
C1326	Q1327	D1328	M1329	Y1330	E1333	E1339	V1341	Y1345	H1346	D1347	R1348	A1349	S1350	S1369	P1370	L1371	M1372	Y1373	Y1378	A1382	V1383	C1384	T1385	E1386	G1387	K1388	N1389	Y1390	Y1391	L1400	P1401	L1402	D1403	D1404	I1405	V1408	E1412	D1413	C1414	I1415	E1417	A1421	Y1422	L1426	H1427	H1428						
L1217	L1218	Q1219	I1220	A1225	E1226	Q1231	R1235	L1236	A1237	H1238	L1241	Q1242	N1243	Q1252	L1255	L1275	H1276	F1277	E1269	A1270	V1271	I1276	H1275	C1286	I1287	N1288	E1289	R1290	V1291	V1292	L1299	E1300	T1301	G1302	R1304	N1305	V1306	Q1307	K1310	F1311	E1319	K1324	K1325									
GLN	GLY	PRO	ASP	GLU	PRO	MET	ASP	GLY	ALA	SER	GLY	GLU	LYS	THR	GLU	GLY	THR	SER	LYS	PRO	LEU	LYS	HIS	GLU	THR	SER	SER	ASN	TYR	TYR	ARG	VAL	K1176	E1177	E1178	I1179	L1180	I1181	R1182	R1198	K1199	Q1200	Q1201	Q1202	R1203	H1211	A1212	V1213	V1214	L1215	E1216	
SER	GLY	ASN	SER	SER	GLN	GLY	PRO	MET	THR	ASN	VAL	PRO	G1026	D1029	D1051	L1052	D1053	D1054	H1055	G1056	G1057	L1061	R1062	V1063	L1064	L1080	L1083	F1084	V1093	L1094	Q1095	A1096	Q1099	V1100	S1106	Q1107	I1115	K1116	Q1117	E1127	K1128	S1129	E1130	L1131	R1132	VAL	TYR	LYS	GLY	SER		

Q2206	I2207	V2208	F2209	P2210	V2211	P2212	C2215	E2216	F2217
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.50Å 221.73Å 318.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 7.31 49.15 – 7.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-7.31) 88.5 (49.15-7.31)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.317 , 0.394 0.316 , 0.394	Depositor DCC
R_{free} test set	536 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	209.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 335.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.219 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.48	1/8465 (0.0%)	0.72	6/11786 (0.1%)
1	B	0.49	1/8455 (0.0%)	0.72	1/11772 (0.0%)
All	All	0.48	2/16920 (0.0%)	0.72	7/23558 (0.0%)

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	25
1	B	0	22
All	All	0	47

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ILE	C-O	7.16	1.36	1.23
1	A	1048	THR	C-N	5.11	1.44	1.34

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	999	ARG	N-CA-C	-7.07	91.92	111.00
1	A	177	VAL	N-CA-C	6.68	129.03	111.00
1	B	743	MET	C-N-CA	5.66	135.84	121.70
1	A	176	VAL	C-N-CA	5.44	135.31	121.70
1	A	554	ARG	CA-C-O	-5.28	109.02	120.10

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLY	Peptide
1	A	15	CYS	Peptide
1	A	176	VAL	Peptide
1	A	73	TRP	Peptide
1	A	8	PHE	Peptide

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	8479	0	3697	386	0
1	B	8469	0	3697	360	0
All	All	16948	0	7394	745	0

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 31.

The worst 5 of 745 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:A:1208:MET:O	1:A:1212:ALA:HB3	1.49	1.10
1:A:405:PRO:HA	1:A:416:LEU:HA	1.39	1.04
1:A:162:TYR:O	1:A:184:LEU:C	1.97	1.02
1:B:1682:MET:O	1:B:1686:ARG:N	1.93	1.01
1:A:1472:SER:O	1:A:1476:LYS:CB	2.10	1.00

There are no symmetry-related clashes.

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	1682/2217 (76%)	1265 (75%)	296 (18%)	121 (7%)	1	14
1	B	1680/2217 (76%)	1193 (71%)	337 (20%)	150 (9%)	1	11
All	All	3362/4434 (76%)	2458 (73%)	633 (19%)	271 (8%)	1	12

5 of 271 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ALA
1	A	87	VAL
1	A	213	ASN
1	A	222	LEU
1	A	226	TRP

5.3.2 Protein sidechains [i](#)

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

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 carbohydrates 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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1710/2217 (77%)	0.34	184 (10%) 5 9	0, 157, 428, 888	0
1	B	1708/2217 (77%)	0.29	175 (10%) 6 10	0, 136, 432, 776	0
All	All	3418/4434 (77%)	0.31	359 (10%) 6 9	0, 147, 430, 888	0

The worst 5 of 359 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2102	ARG	18.5
1	A	2103	HIS	16.7
1	A	2101	SER	13.2
1	A	2107	ASN	13.0
1	A	1395	LYS	11.4

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.