



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 2H6R / pdb_00002h6r
Title : Crystal Structure of triosephosphate isomerase (TIM) from *Methanocaldococcus jannaschii*
Authors : Gayathri, P.; Banerjee, M.; Vijayalakshmi, A.; Balaram, H.; Balaram, P.; Murthy, M.R.N.
Deposited on : 2006-06-01
Resolution : 2.30 Å(reported)

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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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

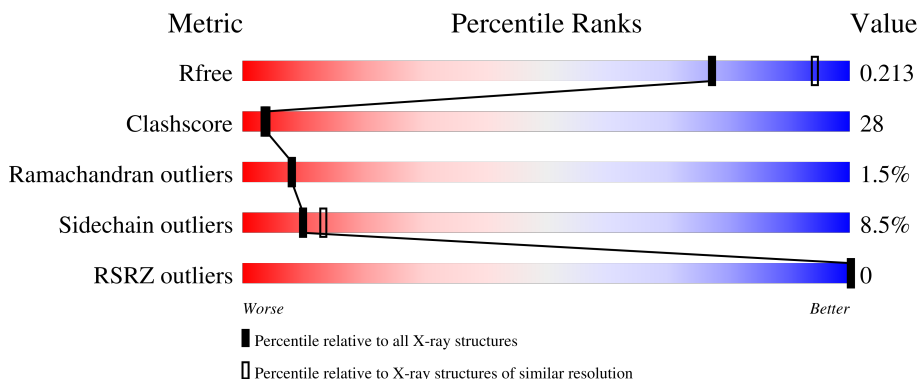
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 of 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	219	
1	B	219	
1	C	219	
1	D	219	
1	E	219	

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Mol	Chain	Length	Quality of chain
1	F	219	 50% 33% 8% 8%
1	G	219	 53% 35% • 9%
1	H	219	 48% 39% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12422 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 Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1504	943	258	294	9			
1	B	209	Total	C	N	O	S	0	0	0
			1548	971	265	303	9			
1	C	204	Total	C	N	O	S	0	0	0
			1508	946	260	293	9			
1	D	200	Total	C	N	O	S	0	0	0
			1480	927	255	289	9			
1	E	207	Total	C	N	O	S	0	0	0
			1538	966	264	299	9			
1	F	201	Total	C	N	O	S	0	0	0
			1490	934	257	290	9			
1	G	200	Total	C	N	O	S	0	0	0
			1477	925	254	289	9			
1	H	201	Total	C	N	O	S	0	0	0
			1493	937	257	290	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q58923
A	134	CYS	TYR	engineered mutation	UNP Q58923
B	2	VAL	LEU	engineered mutation	UNP Q58923
B	134	CYS	TYR	engineered mutation	UNP Q58923
C	2	VAL	LEU	engineered mutation	UNP Q58923
C	134	CYS	TYR	engineered mutation	UNP Q58923
D	2	VAL	LEU	engineered mutation	UNP Q58923
D	134	CYS	TYR	engineered mutation	UNP Q58923
E	2	VAL	LEU	engineered mutation	UNP Q58923
E	134	CYS	TYR	engineered mutation	UNP Q58923
F	2	VAL	LEU	engineered mutation	UNP Q58923
F	134	CYS	TYR	engineered mutation	UNP Q58923
G	2	VAL	LEU	engineered mutation	UNP Q58923

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Chain	Residue	Modelled	Actual	Comment	Reference
G	134	CYS	TYR	engineered mutation	UNP Q58923
H	2	VAL	LEU	engineered mutation	UNP Q58923
H	134	CYS	TYR	engineered mutation	UNP Q58923

- Molecule 2 is water.

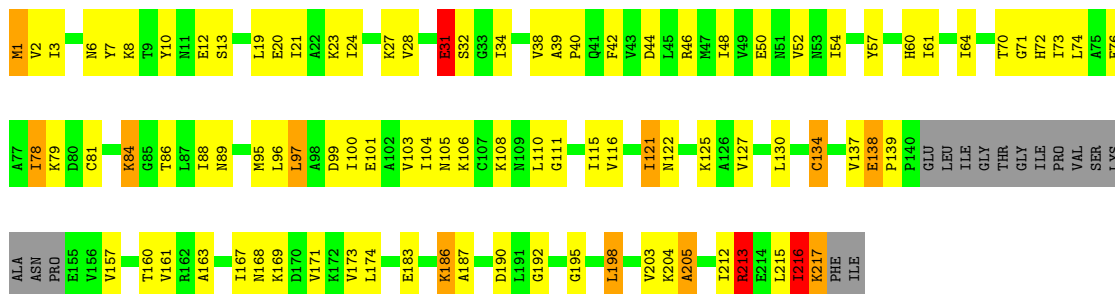
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	58	Total	O	0	0
			58	58		
2	B	55	Total	O	0	0
			55	55		
2	C	45	Total	O	0	0
			45	45		
2	D	46	Total	O	0	0
			46	46		
2	E	53	Total	O	0	0
			53	53		
2	F	34	Total	O	0	0
			34	34		
2	G	36	Total	O	0	0
			36	36		
2	H	57	Total	O	0	0
			57	57		

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.

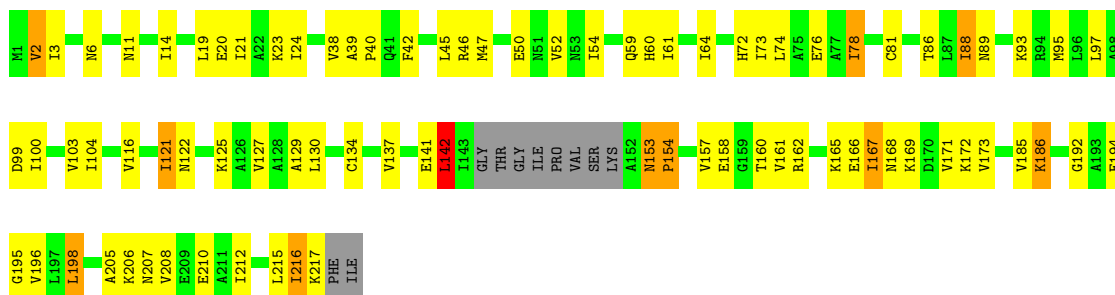
- Molecule 1: Triosephosphate isomerase

Chain A: 



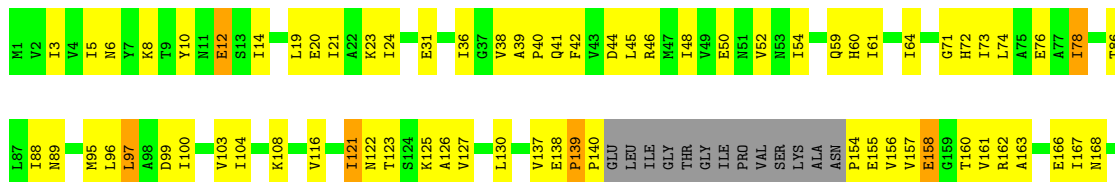
- Molecule 1: Triosephosphate isomerase

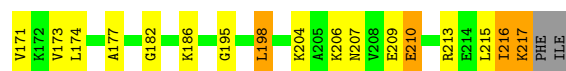
Chain B: 



- Molecule 1: Triosephosphate isomerase

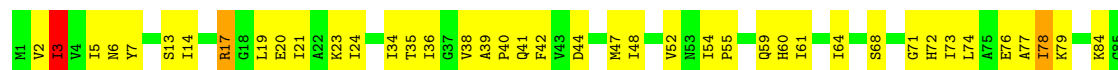
Chain C: 





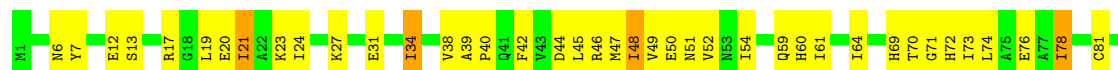
• Molecule 1: Triosephosphate isomerase

Chain D: 49% 36% 5% • 9%



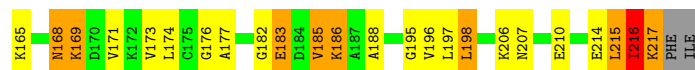
• Molecule 1: Triosephosphate isomerase

Chain E: 47% 39% 7% • 5%



• Molecule 1: Triosephosphate isomerase

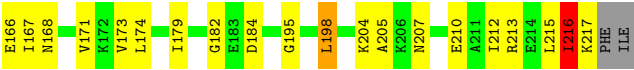
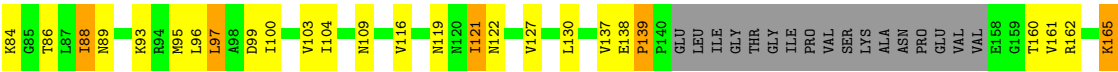
Chain F: 50% 33% 8% 8%



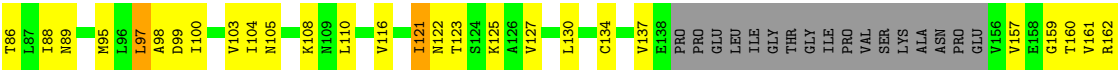
• Molecule 1: Triosephosphate isomerase

Chain G: 53% 35% • 9%





● Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	139.34Å 139.34Å 80.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.28 – 2.30 34.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (34.28-2.30) 96.3 (34.28-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.56 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.278 0.207 , 0.213	Depositor DCC
R_{free} test set	3415 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 26.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.426 for h,-h-k,-l 0.420 for -k,-h,-l	Xtriage
Reported twinning fraction	0.250 for h,k,l 0.250 for k,h,-l 0.250 for -k,-h,-l 0.250 for -h,-k,l	Depositor
Outliers	0 of 75331 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12422	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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	0.41	1/1516 (0.1%)	1.13	11/2051 (0.5%)
1	B	0.31	0/1561	0.89	2/2114 (0.1%)
1	C	0.37	0/1521	0.96	4/2058 (0.2%)
1	D	0.43	1/1490 (0.1%)	1.12	8/2014 (0.4%)
1	E	0.33	0/1552	0.93	7/2100 (0.3%)
1	F	0.39	1/1502 (0.1%)	0.95	8/2031 (0.4%)
1	G	0.31	0/1489	0.93	2/2015 (0.1%)
1	H	0.42	1/1504 (0.1%)	0.98	6/2032 (0.3%)
All	All	0.37	4/12135 (0.0%)	0.99	48/16415 (0.3%)

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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	216	ILE	C-O	-8.67	1.13	1.24
1	D	216	ILE	CA-C	-8.07	1.42	1.52
1	A	216	ILE	CA-C	-6.40	1.44	1.52
1	F	185	VAL	CA-CB	-5.39	1.47	1.55

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	ILE	CA-C-N	17.67	153.51	121.70
1	D	216	ILE	C-N-CA	17.67	153.51	121.70
1	D	216	ILE	O-C-N	14.63	140.86	122.57
1	H	216	ILE	CA-C-N	-14.01	102.24	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	216	ILE	C-N-CA	-14.01	102.24	121.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	ILE	Mainchain

5.2 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 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	1504	0	1560	101	0
1	B	1548	0	1604	71	0
1	C	1508	0	1569	79	0
1	D	1480	0	1538	99	0
1	E	1538	0	1596	110	0
1	F	1490	0	1552	118	0
1	G	1477	0	1525	83	0
1	H	1493	0	1554	86	0
2	A	58	0	0	0	0
2	B	55	0	0	1	0
2	C	45	0	0	0	0
2	D	46	0	0	0	0
2	E	53	0	0	0	0
2	F	34	0	0	0	0
2	G	36	0	0	0	0
2	H	57	0	0	0	0
All	All	12422	0	12498	693	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 28.

The worst 5 of 693 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:F:215:LEU:O	1:F:217:LYS:HD3	1.46	1.13
1:D:217:LYS:HZ3	1:D:217:LYS:HB2	1.01	1.11
1:E:207:ASN:HD21	1:E:210:GLU:HB3	1.07	1.11
1:C:138:GLU:HB3	1:C:139:PRO:HD2	1.12	1.10
1:H:19:LEU:HA	1:H:48:ILE:HD11	1.23	1.09

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	199/219 (91%)	176 (88%)	20 (10%)	3 (2%)	8	8
1	B	205/219 (94%)	177 (86%)	23 (11%)	5 (2%)	4	4
1	C	200/219 (91%)	173 (86%)	26 (13%)	1 (0%)	24	31
1	D	196/219 (90%)	176 (90%)	17 (9%)	3 (2%)	8	8
1	E	203/219 (93%)	181 (89%)	20 (10%)	2 (1%)	12	15
1	F	197/219 (90%)	173 (88%)	20 (10%)	4 (2%)	6	5
1	G	196/219 (90%)	178 (91%)	16 (8%)	2 (1%)	12	15
1	H	197/219 (90%)	174 (88%)	19 (10%)	4 (2%)	6	5
All	All	1593/1752 (91%)	1408 (88%)	161 (10%)	24 (2%)	8	8

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ILE
1	B	142	LEU
1	D	216	ILE
1	G	205	ALA
1	H	205	ALA

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	165/180 (92%)	150 (91%)	15 (9%)	9	11
1	B	170/180 (94%)	157 (92%)	13 (8%)	12	16
1	C	166/180 (92%)	153 (92%)	13 (8%)	11	16
1	D	162/180 (90%)	145 (90%)	17 (10%)	6	8
1	E	169/180 (94%)	150 (89%)	19 (11%)	6	7
1	F	164/180 (91%)	149 (91%)	15 (9%)	9	11
1	G	161/180 (89%)	151 (94%)	10 (6%)	16	24
1	H	164/180 (91%)	154 (94%)	10 (6%)	17	24
All	All	1321/1440 (92%)	1209 (92%)	112 (8%)	10	13

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	217	LYS
1	H	217	LYS
1	E	198	LEU
1	H	216	ILE
1	G	167	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	69	HIS
1	G	105	ASN
1	F	89	ASN
1	F	207	ASN
1	G	168	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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 [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	203/219 (92%)	-1.49	0 100 100	13, 29, 42, 53	0
1	B	209/219 (95%)	-1.47	0 100 100	16, 33, 44, 50	0
1	C	204/219 (93%)	-1.43	0 100 100	17, 32, 50, 57	0
1	D	200/219 (91%)	-1.48	0 100 100	15, 32, 51, 60	0
1	E	207/219 (94%)	-1.40	0 100 100	17, 35, 52, 60	0
1	F	201/219 (91%)	-1.38	0 100 100	21, 37, 55, 61	0
1	G	200/219 (91%)	-1.38	0 100 100	22, 39, 60, 69	0
1	H	201/219 (91%)	-1.47	0 100 100	9, 32, 43, 57	0
All	All	1625/1752 (92%)	-1.44	0 100 100	9, 34, 51, 69	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.