



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:16 AM UTC

PDB ID : 6T9H / pdb_00006t9h
Title : C171S mutant of Linalool Dehydratase Isomerase
Authors : Cuetos, A.; Zukic, E.; Danesh-Azari, H.R.; Grogan, G.
Deposited on : 2019-10-28
Resolution : 2.58 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 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

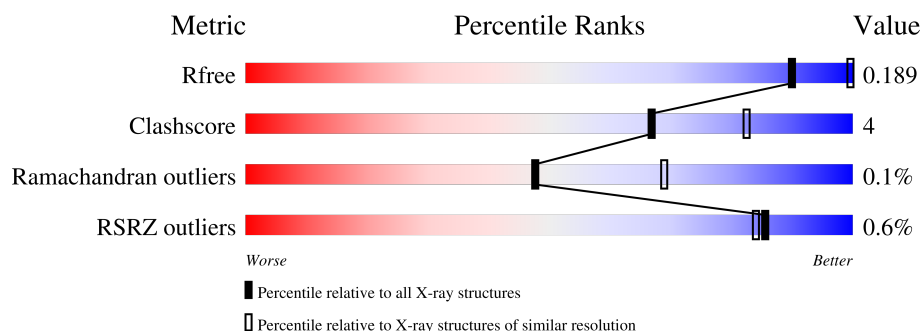
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	372	% 90% 8% .
1	B	372	% 89% 8% ..
1	C	372	% 90% 8% .
1	D	372	89% 8% ..
1	E	372	% 89% 7% ..
1	S	372	% 90% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	T	372	91% 6% .
1	U	372	% 90% 7% .
1	V	372	88% 8% . .
1	W	372	% 89% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29358 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 Linalool dehydratase-isomerase protein LDI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2864	1856	476	520	12			
1	B	363	Total	C	N	O	S	0	0	0
			2862	1855	474	521	12			
1	C	363	Total	C	N	O	S	0	0	0
			2853	1844	476	521	12			
1	D	363	Total	C	N	O	S	0	0	0
			2863	1851	479	521	12			
1	E	362	Total	C	N	O	S	0	0	0
			2855	1848	475	520	12			
1	S	363	Total	C	N	O	S	0	0	0
			2856	1847	478	519	12			
1	T	362	Total	C	N	O	S	0	0	0
			2831	1836	471	512	12			
1	U	362	Total	C	N	O	S	0	0	0
			2807	1820	460	515	12			
1	V	361	Total	C	N	O	S	0	0	0
			2842	1836	477	517	12			
1	W	362	Total	C	N	O	S	0	0	0
			2849	1844	475	518	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP W8X534
A	171	SER	CYS	engineered mutation	UNP W8X534
B	1	MET	-	initiating methionine	UNP W8X534
B	171	SER	CYS	engineered mutation	UNP W8X534
C	1	MET	-	initiating methionine	UNP W8X534
C	171	SER	CYS	engineered mutation	UNP W8X534
D	1	MET	-	initiating methionine	UNP W8X534
D	171	SER	CYS	engineered mutation	UNP W8X534
E	1	MET	-	initiating methionine	UNP W8X534

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	171	SER	CYS	engineered mutation	UNP W8X534
S	1	MET	-	initiating methionine	UNP W8X534
S	171	SER	CYS	engineered mutation	UNP W8X534
T	1	MET	-	initiating methionine	UNP W8X534
T	171	SER	CYS	engineered mutation	UNP W8X534
U	1	MET	-	initiating methionine	UNP W8X534
U	171	SER	CYS	engineered mutation	UNP W8X534
V	1	MET	-	initiating methionine	UNP W8X534
V	171	SER	CYS	engineered mutation	UNP W8X534
W	1	MET	-	initiating methionine	UNP W8X534
W	171	SER	CYS	engineered mutation	UNP W8X534

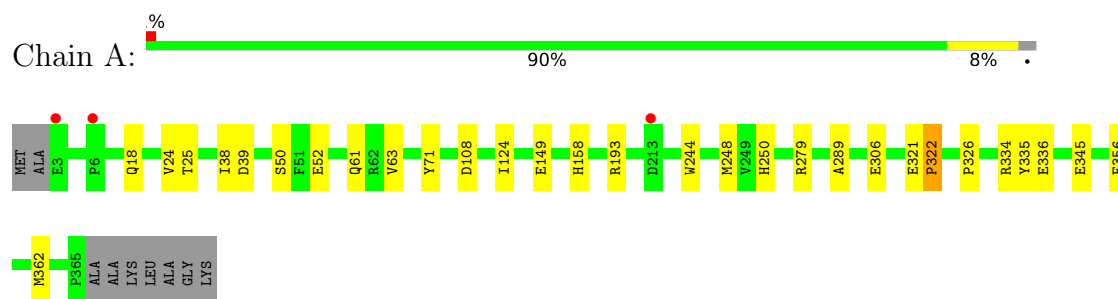
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	108	Total O 108 108	0	0
2	B	92	Total O 92 92	0	0
2	C	87	Total O 87 87	0	0
2	D	102	Total O 102 102	0	0
2	E	102	Total O 102 102	0	0
2	S	84	Total O 84 84	0	0
2	T	66	Total O 66 66	0	0
2	U	59	Total O 59 59	0	0
2	V	94	Total O 94 94	0	0
2	W	82	Total O 82 82	0	0

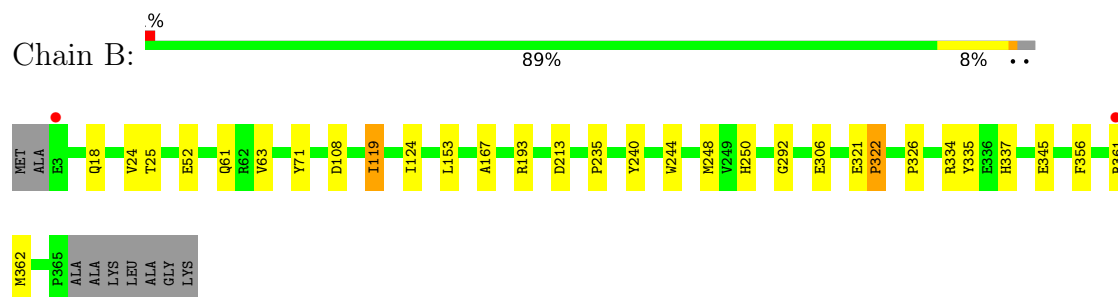
3 Residue-property plots [i](#)

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.

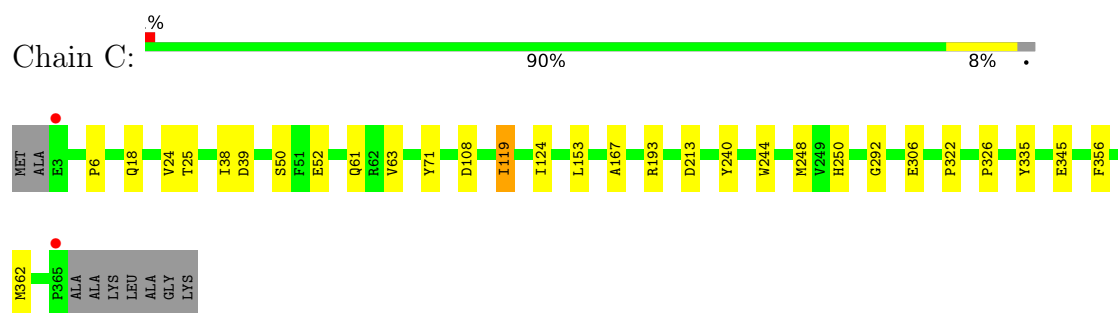
- Molecule 1: Linalool dehydratase-isomerase protein LDI



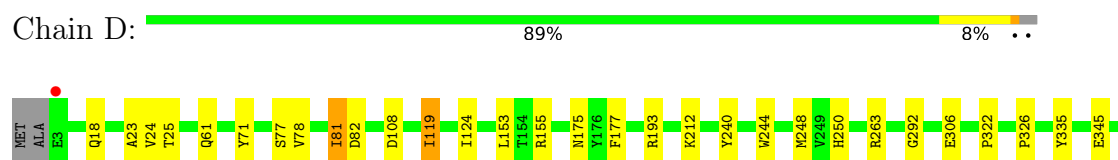
- Molecule 1: Linalool dehydratase-isomerase protein LDI



- Molecule 1: Linalool dehydratase-isomerase protein LDI

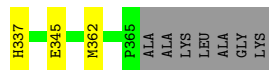
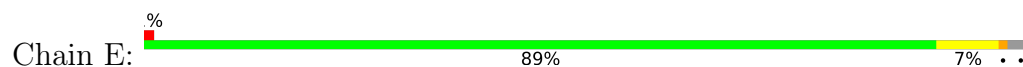


- Molecule 1: Linalool dehydratase-isomerase protein LDI

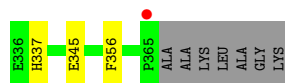




- Molecule 1: Linalool dehydratase-isomerase protein LDI



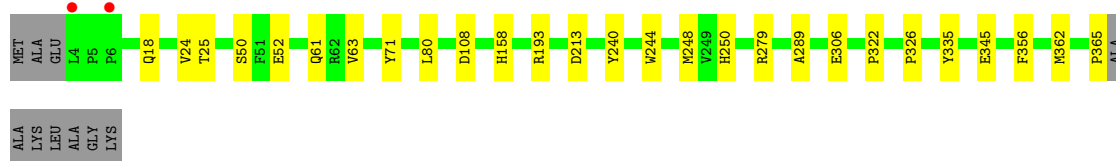
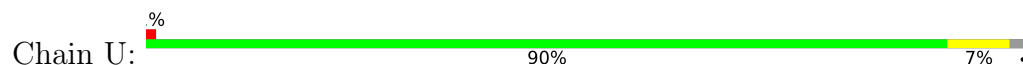
- Molecule 1: Linalool dehydratase-isomerase protein LDI



- Molecule 1: Linalool dehydratase-isomerase protein LDI

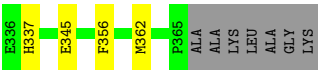


- Molecule 1: Linalool dehydratase-isomerase protein LDI

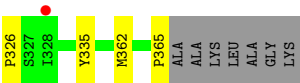
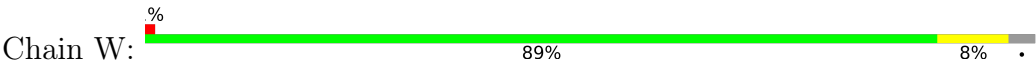


- Molecule 1: Linalool dehydratase-isomerase protein LDI





● Molecule 1: Linalool dehydratase-isomerase protein LDI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.77Å 109.47Å 232.78Å 90.00° 99.53° 90.00°	Depositor
Resolution (Å)	67.99 – 2.58 67.99 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.2 (67.99-2.58) 99.3 (67.99-2.58)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.179 , 0.212 (Not available) , 0.189	Depositor DCC
R_{free} test set	6676 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29358	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.9536e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	1.04	0/2950	1.34	3/4017 (0.1%)
1	B	1.03	1/2948 (0.0%)	1.35	5/4015 (0.1%)
1	C	1.03	0/2939	1.34	3/4008 (0.1%)
1	D	1.05	0/2949	1.36	3/4018 (0.1%)
1	E	1.04	2/2940 (0.1%)	1.35	3/4004 (0.1%)
1	S	1.05	1/2942 (0.0%)	1.34	2/4010 (0.0%)
1	T	1.02	0/2917	1.35	3/3978 (0.1%)
1	U	1.03	0/2892	1.33	2/3948 (0.1%)
1	V	1.04	0/2928	1.34	2/3990 (0.1%)
1	W	1.03	1/2935 (0.0%)	1.34	2/4000 (0.1%)
All	All	1.04	5/29340 (0.0%)	1.34	28/39988 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	158	HIS	CE1-NE2	8.00	1.40	1.32
1	E	158	HIS	CE1-NE2	6.51	1.39	1.32
1	E	91	HIS	CE1-NE2	5.65	1.38	1.32
1	W	158	HIS	CE1-NE2	5.34	1.37	1.32
1	B	235	PRO	C-O	-5.09	1.17	1.24

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	219	ARG	CG-CD-NE	8.31	130.28	112.00
1	T	155	ARG	CG-CD-NE	-7.57	95.35	112.00
1	A	158	HIS	CA-CB-CG	-6.01	107.79	113.80
1	D	119	ILE	CB-CA-C	5.94	116.28	111.06
1	D	81	ILE	CB-CA-C	5.91	119.54	111.97

There are no chirality outliers.

There are no planarity outliers.

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	2864	0	2745	20	0
1	B	2862	0	2740	19	0
1	C	2853	0	2708	21	0
1	D	2863	0	2737	30	0
1	E	2855	0	2738	29	0
1	S	2856	0	2724	18	0
1	T	2831	0	2696	14	0
1	U	2807	0	2650	18	0
1	V	2842	0	2709	24	0
1	W	2849	0	2722	23	0
2	A	108	0	0	4	0
2	B	92	0	0	4	0
2	C	87	0	0	4	0
2	D	102	0	0	4	0
2	E	102	0	0	4	0
2	S	84	0	0	3	0
2	T	66	0	0	3	0
2	U	59	0	0	5	0
2	V	94	0	0	6	0
2	W	82	0	0	2	0
All	All	29358	0	27169	205	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 4.

The worst 5 of 205 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:V:6:PRO:HB2	2:V:467:HOH:O	1.48	1.11
1:W:183:VAL:HG22	1:W:248:MET:HE2	1.50	0.92
1:D:365:PRO:C	2:D:473:HOH:O	2.13	0.90
1:E:183:VAL:HG22	1:E:248:MET:HE2	1.52	0.89
1:E:183:VAL:HA	1:E:248:MET:CE	2.03	0.87

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 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 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	361/372 (97%)	352 (98%)	9 (2%)	0	100	100
1	B	361/372 (97%)	353 (98%)	8 (2%)	0	100	100
1	C	361/372 (97%)	353 (98%)	8 (2%)	0	100	100
1	D	361/372 (97%)	353 (98%)	8 (2%)	0	100	100
1	E	360/372 (97%)	352 (98%)	8 (2%)	0	100	100
1	S	361/372 (97%)	353 (98%)	8 (2%)	0	100	100
1	T	360/372 (97%)	353 (98%)	7 (2%)	0	100	100
1	U	360/372 (97%)	353 (98%)	7 (2%)	0	100	100
1	V	359/372 (96%)	351 (98%)	7 (2%)	1 (0%)	36	56
1	W	360/372 (97%)	352 (98%)	7 (2%)	1 (0%)	36	56
All	All	3604/3720 (97%)	3525 (98%)	77 (2%)	2 (0%)	48	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	W	212	LYS
1	V	212	LYS

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 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	363/372 (97%)	-0.43	3 (0%) 82 81	27, 38, 57, 102	0
1	B	363/372 (97%)	-0.36	2 (0%) 85 84	29, 41, 62, 96	0
1	C	363/372 (97%)	-0.30	2 (0%) 85 84	33, 45, 63, 104	0
1	D	363/372 (97%)	-0.39	1 (0%) 90 89	27, 39, 58, 95	0
1	E	362/372 (97%)	-0.36	3 (0%) 82 81	28, 40, 62, 83	0
1	S	363/372 (97%)	-0.29	4 (1%) 78 75	30, 42, 63, 98	0
1	T	362/372 (97%)	-0.28	1 (0%) 90 89	33, 45, 63, 88	0
1	U	362/372 (97%)	0.00	2 (0%) 85 84	34, 54, 75, 110	0
1	V	361/372 (97%)	-0.31	1 (0%) 90 89	29, 42, 59, 86	0
1	W	362/372 (97%)	-0.33	2 (0%) 85 84	29, 43, 61, 80	0
All	All	3624/3720 (97%)	-0.30	21 (0%) 85 84	27, 43, 65, 110	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	6	PRO	3.5
1	V	5	PRO	3.5
1	S	5	PRO	3.0
1	B	3	GLU	2.9
1	C	3	GLU	2.7

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.