



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:21 PM GMT

PDB ID : 2C7Y
Title : PLANT ENZYME
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Deposited on : 2005-11-30
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

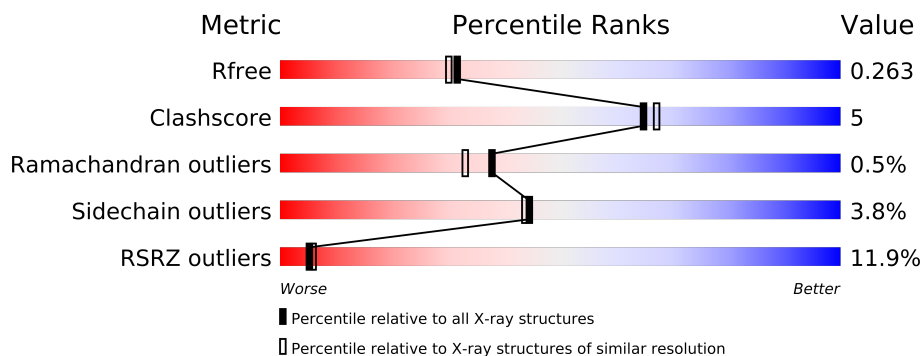
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6285 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-KETOACYL-COA THIOLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	20	1	0
			2871	1796	509	547	19			
1	B	396	Total	C	N	O	S	6	1	0
			2903	1818	514	552	19			

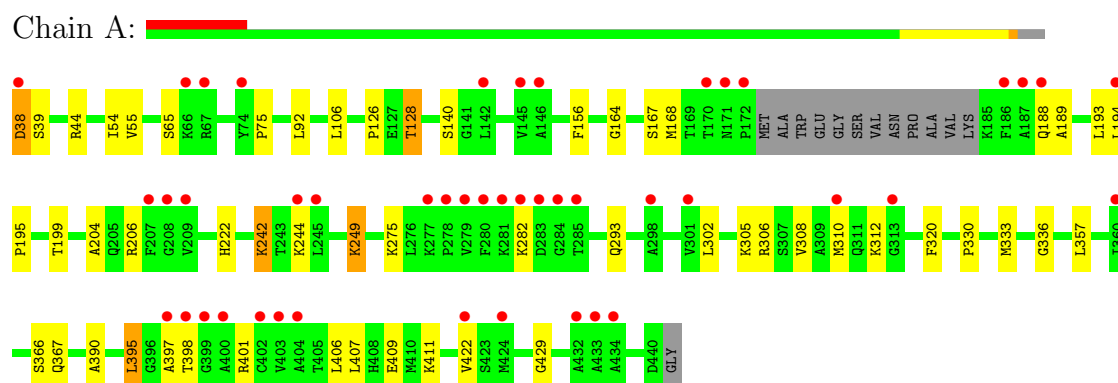
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	228	Total	O	0	0
			228	228		
2	B	283	Total	O	0	0
			283	283		

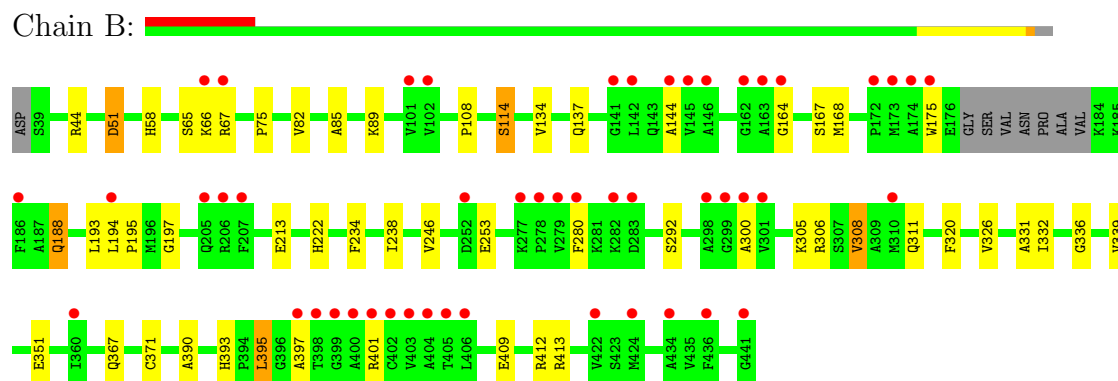
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 3-KETOACYL-COA THIOLASE 2



• Molecule 1: 3-KETOACYL-COA THIOLASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.15Å 94.46Å 111.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.21 – 2.10 29.21 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.21-2.10) 94.9 (29.21-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.201 , 0.263 0.201 , 0.263	Depositor DCC
R_{free} test set	2200 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 43408 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6285	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 64.76 % 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 7.8771e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.53	2/2913 (0.1%)	0.66	3/3940 (0.1%)
1	B	0.54	0/2950	0.66	0/3991
All	All	0.54	2/5863 (0.0%)	0.66	3/7931 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	LYS	CB-CG	-6.67	1.34	1.52
1	A	249	LYS	CB-CG	-5.04	1.39	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	LYS	CA-CB-CG	5.28	125.02	113.40
1	A	38	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	275	LYS	CA-CB-CG	5.18	124.80	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2871	0	2916	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2903	0	2944	27	0
2	A	228	0	0	5	0
2	B	283	0	0	4	0
All	All	6285	0	5860	61	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:ASP:HB2	1:A:39:SER:HA	1.24	1.09
1:A:38:ASP:HB2	1:A:39:SER:CA	1.98	0.92
1:B:371:CYS:HB3	2:B:2246:HOH:O	1.73	0.88
1:A:38:ASP:CB	1:A:39:SER:HA	1.95	0.81
1:B:188:GLN:HG3	2:B:2125:HOH:O	1.85	0.76
1:B:75:PRO:HG3	1:B:167:SER:HB3	1.76	0.67
1:A:65:SER:HB3	1:A:168:MET:HG3	1.77	0.66
1:A:156:PHE:O	2:A:2094:HOH:O	2.14	0.63
1:A:306:ARG:NH2	2:A:2159:HOH:O	2.33	0.62
1:A:330:PRO:HA	1:A:333[A]:MET:HE3	1.82	0.61
1:A:333[B]:MET:H	1:A:333[B]:MET:CE	2.13	0.60
1:B:58:HIS:NE2	1:B:89:LYS:HD2	2.18	0.58
1:B:305:LYS:HB3	1:B:308:VAL:HG12	1.85	0.58
1:B:114:SER:HB2	1:B:175:TRP:HB3	1.85	0.58
1:A:310:MET:CG	2:A:2161:HOH:O	2.53	0.56
1:A:126:PRO:HG2	1:A:128:THR:HG23	1.87	0.55
1:A:305:LYS:HB3	1:A:308:VAL:HG12	1.89	0.55
1:A:92:LEU:CD1	1:A:312:LYS:HE3	2.37	0.54
1:B:194:LEU:HB2	1:B:195:PRO:HD3	1.89	0.54
1:A:92:LEU:HD13	1:A:312:LYS:HE3	1.88	0.54
1:B:222:HIS:CE1	1:B:390:ALA:HA	2.44	0.53
1:B:65:SER:HB3	1:B:168:MET:HG3	1.91	0.53
1:A:106:LEU:CD2	1:A:189:ALA:HB2	2.38	0.52
1:A:333[A]:MET:HE2	1:A:429:GLY:HA2	1.91	0.52
1:B:326:VAL:HG21	1:B:339:VAL:HG12	1.92	0.51
1:A:38:ASP:CB	1:A:39:SER:CA	2.72	0.50
1:A:193:LEU:HD11	1:A:395:LEU:HD21	1.94	0.50
1:A:164:GLY:HA3	1:A:397:ALA:HA	1.93	0.49
1:A:194:LEU:HB2	1:A:195:PRO:HD3	1.94	0.49
1:A:330:PRO:HA	1:A:333[A]:MET:CE	2.42	0.49
1:B:412:ARG:NH2	2:B:2266:HOH:O	2.45	0.49
1:B:82:VAL:HG12	1:B:300:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:PRO:HG3	1:A:167:SER:HB3	1.95	0.48
1:B:197:GLY:HA3	1:B:280:PHE:CZ	2.49	0.47
1:A:401:ARG:HD2	1:A:401:ARG:C	2.35	0.46
1:B:193:LEU:HD11	1:B:395:LEU:HD21	1.97	0.46
1:A:222:HIS:CE1	1:A:390:ALA:HA	2.51	0.46
1:B:292:SER:HB3	1:B:393:HIS:HB2	1.97	0.45
1:B:134:VAL:CG2	1:B:144:ALA:HB2	2.46	0.45
1:B:85:ALA:O	1:B:89:LYS:HG3	2.16	0.45
1:B:234:PHE:HB3	1:B:238:ILE:HD12	1.98	0.45
1:A:406:LEU:HD22	1:A:422:VAL:HG23	1.99	0.45
1:B:409:GLU:O	1:B:413:ARG:HG3	2.17	0.44
1:B:66:LYS:O	1:B:67:ARG:HB2	2.17	0.44
1:B:246:VAL:HG22	1:B:253:GLU:HG2	1.98	0.44
1:A:333[B]:MET:H	1:A:333[B]:MET:HE3	1.83	0.43
1:B:164:GLY:HA3	1:B:397:ALA:HA	1.99	0.43
1:A:55:VAL:HG23	1:A:302:LEU:HD23	2.01	0.43
1:B:51:ASP:OD1	1:B:305:LYS:HG3	2.18	0.43
1:B:306:ARG:NH2	2:B:2209:HOH:O	2.52	0.43
1:A:411:LYS:CD	2:A:2127:HOH:O	2.68	0.42
1:A:54:ILE:HD13	1:A:407:LEU:HD11	2.02	0.42
1:B:331:ALA:C	1:B:332:ILE:HG13	2.40	0.41
1:A:140:SER:HB3	1:A:398:THR:HB	2.02	0.41
1:B:108:PRO:HA	1:B:188:GLN:HE22	1.85	0.41
1:A:242:LYS:HG3	1:A:242:LYS:O	2.20	0.41
1:A:65:SER:HB3	1:A:168:MET:CG	2.48	0.41
1:B:401:ARG:C	1:B:401:ARG:HD2	2.41	0.41
1:A:411:LYS:HD2	2:A:2127:HOH:O	2.20	0.41
1:A:204:ALA:HB2	1:A:366:SER:HB2	2.03	0.41
1:A:357:LEU:HD11	1:A:409:GLU:HG3	2.03	0.41

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	388/404 (96%)	377 (97%)	9 (2%)	2 (0%)	38	33
1	B	393/404 (97%)	383 (98%)	8 (2%)	2 (0%)	38	33
All	All	781/808 (97%)	760 (97%)	17 (2%)	4 (0%)	38	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	395	LEU
1	A	395	LEU
1	A	336	GLY
1	B	336	GLY

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	299/307 (97%)	287 (96%)	12 (4%)	42	41
1	B	301/307 (98%)	290 (96%)	11 (4%)	45	45
All	All	600/614 (98%)	577 (96%)	23 (4%)	44	44

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	128	THR
1	A	188	GLN
1	A	199	THR
1	A	206	ARG
1	A	242	LYS
1	A	244	LYS
1	A	249	LYS
1	A	282	LYS
1	A	293	GLN
1	A	320	PHE
1	A	367	GLN
1	B	44	ARG

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Mol	Chain	Res	Type
1	B	51	ASP
1	B	114	SER
1	B	137	GLN
1	B	188	GLN
1	B	213	GLU
1	B	308	VAL
1	B	311	GLN
1	B	320	PHE
1	B	351	GLU
1	B	367	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	293	GLN
1	A	311	GLN
1	A	361	ASN
1	A	367	GLN
1	B	137	GLN
1	B	188	GLN
1	B	190	GLN
1	B	191	ASN
1	B	212	GLN
1	B	311	GLN
1	B	361	ASN
1	B	393	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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 ⓘ

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	391/404 (96%)	0.73	45 (11%) 5 6	8, 18, 29, 35	5 (1%)
1	B	396/404 (98%)	0.75	49 (12%) 5 5	12, 18, 28, 38	2 (0%)
All	All	787/808 (97%)	0.74	94 (11%) 5 6	8, 18, 29, 38	7 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	PRO	4.7
1	A	38	ASP	4.4
1	A	279	VAL	4.3
1	B	403	VAL	4.3
1	B	402	CYS	4.1
1	A	403	VAL	3.9
1	A	402	CYS	3.7
1	B	173	MET	3.6
1	B	145	VAL	3.6
1	A	400	ALA	3.6
1	B	207	PHE	3.5
1	A	422	VAL	3.5
1	A	145	VAL	3.5
1	A	313	GLY	3.5
1	B	406	LEU	3.4
1	B	400	ALA	3.4
1	A	208	GLY	3.4
1	B	142	LEU	3.3
1	B	282	LYS	3.3
1	B	279	VAL	3.2
1	B	67	ARG	3.2
1	B	301	VAL	3.1
1	A	207	PHE	3.1
1	B	194	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	398	THR	3.1
1	A	74	TYR	3.0
1	B	277	LYS	3.0
1	B	422	VAL	3.0
1	A	142	LEU	3.0
1	B	399	GLY	3.0
1	A	171	ASN	3.0
1	B	186	PHE	2.9
1	B	280	PHE	2.9
1	A	399	GLY	2.9
1	A	398	THR	2.9
1	A	277	LYS	2.8
1	A	280	PHE	2.8
1	A	282	LYS	2.7
1	B	174	ALA	2.7
1	B	163	ALA	2.7
1	B	172	PRO	2.7
1	A	404	ALA	2.7
1	B	102	VAL	2.6
1	B	175	TRP	2.6
1	A	301	VAL	2.6
1	A	66	LYS	2.6
1	A	283	ASP	2.5
1	B	162	GLY	2.5
1	B	66	LYS	2.5
1	B	146	ALA	2.5
1	B	397	ALA	2.5
1	A	360	ILE	2.5
1	A	281	LYS	2.5
1	B	141	GLY	2.5
1	A	187	ALA	2.5
1	A	194	LEU	2.5
1	A	278	PRO	2.4
1	A	284	GLY	2.4
1	B	299	GLY	2.4
1	B	436	PHE	2.4
1	A	67	ARG	2.4
1	A	245	LEU	2.3
1	B	401	ARG	2.3
1	B	404	ALA	2.3
1	B	360	ILE	2.3
1	B	424	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	2.3
1	A	146	ALA	2.3
1	B	298	ALA	2.3
1	A	424	MET	2.3
1	A	186	PHE	2.2
1	A	285	THR	2.2
1	B	441	GLY	2.2
1	B	434	ALA	2.2
1	A	188	GLN	2.2
1	B	205	GLN	2.2
1	A	310	MET	2.2
1	A	397	ALA	2.2
1	B	300	ALA	2.2
1	B	164	GLY	2.2
1	A	244	LYS	2.1
1	A	433	ALA	2.1
1	A	434	ALA	2.1
1	A	298	ALA	2.1
1	B	101	VAL	2.1
1	A	170	THR	2.1
1	B	405	THR	2.1
1	A	209	VAL	2.1
1	B	283	ASP	2.1
1	B	206	ARG	2.1
1	A	432	ALA	2.1
1	B	252	ASP	2.1
1	B	278	PRO	2.0
1	B	310	MET	2.0

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 carbohydrates 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.