



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:31 AM GMT

PDB ID : 2C3T
Title : HUMAN GLUTATHIONE-S-TRANSFERASET1-1, W234R MUTANT, APO FORM
Authors : Tars, K.; Larsson, A.-K.; Shokeer, A.; Olin, B.; Mannervik, B.; Kleywegt, G.J.
Deposited on : 2005-10-12
Resolution : 2.40 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>

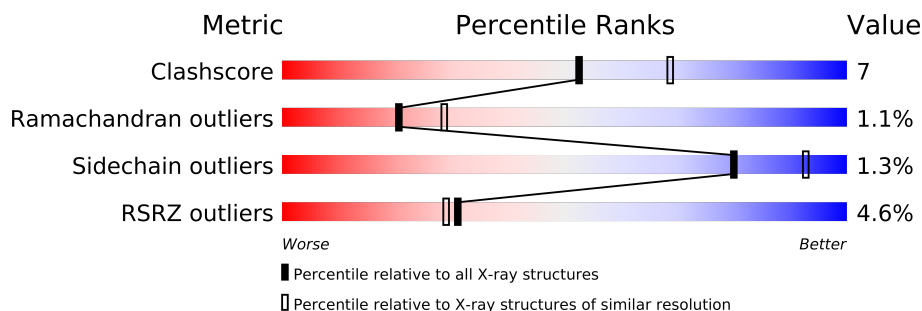
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. 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	247	
1	B	247	
1	C	247	
1	D	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7943 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 GLUTATHIONE S-TRANSFERASE THETA 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1919	1249	326	337	7			
1	B	239	Total	C	N	O	S	0	0	0
			1919	1249	326	337	7			
1	C	239	Total	C	N	O	S	0	0	0
			1919	1249	326	337	7			
1	D	239	Total	C	N	O	S	0	0	0
			1919	1249	326	337	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ARG	TRP	ENGINEERED MUTATION	UNP P30711
B	234	ARG	TRP	ENGINEERED MUTATION	UNP P30711
C	234	ARG	TRP	ENGINEERED MUTATION	UNP P30711
D	234	ARG	TRP	ENGINEERED MUTATION	UNP P30711

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	68	Total	O	0	0
			68	68		
2	C	79	Total	O	0	0
			79	79		
2	D	71	Total	O	0	0
			71	71		

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	164.52Å 111.82Å 55.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.36 – 2.40 28.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.3 (28.36-2.40) 86.3 (28.36-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.267 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 35566 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7943	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 6.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.92	1/1966 (0.1%)	0.58	0/2672
1	B	0.90	0/1966	0.59	1/2672 (0.0%)
1	C	0.95	0/1966	0.59	0/2672
1	D	0.90	0/1966	0.58	0/2672
All	All	0.92	1/7864 (0.0%)	0.59	1/10688 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	GLN	CB-CG	5.60	1.67	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	LEU	CA-CB-CG	6.02	129.14	115.30

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	1919	0	1972	25	0
1	B	1919	0	1972	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1919	0	1972	39	0
1	D	1919	0	1972	26	0
2	A	49	0	0	0	0
2	B	68	0	0	0	1
2	C	79	0	0	1	1
2	D	71	0	0	1	0
All	All	7943	0	7888	111	1

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 7.

All (111) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:193:THR:HG22	1:A:197:ARG:NH1	1.74	1.02
1:B:193:THR:HG22	1:B:197:ARG:NH1	1.83	0.93
1:A:193:THR:HG22	1:A:197:ARG:HH12	1.39	0.85
1:C:232:MET:HB3	1:C:233:PRO:HD3	1.69	0.75
1:C:224:ASP:C	1:C:226:THR:H	1.91	0.74
1:C:36:ILE:HG23	1:C:123:PHE:CE1	2.25	0.71
1:A:193:THR:CG2	1:A:197:ARG:HH12	2.03	0.70
1:C:225:PRO:HA	1:C:228:LYS:HB3	1.74	0.70
1:C:36:ILE:HG23	1:C:123:PHE:HE1	1.56	0.70
1:C:217:ALA:HA	1:C:220:PHE:CE1	2.30	0.67
1:D:12:GLN:HG3	1:D:176:HIS:CE1	2.31	0.66
1:A:196:GLN:HA	1:A:196:GLN:HE21	1.61	0.65
1:B:193:THR:HG22	1:B:197:ARG:HH12	1.59	0.64
1:D:4:GLU:HB2	1:D:58:LYS:HB3	1.80	0.63
1:D:229:GLN:HE21	1:D:229:GLN:H	1.44	0.63
1:A:12:GLN:HG3	1:A:173:GLU:HA	1.81	0.62
1:D:217:ALA:HA	1:D:220:PHE:CE1	2.34	0.62
1:C:41:LEU:HD13	1:C:230:LYS:HG2	1.82	0.62
1:C:225:PRO:HA	1:C:228:LYS:HD3	1.82	0.61
1:D:120:PHE:HB2	1:D:121:PRO:HD3	1.81	0.61
1:A:193:THR:CG2	1:A:197:ARG:NH1	2.59	0.61
1:B:193:THR:CG2	1:B:197:ARG:NH1	2.62	0.61
1:B:115:TRP:HA	1:B:119:MET:HB2	1.81	0.61
1:B:193:THR:CG2	1:B:197:ARG:HH12	2.14	0.60
1:A:217:ALA:HA	1:A:220:PHE:CE1	2.38	0.59
1:C:124:LEU:O	1:C:228:LYS:NZ	2.21	0.58
1:C:224:ASP:C	1:C:226:THR:N	2.53	0.58
1:C:8:ASP:HB2	1:C:33:VAL:O	2.04	0.58
1:D:115:TRP:HA	1:D:119:MET:HB2	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:41:LEU:HA	1:A:52:LYS:HD2	1.86	0.57
1:D:29:GLU:HG2	1:D:31:ARG:HH12	1.69	0.57
1:B:34:ASP:OD2	1:B:36:ILE:HG12	2.04	0.57
1:D:117:LYS:NZ	2:D:2038:HOH:O	2.37	0.57
1:C:41:LEU:HB3	1:C:230:LYS:HE2	1.87	0.56
1:C:48:VAL:O	1:C:49:ASN:HB2	2.04	0.56
1:D:29:GLU:HG2	1:D:31:ARG:NH1	2.19	0.56
1:D:135:ALA:O	1:D:139:GLU:HG2	2.06	0.55
1:C:12:GLN:HG3	1:C:173:GLU:HA	1.87	0.55
1:A:32:ILE:HD12	1:A:32:ILE:N	2.22	0.55
1:C:224:ASP:O	1:C:226:THR:N	2.41	0.54
1:D:108:ARG:NE	1:D:240:ARG:OXT	2.36	0.54
1:A:86:PRO:O	1:A:92:ARG:HB2	2.08	0.54
1:A:186:GLU:OE1	1:A:186:GLU:N	2.40	0.54
1:D:232:MET:HB3	1:D:233:PRO:HD3	1.90	0.53
1:A:217:ALA:HA	1:A:220:PHE:CD1	2.43	0.53
1:A:32:ILE:HD12	1:A:32:ILE:H	1.73	0.53
1:B:114:LEU:HG	1:B:119:MET:HG2	1.91	0.53
1:B:109:SER:HA	1:B:139:GLU:OE2	2.10	0.52
1:C:48:VAL:O	1:C:49:ASN:CB	2.58	0.51
1:C:115:TRP:HA	1:C:119:MET:HB2	1.91	0.51
1:B:41:LEU:HA	1:B:52:LYS:HD3	1.91	0.51
1:C:108:ARG:CZ	1:D:240:ARG:HD3	2.40	0.51
1:B:171:ILE:HD11	1:B:195:ARG:HG3	1.92	0.50
1:D:117:LYS:HG3	1:D:118:VAL:HG23	1.94	0.50
1:B:217:ALA:HA	1:B:220:PHE:CD1	2.46	0.49
1:A:8:ASP:OD2	1:A:35:LEU:HG	2.12	0.49
1:D:229:GLN:H	1:D:229:GLN:NE2	2.08	0.49
1:D:7:LEU:O	1:D:32:ILE:HA	2.12	0.49
1:A:150:LYS:HG2	1:B:51:LEU:HD11	1.94	0.49
1:A:196:GLN:HE21	1:A:196:GLN:CA	2.25	0.48
1:C:48:VAL:HG12	1:C:48:VAL:O	2.13	0.48
1:D:113:ALA:O	1:D:117:LYS:HB3	2.13	0.48
1:A:163:ILE:HG13	1:A:167:ASP:HB2	1.95	0.48
1:D:217:ALA:HA	1:D:220:PHE:CD1	2.48	0.48
1:D:12:GLN:HB2	1:D:13:PRO:CD	2.43	0.47
1:C:57:LEU:HD23	1:C:58:LYS:N	2.29	0.47
1:B:12:GLN:HG3	1:B:173:GLU:HA	1.96	0.47
1:D:229:GLN:NE2	1:D:229:GLN:N	2.63	0.47
1:A:80:VAL:HB	1:A:81:PRO:HD2	1.98	0.46
1:B:41:LEU:HD11	1:B:234:ARG:HG3	1.98	0.46
1:A:13:PRO:HB2	1:A:55:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:ILE:O	1:B:175:MET:HG2	2.16	0.46
1:C:218:LYS:H	1:C:218:LYS:HD2	1.80	0.46
1:C:39:GLN:C	1:C:41:LEU:H	2.19	0.45
1:A:112:ARG:HG2	1:A:239:ILE:HB	1.98	0.45
1:D:12:GLN:HB2	1:D:13:PRO:HD3	1.98	0.45
1:D:237:ALA:O	1:D:240:ARG:HG3	2.15	0.45
1:C:57:LEU:HD12	1:C:70:ILE:HG23	1.96	0.45
1:C:193:THR:HG22	1:C:197:ARG:NH1	2.32	0.45
1:A:11:SER:OG	1:A:14:CYS:SG	2.73	0.45
1:B:169:VAL:O	1:B:173:GLU:HG3	2.17	0.45
1:D:58:LYS:NZ	1:D:60:GLY:O	2.40	0.45
1:A:51:LEU:HD11	1:B:150:LYS:NZ	2.32	0.44
1:A:117:LYS:O	1:A:117:LYS:HD3	2.17	0.44
1:B:220:PHE:HA	1:B:221:PRO:HD3	1.85	0.44
1:D:7:LEU:HD13	1:D:18:TYR:HB2	2.00	0.44
1:C:217:ALA:HA	1:C:220:PHE:CD1	2.53	0.43
1:C:65:THR:O	1:C:66:GLU:HB2	2.18	0.43
1:C:114:LEU:HD22	1:C:176:HIS:CD2	2.53	0.43
1:C:26:ILE:HA	1:C:27:PRO:HD3	1.92	0.43
1:A:171:ILE:O	1:A:175:MET:HG2	2.19	0.43
1:B:8:ASP:OD2	1:B:35:LEU:HG	2.18	0.43
1:D:30:LEU:HD21	1:D:32:ILE:HD11	2.00	0.42
1:B:119:MET:O	1:B:123:PHE:HB3	2.19	0.42
1:B:124:LEU:HD22	1:B:228:LYS:HG3	2.01	0.42
1:A:8:ASP:HB2	1:A:33:VAL:O	2.20	0.42
1:C:40:HIS:HA	1:C:45:PHE:CD2	2.55	0.41
1:D:225:PRO:O	1:D:229:GLN:NE2	2.53	0.41
1:C:41:LEU:HD11	1:C:231:LEU:HD23	2.03	0.41
1:C:169:VAL:O	1:C:173:GLU:HG3	2.21	0.41
1:C:86:PRO:O	1:C:92:ARG:HB2	2.20	0.41
1:B:114:LEU:HD22	1:B:176:HIS:CD2	2.55	0.41
1:C:20:PHE:HB2	1:C:168:LEU:HD21	2.01	0.41
1:B:8:ASP:HB2	1:B:33:VAL:O	2.20	0.41
1:C:126:GLU:HG2	1:C:228:LYS:NZ	2.36	0.41
1:C:12:GLN:HB2	1:C:176:HIS:CE1	2.56	0.41
1:C:108:ARG:O	1:C:112:ARG:HG3	2.21	0.41
1:C:151:PHE:O	1:C:155:LYS:NZ	2.52	0.41
1:C:37:LYS:O	1:C:227:ILE:HG21	2.21	0.40
1:B:20:PHE:HB2	1:B:168:LEU:HD21	2.04	0.40
1:C:111:LEU:CD1	2:C:2005:HOH:O	2.68	0.40

All (1) 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	Distance(Å)	Clash(Å)
2:B:2036:HOH:O	2:C:2065:HOH:O[4.457]	1.79	0.41

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	237/247 (96%)	226 (95%)	8 (3%)	3 (1%)	18	24
1	B	237/247 (96%)	228 (96%)	7 (3%)	2 (1%)	27	39
1	C	237/247 (96%)	221 (93%)	13 (6%)	3 (1%)	18	24
1	D	237/247 (96%)	226 (95%)	9 (4%)	2 (1%)	27	39
All	All	948/988 (96%)	901 (95%)	37 (4%)	10 (1%)	21	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	C	49	ASN
1	B	225	PRO
1	A	225	PRO
1	C	217	ALA
1	C	225	PRO
1	D	225	PRO
1	B	66	GLU
1	D	79	LYS
1	A	122	VAL

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	206/214 (96%)	202 (98%)	4 (2%)	69	87
1	B	206/214 (96%)	203 (98%)	3 (2%)	76	90
1	C	206/214 (96%)	204 (99%)	2 (1%)	85	95
1	D	206/214 (96%)	204 (99%)	2 (1%)	85	95
All	All	824/856 (96%)	813 (99%)	11 (1%)	80	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	79	LYS
1	A	176	HIS
1	A	196	GLN
1	B	139	GLU
1	B	176	HIS
1	B	240	ARG
1	C	176	HIS
1	C	218	LYS
1	D	176	HIS
1	D	229	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	A	196	GLN
1	B	131	GLN
1	B	229	GLN
1	C	131	GLN
1	D	12	GLN
1	D	229	GLN

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	239/247 (96%)	0.14	14 (5%) 22 20	14, 32, 72, 75	0
1	B	239/247 (96%)	-0.06	8 (3%) 44 42	12, 28, 67, 72	0
1	C	239/247 (96%)	0.07	18 (7%) 14 12	12, 26, 84, 87	0
1	D	239/247 (96%)	-0.03	4 (1%) 67 65	14, 31, 60, 67	0
All	All	956/988 (96%)	0.03	44 (4%) 31 29	12, 30, 70, 87	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	PRO	3.8
1	A	44	ALA	3.7
1	C	47	GLN	3.7
1	B	43	ASP	3.6
1	C	48	VAL	3.6
1	A	47	GLN	3.6
1	B	47	GLN	3.6
1	C	230	LYS	3.3
1	A	42	SER	3.0
1	C	42	SER	3.0
1	D	36	ILE	3.0
1	B	183	GLN	3.0
1	C	226	THR	3.0
1	A	43	ASP	2.9
1	C	49	ASN	2.9
1	C	233	PRO	2.9
1	A	186	GLU	2.9
1	D	44	ALA	2.8
1	A	225	PRO	2.8
1	B	44	ALA	2.8
1	C	223	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	227	ILE	2.7
1	C	46	ALA	2.7
1	C	229	GLN	2.6
1	C	44	ALA	2.6
1	C	225	PRO	2.5
1	C	123	PHE	2.5
1	C	43	ASP	2.5
1	A	48	VAL	2.3
1	B	41	LEU	2.3
1	A	234	ARG	2.3
1	A	41	LEU	2.2
1	B	42	SER	2.2
1	C	234	ARG	2.2
1	A	229	GLN	2.2
1	D	34	ASP	2.2
1	A	2	GLY	2.2
1	A	52	LYS	2.1
1	B	230	LYS	2.1
1	A	217	ALA	2.1
1	C	45	PHE	2.1
1	B	226	THR	2.1
1	D	47	GLN	2.0
1	A	46	ALA	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.