



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 25, 2017 – 06:05 PM EDT

PDB ID : 1PVN
Title : The crystal structure of the complex between IMP dehydrogenase catalytic domain and a transition state analogue MZP
Authors : Gan, L.; Seyedsayamdost, M.; Shuto, S.; Matsuda, A.; Petsko, G.A.; Hedstrom, L.
Deposited on : unknown
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

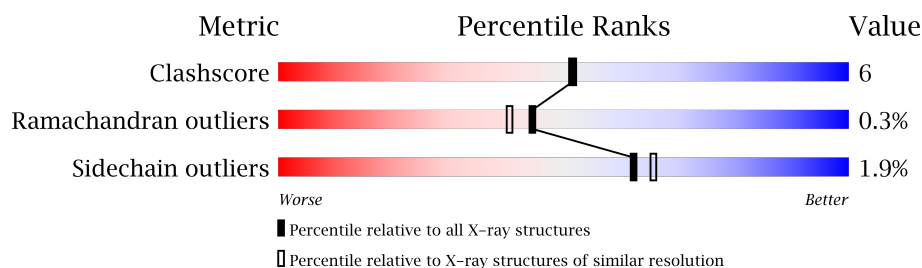
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	376	
1	B	376	
1	C	376	
1	D	376	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	A	993	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12198 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.

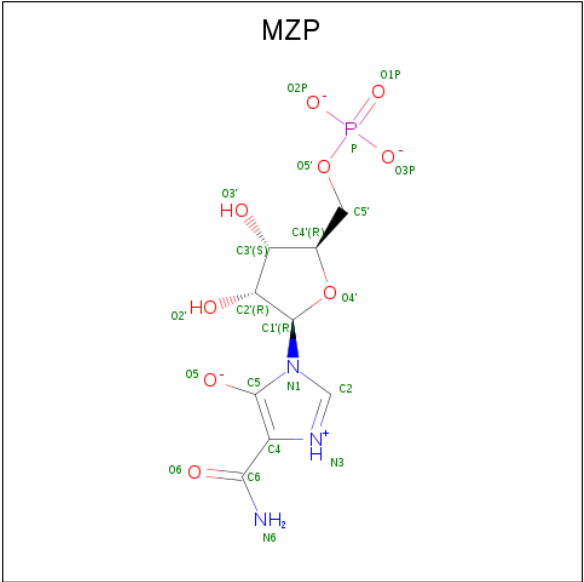
- Molecule 1 is a protein called Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	B	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	C	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			
1	D	362	Total	C	N	O	S	0	0	0
			2771	1757	473	526	15			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

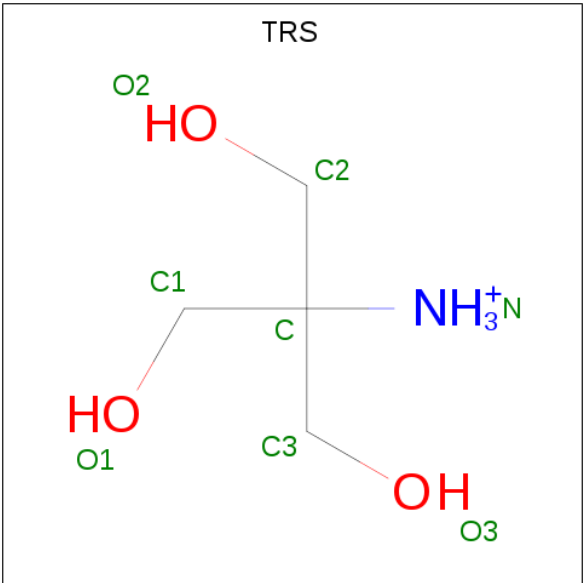
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	K	0	0
			2	2		
2	A	3	Total	K	0	0
			3	3		
2	D	1	Total	K	0	0
			1	1		
2	C	2	Total	K	0	0
			2	2		

- Molecule 3 is 4-CARBAMOYL-1-BETA-D-RIBOFURANOSYL-IMIDAZOLIUM-5-OLAT E-5'-PHOSPHATE (three-letter code: MZP) (formula: C₉H₁₂N₃O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	22	9	3	9	1	0	0
3	B	1	22	9	3	9	1	0	0
3	C	1	22	9	3	9	1	0	0
3	D	1	22	9	3	9	1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is water.

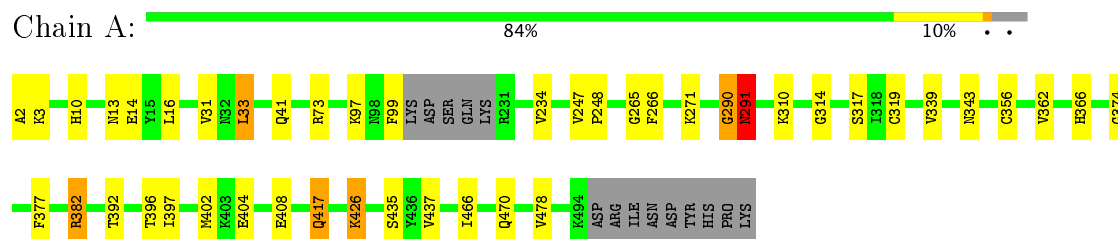
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	260	Total	O	0	0
			260	260		
5	B	249	Total	O	0	0
			249	249		
5	C	232	Total	O	0	0
			232	232		
5	D	229	Total	O	0	0
			229	229		

3 Residue-property plots

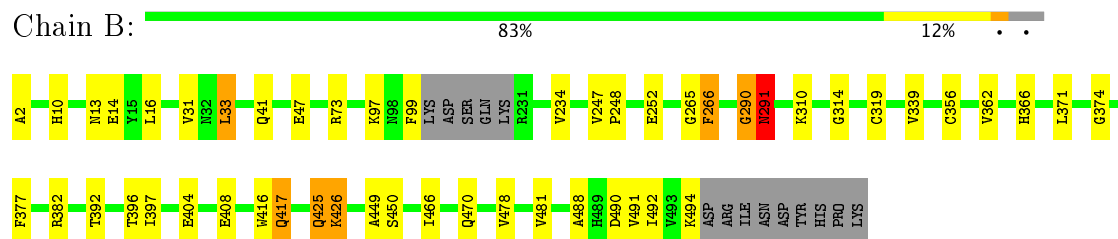
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

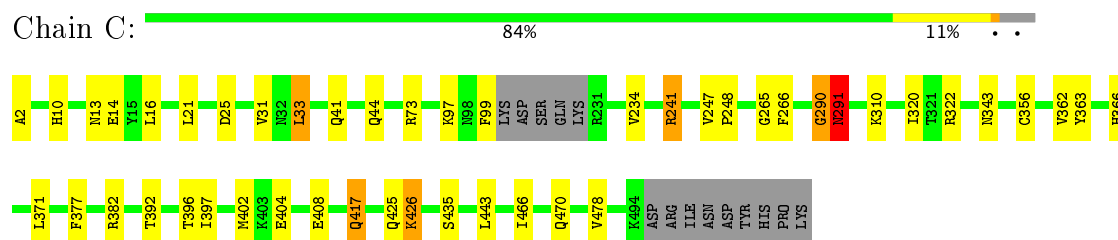
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



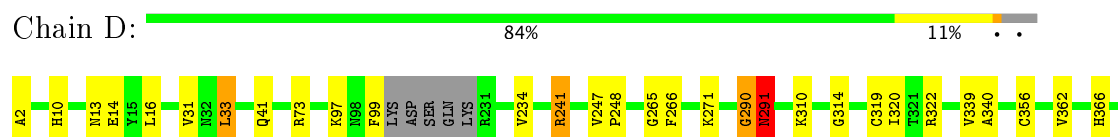
• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



• Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.75 Å 112.57 Å 159.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.00	Depositor
% Data completeness (in resolution range)	97.4 (29.71-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.196 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12198	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MZP, TRS

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	0.31	0/2820	0.62	4/3802 (0.1%)
1	B	0.31	0/2820	0.62	4/3802 (0.1%)
1	C	0.32	0/2820	0.61	3/3802 (0.1%)
1	D	0.32	0/2820	0.68	5/3802 (0.1%)
All	All	0.32	0/11280	0.63	16/15208 (0.1%)

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	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	382	ARG	NE-CZ-NH1	-14.32	113.14	120.30
1	D	382	ARG	NE-CZ-NH2	12.87	126.73	120.30
1	B	382	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	382	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	382	ARG	CD-NE-CZ	5.81	131.74	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	241	ARG	Sidechain
1	D	241	ARG	Sidechain

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	2771	0	2770	38	0
1	B	2771	0	2770	41	0
1	C	2771	0	2770	37	0
1	D	2771	0	2770	37	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	12	1	0
3	B	22	0	12	1	0
3	C	22	0	12	1	0
3	D	22	0	12	1	0
4	A	16	0	24	6	0
4	B	16	0	24	4	0
4	C	8	0	12	4	0
4	D	8	0	12	3	0
5	A	260	0	0	5	0
5	B	249	0	0	4	0
5	C	232	0	0	3	0
5	D	229	0	0	5	0
All	All	12198	0	11200	144	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 6.

The worst 5 of 144 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:D:241:ARG:HH21	1:D:425:GLN:HG2	1.31	0.93
1:D:408:GLU:H	3:D:974:MZP:HN3	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:408:GLU:H	3:B:972:MZP:HN3	1.20	0.90
1:C:408:GLU:H	3:C:973:MZP:HN3	1.20	0.88
1:D:417:GLN:HE21	1:D:417:GLN:H	1.21	0.88

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	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	44	40
1	B	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	44	40
1	C	358/376 (95%)	350 (98%)	7 (2%)	1 (0%)	44	40
1	D	358/376 (95%)	349 (98%)	8 (2%)	1 (0%)	44	40
All	All	1432/1504 (95%)	1397 (98%)	31 (2%)	4 (0%)	44	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	291	ASN
1	C	291	ASN
1	D	291	ASN

5.3.2 Protein sidechains [i](#)

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	294/308 (96%)	289 (98%)	5 (2%)	66	70
1	B	294/308 (96%)	288 (98%)	6 (2%)	60	64
1	C	294/308 (96%)	288 (98%)	6 (2%)	60	64
1	D	294/308 (96%)	289 (98%)	5 (2%)	66	70
All	All	1176/1232 (96%)	1154 (98%)	22 (2%)	62	66

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	425	GLN
1	C	33	LEU
1	D	417	GLN
1	B	426	LYS
1	C	25	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	366	HIS
1	C	13	ASN
1	D	366	HIS
1	C	10	HIS
1	C	41	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	MZP	A	971	-	18,23,23	1.73	4 (22%)	21,35,35	1.30	2 (9%)
4	TRS	A	993	-	7,7,7	1.09	1 (14%)	9,9,9	2.05	2 (22%)
4	TRS	A	996	-	7,7,7	1.03	0	9,9,9	2.27	2 (22%)
3	MZP	B	972	-	18,23,23	1.70	3 (16%)	21,35,35	1.29	2 (9%)
4	TRS	B	991	-	7,7,7	0.96	0	9,9,9	2.19	2 (22%)
4	TRS	B	994	-	7,7,7	0.96	0	9,9,9	2.15	2 (22%)
3	MZP	C	973	-	18,23,23	1.77	4 (22%)	21,35,35	1.33	2 (9%)
4	TRS	C	992	-	7,7,7	0.98	0	9,9,9	2.11	3 (33%)
3	MZP	D	974	-	18,23,23	1.78	4 (22%)	21,35,35	1.32	2 (9%)
4	TRS	D	995	-	7,7,7	0.98	0	9,9,9	2.18	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MZP	A	971	-	-	0/6/30/30	0/2/2/2
4	TRS	A	993	-	-	0/9/9/9	0/0/0/0
4	TRS	A	996	-	-	0/9/9/9	0/0/0/0
3	MZP	B	972	-	-	0/6/30/30	0/2/2/2
4	TRS	B	991	-	-	0/9/9/9	0/0/0/0
4	TRS	B	994	-	-	0/9/9/9	0/0/0/0
3	MZP	C	973	-	-	0/6/30/30	0/2/2/2
4	TRS	C	992	-	-	0/9/9/9	0/0/0/0
3	MZP	D	974	-	-	0/6/30/30	0/2/2/2
4	TRS	D	995	-	-	0/9/9/9	0/0/0/0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	971	MZP	C2-N3	-3.74	1.28	1.35
3	C	973	MZP	C2-N3	-3.70	1.28	1.35
3	D	974	MZP	C2-N3	-3.55	1.28	1.35
3	B	972	MZP	C2-N3	-3.52	1.28	1.35
3	D	974	MZP	P-O5'	-2.22	1.53	1.60

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	973	MZP	O6-C6-N6	-3.82	117.15	122.58
3	A	971	MZP	O6-C6-N6	-3.71	117.30	122.58
3	D	974	MZP	O6-C6-N6	-3.69	117.34	122.58
3	B	972	MZP	O6-C6-N6	-3.67	117.36	122.58
4	A	996	TRS	C1-C-N	-2.66	102.07	107.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	971	MZP	1	0
4	A	993	TRS	6	0
3	B	972	MZP	1	0
4	B	991	TRS	2	0
4	B	994	TRS	2	0
3	C	973	MZP	1	0
4	C	992	TRS	4	0
3	D	974	MZP	1	0
4	D	995	TRS	3	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.