



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:18 PM UTC

PDB ID : 3ICD / pdb_00003icd
Title : STRUCTURE OF A BACTERIAL ENZYME REGULATED BY PHOSPHORYLATION, ISOCITRATE DEHYDROGENASE
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Deposited on : 1989-12-28
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

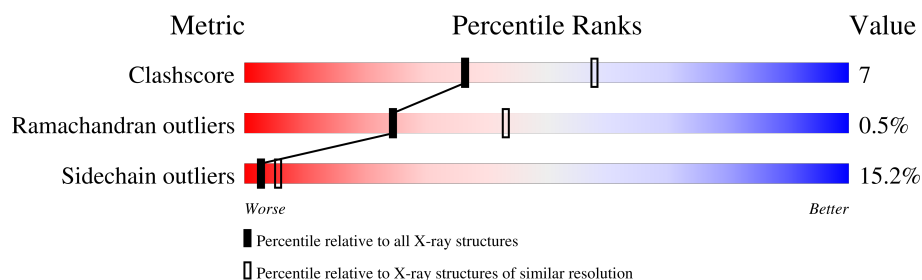
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3254 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 ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3146	2007	531	590	18			

- Molecule 2 is water.

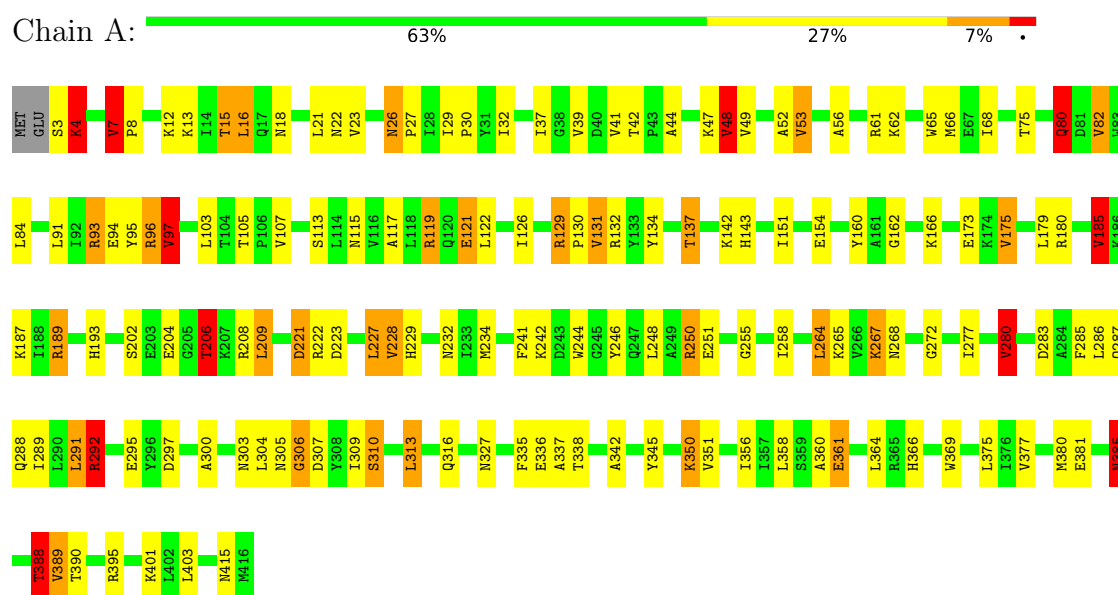
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	108	Total	O	0	0
			108	108		

3 Residue-property plots

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. 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. 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: ISOCITRATE DEHYDROGENASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3254	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

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	1.10	16/3207 (0.5%)	1.95	89/4345 (2.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	VAL	CA-CB	7.62	1.64	1.54
1	A	193	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	229	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	143	HIS	CD2-NE2	-6.57	1.30	1.37
1	A	366	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	23	VAL	CA-CB	5.85	1.59	1.53
1	A	82	VAL	CA-CB	5.78	1.60	1.53
1	A	280	VAL	CA-CB	5.74	1.62	1.54
1	A	185	VAL	CA-CB	5.45	1.60	1.54
1	A	175	VAL	CA-CB	5.44	1.62	1.54
1	A	48	VAL	CA-CB	5.32	1.61	1.54
1	A	97	VAL	CA-CB	5.32	1.62	1.54
1	A	228	VAL	CA-CB	5.32	1.61	1.54
1	A	193	HIS	CG-ND1	-5.23	1.32	1.38
1	A	41	VAL	CA-CB	5.13	1.61	1.54
1	A	206	THR	CA-CB	5.05	1.61	1.53

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	12.62	125.22	112.60
1	A	389	VAL	N-CA-CB	-9.32	95.12	112.36
1	A	361	GLU	CA-CB-CG	8.18	130.46	114.10
1	A	119	ARG	NE-CZ-NH1	-7.86	113.64	121.50
1	A	390	THR	N-CA-CB	-7.43	99.74	110.36
1	A	287	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	A	94	GLU	N-CA-C	6.92	118.61	111.14
1	A	160	TYR	CA-C-O	-6.88	110.11	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	GLU	N-CA-C	6.87	119.61	108.76
1	A	15	THR	CA-CB-OG1	-6.83	99.36	109.60
1	A	389	VAL	CB-CA-C	6.74	121.70	110.30
1	A	26	ASN	CA-CB-CG	6.71	119.31	112.60
1	A	47	LYS	CA-C-O	-6.69	113.80	120.82
1	A	385	ASN	CA-CB-CG	-6.64	105.96	112.60
1	A	335	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	244	TRP	CG-CD2-CE3	6.43	140.33	133.90
1	A	131	VAL	CA-C-O	6.38	126.72	120.27
1	A	204	GLU	CA-C-N	6.27	126.94	119.98
1	A	204	GLU	C-N-CA	6.27	126.94	119.98
1	A	80	GLN	N-CA-C	6.26	120.48	112.34
1	A	277	ILE	N-CA-C	-6.25	98.86	107.99
1	A	129	ARG	NE-CZ-NH1	-6.12	115.38	121.50
1	A	132	ARG	CB-CG-CD	-6.07	97.34	111.30
1	A	388	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	208	ARG	NE-CZ-NH2	6.02	124.61	119.20
1	A	316	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	65	TRP	CB-CG-CD1	-5.98	117.93	126.90
1	A	366	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	A	7	VAL	CA-C-N	5.91	126.22	119.83
1	A	7	VAL	C-N-CA	5.91	126.22	119.83
1	A	342	ALA	CB-CA-C	-5.86	107.04	111.20
1	A	4	LYS	CA-CB-CG	-5.84	102.42	114.10
1	A	193	HIS	CB-CG-CD2	-5.82	123.63	131.20
1	A	84	LEU	CA-C-N	5.81	125.83	119.90
1	A	84	LEU	C-N-CA	5.81	125.83	119.90
1	A	22	ASN	CA-C-N	5.78	126.75	122.59
1	A	22	ASN	C-N-CA	5.78	126.75	122.59
1	A	221	ASP	CB-CA-C	-5.68	103.14	112.06
1	A	223	ASP	N-CA-C	5.67	120.27	113.23
1	A	234	MET	CA-CB-CG	-5.67	102.75	114.10
1	A	246	TYR	CA-C-N	5.67	128.13	120.65
1	A	246	TYR	C-N-CA	5.67	128.13	120.65
1	A	119	ARG	CB-CG-CD	5.66	124.33	111.30
1	A	303	ASN	N-CA-C	5.66	117.92	111.02
1	A	283	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	130	PRO	N-CA-CB	5.64	107.81	103.30
1	A	105	THR	CA-C-N	5.64	125.54	119.85
1	A	105	THR	C-N-CA	5.64	125.54	119.85
1	A	119	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	15	THR	CA-CB-CG2	5.62	120.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	ASN	OD1-CG-ND2	-5.59	117.01	122.60
1	A	337	ALA	N-CA-C	-5.55	101.63	109.96
1	A	380	MET	CG-SD-CE	-5.55	88.69	100.90
1	A	415	ASN	CA-CB-CG	-5.55	107.05	112.60
1	A	42	THR	CA-C-N	5.53	125.62	119.32
1	A	42	THR	C-N-CA	5.53	125.62	119.32
1	A	47	LYS	CG-CD-CE	5.53	124.01	111.30
1	A	209	LEU	CD1-CG-CD2	5.50	122.90	110.80
1	A	360	ALA	N-CA-C	-5.47	105.47	111.82
1	A	52	ALA	CA-C-O	-5.47	114.62	120.42
1	A	26	ASN	OD1-CG-ND2	-5.45	117.16	122.60
1	A	338	THR	CA-CB-OG1	-5.45	101.43	109.60
1	A	369	TRP	CG-CD1-NE1	-5.45	103.12	110.20
1	A	222	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	A	297	ASP	N-CA-CB	-5.39	101.37	110.49
1	A	61	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	189	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	250	ARG	CA-C-N	5.32	127.72	120.54
1	A	250	ARG	C-N-CA	5.32	127.72	120.54
1	A	96	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	142	LYS	CB-CA-C	-5.31	101.98	110.79
1	A	388	THR	N-CA-CB	-5.31	100.69	110.56
1	A	26	ASN	CB-CG-ND2	5.28	124.31	116.40
1	A	56	ALA	N-CA-C	5.22	116.97	111.28
1	A	244	TRP	CE2-CD2-CG	-5.20	100.96	107.20
1	A	306	GLY	O-C-N	5.20	127.18	122.19
1	A	395	ARG	CB-CA-C	-5.18	102.19	110.79
1	A	180	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	244	TRP	CA-C-N	5.14	125.66	120.00
1	A	244	TRP	C-N-CA	5.14	125.66	120.00
1	A	292	ARG	CA-C-N	5.13	124.63	119.19
1	A	292	ARG	C-N-CA	5.13	124.63	119.19
1	A	232	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	137	THR	CA-C-N	5.10	125.33	119.83
1	A	137	THR	C-N-CA	5.10	125.33	119.83
1	A	3	SER	CA-C-N	-5.09	114.61	122.49
1	A	3	SER	C-N-CA	-5.09	114.61	122.49
1	A	232	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	65	TRP	CG-CD2-CE3	5.01	138.91	133.90

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	3146	0	3141	45	0
2	A	108	0	0	3	0
All	All	3254	0	3141	45	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 7.

All (45) 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:A:16:LEU:HD23	1:A:96:ARG:HD2	1.75	0.68
1:A:162:GLY:HA2	2:A:519:HOH:O	1.93	0.67
1:A:305:ASN:O	1:A:309:ILE:HG12	1.97	0.65
1:A:401:LYS:HE3	1:A:403:LEU:HD11	1.78	0.64
1:A:288:GLN:HE22	1:A:292:ARG:HD3	1.63	0.63
1:A:154:GLU:HA	1:A:209:LEU:HD13	1.85	0.57
1:A:16:LEU:HD22	1:A:21:LEU:HD23	1.86	0.57
1:A:49:VAL:O	1:A:53:VAL:HG13	2.05	0.56
1:A:202:SER:O	1:A:206:THR:HG23	2.05	0.55
1:A:206:THR:HB	1:A:241:PHE:CD2	2.42	0.55
1:A:267:LYS:HE2	1:A:272:GLY:HA2	1.88	0.55
1:A:179:LEU:O	1:A:185:VAL:HG13	2.08	0.54
1:A:26:ASN:HA	1:A:62:LYS:O	2.07	0.53
1:A:4:LYS:HB2	1:A:4:LYS:NZ	2.23	0.53
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.91	0.53
1:A:280:VAL:HG22	1:A:285:PHE:HB2	1.90	0.52
1:A:115:ASN:O	1:A:119:ARG:HG3	2.11	0.51
1:A:401:LYS:HE3	1:A:403:LEU:CD1	2.43	0.49
1:A:117:ALA:O	1:A:121:GLU:HB2	2.12	0.49
1:A:134:TYR:O	1:A:137:THR:HG23	2.14	0.48
1:A:345:TYR:CD2	1:A:350:LYS:HD2	2.49	0.47
1:A:227:LEU:HD12	1:A:300:ALA:HB3	1.96	0.47
1:A:44:ALA:O	1:A:48:VAL:HG13	2.15	0.46
1:A:129:ARG:HB2	1:A:151:ILE:HB	1.97	0.46
1:A:37:ILE:HB	1:A:351:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:O	1:A:307:ASP:HB3	2.16	0.46
1:A:166:LYS:HE2	1:A:166:LYS:HB3	1.84	0.45
1:A:388:THR:HG21	2:A:470:HOH:O	2.17	0.45
1:A:30:PRO:HA	1:A:66:MET:O	2.18	0.44
1:A:255:GLY:HA2	1:A:265:LYS:O	2.17	0.44
1:A:93:ARG:HD2	2:A:549:HOH:O	2.18	0.44
1:A:126:ILE:O	1:A:327:ASN:HA	2.17	0.44
1:A:29:ILE:HD12	1:A:97:VAL:HG22	2.00	0.43
1:A:381:GLU:O	1:A:385:ASN:HB2	2.18	0.43
1:A:258:ILE:HD11	1:A:265:LYS:HG3	2.01	0.43
1:A:7:VAL:HA	1:A:8:PRO:HD3	1.89	0.43
1:A:32:ILE:HG13	1:A:68:ILE:HG13	2.01	0.43
1:A:75:THR:HB	1:A:80:GLN:HA	2.01	0.43
1:A:291:LEU:O	1:A:292:ARG:HG3	2.19	0.42
1:A:93:ARG:HD3	1:A:122:LEU:CD2	2.50	0.42
1:A:13:LYS:HG2	1:A:95:TYR:CE1	2.55	0.42
1:A:280:VAL:CG2	1:A:285:PHE:HB2	2.50	0.42
1:A:250:ARG:HG3	1:A:264:LEU:HD21	2.02	0.42
1:A:288:GLN:NE2	1:A:292:ARG:HD3	2.34	0.40
1:A:306:GLY:O	1:A:310:SER:OG	2.40	0.40

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	412/416 (99%)	395 (96%)	15 (4%)	2 (0%)	24 43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASN

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Mol	Chain	Res	Type
1	A	113	SER

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	323/338 (96%)	274 (85%)	49 (15%)	3 5

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	7	VAL
1	A	12	LYS
1	A	15	THR
1	A	16	LEU
1	A	27	PRO
1	A	39	VAL
1	A	48	VAL
1	A	53	VAL
1	A	80	GLN
1	A	82	VAL
1	A	91	LEU
1	A	93	ARG
1	A	97	VAL
1	A	103	LEU
1	A	107	VAL
1	A	121	GLU
1	A	131	VAL
1	A	173	GLU
1	A	175	VAL
1	A	185	VAL
1	A	187	LYS
1	A	189	ARG
1	A	206	THR
1	A	221	ASP

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	228	VAL
1	A	242	LYS
1	A	248	LEU
1	A	251	GLU
1	A	264	LEU
1	A	267	LYS
1	A	280	VAL
1	A	286	LEU
1	A	291	LEU
1	A	292	ARG
1	A	295	GLU
1	A	310	SER
1	A	313	LEU
1	A	350	LYS
1	A	356	ILE
1	A	358	LEU
1	A	361	GLU
1	A	364	LEU
1	A	375	LEU
1	A	377	VAL
1	A	385	ASN
1	A	388	THR
1	A	389	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	115	ASN
1	A	287	GLN
1	A	288	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 [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 ⓘ

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.