



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:48 PM GMT

PDB ID : 1OXY
Title : CRYSTALLOGRAPHIC ANALYSIS OF OXYGENATED AND DEOXY-
GENATED STATES OF ARTHROPOD HEMOCYANIN SHOWS UNUSUAL
DIFFERENCES
Authors : Ton-that, H.; Magnus, K.
Deposited on : 1995-01-06
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>

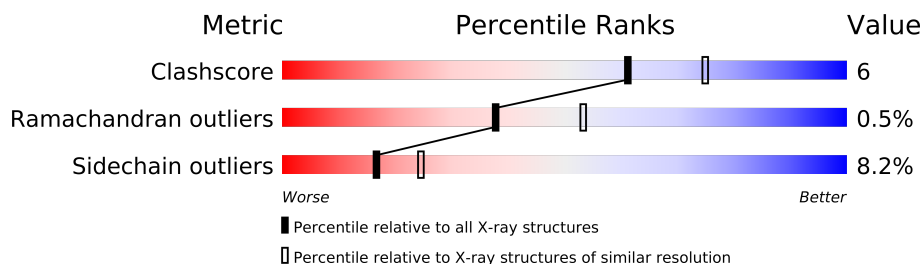
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	628	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	OXY	A	631	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5006 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 HEMOCYANIN (SUBUNIT TYPE II).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4669	2986	812	849	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ILE	VAL	CONFLICT	UNP P04253
A	408	THR	PHE	CONFLICT	UNP P04253
A	409	PHE	THR	CONFLICT	UNP P04253
A	432	LYS	ARG	CONFLICT	UNP P04253
A	549	VAL	ILE	CONFLICT	UNP P04253
A	550	ALA	LYS	CONFLICT	UNP P04253

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).

○ _____ ○

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	333	Total	O	0	0
			333	333		

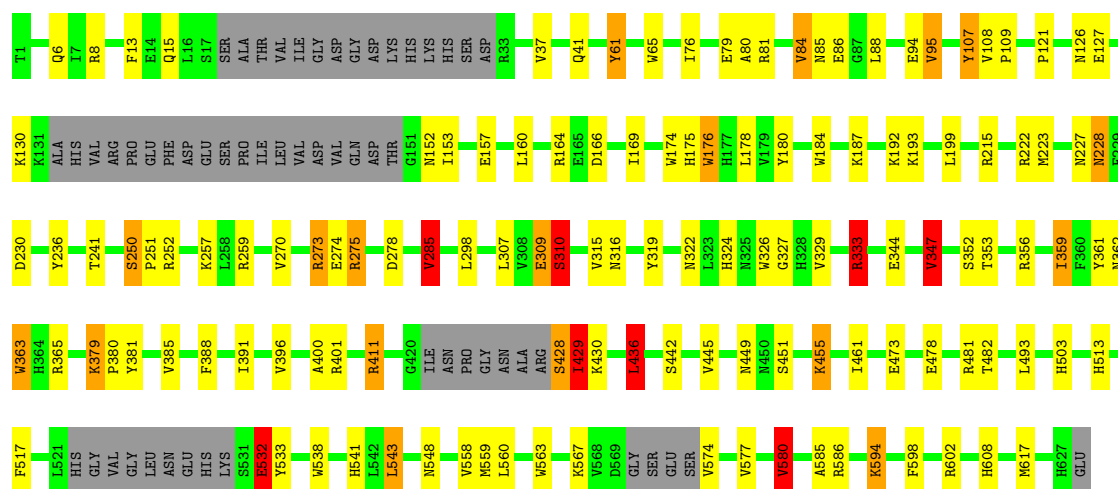
3 Residue-property plots

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.

Note EDS was not executed.

• Molecule 1: HEMOCYANIN (SUBUNIT TYPE II)

Chain A: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	117.24Å 117.24Å 285.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5006	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: OXY, CU

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	0.78	0/4807	1.41	60/6514 (0.9%)

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	A	0	1

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	GLU	N-CA-C	9.78	137.40	111.00
1	A	563	TRP	CD1-CG-CD2	8.09	112.77	106.30
1	A	176	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	586	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	326	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	309	GLU	CA-C-N	-7.82	100.00	117.20
1	A	326	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	176	TRP	CE2-CD2-CG	-7.52	101.28	107.30
1	A	65	TRP	CD1-CG-CD2	7.47	112.28	106.30
1	A	309	GLU	O-C-N	7.47	134.65	122.70
1	A	356	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	A	363	TRP	CD1-CG-CD2	7.30	112.14	106.30
1	A	275	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	184	TRP	CD1-CG-CD2	7.17	112.04	106.30
1	A	184	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	252	ARG	NE-CZ-NH2	-7.06	116.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	TRP	CD1-CG-CD2	7.04	111.93	106.30
1	A	563	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	174	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	A	363	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	65	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	174	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	538	TRP	CE2-CD2-CG	-6.42	102.17	107.30
1	A	61	TYR	CA-CB-CG	6.41	125.58	113.40
1	A	347	VAL	N-CA-CB	-6.38	97.47	111.50
1	A	252	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	594	LYS	CA-CB-CG	-6.23	99.69	113.40
1	A	273	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	326	TRP	CG-CD2-CE3	6.01	139.31	133.90
1	A	222	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	326	TRP	CB-CG-CD1	-5.86	119.38	127.00
1	A	275	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	307	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	107	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	436	LEU	CA-CB-CG	5.77	128.56	115.30
1	A	429	ILE	CA-C-N	5.68	129.70	117.20
1	A	580	VAL	CB-CA-C	-5.63	100.70	111.40
1	A	180	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	310	SER	CA-C-N	-5.57	104.95	117.20
1	A	478	GLU	CA-CB-CG	5.51	125.52	113.40
1	A	401	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	81	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	333	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	95	VAL	CG1-CB-CG2	-5.43	102.20	110.90
1	A	222	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	285	VAL	N-CA-CB	-5.43	99.55	111.50
1	A	176	TRP	CB-CG-CD1	-5.42	119.95	127.00
1	A	429	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	A	130	LYS	C-N-CA	5.37	135.13	121.70
1	A	563	TRP	CG-CD1-NE1	-5.25	104.85	110.10
1	A	347	VAL	CB-CA-C	5.15	121.18	111.40
1	A	8	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	193	LYS	N-CA-C	-5.10	97.23	111.00
1	A	481	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	309	GLU	C-N-CA	5.08	134.40	121.70
1	A	236	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	411	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	176	TRP	CG-CD1-NE1	-5.03	105.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	A	543	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	388	PHE	Peptide

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	4669	0	4417	53	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	333	0	0	4	0
All	All	5006	0	4417	53	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 6.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:GLU:HG3	1:A:108:VAL:HG21	1.67	0.75
1:A:347:VAL:HG22	1:A:353:THR:HB	1.68	0.74
1:A:223:MET:SD	1:A:361:TYR:HB3	2.33	0.68
1:A:310:SER:HB2	1:A:322:ASN:HA	1.77	0.67
1:A:359:ILE:HA	1:A:362:ASN:HD22	1.65	0.61
1:A:157:GLU:HG3	1:A:164:ARG:HH12	1.66	0.61
1:A:94:GLU:HB3	1:A:178:LEU:HD13	1.85	0.58
1:A:13:PHE:HB2	4:A:884:HOH:O	2.04	0.57
1:A:6:GLN:HE22	1:A:107:TYR:H	1.53	0.56
1:A:95:VAL:HG23	1:A:178:LEU:HD22	1.88	0.55
1:A:157:GLU:HG3	1:A:164:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:309:GLU:HA	1:A:324:HIS:HB3	1.89	0.55
1:A:275:ARG:HG2	1:A:319:TYR:CZ	2.42	0.55
1:A:559:MET:HG3	1:A:617:MET:HG2	1.88	0.54
1:A:396:VAL:HG22	1:A:445:VAL:HG13	1.89	0.54
1:A:428:SER:O	1:A:429:ILE:HG13	2.08	0.53
1:A:327:GLY:HA3	1:A:363:TRP:CZ2	2.45	0.51
1:A:436:LEU:O	1:A:541:HIS:HB2	2.09	0.51
1:A:429:ILE:HG22	1:A:430:LYS:H	1.75	0.51
1:A:449:ASN:OD1	1:A:451:SER:HB3	2.11	0.51
1:A:577:VAL:O	1:A:580:VAL:HG22	2.11	0.51
1:A:270:VAL:O	1:A:274:GLU:HG2	2.09	0.51
1:A:329:VAL:O	1:A:333:ARG:HG2	2.10	0.51
1:A:347:VAL:HG22	1:A:353:THR:CB	2.38	0.50
1:A:285:VAL:HG13	1:A:315:VAL:HG21	1.94	0.49
1:A:160:LEU:HD11	1:A:215:ARG:HG2	1.96	0.48
1:A:391:ILE:HD11	1:A:455:LYS:HG3	1.97	0.47
1:A:381:TYR:CE2	1:A:602:ARG:HG3	2.50	0.47
1:A:37:VAL:HG13	1:A:84:VAL:HG21	1.97	0.46
1:A:85:ASN:HD22	1:A:88:LEU:H	1.62	0.46
1:A:429:ILE:HG22	1:A:430:LYS:N	2.31	0.46
1:A:166:ASP:O	1:A:169:ILE:HG22	2.16	0.45
1:A:259:ARG:HA	1:A:259:ARG:HD2	1.76	0.45
1:A:176:TRP:HH2	4:A:876:HOH:O	2.00	0.45
1:A:594:LYS:HD3	1:A:598:PHE:CE1	2.52	0.45
1:A:379:LYS:HA	1:A:380:PRO:HD3	1.78	0.45
1:A:86:GLU:H	1:A:86:GLU:CD	2.20	0.45
1:A:532:GLU:HB2	1:A:533:TYR:H	1.59	0.44
1:A:126:ASN:HB2	4:A:789:HOH:O	2.18	0.44
1:A:442:SER:HB3	1:A:503:HIS:HD2	1.83	0.43
1:A:461:ILE:HG12	1:A:558:VAL:HG22	1.99	0.43
1:A:270:VAL:HG13	1:A:273:ARG:NH2	2.33	0.43
1:A:80:ALA:O	1:A:84:VAL:HB	2.19	0.43
1:A:250:SER:HA	1:A:251:PRO:HD3	1.82	0.42
1:A:94:GLU:OE2	1:A:175:HIS:HD2	2.02	0.42
1:A:228:ASN:ND2	1:A:230:ASP:H	2.17	0.42
1:A:109:PRO:HB2	4:A:884:HOH:O	2.19	0.42
1:A:250:SER:HB2	1:A:344:GLU:O	2.20	0.41
1:A:574:VAL:CG2	1:A:585:ALA:HB1	2.51	0.41
1:A:365:ARG:HA	1:A:365:ARG:HD2	1.87	0.41
1:A:473:GLU:OE2	1:A:608:HIS:HD2	2.04	0.40
1:A:153:ILE:O	1:A:153:ILE:HG13	2.21	0.40
1:A:379:LYS:HE3	1:A:379:LYS:H	1.86	0.40

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	561/628 (89%)	535 (95%)	23 (4%)	3 (0%)	38 53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ILE
1	A	152	ASN
1	A	400	ALA

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	499/557 (90%)	458 (92%)	41 (8%)	17 24

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	41	GLN
1	A	61	TYR
1	A	76	ILE
1	A	79	GLU
1	A	84	VAL
1	A	121	PRO
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	187	LYS
1	A	192	LYS
1	A	199	LEU
1	A	227	ASN
1	A	228	ASN
1	A	241	THR
1	A	250	SER
1	A	257	LYS
1	A	278	ASP
1	A	285	VAL
1	A	298	LEU
1	A	310	SER
1	A	316	ASN
1	A	333	ARG
1	A	347	VAL
1	A	352	SER
1	A	359	ILE
1	A	379	LYS
1	A	385	VAL
1	A	411	ARG
1	A	428	SER
1	A	436	LEU
1	A	455	LYS
1	A	482	THR
1	A	493	LEU
1	A	513	HIS
1	A	517	PHE
1	A	532	GLU
1	A	543	LEU
1	A	548	ASN
1	A	560	LEU
1	A	567	LYS
1	A	580	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	15	GLN
1	A	85	ASN
1	A	172	HIS
1	A	175	HIS

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	228	ASN
1	A	362	ASN
1	A	376	ASN
1	A	387	ASN
1	A	407	HIS
1	A	438	HIS
1	A	503	HIS
1	A	513	HIS
1	A	608	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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	OXY	A	631	2	1,1,1	2.21	1 (100%)	0,0,0	0.00	-

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	OXY	A	631	2	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	631	OXY	O2-O1	2.21	1.41	1.16

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.