



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 16, 2018 – 12:18 AM EST

PDB ID : 1KXQ
Title : Camelid VHH Domain in Complex with Porcine Pancreatic alpha-Amylase
Authors : Desmyter, A.; Spinelli, S.; Payan, F.; Lauwereys, M.; Wyns, L.; Muyldermans, S.; Cambillau, C.
Deposited on : 2002-02-01
Resolution : 1.60 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
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-20030736

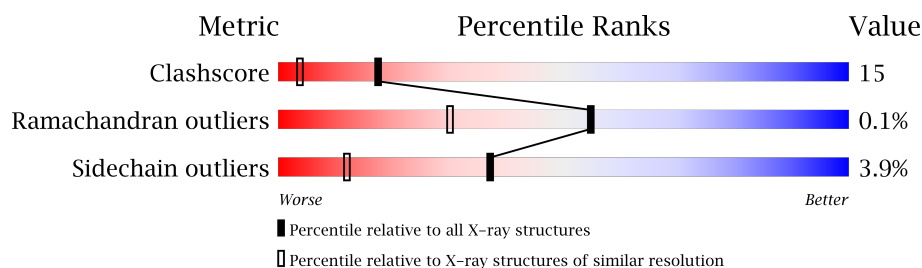
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)


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	496	
1	B	496	
1	C	496	
1	D	496	
2	E	120	
2	F	120	
2	G	120	

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Mol	Chain	Length	Quality of chain
2	H	120	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment representing 74%, a yellow segment representing 23%, and a small orange segment at the end. A small black dot is visible at the far right end of the bar.

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22119 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 alpha-amylase, pancreatic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			
1	B	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			
1	C	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			
1	D	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LYS	GLN	SEE REMARK 999	UNP P00690
A	310	SER	ALA	SEE REMARK 999	UNP P00690
A	323	ILE	VAL	SEE REMARK 999	UNP P00690
A	404	GLN	GLU	SEE REMARK 999	UNP P00690
B	243	LYS	GLN	SEE REMARK 999	UNP P00690
B	310	SER	ALA	SEE REMARK 999	UNP P00690
B	323	ILE	VAL	SEE REMARK 999	UNP P00690
B	404	GLN	GLU	SEE REMARK 999	UNP P00690
C	243	LYS	GLN	SEE REMARK 999	UNP P00690
C	310	SER	ALA	SEE REMARK 999	UNP P00690
C	323	ILE	VAL	SEE REMARK 999	UNP P00690
C	404	GLN	GLU	SEE REMARK 999	UNP P00690
D	243	LYS	GLN	SEE REMARK 999	UNP P00690
D	310	SER	ALA	SEE REMARK 999	UNP P00690
D	323	ILE	VAL	SEE REMARK 999	UNP P00690
D	404	GLN	GLU	SEE REMARK 999	UNP P00690

- Molecule 2 is a protein called antibody VHH fragment CABAMD9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	120	Total	C	N	O	S	0	0	0
			916	570	158	185	3			
2	F	120	Total	C	N	O	S	0	0	0
			916	570	158	185	3			
2	G	120	Total	C	N	O	S	0	0	0
			916	570	158	185	3			
2	H	120	Total	C	N	O	S	0	0	0
			916	570	158	185	3			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	586	Total	O	0	0
			586	586		
5	B	540	Total	O	0	0
			540	540		
5	C	508	Total	O	0	0
			508	508		

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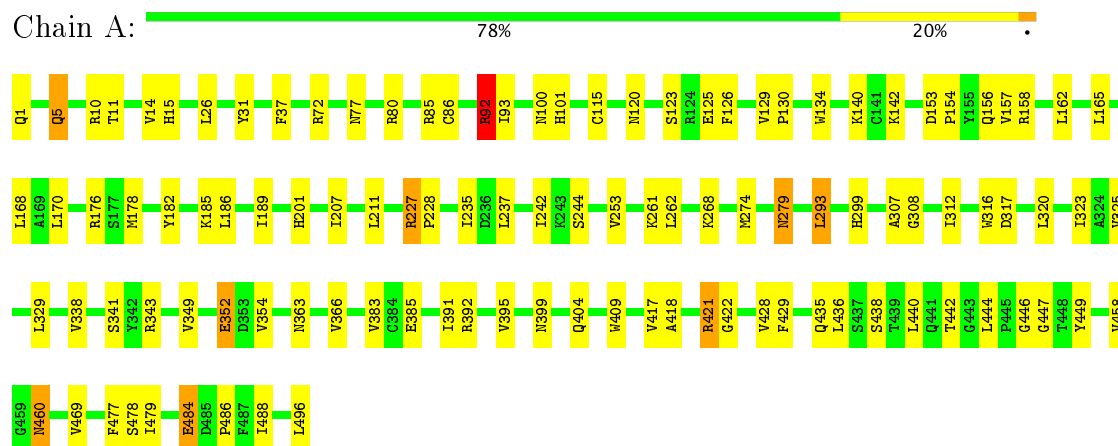
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	635	Total 635	O 635	0	0
5	E	143	Total 143	O 143	0	0
5	F	137	Total 137	O 137	0	0
5	G	144	Total 144	O 144	0	0
5	H	114	Total 114	O 114	0	0

3 Residue-property plots [i](#)

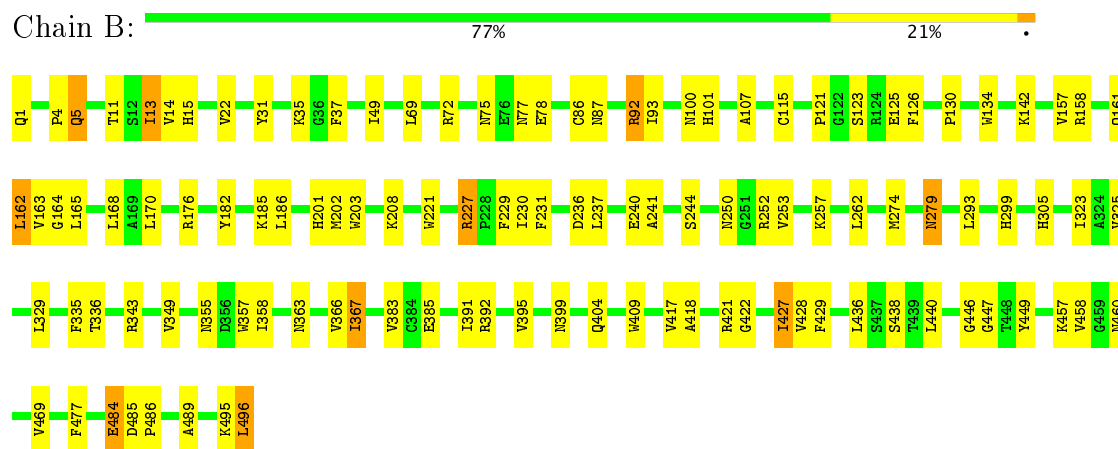
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

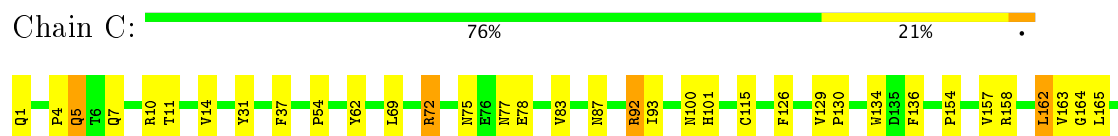
- Molecule 1: alpha-amylase, pancreatic

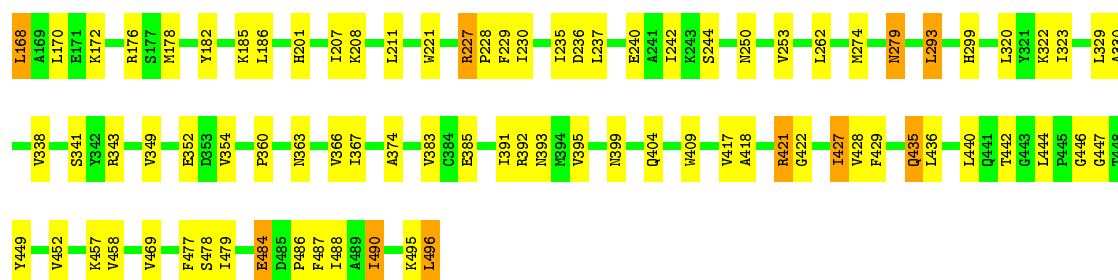


- Molecule 1: alpha-amylase, pancreatic

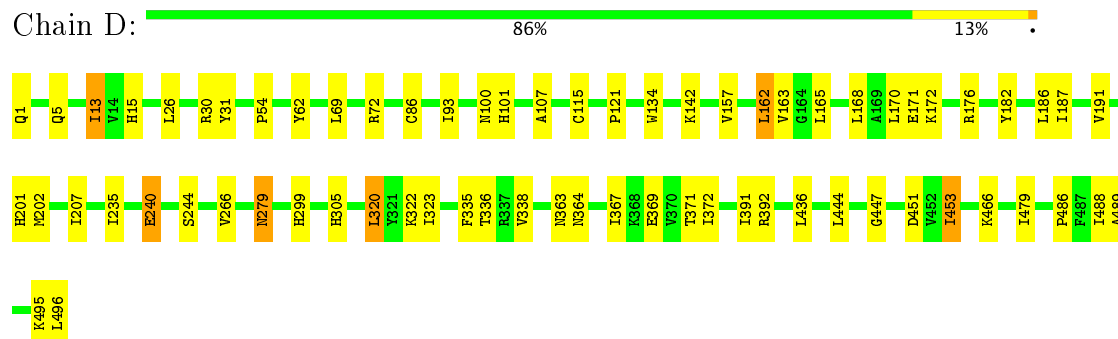


- Molecule 1: alpha-amylase, pancreatic

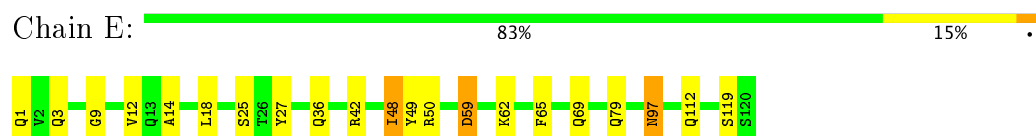




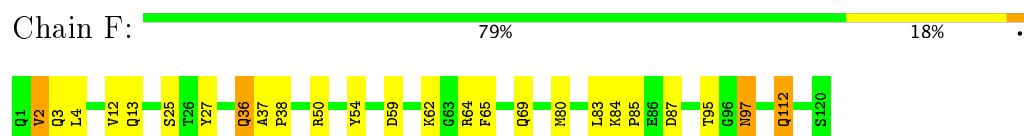
- Molecule 1: alpha-amylase, pancreatic



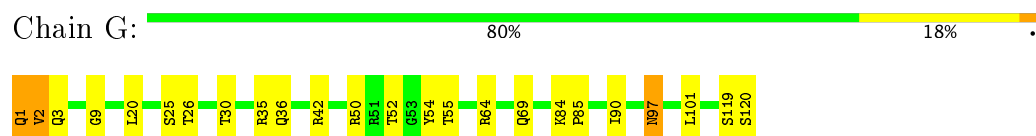
- Molecule 2: antibody VHH fragment CABAMD9



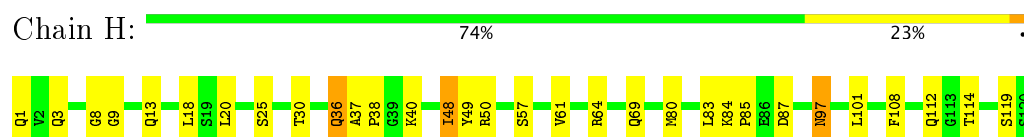
- Molecule 2: antibody VHH fragment CABAMD9



- Molecule 2: antibody VHH fragment CABAMD9



- Molecule 2: antibody VHH fragment CABAMD9



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.17Å 100.92Å 103.74Å 79.31° 72.63° 86.11°	Depositor
Resolution (Å)	29.79 – 1.60	Depositor
% Data completeness (in resolution range)	96.8 (29.79-1.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.197 , 0.219	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22119	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CA, CL

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	0.47	0/4020	0.76	6/5461 (0.1%)
1	B	0.45	0/4020	0.72	0/5461
1	C	0.42	0/4020	0.71	3/5461 (0.1%)
1	D	0.45	0/4020	0.73	0/5461
2	E	0.39	0/935	0.67	0/1267
2	F	0.44	0/935	0.68	0/1267
2	G	0.42	0/935	0.69	1/1267 (0.1%)
2	H	0.39	0/935	0.64	0/1267
All	All	0.44	0/19820	0.72	10/26912 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	LEU	CA-CB-CG	-7.05	99.09	115.30
1	C	72	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	92	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	C	72	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	A	72	ARG	NE-CZ-NH1	-5.88	117.36	120.30

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	3910	0	3693	128	0
1	B	3910	0	3693	135	0
1	C	3910	0	3693	145	0
1	D	3910	0	3693	84	0
2	E	916	0	864	16	0
2	F	916	0	864	38	0
2	G	916	0	864	17	0
2	H	916	0	864	27	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	586	0	0	16	0
5	B	540	0	0	17	0
5	C	508	0	0	12	0
5	D	635	0	0	16	0
5	E	143	0	0	2	0
5	F	137	0	0	15	0
5	G	144	0	0	4	0
5	H	114	0	0	7	0
All	All	22119	0	18228	577	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 15.

The worst 5 of 577 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)
2:F:3:GLN:HG2	2:F:25:SER:HB3	1.29	1.12
1:A:26:LEU:HD21	5:A:4489:HOH:O	1.52	1.09
1:A:352:GLU:OE2	2:H:97:ASN:OD1	1.75	1.04
1:C:1:GLN:HG3	1:C:230:ILE:HD12	1.36	1.03
1:D:453:ILE:HD11	1:D:489:ALA:HB3	1.39	1.02

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	494/496 (100%)	485 (98%)	9 (2%)	0	100	100
1	B	494/496 (100%)	483 (98%)	11 (2%)	0	100	100
1	C	494/496 (100%)	483 (98%)	11 (2%)	0	100	100
1	D	494/496 (100%)	484 (98%)	10 (2%)	0	100	100
2	E	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
2	F	118/120 (98%)	114 (97%)	2 (2%)	2 (2%)	11	1
2	G	118/120 (98%)	115 (98%)	2 (2%)	1 (1%)	22	6
2	H	118/120 (98%)	111 (94%)	7 (6%)	0	100	100
All	All	2448/2464 (99%)	2389 (98%)	56 (2%)	3 (0%)	55	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	2	VAL
2	G	2	VAL
2	F	38	PRO

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	413/413 (100%)	395 (96%)	18 (4%)	33	10
1	B	413/413 (100%)	396 (96%)	17 (4%)	35	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	413/413 (100%)	395 (96%)	18 (4%)	33	10
1	D	413/413 (100%)	400 (97%)	13 (3%)	45	18
2	E	95/96 (99%)	91 (96%)	4 (4%)	34	11
2	F	95/96 (99%)	92 (97%)	3 (3%)	44	17
2	G	95/96 (99%)	92 (97%)	3 (3%)	44	17
2	H	95/96 (99%)	91 (96%)	4 (4%)	34	11
All	All	2032/2036 (100%)	1952 (96%)	80 (4%)	37	12

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	69	LEU
1	C	279	ASN
2	G	1	GLN
1	C	92	ARG
1	C	162	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	5	GLN
1	C	279	ASN
2	G	3	GLN
1	C	101	HIS
1	C	350	ASN

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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 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.