



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 1A6W / pdb_00001a6w
Title : B1-8 FV FRAGMENT COMPLEXED WITH A (4-HYDROXY-5-iodo-3-NITROPHENYL) ACETATE COMPOUND
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Deposited on : 1998-03-03
Resolution : 2.00 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

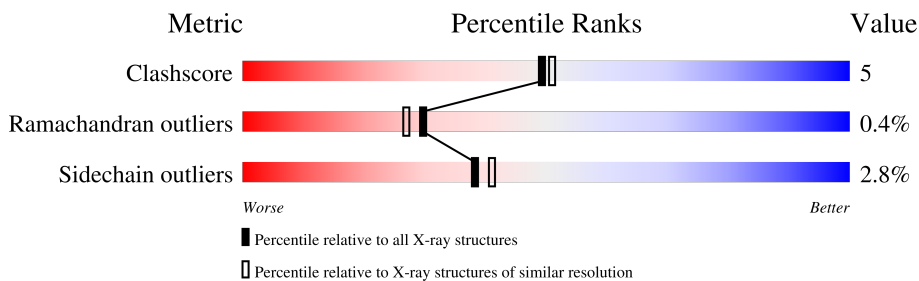
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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	L	109	
2	H	120	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1973 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 B1-8 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	109	Total	C	N	O	S	0	10	0
			835	523	143	166	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	40	GLU	GLN	variant	UNP P01724

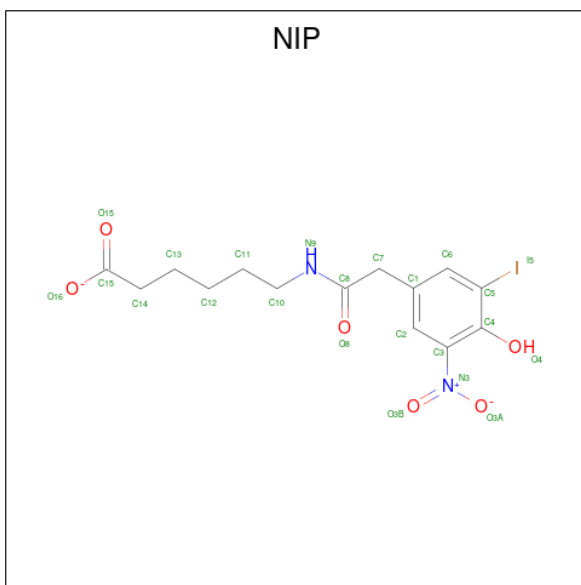
- Molecule 2 is a protein called B1-8 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	120	Total	C	N	O	S	0	3	0
			939	601	149	185	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	416	VAL	LEU	variant	UNP P01751

- Molecule 3 is 4-HYDROXY-5-iodo-3-nitrophenylacetyl-epsilon-aminocaproic acid anion (CCD ID: NIP) (formula: C₁₄H₁₆IN₂O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	I	N	O	0	0
			17	10	1	2	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	92	Total O 92 92	0	0
4	H	90	Total O 90 90	2	0

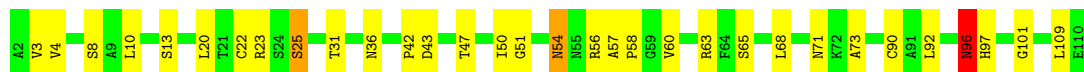
3 Residue-property plots [i](#)

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: B1-8 FV (LIGHT CHAIN)

Chain L:  71% 27% ..



- Molecule 2: B1-8 FV (HEAVY CHAIN)

Chain H:  74% 23% .



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	72.27Å 83.51Å 40.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.171 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1973	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: NIP

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	L	1.16	1/891 (0.1%)	1.90	23/1216 (1.9%)
2	H	1.07	1/981 (0.1%)	1.82	21/1332 (1.6%)
All	All	1.12	2/1872 (0.1%)	1.86	44/2548 (1.7%)

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	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	333	TRP	NE1-CE2	-5.41	1.31	1.37
1	L	96	ASN	CG-ND2	-5.09	1.22	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	23	ARG	NE-CZ-NH1	9.42	130.92	121.50
2	H	308	GLY	N-CA-C	9.39	124.00	112.73
1	L	96	ASN	CB-CG-ND2	8.57	129.26	116.40
2	H	373	ASP	CA-CB-CG	-8.37	104.23	112.60
1	L	96	ASN	OD1-CG-ND2	-7.97	114.63	122.60
2	H	354	ASN	OD1-CG-ND2	7.38	129.98	122.60
1	L	23	ARG	CD-NE-CZ	7.32	134.65	124.40
2	H	405	SER	N-CA-C	7.22	121.48	111.74
2	H	404	SER	N-CA-C	7.08	121.62	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	54	ASN	CB-CG-ND2	6.88	126.71	116.40
2	H	411	GLY	N-CA-C	-6.80	101.64	112.66
1	L	13	SER	O-C-N	6.74	126.81	121.55
2	H	340	ARG	NE-CZ-NH2	-6.71	113.16	119.20
2	H	396	CYS	N-CA-C	-6.59	99.48	109.95
1	L	8	SER	CA-CB-OG	-6.52	98.06	111.10
2	H	343	ARG	CA-C-O	6.23	127.30	119.95
2	H	329	PHE	CA-CB-CG	6.14	119.94	113.80
1	L	42	PRO	O-C-N	5.88	130.35	122.89
2	H	303	GLN	OE1-CD-NE2	5.78	128.38	122.60
1	L	68	LEU	CA-C-O	-5.73	114.02	120.32
2	H	348	ILE	N-CA-C	-5.71	106.25	111.67
2	H	407	PHE	CA-CB-CG	5.70	119.50	113.80
1	L	109	LEU	N-CA-C	5.64	117.27	109.15
1	L	23	ARG	CA-CB-CG	5.59	125.29	114.10
1	L	101	GLY	N-CA-C	-5.58	103.87	112.85
2	H	312	VAL	CA-C-O	5.41	127.35	121.67
1	L	65[A]	SER	CA-C-N	-5.39	117.38	122.66
1	L	65[A]	SER	C-N-CA	-5.39	117.38	122.66
1	L	65[B]	SER	CA-C-N	-5.39	117.38	122.66
1	L	65[B]	SER	C-N-CA	-5.39	117.38	122.66
1	L	54	ASN	CA-C-O	-5.36	113.50	119.34
2	H	371	THR	CA-CB-CG2	5.35	119.60	110.50
1	L	63	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	H	371	THR	CA-CB-OG1	-5.26	101.70	109.60
1	L	90[A]	CYS	N-CA-C	-5.26	101.99	110.14
1	L	90[B]	CYS	N-CA-C	-5.26	101.99	110.14
1	L	31	THR	CA-CB-OG1	-5.20	101.79	109.60
1	L	60	VAL	CB-CA-C	5.20	115.78	110.94
2	H	302	VAL	O-C-N	5.16	128.29	122.67
2	H	365	LYS	CA-CB-CG	5.14	124.38	114.10
2	H	408	ASP	N-CA-C	5.14	116.73	111.03
1	L	50	ILE	O-C-N	5.13	128.59	123.10
2	H	378	THR	O-C-N	5.03	129.77	123.23
2	H	382	GLN	OE1-CD-NE2	-5.01	117.58	122.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	71[A]	ASN	Mainchain

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	L	835	0	805	10	0
2	H	939	0	874	10	0
3	H	17	0	8	0	0
4	H	90	0	0	2	0
4	L	92	0	0	1	0
All	All	1973	0	1687	19	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 5.

All (19) 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:H:313:LYS:HE2	4:H:97:HOH:O	1.83	0.79
2:H:312:VAL:HG11	2:H:318:VAL:HG12	1.82	0.60
2:H:338:LYS:HE2	2:H:340:ARG:HD2	1.84	0.57
2:H:306:GLN:H	2:H:412[B]:GLN:HE22	1.56	0.53
1:L:22:CYS:HB3	1:L:73:ALA:HB3	1.92	0.52
1:L:47[B]:THR:HG22	4:L:138:HOH:O	2.08	0.52
1:L:3:VAL:H	1:L:25[A]:SER:HB2	1.76	0.50
2:H:318:VAL:HG13	2:H:386:LEU:HD11	1.94	0.49
1:L:51:GLY:HA3	2:H:406:TYR:HB3	2.01	0.43
1:L:56[A]:ARG:HH11	1:L:56[A]:ARG:HD3	1.41	0.43
2:H:313:LYS:HD3	2:H:419:SER:O	2.20	0.42
1:L:4:VAL:HG22	1:L:92:LEU:HD12	2.02	0.41
1:L:57:ALA:HA	1:L:58:PRO:HD3	1.88	0.41
1:L:10:LEU:HD12	1:L:20[B]:LEU:HD22	2.02	0.41
1:L:96:ASN:ND2	1:L:97:HIS:ND1	2.69	0.41
2:H:374:LYS:HE2	4:H:124:HOH:O	2.21	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	L	117/109 (107%)	107 (92%)	9 (8%)	1 (1%)	14	9
2	H	121/120 (101%)	120 (99%)	1 (1%)	0	100	100
All	All	238/229 (104%)	227 (95%)	10 (4%)	1 (0%)	30	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	43	ASP

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	L	92/86 (107%)	88 (96%)	4 (4%)	26	25
2	H	98/102 (96%)	95 (97%)	3 (3%)	35	37
All	All	190/188 (101%)	183 (96%)	7 (4%)	38	30

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	25[A]	SER
1	L	25[B]	SER
1	L	54	ASN
1	L	96	ASN
2	H	406	TYR

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Mol	Chain	Res	Type
2	H	417[A]	THR
2	H	417[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	96	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

1 ligand is modelled in this entry.

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	NIP	H	430	-	17,17,23	1.26	1 (5%)	19,23,30	2.34	9 (47%)

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	NIP	H	430	-	-	0/9/11/17	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	430	NIP	O3B-N3	2.14	1.26	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	430	NIP	C3-C4-C5	4.08	123.78	119.12
3	H	430	NIP	C6-C5-C4	-4.07	113.66	121.33
3	H	430	NIP	C7-C1-C6	4.05	126.53	120.38
3	H	430	NIP	C7-C1-C2	-3.64	114.86	120.38
3	H	430	NIP	C4-C5-I5	3.06	123.81	119.35
3	H	430	NIP	C2-C3-C4	-2.91	118.58	121.54
3	H	430	NIP	C1-C6-C5	2.53	125.08	120.45
3	H	430	NIP	O3B-N3-C3	-2.38	114.97	119.03
3	H	430	NIP	C6-C5-I5	2.16	122.52	118.46

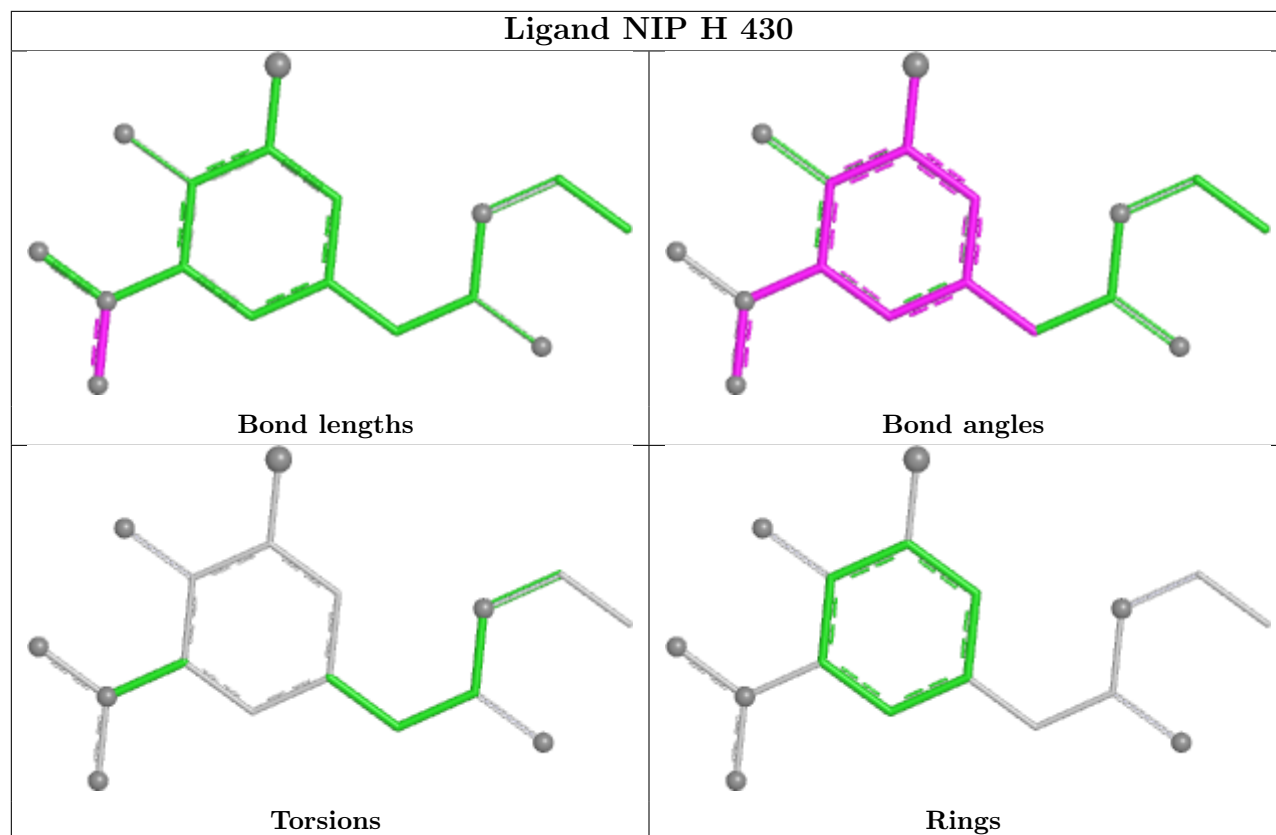
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.