



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:00 PM UTC

PDB ID : 5H72 / pdb_00005h72
Title : Structure of the periplasmic domain of FliP
Authors : Fukumura, T.; Kawaguchi, T.; Saijo-Hamano, Y.; Namba, K.; Minamino, T.; Imada, K.
Deposited on : 2016-11-16
Resolution : 2.40 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

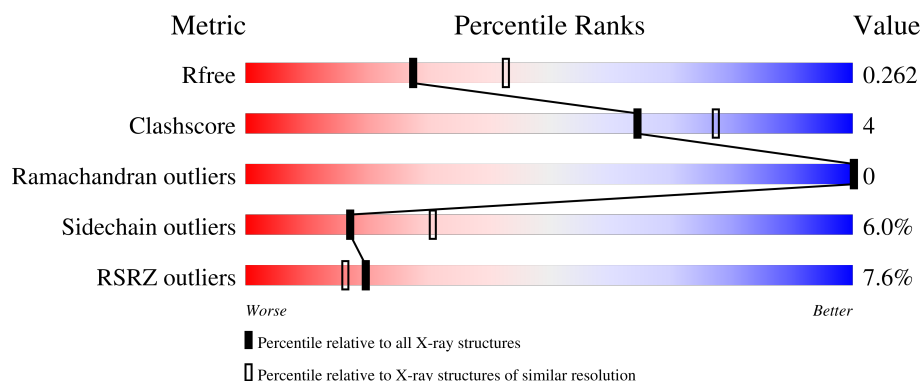
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	82	2% 73% 9% 18%
1	B	82	9% 73% 6% 18%
1	C	82	7% 71% 10% 18%
1	D	82	6% 78% 18%
1	E	82	7% 68% 12% 18%

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Mol	Chain	Length	Quality of chain
1	F	82	7% 68% 10% • 18%
1	G	82	7% 72% 9% • 18%
1	H	82	4% 71% 10% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4729 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 Flagellar biosynthetic protein FlpP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	B	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	C	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	D	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	E	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	F	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	G	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			
1	H	67	Total	C	N	O	S	0	0	0
			542	346	93	100	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	expression tag	UNP Q9WZG2
A	108	SER	-	expression tag	UNP Q9WZG2
A	109	HIS	-	expression tag	UNP Q9WZG2
B	107	GLY	-	expression tag	UNP Q9WZG2
B	108	SER	-	expression tag	UNP Q9WZG2
B	109	HIS	-	expression tag	UNP Q9WZG2
C	107	GLY	-	expression tag	UNP Q9WZG2
C	108	SER	-	expression tag	UNP Q9WZG2
C	109	HIS	-	expression tag	UNP Q9WZG2
D	107	GLY	-	expression tag	UNP Q9WZG2
D	108	SER	-	expression tag	UNP Q9WZG2
D	109	HIS	-	expression tag	UNP Q9WZG2
E	107	GLY	-	expression tag	UNP Q9WZG2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	108	SER	-	expression tag	UNP Q9WZG2
E	109	HIS	-	expression tag	UNP Q9WZG2
F	107	GLY	-	expression tag	UNP Q9WZG2
F	108	SER	-	expression tag	UNP Q9WZG2
F	109	HIS	-	expression tag	UNP Q9WZG2
G	107	GLY	-	expression tag	UNP Q9WZG2
G	108	SER	-	expression tag	UNP Q9WZG2
G	109	HIS	-	expression tag	UNP Q9WZG2
H	107	GLY	-	expression tag	UNP Q9WZG2
H	108	SER	-	expression tag	UNP Q9WZG2
H	109	HIS	-	expression tag	UNP Q9WZG2

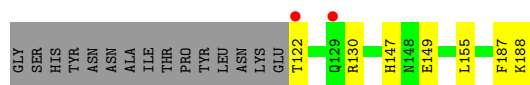
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	44	Total O 44 44	0	0
2	B	47	Total O 47 47	0	0
2	C	43	Total O 43 43	0	0
2	D	50	Total O 50 50	0	0
2	E	55	Total O 55 55	0	0
2	F	37	Total O 37 37	0	0
2	G	62	Total O 62 62	0	0
2	H	55	Total O 55 55	0	0

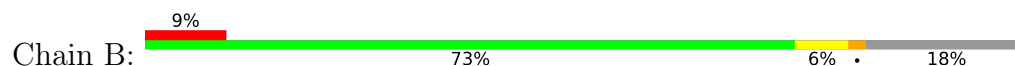
3 Residue-property plots [i](#)

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 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.

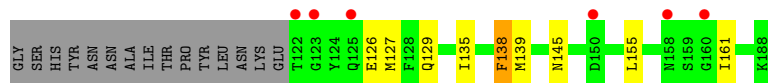
- Molecule 1: Flagellar biosynthetic protein FliP



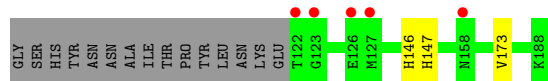
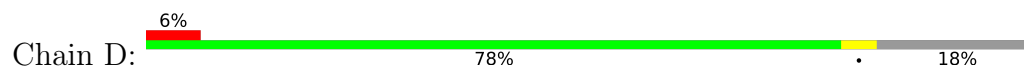
- Molecule 1: Flagellar biosynthetic protein FliP



- Molecule 1: Flagellar biosynthetic protein FliP



- Molecule 1: Flagellar biosynthetic protein FliP



- Molecule 1: Flagellar biosynthetic protein FliP



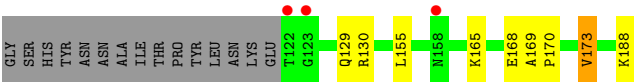
- Molecule 1: Flagellar biosynthetic protein FliP



• Molecule 1: Flagellar biosynthetic protein FliP



• Molecule 1: Flagellar biosynthetic protein FliP



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.88Å 114.88Å 193.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.92 – 2.40 42.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.92-2.40) 99.3 (42.92-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 2.39Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.211 , 0.261 0.214 , 0.262	Depositor DCC
R_{free} test set	1529 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4729	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1659e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/551	0.70	0/741
1	B	0.40	0/551	0.78	0/741
1	C	0.41	0/551	0.72	0/741
1	D	0.46	0/551	0.69	0/741
1	E	0.41	0/551	0.75	0/741
1	F	0.43	0/551	0.71	0/741
1	G	0.46	0/551	0.74	0/741
1	H	0.47	0/551	0.72	0/741
All	All	0.44	0/4408	0.73	0/5928

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	542	0	539	4	0
1	B	542	0	539	3	0
1	C	542	0	539	4	0
1	D	542	0	539	2	0
1	E	542	0	539	5	0
1	F	542	0	539	7	0
1	G	542	0	539	4	0
1	H	542	0	539	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	0	3	0
2	B	47	0	0	3	0
2	C	43	0	0	2	0
2	D	50	0	0	1	0
2	E	55	0	0	0	0
2	F	37	0	0	1	0
2	G	62	0	0	0	0
2	H	55	0	0	3	0
All	All	4729	0	4312	34	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 4.

All (34) 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:147:HIS:ND1	2:A:201:HOH:O	2.18	0.74
1:B:147:HIS:ND1	2:B:203:HOH:O	2.21	0.74
1:H:129:GLN:NE2	2:H:201:HOH:O	2.19	0.73
1:B:150:ASP:OD1	2:B:201:HOH:O	2.12	0.67
1:D:147:HIS:ND1	2:D:201:HOH:O	2.28	0.65
1:D:146:HIS:ND1	1:H:188:LYS:HG3	2.15	0.62
1:H:130:ARG:NH1	2:H:204:HOH:O	2.33	0.61
1:C:145:ASN:ND2	2:C:202:HOH:O	2.34	0.59
1:B:129:GLN:OE1	2:B:202:HOH:O	2.17	0.56
1:H:130:ARG:NH2	2:H:206:HOH:O	2.39	0.55
1:A:130:ARG:NH1	2:A:204:HOH:O	2.40	0.55
1:H:165:LYS:NZ	1:H:168:GLU:OE2	2.39	0.54
1:H:169:ALA:HB1	1:H:173:VAL:HG22	1.92	0.51
1:A:149:GLU:OE2	2:A:202:HOH:O	2.19	0.51
1:F:135:ILE:HG22	1:F:139:MET:HE2	1.93	0.49
1:F:145:ASN:ND2	2:F:202:HOH:O	2.43	0.48
1:G:169:ALA:HB1	1:G:173:VAL:HG22	1.95	0.47
1:G:135:ILE:HG22	1:G:139:MET:HE2	1.96	0.46
1:F:188:LYS:HA	1:F:188:LYS:HD3	1.73	0.46
1:H:170:PRO:HG2	1:H:173:VAL:HG13	1.97	0.46
1:F:169:ALA:HB1	1:F:173:VAL:HG22	1.98	0.45
1:F:138:PHE:C	1:F:138:PHE:CD1	2.95	0.45
1:A:187:PHE:O	1:A:188:LYS:HB3	2.17	0.44
1:G:126:GLU:O	1:G:130:ARG:HG3	2.17	0.44
1:G:170:PRO:HG2	1:G:173:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ILE:HG22	1:C:139:MET:HE2	2.01	0.42
1:C:138:PHE:C	1:C:138:PHE:CD1	2.98	0.42
1:E:125:GLN:O	1:E:129:GLN:HB3	2.19	0.42
1:E:135:ILE:HG22	1:E:139:MET:HE2	2.01	0.41
1:C:129:GLN:NE2	2:C:201:HOH:O	2.19	0.41
1:E:138:PHE:C	1:E:138:PHE:CD1	2.99	0.41
1:E:161:ILE:HG22	1:E:163:ILE:HG23	2.03	0.41
1:F:139:MET:HG2	1:F:178:PHE:CG	2.56	0.40
1:E:125:GLN:HE22	1:F:158:ASN:HB2	1.87	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	65/82 (79%)	64 (98%)	1 (2%)	0	100	100
1	B	65/82 (79%)	64 (98%)	1 (2%)	0	100	100
1	C	65/82 (79%)	63 (97%)	2 (3%)	0	100	100
1	D	65/82 (79%)	65 (100%)	0	0	100	100
1	E	65/82 (79%)	65 (100%)	0	0	100	100
1	F	65/82 (79%)	65 (100%)	0	0	100	100
1	G	65/82 (79%)	64 (98%)	1 (2%)	0	100	100
1	H	65/82 (79%)	64 (98%)	1 (2%)	0	100	100
All	All	520/656 (79%)	514 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	58/71 (82%)	56 (97%)	2 (3%)	32	54
1	B	58/71 (82%)	52 (90%)	6 (10%)	7	11
1	C	58/71 (82%)	53 (91%)	5 (9%)	10	16
1	D	58/71 (82%)	57 (98%)	1 (2%)	53	74
1	E	58/71 (82%)	53 (91%)	5 (9%)	10	16
1	F	58/71 (82%)	53 (91%)	5 (9%)	10	16
1	G	58/71 (82%)	56 (97%)	2 (3%)	32	54
1	H	58/71 (82%)	56 (97%)	2 (3%)	32	54
All	All	464/568 (82%)	436 (94%)	28 (6%)	17	31

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	155	LEU
1	B	125	GLN
1	B	129	GLN
1	B	150	ASP
1	B	163	ILE
1	B	173	VAL
1	B	188	LYS
1	C	126	GLU
1	C	127	MET
1	C	138	PHE
1	C	155	LEU
1	C	161	ILE
1	D	173	VAL
1	E	122	THR
1	E	129	GLN
1	E	150	ASP
1	E	157	LYS
1	E	173	VAL

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Mol	Chain	Res	Type
1	F	138	PHE
1	F	150	ASP
1	F	165	LYS
1	F	173	VAL
1	F	188	LYS
1	G	158	ASN
1	G	173	VAL
1	H	155	LEU
1	H	173	VAL

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

Mol	Chain	Res	Type
1	A	125	GLN
1	A	147	HIS
1	A	148	ASN
1	B	148	ASN
1	B	158	ASN
1	C	141	ASN
1	D	147	HIS
1	D	148	ASN
1	E	125	GLN
1	E	147	HIS
1	E	148	ASN
1	F	141	ASN
1	G	141	ASN
1	G	148	ASN
1	H	148	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	67/82 (81%)	0.23	2 (2%) 52 48	29, 39, 68, 87	0
1	B	67/82 (81%)	0.57	7 (10%) 11 9	31, 43, 81, 88	0
1	C	67/82 (81%)	0.50	6 (8%) 15 12	31, 44, 82, 89	0
1	D	67/82 (81%)	0.30	5 (7%) 20 17	28, 40, 66, 86	0
1	E	67/82 (81%)	0.66	6 (8%) 15 12	32, 48, 84, 88	0
1	F	67/82 (81%)	0.53	6 (8%) 15 12	33, 50, 82, 90	0
1	G	67/82 (81%)	0.25	6 (8%) 15 12	28, 38, 64, 84	0
1	H	67/82 (81%)	0.18	3 (4%) 38 34	28, 37, 66, 84	0
All	All	536/656 (81%)	0.40	41 (7%) 20 16	28, 43, 81, 90	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	122	THR	3.9
1	D	122	THR	3.9
1	B	158	ASN	3.7
1	C	158	ASN	3.6
1	C	125	GLN	3.5
1	E	123	GLY	3.3
1	C	122	THR	3.3
1	B	188	LYS	3.2
1	F	150	ASP	3.2
1	B	125	GLN	3.2
1	E	122	THR	3.2
1	A	122	THR	3.1
1	H	122	THR	3.0
1	D	127	MET	2.8
1	E	156	ALA	2.8
1	E	154	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	158	ASN	2.7
1	F	122	THR	2.7
1	C	150	ASP	2.6
1	E	160	GLY	2.6
1	B	154	MET	2.6
1	B	122	THR	2.6
1	D	158	ASN	2.5
1	H	123	GLY	2.4
1	E	150	ASP	2.4
1	G	127	MET	2.4
1	G	188	LYS	2.4
1	C	123	GLY	2.3
1	B	150	ASP	2.3
1	D	126	GLU	2.3
1	C	160	GLY	2.3
1	F	159	SER	2.3
1	F	126	GLU	2.3
1	F	154	MET	2.2
1	H	158	ASN	2.2
1	D	123	GLY	2.2
1	A	129	GLN	2.2
1	G	138	PHE	2.2
1	G	129	GLN	2.1
1	B	160	GLY	2.1
1	F	123	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.