



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:37 PM UTC

PDB ID : 4ZJD / pdb_00004zjd
Title : Small heat shock protein AgsA from Salmonella typhimurium: Truncations at N- and C- termini
Authors : Mani, N.; Suguna, K.
Deposited on : 2015-04-29
Resolution : 7.50 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

<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

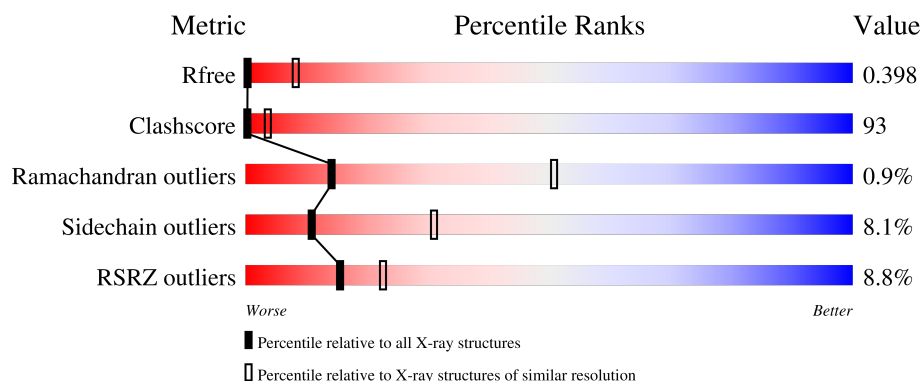
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.50 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))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. 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	137	3% 22% 33% 12% • 32%
1	B	137	5% 16% 38% 13% • 32%
1	C	137	3% 14% 37% 15% • 32%
1	D	137	12% 14% 39% 13% • 32%
1	E	137	4% 16% 36% 12% • 32%

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Mol	Chain	Length	Quality of chain
1	F	137	8% 20% 36% 12% 32%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4294 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 Aggregation suppressing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	0	0	0
			714	458	117	139			
1	B	93	Total	C	N	O	0	0	0
			717	459	117	141			
1	C	93	Total	C	N	O	0	0	0
			713	456	116	141			
1	D	93	Total	C	N	O	0	0	0
			716	458	117	141			
1	E	93	Total	C	N	O	0	0	0
			717	459	117	141			
1	F	93	Total	C	N	O	0	0	0
			717	459	117	141			

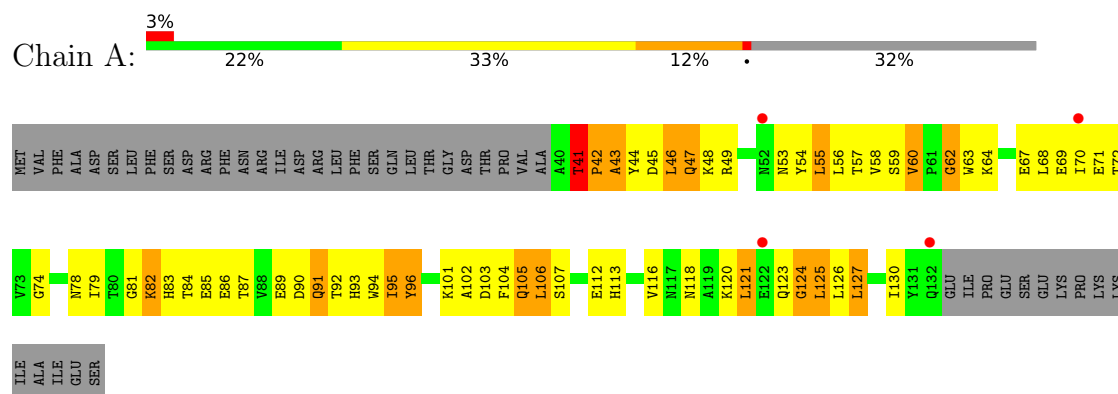
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP D1MC98
B	11	MET	-	expression tag	UNP D1MC98
C	11	MET	-	expression tag	UNP D1MC98
D	11	MET	-	expression tag	UNP D1MC98
E	11	MET	-	expression tag	UNP D1MC98
F	11	MET	-	expression tag	UNP D1MC98

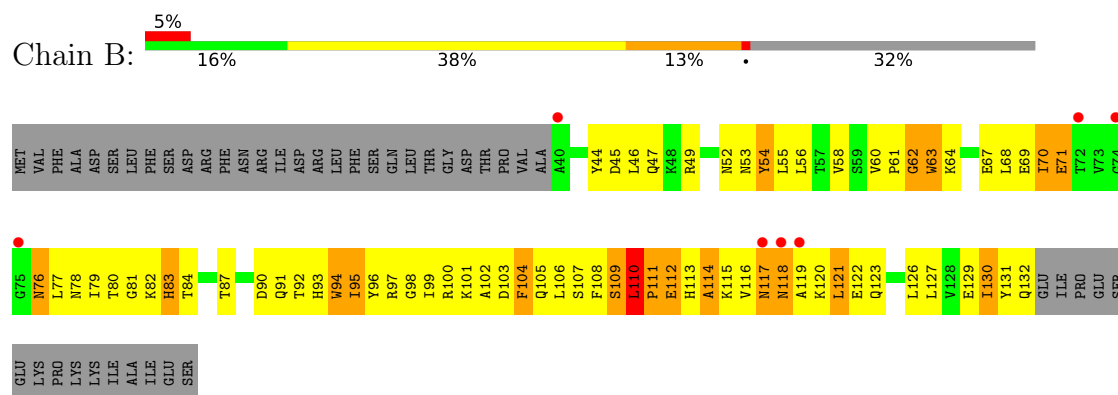
3 Residue-property plots [i](#)

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.

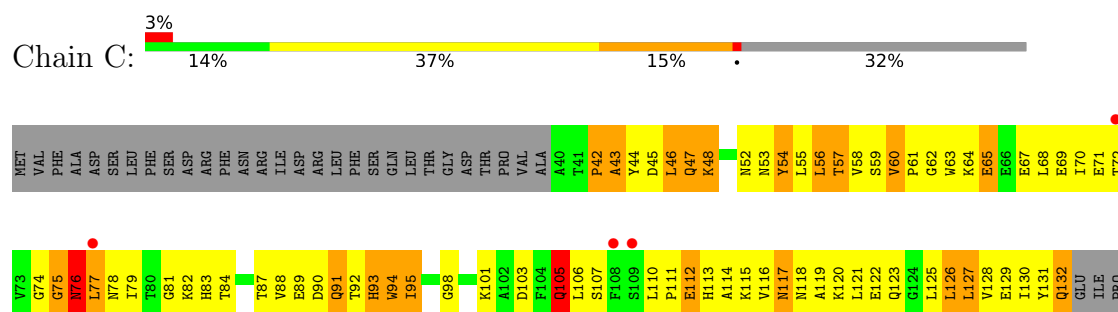
• Molecule 1: Aggregation suppressing protein



• Molecule 1: Aggregation suppressing protein



• Molecule 1: Aggregation suppressing protein



GLU
SER
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PRO
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● Molecule 1: Aggregation suppressing protein



MET VAL PHE ALA ASP SER LEU PHE SER ASP ARG PHE ASN ARG ILE ILE ASP ARG LEU PHE SER GLN LEU THR GLY ASP THR PRO VAL ALA A40 T41 Y44 Y45 L46 Q47 K48 R49 D50 A51 N52 N53 Y54 L55 L56 L57 V60 P61 G62 W63 K64 E65 E66 E67 L68 E69 I70 I71 T72

V73 G74 G75 N76 L77 N78 G81 K82 H83 V88 E89 D90 Q91 T92 H93 Q94 Y95 Y96 T99 R100 K101 A102 S103 F104 Q105 L106 S107 F108 S109 L110 P111 E112 H113 A114 K115 V116 M117 N118 A119 K120 L121 E122 Q123 G124 L125 L126 L127 V128 E129 I130 Y131 Q132 GLU ILE PRO GLU SER

GLU
LYS
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● Molecule 1: Aggregation suppressing protein

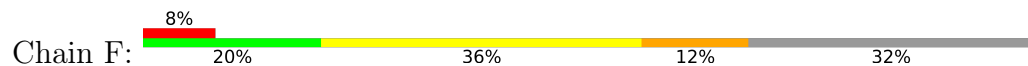


MET VAL PHE ALA ASP SER LEU PHE SER ASP ARG PHE ASN ARG ILE ILE ASP ARG LEU PHE SER GLN LEU THR GLY ASP THR PRO VAL ALA A40 T41 P42 A43 Y44 D45 L46 Q47 K48 Y54 L55 L56 T57 V58 S59 V60 P61 G62 W63 K64 E65 E66 E67 L68 E69 I70 E71 T72 V73 G74

G75 N76 N78 I79 T80 G81 K82 H83 T84 E85 E86 T87 V88 E89 D90 Q91 T92 H93 Q94 Y95 Y96 Y98 G98 T99 R100 K101 A102 S103 F104 Q105 L106 S107 F108 L110 H113 A114 V115 V116 N117 N118 L121 E122 L125 L126 L127 V128 E129 I130 Y131 Q132 GLU ILE PRO GLU SER

GLU
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● Molecule 1: Aggregation suppressing protein



MET VAL PHE ALA ASP SER LEU PHE SER ASP ARG PHE ASN ARG ILE ILE ASP ARG LEU PHE SER GLN LEU THR GLY ASP THR PRO VAL ALA A40 Y44 D45 L46 Q47 K48 L56 T57 V58 S59 V60 P61 G62 W63 K64 E67 L68 E69 I70 E71 T72 V73 G74 G75 N76 L77 N78 I79

T80 G81 H83 T84 T87 V88 E89 D90 Q91 T92 H93 Q94 Y95 Y96 Y98 R97 G98 T99 R100 K101 A102 S103 F104 Q105 L106 S107 F108 S109 L110 P111 E112 H113 A114 K115 V116 N117 N118 A119 K120 Q123 G124 L125 L126 Y131 Q132 GLU ILE PRO GLU SER GLU LYS PRO LYS ILE ALA

ILE
GLU
SER

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	89.78Å 89.78Å 707.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	68.14 – 7.50 68.14 – 7.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (68.14-7.50) 99.6 (68.14-7.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 7.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.351 , 0.396 0.388 , 0.398	Depositor DCC
R_{free} test set	74 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	574.3	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	4294	wwPDB-VP
Average B, all atoms (Å ²)	333.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	1.07	2/728 (0.3%)	1.91	29/992 (2.9%)
1	B	1.04	1/731 (0.1%)	1.98	34/996 (3.4%)
1	C	1.01	2/727 (0.3%)	1.92	38/992 (3.8%)
1	D	1.27	3/730 (0.4%)	2.01	41/995 (4.1%)
1	E	1.12	1/731 (0.1%)	2.02	36/996 (3.6%)
1	F	1.11	3/731 (0.4%)	2.00	34/996 (3.4%)
All	All	1.11	12/4378 (0.3%)	1.97	212/5967 (3.6%)

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	B	0	1
1	D	0	1
1	E	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	TYR	CA-C	9.36	1.63	1.52
1	D	131	TYR	N-CA	7.93	1.55	1.46
1	F	100	ARG	CA-C	-6.13	1.45	1.52
1	C	77	LEU	N-CA	5.74	1.53	1.46
1	A	82	LYS	C-O	-5.51	1.17	1.23

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	116	VAL	N-CA-C	12.36	126.63	109.45
1	D	112	GLU	N-CA-C	11.37	126.64	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	GLN	N-CA-C	10.56	123.86	108.34
1	A	46	LEU	CB-CA-C	10.51	132.45	111.22
1	F	110	LEU	N-CA-C	-10.46	96.65	109.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	76	ASN	Mainchain
1	D	56	LEU	Mainchain
1	E	108	PHE	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	A	714	0	675	248	0
1	B	717	0	676	251	0
1	C	713	0	668	98	0
1	D	716	0	676	143	0
1	E	717	0	679	197	0
1	F	717	0	679	171	0
All	All	4294	0	4053	779	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 93.

The worst 5 of 779 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:E:48:LYS:HB3	1:F:93:HIS:CG	1.12	1.64
1:E:44:TYR:CZ	1:F:96:TYR:CD2	1.75	1.63
1:A:47:GLN:CG	1:B:94:TRP:HA	1.26	1.61
1:A:47:GLN:HG2	1:B:94:TRP:CA	1.24	1.59
1:A:47:GLN:C	1:B:95:ILE:HG13	1.24	1.58

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	91/137 (66%)	86 (94%)	5 (6%)	0	100	100
1	B	91/137 (66%)	83 (91%)	8 (9%)	0	100	100
1	C	91/137 (66%)	80 (88%)	7 (8%)	4 (4%)	2	17
1	D	91/137 (66%)	80 (88%)	11 (12%)	0	100	100
1	E	91/137 (66%)	81 (89%)	9 (10%)	1 (1%)	11	46
1	F	91/137 (66%)	84 (92%)	7 (8%)	0	100	100
All	All	546/822 (66%)	494 (90%)	47 (9%)	5 (1%)	14	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	76	ASN
1	C	75	GLY
1	E	116	VAL
1	C	77	LEU
1	C	95	ILE

5.3.2 Protein sidechains [i](#)

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	71/121 (59%)	68 (96%)	3 (4%)	26	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	72/121 (60%)	69 (96%)	3 (4%)	26	48
1	C	71/121 (59%)	63 (89%)	8 (11%)	5	19
1	D	72/121 (60%)	62 (86%)	10 (14%)	3	14
1	E	72/121 (60%)	66 (92%)	6 (8%)	10	30
1	F	72/121 (60%)	67 (93%)	5 (7%)	14	36
All	All	430/726 (59%)	395 (92%)	35 (8%)	11	31

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	128	VAL
1	E	132	GLN
1	F	97	ARG
1	C	127	LEU
1	C	105	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	78	ASN
1	F	113	HIS
1	F	132	GLN
1	D	47	GLN
1	D	123	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	93/137 (67%)	0.10	4 (4%)	40 40	222, 279, 381, 446	0
1	B	93/137 (67%)	0.03	7 (7%)	20 26	140, 238, 330, 378	0
1	C	93/137 (67%)	0.07	4 (4%)	40 40	276, 357, 469, 550	0
1	D	93/137 (67%)	1.07	17 (18%)	3 11	343, 465, 550, 550	0
1	E	93/137 (67%)	0.31	6 (6%)	25 30	241, 317, 431, 505	0
1	F	93/137 (67%)	0.62	11 (11%)	9 17	211, 303, 379, 477	0
All	All	558/822 (67%)	0.37	49 (8%)	15 22	140, 317, 521, 550	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	80	THR	7.4
1	D	122	GLU	6.6
1	F	68	LEU	5.5
1	C	108	PHE	5.0
1	F	70	ILE	4.9

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.