



wwPDB EM Validation Summary Report ⓘ

Jul 8, 2025 – 02:53 PM JST

PDB ID : 8YGA / pdb_00008yga
EMDB ID : EMD-39240
Title : The tetramer Structure of DSR2 alone
Authors : Gao, X.; Zhu, H.; Cui, S.
Deposited on : 2024-02-26
Resolution : 4.53 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

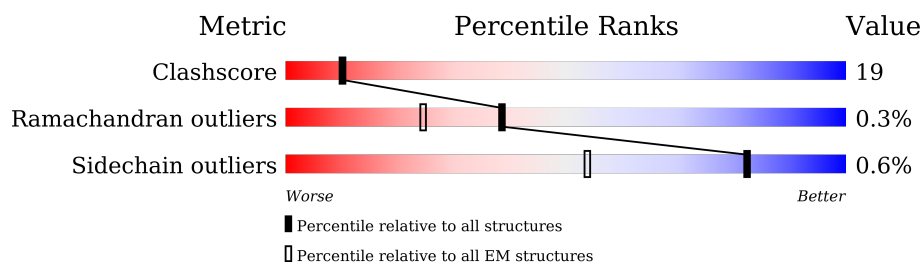
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.53 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1005	
1	B	1005	
1	C	1005	
1	D	1005	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33140 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	B	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	C	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		
1	D	995	Total	C	N	O	S	0	0
			8285	5362	1336	1555	32		

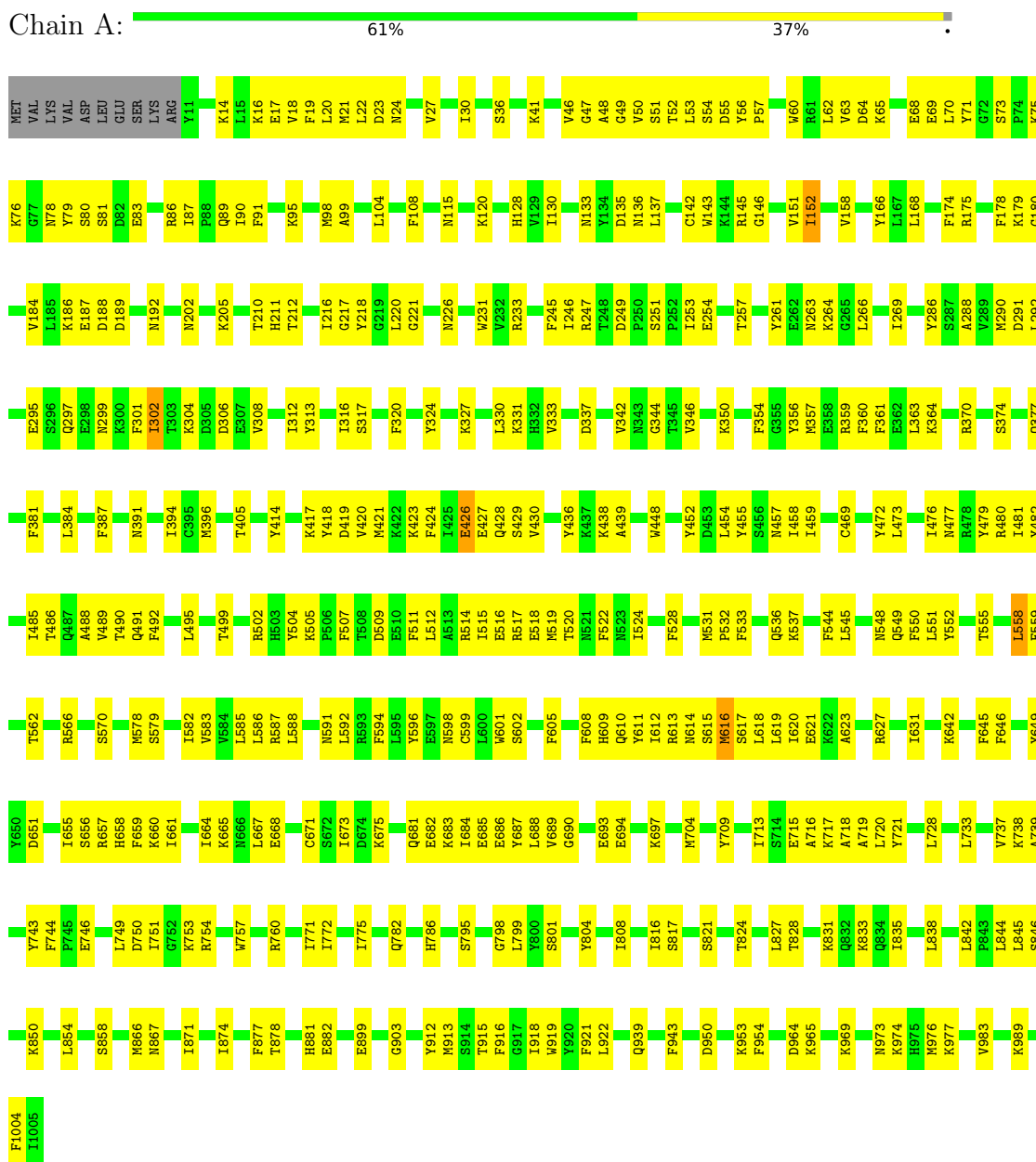
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	HIS	engineered mutation	UNP D4G637
B	171	ALA	HIS	engineered mutation	UNP D4G637
C	171	ALA	HIS	engineered mutation	UNP D4G637
D	171	ALA	HIS	engineered mutation	UNP D4G637

3 Residue-property plots

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.

- Molecule 1: SIR2-like domain-containing protein



- Molecule 1: SIR2-like domain-containing protein

Chain B:



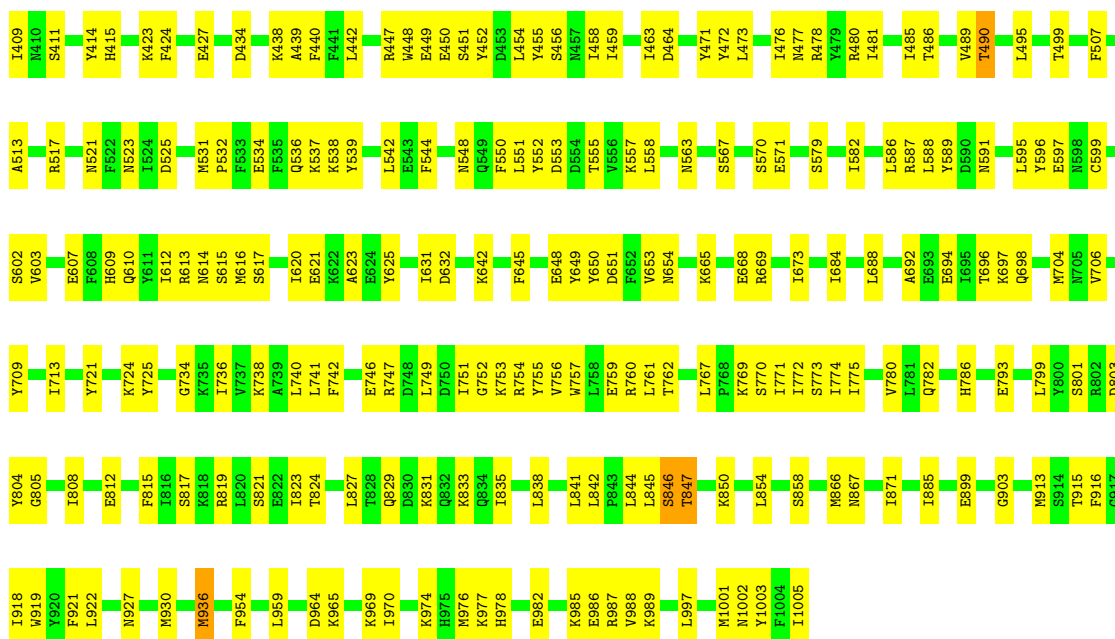
MET	VAL	LYS	VAL	ASP	LEU	GLU	SER	LYS	ARG	Y11	G12	E13	K14	V18	V26	E28	C29	I30	K31	T34	E35	R38	V43	G47	T52	L53	Y66	P57	Q58	W59	R61	L62	V63	D64	K65	Y66	E69	K75	Y79	D82	F83	Y84	L85	R86	I87	
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• Molecule 1: SIR2-like domain-containing protein

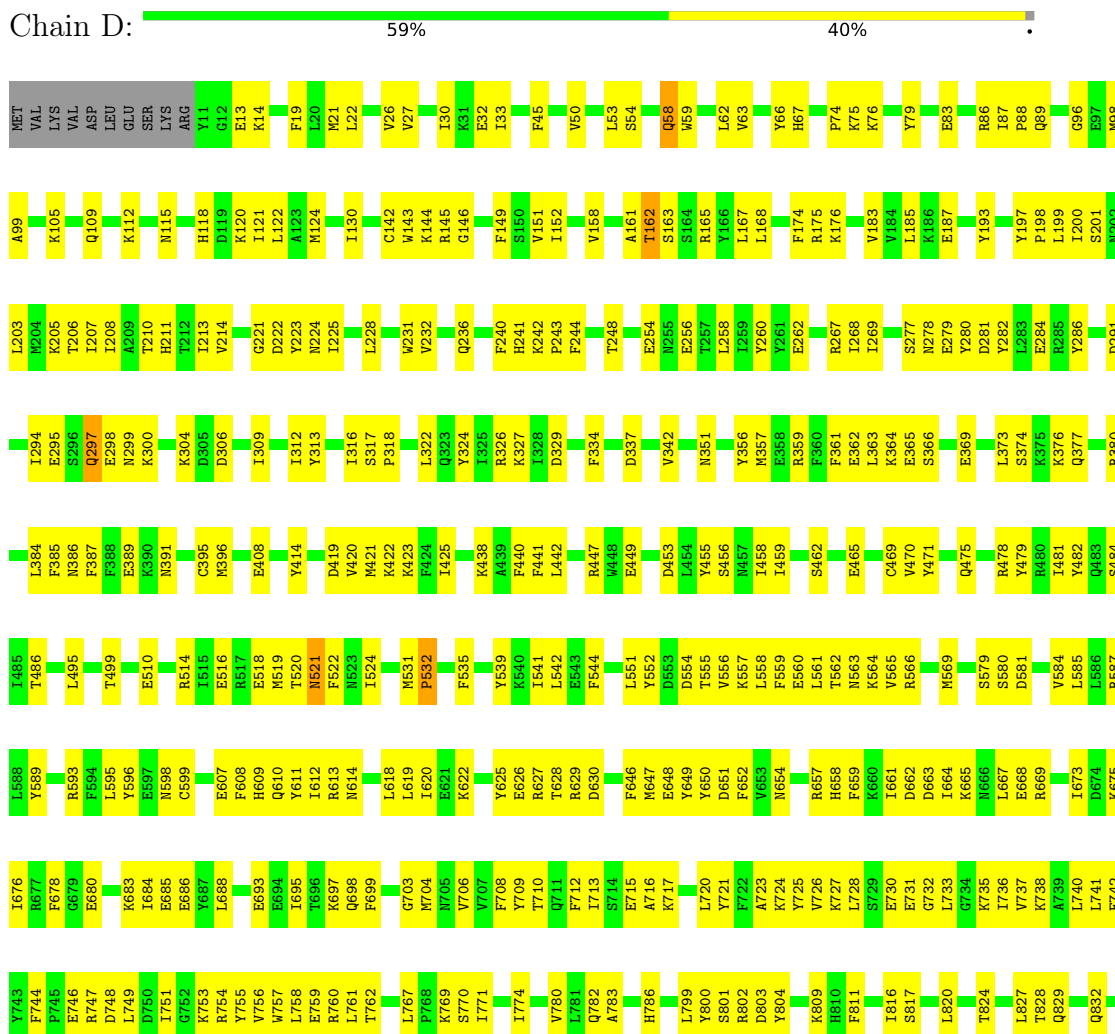
Chain C:

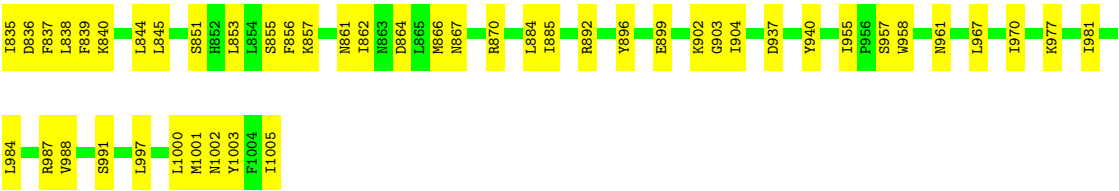


MET	VAL	LYS	VAL	ASP	LEU	GLU	SER	LYS	ARG	Y11	L15	K16	E17	V18	F19	L20	M21	L22	N25	V26	E28	C29	I30	K31	E32	I33	T34	E35	N39	G40	K41	G47	A48	G49	T52	L53	Y56	P57	D64	K65	N78	Y79	S80	S81	D82	E83	Y84	L85	R86	I87																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
	I90	K95	F107	F108	T114	N115	P116	I117	H118	M124	V128	W129	I130	N133	N136	D139	R145	G146	K147	S150	Y151	I152	D157	S163	S164	R165	Y166	L167	L168	D173	F174	R175	Y190	L199	N202	S206	T206	T210	H211	T212	F215																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
	G219	L220	G221	D222	Y223	N224	I225	N226	L227	L228	L229	R233	Q236	F245	T246	R247	T248	I253	E256	T257	L258	I259	E262	N263	T264	R267	S277	N278	D281	Y282	L283	E284	R285	Y286	V289	N290	L292	L293	I294	E295	S296	Q297	E298	N299	K300	F301	I302	T303																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
	K304	E307	D310	Y311	I312	I316	L322	I325	R326	K327	L330	Y338	E341	V342	N351	G355	Y356	K357	E358	R359	F360	F361	E362	L363	K364	E365	S366	E369	R370	S371	K372	Q377	R380	F387	F388	N391	G392	V393	N396	A397	K398	I407	L408	E409																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											



• Molecule 1: SIR2-like domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

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	0.19	0/8478	0.49	1/11418 (0.0%)
1	B	0.19	0/8478	0.49	1/11418 (0.0%)
1	C	0.18	0/8478	0.46	1/11418 (0.0%)
1	D	0.20	0/8478	0.52	1/11418 (0.0%)
All	All	0.19	0/33912	0.49	4/45672 (0.0%)

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	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	299	ASN	N-CA-C	-7.26	102.91	112.34
1	D	532	PRO	CA-N-CD	-6.28	103.22	112.00
1	A	616	MET	CB-CG-SD	-5.38	96.57	112.70
1	B	565	VAL	N-CA-C	-5.35	108.06	113.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	297	GLN	Peptide
1	D	297	GLN	Peptide
1	D	58	GLN	Peptide

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	8285	0	8120	306	0
1	B	8285	0	8120	313	0
1	C	8285	0	8120	293	0
1	D	8285	0	8120	356	0
All	All	33140	0	32480	1238	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 19.

The worst 5 of 1238 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:C:866:MET:HE3	1:C:866:MET:H	1.42	0.84
1:B:627:ARG:HH12	1:B:675:LYS:HG2	1.43	0.82
1:D:425:ILE:HD11	1:D:442:LEU:HG	1.59	0.82
1:C:588:LEU:HD11	1:C:612:ILE:HD12	1.61	0.82
1:D:45:PHE:HB2	1:D:213:ILE:HD11	1.61	0.82

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 PDB entries followed by that with respect to all EM entries.

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	993/1005 (99%)	927 (93%)	65 (6%)	1 (0%)	48 83
1	B	993/1005 (99%)	919 (92%)	73 (7%)	1 (0%)	48 83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	993/1005 (99%)	932 (94%)	56 (6%)	5 (0%)	25 64
1	D	993/1005 (99%)	906 (91%)	81 (8%)	6 (1%)	22 59
All	All	3972/4020 (99%)	3684 (93%)	275 (7%)	13 (0%)	38 72

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	521	ASN
1	C	846	SER
1	C	847	THR
1	D	223	TYR
1	D	521	ASN

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 PDB entries followed by that with respect to all EM entries.

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	912/922 (99%)	906 (99%)	6 (1%)	81 87
1	B	912/922 (99%)	903 (99%)	9 (1%)	73 81
1	C	912/922 (99%)	906 (99%)	6 (1%)	81 87
1	D	912/922 (99%)	910 (100%)	2 (0%)	92 93
All	All	3648/3688 (99%)	3625 (99%)	23 (1%)	82 88

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	866	MET
1	C	108	PHE
1	C	107	PHE
1	C	173	ASP
1	B	182	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	609	HIS
1	D	895	ASN
1	B	782	GLN
1	B	609	HIS
1	D	973	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](#)

There are no ligands in this entry.

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.