



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:03 PM GMT

PDB ID : 4B8C
Title : nuclease module of the yeast Ccr4-Not complex
Authors : Basquin, J.; Conti, E.
Deposited on : 2012-08-26
Resolution : 3.41 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

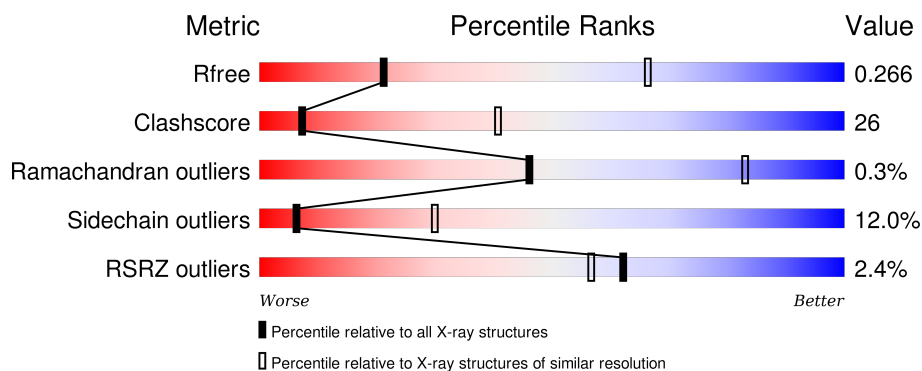
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>2%</div> <div>60%</div> <div>27%</div> <div>6%</div> <div>7%</div> </div>
1	C	288	<div> <div>59%</div> <div>28%</div> <div>6%</div> <div>7%</div> </div>
1	E	288	<div> <div>61%</div> <div>27%</div> <div>•</div> <div>7%</div> </div>
1	F	288	<div> <div>64%</div> <div>24%</div> <div>5%</div> <div>7%</div> </div>
2	B	249	<div> <div>2%</div> <div>65%</div> <div>27%</div> <div>•</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	249	<div><div><div></div><div></div><div></div></div><div><div>61%</div><div>30%</div><div>6%</div></div></div>
2	H	249	<div><div><div></div><div></div><div></div></div><div><div>61%</div><div>31%</div><div>6%</div></div></div>
2	I	249	<div><div><div></div><div></div><div></div></div><div><div>62%</div><div>29%</div><div>6%</div></div></div>
3	D	727	<div><div><div></div><div></div><div></div></div><div><div>16%</div><div>23%</div><div>56%</div></div></div>
3	J	727	<div><div><div></div><div></div><div></div></div><div><div>11%</div><div>14%</div><div>71%</div></div></div>
3	K	727	<div><div><div></div><div></div><div></div></div><div><div>18%</div><div>21%</div><div>5%</div><div>56%</div></div></div>
3	L	727	<div><div><div></div><div></div><div></div></div><div><div>11%</div><div>14%</div><div>71%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24298 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 POLY(A) RIBONUCLEASE POP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			
1	C	267	Total	C	N	O	S	0	0	0
			2174	1412	347	404	11			
1	E	267	Total	C	N	O	S	0	0	0
			2174	1411	347	405	11			
1	F	267	Total	C	N	O	S	0	0	0
			2170	1409	346	404	11			

- Molecule 2 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	G	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	H	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			
2	I	233	Total	C	N	O	S	0	0	0
			1869	1221	309	333	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	752	ARG	-	EXPRESSION TAG	UNP P25655
B	753	SER	-	EXPRESSION TAG	UNP P25655
B	754	MET	-	EXPRESSION TAG	UNP P25655
G	752	ARG	-	EXPRESSION TAG	UNP P25655
G	753	SER	-	EXPRESSION TAG	UNP P25655
G	754	MET	-	EXPRESSION TAG	UNP P25655
H	752	ARG	-	EXPRESSION TAG	UNP P25655
H	753	SER	-	EXPRESSION TAG	UNP P25655

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Chain	Residue	Modelled	Actual	Comment	Reference
H	754	MET	-	EXPRESSION TAG	UNP P25655
I	752	ARG	-	EXPRESSION TAG	UNP P25655
I	753	SER	-	EXPRESSION TAG	UNP P25655
I	754	MET	-	EXPRESSION TAG	UNP P25655

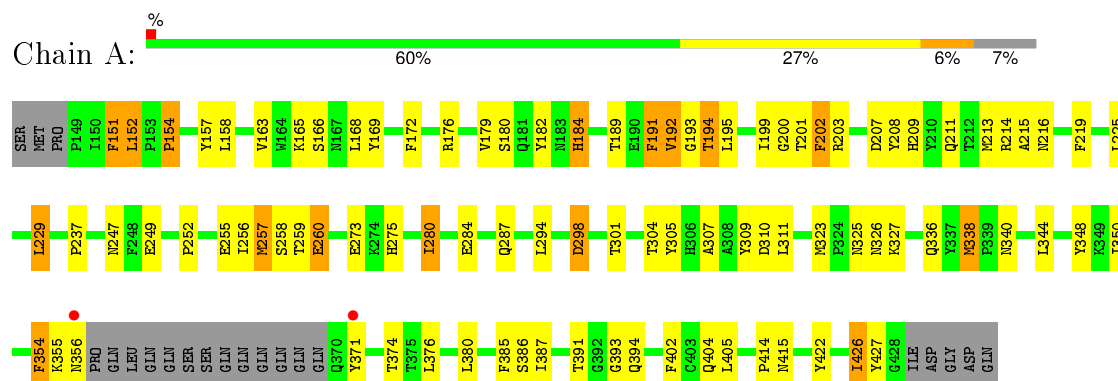
- Molecule 3 is a protein called GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	318	Total	C	N	O	S	0	0	0
			2456	1599	387	459	11			
3	J	210	Total	C	N	O	S	0	0	0
			1604	1034	266	298	6			
3	K	318	Total	C	N	O	S	0	0	0
			2470	1608	392	459	11			
3	L	210	Total	C	N	O	S	0	0	0
			1604	1034	266	298	6			

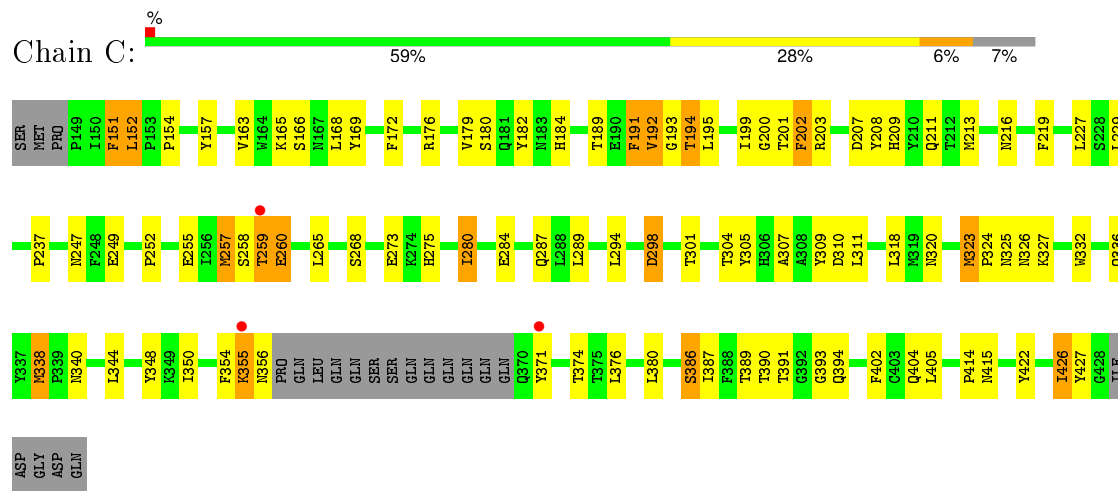
3 Residue-property plots [\(i\)](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

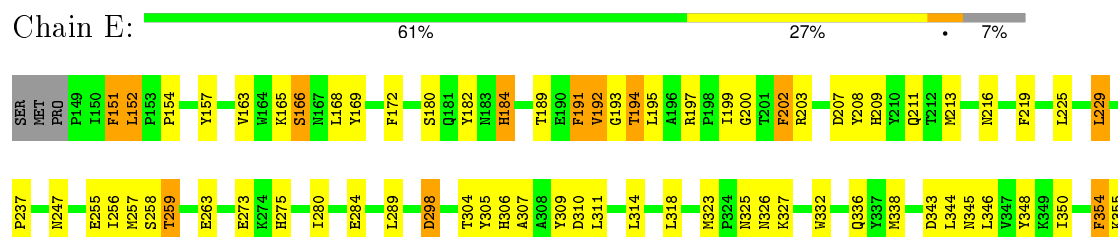
• Molecule 1: POLY(A) RIBONUCLEASE POP2

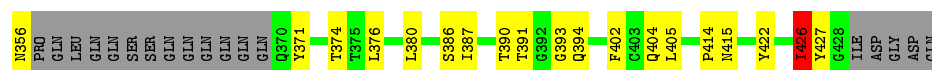


• Molecule 1: POLY(A) RIBONUCLEASE POP2



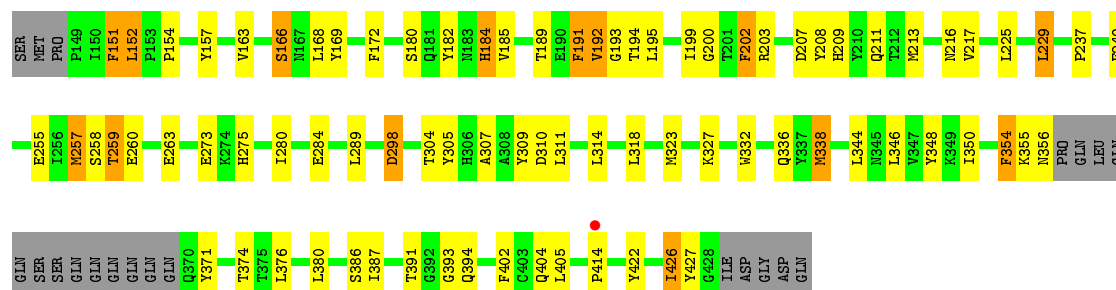
• Molecule 1: POLY(A) RIBONUCLEASE POP2





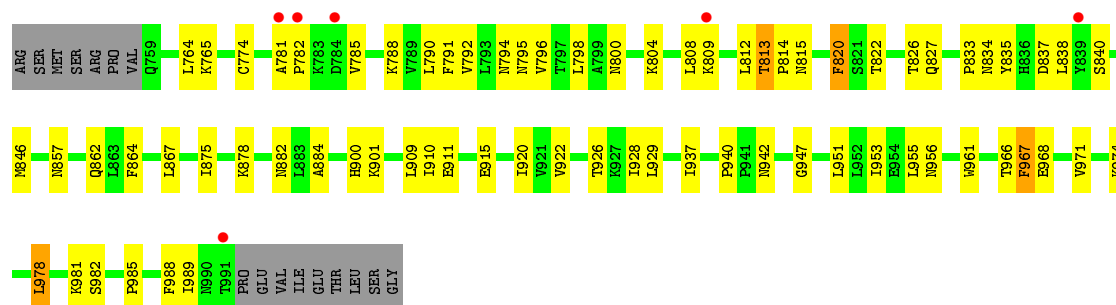
• Molecule 1: POLY(A) RIBONUCLEASE POP2

Chain F: 64% 24% 5% 7%



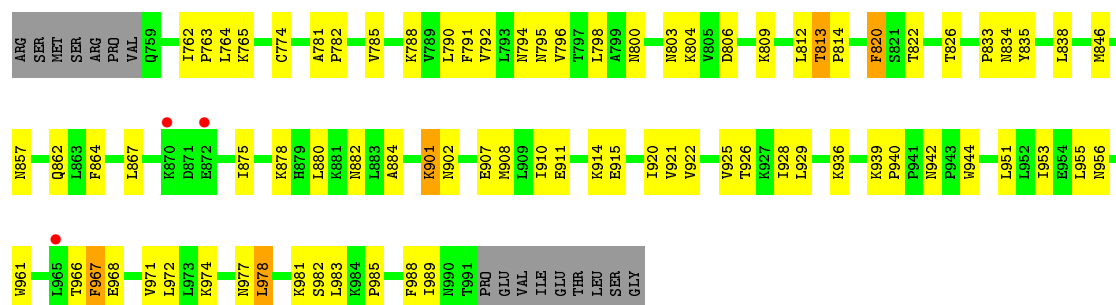
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain B: 65% 27% 2% 6%



• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

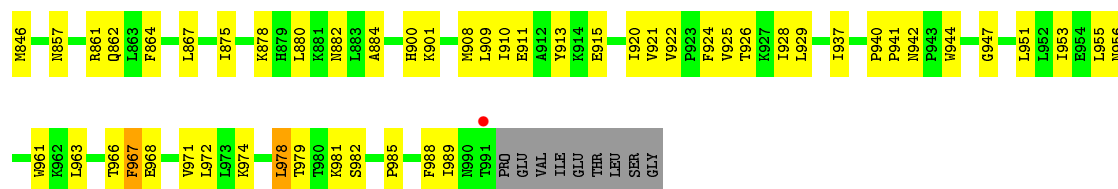
Chain G: 61% 30% 2% 6%



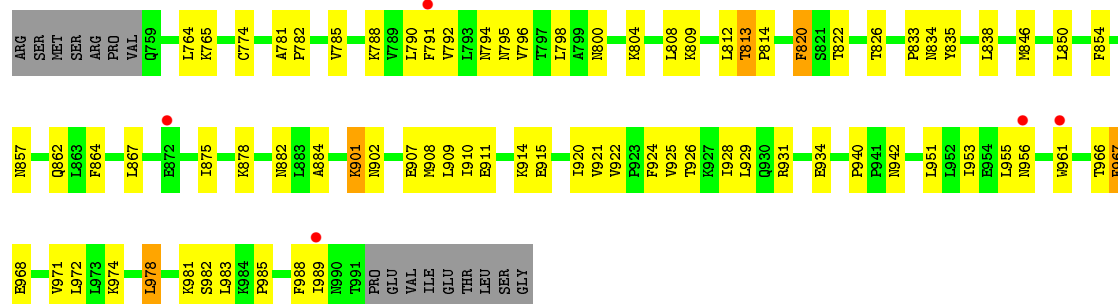
• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1

Chain H: 61% 31% 2% 6%

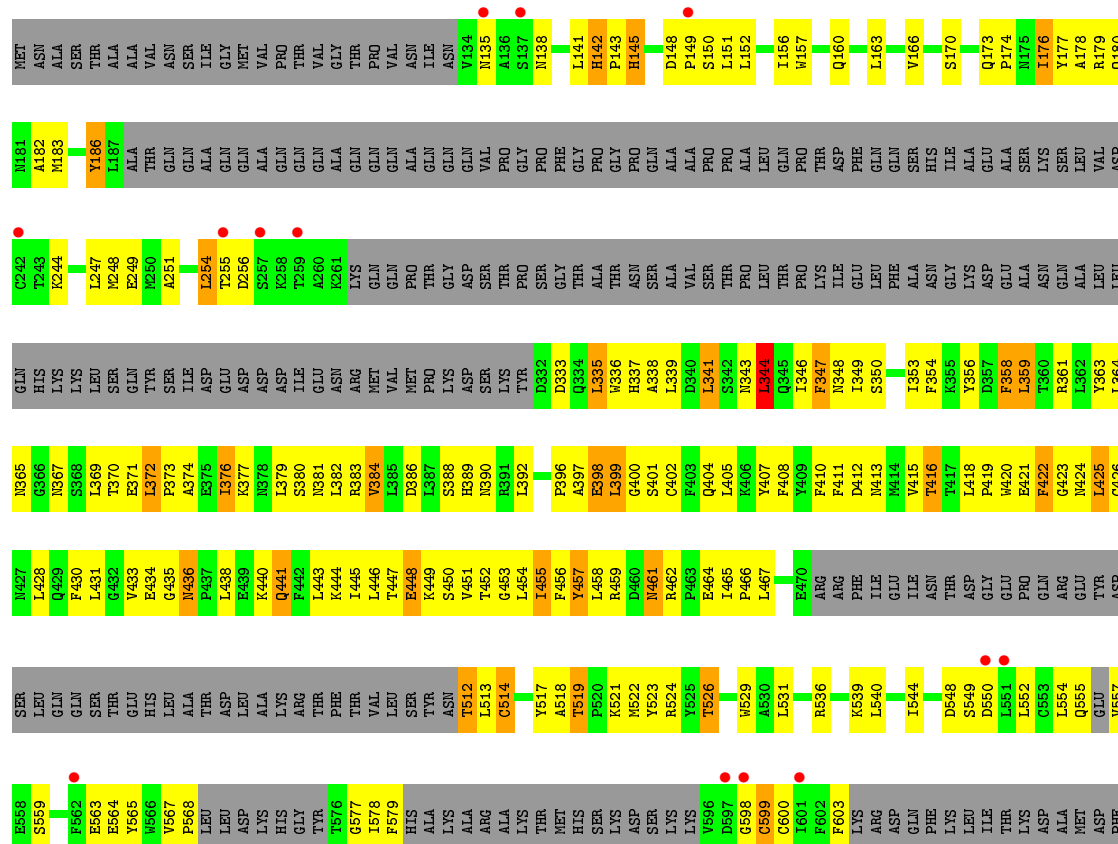


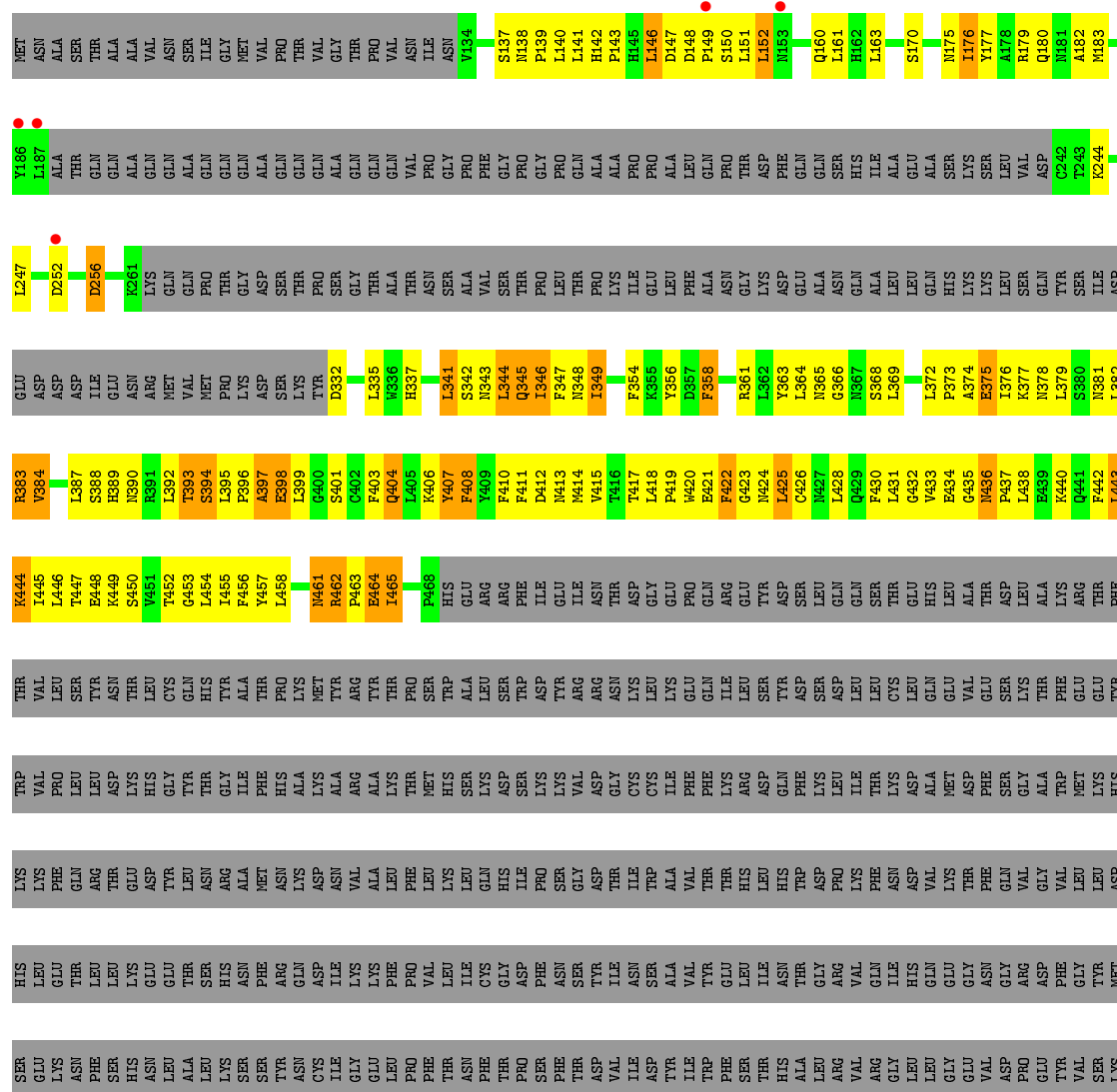


• Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 1



• Molecule 3: GLUCOSE-REPRESSIBLE ALCOHOL DEHYDROGENASE TRANSCRIPTIONAL EFFECTOR





VAL	SER	GLY	LEU	MET	GLU	ARG	F442	S380	ASP	D246	ASN	MET
LYS	PHE	MET	ASP	HIS	GLU	THR	L443	N381	GLU	L247	ALA	THR
ILE	GLU	SER	HIS	LYS	TRP	THR	K444	L382	ASP	D252	THR	GLN
GLY	ILE	GLU	LEU	LYS	VAL	VAL	I446	R383	ASP	D266	ALA	ALA
PHE	ASN	ASN	THR	PHE	PRO	LEU	T447	S384	ILE	K261	GLN	GLN
PRO	PRO	PHE	LEU	ARG	LEU	SER	E448	L387	GLU	L261	ALA	ALA
ASN	ASN	THR	LEU	THR	LEU	THR	K449	S388	ASN	K261	GLN	GLN
SER	SER	GLU	LYS	GLU	LYS	VAL	V451	H389	ARG	LYS	ASN	ASN
ASN	ASN	ASP	LYS	ASP	LYS	THR	T452	L392	MET	GLN	GLN	ILE
LEU	LEU	GLY	GLU	CYS	GLY	CYS	G453	T393	VAL	GLN	ILE	GLY
PRO	PRO	THR	THR	GLN	TRP	GLN	L454	S394	PRO	PRO	GLN	MET
SER	SER	THR	SER	ASN	THR	HIS	L455	L395	LYS	GLY	GLN	VAL
ASP	ASP	ARG	GLY	ARG	THR	THR	F456	P396	ASP	ASP	PRO	PRO
HIS	HIS	ASN	HIS	ALA	ILE	ALA	Y457	A397	SER	SER	GLN	THR
ILE	ILE	PHE	PHE	THR	PHE	THR	L458	E398	LYS	THR	GLN	VAL
PRO	PRO	ARG	ARG	ASN	HIS	PRO		L399	TYR	PRO	ALA	GLY
LEU	LEU	GLN	LYS	LYS	ALA	LYS	M461	G400	D332	SER	GLN	THR
LEU	LEU	ASP	ASP	ASP	LYS	MET	R462	S401	D333	GLY	GLN	PRO
ALA	ALA	ILE	ILE	ASN	ALA	ALA	P463	F403	L334	THR	GLN	VAL
ARG	ARG	LYS	LYS	VAL	ARG	ARG	E464	C402	L335	ALA	VAL	ASN
PHE	PHE	GLU	LYS	ALA	ALA	ALA	I465	Q404	W336	THR	PRO	ILE
GLU	GLU	LEU	PHE	LEU	LYS	THR	I466	L405	H337	ASN	GLY	ASN
PRO	PRO	PRO	PRO	PHE	THR	THR	P467	K406	A338	SER	PRO	GLY
PHE	PHE	VAL	VAL	LEU	MET	SER	L468	Y407	D340	ALA	PHE	GLY
LYS	LYS	THR	ILE	LYS	THR	ALA	HIS	F408	L341	VAL	GLY	GLY
ASN	ASN	GLN	CYS	LEU	LYS	LEU	ARG	Y409	S342	SER	PRO	ASN
ASN	ASN	THR	GLY	HIS	ASP	SER	ARG	F410	N343	THR	GLY	GLY
THR	THR	THR	ASP	ILE	TRP	THR	THR	F411	L344	PRO	PRO	L140
GLY	GLY	PRO	ASP	ILE	SER	THR	PHE	D412	L344	LEU	GLN	L141
SER	SER	PHE	PHE	PRO	LYS	ASP	ILE	N413	Q345	THR	ALA	H142
LYS	LYS	PHE	SER	GLY	LYS	THR	GLU	M414	I346	PRO	ALA	P143
VAL	VAL	ASP	THR	ASP	VAL	ARG	ILE	V415	F347	LYS	PRO	H145
		ASP	THR	ASP	ASP	ARG	ASN	T416	N348	ILE	PRO	L146
VAL	VAL	VAL	ILE	THR	GLY	ASN	THR	T417	I349	GLU	ALA	D147
ILE	ILE	ASN	ASN	ILE	CYS	LYS	ASP	L418		LEU	LEU	D148
ASP	ASP	SER	SER	TRP	CYS	LEU	GLY	K354	F354	PHE	GLN	P149
TYR	TYR	ALA	ALA	ALA	ILE	LYS	GLU	W420	K355	ALA	PRO	S150
TRP	TRP	VAL	VAL	VAL	PHE	GLU	PRO	E421	Y356	ASN	THR	L151
PHE	PHE	THR	THR	THR	PHE	THR	GLN	F422	D357	GLY	ASP	L152
SER	SER	THR	THR	THR	LYS	ILE	ARG	G423	F358	LYS	PHE	L152
THR	THR	LEU	LEU	LEU	GLU	LEU	GLU	N424		ASP	GLN	Q160
HIS	HIS	ASN	ASN	ASN	ASP	SER	TYR	L425	R361	GLU	GLN	L161
ALA	ALA	THR	THR	THR	PHE	THR	ASP	C426	L362	ALA	SER	H162
LEU	LEU	ASP	GLY	ASP	LYS	SER	SER	N427	Y363	ASN	HIS	L163
ARG	ARG	ARG	ARG	PRO	LEU	ASP	LEU	L428	L364	GLN	ILE	L163
VAL	VAL	VAL	VAL	LEU	GLN	LEU	GLN	Q429	N365	ALA	ALA	L163
ARG	ARG	GLN	GLN	LEU	LEU	LEU	GLN	F430	G366	LEU	GLU	L163
GLY	GLY	ARG	GLN	LEU	SER	LEU	GLN	L431	N367	LEU	GLU	L163
GLY	GLY	ILE	ILE	ASN	THR	CYS	THR	G432	S368	GLN	SER	S170
LEU	LEU	HIS	HIS	ASP	LEU	LEU	GLU	V433	L372	HIS	LYS	N176
LEU	LEU	GLN	GLN	VAL	ASP	GLN	HIS	E434	P373	LYS	LYS	L176
GLY	GLY	GLU	GLU	LYS	MET	GLU	LEU	G435	A374	LYS	LEU	Y177
VAL	VAL	ASN	ASN	PHE	THR	GLU	ALA	N436	E375	SER	ASP	A178
ASP	ASP	PHE	PHE	THR	ASP	VAL	THR	P437	L376	LEU	VAL	R179
PRO	PRO	GLY	GLY	GLY	SER	LYS	ASP	L438	K377	GLN	GLN	Q180
GLU	GLU	VAL	VAL	VAL	LEU	THR	LEU	E439	L377	TYR	T243	N181
THR	THR	PHE	PHE	THR	ALA	THR	ALA	K440	N378	SER	K244	M182
		THR	THR	THR	LYS	PHE	LYS	E441	L370	ILE	THR	M182

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	122.65Å 122.91Å 126.42Å 89.47° 89.74° 64.22°	Depositor
Resolution (Å)	47.95 – 3.41 48.23 – 3.28	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.95-3.41) 97.4 (48.23-3.28)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.270 0.229 , 0.266	Depositor DCC
R_{free} test set	4463 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.1	EDS
Estimated twinning fraction	0.026 for -h,-k,l 0.018 for k,h,-l 0.022 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 98830 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	24298	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.56	0/2231	0.67	0/3028
1	C	0.54	0/2235	0.67	0/3032
1	E	0.50	0/2235	0.66	0/3033
1	F	0.52	0/2231	0.66	0/3028
2	B	0.43	0/1908	0.58	0/2588
2	G	0.42	0/1908	0.57	0/2588
2	H	0.43	0/1908	0.58	0/2588
2	I	0.44	0/1908	0.58	0/2588
3	D	0.53	0/2520	0.76	2/3446 (0.1%)
3	J	0.62	1/1640 (0.1%)	0.94	4/2240 (0.2%)
3	K	0.54	1/2535 (0.0%)	0.76	1/3463 (0.0%)
3	L	0.63	2/1640 (0.1%)	0.94	3/2240 (0.1%)
All	All	0.52	4/24899 (0.0%)	0.71	10/33862 (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	A	0	1
1	C	0	1
1	E	0	1
3	D	0	1
3	J	0	1
3	K	0	1
3	L	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	462	ARG	C-N	8.80	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	462	ARG	C-N	8.53	1.50	1.34
3	L	332	ASP	CA-CB	5.73	1.66	1.53
3	K	426	CYS	CB-SG	5.22	1.91	1.82

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	462	ARG	O-C-N	13.09	145.96	121.10
3	J	462	ARG	O-C-N	12.95	145.70	121.10
3	J	462	ARG	CA-C-N	-9.27	91.15	117.10
3	L	462	ARG	CA-C-N	-9.18	91.41	117.10
3	J	397	ALA	N-CA-C	-6.26	94.10	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	THR	Peptide
1	C	194	THR	Peptide
3	D	344	LEU	Peptide
1	E	194	THR	Peptide
3	J	332	ASP	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	2170	0	2083	87	0
1	C	2174	0	2094	94	0
1	E	2174	0	2089	86	1
1	F	2170	0	2083	74	1
2	B	1869	0	1936	49	0
2	G	1869	0	1936	51	1
2	H	1869	0	1936	62	0
2	I	1869	0	1936	50	1
3	D	2456	0	2268	226	0
3	J	1604	0	1505	145	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	2470	0	2293	204	0
3	L	1604	0	1505	157	1
All	All	24298	0	23664	1240	3

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 26.

The worst 5 of 1240 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)
3:D:176:ILE:HD11	3:D:343:ASN:HD22	1.20	1.04
3:J:422:PHE:HD1	3:J:422:PHE:O	1.42	1.00
3:K:176:ILE:HD11	3:K:343:ASN:HD22	1.21	1.00
3:K:567:VAL:HG13	3:K:568:PRO:HD3	1.41	0.99
3:D:424:ASN:HD21	3:D:807:ILE:HG21	1.29	0.98

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:SER:OG	3:L:146:LEU:O[1_554]	2.08	0.12
2:G:835:TYR:OH	2:I:800:ASN:CA[1_465]	2.10	0.10
1:E:166:SER:OG	3:J:146:LEU:O[1_455]	2.14	0.06

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	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	39	79
1	C	263/288 (91%)	250 (95%)	12 (5%)	1 (0%)	39	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	263/288 (91%)	249 (95%)	13 (5%)	1 (0%)	39	79
1	F	263/288 (91%)	250 (95%)	13 (5%)	0	100	100
2	B	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	G	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
2	H	231/249 (93%)	221 (96%)	10 (4%)	0	100	100
2	I	231/249 (93%)	222 (96%)	9 (4%)	0	100	100
3	D	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	46	83
3	J	204/727 (28%)	168 (82%)	34 (17%)	2 (1%)	19	64
3	K	300/727 (41%)	253 (84%)	46 (15%)	1 (0%)	46	83
3	L	204/727 (28%)	171 (84%)	31 (15%)	2 (1%)	19	64
All	All	2984/5056 (59%)	2731 (92%)	244 (8%)	9 (0%)	46	83

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	380	SER
3	K	380	SER
3	J	464	GLU
3	J	465	ILE
3	L	465	ILE

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	241/264 (91%)	216 (90%)	25 (10%)	9	38
1	C	242/264 (92%)	218 (90%)	24 (10%)	10	41
1	E	242/264 (92%)	220 (91%)	22 (9%)	12	45
1	F	241/264 (91%)	218 (90%)	23 (10%)	11	43
2	B	211/231 (91%)	199 (94%)	12 (6%)	25	66
2	G	211/231 (91%)	198 (94%)	13 (6%)	23	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	211/231 (91%)	199 (94%)	12 (6%)	25	66
2	I	211/231 (91%)	198 (94%)	13 (6%)	23	63
3	D	258/648 (40%)	206 (80%)	52 (20%)	1	7
3	J	165/648 (26%)	129 (78%)	36 (22%)	1	6
3	K	261/648 (40%)	208 (80%)	53 (20%)	1	7
3	L	165/648 (26%)	130 (79%)	35 (21%)	1	6
All	All	2659/4572 (58%)	2339 (88%)	320 (12%)	6	30

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	209	HIS
2	H	961	TRP
3	L	345	GLN
1	F	298	ASP
2	G	822	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	424	ASN
3	L	175	ASN
3	K	413	ASN
3	D	343	ASN
3	K	352	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 [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.

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	267/288 (92%)	-0.16	2 (0%) 89 84	36, 58, 98, 121	0
1	C	267/288 (92%)	-0.16	3 (1%) 82 76	36, 58, 99, 121	0
1	E	267/288 (92%)	-0.23	0 100 100	35, 58, 100, 121	0
1	F	267/288 (92%)	-0.19	1 (0%) 93 91	36, 59, 98, 124	0
2	B	233/249 (93%)	0.02	6 (2%) 59 54	48, 79, 115, 146	0
2	G	233/249 (93%)	-0.08	3 (1%) 79 73	49, 81, 112, 146	0
2	H	233/249 (93%)	0.07	4 (1%) 73 67	48, 80, 115, 145	0
2	I	233/249 (93%)	-0.03	5 (2%) 67 62	50, 81, 114, 145	0
3	D	318/727 (43%)	0.14	16 (5%) 32 28	50, 87, 136, 160	0
3	J	210/727 (28%)	-0.28	5 (2%) 62 57	35, 61, 101, 127	0
3	K	318/727 (43%)	0.21	25 (7%) 15 15	50, 87, 136, 160	0
3	L	210/727 (28%)	-0.22	3 (1%) 78 72	35, 62, 102, 131	0
All	All	3056/5056 (60%)	-0.06	73 (2%) 62 57	35, 72, 115, 160	0

The worst 5 of 73 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	597	ASP	5.6
3	K	135	ASN	4.5
2	B	991	THR	4.4
3	L	466	PRO	4.0
2	H	991	THR	3.9

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.