



wwPDB X-ray Structure Validation Summary Report ⓘ

May 1, 2021 – 09:46 PM EDT

PDB ID : 5QU6
Title : Crystal Structure of swapped human Nck SH3.1 domain, 1.8A, triclinic
Authors : Rudolph, M.G.
Deposited on : 2019-12-13
Resolution : 1.82 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

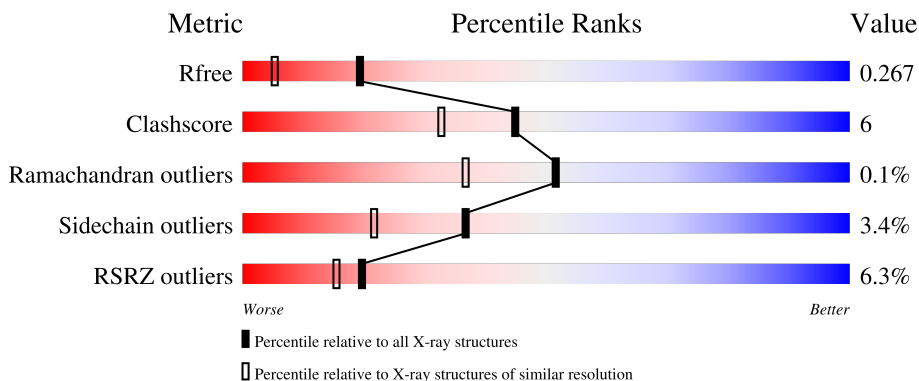
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	1	87	
1	2	87	
1	A	87	
1	B	87	
1	C	87	

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Mol	Chain	Length	Quality of chain
1	D	87	2% 56% 7% 37%
1	E	87	59% 9% 32%
1	F	87	61% 5% 34%
1	G	87	47% 17% 36%
1	H	87	56% 8% 33%
1	I	87	56% 8% 36%
1	J	87	55% 11% 33%
1	K	87	45% 17% 5% 33%
1	L	87	60% 8% 32%
1	M	87	61% 37%
1	N	87	2% 56% 8% 36%
1	O	87	57% 9% 33%
1	P	87	2% 57% 6% 37%
1	Q	87	54% 10% 36%
1	R	87	2% 56% 6% 37%
1	S	87	55% 8% 36%
1	T	87	2% 49% 14% 37%
1	U	87	9% 48% 13% 39%
1	V	87	2% 48% 9% 39%
1	W	87	21% 37% 26% 37%
1	X	87	8% 43% 18% 38%
1	Y	87	16% 36% 21% 43%
1	Z	87	14% 43% 17% 38%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13353 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 Cytoplasmic protein NCK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	55	469	299	82	87	1	0	0	0
1	B	55	469	299	82	87	1	0	0	0
1	C	55	470	300	82	87	1	0	0	0
1	D	55	469	299	82	87	1	0	0	0
1	E	59	497	315	86	94	2	0	0	0
1	F	57	486	309	86	90	1	0	0	0
1	G	56	478	305	84	88	1	0	0	0
1	H	58	492	312	87	92	1	0	0	0
1	I	56	472	301	80	90	1	0	0	0
1	J	58	492	312	87	92	1	0	0	0
1	K	58	494	314	85	93	2	0	1	0
1	L	59	497	315	86	94	2	0	0	0
1	M	55	469	299	82	87	1	0	0	0
1	N	56	472	301	80	90	1	0	0	0
1	O	58	486	309	82	93	2	0	0	0
1	P	55	469	299	82	87	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	56	478	305	84	88	1	0	0	0
1	R	55	469	299	82	87	1	0	0	0
1	S	56	478	305	84	88	1	0	0	0
1	T	55	469	299	82	87	1	0	0	0
1	U	53	456	294	81	80	1	0	0	0
1	V	53	449	288	77	83	1	0	0	0
1	W	55	469	300	83	85	1	0	0	0
1	X	54	458	293	78	86	1	0	0	0
1	Y	50	425	273	75	76	1	0	0	0
1	Z	54	458	293	78	86	1	0	0	0
1	1	54	458	293	78	86	1	0	0	0
1	2	46	392	255	67	69	1	0	0	0

There are 728 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	SER	-	expression tag	UNP P16333
A	-23	GLY	-	expression tag	UNP P16333
A	-22	GLY	-	expression tag	UNP P16333
A	-21	LEU	-	expression tag	UNP P16333
A	-20	ASN	-	expression tag	UNP P16333
A	-19	ASP	-	expression tag	UNP P16333
A	-18	ILE	-	expression tag	UNP P16333
A	-17	PHE	-	expression tag	UNP P16333
A	-16	GLU	-	expression tag	UNP P16333
A	-15	ALA	-	expression tag	UNP P16333
A	-14	GLN	-	expression tag	UNP P16333
A	-13	LYS	-	expression tag	UNP P16333
A	-12	ILE	-	expression tag	UNP P16333
A	-11	GLU	-	expression tag	UNP P16333
A	-10	TRP	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP P16333
A	-8	GLU	-	expression tag	UNP P16333
A	-7	GLY	-	expression tag	UNP P16333
A	-6	SER	-	expression tag	UNP P16333
A	-5	GLU	-	expression tag	UNP P16333
A	-4	ASN	-	expression tag	UNP P16333
A	-3	LEU	-	expression tag	UNP P16333
A	-2	TYR	-	expression tag	UNP P16333
A	-1	PHE	-	expression tag	UNP P16333
A	0	GLN	-	expression tag	UNP P16333
A	1	SER	-	expression tag	UNP P16333
B	-24	SER	-	expression tag	UNP P16333
B	-23	GLY	-	expression tag	UNP P16333
B	-22	GLY	-	expression tag	UNP P16333
B	-21	LEU	-	expression tag	UNP P16333
B	-20	ASN	-	expression tag	UNP P16333
B	-19	ASP	-	expression tag	UNP P16333
B	-18	ILE	-	expression tag	UNP P16333
B	-17	PHE	-	expression tag	UNP P16333
B	-16	GLU	-	expression tag	UNP P16333
B	-15	ALA	-	expression tag	UNP P16333
B	-14	GLN	-	expression tag	UNP P16333
B	-13	LYS	-	expression tag	UNP P16333
B	-12	ILE	-	expression tag	UNP P16333
B	-11	GLU	-	expression tag	UNP P16333
B	-10	TRP	-	expression tag	UNP P16333
B	-9	HIS	-	expression tag	UNP P16333
B	-8	GLU	-	expression tag	UNP P16333
B	-7	GLY	-	expression tag	UNP P16333
B	-6	SER	-	expression tag	UNP P16333
B	-5	GLU	-	expression tag	UNP P16333
B	-4	ASN	-	expression tag	UNP P16333
B	-3	LEU	-	expression tag	UNP P16333
B	-2	TYR	-	expression tag	UNP P16333
B	-1	PHE	-	expression tag	UNP P16333
B	0	GLN	-	expression tag	UNP P16333
B	1	SER	-	expression tag	UNP P16333
C	-24	SER	-	expression tag	UNP P16333
C	-23	GLY	-	expression tag	UNP P16333
C	-22	GLY	-	expression tag	UNP P16333
C	-21	LEU	-	expression tag	UNP P16333
C	-20	ASN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	ASP	-	expression tag	UNP P16333
C	-18	ILE	-	expression tag	UNP P16333
C	-17	PHE	-	expression tag	UNP P16333
C	-16	GLU	-	expression tag	UNP P16333
C	-15	ALA	-	expression tag	UNP P16333
C	-14	GLN	-	expression tag	UNP P16333
C	-13	LYS	-	expression tag	UNP P16333
C	-12	ILE	-	expression tag	UNP P16333
C	-11	GLU	-	expression tag	UNP P16333
C	-10	TRP	-	expression tag	UNP P16333
C	-9	HIS	-	expression tag	UNP P16333
C	-8	GLU	-	expression tag	UNP P16333
C	-7	GLY	-	expression tag	UNP P16333
C	-6	SER	-	expression tag	UNP P16333
C	-5	GLU	-	expression tag	UNP P16333
C	-4	ASN	-	expression tag	UNP P16333
C	-3	LEU	-	expression tag	UNP P16333
C	-2	TYR	-	expression tag	UNP P16333
C	-1	PHE	-	expression tag	UNP P16333
C	0	GLN	-	expression tag	UNP P16333
C	1	SER	-	expression tag	UNP P16333
D	-24	SER	-	expression tag	UNP P16333
D	-23	GLY	-	expression tag	UNP P16333
D	-22	GLY	-	expression tag	UNP P16333
D	-21	LEU	-	expression tag	UNP P16333
D	-20	ASN	-	expression tag	UNP P16333
D	-19	ASP	-	expression tag	UNP P16333
D	-18	ILE	-	expression tag	UNP P16333
D	-17	PHE	-	expression tag	UNP P16333
D	-16	GLU	-	expression tag	UNP P16333
D	-15	ALA	-	expression tag	UNP P16333
D	-14	GLN	-	expression tag	UNP P16333
D	-13	LYS	-	expression tag	UNP P16333
D	-12	ILE	-	expression tag	UNP P16333
D	-11	GLU	-	expression tag	UNP P16333
D	-10	TRP	-	expression tag	UNP P16333
D	-9	HIS	-	expression tag	UNP P16333
D	-8	GLU	-	expression tag	UNP P16333
D	-7	GLY	-	expression tag	UNP P16333
D	-6	SER	-	expression tag	UNP P16333
D	-5	GLU	-	expression tag	UNP P16333
D	-4	ASN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	LEU	-	expression tag	UNP P16333
D	-2	TYR	-	expression tag	UNP P16333
D	-1	PHE	-	expression tag	UNP P16333
D	0	GLN	-	expression tag	UNP P16333
D	1	SER	-	expression tag	UNP P16333
E	-24	SER	-	expression tag	UNP P16333
E	-23	GLY	-	expression tag	UNP P16333
E	-22	GLY	-	expression tag	UNP P16333
E	-21	LEU	-	expression tag	UNP P16333
E	-20	ASN	-	expression tag	UNP P16333
E	-19	ASP	-	expression tag	UNP P16333
E	-18	ILE	-	expression tag	UNP P16333
E	-17	PHE	-	expression tag	UNP P16333
E	-16	GLU	-	expression tag	UNP P16333
E	-15	ALA	-	expression tag	UNP P16333
E	-14	GLN	-	expression tag	UNP P16333
E	-13	LYS	-	expression tag	UNP P16333
E	-12	ILE	-	expression tag	UNP P16333
E	-11	GLU	-	expression tag	UNP P16333
E	-10	TRP	-	expression tag	UNP P16333
E	-9	HIS	-	expression tag	UNP P16333
E	-8	GLU	-	expression tag	UNP P16333
E	-7	GLY	-	expression tag	UNP P16333
E	-6	SER	-	expression tag	UNP P16333
E	-5	GLU	-	expression tag	UNP P16333
E	-4	ASN	-	expression tag	UNP P16333
E	-3	LEU	-	expression tag	UNP P16333
E	-2	TYR	-	expression tag	UNP P16333
E	-1	PHE	-	expression tag	UNP P16333
E	0	GLN	-	expression tag	UNP P16333
E	1	SER	-	expression tag	UNP P16333
F	-24	SER	-	expression tag	UNP P16333
F	-23	GLY	-	expression tag	UNP P16333
F	-22	GLY	-	expression tag	UNP P16333
F	-21	LEU	-	expression tag	UNP P16333
F	-20	ASN	-	expression tag	UNP P16333
F	-19	ASP	-	expression tag	UNP P16333
F	-18	ILE	-	expression tag	UNP P16333
F	-17	PHE	-	expression tag	UNP P16333
F	-16	GLU	-	expression tag	UNP P16333
F	-15	ALA	-	expression tag	UNP P16333
F	-14	GLN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	LYS	-	expression tag	UNP P16333
F	-12	ILE	-	expression tag	UNP P16333
F	-11	GLU	-	expression tag	UNP P16333
F	-10	TRP	-	expression tag	UNP P16333
F	-9	HIS	-	expression tag	UNP P16333
F	-8	GLU	-	expression tag	UNP P16333
F	-7	GLY	-	expression tag	UNP P16333
F	-6	SER	-	expression tag	UNP P16333
F	-5	GLU	-	expression tag	UNP P16333
F	-4	ASN	-	expression tag	UNP P16333
F	-3	LEU	-	expression tag	UNP P16333
F	-2	TYR	-	expression tag	UNP P16333
F	-1	PHE	-	expression tag	UNP P16333
F	0	GLN	-	expression tag	UNP P16333
F	1	SER	-	expression tag	UNP P16333
G	-24	SER	-	expression tag	UNP P16333
G	-23	GLY	-	expression tag	UNP P16333
G	-22	GLY	-	expression tag	UNP P16333
G	-21	LEU	-	expression tag	UNP P16333
G	-20	ASN	-	expression tag	UNP P16333
G	-19	ASP	-	expression tag	UNP P16333
G	-18	ILE	-	expression tag	UNP P16333
G	-17	PHE	-	expression tag	UNP P16333
G	-16	GLU	-	expression tag	UNP P16333
G	-15	ALA	-	expression tag	UNP P16333
G	-14	GLN	-	expression tag	UNP P16333
G	-13	LYS	-	expression tag	UNP P16333
G	-12	ILE	-	expression tag	UNP P16333
G	-11	GLU	-	expression tag	UNP P16333
G	-10	TRP	-	expression tag	UNP P16333
G	-9	HIS	-	expression tag	UNP P16333
G	-8	GLU	-	expression tag	UNP P16333
G	-7	GLY	-	expression tag	UNP P16333
G	-6	SER	-	expression tag	UNP P16333
G	-5	GLU	-	expression tag	UNP P16333
G	-4	ASN	-	expression tag	UNP P16333
G	-3	LEU	-	expression tag	UNP P16333
G	-2	TYR	-	expression tag	UNP P16333
G	-1	PHE	-	expression tag	UNP P16333
G	0	GLN	-	expression tag	UNP P16333
G	1	SER	-	expression tag	UNP P16333
H	-24	SER	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-23	GLY	-	expression tag	UNP P16333
H	-22	GLY	-	expression tag	UNP P16333
H	-21	LEU	-	expression tag	UNP P16333
H	-20	ASN	-	expression tag	UNP P16333
H	-19	ASP	-	expression tag	UNP P16333
H	-18	ILE	-	expression tag	UNP P16333
H	-17	PHE	-	expression tag	UNP P16333
H	-16	GLU	-	expression tag	UNP P16333
H	-15	ALA	-	expression tag	UNP P16333
H	-14	GLN	-	expression tag	UNP P16333
H	-13	LYS	-	expression tag	UNP P16333
H	-12	ILE	-	expression tag	UNP P16333
H	-11	GLU	-	expression tag	UNP P16333
H	-10	TRP	-	expression tag	UNP P16333
H	-9	HIS	-	expression tag	UNP P16333
H	-8	GLU	-	expression tag	UNP P16333
H	-7	GLY	-	expression tag	UNP P16333
H	-6	SER	-	expression tag	UNP P16333
H	-5	GLU	-	expression tag	UNP P16333
H	-4	ASN	-	expression tag	UNP P16333
H	-3	LEU	-	expression tag	UNP P16333
H	-2	TYR	-	expression tag	UNP P16333
H	-1	PHE	-	expression tag	UNP P16333
H	0	GLN	-	expression tag	UNP P16333
H	1	SER	-	expression tag	UNP P16333
I	-24	SER	-	expression tag	UNP P16333
I	-23	GLY	-	expression tag	UNP P16333
I	-22	GLY	-	expression tag	UNP P16333
I	-21	LEU	-	expression tag	UNP P16333
I	-20	ASN	-	expression tag	UNP P16333
I	-19	ASP	-	expression tag	UNP P16333
I	-18	ILE	-	expression tag	UNP P16333
I	-17	PHE	-	expression tag	UNP P16333
I	-16	GLU	-	expression tag	UNP P16333
I	-15	ALA	-	expression tag	UNP P16333
I	-14	GLN	-	expression tag	UNP P16333
I	-13	LYS	-	expression tag	UNP P16333
I	-12	ILE	-	expression tag	UNP P16333
I	-11	GLU	-	expression tag	UNP P16333
I	-10	TRP	-	expression tag	UNP P16333
I	-9	HIS	-	expression tag	UNP P16333
I	-8	GLU	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-7	GLY	-	expression tag	UNP P16333
I	-6	SER	-	expression tag	UNP P16333
I	-5	GLU	-	expression tag	UNP P16333
I	-4	ASN	-	expression tag	UNP P16333
I	-3	LEU	-	expression tag	UNP P16333
I	-2	TYR	-	expression tag	UNP P16333
I	-1	PHE	-	expression tag	UNP P16333
I	0	GLN	-	expression tag	UNP P16333
I	1	SER	-	expression tag	UNP P16333
J	-24	SER	-	expression tag	UNP P16333
J	-23	GLY	-	expression tag	UNP P16333
J	-22	GLY	-	expression tag	UNP P16333
J	-21	LEU	-	expression tag	UNP P16333
J	-20	ASN	-	expression tag	UNP P16333
J	-19	ASP	-	expression tag	UNP P16333
J	-18	ILE	-	expression tag	UNP P16333
J	-17	PHE	-	expression tag	UNP P16333
J	-16	GLU	-	expression tag	UNP P16333
J	-15	ALA	-	expression tag	UNP P16333
J	-14	GLN	-	expression tag	UNP P16333
J	-13	LYS	-	expression tag	UNP P16333
J	-12	ILE	-	expression tag	UNP P16333
J	-11	GLU	-	expression tag	UNP P16333
J	-10	TRP	-	expression tag	UNP P16333
J	-9	HIS	-	expression tag	UNP P16333
J	-8	GLU	-	expression tag	UNP P16333
J	-7	GLY	-	expression tag	UNP P16333
J	-6	SER	-	expression tag	UNP P16333
J	-5	GLU	-	expression tag	UNP P16333
J	-4	ASN	-	expression tag	UNP P16333
J	-3	LEU	-	expression tag	UNP P16333
J	-2	TYR	-	expression tag	UNP P16333
J	-1	PHE	-	expression tag	UNP P16333
J	0	GLN	-	expression tag	UNP P16333
J	1	SER	-	expression tag	UNP P16333
K	-24	SER	-	expression tag	UNP P16333
K	-23	GLY	-	expression tag	UNP P16333
K	-22	GLY	-	expression tag	UNP P16333
K	-21	LEU	-	expression tag	UNP P16333
K	-20	ASN	-	expression tag	UNP P16333
K	-19	ASP	-	expression tag	UNP P16333
K	-18	ILE	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-17	PHE	-	expression tag	UNP P16333
K	-16	GLU	-	expression tag	UNP P16333
K	-15	ALA	-	expression tag	UNP P16333
K	-14	GLN	-	expression tag	UNP P16333
K	-13	LYS	-	expression tag	UNP P16333
K	-12	ILE	-	expression tag	UNP P16333
K	-11	GLU	-	expression tag	UNP P16333
K	-10	TRP	-	expression tag	UNP P16333
K	-9	HIS	-	expression tag	UNP P16333
K	-8	GLU	-	expression tag	UNP P16333
K	-7	GLY	-	expression tag	UNP P16333
K	-6	SER	-	expression tag	UNP P16333
K	-5	GLU	-	expression tag	UNP P16333
K	-4	ASN	-	expression tag	UNP P16333
K	-3	LEU	-	expression tag	UNP P16333
K	-2	TYR	-	expression tag	UNP P16333
K	-1	PHE	-	expression tag	UNP P16333
K	0	GLN	-	expression tag	UNP P16333
K	1	SER	-	expression tag	UNP P16333
L	-24	SER	-	expression tag	UNP P16333
L	-23	GLY	-	expression tag	UNP P16333
L	-22	GLY	-	expression tag	UNP P16333
L	-21	LEU	-	expression tag	UNP P16333
L	-20	ASN	-	expression tag	UNP P16333
L	-19	ASP	-	expression tag	UNP P16333
L	-18	ILE	-	expression tag	UNP P16333
L	-17	PHE	-	expression tag	UNP P16333
L	-16	GLU	-	expression tag	UNP P16333
L	-15	ALA	-	expression tag	UNP P16333
L	-14	GLN	-	expression tag	UNP P16333
L	-13	LYS	-	expression tag	UNP P16333
L	-12	ILE	-	expression tag	UNP P16333
L	-11	GLU	-	expression tag	UNP P16333
L	-10	TRP	-	expression tag	UNP P16333
L	-9	HIS	-	expression tag	UNP P16333
L	-8	GLU	-	expression tag	UNP P16333
L	-7	GLY	-	expression tag	UNP P16333
L	-6	SER	-	expression tag	UNP P16333
L	-5	GLU	-	expression tag	UNP P16333
L	-4	ASN	-	expression tag	UNP P16333
L	-3	LEU	-	expression tag	UNP P16333
L	-2	TYR	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	PHE	-	expression tag	UNP P16333
L	0	GLN	-	expression tag	UNP P16333
L	1	SER	-	expression tag	UNP P16333
M	-24	SER	-	expression tag	UNP P16333
M	-23	GLY	-	expression tag	UNP P16333
M	-22	GLY	-	expression tag	UNP P16333
M	-21	LEU	-	expression tag	UNP P16333
M	-20	ASN	-	expression tag	UNP P16333
M	-19	ASP	-	expression tag	UNP P16333
M	-18	ILE	-	expression tag	UNP P16333
M	-17	PHE	-	expression tag	UNP P16333
M	-16	GLU	-	expression tag	UNP P16333
M	-15	ALA	-	expression tag	UNP P16333
M	-14	GLN	-	expression tag	UNP P16333
M	-13	LYS	-	expression tag	UNP P16333
M	-12	ILE	-	expression tag	UNP P16333
M	-11	GLU	-	expression tag	UNP P16333
M	-10	TRP	-	expression tag	UNP P16333
M	-9	HIS	-	expression tag	UNP P16333
M	-8	GLU	-	expression tag	UNP P16333
M	-7	GLY	-	expression tag	UNP P16333
M	-6	SER	-	expression tag	UNP P16333
M	-5	GLU	-	expression tag	UNP P16333
M	-4	ASN	-	expression tag	UNP P16333
M	-3	LEU	-	expression tag	UNP P16333
M	-2	TYR	-	expression tag	UNP P16333
M	-1	PHE	-	expression tag	UNP P16333
M	0	GLN	-	expression tag	UNP P16333
M	1	SER	-	expression tag	UNP P16333
N	-24	SER	-	expression tag	UNP P16333
N	-23	GLY	-	expression tag	UNP P16333
N	-22	GLY	-	expression tag	UNP P16333
N	-21	LEU	-	expression tag	UNP P16333
N	-20	ASN	-	expression tag	UNP P16333
N	-19	ASP	-	expression tag	UNP P16333
N	-18	ILE	-	expression tag	UNP P16333
N	-17	PHE	-	expression tag	UNP P16333
N	-16	GLU	-	expression tag	UNP P16333
N	-15	ALA	-	expression tag	UNP P16333
N	-14	GLN	-	expression tag	UNP P16333
N	-13	LYS	-	expression tag	UNP P16333
N	-12	ILE	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-11	GLU	-	expression tag	UNP P16333
N	-10	TRP	-	expression tag	UNP P16333
N	-9	HIS	-	expression tag	UNP P16333
N	-8	GLU	-	expression tag	UNP P16333
N	-7	GLY	-	expression tag	UNP P16333
N	-6	SER	-	expression tag	UNP P16333
N	-5	GLU	-	expression tag	UNP P16333
N	-4	ASN	-	expression tag	UNP P16333
N	-3	LEU	-	expression tag	UNP P16333
N	-2	TYR	-	expression tag	UNP P16333
N	-1	PHE	-	expression tag	UNP P16333
N	0	GLN	-	expression tag	UNP P16333
N	1	SER	-	expression tag	UNP P16333
O	-24	SER	-	expression tag	UNP P16333
O	-23	GLY	-	expression tag	UNP P16333
O	-22	GLY	-	expression tag	UNP P16333
O	-21	LEU	-	expression tag	UNP P16333
O	-20	ASN	-	expression tag	UNP P16333
O	-19	ASP	-	expression tag	UNP P16333
O	-18	ILE	-	expression tag	UNP P16333
O	-17	PHE	-	expression tag	UNP P16333
O	-16	GLU	-	expression tag	UNP P16333
O	-15	ALA	-	expression tag	UNP P16333
O	-14	GLN	-	expression tag	UNP P16333
O	-13	LYS	-	expression tag	UNP P16333
O	-12	ILE	-	expression tag	UNP P16333
O	-11	GLU	-	expression tag	UNP P16333
O	-10	TRP	-	expression tag	UNP P16333
O	-9	HIS	-	expression tag	UNP P16333
O	-8	GLU	-	expression tag	UNP P16333
O	-7	GLY	-	expression tag	UNP P16333
O	-6	SER	-	expression tag	UNP P16333
O	-5	GLU	-	expression tag	UNP P16333
O	-4	ASN	-	expression tag	UNP P16333
O	-3	LEU	-	expression tag	UNP P16333
O	-2	TYR	-	expression tag	UNP P16333
O	-1	PHE	-	expression tag	UNP P16333
O	0	GLN	-	expression tag	UNP P16333
O	1	SER	-	expression tag	UNP P16333
P	-24	SER	-	expression tag	UNP P16333
P	-23	GLY	-	expression tag	UNP P16333
P	-22	GLY	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-21	LEU	-	expression tag	UNP P16333
P	-20	ASN	-	expression tag	UNP P16333
P	-19	ASP	-	expression tag	UNP P16333
P	-18	ILE	-	expression tag	UNP P16333
P	-17	PHE	-	expression tag	UNP P16333
P	-16	GLU	-	expression tag	UNP P16333
P	-15	ALA	-	expression tag	UNP P16333
P	-14	GLN	-	expression tag	UNP P16333
P	-13	LYS	-	expression tag	UNP P16333
P	-12	ILE	-	expression tag	UNP P16333
P	-11	GLU	-	expression tag	UNP P16333
P	-10	TRP	-	expression tag	UNP P16333
P	-9	HIS	-	expression tag	UNP P16333
P	-8	GLU	-	expression tag	UNP P16333
P	-7	GLY	-	expression tag	UNP P16333
P	-6	SER	-	expression tag	UNP P16333
P	-5	GLU	-	expression tag	UNP P16333
P	-4	ASN	-	expression tag	UNP P16333
P	-3	LEU	-	expression tag	UNP P16333
P	-2	TYR	-	expression tag	UNP P16333
P	-1	PHE	-	expression tag	UNP P16333
P	0	GLN	-	expression tag	UNP P16333
P	1	SER	-	expression tag	UNP P16333
Q	-24	SER	-	expression tag	UNP P16333
Q	-23	GLY	-	expression tag	UNP P16333
Q	-22	GLY	-	expression tag	UNP P16333
Q	-21	LEU	-	expression tag	UNP P16333
Q	-20	ASN	-	expression tag	UNP P16333
Q	-19	ASP	-	expression tag	UNP P16333
Q	-18	ILE	-	expression tag	UNP P16333
Q	-17	PHE	-	expression tag	UNP P16333
Q	-16	GLU	-	expression tag	UNP P16333
Q	-15	ALA	-	expression tag	UNP P16333
Q	-14	GLN	-	expression tag	UNP P16333
Q	-13	LYS	-	expression tag	UNP P16333
Q	-12	ILE	-	expression tag	UNP P16333
Q	-11	GLU	-	expression tag	UNP P16333
Q	-10	TRP	-	expression tag	UNP P16333
Q	-9	HIS	-	expression tag	UNP P16333
Q	-8	GLU	-	expression tag	UNP P16333
Q	-7	GLY	-	expression tag	UNP P16333
Q	-6	SER	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-5	GLU	-	expression tag	UNP P16333
Q	-4	ASN	-	expression tag	UNP P16333
Q	-3	LEU	-	expression tag	UNP P16333
Q	-2	TYR	-	expression tag	UNP P16333
Q	-1	PHE	-	expression tag	UNP P16333
Q	0	GLN	-	expression tag	UNP P16333
Q	1	SER	-	expression tag	UNP P16333
R	-24	SER	-	expression tag	UNP P16333
R	-23	GLY	-	expression tag	UNP P16333
R	-22	GLY	-	expression tag	UNP P16333
R	-21	LEU	-	expression tag	UNP P16333
R	-20	ASN	-	expression tag	UNP P16333
R	-19	ASP	-	expression tag	UNP P16333
R	-18	ILE	-	expression tag	UNP P16333
R	-17	PHE	-	expression tag	UNP P16333
R	-16	GLU	-	expression tag	UNP P16333
R	-15	ALA	-	expression tag	UNP P16333
R	-14	GLN	-	expression tag	UNP P16333
R	-13	LYS	-	expression tag	UNP P16333
R	-12	ILE	-	expression tag	UNP P16333
R	-11	GLU	-	expression tag	UNP P16333
R	-10	TRP	-	expression tag	UNP P16333
R	-9	HIS	-	expression tag	UNP P16333
R	-8	GLU	-	expression tag	UNP P16333
R	-7	GLY	-	expression tag	UNP P16333
R	-6	SER	-	expression tag	UNP P16333
R	-5	GLU	-	expression tag	UNP P16333
R	-4	ASN	-	expression tag	UNP P16333
R	-3	LEU	-	expression tag	UNP P16333
R	-2	TYR	-	expression tag	UNP P16333
R	-1	PHE	-	expression tag	UNP P16333
R	0	GLN	-	expression tag	UNP P16333
R	1	SER	-	expression tag	UNP P16333
S	-24	SER	-	expression tag	UNP P16333
S	-23	GLY	-	expression tag	UNP P16333
S	-22	GLY	-	expression tag	UNP P16333
S	-21	LEU	-	expression tag	UNP P16333
S	-20	ASN	-	expression tag	UNP P16333
S	-19	ASP	-	expression tag	UNP P16333
S	-18	ILE	-	expression tag	UNP P16333
S	-17	PHE	-	expression tag	UNP P16333
S	-16	GLU	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-15	ALA	-	expression tag	UNP P16333
S	-14	GLN	-	expression tag	UNP P16333
S	-13	LYS	-	expression tag	UNP P16333
S	-12	ILE	-	expression tag	UNP P16333
S	-11	GLU	-	expression tag	UNP P16333
S	-10	TRP	-	expression tag	UNP P16333
S	-9	HIS	-	expression tag	UNP P16333
S	-8	GLU	-	expression tag	UNP P16333
S	-7	GLY	-	expression tag	UNP P16333
S	-6	SER	-	expression tag	UNP P16333
S	-5	GLU	-	expression tag	UNP P16333
S	-4	ASN	-	expression tag	UNP P16333
S	-3	LEU	-	expression tag	UNP P16333
S	-2	TYR	-	expression tag	UNP P16333
S	-1	PHE	-	expression tag	UNP P16333
S	0	GLN	-	expression tag	UNP P16333
S	1	SER	-	expression tag	UNP P16333
T	-24	SER	-	expression tag	UNP P16333
T	-23	GLY	-	expression tag	UNP P16333
T	-22	GLY	-	expression tag	UNP P16333
T	-21	LEU	-	expression tag	UNP P16333
T	-20	ASN	-	expression tag	UNP P16333
T	-19	ASP	-	expression tag	UNP P16333
T	-18	ILE	-	expression tag	UNP P16333
T	-17	PHE	-	expression tag	UNP P16333
T	-16	GLU	-	expression tag	UNP P16333
T	-15	ALA	-	expression tag	UNP P16333
T	-14	GLN	-	expression tag	UNP P16333
T	-13	LYS	-	expression tag	UNP P16333
T	-12	ILE	-	expression tag	UNP P16333
T	-11	GLU	-	expression tag	UNP P16333
T	-10	TRP	-	expression tag	UNP P16333
T	-9	HIS	-	expression tag	UNP P16333
T	-8	GLU	-	expression tag	UNP P16333
T	-7	GLY	-	expression tag	UNP P16333
T	-6	SER	-	expression tag	UNP P16333
T	-5	GLU	-	expression tag	UNP P16333
T	-4	ASN	-	expression tag	UNP P16333
T	-3	LEU	-	expression tag	UNP P16333
T	-2	TYR	-	expression tag	UNP P16333
T	-1	PHE	-	expression tag	UNP P16333
T	0	GLN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
T	1	SER	-	expression tag	UNP P16333
U	-24	SER	-	expression tag	UNP P16333
U	-23	GLY	-	expression tag	UNP P16333
U	-22	GLY	-	expression tag	UNP P16333
U	-21	LEU	-	expression tag	UNP P16333
U	-20	ASN	-	expression tag	UNP P16333
U	-19	ASP	-	expression tag	UNP P16333
U	-18	ILE	-	expression tag	UNP P16333
U	-17	PHE	-	expression tag	UNP P16333
U	-16	GLU	-	expression tag	UNP P16333
U	-15	ALA	-	expression tag	UNP P16333
U	-14	GLN	-	expression tag	UNP P16333
U	-13	LYS	-	expression tag	UNP P16333
U	-12	ILE	-	expression tag	UNP P16333
U	-11	GLU	-	expression tag	UNP P16333
U	-10	TRP	-	expression tag	UNP P16333
U	-9	HIS	-	expression tag	UNP P16333
U	-8	GLU	-	expression tag	UNP P16333
U	-7	GLY	-	expression tag	UNP P16333
U	-6	SER	-	expression tag	UNP P16333
U	-5	GLU	-	expression tag	UNP P16333
U	-4	ASN	-	expression tag	UNP P16333
U	-3	LEU	-	expression tag	UNP P16333
U	-2	TYR	-	expression tag	UNP P16333
U	-1	PHE	-	expression tag	UNP P16333
U	0	GLN	-	expression tag	UNP P16333
U	1	SER	-	expression tag	UNP P16333
V	-24	SER	-	expression tag	UNP P16333
V	-23	GLY	-	expression tag	UNP P16333
V	-22	GLY	-	expression tag	UNP P16333
V	-21	LEU	-	expression tag	UNP P16333
V	-20	ASN	-	expression tag	UNP P16333
V	-19	ASP	-	expression tag	UNP P16333
V	-18	ILE	-	expression tag	UNP P16333
V	-17	PHE	-	expression tag	UNP P16333
V	-16	GLU	-	expression tag	UNP P16333
V	-15	ALA	-	expression tag	UNP P16333
V	-14	GLN	-	expression tag	UNP P16333
V	-13	LYS	-	expression tag	UNP P16333
V	-12	ILE	-	expression tag	UNP P16333
V	-11	GLU	-	expression tag	UNP P16333
V	-10	TRP	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-9	HIS	-	expression tag	UNP P16333
V	-8	GLU	-	expression tag	UNP P16333
V	-7	GLY	-	expression tag	UNP P16333
V	-6	SER	-	expression tag	UNP P16333
V	-5	GLU	-	expression tag	UNP P16333
V	-4	ASN	-	expression tag	UNP P16333
V	-3	LEU	-	expression tag	UNP P16333
V	-2	TYR	-	expression tag	UNP P16333
V	-1	PHE	-	expression tag	UNP P16333
V	0	GLN	-	expression tag	UNP P16333
V	1	SER	-	expression tag	UNP P16333
W	-24	SER	-	expression tag	UNP P16333
W	-23	GLY	-	expression tag	UNP P16333
W	-22	GLY	-	expression tag	UNP P16333
W	-21	LEU	-	expression tag	UNP P16333
W	-20	ASN	-	expression tag	UNP P16333
W	-19	ASP	-	expression tag	UNP P16333
W	-18	ILE	-	expression tag	UNP P16333
W	-17	PHE	-	expression tag	UNP P16333
W	-16	GLU	-	expression tag	UNP P16333
W	-15	ALA	-	expression tag	UNP P16333
W	-14	GLN	-	expression tag	UNP P16333
W	-13	LYS	-	expression tag	UNP P16333
W	-12	ILE	-	expression tag	UNP P16333
W	-11	GLU	-	expression tag	UNP P16333
W	-10	TRP	-	expression tag	UNP P16333
W	-9	HIS	-	expression tag	UNP P16333
W	-8	GLU	-	expression tag	UNP P16333
W	-7	GLY	-	expression tag	UNP P16333
W	-6	SER	-	expression tag	UNP P16333
W	-5	GLU	-	expression tag	UNP P16333
W	-4	ASN	-	expression tag	UNP P16333
W	-3	LEU	-	expression tag	UNP P16333
W	-2	TYR	-	expression tag	UNP P16333
W	-1	PHE	-	expression tag	UNP P16333
W	0	GLN	-	expression tag	UNP P16333
W	1	SER	-	expression tag	UNP P16333
X	-24	SER	-	expression tag	UNP P16333
X	-23	GLY	-	expression tag	UNP P16333
X	-22	GLY	-	expression tag	UNP P16333
X	-21	LEU	-	expression tag	UNP P16333
X	-20	ASN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-19	ASP	-	expression tag	UNP P16333
X	-18	ILE	-	expression tag	UNP P16333
X	-17	PHE	-	expression tag	UNP P16333
X	-16	GLU	-	expression tag	UNP P16333
X	-15	ALA	-	expression tag	UNP P16333
X	-14	GLN	-	expression tag	UNP P16333
X	-13	LYS	-	expression tag	UNP P16333
X	-12	ILE	-	expression tag	UNP P16333
X	-11	GLU	-	expression tag	UNP P16333
X	-10	TRP	-	expression tag	UNP P16333
X	-9	HIS	-	expression tag	UNP P16333
X	-8	GLU	-	expression tag	UNP P16333
X	-7	GLY	-	expression tag	UNP P16333
X	-6	SER	-	expression tag	UNP P16333
X	-5	GLU	-	expression tag	UNP P16333
X	-4	ASN	-	expression tag	UNP P16333
X	-3	LEU	-	expression tag	UNP P16333
X	-2	TYR	-	expression tag	UNP P16333
X	-1	PHE	-	expression tag	UNP P16333
X	0	GLN	-	expression tag	UNP P16333
X	1	SER	-	expression tag	UNP P16333
Y	-24	SER	-	expression tag	UNP P16333
Y	-23	GLY	-	expression tag	UNP P16333
Y	-22	GLY	-	expression tag	UNP P16333
Y	-21	LEU	-	expression tag	UNP P16333
Y	-20	ASN	-	expression tag	UNP P16333
Y	-19	ASP	-	expression tag	UNP P16333
Y	-18	ILE	-	expression tag	UNP P16333
Y	-17	PHE	-	expression tag	UNP P16333
Y	-16	GLU	-	expression tag	UNP P16333
Y	-15	ALA	-	expression tag	UNP P16333
Y	-14	GLN	-	expression tag	UNP P16333
Y	-13	LYS	-	expression tag	UNP P16333
Y	-12	ILE	-	expression tag	UNP P16333
Y	-11	GLU	-	expression tag	UNP P16333
Y	-10	TRP	-	expression tag	UNP P16333
Y	-9	HIS	-	expression tag	UNP P16333
Y	-8	GLU	-	expression tag	UNP P16333
Y	-7	GLY	-	expression tag	UNP P16333
Y	-6	SER	-	expression tag	UNP P16333
Y	-5	GLU	-	expression tag	UNP P16333
Y	-4	ASN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	LEU	-	expression tag	UNP P16333
Y	-2	TYR	-	expression tag	UNP P16333
Y	-1	PHE	-	expression tag	UNP P16333
Y	0	GLN	-	expression tag	UNP P16333
Y	1	SER	-	expression tag	UNP P16333
Z	-24	SER	-	expression tag	UNP P16333
Z	-23	GLY	-	expression tag	UNP P16333
Z	-22	GLY	-	expression tag	UNP P16333
Z	-21	LEU	-	expression tag	UNP P16333
Z	-20	ASN	-	expression tag	UNP P16333
Z	-19	ASP	-	expression tag	UNP P16333
Z	-18	ILE	-	expression tag	UNP P16333
Z	-17	PHE	-	expression tag	UNP P16333
Z	-16	GLU	-	expression tag	UNP P16333
Z	-15	ALA	-	expression tag	UNP P16333
Z	-14	GLN	-	expression tag	UNP P16333
Z	-13	LYS	-	expression tag	UNP P16333
Z	-12	ILE	-	expression tag	UNP P16333
Z	-11	GLU	-	expression tag	UNP P16333
Z	-10	TRP	-	expression tag	UNP P16333
Z	-9	HIS	-	expression tag	UNP P16333
Z	-8	GLU	-	expression tag	UNP P16333
Z	-7	GLY	-	expression tag	UNP P16333
Z	-6	SER	-	expression tag	UNP P16333
Z	-5	GLU	-	expression tag	UNP P16333
Z	-4	ASN	-	expression tag	UNP P16333
Z	-3	LEU	-	expression tag	UNP P16333
Z	-2	TYR	-	expression tag	UNP P16333
Z	-1	PHE	-	expression tag	UNP P16333
Z	0	GLN	-	expression tag	UNP P16333
Z	1	SER	-	expression tag	UNP P16333
1	-24	SER	-	expression tag	UNP P16333
1	-23	GLY	-	expression tag	UNP P16333
1	-22	GLY	-	expression tag	UNP P16333
1	-21	LEU	-	expression tag	UNP P16333
1	-20	ASN	-	expression tag	UNP P16333
1	-19	ASP	-	expression tag	UNP P16333
1	-18	ILE	-	expression tag	UNP P16333
1	-17	PHE	-	expression tag	UNP P16333
1	-16	GLU	-	expression tag	UNP P16333
1	-15	ALA	-	expression tag	UNP P16333
1	-14	GLN	-	expression tag	UNP P16333

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-13	LYS	-	expression tag	UNP P16333
1	-12	ILE	-	expression tag	UNP P16333
1	-11	GLU	-	expression tag	UNP P16333
1	-10	TRP	-	expression tag	UNP P16333
1	-9	HIS	-	expression tag	UNP P16333
1	-8	GLU	-	expression tag	UNP P16333
1	-7	GLY	-	expression tag	UNP P16333
1	-6	SER	-	expression tag	UNP P16333
1	-5	GLU	-	expression tag	UNP P16333
1	-4	ASN	-	expression tag	UNP P16333
1	-3	LEU	-	expression tag	UNP P16333
1	-2	TYR	-	expression tag	UNP P16333
1	-1	PHE	-	expression tag	UNP P16333
1	0	GLN	-	expression tag	UNP P16333
1	1	SER	-	expression tag	UNP P16333
2	-24	SER	-	expression tag	UNP P16333
2	-23	GLY	-	expression tag	UNP P16333
2	-22	GLY	-	expression tag	UNP P16333
2	-21	LEU	-	expression tag	UNP P16333
2	-20	ASN	-	expression tag	UNP P16333
2	-19	ASP	-	expression tag	UNP P16333
2	-18	ILE	-	expression tag	UNP P16333
2	-17	PHE	-	expression tag	UNP P16333
2	-16	GLU	-	expression tag	UNP P16333
2	-15	ALA	-	expression tag	UNP P16333
2	-14	GLN	-	expression tag	UNP P16333
2	-13	LYS	-	expression tag	UNP P16333
2	-12	ILE	-	expression tag	UNP P16333
2	-11	GLU	-	expression tag	UNP P16333
2	-10	TRP	-	expression tag	UNP P16333
2	-9	HIS	-	expression tag	UNP P16333
2	-8	GLU	-	expression tag	UNP P16333
2	-7	GLY	-	expression tag	UNP P16333
2	-6	SER	-	expression tag	UNP P16333
2	-5	GLU	-	expression tag	UNP P16333
2	-4	ASN	-	expression tag	UNP P16333
2	-3	LEU	-	expression tag	UNP P16333
2	-2	TYR	-	expression tag	UNP P16333
2	-1	PHE	-	expression tag	UNP P16333
2	0	GLN	-	expression tag	UNP P16333
2	1	SER	-	expression tag	UNP P16333

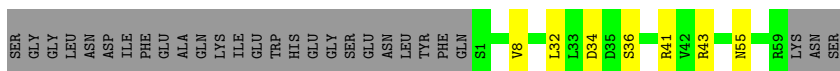
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	20	Total O 20 20	0	0
2	C	8	Total O 8 8	0	0
2	D	11	Total O 11 11	0	0
2	E	22	Total O 22 22	0	0
2	F	8	Total O 8 8	0	0
2	G	18	Total O 18 18	0	0
2	H	12	Total O 12 12	0	0
2	I	14	Total O 14 14	0	0
2	J	6	Total O 6 6	0	0
2	K	16	Total O 16 16	0	0
2	L	9	Total O 9 9	0	0
2	M	6	Total O 6 6	0	0
2	N	5	Total O 5 5	0	0
2	O	4	Total O 4 4	0	0
2	P	7	Total O 7 7	0	0
2	Q	8	Total O 8 8	0	0
2	R	6	Total O 6 6	0	0
2	S	6	Total O 6 6	0	0
2	T	4	Total O 4 4	0	0
2	U	3	Total O 3 3	0	0
2	V	3	Total O 3 3	0	0

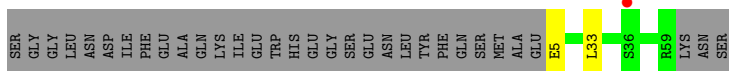
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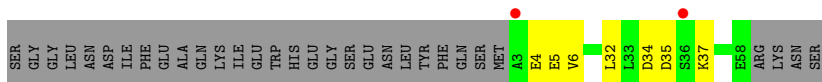
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	W	3	Total O 3 3	0	0
2	X	2	Total O 2 2	0	0



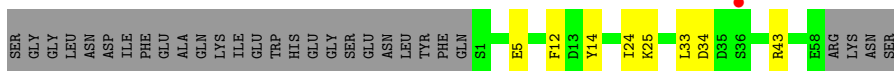
- Molecule 1: Cytoplasmic protein NCK1



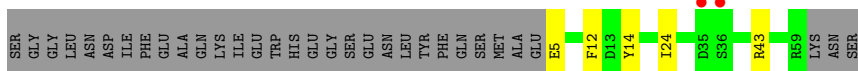
- Molecule 1: Cytoplasmic protein NCK1



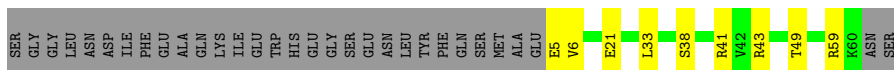
- Molecule 1: Cytoplasmic protein NCK1



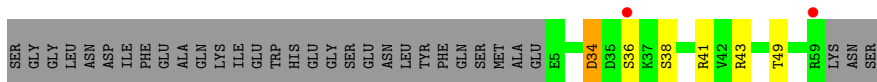
- Molecule 1: Cytoplasmic protein NCK1



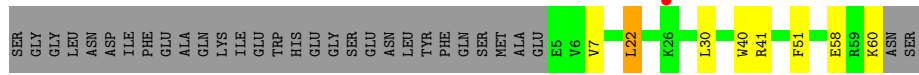
- Molecule 1: Cytoplasmic protein NCK1



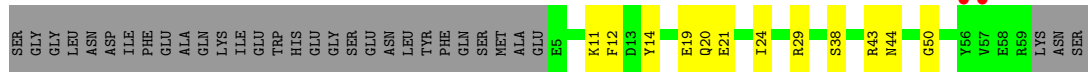
- Molecule 1: Cytoplasmic protein NCK1



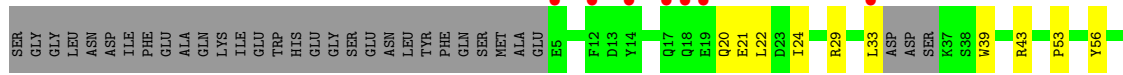
- Molecule 1: Cytoplasmic protein NCK1



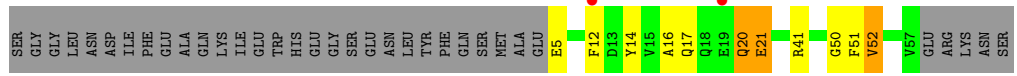
● Molecule 1: Cytoplasmic protein NCK1



● Molecule 1: Cytoplasmic protein NCK1



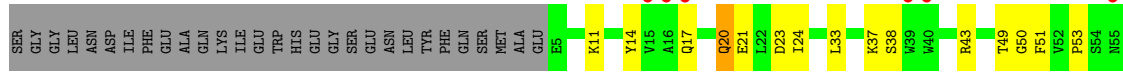
● Molecule 1: Cytoplasmic protein NCK1



● Molecule 1: Cytoplasmic protein NCK1

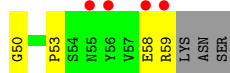
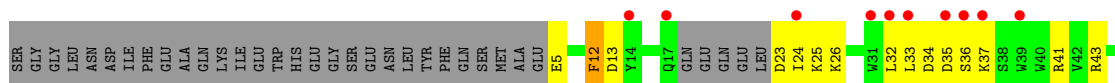
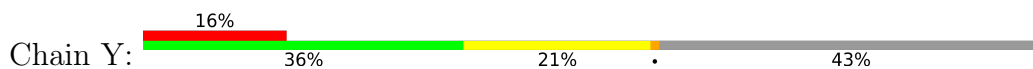


● Molecule 1: Cytoplasmic protein NCK1

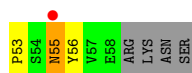
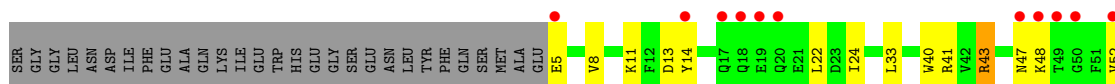




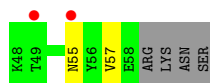
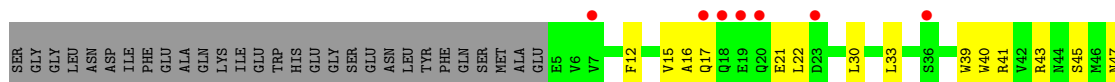
- Molecule 1: Cytoplasmic protein NCK1



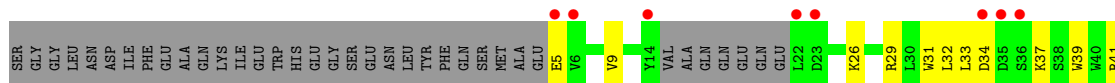
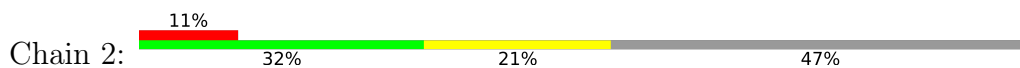
- Molecule 1: Cytoplasmic protein NCK1



- Molecule 1: Cytoplasmic protein NCK1



- Molecule 1: Cytoplasmic protein NCK1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.08Å 92.05Å 114.75Å 103.02° 91.63° 88.57°	Depositor
Resolution (Å)	53.08 – 1.82 55.88 – 1.82	Depositor EDS
% Data completeness (in resolution range)	62.1 (53.08-1.82) 59.5 (55.88-1.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.82Å)	Xtrriage
Refinement program	PHENIX 1.12rc1_2801	Depositor
R, R_{free}	0.208 , 0.263 0.210 , 0.267	Depositor DCC
R_{free} test set	5423 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.079 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13353	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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	1	0.32	0/468	0.54	0/633
1	2	0.33	0/401	0.52	0/541
1	A	0.42	0/479	0.62	0/647
1	B	0.48	0/479	0.66	0/647
1	C	0.45	0/479	0.67	0/645
1	D	0.46	0/479	0.62	0/647
1	E	0.44	0/507	0.63	0/684
1	F	0.45	0/496	0.58	0/669
1	G	0.45	0/488	0.62	0/658
1	H	0.45	0/502	0.54	0/677
1	I	0.46	0/482	0.58	0/652
1	J	0.41	0/502	0.59	0/677
1	K	0.43	0/507	0.57	0/684
1	L	0.43	0/507	0.56	0/684
1	M	0.39	0/479	0.55	0/647
1	N	0.42	0/482	0.63	0/652
1	O	0.41	0/496	0.56	0/670
1	P	0.43	0/479	0.63	0/647
1	Q	0.36	0/488	0.54	0/658
1	R	0.42	0/479	0.60	0/647
1	S	0.38	0/488	0.52	0/658
1	T	0.41	0/479	0.59	0/647
1	U	0.37	0/465	0.55	0/625
1	V	0.34	0/459	0.51	0/621
1	W	0.32	0/479	0.50	0/646
1	X	0.35	0/468	0.53	0/633
1	Y	0.32	0/434	0.50	0/585
1	Z	0.35	0/468	0.57	0/633
All	All	0.41	0/13419	0.58	0/18114

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	1	458	0	446	12	0
1	2	392	0	389	16	0
1	A	469	0	459	6	0
1	B	469	0	459	4	0
1	C	470	0	460	4	0
1	D	469	0	459	3	0
1	E	497	0	487	7	0
1	F	486	0	478	4	0
1	G	478	0	472	10	0
1	H	492	0	483	4	0
1	I	472	0	457	7	0
1	J	492	0	483	7	0
1	K	494	0	487	16	0
1	L	497	0	487	6	0
1	M	469	0	459	1	0
1	N	472	0	457	3	0
1	O	486	0	474	5	0
1	P	469	0	459	4	0
1	Q	478	0	472	6	0
1	R	469	0	459	5	0
1	S	478	0	472	7	0
1	T	469	0	459	8	0
1	U	456	0	458	14	0
1	V	449	0	440	12	0
1	W	469	0	466	25	0
1	X	458	0	446	19	0
1	Y	425	0	419	14	0
1	Z	458	0	446	14	0
2	A	12	0	0	0	0
2	B	20	0	0	0	0
2	C	8	0	0	0	0
2	D	11	0	0	0	0
2	E	22	0	0	0	0
2	F	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	18	0	0	0	0
2	H	12	0	0	0	0
2	I	14	0	0	1	0
2	J	6	0	0	0	0
2	K	16	0	0	1	0
2	L	9	0	0	0	0
2	M	6	0	0	0	0
2	N	5	0	0	0	0
2	O	4	0	0	0	0
2	P	7	0	0	0	0
2	Q	8	0	0	0	0
2	R	6	0	0	0	0
2	S	6	0	0	1	0
2	T	4	0	0	0	0
2	U	3	0	0	0	0
2	V	3	0	0	0	0
2	W	3	0	0	0	0
2	X	2	0	0	0	0
All	All	13353	0	12892	169	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 6.

The worst 5 of 169 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:W:21:GLU:HA	1:X:51:PHE:H	1.38	0.89
1:X:43:ARG:HB2	1:X:49:THR:HG22	1.61	0.83
1:W:20:GLN:NE2	1:X:20:GLN:O	2.13	0.80
1:U:20:GLN:HE21	1:V:20:GLN:HA	1.46	0.78
1:2:43:ARG:HB2	1:2:49:THR:HG22	1.66	0.76

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	1	52/87 (60%)	52 (100%)	0	0	100	100
1	2	42/87 (48%)	39 (93%)	3 (7%)	0	100	100
1	A	53/87 (61%)	53 (100%)	0	0	100	100
1	B	53/87 (61%)	52 (98%)	1 (2%)	0	100	100
1	C	51/87 (59%)	50 (98%)	1 (2%)	0	100	100
1	D	53/87 (61%)	52 (98%)	1 (2%)	0	100	100
1	E	57/87 (66%)	56 (98%)	1 (2%)	0	100	100
1	F	55/87 (63%)	54 (98%)	1 (2%)	0	100	100
1	G	54/87 (62%)	54 (100%)	0	0	100	100
1	H	56/87 (64%)	54 (96%)	2 (4%)	0	100	100
1	I	54/87 (62%)	53 (98%)	1 (2%)	0	100	100
1	J	56/87 (64%)	54 (96%)	2 (4%)	0	100	100
1	K	57/87 (66%)	56 (98%)	1 (2%)	0	100	100
1	L	57/87 (66%)	55 (96%)	2 (4%)	0	100	100
1	M	53/87 (61%)	50 (94%)	3 (6%)	0	100	100
1	N	54/87 (62%)	52 (96%)	2 (4%)	0	100	100
1	O	56/87 (64%)	55 (98%)	1 (2%)	0	100	100
1	P	53/87 (61%)	51 (96%)	2 (4%)	0	100	100
1	Q	54/87 (62%)	54 (100%)	0	0	100	100
1	R	53/87 (61%)	51 (96%)	2 (4%)	0	100	100
1	S	54/87 (62%)	52 (96%)	2 (4%)	0	100	100
1	T	53/87 (61%)	53 (100%)	0	0	100	100
1	U	49/87 (56%)	48 (98%)	1 (2%)	0	100	100
1	V	51/87 (59%)	50 (98%)	1 (2%)	0	100	100
1	W	53/87 (61%)	52 (98%)	1 (2%)	0	100	100
1	X	52/87 (60%)	47 (90%)	5 (10%)	0	100	100
1	Y	46/87 (53%)	41 (89%)	4 (9%)	1 (2%)	6	1
1	Z	52/87 (60%)	48 (92%)	4 (8%)	0	100	100
All	All	1483/2436 (61%)	1438 (97%)	44 (3%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	35	ASP

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	1	51/79 (65%)	49 (96%)	2 (4%)	32	17
1	2	44/79 (56%)	44 (100%)	0	100	100
1	A	52/79 (66%)	52 (100%)	0	100	100
1	B	52/79 (66%)	50 (96%)	2 (4%)	33	18
1	C	52/79 (66%)	49 (94%)	3 (6%)	20	7
1	D	52/79 (66%)	49 (94%)	3 (6%)	20	7
1	E	55/79 (70%)	55 (100%)	0	100	100
1	F	54/79 (68%)	54 (100%)	0	100	100
1	G	53/79 (67%)	52 (98%)	1 (2%)	57	45
1	H	55/79 (70%)	50 (91%)	5 (9%)	9	2
1	I	52/79 (66%)	52 (100%)	0	100	100
1	J	55/79 (70%)	54 (98%)	1 (2%)	59	48
1	K	55/79 (70%)	50 (91%)	5 (9%)	9	2
1	L	55/79 (70%)	54 (98%)	1 (2%)	59	48
1	M	52/79 (66%)	52 (100%)	0	100	100
1	N	52/79 (66%)	49 (94%)	3 (6%)	20	7
1	O	54/79 (68%)	52 (96%)	2 (4%)	34	19
1	P	52/79 (66%)	51 (98%)	1 (2%)	57	45
1	Q	53/79 (67%)	51 (96%)	2 (4%)	33	18
1	R	52/79 (66%)	50 (96%)	2 (4%)	33	18
1	S	53/79 (67%)	52 (98%)	1 (2%)	57	45
1	T	52/79 (66%)	50 (96%)	2 (4%)	33	18
1	U	50/79 (63%)	49 (98%)	1 (2%)	55	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	V	50/79 (63%)	46 (92%)	4 (8%)	12 3
1	W	52/79 (66%)	51 (98%)	1 (2%)	57 45
1	X	51/79 (65%)	49 (96%)	2 (4%)	32 17
1	Y	47/79 (60%)	44 (94%)	3 (6%)	17 6
1	Z	51/79 (65%)	48 (94%)	3 (6%)	19 7
All	All	1458/2212 (66%)	1408 (97%)	50 (3%)	37 22

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	38	SER
1	V	17	GLN
1	1	57	VAL
1	R	34	ASP
1	T	12	PHE

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

Mol	Chain	Res	Type
1	U	20	GLN

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 monosaccharides 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 [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	1	54/87 (62%)	0.88	9 (16%) 1 1	62, 81, 122, 144	0
1	2	46/87 (52%)	1.20	10 (21%) 0 0	61, 83, 126, 161	0
1	A	55/87 (63%)	-0.13	0 100 100	25, 37, 68, 102	0
1	B	55/87 (63%)	-0.10	0 100 100	20, 33, 60, 77	0
1	C	55/87 (63%)	-0.13	1 (1%) 68 64	23, 39, 72, 85	0
1	D	55/87 (63%)	0.10	2 (3%) 42 37	22, 39, 80, 117	0
1	E	59/87 (67%)	-0.24	0 100 100	22, 34, 64, 85	0
1	F	57/87 (65%)	-0.15	1 (1%) 68 64	21, 41, 84, 89	0
1	G	56/87 (64%)	0.01	1 (1%) 68 64	19, 39, 73, 99	0
1	H	58/87 (66%)	0.09	0 100 100	19, 51, 88, 93	0
1	I	56/87 (64%)	-0.34	0 100 100	23, 42, 69, 90	0
1	J	58/87 (66%)	-0.05	1 (1%) 70 66	24, 43, 92, 112	0
1	K	58/87 (66%)	-0.11	1 (1%) 70 66	26, 46, 77, 106	0
1	L	59/87 (67%)	-0.20	0 100 100	29, 42, 81, 99	0
1	M	55/87 (63%)	-0.16	1 (1%) 68 64	32, 50, 73, 122	0
1	N	56/87 (64%)	-0.00	2 (3%) 42 37	32, 47, 93, 123	0
1	O	58/87 (66%)	-0.11	1 (1%) 70 66	34, 47, 78, 118	0
1	P	55/87 (63%)	-0.09	2 (3%) 42 37	32, 51, 84, 128	0
1	Q	56/87 (64%)	-0.25	0 100 100	28, 48, 83, 95	0
1	R	55/87 (63%)	-0.02	2 (3%) 42 37	27, 51, 86, 113	0
1	S	56/87 (64%)	0.21	1 (1%) 68 64	24, 61, 95, 106	0
1	T	55/87 (63%)	-0.00	2 (3%) 42 37	27, 49, 81, 96	0
1	U	53/87 (60%)	0.67	8 (15%) 2 1	44, 72, 104, 125	0
1	V	53/87 (60%)	0.25	2 (3%) 40 35	33, 64, 101, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	W	55/87 (63%)	1.59	18 (32%) 0 0	54, 92, 136, 155	0
1	X	54/87 (62%)	0.79	7 (12%) 3 2	36, 81, 112, 124	0
1	Y	50/87 (57%)	1.48	14 (28%) 0 0	73, 98, 129, 146	0
1	Z	54/87 (62%)	1.17	12 (22%) 0 0	68, 91, 113, 127	0
All	All	1546/2436 (63%)	0.21	98 (6%) 20 15	19, 51, 105, 161	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	36	SER	9.4
1	2	36	SER	8.9
1	X	15	VAL	7.2
1	2	35	ASP	7.0
1	D	36	SER	6.7

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 monosaccharides 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.