

wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 05:41 am BST

PDB ID	:	40SW
Title	:	Crystal structure of the S505E mutant of TAL effector dHax3
Authors	:	Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.
Deposited on	:	2014-02-13
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

:	4.02b-467
:	1.13
:	2.11
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.11
	: : : : : : : : : : : : : : : : : : :

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	5042(2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575(2.30-2.30)
Sidechain outliers	138945	5575(2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 <=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	А	499	83%	15% ••
1	В	499	^{2%} 78%	18% ••
2	G	17	6% 53% 47%	
2	Ι	17	65%	35%
3	Н	17	18% 53% 41%	6%
3	J	17	47% 47%	6%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8831 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	491	Total 3577	C 2237	N 664	O 664	S 12	5	3	0
1	В	487	Total 3552	C 2218	N 659	O 663	S 12	5	3	0

• Molecule 1 is a protein called Hax3.

A230MET-EXPRESSION TAGUNP Q3ZD72A300HISASNENGINEERED MUTATIONUNP Q3ZD72A301ASPILEENGINEERED MUTATIONUNP Q3ZD72A368HISASNENGINEERED MUTATIONUNP Q3ZD72A369ASPILEENGINEERED MUTATIONUNP Q3ZD72A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72<	Chain	Residue	Modelled	Actual	Comment	Reference
A300HISASNENGINEERED MUTATIONUNP Q3ZD72A301ASPILEENGINEERED MUTATIONUNP Q3ZD72A368HISASNENGINEERED MUTATIONUNP Q3ZD72A369ASPILEENGINEERED MUTATIONUNP Q3ZD72A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72 <td>А</td> <td>230</td> <td>MET</td> <td>-</td> <td>EXPRESSION TAG</td> <td>UNP Q3ZD72</td>	А	230	MET	-	EXPRESSION TAG	UNP Q3ZD72
A301ASPILEENGINEERED MUTATIONUNP Q3ZD72A368HISASNENGINEERED MUTATIONUNP Q3ZD72A369ASPILEENGINEERED MUTATIONUNP Q3ZD72A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A4470ASNHISENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A </td <td>A</td> <td>300</td> <td>HIS</td> <td>ASN</td> <td>ENGINEERED MUTATION</td> <td>UNP Q3ZD72</td>	A	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A368HISASNENGINEERED MUTATIONUNP Q3ZD72A369ASPILEENGINEERED MUTATIONUNP Q3ZD72A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A4470ASNHISENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A </td <td>А</td> <td>301</td> <td>ASP</td> <td>ILE</td> <td>ENGINEERED MUTATION</td> <td>UNP Q3ZD72</td>	А	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A369ASPILEENGINEERED MUTATIONUNP Q3ZD72A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A4470ASNHISENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A505GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A402ASNHISENGINEERED MUTATIONUNP Q3ZD72A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A4470ASNHISENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726 <td>А</td> <td>369</td> <td>ASP</td> <td>ILE</td> <td>ENGINEERED MUTATION</td> <td>UNP Q3ZD72</td>	А	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A403GLYASPENGINEERED MUTATIONUNP Q3ZD72A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A436ASNHISENGINEERED MUTATIONUNP Q3ZD72A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A437GLYASPENGINEERED MUTATIONUNP Q3ZD72A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A470ASNHISENGINEERED MUTATIONUNP Q3ZD72A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	A	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A471GLYASPENGINEERED MUTATIONUNP Q3ZD72A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A505GLUSERENGINEERED MUTATIONUNP Q3ZD72A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A539GLYSERENGINEERED MUTATIONUNP Q3ZD72A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	A	505	GLU	SER	ENGINEERED MUTATION	UNP Q3ZD72
A572HISASNENGINEERED MUTATIONUNP Q3ZD72A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
A573ASPSERENGINEERED MUTATIONUNP Q3ZD72A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	A	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A606ASNHISENGINEERED MUTATIONUNP Q3ZD72A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
A607GLYASPENGINEERED MUTATIONUNP Q3ZD72A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
A640HISASNENGINEERED MUTATIONUNP Q3ZD72A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
A641ASPILEENGINEERED MUTATIONUNP Q3ZD72A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
A721LEU-EXPRESSION TAGUNP Q3ZD72A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	A	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
A722GLU-EXPRESSION TAGUNP Q3ZD72A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
A723HIS-EXPRESSION TAGUNP Q3ZD72A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	A	722	GLU	-	EXPRESSION TAG	UNP Q3ZD72
A724HIS-EXPRESSION TAGUNP Q3ZD72A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A725HIS-EXPRESSION TAGUNP Q3ZD72A726HIS-EXPRESSION TAGUNP Q3ZD72	А	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
A 726 HIS - EXPRESSION TAG UNP Q3ZD72	А	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
	A	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72

There are 54 discrepancies between the modelled and reference sequences:

Continued on next page...



Chain	Residue	Modelled	Actual	Comment	Reference
А	727	HIS	_	EXPRESSION TAG	UNP Q3ZD72
A	728	HIS	_	EXPRESSION TAG	UNP Q3ZD72
В	230	MET	_	EXPRESSION TAG	UNP Q3ZD72
В	300	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
В	301	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
В	368	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
В	369	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
В	402	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
В	403	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
В	436	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
В	437	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
В	470	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
В	471	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
В	505	GLU	SER	ENGINEERED MUTATION	UNP Q3ZD72
В	539	GLY	SER	ENGINEERED MUTATION	UNP Q3ZD72
В	572	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
В	573	ASP	SER	ENGINEERED MUTATION	UNP Q3ZD72
В	606	ASN	HIS	ENGINEERED MUTATION	UNP Q3ZD72
В	607	GLY	ASP	ENGINEERED MUTATION	UNP Q3ZD72
В	640	HIS	ASN	ENGINEERED MUTATION	UNP Q3ZD72
В	641	ASP	ILE	ENGINEERED MUTATION	UNP Q3ZD72
В	721	LEU	-	EXPRESSION TAG	UNP Q3ZD72
В	722	GLU	_	EXPRESSION TAG	UNP Q3ZD72
В	723	HIS	-	EXPRESSION TAG	UNP Q3ZD72
В	724	HIS	-	EXPRESSION TAG	UNP Q3ZD72
В	725	HIS	-	EXPRESSION TAG	UNP Q3ZD72
В	726	HIS	-	EXPRESSION TAG	UNP Q3ZD72
В	727	HIS	-	EXPRESSION TAG	UNP Q3ZD72
В	728	HIS	-	EXPRESSION TAG	UNP Q3ZD72

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• Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP* TP*CP*TP*CP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
9	C	17	Total	С	Ν	0	Р	0	0	0
2	G	11	333	163	46	108	16	0	0	0
9	Т	17	Total	С	Ν	0	Р	0	0	0
		17	334	164	46	108	16	0	0	0

• Molecule 3 is a DNA chain called DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*TP*AP*AP* AP*GP*GP*GP*AP*CP*A)-3').



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	п	17	Total	С	Ν	Ο	Р	0	0	0
J J	11	11	357	169	80	92	16	0	0	0
2	т	17	Total	С	Ν	Ο	Р	0	0	0
J J	J	11	357	169	80	92	16	0	0	0

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	1	Total Mg 1 1	0	0
4	А	1	Total Mg 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	132	Total O 132 132	0	0
5	В	118	Total O 118 118	0	0
5	G	19	Total O 19 19	0	0
5	Н	9	Total O 9 9	0	0
5	Ι	30	Total O 30 30	0	0
5	J	11	Total O 11 11	0	0



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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: Hax3

6%

53%

Chain G:



47%

T-2 G-1 C3 T4 T4 C9 C9 C9 T14

• Molecule 2: DNA (5'-D(*TP*GP*TP*CP*CP*CP*TP*TP*TP*AP*TP*CP*TP*CP*TP*CP*TP*CP*T)-3')

Chain I:	65%	35%
112 114 114 115 115 115 115 115 115		

• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*TP*AP*AP*AP*GP*GP*GP*AP*CP *A)-3')

_	18%			
Chain H:		53%	41%	6%
4° M N	<u> </u>			
A-1 6-1 A-6 A-6 G-2	C1 A2			

• Molecule 3: DNA (5'-D(*AP*GP*AP*GP*AP*GP*AP*TP*AP*AP*AP*GP*GP*GP*AP*CP *A)-3')

Chain J:	47%	47%	6%
A 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4 4			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	81.95Å 87.65 Å 87.44 Å	Depositor
a, b, c, α , β , γ	90.00° 102.55° 90.00°	Depositor
Bosolution (Å)	30.86 - 2.30	Depositor
	30.86 - 2.30	EDS
% Data completeness	99.8 (30.86-2.30)	Depositor
(in resolution range)	99.8 (30.86 - 2.30)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.52 (at 2.31 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
D D.	0.198 , 0.243	Depositor
Π, Π_{free}	0.195 , 0.236	DCC
R_{free} test set	2718 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.30 , 33.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8831	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.66% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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).

Mal	Chain	Bond	lengths	Bond angles	
TATOL	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/3630	0.59	3/4960~(0.1%)
1	В	0.41	0/3601	0.56	1/4915~(0.0%)
2	G	1.08	0/368	1.62	4/564~(0.7%)
2	Ι	1.00	0/369	1.58	1/566~(0.2%)
3	Н	0.94	0/405	1.55	8/625~(1.3%)
3	J	0.86	0/405	1.48	6/625~(1.0%)
All	All	0.56	0/8778	0.86	23/12255~(0.2%)

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	В	0	3

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
3	Н	-2	DG	O4'-C1'-N9	10.10	115.07	108.00
2	G	9	DC	O4'-C1'-N1	-8.36	102.15	108.00
1	А	470	ASN	CB-CA-C	-7.76	94.88	110.40
2	Ι	12	DT	O4'-C1'-N1	-7.50	102.75	108.00
3	J	-9	DG	O4'-C1'-N9	7.29	113.11	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	В	420	CYS	Mainchain,Peptide
1	В	421[B]	GLN	Peptide

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	${ m H(model)}$	H(added)	Clashes	Symm-Clashes
1	А	3577	0	3711	43	0
1	В	3552	0	3687	55	0
2	G	333	0	195	12	0
2	Ι	334	0	198	4	0
3	Н	357	0	190	3	0
3	J	357	0	190	4	0
4	А	1	0	0	1	0
4	J	1	0	0	0	0
5	А	132	0	0	10	0
5	В	118	0	0	4	0
5	G	19	0	0	0	0
5	Н	9	0	0	2	0
5	Ι	30	0	0	3	0
5	J	11	0	0	3	0
All	All	8831	0	8171	119	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 7.

The worst 5 of 119 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)
2:G:-2:DT:H6	2:G:-2:DT:C5'	1.38	1.35
1:A:266:ARG:HB2	5:A:1027:HOH:O	1.40	1.20
2:G:-2:DT:C5'	2:G:-2:DT:C6	2.30	1.13
2:G:-2:DT:H5'	2:G:-2:DT:C6	1.88	1.07
2:G:-2:DT:H5'	2:G:-2:DT:H6	1.15	1.05

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	Perce	entiles
1	А	492/499~(99%)	465~(94%)	23~(5%)	4 (1%)	19	23
1	В	486/499~(97%)	465~(96%)	18 (4%)	3~(1%)	25	31
All	All	978/998~(98%)	930~(95%)	41 (4%)	7 (1%)	22	26

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	437	GLY
1	В	438	GLY
1	В	456	ALA
1	А	234	GLY
1	А	257	THR

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	А	376/383~(98%)	359~(96%)	17~(4%)	27 39
1	В	375/383~(98%)	358~(96%)	17~(4%)	27 39
All	All	751/766~(98%)	717~(96%)	34~(4%)	27 39

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	678	ARG
	a	7	

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40SW

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Mol	Chain	Res	Type
1	В	323	LEU
1	В	701	ASP
1	В	253	LEU
1	А	353	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	288	ASN
1	В	402	ASN
1	В	436	ASN
1	В	447	GLN
1	В	702	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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, 95^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	491/499~(98%)	-0.21	8 (1%) 72 77	24, 39, 76, 148	12 (2%)
1	В	487/499~(97%)	-0.00	8 (1%) 72 77	27, 45, 74, 108	9 (1%)
2	G	17/17~(100%)	-0.28	1 (5%) 22 28	30, 34, 89, 96	0
2	Ι	17/17~(100%)	-0.65	0 100 100	25, 30, 76, 78	0
3	Н	17/17~(100%)	0.25	3(17%) 1 1	40, 49, 92, 105	0
3	J	17/17~(100%)	-0.22	0 100 100	36, 48, 74, 80	0
All	All	1046/1066~(98%)	-0.12	20 (1%) 66 73	24, 42, 76, 148	21 (2%)

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	524	ALA	6.5
1	В	438	GLY	6.0
3	Н	-14	DA	3.9
1	А	695	LEU	3.2
1	В	255	LEU	2.9

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	MG	А	801	1/1	0.66	0.09	$93,\!93,\!93,\!93$	0
4	MG	J	101	1/1	0.72	0.11	$71,\!71,\!71,\!71$	0

6.5 Other polymers (i)

There are no such residues in this entry.

