



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 PM GMT

PDB ID : 4OSW  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

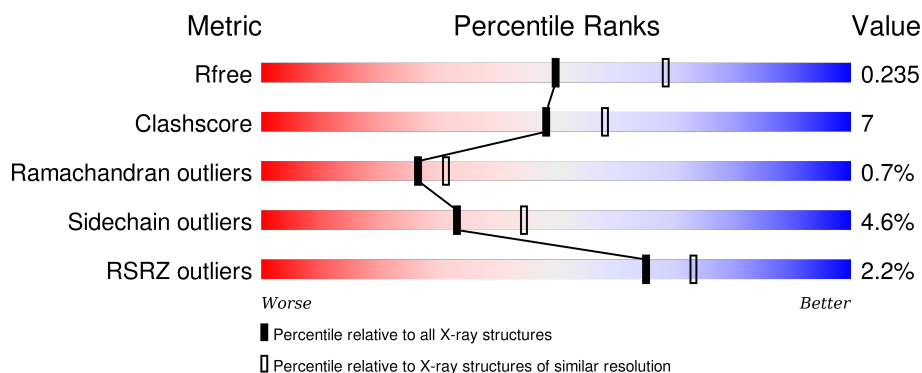
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



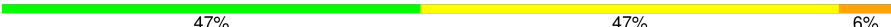
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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	499	<div> <div>2%</div> <div>83%</div> <div>15%</div> <div>••</div> </div>
1	B	499	<div> <div>2%</div> <div>78%</div> <div>18%</div> <div>••</div> </div>
2	G	17	<div> <div>6%</div> <div>53%</div> <div>47%</div> </div>
2	I	17	<div> <div>65%</div> <div>35%</div> </div>
3	H	17	<div> <div>18%</div> <div>53%</div> <div>41%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	17	 A horizontal bar chart showing the quality of chain J. The bar is divided into three segments: a green segment on the left labeled '47%', a yellow segment in the middle labeled '47%', and a small orange segment on the right labeled '6%'. The segments represent different quality metrics, with green indicating good, yellow indicating average, and orange indicating poor quality.

## 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.

- Molecule 1 is a protein called Hax3.

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

There are 54 discrepancies between the modelled and reference sequences:

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

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

- 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
2	G	17	Total	C	N	O	P	0	0	0
			333	163	46	108	16			
2	I	17	Total	C	N	O	P	0	0	0
			334	164	46	108	16			

- 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
3	H	17	Total	C	N	O	P	0	0	0
			357	169	80	92	16			
3	J	17	Total	C	N	O	P	0	0	0
			357	169	80	92	16			

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

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

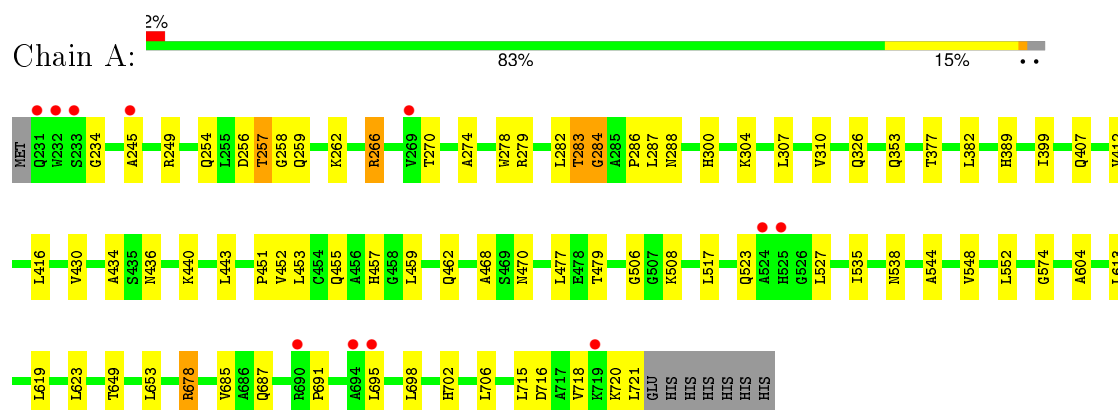
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	118	Total	O	0	0
			118	118		
5	G	19	Total	O	0	0
			19	19		
5	H	9	Total	O	0	0
			9	9		
5	I	30	Total	O	0	0
			30	30		
5	J	11	Total	O	0	0
			11	11		

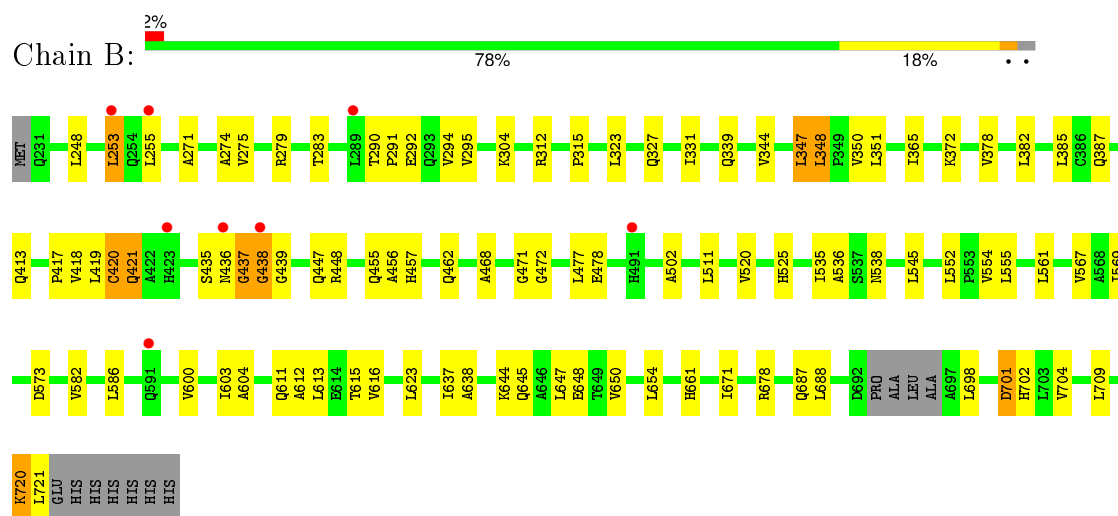
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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



#### • Molecule 1: Hax3

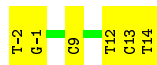


#### • Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*CP\*TP\*CP\*T)-3')



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

Chain I:  65% 35%



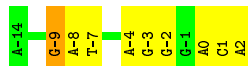
- Molecule 3: DNA (5'-D(\*AP\*GP\*AP\*GP\*AP\*GP\*AP\*TP\*AP\*AP\*AP\*GP\*GP\*GP\*AP\*CP\*A)-3')

Chain H:  18% 53% 41% 6%



- 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%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.95Å 87.65Å 87.44Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	30.86 – 2.30 30.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.86-2.30) 99.8 (30.86-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.198 , 0.243 0.197 , 0.235	Depositor DCC
$R_{free}$ test set	2718 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.3	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 33.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53517 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.43	0/3630	0.59	3/4960 (0.1%)
1	B	0.41	0/3601	0.56	1/4915 (0.0%)
2	G	1.08	0/368	1.62	4/564 (0.7%)
2	I	1.00	0/369	1.58	1/566 (0.2%)
3	H	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	B	0	3

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	-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	A	470	ASN	CB-CA-C	-7.76	94.88	110.40
2	I	12	DT	O4'-C1'-N1	-7.50	102.75	108.00
3	J	-9	DG	O4'-C1'-N9	7.29	113.11	108.00
3	H	1	DC	C1'-O4'-C4'	-6.65	103.45	110.10
3	H	-14	DA	C3'-C2'-C1'	-6.36	94.87	102.50
2	G	10	DT	C6-C5-C7	-6.20	119.18	122.90
3	H	-7	DT	N3-C4-O4	6.01	123.51	119.90
1	B	420	CYS	O-C-N	-5.95	113.18	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	-3	DG	O4'-C1'-N9	5.91	112.14	108.00
3	H	-7	DT	C5-C4-O4	-5.89	120.77	124.90
3	J	0	DA	O4'-C1'-N9	-5.85	103.91	108.00
1	A	470	ASN	N-CA-C	-5.61	95.84	111.00
2	G	14	DT	O4'-C1'-N1	5.59	111.91	108.00
3	J	-4	DA	O4'-C1'-N9	5.46	111.83	108.00
3	H	-13	DG	O4'-C1'-N9	5.44	111.81	108.00
3	H	-12	DA	O4'-C1'-N9	5.35	111.74	108.00
3	H	-6	DA	C1'-O4'-C4'	-5.35	104.75	110.10
2	G	8	DT	N3-C4-O4	5.32	123.09	119.90
1	A	552	LEU	CA-CB-CG	5.26	127.41	115.30
3	J	-7	DT	O4'-C1'-N1	-5.11	104.42	108.00
3	J	-2	DG	O4'-C1'-N9	5.10	111.57	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3577	0	3711	43	0
1	B	3552	0	3687	55	0
2	G	333	0	195	12	0
2	I	334	0	198	4	0
3	H	357	0	190	3	0
3	J	357	0	190	4	0
4	A	1	0	0	1	0
4	J	1	0	0	0	0
5	A	132	0	0	10	0
5	B	118	0	0	4	0
5	G	19	0	0	0	0
5	H	9	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	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.

All (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:C6	2:G:-2:DT:C5'	2.30	1.13
2:G:-2:DT:C6	2:G:-2:DT:H5'	1.88	1.07
2:G:-2:DT:H5'	2:G:-2:DT:H6	1.15	1.05
2:G:-2:DT:H6	2:G:-2:DT:H5''	1.22	1.01
2:G:-2:DT:C6	2:G:-2:DT:H5''	2.07	0.84
1:A:284:GLY:O	1:A:288:ASN:ND2	2.10	0.83
1:A:407:GLN:HB3	1:A:440:LYS:HD2	1.68	0.75
1:A:523:GLN:O	5:A:1011:HOH:O	2.05	0.75
3:H:-2:DG:N7	5:H:109:HOH:O	2.21	0.74
1:A:687:GLN:HG2	1:A:695:LEU:HD22	1.68	0.73
1:B:339:GLN:HB3	1:B:372:LYS:HD3	1.73	0.71
1:A:436:ASN:HB2	5:A:1024:HOH:O	1.90	0.70
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.74	0.69
1:B:648:GLU:OE1	5:B:832:HOH:O	2.12	0.68
3:H:-2:DG:N3	5:H:101:HOH:O	2.26	0.67
2:G:-2:DT:H3	3:H:2:DA:H2	1.43	0.67
1:A:535:ILE:HD13	1:A:548:VAL:HG21	1.76	0.66
1:A:721:LEU:O	5:A:1021:HOH:O	2.14	0.66
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.78	0.66
1:B:701:ASP:OD1	5:B:887:HOH:O	2.13	0.66
4:A:801:MG:MG	5:J:209:HOH:O	1.37	0.65
1:B:435:SER:O	1:B:436:ASN:ND2	2.30	0.65
1:A:574:GLY:HA3	5:I:127:HOH:O	1.96	0.65
2:G:-2:DT:H2''	2:G:-1:DG:H5'	1.77	0.65
1:B:436:ASN:O	1:B:437:GLY:C	2.34	0.64
3:J:-9:DG:OP2	5:J:211:HOH:O	2.16	0.62
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.82	0.60
1:A:279:ARG:O	1:A:283:THR:OG1	2.20	0.59
1:B:248:LEU:HD13	1:B:255:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:ILE:HD13	1:B:378:VAL:HG21	1.85	0.57
1:B:720:LYS:HB3	1:B:720:LYS:NZ	2.19	0.57
1:B:448:ARG:NH2	1:B:478:GLU:OE1	2.36	0.57
1:B:637:ILE:HD13	1:B:650:VAL:HG21	1.87	0.55
1:A:452:VAL:HG23	5:A:926:HOH:O	2.06	0.55
1:A:377:THR:OG1	5:A:954:HOH:O	2.17	0.55
2:I:13:DC:H2"	2:I:14:DT:H5"	1.90	0.54
1:A:538:ASN:HB2	5:A:1018:HOH:O	2.07	0.54
1:B:455:GLN:O	1:B:457:HIS:N	2.40	0.54
1:A:256:ASP:O	1:A:259:GLN:N	2.42	0.53
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.90	0.53
2:G:-2:DT:H2'	2:G:-1:DG:C8	2.44	0.53
1:B:418:VAL:HG11	1:B:447:GLN:HE21	1.74	0.52
1:A:256:ASP:O	1:A:257:THR:C	2.48	0.52
1:B:586:LEU:HD13	1:B:600:VAL:HG11	1.91	0.52
1:B:720:LYS:O	1:B:720:LYS:HG3	2.11	0.51
1:B:569:ILE:HD13	1:B:582:VAL:HG21	1.93	0.51
1:B:720:LYS:CB	1:B:720:LYS:NZ	2.73	0.51
1:B:271:ALA:O	1:B:275:VAL:HG23	2.10	0.51
3:J:-9:DG:H2"	3:J:-8:DA:H5"	1.93	0.51
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.94	0.50
1:A:468:ALA:HB2	1:A:477:LEU:HD11	1.94	0.50
2:G:-2:DT:C6	2:G:-2:DT:C4'	2.89	0.50
2:I:9:DC:OP2	5:I:127:HOH:O	2.20	0.50
1:A:274:ALA:HB2	1:A:304:LYS:HG3	1.94	0.50
1:B:472:GLY:N	5:B:811:HOH:O	2.08	0.50
1:A:282:LEU:HA	1:A:287:LEU:HD12	1.94	0.49
1:B:436:ASN:O	1:B:437:GLY:O	2.30	0.49
1:B:661:HIS:ND1	1:B:688:LEU:HB3	2.26	0.49
1:B:253:LEU:HD21	1:B:294:VAL:HG11	1.93	0.49
1:A:702:HIS:HB3	1:B:702:HIS:CE1	2.47	0.49
1:A:389:HIS:HB3	1:A:416:LEU:HD23	1.96	0.48
1:B:720:LYS:HB3	1:B:720:LYS:HZ3	1.78	0.48
1:B:419:LEU:HD21	1:B:447:GLN:HB2	1.95	0.48
1:A:716:ASP:O	1:A:720:LYS:HG2	2.14	0.48
1:B:603:ILE:HD13	1:B:616:VAL:HG21	1.94	0.47
1:B:638:ALA:O	5:B:815:HOH:O	2.20	0.47
1:B:535:ILE:HD11	1:B:567:VAL:HG22	1.97	0.47
2:G:-2:DT:H2"	2:G:-1:DG:C5'	2.45	0.47
1:A:451:PRO:O	1:A:455:GLN:HG2	2.14	0.47
1:A:457:HIS:O	5:A:986:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:ILE:HD11	1:B:704:VAL:HG13	1.97	0.46
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.96	0.46
1:A:249:ARG:NH1	1:A:257:THR:OG1	2.32	0.45
1:A:256:ASP:O	1:A:258:GLY:N	2.49	0.45
1:B:615:THR:OG1	1:B:644:LYS:HG3	2.16	0.45
1:B:421[B]:GLN:HB2	1:B:421[B]:GLN:HE21	1.57	0.45
1:A:506:GLY:N	5:A:1014:HOH:O	2.35	0.45
1:B:502:ALA:HB2	1:B:511:LEU:HD11	1.99	0.45
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.98	0.44
1:B:525:HIS:HB3	1:B:552:LEU:HD22	1.99	0.44
1:A:270:THR:HG23	5:I:108:HOH:O	2.16	0.44
1:B:538:ASN:HB3	1:B:573:ASP:OD1	2.18	0.43
1:B:468:ALA:HB2	1:B:477:LEU:HD11	2.00	0.43
1:B:438:GLY:HA2	1:B:439:GLY:HA3	1.74	0.43
1:A:649:THR:OG1	1:A:678:ARG:HD3	2.18	0.43
1:B:344:VAL:O	1:B:348:LEU:HB2	2.19	0.43
3:J:1:DC:H2''	3:J:2:DA:C8	2.54	0.43
1:B:612:ALA:O	1:B:616:VAL:HG23	2.17	0.43
2:G:3:DC:H2''	2:G:4:DT:O5'	2.19	0.43
1:A:604:ALA:HB2	1:A:613:LEU:HD11	2.01	0.42
1:B:555:LEU:HB3	1:B:561:LEU:HD23	2.01	0.42
1:B:312:ARG:O	1:B:315:PRO:HD2	2.19	0.42
1:A:434:ALA:HB2	1:A:443:LEU:HD11	2.01	0.42
1:A:687:GLN:O	1:A:691:PRO:HA	2.20	0.42
1:B:327:GLN:O	1:B:331:ILE:HG13	2.20	0.42
1:B:638:ALA:HB2	1:B:647:LEU:HD11	2.01	0.42
1:A:479:THR:OG1	1:A:508:LYS:HG3	2.20	0.42
1:B:347:LEU:HA	1:B:350:VAL:HG12	2.00	0.42
1:A:399:ILE:HD13	1:A:412:VAL:HG21	2.01	0.42
1:A:278[B]:TRP:HD1	1:A:282:LEU:HD11	1.84	0.42
1:B:417:PRO:O	1:B:421[A]:GLN:HG2	2.19	0.42
1:A:416:LEU:HD13	1:A:430:VAL:HG11	2.02	0.41
1:A:245:ALA:O	1:A:249:ARG:HG3	2.19	0.41
1:B:437:GLY:O	1:B:471:GLY:HA2	2.20	0.41
1:B:721:LEU:HA	2:I:14:DT:H72	2.02	0.41
1:B:604:ALA:HB2	1:B:613:LEU:HD11	2.03	0.41
1:B:623:LEU:HA	1:B:623:LEU:HD23	1.90	0.41
1:B:253:LEU:HD13	1:B:283:THR:HG21	2.02	0.41
1:A:266:ARG:HD2	1:A:266:ARG:HA	1.70	0.41
1:A:262:LYS:HG3	5:J:208:HOH:O	2.19	0.41
1:B:291:PRO:O	1:B:295:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:HD21	1:B:413:GLN:HB2	2.03	0.41
2:I:-2:DT:H2''	2:I:-1:DG:C8	2.56	0.40
1:B:290:THR:OG1	1:B:292:GLU:HG2	2.21	0.40
3:J:2:DA:OP2	3:J:2:DA:H2'	2.22	0.40
1:A:544:ALA:O	1:A:548:VAL:HG23	2.22	0.40
1:A:698:LEU:HA	5:A:905:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	492/499 (99%)	465 (94%)	23 (5%)	4 (1%)	24	27
1	B	486/499 (97%)	465 (96%)	18 (4%)	3 (1%)	30	36
All	All	978/998 (98%)	930 (95%)	41 (4%)	7 (1%)	26	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	437	GLY
1	B	438	GLY
1	B	456	ALA
1	A	234	GLY
1	A	257	THR
1	A	284	GLY
1	A	286	PRO

### 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	376/383 (98%)	359 (96%)	17 (4%)	34	46
1	B	375/383 (98%)	358 (96%)	17 (4%)	34	46
All	All	751/766 (98%)	717 (96%)	34 (4%)	33	46

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	266	ARG
1	A	283	THR
1	A	307	LEU
1	A	310	VAL
1	A	326	GLN
1	A	353	GLN
1	A	382	LEU
1	A	453	LEU
1	A	459	LEU
1	A	462	GLN
1	A	517	LEU
1	A	527	LEU
1	A	619	LEU
1	A	623	LEU
1	A	678	ARG
1	A	715	LEU
1	B	253	LEU
1	B	279	ARG
1	B	323	LEU
1	B	347	LEU
1	B	348	LEU
1	B	351	LEU
1	B	382	LEU
1	B	387	GLN
1	B	462	GLN
1	B	520	VAL

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Mol	Chain	Res	Type
1	B	554	VAL
1	B	654	LEU
1	B	687	GLN
1	B	698	LEU
1	B	701	ASP
1	B	709	LEU
1	B	720	LYS

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

Mol	Chain	Res	Type
1	A	288	ASN
1	B	402	ASN
1	B	436	ASN
1	B	447	GLN
1	B	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	491/499 (98%)	-0.16	11 (2%) 65 73	24, 39, 76, 148	12 (2%)
1	B	487/499 (97%)	0.05	8 (1%) 74 80	27, 45, 74, 108	9 (1%)
2	G	17/17 (100%)	-0.22	1 (5%) 26 34	30, 34, 89, 96	0
2	I	17/17 (100%)	-0.60	0 100 100	25, 30, 76, 78	0
3	H	17/17 (100%)	0.33	3 (17%) 2 3	40, 49, 92, 105	0
3	J	17/17 (100%)	-0.16	0 100 100	36, 48, 74, 80	0
All	All	1046/1066 (98%)	-0.06	23 (2%) 65 73	24, 42, 76, 148	21 (2%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	524	ALA	6.7
1	B	438	GLY	6.2
3	H	-14	DA	4.1
1	A	695	LEU	3.3
1	B	255	LEU	3.0
1	B	491	HIS	2.8
3	H	-13	DG	2.7
1	B	423	HIS	2.6
1	A	719	LYS	2.6
1	B	253	LEU	2.6
1	B	436	ASN	2.5
1	A	269	VAL	2.4
1	A	690	ARG	2.4
1	A	245	ALA	2.3
3	H	2	DA	2.2
1	A	232	TRP	2.2
1	A	694	ALA	2.1
1	A	231	GLN	2.1
2	G	14	DT	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	289	LEU	2.1
1	B	591	GLN	2.1
1	A	525	HIS	2.1
1	A	233	SER	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	J	101	1/1	0.72	0.11	0.00	71,71,71,71	0
4	MG	A	801	1/1	0.66	0.09	-1.33	93,93,93,93	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.