



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 PM GMT

PDB ID : 4OST  
Title : Crystal structure of the S505C 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 : 2.00 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

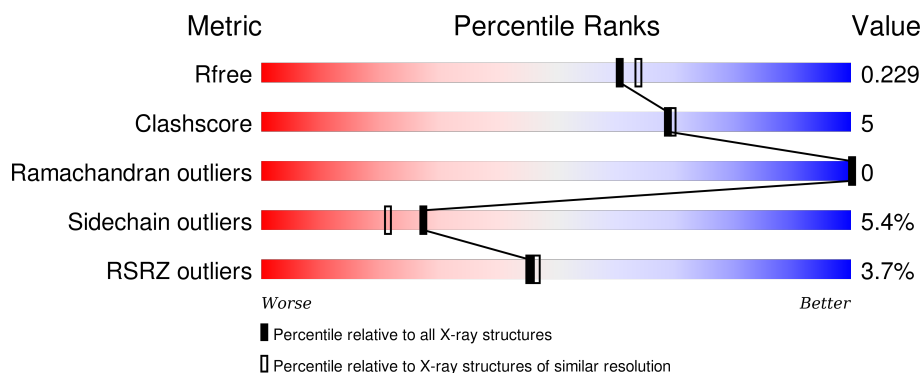
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>4%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	B	499	<div> <div>3%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
2	G	17	<div> <div>53%</div> <div>29%</div> <div>12%</div> <div>6%</div> </div>
2	I	17	<div> <div>6%</div> <div>71%</div> <div>29%</div> </div>
3	H	17	<div> <div>12%</div> <div>53%</div> <div>41%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	J	17	<div><div></div><div>65%</div><div>29%</div><div>6%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9075 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	493	Total	C	N	O	S	0	6	0
			3618	2262	675	668	13			
1	B	488	Total	C	N	O	S	0	8	0
			3587	2239	667	667	14			

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	CYS	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	CYS	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	16	Total	C	N	O	P	0	0	0
			314	154	44	101	15			
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	16	Total 339	C 159	N 75	O 89	P 16	0	0	0
3	J	17	Total 357	C 169	N 80	O 92	P 16	0	0	0

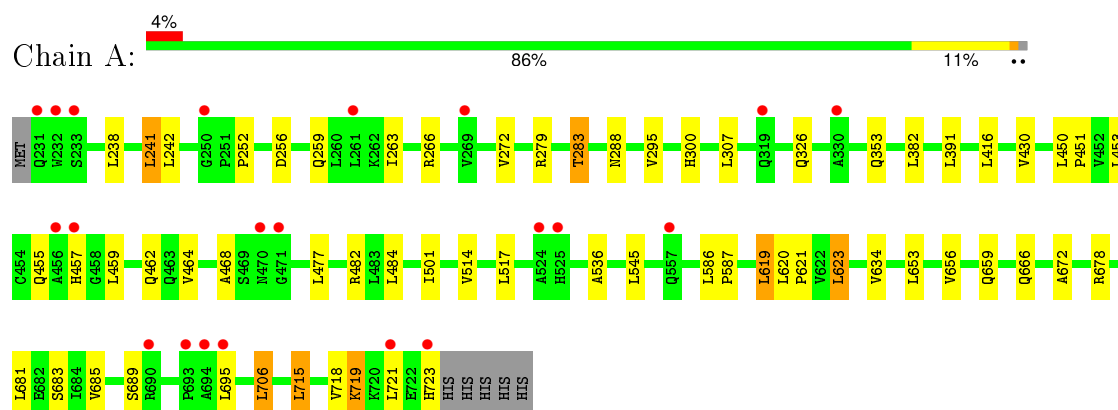
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	201	Total 201	O 201	0	0
4	B	195	Total 195	O 195	0	0
4	G	46	Total 46	O 46	0	0
4	H	19	Total 19	O 19	0	0
4	I	43	Total 43	O 43	0	0
4	J	22	Total 22	O 22	0	0

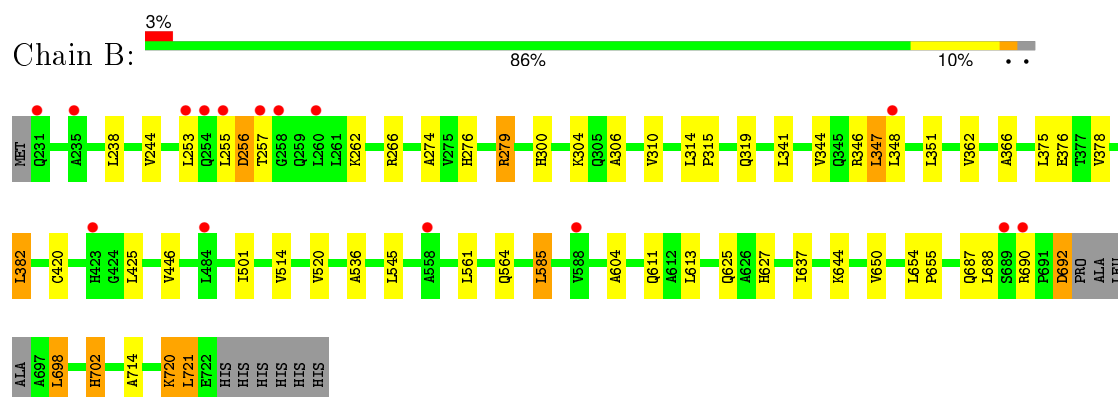
### 3 Residue-property plots [i](#)

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

- Molecule 1: Hax3



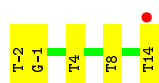
- Molecule 1: Hax3



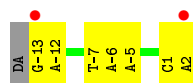
- Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*CP\*TP\*CP\*T)-3')



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



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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.12Å 87.02Å 87.91Å 90.00° 102.78° 90.00°	Depositor
Resolution (Å)	39.38 – 2.00 39.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.38-2.00) 99.5 (39.38-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.201 , 0.233 0.196 , 0.229	Depositor DCC
$R_{free}$ test set	4031 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80640 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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

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	0.36	0/3672	0.53	0/5016
1	B	0.36	0/3637	0.53	0/4964
2	G	0.75	0/347	1.55	8/532 (1.5%)
2	I	0.73	0/369	1.46	2/566 (0.4%)
3	H	0.64	0/384	1.17	0/592
3	J	0.71	1/405 (0.2%)	1.34	3/625 (0.5%)
All	All	0.44	1/8814 (0.0%)	0.77	13/12295 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	-2	DG	C3'-O3'	-5.06	1.37	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	-2	DG	O4'-C1'-N9	8.92	114.24	108.00
3	J	-13	DG	C3'-C2'-C1'	-6.45	94.76	102.50
2	G	-2	DT	N3-C4-O4	6.25	123.65	119.90
2	G	9	DC	O4'-C1'-N1	-5.93	103.85	108.00
2	G	12	DT	O4'-C1'-N1	-5.78	103.95	108.00
2	G	10	DT	N3-C4-O4	5.70	123.32	119.90
2	I	4	DT	O4'-C1'-N1	-5.59	104.08	108.00
2	G	13	DC	C3'-C2'-C1'	-5.55	95.84	102.50
2	G	-2	DT	C5-C4-O4	-5.40	121.12	124.90
2	G	2	DC	C1'-O4'-C4'	-5.28	104.82	110.10
2	G	12	DT	N3-C4-O4	5.23	123.04	119.90
2	I	8	DT	C1'-O4'-C4'	-5.05	105.05	110.10
3	J	-2	DG	C5-C6-O6	-5.04	125.58	128.60

There are no chirality outliers.

There are no planarity outliers.

## 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	3618	0	3758	29	0
1	B	3587	0	3719	37	0
2	G	314	0	186	3	0
2	I	334	0	198	3	0
3	H	339	0	178	5	0
3	J	357	0	190	4	0
4	A	201	0	0	1	0
4	B	195	0	0	1	0
4	G	46	0	0	0	0
4	H	19	0	0	0	0
4	I	43	0	0	0	0
4	J	22	0	0	0	0
All	All	9075	0	8229	75	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 5.

All (75) 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:H3	3:H:2:DA:H2	1.17	0.91
1:B:720:LYS:HG3	1:B:720:LYS:O	1.88	0.73
1:B:256:ASP:OD1	1:B:256:ASP:N	2.22	0.72
1:B:692:ASP:OD2	1:B:692:ASP:N	2.25	0.69
1:A:468:ALA:HB2	1:A:477:LEU:HD11	1.74	0.68
1:A:451:PRO:O	1:A:455:GLN:HG2	1.99	0.63
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.82	0.62
1:B:306:ALA:O	1:B:310:VAL:HG13	2.01	0.60
1:B:266:ARG:HG2	1:B:300:HIS:HA	1.83	0.60
1:B:721:LEU:HD12	2:I:14:DT:H72	1.84	0.60
1:B:698:LEU:HG	1:B:702:HIS:CD2	2.38	0.59
1:A:450:LEU:HD13	1:A:464:VAL:HG11	1.84	0.59
3:J:1:DC:H2"	3:J:2:DA:C8	2.39	0.58
1:A:238:LEU:O	1:A:242:LEU:HG	2.04	0.57
1:B:720:LYS:HB3	1:B:720:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ALA:HB2	1:B:304:LYS:HG3	1.88	0.55
1:B:425[A]:LEU:HD11	1:B:446:VAL:HG11	1.89	0.54
1:A:706:LEU:HD21	1:A:718:VAL:HG21	1.88	0.54
1:B:425[B]:LEU:HD11	1:B:446:VAL:HG11	1.90	0.54
1:A:619:LEU:HB3	1:A:623:LEU:HD22	1.88	0.54
1:A:672:ALA:HB2	1:A:681:LEU:HD11	1.90	0.53
1:A:721:LEU:HD13	1:B:714:ALA:HA	1.88	0.53
1:B:720:LYS:CG	1:B:720:LYS:O	2.56	0.53
2:I:-2:DT:H2''	2:I:-1:DG:C8	2.45	0.52
1:B:310:VAL:HG12	1:B:341:LEU:HD11	1.92	0.51
1:B:253:LEU:HD22	1:B:279:ARG:HB3	1.93	0.51
1:A:266:ARG:HG3	1:A:300:HIS:HA	1.93	0.51
1:B:501:ILE:HD13	1:B:514:VAL:HG21	1.94	0.50
1:B:611:GLN:HB3	1:B:644:LYS:HD2	1.94	0.50
1:B:720:LYS:O	2:I:14:DT:H3'	2.11	0.50
1:A:241:LEU:HD21	1:A:272:VAL:HG21	1.94	0.49
1:A:501:ILE:HD13	1:A:514:VAL:HG21	1.93	0.49
1:A:536:ALA:HB2	1:A:545:LEU:HD11	1.94	0.49
1:A:695:LEU:HD13	1:A:719:LYS:HG3	1.95	0.49
1:A:416:LEU:HD13	1:A:430:VAL:HG11	1.94	0.47
1:B:315:PRO:O	1:B:319:GLN:HB2	2.15	0.47
1:B:627:HIS:HB3	1:B:654:LEU:HD23	1.96	0.47
1:B:262:LYS:HE3	3:H:-5:DA:OP1	2.15	0.47
1:A:252:PRO:HD2	1:A:279[A]:ARG:NE	2.29	0.46
3:J:-8:DA:C8	3:J:-8:DA:H5'	2.51	0.46
2:G:-2:DT:H2'	2:G:-1:DG:C8	2.51	0.46
3:J:-8:DA:H5'	3:J:-8:DA:H8	1.81	0.46
1:B:604:ALA:HB2	1:B:613:LEU:HD11	1.97	0.46
1:B:344:VAL:O	1:B:348:LEU:HB2	2.16	0.46
1:B:244:VAL:HG13	1:B:276:HIS:HB2	1.98	0.46
1:B:378:VAL:O	1:B:382:LEU:HB2	2.16	0.46
1:A:263:ILE:HD11	1:A:295:VAL:HG22	1.99	0.45
1:B:654:LEU:HB3	1:B:655:PRO:HD3	1.98	0.45
1:A:482:ARG:NE	4:A:844:HOH:O	2.39	0.45
3:H:-7:DT:H2''	3:H:-6:DA:C8	2.52	0.45
1:A:620:LEU:HD13	1:A:634:VAL:HG11	1.99	0.45
1:B:420[B]:CYS:HA	1:B:425[B]:LEU:O	2.16	0.45
1:B:348:LEU:HD23	1:B:362:VAL:HG11	1.99	0.44
1:B:637:ILE:HD13	1:B:650:VAL:HG21	2.00	0.43
1:A:723:HIS:O	2:G:13:DC:C6	2.71	0.43
1:B:346:ARG:NH1	1:B:376:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:-14:DA:H2"	3:J:-13:DG:C8	2.54	0.43
1:B:366:ALA:HB2	1:B:375:LEU:HD11	2.01	0.43
1:B:319:GLN:NE2	4:B:968:HOH:O	2.51	0.43
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.87	0.43
1:A:256:ASP:OD2	1:A:259:GLN:HG3	2.19	0.42
3:H:1:DC:H2"	3:H:2:DA:C8	2.54	0.42
1:B:536:ALA:HB2	1:B:545:LEU:HD11	2.01	0.42
1:B:720:LYS:CB	1:B:720:LYS:NZ	2.82	0.42
1:B:585:LEU:HA	1:B:585:LEU:HD12	1.83	0.42
1:A:666:GLN:H	1:A:666:GLN:CD	2.22	0.42
1:A:683:SER:HB3	1:A:715:LEU:HD23	2.03	0.41
1:A:620:LEU:HB3	1:A:621:PRO:HD3	2.02	0.41
1:A:450:LEU:HB3	1:A:451:PRO:HD3	2.02	0.41
3:H:-13:DG:H2"	3:H:-12:DA:H5"	2.02	0.41
1:A:457:HIS:HB3	1:A:484:LEU:CD2	2.51	0.41
1:A:586:LEU:N	1:A:587:PRO:HD2	2.35	0.40
1:B:314:LEU:HB3	1:B:315:PRO:HD3	2.03	0.40
1:A:283:THR:O	1:A:288:ASN:HA	2.22	0.40
1:A:391:LEU:HD21	1:A:416:LEU:HD21	2.04	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	497/499 (100%)	483 (97%)	14 (3%)	0	100	100
1	B	492/499 (99%)	472 (96%)	20 (4%)	0	100	100
All	All	989/998 (99%)	955 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	381/383 (100%)	362 (95%)	19 (5%)	30	24
1	B	378/383 (99%)	357 (94%)	21 (6%)	26	20
All	All	759/766 (99%)	719 (95%)	40 (5%)	27	22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	283	THR
1	A	307	LEU
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	619	LEU
1	A	623	LEU
1	A	656	VAL
1	A	659	GLN
1	A	678	ARG
1	A	689	SER
1	A	706	LEU
1	A	715	LEU
1	A	719	LYS
1	B	238	LEU
1	B	255	LEU
1	B	256	ASP
1	B	257	THR
1	B	279	ARG
1	B	347	LEU
1	B	351	LEU
1	B	382	LEU

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Mol	Chain	Res	Type
1	B	520	VAL
1	B	561	LEU
1	B	564	GLN
1	B	585	LEU
1	B	625	GLN
1	B	687	GLN
1	B	688	LEU
1	B	690	ARG
1	B	692	ASP
1	B	698	LEU
1	B	702	HIS
1	B	720	LYS
1	B	721	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	436	ASN
1	A	470	ASN
1	A	723	HIS
1	B	702	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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	493/499 (98%)	0.12	21 (4%) 39 40	15, 29, 58, 94	14 (2%)
1	B	488/499 (97%)	0.07	15 (3%) 52 53	15, 28, 58, 93	13 (2%)
2	G	16/17 (94%)	-0.31	0 100 100	18, 21, 56, 56	0
2	I	17/17 (100%)	-0.03	1 (5%) 26 27	17, 21, 72, 105	0
3	H	16/17 (94%)	0.13	2 (12%) 5 5	31, 37, 76, 89	0
3	J	17/17 (100%)	0.39	0 100 100	25, 41, 85, 85	0
All	All	1047/1066 (98%)	0.10	39 (3%) 45 47	15, 28, 60, 105	27 (2%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423[A]	HIS	4.8
1	A	470	ASN	3.9
1	B	231	GLN	3.8
1	B	255	LEU	3.5
1	A	721	LEU	3.5
1	A	232	TRP	3.4
1	A	524	ALA	3.4
1	B	253	LEU	3.3
1	A	269[A]	VAL	3.2
1	B	260	LEU	2.9
1	A	456	ALA	2.8
1	B	257	THR	2.8
1	A	231	GLN	2.8
1	B	484	LEU	2.7
3	H	-13	DG	2.7
1	A	250	GLY	2.6
1	A	557	GLN	2.6
1	A	694	ALA	2.5
1	B	690	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	I	14	DT	2.4
1	A	261	LEU	2.4
1	B	254	GLN	2.4
1	A	233	SER	2.4
1	A	330	ALA	2.3
1	A	690	ARG	2.3
1	B	348	LEU	2.2
1	A	695	LEU	2.2
1	B	588	VAL	2.2
1	B	235	ALA	2.2
1	A	319	GLN	2.1
1	A	457	HIS	2.1
1	A	471	GLY	2.1
1	B	558	ALA	2.1
1	A	693	PRO	2.1
3	H	2	DA	2.0
1	B	689	SER	2.0
1	A	525	HIS	2.0
1	A	723	HIS	2.0
1	B	258	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.