



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 PM GMT

PDB ID : 4OSJ  
Title : Crystal structure of TAL effector reveals the recognition between asparagine and adenine  
Authors : Deng, D.; Wu, J.P.; Yan, C.Y.; Pan, X.J.; Yan, N.  
Deposited on : 2014-02-13  
Resolution : 2.79 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

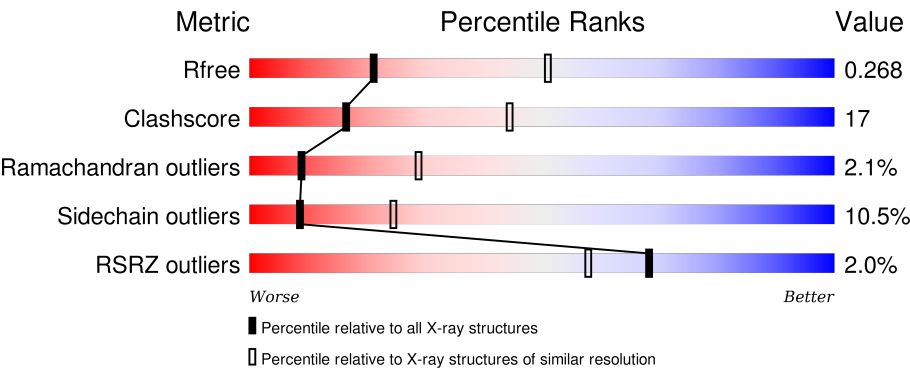
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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 <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 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	
1	B	499	
2	G	17	
2	I	17	
3	H	17	

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Mol	Chain	Length	Quality of chain
3	J	17	<div><div></div><div>65%</div><div>24%</div><div>6%</div><div>6%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8390 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	487	Total	C	N	O	S	15	0	0
			3514	2197	650	655	12			
1	B	489	Total	C	N	O	S	13	0	0
			3532	2206	658	656	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	ASN	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	ASN	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	I	16	Total	C	N	O	P	0	0	0
			316	153	44	103	16			
2	G	16	Total	C	N	O	P	0	0	0
			314	154	44	101	15			

- 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	J	16	Total 336	C 159	N 75	O 87	P 15	0	0	0
3	H	16	Total 339	C 159	N 75	O 89	P 16	0	0	0

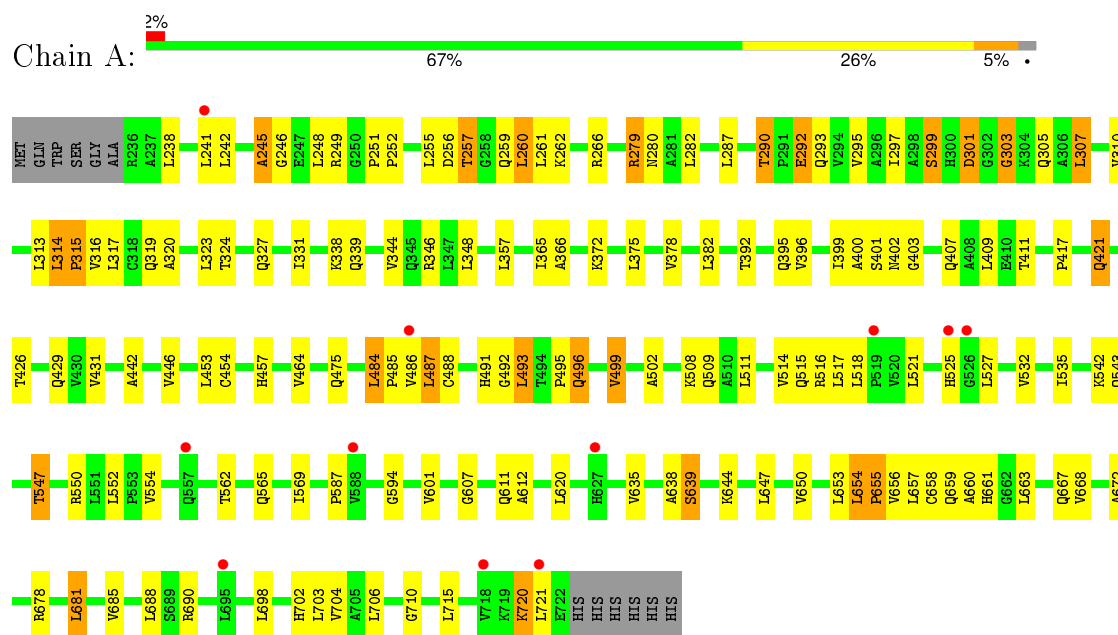
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total 8	O 8	0	0
4	I	4	Total 4	O 4	0	0
4	B	20	Total 20	O 20	0	0
4	G	7	Total 7	O 7	0	0

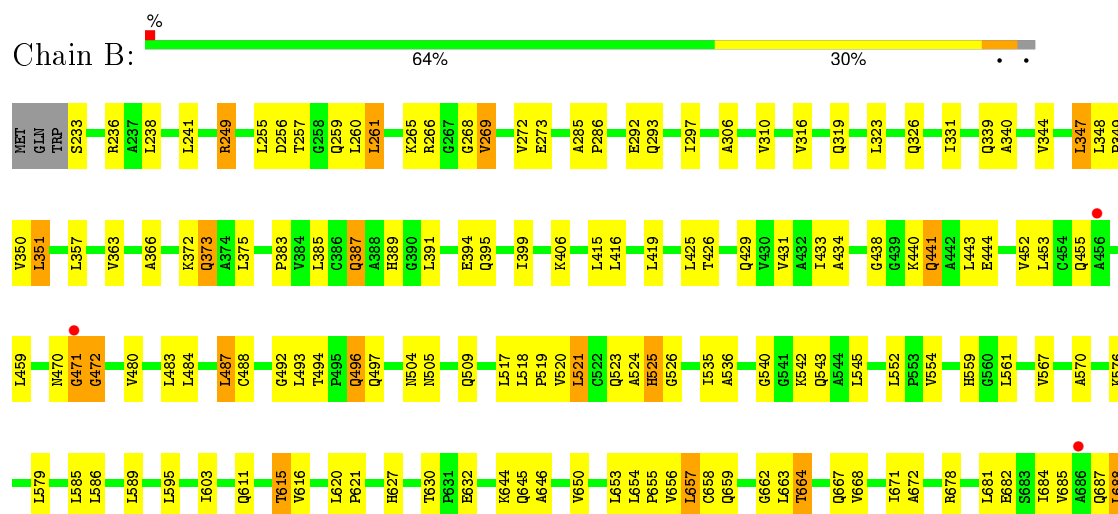
### 3 Residue-property plots

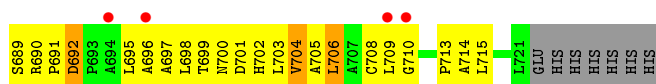
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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')



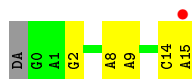
- Molecule 2: DNA (5'-D(\*TP\*GP\*TP\*CP\*CP\*CP\*TP\*TP\*TP\*AP\*TP\*CP\*TP\*CP\*TP\*CP\*T)-3')



- 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, $\alpha$ , $\beta$ , $\gamma$	84.41Å 80.81Å 88.82Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	38.06 – 2.79 38.06 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.06-2.79) 98.1 (38.06-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.214 , 0.271 0.212 , 0.268	Depositor DCC
$R_{free}$ test set	1442 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.4	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 28520 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8390	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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	0.40	0/3563	0.61	3/4868 (0.1%)
1	B	0.45	0/3581	0.66	3/4890 (0.1%)
2	G	0.78	0/347	1.56	7/532 (1.3%)
2	I	0.77	0/349	1.58	4/534 (0.7%)
3	H	0.73	0/384	1.48	2/592 (0.3%)
3	J	0.90	0/381	1.67	5/588 (0.9%)
All	All	0.51	0/8605	0.89	24/12004 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	LEU	O-C-N	15.47	147.44	122.70
1	A	245	ALA	N-CA-C	12.38	144.43	111.00
1	B	698	LEU	CA-C-N	-11.99	90.81	117.20
3	J	10	DG	O4'-C1'-N9	9.73	114.81	108.00
3	J	13	DA	O4'-C4'-C3'	-8.93	100.64	106.00
1	A	245	ALA	CB-CA-C	-8.12	97.93	110.10
2	G	10	DA	O4'-C1'-N9	7.93	113.55	108.00
3	H	8	DA	O4'-C1'-N9	7.86	113.50	108.00
2	G	8	DT	N3-C4-O4	7.25	124.25	119.90
2	I	13	DT	N3-C4-O4	7.05	124.13	119.90
1	B	698	LEU	C-N-CA	-6.40	105.71	121.70
2	I	9	DT	C1'-O4'-C4'	-5.93	104.17	110.10
2	I	13	DT	C5-C4-O4	-5.92	120.76	124.90
3	J	3	DA	O4'-C1'-C2'	-5.65	101.38	105.90
3	J	13	DA	O4'-C1'-N9	-5.58	104.10	108.00
2	G	13	DT	N3-C4-O4	5.56	123.23	119.90
2	G	5	DC	C1'-O4'-C4'	-5.48	104.62	110.10
3	J	13	DA	C1'-O4'-C4'	-5.43	104.67	110.10
2	G	4	DC	C1'-O4'-C4'	-5.42	104.69	110.10
2	G	8	DT	C5-C4-O4	-5.29	121.20	124.90
2	G	11	DT	C5-C4-O4	-5.18	121.27	124.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	7	DT	C1'-O4'-C4'	-5.14	104.96	110.10
3	H	9	DA	O4'-C1'-N9	5.10	111.57	108.00
1	A	246	GLY	N-CA-C	-5.09	100.38	113.10

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	3514	0	3661	138	0
1	B	3532	0	3690	128	0
2	G	314	0	186	13	0
2	I	316	0	182	3	0
3	H	339	0	178	4	0
3	J	336	0	179	2	0
4	A	8	0	0	0	0
4	B	20	0	0	6	0
4	G	7	0	0	0	0
4	I	4	0	0	0	0
All	All	8390	0	8076	271	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 17.

All (271) 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:A:262:LYS:HZ1	1:A:295:VAL:CG1	1.44	1.31
1:A:262:LYS:NZ	1:A:295:VAL:CG1	1.98	1.22
1:A:314:LEU:HD13	1:A:314:LEU:O	1.35	1.20
1:A:486:VAL:O	1:A:487:LEU:HD23	1.51	1.10
1:A:720:LYS:O	2:G:16:DC:H2'	1.57	1.03
1:A:262:LYS:HZ1	1:A:295:VAL:HG12	1.27	1.00
1:A:486:VAL:O	1:A:486:VAL:HG12	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HZ1	1:A:295:VAL:HG11	1.28	0.95
1:A:314:LEU:HD13	1:A:314:LEU:C	1.90	0.90
1:A:657:LEU:HD11	1:A:685:VAL:CG2	2.02	0.89
1:A:655:PRO:O	1:A:659:GLN:HB2	1.74	0.88
1:B:710:GLY:O	1:B:713:PRO:HG2	1.74	0.88
1:A:262:LYS:NZ	1:A:295:VAL:HG12	1.84	0.87
1:A:314:LEU:H	1:A:315:PRO:HD2	1.40	0.87
1:A:657:LEU:HD11	1:A:685:VAL:HG22	1.56	0.86
1:B:657:LEU:HD13	1:B:668:VAL:CG2	2.05	0.86
1:A:262:LYS:NZ	1:A:295:VAL:HG13	1.90	0.84
1:A:654:LEU:H	1:A:655:PRO:HD2	1.42	0.84
1:A:262:LYS:HZ3	1:A:295:VAL:CG1	1.87	0.84
1:A:262:LYS:HZ3	1:A:295:VAL:HG13	1.40	0.83
1:A:656:VAL:O	1:A:660:ALA:HB3	1.77	0.83
1:B:657:LEU:CD1	1:B:668:VAL:HG22	2.09	0.83
1:B:687:GLN:HE22	1:B:692:ASP:H	1.26	0.83
1:A:653:LEU:HD13	1:A:685:VAL:HG21	1.61	0.82
1:A:721:LEU:HD13	1:B:714:ALA:HA	1.62	0.81
1:B:703:LEU:O	1:B:703:LEU:HD23	1.80	0.80
1:B:657:LEU:O	1:B:657:LEU:CD2	2.30	0.80
1:A:657:LEU:HD21	1:A:685:VAL:HG22	1.62	0.80
1:A:486:VAL:O	1:A:487:LEU:CD2	2.31	0.78
3:H:15:DA:H4'	3:H:15:DA:OP1	1.83	0.78
1:A:314:LEU:N	1:A:315:PRO:HD2	1.97	0.78
1:A:486:VAL:O	1:A:486:VAL:CG1	2.30	0.78
1:B:657:LEU:HD13	1:B:668:VAL:HG22	1.65	0.78
1:B:373:GLN:HG3	1:B:406:LYS:HD3	1.66	0.77
2:G:1:DT:H2''	2:G:2:DG:OP2	1.84	0.77
1:B:525:HIS:HB3	1:B:552:LEU:HD23	1.65	0.77
1:A:454:CYS:SG	1:A:464:VAL:HG21	2.25	0.77
1:B:655:PRO:O	1:B:659:GLN:HG2	1.86	0.76
1:A:245:ALA:O	1:A:249:ARG:HG3	1.86	0.75
1:A:661:HIS:HB3	1:A:688:LEU:HD13	1.69	0.74
2:G:1:DT:H4'	2:G:2:DG:H5'	1.71	0.73
1:B:366:ALA:HB2	1:B:375:LEU:HD11	1.68	0.73
1:A:667:GLN:HG2	1:A:704:VAL:HG11	1.68	0.73
1:B:615:THR:HG21	1:B:644:LYS:HG3	1.71	0.73
3:H:15:DA:OP1	3:H:15:DA:C4'	2.37	0.72
1:A:668:VAL:HG13	1:A:681:LEU:HD21	1.69	0.72
1:A:720:LYS:O	2:G:16:DC:C2'	2.38	0.71
1:B:472:GLY:HA2	4:B:819:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:14:DC:H2"	3:H:15:DA:C8	2.26	0.71
1:B:419:LEU:HB3	1:B:425:LEU:HD22	1.71	0.70
1:A:314:LEU:C	1:A:314:LEU:CD1	2.60	0.70
1:B:657:LEU:O	1:B:657:LEU:HD22	1.90	0.70
1:A:657:LEU:CD1	1:A:685:VAL:HG22	2.21	0.70
1:A:484:LEU:HB3	1:A:485:PRO:HD3	1.74	0.70
1:B:695:LEU:C	1:B:697:ALA:H	1.93	0.70
1:A:287:LEU:HD23	1:A:314:LEU:HG	1.72	0.69
1:B:657:LEU:HD13	1:B:668:VAL:HG21	1.74	0.69
1:A:672:ALA:HB2	1:A:681:LEU:HD11	1.73	0.69
1:B:706:LEU:O	1:B:709:LEU:N	2.25	0.68
1:B:504:ASN:HB2	4:B:810:HOH:O	1.93	0.68
1:A:314:LEU:N	1:A:315:PRO:CD	2.57	0.67
1:B:657:LEU:O	1:B:657:LEU:HD23	1.94	0.67
1:A:698:LEU:HD23	1:A:702:HIS:ND1	2.07	0.67
1:A:654:LEU:N	1:A:655:PRO:HD2	2.09	0.67
1:A:654:LEU:H	1:A:655:PRO:CD	2.07	0.66
1:A:657:LEU:CD2	1:A:685:VAL:HG22	2.25	0.66
1:A:657:LEU:CG	1:A:685:VAL:HG22	2.26	0.66
1:A:638:ALA:HB2	1:A:647:LEU:HD11	1.76	0.66
1:B:249:ARG:HD2	1:B:255:LEU:O	1.96	0.66
2:G:1:DT:C4'	2:G:2:DG:H5'	2.26	0.66
1:B:645:GLN:HB3	1:B:678:ARG:HD2	1.77	0.65
1:A:721:LEU:HD22	1:B:713:PRO:HB2	1.78	0.65
1:B:441:GLN:NE2	2:G:7:DT:OP1	2.29	0.65
1:B:695:LEU:O	1:B:697:ALA:N	2.30	0.64
1:B:704:VAL:HG12	1:B:705:ALA:N	2.12	0.64
1:B:687:GLN:O	1:B:691:PRO:HB3	1.97	0.64
1:A:475:GLN:HB3	1:A:508:LYS:HD2	1.79	0.64
1:B:351:LEU:HG	1:B:357:LEU:HD12	1.80	0.64
1:A:654:LEU:O	1:A:654:LEU:HD12	1.98	0.64
1:A:654:LEU:N	1:A:655:PRO:CD	2.58	0.62
1:B:704:VAL:CG1	1:B:705:ALA:N	2.63	0.62
1:B:687:GLN:HE22	1:B:692:ASP:N	1.98	0.61
1:A:426:THR:HG21	1:B:387:GLN:HB2	1.83	0.61
1:A:487:LEU:HD21	1:A:515:GLN:HG3	1.82	0.61
2:G:1:DT:C2'	2:G:2:DG:OP2	2.48	0.61
1:A:417:PRO:O	1:A:421:GLN:HB2	2.01	0.61
1:B:535:ILE:HD11	1:B:567:VAL:HG22	1.83	0.61
1:A:315:PRO:O	1:A:319:GLN:HB3	2.01	0.61
1:A:316:VAL:O	1:A:320:ALA:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:CYS:HA	1:A:493:LEU:O	2.00	0.61
1:A:668:VAL:CG1	1:A:681:LEU:HD21	2.31	0.61
1:A:509:GLN:HB3	1:A:542:LYS:HD2	1.82	0.61
1:B:415:LEU:O	1:B:419:LEU:HG	2.02	0.60
2:I:17:DT:H3	3:J:-1:DA:H61	1.47	0.60
1:A:721:LEU:HD13	1:B:714:ALA:CA	2.32	0.60
1:B:630:THR:HG22	1:B:632:GLU:H	1.66	0.60
1:A:314:LEU:O	1:A:314:LEU:CD1	2.30	0.59
1:B:261:LEU:HD12	1:B:265:LYS:HE2	1.83	0.59
1:B:399:ILE:HD11	1:B:431:VAL:HG22	1.84	0.59
1:A:495:PRO:HB2	1:A:496:GLN:HE21	1.68	0.59
1:A:252:PRO:HD2	1:A:279:ARG:HG3	1.85	0.59
1:B:426:THR:OG1	1:B:429:GLN:HG3	2.03	0.59
1:B:657:LEU:HD11	1:B:668:VAL:HG22	1.82	0.58
1:B:630:THR:CG2	1:B:632:GLU:OE2	2.51	0.58
1:B:525:HIS:HB3	1:B:552:LEU:CD2	2.33	0.58
1:A:492:GLY:O	1:A:493:LEU:O	2.22	0.57
1:A:290:THR:HG22	1:A:293:GLN:H	1.70	0.57
1:B:611:GLN:O	1:B:615:THR:HG23	2.04	0.56
1:A:487:LEU:HD22	1:A:491:HIS:ND1	2.20	0.56
1:A:532:VAL:HA	1:A:535:ILE:HD12	1.86	0.56
1:B:438:GLY:N	4:B:806:HOH:O	2.37	0.56
1:A:721:LEU:CD1	1:B:714:ALA:HA	2.35	0.56
1:A:702:HIS:HB2	1:B:702:HIS:CE1	2.41	0.55
1:B:470:ASN:O	1:B:471:GLY:C	2.45	0.55
1:B:487:LEU:O	1:B:493:LEU:HB2	2.05	0.55
1:A:654:LEU:HB3	1:A:655:PRO:HD3	1.87	0.55
1:A:262:LYS:NZ	1:A:295:VAL:HG11	1.95	0.54
1:B:654:LEU:N	1:B:655:PRO:HD2	2.23	0.54
1:B:524:ALA:C	1:B:526:GLY:H	2.09	0.54
1:A:657:LEU:HB3	1:A:663:LEU:HD13	1.90	0.54
1:B:339:GLN:HB3	1:B:372:LYS:HD2	1.88	0.54
1:B:540:GLY:HA2	2:G:10:DA:OP2	2.08	0.54
1:B:620:LEU:HB3	1:B:621:PRO:HD3	1.89	0.54
1:A:365:ILE:HD13	1:A:378:VAL:HG21	1.89	0.53
1:A:569:ILE:HD11	1:A:601:VAL:HG22	1.89	0.53
1:B:543:GLN:HB3	1:B:576:LYS:HD2	1.90	0.53
1:B:627:HIS:HB3	1:B:654:LEU:HD23	1.90	0.53
1:B:630:THR:HG22	1:B:632:GLU:N	2.23	0.53
1:B:383:PRO:O	1:B:387:GLN:HG2	2.09	0.53
1:B:389:HIS:HB3	1:B:416:LEU:CD2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:HIS:NE2	1:B:702:HIS:HB3	2.23	0.52
1:B:306:ALA:HB2	4:B:818:HOH:O	2.08	0.52
1:A:279:ARG:HG2	1:A:280:ASN:N	2.25	0.52
1:A:611:GLN:HB3	1:A:644:LYS:HD3	1.90	0.52
1:A:650:VAL:O	1:A:654:LEU:HB2	2.09	0.52
1:A:681:LEU:O	1:A:685:VAL:HG23	2.10	0.52
1:A:668:VAL:HG13	1:A:681:LEU:CD2	2.37	0.52
1:B:646:ALA:O	1:B:650:VAL:HG23	2.09	0.52
1:A:256:ASP:OD1	1:A:259:GLN:HG3	2.10	0.52
1:A:492:GLY:O	1:A:493:LEU:C	2.48	0.51
1:B:672:ALA:HB2	1:B:681:LEU:HD11	1.92	0.51
1:A:657:LEU:HD21	1:A:685:VAL:HA	1.92	0.51
1:A:305:GLN:HB3	1:A:338:LYS:HD2	1.93	0.51
1:A:339:GLN:HB3	1:A:372:LYS:HD2	1.92	0.51
1:B:389:HIS:HB3	1:B:416:LEU:HD23	1.93	0.51
1:A:484:LEU:HB3	1:A:485:PRO:CD	2.39	0.51
1:A:238:LEU:O	1:A:242:LEU:HG	2.11	0.51
1:B:517:LEU:HB3	1:B:521:LEU:HD22	1.93	0.50
1:B:536:ALA:HB2	1:B:545:LEU:HD11	1.93	0.50
1:A:658:CYS:HA	1:A:663:LEU:O	2.11	0.50
1:B:695:LEU:C	1:B:697:ALA:N	2.60	0.50
1:B:470:ASN:O	1:B:471:GLY:O	2.30	0.50
1:A:400:ALA:HB2	1:A:409:LEU:HD11	1.92	0.50
1:A:502:ALA:HB2	1:A:511:LEU:HD11	1.94	0.50
1:B:453:LEU:HB3	1:B:459:LEU:HD12	1.94	0.50
1:B:687:GLN:NE2	1:B:692:ASP:H	2.02	0.50
1:B:440:LYS:O	1:B:444:GLU:HG3	2.12	0.50
1:A:426:THR:OG1	1:A:429:GLN:HG3	2.12	0.49
1:B:654:LEU:HD13	1:B:668:VAL:HG11	1.94	0.49
1:A:295:VAL:O	1:A:299:SER:OG	2.30	0.49
2:I:16:DC:H2"	2:I:17:DT:H5"	1.94	0.49
1:A:256:ASP:OD1	1:A:259:GLN:OE1	2.30	0.49
1:A:401:SER:O	1:A:402:ASN:ND2	2.45	0.49
1:B:496:GLN:N	1:B:496:GLN:OE1	2.45	0.49
1:A:251:PRO:O	1:A:279:ARG:NH2	2.46	0.49
1:A:297:ILE:HD13	1:A:310:VAL:HG21	1.94	0.49
1:B:524:ALA:O	1:B:526:GLY:N	2.46	0.49
1:B:700:ASN:HA	1:B:703:LEU:HB3	1.94	0.48
1:B:570:ALA:HB2	1:B:579:LEU:HD11	1.94	0.48
1:B:348:LEU:HB3	1:B:349:PRO:HD3	1.95	0.48
1:A:293:GLN:O	1:A:297:ILE:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLN:O	1:B:399:ILE:HG13	2.13	0.48
1:B:293:GLN:O	1:B:297:ILE:HG13	2.14	0.48
1:B:297:ILE:HD13	1:B:310:VAL:HG21	1.94	0.48
1:B:706:LEU:HA	1:B:706:LEU:HD23	1.62	0.48
1:A:484:LEU:CB	1:A:485:PRO:CD	2.92	0.48
1:B:687:GLN:OE1	1:B:687:GLN:HA	2.13	0.48
1:B:385:LEU:HB3	1:B:391:LEU:HD12	1.96	0.48
1:A:290:THR:HG22	1:A:293:GLN:HG3	1.95	0.48
1:B:471:GLY:HA3	1:B:505:ASN:CG	2.34	0.48
1:A:635:VAL:O	1:A:639:SER:HB2	2.14	0.48
1:A:702:HIS:CD2	1:B:702:HIS:HB3	2.49	0.48
1:B:657:LEU:CD1	1:B:668:VAL:CG2	2.76	0.48
1:B:483:LEU:HB3	1:B:487:LEU:HD23	1.95	0.48
1:B:434:ALA:HB2	1:B:443:LEU:HD11	1.94	0.48
1:B:429:GLN:O	1:B:433:ILE:HG13	2.13	0.47
1:A:525:HIS:CG	1:A:552:LEU:HD23	2.49	0.47
1:B:494:THR:OG1	1:B:497:GLN:HG2	2.14	0.47
1:B:483:LEU:HB3	1:B:487:LEU:CD2	2.45	0.47
1:B:488:CYS:HA	1:B:493:LEU:O	2.15	0.47
1:A:303:GLY:O	1:A:307:LEU:HD22	2.15	0.47
1:A:290:THR:HG23	1:A:292:GLU:HG2	1.96	0.47
1:A:287:LEU:CD2	1:A:314:LEU:HG	2.42	0.47
1:B:653:LEU:O	1:B:657:LEU:HB2	2.14	0.47
1:B:704:VAL:HG12	1:B:705:ALA:H	1.81	0.46
1:A:484:LEU:CB	1:A:485:PRO:HD3	2.44	0.46
1:B:509:GLN:HB3	1:B:542:LYS:HD2	1.96	0.46
1:A:257:THR:O	1:A:260:LEU:HD12	2.15	0.46
1:B:706:LEU:HD22	1:B:714:ALA:HB1	1.97	0.46
1:A:366:ALA:HB2	1:A:375:LEU:HD11	1.97	0.46
1:A:255:LEU:HA	1:A:259:GLN:OE1	2.16	0.46
1:A:403:GLY:HA3	2:I:7:DT:H72	1.96	0.46
1:B:480:VAL:HG13	1:B:484:LEU:HD12	1.98	0.46
1:A:457:HIS:CG	1:A:484:LEU:HD23	2.51	0.46
1:A:257:THR:HA	1:A:260:LEU:HD11	1.97	0.46
1:B:682:GLU:HA	1:B:685:VAL:HG12	1.98	0.46
1:B:688:LEU:HA	1:B:688:LEU:HD13	1.76	0.46
1:A:407:GLN:O	1:A:411:THR:OG1	2.29	0.45
1:A:315:PRO:O	1:A:319:GLN:CB	2.64	0.45
2:G:15:DT:O2	3:H:2:DG:N2	2.50	0.45
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.98	0.44
1:B:488:CYS:O	1:B:492:GLY:HA2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:LEU:CD2	1:B:657:LEU:C	2.81	0.44
1:A:657:LEU:HD21	1:A:685:VAL:CG2	2.41	0.44
1:A:565:GLN:O	1:A:569:ILE:HG13	2.18	0.44
1:A:266:ARG:HA	1:A:266:ARG:HD2	1.84	0.44
1:B:255:LEU:HA	1:B:259:GLN:OE1	2.18	0.43
1:B:663:LEU:HD12	1:B:664:THR:H	1.83	0.43
1:A:317:LEU:HB3	1:A:323:LEU:HD12	1.99	0.43
1:B:611:GLN:HB3	1:B:644:LYS:HD2	2.00	0.43
1:A:442:ALA:O	1:A:446:VAL:HG23	2.19	0.43
1:A:495:PRO:O	1:A:499:VAL:HG13	2.19	0.43
1:A:256:ASP:OD1	1:A:259:GLN:CG	2.66	0.43
1:A:399:ILE:HD11	1:A:431:VAL:HG22	2.00	0.43
1:A:324:THR:OG1	1:A:327:GLN:HG3	2.19	0.43
1:B:331:ILE:HD11	1:B:363:VAL:HG22	2.01	0.43
1:B:285:ALA:HA	1:B:286:PRO:HA	1.77	0.43
1:B:654:LEU:H	1:B:655:PRO:HD2	1.83	0.43
1:A:521:LEU:HD22	1:A:525:HIS:HD2	1.82	0.43
1:A:491:HIS:HB3	1:A:518:LEU:CD2	2.48	0.43
1:B:603:ILE:HD13	1:B:616:VAL:HG21	2.00	0.43
2:G:1:DT:H2'	2:G:1:DT:H6	1.70	0.43
1:A:484:LEU:HD12	1:A:484:LEU:HA	1.81	0.43
1:A:392:THR:OG1	1:A:395:GLN:HG3	2.18	0.43
1:B:268:GLY:O	1:B:272:VAL:HG23	2.19	0.43
1:A:382:LEU:HD12	1:A:396:VAL:HG11	2.01	0.43
1:B:480:VAL:O	1:B:484:LEU:HB2	2.19	0.42
1:B:472:GLY:HA3	4:B:820:HOH:O	2.18	0.42
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.89	0.42
1:B:699:THR:HG23	1:B:702:HIS:H	1.84	0.42
1:A:331:ILE:HD13	1:A:344:VAL:HG21	2.01	0.42
1:A:543:GLN:O	1:A:547:THR:OG1	2.31	0.42
2:G:1:DT:H4'	2:G:2:DG:C5'	2.45	0.42
1:A:255:LEU:HD23	1:A:255:LEU:N	2.35	0.42
1:B:700:ASN:O	1:B:704:VAL:N	2.53	0.42
1:A:678:ARG:HH11	1:A:678:ARG:HG3	1.85	0.42
1:B:559:HIS:HB3	1:B:586:LEU:HD22	2.02	0.42
1:B:517:LEU:O	1:B:521:LEU:HB2	2.20	0.41
1:B:655:PRO:C	1:B:657:LEU:H	2.23	0.41
2:G:1:DT:C1'	2:G:2:DG:H5'	2.51	0.41
1:A:491:HIS:HB3	1:A:518:LEU:HD23	2.02	0.41
1:A:262:LYS:HE2	1:A:299:SER:OG	2.20	0.41
1:B:340:ALA:O	1:B:344:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:LEU:HB3	1:B:710:GLY:HA3	2.03	0.41
1:A:348:LEU:HD12	1:A:348:LEU:O	2.20	0.41
1:B:233:SER:HA	1:B:236:ARG:HB3	2.03	0.41
1:B:706:LEU:O	1:B:708:CYS:N	2.54	0.41
1:A:706:LEU:HD21	1:A:715:LEU:HA	2.03	0.41
1:B:269:VAL:O	1:B:273:GLU:HG3	2.21	0.41
1:B:441:GLN:H	1:B:441:GLN:HG2	1.60	0.41
1:B:441:GLN:NE2	2:G:7:DT:H5"	2.36	0.41
1:B:260:LEU:HD13	1:B:260:LEU:HA	1.91	0.41
1:B:671:ILE:HD13	1:B:684:ILE:HD12	2.01	0.41
1:B:347:LEU:O	1:B:351:LEU:HB2	2.22	0.41
3:J:3:DA:H2"	3:J:4:DG:H8	1.86	0.41
1:A:310:VAL:O	1:A:314:LEU:HB2	2.20	0.40
1:A:496:GLN:HG2	1:A:496:GLN:H	1.56	0.40
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.94	0.40
1:B:438:GLY:HA2	4:B:806:HOH:O	2.21	0.40
1:B:496:GLN:H	1:B:496:GLN:CD	2.25	0.40
1:B:348:LEU:HB3	1:B:349:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/499 (97%)	423 (87%)	48 (10%)	14 (3%)	6	19
1	B	487/499 (98%)	448 (92%)	33 (7%)	6 (1%)	16	47
All	All	972/998 (97%)	871 (90%)	81 (8%)	20 (2%)	9	29

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	493	LEU
1	B	696	ALA
1	A	607	GLY
1	A	655	PRO
1	B	471	GLY
1	B	525	HIS
1	B	662	GLY
1	A	257	THR
1	A	303	GLY
1	A	315	PRO
1	A	594	GLY
1	A	639	SER
1	B	472	GLY
1	A	301	ASP
1	A	487	LEU
1	A	690	ARG
1	A	612	ALA
1	B	519	PRO
1	A	587	PRO
1	A	710	GLY

### 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	371/383 (97%)	340 (92%)	31 (8%)	14	37
1	B	373/383 (97%)	326 (87%)	47 (13%)	5	17
All	All	744/766 (97%)	666 (90%)	78 (10%)	8	24

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	260	LEU
1	A	261	LEU
1	A	279	ARG

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Mol	Chain	Res	Type
1	A	282	LEU
1	A	290	THR
1	A	292	GLU
1	A	299	SER
1	A	301	ASP
1	A	307	LEU
1	A	313	LEU
1	A	314	LEU
1	A	346	ARG
1	A	357	LEU
1	A	421	GLN
1	A	453	LEU
1	A	484	LEU
1	A	496	GLN
1	A	499	VAL
1	A	514	VAL
1	A	516	ARG
1	A	517	LEU
1	A	527	LEU
1	A	547	THR
1	A	550	ARG
1	A	554	VAL
1	A	562	THR
1	A	620	LEU
1	A	654	LEU
1	A	681	LEU
1	A	720	LYS
1	B	238	LEU
1	B	241	LEU
1	B	249	ARG
1	B	256	ASP
1	B	257	THR
1	B	261	LEU
1	B	266	ARG
1	B	269	VAL
1	B	292	GLU
1	B	316	VAL
1	B	319	GLN
1	B	323	LEU
1	B	326	GLN
1	B	347	LEU
1	B	350	VAL

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Mol	Chain	Res	Type
1	B	351	LEU
1	B	373	GLN
1	B	387	GLN
1	B	394	GLU
1	B	441	GLN
1	B	452	VAL
1	B	455	GLN
1	B	487	LEU
1	B	496	GLN
1	B	518	LEU
1	B	520	VAL
1	B	521	LEU
1	B	523	GLN
1	B	554	VAL
1	B	561	LEU
1	B	585	LEU
1	B	589	LEU
1	B	595	LEU
1	B	615	THR
1	B	656	VAL
1	B	657	LEU
1	B	658	CYS
1	B	664	THR
1	B	667	GLN
1	B	688	LEU
1	B	689	SER
1	B	690	ARG
1	B	692	ASP
1	B	701	ASP
1	B	704	VAL
1	B	706	LEU
1	B	715	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	525	HIS
1	B	441	GLN
1	B	470	ASN
1	B	687	GLN
1	B	700	ASN

### 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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	487/499 (97%)	0.04	11 (2%) 64 52	29, 56, 92, 126	14 (2%)
1	B	489/499 (97%)	-0.07	7 (1%) 78 69	22, 44, 86, 144	11 (2%)
2	G	16/17 (94%)	-0.26	1 (6%) 23 14	34, 38, 99, 110	0
2	I	16/17 (94%)	-0.42	1 (6%) 23 14	34, 47, 87, 138	0
3	H	16/17 (94%)	0.32	1 (6%) 23 14	37, 54, 116, 138	0
3	J	16/17 (94%)	-0.37	0 100 100	49, 58, 97, 119	0
All	All	1040/1066 (97%)	-0.03	21 (2%) 68 58	22, 50, 92, 144	25 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	15	DA	6.4
1	A	721	LEU	4.2
1	B	696	ALA	3.1
1	A	718	VAL	2.8
1	A	486	VAL	2.6
1	B	709	LEU	2.6
1	A	695	LEU	2.6
1	B	686	ALA	2.5
2	G	1	DT	2.4
1	A	519	PRO	2.3
1	B	694	ALA	2.3
1	B	471	GLY	2.3
1	A	526	GLY	2.2
1	A	241	LEU	2.2
1	A	557	GLN	2.2
1	A	525	HIS	2.1
1	A	588	VAL	2.1
1	B	456	ALA	2.1
1	B	710	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	I	17	DT	2.0
1	A	627	HIS	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.