



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:26 PM GMT

PDB ID : 1P27  
Title : Crystal Structure of the Human Y14/Magoh complex  
Authors : Lau, C.K.; Diem, M.D.; Dreyfuss, G.; Van Duyne, G.D.  
Deposited on : 2003-04-14  
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

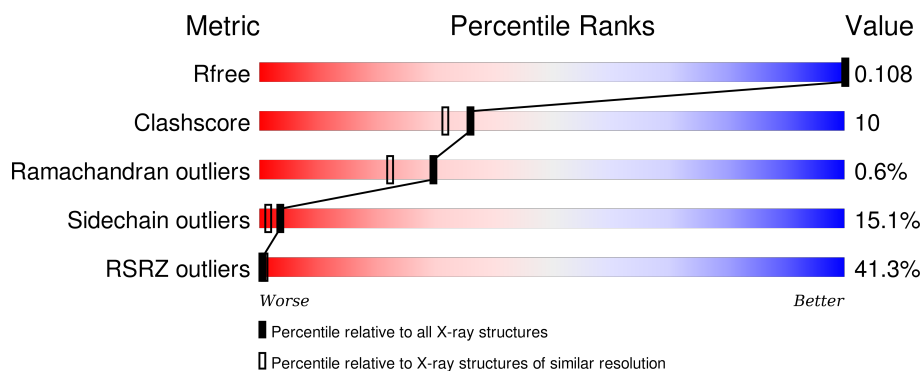
# 1 Overall quality at a glance

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	144	<div> <div>31%</div> <div> <div>73%</div> <div>21%</div> <div>5%</div> </div> </div>
1	C	144	<div> <div>39%</div> <div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>
2	B	106	<div> <div>38%</div> <div> <div>70%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
2	D	106	<div> <div>52%</div> <div> <div>51%</div> <div>29%</div> <div>7%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3966 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 Mago nashi protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total	C	N	O	S	0	0	0
			1196	771	200	222	3			
1	C	144	Total	C	N	O	S	0	0	0
			1196	771	200	222	3			

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			737	468	123	143	3			
2	D	92	Total	C	N	O	S	0	0	0
			737	468	123	143	3			

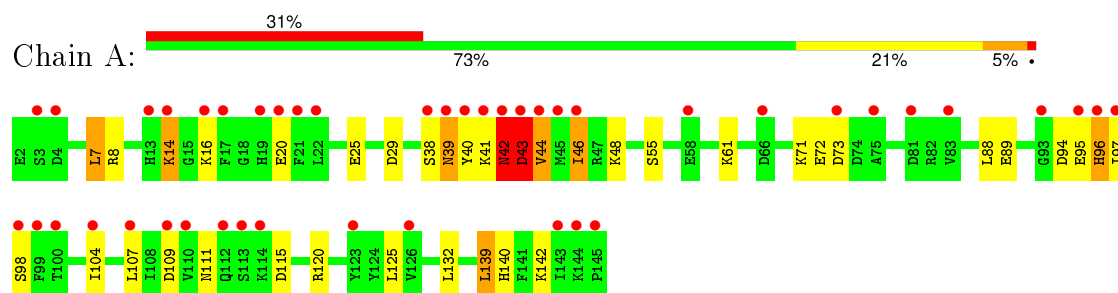
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	12	Total	O	0	0
			12	12		
3	C	41	Total	O	0	0
			41	41		
3	D	14	Total	O	0	0
			14	14		

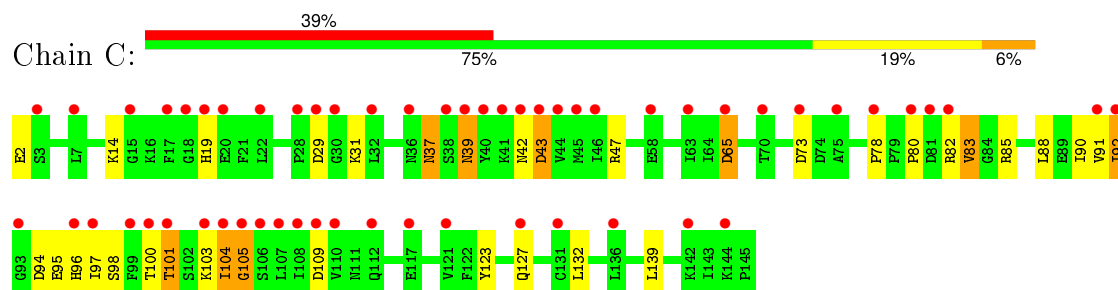
### 3 Residue-property plots [i](#)

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.

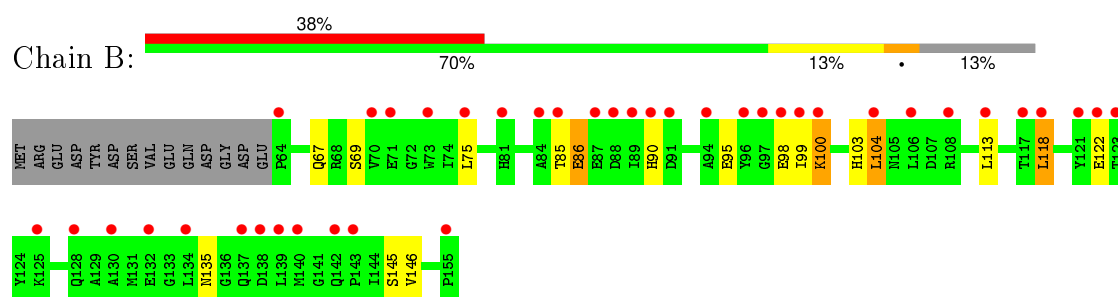
#### • Molecule 1: Mago nashi protein homolog



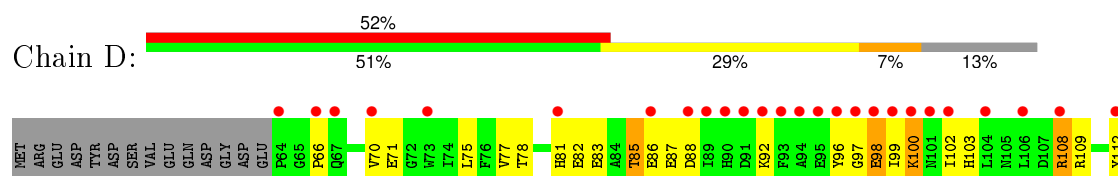
#### • Molecule 1: Mago nashi protein homolog

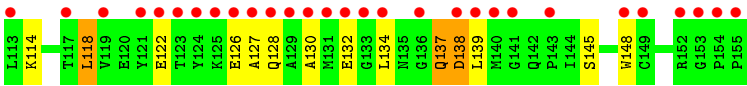


#### • Molecule 2: RNA-binding protein 8A



#### • Molecule 2: RNA-binding protein 8A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.15Å 108.45Å 50.94Å 90.00° 90.24° 90.00°	Depositor
Resolution (Å)	46.11 – 2.00 46.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.8 (46.11-2.00) 97.7 (46.11-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.21 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.220 , 0.268 0.329 , 0.108	Depositor DCC
$R_{free}$ test set	1698 reflections (5.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.8	EDS
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.64$ , $\langle L^2 \rangle = 0.51$	Xtriage
Outliers	0 of 33810 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.74% 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	0.80	0/1225	0.97	6/1649 (0.4%)
1	C	0.73	0/1225	0.98	7/1649 (0.4%)
2	B	0.78	0/756	0.87	1/1024 (0.1%)
2	D	0.78	0/756	0.89	2/1024 (0.2%)
All	All	0.77	0/3962	0.94	16/5346 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	94	ASP	CB-CG-OD2	6.63	124.26	118.30
1	C	85	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	109	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	73	ASP	CB-CG-OD2	6.21	123.89	118.30
2	D	138	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	85	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	29	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	115	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	65	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	118	LEU	CA-CB-CG	5.65	128.30	115.30
2	D	88	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	73	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	29	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	43	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	43	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	94	ASP	CB-CG-OD2	5.04	122.83	118.30

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	1196	0	1177	22	1
1	C	1196	0	1177	23	1
2	B	737	0	697	12	0
2	D	737	0	697	23	0
3	A	33	0	0	1	0
3	B	12	0	0	0	0
3	C	41	0	0	0	0
3	D	14	0	0	1	0
All	All	3966	0	3748	73	1

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 10.

All (73) 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:8:ARG:NH1	1:A:89:GLU:OE1	1.86	1.08
1:C:90:ILE:O	1:C:96:HIS:HD2	1.46	0.99
1:C:90:ILE:O	1:C:96:HIS:CD2	2.34	0.81
1:C:37:ASN:ND2	1:C:37:ASN:O	2.15	0.80
1:C:91:VAL:HG22	1:C:96:HIS:CD2	2.20	0.76
2:D:114:LYS:O	3:D:157:HOH:O	2.08	0.70
1:C:104:ILE:O	1:C:105:GLY:O	2.15	0.65
1:C:37:ASN:C	1:C:37:ASN:ND2	2.49	0.63
2:D:100:LYS:HZ1	2:D:122:GLU:HB2	1.65	0.62
1:A:44:VAL:HG13	1:A:46:ILE:HG22	1.81	0.61
1:C:80:PRO:HG3	1:C:100:THR:HG22	1.83	0.59
1:C:39:ASN:HA	1:C:42:ASN:O	2.03	0.58
1:A:111:ASN:OD1	1:A:120:ARG:NH1	2.37	0.57
1:A:140:HIS:HD2	2:B:69:SER:OG	1.87	0.56
2:B:135:ASN:HD22	2:B:146:VAL:H	1.54	0.55
2:D:98:GLU:HB3	2:D:100:LYS:NZ	2.22	0.55
2:D:118:LEU:N	2:D:118:LEU:HD23	2.22	0.55
1:A:39:ASN:HA	1:A:43:ASP:HA	1.88	0.54
1:C:91:VAL:CG2	1:C:96:HIS:NE2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASN:HD22	1:A:39:ASN:C	2.11	0.53
1:C:78:PRO:O	1:C:101:THR:HG22	2.09	0.52
2:D:96:TYR:HB2	2:D:130:ALA:HB2	1.91	0.52
2:D:99:ILE:HG21	2:D:102:ILE:HG13	1.91	0.52
1:C:91:VAL:CG2	1:C:96:HIS:CD2	2.91	0.52
1:A:44:VAL:CG1	1:A:46:ILE:HG22	2.38	0.52
1:C:123:TYR:CE2	1:C:127:GLN:OE1	2.64	0.50
1:A:43:ASP:N	1:C:14:LYS:HZ1	2.10	0.50
2:B:100:LYS:HB2	2:B:100:LYS:NZ	2.27	0.50
1:C:90:ILE:HG22	1:C:92:ILE:HG13	1.92	0.50
1:A:43:ASP:HB3	1:C:19:HIS:HB2	1.93	0.50
2:D:66:PRO:HB3	2:D:148:TRP:CD2	2.47	0.49
1:C:91:VAL:HG22	1:C:96:HIS:CG	2.48	0.48
1:A:7:LEU:HD13	1:A:8:ARG:N	2.28	0.48
1:A:8:ARG:HH12	1:A:89:GLU:CB	2.27	0.48
2:D:66:PRO:HB3	2:D:148:TRP:CG	2.50	0.47
1:C:91:VAL:HG23	1:C:96:HIS:NE2	2.28	0.47
1:A:8:ARG:NH1	1:A:89:GLU:HB3	2.30	0.46
2:D:85:THR:HG22	2:D:87:GLU:N	2.30	0.46
1:A:8:ARG:NH1	1:A:89:GLU:CB	2.78	0.46
2:D:98:GLU:HB3	2:D:100:LYS:HZ2	1.79	0.46
2:B:104:LEU:HD22	2:B:113:LEU:HD13	1.99	0.45
1:A:96:HIS:CE1	3:A:154:HOH:O	2.70	0.45
2:D:66:PRO:HB3	2:D:148:TRP:CD1	2.52	0.45
2:D:70:VAL:HG12	2:D:71:GLU:HG3	1.99	0.45
2:D:128:GLN:NE2	2:D:132:GLU:OE1	2.50	0.45
1:A:20:GLU:HG2	1:A:38:SER:HA	1.98	0.44
1:A:46:ILE:CD1	1:A:48:LYS:HG2	2.47	0.44
2:D:97:GLY:HA3	2:D:126:GLU:HG2	1.99	0.44
1:A:8:ARG:HH12	1:A:89:GLU:HB2	1.82	0.44
2:B:90:HIS:CD2	2:B:99:ILE:HD12	2.52	0.44
1:A:14:LYS:HD2	1:A:14:LYS:H	1.82	0.44
1:C:83:VAL:CG1	1:C:103:LYS:HE3	2.47	0.43
2:B:135:ASN:HD22	2:B:145:SER:HA	1.84	0.43
2:D:66:PRO:HB3	2:D:148:TRP:CE2	2.54	0.43
2:D:77:VAL:HA	2:D:145:SER:O	2.19	0.43
1:A:43:ASP:HB3	1:C:14:LYS:HZ3	1.84	0.43
1:C:80:PRO:CG	1:C:100:THR:HG22	2.48	0.42
1:C:92:ILE:HD12	1:C:95:GLU:HB2	2.00	0.42
2:B:85:THR:C	2:B:104:LEU:HD11	2.40	0.42
2:D:75:LEU:HD11	2:D:127:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:GLU:HA	2:B:104:LEU:HD12	2.02	0.42
2:D:99:ILE:HG21	2:D:102:ILE:CG1	2.50	0.42
2:B:86:GLU:N	2:B:104:LEU:CD1	2.83	0.42
1:A:42:ASN:ND2	1:C:14:LYS:NZ	2.68	0.41
2:D:96:TYR:CG	2:D:130:ALA:HA	2.54	0.41
2:D:81:HIS:CD2	2:D:83:GLU:H	2.39	0.41
2:B:104:LEU:CD2	2:B:113:LEU:HD13	2.51	0.41
1:A:42:ASN:O	1:A:44:VAL:N	2.53	0.41
2:D:82:GLU:HB3	2:D:112:TYR:HB3	2.03	0.41
1:A:139:LEU:HD21	2:B:103:HIS:ND1	2.36	0.41
2:B:86:GLU:N	2:B:104:LEU:HD12	2.35	0.40
1:C:127:GLN:HE22	2:D:108:ARG:HE	1.68	0.40
2:D:134:LEU:HA	2:D:137:GLN:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	1:C:109:ASP:OD1[1_556]	1.98	0.22

## 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	142/144 (99%)	136 (96%)	4 (3%)	2 (1%)	14	6
1	C	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	26	19
2	B	90/106 (85%)	89 (99%)	1 (1%)	0	100	100
2	D	90/106 (85%)	88 (98%)	2 (2%)	0	100	100
All	All	464/500 (93%)	447 (96%)	14 (3%)	3 (1%)	30	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	43	ASP
1	C	105	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	132/132 (100%)	108 (82%)	24 (18%)	2	1
1	C	132/132 (100%)	115 (87%)	17 (13%)	5	3
2	B	77/90 (86%)	68 (88%)	9 (12%)	7	3
2	D	77/90 (86%)	64 (83%)	13 (17%)	2	1
All	All	418/444 (94%)	355 (85%)	63 (15%)	3	1

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	LYS
1	A	16	LYS
1	A	25	GLU
1	A	39	ASN
1	A	40	TYR
1	A	41	LYS
1	A	42	ASN
1	A	44	VAL
1	A	46	ILE
1	A	55	SER
1	A	71	LYS
1	A	72	GLU
1	A	88	LEU
1	A	95	GLU
1	A	96	HIS
1	A	97	ILE
1	A	98	SER
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	107	LEU
1	A	125	LEU
1	A	132	LEU
1	A	139	LEU
1	A	142	LYS
2	B	67	GLN
2	B	75	LEU
2	B	86	GLU
2	B	95	GLU
2	B	98	GLU
2	B	100	LYS
2	B	104	LEU
2	B	118	LEU
2	B	122	GLU
1	C	2	GLU
1	C	31	LYS
1	C	37	ASN
1	C	39	ASN
1	C	43	ASP
1	C	47	ARG
1	C	65	ASP
1	C	82	ARG
1	C	83	VAL
1	C	88	LEU
1	C	92	ILE
1	C	97	ILE
1	C	98	SER
1	C	101	THR
1	C	104	ILE
1	C	132	LEU
1	C	139	LEU
2	D	78	THR
2	D	85	THR
2	D	86	GLU
2	D	92	LYS
2	D	98	GLU
2	D	100	LYS
2	D	103	HIS
2	D	108	ARG
2	D	109	ARG
2	D	118	LEU
2	D	137	GLN

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Mol	Chain	Res	Type
2	D	138	ASP
2	D	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	39	ASN
1	A	42	ASN
1	A	86	GLN
1	A	140	HIS
2	B	67	GLN
2	B	90	HIS
2	B	103	HIS
2	B	135	ASN
1	C	37	ASN
1	C	86	GLN
1	C	96	HIS
1	C	140	HIS
2	D	81	HIS
2	D	103	HIS
2	D	135	ASN

### 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 [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	144/144 (100%)	2.37	44 (30%)  	8, 16, 34, 53	0
1	C	144/144 (100%)	2.18	56 (38%)  	7, 16, 34, 49	0
2	B	92/106 (86%)	2.35	40 (43%)  	18, 27, 35, 38	0
2	D	92/106 (86%)	3.09	55 (59%)  	21, 32, 41, 45	0
All	All	472/500 (94%)	2.45	195 (41%)  	7, 21, 38, 53	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	TYR	28.2
1	A	42	ASN	19.4
1	A	41	LYS	18.9
1	A	43	ASP	17.8
1	A	40	TYR	14.5
2	D	133	GLY	12.3
1	A	39	ASN	10.8
1	A	17	PHE	9.5
1	A	44	VAL	8.9
2	D	64	PRO	8.7
1	C	41	LYS	8.3
2	D	98	GLU	8.3
1	C	44	VAL	8.1
2	B	97	GLY	8.0
1	C	18	GLY	7.9
1	C	39	ASN	7.9
2	D	96	TYR	7.8
2	B	132	GLU	7.8
2	D	154	PRO	7.8
2	B	94	ALA	7.6
1	C	96	HIS	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	114	LYS	6.6
2	B	89	ILE	6.4
1	C	38	SER	6.2
2	D	125	LYS	6.2
2	D	119	VAL	5.9
2	D	155	PRO	5.8
2	D	86	GLU	5.8
2	D	91	ASP	5.6
1	C	19	HIS	5.5
2	D	141	GLY	5.4
1	A	98	SER	5.4
2	D	108	ARG	5.4
2	D	138	ASP	5.2
2	D	89	ILE	5.2
1	C	110	VAL	5.0
1	C	43	ASP	4.9
1	C	82	ARG	4.9
2	B	108	ARG	4.9
2	D	139	LEU	4.8
2	B	96	TYR	4.8
2	D	95	GLU	4.7
2	B	100	LYS	4.7
1	A	19	HIS	4.6
2	D	94	ALA	4.6
2	D	104	LEU	4.6
2	D	123	THR	4.6
2	B	98	GLU	4.5
2	D	148	TRP	4.5
2	B	140	MET	4.5
2	B	143	PRO	4.4
1	C	97	ILE	4.4
1	C	15	GLY	4.4
1	A	66	ASP	4.3
2	B	122	GLU	4.3
1	A	145	PRO	4.3
2	D	124	TYR	4.2
2	D	121	TYR	4.2
2	B	91	ASP	4.2
2	D	99	ILE	4.2
2	B	128	GLN	4.1
1	C	108	ILE	4.1
1	A	144	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	100	THR	4.0
1	A	113	SER	4.0
2	D	97	GLY	4.0
1	A	96	HIS	4.0
2	D	130	ALA	4.0
2	D	122	GLU	4.0
1	A	104	ILE	4.0
1	C	45	MET	3.9
1	C	75	ALA	3.9
2	D	152	ARG	3.9
1	C	20	GLU	3.9
2	B	138	ASP	3.8
2	D	73	TRP	3.8
1	C	105	GLY	3.8
2	B	125	LYS	3.8
1	C	30	GLY	3.8
1	A	97	ILE	3.7
2	B	155	PRO	3.7
2	D	127	ALA	3.7
1	A	58	GLU	3.7
2	D	92	LYS	3.6
1	A	14	LYS	3.6
1	C	104	ILE	3.6
2	B	123	THR	3.6
1	C	117	GLU	3.5
1	A	21	PHE	3.5
1	A	81	ASP	3.5
2	B	139	LEU	3.5
1	C	42	ASN	3.5
2	D	136	GLY	3.5
2	D	117	THR	3.5
1	A	110	VAL	3.4
1	A	38	SER	3.4
2	D	90	HIS	3.4
2	B	142	GLN	3.4
1	C	107	LEU	3.4
2	D	132	GLU	3.3
1	C	92	ILE	3.3
2	D	128	GLN	3.3
1	C	17	PHE	3.3
1	A	107	LEU	3.3
2	B	85	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	100	LYS	3.3
1	A	46	ILE	3.3
1	C	73	ASP	3.3
1	C	109	ASP	3.3
2	D	131	MET	3.3
1	A	13	HIS	3.2
1	C	58	GLU	3.2
2	B	121	TYR	3.2
2	B	90	HIS	3.2
1	A	20	GLU	3.1
2	B	137	GLN	3.1
2	B	87	GLU	3.1
2	D	101	ASN	3.1
2	D	134	LEU	3.1
1	C	46	ILE	3.1
2	B	71	GLU	3.0
1	A	75	ALA	3.0
2	B	130	ALA	3.0
1	C	65	ASP	3.0
2	D	140	MET	3.0
2	B	99	ILE	3.0
1	C	81	ASP	3.0
2	D	93	PHE	3.0
1	C	3	SER	3.0
1	A	4	ASP	2.9
1	A	95	GLU	2.8
2	D	106	LEU	2.8
2	D	153	GLY	2.8
1	A	112	GLN	2.8
2	B	75	LEU	2.8
2	B	113	LEU	2.8
2	D	81	HIS	2.8
2	D	70	VAL	2.8
2	D	112	TYR	2.7
1	C	93	GLY	2.7
2	B	118	LEU	2.7
2	B	81	HIS	2.7
1	C	80	PRO	2.7
1	A	45	MET	2.6
1	A	22	LEU	2.6
2	B	88	ASP	2.6
1	A	123	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	134	LEU	2.6
1	C	127	GLN	2.6
1	C	99	PHE	2.5
2	D	66	PRO	2.5
2	B	117	THR	2.5
2	D	149	CYS	2.5
2	D	126	GLU	2.5
1	C	32	LEU	2.5
1	A	16	LYS	2.5
1	C	112	GLN	2.5
2	D	129	ALA	2.4
1	C	106	SER	2.4
2	B	104	LEU	2.4
2	D	113	LEU	2.4
1	A	73	ASP	2.4
2	D	102	ILE	2.4
2	B	106	LEU	2.4
1	C	36	ASN	2.4
1	A	3	SER	2.4
2	D	143	PRO	2.3
1	C	100	THR	2.3
1	C	121	VAL	2.3
1	C	70	THR	2.3
1	C	63	ILE	2.3
1	C	101	THR	2.3
1	C	29	ASP	2.3
1	A	99	PHE	2.2
2	B	70	VAL	2.2
1	C	103	LYS	2.2
1	C	144	LYS	2.2
2	D	67	GLN	2.2
2	D	88	ASP	2.2
2	B	73	TRP	2.2
1	C	7	LEU	2.1
1	A	83	VAL	2.1
1	C	91	VAL	2.1
2	B	64	PRO	2.1
2	B	84	ALA	2.1
1	A	126	VAL	2.1
1	C	78	PRO	2.1
1	C	131	CYS	2.1
1	A	143	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	22	LEU	2.0
1	C	136	LEU	2.0
1	A	93	GLY	2.0
1	A	109	ASP	2.0
1	C	142	LYS	2.0
1	C	28	PRO	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.