



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:38 pm BST

PDB ID : 1P27
Title : Crystal Structure of the Human Y14/Magoh complex
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

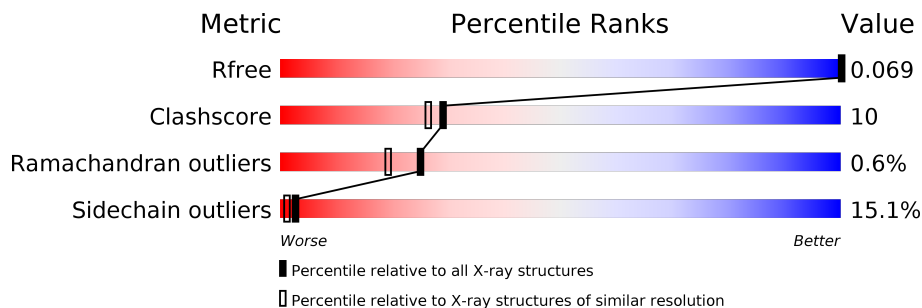
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	144	73% (green), 21% (yellow), 5% (red)
1	C	144	75% (green), 19% (yellow), 6% (red)
2	B	106	70% (green), 13% (yellow), 13% (grey)
2	D	106	51% (green), 29% (yellow), 7% (red), 13% (grey)

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
			Total	C	N	O	S			
1	A	144	1196	771	200	222	3	0	0	0
1	C	144	1196	771	200	222	3	0	0	0

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

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

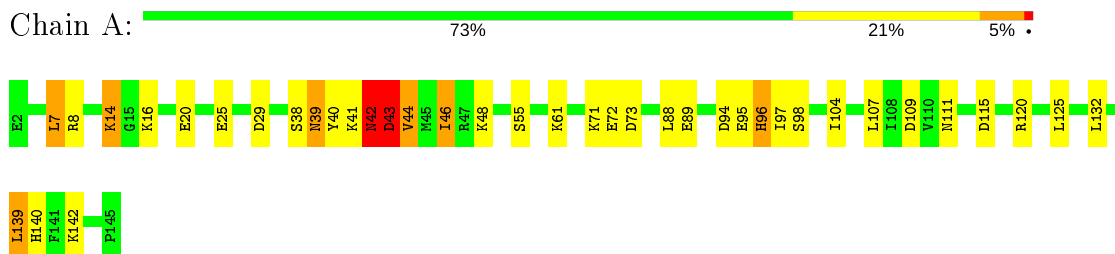
- Molecule 3 is water.

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

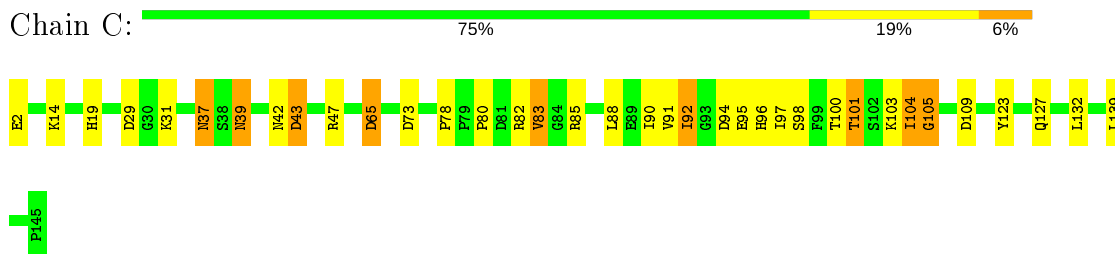
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

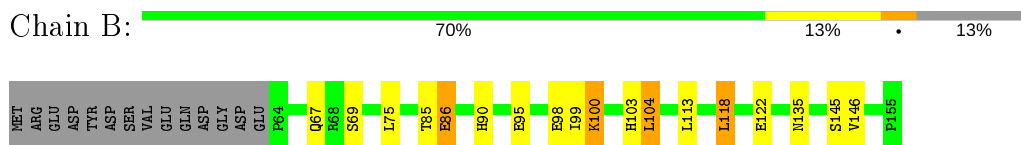
- Molecule 1: Mago nashi protein homolog



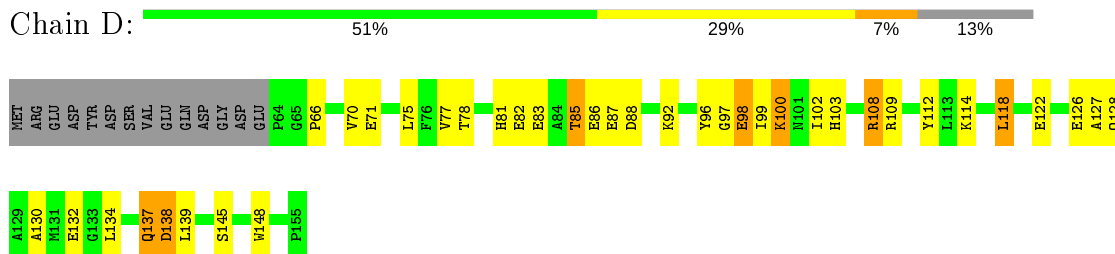
- Molecule 1: Mago nashi protein homolog



- 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.220 , 0.268 0.390 , 0.069	Depositor DCC
R_{free} test set	1701 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.079	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.64$, $\langle L^2 \rangle = 0.51$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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 [i](#)

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

Mol	Chain	Non-H	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:O	1:C:37:ASN:ND2	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:A:39:ASN:HD22	1:A:39:ASN:C	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:VAL:CG2	1:C:96:HIS:NE2	2.71	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
2:B:100:LYS:HB2	2:B:100:LYS:NZ	2.27	0.50
1:A:43:ASP:N	1:C:14:LYS:HZ1	2.10	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
1:A:96:HIS:CE1	3:A:154:HOH:O	2.70	0.45
2:B:104:LEU:HD22	2:B:113:LEU:HD13	1.99	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:B:86:GLU:N	2:B:104:LEU:CD1	2.83	0.42
2:D:99:ILE:HG21	2:D:102:ILE:CG1	2.50	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 [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	142/144 (99%)	136 (96%)	4 (3%)	2 (1%)	11	5
1	C	142/144 (99%)	134 (94%)	7 (5%)	1 (1%)	22	16
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%)	25	19

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	132/132 (100%)	108 (82%)	24 (18%)	1 1
1	C	132/132 (100%)	115 (87%)	17 (13%)	4 2
2	B	77/90 (86%)	68 (88%)	9 (12%)	5 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 [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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.