Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 11:51 AM EST

PDB ID	:	1RDD
Title	:	CRYSTAL STRUCTURE OF ESCHERICHIA COLI RNASE HI IN COMPLEX WITH MG2+ AT 2.8 ANGSTROMS RESOLUTION: PROOF FOR A SINGLE MG2+ SITE
Authors	:	Katayanagi, K.; Morikawa, K.
Deposited on	:	1993-06-23
Resolution	:	2.80 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

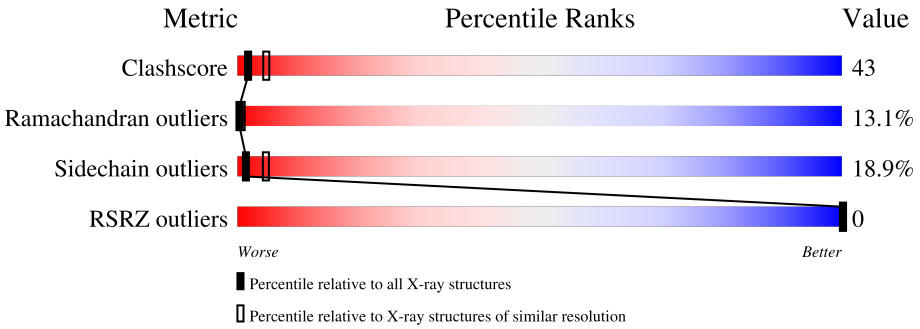
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 of 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 <=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	155	26% 43% 23% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1274 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 RIBONUCLEASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1238	776	227	228	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

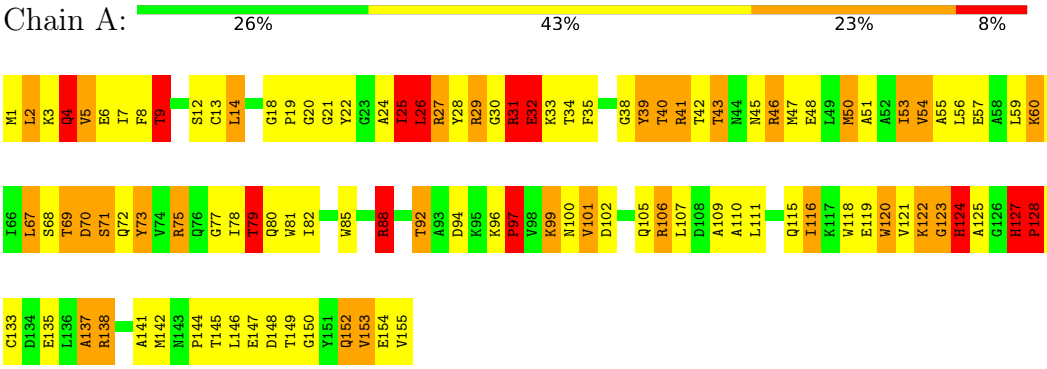
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: RIBONUCLEASE H

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	63.20Å 63.20Å 80.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 9.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 90.3 (9.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available) 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.09 , 83.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	1274	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	1.02	0/1266	2.30	50/1710 (2.9%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	138	ARG	NE-CZ-NH1	16.31	128.46	120.30
1	A	138	ARG	CD-NE-CZ	15.41	145.18	123.60
1	A	132	ARG	NE-CZ-NH2	-14.85	112.88	120.30
1	A	27	ARG	NE-CZ-NH1	13.87	127.24	120.30
1	A	41	ARG	NE-CZ-NH2	13.82	127.21	120.30
1	A	29	ARG	CD-NE-CZ	12.31	140.83	123.60
1	A	27	ARG	CD-NE-CZ	11.51	139.71	123.60
1	A	132	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	127	HIS	CA-CB-CG	10.87	132.07	113.60
1	A	31	ARG	NE-CZ-NH1	10.23	125.42	120.30
1	A	127	HIS	N-CA-CB	10.23	129.01	110.60
1	A	27	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	41	ARG	CD-NE-CZ	8.94	136.12	123.60
1	A	29	ARG	NE-CZ-NH1	8.59	124.60	120.30
1	A	59	LEU	C-N-CA	8.08	141.91	121.70
1	A	22	TYR	CB-CG-CD1	7.96	125.78	121.00
1	A	73	TYR	CB-CG-CD1	-7.79	116.32	121.00
1	A	39	TYR	CB-CA-C	7.54	125.49	110.40
1	A	88	ARG	CD-NE-CZ	7.49	134.08	123.60
1	A	31	ARG	CA-CB-CG	7.06	128.93	113.40
1	A	22	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	A	109	ALA	N-CA-CB	6.99	119.88	110.10
1	A	50	MET	CA-CB-CG	6.70	124.69	113.30
1	A	137	ALA	CB-CA-C	6.57	119.95	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ALA	CB-CA-C	6.47	119.81	110.10
1	A	4	GLN	CB-CG-CD	6.37	128.17	111.60
1	A	122	LYS	N-CA-C	-6.36	93.82	111.00
1	A	26	LEU	CA-CB-CG	6.32	129.84	115.30
1	A	88	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	64	GLU	CA-CB-CG	6.26	127.17	113.40
1	A	39	TYR	CB-CG-CD1	6.16	124.69	121.00
1	A	6	GLU	N-CA-CB	5.97	121.34	110.60
1	A	46	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	41	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	A	73	TYR	CB-CG-CD2	5.77	124.46	121.00
1	A	61	GLU	CG-CD-OE1	5.63	129.56	118.30
1	A	138	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	25	ILE	CB-CA-C	-5.45	100.70	111.60
1	A	31	ARG	N-CA-CB	5.43	120.37	110.60
1	A	106	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	A	128	PRO	N-CD-CG	-5.31	95.23	103.20
1	A	75	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	70	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	34	THR	CA-CB-CG2	5.26	119.77	112.40
1	A	31	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	2	LEU	O-C-N	5.18	130.99	122.70
1	A	4	GLN	C-N-CA	5.18	134.65	121.70
1	A	50	MET	CA-C-N	-5.06	106.06	117.20
1	A	27	ARG	CG-CD-NE	5.06	122.42	111.80
1	A	9	THR	C-N-CA	5.01	134.23	121.70

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	1238	0	1216	106	1
2	A	1	0	0	0	0
3	A	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1274	0	1216	106	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 43.

All (106) 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:111:LEU:HD23	1:A:116:ILE:HD13	1.37	1.05
1:A:4:GLN:HG3	1:A:64:GLU:HB3	1.47	0.93
1:A:8:PHE:HB2	1:A:25:ILE:HD12	1.53	0.89
1:A:46:ARG:O	1:A:50:MET:HB2	1.76	0.86
1:A:88:ARG:HG2	1:A:88:ARG:HH21	1.42	0.84
1:A:7:ILE:HG21	1:A:67:LEU:HG	1.59	0.83
1:A:111:LEU:HD11	1:A:118:TRP:HZ2	1.42	0.83
1:A:13:CYS:HA	1:A:20:GLY:HA2	1.69	0.74
1:A:70:ASP:HA	1:A:121:VAL:O	1.90	0.72
1:A:56:LEU:HB3	1:A:110:ALA:HB1	1.73	0.71
1:A:101:VAL:HG22	1:A:105:GLN:HE21	1.57	0.69
1:A:12:SER:H	1:A:137:ALA:HB1	1.61	0.64
1:A:8:PHE:HE2	1:A:27:ARG:HD2	1.61	0.64
1:A:4:GLN:CG	1:A:64:GLU:HB3	2.27	0.62
1:A:43:THR:O	1:A:47:MET:HG2	1.99	0.62
1:A:129:GLU:HA	1:A:132:ARG:HG3	1.82	0.62
1:A:7:ILE:CG2	1:A:67:LEU:HG	2.27	0.61
1:A:111:LEU:HD11	1:A:118:TRP:CZ2	2.31	0.61
1:A:92:THR:HG23	1:A:96:LYS:O	2.01	0.60
1:A:2:LEU:N	1:A:29:ARG:O	2.31	0.60
1:A:107:LEU:O	1:A:111:LEU:HB2	2.02	0.59
1:A:57:GLU:OE1	1:A:106:ARG:NH2	2.36	0.59
1:A:40:THR:HG22	1:A:146:LEU:O	2.03	0.58
1:A:26:LEU:CD1	1:A:33:LYS:HD2	2.33	0.58
1:A:25:ILE:CG2	1:A:32:GLU:HG3	2.32	0.58
1:A:69:THR:CG2	1:A:71:SER:HB3	2.33	0.58
1:A:25:ILE:HD11	1:A:129:GLU:HB3	1.86	0.58
1:A:24:ALA:O	1:A:35:PHE:N	2.34	0.57
1:A:25:ILE:CD1	1:A:129:GLU:HB3	2.35	0.57
1:A:65:VAL:HG23	1:A:116:ILE:HG13	1.85	0.56
1:A:75:ARG:HA	1:A:120:TRP:CZ2	2.40	0.56
1:A:99:LYS:O	1:A:100:ASN:HB2	2.06	0.56
1:A:31:ARG:O	1:A:32:GLU:HB3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:O	1:A:56:LEU:N	2.39	0.55
1:A:123:GLY:O	1:A:125:ALA:N	2.40	0.55
1:A:38:GLY:HA3	1:A:144:PRO:HA	1.87	0.55
1:A:8:PHE:CE2	1:A:27:ARG:HD2	2.42	0.54
1:A:85:TRP:O	1:A:88:ARG:N	2.41	0.53
1:A:4:GLN:HB3	1:A:64:GLU:O	2.08	0.53
1:A:45:ASN:HB3	1:A:73:TYR:CE2	2.44	0.53
1:A:128:PRO:HG2	1:A:129:GLU:OE1	2.09	0.53
1:A:132:ARG:O	1:A:135:GLU:HG3	2.09	0.53
1:A:53:ILE:O	1:A:55:ALA:N	2.43	0.52
1:A:5:VAL:HG12	1:A:65:VAL:HG12	1.90	0.52
1:A:28:TYR:C	1:A:30:GLY:H	2.09	0.52
1:A:5:VAL:HG22	1:A:28:TYR:HA	1.92	0.51
1:A:56:LEU:CB	1:A:110:ALA:HB1	2.39	0.51
1:A:137:ALA:O	1:A:138:ARG:C	2.47	0.51
1:A:20:GLY:HA3	1:A:42:THR:CG2	2.41	0.51
1:A:127:HIS:O	1:A:129:GLU:N	2.44	0.50
1:A:27:ARG:HA	1:A:32:GLU:HA	1.94	0.49
1:A:4:GLN:HG2	1:A:64:GLU:OE1	2.13	0.49
1:A:68:SER:HB2	1:A:119:GLU:OE1	2.13	0.49
1:A:129:GLU:HA	1:A:132:ARG:HB2	1.95	0.49
1:A:78:ILE:HG21	1:A:120:TRP:HZ2	1.78	0.48
1:A:3:LYS:O	1:A:4:GLN:HB2	2.13	0.48
1:A:45:ASN:ND2	1:A:45:ASN:N	2.59	0.48
1:A:152:GLN:O	1:A:154:GLU:N	2.47	0.47
1:A:53:ILE:O	1:A:54:VAL:C	2.53	0.47
1:A:14:LEU:HD12	1:A:141:ALA:HB1	1.96	0.47
1:A:18:GLY:HA2	1:A:41:ARG:HG3	1.96	0.46
1:A:2:LEU:O	1:A:29:ARG:HA	2.16	0.46
1:A:127:HIS:O	1:A:130:ASN:N	2.48	0.46
1:A:8:PHE:CB	1:A:25:ILE:HD12	2.34	0.46
1:A:19:PRO:HG3	1:A:40:THR:O	2.15	0.46
1:A:96:LYS:HE2	1:A:155:VAL:HG13	1.98	0.46
1:A:8:PHE:HB3	1:A:133:CYS:SG	2.55	0.46
1:A:45:ASN:N	1:A:45:ASN:HD22	2.11	0.45
1:A:79:THR:O	1:A:80:GLN:HG3	2.16	0.45
1:A:39:TYR:HA	1:A:146:LEU:O	2.17	0.45
1:A:40:THR:HG22	1:A:147:GLU:HA	1.98	0.45
1:A:122:LYS:O	1:A:124:HIS:N	2.49	0.45
1:A:18:GLY:CA	1:A:41:ARG:HG3	2.47	0.45
1:A:31:ARG:HH21	1:A:33:LYS:CE	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG22	1:A:79:THR:N	2.31	0.45
1:A:75:ARG:O	1:A:77:GLY:N	2.50	0.44
1:A:100:ASN:O	1:A:102:ASP:N	2.51	0.44
1:A:79:THR:HG21	1:A:120:TRP:HE1	1.83	0.44
1:A:127:HIS:HA	1:A:128:PRO:HD2	1.72	0.44
1:A:1:MET:HB2	1:A:3:LYS:HE3	1.99	0.44
1:A:4:GLN:CG	1:A:64:GLU:OE1	2.66	0.43
1:A:21:GLY:O	1:A:137:ALA:HB1	2.18	0.43
1:A:1:MET:HB2	1:A:3:LYS:NZ	2.33	0.43
1:A:40:THR:CG2	1:A:147:GLU:HA	2.48	0.43
1:A:27:ARG:NH2	1:A:129:GLU:OE2	2.52	0.43
1:A:26:LEU:CD2	1:A:28:TYR:HB2	2.49	0.43
1:A:111:LEU:HD21	1:A:116:ILE:HG21	2.00	0.42
1:A:54:VAL:O	1:A:55:ALA:C	2.56	0.42
1:A:81:TRP:HB3	1:A:85:TRP:CZ2	2.55	0.42
1:A:4:GLN:CB	1:A:64:GLU:HB3	2.49	0.42
1:A:28:TYR:CZ	1:A:60:LYS:HD3	2.54	0.42
1:A:50:MET:O	1:A:54:VAL:HG23	2.19	0.42
1:A:46:ARG:HH22	1:A:150:GLY:HA3	1.84	0.42
1:A:46:ARG:O	1:A:47:MET:HE1	2.20	0.41
1:A:82:ILE:O	1:A:85:TRP:N	2.53	0.41
1:A:131:GLU:O	1:A:132:ARG:C	2.58	0.41
1:A:8:PHE:O	1:A:9:THR:HG22	2.21	0.41
1:A:78:ILE:CG2	1:A:120:TRP:HZ2	2.34	0.41
1:A:96:LYS:O	1:A:97:PRO:O	2.38	0.41
1:A:56:LEU:HD13	1:A:110:ALA:O	2.21	0.41
1:A:88:ARG:HG2	1:A:88:ARG:NH2	2.21	0.40
1:A:5:VAL:CG1	1:A:26:LEU:HD23	2.51	0.40
1:A:115:GLN:HE21	1:A:115:GLN:HB3	1.74	0.40
1:A:7:ILE:CD1	1:A:55:ALA:HB1	2.51	0.40
1:A:88:ARG:HH21	1:A:88:ARG:CG	2.21	0.40
1:A:18:GLY:C	1:A:41:ARG:HA	2.42	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:124:HIS:CE1	1:A:124:HIS:CE1[5_555]	2.15	0.05

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	153/155 (99%)	99 (65%)	34 (22%)	20 (13%)	0 1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	53	ILE
1	A	54	VAL
1	A	71	SER
1	A	120	TRP
1	A	123	GLY
1	A	124	HIS
1	A	4	GLN
1	A	5	VAL
1	A	14	LEU
1	A	32	GLU
1	A	97	PRO
1	A	128	PRO
1	A	153	VAL
1	A	79	THR
1	A	127	HIS
1	A	142	MET
1	A	92	THR
1	A	148	ASP
1	A	101	VAL

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	127/127 (100%)	103 (81%)	24 (19%)	1 5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	9	THR
1	A	25	ILE
1	A	26	LEU
1	A	32	GLU
1	A	40	THR
1	A	43	THR
1	A	48	GLU
1	A	60	LYS
1	A	65	VAL
1	A	67	LEU
1	A	69	THR
1	A	72	GLN
1	A	79	THR
1	A	88	ARG
1	A	94	ASP
1	A	97	PRO
1	A	99	LYS
1	A	116	ILE
1	A	124	HIS
1	A	145	THR
1	A	149	THR
1	A	152	GLN
1	A	153	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	72	GLN
1	A	105	GLN
1	A	113	GLN
1	A	127	HIS
1	A	130	ASN
1	A	152	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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^{th} 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^2)	Q<0.9
1	A	155/155 (100%)	-0.78	0 100 100	5, 9, 17, 24	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	MG	A	300	1/1	0.94	0.12	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.