Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 12:47 PM JST

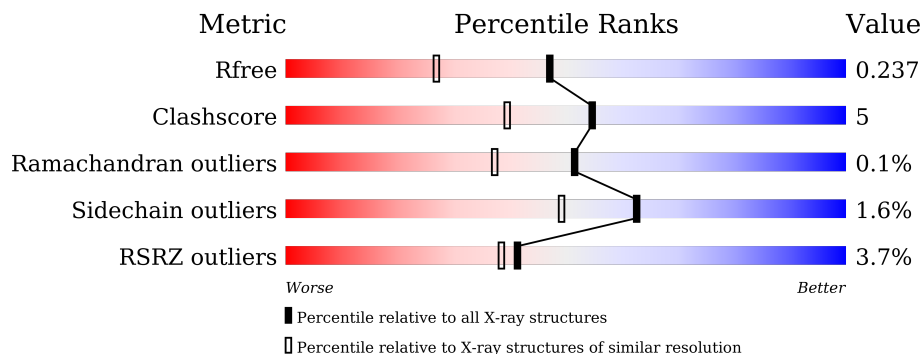|		
PDB ID	:	5XGU
Title	:	Escherichia coli. RNase R
Authors	:	Chu, L.Y.; Hsieh, T.J.; Yuan, H.S.
Deposited on	:	2017-04-17
Resolution	:	1.85 Å(reported)

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 1.85 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	Percentile Ranks	Value
Rfree		0.237
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		3.7%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	645	4% — 87% ... 10% ..
1	B	645	3% — 86% ... 10% .

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11642 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 R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	619	Total 4926	C 3100	N 872	O 927	S 27	0	0	0
1	A	631	Total 5033	C 3167	N 900	O 939	S 27	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP H4USN4
B	-4	HIS	-	expression tag	UNP H4USN4
B	-3	HIS	-	expression tag	UNP H4USN4
B	-2	HIS	-	expression tag	UNP H4USN4
B	-1	HIS	-	expression tag	UNP H4USN4
B	0	HIS	-	expression tag	UNP H4USN4
B	45	VAL	ALA	engineered mutation	UNP H4USN4
A	-5	HIS	-	expression tag	UNP H4USN4
A	-4	HIS	-	expression tag	UNP H4USN4
A	-3	HIS	-	expression tag	UNP H4USN4
A	-2	HIS	-	expression tag	UNP H4USN4
A	-1	HIS	-	expression tag	UNP H4USN4
A	0	HIS	-	expression tag	UNP H4USN4
A	45	VAL	ALA	engineered mutation	UNP H4USN4

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	870	Total 870	O 870	0	0
3	A	811	Total 811	O 811	0	0

3 Residue-property plots ⓘ

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 R
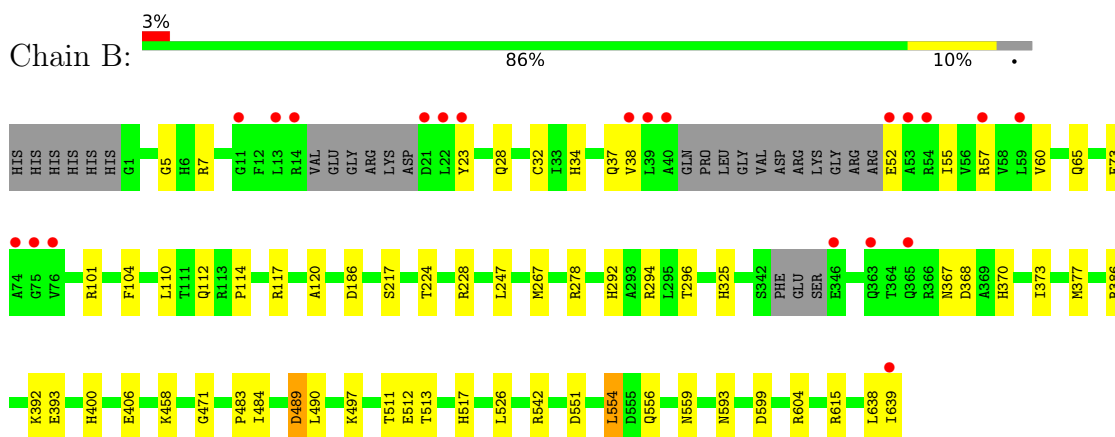
• Molecule 1: Ribonuclease R
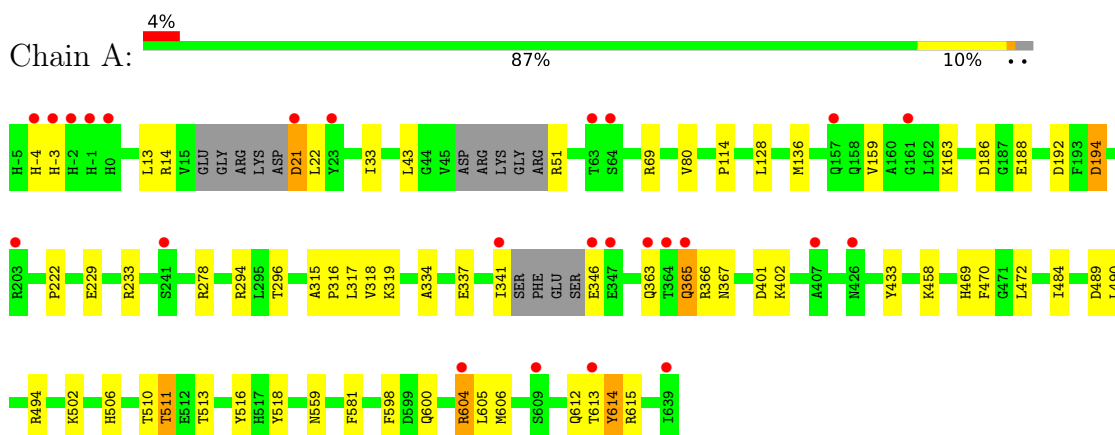
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.69Å 120.86Å 83.63Å 90.00° 91.61° 90.00°	Depositor
Resolution (Å)	29.67 – 1.85 29.67 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.67-1.85) 99.1 (29.67-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.187 , 0.236 0.187 , 0.237	Depositor DCC
R_{free} test set	2005 reflections (1.61%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11642	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]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	0.40	4/5133 (0.1%)	0.56	6/6933 (0.1%)
1	B	0.36	2/5019 (0.0%)	0.47	0/6777
All	All	0.38	6/10152 (0.1%)	0.52	6/13710 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	GLU	CD-OE1	-11.67	1.12	1.25
1	A	604	ARG	CD-NE	-10.80	1.28	1.46
1	B	73	GLU	CD-OE2	-9.98	1.14	1.25
1	A	604	ARG	NE-CZ	-9.91	1.20	1.33
1	A	604	ARG	CG-CD	-8.97	1.29	1.51
1	A	614	TYR	CB-CG	-7.42	1.40	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	ARG	NE-CZ-NH2	-17.29	111.66	120.30
1	A	604	ARG	NH1-CZ-NH2	9.54	129.90	119.40
1	A	604	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	A	604	ARG	CB-CG-CD	-6.53	94.63	111.60
1	A	604	ARG	CD-NE-CZ	-6.12	115.03	123.60
1	A	319	LYS	CD-CE-NZ	-5.50	99.05	111.70

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	5033	0	4976	60	0
1	B	4926	0	4879	43	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	811	0	0	12	1
3	B	870	0	0	8	1
All	All	11642	0	9855	103	2

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 (103) 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:315:ALA:O	3:A:801:HOH:O	1.84	0.93
1:A:604:ARG:HD3	1:A:604:ARG:C	1.83	0.92
1:A:604:ARG:HD3	1:A:605:LEU:N	1.91	0.85
1:B:400:HIS:HD2	1:B:471:GLY:H	1.23	0.83
1:A:604:ARG:HH12	1:A:614:TYR:N	1.75	0.83
1:B:392:LYS:NZ	3:B:801:HOH:O	2.09	0.83
1:B:5:GLY:H	1:B:34:HIS:HD2	1.25	0.81
1:A:604:ARG:HD2	1:A:606:MET:HG3	1.65	0.78
1:A:604:ARG:HH12	1:A:614:TYR:H	1.35	0.75
1:A:469:HIS:HD2	1:A:472:LEU:H	1.33	0.74
1:A:80:VAL:O	3:A:802:HOH:O	2.07	0.71
1:B:5:GLY:H	1:B:34:HIS:CD2	2.10	0.70
1:B:367:ASN:H	1:B:370:HIS:HD2	1.39	0.69
1:A:604:ARG:NH1	1:A:605:LEU:O	2.27	0.67
1:A:334:ALA:O	1:A:337:GLU:HG3	1.95	0.66
1:B:65:GLN:OE1	3:B:803:HOH:O	2.14	0.65
1:A:316:PRO:C	3:A:801:HOH:O	2.36	0.64
1:A:69:ARG:N	3:A:802:HOH:O	2.32	0.63
1:A:604:ARG:NH2	1:A:613:THR:HG22	2.12	0.62
1:B:400:HIS:CD2	1:B:471:GLY:H	2.13	0.62
1:A:612:GLN:OE1	1:A:614:TYR:OH	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD11	1:A:114:PRO:HD2	1.82	0.61
1:B:511:THR:HG22	1:B:513:THR:H	1.65	0.60
1:B:386:ARG:NH1	3:B:812:HOH:O	2.30	0.60
1:B:38:VAL:HG21	1:B:55:ILE:HD12	1.84	0.60
1:B:393:GLU:OE1	1:B:517:HIS:ND1	2.32	0.60
1:A:604:ARG:HG3	1:A:606:MET:SD	2.43	0.59
1:A:366:ARG:NH1	3:A:807:HOH:O	2.29	0.58
1:A:469:HIS:CD2	1:A:472:LEU:H	2.16	0.58
1:A:318:VAL:N	3:A:801:HOH:O	2.37	0.56
1:B:400:HIS:HD2	1:B:471:GLY:N	1.99	0.56
1:B:37:GLN:HB2	1:B:60:VAL:HB	1.87	0.55
1:A:13:LEU:O	1:A:21:ASP:N	2.39	0.55
1:A:341:ILE:HD11	1:A:433:TYR:HB2	1.89	0.55
1:B:325:HIS:HE1	1:B:368:ASP:OD2	1.90	0.55
1:B:267:MET:CE	1:B:497:LYS:HE2	2.37	0.54
1:B:278:ARG:NH1	3:B:822:HOH:O	2.41	0.54
1:B:23:TYR:HD2	1:B:52:GLU:HG2	1.73	0.53
1:B:556:GLN:NE2	1:B:559:ASN:HD22	2.06	0.53
1:A:604:ARG:NH2	1:A:615:ARG:N	2.56	0.53
1:A:604:ARG:HH21	1:A:615:ARG:HB2	1.74	0.52
1:A:604:ARG:NH1	1:A:614:TYR:N	2.52	0.52
1:B:247:LEU:HD12	1:B:484:ILE:HD12	1.92	0.52
1:B:367:ASN:H	1:B:370:HIS:CD2	2.23	0.52
1:A:317:LEU:N	3:A:801:HOH:O	2.44	0.51
1:B:186:ASP:O	1:B:296:THR:HA	2.12	0.50
1:B:497:LYS:NZ	1:B:513:THR:O	2.44	0.50
1:B:542:ARG:NH1	3:B:802:HOH:O	2.11	0.50
1:B:32:CYS:SG	1:B:55:ILE:HG13	2.51	0.49
1:B:638:LEU:O	1:B:639:ILE:HG13	2.13	0.49
1:B:217:SER:OG	1:B:497:LYS:HE3	2.12	0.49
1:B:114:PRO:HD3	1:B:120:ALA:HB2	1.94	0.49
1:B:400:HIS:HE1	1:B:458:LYS:O	1.95	0.49
1:A:229:GLU:O	1:A:233:ARG:HG3	2.12	0.49
1:A:346:GLU:HG3	1:A:581:PHE:CE2	2.48	0.49
1:A:402:LYS:HD3	1:A:470:PHE:CD1	2.48	0.49
1:A:402:LYS:O	1:A:458:LYS:NZ	2.38	0.48
1:B:512:GLU:H	1:B:512:GLU:CD	2.16	0.48
1:A:43:LEU:O	1:A:51:ARG:NH1	2.38	0.48
1:B:28:GLN:OE1	1:B:55:ILE:HG12	2.12	0.48
1:A:506:HIS:HE1	1:A:510:THR:O	1.96	0.48
1:B:599:ASP:HB3	1:B:604:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ARG:N	3:A:824:HOH:O	2.47	0.48
1:A:365:GLN:NE2	1:A:367:ASN:HD22	2.12	0.48
1:A:341:ILE:O	3:A:803:HOH:O	2.20	0.47
1:B:5:GLY:N	1:B:34:HIS:HD2	2.04	0.47
1:A:128:LEU:HB3	1:A:136:MET:HE3	1.95	0.47
1:A:-4:HIS:HA	1:A:-3:HIS:HA	1.57	0.47
1:A:604:ARG:NH2	1:A:615:ARG:HB2	2.29	0.47
1:A:598:PHE:CE2	1:A:600:GLN:HG2	2.50	0.46
1:A:194:ASP:OD1	1:A:484:ILE:HG13	2.15	0.46
1:A:559:ASN:ND2	3:A:827:HOH:O	2.48	0.46
1:A:511:THR:HG22	1:A:513:THR:H	1.81	0.45
1:A:13:LEU:HB3	1:A:22:LEU:HB2	1.98	0.45
1:A:14:ARG:NH1	1:A:21:ASP:OD1	2.50	0.45
1:B:373:ILE:O	1:B:377:MET:HG2	2.18	0.44
1:A:494:ARG:NH1	1:A:518:TYR:OH	2.51	0.44
1:B:551:ASP:HA	1:B:554:LEU:HD22	1.99	0.44
1:A:186:ASP:O	1:A:296:THR:HA	2.18	0.44
1:A:21:ASP:N	1:A:21:ASP:OD1	2.50	0.43
1:A:188:GLU:HG3	1:A:296:THR:HG21	2.00	0.43
1:A:502:LYS:NZ	3:A:838:HOH:O	2.51	0.43
1:B:110:LEU:HD12	3:B:808:HOH:O	2.18	0.42
1:A:192:ASP:OD1	1:A:192:ASP:N	2.52	0.42
1:A:402:LYS:HD3	1:A:470:PHE:HD1	1.85	0.42
1:A:604:ARG:NH1	1:A:613:THR:HA	2.34	0.42
1:A:604:ARG:CZ	1:A:614:TYR:C	2.87	0.42
1:B:28:GLN:HE22	1:B:55:ILE:H	1.67	0.42
1:A:346:GLU:HB2	1:A:363:GLN:NE2	2.34	0.42
1:A:401:ASP:HB2	1:A:458:LYS:HD2	2.01	0.41
1:A:469:HIS:HE1	3:A:1145:HOH:O	2.04	0.41
1:A:604:ARG:NH2	1:A:613:THR:CG2	2.81	0.41
3:B:919:HOH:O	1:A:278:ARG:HD3	2.21	0.41
1:B:406:GLU:HG3	3:B:1201:HOH:O	2.20	0.41
1:B:101:ARG:HD2	1:B:104:PHE:CZ	2.56	0.41
1:B:267:MET:HE1	1:B:497:LYS:HG2	2.02	0.41
1:B:373:ILE:HD13	1:B:373:ILE:HA	1.95	0.41
1:B:604:ARG:HB3	1:B:615:ARG:HG3	2.03	0.41
1:B:224:THR:O	1:B:228:ARG:HG3	2.20	0.41
1:B:483:PRO:HA	1:B:489:ASP:HB2	2.03	0.40
1:A:222:PRO:HG2	1:A:516:TYR:CD1	2.56	0.40
1:A:128:LEU:HB3	1:A:136:MET:CE	2.52	0.40
1:A:604:ARG:CZ	1:A:613:THR:HG23	2.52	0.40

All (2) 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:B:117:ARG:NH1	3:A:1364:HOH:O[2_443]	2.07	0.13
1:B:112:GLN:NE2	3:B:1433:HOH:O[2_444]	2.19	0.01

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	623/645 (97%)	614 (99%)	9 (1%)	0	100	100
1	B	611/645 (95%)	606 (99%)	4 (1%)	1 (0%)	47	33
All	All	1234/1290 (96%)	1220 (99%)	13 (1%)	1 (0%)	51	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	593	ASN

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	541/553 (98%)	532 (98%)	9 (2%)	60	47
1	B	530/553 (96%)	522 (98%)	8 (2%)	65	52
All	All	1071/1106 (97%)	1054 (98%)	17 (2%)	62	49

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ARG
1	B	57	ARG
1	B	292	HIS
1	B	294	ARG
1	B	489	ASP
1	B	490	LEU
1	B	526	LEU
1	B	554	LEU
1	A	21	ASP
1	A	159	VAL
1	A	163	LYS
1	A	194	ASP
1	A	294	ARG
1	A	365	GLN
1	A	489	ASP
1	A	490	LEU
1	A	511	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	34	HIS
1	B	65	GLN
1	B	325	HIS
1	B	370	HIS
1	B	400	HIS
1	B	466	ASN
1	B	509	ASN
1	B	556	GLN
1	A	0	HIS
1	A	37	GLN
1	A	65	GLN
1	A	96	GLN
1	A	157	GLN
1	A	365	GLN
1	A	469	HIS
1	A	506	HIS
1	A	509	ASN
1	A	556	GLN
1	A	559	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are 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, 95th 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	631/645 (97%)	0.09	25 (3%)	38	35	11, 24, 50, 78	0
1	B	619/645 (95%)	0.03	21 (3%)	45	41	11, 21, 46, 76	0
All	All	1250/1290 (96%)	0.06	46 (3%)	41	38	11, 22, 48, 78	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	LEU	6.1
1	A	604	ARG	5.9
1	B	22	LEU	5.7
1	A	-3	HIS	4.8
1	B	365	GLN	4.3
1	A	341	ILE	4.2
1	B	38	VAL	4.0
1	A	64	SER	4.0
1	B	39	LEU	3.7
1	A	63	THR	3.4
1	B	59	LEU	3.4
1	A	-2	HIS	3.3
1	A	203	ARG	3.2
1	A	346	GLU	3.1
1	A	363	GLN	3.1
1	B	21	ASP	3.0
1	B	14	ARG	2.8
1	A	613	THR	2.7
1	A	0	HIS	2.7
1	A	21	ASP	2.7
1	B	40	ALA	2.6
1	B	52	GLU	2.6
1	A	-4	HIS	2.5
1	A	241	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	407	ALA	2.4
1	B	54	ARG	2.4
1	B	76	VAL	2.4
1	A	347	GLU	2.4
1	A	609	SER	2.3
1	A	161	GLY	2.3
1	B	639	ILE	2.3
1	A	364	THR	2.3
1	B	11	GLY	2.3
1	A	365	GLN	2.3
1	A	639	ILE	2.2
1	B	363	GLN	2.2
1	B	346	GLU	2.1
1	B	23	TYR	2.1
1	B	53	ALA	2.1
1	B	74	ALA	2.1
1	B	75	GLY	2.1
1	A	157	GLN	2.0
1	A	426	ASN	2.0
1	A	23	TYR	2.0
1	A	-1	HIS	2.0
1	B	57	ARG	2.0

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, 95th 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(Å²)	Q<0.9
2	MG	B	701	1/1	0.98	0.04	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	701	1/1	0.99	0.06	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.