



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:33 am BST

PDB ID : 3UXO
Title : Crystal Structure of Rat DNA Polymerase Beta Mutator I260Q Apoenzyme
Authors : Gridley, C.L.; Jaeger, J.
Deposited on : 2011-12-05
Resolution : 2.10 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

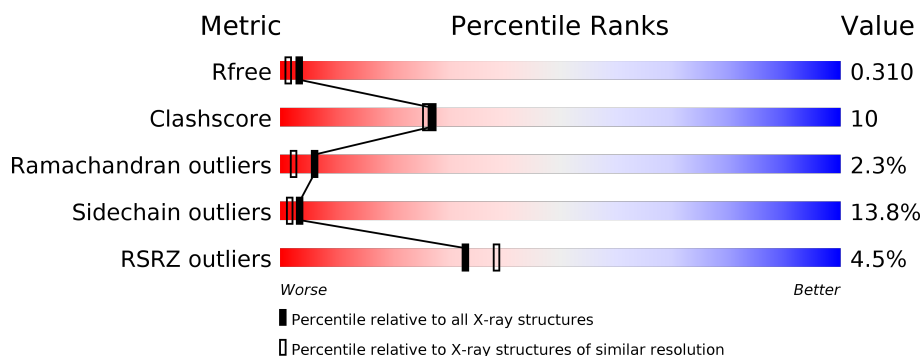
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	335	 3% 72% 23% . .
1	B	335	 6% 62% 28% 7% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5488 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 DNA polymerase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	65	0	0
			2611	1646	462	494	9			
1	B	325	Total	C	N	O	S	92	0	0
			2611	1646	462	494	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	GLN	ILE	ENGINEERED MUTATION	UNP P06766
B	260	GLN	ILE	ENGINEERED MUTATION	UNP P06766

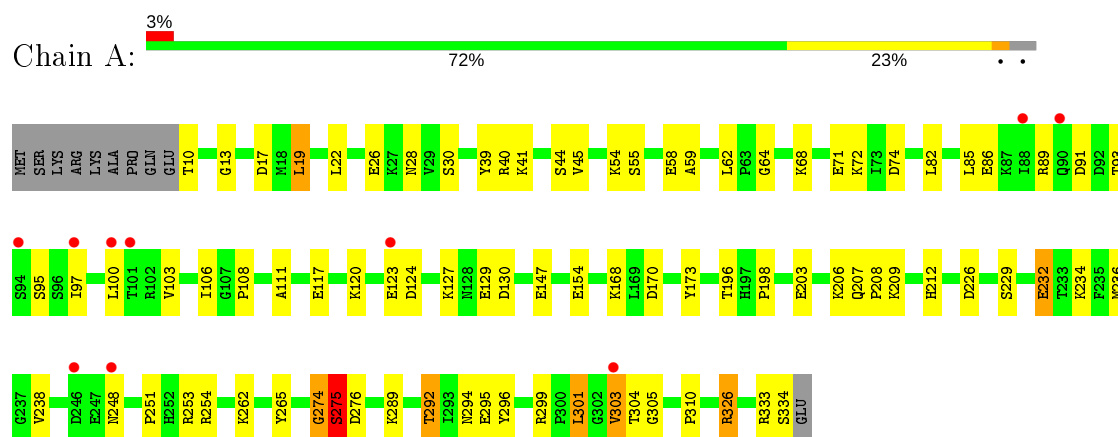
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	162	Total	O	0	0
			162	162		
2	B	104	Total	O	0	0
			104	104		

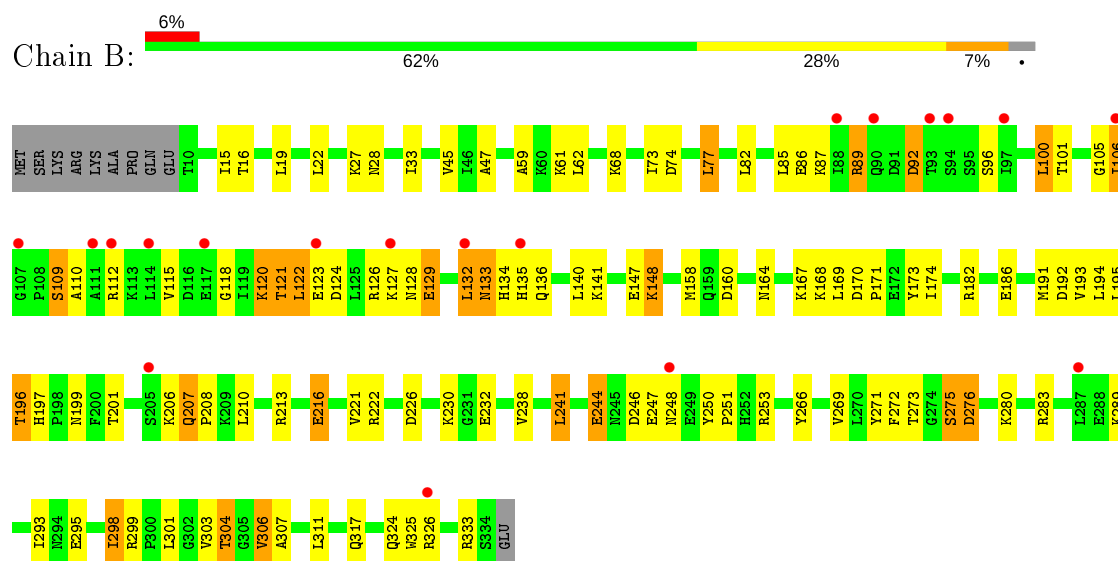
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA polymerase beta



- Molecule 1: DNA polymerase beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.91Å 67.40Å 82.46Å 90.00° 115.81° 90.00°	Depositor
Resolution (Å)	24.05 – 2.10 24.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.05-2.10) 92.5 (24.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.257 , 0.318 0.250 , 0.310	Depositor DCC
R_{free} test set	1873 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.066 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5488	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.76 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7556e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.53	0/2659	0.63	0/3578
1	B	0.40	0/2659	0.58	0/3578
All	All	0.47	0/5318	0.60	0/7156

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	GLY	Peptide
1	B	244	GLU	Peptide
1	B	247	GLU	Peptide

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	2611	0	2626	45	0
1	B	2611	0	2626	62	0
2	A	162	0	0	9	0
2	B	104	0	0	9	0
All	All	5488	0	5252	103	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 10.

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:B:216:GLU:OE2	2:B:496:HOH:O	1.98	0.81
1:B:250:TYR:OH	2:B:455:HOH:O	1.99	0.81
1:B:266:TYR:HA	1:B:269:VAL:HG22	1.68	0.76
1:B:304:THR:HG22	1:B:306:VAL:HG22	1.70	0.74
1:B:86:GLU:OE1	1:B:89:ARG:NH1	2.21	0.74
1:B:192:ASP:OD2	2:B:499:HOH:O	2.06	0.72
1:A:294:ASN:HB3	1:A:296:TYR:H	1.58	0.68
1:B:147:GLU:O	2:B:474:HOH:O	2.14	0.65
1:A:334:SER:O	2:A:477:HOH:O	2.14	0.65
1:B:109:SER:OG	1:B:110:ALA:N	2.32	0.63
1:B:207:GLN:HB3	1:B:210:LEU:HD12	1.80	0.63
1:B:164:ASN:ND2	2:B:487:HOH:O	2.30	0.63
1:B:112:ARG:NH1	2:B:503:HOH:O	2.34	0.60
1:B:92:ASP:O	1:B:96:SER:OG	2.18	0.60
1:B:106:ILE:HG21	1:B:110:ALA:HB3	1.82	0.60
1:B:324:GLN:O	2:B:457:HOH:O	2.16	0.59
1:B:174:ILE:HB	1:B:196:THR:HG22	1.84	0.59
1:B:133:ASN:HD22	1:B:133:ASN:N	2.01	0.58
1:B:304:THR:HG22	1:B:306:VAL:H	1.69	0.58
1:B:82:LEU:HB3	1:B:85:LEU:HB2	1.85	0.57
1:A:326:ARG:HH11	1:A:326:ARG:H	1.52	0.56
1:A:59:ALA:HA	1:A:62:LEU:HD12	1.86	0.56
1:B:115:VAL:HG13	1:B:120:LYS:HA	1.88	0.55
1:B:135:HIS:HD2	1:B:136:GLN:HG3	1.70	0.55
1:B:275:SER:OG	1:B:333:ARG:O	2.25	0.55
1:B:105:GLY:HA3	1:B:136:GLN:HG2	1.88	0.54
1:B:45:VAL:HG12	1:B:62:LEU:HD23	1.90	0.54
1:A:26:GLU:HA	1:A:30:SER:HB2	1.89	0.54
1:B:299:ARG:HG3	1:B:307:ALA:HB1	1.90	0.54
1:A:208:PRO:HB3	1:A:232:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HA	1:A:111:ALA:HB3	1.91	0.53
1:B:276:ASP:O	1:B:280:LYS:HG2	2.09	0.53
1:A:275:SER:HB3	1:A:333:ARG:O	2.09	0.53
1:B:182:ARG:HD3	1:B:273:THR:OG1	2.09	0.52
1:A:17:ASP:OD2	2:A:476:HOH:O	2.19	0.52
1:A:304:THR:HG21	1:B:182:ARG:HG3	1.91	0.52
1:A:68:LYS:HA	1:A:71:GLU:HB2	1.91	0.52
1:A:59:ALA:N	2:A:464:HOH:O	2.41	0.51
1:A:299:ARG:HG3	1:A:310:PRO:HA	1.94	0.50
1:A:304:THR:HG23	1:B:182:ARG:HA	1.94	0.49
1:B:123:GLU:HA	1:B:126:ARG:HG3	1.93	0.49
1:B:16:THR:HG21	1:B:47:ALA:HB2	1.93	0.49
1:A:304:THR:HG22	1:A:305:GLY:H	1.78	0.49
1:B:271:TYR:HD1	1:B:283:ARG:HH22	1.60	0.49
1:A:304:THR:CG2	1:B:182:ARG:HG3	2.43	0.49
1:B:148:LYS:HB3	1:B:253:ARG:HH12	1.78	0.49
1:A:262:LYS:NZ	2:A:549:HOH:O	2.40	0.48
1:B:194:LEU:HD11	1:B:272:PHE:HB2	1.96	0.48
1:A:39:TYR:OH	1:A:72:LYS:NZ	2.46	0.48
1:A:124:ASP:HA	1:A:127:LYS:HB2	1.95	0.47
1:B:158:MET:HB3	1:B:191:MET:HE1	1.96	0.47
1:A:22:LEU:HD13	1:A:39:TYR:CE2	2.50	0.47
1:B:251:PRO:HG2	1:B:253:ARG:CZ	2.45	0.46
1:B:121:THR:OG1	1:B:122:LEU:N	2.47	0.46
1:A:304:THR:HG22	1:A:305:GLY:N	2.30	0.46
1:A:299:ARG:NH2	1:B:160:ASP:OD1	2.49	0.46
1:A:251:PRO:HG2	1:A:253:ARG:CZ	2.45	0.46
1:A:234:LYS:NZ	2:A:500:HOH:O	2.49	0.46
1:B:129:GLU:HG2	1:B:129:GLU:H	1.45	0.45
1:A:103:VAL:HB	1:A:106:ILE:HD12	1.99	0.45
1:A:10:THR:N	2:A:453:HOH:O	2.50	0.45
1:B:208:PRO:HB3	1:B:232:GLU:HB3	1.99	0.45
1:A:229:SER:HB3	1:A:236:MET:HB2	1.98	0.45
1:B:133:ASN:HD22	1:B:133:ASN:H	1.64	0.45
1:A:45:VAL:HG11	1:A:62:LEU:HB3	1.99	0.45
1:A:82:LEU:O	1:A:86:GLU:HG2	2.17	0.44
1:A:28:ASN:ND2	2:A:450:HOH:O	2.50	0.44
1:B:122:LEU:HD21	1:B:126:ARG:NH2	2.32	0.44
1:A:226:ASP:HB2	1:A:238:VAL:HB	1.99	0.44
1:B:304:THR:CG2	1:B:306:VAL:HG22	2.44	0.44
1:A:196:THR:HB	1:A:265:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:THR:OG1	1:A:13:GLY:N	2.50	0.44
1:A:154:GLU:OE2	2:A:434:HOH:O	2.21	0.44
1:B:226:ASP:HB2	1:B:238:VAL:HB	1.99	0.44
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.73	0.43
1:A:54:LYS:HB2	1:A:54:LYS:HE3	1.72	0.43
1:B:293:ILE:HG12	1:B:298:ILE:HG13	2.01	0.43
1:B:194:LEU:HD12	1:B:269:VAL:HA	2.01	0.43
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.89	0.42
1:A:170:ASP:HB3	1:A:173:TYR:CD1	2.54	0.42
1:B:230:LYS:HE3	1:B:230:LYS:HB2	1.68	0.42
1:B:73:ILE:O	1:B:77:LEU:HB2	2.18	0.42
1:B:92:ASP:HB2	2:B:501:HOH:O	2.19	0.42
1:A:68:LYS:HB3	1:A:68:LYS:HE2	1.75	0.42
1:A:236:MET:HE3	1:A:254:ARG:NH2	2.35	0.42
1:A:234:LYS:HE3	1:A:234:LYS:HB3	1.92	0.41
1:B:197:HIS:CD2	1:B:199:ASN:H	2.38	0.41
1:A:289:LYS:HB3	1:A:289:LYS:HE3	1.94	0.41
1:B:133:ASN:ND2	1:B:133:ASN:N	2.68	0.41
1:A:209:LYS:HA	1:A:212:HIS:HB2	2.02	0.41
1:B:148:LYS:HB2	1:B:148:LYS:HE3	1.53	0.41
1:B:132:LEU:O	2:B:460:HOH:O	2.22	0.41
1:B:15:ILE:HD13	1:B:73:ILE:HG23	2.02	0.41
1:A:198:PRO:HA	1:A:262:LYS:HD3	2.03	0.41
1:B:59:ALA:O	1:B:62:LEU:HB2	2.20	0.41
1:B:170:ASP:HB3	1:B:173:TYR:CD1	2.56	0.41
1:A:292:THR:OG1	1:A:301:LEU:HG	2.21	0.41
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.75	0.41
1:B:170:ASP:HA	1:B:171:PRO:HD3	1.94	0.40
1:B:173:TYR:CD2	1:B:195:LEU:HD11	2.57	0.40
1:B:241:LEU:HB3	1:B:250:TYR:CD1	2.56	0.40
1:A:209:LYS:HB2	2:A:555:HOH:O	2.21	0.40
1:B:27:LYS:HE3	1:B:28:ASN:OD1	2.22	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	323/335 (96%)	289 (90%)	28 (9%)	6 (2%)	8	3
1	B	323/335 (96%)	286 (88%)	28 (9%)	9 (3%)	5	1
All	All	646/670 (96%)	575 (89%)	56 (9%)	15 (2%)	6	2

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	GLY
1	A	303	VAL
1	B	106	ILE
1	B	129	GLU
1	A	64	GLY
1	B	109	SER
1	B	132	LEU
1	B	134	HIS
1	B	248	ASN
1	A	206	LYS
1	A	275	SER
1	A	248	ASN
1	B	118	GLY
1	B	121	THR
1	B	206	LYS

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	286/296 (97%)	255 (89%)	31 (11%)	6	3
1	B	286/296 (97%)	238 (83%)	48 (17%)	2	1
All	All	572/592 (97%)	493 (86%)	79 (14%)	3	2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	40	ARG
1	A	41	LYS
1	A	44	SER
1	A	55	SER
1	A	58	GLU
1	A	74	ASP
1	A	85	LEU
1	A	89	ARG
1	A	91	ASP
1	A	93	THR
1	A	95	SER
1	A	97	ILE
1	A	100	LEU
1	A	117	GLU
1	A	120	LYS
1	A	123	GLU
1	A	129	GLU
1	A	130	ASP
1	A	147	GLU
1	A	168	LYS
1	A	203	GLU
1	A	207	GLN
1	A	232	GLU
1	A	275	SER
1	A	276	ASP
1	A	292	THR
1	A	295	GLU
1	A	301	LEU
1	A	303	VAL
1	A	326	ARG
1	B	19	LEU
1	B	33	ILE
1	B	61	LYS
1	B	68	LYS
1	B	74	ASP
1	B	77	LEU
1	B	87	LYS
1	B	89	ARG
1	B	92	ASP
1	B	100	LEU
1	B	101	THR

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Mol	Chain	Res	Type
1	B	120	LYS
1	B	122	LEU
1	B	124	ASP
1	B	127	LYS
1	B	128	ASN
1	B	133	ASN
1	B	140	LEU
1	B	141	LYS
1	B	148	LYS
1	B	167	LYS
1	B	168	LYS
1	B	169	LEU
1	B	186	GLU
1	B	193	VAL
1	B	196	THR
1	B	201	THR
1	B	207	GLN
1	B	213	ARG
1	B	216	GLU
1	B	221	VAL
1	B	222	ARG
1	B	241	LEU
1	B	244	GLU
1	B	246	ASP
1	B	275	SER
1	B	276	ASP
1	B	289	LYS
1	B	295	GLU
1	B	298	ILE
1	B	301	LEU
1	B	303	VAL
1	B	304	THR
1	B	306	VAL
1	B	311	LEU
1	B	317	GLN
1	B	325	TRP
1	B	326	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	HIS

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Mol	Chain	Res	Type
1	B	197	HIS

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, 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	325/335 (97%)	-0.04	10 (3%) 49 55	21, 41, 81, 94	87 (26%)
1	B	325/335 (97%)	0.17	19 (5%) 23 28	33, 53, 95, 104	110 (33%)
All	All	650/670 (97%)	0.07	29 (4%) 33 38	21, 50, 88, 104	197 (30%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	ASN	9.9
1	B	248	ASN	6.6
1	B	107	GLY	3.6
1	A	303	VAL	3.5
1	A	90	GLN	3.4
1	A	246	ASP	3.3
1	B	123	GLU	3.3
1	B	90	GLN	3.2
1	B	127	LYS	3.2
1	B	106	ILE	3.2
1	B	326	ARG	3.1
1	A	100	LEU	3.1
1	B	114	LEU	3.0
1	B	88	ILE	3.0
1	B	93	THR	2.8
1	A	97	ILE	2.8
1	B	94	SER	2.6
1	B	132	LEU	2.5
1	B	287	LEU	2.4
1	A	94	SER	2.4
1	B	205	SER	2.3
1	B	117	GLU	2.2
1	A	101	THR	2.2
1	B	111	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	HIS	2.1
1	A	123	GLU	2.1
1	B	112	ARG	2.0
1	B	97	ILE	2.0
1	A	88	ILE	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.