



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:31 PM UTC

PDB ID : 9DR9 / pdb_00009dr9
Title : Binary product complex of DNA polymerase iota with DNA
Authors : Frevert, Z.; Reusch, D.; Freudenthal, B.; Washington, M.T.
Deposited on : 2024-09-25
Resolution : 2.21 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

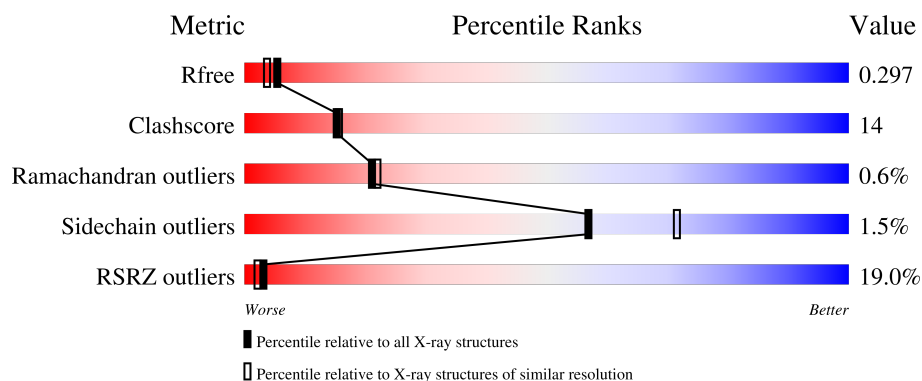
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 $\leq 5\%$. 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	420	17% 67% 19% • 13%
2	B	19	5% 42% 37% 11% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6877 atoms, of which 3485 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 iota.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	H	N	O	S	2	0	0
			5884	1825	2992	504	542	21			

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	17	Total	C	H	N	O	P	0	0	0
			540	165	191	66	101	17			

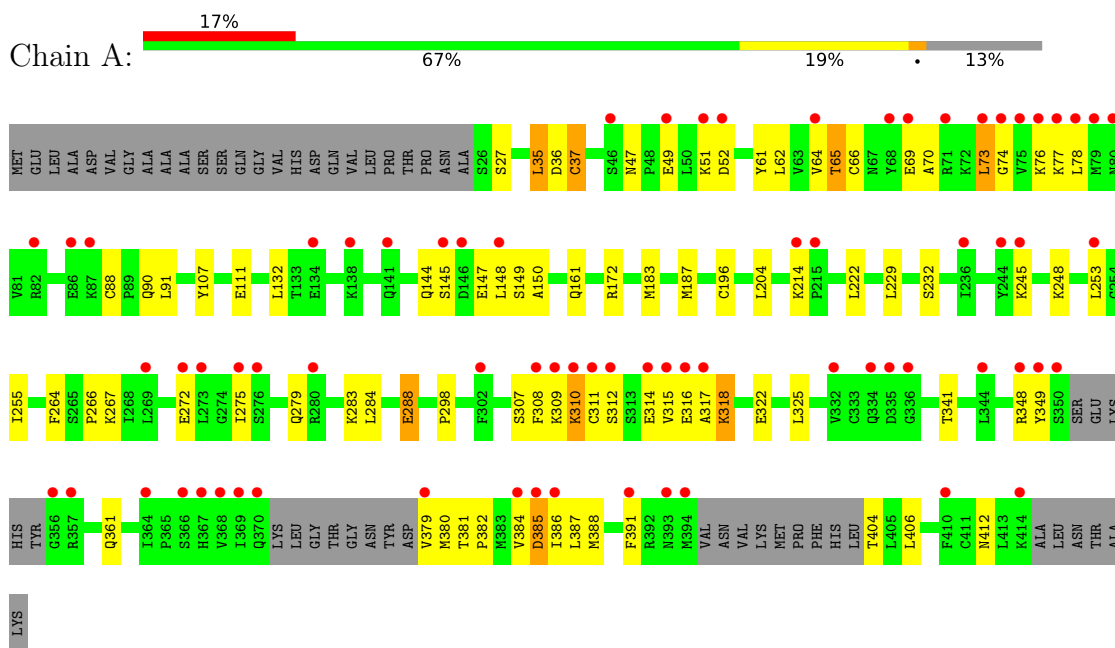
- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	132	Total	H	O	0	0
			396	264	132		
3	B	19	Total	H	O	0	0
			57	38	19		

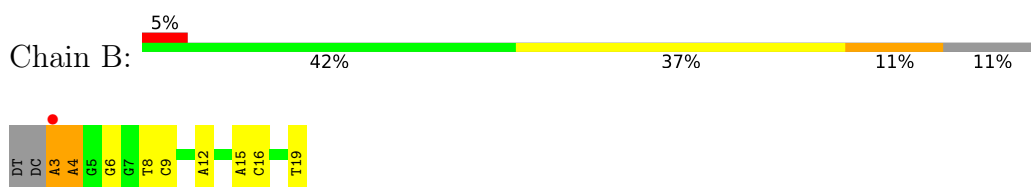
3 Residue-property plots [i](#)

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: DNA polymerase iota



- Molecule 2: DNA (5'-D(P*AP*AP*GP*GP*GP*TP*CP*CP*TP*AP*GP*GP*AP*CP*CP*C P*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	97.10Å 97.10Å 202.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.76 – 2.21 43.76 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.3 (43.76-2.21) 97.2 (43.76-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.297 0.255 , 0.297	Depositor DCC
R_{free} test set	1405 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6877	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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	0.66	2/2931 (0.1%)	0.97	3/3948 (0.1%)
2	B	1.26	5/391 (1.3%)	1.36	6/601 (1.0%)
All	All	0.76	7/3322 (0.2%)	1.03	9/4549 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	DA	C1'-N9	8.63	1.63	1.46
2	B	3	DA	C4'-C3'	6.03	1.64	1.52
1	A	298	PRO	CA-C	-5.85	1.48	1.52
2	B	4	DA	P-O5'	-5.64	1.49	1.60
1	A	348	ARG	CG-CD	5.37	1.68	1.52
2	B	3	DA	C5'-C4'	5.09	1.62	1.52
2	B	3	DA	N9-C4	5.03	1.48	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	DA	C4'-C3'-O3'	-12.70	90.95	110.00
2	B	3	DA	C2'-C3'-O3'	9.40	125.60	111.50
2	B	3	DA	P-O3'-C3'	9.16	133.94	120.20
2	B	3	DA	O3'-P-O5'	-6.71	93.93	104.00
2	B	3	DA	O4'-C1'-N9	-5.96	99.46	108.40
1	A	385	ASP	N-CA-CB	5.56	118.39	110.16
1	A	288	GLU	CB-CG-CD	-5.54	103.18	112.60
1	A	348	ARG	CG-CD-NE	5.21	123.47	112.00
2	B	4	DA	O5'-C5'-C4'	-5.01	103.29	110.80

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	2892	2992	2980	79	0
2	B	349	191	191	11	0
3	A	132	264	0	2	0
3	B	19	38	0	2	0
All	All	3392	3485	3171	87	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 14.

All (87) 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:245:LYS:HE3	2:B:15:DA:H5''	1.53	0.90
1:A:62:LEU:HD13	1:A:78:LEU:HD23	1.60	0.80
1:A:64:VAL:HG13	1:A:65:THR:HG22	1.64	0.77
2:B:6:DG:H4'	3:B:101:HOH:O	1.87	0.74
1:A:325:LEU:HD21	1:A:387:LEU:HD11	1.69	0.73
1:A:325:LEU:HD21	1:A:387:LEU:CD1	2.23	0.69
1:A:69:GLU:O	1:A:73:LEU:HD13	1.94	0.67
1:A:312:SER:OG	1:A:317:ALA:HB2	1.94	0.66
1:A:69:GLU:O	1:A:73:LEU:CD1	2.43	0.66
1:A:35:LEU:HD21	1:A:187:MET:CE	2.25	0.66
1:A:27:SER:O	1:A:172:ARG:NH2	2.30	0.64
1:A:47:ASN:OD1	1:A:49:GLU:HB2	1.98	0.63
1:A:382:PRO:O	1:A:386:ILE:HD12	1.98	0.63
1:A:283:LYS:HE3	1:A:288:GLU:OE1	1.98	0.63
1:A:317:ALA:HA	3:A:512:HOH:O	1.99	0.62
1:A:310:LYS:HD3	1:A:349:TYR:HB2	1.80	0.62
1:A:267:LYS:HD3	1:A:267:LYS:H	1.67	0.60
1:A:148:LEU:O	1:A:148:LEU:HD23	2.03	0.58
1:A:229:LEU:O	1:A:232:SER:OG	2.21	0.57
1:A:308:PHE:HB2	1:A:311:CYS:HB2	1.85	0.56
1:A:35:LEU:HD21	1:A:187:MET:HE1	1.88	0.55
1:A:196:CYS:SG	1:A:214:LYS:O	2.65	0.55
2:B:4:DA:H5'	2:B:4:DA:N3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LYS:O	1:A:311:CYS:N	2.40	0.55
1:A:65:THR:HB	2:B:19:DT:O3'	2.06	0.54
1:A:267:LYS:HD3	1:A:267:LYS:N	2.23	0.54
1:A:77:LYS:O	1:A:78:LEU:HB2	2.07	0.54
1:A:315:VAL:CG1	1:A:315:VAL:O	2.56	0.53
1:A:275:ILE:HD12	1:A:275:ILE:H	1.73	0.53
1:A:380:MET:O	1:A:384:VAL:HG23	2.10	0.52
1:A:388:MET:HE3	1:A:388:MET:HA	1.92	0.52
1:A:35:LEU:HD21	1:A:187:MET:HE3	1.93	0.51
1:A:74:GLY:O	1:A:76:LYS:HG2	2.11	0.50
1:A:90:GLN:OE1	1:A:90:GLN:N	2.35	0.50
1:A:308:PHE:CD1	1:A:404:THR:HA	2.47	0.50
1:A:73:LEU:HD12	1:A:73:LEU:N	2.27	0.50
1:A:148:LEU:HD23	1:A:148:LEU:C	2.37	0.49
1:A:266:PRO:HD2	1:A:267:LYS:NZ	2.28	0.49
1:A:315:VAL:O	1:A:315:VAL:HG12	2.12	0.49
1:A:384:VAL:O	1:A:388:MET:HG2	2.11	0.49
1:A:379:VAL:C	1:A:382:PRO:HD2	2.39	0.48
2:B:6:DG:C4'	3:B:101:HOH:O	2.53	0.48
1:A:161:GLN:OE1	1:A:222:LEU:HB2	2.15	0.47
1:A:385:ASP:CB	3:A:523:HOH:O	2.63	0.47
1:A:36:ASP:O	1:A:37:CYS:C	2.57	0.47
1:A:66:CYS:HB2	1:A:70:ALA:HB3	1.97	0.47
1:A:309:LYS:O	1:A:310:LYS:C	2.57	0.47
2:B:3:DA:O5'	2:B:3:DA:N3	2.48	0.46
1:A:361:GLN:HG2	2:B:12:DA:OP2	2.15	0.46
2:B:8:DT:H2''	2:B:9:DC:H5'	1.96	0.46
1:A:267:LYS:H	1:A:267:LYS:CD	2.29	0.46
1:A:35:LEU:CD2	1:A:187:MET:HE1	2.45	0.45
1:A:318:LYS:O	1:A:322:GLU:HG3	2.17	0.45
1:A:325:LEU:CD2	1:A:387:LEU:CD1	2.94	0.45
2:B:15:DA:H2'	2:B:16:DC:C6	2.52	0.45
1:A:107:TYR:O	1:A:111:GLU:HG3	2.16	0.45
1:A:69:GLU:O	1:A:73:LEU:HD12	2.17	0.44
1:A:245:LYS:HD2	1:A:245:LYS:C	2.42	0.44
1:A:222:LEU:HD23	1:A:222:LEU:N	2.32	0.44
1:A:325:LEU:HB3	1:A:380:MET:HE1	1.99	0.44
1:A:255:ILE:HD11	1:A:264:PHE:CG	2.53	0.44
2:B:3:DA:N3	2:B:3:DA:C5'	2.81	0.44
2:B:8:DT:H2'	2:B:9:DC:C6	2.53	0.44
1:A:144:GLN:H	1:A:147:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:HG	1:A:317:ALA:HB2	1.81	0.43
1:A:309:LYS:C	1:A:311:CYS:N	2.76	0.43
1:A:316:GLU:O	1:A:316:GLU:OE1	2.37	0.43
1:A:275:ILE:O	1:A:279:GLN:HB2	2.19	0.43
1:A:204:LEU:HD22	1:A:284:LEU:CD2	2.48	0.42
1:A:147:GLU:O	1:A:150:ALA:N	2.44	0.42
1:A:314:GLU:HB3	1:A:316:GLU:HG3	2.01	0.42
1:A:51:LYS:O	1:A:52:ASP:HB2	2.20	0.42
1:A:248:LYS:HE3	1:A:248:LYS:HB3	1.65	0.42
1:A:307:SER:O	1:A:308:PHE:HB3	2.20	0.42
1:A:309:LYS:O	1:A:311:CYS:SG	2.76	0.42
1:A:266:PRO:HD2	1:A:267:LYS:HZ1	1.83	0.42
1:A:88:CYS:SG	1:A:91:LEU:HB2	2.60	0.42
1:A:341:THR:OG1	1:A:412:ASN:HB2	2.20	0.41
1:A:253:LEU:HD11	1:A:272:GLU:HG2	2.01	0.41
1:A:61:TYR:CD2	1:A:62:LEU:HD23	2.56	0.41
1:A:132:LEU:HD21	1:A:183:MET:HE1	2.03	0.41
1:A:144:GLN:O	1:A:145:SER:C	2.61	0.41
1:A:204:LEU:HD22	1:A:284:LEU:HD22	2.03	0.41
1:A:317:ALA:HB1	1:A:406:LEU:HD11	2.03	0.41
1:A:381:THR:N	1:A:382:PRO:CD	2.85	0.40
1:A:385:ASP:O	1:A:386:ILE:C	2.63	0.40
1:A:391:PHE:CD1	1:A:391:PHE:C	2.98	0.40

There are no symmetry-related clashes.

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	359/420 (86%)	338 (94%)	19 (5%)	2 (1%)	21	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	LYS
1	A	37	CYS

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	334/376 (89%)	329 (98%)	5 (2%)	57 71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	65	THR
1	A	73	LEU
1	A	149	SER
1	A	318	LYS

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

Mol	Chain	Res	Type
1	A	80	ASN
1	A	256	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 oligosaccharides 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	367/420 (87%)	1.11	72 (19%) 3 2	31, 54, 92, 107	0
2	B	17/19 (89%)	0.57	1 (5%) 28 25	36, 44, 59, 88	0
All	All	384/439 (87%)	1.08	73 (19%) 3 2	31, 53, 91, 107	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3	DA	4.9
1	A	315	VAL	4.6
1	A	317	ALA	4.5
1	A	244	TYR	4.4
1	A	68	TYR	4.4
1	A	350	SER	4.3
1	A	349	TYR	4.2
1	A	316	GLU	4.2
1	A	311	CYS	4.1
1	A	370	GLN	4.1
1	A	367	HIS	4.0
1	A	275	ILE	4.0
1	A	215	PRO	4.0
1	A	336	GLY	4.0
1	A	77	LYS	4.0
1	A	385	ASP	4.0
1	A	214	LYS	3.9
1	A	314	GLU	3.9
1	A	309	LYS	3.7
1	A	86	GLU	3.6
1	A	73	LEU	3.6
1	A	348	ARG	3.6
1	A	379	VAL	3.6
1	A	368	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLN	3.4
1	A	46	SER	3.4
1	A	394	MET	3.3
1	A	356	GLY	3.2
1	A	87	LYS	3.1
1	A	414	LYS	3.1
1	A	78	LEU	3.1
1	A	310	LYS	3.0
1	A	134	GLU	3.0
1	A	76	LYS	2.9
1	A	369	ILE	2.9
1	A	276	SER	2.9
1	A	236	ILE	2.9
1	A	245	LYS	2.8
1	A	272	GLU	2.8
1	A	280	ARG	2.8
1	A	71	ARG	2.8
1	A	148	LEU	2.8
1	A	344	LEU	2.7
1	A	332	VAL	2.7
1	A	269	LEU	2.5
1	A	64	VAL	2.5
1	A	386	ILE	2.5
1	A	75	VAL	2.5
1	A	312	SER	2.5
1	A	52	ASP	2.5
1	A	145	SER	2.4
1	A	273	LEU	2.4
1	A	366	SER	2.4
1	A	302	PHE	2.4
1	A	391	PHE	2.4
1	A	80	ASN	2.3
1	A	335	ASP	2.3
1	A	82	ARG	2.3
1	A	334	GLN	2.3
1	A	79	MET	2.3
1	A	146	ASP	2.2
1	A	357	ARG	2.2
1	A	364	ILE	2.2
1	A	308	PHE	2.2
1	A	138	LYS	2.2
1	A	74	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	LYS	2.1
1	A	49	GLU	2.1
1	A	384	VAL	2.1
1	A	410	PHE	2.1
1	A	69	GLU	2.0
1	A	253	LEU	2.0
1	A	393	ASN	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 oligosaccharides 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.