



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 09:40 pm GMT

PDB ID : 2BPC  
Title : CRYSTAL STRUCTURE OF RAT DNA POLYMERASE BETA: EVIDENCE FOR A COMMON POLYMERASE MECHANISM  
Authors : Sawaya, M.R.; Pelletier, H.; Kumar, A.; Wilson, S.H.; Kraut, J.  
Deposited on : 1994-07-08  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

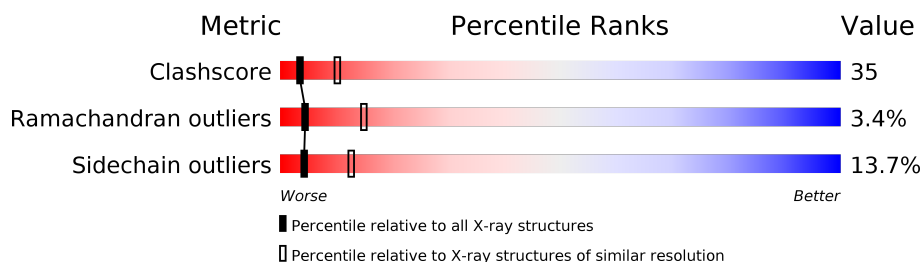
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2016 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	242	Total	C	N	O	S	0	0	0
			1923	1211	338	366	8			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

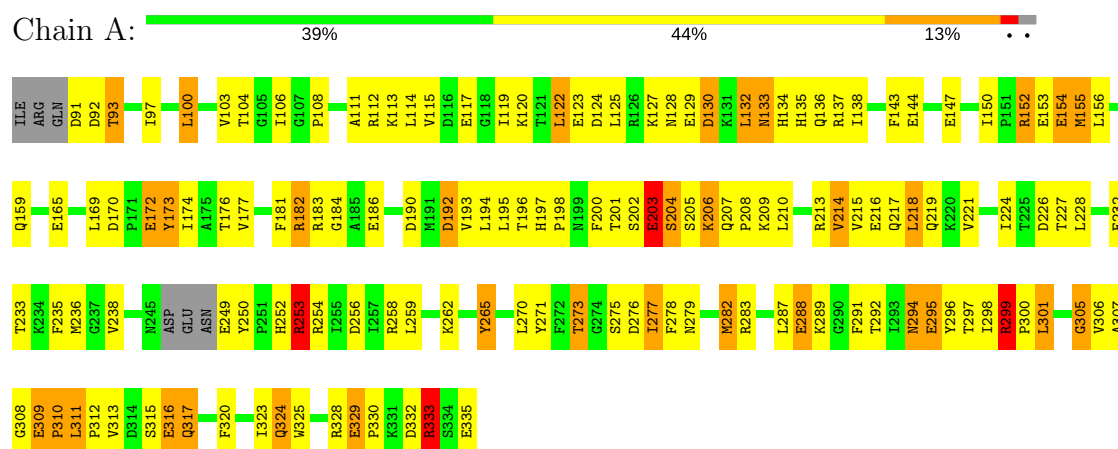
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		

### 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 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.

Note EDS was not executed.

#### • Molecule 1: DNA POLYMERASE BETA



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.81Å 62.63Å 37.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2016	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.31	19/1961 (1.0%)	1.63	20/2646 (0.8%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	144	GLU	CD-OE2	8.86	1.35	1.25
1	A	335	GLU	CD-OE2	8.67	1.35	1.25
1	A	154	GLU	CD-OE2	8.49	1.34	1.25
1	A	216	GLU	CD-OE2	8.09	1.34	1.25
1	A	153	GLU	CD-OE2	7.97	1.34	1.25
1	A	295	GLU	CD-OE2	7.90	1.34	1.25
1	A	232	GLU	CD-OE2	7.82	1.34	1.25
1	A	129	GLU	CD-OE2	7.79	1.34	1.25
1	A	172	GLU	CD-OE2	7.61	1.34	1.25
1	A	203	GLU	CD-OE2	7.58	1.33	1.25
1	A	117	GLU	CD-OE2	7.55	1.33	1.25
1	A	147	GLU	CD-OE2	7.45	1.33	1.25
1	A	288	GLU	CD-OE2	7.40	1.33	1.25
1	A	165	GLU	CD-OE2	7.39	1.33	1.25
1	A	329	GLU	CD-OE2	7.34	1.33	1.25
1	A	249	GLU	CD-OE2	7.09	1.33	1.25
1	A	186	GLU	CD-OE2	7.07	1.33	1.25
1	A	316	GLU	CD-OE2	6.12	1.32	1.25
1	A	309	GLU	CD-OE2	5.88	1.32	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	192	ASP	N-CA-CB	9.60	127.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ASP	CB-CG-OD2	-9.03	110.18	118.30
1	A	253	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	258	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	226	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	190	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	226	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	258	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	265	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	299	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	276	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	276	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	282	MET	CA-CB-CG	-5.60	103.78	113.30
1	A	299	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	113	LYS	N-CA-CB	5.33	120.19	110.60
1	A	236	MET	CA-CB-CG	-5.24	104.40	113.30
1	A	233	THR	CA-CB-CG2	-5.22	105.10	112.40
1	A	132	LEU	CB-CA-C	-5.14	100.44	110.20
1	A	333	ARG	NE-CZ-NH1	5.07	122.84	120.30

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	1923	0	1853	132	0
2	A	1	0	0	0	0
3	A	92	0	0	15	0
All	All	2016	0	1853	132	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 35.

All (132) 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:270:LEU:HD21	1:A:282:MET:HE1	1.32	1.10
1:A:317:GLN:NE2	1:A:317:GLN:H	1.57	1.02
1:A:317:GLN:HE21	1:A:317:GLN:N	1.61	0.98
1:A:294:ASN:ND2	1:A:296:TYR:H	1.61	0.98
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.29	0.96
1:A:294:ASN:HD22	1:A:296:TYR:H	1.12	0.94
1:A:133:ASN:ND2	1:A:136:GLN:HG3	1.86	0.90
1:A:270:LEU:HD21	1:A:282:MET:CE	2.05	0.87
1:A:152:ARG:HA	1:A:155:MET:HB2	1.59	0.83
1:A:289:LYS:NZ	1:A:324:GLN:HG3	1.95	0.81
1:A:215:VAL:O	1:A:219:GLN:HG3	1.80	0.81
1:A:172:GLU:HG2	1:A:198:PRO:HG2	1.66	0.78
1:A:254:ARG:NH1	1:A:254:ARG:HB3	2.01	0.75
1:A:279:ASN:O	1:A:283:ARG:HB2	1.87	0.75
1:A:193:VAL:C	1:A:194:LEU:HD12	2.08	0.74
1:A:316:GLU:HB2	3:A:466:HOH:O	1.86	0.74
1:A:208:PRO:HD2	3:A:473:HOH:O	1.87	0.73
1:A:170:ASP:OD2	1:A:197:HIS:NE2	2.23	0.71
1:A:299:ARG:HG3	1:A:299:ARG:NH1	2.03	0.69
1:A:328:ARG:HD3	1:A:332:ASP:O	1.92	0.69
1:A:134:HIS:O	1:A:138:ILE:HG12	1.93	0.68
1:A:204:SER:O	1:A:206:LYS:HD3	1.93	0.68
1:A:294:ASN:HD22	1:A:295:GLU:N	1.92	0.68
1:A:287:LEU:HA	1:A:291:PHE:O	1.94	0.68
1:A:133:ASN:HD21	1:A:136:GLN:HG3	1.59	0.66
1:A:194:LEU:HD12	1:A:194:LEU:N	2.09	0.66
1:A:328:ARG:HG3	3:A:430:HOH:O	1.96	0.66
1:A:136:GLN:NE2	3:A:471:HOH:O	2.28	0.66
1:A:270:LEU:CD2	1:A:282:MET:HE1	2.18	0.66
1:A:200:PHE:CE2	1:A:259:LEU:HG	2.31	0.65
1:A:329:GLU:HB3	3:A:429:HOH:O	1.96	0.65
1:A:169:LEU:HD21	1:A:217:GLN:HG2	1.79	0.65
1:A:305:GLY:O	1:A:307:ALA:N	2.29	0.65
1:A:253:ARG:NH1	3:A:402:HOH:O	2.26	0.64
1:A:224:ILE:HD13	1:A:235:PHE:CE2	2.32	0.64
1:A:143:PHE:HA	3:A:465:HOH:O	1.96	0.64
1:A:159:GLN:HB2	1:A:177:VAL:HG11	1.80	0.64
1:A:289:LYS:HZ3	1:A:324:GLN:HG3	1.60	0.63
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.63	0.62
1:A:224:ILE:HD13	1:A:235:PHE:HE2	1.64	0.61
1:A:289:LYS:HZ2	1:A:324:GLN:HG3	1.64	0.61
1:A:137:ARG:HD3	3:A:434:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:HG3	3:A:443:HOH:O	2.01	0.60
1:A:152:ARG:NH2	1:A:181:PHE:O	2.35	0.60
1:A:214:VAL:HG23	1:A:218:LEU:HD22	1.84	0.60
1:A:200:PHE:HE1	1:A:205:SER:HA	1.67	0.59
1:A:122:LEU:HD12	1:A:122:LEU:H	1.67	0.59
1:A:132:LEU:HA	3:A:471:HOH:O	2.01	0.59
1:A:182:ARG:HD3	1:A:273:THR:OG1	2.03	0.59
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.18	0.58
1:A:315:SER:HB2	1:A:317:GLN:NE2	2.18	0.58
1:A:317:GLN:HE21	1:A:317:GLN:H	0.78	0.58
1:A:273:THR:HG22	3:A:414:HOH:O	2.04	0.57
1:A:294:ASN:C	1:A:294:ASN:HD22	2.07	0.57
1:A:182:ARG:NH1	1:A:316:GLU:OE2	2.29	0.57
1:A:200:PHE:HE2	1:A:259:LEU:HG	1.69	0.57
1:A:200:PHE:HB2	1:A:210:LEU:CD1	2.34	0.56
1:A:238:VAL:HG13	1:A:252:HIS:HB3	1.87	0.56
1:A:97:ILE:HD12	1:A:97:ILE:N	2.19	0.56
1:A:174:ILE:HB	1:A:196:THR:HG22	1.88	0.55
1:A:174:ILE:HG21	1:A:265:TYR:CE2	2.42	0.54
1:A:182:ARG:HH12	1:A:316:GLU:CD	2.11	0.53
1:A:103:VAL:HB	1:A:106:ILE:HD12	1.91	0.53
1:A:133:ASN:ND2	1:A:135:HIS:HB3	2.23	0.53
1:A:192:ASP:HA	1:A:256:ASP:O	2.09	0.52
1:A:254:ARG:HH11	1:A:254:ARG:HB3	1.74	0.52
1:A:201:THR:C	1:A:203:GLU:H	2.12	0.52
1:A:125:LEU:O	1:A:128:ASN:N	2.37	0.52
1:A:228:LEU:HD13	1:A:238:VAL:HG23	1.92	0.51
1:A:330:PRO:HD3	1:A:333:ARG:HH21	1.75	0.51
1:A:174:ILE:HG22	1:A:265:TYR:OH	2.10	0.51
1:A:176:THR:HA	3:A:424:HOH:O	2.10	0.51
1:A:133:ASN:ND2	1:A:136:GLN:H	2.09	0.51
1:A:172:GLU:HG2	1:A:198:PRO:CG	2.39	0.50
1:A:328:ARG:HA	3:A:460:HOH:O	2.11	0.50
1:A:297:THR:OG1	1:A:299:ARG:NH1	2.45	0.50
1:A:100:LEU:HD23	1:A:111:ALA:O	2.12	0.49
1:A:227:THR:HG23	1:A:235:PHE:CE1	2.48	0.49
1:A:228:LEU:CD1	1:A:238:VAL:HG23	2.45	0.47
1:A:271:TYR:CD2	1:A:295:GLU:HB3	2.49	0.47
1:A:104:THR:HG22	3:A:435:HOH:O	2.13	0.47
1:A:122:LEU:CD1	1:A:123:GLU:H	2.27	0.47
1:A:294:ASN:HD22	1:A:296:TYR:N	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG23	1:A:235:PHE:HE1	1.79	0.47
1:A:170:ASP:O	1:A:173:TYR:HB2	2.15	0.47
1:A:330:PRO:O	1:A:333:ARG:HG3	2.15	0.47
1:A:254:ARG:HB3	1:A:254:ARG:CZ	2.45	0.47
1:A:323:ILE:C	1:A:324:GLN:HG2	2.35	0.47
1:A:309:GLU:HA	1:A:310:PRO:HD3	1.40	0.46
1:A:115:VAL:HG13	1:A:120:LYS:HG2	1.96	0.46
1:A:218:LEU:O	1:A:221:VAL:HG23	2.16	0.46
1:A:201:THR:O	1:A:203:GLU:N	2.49	0.46
1:A:275:SER:OG	1:A:277:ILE:HG12	2.15	0.46
1:A:152:ARG:NH2	1:A:184:GLY:CA	2.78	0.46
1:A:122:LEU:HD12	1:A:122:LEU:N	2.31	0.46
1:A:154:GLU:HG2	1:A:250:TYR:HE2	1.81	0.45
1:A:192:ASP:HB3	1:A:256:ASP:HB2	1.99	0.45
1:A:137:ARG:HB2	3:A:434:HOH:O	2.16	0.45
1:A:127:LYS:HA	1:A:127:LYS:HD3	1.82	0.44
1:A:294:ASN:HD21	1:A:296:TYR:HB2	1.82	0.44
1:A:194:LEU:N	1:A:194:LEU:CD1	2.78	0.44
1:A:311:LEU:HA	1:A:312:PRO:HD3	1.82	0.44
1:A:324:GLN:HB3	1:A:324:GLN:HE21	1.59	0.44
1:A:112:ARG:O	1:A:115:VAL:N	2.49	0.43
1:A:152:ARG:O	1:A:156:LEU:HB2	2.17	0.43
1:A:207:GLN:O	1:A:210:LEU:HB2	2.17	0.43
1:A:207:GLN:HB2	1:A:210:LEU:HD12	2.00	0.43
1:A:294:ASN:ND2	1:A:297:THR:H	2.17	0.43
1:A:298:ILE:O	1:A:298:ILE:HG23	2.18	0.43
1:A:97:ILE:H	1:A:97:ILE:HD12	1.83	0.43
1:A:174:ILE:CG2	1:A:265:TYR:CE2	3.02	0.43
1:A:278:PHE:CG	1:A:333:ARG:HB3	2.54	0.43
1:A:130:ASP:N	1:A:130:ASP:OD1	2.52	0.42
1:A:119:ILE:HA	1:A:124:ASP:HB3	2.02	0.42
1:A:183:ARG:NH1	1:A:275:SER:CA	2.83	0.42
1:A:209:LYS:O	1:A:213:ARG:HB2	2.19	0.42
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.84	0.42
1:A:292:THR:O	1:A:292:THR:HG23	2.19	0.42
1:A:300:PRO:O	1:A:308:GLY:HA2	2.19	0.42
1:A:320:PHE:O	1:A:324:GLN:N	2.53	0.42
1:A:299:ARG:CG	1:A:299:ARG:NH1	2.79	0.41
1:A:295:GLU:CD	1:A:295:GLU:H	2.23	0.41
1:A:262:LYS:O	1:A:262:LYS:HG3	2.21	0.41
1:A:294:ASN:ND2	1:A:296:TYR:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:O	1:A:93:THR:N	2.42	0.41
1:A:201:THR:C	1:A:203:GLU:N	2.74	0.41
1:A:214:VAL:HG23	1:A:218:LEU:CD2	2.48	0.41
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.83	0.41
1:A:294:ASN:ND2	1:A:294:ASN:C	2.73	0.41
1:A:292:THR:HG23	1:A:299:ARG:HB2	2.03	0.40
1:A:122:LEU:HD12	1:A:123:GLU:H	1.86	0.40
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.56	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	238/248 (96%)	197 (83%)	33 (14%)	8 (3%)	4	15

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	306	VAL
1	A	202	SER
1	A	324	GLN
1	A	301	LEU
1	A	305	GLY
1	A	310	PRO
1	A	108	PRO

### 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	205/226 (91%)	177 (86%)	28 (14%)	4 13

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	A	100	LEU
1	A	114	LEU
1	A	122	LEU
1	A	130	ASP
1	A	133	ASN
1	A	150	ILE
1	A	152	ARG
1	A	155	MET
1	A	173	TYR
1	A	195	LEU
1	A	203	GLU
1	A	204	SER
1	A	206	LYS
1	A	214	VAL
1	A	218	LEU
1	A	253	ARG
1	A	273	THR
1	A	277	ILE
1	A	288	GLU
1	A	294	ASN
1	A	299	ARG
1	A	301	LEU
1	A	311	LEU
1	A	313	VAL
1	A	317	GLN
1	A	325	TRP
1	A	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
1	A	136	GLN
1	A	164	ASN
1	A	281	ASN
1	A	294	ASN
1	A	317	GLN
1	A	324	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 carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.