



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:15 PM UTC

PDB ID : 3K5N / pdb_00003k5n
Title : Crystal structure of E.coli Pol II-abasic DNA binary complex
Authors : Yang, W.; Wang, F.
Deposited on : 2009-10-07
Resolution : 3.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

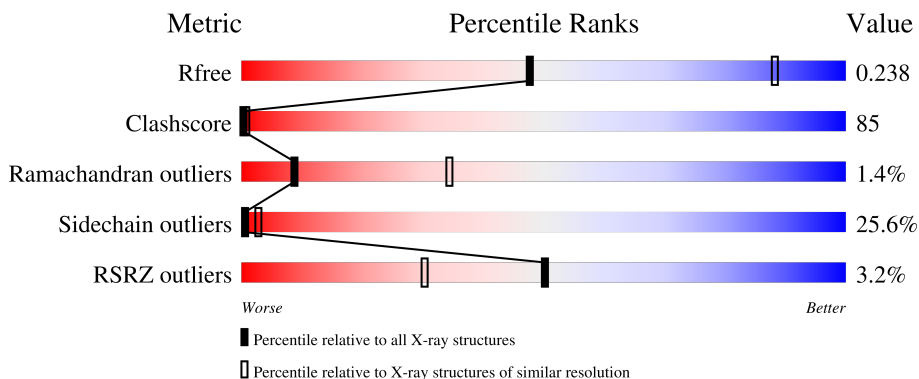
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	786	2% 24% 45% 22% 5%
1	B	786	2% 21% 45% 23% 5% 6%
2	T	20	35% 55% 10% 35%
3	P	13	54% 77% 23%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12722 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			6169	3934	1093	1117	25			
1	B	738	Total	C	N	O	S	0	0	0
			6007	3832	1066	1086	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189
B	-2	GLY	-	expression tag	UNP P21189
B	-1	PRO	-	expression tag	UNP P21189
B	0	HIS	-	expression tag	UNP P21189
B	335	ASN	ASP	engineered mutation	UNP P21189

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*C P*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	13	Total	C	N	O	P	0	0	0
			263	126	51	74	12			

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	13	Total	C	N	O	P	0	0	0
			255	122	45	76	12			

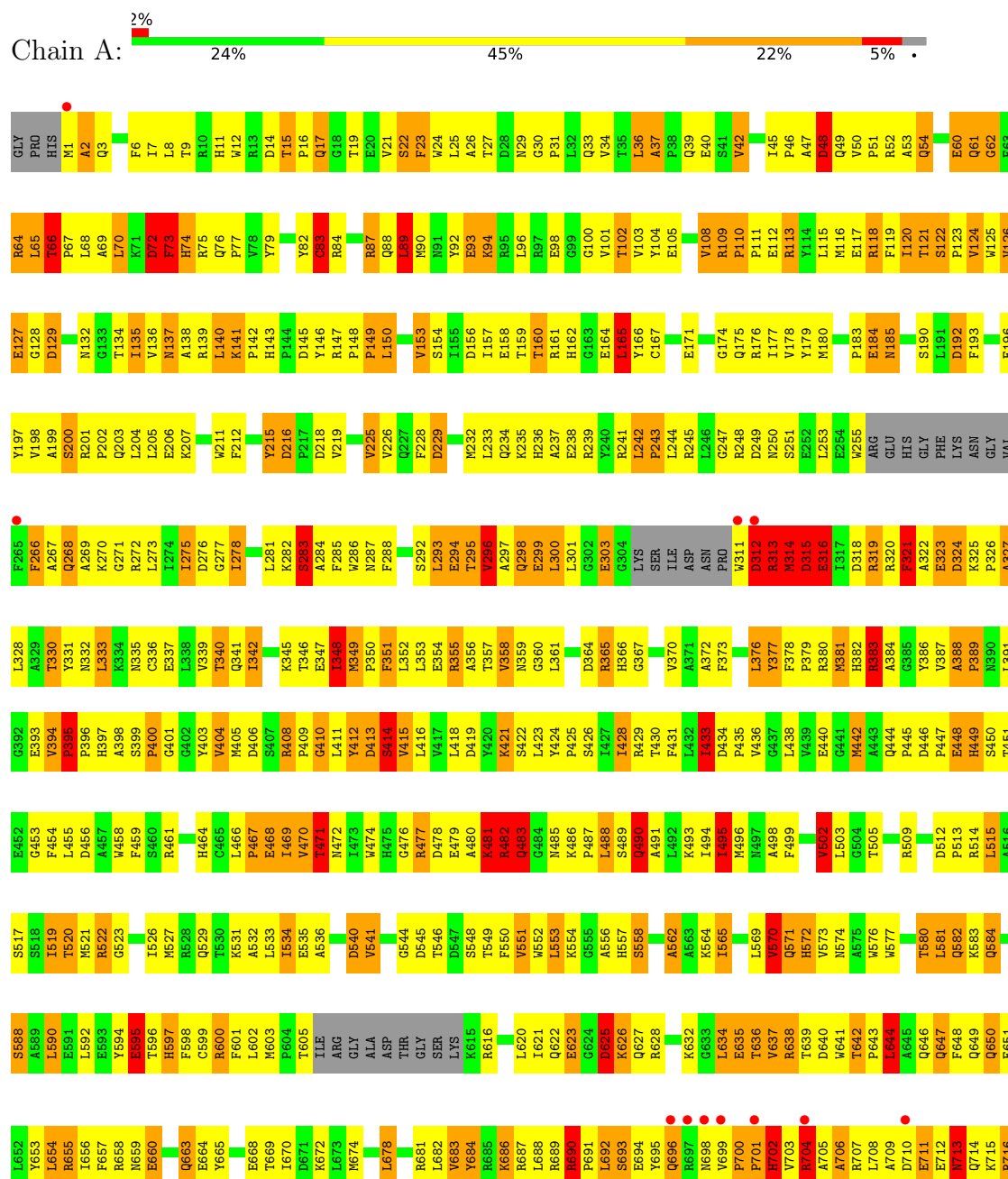
- Molecule 4 is water.

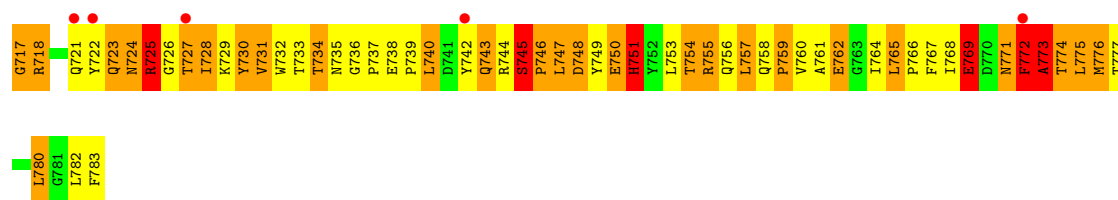
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	10	Total 10	O 10	0	0

3 Residue-property plots

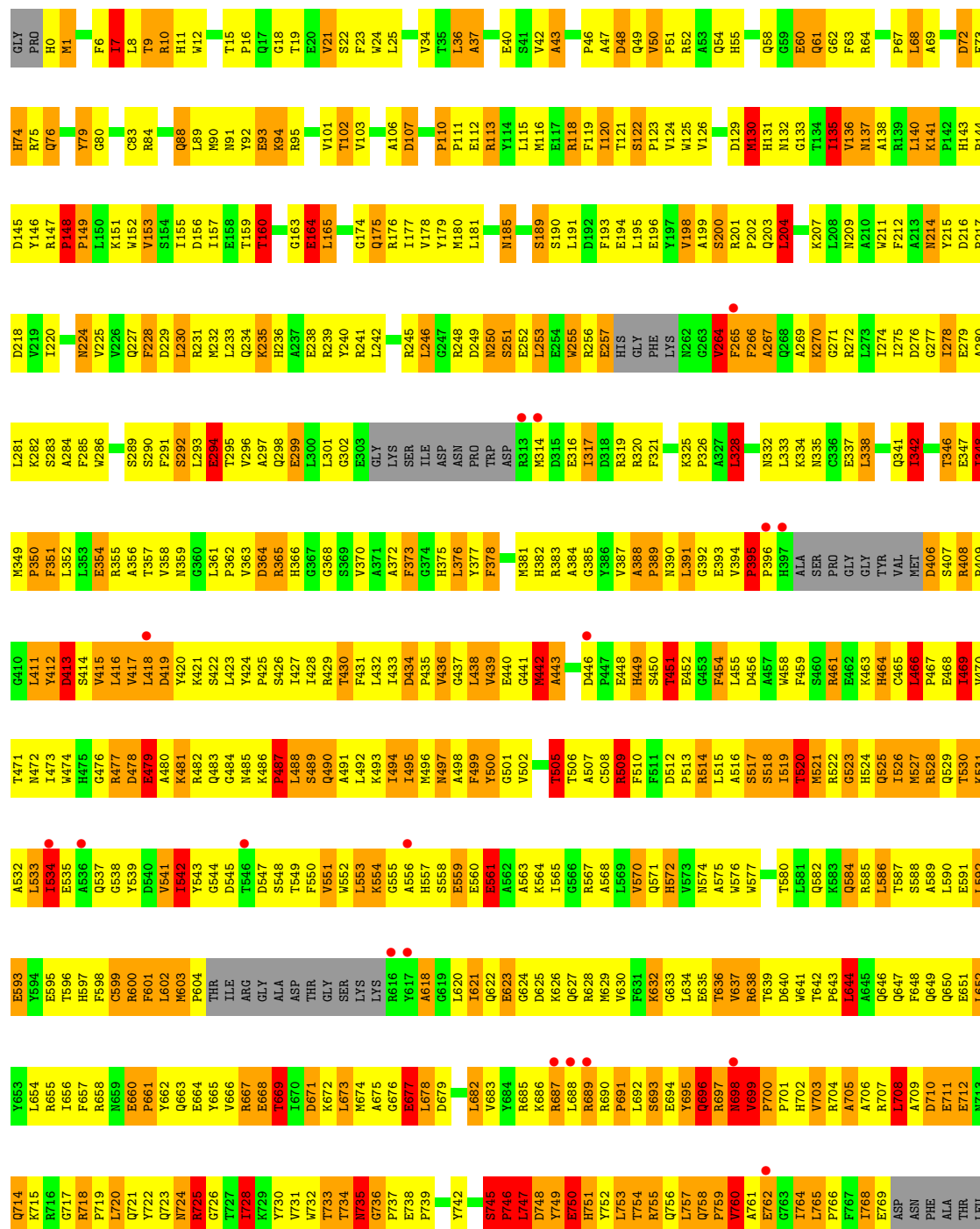
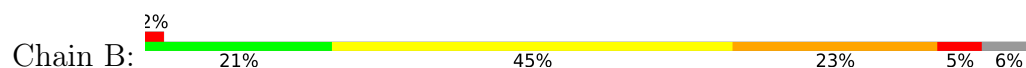
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase II





● Molecule 1: DNA polymerase II



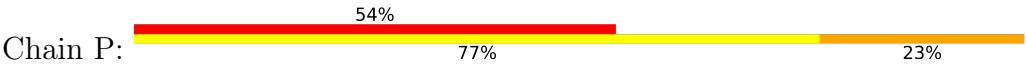
MET
THR
GLY
GLN
LEU
GLY
LEU
PHE

● Molecule 2: DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3')



DG	DT	DC	DC	DT	DG	3DR	T808	A809	C810	G811	C812	T813	A814	G815	G816	C817	A818	C819	A820

● Molecule 3: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3')



G901	T902	G903	C904	C905	T906	A907	G908	C909	G910	T911	A912	G913

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.41Å 147.55Å 96.28Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	31.31 – 3.15 31.31 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (31.31-3.15) 95.2 (31.31-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.236 0.232 , 0.238	Depositor DCC
R_{free} test set	1696 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12722	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	1.27	22/6331 (0.3%)	1.60	141/8587 (1.6%)
1	B	1.24	26/6163 (0.4%)	1.57	142/8359 (1.7%)
2	T	0.69	0/295	1.49	5/453 (1.1%)
3	P	0.80	0/285	1.56	6/438 (1.4%)
All	All	1.24	48/13074 (0.4%)	1.58	294/17837 (1.6%)

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	B	0	1

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	ARG	CG-CD	-14.96	1.07	1.52
1	B	50	VAL	CA-CB	-9.07	1.49	1.54
1	B	130	MET	SD-CE	-8.23	1.58	1.79
1	B	220	ILE	CA-CB	-7.37	1.45	1.54
1	A	433	ILE	CA-CB	-7.31	1.45	1.54

The worst 5 of 294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	HIS	N-CA-C	-14.31	95.37	110.97
1	A	725	ARG	CA-CB-CG	13.95	142.00	114.10
1	A	702	HIS	N-CA-C	-13.77	95.88	111.71
1	B	623	GLU	N-CA-C	-13.61	91.31	110.50
1	A	725	ARG	NE-CZ-NH1	-13.27	108.23	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	745	SER	Mainchain

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	6169	0	6040	889	2
1	B	6007	0	5881	1097	4
2	T	263	0	147	67	0
3	P	255	0	143	59	0
4	A	18	0	0	2	0
4	B	10	0	0	0	0
All	All	12722	0	12211	2103	4

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 85.

The worst 5 of 2103 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:688:LEU:CD1	1:B:728:ILE:HD11	1.34	1.51
1:B:231:ARG:HD2	1:B:265:PHE:CE1	1.42	1.51
1:B:688:LEU:HD11	1:B:728:ILE:CD1	1.45	1.44
1:B:642:THR:CB	1:B:756:GLN:NE2	1.85	1.37
1:A:14:ASP:OD2	1:A:87:ARG:HG2	1.20	1.35

All (4) 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:79:TYR:OH	1:B:671:ASP:OD1[2_554]	1.81	0.39
1:B:79:TYR:OH	1:B:667:ARG:NH1[2_554]	1.85	0.35
1:A:241:ARG:NH2	1:B:585:ARG:NH1[1_556]	2.14	0.06
1:A:201:ARG:NH1	1:B:714:GLN:O[2_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	751/786 (96%)	698 (93%)	42 (6%)	11 (2%)	8	33
1	B	728/786 (93%)	678 (93%)	41 (6%)	9 (1%)	10	37
All	All	1479/1572 (94%)	1376 (93%)	83 (6%)	20 (1%)	9	34

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ASP
1	A	483	GLN
1	A	690	ARG
1	A	769	GLU
1	B	1	MET

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	649/672 (97%)	478 (74%)	171 (26%)	0	2
1	B	632/672 (94%)	475 (75%)	157 (25%)	1	3
All	All	1281/1344 (95%)	953 (74%)	328 (26%)	0	3

5 of 328 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	LEU

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Mol	Chain	Res	Type
1	B	603	MET
1	B	442	MET
1	B	514	ARG
1	B	687	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	HIS
1	B	185	ASN
1	B	721	GLN
1	B	49	GLN
1	B	88	GLN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	759/786 (96%)	-0.07	16 (2%) 63 42	3, 29, 70, 98	0
1	B	738/786 (93%)	0.15	18 (2%) 59 39	9, 46, 78, 93	0
2	T	13/20 (65%)	1.86	7 (53%) 0 0	85, 100, 131, 134	0
3	P	13/13 (100%)	1.81	7 (53%) 0 0	60, 97, 131, 131	0
All	All	1523/1605 (94%)	0.07	48 (3%) 50 30	3, 36, 78, 134	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	699	VAL	5.0
1	A	772	PHE	4.7
2	T	820	DA	4.0
1	A	311	TRP	3.5
1	A	710	ASP	3.1

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.