



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 8, 2026 – 11:49 PM JST

PDB ID : 25EC / pdb_000025ec
Title : Crystal Structure of a Human Topoisomerase II Beta-DNA Cleavage Complex
Trapped in N-gate Dissociated State
Authors : Ali, M.S.; Zhao, W.
Deposited on : 2026-03-30
Resolution : 2.90 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

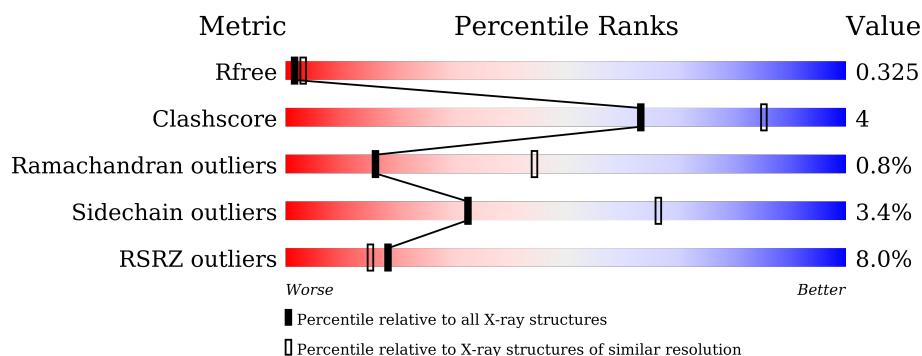
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	757	7% 79% 11% 10%
2	D	12	8% 83% 17%
3	E	8	12% 88% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5597 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 topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	683	Total	C	N	O	S	0	0	0
			5160	3284	871	983	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			

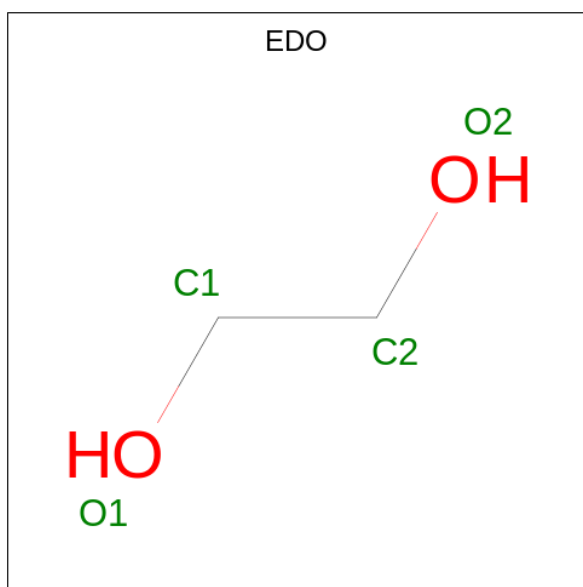
- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

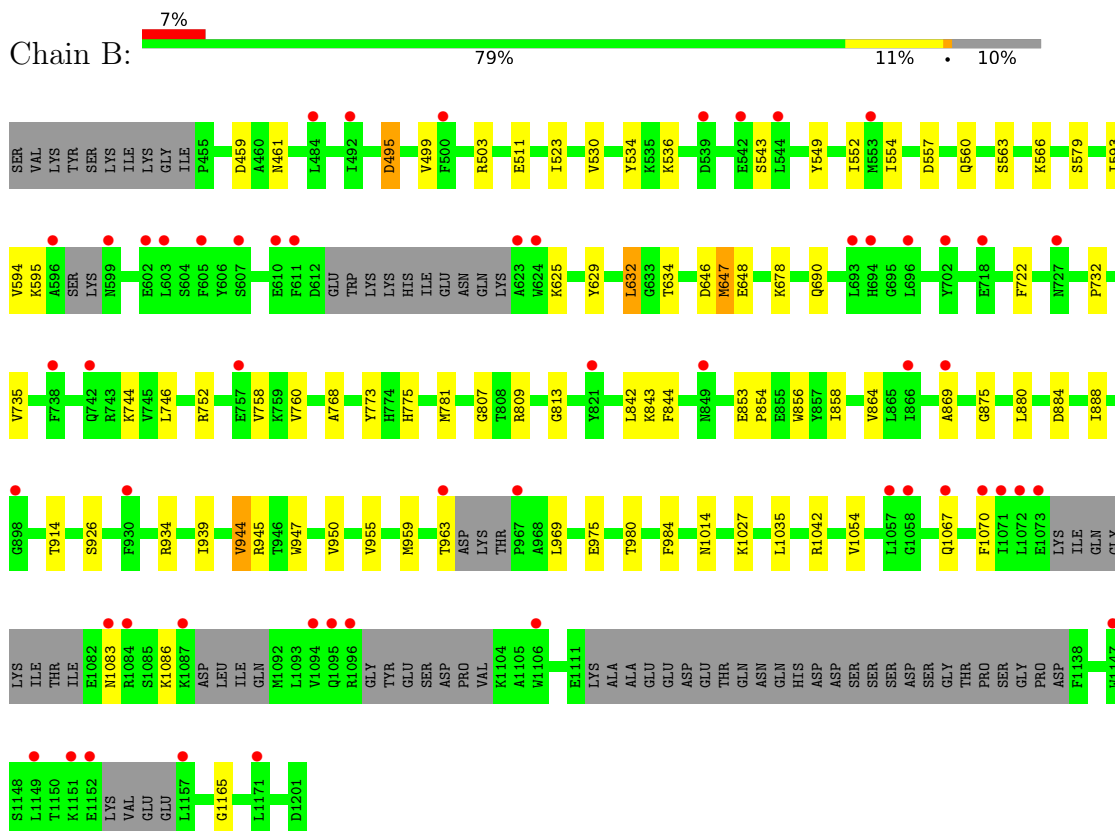
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	6	Total	O	0	0
			6	6		
6	D	2	Total	O	0	0
			2	2		

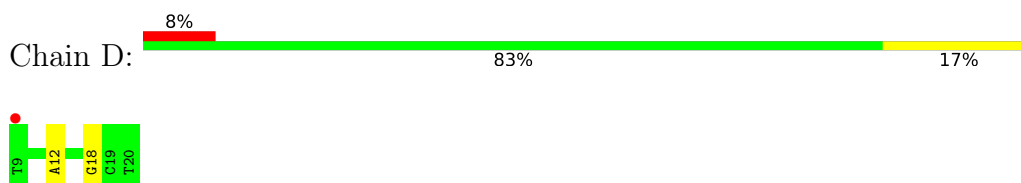
3 Residue-property plots [i](#)

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.

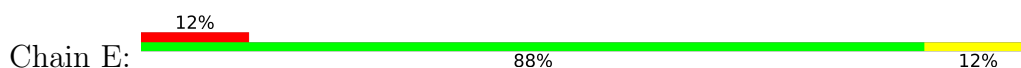
- Molecule 1: DNA topoisomerase 2-beta



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



- Molecule 3: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.31Å 92.31Å 232.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.17 – 2.90 40.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.17-2.90) 99.3 (40.17-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.289 , 0.329 0.283 , 0.325	Depositor DCC
R_{free} test set	1326 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5597	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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](#)

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

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	B	0.11	0/5258	0.30	0/7136
2	D	0.21	0/273	0.45	0/419
3	E	0.21	0/185	0.38	0/283
All	All	0.12	0/5716	0.31	0/7838

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	5160	0	4787	40	0
2	D	245	0	136	2	0
3	E	165	0	89	1	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
5	B	16	0	24	0	0
6	B	6	0	0	0	0
6	D	2	0	0	0	0
All	All	5597	0	5036	41	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 4.

All (41) 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:944:VAL:HG13	1:B:945:ARG:HG3	1.73	0.69
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.73	0.69
1:B:844:PHE:HA	1:B:854:PRO:HA	1.82	0.60
1:B:557:ASP:HA	1:B:632:LEU:HD13	1.87	0.56
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.89	0.55
1:B:807:GLY:HA3	1:B:813:GLY:HA2	1.90	0.53
1:B:768:ALA:HA	1:B:773:TYR:HB3	1.90	0.53
1:B:595:LYS:HB2	1:B:629:TYR:HE1	1.74	0.53
1:B:1014:ASN:O	1:B:1027:LYS:NZ	2.42	0.52
1:B:955:VAL:HG12	1:B:959:MET:HE2	1.90	0.52
2:D:18:DG:H1	3:E:3:DC:H42	1.59	0.51
1:B:536:LYS:HZ3	1:B:543:SER:HB2	1.76	0.50
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.95	0.49
1:B:503:ARG:HB3	2:D:12:DA:C2	2.48	0.48
1:B:975:GLU:HG2	1:B:984:PHE:CE1	2.49	0.48
1:B:459:ASP:OD1	1:B:549:TYR:OH	2.21	0.48
1:B:678:LYS:NZ	1:B:875:GLY:O	2.42	0.47
1:B:760:VAL:HG12	1:B:781:MET:HG2	1.97	0.47
1:B:554:ILE:HG21	1:B:566:LYS:HG2	1.97	0.47
1:B:534:TYR:C	1:B:536:LYS:H	2.23	0.47
1:B:752:ARG:NH2	1:B:758:VAL:HG11	2.30	0.46
1:B:629:TYR:HA	1:B:634:THR:HG21	1.98	0.46
1:B:530:VAL:HG21	1:B:552:ILE:HD11	1.99	0.45
1:B:809:ARG:NH1	1:B:980:THR:O	2.43	0.45
1:B:842:LEU:HD21	1:B:858:ILE:HG22	1.98	0.45
1:B:563:SER:HA	1:B:566:LYS:HE3	2.00	0.44
1:B:595:LYS:HB2	1:B:629:TYR:CE1	2.52	0.44
1:B:884:ASP:O	1:B:888:ILE:HG12	2.17	0.44
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.99	0.44
1:B:864:VAL:HG22	1:B:880:LEU:HD22	1.98	0.44
1:B:593:ILE:HG23	1:B:594:VAL:HG23	1.99	0.44
1:B:744:LYS:HZ3	1:B:853:GLU:CD	2.26	0.43
1:B:735:VAL:HG11	1:B:856:TRP:CE3	2.53	0.43
1:B:773:TYR:CZ	1:B:775:HIS:HB2	2.54	0.43
1:B:939:ILE:HB	1:B:984:PHE:HB2	2.00	0.43
1:B:646:ASP:C	1:B:648:GLU:H	2.27	0.42
1:B:843:LYS:HA	1:B:843:LYS:HD2	1.81	0.42
1:B:947:TRP:HB2	1:B:950:VAL:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ILE:HG23	1:B:858:ILE:O	2.21	0.41
1:B:1070:PHE:O	1:B:1070:PHE:CG	2.74	0.41
1:B:1067:GLN:O	1:B:1070:PHE:HD2	2.03	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	B	665/757 (88%)	625 (94%)	35 (5%)	5 (1%)	16	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	625	LYS
1	B	1083	ASN
1	B	647	MET
1	B	1086	LYS
1	B	1165	GLY

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	B	506/665 (76%)	489 (97%)	17 (3%)	32	66

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

Mol	Chain	Res	Type
1	B	495	ASP
1	B	499	VAL
1	B	511	GLU
1	B	523	ILE
1	B	579	SER
1	B	632	LEU
1	B	647	MET
1	B	690	GLN
1	B	746	LEU
1	B	914	THR
1	B	926	SER
1	B	934	ARG
1	B	944	VAL
1	B	963	THR
1	B	969	LEU
1	B	1035	LEU
1	B	1054	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	650	HIS
1	B	690	GLN
1	B	712	ASN
1	B	922	GLN
1	B	935	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	1303	-	3,3,3	0.47	0	2,2,2	0.27	0
5	EDO	B	1305	-	3,3,3	0.46	0	2,2,2	0.31	0
5	EDO	B	1306	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	B	1304	-	3,3,3	0.46	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1303	-	-	0/1/1/1	-
5	EDO	B	1305	-	-	0/1/1/1	-
5	EDO	B	1306	-	-	0/1/1/1	-
5	EDO	B	1304	-	-	0/1/1/1	-

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	B	683/757 (90%)	0.73	54 (7%) 18 15	40, 55, 87, 115	0
2	D	12/12 (100%)	0.40	1 (8%) 17 14	43, 54, 97, 112	0
3	E	8/8 (100%)	0.25	1 (12%) 8 7	45, 46, 73, 91	0
All	All	703/777 (90%)	0.72	56 (7%) 18 15	40, 55, 89, 115	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1152	GLU	4.8
1	B	1083	ASN	4.4
1	B	611	PHE	4.1
1	B	484	LEU	3.9
1	B	1094	VAL	3.8
2	D	9	DT	3.8
1	B	727	ASN	3.8
1	B	898	GLY	3.3
1	B	1087	LYS	3.2
1	B	930	PHE	3.0
1	B	603	LEU	3.0
1	B	738	PHE	3.0
1	B	1095	GLN	3.0
1	B	623	ALA	3.0
1	B	693	LEU	3.0
1	B	500	PHE	3.0
1	B	1084	ARG	2.9
1	B	602	GLU	2.9
1	B	539	ASP	2.9
1	B	1058	GLY	2.9
1	B	821	TYR	2.8
1	B	1057	LEU	2.7
1	B	1072	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1106	TRP	2.6
1	B	599	ASN	2.6
1	B	1151	LYS	2.6
1	B	866	ILE	2.6
1	B	1096	ARG	2.6
1	B	624	TRP	2.5
1	B	544	LEU	2.5
1	B	1071	ILE	2.5
1	B	849	ASN	2.5
1	B	696	LEU	2.5
1	B	1073	GLU	2.5
1	B	542	GLU	2.4
3	E	1	DA	2.4
1	B	1171	LEU	2.4
1	B	596	ALA	2.4
1	B	1157	LEU	2.4
1	B	757	GLU	2.3
1	B	967	PRO	2.3
1	B	1067	GLN	2.3
1	B	1149	LEU	2.3
1	B	694	HIS	2.3
1	B	607	SER	2.3
1	B	553	MET	2.2
1	B	1070	PHE	2.2
1	B	718	GLU	2.2
1	B	1147	TRP	2.2
1	B	605	PHE	2.2
1	B	702	TYR	2.2
1	B	742	GLN	2.1
1	B	963	THR	2.1
1	B	610	GLU	2.1
1	B	869	ALA	2.0
1	B	492	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
5	EDO	B	1306	4/4	0.72	0.33	59,61,62,67	4
5	EDO	B	1304	4/4	0.73	0.36	52,56,57,58	4
5	EDO	B	1305	4/4	0.78	0.17	50,52,53,54	4
4	MG	D	101	1/1	0.79	0.37	55,55,55,55	0
4	MG	B	1302	1/1	0.80	0.33	51,51,51,51	0
5	EDO	B	1303	4/4	0.84	0.14	48,52,55,57	0
4	MG	B	1301	1/1	0.93	0.28	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.