



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 AM UTC

PDB ID : 4XIU / pdb_00004xiu
Title : Binary complex structure of Klenow fragment of Taq DNA polymerase I707L mutant with DNA containing TTT overhang
Authors : Wu, E.Y.
Deposited on : 2015-01-07
Resolution : 2.50 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	:	2022.3.0, CSD as543be (2022)
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

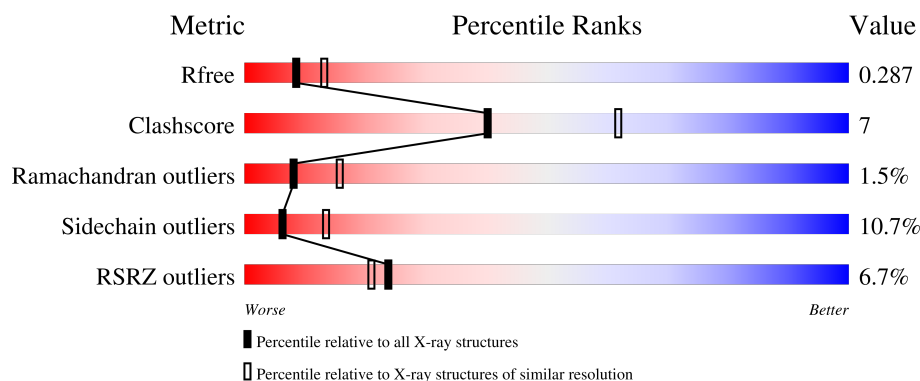
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	12	92% 8%
2	C	14	71% 29%
3	A	539	7% 76% 22% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4723 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 DNA chain called Synthetic oligonucleotide primer strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	12	Total	C	N	O	P	0	0	0
			240	114	48	67	11			

- Molecule 2 is a DNA chain called Synthetic oligonucleotide template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total	C	N	O	P	0	0	0
			290	136	53	87	14			

- Molecule 3 is a protein called DNA polymerase I, thermostable.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	539	Total	C	N	O	S	0	0	0
			4191	2670	748	760	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LEU	ILE	engineered mutation	UNP P19821

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

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

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.

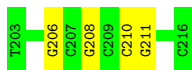
- Molecule 1: Synthetic oligonucleotide primer strand

Chain B:  92% 8%



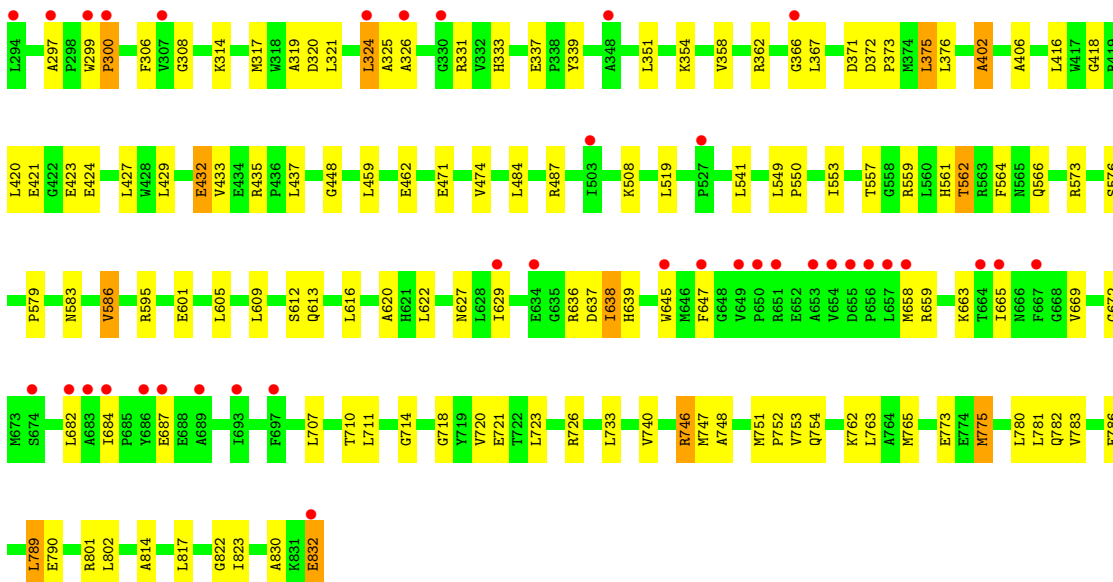
- Molecule 2: Synthetic oligonucleotide template strand

Chain C:  71% 29%



- Molecule 3: DNA polymerase I, thermostable

Chain A:  7% 76% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	110.03Å 110.03Å 90.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.64 – 2.50 47.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.64-2.50) 96.4 (47.64-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.286 0.225 , 0.287	Depositor DCC
R_{free} test set	1075 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: DOC, MG

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	0.36	0/249	0.74	0/382
2	C	0.40	0/324	0.82	0/499
3	A	0.70	0/4281	0.92	3/5813 (0.1%)
All	All	0.67	0/4854	0.91	3/6694 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ALA	N-CA-C	5.29	117.73	111.33
3	A	337	GLU	CA-C-N	5.04	124.48	119.24
3	A	337	GLU	C-N-CA	5.04	124.48	119.24

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	240	0	134	0	0
2	C	290	0	158	3	0
3	A	4191	0	4173	60	1
4	A	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4723	0	4465	61	1

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 7.

All (61) 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)
3:A:474:VAL:HG21	3:A:484:LEU:HD11	1.59	0.83
3:A:317:MET:HE1	3:A:362:ARG:HB3	1.62	0.81
3:A:317:MET:HA	3:A:317:MET:HE2	1.61	0.80
3:A:562:THR:CG2	3:A:579:PRO:O	2.33	0.77
3:A:317:MET:HE3	3:A:358:VAL:HG12	1.75	0.67
3:A:562:THR:HG22	3:A:579:PRO:O	1.95	0.66
3:A:418:GLY:O	3:A:421:GLU:HG3	1.97	0.65
3:A:562:THR:HG21	3:A:576:SER:OG	1.98	0.62
3:A:562:THR:HG23	3:A:579:PRO:O	2.01	0.60
3:A:351:LEU:HG	3:A:373:PRO:HG2	1.84	0.60
2:C:210:DC:H2'	2:C:211:DG:C8	2.38	0.59
3:A:573:ARG:HG3	3:A:754:GLN:HE21	1.69	0.58
3:A:297:ALA:HB2	3:A:331:ARG:HD3	1.86	0.58
2:C:206:DG:OP1	3:A:747:MET:HG2	2.07	0.55
3:A:354:LYS:NZ	3:A:564:PHE:O	2.39	0.54
3:A:299:TRP:O	3:A:300:PRO:C	2.50	0.54
3:A:317:MET:HE1	3:A:362:ARG:CB	2.35	0.53
3:A:595:ARG:HD3	3:A:832:GLU:OE2	2.08	0.53
3:A:822:GLY:HA3	3:A:830:ALA:O	2.10	0.52
3:A:474:VAL:HG21	3:A:484:LEU:CD1	2.34	0.52
3:A:324:LEU:HD23	3:A:325:ALA:N	2.25	0.52
3:A:620:ALA:HB1	3:A:629:ILE:HG22	1.92	0.52
3:A:320:ASP:OD1	3:A:339:TYR:OH	2.14	0.51
3:A:437:LEU:HD22	3:A:762:LYS:HD3	1.93	0.51
3:A:609:LEU:CD1	3:A:789:LEU:HD22	2.40	0.51
3:A:647:PHE:CE2	3:A:658:MET:HG2	2.45	0.51
3:A:317:MET:HE3	3:A:358:VAL:CG1	2.39	0.51
3:A:371:ASP:OD1	3:A:435:ARG:NH1	2.41	0.51
3:A:720:VAL:HG21	3:A:748:ALA:O	2.10	0.51
3:A:672:GLY:HA3	3:A:746:ARG:HG2	1.92	0.50
3:A:317:MET:CE	3:A:362:ARG:HB3	2.39	0.50
3:A:605:LEU:HD13	3:A:823:ILE:HG22	1.94	0.49
3:A:372:ASP:HB3	3:A:375:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:208:DG:H4'	3:A:576:SER:O	2.14	0.48
3:A:721:GLU:HA	3:A:726:ARG:O	2.15	0.47
3:A:376:LEU:HD22	3:A:420:LEU:HD12	1.97	0.47
3:A:429:LEU:O	3:A:433:VAL:HB	2.15	0.46
3:A:306:PHE:O	3:A:326:ALA:HA	2.15	0.46
3:A:308:GLY:O	3:A:402:ALA:HB1	2.16	0.45
3:A:319:ALA:O	3:A:362:ARG:NH1	2.45	0.45
3:A:324:LEU:HD23	3:A:325:ALA:H	1.81	0.45
3:A:751:MET:HB3	3:A:752:PRO:HD3	1.99	0.45
3:A:783:VAL:HB	3:A:786:GLU:HG3	2.00	0.44
3:A:297:ALA:HB3	3:A:333:HIS:CD2	2.52	0.44
3:A:549:LEU:HB2	3:A:550:PRO:HD3	2.00	0.44
3:A:637:ASP:O	3:A:638:ILE:C	2.60	0.43
3:A:376:LEU:HD22	3:A:420:LEU:CD1	2.48	0.43
3:A:637:ASP:O	3:A:639:HIS:N	2.53	0.42
3:A:557:THR:OG1	3:A:561:HIS:HE1	2.03	0.42
3:A:773:GLU:C	3:A:775:MET:H	2.26	0.42
3:A:639:HIS:ND1	3:A:663:LYS:HG3	2.35	0.42
3:A:586:VAL:O	3:A:586:VAL:HG22	2.19	0.42
3:A:471:GLU:O	3:A:474:VAL:HG22	2.20	0.42
3:A:559:ARG:HH22	3:A:790:GLU:CD	2.28	0.42
3:A:780:LEU:HD11	3:A:790:GLU:HB2	2.02	0.42
3:A:714:GLY:O	3:A:718:GLY:N	2.50	0.41
3:A:306:PHE:O	3:A:406:ALA:HB1	2.21	0.40
3:A:765:MET:SD	3:A:782:GLN:HG3	2.61	0.40
3:A:423:GLU:O	3:A:424:GLU:C	2.63	0.40
3:A:573:ARG:HG3	3:A:754:GLN:NE2	2.35	0.40
3:A:448:GLY:O	3:A:780:LEU:HD22	2.20	0.40

All (1) 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)
3:A:432:GLU:OE2	3:A:432:GLU:OE2[6_555]	2.14	0.06

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
3	A	537/539 (100%)	492 (92%)	37 (7%)	8 (2%)	8 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	638	ILE
3	A	366	GLY
3	A	687	GLU
3	A	586	VAL
3	A	814	ALA
3	A	601	GLU
3	A	367	LEU
3	A	300	PRO

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
3	A	419/441 (95%)	374 (89%)	45 (11%)	6 13

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	314	LYS
3	A	321	LEU
3	A	324	LEU

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Mol	Chain	Res	Type
3	A	375	LEU
3	A	416	LEU
3	A	427	LEU
3	A	432	GLU
3	A	459	LEU
3	A	462	GLU
3	A	487	ARG
3	A	508	LYS
3	A	519	LEU
3	A	541	LEU
3	A	553	ILE
3	A	562	THR
3	A	566	GLN
3	A	583	ASN
3	A	612	SER
3	A	613	GLN
3	A	616	LEU
3	A	622	LEU
3	A	627	ASN
3	A	636	ARG
3	A	645	TRP
3	A	659	ARG
3	A	665	ILE
3	A	669	VAL
3	A	682	LEU
3	A	684	ILE
3	A	707	LEU
3	A	710	THR
3	A	711	LEU
3	A	723	LEU
3	A	733	LEU
3	A	740	VAL
3	A	746	ARG
3	A	753	VAL
3	A	763	LEU
3	A	775	MET
3	A	781	LEU
3	A	789	LEU
3	A	801	ARG
3	A	802	LEU
3	A	817	LEU
3	A	832	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	554	HIS
3	A	561	HIS
3	A	566	GLN
3	A	582	GLN
3	A	583	ASN
3	A	613	GLN
3	A	633	GLN
3	A	754	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	DOC	B	112	1,2	16,19,20	0.83	0	20,26,29	1.15	2 (10%)

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
1	DOC	B	112	1,2	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	DOC	O4'-C1'-C2'	2.37	109.22	106.41
1	B	112	DOC	C4'-O4'-C1'	-2.32	107.62	109.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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	B	11/12 (91%)	-0.43	0	100	100	28, 29, 58, 60	0
2	C	14/14 (100%)	-0.23	0	100	100	25, 33, 67, 79	0
3	A	539/539 (100%)	0.56	38 (7%)	22	19	27, 50, 99, 160	0
All	All	564/565 (99%)	0.52	38 (6%)	24	21	25, 50, 98, 160	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	650	PRO	5.2
3	A	654	VAL	4.9
3	A	653	ALA	3.7
3	A	656	PRO	3.6
3	A	299	TRP	3.5
3	A	326	ALA	3.4
3	A	697	PHE	2.9
3	A	658	MET	2.9
3	A	647	PHE	2.9
3	A	657	LEU	2.8
3	A	655	ASP	2.8
3	A	294	LEU	2.8
3	A	649	VAL	2.8
3	A	684	ILE	2.7
3	A	503	ILE	2.6
3	A	307	VAL	2.5
3	A	832	GLU	2.5
3	A	686	TYR	2.4
3	A	651	ARG	2.4
3	A	297	ALA	2.3
3	A	689	ALA	2.3
3	A	330	GLY	2.3
3	A	366	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	665	ILE	2.3
3	A	683	ALA	2.2
3	A	300	PRO	2.2
3	A	348	ALA	2.2
3	A	324	LEU	2.1
3	A	664	THR	2.1
3	A	629	ILE	2.1
3	A	634	GLU	2.1
3	A	687	GLU	2.1
3	A	645	TRP	2.1
3	A	667	PHE	2.1
3	A	693	ILE	2.1
3	A	682	LEU	2.0
3	A	527	PRO	2.0
3	A	674	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	DOC	B	112	18/19	0.97	0.06	29,33,35,35	0

6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
4	MG	A	901	1/1	0.77	0.23	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.