



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 05:50 AM EDT

PDB ID : 3PVX / pdb_00003pvx
Title : Binary complex of Aflatoxin B1 Adduct modified DNA (AFB1-FAPY) with DNA Polymerase IV
Authors : Banerjee, S.
Deposited on : 2010-12-07
Resolution : 3.03 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

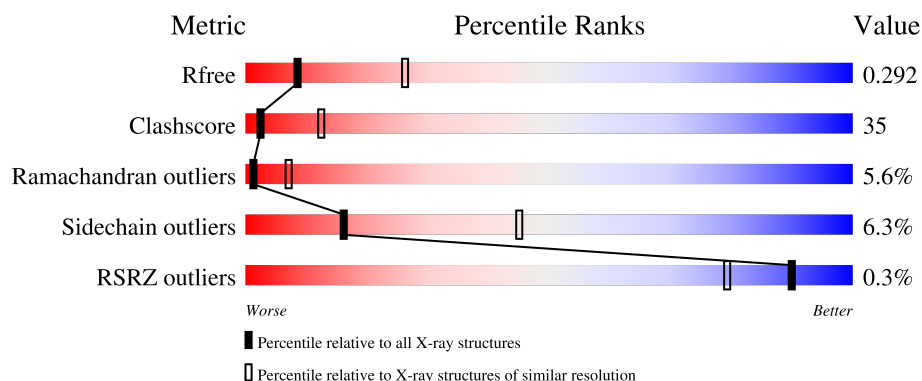
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

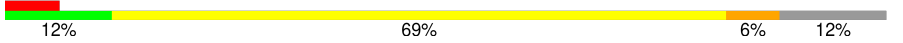
The reported resolution of this entry is 3.03 Å.

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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	347	
2	B	16	
3	C	13	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3402 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2744	1760	472	505	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q97W02
A	-4	HIS	-	expression tag	UNP Q97W02
A	-3	HIS	-	expression tag	UNP Q97W02
A	-2	HIS	-	expression tag	UNP Q97W02
A	-1	HIS	-	expression tag	UNP Q97W02
A	0	HIS	-	expression tag	UNP Q97W02

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	P	0	0	0
			299	150	44	92	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		

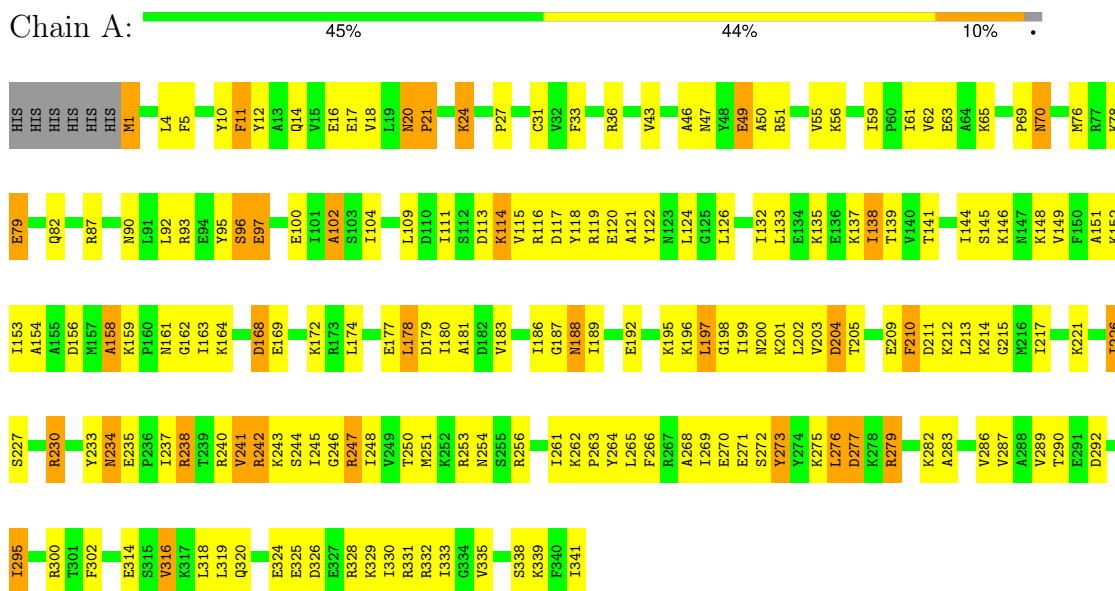
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total 63	O 63	0	0
5	B	14	Total 14	O 14	0	0
5	C	6	Total 6	O 6	0	0

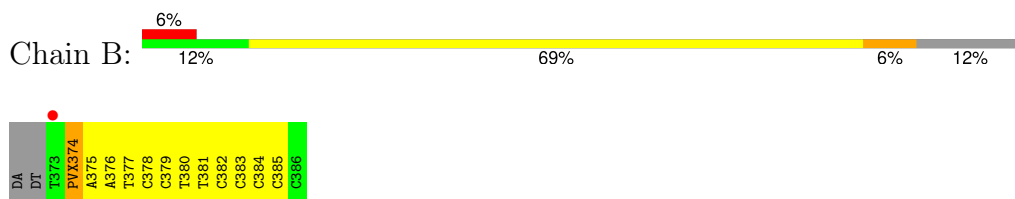
3 Residue-property plots [i](#)

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.

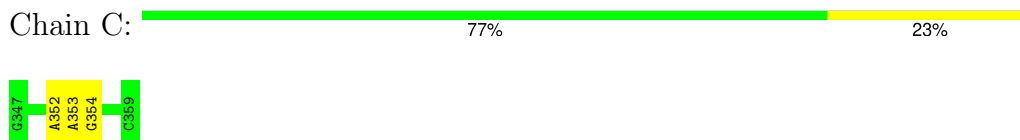
• Molecule 1: DNA polymerase IV



• Molecule 2: DNA (5'-D(*AP*TP*TP*(PVX)P*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3')



• Molecule 3: DNA (5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.75Å 103.91Å 52.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.96 – 3.03 27.96 – 3.03	Depositor EDS
% Data completeness (in resolution range)	88.5 (27.96-3.03) 88.3 (27.96-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.299 0.220 , 0.292	Depositor DCC
R_{free} test set	752 reflections (7.73%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3402	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% 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

5.1 Standard geometry

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

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	0.49	0/2783	0.95	9/3736 (0.2%)
2	B	0.39	0/278	0.79	0/422
3	C	0.36	0/308	0.66	0/476
All	All	0.47	0/3369	0.91	9/4634 (0.2%)

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	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASN	CA-C-N	6.24	127.64	119.84
1	A	20	ASN	C-N-CA	6.24	127.64	119.84
1	A	148	LYS	N-CA-C	5.54	117.32	111.28
1	A	11	PHE	N-CA-C	5.41	122.33	110.80
1	A	295	ILE	N-CA-C	5.40	116.02	108.89
1	A	135	LYS	N-CA-C	5.27	117.70	111.33
1	A	97	GLU	N-CA-C	-5.11	106.20	112.90
1	A	102	ALA	N-CA-C	5.00	116.73	111.28
1	A	256	ARG	N-CA-C	-5.00	108.45	114.75

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

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	2744	0	2889	197	0
2	B	299	0	164	27	0
3	C	273	0	147	12	0
4	A	3	0	0	0	0
5	A	63	0	0	14	0
5	B	14	0	0	5	0
5	C	6	0	0	2	0
All	All	3402	0	3200	228	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 (228) 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:115:VAL:HG13	1:A:120:GLU:HB2	1.47	0.97
2:B:376:DA:H2''	2:B:377:DT:H5'	1.47	0.97
1:A:316:VAL:O	1:A:320:GLN:HG3	1.68	0.94
1:A:69:PRO:C	1:A:70:ASN:HD22	1.77	0.91
1:A:289:VAL:HG21	1:A:332:ARG:HD3	1.54	0.90
1:A:14:GLN:NE2	1:A:139:THR:H	1.73	0.86
1:A:17:GLU:HB3	5:A:2040:HOH:O	1.74	0.86
1:A:339:LYS:NZ	3:C:352:DA:H5'	1.91	0.85
1:A:36:ARG:HH11	1:A:331:ARG:NH1	1.76	0.83
1:A:24:LYS:HD3	5:A:2040:HOH:O	1.79	0.82
1:A:14:GLN:HE22	1:A:139:THR:N	1.75	0.82
1:A:341:ILE:HB	5:A:2050:HOH:O	1.80	0.82
1:A:100:GLU:HB2	1:A:237:ILE:HG23	1.59	0.81
1:A:14:GLN:HE22	1:A:139:THR:H	1.26	0.80
1:A:300:ARG:HD3	1:A:314:GLU:OE1	1.82	0.80
1:A:283:ALA:HB2	1:A:339:LYS:HD2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:MET:HG3	5:A:2048:HOH:O	1.84	0.78
1:A:36:ARG:HH22	1:A:254:ASN:HD22	1.32	0.78
1:A:36:ARG:HH12	1:A:254:ASN:HD21	1.30	0.76
1:A:262:LYS:HB2	1:A:263:PRO:HD3	1.68	0.75
3:C:352:DA:H2'	3:C:353:DA:C8	2.22	0.74
1:A:339:LYS:HZ3	3:C:352:DA:H5'	1.54	0.73
1:A:203:VAL:HG13	1:A:204:ASP:H	1.54	0.72
1:A:79:GLU:CD	1:A:79:GLU:H	1.98	0.71
1:A:36:ARG:HH22	1:A:254:ASN:ND2	1.89	0.71
1:A:233:TYR:CZ	1:A:235:GLU:HG2	2.27	0.70
1:A:116:ARG:HB2	1:A:120:GLU:OE2	1.91	0.69
2:B:375:DA:OP2	5:B:2009:HOH:O	2.09	0.69
2:B:384:DC:H4'	5:B:2011:HOH:O	1.93	0.69
3:C:352:DA:C4'	5:C:2006:HOH:O	2.40	0.69
1:A:248:ILE:HB	5:B:2010:HOH:O	1.92	0.69
1:A:203:VAL:HG13	1:A:204:ASP:N	2.09	0.68
2:B:378:DC:H2''	2:B:379:DC:C5'	2.24	0.68
1:A:116:ARG:HH11	1:A:116:ARG:HB3	1.58	0.68
1:A:287:VAL:O	1:A:333:ILE:HD12	1.94	0.68
2:B:381:DT:H1'	2:B:382:DC:H5''	1.75	0.67
2:B:384:DC:C4'	5:B:2011:HOH:O	2.43	0.67
1:A:244:SER:C	1:A:245:ILE:HD12	2.19	0.67
1:A:156:ASP:HA	1:A:159:LYS:HD2	1.78	0.66
1:A:341:ILE:HA	5:A:2049:HOH:O	1.96	0.65
1:A:210:PHE:CE2	1:A:214:LYS:HE3	2.32	0.64
1:A:21:PRO:O	1:A:24:LYS:HB2	1.98	0.64
1:A:242:ARG:HA	2:B:376:DA:OP1	1.97	0.64
3:C:352:DA:H4'	3:C:352:DA:OP1	1.98	0.64
2:B:376:DA:C2'	2:B:377:DT:H5'	2.26	0.64
1:A:24:LYS:HB2	1:A:24:LYS:HZ2	1.63	0.63
1:A:92:LEU:O	1:A:95:TYR:HB2	1.98	0.63
3:C:352:DA:H2'	3:C:353:DA:H8	1.63	0.63
1:A:12:TYR:OH	1:A:78:LYS:HE3	1.98	0.63
1:A:273:TYR:HA	1:A:276:LEU:HD12	1.79	0.63
1:A:95:TYR:CE1	1:A:124:LEU:HD11	2.34	0.63
1:A:102:ALA:HA	1:A:240:ARG:NH1	2.13	0.63
1:A:97:GLU:N	1:A:97:GLU:CD	2.57	0.62
1:A:253:ARG:HB3	1:A:253:ARG:HH11	1.64	0.62
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.82	0.62
1:A:250:THR:HA	5:A:2048:HOH:O	2.01	0.61
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HA	1:A:59:ILE:CD1	2.32	0.60
1:A:61:ILE:O	1:A:65:LYS:HG3	2.02	0.60
1:A:251:MET:HG2	1:A:264:TYR:CD2	2.36	0.60
1:A:100:GLU:OE1	1:A:238:ARG:HD3	2.02	0.59
1:A:16:GLU:OE1	1:A:16:GLU:HA	2.02	0.59
1:A:199:ILE:HA	1:A:204:ASP:HB3	1.85	0.59
1:A:302:PHE:HZ	1:A:314:GLU:CD	2.11	0.58
1:A:339:LYS:HZ1	3:C:352:DA:H5'	1.68	0.58
1:A:178:LEU:HD13	1:A:179:ASP:O	2.04	0.58
1:A:24:LYS:HB2	1:A:24:LYS:NZ	2.19	0.58
1:A:36:ARG:NH1	1:A:331:ARG:NH1	2.50	0.58
1:A:70:ASN:HD22	1:A:70:ASN:N	1.96	0.58
1:A:251:MET:HA	1:A:264:TYR:CE1	2.39	0.58
1:A:250:THR:HG23	1:A:331:ARG:O	2.04	0.57
1:A:195:LYS:NZ	1:A:200:ASN:HD21	2.02	0.57
1:A:292:ASP:OD1	1:A:328:ARG:NH1	2.31	0.57
1:A:36:ARG:HH11	1:A:331:ARG:HH12	1.52	0.57
1:A:117:ASP:OD1	1:A:119:ARG:HB3	2.04	0.57
1:A:332:ARG:HA	5:A:2048:HOH:O	2.04	0.57
1:A:27:PRO:CA	1:A:49:GLU:HB3	2.34	0.57
1:A:217:ILE:HD12	1:A:221:LYS:HG2	1.87	0.56
1:A:121:ALA:HB1	1:A:144:ILE:HD13	1.87	0.56
1:A:14:GLN:HE21	1:A:138:ILE:HA	1.70	0.56
1:A:62:VAL:HG23	5:A:2043:HOH:O	2.06	0.56
2:B:384:DC:H2''	2:B:385:DC:C5'	2.36	0.55
2:B:378:DC:H2''	2:B:379:DC:H5''	1.89	0.55
2:B:376:DA:H5'	5:B:2004:HOH:O	2.06	0.54
1:A:36:ARG:NH1	1:A:254:ASN:HD21	2.03	0.54
1:A:116:ARG:HB3	1:A:116:ARG:NH1	2.22	0.54
2:B:378:DC:H2''	2:B:379:DC:H5'	1.89	0.54
1:A:33:PHE:HB3	5:A:2005:HOH:O	2.07	0.54
1:A:203:VAL:O	1:A:205:THR:N	2.40	0.54
1:A:196:LYS:C	1:A:198:GLY:H	2.16	0.54
1:A:251:MET:N	5:A:2048:HOH:O	2.40	0.54
1:A:341:ILE:HG22	1:A:341:ILE:OXT	2.06	0.53
1:A:151:ALA:O	1:A:154:ALA:HB3	2.08	0.53
1:A:266:PHE:O	1:A:270:GLU:HG2	2.09	0.53
1:A:14:GLN:NE2	1:A:139:THR:N	2.41	0.53
1:A:275:LYS:O	1:A:276:LEU:C	2.52	0.53
2:B:383:DC:H2''	2:B:384:DC:O5'	2.08	0.53
1:A:210:PHE:HE2	1:A:214:LYS:HE3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:O	1:A:195:LYS:HB2	2.09	0.52
2:B:379:DC:H5'	2:B:379:DC:H6	1.74	0.52
1:A:21:PRO:HB3	1:A:24:LYS:HZ1	1.72	0.52
1:A:27:PRO:O	5:A:2041:HOH:O	2.18	0.52
1:A:1:MET:HE3	1:A:234:ASN:OD1	2.09	0.52
1:A:4:LEU:HD22	1:A:109:LEU:HD12	1.92	0.52
2:B:377:DT:H2''	2:B:378:DC:C6	2.46	0.51
1:A:14:GLN:NE2	1:A:138:ILE:HG23	2.26	0.51
1:A:97:GLU:CD	1:A:97:GLU:H	2.18	0.51
1:A:169:GLU:O	1:A:172:LYS:HB2	2.10	0.51
1:A:247:ARG:HG2	2:B:374:PVX:OP2	2.10	0.51
1:A:92:LEU:O	1:A:93:ARG:C	2.53	0.51
1:A:133:LEU:O	1:A:137:LYS:HA	2.10	0.51
1:A:158:ALA:HB2	1:A:164:LYS:HB2	1.93	0.51
1:A:118:TYR:O	1:A:121:ALA:HB3	2.11	0.51
1:A:27:PRO:HA	1:A:49:GLU:HB3	1.92	0.51
2:B:378:DC:C2'	2:B:379:DC:H5''	2.42	0.50
2:B:381:DT:H2''	2:B:382:DC:C5'	2.41	0.50
1:A:95:TYR:O	1:A:96:SER:HB2	2.11	0.50
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.94	0.50
3:C:353:DA:H2''	3:C:354:DG:C8	2.47	0.50
1:A:102:ALA:HA	1:A:240:ARG:HH11	1.76	0.49
1:A:261:ILE:HG21	1:A:319:LEU:HD21	1.93	0.49
1:A:27:PRO:HB3	1:A:49:GLU:HB3	1.94	0.49
1:A:36:ARG:NH2	1:A:254:ASN:HD22	2.07	0.49
1:A:201:LYS:HB2	1:A:203:VAL:HG12	1.94	0.49
1:A:1:MET:HA	5:A:2009:HOH:O	2.12	0.49
1:A:192:GLU:OE1	1:A:192:GLU:HA	2.13	0.49
1:A:251:MET:HG2	1:A:264:TYR:CE2	2.48	0.49
1:A:261:ILE:O	1:A:262:LYS:C	2.55	0.49
1:A:55:VAL:HA	1:A:59:ILE:HD11	1.95	0.49
1:A:36:ARG:NH2	1:A:254:ASN:ND2	2.61	0.48
1:A:95:TYR:HE1	1:A:124:LEU:HD11	1.78	0.48
1:A:122:TYR:O	1:A:126:LEU:HG	2.13	0.48
1:A:43:VAL:HG23	1:A:59:ILE:O	2.13	0.48
1:A:233:TYR:CE1	1:A:235:GLU:HG2	2.48	0.48
1:A:79:GLU:CD	1:A:79:GLU:N	2.70	0.47
1:A:113:ASP:O	1:A:114:LYS:C	2.57	0.47
1:A:196:LYS:C	1:A:198:GLY:N	2.72	0.47
1:A:254:ASN:HD22	1:A:254:ASN:N	2.12	0.47
1:A:277:ASP:C	1:A:279:ARG:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ALA:HB3	1:A:338:SER:OG	2.14	0.47
1:A:36:ARG:HH12	1:A:254:ASN:ND2	2.04	0.47
1:A:70:ASN:N	1:A:70:ASN:ND2	2.62	0.47
1:A:241:VAL:O	1:A:243:LYS:N	2.48	0.47
1:A:5:PHE:CD2	1:A:152:LYS:HA	2.50	0.47
1:A:269:ILE:CG1	1:A:335:VAL:HG11	2.46	0.47
2:B:381:DT:H2''	2:B:382:DC:H5'	1.96	0.47
1:A:82:GLN:HA	1:A:104:ILE:HD11	1.97	0.46
1:A:226:ILE:HG22	1:A:227:SER:N	2.30	0.46
1:A:210:PHE:HE2	1:A:214:LYS:CE	2.28	0.46
1:A:93:ARG:C	1:A:95:TYR:H	2.23	0.46
1:A:226:ILE:HG22	1:A:230:ARG:HD2	1.98	0.46
1:A:251:MET:HG2	1:A:264:TYR:CG	2.51	0.46
1:A:241:VAL:O	1:A:242:ARG:C	2.58	0.46
1:A:187:GLY:O	1:A:188:ASN:C	2.59	0.46
1:A:27:PRO:HA	1:A:49:GLU:CB	2.46	0.46
1:A:56:LYS:O	1:A:59:ILE:HG12	2.15	0.46
1:A:55:VAL:HG13	1:A:59:ILE:HD11	1.97	0.45
1:A:282:LYS:HD3	5:A:2049:HOH:O	2.14	0.45
1:A:265:LEU:O	1:A:268:ALA:HB3	2.16	0.45
1:A:100:GLU:CB	1:A:237:ILE:HG23	2.38	0.45
1:A:247:ARG:NH1	2:B:374:PVX:OP2	2.50	0.45
2:B:384:DC:H2'	2:B:385:DC:C6	2.50	0.45
1:A:209:GLU:O	1:A:210:PHE:C	2.60	0.45
1:A:251:MET:CE	1:A:330:ILE:HG22	2.46	0.45
1:A:36:ARG:NH1	1:A:331:ARG:HH11	2.15	0.45
1:A:183:VAL:O	1:A:186:ILE:HG12	2.16	0.45
1:A:201:LYS:CB	1:A:203:VAL:HG12	2.47	0.45
1:A:237:ILE:N	1:A:237:ILE:HD12	2.31	0.44
1:A:269:ILE:HG12	1:A:335:VAL:HG11	2.00	0.44
1:A:51:ARG:HA	1:A:55:VAL:O	2.17	0.44
1:A:247:ARG:HE	1:A:271:GLU:CD	2.26	0.44
1:A:203:VAL:CG1	1:A:204:ASP:H	2.26	0.44
3:C:352:DA:C4'	3:C:352:DA:OP1	2.64	0.44
1:A:174:LEU:O	1:A:178:LEU:HB3	2.18	0.44
1:A:300:ARG:CD	1:A:314:GLU:OE1	2.61	0.44
2:B:379:DC:H42	3:C:354:DG:H1	1.66	0.44
1:A:76:MET:HE3	1:A:78:LYS:HD3	1.99	0.44
1:A:180:ILE:HG23	1:A:181:ALA:N	2.33	0.43
1:A:50:ALA:HB1	1:A:55:VAL:HB	2.00	0.43
1:A:139:THR:HB	1:A:161:ASN:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:CG1	1:A:204:ASP:N	2.79	0.43
1:A:180:ILE:CG2	1:A:181:ALA:N	2.81	0.43
1:A:27:PRO:CB	1:A:49:GLU:HB3	2.48	0.43
1:A:289:VAL:CG2	1:A:332:ARG:HD3	2.37	0.43
1:A:87:ARG:O	1:A:90:ASN:HB2	2.18	0.43
1:A:210:PHE:HE2	1:A:214:LYS:NZ	2.16	0.43
1:A:244:SER:O	1:A:245:ILE:HD12	2.18	0.43
1:A:199:ILE:HD13	1:A:205:THR:HG22	2.00	0.43
1:A:76:MET:HE3	1:A:78:LYS:HB2	2.00	0.43
1:A:92:LEU:HD21	1:A:132:ILE:HD11	2.00	0.43
1:A:226:ILE:CG2	1:A:230:ARG:HD2	2.49	0.43
1:A:289:VAL:CG2	1:A:332:ARG:HB2	2.48	0.42
1:A:324:GLU:C	1:A:326:ASP:H	2.27	0.42
2:B:384:DC:H2''	2:B:385:DC:H5'	2.00	0.42
1:A:247:ARG:HD3	1:A:247:ARG:C	2.45	0.42
1:A:202:LEU:HA	1:A:202:LEU:HD23	1.78	0.42
1:A:246:GLY:N	2:B:375:DA:OP1	2.49	0.42
1:A:197:LEU:HD21	1:A:212:LYS:HE2	2.02	0.42
1:A:189:ILE:O	1:A:192:GLU:HB3	2.20	0.42
1:A:199:ILE:HA	1:A:204:ASP:CB	2.48	0.42
1:A:272:SER:O	1:A:276:LEU:HG	2.20	0.42
1:A:314:GLU:OE2	1:A:314:GLU:HA	2.20	0.42
2:B:376:DA:H2''	2:B:377:DT:C5'	2.33	0.42
1:A:196:LYS:O	1:A:198:GLY:N	2.53	0.42
1:A:55:VAL:HA	1:A:59:ILE:HD13	2.00	0.41
1:A:144:ILE:O	1:A:145:SER:HB2	2.18	0.41
1:A:276:LEU:O	1:A:277:ASP:O	2.38	0.41
2:B:377:DT:H2''	2:B:378:DC:H6	1.84	0.41
1:A:341:ILE:OXT	1:A:341:ILE:CG2	2.68	0.41
1:A:246:GLY:O	1:A:247:ARG:HB2	2.18	0.41
1:A:31:CYS:HB2	1:A:33:PHE:CE2	2.55	0.41
1:A:111:ILE:C	1:A:113:ASP:N	2.78	0.41
1:A:47:ASN:HD21	1:A:49:GLU:HB2	1.84	0.41
1:A:290:THR:HA	1:A:329:LYS:O	2.21	0.41
1:A:21:PRO:HB3	1:A:24:LYS:NZ	2.35	0.41
1:A:251:MET:HE1	1:A:330:ILE:HG22	2.03	0.41
1:A:286:VAL:HG21	1:A:318:LEU:HB2	2.03	0.41
2:B:379:DC:H2''	2:B:380:DT:O5'	2.20	0.41
1:A:20:ASN:O	1:A:20:ASN:CG	2.64	0.41
1:A:210:PHE:O	1:A:213:LEU:N	2.45	0.40
3:C:353:DA:H2''	3:C:354:DG:H8	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:HG2	1:A:119:ARG:HH11	1.86	0.40
3:C:352:DA:H4'	5:C:2006:HOH:O	2.13	0.40
1:A:226:ILE:O	1:A:227:SER:C	2.63	0.40
1:A:250:THR:HG22	1:A:251:MET:N	2.36	0.40
1:A:141:THR:HA	1:A:162:GLY:O	2.20	0.40
1:A:149:VAL:O	1:A:153:ILE:HG13	2.21	0.40
1:A:215:GLY:HA2	5:A:2030:HOH:O	2.21	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	339/347 (98%)	287 (85%)	33 (10%)	19 (6%)	1 7

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	LYS
1	A	204	ASP
1	A	277	ASP
1	A	11	PHE
1	A	211	ASP
1	A	242	ARG
1	A	21	PRO
1	A	96	SER
1	A	168	ASP
1	A	210	PHE
1	A	234	ASN
1	A	325	GLU
1	A	197	LEU
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	10	TYR
1	A	158	ALA
1	A	188	ASN
1	A	247	ARG
1	A	226	ILE

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	300/306 (98%)	281 (94%)	19 (6%)	16	45

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	VAL
1	A	24	LYS
1	A	49	GLU
1	A	63	GLU
1	A	70	ASN
1	A	79	GLU
1	A	138	ILE
1	A	146	LYS
1	A	163	ILE
1	A	168	ASP
1	A	177	GLU
1	A	178	LEU
1	A	230	ARG
1	A	238	ARG
1	A	241	VAL
1	A	279	ARG
1	A	295	ILE
1	A	316	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	70	ASN
1	A	123	ASN
1	A	188	ASN
1	A	200	ASN
1	A	254	ASN

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	$\# Z > 2$
2	PVX	B	374	2	46,53,54	2.95	16 (34%)	51,81,84	2.09	18 (35%)

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
2	PVX	B	374	2	-	3/11/66/67	0/7/7/7

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	PVX	C2A-C3	9.09	1.55	1.35
2	B	374	PVX	O-C4B	6.37	1.47	1.37
2	B	374	PVX	P-O5'	5.91	1.79	1.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	PVX	O10-CA1	5.51	1.46	1.38
2	B	374	PVX	O10-C11	5.27	1.45	1.38
2	B	374	PVX	C5B-C4B	4.93	1.47	1.38
2	B	374	PVX	C4A-C4B	4.63	1.48	1.40
2	B	374	PVX	C2-N2	4.61	1.45	1.34
2	B	374	PVX	C2-N3	4.35	1.48	1.37
2	B	374	PVX	C6-N6	4.14	1.44	1.35
2	B	374	PVX	C3-C3A	4.04	1.54	1.43
2	B	374	PVX	O6A-C5M	3.01	1.42	1.37
2	B	374	PVX	CB1-C1	-2.67	1.41	1.50
2	B	374	PVX	C2A-C1	2.47	1.52	1.46
2	B	374	PVX	C5B-C5M	2.38	1.42	1.38
2	B	374	PVX	O3'-C3'	2.29	1.48	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	PVX	C5-C4-N3	5.24	120.16	110.94
2	B	374	PVX	CA1-O10-C11	-4.50	117.32	122.64
2	B	374	PVX	C6A-O7-C8A	4.40	113.90	106.05
2	B	374	PVX	O-C4B-C4A	4.27	121.89	115.84
2	B	374	PVX	O1-C1-C2A	-3.43	121.46	126.74
2	B	374	PVX	C5M-C9B-CA1	3.31	122.77	118.21
2	B	374	PVX	C2A-C3-C3A	-3.27	103.07	109.36
2	B	374	PVX	C3A-CB1-C1	3.25	111.49	108.60
2	B	374	PVX	O6A-C6A-C9A	3.23	110.74	106.71
2	B	374	PVX	O6A-C5M-C5B	2.89	127.05	123.30
2	B	374	PVX	C2-N3-C4	-2.80	120.03	125.11
2	B	374	PVX	C2-N1-C6	2.70	118.12	113.36
2	B	374	PVX	C5B-C5M-C9B	-2.49	120.88	124.00
2	B	374	PVX	CA1-C4A-C3A	-2.48	115.97	118.06
2	B	374	PVX	C5B-C4B-C4A	-2.44	117.53	121.79
2	B	374	PVX	N2-C2-N3	2.13	121.26	116.76
2	B	374	PVX	O-C4B-C5B	-2.03	120.57	124.08
2	B	374	PVX	C6-C5-N7	2.02	123.16	119.28

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	374	PVX	C3'-C4'-C5'-O5'
2	B	374	PVX	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	B	374	PVX	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	374	PVX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are 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 [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	341/347 (98%)	-0.27	0 100 100	30, 60, 86, 98	0
2	B	13/16 (81%)	0.56	1 (7%) 19 10	67, 77, 89, 93	0
3	C	13/13 (100%)	-0.08	0 100 100	51, 61, 79, 85	0
All	All	367/376 (97%)	-0.24	1 (0%) 90 79	30, 61, 86, 98	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	373	DT	2.6

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
2	PVX	B	374	47/48	0.84	0.13	81,90,93,93	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($\text{\AA}^2$)	Q<0.9
4	CA	A	1001	1/1	0.83	0.16	79,79,79,79	0
4	CA	A	1003	1/1	0.83	0.10	93,93,93,93	0
4	CA	A	1002	1/1	0.93	0.10	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.