



## Full wwPDB EM Validation Report ⓘ

Mar 18, 2025 – 12:05 pm GMT

PDB ID : 9EPF  
EMDB ID : EMD-19878  
Title : Human Picobirnavirus CP VLP  
Authors : Rodriguez-Espinosa, M.J.; Novoa, G.; Martinez-Romero, J.M.; de Pablo, P.J.;  
Caston, J.R.  
Deposited on : 2024-03-18  
Resolution : 3.54 Å(reported)

This is a Full wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
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>.

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

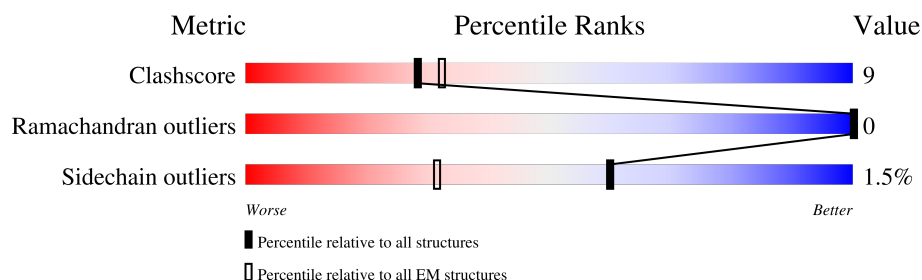
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.54 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	501	 78% 21% .
1	B	501	 76% 24%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Capsid protein precursor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			3943	2546	637	735	25		
1	B	501	Total	C	N	O	S	0	0
			3959	2556	640	738	25		

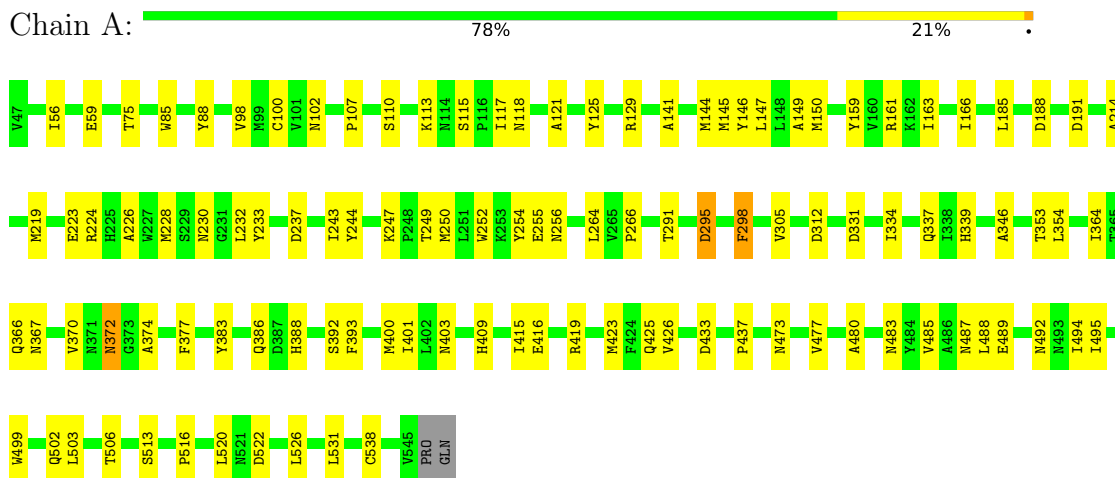
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	546	PRO	-	expression tag	UNP Q50LE5
A	547	GLN	-	expression tag	UNP Q50LE5
B	546	PRO	-	expression tag	UNP Q50LE5
B	547	GLN	-	expression tag	UNP Q50LE5

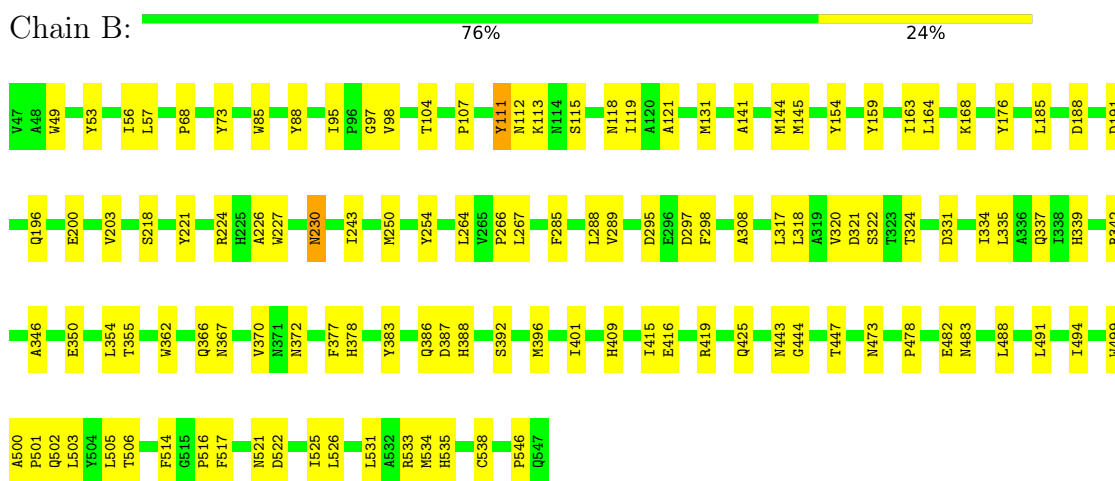
### 3 Residue-property plots

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. 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. 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: Capsid protein precursor



- Molecule 1: Capsid protein precursor



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80582	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS TALOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	29.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

## 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	0.28	0/4053	0.47	0/5534
1	B	0.27	0/4070	0.46	0/5558
All	All	0.27	0/8123	0.47	0/11092

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	A	3943	0	3828	74	0
1	B	3959	0	3843	77	0
All	All	7902	0	7671	145	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 9.

All (145) 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:295:ASP:HB3	1:A:298:PHE:HB2	1.72	0.71
1:B:331:ASP:HB3	1:B:334:ILE:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:HD21	1:A:520:LEU:HA	1.57	0.70
1:B:131:MET:HG2	1:B:308:ALA:HA	1.72	0.69
1:B:367:ASN:HB3	1:B:370:VAL:HG22	1.76	0.68
1:B:491:LEU:HD11	1:B:505:LEU:HD21	1.76	0.66
1:A:339:HIS:HB2	1:A:499:TRP:HB3	1.77	0.66
1:B:226:ALA:O	1:B:230:ASN:HB2	1.96	0.65
1:A:141:ALA:O	1:A:145:MET:HG2	1.96	0.64
1:A:473:ASN:ND2	1:A:502:GLN:O	2.27	0.64
1:A:331:ASP:HB3	1:A:334:ILE:HG22	1.78	0.64
1:A:150:MET:HE3	1:A:150:MET:HA	1.82	0.62
1:B:401:ILE:HD12	1:B:516:PRO:HG2	1.81	0.62
1:A:425:GLN:HG2	1:A:426:VAL:HG13	1.81	0.61
1:B:346:ALA:N	1:B:383:TYR:O	2.32	0.61
1:B:482:GLU:N	1:B:482:GLU:OE2	2.34	0.60
1:A:264:LEU:HD12	1:A:364:ILE:HD12	1.83	0.60
1:B:111:TYR:O	1:B:112:ASN:ND2	2.34	0.60
1:A:147:LEU:HD13	1:A:219:MET:HE1	1.84	0.59
1:A:492:ASN:HD22	1:B:514:PHE:HE2	1.50	0.59
1:A:98:VAL:HG23	1:A:243:ILE:HB	1.84	0.59
1:B:473:ASN:HD21	1:B:501:PRO:HB2	1.69	0.57
1:B:318:LEU:H	1:B:318:LEU:HD23	1.70	0.56
1:B:98:VAL:HG23	1:B:243:ILE:HB	1.88	0.55
1:B:409:HIS:NE2	1:B:522:ASP:OD2	2.37	0.55
1:A:161:ARG:HE	1:A:230:ASN:HD21	1.53	0.55
1:A:146:TYR:HD1	1:A:298:PHE:CE2	2.24	0.55
1:A:403:ASN:ND2	1:A:520:LEU:HA	2.21	0.55
1:B:141:ALA:O	1:B:145:MET:HG2	2.08	0.54
1:B:159:TYR:OH	1:B:185:LEU:O	2.25	0.54
1:B:254:TYR:HA	1:B:264:LEU:HD22	1.89	0.54
1:A:401:ILE:HD12	1:A:516:PRO:HG2	1.89	0.54
1:A:494:ILE:HD13	1:A:503:LEU:HD21	1.90	0.54
1:B:355:THR:OG1	1:B:387:ASP:OD2	2.23	0.54
1:A:159:TYR:OH	1:A:185:LEU:O	2.26	0.54
1:A:223:GLU:OE1	1:A:223:GLU:N	2.35	0.53
1:A:141:ALA:HB1	1:A:366:GLN:HG3	1.89	0.53
1:A:409:HIS:NE2	1:A:522:ASP:OD2	2.37	0.53
1:B:113:LYS:NZ	1:B:372:ASN:O	2.38	0.52
1:B:250:MET:SD	1:B:266:PRO:HB3	2.50	0.52
1:A:416:GLU:OE2	1:A:419:ARG:NH1	2.42	0.52
1:B:49:TRP:CH2	1:B:56:ILE:HD11	2.45	0.52
1:A:346:ALA:N	1:A:383:TYR:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:HD13	1:B:499:TRP:HD1	1.75	0.52
1:A:254:TYR:CZ	1:A:256:ASN:HB2	2.45	0.51
1:B:494:ILE:HD13	1:B:503:LEU:HD21	1.93	0.51
1:B:526:LEU:HD13	1:B:531:LEU:HD13	1.92	0.51
1:A:161:ARG:HH21	1:A:230:ASN:HD21	1.58	0.51
1:A:115:SER:HB2	1:A:118:ASN:HD22	1.75	0.50
1:A:85:TRP:HB3	1:A:88:TYR:HB2	1.94	0.50
1:A:146:TYR:O	1:A:147:LEU:C	2.49	0.49
1:A:113:LYS:NZ	1:A:372:ASN:O	2.38	0.49
1:A:252:TRP:HB3	1:A:264:LEU:HD13	1.93	0.49
1:A:121:ALA:HB2	1:A:144:MET:HG3	1.95	0.49
1:A:75:THR:HA	1:B:525:ILE:HD13	1.94	0.49
1:A:214:ALA:HB3	1:A:305:VAL:HG23	1.95	0.48
1:B:320:VAL:HA	1:B:324:THR:HG21	1.95	0.48
1:A:254:TYR:CE2	1:A:256:ASN:HB2	2.48	0.48
1:A:367:ASN:HB3	1:A:370:VAL:HB	1.95	0.48
1:A:159:TYR:HE1	1:A:185:LEU:HD22	1.79	0.48
1:A:386:GLN:HB2	1:A:388:HIS:ND1	2.28	0.48
1:A:392:SER:HA	1:A:506:THR:HG21	1.94	0.48
1:B:250:MET:HE1	1:B:362:TRP:CE3	2.49	0.48
1:A:354:LEU:HD22	1:A:437:PRO:HG3	1.95	0.48
1:B:53:TYR:HB3	1:B:56:ILE:HG12	1.95	0.48
1:B:321:ASP:H	1:B:324:THR:CG2	2.27	0.47
1:A:110:SER:HB2	1:A:117:ILE:HG21	1.96	0.47
1:A:146:TYR:O	1:A:149:ALA:N	2.47	0.47
1:A:113:LYS:HD2	1:A:374:ALA:HB2	1.95	0.47
1:B:121:ALA:HB2	1:B:144:MET:HG2	1.96	0.47
1:A:254:TYR:CZ	1:A:298:PHE:HE1	2.33	0.47
1:A:250:MET:CE	1:A:266:PRO:HB3	2.45	0.46
1:A:415:ILE:HG13	1:B:57:LEU:HD11	1.96	0.46
1:B:473:ASN:ND2	1:B:502:GLN:O	2.36	0.46
1:B:444:GLY:O	1:B:535:HIS:ND1	2.48	0.46
1:A:59:GLU:OE2	1:B:533:ARG:NH2	2.49	0.46
1:A:485:VAL:O	1:A:489:GLU:HG3	2.16	0.46
1:B:107:PRO:HD2	1:B:377:PHE:CD2	2.51	0.46
1:A:506:THR:HA	1:A:513:SER:HA	1.99	0.46
1:B:221:TYR:HE1	1:B:447:THR:HB	1.81	0.45
1:B:250:MET:HE1	1:B:362:TRP:HE3	1.80	0.45
1:A:56:ILE:HA	1:A:59:GLU:HG2	1.98	0.45
1:A:233:TYR:O	1:A:244:TYR:N	2.41	0.45
1:A:477:VAL:HG11	1:A:487:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:ASP:HB3	1:B:298:PHE:HB2	1.99	0.45
1:B:478:PRO:HD2	1:B:483:ASN:ND2	2.31	0.45
1:A:334:ILE:HA	1:A:337:GLN:HG2	1.99	0.45
1:B:168:LYS:NZ	1:B:322:SER:O	2.34	0.45
1:B:159:TYR:CZ	1:B:163:ILE:HD11	2.53	0.44
1:B:425:GLN:OE1	1:B:443:ASN:ND2	2.50	0.44
1:B:339:HIS:HB2	1:B:499:TRP:HB3	1.98	0.44
1:B:354:LEU:HD23	1:B:354:LEU:HA	1.88	0.44
1:A:107:PRO:HD2	1:A:377:PHE:CD2	2.53	0.44
1:A:166:ILE:HD11	1:A:232:LEU:HD21	1.99	0.44
1:B:334:ILE:HA	1:B:337:GLN:HG2	2.00	0.44
1:B:342:ARG:NH2	1:B:396:MET:SD	2.90	0.44
1:A:188:ASP:HB3	1:A:191:ASP:HB3	1.99	0.44
1:B:159:TYR:HE1	1:B:185:LEU:HD22	1.83	0.44
1:B:350:GLU:H	1:B:350:GLU:CD	2.21	0.44
1:B:97:GLY:HA3	1:B:176:TYR:CD2	2.52	0.44
1:A:226:ALA:O	1:A:230:ASN:HB3	2.18	0.44
1:B:531:LEU:HD12	1:B:531:LEU:HA	1.87	0.44
1:B:392:SER:HA	1:B:506:THR:HG21	1.99	0.43
1:A:433:ASP:OD1	1:A:433:ASP:N	2.46	0.43
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.89	0.43
1:B:230:ASN:HD22	1:B:230:ASN:HA	1.56	0.43
1:A:159:TYR:CZ	1:A:163:ILE:HD11	2.53	0.43
1:B:115:SER:O	1:B:119:ILE:HG12	2.18	0.43
1:B:267:LEU:HD22	1:B:288:LEU:HD13	1.99	0.43
1:B:68:PRO:O	1:B:73:TYR:OH	2.24	0.43
1:A:100:CYS:SG	1:A:247:LYS:HB2	2.59	0.43
1:B:415:ILE:HD12	1:B:534:MET:HG2	2.00	0.43
1:A:526:LEU:HD23	1:A:526:LEU:HA	1.92	0.43
1:B:188:ASP:HB3	1:B:191:ASP:HB3	2.00	0.43
1:B:526:LEU:HD23	1:B:526:LEU:HA	1.90	0.43
1:B:503:LEU:HB2	1:B:517:PHE:HB3	2.01	0.42
1:A:400:MET:HG2	1:A:423:MET:SD	2.59	0.42
1:B:321:ASP:H	1:B:324:THR:HG23	1.84	0.42
1:B:115:SER:HB2	1:B:118:ASN:HD22	1.84	0.42
1:B:154:TYR:CD1	1:B:317:LEU:HD21	2.55	0.42
1:B:141:ALA:HB1	1:B:366:GLN:HG3	2.02	0.42
1:B:196:GLN:O	1:B:200:GLU:HG3	2.18	0.42
1:B:285:PHE:O	1:B:289:VAL:HG22	2.20	0.42
1:B:488:LEU:HA	1:B:488:LEU:HD23	1.85	0.42
1:A:489:GLU:HG2	1:B:514:PHE:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:GLN:HB2	1:B:388:HIS:ND1	2.35	0.41
1:A:423:MET:SD	1:A:531:LEU:HD22	2.60	0.41
1:A:312:ASP:N	1:A:312:ASP:OD1	2.54	0.41
1:B:339:HIS:ND1	1:B:500:ALA:O	2.50	0.41
1:B:104:THR:HG21	1:B:250:MET:HE3	2.03	0.41
1:B:164:LEU:HD22	1:B:203:VAL:HG11	2.03	0.41
1:B:224:ARG:HE	1:B:227:TRP:HZ3	1.68	0.41
1:A:125:TYR:CZ	1:A:129:ARG:HG3	2.55	0.41
1:A:488:LEU:HA	1:A:488:LEU:HD23	1.86	0.41
1:A:520:LEU:HD12	1:B:95:ILE:HD11	2.03	0.41
1:A:102:ASN:HB3	1:A:249:THR:OG1	2.21	0.41
1:B:254:TYR:CD2	1:B:298:PHE:HZ	2.39	0.41
1:A:145:MET:O	1:A:146:TYR:C	2.59	0.40
1:A:255:GLU:H	1:A:291:THR:HG21	1.85	0.40
1:A:492:ASN:HA	1:A:495:ILE:HD12	2.03	0.40
1:B:85:TRP:HB3	1:B:88:TYR:HB2	2.03	0.40
1:A:480:ALA:HB3	1:A:483:ASN:HB2	2.01	0.40
1:B:218:SER:OG	1:B:546:PRO:HD3	2.22	0.40
1:A:224:ARG:NH2	1:A:228:MET:SD	2.95	0.40
1:B:416:GLU:OE1	1:B:419:ARG:HD2	2.22	0.40

There are no symmetry-related clashes.

## 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 PDB entries followed by that with respect to all EM entries.

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	497/501 (99%)	481 (97%)	16 (3%)	0	100	100
1	B	499/501 (100%)	484 (97%)	15 (3%)	0	100	100
All	All	996/1002 (99%)	965 (97%)	31 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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 PDB entries followed by that with respect to all EM entries.

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	423/425 (100%)	416 (98%)	7 (2%)	56	76
1	B	425/425 (100%)	419 (99%)	6 (1%)	62	80
All	All	848/850 (100%)	835 (98%)	13 (2%)	60	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	ASP
1	A	295	ASP
1	A	298	PHE
1	A	353	THR
1	A	372	ASN
1	A	393	PHE
1	A	538	CYS
1	B	111	TYR
1	B	230	ASN
1	B	297	ASP
1	B	378	HIS
1	B	521	ASN
1	B	538	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	ASN
1	B	112	ASN
1	B	443	ASN

### 5.3.3 RNA ⓘ

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.