



Full wwPDB EM Model Validation Report ⓘ

Apr 7, 2020 – 09:43 PM EDT

PDB ID : 6T2C
EMDB ID : EMD-10368
Title : Bat Influenza A polymerase recycling complex
Authors : Wandzik, J.M.; Kouba, T.; Cusack, S.
Deposited on : 2019-10-08
Resolution : 3.52 Å(reported)

This is a Full wwPDB EM Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

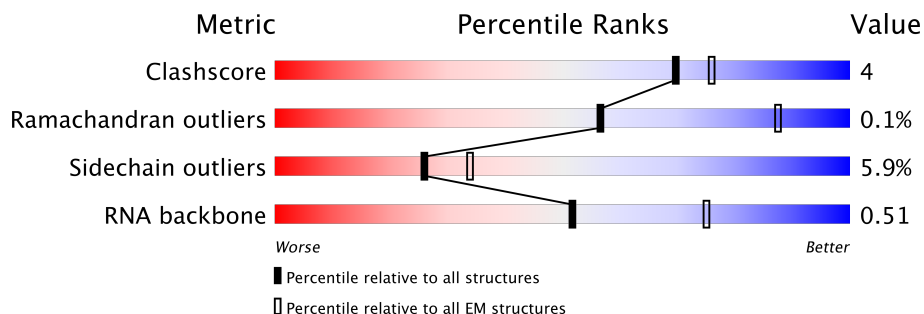
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.52 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	738	61% 8% 30%
2	B	776	69% 10% 19%
3	C	809	11% 86%
4	V	34	53% 26% 6% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10700 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	513	4145	2640	700	778	27	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	626	Total	C	N	O	S	0	0
			4996	3152	880	933	31		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total	C	N	O	S	0	0
			941	602	164	168	7		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	29	Total	C	N	O	P	0	0
			617	276	109	203	29		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	

ASN	THR	CYS	LYS	ALA	ILE	GLU	ALA	LEU	LYS	ARG	GLN	GLY	SER	GLY	SER	GLY	GLU	ASN	LEU	TYR	PHE	GLN
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- Molecule 3: Polymerase basic protein 2

Chain C:  11% . 86%

[illegible]

- Molecule 4: vRNA

Chain V:  53% 26% 6% 15%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	16301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	31	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

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

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	0.42	0/4235	0.49	0/5707
2	B	0.39	0/5097	0.50	0/6887
3	C	0.30	0/970	0.48	0/1320
4	V	0.69	1/687 (0.1%)	0.95	1/1061 (0.1%)
All	All	0.42	1/10989 (0.0%)	0.54	1/14975 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-11.20	1.47	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	7	A	O4'-C1'-N9	5.24	112.39	108.20

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	4145	0	4121	34	0
2	B	4996	0	4988	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	941	0	902	11	0
4	V	617	0	314	6	0
5	B	1	0	0	0	0
All	All	10700	0	10325	84	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 (84) 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:544:GLU:HG2	1:A:553:MET:SD	1.74	1.26
1:A:546:ARG:HG2	1:A:551:THR:HG23	1.42	1.02
1:A:544:GLU:CG	1:A:553:MET:SD	2.55	0.93
2:B:48:ASP:OD1	2:B:48:ASP:O	2.10	0.70
2:B:292:LYS:HG2	2:B:292:LYS:O	1.98	0.64
1:A:546:ARG:HG2	1:A:551:THR:CG2	2.24	0.63
4:V:24:C:H2'	4:V:25:U:H6	1.63	0.63
1:A:382:VAL:HG12	1:A:384:ASP:H	1.65	0.62
1:A:347:GLU:HG2	1:A:347:GLU:O	1.99	0.62
2:B:619:ASP:OD1	2:B:619:ASP:N	2.32	0.60
2:B:617:ASP:OD1	2:B:617:ASP:N	2.30	0.60
1:A:324:LYS:NZ	1:A:532:TRP:O	2.36	0.59
1:A:448:CYS:SG	1:A:449:ARG:N	2.77	0.58
1:A:357:LYS:HB3	1:A:362:LYS:HE3	1.87	0.57
1:A:610:ARG:O	1:A:611:GLU:HG3	2.05	0.57
2:B:127:GLN:O	2:B:249:ARG:NH2	2.38	0.57
2:B:225:ASN:OD1	2:B:350:ARG:NH1	2.39	0.56
1:A:457:ALA:O	1:A:461:ASN:ND2	2.38	0.56
1:A:431:GLU:OE1	2:B:600:ASN:ND2	2.39	0.56
2:B:625:CYS:HB2	3:C:108:VAL:HG11	1.88	0.54
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.41	0.53
1:A:246:LEU:HD22	2:B:468:ARG:HB3	1.90	0.53
2:B:283:ALA:O	2:B:287:LYS:HG3	2.08	0.53
1:A:547:THR:OG1	1:A:548:SER:N	2.42	0.53
3:C:71:ASP:HB2	3:C:75:ASN:H	1.75	0.52
4:V:24:C:H2'	4:V:25:U:C6	2.45	0.52
2:B:372:ASN:N	2:B:372:ASN:OD1	2.43	0.51
2:B:571:ARG:NH2	4:V:31:U:OP1	2.42	0.51
2:B:374:SER:OG	2:B:375:ASP:OD1	2.27	0.50
2:B:177:ASP:N	2:B:177:ASP:OD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LYS:HG2	1:A:475:TYR:CE2	2.47	0.50
1:A:326:HIS:HB2	1:A:536:CYS:HB2	1.94	0.50
1:A:234:SER:HB2	2:B:334:ARG:HH22	1.76	0.49
1:A:485:ARG:NH1	1:A:489:GLY:O	2.46	0.49
1:A:538:LEU:HD12	1:A:558:LEU:HD23	1.94	0.49
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.31	0.49
1:A:380:LYS:O	2:B:380:TYR:OH	2.28	0.48
2:B:558:THR:HG23	3:C:48:LYS:HG2	1.96	0.48
2:B:309:TRP:HZ3	2:B:475:ILE:HG23	1.78	0.48
2:B:177:ASP:HA	2:B:214:LYS:HB2	1.96	0.48
2:B:369:SER:OG	2:B:372:ASN:OD1	2.31	0.47
2:B:474:GLY:O	2:B:476:ASN:ND2	2.48	0.47
2:B:315:PRO:HA	2:B:318:PHE:HD2	1.80	0.47
2:B:155:TYR:OH	2:B:176:ASN:ND2	2.44	0.47
1:A:367:GLU:OE1	1:A:475:TYR:OH	2.33	0.47
1:A:642:ASN:OD1	1:A:694:TRP:NE1	2.40	0.47
1:A:426:ASP:OD1	2:B:600:ASN:ND2	2.48	0.47
1:A:298:GLU:O	1:A:298:GLU:HG2	2.15	0.46
2:B:86:ASP:OD1	2:B:86:ASP:N	2.35	0.46
2:B:446:ASP:CB	2:B:493:THR:HG22	2.45	0.46
2:B:354:GLY:HA3	2:B:368:ILE:O	2.15	0.46
2:B:50:SER:HB3	2:B:68:PRO:HB3	1.97	0.46
2:B:269:SER:O	2:B:281:LYS:NZ	2.41	0.46
2:B:302:ILE:HG12	2:B:484:ILE:HB	1.98	0.46
2:B:519:GLU:HB2	2:B:664:HIS:HB3	1.98	0.45
1:A:300:GLU:O	4:V:32:G:N2	2.49	0.45
2:B:371:GLU:O	2:B:371:GLU:HG2	2.16	0.45
2:B:525:ILE:HG13	2:B:657:TYR:HB3	1.99	0.45
3:C:235:THR:OG1	3:C:242:GLN:O	2.33	0.45
2:B:362:MET:HB2	2:B:364:LEU:HD22	1.98	0.44
2:B:43:VAL:HG22	2:B:403:LEU:HD13	2.00	0.44
2:B:443:SER:HB2	2:B:492:PHE:HZ	1.83	0.44
3:C:46:ARG:HA	3:C:49:TRP:CD1	2.53	0.44
1:A:260:PHE:HB3	1:A:673:PRO:HG2	1.99	0.43
2:B:266:LEU:HD13	2:B:421:VAL:HG11	2.00	0.43
3:C:56:PRO:HG2	3:C:57:ILE:HG13	2.00	0.43
4:V:19:U:H4'	4:V:20:A:C8	2.53	0.43
2:B:18:ILE:HA	2:B:18:ILE:HD12	1.90	0.43
2:B:5:PRO:O	2:B:8:ILE:HB	2.19	0.43
3:C:239:CYS:SG	3:C:240:TRP:N	2.91	0.43
3:C:106:SER:OG	3:C:107:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:THR:HA	2:B:497:TYR:O	2.18	0.43
2:B:63:ALA:HB1	2:B:402:SER:HB2	2.00	0.43
3:C:132:PRO:HD2	3:C:243:GLN:HB3	2.01	0.43
1:A:448:CYS:HB2	1:A:633:ARG:HD2	2.00	0.42
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.84	0.42
1:A:434:ALA:HB2	2:B:541:PRO:HB2	2.00	0.42
1:A:428:ALA:HB1	3:C:242:GLN:HE22	1.85	0.41
3:C:72:GLU:OE1	3:C:101:ARG:NH2	2.42	0.41
1:A:224:LYS:O	1:A:224:LYS:HG2	2.20	0.41
1:A:588:GLU:OE1	2:B:543:THR:OG1	2.34	0.41
1:A:471:ALA:O	1:A:501:LYS:NZ	2.54	0.40
1:A:485:ARG:NH2	4:V:34:U:O2	2.55	0.40
1:A:445:VAL:HG22	1:A:636:LEU:HD22	2.04	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 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	511/738 (69%)	483 (94%)	28 (6%)	0	100	100
2	B	620/776 (80%)	588 (95%)	31 (5%)	1 (0%)	49	83
3	C	112/809 (14%)	100 (89%)	12 (11%)	0	100	100
All	All	1243/2323 (54%)	1171 (94%)	71 (6%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	444	SER

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	456/657 (69%)	437 (96%)	19 (4%)	32	68
2	B	548/676 (81%)	513 (94%)	35 (6%)	19	55
3	C	100/706 (14%)	89 (89%)	11 (11%)	7	33
All	All	1104/2039 (54%)	1039 (94%)	65 (6%)	26	58

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	THR
1	A	278	GLN
1	A	279	ARG
1	A	294	ASN
1	A	315	TRP
1	A	324	LYS
1	A	388	TYR
1	A	445	VAL
1	A	455	MET
1	A	465	LEU
1	A	468	SER
1	A	476	GLN
1	A	486	ASP
1	A	507	ARG
1	A	513	VAL
1	A	518	LEU
1	A	547	THR
1	A	585	GLN
1	A	660	LEU
2	B	15	GLN
2	B	19	SER
2	B	86	ASP
2	B	108	GLN
2	B	148	GLU
2	B	171	LEU
2	B	175	GLU

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Mol	Chain	Res	Type
2	B	176	ASN
2	B	177	ASP
2	B	182	THR
2	B	207	LYS
2	B	209	ARG
2	B	227	MET
2	B	249	ARG
2	B	276	ASN
2	B	294	THR
2	B	305	ASP
2	B	344	PHE
2	B	364	LEU
2	B	368	ILE
2	B	372	ASN
2	B	375	ASP
2	B	397	VAL
2	B	425	ASN
2	B	435	THR
2	B	444	SER
2	B	468	ARG
2	B	573	THR
2	B	583	THR
2	B	610	CYS
2	B	617	ASP
2	B	619	ASP
2	B	624	LEU
2	B	632	VAL
2	B	658	ASP
3	C	67	ILE
3	C	81	THR
3	C	87	ASN
3	C	108	VAL
3	C	117	MET
3	C	123	GLU
3	C	126	THR
3	C	127	HIS
3	C	129	THR
3	C	133	VAL
3	C	245	THR

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

Mol	Chain	Res	Type
1	A	414	ASN
2	B	108	GLN
2	B	176	ASN
2	B	567	ASN
3	C	87	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	26/34 (76%)	4 (15%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	7	A
4	V	11	A
4	V	17	A
4	V	34	U

There are no RNA pucker outliers to report.

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 carbohydrates 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.