



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 05:43 PM EDT

PDB ID : 3P0S  
Title : Crystal structure of Bombyx mori densovirus 1 capsid  
Authors : Kaufmann, B.; Rossmann, M.G.  
Deposited on : unknown  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

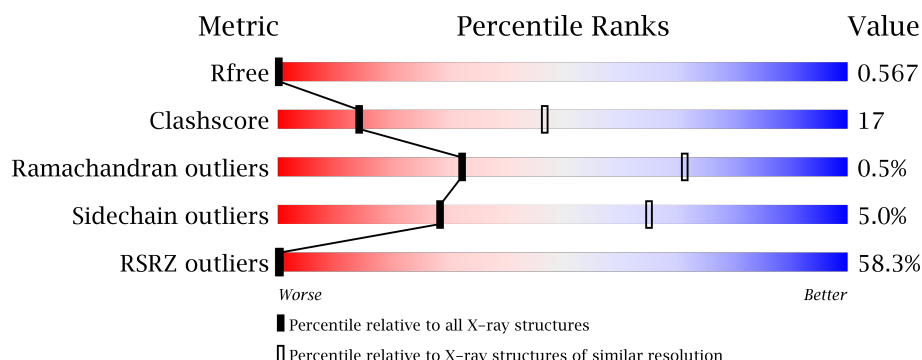
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	494	<div> <div>49%</div> <div>55%</div> <div>27%</div> <div>•</div> <div>17%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3290 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.

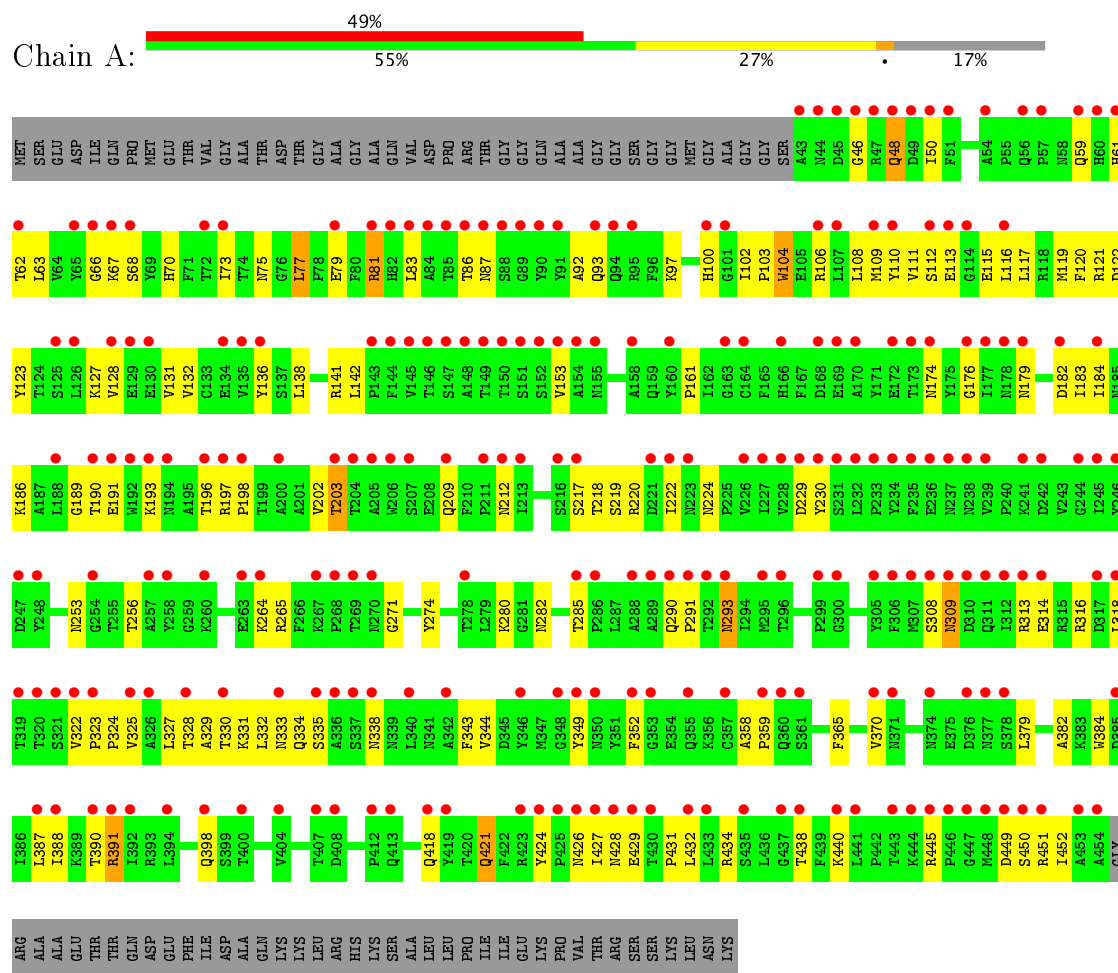
- Molecule 1 is a protein called Capsid protein VP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3290	2090	568	620	12	0	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Capsid protein VP



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	245.40 Å   245.60 Å   245.70 Å 59.98°   67.93°   72.27°	Depositor
Resolution (Å)	45.00 – 3.10 45.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.00-3.10) 81.4 (45.58-3.10)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 3.12 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , (Not available) 0.567 , 0.567	Depositor DCC
$R_{free}$ test set	65598 reflections (8.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 12.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.09	EDS
Total number of atoms	3290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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](#)

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	0.30	0/3376	0.60	0/4599

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	3290	0	3207	113	0
All	All	3290	0	3207	113	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 17.

All (113) 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:81:ARG:HH11	1:A:93:GLN:HE22	1.13	0.92
1:A:81:ARG:HH11	1:A:93:GLN:NE2	1.69	0.90
1:A:111:VAL:HG13	1:A:115:GLU:HB2	1.54	0.89
1:A:141:ARG:HB3	1:A:153:VAL:HG12	1.55	0.86
1:A:190:THR:HG23	1:A:212:ASN:HD22	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG22	1:A:332:LEU:H	1.45	0.81
1:A:100:HIS:HD2	1:A:224:ASN:H	1.29	0.80
1:A:81:ARG:NH1	1:A:93:GLN:HE22	1.80	0.79
1:A:75:ASN:HD22	1:A:382:ALA:N	1.80	0.79
1:A:75:ASN:HD22	1:A:382:ALA:H	1.32	0.78
1:A:324:PRO:HG2	1:A:432:LEU:HD13	1.65	0.77
1:A:253:ASN:HD22	1:A:256:THR:H	1.29	0.76
1:A:161:PRO:HB2	1:A:370:VAL:HB	1.70	0.73
1:A:128:VAL:HG11	1:A:344:VAL:HG13	1.70	0.73
1:A:391:ARG:HG2	1:A:391:ARG:HH11	1.52	0.72
1:A:66:GLY:O	1:A:67:LYS:HD2	1.90	0.71
1:A:293:ASN:H	1:A:293:ASN:HD22	1.40	0.70
1:A:75:ASN:HB3	1:A:379:LEU:HD11	1.72	0.70
1:A:325:VAL:HG13	1:A:327:LEU:HG	1.73	0.69
1:A:318:LEU:HB2	1:A:323:PRO:HG3	1.75	0.67
1:A:330:THR:HG22	1:A:332:LEU:N	2.12	0.65
1:A:308:SER:HB3	1:A:313:ARG:HH11	1.63	0.64
1:A:66:GLY:C	1:A:67:LYS:HD2	2.19	0.63
1:A:329:ALA:HA	1:A:421:GLN:HG2	1.79	0.62
1:A:81:ARG:HD2	1:A:93:GLN:HE21	1.65	0.62
1:A:111:VAL:CG1	1:A:115:GLU:HB2	2.30	0.62
1:A:217:SER:O	1:A:218:THR:HG23	1.99	0.62
1:A:220:ARG:HH11	1:A:220:ARG:HG2	1.63	0.62
1:A:92:ALA:HB3	1:A:230:TYR:HB2	1.82	0.62
1:A:335:SER:H	1:A:338:ASN:HD22	1.50	0.60
1:A:293:ASN:HD22	1:A:293:ASN:N	2.00	0.59
1:A:131:VAL:HG11	1:A:344:VAL:HG11	1.83	0.59
1:A:59:GLN:HB2	1:A:398:GLN:HB2	1.84	0.59
1:A:182:ASP:OD1	1:A:186:LYS:HE3	2.03	0.59
1:A:432:LEU:HD12	1:A:449:ASP:O	2.02	0.59
1:A:81:ARG:HD2	1:A:93:GLN:NE2	2.19	0.58
1:A:426:ASN:HB3	1:A:429:GLU:HG2	1.86	0.58
1:A:106:ARG:HG3	1:A:184:ILE:HD11	1.84	0.58
1:A:176:GLY:HA3	1:A:179:ASN:HD22	1.69	0.57
1:A:314:GLU:OE1	1:A:316:ARG:HD3	2.04	0.57
1:A:128:VAL:HG11	1:A:344:VAL:CG1	2.35	0.56
1:A:77:LEU:HD13	1:A:379:LEU:HB2	1.87	0.56
1:A:330:THR:HG22	1:A:331:LYS:N	2.20	0.56
1:A:282:ASN:O	1:A:332:LEU:HD13	2.04	0.56
1:A:434:ARG:HH11	1:A:434:ARG:HG3	1.70	0.56
1:A:75:ASN:ND2	1:A:382:ALA:N	2.50	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ILE:HG23	1:A:452:ILE:O	2.07	0.55
1:A:280:LYS:HE3	1:A:285:THR:O	2.08	0.54
1:A:138:LEU:O	1:A:141:ARG:NH2	2.40	0.54
1:A:426:ASN:HB3	1:A:429:GLU:CG	2.38	0.53
1:A:141:ARG:CB	1:A:153:VAL:HG12	2.34	0.53
1:A:63:LEU:N	1:A:63:LEU:HD12	2.23	0.53
1:A:391:ARG:HG2	1:A:391:ARG:NH1	2.22	0.53
1:A:75:ASN:CB	1:A:379:LEU:HD11	2.39	0.52
1:A:343:PHE:CD2	1:A:434:ARG:HG2	2.44	0.52
1:A:450:SER:O	1:A:452:ILE:N	2.42	0.52
1:A:220:ARG:NH1	1:A:220:ARG:HG2	2.25	0.52
1:A:112:SER:OG	1:A:115:GLU:HG3	2.10	0.51
1:A:324:PRO:CG	1:A:432:LEU:HD13	2.38	0.50
1:A:280:LYS:HE2	1:A:282:ASN:O	2.11	0.50
1:A:202:VAL:HG22	1:A:203:THR:N	2.27	0.49
1:A:79:GLU:CD	1:A:97:LYS:HD2	2.33	0.48
1:A:127:LYS:NZ	1:A:271:GLY:H	2.11	0.48
1:A:330:THR:OG1	1:A:427:ILE:HD11	2.13	0.48
1:A:121:ARG:NH1	1:A:122:ASP:OD1	2.47	0.48
1:A:308:SER:O	1:A:309:ASN:HB2	2.13	0.48
1:A:67:LYS:NZ	1:A:115:GLU:OE1	2.46	0.47
1:A:290:GLN:HB3	1:A:291:PRO:HD2	1.95	0.47
1:A:68:SER:HA	1:A:388:ILE:O	2.15	0.47
1:A:136:TYR:HB2	1:A:387:LEU:HB2	1.96	0.47
1:A:333:ASN:HB3	1:A:431:PRO:CG	2.45	0.46
1:A:191:GLU:OE2	1:A:193:LYS:HG3	2.15	0.46
1:A:391:ARG:CG	1:A:391:ARG:HH11	2.26	0.46
1:A:174:ASN:ND2	1:A:229:ASP:OD2	2.49	0.46
1:A:293:ASN:H	1:A:293:ASN:ND2	2.11	0.46
1:A:111:VAL:HG12	1:A:112:SER:O	2.17	0.45
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.87	0.45
1:A:280:LYS:NZ	1:A:428:ASN:ND2	2.65	0.45
1:A:318:LEU:HB2	1:A:323:PRO:CG	2.46	0.45
1:A:116:LEU:C	1:A:116:LEU:HD23	2.37	0.45
1:A:110:TYR:CD1	1:A:390:THR:HB	2.52	0.45
1:A:189:GLY:HA2	1:A:212:ASN:ND2	2.32	0.44
1:A:325:VAL:HG13	1:A:327:LEU:CG	2.45	0.44
1:A:333:ASN:HB3	1:A:431:PRO:HG2	1.99	0.44
1:A:424:TYR:CZ	1:A:452:ILE:HG21	2.53	0.44
1:A:50:ILE:HD13	1:A:50:ILE:HA	1.84	0.44
1:A:103:PRO:O	1:A:109:MET:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:SER:C	1:A:452:ILE:H	2.21	0.44
1:A:70:HIS:CE1	1:A:219:SER:HB2	2.53	0.44
1:A:352:PHE:HB2	1:A:418:GLN:O	2.17	0.43
1:A:93:GLN:HG2	1:A:229:ASP:OD1	2.18	0.43
1:A:86:THR:O	1:A:87:ASN:HB2	2.17	0.43
1:A:349:TYR:CD1	1:A:421:GLN:HB3	2.53	0.43
1:A:67:LYS:HD3	1:A:110:TYR:O	2.19	0.42
1:A:358:ALA:HA	1:A:359:PRO:HD3	1.88	0.42
1:A:73:ILE:HD11	1:A:384:TRP:CE3	2.55	0.42
1:A:102:ILE:N	1:A:102:ILE:HD12	2.35	0.42
1:A:322:VAL:HB	1:A:452:ILE:HG23	2.02	0.42
1:A:132:VAL:HG22	1:A:265:ARG:HG2	2.01	0.41
1:A:438:THR:HG22	1:A:438:THR:O	2.20	0.41
1:A:113:GLU:O	1:A:117:LEU:HG	2.20	0.41
1:A:48:GLN:CD	1:A:48:GLN:H	2.23	0.41
1:A:61:HIS:HD2	1:A:123:TYR:HE1	1.66	0.41
1:A:142:LEU:HD12	1:A:142:LEU:O	2.20	0.41
1:A:391:ARG:CG	1:A:391:ARG:NH1	2.83	0.41
1:A:111:VAL:HG11	1:A:119:MET:HE3	2.03	0.41
1:A:183:ILE:HG12	1:A:222:ILE:HB	2.02	0.41
1:A:142:LEU:HA	1:A:153:VAL:HG13	2.03	0.41
1:A:104:TRP:CH2	1:A:264:LYS:HB3	2.56	0.40
1:A:46:GLY:H	1:A:48:GLN:HE21	1.69	0.40
1:A:253:ASN:ND2	1:A:256:THR:HG23	2.36	0.40
1:A:274:TYR:HA	1:A:349:TYR:CE2	2.57	0.40
1:A:358:ALA:O	1:A:445:ARG:NH1	2.55	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	410/494 (83%)	379 (92%)	29 (7%)	2 (0%)	32 71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	ARG
1	A	309	ASN

### 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	359/418 (86%)	341 (95%)	18 (5%)	28 65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	62	THR
1	A	77	LEU
1	A	81	ARG
1	A	83	LEU
1	A	104	TRP
1	A	108	LEU
1	A	120	PHE
1	A	196	THR
1	A	203	THR
1	A	209	GLN
1	A	293	ASN
1	A	328	THR
1	A	334	GLN
1	A	365	PHE
1	A	391	ARG
1	A	421	GLN
1	A	440	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	61	HIS
1	A	75	ASN
1	A	87	ASN
1	A	93	GLN
1	A	100	HIS
1	A	159	GLN
1	A	174	ASN
1	A	179	ASN
1	A	212	ASN
1	A	253	ASN
1	A	282	ASN
1	A	293	ASN
1	A	311	GLN
1	A	333	ASN
1	A	334	GLN
1	A	338	ASN
1	A	360	GLN
1	A	377	ASN
1	A	413	GLN
1	A	421	GLN
1	A	428	ASN

### 5.3.3 RNA [i](#)

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 carbohydrates 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.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	412/494 (83%)	2.69	240 (58%) 0 0	5, 16, 31, 65	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	SER	12.3
1	A	454	ALA	9.8
1	A	323	PRO	9.8
1	A	231	SER	8.2
1	A	204	THR	7.8
1	A	449	ASP	7.7
1	A	149	THR	7.5
1	A	320	THR	7.3
1	A	317	ASP	7.3
1	A	233	PRO	6.8
1	A	311	GLN	6.8
1	A	44	ASN	6.8
1	A	147	SER	6.8
1	A	227	ILE	6.7
1	A	164	CYS	6.6
1	A	337	SER	6.5
1	A	150	THR	6.3
1	A	89	GLY	6.2
1	A	229	ASP	6.2
1	A	238	ASN	6.2
1	A	217	SER	6.2
1	A	205	ALA	6.2
1	A	335	SER	6.1
1	A	309	ASN	6.0
1	A	361	SER	6.0
1	A	308	SER	6.0
1	A	223	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	88	SER	5.7
1	A	236	GLU	5.7
1	A	288	ALA	5.6
1	A	237	ASN	5.5
1	A	268	PRO	5.4
1	A	60	HIS	5.4
1	A	196	THR	5.3
1	A	245	ILE	5.3
1	A	112	SER	5.3
1	A	45	ASP	5.3
1	A	49	ASP	5.2
1	A	267	LYS	5.1
1	A	148	ALA	5.1
1	A	270	ASN	5.1
1	A	426	ASN	5.1
1	A	378	SER	5.1
1	A	145	VAL	5.1
1	A	428	ASN	5.0
1	A	246	TYR	5.0
1	A	179	ASN	5.0
1	A	310	ASP	5.0
1	A	293	ASN	4.9
1	A	453	ALA	4.9
1	A	116	LEU	4.8
1	A	46	GLY	4.8
1	A	86	THR	4.7
1	A	430	THR	4.7
1	A	172	GLU	4.6
1	A	93	GLN	4.6
1	A	244	GLY	4.6
1	A	447	GLY	4.6
1	A	260	LYS	4.6
1	A	62	THR	4.6
1	A	385	ASP	4.5
1	A	360	GLN	4.5
1	A	107	LEU	4.5
1	A	314	GLU	4.5
1	A	178	ASN	4.4
1	A	388	ILE	4.4
1	A	286	PRO	4.4
1	A	400	THR	4.3
1	A	285	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	263	GLU	4.2
1	A	68	SER	4.2
1	A	57	PRO	4.1
1	A	135	VAL	4.1
1	A	342	ALA	4.1
1	A	328	THR	4.0
1	A	160	TYR	4.0
1	A	232	LEU	3.9
1	A	376	ASP	3.9
1	A	152	SER	3.9
1	A	313	ARG	3.9
1	A	340	LEU	3.9
1	A	191	GLU	3.8
1	A	336	ALA	3.8
1	A	43	ALA	3.8
1	A	48	GLN	3.8
1	A	234	TYR	3.8
1	A	226	VAL	3.8
1	A	443	THR	3.8
1	A	82	HIS	3.8
1	A	66	GLY	3.7
1	A	106	ARG	3.7
1	A	306	PHE	3.7
1	A	418	GLN	3.7
1	A	437	GLY	3.7
1	A	198	PRO	3.7
1	A	51	PHE	3.7
1	A	300	GLY	3.7
1	A	318	LEU	3.6
1	A	194	ASN	3.6
1	A	247	ASP	3.6
1	A	221	ASP	3.6
1	A	73	ILE	3.6
1	A	321	SER	3.6
1	A	163	GLY	3.6
1	A	125	SER	3.5
1	A	448	MET	3.5
1	A	190	THR	3.5
1	A	349	TYR	3.5
1	A	305	TYR	3.5
1	A	371	ASN	3.5
1	A	355	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	446	PRO	3.5
1	A	79	GLU	3.4
1	A	445	ARG	3.4
1	A	333	ASN	3.4
1	A	61	HIS	3.4
1	A	168	ASP	3.4
1	A	54	ALA	3.4
1	A	235	PHE	3.4
1	A	72	THR	3.3
1	A	130	GLU	3.3
1	A	325	VAL	3.3
1	A	101	GLY	3.3
1	A	392	ILE	3.3
1	A	95	ARG	3.3
1	A	47	ARG	3.3
1	A	173	THR	3.3
1	A	239	VAL	3.2
1	A	177	ILE	3.2
1	A	441	LEU	3.2
1	A	100	HIS	3.2
1	A	192	TRP	3.2
1	A	230	TYR	3.2
1	A	338	ASN	3.2
1	A	291	PRO	3.2
1	A	128	VAL	3.2
1	A	182	ASP	3.2
1	A	50	ILE	3.1
1	A	357	CYS	3.1
1	A	312	ILE	3.1
1	A	85	THR	3.1
1	A	211	PRO	3.1
1	A	114	GLY	3.0
1	A	203	THR	3.0
1	A	200	ALA	3.0
1	A	429	GLU	3.0
1	A	84	ALA	3.0
1	A	241	LYS	3.0
1	A	407	THR	3.0
1	A	290	GLN	3.0
1	A	359	PRO	3.0
1	A	394	LEU	3.0
1	A	144	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	91	TYR	3.0
1	A	207	SER	3.0
1	A	319	THR	3.0
1	A	346	TYR	2.9
1	A	158	ALA	2.9
1	A	197	ARG	2.9
1	A	424	TYR	2.9
1	A	216	SER	2.9
1	A	166	HIS	2.9
1	A	206	TRP	2.8
1	A	151	SER	2.8
1	A	126	LEU	2.8
1	A	169	GLU	2.8
1	A	143	PRO	2.8
1	A	254	GLY	2.8
1	A	193	LYS	2.8
1	A	292	THR	2.8
1	A	433	LEU	2.8
1	A	435	SER	2.8
1	A	264	LYS	2.7
1	A	350	ASN	2.7
1	A	413	GLN	2.7
1	A	184	ILE	2.7
1	A	440	LYS	2.7
1	A	295	MET	2.7
1	A	307	MET	2.7
1	A	374	ASN	2.7
1	A	176	GLY	2.7
1	A	67	LYS	2.6
1	A	170	ALA	2.6
1	A	87	ASN	2.6
1	A	377	ASN	2.6
1	A	90	TYR	2.6
1	A	136	TYR	2.6
1	A	248	TYR	2.6
1	A	228	VAL	2.6
1	A	278	THR	2.6
1	A	353	GLY	2.6
1	A	213	ILE	2.5
1	A	242	ASP	2.5
1	A	129	GLU	2.5
1	A	155	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	ARG	2.5
1	A	322	VAL	2.5
1	A	352	PHE	2.5
1	A	188	LEU	2.5
1	A	299	PRO	2.5
1	A	432	LEU	2.4
1	A	146	THR	2.4
1	A	425	PRO	2.4
1	A	154	ALA	2.4
1	A	296	THR	2.4
1	A	65	TYR	2.4
1	A	153	VAL	2.4
1	A	212	ASN	2.4
1	A	134	GLU	2.4
1	A	444	LYS	2.3
1	A	408	ASP	2.3
1	A	423	ARG	2.3
1	A	269	THR	2.3
1	A	348	GLY	2.3
1	A	56	GLN	2.3
1	A	113	GLU	2.3
1	A	174	ASN	2.3
1	A	258	TYR	2.3
1	A	451	ARG	2.3
1	A	326	ALA	2.2
1	A	427	ILE	2.2
1	A	209	GLN	2.2
1	A	257	ALA	2.2
1	A	110	TYR	2.2
1	A	387	LEU	2.2
1	A	109	MET	2.2
1	A	390	THR	2.2
1	A	391	ARG	2.1
1	A	59	GLN	2.1
1	A	222	ILE	2.1
1	A	330	THR	2.1
1	A	370	VAL	2.1
1	A	83	LEU	2.1
1	A	398	GLN	2.1
1	A	412	PRO	2.1
1	A	289	ALA	2.1
1	A	419	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	438	THR	2.0
1	A	94	GLN	2.0
1	A	404	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.