Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:26 AM GMT

PDB ID	:	3P0S
Title	:	Crystal structure of Bombyx mori densovirus 1 capsid
Authors	:	Kaufmann, B.; Rossmann, M.G.
Deposited on	:	2010-09-29
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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

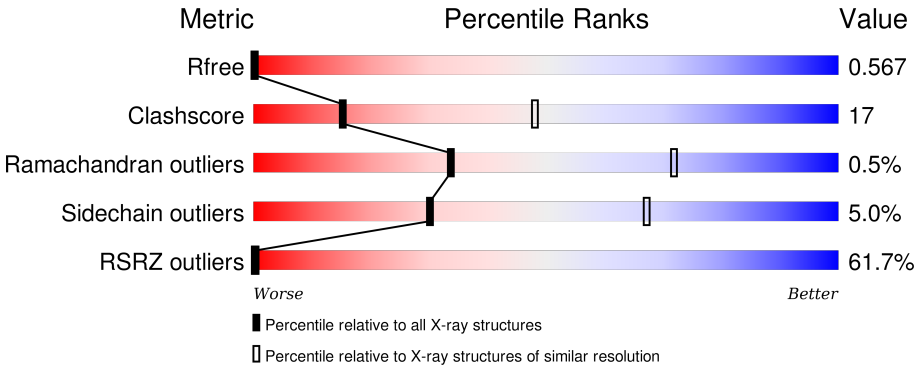
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 >=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 <=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	51% 55% 27% • 17%

2 Entry composition (i)

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.

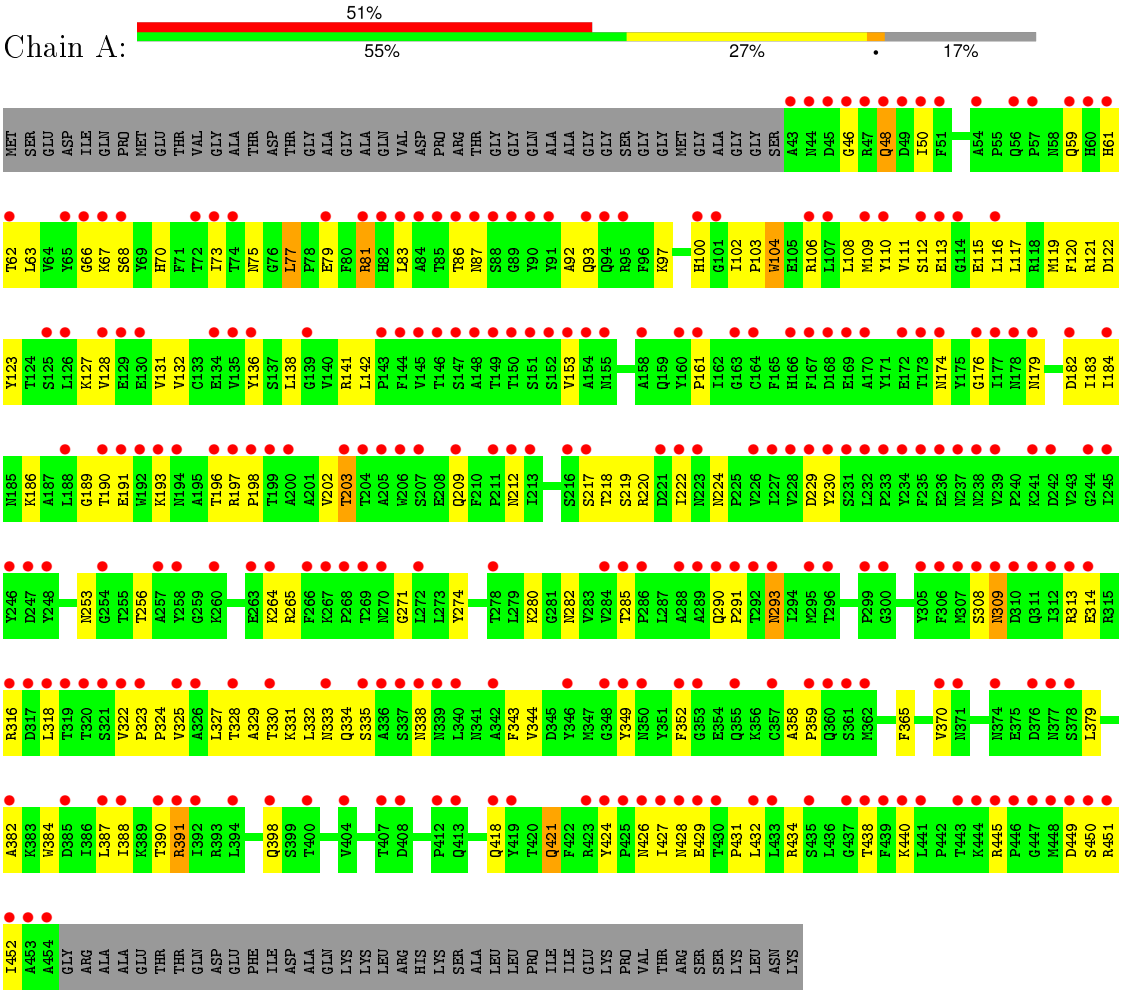
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	412	3290	2090	568	620	12	0	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	245.40Å 245.60Å 245.70Å 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
$< I/\sigma(I) >$ [1]	4.87 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.209 , (Not available) 0.567 , 0.567	Depositor DCC
R_{free} test set	65671 reflections (9.09%)	DCC
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 12.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 788408 reflections	Xtriage
F_o,F_c correlation	0.09	EDS
Total number of atoms	3290	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:75:ASN:HB3	1:A:379:LEU:HD11	1.72	0.70
1:A:293:ASN:H	1:A:293:ASN:HD22	1.40	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:220:ARG:HH11	1:A:220:ARG:HG2	1.63	0.62
1:A:217:SER:O	1:A:218:THR:HG23	1.99	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:N	1:A:293:ASN:HD22	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:432:LEU:HD12	1:A:449:ASP:O	2.02	0.59
1:A:182:ASP:OD1	1:A:186:LYS:HE3	2.03	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:314:GLU:OE1	1:A:316:ARG:HD3	2.04	0.57
1:A:176:GLY:HA3	1:A:179:ASN:HD22	1.69	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:280:LYS:NZ	1:A:428:ASN:ND2	2.65	0.45
1:A:197:ARG:HA	1:A:198:PRO:HD3	1.87	0.45
1:A:318:LEU:HB2	1:A:323:PRO:CG	2.46	0.45
1:A:110:TYR:CD1	1:A:390:THR:HB	2.52	0.45
1:A:116:LEU:C	1:A:116:LEU:HD23	2.37	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:450:SER:C	1:A:452:ILE:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:HIS:CE1	1:A:219:SER:HB2	2.53	0.44
1:A:103:PRO:O	1:A:109:MET:HG3	2.17	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:HD12	1:A:102:ILE:N	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:46:GLY:H	1:A:48:GLN:HE21	1.69	0.40
1:A:104:TRP:CH2	1:A:264:LYS:HB3	2.56	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%)	34 72

All (2) Ramachandran outliers are listed below:

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

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
1	A	359/418 (86%)	341 (95%)	18 (5%)	30 67

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

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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^{th} 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	412/494 (83%)	2.77	254 (61%)	0	0	5, 16, 31, 65	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	450	SER	12.6
1	A	323	PRO	10.1
1	A	454	ALA	10.0
1	A	231	SER	8.4
1	A	204	THR	8.0
1	A	449	ASP	7.8
1	A	149	THR	7.7
1	A	320	THR	7.5
1	A	317	ASP	7.5
1	A	233	PRO	7.0
1	A	147	SER	6.9
1	A	311	GLN	6.9
1	A	44	ASN	6.9
1	A	227	ILE	6.8
1	A	164	CYS	6.8
1	A	337	SER	6.7
1	A	150	THR	6.5
1	A	89	GLY	6.4
1	A	217	SER	6.4
1	A	229	ASP	6.4
1	A	205	ALA	6.3
1	A	238	ASN	6.3
1	A	335	SER	6.3
1	A	309	ASN	6.1
1	A	361	SER	6.1
1	A	308	SER	6.1
1	A	88	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	223	ASN	5.8
1	A	236	GLU	5.8
1	A	288	ALA	5.8
1	A	237	ASN	5.6
1	A	268	PRO	5.6
1	A	60	HIS	5.5
1	A	196	THR	5.5
1	A	112	SER	5.4
1	A	245	ILE	5.4
1	A	45	ASP	5.4
1	A	49	ASP	5.3
1	A	267	LYS	5.3
1	A	148	ALA	5.2
1	A	246	TYR	5.2
1	A	378	SER	5.2
1	A	270	ASN	5.2
1	A	145	VAL	5.2
1	A	426	ASN	5.2
1	A	428	ASN	5.1
1	A	310	ASP	5.1
1	A	179	ASN	5.1
1	A	293	ASN	5.0
1	A	453	ALA	5.0
1	A	116	LEU	5.0
1	A	46	GLY	4.9
1	A	86	THR	4.8
1	A	430	THR	4.8
1	A	244	GLY	4.8
1	A	172	GLU	4.7
1	A	447	GLY	4.7
1	A	93	GLN	4.7
1	A	62	THR	4.7
1	A	260	LYS	4.7
1	A	385	ASP	4.7
1	A	360	GLN	4.6
1	A	107	LEU	4.6
1	A	314	GLU	4.6
1	A	178	ASN	4.5
1	A	286	PRO	4.5
1	A	388	ILE	4.5
1	A	400	THR	4.5
1	A	285	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	263	GLU	4.3
1	A	68	SER	4.3
1	A	57	PRO	4.3
1	A	135	VAL	4.2
1	A	342	ALA	4.2
1	A	328	THR	4.1
1	A	160	TYR	4.1
1	A	232	LEU	4.1
1	A	313	ARG	4.1
1	A	152	SER	4.0
1	A	376	ASP	4.0
1	A	340	LEU	4.0
1	A	234	TYR	4.0
1	A	191	GLU	3.9
1	A	336	ALA	3.9
1	A	43	ALA	3.9
1	A	48	GLN	3.9
1	A	443	THR	3.9
1	A	226	VAL	3.9
1	A	106	ARG	3.9
1	A	66	GLY	3.9
1	A	306	PHE	3.8
1	A	82	HIS	3.8
1	A	437	GLY	3.8
1	A	198	PRO	3.8
1	A	51	PHE	3.8
1	A	418	GLN	3.8
1	A	300	GLY	3.8
1	A	318	LEU	3.8
1	A	247	ASP	3.7
1	A	194	ASN	3.7
1	A	221	ASP	3.7
1	A	321	SER	3.7
1	A	163	GLY	3.7
1	A	73	ILE	3.7
1	A	448	MET	3.7
1	A	349	TYR	3.6
1	A	305	TYR	3.6
1	A	125	SER	3.6
1	A	190	THR	3.6
1	A	446	PRO	3.6
1	A	445	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLN	3.5
1	A	371	ASN	3.5
1	A	79	GLU	3.5
1	A	235	PHE	3.5
1	A	168	ASP	3.5
1	A	333	ASN	3.5
1	A	54	ALA	3.5
1	A	61	HIS	3.4
1	A	72	THR	3.4
1	A	95	ARG	3.4
1	A	101	GLY	3.4
1	A	325	VAL	3.4
1	A	130	GLU	3.4
1	A	47	ARG	3.4
1	A	173	THR	3.4
1	A	392	ILE	3.4
1	A	230	TYR	3.3
1	A	192	TRP	3.3
1	A	239	VAL	3.3
1	A	441	LEU	3.3
1	A	177	ILE	3.3
1	A	100	HIS	3.3
1	A	291	PRO	3.3
1	A	357	CYS	3.3
1	A	128	VAL	3.2
1	A	338	ASN	3.2
1	A	182	ASP	3.2
1	A	50	ILE	3.2
1	A	312	ILE	3.2
1	A	85	THR	3.2
1	A	211	PRO	3.2
1	A	114	GLY	3.1
1	A	203	THR	3.1
1	A	91	TYR	3.1
1	A	407	THR	3.1
1	A	359	PRO	3.1
1	A	241	LYS	3.1
1	A	200	ALA	3.1
1	A	429	GLU	3.1
1	A	84	ALA	3.1
1	A	394	LEU	3.1
1	A	144	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	GLN	3.1
1	A	346	TYR	3.1
1	A	319	THR	3.0
1	A	207	SER	3.0
1	A	424	TYR	3.0
1	A	197	ARG	3.0
1	A	158	ALA	3.0
1	A	216	SER	3.0
1	A	206	TRP	3.0
1	A	166	HIS	2.9
1	A	151	SER	2.9
1	A	126	LEU	2.9
1	A	143	PRO	2.9
1	A	254	GLY	2.9
1	A	193	LYS	2.9
1	A	292	THR	2.9
1	A	433	LEU	2.9
1	A	169	GLU	2.9
1	A	435	SER	2.8
1	A	264	LYS	2.8
1	A	295	MET	2.8
1	A	307	MET	2.8
1	A	440	LYS	2.8
1	A	413	GLN	2.8
1	A	176	GLY	2.8
1	A	350	ASN	2.8
1	A	184	ILE	2.8
1	A	374	ASN	2.8
1	A	90	TYR	2.7
1	A	136	TYR	2.7
1	A	248	TYR	2.7
1	A	67	LYS	2.7
1	A	170	ALA	2.7
1	A	87	ASN	2.7
1	A	228	VAL	2.7
1	A	377	ASN	2.7
1	A	278	THR	2.7
1	A	353	GLY	2.7
1	A	81	ARG	2.6
1	A	242	ASP	2.6
1	A	129	GLU	2.6
1	A	213	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	155	ASN	2.6
1	A	352	PHE	2.6
1	A	322	VAL	2.6
1	A	188	LEU	2.5
1	A	299	PRO	2.5
1	A	432	LEU	2.5
1	A	146	THR	2.5
1	A	65	TYR	2.5
1	A	425	PRO	2.5
1	A	296	THR	2.5
1	A	154	ALA	2.5
1	A	153	VAL	2.5
1	A	134	GLU	2.5
1	A	212	ASN	2.4
1	A	423	ARG	2.4
1	A	444	LYS	2.4
1	A	408	ASP	2.4
1	A	269	THR	2.4
1	A	348	GLY	2.4
1	A	258	TYR	2.4
1	A	451	ARG	2.4
1	A	113	GLU	2.4
1	A	56	GLN	2.4
1	A	174	ASN	2.3
1	A	110	TYR	2.3
1	A	326	ALA	2.3
1	A	109	MET	2.3
1	A	387	LEU	2.3
1	A	257	ALA	2.3
1	A	209	GLN	2.3
1	A	427	ILE	2.3
1	A	390	THR	2.2
1	A	391	ARG	2.2
1	A	330	THR	2.2
1	A	59	GLN	2.2
1	A	222	ILE	2.2
1	A	370	VAL	2.2
1	A	419	TYR	2.2
1	A	83	LEU	2.2
1	A	412	PRO	2.2
1	A	289	ALA	2.1
1	A	398	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	438	THR	2.1
1	A	94	GLN	2.1
1	A	404	VAL	2.1
1	A	161	PRO	2.1
1	A	74	THR	2.0
1	A	199	THR	2.0
1	A	439	PHE	2.0
1	A	284	VAL	2.0
1	A	382	ALA	2.0
1	A	452	ILE	2.0
1	A	167	PHE	2.0
1	A	266	PHE	2.0
1	A	272	LEU	2.0
1	A	362	MET	2.0
1	A	139	GLY	2.0
1	A	316	ARG	2.0
1	A	339	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.