



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 05:15 AM UTC

PDB ID : 5A00 / pdb_00005a00
Title : X-ray structure of a human Kobuvirus: Aichi virus A (AiV)
Authors : Sabin, C.; Palkova, L.; Plevka, P.
Deposited on : 2015-09-11
Resolution : 2.10 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

<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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.48.1

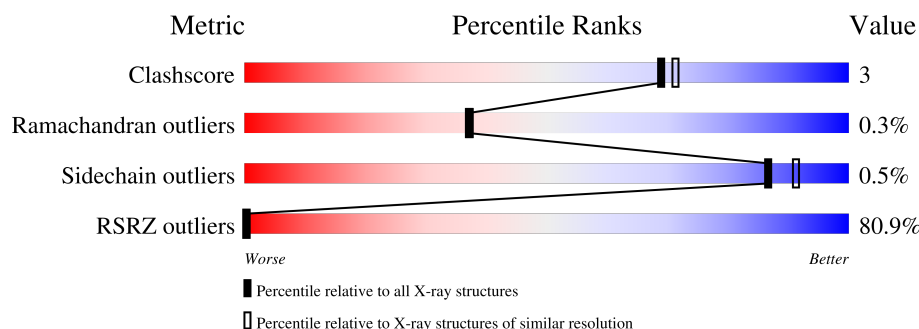
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	253	76% 78% 12% 9%
2	B	370	71% 75% 9% 15%
3	C	223	73% 89% 9% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5938 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 VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1746	1130	276	331	9			

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2366	1506	390	464	6			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	220	Total	C	N	O	S	0	0	0
			1679	1085	283	304	7			

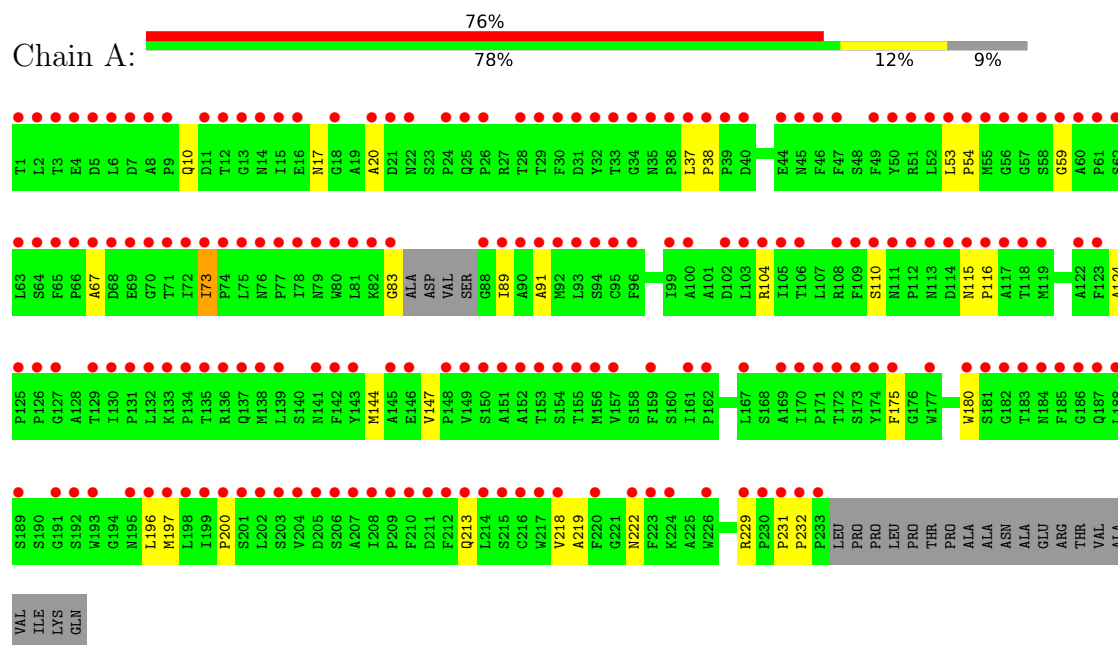
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	58	Total	O	0	0
			58	58		
4	C	37	Total	O	0	0
			37	37		

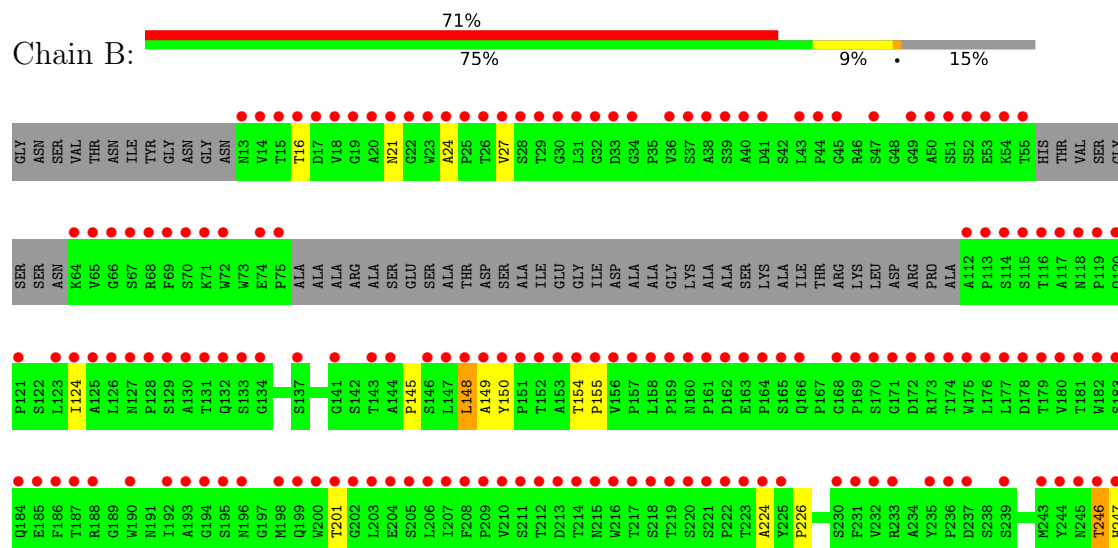
3 Residue-property plots [i](#)

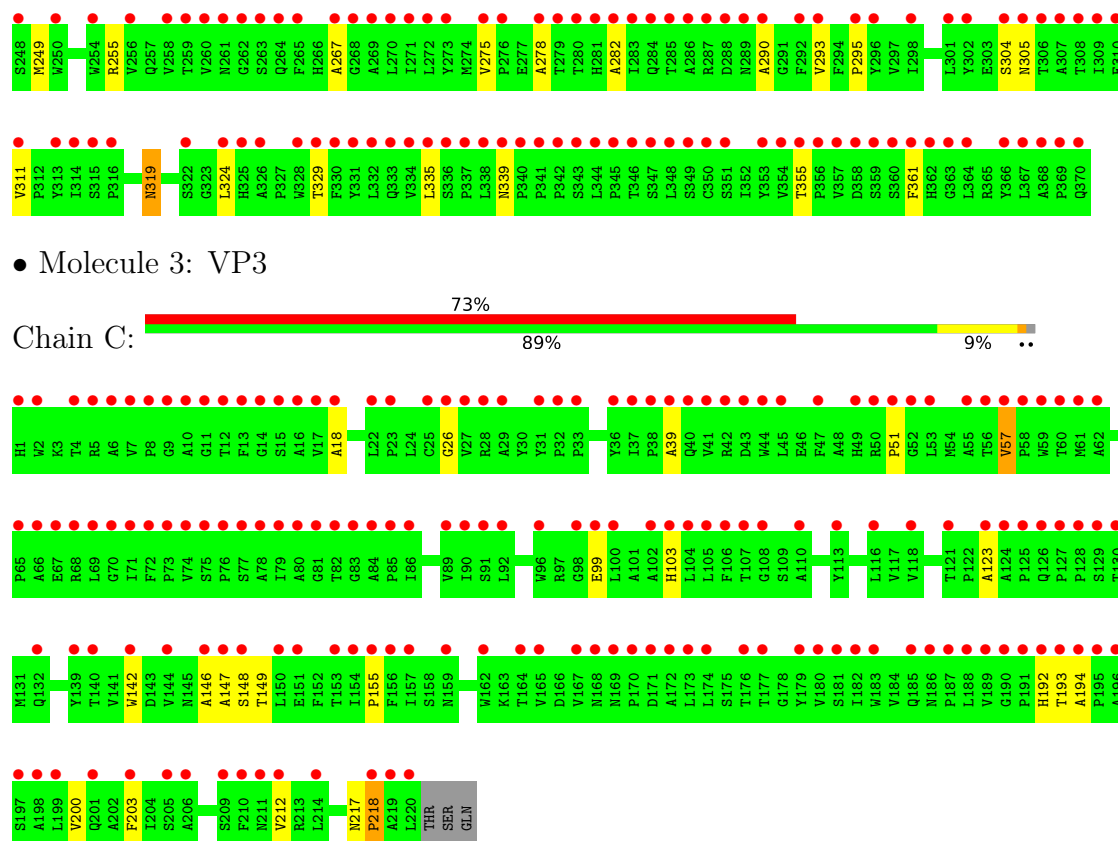
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: VP0



• Molecule 2: VP1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	350.82Å 350.82Å 350.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.46 – 2.10 71.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (71.46-2.10) 89.6 (71.46-2.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1494.23 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.330 , (Not available) 0.364 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 7.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.50	EDS
Total number of atoms	5938	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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

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	0.72	0/1806	0.87	3/2481 (0.1%)
2	B	0.80	3/2448 (0.1%)	0.93	11/3379 (0.3%)
3	C	0.76	0/1736	0.93	7/2389 (0.3%)
All	All	0.76	3/5990 (0.1%)	0.91	21/8249 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	246	THR	CB-CG2	-8.67	1.24	1.52
2	B	246	THR	CA-CB	-8.03	1.42	1.54
2	B	319	ASN	C-O	-6.52	1.16	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	148	SER	N-CA-C	8.63	120.69	111.28
3	C	147	ALA	N-CA-C	-8.03	97.98	110.42
2	B	148	LEU	N-CA-C	-7.90	97.16	109.25
3	C	26	GLY	N-CA-C	6.97	121.69	112.77
2	B	293	VAL	N-CA-C	-6.75	102.40	111.44
2	B	304	SER	N-CA-C	6.69	120.59	109.95
3	C	57	VAL	N-CA-C	6.57	114.40	107.76
2	B	124	ILE	N-CA-C	6.42	116.59	110.42
2	B	305	ASN	N-CA-C	-6.12	105.61	114.12
2	B	246	THR	CA-CB-CG2	-6.06	100.19	110.50
3	C	194	ALA	N-CA-C	-5.99	102.56	110.40
2	B	275	VAL	N-CA-C	5.87	114.34	107.77
3	C	142	TRP	N-CA-C	5.74	118.09	108.73
2	B	201	THR	N-CA-C	-5.66	106.42	113.38
1	A	73	ILE	N-CA-C	5.42	113.40	107.60
1	A	144	MET	N-CA-C	5.23	117.82	110.14
2	B	278	ALA	N-CA-C	5.16	116.58	109.15
1	A	147	VAL	N-CA-C	5.16	113.61	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	224	ALA	N-CA-C	5.15	117.69	109.81
2	B	335	LEU	N-CA-C	-5.14	104.71	111.96
3	C	123	ALA	N-CA-C	5.12	117.73	110.10

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	1746	0	1681	19	0
2	B	2366	0	2246	20	0
3	C	1679	0	1635	8	0
4	A	52	0	0	0	0
4	B	58	0	0	0	0
4	C	37	0	0	0	0
All	All	5938	0	5562	39	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 3.

All (39) 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)
2:B:246:THR:O	2:B:246:THR:HG22	1.83	0.77
3:C:192:HIS:O	3:C:193:THR:HG22	1.96	0.66
2:B:149:ALA:CB	2:B:295:PRO:HB3	2.29	0.63
2:B:255:ARG:HB3	2:B:355:THR:HB	1.81	0.62
2:B:149:ALA:HB3	2:B:311:VAL:HG12	1.83	0.60
1:A:20:ALA:HB2	3:C:51:PRO:HG3	1.88	0.56
1:A:180:TRP:HA	2:B:324:LEU:HD21	1.89	0.54
1:A:110:SER:HB2	1:A:213:GLN:HB2	1.90	0.54
2:B:226:PRO:HA	2:B:329:THR:HG22	1.91	0.53
2:B:267:ALA:HB3	2:B:339:ASN:HB3	1.90	0.53
1:A:89:ILE:HD13	1:A:218:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:ND2	2:B:21:ASN:OD1	2.45	0.50
2:B:149:ALA:HB1	2:B:295:PRO:HB3	1.95	0.48
3:C:57:VAL:HG13	3:C:200:VAL:HB	1.95	0.48
1:A:231:PRO:HD2	2:B:290:ALA:HB1	1.96	0.47
1:A:175:PHE:C	1:A:175:PHE:CD1	2.93	0.47
1:A:229:ARG:HH21	2:B:282:ALA:HB2	1.80	0.46
1:A:124:ALA:HB2	1:A:197:MET:HE2	1.97	0.46
1:A:91:ALA:HB1	1:A:232:PRO:HG3	1.97	0.46
2:B:247:HIS:CG	2:B:361:PHE:HB3	2.50	0.46
1:A:104:ARG:HB2	1:A:219:ALA:HB3	1.98	0.45
2:B:149:ALA:HB2	2:B:295:PRO:HB3	1.98	0.45
1:A:53:LEU:HD12	1:A:54:PRO:HD2	1.99	0.44
3:C:103:HIS:HB2	3:C:203:PHE:HB2	1.99	0.44
3:C:217:ASN:O	3:C:218:PRO:C	2.60	0.44
2:B:150:TYR:CD2	3:C:39:ALA:HB2	2.52	0.43
1:A:73:ILE:HG13	1:A:196:LEU:HB2	2.00	0.43
2:B:148:LEU:HG	2:B:150:TYR:O	2.17	0.43
3:C:99:GLU:HG3	3:C:155:PRO:HA	2.01	0.42
1:A:59:GLY:HA3	1:A:83:GLY:HA3	2.02	0.42
1:A:175:PHE:C	1:A:175:PHE:HD1	2.27	0.42
2:B:24:ALA:HB3	2:B:27:VAL:HG23	2.00	0.42
1:A:17:ASN:HA	2:B:145:PRO:HB3	2.02	0.42
1:A:115:ASN:HA	1:A:116:PRO:HD3	1.94	0.41
2:B:249:MET:HB2	2:B:319:ASN:HB3	2.01	0.41
1:A:67:ALA:HA	1:A:200:PRO:HG2	2.03	0.41
1:A:37:LEU:HA	1:A:38:PRO:HD3	1.96	0.40
2:B:16:THR:HA	3:C:18:ALA:HB2	2.03	0.40
2:B:154:THR:HA	2:B:155:PRO:HD3	1.92	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 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	225/253 (89%)	216 (96%)	9 (4%)	0	100	100
2	B	308/370 (83%)	295 (96%)	13 (4%)	0	100	100
3	C	218/223 (98%)	208 (95%)	8 (4%)	2 (1%)	14	11
All	All	751/846 (89%)	719 (96%)	30 (4%)	2 (0%)	37	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	146	ALA
3	C	218	PRO

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	193/212 (91%)	192 (100%)	1 (0%)	86	91
2	B	264/302 (87%)	264 (100%)	0	100	100
3	C	175/178 (98%)	173 (99%)	2 (1%)	70	77
All	All	632/692 (91%)	629 (100%)	3 (0%)	86	91

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
3	C	149	THR
3	C	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	17	ASN
1	A	25	GLN

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Mol	Chain	Res	Type
1	A	35	ASN
1	A	222	ASN
2	B	21	ASN
2	B	120	GLN
3	C	20	GLN
3	C	111	GLN
3	C	201	GLN

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 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.

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, 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	229/253 (90%)	3.52	192 (83%) 0 0	15, 22, 42, 51	0
2	B	314/370 (84%)	3.47	263 (83%) 0 0	15, 20, 39, 56	0
3	C	220/223 (98%)	2.93	162 (73%) 0 0	15, 20, 30, 42	0
All	All	763/846 (90%)	3.33	617 (80%) 0 0	15, 20, 39, 56	0

All (617) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	20	ALA	16.1
1	A	56	GLY	12.6
1	A	206	SER	12.5
2	B	112	ALA	11.9
1	A	205	ASP	11.1
1	A	1	THR	10.8
2	B	64	LYS	10.6
2	B	21	ASN	10.5
2	B	65	VAL	10.0
2	B	220	SER	9.3
2	B	342	PRO	9.1
1	A	208	ILE	9.1
2	B	113	PRO	9.0
1	A	207	ALA	9.0
2	B	219	THR	8.7
1	A	58	SER	8.7
1	A	57	GLY	8.4
2	B	214	THR	8.1
2	B	281	HIS	7.9
1	A	83	GLY	7.6
3	C	9	GLY	7.5
3	C	170	PRO	7.5
3	C	80	ALA	7.5

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Mol	Chain	Res	Type	RSRZ
3	C	192	HIS	7.3
1	A	210	PHE	7.3
2	B	22	GLY	7.3
1	A	64	SER	7.0
2	B	24	ALA	6.9
2	B	344	LEU	6.9
2	B	285	THR	6.9
2	B	19	GLY	6.9
3	C	57	VAL	6.7
2	B	67	SER	6.7
3	C	78	ALA	6.7
1	A	114	ASP	6.6
2	B	163	GLU	6.6
3	C	81	GLY	6.6
3	C	79	ILE	6.6
1	A	132	LEU	6.5
1	A	54	PRO	6.5
2	B	290	ALA	6.5
2	B	55	THR	6.4
1	A	204	VAL	6.4
1	A	202	LEU	6.4
3	C	169	ASN	6.4
1	A	55	MET	6.3
2	B	337	PRO	6.2
2	B	207	ILE	6.2
2	B	114	SER	6.2
1	A	2	LEU	6.1
2	B	208	PHE	6.1
2	B	203	LEU	6.0
1	A	60	ALA	6.0
1	A	68	ASP	5.9
2	B	185	GLU	5.9
1	A	110	SER	5.9
2	B	68	ARG	5.9
1	A	209	PRO	5.9
2	B	157	PRO	5.8
1	A	133	LYS	5.7
2	B	202	GLY	5.7
2	B	147	LEU	5.7
1	A	188	LEU	5.7
3	C	77	SER	5.7
1	A	135	THR	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	199	GLN	5.6
1	A	59	GLY	5.6
2	B	343	SER	5.6
1	A	61	PRO	5.5
2	B	75	PRO	5.5
2	B	28	SER	5.5
2	B	23	TRP	5.5
2	B	345	PRO	5.5
1	A	63	LEU	5.5
1	A	62	SER	5.4
2	B	116	THR	5.4
3	C	82	THR	5.3
3	C	71	ILE	5.3
1	A	71	THR	5.3
2	B	190	TRP	5.3
2	B	221	SER	5.2
2	B	210	VAL	5.2
1	A	67	ALA	5.2
2	B	270	LEU	5.1
2	B	115	SER	5.1
1	A	134	PRO	5.1
2	B	356	PRO	5.1
1	A	136	ARG	5.1
2	B	40	ALA	5.1
2	B	124	ILE	5.1
2	B	160	ASN	5.1
2	B	293	VAL	5.1
2	B	17	ASP	5.1
2	B	206	LEU	5.0
2	B	201	THR	5.0
3	C	144	VAL	5.0
2	B	53	GLU	5.0
2	B	177	LEU	5.0
2	B	18	VAL	5.0
1	A	65	PHE	4.9
3	C	23	PRO	4.9
2	B	150	TYR	4.9
3	C	191	PRO	4.9
1	A	82	LYS	4.9
1	A	93	LEU	4.9
3	C	6	ALA	4.8
2	B	126	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	88	GLY	4.8
2	B	280	THR	4.8
3	C	193	THR	4.8
2	B	121	PRO	4.8
2	B	218	SER	4.8
2	B	211	SER	4.8
1	A	81	LEU	4.7
3	C	76	PRO	4.7
3	C	83	GLY	4.7
1	A	232	PRO	4.7
2	B	265	PHE	4.7
3	C	62	ALA	4.7
3	C	220	LEU	4.7
3	C	8	PRO	4.6
1	A	100	ALA	4.6
3	C	47	PHE	4.6
3	C	164	THR	4.6
1	A	73	ILE	4.6
1	A	131	PRO	4.6
2	B	148	LEU	4.6
3	C	194	ALA	4.6
1	A	115	ASN	4.6
3	C	127	PRO	4.6
3	C	196	ALA	4.6
2	B	47	SER	4.6
2	B	194	GLY	4.5
3	C	199	LEU	4.5
1	A	217	TRP	4.5
3	C	108	GLY	4.5
1	A	183	THR	4.5
1	A	126	PRO	4.5
1	A	69	GLU	4.5
2	B	217	THR	4.5
1	A	112	PRO	4.4
3	C	155	PRO	4.4
1	A	52	LEU	4.4
1	A	211	ASP	4.4
3	C	52	GLY	4.4
2	B	144	ALA	4.4
1	A	34	GLY	4.4
1	A	137	GLN	4.4
2	B	26	THR	4.4

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Mol	Chain	Res	Type	RSRZ
3	C	7	VAL	4.4
1	A	24	PRO	4.4
2	B	161	PRO	4.4
3	C	128	PRO	4.4
2	B	43	LEU	4.4
3	C	168	ASN	4.4
2	B	282	ALA	4.4
1	A	212	PHE	4.3
3	C	65	PRO	4.3
3	C	188	LEU	4.3
2	B	353	TYR	4.3
2	B	158	LEU	4.3
2	B	338	LEU	4.3
1	A	18	GLY	4.3
1	A	153	THR	4.3
1	A	26	PRO	4.3
1	A	215	SER	4.3
2	B	44	PRO	4.3
3	C	104	LEU	4.3
2	B	117	ALA	4.3
2	B	368	ALA	4.3
2	B	181	THR	4.3
2	B	25	PRO	4.2
3	C	27	VAL	4.2
2	B	192	ILE	4.2
1	A	152	ALA	4.2
3	C	10	ALA	4.2
2	B	152	THR	4.2
2	B	246	THR	4.2
1	A	32	TYR	4.2
2	B	324	LEU	4.2
1	A	117	ALA	4.2
2	B	279	THR	4.2
2	B	287	ARG	4.1
1	A	230	PRO	4.1
1	A	159	PHE	4.1
1	A	218	VAL	4.1
3	C	68	ARG	4.1
1	A	203	SER	4.1
3	C	171	ASP	4.1
2	B	164	PRO	4.1
2	B	216	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	66	GLY	4.1
1	A	157	VAL	4.1
2	B	357	VAL	4.1
3	C	147	ALA	4.1
3	C	195	PRO	4.1
2	B	348	LEU	4.1
2	B	284	GLN	4.1
2	B	340	PRO	4.0
2	B	370	GLN	4.0
1	A	199	ILE	4.0
3	C	5	ARG	4.0
2	B	369	PRO	4.0
1	A	79	ASN	4.0
2	B	118	ASN	4.0
2	B	278	ALA	4.0
2	B	316	PRO	4.0
2	B	268	GLY	4.0
3	C	67	GLU	4.0
3	C	15	SER	4.0
2	B	346	THR	4.0
1	A	75	LEU	4.0
3	C	173	LEU	4.0
3	C	174	LEU	3.9
2	B	175	TRP	3.9
2	B	182	TRP	3.9
3	C	107	THR	3.9
1	A	182	GLY	3.9
1	A	37	LEU	3.9
1	A	109	PHE	3.9
2	B	130	ALA	3.9
2	B	307	ALA	3.9
3	C	49	HIS	3.9
2	B	120	GLN	3.9
1	A	53	LEU	3.9
1	A	220	PHE	3.9
2	B	351	SER	3.8
3	C	55	ALA	3.8
1	A	231	PRO	3.8
2	B	341	PRO	3.8
3	C	86	ILE	3.8
2	B	149	ALA	3.8
2	B	269	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	C	39	ALA	3.8
2	B	27	VAL	3.8
1	A	66	PRO	3.8
2	B	151	PRO	3.8
1	A	99	ILE	3.8
1	A	142	PHE	3.7
2	B	69	PHE	3.7
2	B	209	PRO	3.7
1	A	130	ILE	3.7
2	B	362	HIS	3.7
3	C	2	TRP	3.7
2	B	16	THR	3.7
2	B	288	ASP	3.7
1	A	72	ILE	3.7
2	B	51	SER	3.7
2	B	225	TYR	3.7
1	A	13	GLY	3.7
3	C	12	THR	3.7
1	A	36	PRO	3.7
1	A	233	PRO	3.7
2	B	54	LYS	3.7
2	B	272	LEU	3.7
1	A	177	TRP	3.7
1	A	150	SER	3.6
1	A	184	ASN	3.6
3	C	180	VAL	3.6
1	A	201	SER	3.6
2	B	205	SER	3.6
3	C	42	ARG	3.6
2	B	308	THR	3.6
1	A	169	ALA	3.6
1	A	77	PRO	3.6
3	C	14	GLY	3.6
1	A	102	ASP	3.6
1	A	8	ALA	3.6
1	A	116	PRO	3.6
2	B	361	PHE	3.6
1	A	187	GLN	3.5
3	C	140	THR	3.5
3	C	139	TYR	3.5
3	C	219	ALA	3.5
2	B	159	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	35	ASN	3.5
2	B	304	SER	3.5
2	B	166	GLN	3.5
3	C	190	GLY	3.5
2	B	38	ALA	3.5
2	B	256	VAL	3.5
1	A	180	TRP	3.5
2	B	298	ILE	3.5
1	A	39	PRO	3.5
3	C	32	PRO	3.5
2	B	347	SER	3.5
3	C	72	PHE	3.5
2	B	154	THR	3.5
1	A	151	ALA	3.4
3	C	118	VAL	3.4
2	B	233	ARG	3.4
1	A	129	THR	3.4
2	B	141	GLY	3.4
2	B	200	TRP	3.4
3	C	33	PRO	3.4
3	C	73	PRO	3.4
2	B	336	SER	3.4
2	B	231	PHE	3.4
2	B	179	THR	3.4
3	C	4	THR	3.4
1	A	214	LEU	3.4
2	B	125	ALA	3.4
1	A	47	PHE	3.3
2	B	329	THR	3.3
1	A	216	CYS	3.3
3	C	100	LEU	3.3
2	B	276	PRO	3.3
3	C	38	PRO	3.3
1	A	4	GLU	3.3
2	B	204	GLU	3.3
2	B	171	GLY	3.3
1	A	143	TYR	3.3
3	C	159	ASN	3.3
3	C	45	LEU	3.3
1	A	200	PRO	3.3
1	A	5	ASP	3.3
3	C	132	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	195	ASN	3.3
2	B	296	TYR	3.3
2	B	302	TYR	3.3
1	A	192	SER	3.3
1	A	198	LEU	3.3
2	B	315	SER	3.3
2	B	30	GLY	3.2
2	B	72	TRP	3.2
3	C	50	ARG	3.2
1	A	33	THR	3.2
3	C	22	LEU	3.2
1	A	89	ILE	3.2
2	B	289	ASN	3.2
3	C	186	ASN	3.2
2	B	310	GLU	3.2
2	B	36	VAL	3.2
3	C	167	VAL	3.2
3	C	212	VAL	3.2
1	A	175	PHE	3.2
2	B	186	PHE	3.2
3	C	75	SER	3.2
3	C	187	PRO	3.2
3	C	214	LEU	3.2
2	B	358	ASP	3.2
3	C	218	PRO	3.2
3	C	146	ALA	3.2
2	B	367	LEU	3.1
1	A	108	ARG	3.1
3	C	18	ALA	3.1
1	A	12	THR	3.1
1	A	118	THR	3.1
2	B	162	ASP	3.1
2	B	195	SER	3.1
1	A	20	ALA	3.1
2	B	215	ASN	3.1
1	A	170	ILE	3.1
1	A	173	SER	3.1
2	B	29	THR	3.1
2	B	173	ARG	3.1
2	B	335	LEU	3.1
3	C	142	TRP	3.1
2	B	261	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	16	ALA	3.1
2	B	170	SER	3.1
2	B	248	SER	3.1
1	A	167	LEU	3.0
3	C	84	ALA	3.0
1	A	105	ILE	3.0
1	A	171	PRO	3.0
2	B	169	PRO	3.0
2	B	31	LEU	3.0
2	B	331	TYR	3.0
1	A	138	MET	3.0
2	B	52	SER	3.0
2	B	143	THR	3.0
1	A	9	PRO	3.0
3	C	13	PHE	3.0
3	C	162	TRP	3.0
3	C	148	SER	3.0
2	B	168	GLY	3.0
2	B	332	LEU	3.0
1	A	146	GLU	3.0
1	A	50	TYR	2.9
3	C	25	CYS	2.9
3	C	130	THR	2.9
1	A	70	GLY	2.9
2	B	14	VAL	2.9
2	B	258	VAL	2.9
1	A	196	LEU	2.9
3	C	61	MET	2.9
1	A	213	GLN	2.9
3	C	11	GLY	2.9
2	B	275	VAL	2.9
3	C	105	LEU	2.9
1	A	123	PHE	2.9
2	B	183	SER	2.9
3	C	91	SER	2.9
1	A	155	THR	2.9
2	B	187	THR	2.9
1	A	104	ARG	2.9
2	B	250	TRP	2.9
2	B	119	PRO	2.9
3	C	17	VAL	2.9
2	B	247	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	264	GLN	2.9
3	C	157	ILE	2.9
1	A	76	ASN	2.9
3	C	177	THR	2.9
2	B	325	HIS	2.8
1	A	22	ASN	2.8
1	A	139	LEU	2.8
2	B	176	LEU	2.8
2	B	333	GLN	2.8
2	B	305	ASN	2.8
3	C	56	THR	2.8
3	C	121	THR	2.8
2	B	222	PRO	2.8
1	A	46	PHE	2.8
1	A	154	SER	2.8
3	C	129	SER	2.8
1	A	222	ASN	2.8
3	C	151	GLU	2.8
3	C	185	GLN	2.8
1	A	226	TRP	2.8
2	B	74	GLU	2.8
2	B	260	VAL	2.8
2	B	354	VAL	2.8
3	C	74	VAL	2.8
1	A	189	SER	2.8
2	B	153	ALA	2.7
1	A	161	ILE	2.7
1	A	95	CYS	2.7
2	B	128	PRO	2.7
2	B	244	TYR	2.7
2	B	273	TYR	2.7
3	C	150	LEU	2.7
1	A	149	VAL	2.7
3	C	29	ALA	2.7
3	C	203	PHE	2.7
1	A	172	THR	2.7
2	B	283	ILE	2.7
3	C	90	ILE	2.7
3	C	182	ILE	2.7
2	B	155	PRO	2.7
3	C	51	PRO	2.7
3	C	92	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	123	ALA	2.7
1	A	223	PHE	2.7
1	A	11	ASP	2.7
3	C	43	ASP	2.7
1	A	74	PRO	2.7
2	B	134	GLY	2.7
2	B	306	THR	2.7
3	C	183	TRP	2.7
1	A	78	ILE	2.7
3	C	154	ILE	2.7
1	A	125	PRO	2.6
2	B	245	ASN	2.6
1	A	6	LEU	2.6
3	C	181	SER	2.6
2	B	313	TYR	2.6
3	C	36	TYR	2.6
1	A	91	ALA	2.6
2	B	132	GLN	2.6
3	C	126	GLN	2.6
2	B	49	GLY	2.6
3	C	59	TRP	2.6
2	B	180	VAL	2.6
2	B	311	VAL	2.6
3	C	124	ALA	2.6
3	C	165	VAL	2.6
3	C	172	ALA	2.6
3	C	99	GLU	2.6
1	A	49	PHE	2.6
3	C	210	PHE	2.6
2	B	236	PRO	2.6
1	A	197	MET	2.6
1	A	113	ASN	2.6
2	B	188	ARG	2.6
3	C	66	ALA	2.6
3	C	110	ALA	2.6
2	B	235	TYR	2.6
3	C	106	PHE	2.6
1	A	14	ASN	2.6
1	A	94	SER	2.6
1	A	40	ASP	2.5
2	B	41	ASP	2.5
1	A	111	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	181	SER	2.5
2	B	172	ASP	2.5
1	A	174	TYR	2.5
2	B	292	PHE	2.5
3	C	85	PRO	2.5
3	C	156	PHE	2.5
1	A	15	ILE	2.5
2	B	146	SER	2.5
3	C	116	LEU	2.5
2	B	232	VAL	2.5
3	C	40	GLN	2.5
2	B	309	ILE	2.5
1	A	7	ASP	2.5
1	A	156	MET	2.5
2	B	131	THR	2.5
2	B	37	SER	2.4
3	C	37	ILE	2.4
1	A	186	GLY	2.4
2	B	198	MET	2.4
2	B	213	ASP	2.4
3	C	28	ARG	2.4
1	A	3	THR	2.4
1	A	29	THR	2.4
3	C	211	ASN	2.4
1	A	148	PRO	2.4
2	B	137	SER	2.4
2	B	263	SER	2.4
2	B	322	SER	2.4
3	C	31	TYR	2.4
1	A	96	PHE	2.4
2	B	259	THR	2.4
2	B	156	VAL	2.4
3	C	1	HIS	2.4
2	B	359	SER	2.4
3	C	26	GLY	2.4
1	A	31	ASP	2.4
2	B	237	ASP	2.4
1	A	103	LEU	2.4
3	C	206	ALA	2.4
2	B	70	SER	2.4
3	C	205	SER	2.4
1	A	30	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	21	ASP	2.4
2	B	33	ASP	2.4
2	B	34	GLY	2.4
2	B	364	LEU	2.3
2	B	339	ASN	2.3
1	A	122	ALA	2.3
2	B	50	ALA	2.3
1	A	162	PRO	2.3
2	B	129	SER	2.3
1	A	185	PHE	2.3
3	C	179	TYR	2.3
2	B	271	ILE	2.3
2	B	123	LEU	2.3
1	A	28	THR	2.3
2	B	193	ALA	2.3
1	A	119	MET	2.3
2	B	243	MET	2.3
3	C	197	SER	2.3
1	A	127	GLY	2.3
3	C	96	TRP	2.3
3	C	103	HIS	2.3
2	B	301	LEU	2.3
1	A	145	ALA	2.3
2	B	212	THR	2.3
2	B	286	ALA	2.3
3	C	153	THR	2.3
1	A	25	GLN	2.3
1	A	191	GLY	2.3
1	A	80	TRP	2.3
2	B	328	TRP	2.3
3	C	113	TYR	2.3
2	B	223	THR	2.3
3	C	176	THR	2.3
2	B	133	SER	2.3
2	B	45	GLY	2.2
2	B	363	GLY	2.2
2	B	127	ASN	2.2
2	B	254	TRP	2.2
2	B	15	THR	2.2
3	C	60	THR	2.2
2	B	224	ALA	2.2
2	B	326	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	239	SER	2.2
2	B	262	GLY	2.2
3	C	89	VAL	2.2
1	A	44	GLU	2.2
1	A	224	LYS	2.2
2	B	350	CYS	2.2
3	C	70	GLY	2.2
1	A	229	ARG	2.2
3	C	201	GLN	2.2
2	B	355	THR	2.2
2	B	366	TYR	2.2
2	B	360	SER	2.2
3	C	102	ALA	2.2
1	A	45	ASN	2.2
2	B	184	GLN	2.2
2	B	314	ILE	2.1
3	C	69	LEU	2.1
1	A	106	THR	2.1
2	B	71	LYS	2.1
2	B	165	SER	2.1
3	C	44	TRP	2.1
3	C	209	SER	2.1
2	B	267	ALA	2.1
2	B	334	VAL	2.1
2	B	349	SER	2.1
1	A	90	ALA	2.1
3	C	198	ALA	2.1
1	A	92	MET	2.1
3	C	53	LEU	2.1
2	B	39	SER	2.1
1	A	38	PRO	2.1
2	B	295	PRO	2.1
3	C	58	PRO	2.1
3	C	125	PRO	2.1
1	A	193	TRP	2.1
1	A	16	GLU	2.1
1	A	51	ARG	2.1
2	B	230	SER	2.1
2	B	330	PHE	2.1
2	B	32	GLY	2.0
2	B	13	ASN	2.0
3	C	41	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	189	VAL	2.0
2	B	174	THR	2.0
1	A	141	ASN	2.0
2	B	196	ASN	2.0
3	C	98	GLY	2.0
2	B	178	ASP	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 oligosaccharides 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.