



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:43 AM UTC

PDB ID : 5JHM / pdb_00005jhm
Title : Crystal structure of Zika virus Envelope protein
Authors : Dai, L.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2016-04-21
Resolution : 2.00 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	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

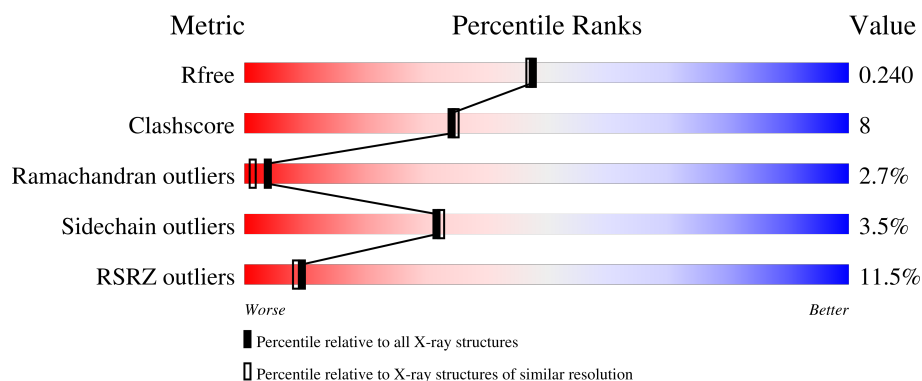
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	416	13% 72% 18% • 6%
1	B	416	8% 79% 13% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6236 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 Envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	1	0
			2988	1867	521	575	25			
1	B	390	Total	C	N	O	S	0	0	0
			2975	1860	519	571	25			

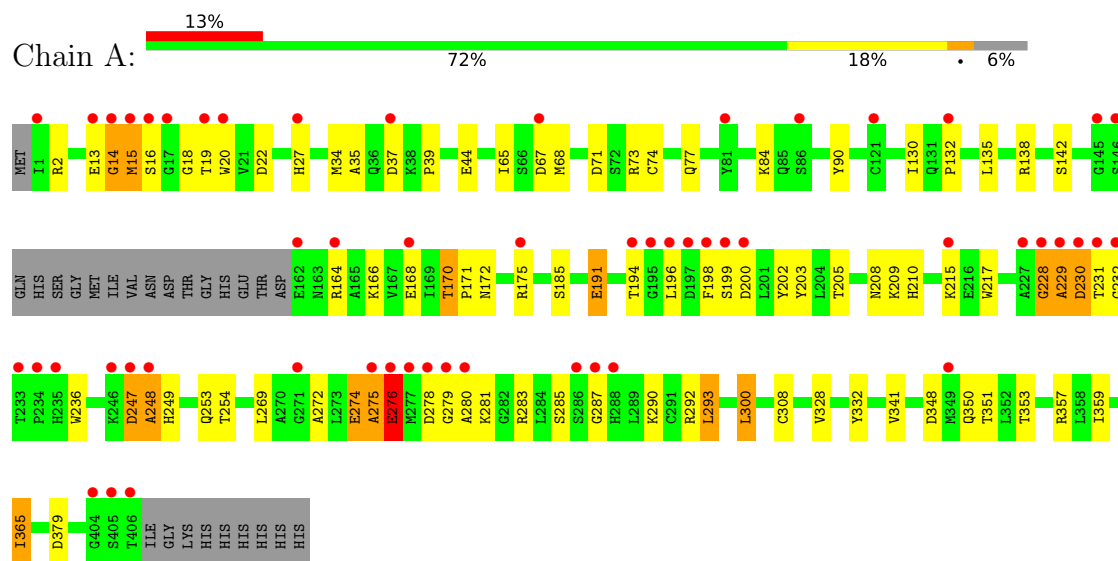
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	128	Total	O	0	0
			128	128		
2	B	145	Total	O	0	0
			145	145		

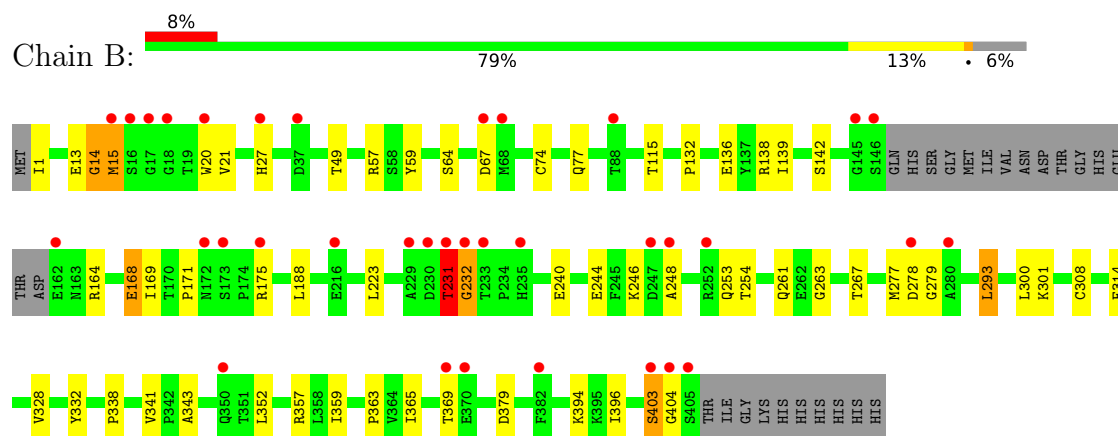
3 Residue-property plots

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 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: Envelope protein



• Molecule 1: Envelope protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.45Å 59.06Å 103.67Å 90.00° 103.72° 90.00°	Depositor
Resolution (Å)	33.98 – 2.00 33.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (33.98-2.00) 86.1 (33.98-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.208 , 0.237 0.213 , 0.240	Depositor DCC
R_{free} test set	2901 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6236	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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 [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	0.42	0/3050	0.86	6/4130 (0.1%)
1	B	0.42	0/3037	0.80	1/4112 (0.0%)
All	All	0.42	0/6087	0.83	7/8242 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	GLY	N-CA-C	-11.93	99.87	112.04
1	A	228	GLY	CA-C-N	7.22	134.70	121.70
1	A	228	GLY	C-N-CA	7.22	134.70	121.70
1	B	231	THR	N-CA-C	-6.03	97.95	110.80
1	A	228	GLY	CA-C-O	-5.51	115.80	120.98
1	A	274	GLU	CA-C-N	5.45	131.50	121.70
1	A	274	GLU	C-N-CA	5.45	131.50	121.70

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	2988	0	2926	55	0
1	B	2975	0	2915	36	0
2	A	128	0	0	4	0
2	B	145	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6236	0	5841	90	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 8.

All (90) 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:B:27:HIS:ND1	2:B:502:HOH:O	1.99	0.92
1:A:67:ASP:OD2	1:A:90:TYR:OH	1.93	0.85
1:A:274:GLU:HB3	1:A:275:ALA:HB2	1.58	0.83
1:B:64:SER:OG	2:B:501:HOH:O	1.96	0.82
1:A:37:ASP:OD2	2:A:501:HOH:O	1.97	0.81
1:B:244:GLU:OE2	1:B:246:LYS:HE2	1.85	0.76
1:A:253:GLN:OE1	2:A:502:HOH:O	2.03	0.76
1:B:277:MET:SD	2:B:595:HOH:O	2.45	0.75
1:A:74:CYS:HB2	1:A:77:GLN:HG3	1.73	0.70
1:A:205:THR:HG23	2:A:544:HOH:O	1.92	0.69
1:A:228:GLY:HA2	1:A:229:ALA:CB	2.24	0.68
1:B:246:LYS:O	2:B:505:HOH:O	2.14	0.66
1:A:276:GLU:OE2	1:A:285:SER:HB3	1.97	0.64
1:A:170:THR:HG22	1:A:172:ASN:H	1.64	0.62
1:A:2:ARG:NE	1:A:44:GLU:OE2	2.23	0.62
1:A:194:THR:HG21	1:A:290:LYS:H	1.66	0.60
1:B:254:THR:N	2:B:505:HOH:O	2.16	0.60
1:B:343:ALA:O	2:B:506:HOH:O	2.16	0.60
1:A:138:ARG:NH2	1:A:168:GLU:OE2	2.35	0.59
1:A:14:GLY:N	1:A:34:MET:O	2.31	0.58
1:B:14:GLY:O	1:B:15:MET:HB2	2.01	0.58
1:A:166:LYS:NZ	2:A:504:HOH:O	2.37	0.57
1:A:228:GLY:HA2	1:A:229:ALA:HB3	1.86	0.56
1:B:308:CYS:HB3	1:B:332:TYR:CZ	2.40	0.56
1:A:135:LEU:HD13	1:A:198:PHE:HZ	1.71	0.56
1:A:274:GLU:HB3	1:A:275:ALA:CB	2.34	0.55
1:B:359:ILE:HD11	1:B:379:ASP:HB2	1.88	0.55
1:A:198:PHE:O	1:A:200:ASP:N	2.31	0.55
1:A:13:GLU:OE2	1:A:357:ARG:NH1	2.40	0.54
1:A:65:ILE:HG13	1:A:68:MET:HE2	1.90	0.54
1:A:22:ASP:OD1	1:A:292:ARG:NH1	2.41	0.54
1:A:13:GLU:CD	1:A:357:ARG:HH12	2.17	0.53
1:A:348:ASP:OD2	1:A:351:THR:HG22	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ILE:HD12	1:B:169:ILE:HD12	1.90	0.52
1:A:194:THR:CG2	1:A:290:LYS:H	2.22	0.52
1:A:274:GLU:OE2	1:B:246:LYS:HE3	2.10	0.51
1:B:74:CYS:HB2	1:B:77:GLN:HG3	1.93	0.51
1:B:403:SER:OG	1:B:404:GLY:N	2.44	0.50
1:A:142:SER:HB3	1:A:164:ARG:HG2	1.92	0.50
1:A:247:ASP:OD2	1:A:249:HIS:CE1	2.65	0.50
1:A:274:GLU:CB	1:A:275:ALA:HB2	2.37	0.50
1:B:301:LYS:HB2	2:B:518:HOH:O	2.13	0.49
1:A:308:CYS:HB3	1:A:332:TYR:CZ	2.47	0.49
1:B:20:TRP:HA	1:B:293:LEU:O	2.13	0.48
1:B:263:GLY:O	1:B:267:THR:HG23	2.13	0.48
1:B:142:SER:HB3	1:B:164:ARG:HG2	1.95	0.48
1:B:341:VAL:HB	1:B:363:PRO:HG2	1.95	0.48
1:B:138:ARG:HH12	1:B:168:GLU:CD	2.21	0.47
1:A:229:ALA:HA	1:A:230:ASP:HB3	1.95	0.47
1:A:279:GLY:C	1:A:281:LYS:H	2.21	0.47
1:B:338:PRO:HA	1:B:365:ILE:O	2.13	0.47
1:A:27:HIS:HD2	1:A:287:GLY:HA3	1.79	0.46
1:B:138:ARG:NH1	1:B:168:GLU:OE2	2.48	0.45
1:A:130:ILE:HD11	1:A:203:TYR:HB2	1.98	0.45
1:A:228:GLY:HA2	1:A:229:ALA:HB2	1.98	0.45
1:A:15:MET:HG3	1:A:18:GLY:HA3	1.98	0.45
1:B:115:THR:OG1	1:B:253:GLN:HB2	2.16	0.45
1:A:217:TRP:CH2	1:A:269:LEU:HD21	2.51	0.45
1:B:223:LEU:HD21	1:B:261:GLN:HG3	1.99	0.44
1:B:164:ARG:HG2	1:B:164:ARG:HH11	1.83	0.44
1:A:71:ASP:OD2	1:A:73:ARG:NH1	2.51	0.44
1:A:247:ASP:O	1:A:248:ALA:CB	2.66	0.43
1:B:175:ARG:HA	1:B:188:LEU:O	2.17	0.43
1:A:359:ILE:HD11	1:A:379:ASP:HB2	2.01	0.43
1:B:231:THR:O	1:B:232:GLY:C	2.62	0.43
1:B:14:GLY:HA2	1:B:21:VAL:CG1	2.48	0.43
1:B:136:GLU:OE2	1:B:168:GLU:HG2	2.18	0.43
1:A:247:ASP:CG	1:A:248:ALA:N	2.76	0.43
1:A:341:VAL:HG22	1:A:365:ILE:HD12	1.99	0.43
1:A:132:PRO:O	1:A:171:PRO:HG2	2.19	0.42
1:A:351:THR:HG23	1:A:353:THR:HG23	2.01	0.42
1:B:57:ARG:NH1	1:B:59:TYR:OH	2.52	0.42
1:B:14:GLY:HA2	1:B:21:VAL:HG11	2.00	0.42
1:A:175:ARG:HA	1:A:175:ARG:HD2	1.61	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:HA3	1:A:35:ALA:HB2	2.01	0.42
1:A:194:THR:HG21	1:A:290:LYS:HB2	2.02	0.42
1:A:20:TRP:HA	1:A:293:LEU:O	2.20	0.41
1:B:13:GLU:HG2	1:B:357:ARG:HH12	1.85	0.41
1:B:314:PHE:CZ	1:B:396:ILE:HG21	2.55	0.41
1:A:202:TYR:CE1	1:A:215:LYS:HE2	2.55	0.41
1:A:205:THR:HG22	1:A:210:HIS:ND1	2.36	0.41
1:A:276:GLU:HG3	1:A:283:ARG:O	2.19	0.41
1:A:278:ASP:HA	1:A:279:GLY:HA2	1.70	0.41
1:B:132:PRO:O	1:B:171:PRO:HG2	2.20	0.41
1:B:1:ILE:HD13	1:B:1:ILE:HG21	1.88	0.41
1:A:39:PRO:HD3	1:A:300:LEU:HD13	2.03	0.40
1:A:196:LEU:HD23	1:A:198:PHE:HE1	1.86	0.40
1:A:191:GLU:O	1:A:194:THR:HG22	2.22	0.40
1:A:210:HIS:O	1:A:275:ALA:HA	2.21	0.40
1:B:278:ASP:HA	1:B:279:GLY:HA2	1.81	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	388/416 (93%)	366 (94%)	8 (2%)	14 (4%)	2	1
1	B	386/416 (93%)	366 (95%)	13 (3%)	7 (2%)	6	3
All	All	774/832 (93%)	732 (95%)	21 (3%)	21 (3%)	4	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	229	ALA
1	A	231	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	ALA
1	A	272	ALA
1	A	276	GLU
1	B	15	MET
1	B	231	THR
1	A	14	GLY
1	A	15	MET
1	A	16	SER
1	A	275	ALA
1	B	14	GLY
1	B	232	GLY
1	A	199	SER
1	A	230	ASP
1	A	247	ASP
1	B	67	ASP
1	B	403	SER
1	A	236	TRP
1	A	280	ALA
1	B	248	ALA

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	327/348 (94%)	312 (95%)	15 (5%)	24	22
1	B	325/348 (93%)	316 (97%)	9 (3%)	38	41
All	All	652/696 (94%)	628 (96%)	24 (4%)	32	30

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	84	LYS
1	A	170	THR
1	A	185[A]	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	185[B]	SER
1	A	191	GLU
1	A	208	ASN
1	A	209	LYS
1	A	254	THR
1	A	276	GLU
1	A	293	LEU
1	A	300	LEU
1	A	328	VAL
1	A	350	GLN
1	A	365	ILE
1	B	49	THR
1	B	168	GLU
1	B	240	GLU
1	B	293	LEU
1	B	300	LEU
1	B	328	VAL
1	B	352	LEU
1	B	369	THR
1	B	394	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	134	ASN
1	A	172	ASN
1	A	261	GLN
1	A	350	GLN
1	B	77	GLN
1	B	134	ASN
1	B	399	HIS

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 [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	391/416 (93%)	0.79	55 (14%) 6 5	16, 37, 74, 124	1 (0%)
1	B	390/416 (93%)	0.56	35 (8%) 15 14	19, 31, 67, 133	0
All	All	781/832 (93%)	0.67	90 (11%) 9 8	16, 34, 70, 133	1 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	229	ALA	6.4
1	A	196	LEU	5.1
1	A	198	PHE	5.1
1	B	405	SER	4.9
1	B	231	THR	4.7
1	A	15	MET	4.5
1	A	279	GLY	4.5
1	B	278	ASP	4.4
1	A	235	HIS	4.4
1	A	229	ALA	4.4
1	B	404	GLY	4.3
1	A	16	SER	4.3
1	A	247	ASP	4.2
1	B	230	ASP	4.2
1	A	14	GLY	4.1
1	B	247	ASP	4.1
1	B	20	TRP	3.7
1	A	194	THR	3.7
1	A	231	THR	3.7
1	A	17	GLY	3.7
1	A	248	ALA	3.7
1	A	228	GLY	3.6
1	A	287	GLY	3.6
1	A	278	ASP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	406	THR	3.5
1	B	370	GLU	3.4
1	B	15	MET	3.4
1	A	280	ALA	3.4
1	A	276	GLU	3.3
1	B	146	SER	3.2
1	A	1	ILE	3.2
1	A	162	GLU	3.0
1	A	288	HIS	3.0
1	B	280	ALA	3.0
1	B	162	GLU	2.9
1	B	172	ASN	2.9
1	A	246	LYS	2.7
1	B	233	THR	2.7
1	A	200	ASP	2.7
1	B	68	MET	2.7
1	A	199	SER	2.7
1	A	145	GLY	2.7
1	B	235	HIS	2.7
1	B	67	ASP	2.7
1	B	248	ALA	2.6
1	B	369	THR	2.6
1	A	230	ASP	2.6
1	B	403	SER	2.6
1	A	121	CYS	2.6
1	A	197	ASP	2.5
1	B	382	PHE	2.5
1	A	175	ARG	2.5
1	B	350	GLN	2.4
1	A	405	SER	2.4
1	B	173	SER	2.4
1	A	13	GLU	2.4
1	A	146	SER	2.4
1	B	232	GLY	2.4
1	B	16	SER	2.4
1	B	27	HIS	2.4
1	A	227	ALA	2.4
1	B	18	GLY	2.4
1	A	67	ASP	2.4
1	A	164	ARG	2.4
1	A	86	SER	2.4
1	B	175	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	37	ASP	2.3
1	B	145	GLY	2.3
1	B	17	GLY	2.2
1	A	19	THR	2.2
1	A	234	PRO	2.2
1	B	252	ARG	2.2
1	A	215	LYS	2.2
1	A	275	ALA	2.2
1	A	27	HIS	2.2
1	A	277	MET	2.2
1	A	349	MET	2.2
1	B	37	ASP	2.2
1	A	404	GLY	2.1
1	A	168	GLU	2.1
1	A	132	PRO	2.1
1	A	20	TRP	2.1
1	A	195	GLY	2.1
1	B	216	GLU	2.1
1	A	81	TYR	2.1
1	B	88	THR	2.1
1	A	232	GLY	2.1
1	A	271	GLY	2.1
1	A	233	THR	2.0
1	A	286	SER	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.