



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:21 AM UTC

PDB ID : 4KVC / pdb_00004kvc
Title : 2H2 Fab fragment of immature Dengue virus
Authors : Wang, Z.; Rossmann, M.G.
Deposited on : 2013-05-22
Resolution : 2.31 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

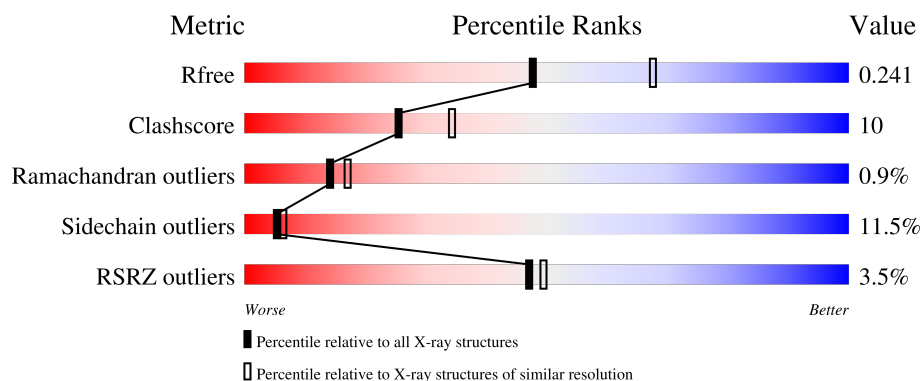
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	H	220	4% 75% 17% 6%
2	L	212	3% 72% 22% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6647 atoms, of which 3186 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 Ig heavy chain V region MOPC 21, Igh protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	220	Total	C	H	N	O	S	0	0	0
			3270	1048	1609	278	326	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	104	HIS	-	linker	UNP Q6PIP8
H	105	TYR	-	linker	UNP Q6PIP8
H	136	ASP	GLY	conflict	UNP Q6PIP8
H	137	GLY	ASP	conflict	UNP Q6PIP8

- Molecule 2 is a protein called Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	212	Total	C	H	N	O	S	0	0	0
			3221	1024	1577	275	337	8			

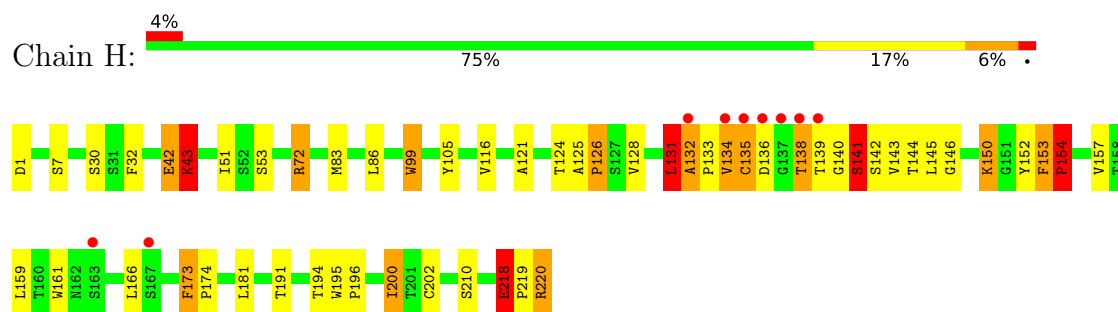
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	76	Total	O	0	0
			76	76		
3	L	80	Total	O	0	0
			80	80		

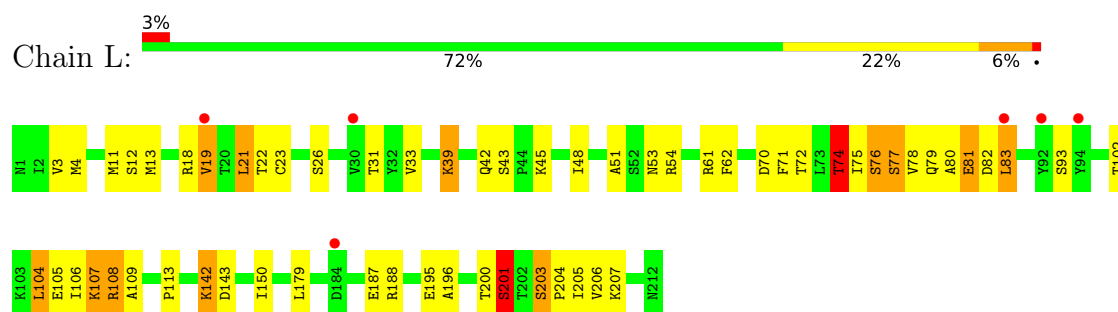
3 Residue-property plots [i](#)

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: Ig heavy chain V region MOPC 21, Igh protein



- Molecule 2: Ig kappa chain V-V region MOPC 21, Anti-colorectal carcinoma light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.55Å 81.71Å 85.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 2.31 44.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.00-2.31) 99.6 (44.00-2.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.179 , 0.234 0.196 , 0.241	Depositor DCC
R_{free} test set	832 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 40.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6647	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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	H	0.89	11/1707 (0.6%)	1.04	10/2331 (0.4%)
2	L	1.09	12/1681 (0.7%)	1.01	7/2283 (0.3%)
All	All	1.00	23/3388 (0.7%)	1.02	17/4614 (0.4%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	128	VAL	C-O	-9.07	1.14	1.24
1	H	131	LEU	C-O	-7.33	1.15	1.23
2	L	104	LEU	C-O	-6.79	1.15	1.24
2	L	201	SER	CA-C	-6.60	1.44	1.52
2	L	201	SER	C-O	-6.46	1.16	1.23
1	H	126	PRO	C-O	-6.28	1.15	1.23
1	H	144	THR	C-O	-6.02	1.16	1.24
1	H	125	ALA	C-N	5.98	1.40	1.33
1	H	124	THR	C-O	-5.96	1.17	1.24
2	L	76	SER	C-O	-5.84	1.17	1.24
2	L	72	THR	C-O	-5.83	1.16	1.23
2	L	107	LYS	C-O	-5.83	1.17	1.24
1	H	141	SER	C-O	-5.81	1.16	1.24
2	L	51	ALA	C-O	-5.76	1.16	1.24
2	L	200	THR	C-O	-5.61	1.16	1.24
2	L	82	ASP	C-O	-5.42	1.16	1.24
2	L	53	ASN	C-O	-5.24	1.17	1.24
1	H	150	LYS	C-O	-5.21	1.17	1.24
2	L	62	PHE	C-O	-5.11	1.17	1.24
1	H	154	PRO	N-CD	5.08	1.54	1.47
1	H	218	GLU	C-O	-5.07	1.17	1.24
2	L	204	PRO	C-O	-5.05	1.17	1.23
1	H	153	PHE	C-O	-5.02	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	153	PHE	C-N-CD	8.58	139.49	120.60
1	H	131	LEU	CA-C-N	7.66	135.48	121.70
1	H	131	LEU	C-N-CA	7.66	135.48	121.70
1	H	125	ALA	CA-C-N	-6.74	113.84	120.52
1	H	125	ALA	C-N-CA	-6.74	113.84	120.52
1	H	150	LYS	N-CA-C	6.67	120.28	109.40
2	L	203	SER	CA-C-N	-6.28	113.31	119.78
2	L	203	SER	C-N-CA	-6.28	113.31	119.78
2	L	42	GLN	N-CA-C	6.26	119.73	110.46
1	H	173	PHE	CA-C-N	6.08	126.10	119.90
1	H	173	PHE	C-N-CA	6.08	126.10	119.90
2	L	39	LYS	CA-C-N	5.84	127.14	119.84
2	L	39	LYS	C-N-CA	5.84	127.14	119.84
2	L	74	THR	CB-CA-C	5.32	118.95	109.65
2	L	200	THR	N-CA-C	5.07	118.56	112.38
1	H	131	LEU	O-C-N	-5.05	115.31	122.99
1	H	143	VAL	N-CA-C	5.01	115.70	108.48

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	H	1661	1609	1604	36	3
2	L	1644	1577	1574	26	4
3	H	76	0	0	2	0
3	L	80	0	0	1	0
All	All	3461	3186	3178	62	5

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 10.

All (62) 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:H:218:GLU:N	1:H:218:GLU:OE1	1.97	0.97
1:H:134:VAL:HG12	1:H:135:CYS:H	1.28	0.96
1:H:131:LEU:HA	1:H:132:ALA:HB3	1.53	0.91
1:H:138:THR:O	1:H:139:THR:OG1	1.94	0.85
1:H:219:PRO:O	1:H:220:ARG:HB2	1.76	0.83
1:H:131:LEU:HA	1:H:132:ALA:CB	2.16	0.76
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.69	0.75
1:H:134:VAL:CG1	1:H:135:CYS:H	2.02	0.71
1:H:126:PRO:HB3	1:H:152:TYR:HB3	1.73	0.71
1:H:131:LEU:O	1:H:146:GLY:N	2.24	0.70
2:L:201:SER:HB2	2:L:203:SER:O	2.03	0.57
1:H:134:VAL:HG12	1:H:135:CYS:N	2.11	0.57
1:H:135:CYS:O	1:H:220:ARG:HA	2.05	0.56
2:L:19:VAL:HG23	2:L:75:ILE:O	2.07	0.55
1:H:138:THR:C	1:H:139:THR:HG23	2.31	0.55
2:L:80:ALA:HA	2:L:106:ILE:HD11	1.88	0.54
1:H:132:ALA:CB	3:H:313:HOH:O	2.54	0.54
1:H:133:PRO:HD3	1:H:145:LEU:HD23	1.90	0.54
2:L:83:LEU:HD13	2:L:104:LEU:O	2.09	0.53
2:L:196:ALA:HB3	2:L:205:ILE:CG2	2.39	0.52
1:H:83:MET:HE1	1:H:116:VAL:HG21	1.90	0.52
2:L:206:VAL:HG12	2:L:207:LYS:N	2.25	0.52
1:H:140:GLY:O	1:H:141:SER:HB3	2.10	0.52
2:L:19:VAL:HG11	2:L:104:LEU:CD1	2.40	0.51
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.91	0.51
2:L:74:THR:HB	3:L:313:HOH:O	2.11	0.50
1:H:30:SER:O	1:H:53:SER:HB2	2.12	0.50
1:H:195:TRP:CD1	1:H:196:PRO:HA	2.47	0.49
2:L:83:LEU:HD21	2:L:106:ILE:HG13	1.93	0.49
1:H:42:GLU:HA	1:H:43:LYS:HG2	1.94	0.49
1:H:131:LEU:CA	1:H:132:ALA:CB	2.84	0.48
1:H:99:TRP:CZ2	1:H:105:TYR:HB3	2.49	0.47
1:H:210:SER:O	1:H:210:SER:OG	2.29	0.47
1:H:32:PHE:O	1:H:72:ARG:NH2	2.39	0.47
1:H:132:ALA:HB2	3:H:313:HOH:O	2.14	0.47
1:H:121:ALA:HB3	1:H:153:PHE:CE2	2.50	0.47
2:L:83:LEU:CD2	2:L:106:ILE:HG13	2.45	0.46
2:L:142:LYS:HD3	2:L:142:LYS:H	1.80	0.46
1:H:42:GLU:HA	1:H:43:LYS:CB	2.45	0.46
2:L:113:PRO:HG2	2:L:205:ILE:HD13	1.96	0.45
2:L:108:ARG:HD3	2:L:109:ALA:O	2.16	0.45
1:H:218:GLU:N	1:H:218:GLU:CD	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:140:GLY:O	1:H:142:SER:N	2.46	0.45
1:H:195:TRP:CD1	1:H:200:ILE:HD12	2.52	0.45
2:L:21:LEU:HD21	2:L:102:THR:OG1	2.17	0.44
1:H:219:PRO:O	1:H:220:ARG:CB	2.56	0.44
2:L:4:MET:HE3	2:L:23:CYS:SG	2.57	0.44
1:H:161:TRP:CZ3	1:H:202:CYS:HB3	2.52	0.44
2:L:206:VAL:CG1	2:L:207:LYS:N	2.81	0.43
2:L:19:VAL:HG11	2:L:104:LEU:HD13	2.00	0.43
1:H:153:PHE:HA	1:H:154:PRO:HA	1.75	0.43
1:H:135:CYS:O	1:H:220:ARG:CA	2.66	0.43
1:H:173:PHE:HA	1:H:174:PRO:HD3	1.88	0.43
1:H:195:TRP:HD1	1:H:200:ILE:HD12	1.83	0.42
1:H:51:ILE:HD13	1:H:72:ARG:HG2	2.02	0.42
2:L:71:PHE:CD2	2:L:71:PHE:N	2.87	0.42
2:L:142:LYS:HE3	2:L:143:ASP:CG	2.45	0.41
2:L:3:VAL:HB	2:L:26:SER:HB3	2.02	0.41
2:L:12:SER:HA	2:L:105:GLU:HG2	2.03	0.41
2:L:13:MET:HG2	2:L:19:VAL:HG22	2.02	0.41
2:L:188:ARG:HD3	2:L:188:ARG:HA	1.76	0.40
2:L:76:SER:HA	2:L:77:SER:HA	1.87	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:7:SER:HG	1:H:194:THR:HG1[2_555]	1.01	0.59
2:L:61:ARG:HE	2:L:79:GLN:HE22[2_555]	1.10	0.50
2:L:81:GLU:HG2	2:L:81:GLU:HG2[2_555]	1.16	0.44
1:H:1:ASP:OD1	2:L:108:ARG:HH22[2_555]	1.46	0.14
1:H:1:ASP:OD1	2:L:108:ARG:NH2[2_555]	2.08	0.12

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	H	218/220 (99%)	207 (95%)	7 (3%)	4 (2%)	6	6
2	L	210/212 (99%)	202 (96%)	8 (4%)	0	100	100
All	All	428/432 (99%)	409 (96%)	15 (4%)	4 (1%)	14	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	134	VAL
1	H	132	ALA
1	H	136	ASP
1	H	43	LYS

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	H	187/187 (100%)	168 (90%)	19 (10%)	7	8
2	L	188/188 (100%)	164 (87%)	24 (13%)	4	4
All	All	375/375 (100%)	332 (88%)	43 (12%)	5	6

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	42	GLU
1	H	43	LYS
1	H	72	ARG
1	H	86	LEU
1	H	99	TRP
1	H	131	LEU
1	H	135	CYS
1	H	138	THR
1	H	141	SER
1	H	150	LYS

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Mol	Chain	Res	Type
1	H	154	PRO
1	H	157	VAL
1	H	159	LEU
1	H	166	LEU
1	H	181	LEU
1	H	191	THR
1	H	200	ILE
1	H	218	GLU
1	H	220	ARG
2	L	11	MET
2	L	18	ARG
2	L	19	VAL
2	L	21	LEU
2	L	22	THR
2	L	31	THR
2	L	33	VAL
2	L	39	LYS
2	L	43	SER
2	L	45	LYS
2	L	48	ILE
2	L	54	ARG
2	L	70	ASP
2	L	74	THR
2	L	77	SER
2	L	78	VAL
2	L	81	GLU
2	L	83	LEU
2	L	93	SER
2	L	107	LYS
2	L	108	ARG
2	L	142	LYS
2	L	187	GLU
2	L	201	SER

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

Mol	Chain	Res	Type
1	H	82	GLN
1	H	171	HIS
2	L	137	ASN
2	L	145	ASN
2	L	210	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	H	220/220 (100%)	0.09	9 (4%) 41 43	9, 20, 41, 58	0
2	L	212/212 (100%)	-0.00	6 (2%) 55 57	10, 21, 35, 48	1 (0%)
All	All	432/432 (100%)	0.05	15 (3%) 47 49	9, 21, 37, 58	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	134	VAL	5.6
1	H	136	ASP	5.3
1	H	138	THR	4.4
2	L	30	VAL	4.3
1	H	135	CYS	4.3
1	H	139	THR	4.2
2	L	94	TYR	3.9
1	H	137	GLY	3.8
1	H	167	SER	2.7
1	H	132	ALA	2.7
1	H	163	SER	2.6
2	L	184	ASP	2.4
2	L	83	LEU	2.2
2	L	19	VAL	2.2
2	L	92	TYR	2.1

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.