Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 01:37 PM EDT

PDB ID	:	6RNN
Title	:	P46, an immunodominant surface protein from Mycoplasma hyopneumoniae
Authors	:	Guasch, A.; Gonzalez-Gonzalez, L.; Fita, I.
Deposited on	:	2019-05-09
Resolution	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

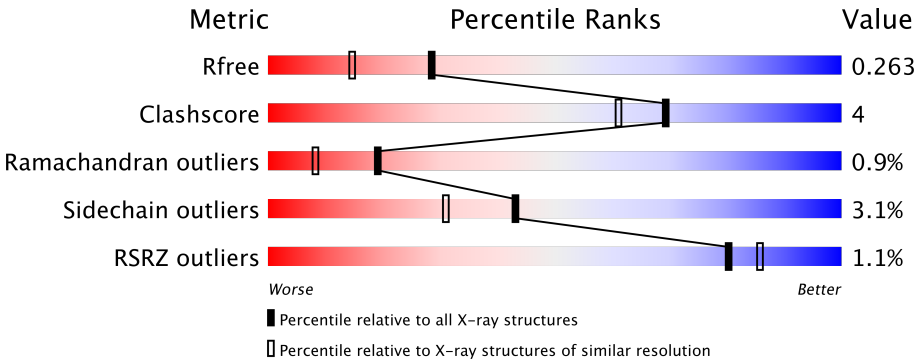
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.10.1
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.10.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

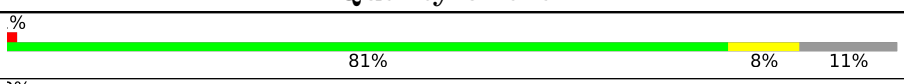
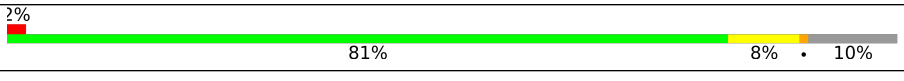
The reported resolution of this entry is 1.95 Å.

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}	111664	2220 (1.96-1.96)
Clashscore	122126	2333 (1.96-1.96)
Ramachandran outliers	120053	2314 (1.96-1.96)
Sidechain outliers	120020	2314 (1.96-1.96)
RSRZ outliers	108989	2174 (1.96-1.96)

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 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 <=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	C	238	
1	L	238	
2	D	474	
2	H	474	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7125 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 Immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	1	0
			1677	1049	283	338	7			
1	C	211	Total	C	N	O	S	0	0	0
			1643	1028	276	333	6			

- Molecule 2 is a protein called Immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	204	Total	C	N	O	S	0	2	0
			1578	1006	255	308	9			
2	H	205	Total	C	N	O	S	0	1	0
			1580	1007	255	310	8			

- Molecule 3 is water.

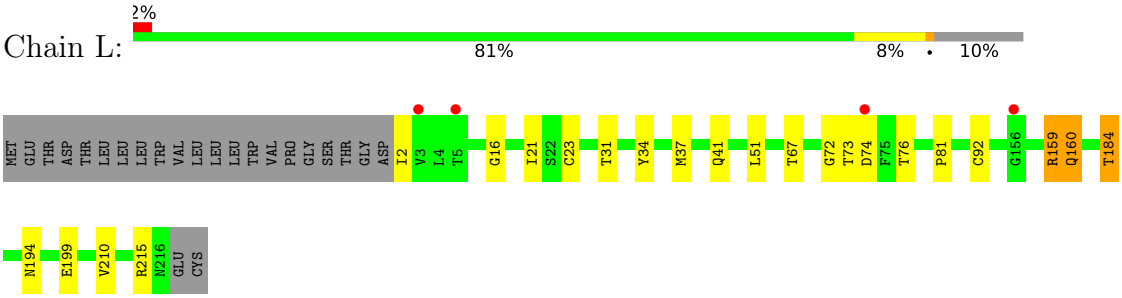
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	140	Total	O	0	0
			140	140		
3	D	166	Total	O	0	0
			166	166		
3	C	181	Total	O	0	0
			181	181		
3	H	160	Total	O	0	0
			160	160		

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 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.

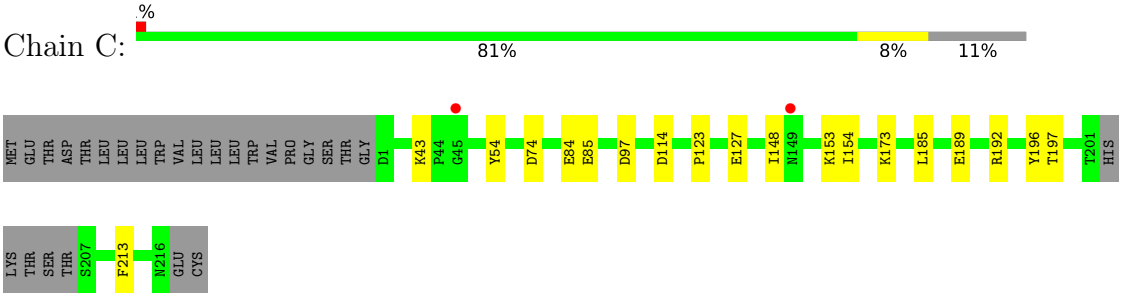
• Molecule 1: Immunoglobulin light chain

Chain L:



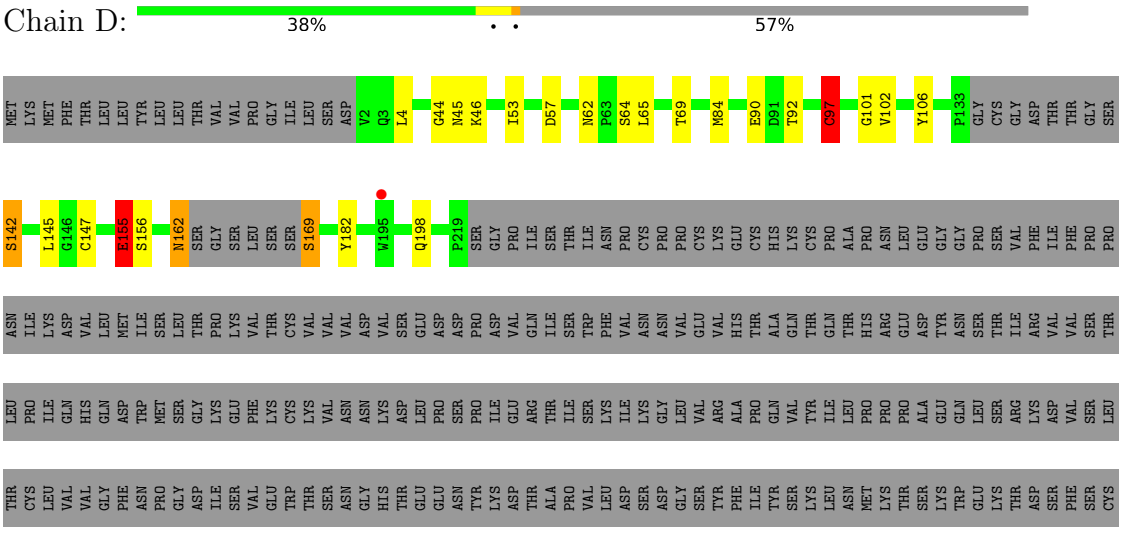
• Molecule 1: Immunoglobulin light chain

Chain C:



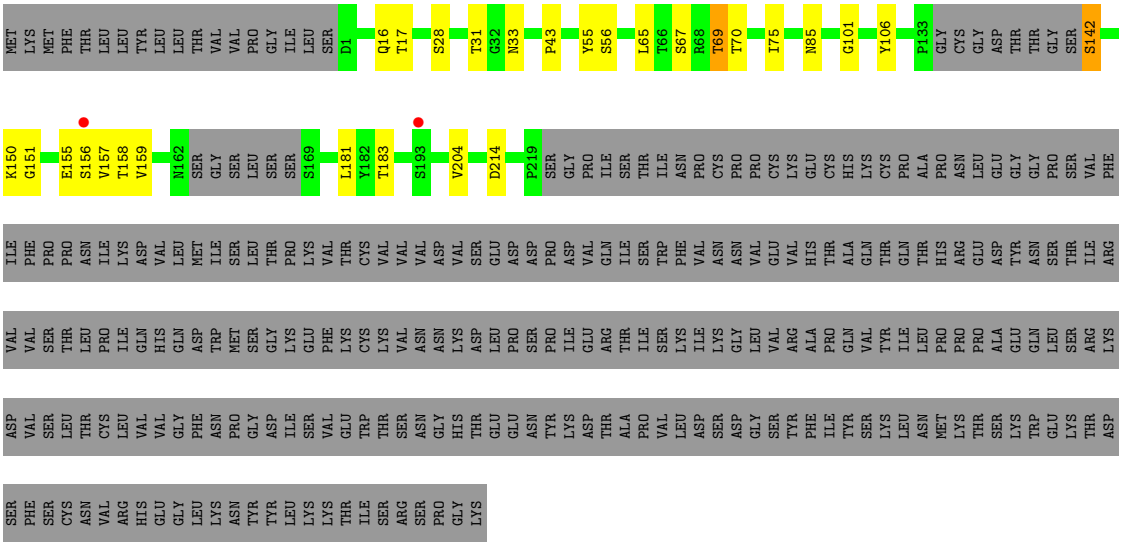
• Molecule 2: Immunoglobulin heavy chain

Chain D:



• Molecule 2: Immunoglobulin heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.21Å 88.38Å 123.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.00 – 1.95 60.97 – 1.73	Depositor EDS
% Data completeness (in resolution range)	98.3 (61.00-1.95) 97.7 (60.97-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 1.73Å)	Xtriage
Refinement program	PHENIX (dev_2880: ???)	Depositor
R, R_{free}	0.207 , 0.261 0.213 , 0.263	Depositor DCC
R_{free} test set	4667 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7125	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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, 0.333 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	C	0.41	0/1684	0.59	1/2295 (0.0%)
1	L	0.38	0/1723	0.56	0/2349
2	D	0.40	0/1624	0.65	4/2230 (0.2%)
2	H	0.36	0/1626	0.59	0/2233
All	All	0.39	0/6657	0.60	5/9107 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	H	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	147[A]	CYS	CA-CB-SG	5.44	123.79	114.00
2	D	147[B]	CYS	CA-CB-SG	5.44	123.79	114.00
2	D	97[A]	CYS	CA-CB-SG	5.20	123.36	114.00
2	D	97[B]	CYS	CA-CB-SG	5.20	123.36	114.00
1	C	97	ASP	CB-CG-OD1	5.10	122.89	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	155	GLU	Peptide
2	H	31	THR	Peptide

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	C	1643	0	1563	12	0
1	L	1677	0	1600	11	0
2	D	1578	0	1539	15	0
2	H	1580	0	1543	15	0
3	C	181	0	0	4	0
3	D	166	0	0	5	0
3	H	160	0	0	3	0
3	L	140	0	0	3	0
All	All	7125	0	6245	51	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 4.

All (51) 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:D:69:THR:HG22	2:D:84:MET:HG3	1.69	0.74
1:C:114:ASP:O	3:C:302:HOH:O	2.09	0.69
2:D:169:SER:OG	3:D:505:HOH:O	2.13	0.66
1:L:37:MET:HE3	1:L:92:CYS:HB2	1.79	0.65
1:L:2:ILE:N	3:L:305:HOH:O	2.31	0.63
1:C:84:GLU:CD	1:C:84:GLU:H	2.01	0.62
1:C:127:GLU:OE2	1:C:127:GLU:N	2.30	0.61
1:C:154:ILE:HD12	1:C:196:TYR:CD2	2.36	0.60
2:H:43:PRO:O	3:H:528:HOH:O	2.17	0.60
2:H:101:GLY:HA3	2:H:106:TYR:CE2	2.38	0.59
2:D:162:ASN:O	3:D:514:HOH:O	2.17	0.59
2:H:142:SER:N	3:H:510:HOH:O	2.35	0.58
1:C:185:LEU:HB3	1:C:189:GLU:HG3	1.86	0.57
1:L:21:ILE:HG23	3:L:307:HOH:O	2.05	0.55
1:L:159:ARG:HG3	1:L:160:GLN:N	2.22	0.55
1:C:43:LYS:NZ	1:C:85:GLU:O	2.29	0.55
2:H:158:THR:OG1	3:H:503:HOH:O	2.10	0.54
2:D:64:SER:OG	2:D:65:LEU:HD12	2.07	0.54
2:H:65:LEU:O	2:H:69:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:THR:HG22	2:H:85:ASN:HB3	1.91	0.53
2:D:65:LEU:HD23	2:D:84:MET:HE3	1.91	0.52
2:D:4:LEU:HD23	2:D:97[A]:CYS:SG	2.50	0.52
2:D:92:THR:HG21	2:H:75:ILE:HD11	1.92	0.51
1:L:16:GLY:HA2	1:L:81:PRO:HB2	1.93	0.51
2:D:101:GLY:HA3	2:D:106:TYR:CE2	2.46	0.50
2:H:33:ASN:HA	2:H:55:TYR:CD1	2.47	0.50
2:D:90:GLU:HB3	3:D:593:HOH:O	2.13	0.49
1:C:54:TYR:OH	3:C:306:HOH:O	2.16	0.48
1:L:184:THR:OG1	3:L:302:HOH:O	2.20	0.48
2:H:151:GLY:HA2	2:H:181:LEU:HB3	1.96	0.47
1:L:23:CYS:SG	1:L:37:MET:HE2	2.55	0.47
1:C:74:ASP:OD1	3:C:305:HOH:O	2.21	0.46
1:L:41:GLN:HB2	1:L:51:LEU:HD11	1.96	0.46
2:D:44:GLY:O	2:D:45:ASN:HB2	2.16	0.45
1:L:37:MET:CE	1:L:92:CYS:HB2	2.45	0.45
1:L:199:GLU:HG3	1:L:210:VAL:HG22	1.98	0.45
3:D:558:HOH:O	2:H:28:SER:HB2	2.17	0.44
2:D:142:SER:N	3:D:509:HOH:O	2.51	0.44
2:H:65:LEU:HB3	2:H:69:THR:HG21	2.01	0.42
2:H:159:VAL:HG22	2:H:204:VAL:HG22	2.00	0.42
2:D:53:ILE:HD11	2:D:57:ASP:OD1	2.19	0.42
2:D:62:ASN:HB3	2:D:65:LEU:HD13	2.01	0.42
2:H:65:LEU:HB3	2:H:69:THR:CG2	2.49	0.42
1:C:123:PRO:HB3	1:C:213:PHE:CE1	2.55	0.42
1:C:153:LYS:HB3	1:C:197:THR:HB	2.02	0.41
1:C:173:LYS:HD3	1:C:173:LYS:HA	1.85	0.41
1:C:192:ARG:NH2	3:C:432:HOH:O	2.53	0.41
2:D:46:LYS:HG3	2:H:56:SER:HB2	2.01	0.41
1:L:31:THR:HG22	1:L:34:TYR:O	2.21	0.41
2:D:155:GLU:HG3	2:D:182:TYR:CZ	2.56	0.41
2:H:150:LYS:HG3	2:H:183:THR:OG1	2.21	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	C	207/238 (87%)	200 (97%)	6 (3%)	1 (0%)	31 18
1	L	214/238 (90%)	204 (95%)	8 (4%)	2 (1%)	19 8
2	D	200/474 (42%)	193 (96%)	5 (2%)	2 (1%)	17 7
2	H	200/474 (42%)	193 (96%)	5 (2%)	2 (1%)	17 7
All	All	821/1424 (58%)	790 (96%)	24 (3%)	7 (1%)	19 8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	156	SER
2	H	156	SER
1	L	215	ARG
1	L	72	GLY
2	D	155	GLU
2	H	16	GLN
1	C	148	ILE

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	C	187/212 (88%)	187 (100%)	0	100 100
1	L	192/212 (91%)	184 (96%)	8 (4%)	32 18
2	D	184/431 (43%)	175 (95%)	9 (5%)	27 13
2	H	184/431 (43%)	177 (96%)	7 (4%)	36 23
All	All	747/1286 (58%)	723 (97%)	24 (3%)	43 30

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

Mol	Chain	Res	Type
1	L	67	THR
1	L	73	THR
1	L	74	ASP
1	L	76	THR
1	L	159	ARG
1	L	160	GLN
1	L	184	THR
1	L	194	ASN
2	D	97[A]	CYS
2	D	97[B]	CYS
2	D	102	VAL
2	D	142	SER
2	D	145	LEU
2	D	155	GLU
2	D	162	ASN
2	D	169	SER
2	D	198	GLN
2	H	67	SER
2	H	69	THR
2	H	70	THR
2	H	142	SER
2	H	155	GLU
2	H	157	VAL
2	H	214	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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^{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	C	211/238 (88%)	-0.14	2 (0%)	84	89	12, 26, 44, 54	0
1	L	215/238 (90%)	0.21	4 (1%)	66	75	17, 33, 53, 75	0
2	D	204/474 (43%)	-0.17	1 (0%)	90	94	14, 26, 47, 68	0
2	H	205/474 (43%)	-0.08	2 (0%)	82	87	17, 32, 49, 60	0
All	All	835/1424 (58%)	-0.04	9 (1%)	80	86	12, 29, 51, 75	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	156	GLY	3.7
1	C	45	GLY	2.6
1	L	3	VAL	2.6
2	H	156	SER	2.5
1	C	149	ASN	2.3
1	L	74	ASP	2.2
1	L	5	THR	2.2
2	H	193	SER	2.0
2	D	195	TRP	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.