Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2025 – 10:02 AM EST

PDB ID	:	9CQB
Title	:	Antibody 1G8 bound to the central conserved domain of RSV G
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Deposited on	:	2024-07-19
Resolution	:	2.50 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:

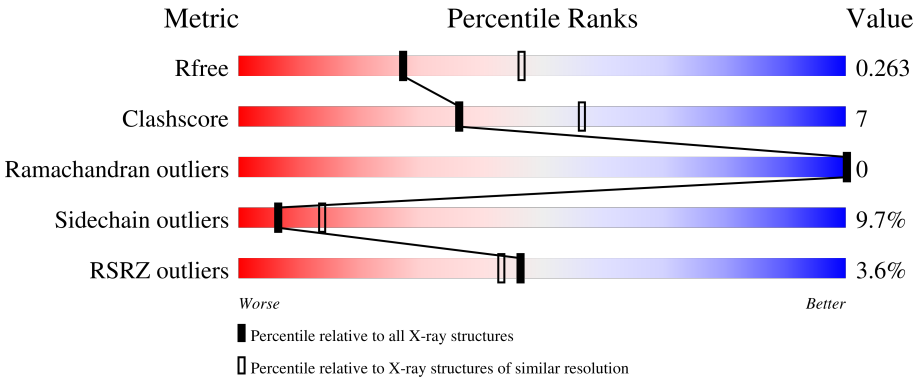
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

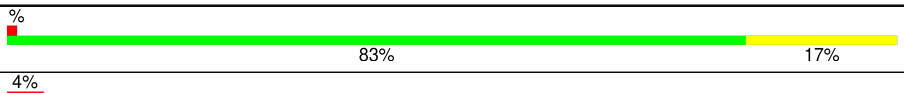
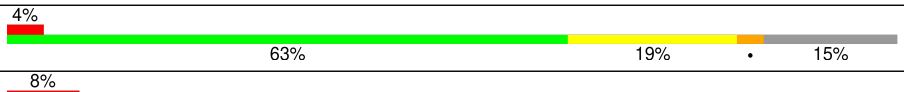
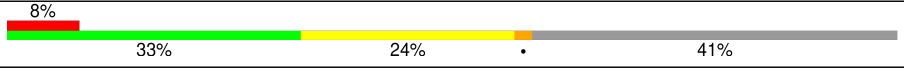
The reported resolution of this entry is 2.50 Å.

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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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 <=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	216	
2	B	266	
3	D	49	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3594 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 Fab 1G8 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1658	1040	282	331	5			

- Molecule 2 is a protein called Fab 1G8 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	225	Total	C	N	O	S	0	0	0
			1684	1065	277	337	5			

- Molecule 3 is a protein called Mature secreted glycoprotein G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	29	Total	C	N	O	S	0	0	0
			236	154	39	39	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	155	MET	-	initiating methionine	UNP P03423
D	156	GLY	-	expression tag	UNP P03423
D	198	HIS	-	expression tag	UNP P03423
D	199	HIS	-	expression tag	UNP P03423
D	200	HIS	-	expression tag	UNP P03423
D	201	HIS	-	expression tag	UNP P03423
D	202	HIS	-	expression tag	UNP P03423
D	203	HIS	-	expression tag	UNP P03423

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		

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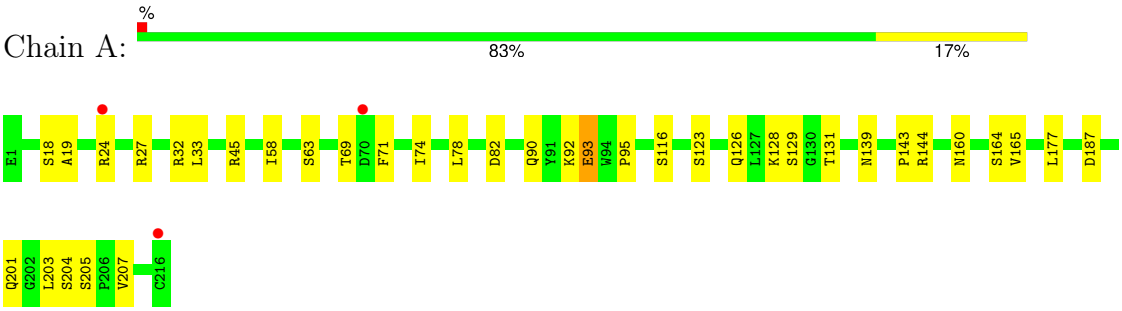
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0

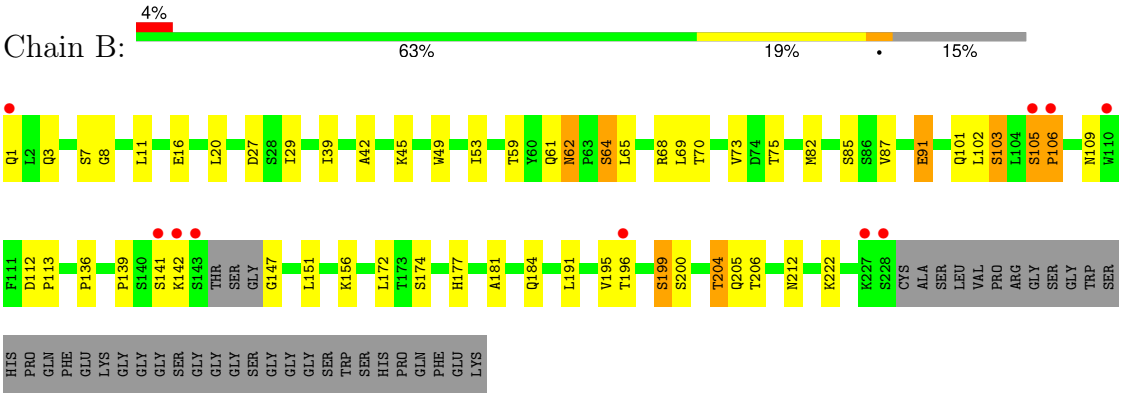
3 Residue-property plots (i)

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.

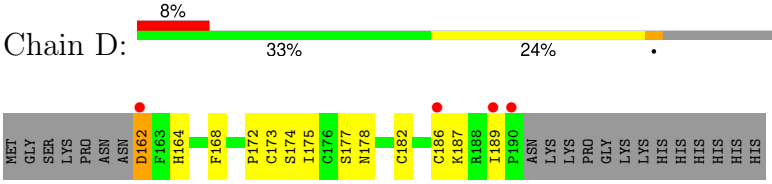
• Molecule 1: Fab 1G8 Light Chain



• Molecule 2: Fab 1G8 Heavy Chain



• Molecule 3: Mature secreted glycoprotein G



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	67.39Å 67.39Å 286.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.37 – 2.50 58.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (58.37-2.50) 99.9 (58.37-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.226 , 0.263 0.226 , 0.263	Depositor DCC
R_{free} test set	25215 reflections (7.38%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.076 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3594	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	A	0.47	0/1696	0.65	0/2305
2	B	0.46	0/1725	0.63	0/2356
3	D	0.56	0/245	0.60	0/334
All	All	0.47	0/3666	0.64	0/4995

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	1658	0	1615	19	0
2	B	1684	0	1665	30	0
3	D	236	0	216	8	0
4	A	11	0	0	0	0
4	B	4	0	0	0	0
4	D	1	0	0	0	0
All	All	3594	0	3496	50	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 7.

All (50) 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:87:VAL:HG22	2:B:91:GLU:HG2	1.65	0.77
2:B:139:PRO:HG3	2:B:151:LEU:HB3	1.78	0.66
2:B:147:GLY:N	2:B:199:SER:HG	1.96	0.64
1:A:92:LYS:HD3	1:A:93:GLU:OE1	2.01	0.61
1:A:139:ASN:HD21	2:B:177:HIS:HD2	1.49	0.60
2:B:105:SER:CB	2:B:106:PRO:HD3	2.35	0.56
2:B:101:GLN:O	2:B:109:ASN:HA	2.06	0.56
3:D:162:ASP:OD1	3:D:162:ASP:N	2.39	0.55
1:A:95:PRO:HG3	3:D:168:PHE:CE1	2.41	0.55
1:A:165:VAL:HG22	1:A:177:LEU:HD12	1.88	0.54
2:B:105:SER:HB2	2:B:106:PRO:HD3	1.88	0.54
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.89	0.53
1:A:139:ASN:HD21	2:B:177:HIS:CD2	2.27	0.52
2:B:68:ARG:HD2	2:B:85:SER:O	2.08	0.52
1:A:203:LEU:HD13	1:A:207:VAL:HG12	1.91	0.52
1:A:78:LEU:HD22	1:A:82:ASP:HB2	1.92	0.51
1:A:93:GLU:HG2	3:D:164:HIS:NE2	2.25	0.51
1:A:144:ARG:NH2	1:A:165:VAL:HG21	2.28	0.49
2:B:172:LEU:HD21	2:B:195:VAL:HG21	1.95	0.48
2:B:42:ALA:O	2:B:45:LYS:HB2	2.14	0.48
2:B:181:ALA:HA	2:B:191:LEU:HB3	1.95	0.48
2:B:102:LEU:HD23	2:B:102:LEU:HA	1.75	0.48
2:B:204:THR:OG1	2:B:205:GLN:N	2.48	0.47
2:B:39:ILE:HG23	2:B:49:TRP:HA	1.98	0.46
2:B:70:THR:O	2:B:82:MET:HA	2.15	0.46
2:B:156:LYS:NZ	2:B:184:GLN:OE1	2.31	0.45
1:A:33:LEU:HD22	1:A:71:PHE:CG	2.51	0.45
1:A:19:ALA:O	1:A:74:ILE:HA	2.16	0.45
1:A:27:ARG:O	1:A:69:THR:HG22	2.18	0.44
2:B:8:GLY:HA3	2:B:20:LEU:CD2	2.46	0.44
1:A:139:ASN:ND2	2:B:177:HIS:HD2	2.13	0.44
1:A:93:GLU:HB3	3:D:164:HIS:CD2	2.53	0.44
3:D:177:SER:OG	3:D:178:ASN:N	2.51	0.43
2:B:62:ASN:C	2:B:62:ASN:HD22	2.21	0.43
2:B:103:SER:OG	2:B:106:PRO:O	2.37	0.42
1:A:126:GLN:HG2	1:A:131:THR:O	2.18	0.42
1:A:123:SER:HB2	2:B:136:PRO:HD2	2.02	0.42
2:B:112:ASP:HA	2:B:113:PRO:HA	1.75	0.42
1:A:160:ASN:OD1	1:A:160:ASN:N	2.51	0.42
1:A:58:ILE:HD13	1:A:58:ILE:HA	1.88	0.41
2:B:61:GLN:HB3	2:B:69:LEU:HD23	2.02	0.41
2:B:62:ASN:ND2	2:B:64:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PRO:HG2	1:A:201:GLN:NE2	2.35	0.41
2:B:29:ILE:HD11	2:B:75:THR:HG22	2.02	0.41
3:D:182:CYS:O	3:D:186:CYS:HB2	2.20	0.41
2:B:16:GLU:O	2:B:87:VAL:HB	2.20	0.40
3:D:172:PRO:O	3:D:175:ILE:HG12	2.21	0.40
2:B:62:ASN:HB3	2:B:65:LEU:HD12	2.03	0.40
3:D:173:CYS:N	3:D:186:CYS:SG	2.86	0.40
2:B:53:ILE:HD13	2:B:73:VAL:HB	2.04	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	214/216 (99%)	203 (95%)	11 (5%)	0	100	100
2	B	221/266 (83%)	202 (91%)	19 (9%)	0	100	100
3	D	27/49 (55%)	25 (93%)	2 (7%)	0	100	100
All	All	462/531 (87%)	430 (93%)	32 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	187/187 (100%)	173 (92%)	14 (8%)	11 23
2	B	196/224 (88%)	174 (89%)	22 (11%)	5 10
3	D	28/46 (61%)	24 (86%)	4 (14%)	2 5
All	All	411/457 (90%)	371 (90%)	40 (10%)	6 14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	SER
1	A	24	ARG
1	A	32	ARG
1	A	45	ARG
1	A	63	SER
1	A	90	GLN
1	A	93	GLU
1	A	116	SER
1	A	128	LYS
1	A	129	SER
1	A	164	SER
1	A	187	ASP
1	A	204	SER
1	A	205	SER
2	B	1	GLN
2	B	3	GLN
2	B	7	SER
2	B	11	LEU
2	B	27	ASP
2	B	59	THR
2	B	62	ASN
2	B	64	SER
2	B	91	GLU
2	B	103	SER
2	B	105	SER
2	B	106	PRO
2	B	141	SER
2	B	142	LYS
2	B	174	SER
2	B	196	THR
2	B	199	SER
2	B	200	SER
2	B	204	THR
2	B	206	THR

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Mol	Chain	Res	Type
2	B	212	ASN
2	B	222	LYS
3	D	162	ASP
3	D	174	SER
3	D	187	LYS
3	D	189	ILE

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

Mol	Chain	Res	Type
1	A	139	ASN
1	A	149	GLN
1	A	201	GLN
2	B	62	ASN
2	B	212	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

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	216/216 (100%)	0.05	3 (1%)	73	70	32, 52, 69, 93	0
2	B	225/266 (84%)	0.27	10 (4%)	39	36	35, 54, 73, 93	0
3	D	29/49 (59%)	1.04	4 (13%)	8	7	53, 69, 89, 94	0
All	All	470/531 (88%)	0.22	17 (3%)	46	43	32, 54, 73, 94	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	228	SER	7.0
1	A	216	CYS	4.8
3	D	190	PRO	3.9
2	B	227	LYS	3.6
2	B	143	SER	3.3
2	B	106	PRO	3.0
2	B	1	GLN	2.8
2	B	142	LYS	2.6
3	D	189	ILE	2.5
2	B	110	TRP	2.5
2	B	105	SER	2.3
3	D	186	CYS	2.3
2	B	141	SER	2.3
3	D	162	ASP	2.2
1	A	24	ARG	2.1
2	B	196	THR	2.1
1	A	70	ASP	2.1

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 (i)

There are no monosaccharides 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.