wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 11:47 am BST

PDB ID	:	6APD
Title	:	Crystal structure of RSV F bound by AM22 and the infant antibody ADI-19425
Authors	:	Wrapp, D.; McLellan, J.S.
Deposited on	:	2017-08-17
Resolution	:	4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

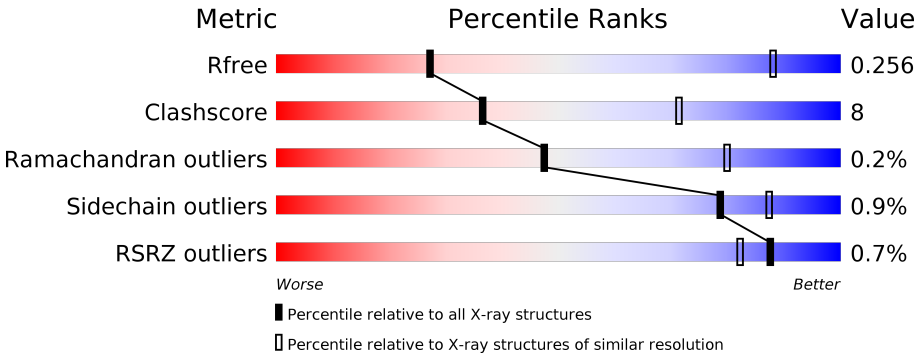
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 4.10 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))
R_{free}	130704	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	A	573	61% 18% • 21%
1	B	573	63% 16% 21%
1	C	573	63% 16% 21%
2	D	228	% 86% 11% •
2	F	228	81% 16% •
2	H	228	% 82% 15% •

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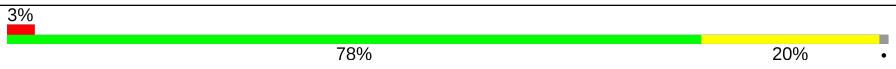
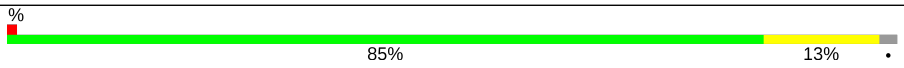
Mol	Chain	Length	Quality of chain
3	E	215	
3	G	215	
3	I	215	
4	J	226	
4	K	226	
4	N	226	
5	L	218	
5	M	218	
5	O	218	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 30005 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 Fusion glycoprotein F0,Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3488	2205	574	688	21			
1	B	453	Total	C	N	O	S	0	0	0
			3500	2213	576	690	21			
1	C	452	Total	C	N	O	S	0	0	0
			3491	2208	574	688	21			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GLU	LYS	conflict	UNP C3UPB8
A	67	ILE	ASN	engineered mutation	UNP C3UPB8
A	76	VAL	ILE	conflict	UNP C3UPB8
A	215	PRO	SER	engineered mutation	UNP C3UPB8
A	514	SER	-	linker	UNP C3UPB8
A	515	ALA	-	linker	UNP C3UPB8
A	516	ILE	-	linker	UNP C3UPB8
A	517	GLY	-	linker	UNP C3UPB8
A	547	MET	-	expression tag	UNP M1E1E4
A	548	GLU	-	expression tag	UNP M1E1E4
A	549	VAL	-	expression tag	UNP M1E1E4
A	550	LEU	-	expression tag	UNP M1E1E4
A	551	PHE	-	expression tag	UNP M1E1E4
A	552	GLN	-	expression tag	UNP M1E1E4
A	553	GLY	-	expression tag	UNP M1E1E4
A	554	PRO	-	expression tag	UNP M1E1E4
A	555	GLY	-	expression tag	UNP M1E1E4
A	556	HIS	-	expression tag	UNP M1E1E4
A	557	HIS	-	expression tag	UNP M1E1E4
A	558	HIS	-	expression tag	UNP M1E1E4
A	559	HIS	-	expression tag	UNP M1E1E4
A	560	HIS	-	expression tag	UNP M1E1E4
A	561	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	562	HIS	-	expression tag	UNP M1E1E4
A	563	HIS	-	expression tag	UNP M1E1E4
A	564	SER	-	expression tag	UNP M1E1E4
A	565	ALA	-	expression tag	UNP M1E1E4
A	566	TRP	-	expression tag	UNP M1E1E4
A	567	SER	-	expression tag	UNP M1E1E4
A	568	HIS	-	expression tag	UNP M1E1E4
A	569	PRO	-	expression tag	UNP M1E1E4
A	570	GLN	-	expression tag	UNP M1E1E4
A	571	PHE	-	expression tag	UNP M1E1E4
A	572	GLU	-	expression tag	UNP M1E1E4
A	573	LYS	-	expression tag	UNP M1E1E4
B	66	GLU	LYS	conflict	UNP C3UPB8
B	67	ILE	ASN	engineered mutation	UNP C3UPB8
B	76	VAL	ILE	conflict	UNP C3UPB8
B	215	PRO	SER	engineered mutation	UNP C3UPB8
B	514	SER	-	linker	UNP C3UPB8
B	515	ALA	-	linker	UNP C3UPB8
B	516	ILE	-	linker	UNP C3UPB8
B	517	GLY	-	linker	UNP C3UPB8
B	547	MET	-	expression tag	UNP M1E1E4
B	548	GLU	-	expression tag	UNP M1E1E4
B	549	VAL	-	expression tag	UNP M1E1E4
B	550	LEU	-	expression tag	UNP M1E1E4
B	551	PHE	-	expression tag	UNP M1E1E4
B	552	GLN	-	expression tag	UNP M1E1E4
B	553	GLY	-	expression tag	UNP M1E1E4
B	554	PRO	-	expression tag	UNP M1E1E4
B	555	GLY	-	expression tag	UNP M1E1E4
B	556	HIS	-	expression tag	UNP M1E1E4
B	557	HIS	-	expression tag	UNP M1E1E4
B	558	HIS	-	expression tag	UNP M1E1E4
B	559	HIS	-	expression tag	UNP M1E1E4
B	560	HIS	-	expression tag	UNP M1E1E4
B	561	HIS	-	expression tag	UNP M1E1E4
B	562	HIS	-	expression tag	UNP M1E1E4
B	563	HIS	-	expression tag	UNP M1E1E4
B	564	SER	-	expression tag	UNP M1E1E4
B	565	ALA	-	expression tag	UNP M1E1E4
B	566	TRP	-	expression tag	UNP M1E1E4
B	567	SER	-	expression tag	UNP M1E1E4
B	568	HIS	-	expression tag	UNP M1E1E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	569	PRO	-	expression tag	UNP M1E1E4
B	570	GLN	-	expression tag	UNP M1E1E4
B	571	PHE	-	expression tag	UNP M1E1E4
B	572	GLU	-	expression tag	UNP M1E1E4
B	573	LYS	-	expression tag	UNP M1E1E4
C	66	GLU	LYS	conflict	UNP C3UPB8
C	67	ILE	ASN	engineered mutation	UNP C3UPB8
C	76	VAL	ILE	conflict	UNP C3UPB8
C	215	PRO	SER	engineered mutation	UNP C3UPB8
C	514	SER	-	linker	UNP C3UPB8
C	515	ALA	-	linker	UNP C3UPB8
C	516	ILE	-	linker	UNP C3UPB8
C	517	GLY	-	linker	UNP C3UPB8
C	547	MET	-	expression tag	UNP M1E1E4
C	548	GLU	-	expression tag	UNP M1E1E4
C	549	VAL	-	expression tag	UNP M1E1E4
C	550	LEU	-	expression tag	UNP M1E1E4
C	551	PHE	-	expression tag	UNP M1E1E4
C	552	GLN	-	expression tag	UNP M1E1E4
C	553	GLY	-	expression tag	UNP M1E1E4
C	554	PRO	-	expression tag	UNP M1E1E4
C	555	GLY	-	expression tag	UNP M1E1E4
C	556	HIS	-	expression tag	UNP M1E1E4
C	557	HIS	-	expression tag	UNP M1E1E4
C	558	HIS	-	expression tag	UNP M1E1E4
C	559	HIS	-	expression tag	UNP M1E1E4
C	560	HIS	-	expression tag	UNP M1E1E4
C	561	HIS	-	expression tag	UNP M1E1E4
C	562	HIS	-	expression tag	UNP M1E1E4
C	563	HIS	-	expression tag	UNP M1E1E4
C	564	SER	-	expression tag	UNP M1E1E4
C	565	ALA	-	expression tag	UNP M1E1E4
C	566	TRP	-	expression tag	UNP M1E1E4
C	567	SER	-	expression tag	UNP M1E1E4
C	568	HIS	-	expression tag	UNP M1E1E4
C	569	PRO	-	expression tag	UNP M1E1E4
C	570	GLN	-	expression tag	UNP M1E1E4
C	571	PHE	-	expression tag	UNP M1E1E4
C	572	GLU	-	expression tag	UNP M1E1E4
C	573	LYS	-	expression tag	UNP M1E1E4

- Molecule 2 is a protein called AM22 Fab Heavy Chain,IGH@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	221	Total	C	N	O	S	0	0	0
			1646	1046	271	323	6			
2	F	222	Total	C	N	O	S	0	0	0
			1652	1049	272	324	7			
2	H	221	Total	C	N	O	S	0	0	0
			1646	1046	271	323	6			

- Molecule 3 is a protein called AM22 Fab Light Chain,Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1624	1019	278	323	4			
3	G	215	Total	C	N	O	S	0	0	0
			1639	1027	280	327	5			
3	I	212	Total	C	N	O	S	0	0	0
			1620	1017	277	322	4			

- Molecule 4 is a protein called Immunoglobulin heavy variable 3-21,Immunoglobulin gamma-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	223	Total	C	N	O	S	0	0	0
			1656	1043	277	328	8			
4	K	223	Total	C	N	O	S	0	0	0
			1656	1043	277	328	8			
4	N	223	Total	C	N	O	S	0	0	0
			1656	1043	277	328	8			

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	95	LEU	-	linker	UNP A0A0B4J1V1
J	96	GLY	-	linker	UNP A0A0B4J1V1
J	97	TYR	-	linker	UNP A0A0B4J1V1
J	98	CYS	-	linker	UNP A0A0B4J1V1
J	99	SER	-	linker	UNP A0A0B4J1V1
J	100	GLY	-	linker	UNP A0A0B4J1V1
J	100A	GLY	-	linker	UNP A0A0B4J1V1
J	100B	SER	-	linker	UNP A0A0B4J1V1
J	100C	CYS	-	linker	UNP A0A0B4J1V1
J	100D	HIS	-	linker	UNP A0A0B4J1V1
J	100E	PHE	-	linker	UNP A0A0B4J1V1
J	101	ASP	-	linker	UNP A0A0B4J1V1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	102	TYR	-	linker	UNP A0A0B4J1V1
K	95	LEU	-	linker	UNP A0A0B4J1V1
K	96	GLY	-	linker	UNP A0A0B4J1V1
K	97	TYR	-	linker	UNP A0A0B4J1V1
K	98	CYS	-	linker	UNP A0A0B4J1V1
K	99	SER	-	linker	UNP A0A0B4J1V1
K	100	GLY	-	linker	UNP A0A0B4J1V1
K	100A	GLY	-	linker	UNP A0A0B4J1V1
K	100B	SER	-	linker	UNP A0A0B4J1V1
K	100C	CYS	-	linker	UNP A0A0B4J1V1
K	100D	HIS	-	linker	UNP A0A0B4J1V1
K	100E	PHE	-	linker	UNP A0A0B4J1V1
K	101	ASP	-	linker	UNP A0A0B4J1V1
K	102	TYR	-	linker	UNP A0A0B4J1V1
N	95	LEU	-	linker	UNP A0A0B4J1V1
N	96	GLY	-	linker	UNP A0A0B4J1V1
N	97	TYR	-	linker	UNP A0A0B4J1V1
N	98	CYS	-	linker	UNP A0A0B4J1V1
N	99	SER	-	linker	UNP A0A0B4J1V1
N	100	GLY	-	linker	UNP A0A0B4J1V1
N	100A	GLY	-	linker	UNP A0A0B4J1V1
N	100B	SER	-	linker	UNP A0A0B4J1V1
N	100C	CYS	-	linker	UNP A0A0B4J1V1
N	100D	HIS	-	linker	UNP A0A0B4J1V1
N	100E	PHE	-	linker	UNP A0A0B4J1V1
N	101	ASP	-	linker	UNP A0A0B4J1V1
N	102	TYR	-	linker	UNP A0A0B4J1V1

- Molecule 5 is a protein called IGL@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	213	Total	C	N	O	S	0	0	0
			1577	988	262	323	4			
5	M	213	Total	C	N	O	S	0	0	0
			1577	988	262	323	4			
5	O	213	Total	C	N	O	S	0	0	0
			1577	988	262	323	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	45	LYS	ARG	conflict	UNP Q6GMX4

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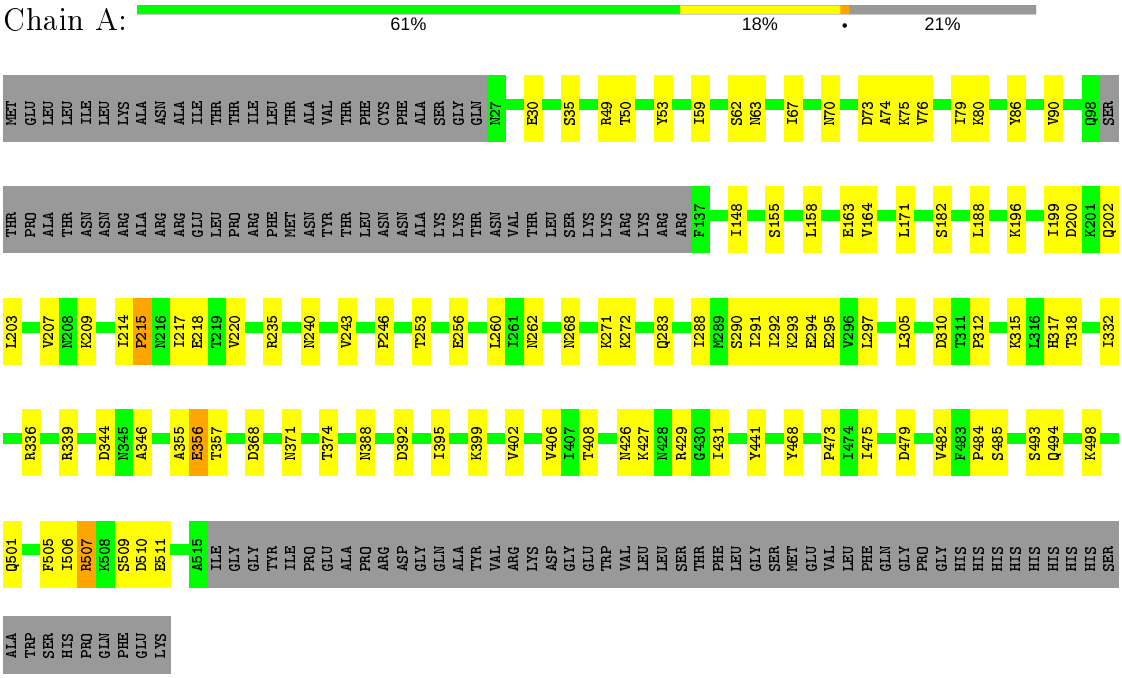
Chain	Residue	Modelled	Actual	Comment	Reference
L	95C	PHE	-	insertion	UNP Q6GMX4
L	96	TYR	VAL	conflict	UNP Q6GMX4
L	97	VAL	MET	conflict	UNP Q6GMX4
L	100	THR	GLY	conflict	UNP Q6GMX4
L	104	VAL	LEU	conflict	UNP Q6GMX4
M	45	LYS	ARG	conflict	UNP Q6GMX4
M	95C	PHE	-	insertion	UNP Q6GMX4
M	96	TYR	VAL	conflict	UNP Q6GMX4
M	97	VAL	MET	conflict	UNP Q6GMX4
M	100	THR	GLY	conflict	UNP Q6GMX4
M	104	VAL	LEU	conflict	UNP Q6GMX4
O	45	LYS	ARG	conflict	UNP Q6GMX4
O	95C	PHE	-	insertion	UNP Q6GMX4
O	96	TYR	VAL	conflict	UNP Q6GMX4
O	97	VAL	MET	conflict	UNP Q6GMX4
O	100	THR	GLY	conflict	UNP Q6GMX4
O	104	VAL	LEU	conflict	UNP Q6GMX4

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.

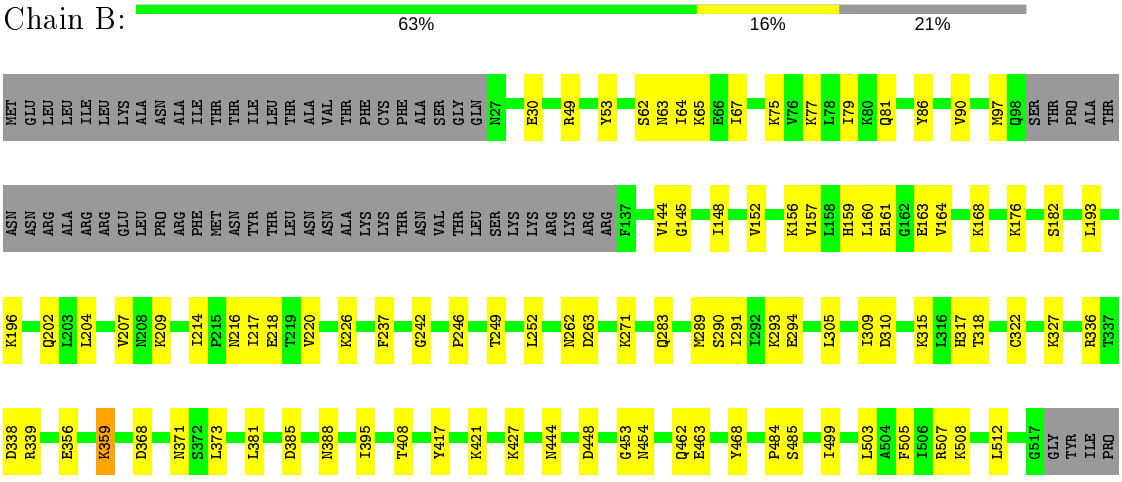
- Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

Chain A:



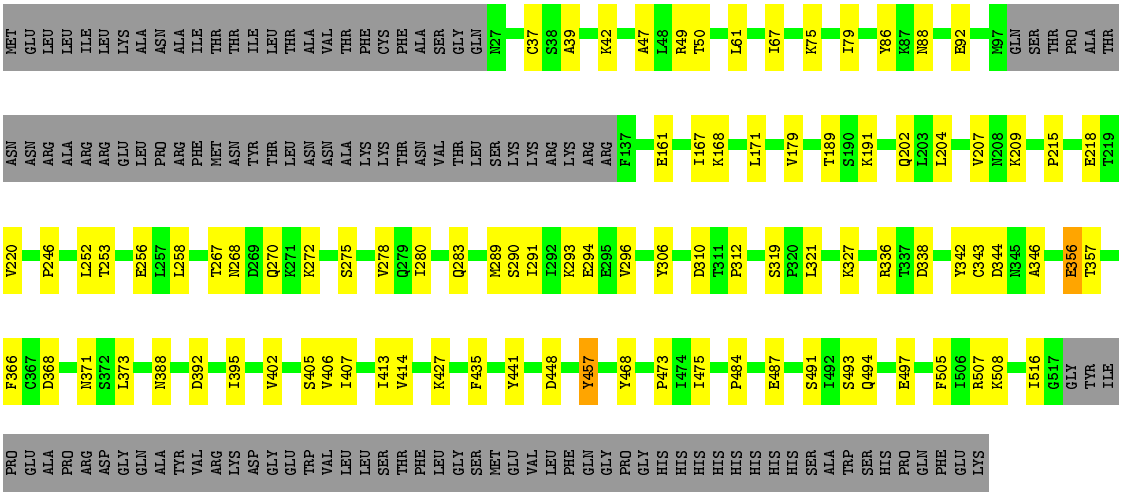
- Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

Chain B:



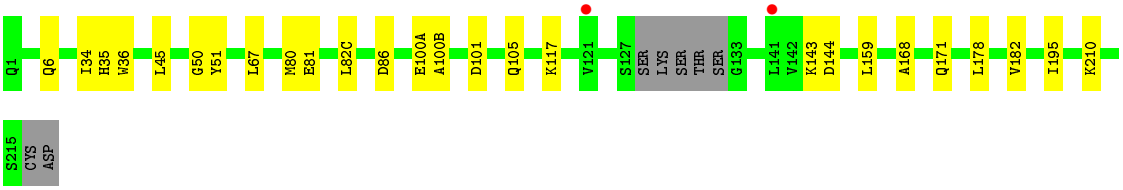
• Molecule 1: Fusion glycoprotein F0,Envelope glycoprotein

Chain C:



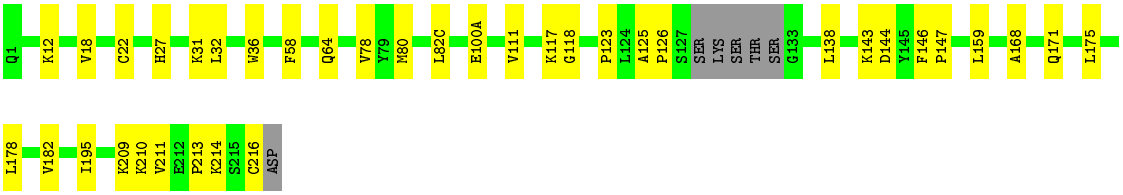
• Molecule 2: AM22 Fab Heavy Chain,IGH@ protein

Chain D:



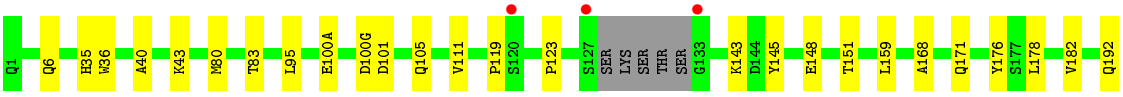
• Molecule 2: AM22 Fab Heavy Chain,IGH@ protein

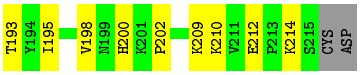
Chain F:



• Molecule 2: AM22 Fab Heavy Chain,IGH@ protein

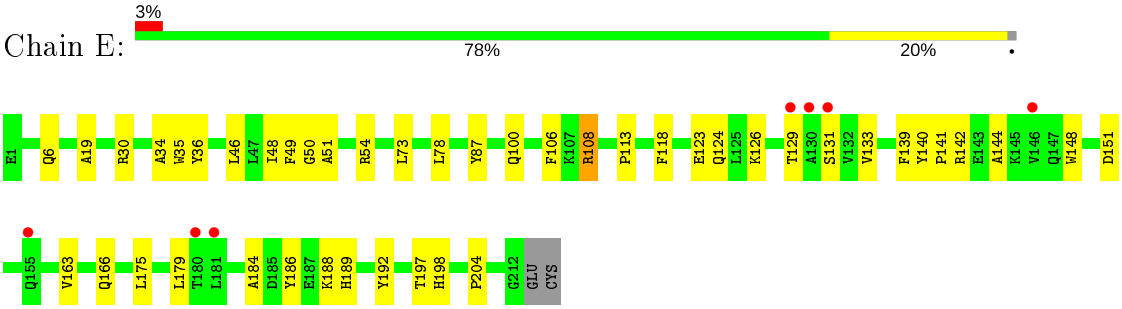
Chain H:





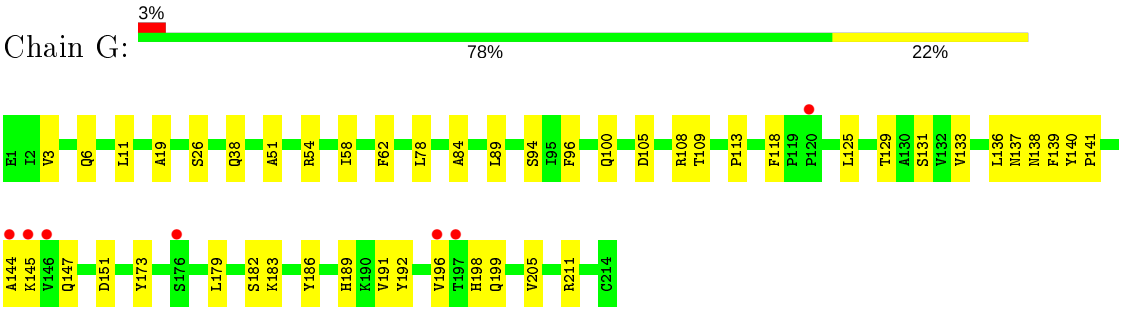
• Molecule 3: AM22 Fab Light Chain,Uncharacterized protein

Chain E:



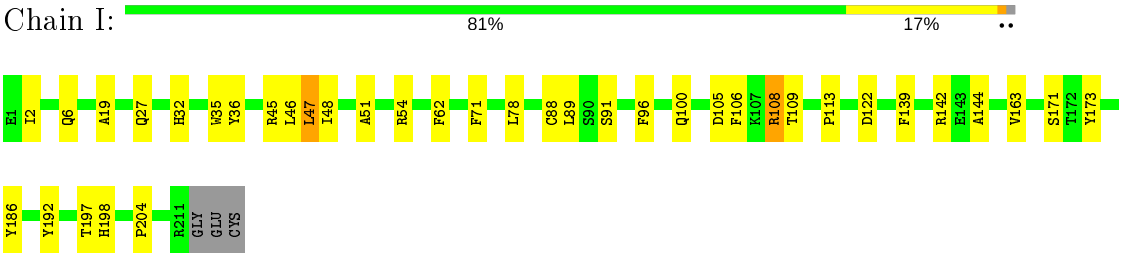
• Molecule 3: AM22 Fab Light Chain,Uncharacterized protein

Chain G:



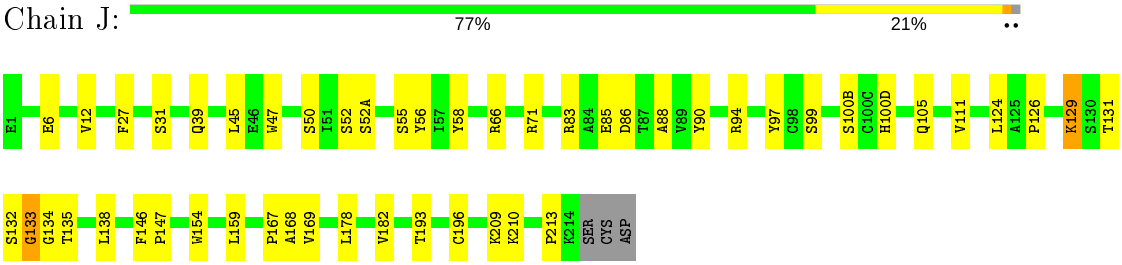
• Molecule 3: AM22 Fab Light Chain,Uncharacterized protein

Chain I:



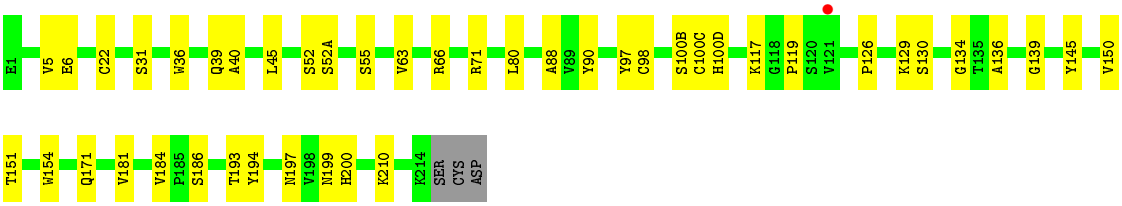
• Molecule 4: Immunoglobulin heavy variable 3-21,Immunoglobulin gamma-1 heavy chain

Chain J:

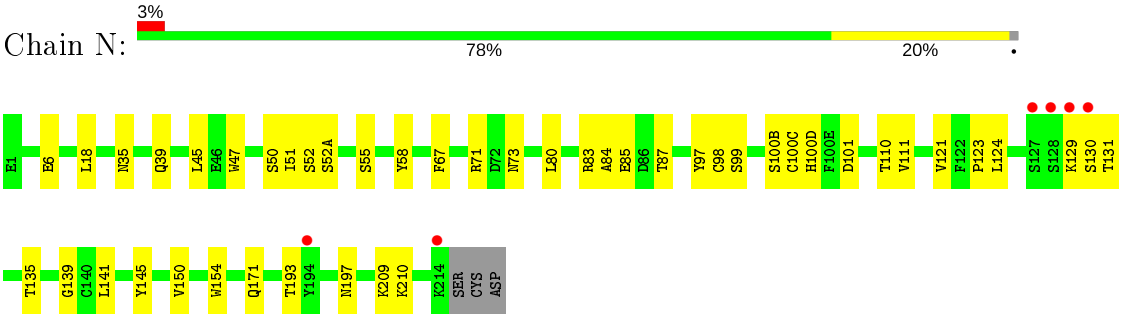


• Molecule 4: Immunoglobulin heavy variable 3-21,Immunoglobulin gamma-1 heavy chain

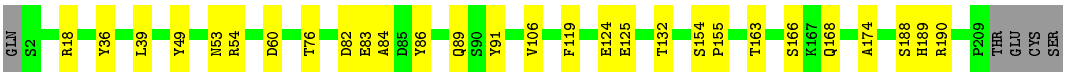
Chain K:



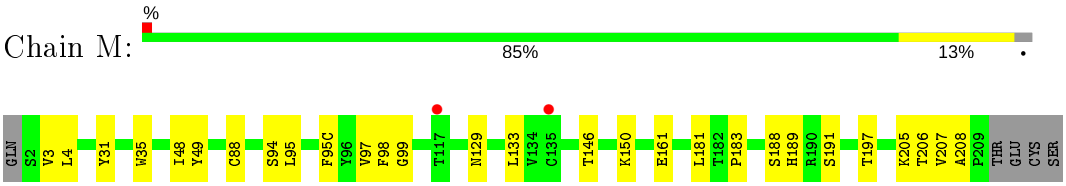
• Molecule 4: Immunoglobulin heavy variable 3-21,Immunoglobulin gamma-1 heavy chain



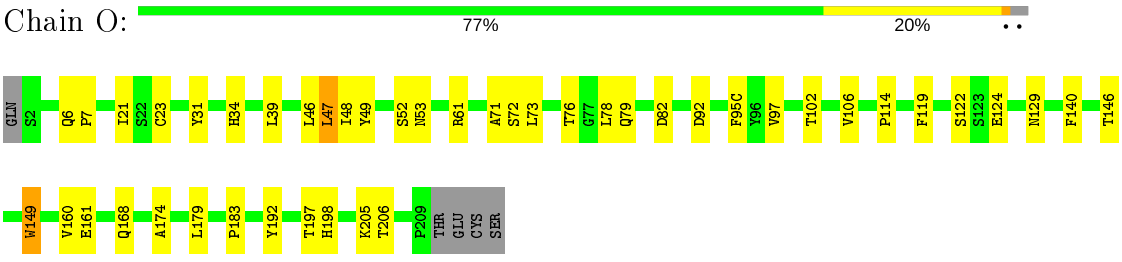
• Molecule 5: IGL@ protein



• Molecule 5: IGL@ protein



• Molecule 5: IGL@ protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	229.47Å 229.47Å 304.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.96 – 4.10 50.96 – 4.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.96-4.10) 100.0 (50.96-4.10)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.256 0.203 , 0.256	Depositor DCC
R_{free} test set	3297 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	117.3	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 86.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30005	wwPDB-VP
Average B, all atoms (Å^2)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% 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	0.28	0/3538	0.49	1/4794 (0.0%)
1	B	0.28	0/3550	0.49	0/4810
1	C	0.29	0/3541	0.49	0/4798
2	D	0.25	0/1682	0.48	0/2292
2	F	0.26	0/1688	0.50	0/2300
2	H	0.27	0/1682	0.50	0/2292
3	E	0.27	0/1659	0.48	0/2252
3	G	0.26	0/1674	0.46	0/2272
3	I	0.28	0/1655	0.49	0/2247
4	J	0.29	0/1696	0.51	0/2306
4	K	0.27	0/1696	0.50	0/2306
4	N	0.30	0/1696	0.49	0/2306
5	L	0.28	0/1617	0.48	0/2210
5	M	0.27	0/1617	0.46	0/2210
5	O	0.27	0/1617	0.46	0/2210
All	All	0.28	0/30608	0.49	1/41605 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	LEU	CA-CB-CG	5.93	128.94	115.30

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	3488	0	3539	73	0
1	B	3500	0	3553	65	0
1	C	3491	0	3545	63	1
2	D	1646	0	1637	16	0
2	F	1652	0	1641	22	1
2	H	1646	0	1637	23	0
3	E	1624	0	1590	29	0
3	G	1639	0	1600	28	0
3	I	1620	0	1587	30	0
4	J	1656	0	1615	36	0
4	K	1656	0	1615	34	0
4	N	1656	0	1615	39	0
5	L	1577	0	1521	18	0
5	M	1577	0	1521	22	0
5	O	1577	0	1521	38	0
All	All	30005	0	29737	474	1

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.

The worst 5 of 474 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:H:214:LYS:NZ	3:I:122:ASP:OD2	1.82	1.12
3:I:36:TYR:CZ	3:I:46:LEU:HD22	1.88	1.07
1:A:218:GLU:OE2	1:C:75:LYS:NZ	1.91	1.02
3:G:108:ARG:NH1	3:G:109:THR:O	1.96	0.96
4:N:129:LYS:NZ	5:O:206:THR:O	1.99	0.96

All (1) 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:C:327:LYS:NZ	2:F:64:GLN:O[6_554]	2.17	0.03

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	447/573 (78%)	422 (94%)	24 (5%)	1 (0%)	47	80
1	B	449/573 (78%)	423 (94%)	25 (6%)	1 (0%)	47	80
1	C	448/573 (78%)	424 (95%)	23 (5%)	1 (0%)	47	80
2	D	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
2	F	218/228 (96%)	209 (96%)	9 (4%)	0	100	100
2	H	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
3	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	29	67
3	G	213/215 (99%)	203 (95%)	9 (4%)	1 (0%)	29	67
3	I	210/215 (98%)	201 (96%)	8 (4%)	1 (0%)	29	67
4	J	221/226 (98%)	210 (95%)	9 (4%)	2 (1%)	17	54
4	K	221/226 (98%)	211 (96%)	10 (4%)	0	100	100
4	N	221/226 (98%)	210 (95%)	11 (5%)	0	100	100
5	L	211/218 (97%)	197 (93%)	14 (7%)	0	100	100
5	M	211/218 (97%)	201 (95%)	10 (5%)	0	100	100
5	O	211/218 (97%)	200 (95%)	11 (5%)	0	100	100
All	All	3926/4380 (90%)	3734 (95%)	184 (5%)	8 (0%)	47	80

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	PRO
1	C	215	PRO
3	E	51	ALA
3	G	51	ALA
3	I	51	ALA

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	411/515 (80%)	406 (99%)	5 (1%)	71 83
1	B	412/515 (80%)	408 (99%)	4 (1%)	76 85
1	C	411/515 (80%)	401 (98%)	10 (2%)	49 69
2	D	184/191 (96%)	184 (100%)	0	100 100
2	F	185/191 (97%)	183 (99%)	2 (1%)	73 84
2	H	184/191 (96%)	184 (100%)	0	100 100
3	E	183/185 (99%)	181 (99%)	2 (1%)	73 84
3	G	185/185 (100%)	185 (100%)	0	100 100
3	I	183/185 (99%)	180 (98%)	3 (2%)	62 78
4	J	187/190 (98%)	186 (100%)	1 (0%)	88 93
4	K	187/190 (98%)	186 (100%)	1 (0%)	88 93
4	N	187/190 (98%)	186 (100%)	1 (0%)	88 93
5	L	177/182 (97%)	177 (100%)	0	100 100
5	M	177/182 (97%)	177 (100%)	0	100 100
5	O	177/182 (97%)	175 (99%)	2 (1%)	73 84
All	All	3430/3789 (90%)	3399 (99%)	31 (1%)	78 87

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	388	ASN
1	C	505	PHE
4	N	197	ASN
1	C	457	TYR
1	C	507	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	159	HIS
4	N	35	ASN
3	G	137	ASN
1	A	380	ASN
4	J	39	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	451/573 (78%)	-0.52	0 100 100	90, 130, 193, 298	0
1	B	453/573 (79%)	-0.51	0 100 100	84, 119, 182, 368	0
1	C	452/573 (78%)	-0.49	0 100 100	77, 122, 176, 301	0
2	D	221/228 (96%)	-0.29	2 (0%) 84 77	111, 177, 258, 342	0
2	F	222/228 (97%)	-0.25	0 100 100	107, 178, 350, 493	0
2	H	221/228 (96%)	-0.37	3 (1%) 75 65	108, 182, 249, 283	0
3	E	213/215 (99%)	-0.07	7 (3%) 46 37	101, 189, 285, 341	0
3	G	215/215 (100%)	-0.14	7 (3%) 46 37	105, 223, 385, 471	0
3	I	212/215 (98%)	-0.27	0 100 100	96, 172, 290, 329	0
4	J	223/226 (98%)	-0.49	0 100 100	90, 131, 170, 381	0
4	K	223/226 (98%)	-0.25	1 (0%) 92 87	91, 165, 323, 368	0
4	N	223/226 (98%)	-0.18	6 (2%) 54 44	113, 181, 252, 389	0
5	L	213/218 (97%)	-0.44	0 100 100	99, 136, 183, 207	0
5	M	213/218 (97%)	-0.29	2 (0%) 84 77	106, 196, 316, 371	0
5	O	213/218 (97%)	-0.34	0 100 100	107, 171, 243, 270	0
All	All	3968/4380 (90%)	-0.36	28 (0%) 87 82	77, 150, 301, 493	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	128	SER	6.5
3	G	144	ALA	5.7
3	G	120	PRO	4.1
4	K	121	VAL	3.5
3	E	180	THR	3.3

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.