wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2020 – 06:49 PM BST

PDB ID	:	4HG4
Title	:	Crystal structure of Fab 2G1 in complex with a H2N2 influenza virus hemagglutinin
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2012-10-06
Resolution	:	3.20 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:

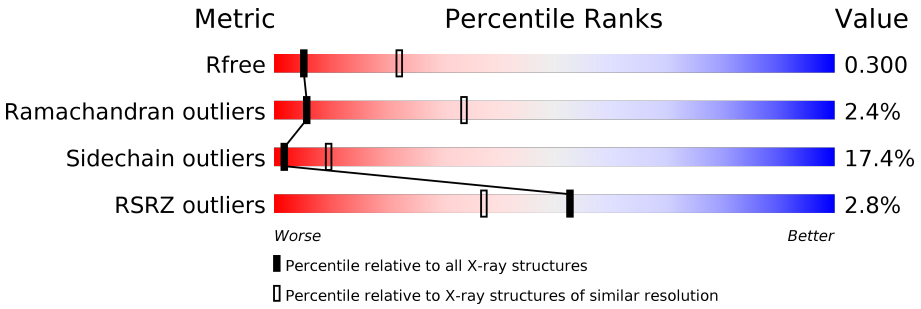
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 3.20 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.



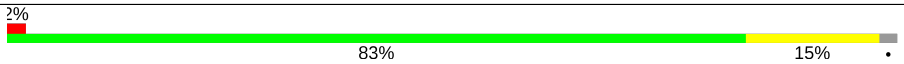
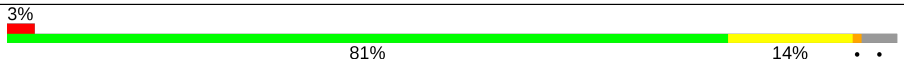
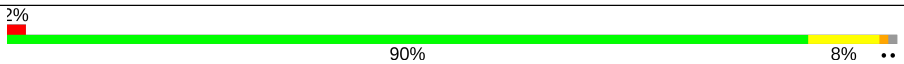
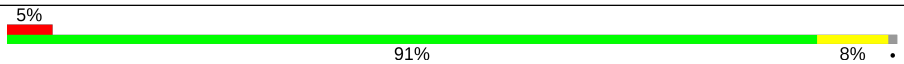
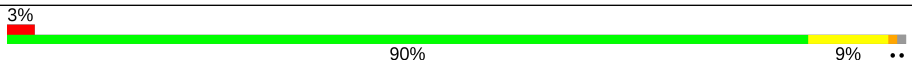
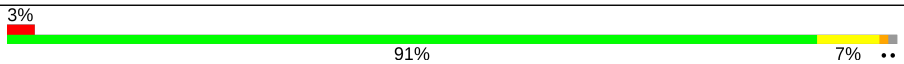
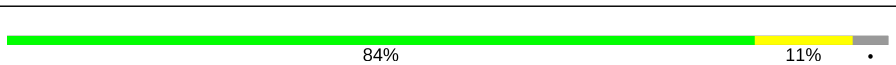
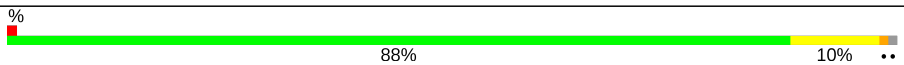
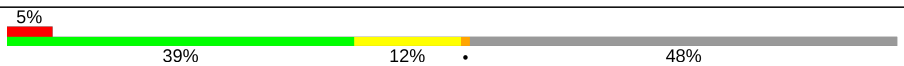
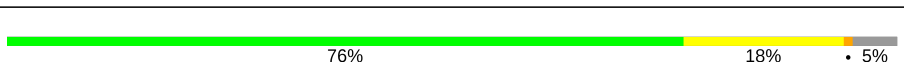
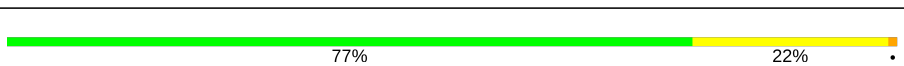
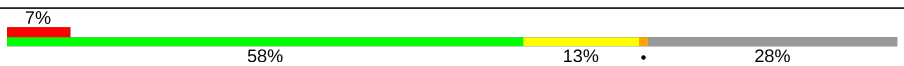
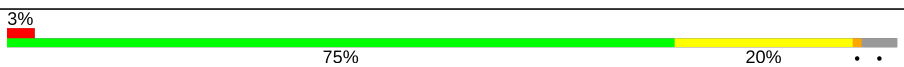
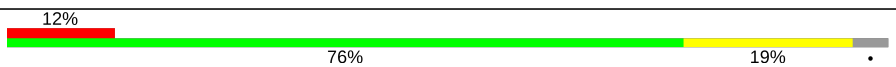
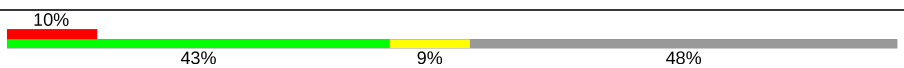
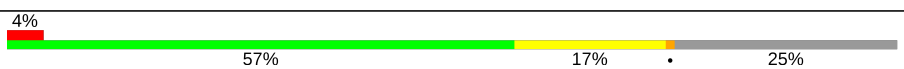
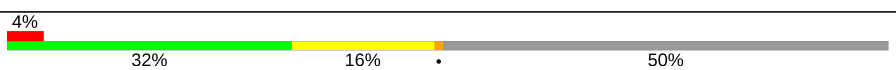
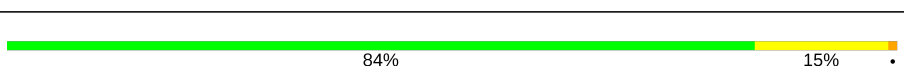
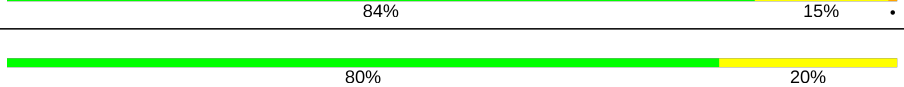
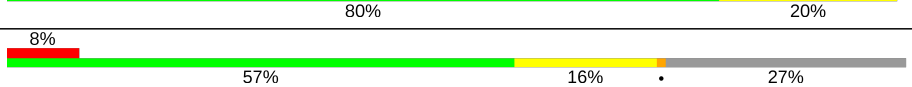
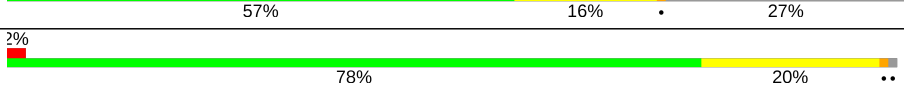
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	327	83% 15%
1	B	327	% 81% 16%
1	C	327	% 83% 16%
1	D	327	% 83% 16%
1	E	327	83% 16%
1	F	327	% 82% 17%
1	G	327	2% 83% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	327	
1	I	327	
2	a	174	
2	b	174	
2	c	174	
2	d	174	
2	e	174	
2	f	174	
2	g	174	
2	h	174	
2	i	174	
3	J	223	
3	L	223	
3	N	223	
3	P	223	
3	R	223	
3	T	223	
3	V	223	
3	X	223	
3	Z	223	
4	K	214	
4	M	214	
4	O	214	
4	Q	214	
4	S	214	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	U	214	5% 74% 24%
4	W	214	38% 10% 51%
4	Y	214	40% 10% 49%
4	z	214	3% 42% 13% 44%
5	j	2	50% 50%
5	k	2	100%
5	m	2	50% 50%
5	n	2	50% 50%
5	o	2	100%
5	q	2	50% 50%
5	r	2	100%
5	s	2	50% 50%
5	t	2	100%
6	l	3	33% 67%
6	p	3	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	s	2	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 58742 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 Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2531	1593	438	485	15			
1	B	319	Total	C	N	O	S	0	0	0
			2503	1577	433	478	15			
1	C	324	Total	C	N	O	S	0	0	0
			2539	1599	439	486	15			
1	D	324	Total	C	N	O	S	0	0	0
			2539	1599	439	486	15			
1	E	323	Total	C	N	O	S	0	0	0
			2531	1593	438	485	15			
1	F	324	Total	C	N	O	S	0	0	0
			2539	1599	439	486	15			
1	G	324	Total	C	N	O	S	0	0	0
			2539	1599	439	486	15			
1	H	325	Total	C	N	O	S	0	0	0
			2548	1604	440	489	15			
1	I	324	Total	C	N	O	S	0	0	0
			2539	1599	439	486	15			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP Q67085
B	9	PRO	-	expression tag	UNP Q67085
C	9	PRO	-	expression tag	UNP Q67085
D	9	PRO	-	expression tag	UNP Q67085
E	9	PRO	-	expression tag	UNP Q67085
F	9	PRO	-	expression tag	UNP Q67085
G	9	PRO	-	expression tag	UNP Q67085
H	9	PRO	-	expression tag	UNP Q67085
I	9	PRO	-	expression tag	UNP Q67085

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	171	Total	C	N	O	S	0	0	0
			1387	866	236	276	9			
2	b	167	Total	C	N	O	S	0	0	0
			1345	836	229	271	9			
2	c	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			
2	d	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			
2	e	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			
2	f	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			
2	g	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			
2	h	167	Total	C	N	O	S	0	0	0
			1355	845	231	270	9			
2	i	172	Total	C	N	O	S	0	0	0
			1396	871	237	279	9			

- Molecule 3 is a protein called Fab 2G1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	115	Total	C	N	O	S	0	0	0
			871	555	142	171	3			
3	L	212	Total	C	N	O	S	0	0	0
			1578	1004	258	311	5			
3	N	223	Total	C	N	O	S	0	0	0
			1648	1043	271	328	6			
3	P	161	Total	C	N	O	S	0	0	0
			1207	770	195	239	3			
3	R	214	Total	C	N	O	S	0	0	0
			1589	1010	260	314	5			
3	T	213	Total	C	N	O	S	0	0	0
			1580	1005	259	311	5			
3	V	117	Total	C	N	O	S	0	0	0
			883	564	144	172	3			
3	X	164	Total	C	N	O	S	0	0	0
			1232	785	201	242	4			
3	Z	167	Total	C	N	O	S	0	0	0
			1262	807	205	246	4			

- Molecule 4 is a protein called Fab 2G1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	106	Total	C	N	O	S	0	0	0
			826	518	140	166	2			
4	M	214	Total	C	N	O	S	0	0	0
			1661	1037	282	337	5			
4	O	214	Total	C	N	O	S	0	0	0
			1661	1037	282	337	5			
4	Q	157	Total	C	N	O	S	0	0	0
			1217	760	206	248	3			
4	S	211	Total	C	N	O	S	0	0	0
			1642	1027	279	332	4			
4	U	211	Total	C	N	O	S	0	0	0
			1642	1027	279	332	4			
4	W	105	Total	C	N	O	S	0	0	0
			818	512	139	165	2			
4	Y	109	Total	C	N	O	S	0	0	0
			853	534	147	170	2			
4	z	119	Total	C	N	O	S	0	0	0
			915	568	155	190	2			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

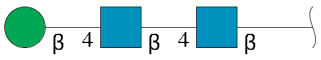
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	j	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	k	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	m	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	n	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	o	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	q	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	r	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	s	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

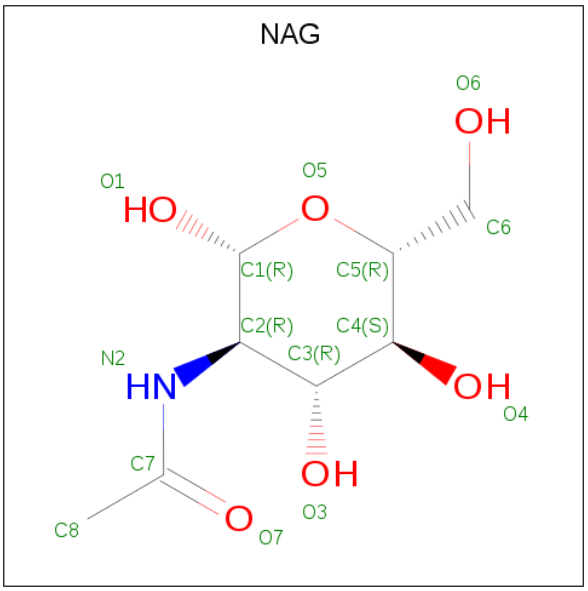
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	t	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	l	3	Total C N O 39 22 2 15	0	0	0
6	p	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 14 8 1 5	0	0
7	C	1	Total C N O 14 8 1 5	0	0
7	E	1	Total C N O 14 8 1 5	0	0

Continued on next page...

Continued from previous page...

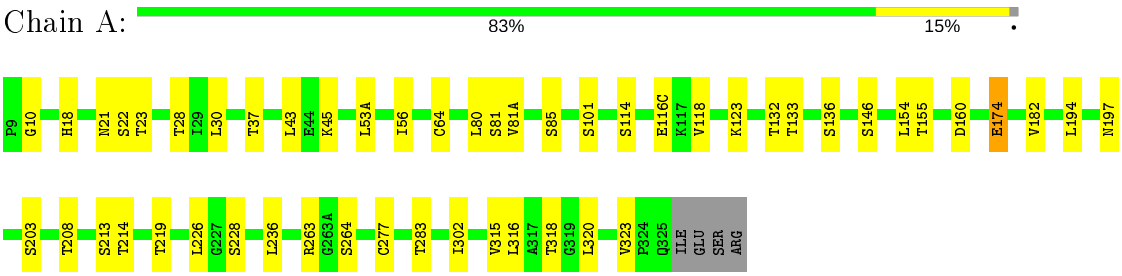
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			14	8	1	5		

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.

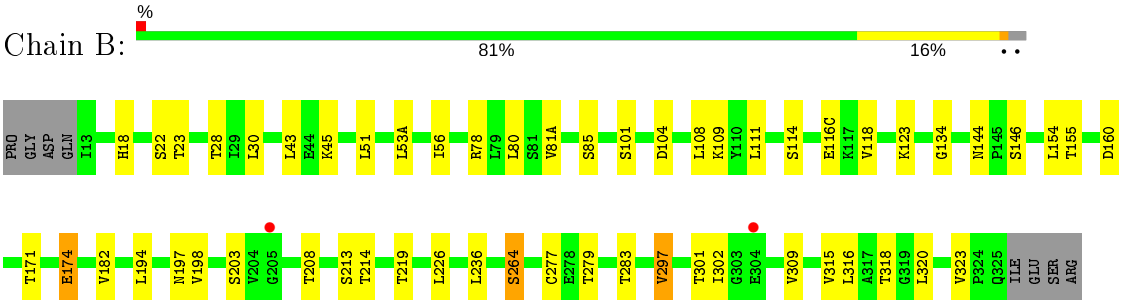
- Molecule 1: Hemagglutinin HA1

Chain A:



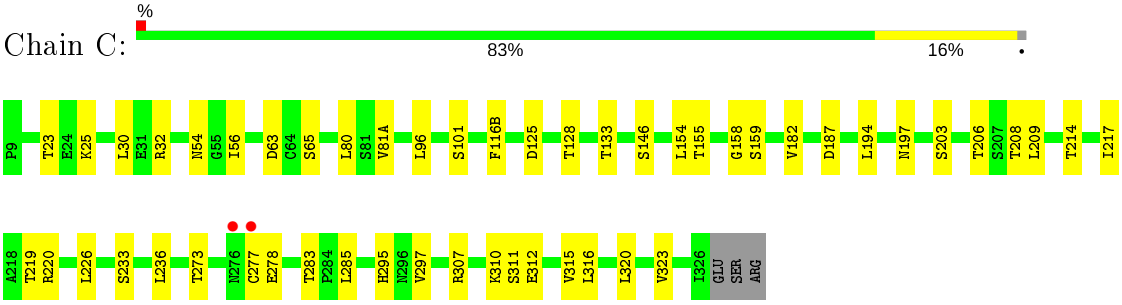
- Molecule 1: Hemagglutinin HA1

Chain B:



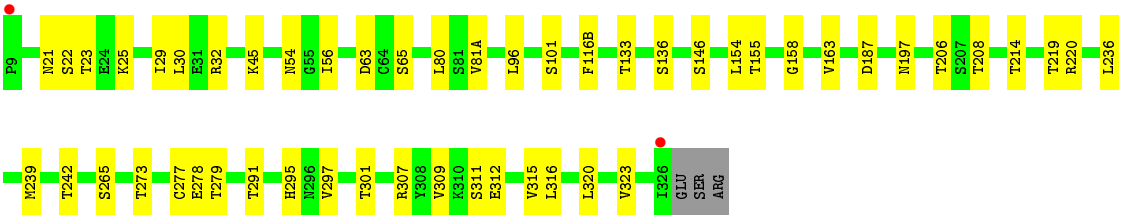
- Molecule 1: Hemagglutinin HA1

Chain C:

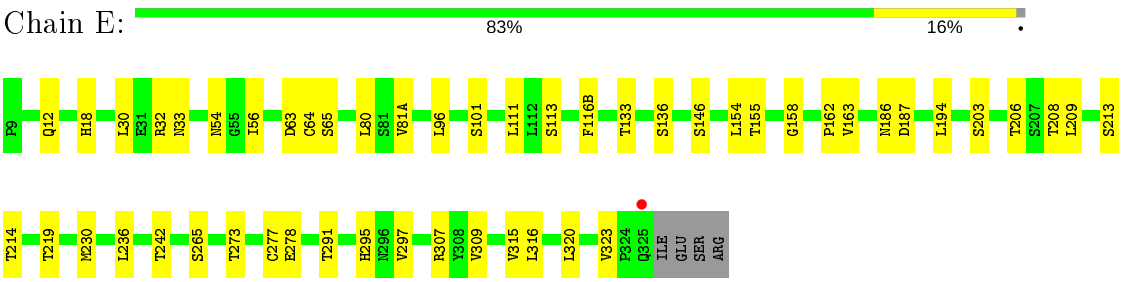


- Molecule 1: Hemagglutinin HA1

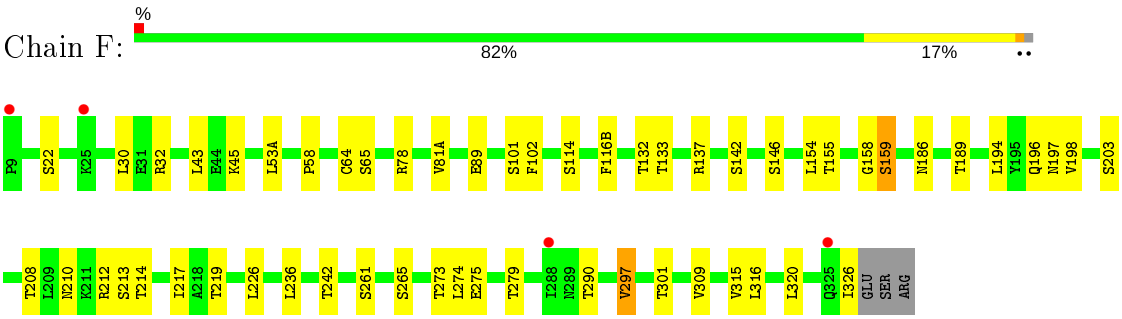
Chain D:



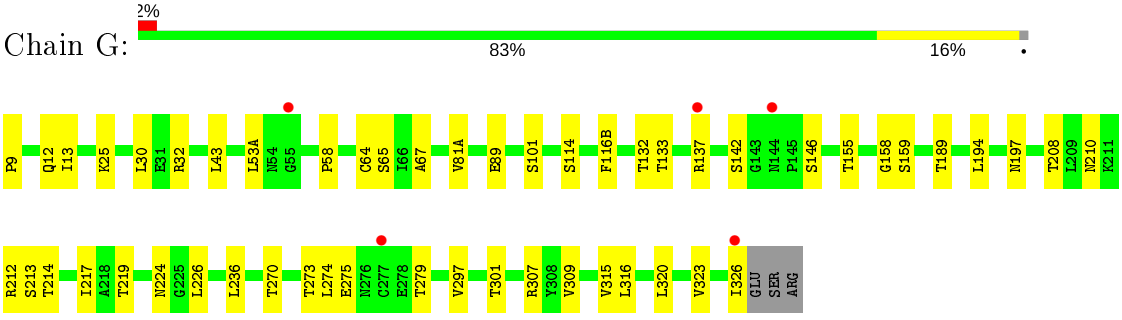
• Molecule 1: Hemagglutinin HA1



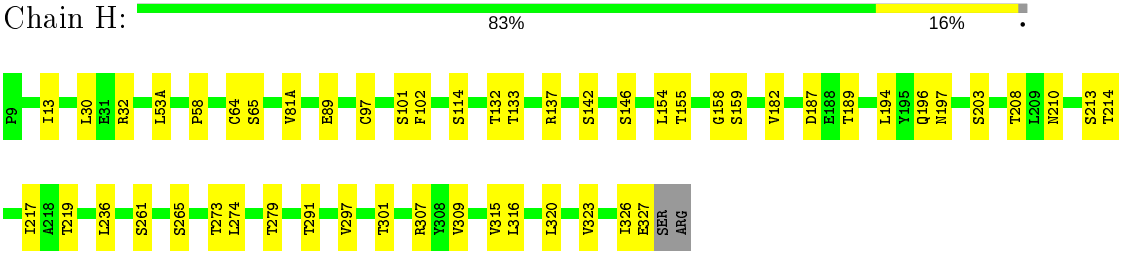
• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1

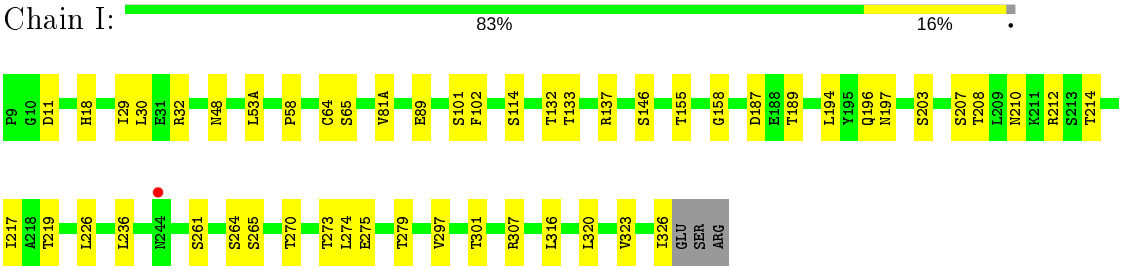


• Molecule 1: Hemagglutinin HA1



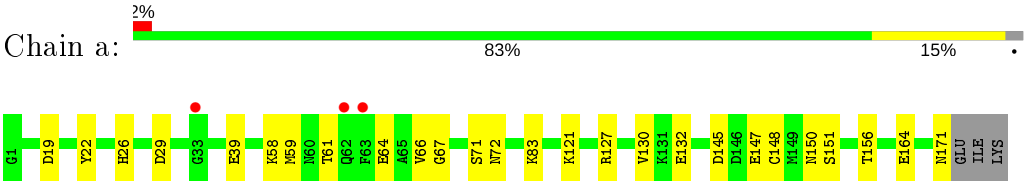
• Molecule 1: Hemagglutinin HA1

Chain I:



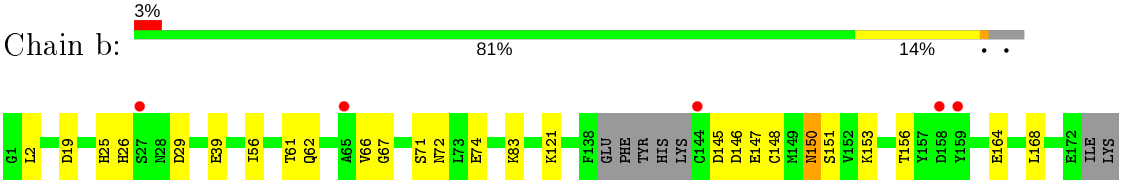
• Molecule 2: Hemagglutinin HA2

Chain a:



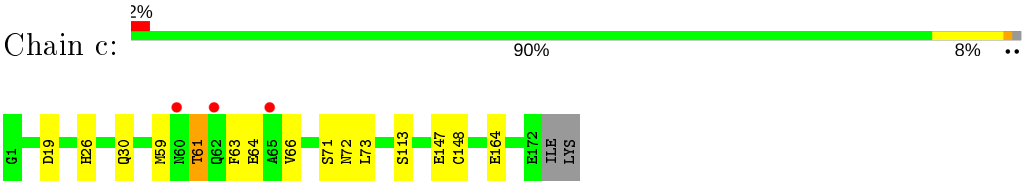
• Molecule 2: Hemagglutinin HA2

Chain b:



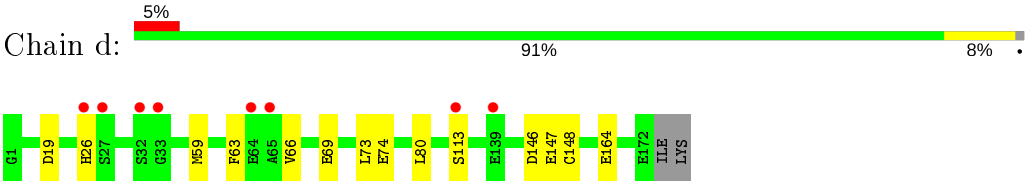
• Molecule 2: Hemagglutinin HA2

Chain c:



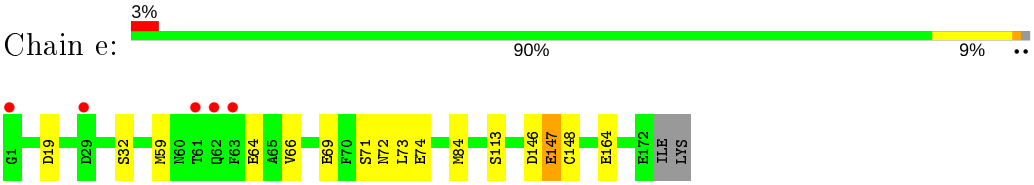
• Molecule 2: Hemagglutinin HA2

Chain d:



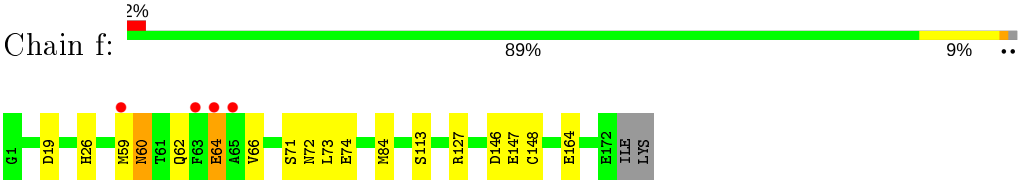
• Molecule 2: Hemagglutinin HA2

Chain e:



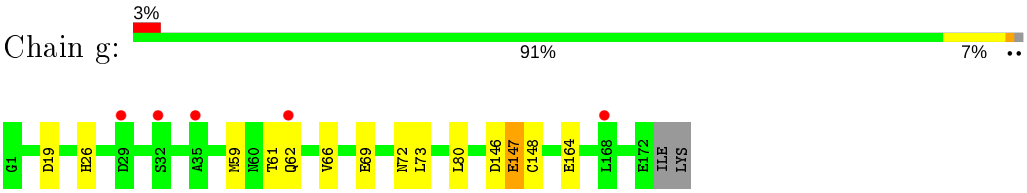
• Molecule 2: Hemagglutinin HA2

Chain f:



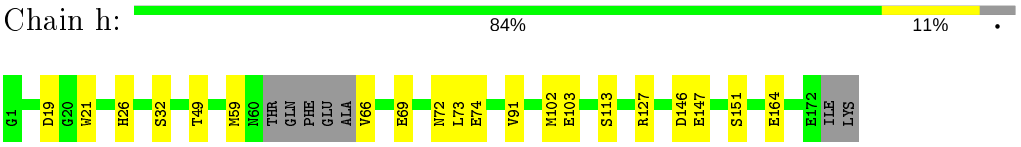
• Molecule 2: Hemagglutinin HA2

Chain g:



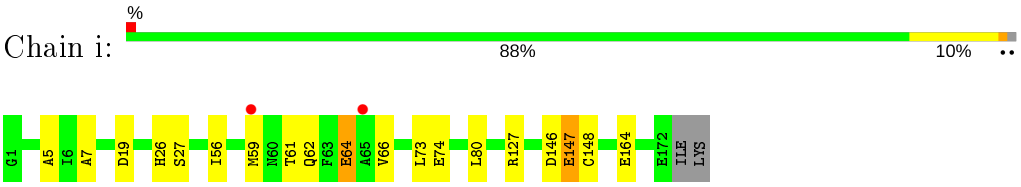
• Molecule 2: Hemagglutinin HA2

Chain h:



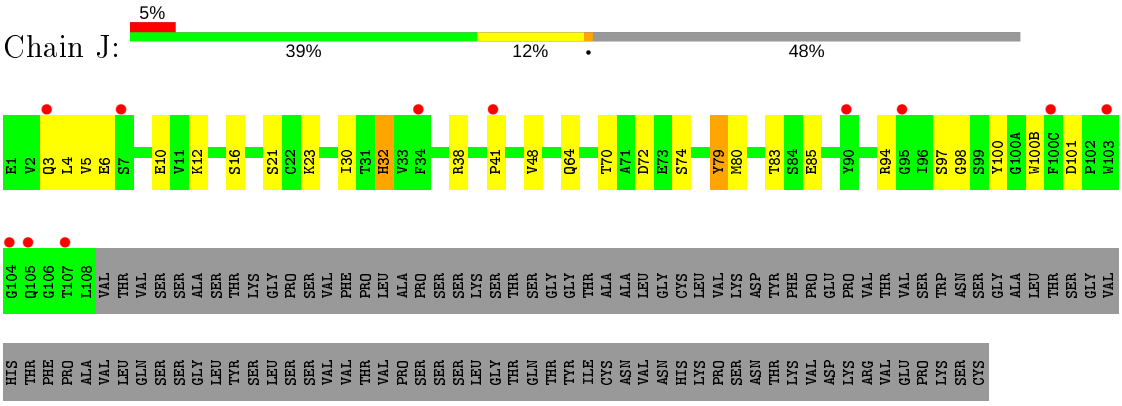
• Molecule 2: Hemagglutinin HA2

Chain i:



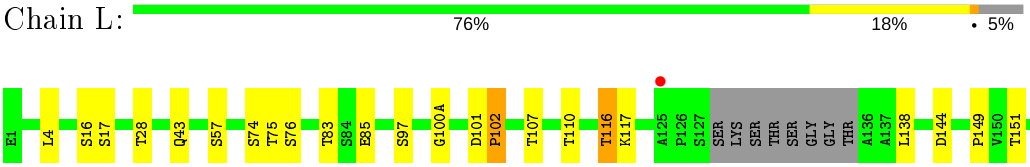
• Molecule 3: Fab 2G1 heavy chain

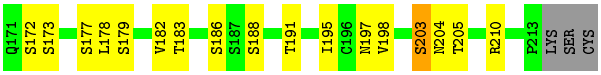
Chain J:



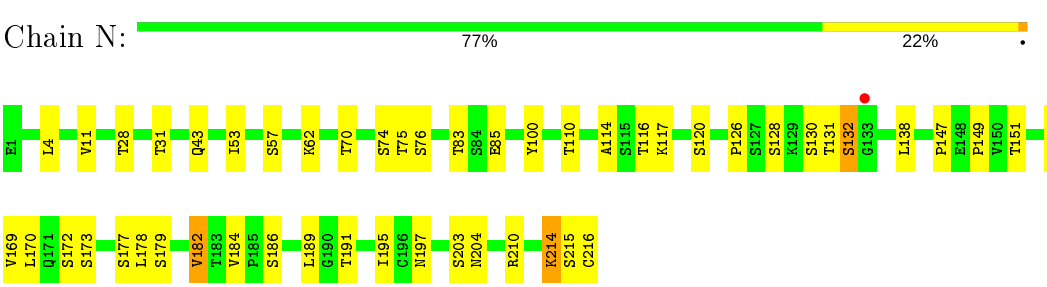
• Molecule 3: Fab 2G1 heavy chain

Chain L:

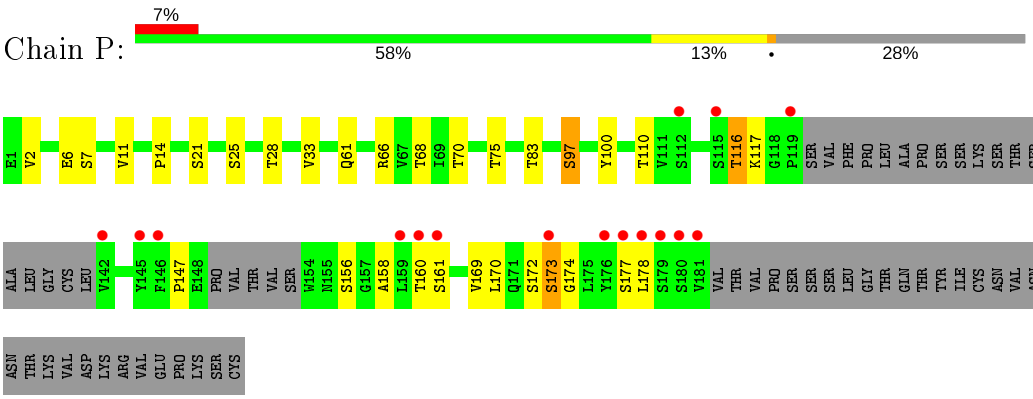




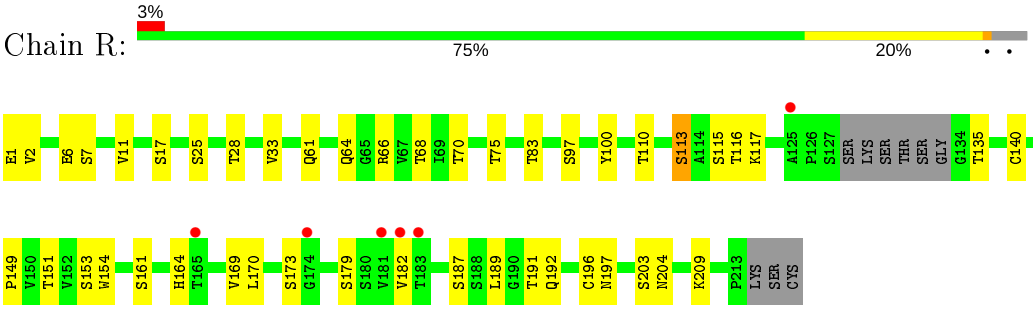
• Molecule 3: Fab 2G1 heavy chain



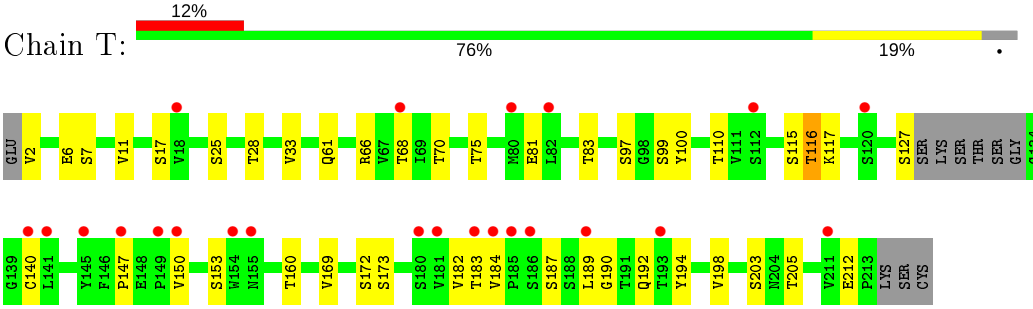
• Molecule 3: Fab 2G1 heavy chain



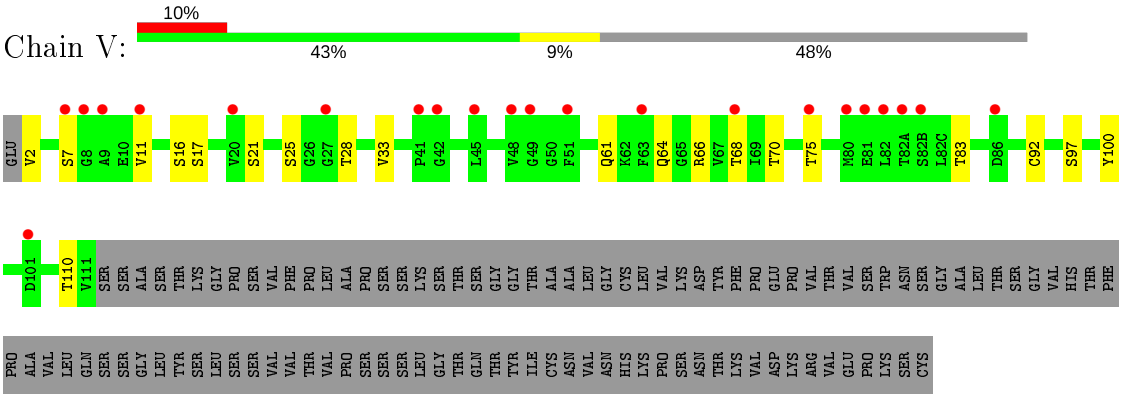
• Molecule 3: Fab 2G1 heavy chain



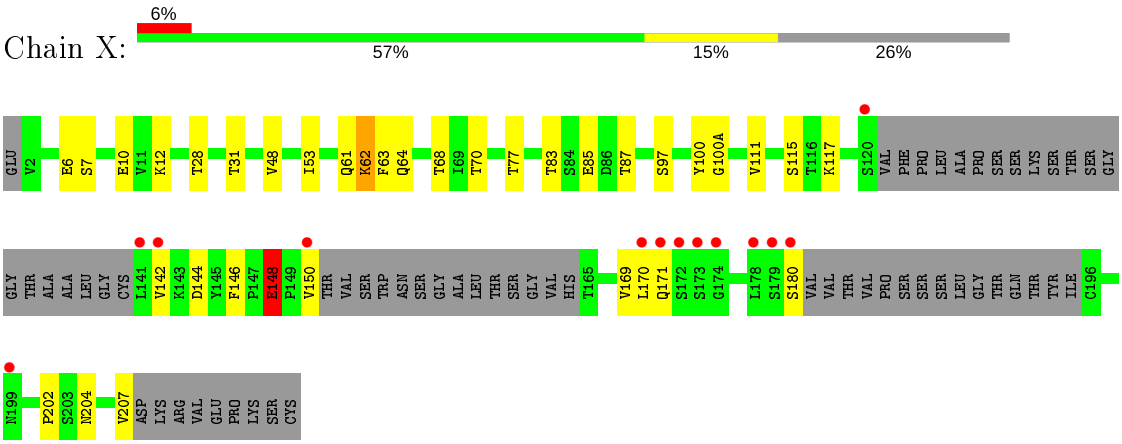
• Molecule 3: Fab 2G1 heavy chain



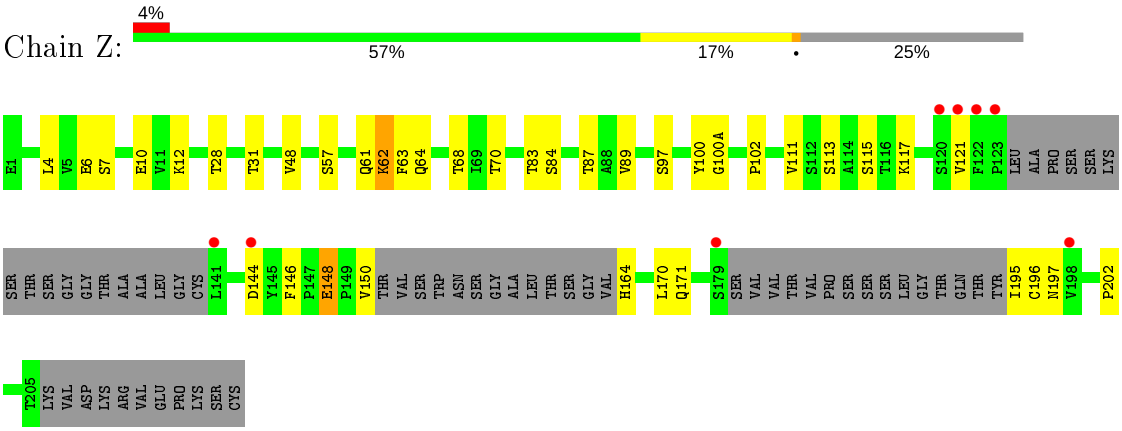
• Molecule 3: Fab 2G1 heavy chain



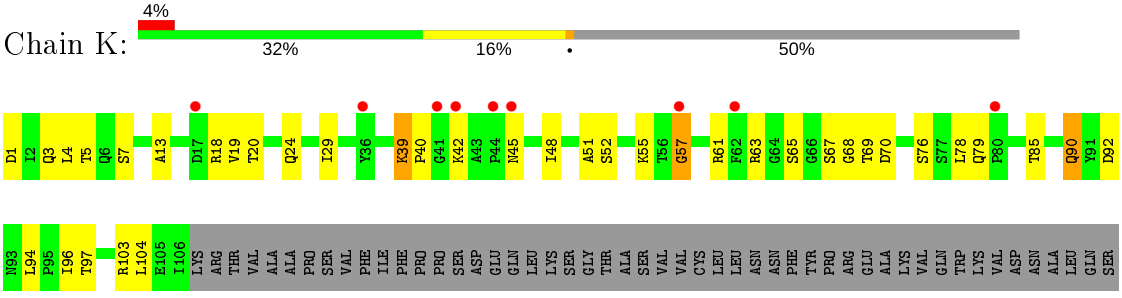
• Molecule 3: Fab 2G1 heavy chain



• Molecule 3: Fab 2G1 heavy chain

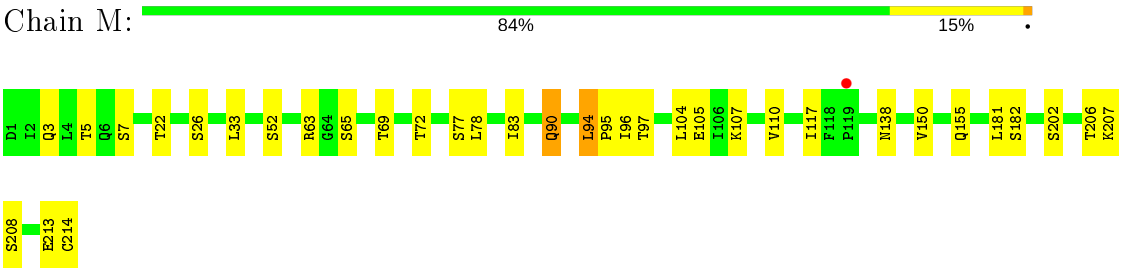


• Molecule 4: Fab 2G1 light chain



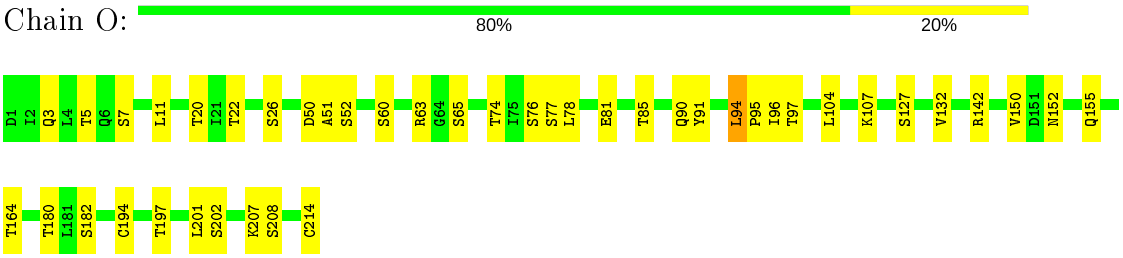
• Molecule 4: Fab 2G1 light chain

Chain M:



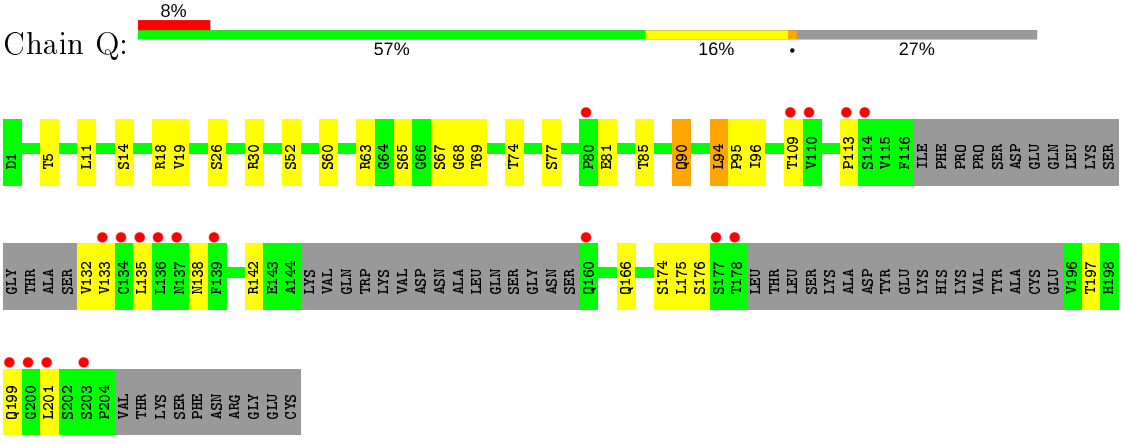
• Molecule 4: Fab 2G1 light chain

Chain O:



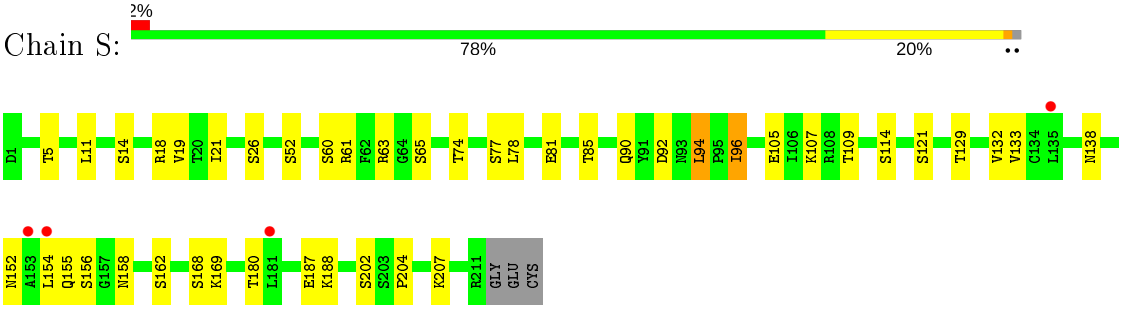
• Molecule 4: Fab 2G1 light chain

Chain Q:



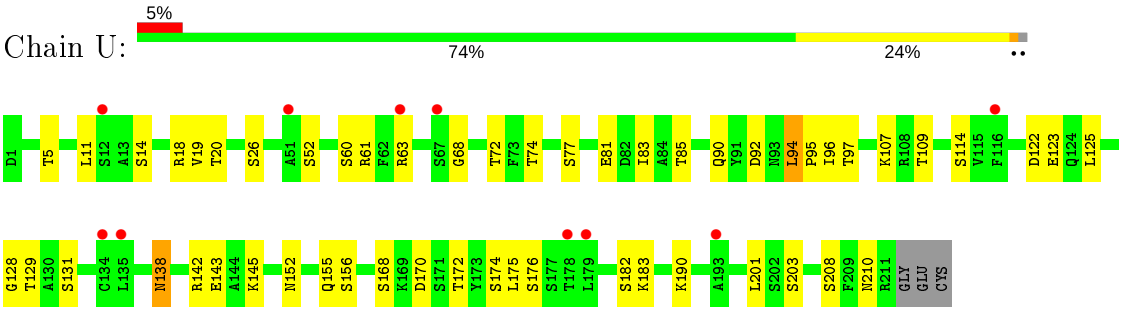
• Molecule 4: Fab 2G1 light chain

Chain S:



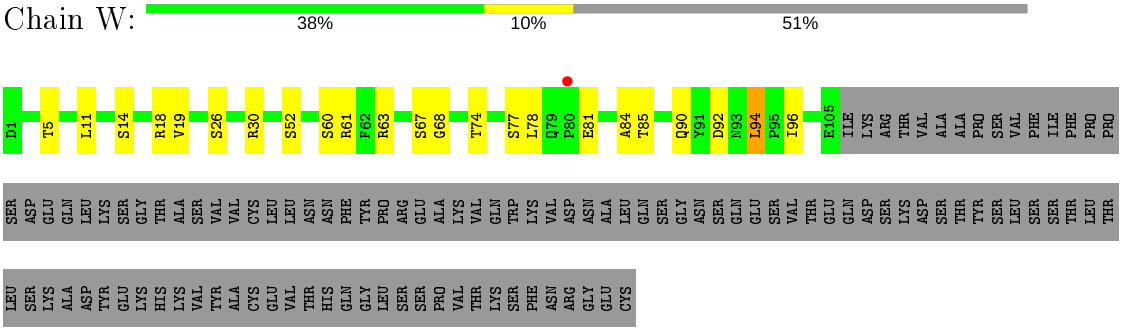
• Molecule 4: Fab 2G1 light chain

Chain U:



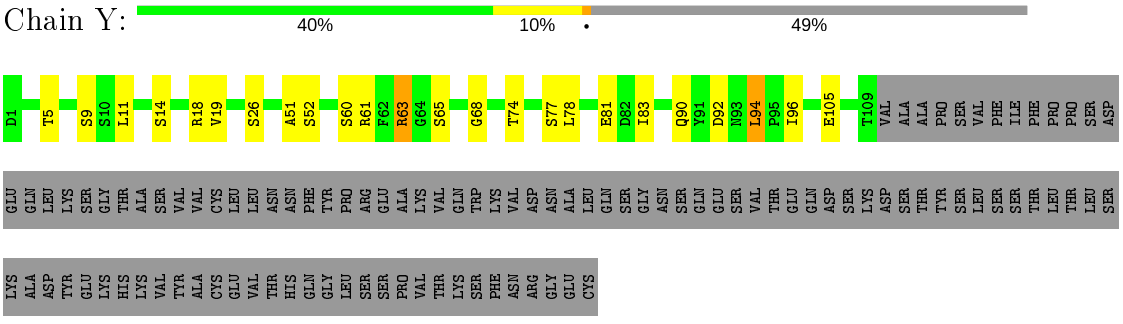
• Molecule 4: Fab 2G1 light chain

Chain W:



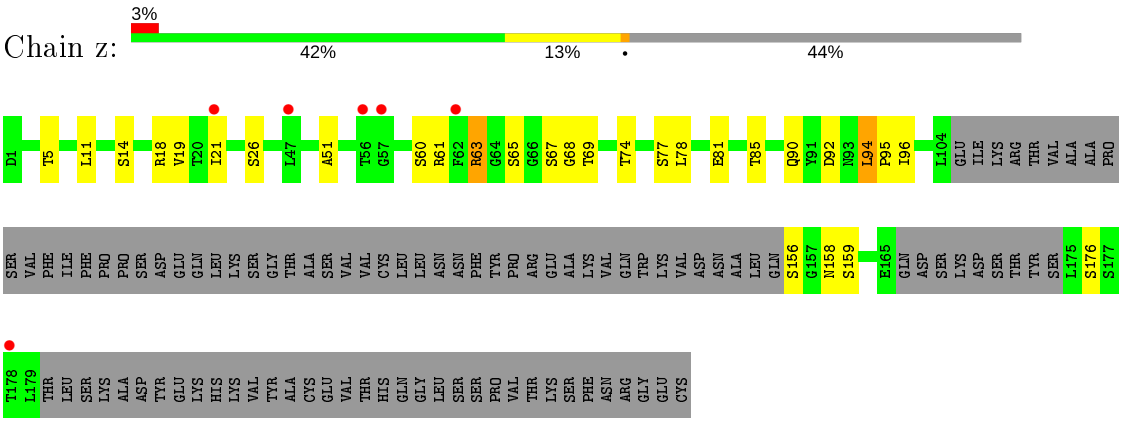
• Molecule 4: Fab 2G1 light chain

Chain Y:



• Molecule 4: Fab 2G1 light chain

Chain z:

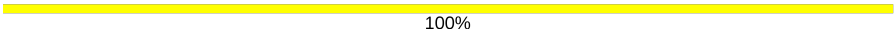


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

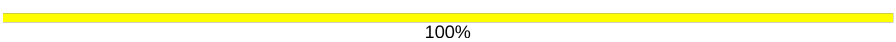
Chain o:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain q:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:

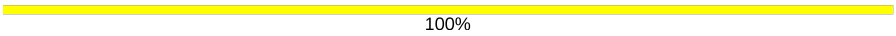


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:

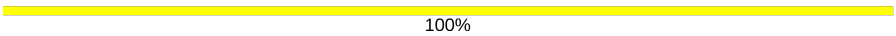


• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:

• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	126.84Å 133.14Å 812.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 3.20 50.01 – 3.16	Depositor EDS
% Data completeness (in resolution range)	90.2 (48.13-3.20) 87.4 (50.01-3.16)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.22 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.249 , 0.302 0.244 , 0.300	Depositor DCC
R_{free} test set	10355 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	58742	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG

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	0.51	1/2591 (0.0%)	0.68	0/3517
1	B	0.49	0/2562	0.69	0/3478
1	C	0.53	0/2599	0.74	1/3528 (0.0%)
1	D	0.44	0/2599	0.64	1/3528 (0.0%)
1	E	0.48	1/2591 (0.0%)	0.65	0/3517
1	F	0.44	1/2599 (0.0%)	0.62	0/3528
1	G	0.42	1/2599 (0.0%)	0.63	0/3528
1	H	0.50	1/2608 (0.0%)	0.69	0/3540
1	I	0.45	1/2599 (0.0%)	0.65	0/3528
2	a	0.44	0/1415	0.63	0/1900
2	b	0.45	0/1369	0.64	0/1837
2	c	0.44	0/1424	0.60	0/1912
2	d	0.43	0/1424	0.58	0/1912
2	e	0.48	0/1424	0.62	0/1912
2	f	0.47	0/1424	0.62	0/1912
2	g	0.45	0/1424	0.62	0/1912
2	h	0.55	0/1381	0.65	0/1852
2	i	0.56	0/1424	0.67	0/1912
3	J	0.49	0/893	0.69	0/1213
3	L	0.60	0/1618	0.78	1/2209 (0.0%)
3	N	0.63	0/1689	0.83	1/2304 (0.0%)
3	P	0.42	0/1237	0.59	0/1682
3	R	0.45	0/1629	0.66	0/2224
3	T	0.39	0/1620	0.61	0/2212
3	V	0.44	0/905	0.60	0/1231
3	X	0.51	0/1261	0.70	0/1713
3	Z	0.42	0/1294	0.64	0/1760
4	K	0.43	0/843	0.72	1/1146 (0.1%)
4	M	0.57	0/1695	0.75	0/2302
4	O	0.67	0/1695	0.85	1/2302 (0.0%)
4	Q	0.44	0/1239	0.65	0/1682
4	S	0.45	0/1676	0.66	1/2277 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
4	U	0.40	0/1676	0.60	0/2277
4	W	0.45	0/835	0.62	0/1135
4	Y	0.51	0/870	0.75	1/1181 (0.1%)
4	z	0.40	0/930	0.62	1/1261 (0.1%)
All	All	0.48	6/59661 (0.0%)	0.67	9/80864 (0.0%)

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
1	A	0	1
1	G	0	1
2	b	0	2
2	f	0	1
2	i	0	2
3	J	0	2
3	L	0	2
3	N	0	3
3	R	0	1
3	X	0	1
3	Z	0	1
4	K	0	4
4	M	0	2
4	O	0	1
4	Q	0	2
4	S	0	1
4	U	0	1
4	W	0	1
4	Y	0	1
4	z	0	1
All	All	0	31

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	CYS	CB-SG	-7.01	1.70	1.82
1	E	64	CYS	CB-SG	-5.99	1.72	1.81
1	G	64	CYS	CB-SG	-5.53	1.72	1.81
1	F	64	CYS	CB-SG	-5.51	1.72	1.81
1	I	64	CYS	CB-SG	-5.20	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	220	ARG	NE-CZ-NH2	6.90	123.75	120.30
4	K	57	GLY	N-CA-C	-6.43	97.01	113.10
4	z	63	ARG	NE-CZ-NH1	-6.29	117.16	120.30
4	Y	63	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	L	102	PRO	N-CA-C	-5.32	98.28	112.10

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	GLY	Peptide
1	G	9	PRO	Peptide
2	b	61	THR	Peptide
2	b	62	GLN	Peptide
2	f	60	ASN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	321/327 (98%)	292 (91%)	28 (9%)	1 (0%)	41 74
1	B	317/327 (97%)	283 (89%)	30 (10%)	4 (1%)	12 47
1	C	322/327 (98%)	288 (89%)	29 (9%)	5 (2%)	9 43
1	D	322/327 (98%)	293 (91%)	26 (8%)	3 (1%)	17 56
1	E	321/327 (98%)	291 (91%)	26 (8%)	4 (1%)	13 49
1	F	322/327 (98%)	288 (89%)	28 (9%)	6 (2%)	8 39

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	322/327 (98%)	285 (88%)	32 (10%)	5 (2%)	9 43
1	H	323/327 (99%)	286 (88%)	34 (10%)	3 (1%)	17 56
1	I	322/327 (98%)	287 (89%)	32 (10%)	3 (1%)	17 56
2	a	169/174 (97%)	143 (85%)	20 (12%)	6 (4%)	3 23
2	b	163/174 (94%)	135 (83%)	24 (15%)	4 (2%)	5 32
2	c	170/174 (98%)	147 (86%)	19 (11%)	4 (2%)	6 34
2	d	170/174 (98%)	147 (86%)	21 (12%)	2 (1%)	13 49
2	e	170/174 (98%)	154 (91%)	14 (8%)	2 (1%)	13 49
2	f	170/174 (98%)	144 (85%)	22 (13%)	4 (2%)	6 34
2	g	170/174 (98%)	148 (87%)	20 (12%)	2 (1%)	13 49
2	h	163/174 (94%)	143 (88%)	15 (9%)	5 (3%)	4 26
2	i	170/174 (98%)	144 (85%)	21 (12%)	5 (3%)	4 28
3	J	113/223 (51%)	80 (71%)	26 (23%)	7 (6%)	1 11
3	L	208/223 (93%)	186 (89%)	13 (6%)	9 (4%)	2 20
3	N	221/223 (99%)	200 (90%)	14 (6%)	7 (3%)	4 26
3	P	155/223 (70%)	134 (86%)	12 (8%)	9 (6%)	1 13
3	R	210/223 (94%)	185 (88%)	18 (9%)	7 (3%)	4 25
3	T	209/223 (94%)	184 (88%)	19 (9%)	6 (3%)	4 28
3	V	115/223 (52%)	106 (92%)	8 (7%)	1 (1%)	17 56
3	X	156/223 (70%)	129 (83%)	19 (12%)	8 (5%)	2 15
3	Z	159/223 (71%)	133 (84%)	16 (10%)	10 (6%)	1 10
4	K	104/214 (49%)	77 (74%)	17 (16%)	10 (10%)	0 3
4	M	212/214 (99%)	191 (90%)	18 (8%)	3 (1%)	11 46
4	O	212/214 (99%)	190 (90%)	18 (8%)	4 (2%)	8 39
4	Q	149/214 (70%)	125 (84%)	20 (13%)	4 (3%)	5 30
4	S	209/214 (98%)	182 (87%)	20 (10%)	7 (3%)	4 25
4	U	209/214 (98%)	177 (85%)	25 (12%)	7 (3%)	4 25
4	W	103/214 (48%)	89 (86%)	10 (10%)	4 (4%)	3 22
4	Y	107/214 (50%)	94 (88%)	9 (8%)	4 (4%)	3 22
4	z	113/214 (53%)	97 (86%)	11 (10%)	5 (4%)	2 19
All	All	7371/8442 (87%)	6457 (88%)	734 (10%)	180 (2%)	6 34

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	a	66	VAL
1	B	264	SER
2	c	61	THR
2	e	146	ASP
2	f	62	GLN

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	285/289 (99%)	236 (83%)	49 (17%)	2 10
1	B	282/289 (98%)	228 (81%)	54 (19%)	1 8
1	C	286/289 (99%)	241 (84%)	45 (16%)	2 12
1	D	286/289 (99%)	239 (84%)	47 (16%)	2 11
1	E	285/289 (99%)	239 (84%)	46 (16%)	2 11
1	F	286/289 (99%)	235 (82%)	51 (18%)	2 9
1	G	286/289 (99%)	241 (84%)	45 (16%)	2 12
1	H	287/289 (99%)	239 (83%)	48 (17%)	2 10
1	I	286/289 (99%)	239 (84%)	47 (16%)	2 11
2	a	148/151 (98%)	128 (86%)	20 (14%)	4 18
2	b	144/151 (95%)	123 (85%)	21 (15%)	3 15
2	c	149/151 (99%)	137 (92%)	12 (8%)	11 42
2	d	149/151 (99%)	137 (92%)	12 (8%)	11 42
2	e	149/151 (99%)	134 (90%)	15 (10%)	7 29
2	f	149/151 (99%)	134 (90%)	15 (10%)	7 29
2	g	149/151 (99%)	136 (91%)	13 (9%)	10 37
2	h	145/151 (96%)	130 (90%)	15 (10%)	7 29
2	i	149/151 (99%)	135 (91%)	14 (9%)	8 33
3	J	91/185 (49%)	70 (77%)	21 (23%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	176/185 (95%)	142 (81%)	34 (19%)	1 8
3	N	185/185 (100%)	142 (77%)	43 (23%)	1 3
3	P	130/185 (70%)	104 (80%)	26 (20%)	1 6
3	R	177/185 (96%)	136 (77%)	41 (23%)	1 3
3	T	176/185 (95%)	138 (78%)	38 (22%)	1 5
3	V	93/185 (50%)	74 (80%)	19 (20%)	1 6
3	X	136/185 (74%)	106 (78%)	30 (22%)	1 4
3	Z	139/185 (75%)	109 (78%)	30 (22%)	1 5
4	K	93/190 (49%)	67 (72%)	26 (28%)	0 1
4	M	190/190 (100%)	158 (83%)	32 (17%)	2 10
4	O	190/190 (100%)	152 (80%)	38 (20%)	1 6
4	Q	140/190 (74%)	108 (77%)	32 (23%)	1 4
4	S	188/190 (99%)	151 (80%)	37 (20%)	1 7
4	U	188/190 (99%)	141 (75%)	47 (25%)	0 2
4	W	92/190 (48%)	73 (79%)	19 (21%)	1 6
4	Y	96/190 (50%)	76 (79%)	20 (21%)	1 6
4	z	105/190 (55%)	81 (77%)	24 (23%)	1 4
All	All	6485/7335 (88%)	5359 (83%)	1126 (17%)	2 10

5 of 1126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	18	HIS
3	L	117	LYS
3	X	115	SER
1	I	146	SER
3	J	5	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	295	HIS
2	i	125	GLN
4	Y	90	GLN
2	h	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	K	34	ASN

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

24 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	j	1	1,5	14,14,15	0.56	0	17,19,21	1.24	1 (5%)
5	NAG	j	2	5	14,14,15	0.62	0	17,19,21	0.81	0
5	NAG	k	1	1,5	14,14,15	0.53	0	17,19,21	1.09	1 (5%)
5	NAG	k	2	5	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
6	NAG	l	1	1,6	14,14,15	0.62	0	17,19,21	1.68	3 (17%)
6	NAG	l	2	6	14,14,15	0.53	0	17,19,21	1.00	0
6	BMA	l	3	6	11,11,12	0.56	0	15,15,17	1.38	1 (6%)
5	NAG	m	1	1,5	14,14,15	0.50	0	17,19,21	1.22	2 (11%)
5	NAG	m	2	5	14,14,15	0.59	0	17,19,21	0.71	0
5	NAG	n	1	1,5	14,14,15	0.62	0	17,19,21	1.50	3 (17%)
5	NAG	n	2	5	14,14,15	0.57	0	17,19,21	0.97	0
5	NAG	o	1	1,5	14,14,15	0.62	0	17,19,21	1.63	2 (11%)
5	NAG	o	2	5	14,14,15	0.42	0	17,19,21	1.19	1 (5%)
6	NAG	p	1	1,6	14,14,15	0.63	0	17,19,21	1.04	1 (5%)
6	NAG	p	2	6	14,14,15	0.54	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	p	3	6	11,11,12	0.67	0	15,15,17	1.15	2 (13%)
5	NAG	q	1	1,5	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
5	NAG	q	2	5	14,14,15	0.55	0	17,19,21	0.84	0
5	NAG	r	1	1,5	14,14,15	0.50	0	17,19,21	1.42	2 (11%)
5	NAG	r	2	5	14,14,15	0.53	0	17,19,21	0.76	1 (5%)
5	NAG	s	1	1,5	14,14,15	0.48	0	17,19,21	1.39	1 (5%)
5	NAG	s	2	5	14,14,15	0.51	0	17,19,21	0.71	0
5	NAG	t	1	1,5	14,14,15	0.47	0	17,19,21	1.03	1 (5%)
5	NAG	t	2	5	14,14,15	0.48	0	17,19,21	1.28	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	j	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	j	2	5	-	4/6/23/26	0/1/1/1
5	NAG	k	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	k	2	5	-	2/6/23/26	0/1/1/1
6	NAG	l	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	l	2	6	-	2/6/23/26	0/1/1/1
6	BMA	l	3	6	-	2/2/19/22	0/1/1/1
5	NAG	m	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	m	2	5	-	2/6/23/26	0/1/1/1
5	NAG	n	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	n	2	5	-	4/6/23/26	0/1/1/1
5	NAG	o	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	o	2	5	-	2/6/23/26	0/1/1/1
6	NAG	p	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	p	2	6	-	2/6/23/26	0/1/1/1
6	BMA	p	3	6	-	2/2/19/22	0/1/1/1
5	NAG	q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	q	2	5	-	0/6/23/26	0/1/1/1
5	NAG	r	1	1,5	-	6/6/23/26	0/1/1/1
5	NAG	r	2	5	-	2/6/23/26	0/1/1/1
5	NAG	s	1	1,5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	s	2	5	-	2/6/23/26	0/1/1/1
5	NAG	t	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	l	1	NAG	C2-N2-C7	-4.92	115.90	122.90
5	o	1	NAG	C2-N2-C7	-4.73	116.16	122.90
6	l	3	BMA	O5-C5-C6	4.37	114.05	107.20
5	n	1	NAG	C2-N2-C7	3.77	128.27	122.90
5	r	1	NAG	C3-C4-C5	3.73	116.89	110.24

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	t	1	NAG	C8-C7-N2-C2
5	t	1	NAG	O7-C7-N2-C2
5	r	1	NAG	C8-C7-N2-C2
5	r	1	NAG	O7-C7-N2-C2
5	o	1	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	E	401	1	14,14,15	0.51	0	17,19,21	1.30	3 (17%)
7	NAG	C	404	1	14,14,15	1.71	2 (14%)	17,19,21	2.63	4 (23%)
7	NAG	A	403	1	14,14,15	0.47	0	17,19,21	1.37	2 (11%)
7	NAG	F	403	1	14,14,15	0.38	0	17,19,21	1.25	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	E	401	1	-	1/6/23/26	0/1/1/1
7	NAG	C	404	1	-	3/6/23/26	0/1/1/1
7	NAG	A	403	1	-	2/6/23/26	0/1/1/1
7	NAG	F	403	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	404	NAG	C1-C2	3.82	1.58	1.52
7	C	404	NAG	O5-C5	3.69	1.50	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	404	NAG	C1-O5-C5	9.67	125.29	112.19
7	A	403	NAG	C1-O5-C5	3.64	117.12	112.19
7	F	403	NAG	C1-O5-C5	3.31	116.67	112.19
7	E	401	NAG	C1-O5-C5	2.93	116.16	112.19
7	F	403	NAG	O5-C5-C6	2.73	111.48	107.20

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	403	NAG	C8-C7-N2-C2
7	A	403	NAG	O7-C7-N2-C2
7	C	404	NAG	O5-C5-C6-O6
7	C	404	NAG	C8-C7-N2-C2
7	F	403	NAG	C8-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	323/327 (98%)	-0.34	0 100 100	20, 53, 91, 130	0
1	B	319/327 (97%)	-0.18	2 (0%) 89 83	25, 60, 101, 142	0
1	C	324/327 (99%)	-0.25	2 (0%) 89 83	21, 58, 98, 133	0
1	D	324/327 (99%)	-0.20	2 (0%) 89 83	38, 66, 99, 168	0
1	E	323/327 (98%)	-0.25	1 (0%) 94 92	45, 68, 97, 125	0
1	F	324/327 (99%)	-0.07	4 (1%) 79 67	45, 76, 107, 138	0
1	G	324/327 (99%)	0.17	5 (1%) 73 61	46, 82, 124, 162	0
1	H	325/327 (99%)	-0.40	0 100 100	31, 53, 82, 122	0
1	I	324/327 (99%)	-0.13	1 (0%) 94 92	42, 75, 107, 127	0
2	a	171/174 (98%)	-0.02	3 (1%) 68 55	25, 75, 130, 168	0
2	b	167/174 (95%)	0.02	5 (2%) 50 34	24, 79, 138, 179	0
2	c	172/174 (98%)	-0.02	3 (1%) 70 57	30, 79, 134, 176	0
2	d	172/174 (98%)	0.32	8 (4%) 31 19	43, 91, 149, 196	0
2	e	172/174 (98%)	-0.05	5 (2%) 51 36	38, 69, 123, 176	0
2	f	172/174 (98%)	-0.03	4 (2%) 60 47	46, 74, 125, 195	0
2	g	172/174 (98%)	0.09	5 (2%) 51 36	43, 81, 145, 169	0
2	h	167/174 (95%)	-0.28	0 100 100	35, 49, 85, 134	0
2	i	172/174 (98%)	-0.27	2 (1%) 79 67	33, 55, 122, 187	0
3	J	115/223 (51%)	0.68	11 (9%) 8 4	46, 94, 132, 166	0
3	L	212/223 (95%)	-0.34	1 (0%) 91 86	20, 38, 99, 134	0
3	N	223/223 (100%)	-0.37	1 (0%) 92 89	14, 28, 73, 129	0
3	P	161/223 (72%)	0.40	16 (9%) 7 4	52, 90, 147, 172	0
3	R	214/223 (95%)	0.17	7 (3%) 46 30	45, 83, 114, 128	0
3	T	213/223 (95%)	0.76	26 (12%) 4 2	62, 107, 153, 233	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	V	117/223 (52%)	1.22	22 (18%) 1 1	66, 122, 174, 221	0
3	X	164/223 (73%)	0.16	13 (7%) 12 6	35, 67, 110, 147	0
3	Z	167/223 (74%)	0.05	8 (4%) 30 18	59, 95, 128, 180	0
4	K	106/214 (49%)	0.48	9 (8%) 10 6	63, 111, 145, 173	0
4	M	214/214 (100%)	-0.22	1 (0%) 91 86	19, 42, 96, 150	0
4	O	214/214 (100%)	-0.50	0 100 100	16, 30, 52, 70	0
4	Q	157/214 (73%)	0.33	18 (11%) 4 3	49, 90, 134, 161	0
4	S	211/214 (98%)	0.00	4 (1%) 66 53	52, 77, 123, 185	0
4	U	211/214 (98%)	0.46	10 (4%) 31 19	66, 104, 141, 162	0
4	W	105/214 (49%)	0.05	1 (0%) 82 72	57, 88, 125, 148	0
4	Y	109/214 (50%)	-0.42	0 100 100	36, 51, 76, 98	0
4	z	119/214 (55%)	0.46	6 (5%) 28 16	61, 98, 140, 161	0
All	All	7479/8442 (88%)	-0.02	206 (2%) 53 37	14, 70, 129, 233	0

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	134	CYS	7.3
3	T	185	PRO	6.4
3	T	180	SER	6.3
3	T	183	THR	5.8
3	V	48	VAL	5.6

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	BMA	l	3	11/12	0.61	0.31	109,140,145,148	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	s	2	14/15	0.72	0.46	148,157,164,167	0
5	NAG	o	2	14/15	0.81	0.30	97,113,122,124	0
5	NAG	t	2	14/15	0.82	0.22	82,103,118,122	0
5	NAG	n	2	14/15	0.83	0.25	101,113,121,122	0
5	NAG	k	2	14/15	0.84	0.22	125,133,136,140	0
6	BMA	p	3	11/12	0.85	0.15	117,121,132,137	0
5	NAG	j	2	14/15	0.85	0.26	90,107,119,121	0
5	NAG	r	2	14/15	0.86	0.34	94,108,128,135	0
5	NAG	s	1	14/15	0.86	0.26	88,112,125,131	0
5	NAG	k	1	14/15	0.86	0.17	63,92,107,114	0
6	NAG	l	2	14/15	0.86	0.34	88,117,138,139	0
5	NAG	q	2	14/15	0.88	0.41	98,107,122,125	0
6	NAG	p	2	14/15	0.88	0.18	93,112,127,132	0
5	NAG	m	2	14/15	0.88	0.17	85,111,119,120	0
5	NAG	o	1	14/15	0.89	0.26	60,82,88,96	0
5	NAG	n	1	14/15	0.91	0.17	60,86,97,102	0
6	NAG	l	1	14/15	0.92	0.29	56,81,94,108	0
5	NAG	q	1	14/15	0.92	0.14	50,75,92,93	0
6	NAG	p	1	14/15	0.93	0.18	84,97,101,102	0
5	NAG	t	1	14/15	0.93	0.22	68,81,87,88	0
5	NAG	m	1	14/15	0.93	0.10	61,84,89,97	0
5	NAG	j	1	14/15	0.94	0.24	72,88,97,98	0
5	NAG	r	1	14/15	0.95	0.17	61,80,90,101	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	C	404	14/15	0.75	0.37	116,126,129,130	0
7	NAG	E	401	14/15	0.79	0.24	80,99,105,113	0
7	NAG	A	403	14/15	0.90	0.32	75,97,108,109	0
7	NAG	F	403	14/15	0.93	0.24	68,81,94,96	0

6.5 Other polymers

There are no such residues in this entry.