



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 09:01 am GMT

PDB ID : 4FQR
Title : Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-06-25
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28972

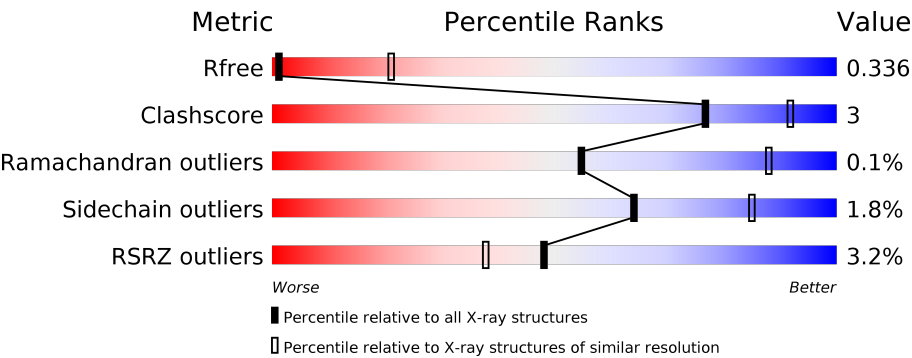
1 Overall quality at a glance i

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}	100719	1153 (4.60-3.60)
Clashscore	112137	1002 (4.54-3.66)
Ramachandran outliers	110173	1000 (4.58-3.62)
Sidechain outliers	110143	1191 (4.60-3.60)
RSRZ outliers	101464	1165 (4.60-3.60)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	323	<div><div>3%</div><div>95%</div><div>6%</div><div>• •</div></div>
1	C	323	<div><div>2%</div><div>95%</div><div>6%</div><div>• •</div></div>
1	E	323	<div><div>3%</div><div>95%</div><div>6%</div><div>• •</div></div>
1	G	323	<div><div>3%</div><div>95%</div><div>6%</div><div>• •</div></div>
1	I	323	<div><div>3%</div><div>92%</div><div>6%</div><div>• •</div></div>
1	K	323	<div><div>0%</div><div>95%</div><div>6%</div><div>• •</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	323	
1	O	323	
1	Q	323	
1	S	323	
1	U	323	
1	W	323	
2	B	174	
2	D	174	
2	F	174	
2	H	174	
2	J	174	
2	L	174	
2	N	174	
2	P	174	
2	R	174	
2	T	174	
2	V	174	
2	X	174	
3	a	241	
3	c	241	
3	e	241	
3	g	241	
3	i	241	
3	k	241	
3	m	241	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	o	241	
3	q	241	
3	s	241	
3	u	241	
3	w	241	
4	b	214	
4	d	214	
4	f	214	
4	h	214	
4	j	214	
4	l	214	
4	n	214	
4	p	214	
4	r	214	
4	t	214	
4	v	214	
4	x	214	

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	A	601	-	-	-	X
5	NAG	C	501	-	-	-	X
5	NAG	D	201	-	-	-	X
5	NAG	G	502	-	-	-	X
5	NAG	O	501	-	-	-	X
5	NAG	S	501	-	-	-	X
5	NAG	T	201	-	-	-	X
6	NAG	A	602	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	K	603	-	-	-	X
6	NAG	O	504	-	-	-	X
7	NAG	U	507	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 90792 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	C	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	E	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	G	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	I	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	K	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	M	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	O	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	Q	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	S	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	U	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	W	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
A	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
A	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
A	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
C	7	ALA	-	EXPRESSION TAG	UNP Q91MA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
C	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
C	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
E	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
E	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
E	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
E	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
G	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
G	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
G	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
G	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
I	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
I	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
I	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
I	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
K	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
K	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
K	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
K	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
M	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
M	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
M	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
M	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
O	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
O	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
O	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
O	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
Q	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
Q	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
Q	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
Q	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
S	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
S	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
S	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
S	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
U	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
U	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
U	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
U	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
W	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
W	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
W	9	PRO	-	EXPRESSION TAG	UNP Q91MA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
W	10	GLY	-	EXPRESSION TAG	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	D	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	F	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	H	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	J	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	L	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	N	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	P	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	R	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	T	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	V	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	X	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
H	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
J	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
L	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
N	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
P	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
R	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
V	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
X	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Broadly neutralizing antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	c	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	e	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	g	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	i	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	k	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	m	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	o	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	q	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	s	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	u	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	w	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			

- Molecule 4 is a protein called Broadly neutralizing antibody C05, light chain.

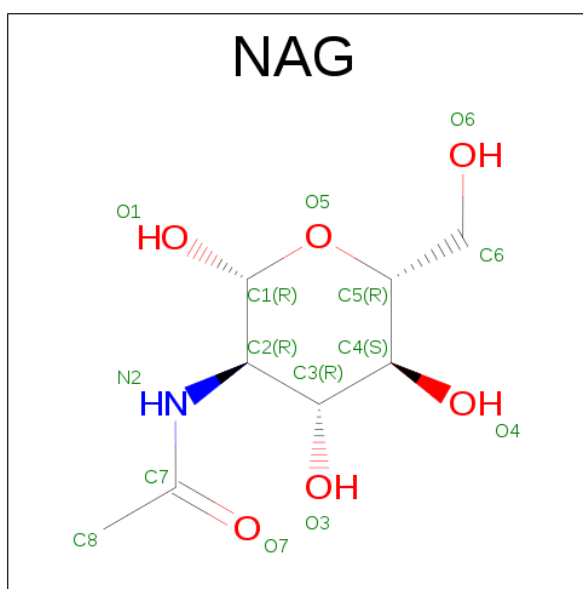
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	d	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	f	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	h	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	l	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	n	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	p	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	r	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	t	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	v	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	x	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	R	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	T	1	Total	C	N	O	0	0
			14	8	1	5		
5	U	1	Total	C	N	O	0	0
			14	8	1	5		
5	U	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	W	1	Total	C	N	O	0	0
			14	8	1	5		
5	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			50	28	2	20		
6	C	4	Total	C	N	O	0	0
			50	28	2	20		
6	E	4	Total	C	N	O	0	0
			50	28	2	20		
6	G	4	Total	C	N	O	0	0
			50	28	2	20		
6	I	4	Total	C	N	O	0	0
			50	28	2	20		
6	K	4	Total	C	N	O	0	0
			50	28	2	20		
6	M	4	Total	C	N	O	0	0
			50	28	2	20		
6	O	4	Total	C	N	O	0	0
			50	28	2	20		
6	Q	4	Total	C	N	O	0	0
			50	28	2	20		
6	S	4	Total	C	N	O	0	0
			50	28	2	20		
6	U	4	Total	C	N	O	0	0
			50	28	2	20		
6	W	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total	C	N	O	0	0
			28	16	2	10		
7	C	2	Total	C	N	O	0	0
			28	16	2	10		
7	E	2	Total	C	N	O	0	0
			28	16	2	10		
7	G	2	Total	C	N	O	0	0
			28	16	2	10		
7	I	2	Total	C	N	O	0	0
			28	16	2	10		
7	K	2	Total	C	N	O	0	0
			28	16	2	10		
7	M	2	Total	C	N	O	0	0
			28	16	2	10		
7	O	2	Total	C	N	O	0	0
			28	16	2	10		
7	Q	2	Total	C	N	O	0	0
			28	16	2	10		
7	S	2	Total	C	N	O	0	0
			28	16	2	10		
7	U	2	Total	C	N	O	0	0
			28	16	2	10		
7	W	2	Total	C	N	O	0	0
			28	16	2	10		

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: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain



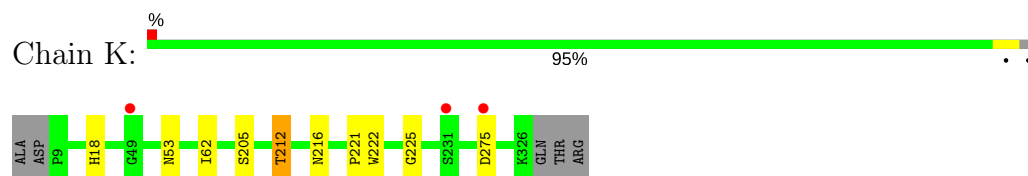
- Molecule 1: Hemagglutinin HA1 chain



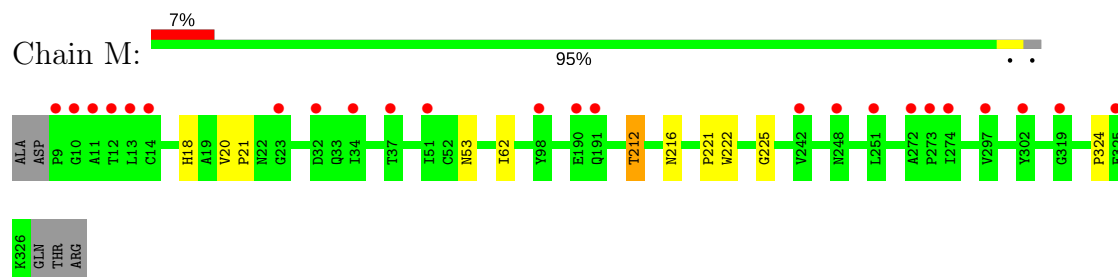
- Molecule 1: Hemagglutinin HA1 chain



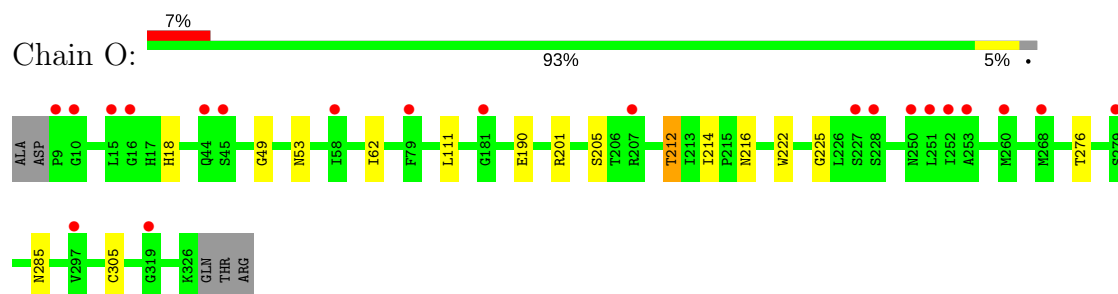
- Molecule 1: Hemagglutinin HA1 chain



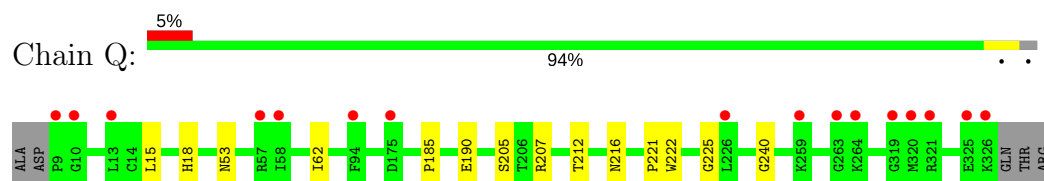
- Molecule 1: Hemagglutinin HA1 chain



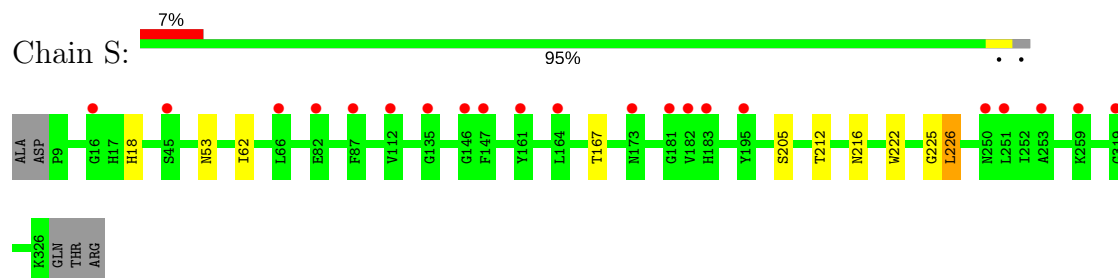
- Molecule 1: Hemagglutinin HA1 chain



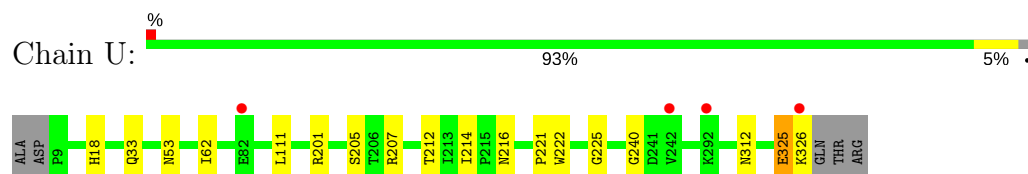
- Molecule 1: Hemagglutinin HA1 chain



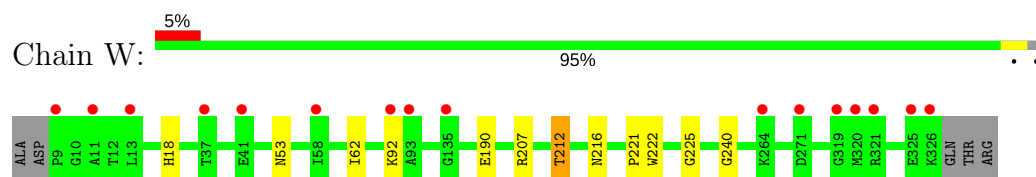
- Molecule 1: Hemagglutinin HA1 chain



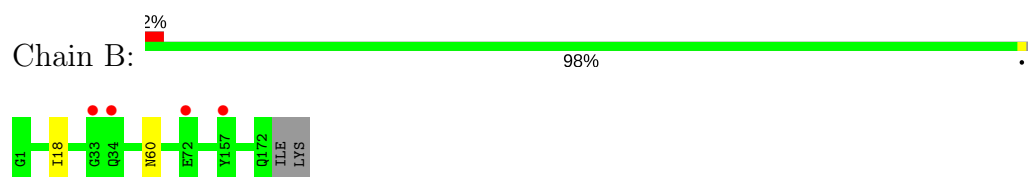
- Molecule 1: Hemagglutinin HA1 chain



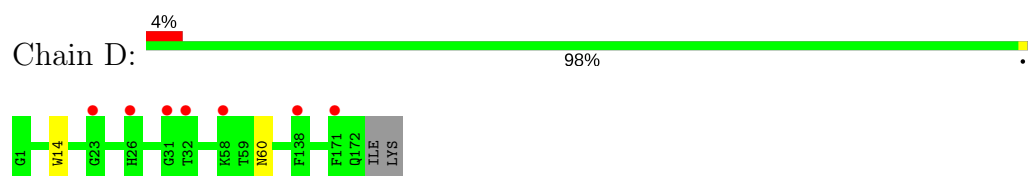
- Molecule 1: Hemagglutinin HA1 chain



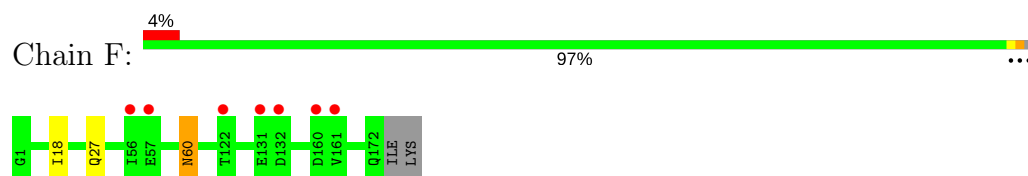
- Molecule 2: Hemagglutinin HA2 chain



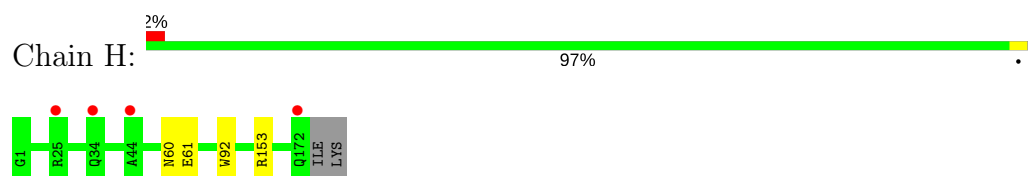
- Molecule 2: Hemagglutinin HA2 chain



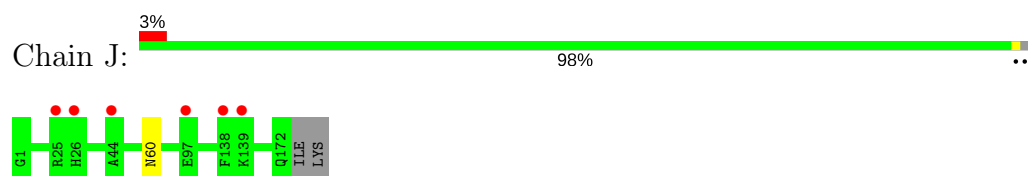
- Molecule 2: Hemagglutinin HA2 chain



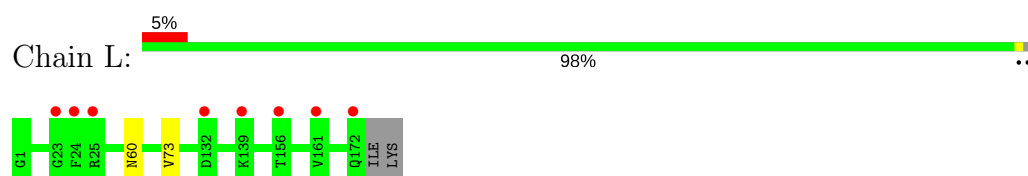
- Molecule 2: Hemagglutinin HA2 chain



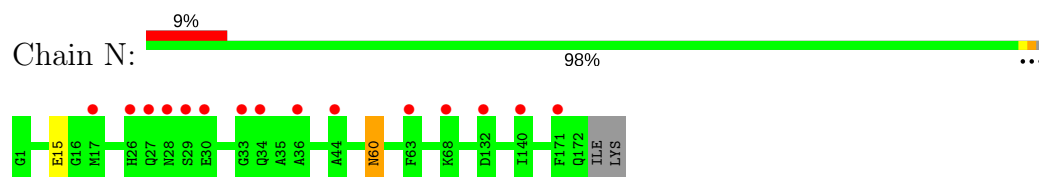
- Molecule 2: Hemagglutinin HA2 chain



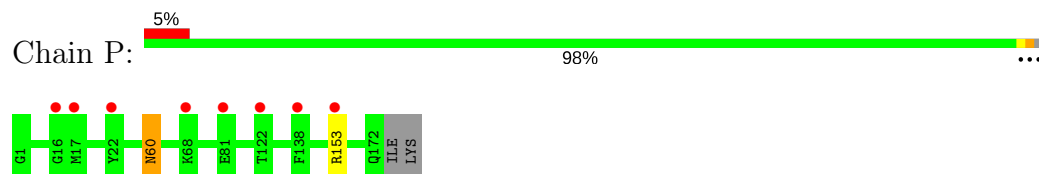
- Molecule 2: Hemagglutinin HA2 chain



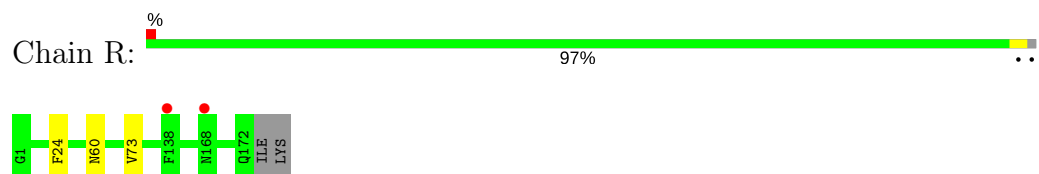
● Molecule 2: Hemagglutinin HA2 chain



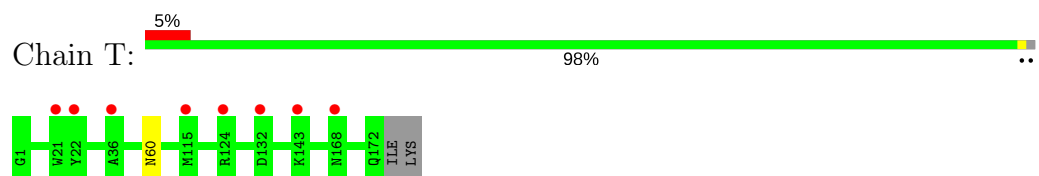
● Molecule 2: Hemagglutinin HA2 chain



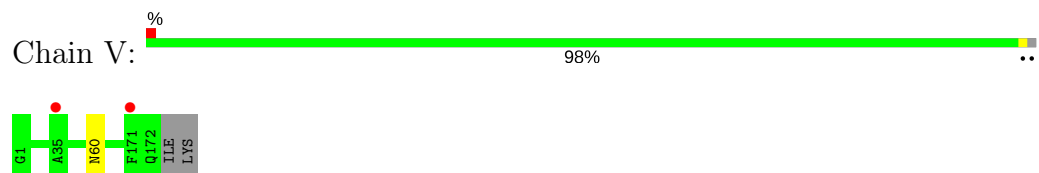
● Molecule 2: Hemagglutinin HA2 chain



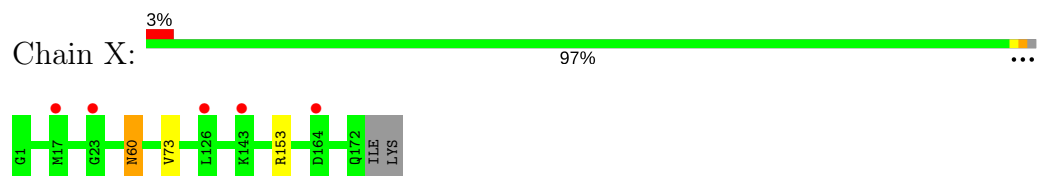
● Molecule 2: Hemagglutinin HA2 chain



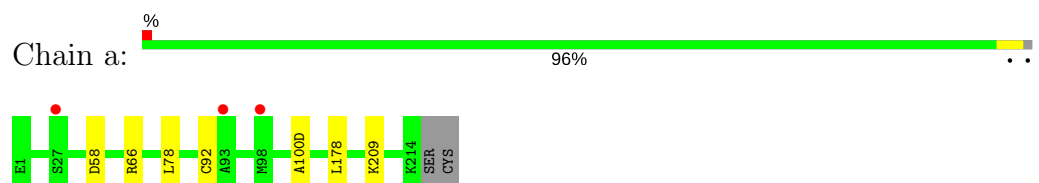
● Molecule 2: Hemagglutinin HA2 chain



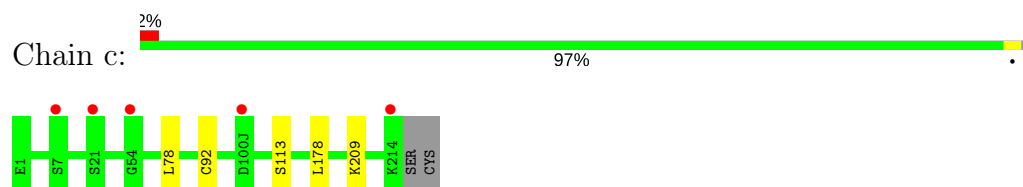
● Molecule 2: Hemagglutinin HA2 chain



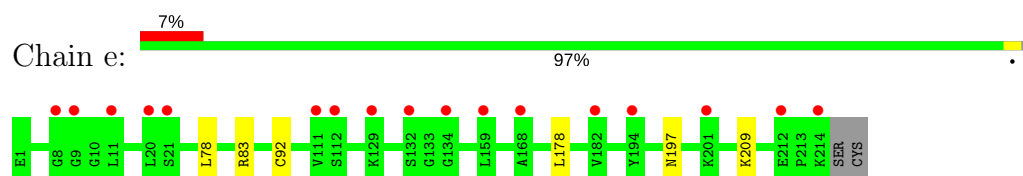
● Molecule 3: Broadly neutralizing antibody C05, heavy chain



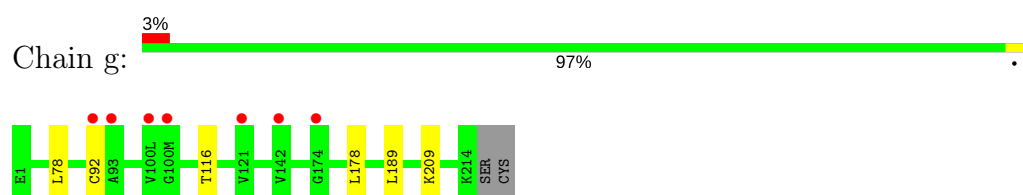
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



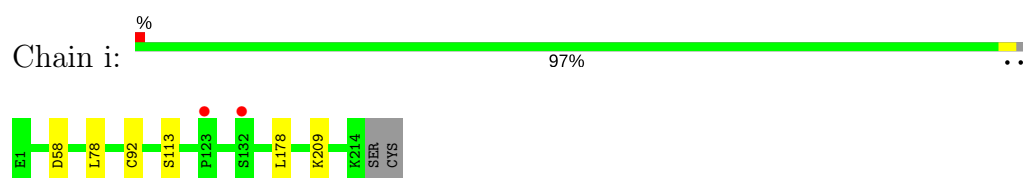
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



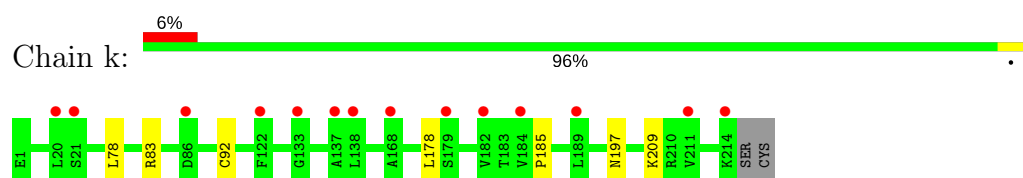
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



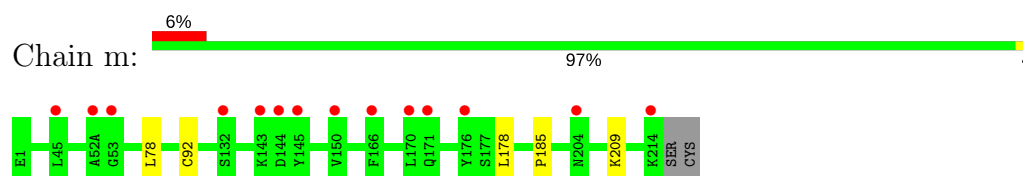
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



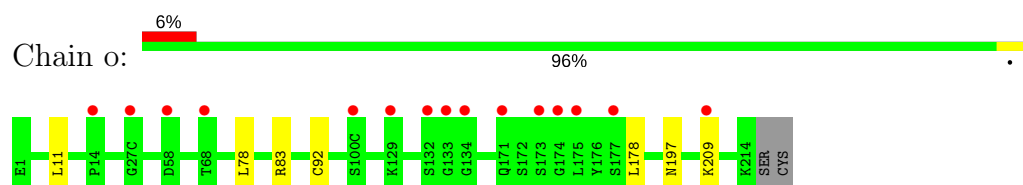
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



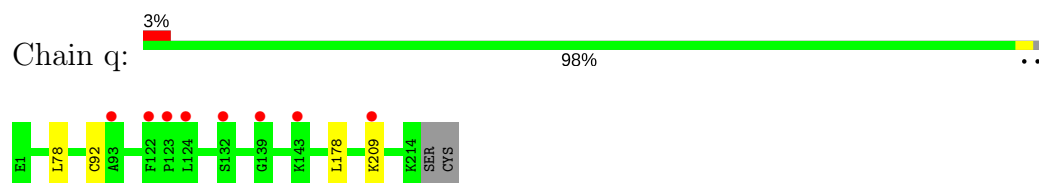
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



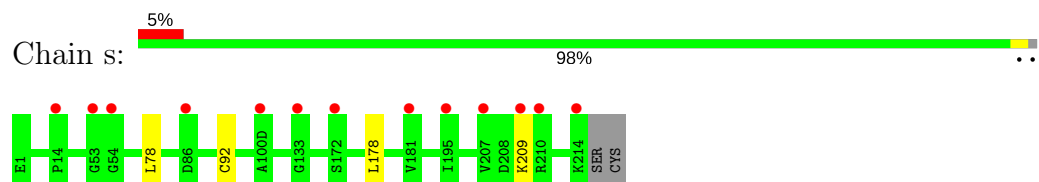
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



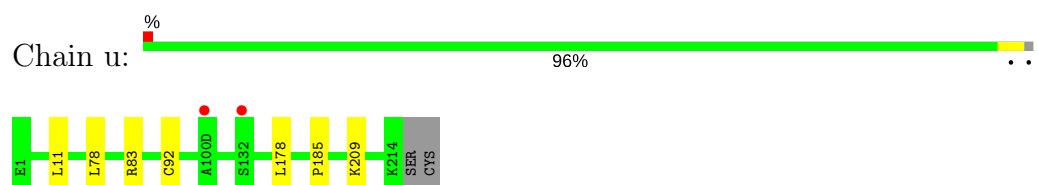
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



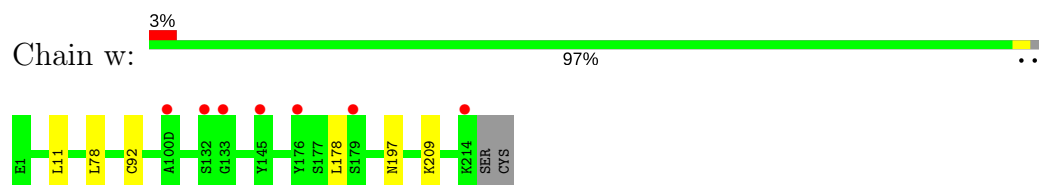
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



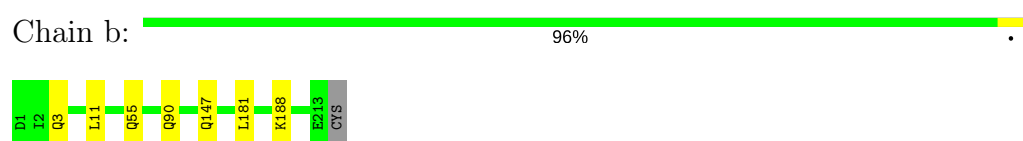
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



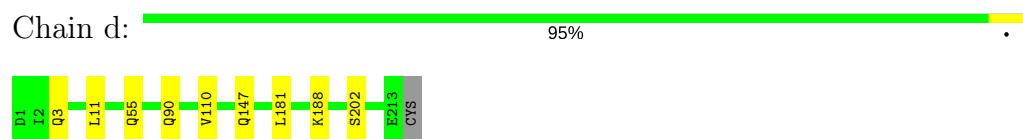
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



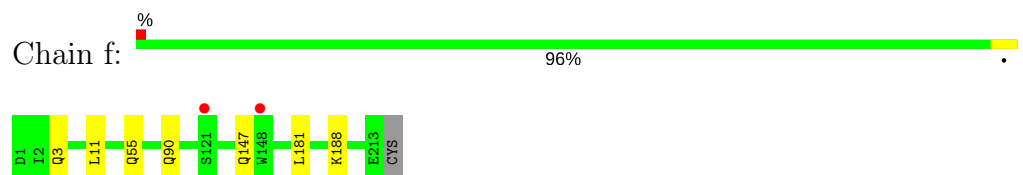
- Molecule 4: Broadly neutralizing antibody C05, light chain



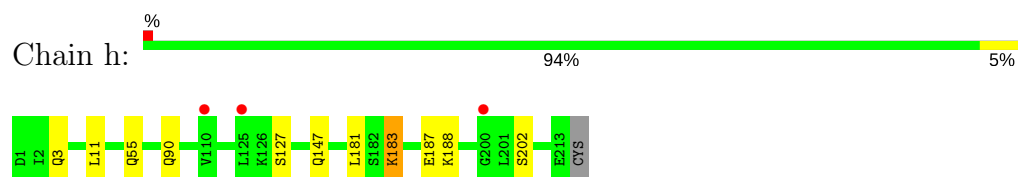
- Molecule 4: Broadly neutralizing antibody C05, light chain



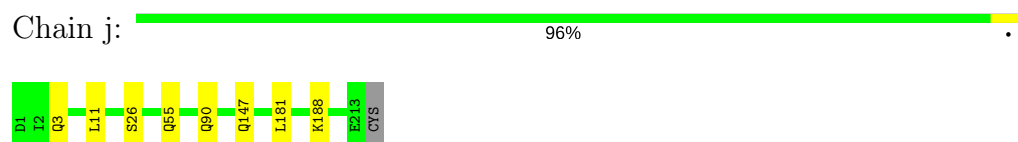
- Molecule 4: Broadly neutralizing antibody C05, light chain



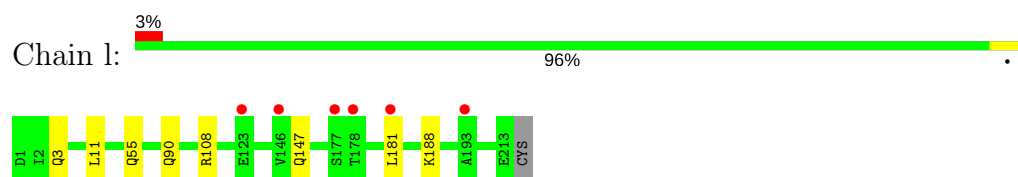
- Molecule 4: Broadly neutralizing antibody C05, light chain



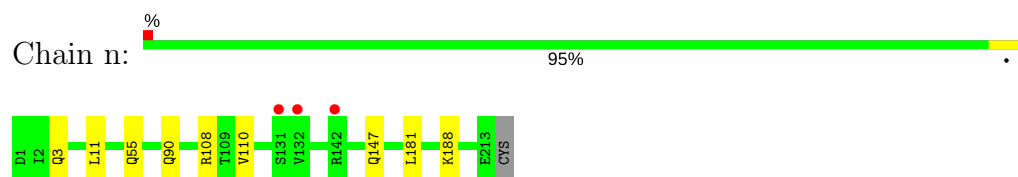
- Molecule 4: Broadly neutralizing antibody C05, light chain



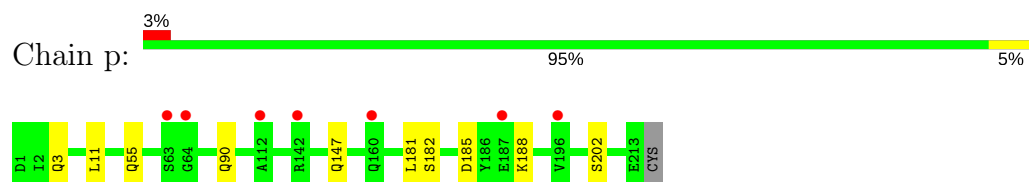
- Molecule 4: Broadly neutralizing antibody C05, light chain



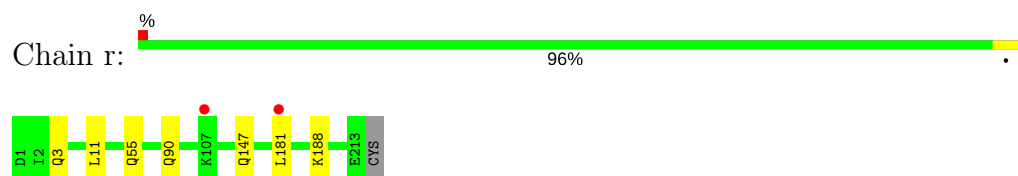
- Molecule 4: Broadly neutralizing antibody C05, light chain



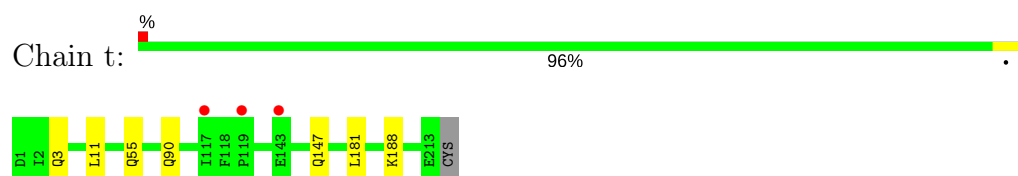
- Molecule 4: Broadly neutralizing antibody C05, light chain



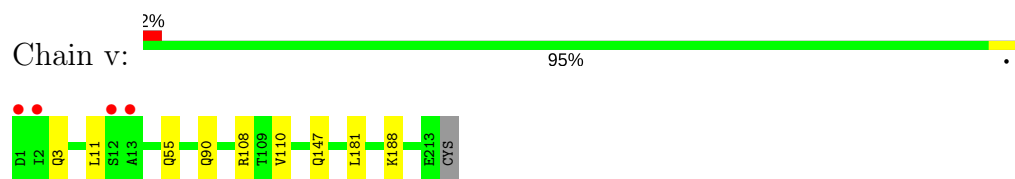
- Molecule 4: Broadly neutralizing antibody C05, light chain



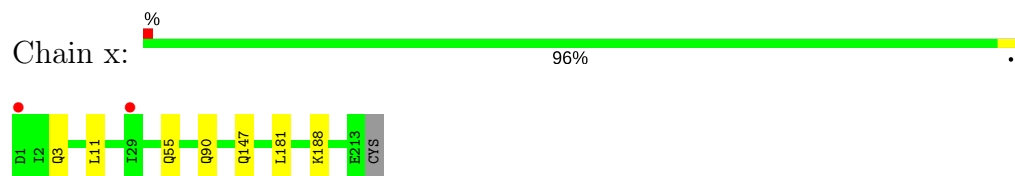
- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	142.02Å 158.62Å 178.50Å 89.95° 85.44° 84.37°	Depositor
Resolution (Å)	49.07 – 4.10 49.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	73.9 (49.07-4.10) 58.9 (49.07-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.309 , 0.334 0.311 , 0.336	Depositor DCC
R_{free} test set	4523 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 8.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	90792	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/2612	0.66	0/3558
1	C	0.39	0/2612	0.65	1/3558 (0.0%)
1	E	0.38	1/2612 (0.0%)	0.65	0/3558
1	G	0.39	0/2612	0.66	0/3558
1	I	0.48	2/2612 (0.1%)	0.69	2/3558 (0.1%)
1	K	0.39	0/2612	0.64	1/3558 (0.0%)
1	M	0.42	0/2612	0.68	2/3558 (0.1%)
1	O	0.41	1/2612 (0.0%)	0.65	1/3558 (0.0%)
1	Q	0.40	0/2612	0.66	0/3558
1	S	0.38	0/2612	0.66	1/3558 (0.0%)
1	U	0.44	1/2612 (0.0%)	0.68	1/3558 (0.0%)
1	W	0.42	1/2612 (0.0%)	0.65	1/3558 (0.0%)
2	B	0.37	0/1470	0.63	0/1975
2	D	0.36	0/1470	0.64	0/1975
2	F	0.41	0/1470	0.66	0/1975
2	H	0.37	0/1470	0.64	1/1975 (0.1%)
2	J	0.37	0/1470	0.63	0/1975
2	L	0.39	0/1470	0.64	0/1975
2	N	0.35	0/1470	0.63	0/1975
2	P	0.38	0/1470	0.63	1/1975 (0.1%)
2	R	0.36	0/1470	0.64	0/1975
2	T	0.36	0/1470	0.63	0/1975
2	V	0.37	0/1470	0.65	0/1975
2	X	0.36	0/1470	0.63	1/1975 (0.1%)
3	a	0.48	1/1837 (0.1%)	0.75	2/2500 (0.1%)
3	c	0.41	0/1837	0.68	0/2500
3	e	0.43	0/1837	0.71	0/2500
3	g	0.46	1/1837 (0.1%)	0.71	1/2500 (0.0%)
3	i	0.53	0/1837	0.79	1/2500 (0.0%)
3	k	0.42	0/1837	0.69	0/2500
3	m	0.41	0/1837	0.69	0/2500
3	o	0.43	0/1837	0.71	1/2500 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.43	0/1837	0.69	0/2500
3	s	0.42	0/1837	0.69	0/2500
3	u	0.41	0/1837	0.70	1/2500 (0.0%)
3	w	0.42	0/1837	0.69	1/2500 (0.0%)
4	b	0.45	0/1682	0.67	0/2280
4	d	0.50	1/1682 (0.1%)	0.72	0/2280
4	f	0.40	0/1682	0.66	0/2280
4	h	0.51	1/1682 (0.1%)	0.71	0/2280
4	j	0.44	0/1682	0.69	0/2280
4	l	0.44	0/1682	0.68	0/2280
4	n	0.48	1/1682 (0.1%)	0.69	0/2280
4	p	0.51	0/1682	0.78	4/2280 (0.2%)
4	r	0.39	0/1682	0.66	0/2280
4	t	0.37	0/1682	0.64	0/2280
4	v	0.48	1/1682 (0.1%)	0.70	0/2280
4	x	0.40	0/1682	0.66	0/2280
All	All	0.42	12/91212 (0.0%)	0.67	24/123756 (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
2	F	0	1
3	k	0	1
3	m	0	1
3	u	0	1
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	GLU	CG-CD	-11.09	1.35	1.51
1	W	190	GLU	CB-CG	-7.77	1.37	1.52
3	a	100(D)	ALA	CA-CB	-7.11	1.37	1.52
3	g	116	THR	CB-CG2	-7.02	1.29	1.52
4	n	110	VAL	CB-CG2	-6.42	1.39	1.52

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	185	ASP	CB-CG-OD2	10.08	127.37	118.30
3	i	58	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	M	20	VAL	N-CA-C	-8.49	88.08	111.00
4	p	185	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	I	190	GLU	OE1-CD-OE2	7.20	131.93	123.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	ILE	Mainchain
3	k	185	PRO	Mainchain
3	m	185	PRO	Mainchain
3	u	185	PRO	Mainchain

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	2553	0	2491	11	1
1	C	2553	0	2491	11	0
1	E	2553	0	2491	11	0
1	G	2553	0	2490	10	0
1	I	2553	0	2491	18	0
1	K	2553	0	2491	13	0
1	M	2553	0	2490	11	0
1	O	2553	0	2490	15	0
1	Q	2553	0	2490	14	0
1	S	2553	0	2490	12	0
1	U	2553	0	2490	15	3
1	W	2553	0	2491	14	0
2	B	1446	0	1370	1	0
2	D	1446	0	1370	1	0
2	F	1446	0	1370	3	0
2	H	1446	0	1370	2	0
2	J	1446	0	1370	0	0
2	L	1446	0	1370	1	0
2	N	1446	0	1370	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1446	0	1370	1	0
2	R	1446	0	1370	2	0
2	T	1446	0	1370	0	0
2	V	1446	0	1370	0	0
2	X	1446	0	1370	2	0
3	a	1806	0	1749	0	0
3	c	1806	0	1749	0	0
3	e	1806	0	1749	0	0
3	g	1806	0	1749	0	0
3	i	1806	0	1749	0	0
3	k	1806	0	1749	0	0
3	m	1806	0	1749	0	0
3	o	1806	0	1749	0	0
3	q	1806	0	1749	0	0
3	s	1806	0	1749	0	0
3	u	1806	0	1749	0	0
3	w	1806	0	1749	0	0
4	b	1648	0	1614	0	0
4	d	1648	0	1614	0	1
4	f	1648	0	1614	0	0
4	h	1648	0	1614	0	4
4	j	1648	0	1614	0	1
4	l	1648	0	1614	0	1
4	n	1648	0	1614	0	1
4	p	1648	0	1614	0	1
4	r	1648	0	1614	0	0
4	t	1648	0	1614	0	0
4	v	1648	0	1614	0	1
4	x	1648	0	1614	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	28	0	26	0	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0
5	L	14	0	13	0	0
5	M	28	0	26	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	N	14	0	13	0	0
5	O	28	0	26	0	0
5	P	14	0	13	0	0
5	Q	28	0	26	0	0
5	R	14	0	13	0	0
5	S	28	0	26	0	0
5	T	14	0	13	0	0
5	U	28	0	26	0	0
5	V	14	0	13	0	0
5	W	14	0	13	0	0
5	X	14	0	13	0	0
6	A	50	0	43	0	0
6	C	50	0	43	0	0
6	E	50	0	43	0	0
6	G	50	0	43	0	0
6	I	50	0	43	0	0
6	K	50	0	43	0	0
6	M	50	0	43	0	0
6	O	50	0	43	0	0
6	Q	50	0	43	0	0
6	S	50	0	43	1	0
6	U	50	0	43	0	0
6	W	50	0	43	0	0
7	A	28	0	25	0	0
7	C	28	0	25	0	0
7	E	28	0	25	0	0
7	G	28	0	25	0	0
7	I	28	0	25	0	0
7	K	28	0	25	0	0
7	M	28	0	25	0	0
7	O	28	0	25	0	0
7	Q	28	0	25	0	0
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
All	All	90792	0	87888	105	7

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 3.

The worst 5 of 105 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:THR:HG21	1:E:216:ASN:ND2	1.99	0.78
1:I:212:THR:HG21	1:K:216:ASN:CG	2.07	0.75
1:O:212:THR:HG21	1:Q:216:ASN:CG	2.11	0.71
1:C:212:THR:HG21	1:E:216:ASN:CG	2.11	0.70
1:I:212:THR:HG21	1:K:216:ASN:ND2	2.09	0.68

The worst 5 of 7 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)
4:d:202:SER:OG	4:v:108:ARG:O[1_545]	1.78	0.42
4:h:202:SER:OG	4:n:108:ARG:O[1_564]	1.83	0.37
4:l:108:ARG:O	4:p:202:SER:OG[1_564]	1.87	0.33
1:U:312:ASN:ND2	4:h:187:GLU:OE2[1_646]	1.93	0.27
1:U:33:GLN:NE2	4:h:127:SER:O[1_646]	2.09	0.11

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	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	C	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	G	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	I	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	K	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	M	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	O	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	Q	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
1	S	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	328/323 (102%)	323 (98%)	4 (1%)	1 (0%)	44	80
1	W	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	44	80
2	B	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	D	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	F	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	H	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	J	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	L	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	N	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	P	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	R	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	T	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	V	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	X	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
3	a	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	c	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	e	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	g	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	i	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	k	241/241 (100%)	235 (98%)	6 (2%)	0	100	100
3	m	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	o	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	q	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	s	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	u	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	w	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
4	b	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	d	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	f	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	h	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	j	212/214 (99%)	209 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	l	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	n	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	p	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	r	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	t	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	v	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	x	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	11496/11424 (101%)	11268 (98%)	216 (2%)	12 (0%)	55	88

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	G	62	ILE
1	I	62	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	C	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	E	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	G	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	I	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	K	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	M	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	O	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	Q	291/283 (103%)	289 (99%)	2 (1%)	87	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	U	291/283 (103%)	289 (99%)	2 (1%)	87	94
1	W	291/283 (103%)	289 (99%)	2 (1%)	87	94
2	B	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	D	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	F	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	H	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	J	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	L	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	N	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	P	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	R	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	T	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	V	153/148 (103%)	152 (99%)	1 (1%)	87	94
2	X	153/148 (103%)	152 (99%)	1 (1%)	87	94
3	a	202/200 (101%)	198 (98%)	4 (2%)	60	83
3	c	202/200 (101%)	197 (98%)	5 (2%)	53	78
3	e	202/200 (101%)	196 (97%)	6 (3%)	46	74
3	g	202/200 (101%)	198 (98%)	4 (2%)	60	83
3	i	202/200 (101%)	197 (98%)	5 (2%)	53	78
3	k	202/200 (101%)	196 (97%)	6 (3%)	46	74
3	m	202/200 (101%)	198 (98%)	4 (2%)	60	83
3	o	202/200 (101%)	196 (97%)	6 (3%)	46	74
3	q	202/200 (101%)	198 (98%)	4 (2%)	60	83
3	s	202/200 (101%)	198 (98%)	4 (2%)	60	83
3	u	202/200 (101%)	197 (98%)	5 (2%)	53	78
3	w	202/200 (101%)	197 (98%)	5 (2%)	53	78
4	b	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	d	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	f	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	h	187/187 (100%)	180 (96%)	7 (4%)	39	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	j	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	l	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	n	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	p	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	r	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	t	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	v	187/187 (100%)	180 (96%)	7 (4%)	39	71
4	x	187/187 (100%)	180 (96%)	7 (4%)	39	71
All	All	9996/9816 (102%)	9818 (98%)	178 (2%)	64	85

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	h	147	GLN
3	k	197	ASN
4	v	181	LEU
4	h	188	LYS
4	j	55	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
2	T	53	ASN
2	X	125	GLN
4	t	199	GLN
2	T	60	ASN
2	V	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
3	PCA	a	1	3	8,8,9	2.11	2 (25%)	9,10,12	2.29	5 (55%)
3	PCA	c	1	3	8,8,9	1.99	2 (25%)	9,10,12	2.31	5 (55%)
3	PCA	e	1	3	8,8,9	1.96	2 (25%)	9,10,12	2.30	5 (55%)
3	PCA	g	1	3	8,8,9	1.86	2 (25%)	9,10,12	2.32	5 (55%)
3	PCA	i	1	3	8,8,9	2.03	2 (25%)	9,10,12	2.21	5 (55%)
3	PCA	k	1	3	8,8,9	1.91	2 (25%)	9,10,12	2.35	6 (66%)
3	PCA	m	1	3	8,8,9	1.97	2 (25%)	9,10,12	2.11	5 (55%)
3	PCA	o	1	3	8,8,9	2.00	2 (25%)	9,10,12	2.24	5 (55%)
3	PCA	q	1	3	8,8,9	1.90	2 (25%)	9,10,12	2.23	5 (55%)
3	PCA	s	1	3	8,8,9	2.12	2 (25%)	9,10,12	2.30	5 (55%)
3	PCA	u	1	3	8,8,9	2.00	2 (25%)	9,10,12	2.30	5 (55%)
3	PCA	w	1	3	8,8,9	1.99	2 (25%)	9,10,12	2.25	5 (55%)

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
3	PCA	a	1	3	-	0/0/11/13	0/1/1/1
3	PCA	c	1	3	-	0/0/11/13	0/1/1/1
3	PCA	e	1	3	-	0/0/11/13	0/1/1/1
3	PCA	g	1	3	-	0/0/11/13	0/1/1/1
3	PCA	i	1	3	-	0/0/11/13	0/1/1/1
3	PCA	k	1	3	-	0/0/11/13	0/1/1/1
3	PCA	m	1	3	-	0/0/11/13	0/1/1/1
3	PCA	o	1	3	-	0/0/11/13	0/1/1/1
3	PCA	q	1	3	-	0/0/11/13	0/1/1/1
3	PCA	s	1	3	-	0/0/11/13	0/1/1/1
3	PCA	u	1	3	-	0/0/11/13	0/1/1/1
3	PCA	w	1	3	-	0/0/11/13	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	1	PCA	CA-N	2.79	1.49	1.46
3	q	1	PCA	CA-N	2.96	1.50	1.46
3	k	1	PCA	CA-N	2.97	1.50	1.46
3	m	1	PCA	CA-N	3.10	1.50	1.46
3	u	1	PCA	CA-N	3.14	1.50	1.46

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	s	1	PCA	CB-CA-C	-3.91	107.32	112.70
3	o	1	PCA	CB-CA-C	-3.59	107.76	112.70
3	a	1	PCA	CB-CA-C	-3.58	107.77	112.70
3	w	1	PCA	CB-CA-C	-3.55	107.81	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

72 carbohydrates 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	$\# Z > 2$
6	NAG	A	602	1,6	14,14,15	0.48	0	15,19,21	1.21	1 (6%)
6	NAG	A	603	6	14,14,15	0.64	0	15,19,21	0.88	1 (6%)
6	BMA	A	604	6	11,11,12	0.73	0	13,15,17	1.33	3 (23%)
6	MAN	A	605	6	11,11,12	0.60	0	13,15,17	0.70	0
7	NAG	A	606	1,7	14,14,15	0.54	0	15,19,21	0.42	0
7	NAG	A	607	7	14,14,15	0.47	0	15,19,21	0.72	0
6	NAG	C	502	1,6	14,14,15	0.52	0	15,19,21	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	503	6	14,14,15	0.53	0	15,19,21	0.55	0
6	BMA	C	504	6	11,11,12	0.69	0	13,15,17	1.20	1 (7%)
6	MAN	C	505	6	11,11,12	0.61	0	13,15,17	0.71	0
7	NAG	C	506	1,7	14,14,15	0.60	0	15,19,21	0.64	0
7	NAG	C	507	7	14,14,15	0.44	0	15,19,21	0.93	1 (6%)
6	NAG	E	602	1,6	14,14,15	0.51	0	15,19,21	1.00	1 (6%)
6	NAG	E	603	6	14,14,15	0.58	0	15,19,21	0.64	0
6	BMA	E	604	6	11,11,12	0.73	0	13,15,17	0.92	1 (7%)
6	MAN	E	605	6	11,11,12	0.66	0	13,15,17	0.87	1 (7%)
7	NAG	E	606	1,7	14,14,15	0.58	0	15,19,21	0.66	0
7	NAG	E	607	7	14,14,15	0.46	0	15,19,21	0.89	1 (6%)
6	NAG	G	503	1,6	14,14,15	0.61	0	15,19,21	1.04	1 (6%)
6	NAG	G	504	6	14,14,15	0.54	0	15,19,21	0.81	0
6	BMA	G	505	6	11,11,12	0.74	0	13,15,17	1.18	1 (7%)
6	MAN	G	506	6	11,11,12	0.58	0	13,15,17	0.83	1 (7%)
7	NAG	G	507	1,7	14,14,15	0.51	0	15,19,21	0.72	0
7	NAG	G	508	7	14,14,15	0.46	0	15,19,21	1.09	1 (6%)
6	NAG	I	502	1,6	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
6	NAG	I	503	6	14,14,15	0.53	0	15,19,21	0.54	0
6	BMA	I	504	6	11,11,12	0.70	0	13,15,17	0.91	1 (7%)
6	MAN	I	505	6	11,11,12	0.62	0	13,15,17	0.95	1 (7%)
7	NAG	I	506	1,7	14,14,15	0.58	0	15,19,21	0.57	0
7	NAG	I	507	7	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
6	NAG	K	602	1,6	14,14,15	0.49	0	15,19,21	1.01	1 (6%)
6	NAG	K	603	6	14,14,15	0.52	0	15,19,21	0.56	0
6	BMA	K	604	6	11,11,12	0.75	0	13,15,17	0.94	1 (7%)
6	MAN	K	605	6	11,11,12	0.60	0	13,15,17	0.64	0
7	NAG	K	606	1,7	14,14,15	0.56	0	15,19,21	0.63	0
7	NAG	K	607	7	14,14,15	0.45	0	15,19,21	0.90	1 (6%)
6	NAG	M	503	1,6	14,14,15	0.44	0	15,19,21	1.17	1 (6%)
6	NAG	M	504	6	14,14,15	0.51	0	15,19,21	0.62	0
6	BMA	M	505	6	11,11,12	0.68	0	13,15,17	0.98	1 (7%)
6	MAN	M	506	6	11,11,12	0.62	0	13,15,17	1.04	1 (7%)
7	NAG	M	507	1,7	14,14,15	0.57	0	15,19,21	0.61	0
7	NAG	M	508	7	14,14,15	0.52	0	15,19,21	0.91	1 (6%)
6	NAG	O	503	1,6	14,14,15	0.59	0	15,19,21	1.00	1 (6%)
6	NAG	O	504	6	14,14,15	0.56	0	15,19,21	0.74	0
6	BMA	O	505	6	11,11,12	0.81	0	13,15,17	0.93	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	O	506	6	11,11,12	0.61	0	13,15,17	0.99	1 (7%)
7	NAG	O	507	1,7	14,14,15	0.54	0	15,19,21	0.60	0
7	NAG	O	508	7	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
6	NAG	Q	503	1,6	14,14,15	0.50	0	15,19,21	0.95	1 (6%)
6	NAG	Q	504	6	14,14,15	0.54	0	15,19,21	0.84	0
6	BMA	Q	505	6	11,11,12	0.77	0	13,15,17	0.97	1 (7%)
6	MAN	Q	506	6	11,11,12	0.61	0	13,15,17	0.84	1 (7%)
7	NAG	Q	507	1,7	14,14,15	0.58	0	15,19,21	0.69	0
7	NAG	Q	508	7	14,14,15	0.51	0	15,19,21	0.88	1 (6%)
6	NAG	S	503	1,6	14,14,15	0.45	0	15,19,21	1.00	1 (6%)
6	NAG	S	504	6	14,14,15	0.53	0	15,19,21	0.89	1 (6%)
6	BMA	S	505	6	11,11,12	0.74	0	13,15,17	1.08	1 (7%)
6	MAN	S	506	6	11,11,12	0.62	0	13,15,17	0.78	1 (7%)
7	NAG	S	507	1,7	14,14,15	0.57	0	15,19,21	0.61	0
7	NAG	S	508	7	14,14,15	0.54	0	15,19,21	0.81	0
6	NAG	U	503	1,6	14,14,15	0.54	0	15,19,21	1.14	0
6	NAG	U	504	6	14,14,15	0.54	0	15,19,21	0.90	0
6	BMA	U	505	6	11,11,12	0.77	0	13,15,17	0.88	1 (7%)
6	MAN	U	506	6	11,11,12	0.61	0	13,15,17	0.77	1 (7%)
7	NAG	U	507	1,7	14,14,15	0.52	0	15,19,21	0.68	0
7	NAG	U	508	7	14,14,15	0.52	0	15,19,21	0.87	1 (6%)
6	NAG	W	602	1,6	14,14,15	0.48	0	15,19,21	0.96	1 (6%)
6	NAG	W	603	6	14,14,15	0.56	0	15,19,21	0.59	0
6	BMA	W	604	6	11,11,12	0.74	0	13,15,17	0.92	1 (7%)
6	MAN	W	605	6	11,11,12	0.58	0	13,15,17	0.84	1 (7%)
7	NAG	W	606	1,7	14,14,15	0.57	0	15,19,21	0.60	0
7	NAG	W	607	7	14,14,15	0.53	0	15,19,21	0.92	1 (6%)

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
6	NAG	A	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	603	6	-	0/6/23/26	0/1/1/1
6	BMA	A	604	6	-	0/2/19/22	0/1/1/1
6	MAN	A	605	6	-	0/2/19/22	0/1/1/1
7	NAG	A	606	1,7	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	607	7	-	0/6/23/26	0/1/1/1
6	NAG	C	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	503	6	-	0/6/23/26	0/1/1/1
6	BMA	C	504	6	-	0/2/19/22	0/1/1/1
6	MAN	C	505	6	-	0/2/19/22	0/1/1/1
7	NAG	C	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	507	7	-	0/6/23/26	0/1/1/1
6	NAG	E	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	603	6	-	0/6/23/26	0/1/1/1
6	BMA	E	604	6	-	0/2/19/22	0/1/1/1
6	MAN	E	605	6	-	0/2/19/22	0/1/1/1
7	NAG	E	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	607	7	-	0/6/23/26	0/1/1/1
6	NAG	G	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	504	6	-	0/6/23/26	0/1/1/1
6	BMA	G	505	6	-	0/2/19/22	0/1/1/1
6	MAN	G	506	6	-	0/2/19/22	0/1/1/1
7	NAG	G	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	508	7	-	0/6/23/26	0/1/1/1
6	NAG	I	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	503	6	-	0/6/23/26	0/1/1/1
6	BMA	I	504	6	-	0/2/19/22	0/1/1/1
6	MAN	I	505	6	-	0/2/19/22	0/1/1/1
7	NAG	I	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	507	7	-	0/6/23/26	0/1/1/1
6	NAG	K	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	603	6	-	0/6/23/26	0/1/1/1
6	BMA	K	604	6	-	0/2/19/22	0/1/1/1
6	MAN	K	605	6	-	0/2/19/22	0/1/1/1
7	NAG	K	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	607	7	-	0/6/23/26	0/1/1/1
6	NAG	M	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	504	6	-	0/6/23/26	0/1/1/1
6	BMA	M	505	6	-	0/2/19/22	0/1/1/1
6	MAN	M	506	6	-	0/2/19/22	0/1/1/1
7	NAG	M	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	508	7	-	0/6/23/26	0/1/1/1
6	NAG	O	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	504	6	-	0/6/23/26	0/1/1/1
6	BMA	O	505	6	-	0/2/19/22	0/1/1/1
6	MAN	O	506	6	-	0/2/19/22	0/1/1/1
7	NAG	O	507	1,7	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	O	508	7	-	0/6/23/26	0/1/1/1
6	NAG	Q	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	504	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	505	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	506	6	-	0/2/19/22	0/1/1/1
7	NAG	Q	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	508	7	-	0/6/23/26	0/1/1/1
6	NAG	S	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	504	6	-	0/6/23/26	0/1/1/1
6	BMA	S	505	6	-	0/2/19/22	0/1/1/1
6	MAN	S	506	6	-	0/2/19/22	0/1/1/1
7	NAG	S	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	508	7	-	0/6/23/26	0/1/1/1
6	NAG	U	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	504	6	-	0/6/23/26	0/1/1/1
6	BMA	U	505	6	-	0/2/19/22	0/1/1/1
6	MAN	U	506	6	-	0/2/19/22	0/1/1/1
7	NAG	U	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	508	7	-	0/6/23/26	0/1/1/1
6	NAG	W	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	603	6	-	0/6/23/26	0/1/1/1
6	BMA	W	604	6	-	0/2/19/22	0/1/1/1
6	MAN	W	605	6	-	0/2/19/22	0/1/1/1
7	NAG	W	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	607	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	NAG	O5-C1-C2	-3.18	107.05	111.47
6	K	602	NAG	O5-C1-C2	-2.93	107.39	111.47
6	M	506	MAN	O5-C1-C2	-2.62	106.68	110.79
6	I	505	MAN	O5-C1-C2	-2.58	106.75	110.79
6	O	503	NAG	O5-C1-C2	-2.54	107.93	111.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	503	NAG	1	0

5.6 Ligand geometry

30 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	$\# Z > 2$
5	NAG	A	601	1	14,14,15	1.50	2 (14%)	15,19,21	4.64	9 (60%)
5	NAG	B	201	2	14,14,15	0.61	0	15,19,21	0.96	1 (6%)
5	NAG	C	501	1	14,14,15	0.45	0	15,19,21	1.19	2 (13%)
5	NAG	D	201	2	14,14,15	0.53	0	15,19,21	1.24	1 (6%)
5	NAG	E	601	1	14,14,15	0.48	0	15,19,21	1.20	1 (6%)
5	NAG	F	201	2	14,14,15	0.50	0	15,19,21	1.09	1 (6%)
5	NAG	G	501	1	14,14,15	0.39	0	15,19,21	1.09	1 (6%)
5	NAG	G	502	1	14,14,15	0.49	0	15,19,21	1.05	1 (6%)
5	NAG	H	201	2	14,14,15	0.57	0	15,19,21	0.99	2 (13%)
5	NAG	I	501	1	14,14,15	0.45	0	15,19,21	1.04	2 (13%)
5	NAG	J	201	2	14,14,15	0.52	0	15,19,21	1.27	1 (6%)
5	NAG	K	601	1	14,14,15	0.48	0	15,19,21	1.26	1 (6%)
5	NAG	L	201	2	14,14,15	0.55	0	15,19,21	0.97	1 (6%)
5	NAG	M	501	1	14,14,15	0.43	0	15,19,21	1.20	2 (13%)
5	NAG	M	502	1	14,14,15	0.46	0	15,19,21	1.03	1 (6%)
5	NAG	N	201	2	14,14,15	0.55	0	15,19,21	1.20	3 (20%)
5	NAG	O	501	1	14,14,15	0.50	0	15,19,21	0.91	0
5	NAG	O	502	1	14,14,15	0.50	0	15,19,21	1.17	2 (13%)
5	NAG	P	201	2	14,14,15	0.56	0	15,19,21	1.02	1 (6%)
5	NAG	Q	501	1	14,14,15	0.43	0	15,19,21	1.00	1 (6%)
5	NAG	Q	502	1	14,14,15	0.58	0	15,19,21	1.11	1 (6%)
5	NAG	R	201	2	14,14,15	0.52	0	15,19,21	1.06	1 (6%)
5	NAG	S	501	1	14,14,15	0.46	0	15,19,21	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	S	502	1	14,14,15	0.53	0	15,19,21	1.37	2 (13%)
5	NAG	T	201	2	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
5	NAG	U	501	1	14,14,15	0.48	0	15,19,21	0.98	1 (6%)
5	NAG	U	502	1	14,14,15	0.47	0	15,19,21	1.14	1 (6%)
5	NAG	V	201	2	14,14,15	0.55	0	15,19,21	0.90	1 (6%)
5	NAG	W	601	1	14,14,15	0.54	0	15,19,21	1.44	3 (20%)
5	NAG	X	201	2	14,14,15	0.53	0	15,19,21	1.07	2 (13%)

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	A	601	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	601	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
5	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	NAG	G	502	1	-	0/6/23/26	0/1/1/1
5	NAG	H	201	2	-	0/6/23/26	0/1/1/1
5	NAG	I	501	1	-	0/6/23/26	0/1/1/1
5	NAG	J	201	2	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1	-	0/6/23/26	0/1/1/1
5	NAG	L	201	2	-	0/6/23/26	0/1/1/1
5	NAG	M	501	1	-	0/6/23/26	0/1/1/1
5	NAG	M	502	1	-	0/6/23/26	0/1/1/1
5	NAG	N	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	501	1	-	0/6/23/26	0/1/1/1
5	NAG	O	502	1	-	0/6/23/26	0/1/1/1
5	NAG	P	201	2	-	0/6/23/26	0/1/1/1
5	NAG	Q	501	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	502	1	-	0/6/23/26	0/1/1/1
5	NAG	R	201	2	-	0/6/23/26	0/1/1/1
5	NAG	S	501	1	-	0/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	T	201	2	-	0/6/23/26	0/1/1/1
5	NAG	U	501	1	-	0/6/23/26	0/1/1/1
5	NAG	U	502	1	-	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	V	201	2	-	0/6/23/26	0/1/1/1
5	NAG	W	601	1	-	0/6/23/26	0/1/1/1
5	NAG	X	201	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	C2-N2	-3.86	1.39	1.46
5	A	601	NAG	C8-C7	-3.35	1.43	1.50

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	O5-C1-C2	-10.01	97.54	111.47
5	A	601	NAG	C2-N2-C7	-7.73	111.67	122.94
5	A	601	NAG	C4-C3-C2	-7.71	99.72	111.02
5	A	601	NAG	C8-C7-N2	-5.50	106.18	116.11
5	A	601	NAG	C3-C4-C5	-4.94	101.51	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	318/323 (98%)	0.22	9 (2%) 53 43	33, 40, 68, 127	0
1	C	318/323 (98%)	0.15	5 (1%) 72 63	24, 43, 70, 106	0
1	E	318/323 (98%)	0.19	9 (2%) 53 43	30, 41, 77, 116	0
1	G	318/323 (98%)	0.08	9 (2%) 53 43	21, 33, 78, 132	0
1	I	318/323 (98%)	0.24	9 (2%) 53 43	25, 42, 64, 102	0
1	K	318/323 (98%)	0.05	3 (0%) 84 77	29, 42, 61, 112	0
1	M	318/323 (98%)	0.52	24 (7%) 15 12	58, 70, 100, 141	0
1	O	318/323 (98%)	0.42	21 (6%) 19 14	38, 61, 90, 116	0
1	Q	318/323 (98%)	0.22	16 (5%) 30 23	40, 49, 72, 115	0
1	S	318/323 (98%)	0.41	21 (6%) 19 14	43, 60, 76, 109	0
1	U	318/323 (98%)	0.13	4 (1%) 77 68	33, 42, 74, 121	0
1	W	318/323 (98%)	0.23	16 (5%) 30 23	31, 38, 91, 159	0
2	B	172/174 (98%)	0.02	4 (2%) 61 51	34, 61, 97, 111	0
2	D	172/174 (98%)	0.27	7 (4%) 38 29	40, 58, 81, 85	0
2	F	172/174 (98%)	0.18	7 (4%) 38 29	46, 61, 92, 97	0
2	H	172/174 (98%)	0.15	4 (2%) 61 51	15, 74, 123, 133	0
2	J	172/174 (98%)	0.22	6 (3%) 44 35	39, 61, 89, 96	0
2	L	172/174 (98%)	0.19	8 (4%) 32 25	23, 54, 94, 102	0
2	N	172/174 (98%)	0.34	15 (8%) 11 9	40, 87, 125, 133	0
2	P	172/174 (98%)	0.30	8 (4%) 32 25	40, 81, 115, 128	0
2	R	172/174 (98%)	0.04	2 (1%) 79 71	33, 61, 100, 111	0
2	T	172/174 (98%)	0.22	8 (4%) 32 25	43, 70, 121, 136	0
2	V	172/174 (98%)	0.01	2 (1%) 79 71	35, 57, 102, 115	0
2	X	172/174 (98%)	0.14	5 (2%) 52 42	36, 76, 130, 139	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	a	238/241 (98%)	-0.02	3 (1%) 77 68	23, 37, 62, 74	0
3	c	238/241 (98%)	0.06	5 (2%) 64 54	26, 36, 54, 59	0
3	e	238/241 (98%)	0.30	17 (7%) 17 12	45, 66, 75, 83	0
3	g	238/241 (98%)	0.17	7 (2%) 52 42	18, 39, 95, 107	0
3	i	238/241 (98%)	0.08	2 (0%) 86 79	23, 30, 59, 70	0
3	k	238/241 (98%)	0.25	14 (5%) 23 17	50, 65, 91, 107	0
3	m	238/241 (98%)	0.14	14 (5%) 23 17	39, 47, 73, 86	0
3	o	238/241 (98%)	0.39	15 (6%) 21 15	70, 85, 107, 124	0
3	q	238/241 (98%)	0.18	8 (3%) 46 36	38, 54, 81, 91	0
3	s	238/241 (98%)	0.34	13 (5%) 26 20	63, 81, 100, 126	0
3	u	238/241 (98%)	0.02	2 (0%) 86 79	42, 57, 74, 86	0
3	w	238/241 (98%)	0.14	7 (2%) 52 42	28, 47, 83, 97	0
4	b	213/214 (99%)	-0.08	0 100 100	17, 28, 62, 66	0
4	d	213/214 (99%)	-0.08	0 100 100	23, 39, 67, 73	0
4	f	213/214 (99%)	-0.13	2 (0%) 84 77	44, 54, 86, 97	0
4	h	213/214 (99%)	0.05	3 (1%) 75 66	20, 33, 85, 91	0
4	j	213/214 (99%)	-0.05	0 100 100	23, 31, 66, 80	0
4	l	213/214 (99%)	-0.02	6 (2%) 53 43	54, 79, 103, 107	0
4	n	213/214 (99%)	0.04	3 (1%) 75 66	33, 44, 55, 62	0
4	p	213/214 (99%)	0.09	7 (3%) 47 37	70, 79, 105, 111	0
4	r	213/214 (99%)	-0.07	2 (0%) 84 77	33, 53, 68, 73	0
4	t	213/214 (99%)	-0.09	3 (1%) 75 66	47, 68, 105, 115	0
4	v	213/214 (99%)	-0.01	4 (1%) 67 58	34, 48, 84, 93	0
4	x	213/214 (99%)	0.03	2 (0%) 84 77	25, 41, 54, 59	0
All	All	11292/11424 (98%)	0.15	361 (3%) 48 38	15, 51, 98, 159	0

The worst 5 of 361 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	133	GLY	8.1
1	Q	10	GLY	7.3
1	W	326	LYS	7.1
3	w	132	SER	7.1
2	N	27	GLN	6.3

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PCA	e	1	8/9	0.86	0.29	-	54,56,59,62	0
3	PCA	g	1	8/9	0.94	0.17	-	35,36,38,38	0
3	PCA	a	1	8/9	0.90	0.21	-	36,36,37,38	0
3	PCA	c	1	8/9	0.88	0.25	-	36,37,38,39	0
3	PCA	m	1	8/9	0.90	0.17	-	40,41,41,41	0
3	PCA	o	1	8/9	0.77	0.26	-	77,78,79,79	0
3	PCA	i	1	8/9	0.82	0.34	-	32,32,33,33	0
3	PCA	k	1	8/9	0.90	0.21	-	50,52,54,57	0
3	PCA	u	1	8/9	0.86	0.30	-	54,55,56,56	0
3	PCA	w	1	8/9	0.91	0.17	-	27,27,27,29	0
3	PCA	q	1	8/9	0.86	0.24	-	57,57,58,58	0
3	PCA	s	1	8/9	0.90	0.18	-	63,64,64,64	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	U	507	14/15	0.82	0.54	3.07	42,44,47,47	0
6	NAG	K	603	14/15	0.72	0.51	2.17	51,60,69,71	0
6	NAG	A	602	14/15	0.72	0.41	1.13	45,48,60,61	0
7	NAG	Q	507	14/15	0.85	0.33	0.80	46,50,54,57	0
6	NAG	O	504	14/15	0.80	0.41	0.42	47,52,59,62	0
7	NAG	I	506	14/15	0.81	0.38	0.23	50,57,61,63	0
6	NAG	E	602	14/15	0.87	0.28	-0.05	40,46,56,56	0
7	NAG	K	606	14/15	0.84	0.30	-0.11	40,47,50,53	0
7	NAG	E	606	14/15	0.78	0.24	-0.28	60,66,70,74	0
7	NAG	C	506	14/15	0.83	0.32	-0.30	43,45,49,50	0
7	NAG	S	507	14/15	0.79	0.28	-0.42	59,63,67,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	K	602	14/15	0.81	0.27	-0.46	49,56,67,67	0
7	NAG	M	507	14/15	0.76	0.37	-0.55	70,73,76,76	0
7	NAG	O	507	14/15	0.72	0.36	-0.58	71,77,82,84	0
7	NAG	A	606	14/15	0.82	0.24	-0.72	37,40,44,49	0
6	NAG	M	503	14/15	0.91	0.26	-0.80	66,67,68,68	0
7	NAG	W	606	14/15	0.85	0.26	-0.81	53,60,66,68	0
6	NAG	Q	503	14/15	0.86	0.23	-0.91	54,60,70,71	0
7	NAG	G	507	14/15	0.85	0.22	-0.93	37,42,47,49	0
6	NAG	C	502	14/15	0.94	0.24	-0.93	30,32,34,34	0
6	NAG	I	502	14/15	0.95	0.25	-1.16	40,47,57,58	0
6	NAG	O	503	14/15	0.91	0.19	-1.21	43,49,57,58	0
6	NAG	U	503	14/15	0.93	0.17	-1.38	41,43,48,48	0
6	NAG	C	503	14/15	0.84	0.21	-1.85	32,34,37,40	0
6	NAG	I	503	14/15	0.89	0.23	-1.85	42,50,60,62	0
6	MAN	U	506	11/12	0.83	0.24	-	74,78,81,82	0
6	MAN	C	505	11/12	0.91	0.20	-	56,59,60,61	0
6	BMA	M	505	11/12	0.48	0.31	-	78,82,85,86	0
6	MAN	M	506	11/12	0.69	0.34	-	88,92,93,93	0
6	MAN	E	605	11/12	0.83	0.27	-	76,78,80,81	0
6	NAG	U	504	14/15	0.84	0.27	-	44,46,55,58	0
6	NAG	G	504	14/15	0.92	0.21	-	30,37,45,47	0
6	NAG	A	603	14/15	0.79	0.28	-	45,54,65,65	0
7	NAG	I	507	14/15	0.78	0.23	-	62,74,81,82	0
7	NAG	S	508	14/15	0.74	0.25	-	70,80,86,87	0
6	NAG	S	503	14/15	0.85	0.19	-	53,58,69,69	0
6	NAG	W	602	14/15	0.73	0.32	-	39,46,56,57	0
7	NAG	O	508	14/15	0.79	0.32	-	82,93,102,102	0
7	NAG	W	607	14/15	0.84	0.28	-	67,78,86,87	0
7	NAG	E	607	14/15	0.70	0.33	-	75,83,89,90	0
7	NAG	A	607	14/15	0.79	0.36	-	51,59,65,65	0
6	MAN	W	605	11/12	0.75	0.26	-	78,81,84,84	0
6	BMA	E	604	11/12	0.60	0.26	-	64,68,72,73	0
6	MAN	I	505	11/12	0.73	0.33	-	75,78,80,80	0
6	MAN	S	506	11/12	0.84	0.29	-	81,83,84,84	0
6	BMA	Q	505	11/12	0.70	0.27	-	82,87,91,92	0
6	BMA	C	504	11/12	0.74	0.23	-	44,48,51,53	0
6	BMA	G	505	11/12	0.76	0.24	-	51,55,58,60	0
7	NAG	U	508	14/15	0.88	0.32	-	48,56,62,63	0
6	MAN	K	605	11/12	0.72	0.34	-	84,87,89,90	0
6	MAN	O	506	11/12	0.45	0.53	-	78,81,81,82	0
6	BMA	O	505	11/12	0.46	0.37	-	66,70,72,75	0
6	BMA	W	604	11/12	0.71	0.27	-	68,73,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	BMA	K	604	11/12	0.77	0.23	-	75,79,82,83	0
6	MAN	G	506	11/12	0.75	0.30	-	62,65,66,67	0
6	NAG	M	504	14/15	0.78	0.21	-	66,69,71,74	0
6	NAG	S	504	14/15	0.79	0.38	-	52,58,68,69	0
6	BMA	S	505	11/12	0.70	0.27	-	72,75,77,79	0
6	NAG	Q	504	14/15	0.82	0.42	-	57,66,77,78	0
6	NAG	G	503	14/15	0.93	0.25	-	26,32,41,42	0
7	NAG	M	508	14/15	0.77	0.30	-	70,79,89,89	0
6	MAN	Q	506	11/12	0.73	0.30	-	92,96,98,98	0
6	NAG	W	603	14/15	0.76	0.32	-	43,52,61,63	0
7	NAG	C	507	14/15	0.82	0.25	-	45,52,59,60	0
6	BMA	I	504	11/12	0.72	0.26	-	65,69,73,73	0
7	NAG	Q	508	14/15	0.83	0.36	-	59,67,73,73	0
6	MAN	A	605	11/12	0.73	0.40	-	78,80,84,84	0
7	NAG	G	508	14/15	0.76	0.54	-	49,58,66,66	0
7	NAG	K	607	14/15	0.61	0.41	-	54,62,69,69	0
6	BMA	U	505	11/12	0.56	0.31	-	62,67,72,72	0
6	NAG	E	603	14/15	0.88	0.25	-	46,50,58,60	0
6	BMA	A	604	11/12	0.77	0.22	-	70,74,78,78	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	G	502	14/15	0.49	0.70	4.38	42,47,49,51	0
5	NAG	D	201	14/15	0.71	0.37	3.72	73,75,77,78	0
5	NAG	T	201	14/15	0.58	0.48	2.17	93,100,105,107	0
5	NAG	C	501	14/15	0.74	0.42	2.15	66,69,74,76	0
5	NAG	N	201	14/15	0.52	0.34	1.51	109,114,121,122	0
5	NAG	O	501	14/15	0.64	0.63	1.50	90,98,105,108	0
5	NAG	X	201	14/15	0.66	0.34	1.28	119,129,138,140	0
5	NAG	S	501	14/15	0.72	0.48	1.08	71,78,84,87	0
5	NAG	P	201	14/15	0.56	0.36	0.80	96,101,106,107	0
5	NAG	J	201	14/15	0.68	0.39	0.29	73,75,79,80	0
5	NAG	L	201	14/15	0.62	0.38	0.10	81,89,95,96	0
5	NAG	A	601	14/15	0.56	0.46	0.02	38,44,45,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	201	14/15	0.76	0.26	0.01	80,89,94,96	0
5	NAG	Q	501	14/15	0.85	0.24	-0.42	66,74,80,83	0
5	NAG	G	501	14/15	0.78	0.30	-0.44	68,75,84,87	0
5	NAG	I	501	14/15	0.68	0.36	-0.44	66,74,81,84	0
5	NAG	U	501	14/15	0.84	0.26	-0.52	66,70,75,78	0
5	NAG	M	501	14/15	0.85	0.23	-1.63	89,92,96,98	0
5	NAG	R	201	14/15	0.36	0.60	-	100,111,117,117	0
5	NAG	V	201	14/15	0.64	0.58	-	83,85,91,93	0
5	NAG	E	601	14/15	0.44	0.42	-	59,64,66,67	0
5	NAG	H	201	14/15	0.69	0.33	-	115,125,133,134	0
5	NAG	O	502	14/15	0.62	0.37	-	74,78,81,83	0
5	NAG	U	502	14/15	0.45	0.61	-	46,48,50,51	0
5	NAG	S	502	14/15	0.57	0.42	-	65,69,74,75	0
5	NAG	W	601	14/15	0.55	0.40	-	45,51,52,54	0
5	NAG	K	601	14/15	0.63	0.34	-	58,64,66,68	0
5	NAG	M	502	14/15	0.40	0.58	-	75,76,77,78	0
5	NAG	Q	502	14/15	0.49	0.66	-	61,67,70,71	0
5	NAG	F	201	14/15	0.76	0.44	-	88,93,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.