



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:24 PM GMT

PDB ID : 3WHE
Title : A new conserved neutralizing epitope at the globular head of hemagglutinin
in H3N2 influenza viruses
Authors : Fujii, Y.; Sumida, T.; Shirouzu, M.; Yokoyama, S.
Deposited on : 2013-08-25
Resolution : 4.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

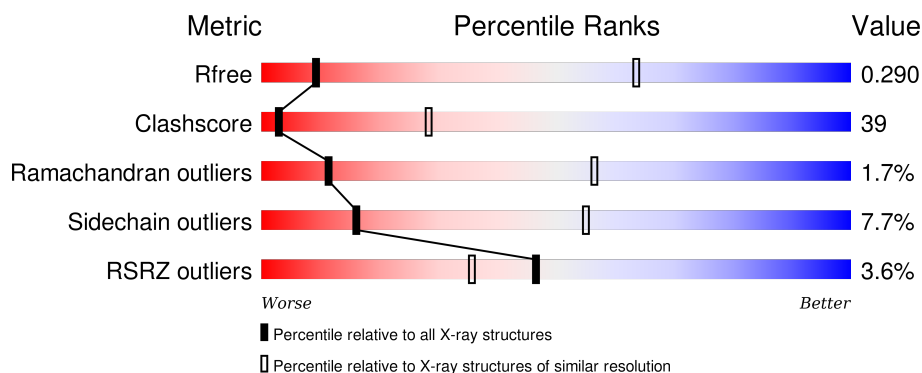
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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	493	<div> <div>2%</div> <div>49%</div> <div>46%</div> <div>.</div> </div>
1	B	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>.</div> </div>
1	C	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>.</div> </div>
1	D	493	<div> <div>2%</div> <div>47%</div> <div>48%</div> <div>.</div> </div>
1	E	493	<div> <div>2%</div> <div>46%</div> <div>49%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	493	% 46% 49% 5%
1	G	493	% 48% 48% .
1	H	493	% 47% 49% .
1	I	493	% 46% 50% .
1	J	493	2% 47% 49% .
1	K	493	% 46% 50% .
1	L	493	3% 47% 48% .
2	1	226	6% 32% 57% 11%
2	3	226	8% 32% 57% 11%
2	5	226	9% 32% 57% 11%
2	7	226	4% 32% 56% 12%
2	9	226	3% 33% 56% 11%
2	M	226	6% 29% 60% 11%
2	O	226	4% 32% 57% 12%
2	Q	226	8% 31% 58% 11%
2	S	226	11% 31% 58% 12%
2	U	226	10% 31% 57% 12%
2	W	226	12% 32% 56% 12%
2	Y	226	8% 31% 58% 11%
3	0	220	39% 52% 5% .
3	2	220	2% 41% 50% 5% .
3	4	220	2% 40% 52% 5% .
3	6	220	7% 40% 52% 5% .
3	8	220	% 43% 49% 5% .
3	N	220	3% 36% 55% 5% .

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Mol	Chain	Length	Quality of chain
3	P	220	
3	R	220	
3	T	220	
3	V	220	
3	X	220	
3	Z	220	

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
4	NAG	K	602	-	-	X	-
5	NAG	H	608	-	-	-	X
5	NAG	H	618	-	-	-	X
6	NAG	C	610	-	-	X	-
6	NAG	F	610	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 88152 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	B	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	C	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	D	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	E	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	F	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	G	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	H	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	I	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	J	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	K	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			
1	L	493	Total	C	N	O	S	0	0	0
			3878	2418	684	757	19			

- Molecule 2 is a protein called immunoglobulin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	O	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Q	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	S	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	U	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	W	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	Y	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	1	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	3	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	5	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	7	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			
2	9	226	Total	C	N	O	S	0	0	0
			1697	1072	284	331	10			

- Molecule 3 is a protein called immunoglobulin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	P	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	R	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	T	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	V	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	X	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	Z	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	2	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	4	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

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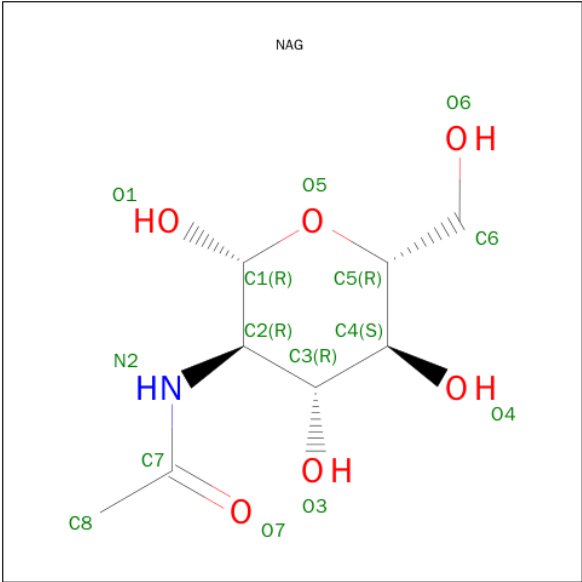
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	6	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	8	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			
3	0	212	Total	C	N	O	S	0	0	0
			1549	965	261	319	4			

- Molecule 4 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	7	Total	C	N	O	0	0
			83	46	2	35		
4	B	7	Total	C	N	O	0	0
			83	46	2	35		
4	C	7	Total	C	N	O	0	0
			83	46	2	35		
4	D	7	Total	C	N	O	0	0
			83	46	2	35		
4	E	7	Total	C	N	O	0	0
			83	46	2	35		
4	F	7	Total	C	N	O	0	0
			83	46	2	35		
4	G	7	Total	C	N	O	0	0
			83	46	2	35		
4	H	7	Total	C	N	O	0	0
			83	46	2	35		
4	I	7	Total	C	N	O	0	0
			83	46	2	35		
4	J	7	Total	C	N	O	0	0
			83	46	2	35		
4	K	7	Total	C	N	O	0	0
			83	46	2	35		
4	L	7	Total	C	N	O	0	0
			83	46	2	35		

- 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	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	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		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
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	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	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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	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	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	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	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	L	1	Total	C	N	O	0	0
			14	8	1	5		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	6	Total	C	N	O	0	0
			72	40	2	30		
6	B	6	Total	C	N	O	0	0
			72	40	2	30		
6	C	6	Total	C	N	O	0	0
			72	40	2	30		
6	D	6	Total	C	N	O	0	0
			72	40	2	30		
6	E	6	Total	C	N	O	0	0
			72	40	2	30		
6	F	6	Total	C	N	O	0	0
			72	40	2	30		
6	G	6	Total	C	N	O	0	0
			72	40	2	30		
6	H	6	Total	C	N	O	0	0
			72	40	2	30		
6	I	6	Total	C	N	O	0	0
			72	40	2	30		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	6	Total	C	N	O	0	0
			72	40	2	30		
6	K	6	Total	C	N	O	0	0
			72	40	2	30		
6	L	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		
7	C	3	Total	C	N	O	0	0
			39	22	2	15		
7	D	3	Total	C	N	O	0	0
			39	22	2	15		
7	E	3	Total	C	N	O	0	0
			39	22	2	15		
7	F	3	Total	C	N	O	0	0
			39	22	2	15		
7	G	3	Total	C	N	O	0	0
			39	22	2	15		
7	H	3	Total	C	N	O	0	0
			39	22	2	15		
7	I	3	Total	C	N	O	0	0
			39	22	2	15		
7	J	3	Total	C	N	O	0	0
			39	22	2	15		
7	K	3	Total	C	N	O	0	0
			39	22	2	15		
7	L	3	Total	C	N	O	0	0
			39	22	2	15		

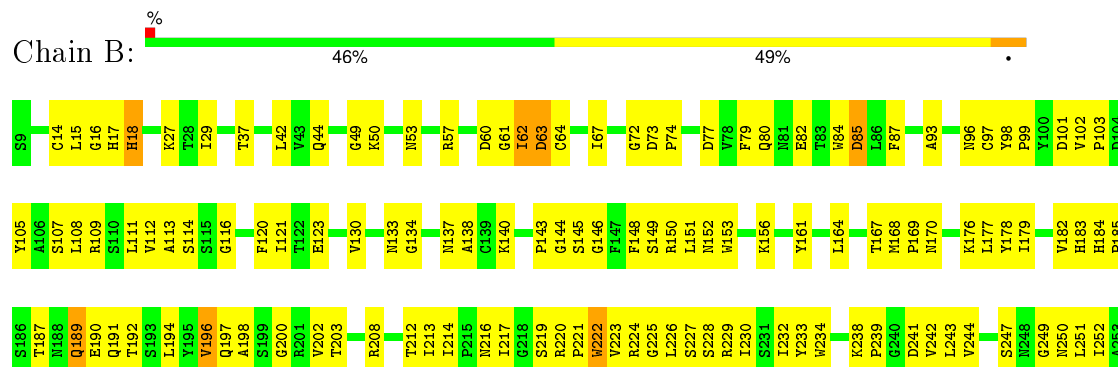
3 Residue-property plots

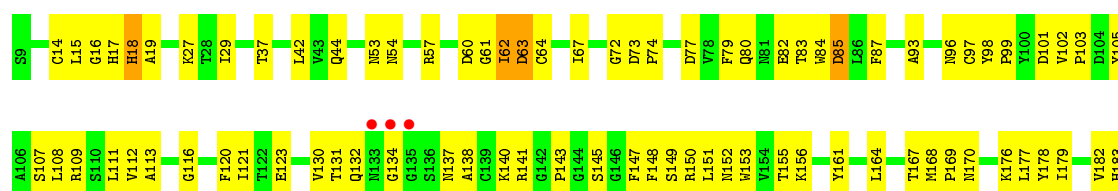
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

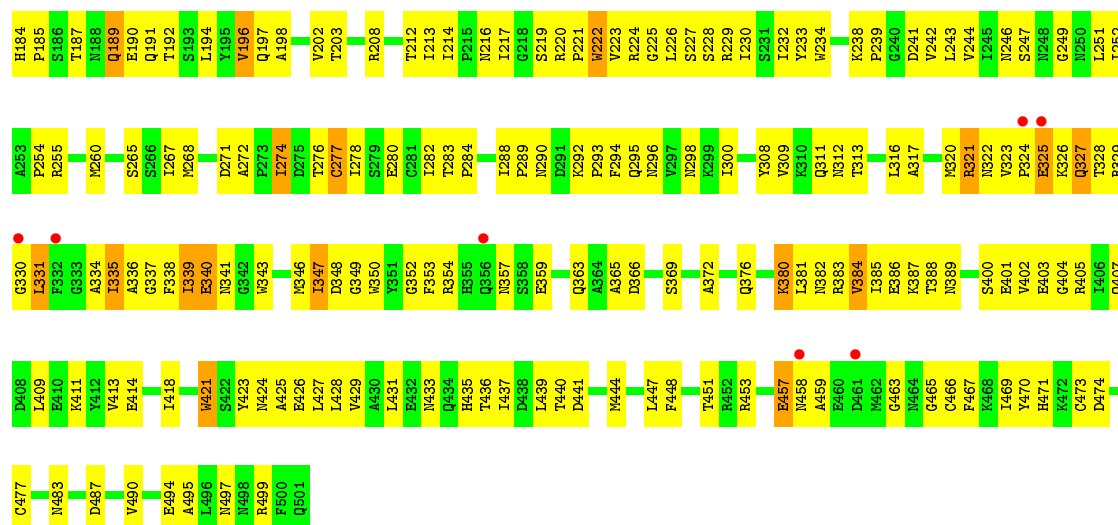
• Molecule 1: Hemagglutinin



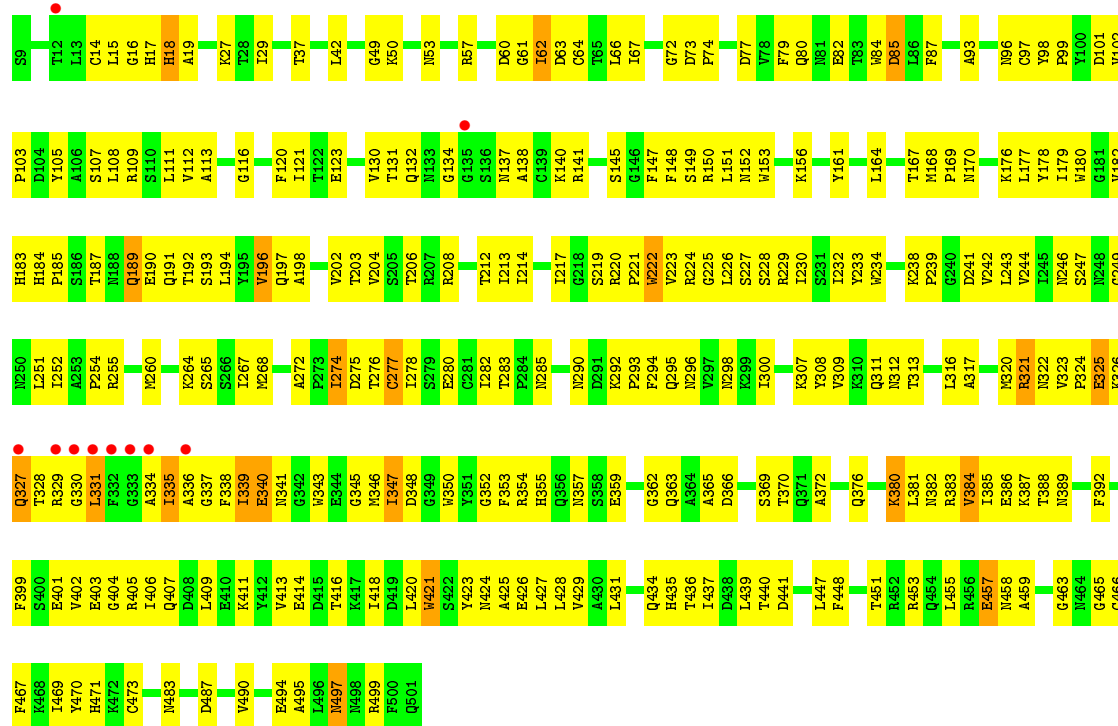
• Molecule 1: Hemagglutinin



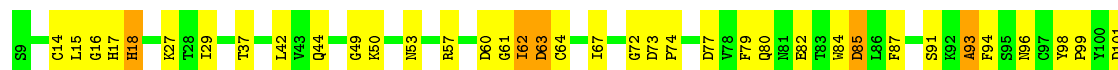


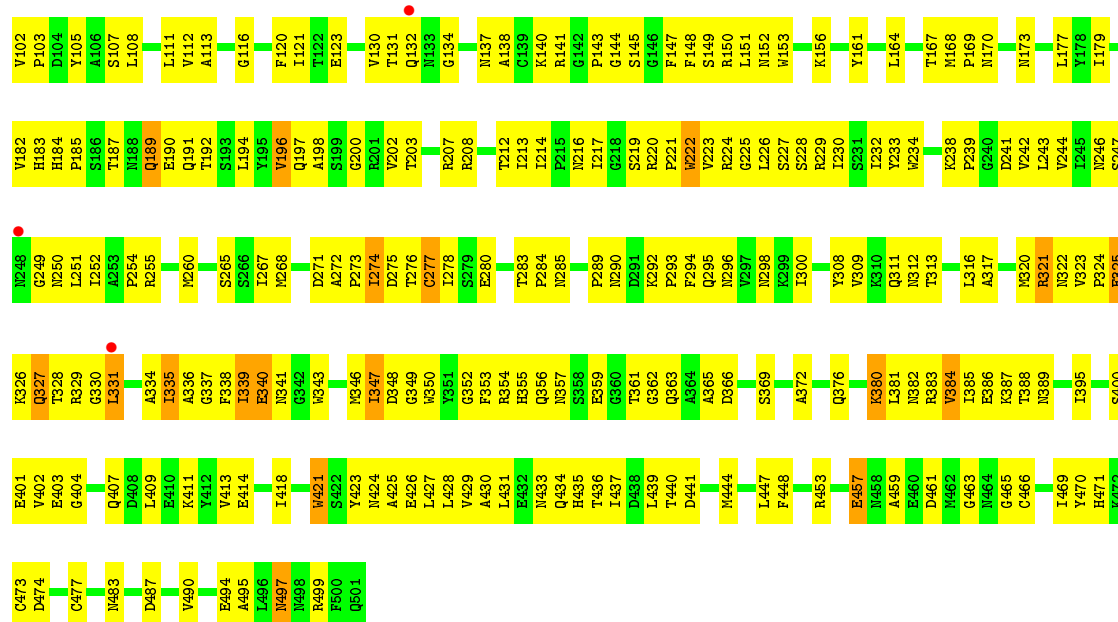


• Molecule 1: Hemagglutinin

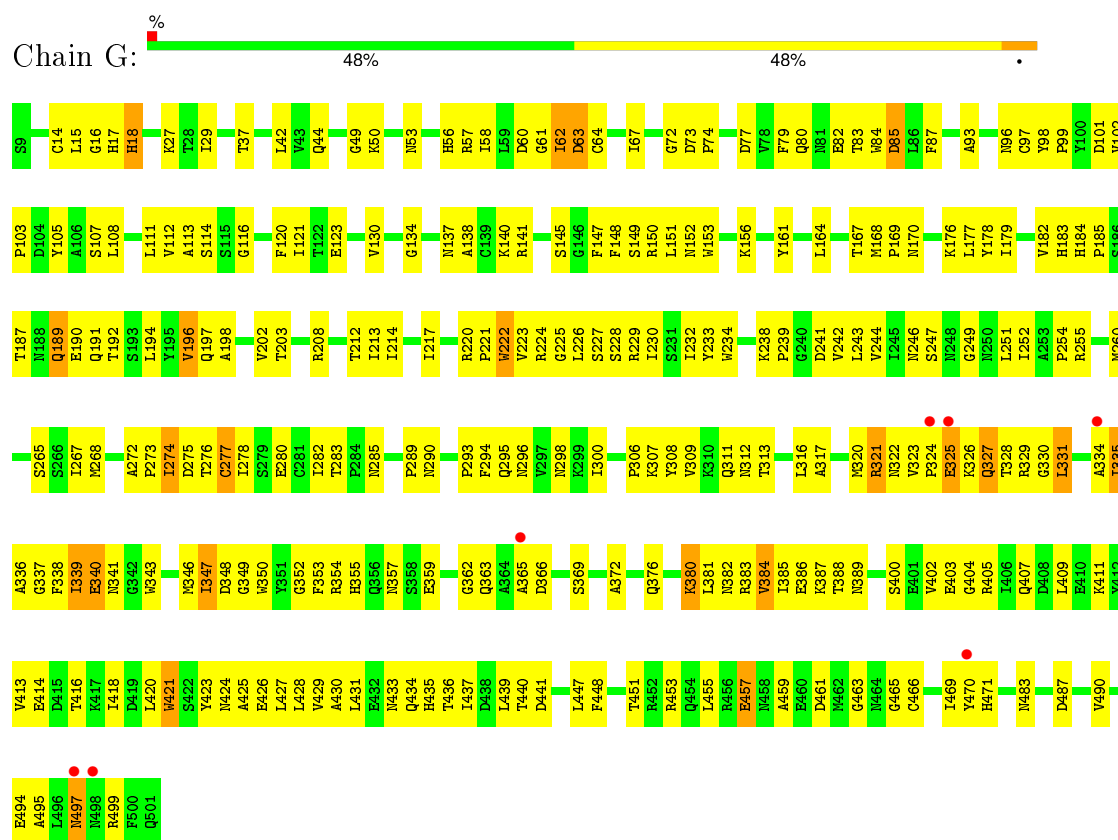


• Molecule 1: Hemagglutinin



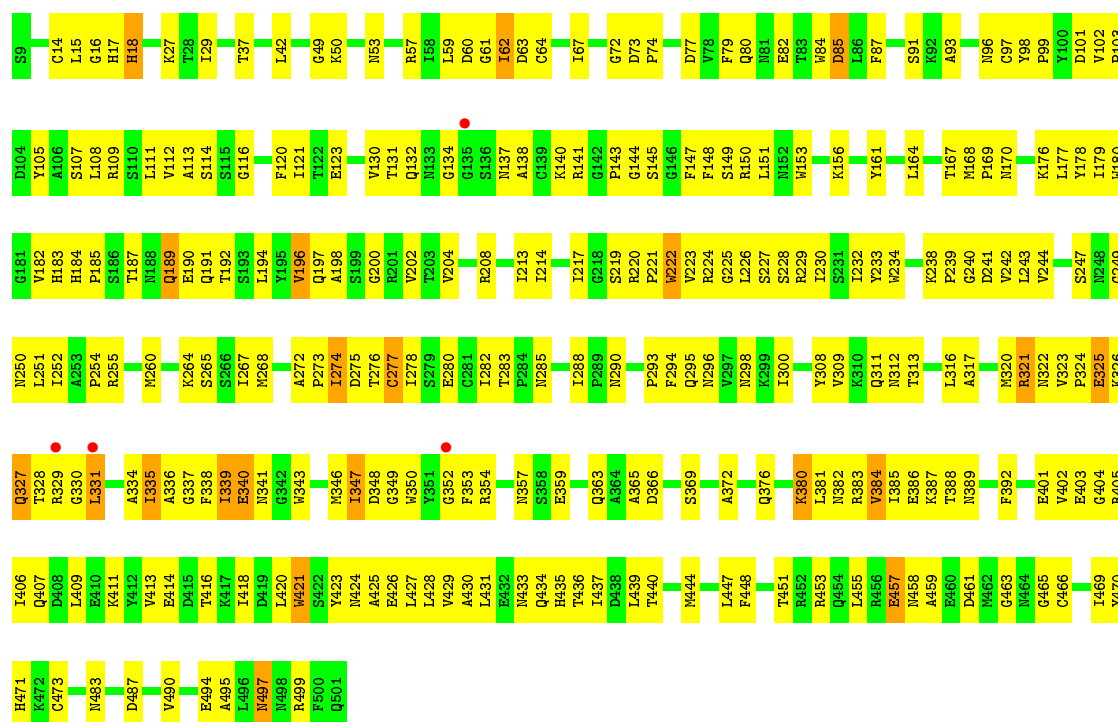


• Molecule 1: Hemagglutinin

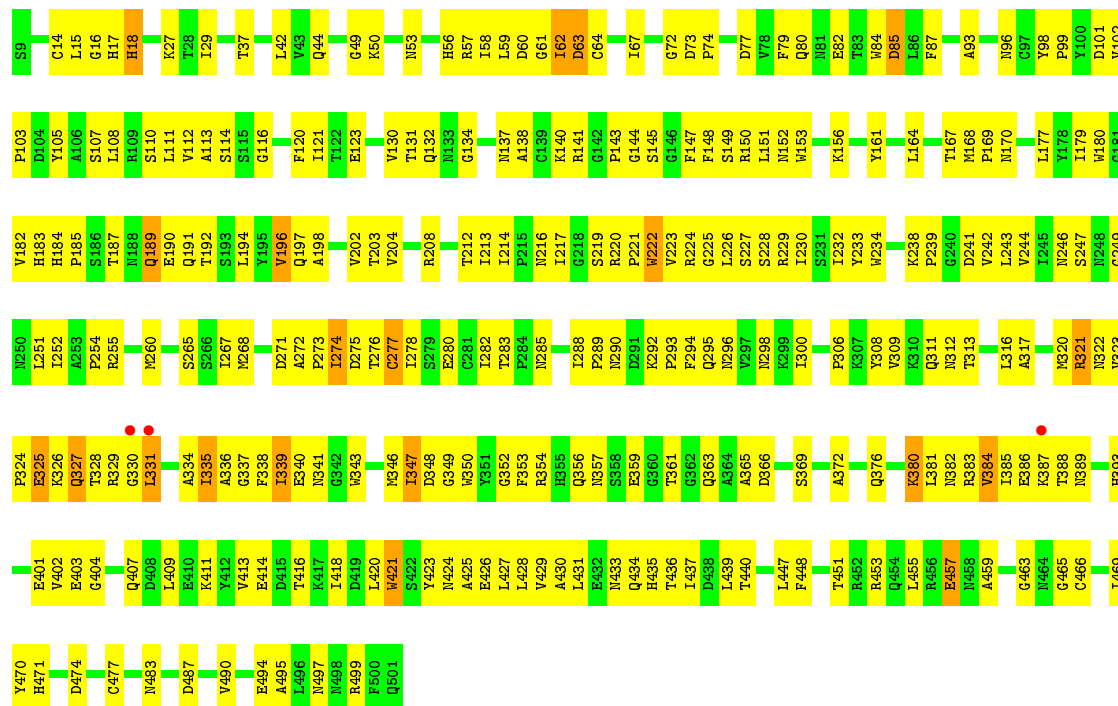


• Molecule 1: Hemagglutinin



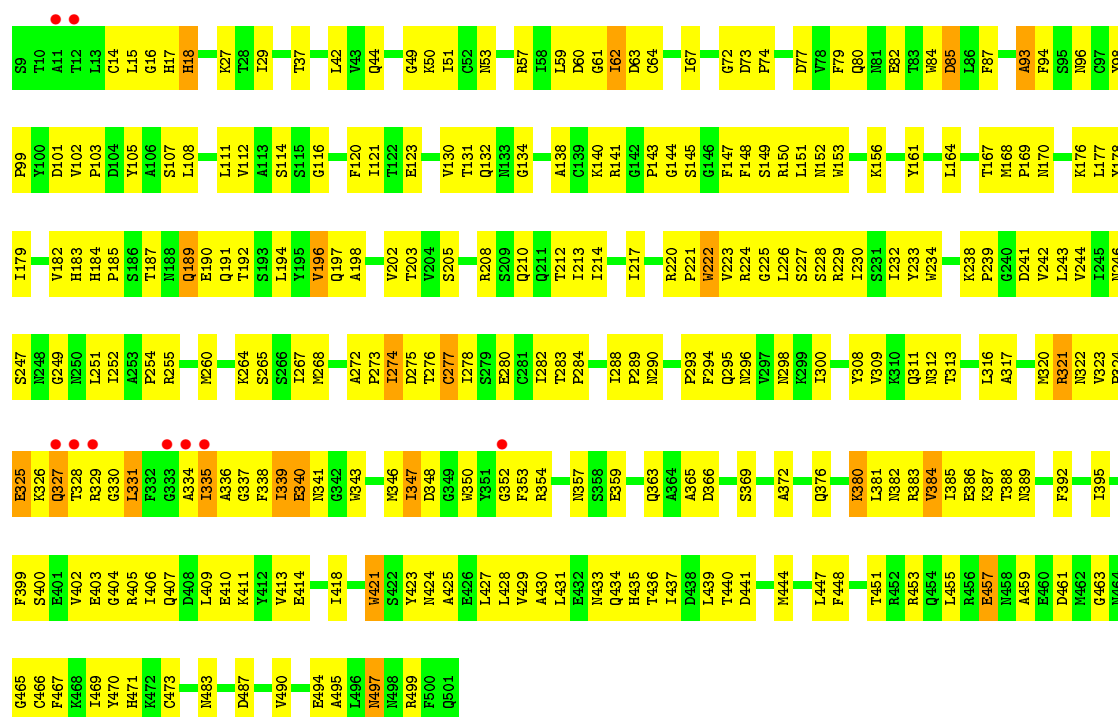


• Molecule 1: Hemagglutinin

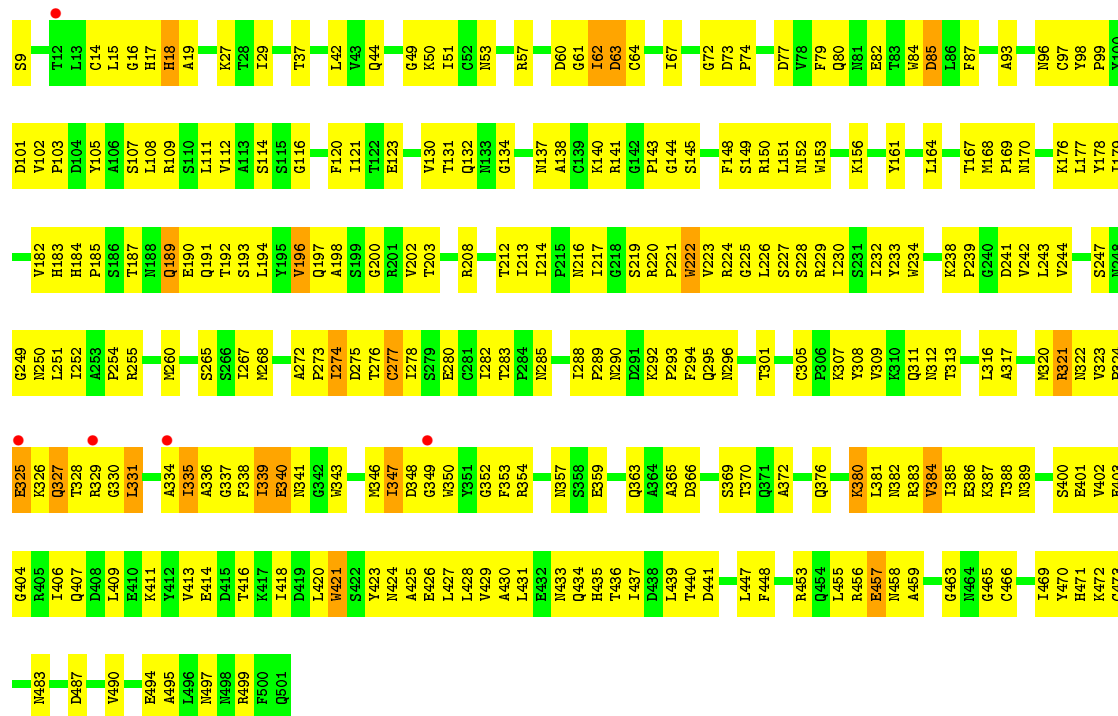


• Molecule 1: Hemagglutinin



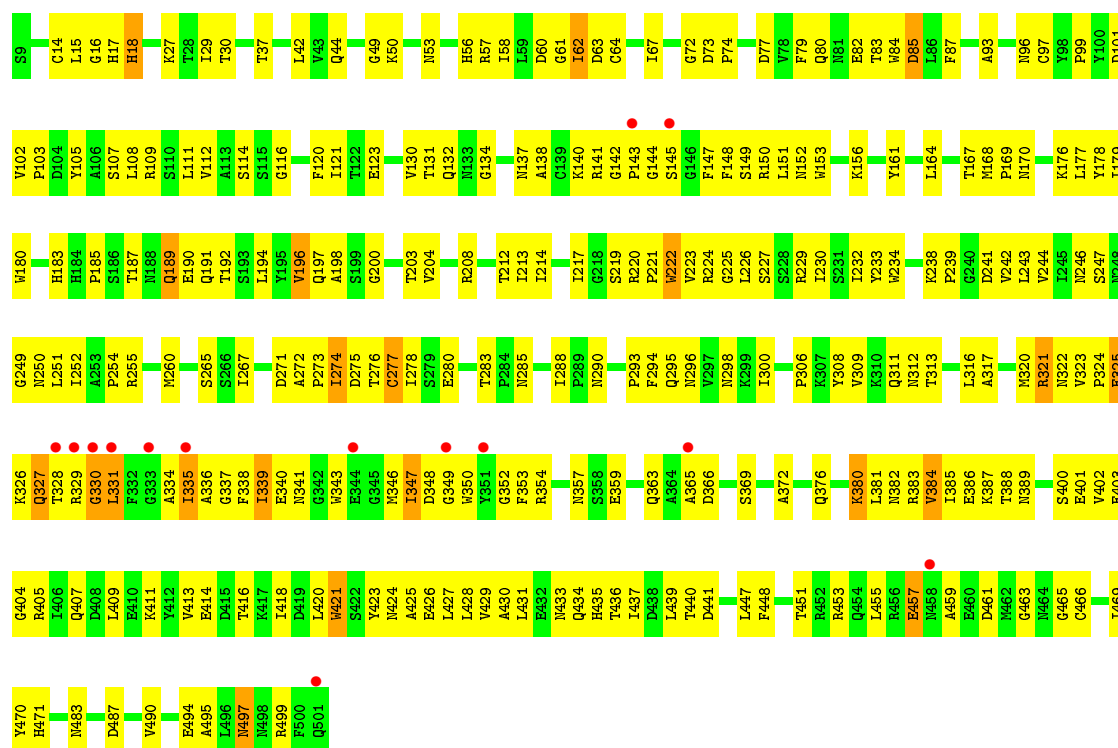


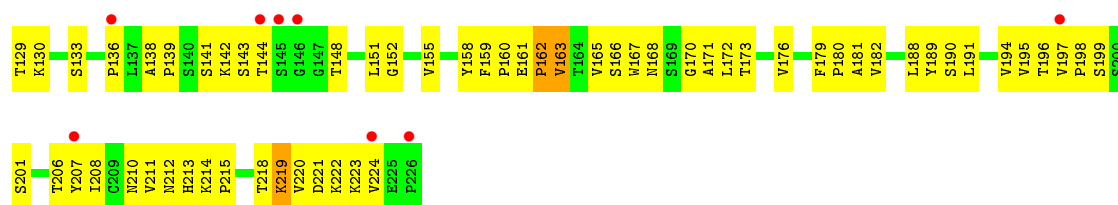
• Molecule 1: Hemagglutinin



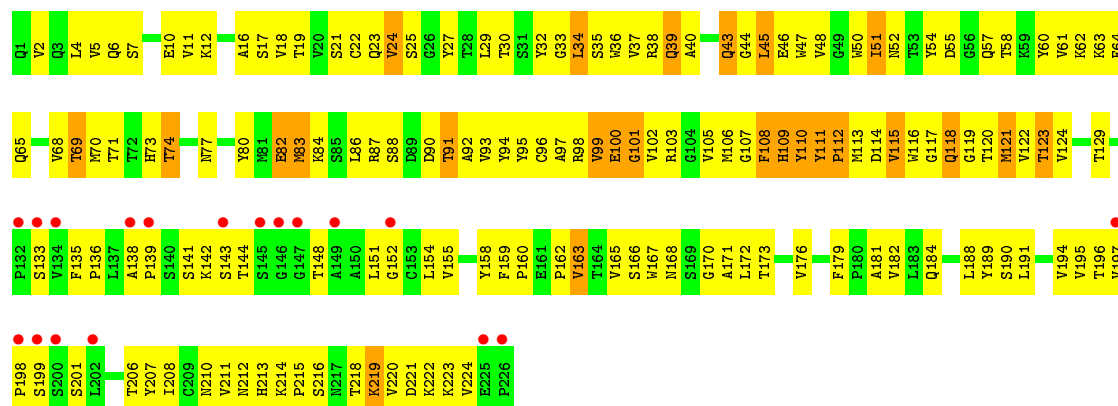
• Molecule 1: Hemagglutinin



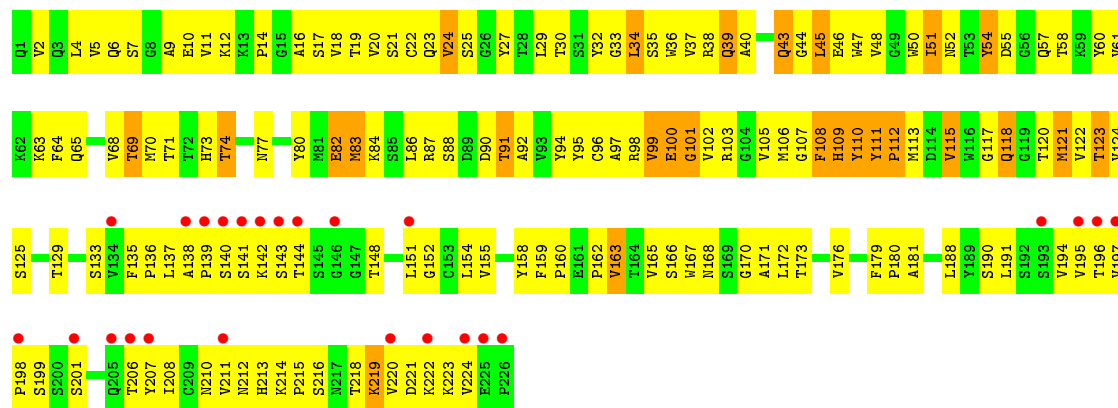




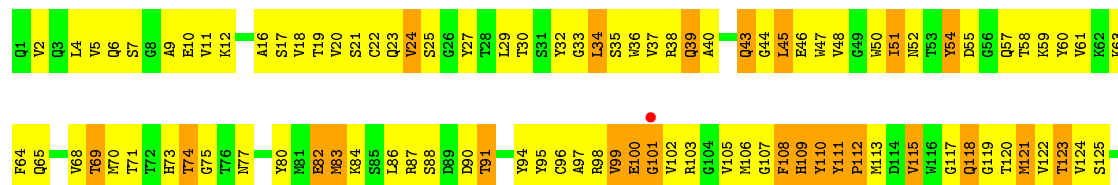
• Molecule 2: immunoglobulin heavy chain

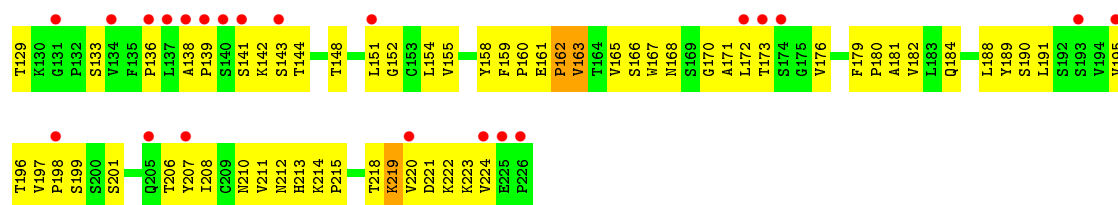


• Molecule 2: immunoglobulin heavy chain

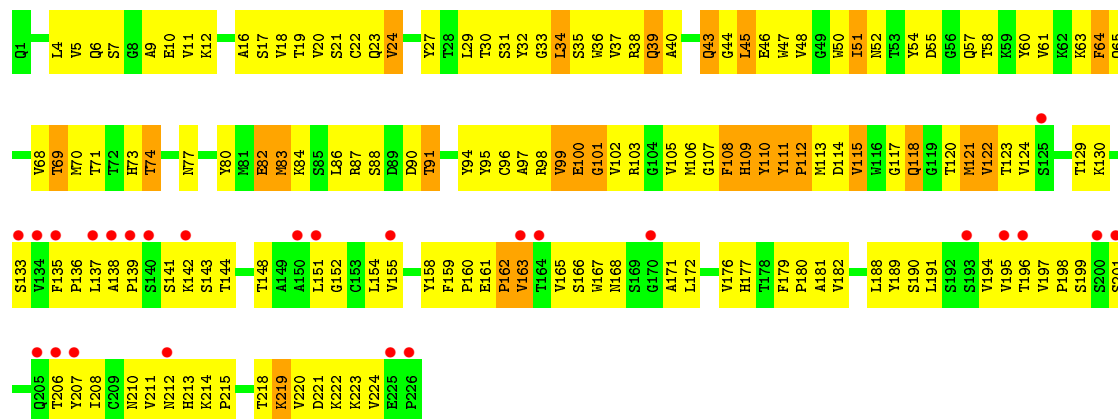


• Molecule 2: immunoglobulin heavy chain

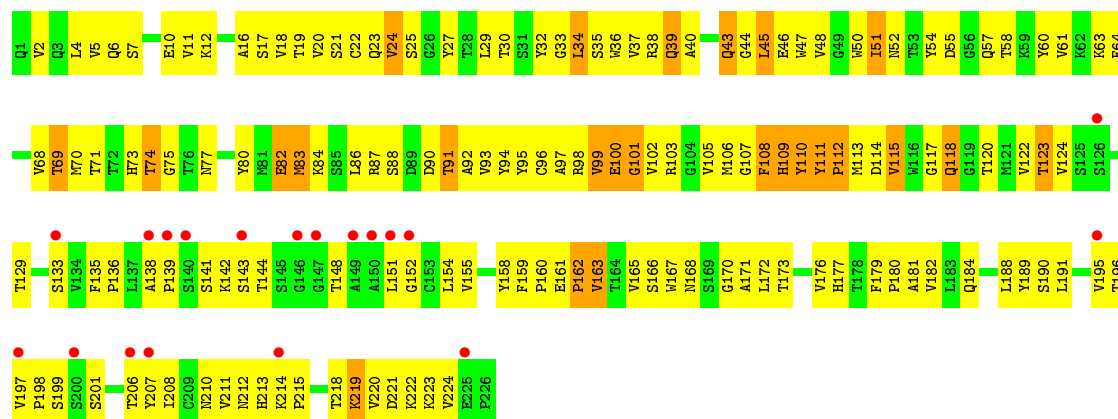




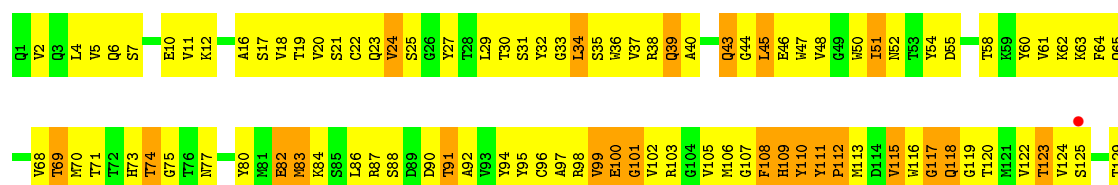
• Molecule 2: immunoglobulin heavy chain



• Molecule 2: immunoglobulin heavy chain

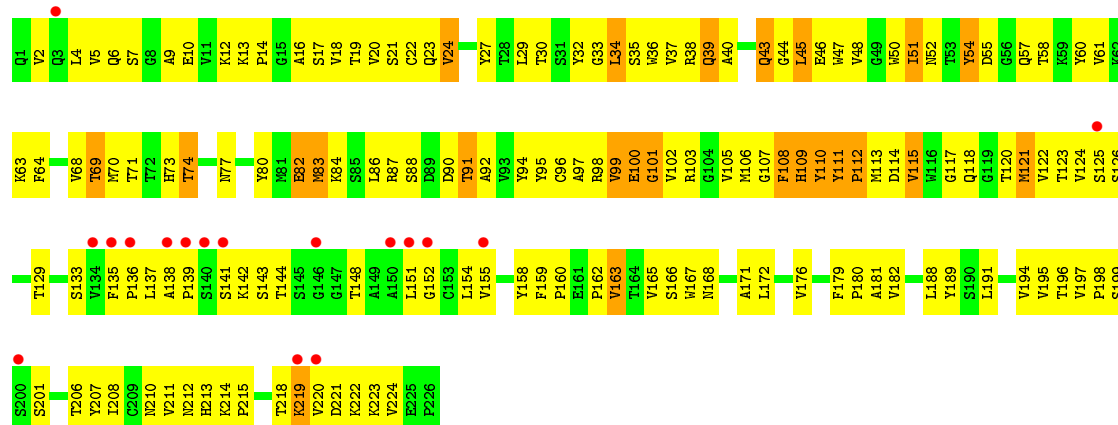


• Molecule 2: immunoglobulin heavy chain

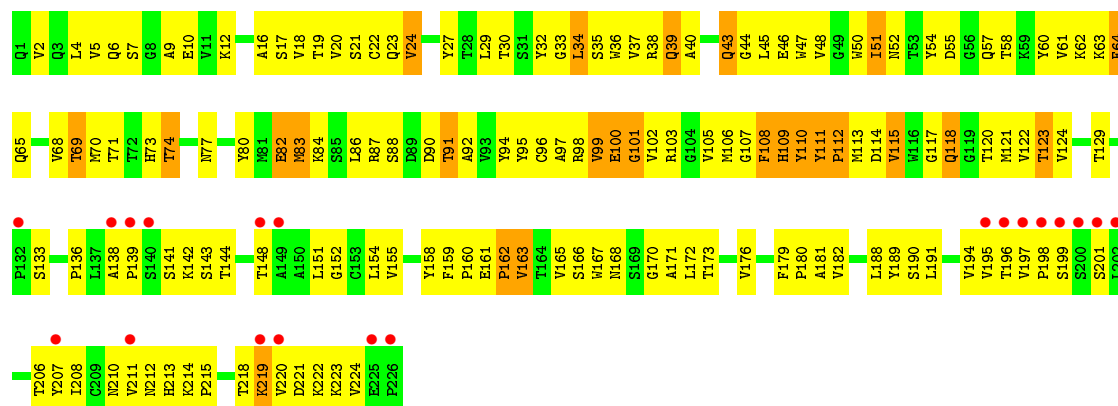




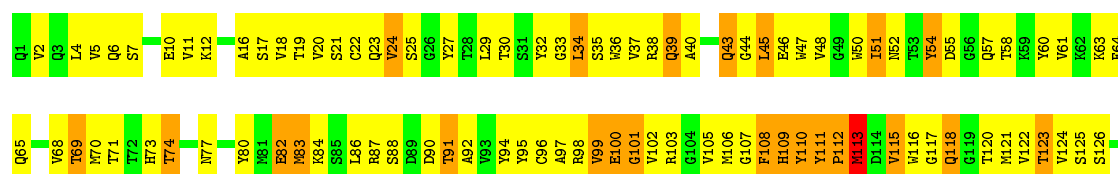
• Molecule 2: immunoglobulin heavy chain

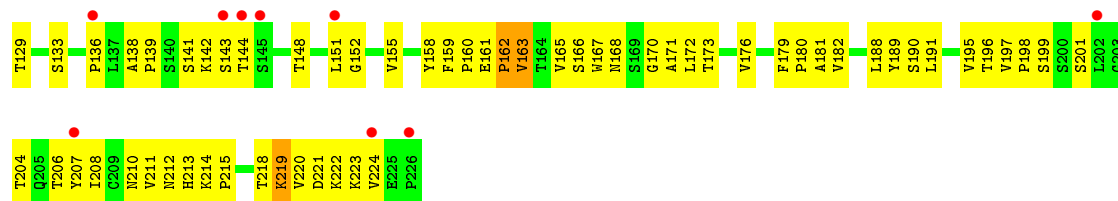


• Molecule 2: immunoglobulin heavy chain

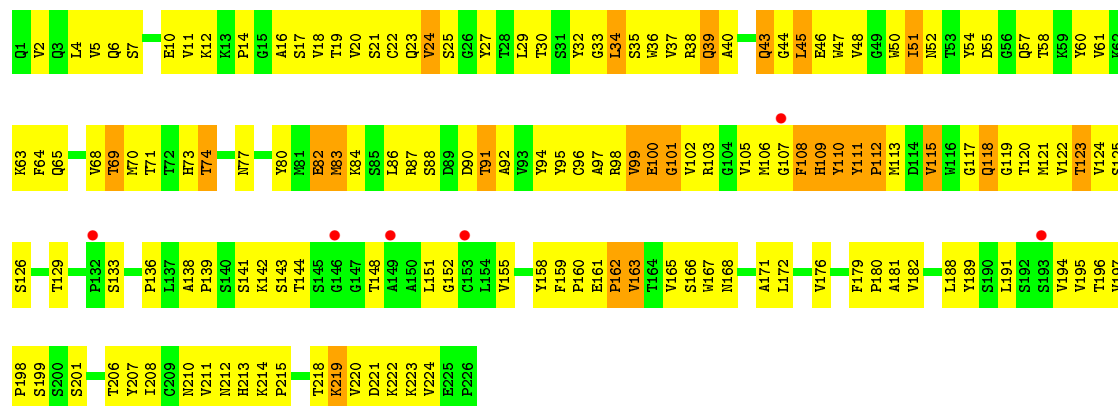


• Molecule 2: immunoglobulin heavy chain

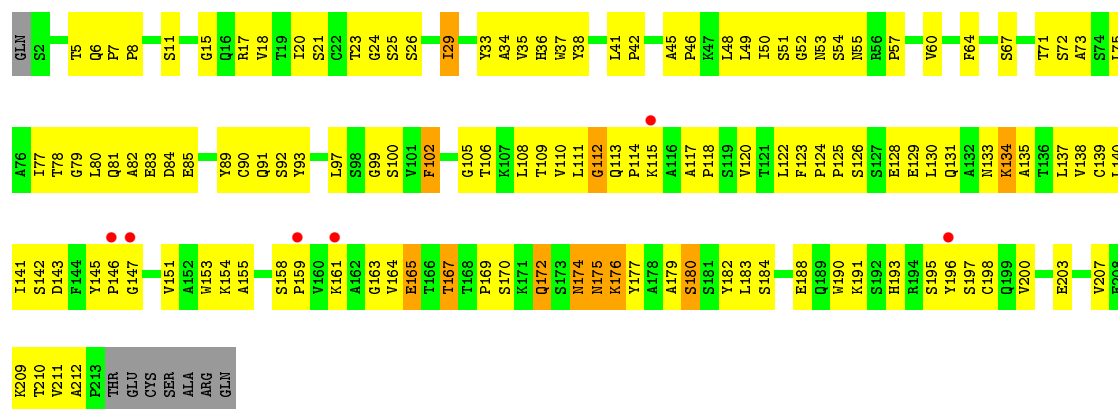




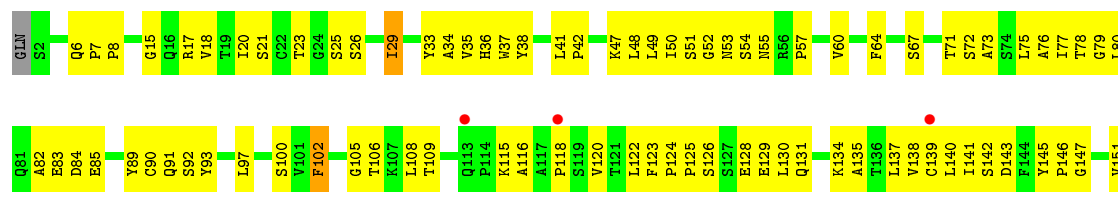
• Molecule 2: immunoglobulin heavy chain

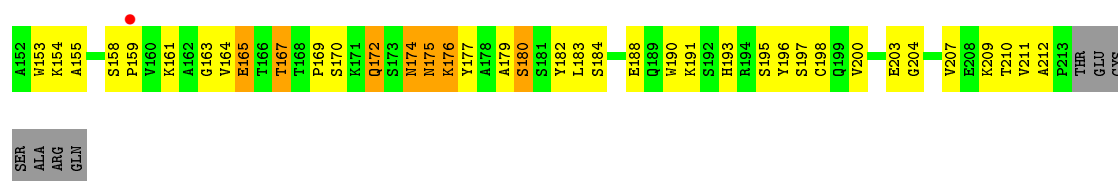


• Molecule 3: immunoglobulin light chain

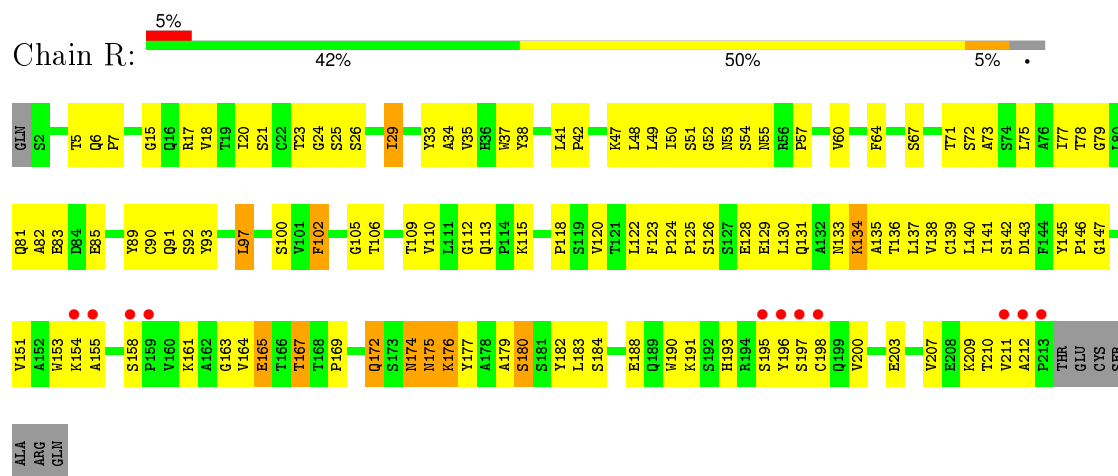


• Molecule 3: immunoglobulin light chain

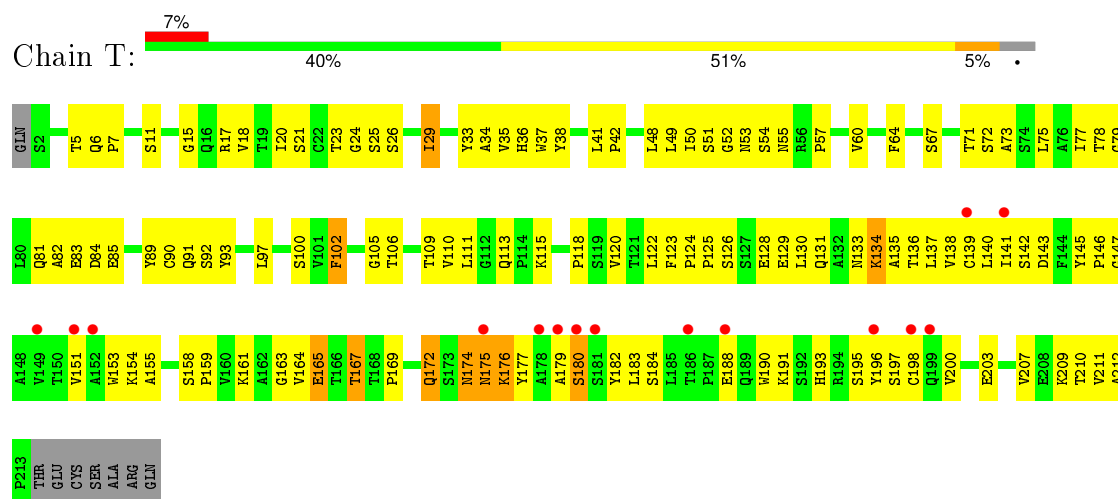




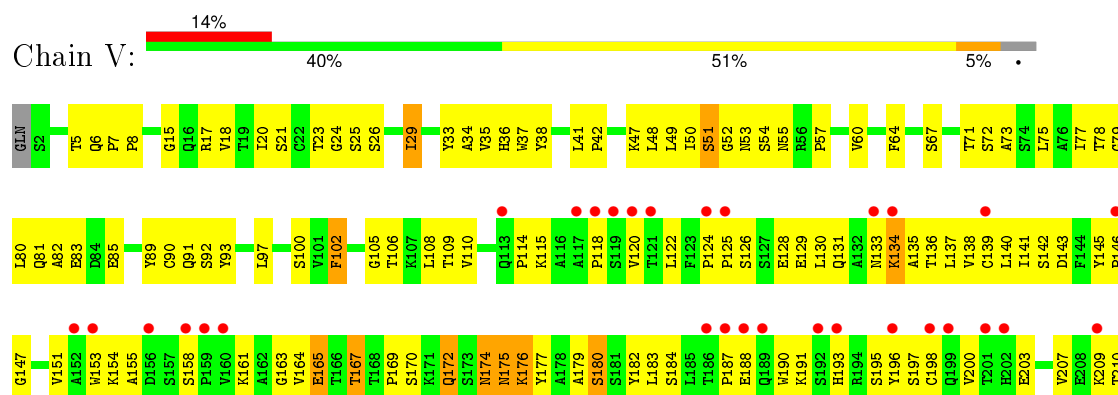
• Molecule 3: immunoglobulin light chain



• Molecule 3: immunoglobulin light chain

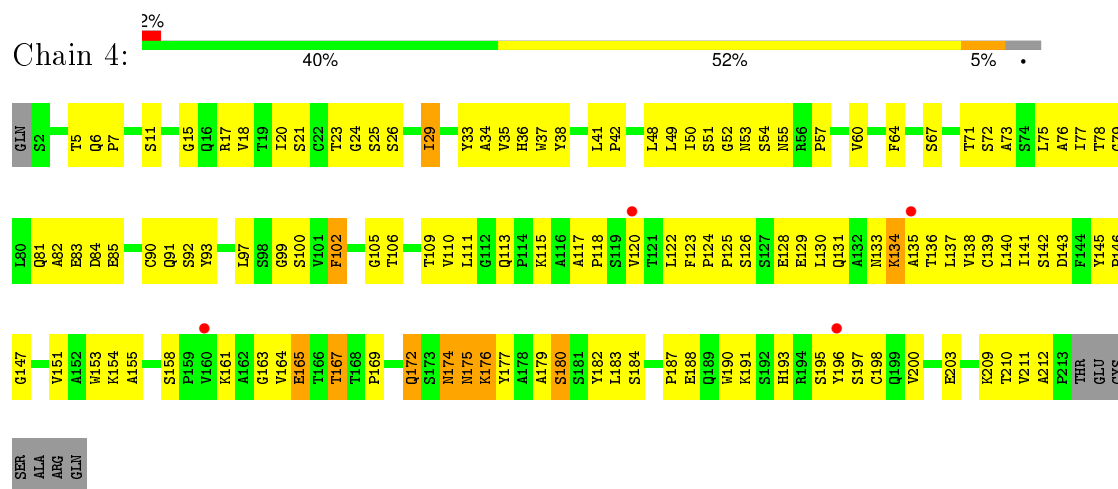


• Molecule 3: immunoglobulin light chain

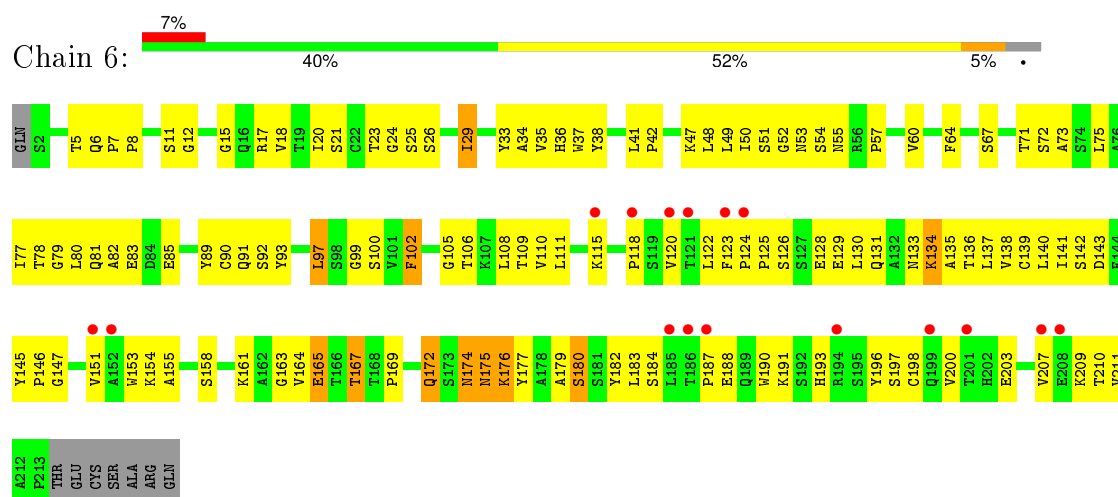


CYS
SER
ALA
ARG
GLN

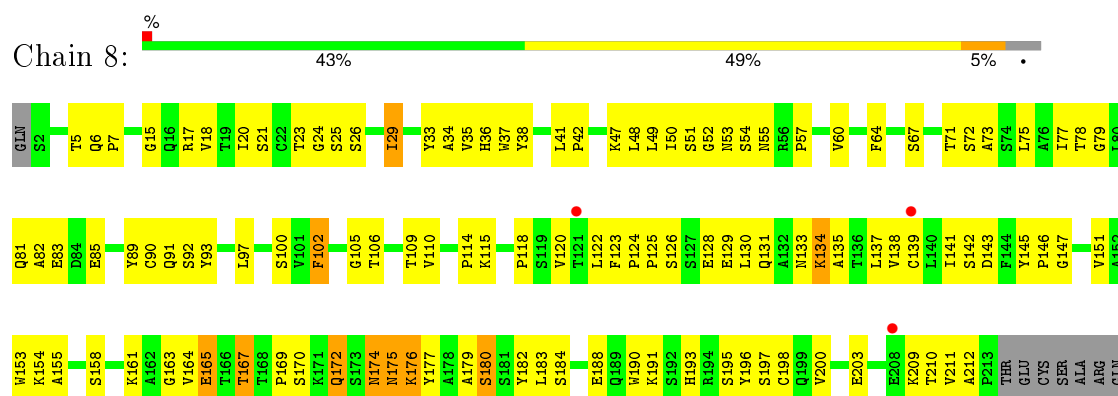
• Molecule 3: immunoglobulin light chain



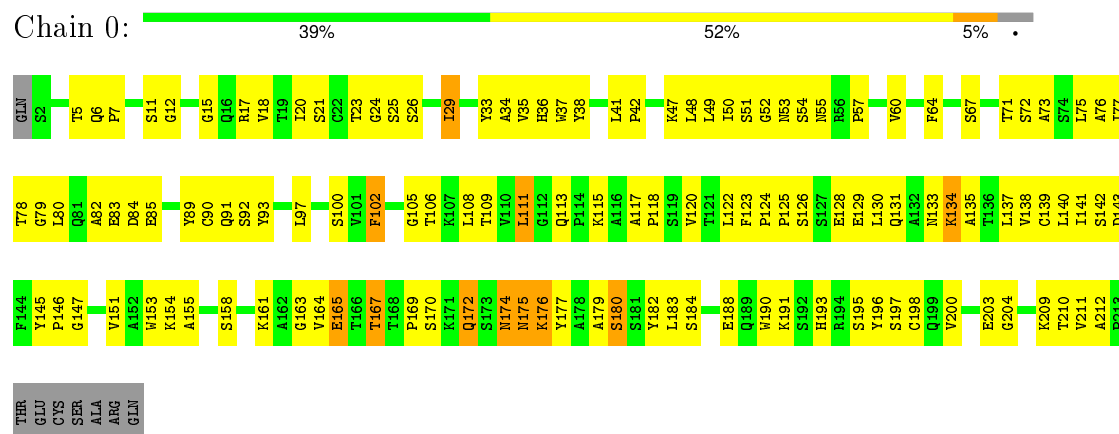
• Molecule 3: immunoglobulin light chain



• Molecule 3: immunoglobulin light chain



• Molecule 3: immunoglobulin light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	391.04Å 241.17Å 223.21Å 90.00° 123.62° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00 29.98 – 4.00	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-4.00) 98.2 (29.98-4.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.308 0.283 , 0.290	Depositor DCC
R_{free} test set	7101 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	180.3	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 149.3	EDS
Estimated twinning fraction	0.063 for -h-2*k,l,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 142111 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	88152	wwPDB-VP
Average B, all atoms (Å ²)	205.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.25	0/3959	0.50	0/5369
1	B	0.25	0/3959	0.50	0/5369
1	C	0.25	0/3959	0.50	0/5369
1	D	0.25	0/3959	0.50	0/5369
1	E	0.25	0/3959	0.50	0/5369
1	F	0.25	0/3959	0.49	0/5369
1	G	0.25	0/3959	0.50	0/5369
1	H	0.25	0/3959	0.50	0/5369
1	I	0.25	0/3959	0.50	0/5369
1	J	0.25	0/3959	0.50	0/5369
1	K	0.25	0/3959	0.50	0/5369
1	L	0.25	0/3959	0.50	0/5369
2	1	0.25	0/1739	0.52	0/2371
2	3	0.26	0/1739	0.52	0/2371
2	5	0.25	0/1739	0.52	0/2371
2	7	0.25	0/1739	0.52	0/2371
2	9	0.26	0/1739	0.52	0/2371
2	M	0.25	0/1739	0.52	0/2371
2	O	0.25	0/1739	0.52	0/2371
2	Q	0.25	0/1739	0.53	0/2371
2	S	0.25	0/1739	0.52	0/2371
2	U	0.25	0/1739	0.52	0/2371
2	W	0.26	0/1739	0.52	0/2371
2	Y	0.25	0/1739	0.52	0/2371
3	0	0.26	0/1586	0.53	0/2166
3	2	0.26	0/1586	0.53	0/2166
3	4	0.26	0/1586	0.53	0/2166
3	6	0.26	0/1586	0.53	0/2166
3	8	0.26	0/1586	0.53	0/2166
3	N	0.26	0/1586	0.55	1/2166 (0.0%)
3	P	0.26	0/1586	0.53	0/2166
3	R	0.26	0/1586	0.55	1/2166 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	T	0.26	0/1586	0.53	0/2166
3	V	0.28	0/1586	0.55	0/2166
3	X	0.26	0/1586	0.53	0/2166
3	Z	0.26	0/1586	0.53	0/2166
All	All	0.25	0/87408	0.51	2/118872 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	112	GLY	N-CA-C	-5.23	100.03	113.10
3	N	112	GLY	N-CA-C	-5.11	100.33	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3878	0	3743	259	0
1	B	3878	0	3743	278	0
1	C	3878	0	3743	277	0
1	D	3878	0	3743	277	0
1	E	3878	0	3743	281	0
1	F	3878	0	3743	283	0
1	G	3878	0	3743	249	0
1	H	3878	0	3743	259	0
1	I	3878	0	3743	256	0
1	J	3878	0	3743	263	0
1	K	3878	0	3743	262	0
1	L	3878	0	3743	268	0
2	1	1697	0	1668	192	0
2	3	1697	0	1668	191	2
2	5	1697	0	1668	193	0
2	7	1697	0	1668	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	1697	0	1668	192	0
2	M	1697	0	1668	217	0
2	O	1697	0	1668	197	0
2	Q	1697	0	1668	191	0
2	S	1697	0	1668	200	0
2	U	1697	0	1668	210	0
2	W	1697	0	1668	211	0
2	Y	1697	0	1668	189	0
3	0	1549	0	1503	133	0
3	2	1549	0	1503	133	0
3	4	1549	0	1503	136	0
3	6	1549	0	1503	137	0
3	8	1549	0	1503	127	0
3	N	1549	0	1503	154	0
3	P	1549	0	1503	132	0
3	R	1549	0	1503	137	0
3	T	1549	0	1503	135	0
3	V	1549	0	1503	144	0
3	X	1549	0	1503	143	0
3	Z	1549	0	1503	133	0
4	A	83	0	70	4	0
4	B	83	0	70	5	0
4	C	83	0	70	1	0
4	D	83	0	70	4	0
4	E	83	0	70	2	0
4	F	83	0	70	2	0
4	G	83	0	70	2	0
4	H	83	0	70	2	0
4	I	83	0	70	1	0
4	J	83	0	70	4	0
4	K	83	0	70	7	0
4	L	83	0	70	5	0
5	A	28	0	26	0	0
5	B	28	0	26	0	0
5	C	28	0	26	0	0
5	D	28	0	26	0	0
5	E	28	0	26	0	0
5	F	28	0	26	0	0
5	G	28	0	26	0	0
5	H	28	0	26	0	0
5	I	28	0	26	0	0
5	J	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	28	0	26	0	0
5	L	28	0	26	0	0
6	A	72	0	61	3	0
6	B	72	0	61	3	0
6	C	72	0	61	9	0
6	D	72	0	61	7	0
6	E	72	0	61	3	0
6	F	72	0	61	11	0
6	G	72	0	61	3	0
6	H	72	0	61	3	0
6	I	72	0	61	4	0
6	J	72	0	61	3	0
6	K	72	0	61	3	0
6	L	72	0	61	4	0
7	A	39	0	34	1	0
7	B	39	0	34	1	0
7	C	39	0	34	1	0
7	D	39	0	34	1	0
7	E	39	0	34	1	0
7	F	39	0	34	1	0
7	G	39	0	34	2	0
7	H	39	0	34	1	0
7	I	39	0	34	1	0
7	J	39	0	34	1	0
7	K	39	0	34	1	0
7	L	39	0	34	1	0
All	All	88152	0	85260	6774	2

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 39.

The worst 5 of 6774 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:136:PRO:O	3:6:126:SER:HB3	1.52	1.09
3:2:143:ASP:HA	3:2:176:LYS:HG3	1.35	1.08
3:T:143:ASP:HA	3:T:176:LYS:HG3	1.35	1.08
3:0:143:ASP:HA	3:0:176:LYS:HG3	1.34	1.08
1:G:331:LEU:H	1:G:331:LEU:HD22	1.19	1.08

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:171:ALA:CB	2:3:171:ALA:CB[2_556]	1.73	0.47
2:3:206:THR:OG1	2:3:206:THR:OG1[2_556]	1.74	0.46

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	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	B	491/493 (100%)	425 (87%)	60 (12%)	6 (1%)	16	62
1	C	491/493 (100%)	427 (87%)	57 (12%)	7 (1%)	14	59
1	D	491/493 (100%)	429 (87%)	55 (11%)	7 (1%)	14	59
1	E	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	14	59
1	F	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	14	59
1	G	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	H	491/493 (100%)	426 (87%)	58 (12%)	7 (1%)	14	59
1	I	491/493 (100%)	431 (88%)	54 (11%)	6 (1%)	16	62
1	J	491/493 (100%)	430 (88%)	54 (11%)	7 (1%)	14	59
1	K	491/493 (100%)	424 (86%)	60 (12%)	7 (1%)	14	59
1	L	491/493 (100%)	429 (87%)	56 (11%)	6 (1%)	16	62
2	1	224/226 (99%)	200 (89%)	18 (8%)	6 (3%)	6	47
2	3	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	8	52
2	5	224/226 (99%)	202 (90%)	17 (8%)	5 (2%)	8	52
2	7	224/226 (99%)	198 (88%)	20 (9%)	6 (3%)	6	47
2	9	224/226 (99%)	201 (90%)	18 (8%)	5 (2%)	8	52
2	M	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52
2	O	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q	224/226 (99%)	203 (91%)	16 (7%)	5 (2%)	8	52
2	S	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	8	52
2	U	224/226 (99%)	199 (89%)	20 (9%)	5 (2%)	8	52
2	W	224/226 (99%)	200 (89%)	19 (8%)	5 (2%)	8	52
2	Y	224/226 (99%)	197 (88%)	22 (10%)	5 (2%)	8	52
3	0	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	7	50
3	2	210/220 (96%)	191 (91%)	16 (8%)	3 (1%)	14	59
3	4	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	6	210/220 (96%)	192 (91%)	15 (7%)	3 (1%)	14	59
3	8	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	N	210/220 (96%)	189 (90%)	16 (8%)	5 (2%)	7	50
3	P	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	10	54
3	R	210/220 (96%)	190 (90%)	17 (8%)	3 (1%)	14	59
3	T	210/220 (96%)	192 (91%)	14 (7%)	4 (2%)	10	54
3	V	210/220 (96%)	190 (90%)	16 (8%)	4 (2%)	10	54
3	X	210/220 (96%)	191 (91%)	15 (7%)	4 (2%)	10	54
3	Z	210/220 (96%)	190 (90%)	15 (7%)	5 (2%)	7	50
All	All	11100/11268 (98%)	9822 (88%)	1089 (10%)	189 (2%)	11	56

5 of 189 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	330	GLY
2	5	115	VAL
3	N	175	ASN
3	P	175	ASN
3	R	175	ASN

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	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	B	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	C	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	D	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	E	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	F	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	G	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	H	430/430 (100%)	407 (95%)	23 (5%)	28	67
1	I	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	J	430/430 (100%)	406 (94%)	24 (6%)	26	65
1	K	430/430 (100%)	405 (94%)	25 (6%)	25	64
1	L	430/430 (100%)	406 (94%)	24 (6%)	26	65
2	1	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	3	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	5	191/191 (100%)	168 (88%)	23 (12%)	6	33
2	7	191/191 (100%)	163 (85%)	28 (15%)	4	26
2	9	191/191 (100%)	165 (86%)	26 (14%)	5	30
2	M	191/191 (100%)	167 (87%)	24 (13%)	5	31
2	O	191/191 (100%)	164 (86%)	27 (14%)	4	28
2	Q	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	S	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	U	191/191 (100%)	165 (86%)	26 (14%)	5	30
2	W	191/191 (100%)	166 (87%)	25 (13%)	5	30
2	Y	191/191 (100%)	167 (87%)	24 (13%)	5	31
3	0	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	2	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	4	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	6	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	8	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	N	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	P	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	R	174/181 (96%)	162 (93%)	12 (7%)	19	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	V	174/181 (96%)	161 (92%)	13 (8%)	17	56
3	X	174/181 (96%)	162 (93%)	12 (7%)	19	59
3	Z	174/181 (96%)	161 (92%)	13 (8%)	17	56
All	All	9540/9624 (99%)	8802 (92%)	738 (8%)	16	55

5 of 738 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	118	GLN
2	U	143	SER
3	2	134	LYS
2	Q	43	GLN
2	S	73	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 369 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	211	GLN
1	K	171	ASN
3	2	133	ASN
1	I	341	ASN
1	J	210	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

192 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
4	NAG	A	601	1,4	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
4	NAG	A	602	4	14,14,15	0.54	0	15,19,21	0.75	1 (6%)
4	BMA	A	603	4	11,11,12	0.92	1 (9%)	14,15,17	0.51	0
4	MAN	A	604	4	11,11,12	0.76	0	14,15,17	0.67	0
4	MAN	A	605	4	11,11,12	1.07	2 (18%)	14,15,17	1.34	1 (7%)
4	MAN	A	606	4	11,11,12	0.72	0	14,15,17	0.96	2 (14%)
4	MAN	A	607	4	11,11,12	0.63	0	14,15,17	0.74	0
6	NAG	A	609	1,6	14,14,15	0.77	0	15,19,21	1.14	2 (13%)
6	NAG	A	610	6	14,14,15	0.83	1 (7%)	15,19,21	1.29	2 (13%)
6	BMA	A	611	6	11,11,12	0.93	1 (9%)	14,15,17	0.82	1 (7%)
6	MAN	A	612	6	11,11,12	0.92	1 (9%)	14,15,17	1.28	1 (7%)
6	MAN	A	613	6	11,11,12	0.66	0	14,15,17	0.92	2 (14%)
6	MAN	A	614	6	11,11,12	0.65	0	14,15,17	0.84	1 (7%)
7	NAG	A	615	1,7	14,14,15	0.76	0	15,19,21	1.25	2 (13%)
7	NAG	A	616	7	14,14,15	0.75	1 (7%)	15,19,21	0.71	1 (6%)
7	BMA	A	617	7	11,11,12	0.74	0	14,15,17	0.33	0
4	NAG	B	601	1,4	14,14,15	0.60	0	15,19,21	0.74	1 (6%)
4	NAG	B	602	4	14,14,15	0.47	0	15,19,21	0.83	1 (6%)
4	BMA	B	603	4	11,11,12	0.91	1 (9%)	14,15,17	0.55	0
4	MAN	B	604	4	11,11,12	0.75	0	14,15,17	0.62	0
4	MAN	B	605	4	11,11,12	1.05	1 (9%)	14,15,17	1.34	1 (7%)
4	MAN	B	606	4	11,11,12	0.80	0	14,15,17	1.01	2 (14%)
4	MAN	B	607	4	11,11,12	0.62	0	14,15,17	0.74	0
6	NAG	B	609	1,6	14,14,15	0.89	0	15,19,21	1.17	2 (13%)
6	NAG	B	610	6	14,14,15	0.93	1 (7%)	15,19,21	1.23	2 (13%)
6	BMA	B	611	6	11,11,12	0.77	0	14,15,17	0.83	1 (7%)
6	MAN	B	612	6	11,11,12	0.93	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	B	613	6	11,11,12	0.69	0	14,15,17	0.88	2 (14%)
6	MAN	B	614	6	11,11,12	0.71	0	14,15,17	0.82	1 (7%)
7	NAG	B	615	1,7	14,14,15	0.79	0	15,19,21	1.27	2 (13%)
7	NAG	B	616	7	14,14,15	0.73	0	15,19,21	0.72	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	B	617	7	11,11,12	0.75	0	14,15,17	0.30	0
4	NAG	C	601	1,4	14,14,15	0.52	0	15,19,21	0.75	1 (6%)
4	NAG	C	602	4	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	BMA	C	603	4	11,11,12	0.91	1 (9%)	14,15,17	0.53	0
4	MAN	C	604	4	11,11,12	0.76	0	14,15,17	0.66	0
4	MAN	C	605	4	11,11,12	1.08	2 (18%)	14,15,17	1.34	1 (7%)
4	MAN	C	606	4	11,11,12	0.73	0	14,15,17	0.96	2 (14%)
4	MAN	C	607	4	11,11,12	0.63	0	14,15,17	0.75	0
6	NAG	C	609	1,6	14,14,15	0.78	0	15,19,21	1.22	2 (13%)
6	NAG	C	610	6	14,14,15	0.84	1 (7%)	15,19,21	1.35	2 (13%)
6	BMA	C	611	6	11,11,12	0.74	0	14,15,17	0.92	1 (7%)
6	MAN	C	612	6	11,11,12	0.84	0	14,15,17	1.35	1 (7%)
6	MAN	C	613	6	11,11,12	0.63	0	14,15,17	0.88	1 (7%)
6	MAN	C	614	6	11,11,12	0.69	0	14,15,17	0.86	1 (7%)
7	NAG	C	615	1,7	14,14,15	0.85	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	C	616	7	14,14,15	0.83	1 (7%)	15,19,21	0.73	1 (6%)
7	BMA	C	617	7	11,11,12	0.75	0	14,15,17	0.33	0
4	NAG	D	601	1,4	14,14,15	0.60	0	15,19,21	0.73	1 (6%)
4	NAG	D	602	4	14,14,15	0.59	0	15,19,21	0.78	1 (6%)
4	BMA	D	603	4	11,11,12	0.84	1 (9%)	14,15,17	0.49	0
4	MAN	D	604	4	11,11,12	0.68	0	14,15,17	0.63	0
4	MAN	D	605	4	11,11,12	1.08	1 (9%)	14,15,17	1.36	1 (7%)
4	MAN	D	606	4	11,11,12	0.75	0	14,15,17	1.00	2 (14%)
4	MAN	D	607	4	11,11,12	0.62	0	14,15,17	0.73	0
6	NAG	D	609	1,6	14,14,15	0.83	0	15,19,21	1.22	2 (13%)
6	NAG	D	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.29	2 (13%)
6	BMA	D	611	6	11,11,12	0.87	1 (9%)	14,15,17	0.85	1 (7%)
6	MAN	D	612	6	11,11,12	0.93	1 (9%)	14,15,17	1.33	1 (7%)
6	MAN	D	613	6	11,11,12	0.67	0	14,15,17	0.89	2 (14%)
6	MAN	D	614	6	11,11,12	0.72	0	14,15,17	0.82	1 (7%)
7	NAG	D	615	1,7	14,14,15	0.83	1 (7%)	15,19,21	1.19	2 (13%)
7	NAG	D	616	7	14,14,15	0.76	1 (7%)	15,19,21	0.69	1 (6%)
7	BMA	D	617	7	11,11,12	0.72	0	14,15,17	0.30	0
4	NAG	E	601	1,4	14,14,15	0.50	0	15,19,21	0.76	1 (6%)
4	NAG	E	602	4	14,14,15	0.40	0	15,19,21	0.79	1 (6%)
4	BMA	E	603	4	11,11,12	0.99	1 (9%)	14,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	E	604	4	11,11,12	0.79	0	14,15,17	0.69	0
4	MAN	E	605	4	11,11,12	1.12	1 (9%)	14,15,17	1.34	1 (7%)
4	MAN	E	606	4	11,11,12	0.72	0	14,15,17	0.95	2 (14%)
4	MAN	E	607	4	11,11,12	0.58	0	14,15,17	0.74	0
6	NAG	E	609	1,6	14,14,15	0.81	0	15,19,21	1.17	2 (13%)
6	NAG	E	610	6	14,14,15	0.84	1 (7%)	15,19,21	1.31	2 (13%)
6	BMA	E	611	6	11,11,12	0.85	0	14,15,17	0.84	1 (7%)
6	MAN	E	612	6	11,11,12	0.90	1 (9%)	14,15,17	1.32	1 (7%)
6	MAN	E	613	6	11,11,12	0.71	0	14,15,17	0.91	2 (14%)
6	MAN	E	614	6	11,11,12	0.65	0	14,15,17	0.84	1 (7%)
7	NAG	E	615	1,7	14,14,15	0.82	0	15,19,21	1.26	2 (13%)
7	NAG	E	616	7	14,14,15	0.70	0	15,19,21	0.74	1 (6%)
7	BMA	E	617	7	11,11,12	0.71	0	14,15,17	0.32	0
4	NAG	F	601	1,4	14,14,15	0.66	0	15,19,21	0.81	1 (6%)
4	NAG	F	602	4	14,14,15	0.44	0	15,19,21	0.84	1 (6%)
4	BMA	F	603	4	11,11,12	0.99	1 (9%)	14,15,17	0.54	0
4	MAN	F	604	4	11,11,12	0.73	0	14,15,17	0.67	0
4	MAN	F	605	4	11,11,12	1.08	2 (18%)	14,15,17	1.37	1 (7%)
4	MAN	F	606	4	11,11,12	0.73	0	14,15,17	1.01	2 (14%)
4	MAN	F	607	4	11,11,12	0.57	0	14,15,17	0.73	0
6	NAG	F	609	1,6	14,14,15	0.84	0	15,19,21	1.12	2 (13%)
6	NAG	F	610	6	14,14,15	0.92	1 (7%)	15,19,21	1.24	2 (13%)
6	BMA	F	611	6	11,11,12	0.86	1 (9%)	14,15,17	0.94	1 (7%)
6	MAN	F	612	6	11,11,12	0.88	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	F	613	6	11,11,12	0.69	0	14,15,17	0.91	2 (14%)
6	MAN	F	614	6	11,11,12	0.66	0	14,15,17	0.83	1 (7%)
7	NAG	F	615	1,7	14,14,15	0.78	0	15,19,21	1.26	2 (13%)
7	NAG	F	616	7	14,14,15	0.67	0	15,19,21	0.74	1 (6%)
7	BMA	F	617	7	11,11,12	0.71	0	14,15,17	0.32	0
4	NAG	G	601	1,4	14,14,15	0.61	0	15,19,21	0.76	1 (6%)
4	NAG	G	602	4	14,14,15	0.53	0	15,19,21	0.82	1 (6%)
4	BMA	G	603	4	11,11,12	0.92	1 (9%)	14,15,17	0.58	0
4	MAN	G	604	4	11,11,12	0.70	0	14,15,17	0.68	0
4	MAN	G	605	4	11,11,12	1.03	1 (9%)	14,15,17	1.33	1 (7%)
4	MAN	G	606	4	11,11,12	0.69	0	14,15,17	0.96	2 (14%)
4	MAN	G	607	4	11,11,12	0.59	0	14,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	G	609	1,6	14,14,15	0.92	0	15,19,21	1.16	2 (13%)
6	NAG	G	610	6	14,14,15	0.89	1 (7%)	15,19,21	1.27	2 (13%)
6	BMA	G	611	6	11,11,12	0.85	1 (9%)	14,15,17	0.80	1 (7%)
6	MAN	G	612	6	11,11,12	0.78	0	14,15,17	1.38	1 (7%)
6	MAN	G	613	6	11,11,12	0.67	0	14,15,17	0.87	2 (14%)
6	MAN	G	614	6	11,11,12	0.70	0	14,15,17	0.82	1 (7%)
7	NAG	G	615	1,7	14,14,15	0.86	1 (7%)	15,19,21	1.26	2 (13%)
7	NAG	G	616	7	14,14,15	0.80	1 (7%)	15,19,21	0.70	1 (6%)
7	BMA	G	617	7	11,11,12	0.77	0	14,15,17	0.36	0
4	NAG	H	601	1,4	14,14,15	0.63	0	15,19,21	0.74	1 (6%)
4	NAG	H	602	4	14,14,15	0.67	0	15,19,21	0.75	1 (6%)
4	BMA	H	603	4	11,11,12	0.89	1 (9%)	14,15,17	0.46	0
4	MAN	H	604	4	11,11,12	0.73	0	14,15,17	0.63	0
4	MAN	H	605	4	11,11,12	1.11	2 (18%)	14,15,17	1.35	1 (7%)
4	MAN	H	606	4	11,11,12	0.72	0	14,15,17	1.01	2 (14%)
4	MAN	H	607	4	11,11,12	0.64	0	14,15,17	0.76	0
6	NAG	H	609	1,6	14,14,15	0.88	0	15,19,21	1.16	2 (13%)
6	NAG	H	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.27	2 (13%)
6	BMA	H	611	6	11,11,12	0.86	0	14,15,17	0.83	1 (7%)
6	MAN	H	612	6	11,11,12	0.90	1 (9%)	14,15,17	1.34	1 (7%)
6	MAN	H	613	6	11,11,12	0.68	0	14,15,17	0.86	2 (14%)
6	MAN	H	614	6	11,11,12	0.64	0	14,15,17	0.81	1 (7%)
7	NAG	H	615	1,7	14,14,15	1.02	1 (7%)	15,19,21	1.14	3 (20%)
7	NAG	H	616	7	14,14,15	0.74	0	15,19,21	0.67	0
7	BMA	H	617	7	11,11,12	0.73	0	14,15,17	0.33	0
4	NAG	I	601	1,4	14,14,15	0.59	0	15,19,21	0.77	1 (6%)
4	NAG	I	602	4	14,14,15	0.43	0	15,19,21	0.80	1 (6%)
4	BMA	I	603	4	11,11,12	1.07	1 (9%)	14,15,17	0.54	0
4	MAN	I	604	4	11,11,12	0.83	0	14,15,17	0.70	0
4	MAN	I	605	4	11,11,12	1.12	2 (18%)	14,15,17	1.39	1 (7%)
4	MAN	I	606	4	11,11,12	0.73	0	14,15,17	1.02	2 (14%)
4	MAN	I	607	4	11,11,12	0.64	0	14,15,17	0.74	0
6	NAG	I	609	1,6	14,14,15	0.88	0	15,19,21	1.18	2 (13%)
6	NAG	I	610	6	14,14,15	0.91	1 (7%)	15,19,21	1.25	2 (13%)
6	BMA	I	611	6	11,11,12	0.74	0	14,15,17	0.85	1 (7%)
6	MAN	I	612	6	11,11,12	0.85	1 (9%)	14,15,17	1.35	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	I	613	6	11,11,12	0.68	0	14,15,17	0.86	1 (7%)
6	MAN	I	614	6	11,11,12	0.70	0	14,15,17	0.84	1 (7%)
7	NAG	I	615	1,7	14,14,15	0.86	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	I	616	7	14,14,15	0.73	0	15,19,21	0.70	0
7	BMA	I	617	7	11,11,12	0.74	0	14,15,17	0.30	0
4	NAG	J	601	1,4	14,14,15	0.61	0	15,19,21	0.76	1 (6%)
4	NAG	J	602	4	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	BMA	J	603	4	11,11,12	0.81	0	14,15,17	0.55	0
4	MAN	J	604	4	11,11,12	0.72	0	14,15,17	0.66	0
4	MAN	J	605	4	11,11,12	1.04	1 (9%)	14,15,17	1.36	1 (7%)
4	MAN	J	606	4	11,11,12	0.76	0	14,15,17	1.01	2 (14%)
4	MAN	J	607	4	11,11,12	0.58	0	14,15,17	0.74	0
6	NAG	J	609	1,6	14,14,15	0.88	0	15,19,21	1.20	2 (13%)
6	NAG	J	610	6	14,14,15	0.87	1 (7%)	15,19,21	1.32	2 (13%)
6	BMA	J	611	6	11,11,12	0.80	0	14,15,17	0.83	1 (7%)
6	MAN	J	612	6	11,11,12	0.84	0	14,15,17	1.36	1 (7%)
6	MAN	J	613	6	11,11,12	0.67	0	14,15,17	0.88	1 (7%)
6	MAN	J	614	6	11,11,12	0.75	0	14,15,17	0.84	1 (7%)
7	NAG	J	615	1,7	14,14,15	0.83	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	J	616	7	14,14,15	0.72	0	15,19,21	0.73	1 (6%)
7	BMA	J	617	7	11,11,12	0.77	0	14,15,17	0.32	0
4	NAG	K	601	1,4	14,14,15	0.53	0	15,19,21	0.75	1 (6%)
4	NAG	K	602	4	14,14,15	0.57	0	15,19,21	0.76	1 (6%)
4	BMA	K	603	4	11,11,12	0.90	1 (9%)	14,15,17	0.53	0
4	MAN	K	604	4	11,11,12	0.65	0	14,15,17	0.69	0
4	MAN	K	605	4	11,11,12	1.09	1 (9%)	14,15,17	1.33	1 (7%)
4	MAN	K	606	4	11,11,12	0.68	0	14,15,17	0.96	2 (14%)
4	MAN	K	607	4	11,11,12	0.62	0	14,15,17	0.77	0
6	NAG	K	609	1,6	14,14,15	0.89	0	15,19,21	1.16	2 (13%)
6	NAG	K	610	6	14,14,15	0.86	1 (7%)	15,19,21	1.25	2 (13%)
6	BMA	K	611	6	11,11,12	0.87	1 (9%)	14,15,17	0.82	1 (7%)
6	MAN	K	612	6	11,11,12	0.87	1 (9%)	14,15,17	1.35	1 (7%)
6	MAN	K	613	6	11,11,12	0.68	0	14,15,17	0.86	1 (7%)
6	MAN	K	614	6	11,11,12	0.72	0	14,15,17	0.79	1 (7%)
7	NAG	K	615	1,7	14,14,15	0.93	1 (7%)	15,19,21	1.21	2 (13%)
7	NAG	K	616	7	14,14,15	0.75	0	15,19,21	0.69	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	K	617	7	11,11,12	0.72	0	14,15,17	0.30	0
4	NAG	L	601	1,4	14,14,15	0.71	0	15,19,21	0.76	1 (6%)
4	NAG	L	602	4	14,14,15	0.54	0	15,19,21	0.77	1 (6%)
4	BMA	L	603	4	11,11,12	0.84	0	14,15,17	0.52	0
4	MAN	L	604	4	11,11,12	0.75	0	14,15,17	0.68	0
4	MAN	L	605	4	11,11,12	1.15	2 (18%)	14,15,17	1.39	1 (7%)
4	MAN	L	606	4	11,11,12	0.76	0	14,15,17	1.01	2 (14%)
4	MAN	L	607	4	11,11,12	0.66	0	14,15,17	0.73	0
6	NAG	L	609	1,6	14,14,15	0.87	0	15,19,21	1.15	2 (13%)
6	NAG	L	610	6	14,14,15	0.88	1 (7%)	15,19,21	1.29	2 (13%)
6	BMA	L	611	6	11,11,12	0.81	0	14,15,17	0.85	1 (7%)
6	MAN	L	612	6	11,11,12	0.87	1 (9%)	14,15,17	1.35	1 (7%)
6	MAN	L	613	6	11,11,12	0.68	0	14,15,17	0.89	2 (14%)
6	MAN	L	614	6	11,11,12	0.69	0	14,15,17	0.82	1 (7%)
7	NAG	L	615	1,7	14,14,15	0.90	1 (7%)	15,19,21	1.20	2 (13%)
7	NAG	L	616	7	14,14,15	0.71	0	15,19,21	0.73	1 (6%)
7	BMA	L	617	7	11,11,12	0.75	0	14,15,17	0.31	0

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
4	NAG	A	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	602	4	-	0/6/23/26	0/1/1/1
4	BMA	A	603	4	-	0/2/19/22	0/1/1/1
4	MAN	A	604	4	-	0/2/19/22	0/1/1/1
4	MAN	A	605	4	-	0/2/19/22	0/1/1/1
4	MAN	A	606	4	-	0/2/19/22	0/1/1/1
4	MAN	A	607	4	-	0/2/19/22	0/1/1/1
6	NAG	A	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	610	6	-	0/6/23/26	0/1/1/1
6	BMA	A	611	6	-	0/2/19/22	0/1/1/1
6	MAN	A	612	6	-	0/2/19/22	0/1/1/1
6	MAN	A	613	6	-	0/2/19/22	0/1/1/1
6	MAN	A	614	6	-	0/2/19/22	0/1/1/1
7	NAG	A	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	616	7	-	1/6/23/26	0/1/1/1
7	BMA	A	617	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	602	4	-	0/6/23/26	0/1/1/1
4	BMA	B	603	4	-	0/2/19/22	0/1/1/1
4	MAN	B	604	4	-	0/2/19/22	0/1/1/1
4	MAN	B	605	4	-	0/2/19/22	0/1/1/1
4	MAN	B	606	4	-	0/2/19/22	0/1/1/1
4	MAN	B	607	4	-	0/2/19/22	0/1/1/1
6	NAG	B	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	610	6	-	0/6/23/26	0/1/1/1
6	BMA	B	611	6	-	0/2/19/22	0/1/1/1
6	MAN	B	612	6	-	0/2/19/22	0/1/1/1
6	MAN	B	613	6	-	0/2/19/22	0/1/1/1
6	MAN	B	614	6	-	0/2/19/22	0/1/1/1
7	NAG	B	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	616	7	-	1/6/23/26	0/1/1/1
7	BMA	B	617	7	-	0/2/19/22	0/1/1/1
4	NAG	C	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	602	4	-	0/6/23/26	0/1/1/1
4	BMA	C	603	4	-	0/2/19/22	0/1/1/1
4	MAN	C	604	4	-	0/2/19/22	0/1/1/1
4	MAN	C	605	4	-	0/2/19/22	0/1/1/1
4	MAN	C	606	4	-	0/2/19/22	0/1/1/1
4	MAN	C	607	4	-	0/2/19/22	0/1/1/1
6	NAG	C	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	610	6	-	0/6/23/26	0/1/1/1
6	BMA	C	611	6	-	0/2/19/22	0/1/1/1
6	MAN	C	612	6	-	0/2/19/22	0/1/1/1
6	MAN	C	613	6	-	0/2/19/22	0/1/1/1
6	MAN	C	614	6	-	0/2/19/22	0/1/1/1
7	NAG	C	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	616	7	-	1/6/23/26	0/1/1/1
7	BMA	C	617	7	-	0/2/19/22	0/1/1/1
4	NAG	D	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	602	4	-	0/6/23/26	0/1/1/1
4	BMA	D	603	4	-	0/2/19/22	0/1/1/1
4	MAN	D	604	4	-	0/2/19/22	0/1/1/1
4	MAN	D	605	4	-	0/2/19/22	0/1/1/1
4	MAN	D	606	4	-	0/2/19/22	0/1/1/1
4	MAN	D	607	4	-	0/2/19/22	0/1/1/1
6	NAG	D	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	610	6	-	0/6/23/26	0/1/1/1
6	BMA	D	611	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	D	612	6	-	0/2/19/22	0/1/1/1
6	MAN	D	613	6	-	0/2/19/22	0/1/1/1
6	MAN	D	614	6	-	0/2/19/22	0/1/1/1
7	NAG	D	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	D	616	7	-	1/6/23/26	0/1/1/1
7	BMA	D	617	7	-	0/2/19/22	0/1/1/1
4	NAG	E	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	602	4	-	0/6/23/26	0/1/1/1
4	BMA	E	603	4	-	0/2/19/22	0/1/1/1
4	MAN	E	604	4	-	0/2/19/22	0/1/1/1
4	MAN	E	605	4	-	0/2/19/22	0/1/1/1
4	MAN	E	606	4	-	0/2/19/22	0/1/1/1
4	MAN	E	607	4	-	0/2/19/22	0/1/1/1
6	NAG	E	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	610	6	-	0/6/23/26	0/1/1/1
6	BMA	E	611	6	-	0/2/19/22	0/1/1/1
6	MAN	E	612	6	-	0/2/19/22	0/1/1/1
6	MAN	E	613	6	-	0/2/19/22	0/1/1/1
6	MAN	E	614	6	-	0/2/19/22	0/1/1/1
7	NAG	E	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	616	7	-	1/6/23/26	0/1/1/1
7	BMA	E	617	7	-	0/2/19/22	0/1/1/1
4	NAG	F	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	602	4	-	0/6/23/26	0/1/1/1
4	BMA	F	603	4	-	0/2/19/22	0/1/1/1
4	MAN	F	604	4	-	0/2/19/22	0/1/1/1
4	MAN	F	605	4	-	0/2/19/22	0/1/1/1
4	MAN	F	606	4	-	0/2/19/22	0/1/1/1
4	MAN	F	607	4	-	0/2/19/22	0/1/1/1
6	NAG	F	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	610	6	-	0/6/23/26	0/1/1/1
6	BMA	F	611	6	-	0/2/19/22	0/1/1/1
6	MAN	F	612	6	-	0/2/19/22	0/1/1/1
6	MAN	F	613	6	-	0/2/19/22	0/1/1/1
6	MAN	F	614	6	-	0/2/19/22	0/1/1/1
7	NAG	F	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	F	616	7	-	1/6/23/26	0/1/1/1
7	BMA	F	617	7	-	0/2/19/22	0/1/1/1
4	NAG	G	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	602	4	-	0/6/23/26	0/1/1/1
4	BMA	G	603	4	-	0/2/19/22	0/1/1/1
4	MAN	G	604	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	605	4	-	0/2/19/22	0/1/1/1
4	MAN	G	606	4	-	0/2/19/22	0/1/1/1
4	MAN	G	607	4	-	0/2/19/22	0/1/1/1
6	NAG	G	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	610	6	-	0/6/23/26	0/1/1/1
6	BMA	G	611	6	-	0/2/19/22	0/1/1/1
6	MAN	G	612	6	-	0/2/19/22	0/1/1/1
6	MAN	G	613	6	-	0/2/19/22	0/1/1/1
6	MAN	G	614	6	-	0/2/19/22	0/1/1/1
7	NAG	G	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	7	-	1/6/23/26	0/1/1/1
7	BMA	G	617	7	-	0/2/19/22	0/1/1/1
4	NAG	H	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	602	4	-	0/6/23/26	0/1/1/1
4	BMA	H	603	4	-	0/2/19/22	0/1/1/1
4	MAN	H	604	4	-	0/2/19/22	0/1/1/1
4	MAN	H	605	4	-	0/2/19/22	0/1/1/1
4	MAN	H	606	4	-	0/2/19/22	0/1/1/1
4	MAN	H	607	4	-	0/2/19/22	0/1/1/1
6	NAG	H	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	610	6	-	0/6/23/26	0/1/1/1
6	BMA	H	611	6	-	0/2/19/22	0/1/1/1
6	MAN	H	612	6	-	0/2/19/22	0/1/1/1
6	MAN	H	613	6	-	0/2/19/22	0/1/1/1
6	MAN	H	614	6	-	0/2/19/22	0/1/1/1
7	NAG	H	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	H	616	7	-	1/6/23/26	0/1/1/1
7	BMA	H	617	7	-	0/2/19/22	0/1/1/1
4	NAG	I	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	602	4	-	0/6/23/26	0/1/1/1
4	BMA	I	603	4	-	0/2/19/22	0/1/1/1
4	MAN	I	604	4	-	0/2/19/22	0/1/1/1
4	MAN	I	605	4	-	0/2/19/22	0/1/1/1
4	MAN	I	606	4	-	0/2/19/22	0/1/1/1
4	MAN	I	607	4	-	0/2/19/22	0/1/1/1
6	NAG	I	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	610	6	-	0/6/23/26	0/1/1/1
6	BMA	I	611	6	-	0/2/19/22	0/1/1/1
6	MAN	I	612	6	-	0/2/19/22	0/1/1/1
6	MAN	I	613	6	-	0/2/19/22	0/1/1/1
6	MAN	I	614	6	-	0/2/19/22	0/1/1/1
7	NAG	I	615	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	I	616	7	-	1/6/23/26	0/1/1/1
7	BMA	I	617	7	-	0/2/19/22	0/1/1/1
4	NAG	J	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	602	4	-	0/6/23/26	0/1/1/1
4	BMA	J	603	4	-	0/2/19/22	0/1/1/1
4	MAN	J	604	4	-	0/2/19/22	0/1/1/1
4	MAN	J	605	4	-	0/2/19/22	0/1/1/1
4	MAN	J	606	4	-	0/2/19/22	0/1/1/1
4	MAN	J	607	4	-	0/2/19/22	0/1/1/1
6	NAG	J	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	610	6	-	0/6/23/26	0/1/1/1
6	BMA	J	611	6	-	0/2/19/22	0/1/1/1
6	MAN	J	612	6	-	0/2/19/22	0/1/1/1
6	MAN	J	613	6	-	0/2/19/22	0/1/1/1
6	MAN	J	614	6	-	0/2/19/22	0/1/1/1
7	NAG	J	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	J	616	7	-	1/6/23/26	0/1/1/1
7	BMA	J	617	7	-	0/2/19/22	0/1/1/1
4	NAG	K	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	602	4	-	0/6/23/26	0/1/1/1
4	BMA	K	603	4	-	0/2/19/22	0/1/1/1
4	MAN	K	604	4	-	0/2/19/22	0/1/1/1
4	MAN	K	605	4	-	0/2/19/22	0/1/1/1
4	MAN	K	606	4	-	0/2/19/22	0/1/1/1
4	MAN	K	607	4	-	0/2/19/22	0/1/1/1
6	NAG	K	609	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	610	6	-	0/6/23/26	0/1/1/1
6	BMA	K	611	6	-	0/2/19/22	0/1/1/1
6	MAN	K	612	6	-	0/2/19/22	0/1/1/1
6	MAN	K	613	6	-	0/2/19/22	0/1/1/1
6	MAN	K	614	6	-	0/2/19/22	0/1/1/1
7	NAG	K	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	616	7	-	1/6/23/26	0/1/1/1
7	BMA	K	617	7	-	0/2/19/22	0/1/1/1
4	NAG	L	601	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	602	4	-	0/6/23/26	0/1/1/1
4	BMA	L	603	4	-	0/2/19/22	0/1/1/1
4	MAN	L	604	4	-	0/2/19/22	0/1/1/1
4	MAN	L	605	4	-	0/2/19/22	0/1/1/1
4	MAN	L	606	4	-	0/2/19/22	0/1/1/1
4	MAN	L	607	4	-	0/2/19/22	0/1/1/1
6	NAG	L	609	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	610	6	-	0/6/23/26	0/1/1/1
6	BMA	L	611	6	-	0/2/19/22	0/1/1/1
6	MAN	L	612	6	-	0/2/19/22	0/1/1/1
6	MAN	L	613	6	-	0/2/19/22	0/1/1/1
6	MAN	L	614	6	-	0/2/19/22	0/1/1/1
7	NAG	L	615	1,7	-	0/6/23/26	0/1/1/1
7	NAG	L	616	7	-	1/6/23/26	0/1/1/1
7	BMA	L	617	7	-	0/2/19/22	0/1/1/1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	611	BMA	C4-C3	2.01	1.57	1.52
4	G	605	MAN	C2-C3	2.02	1.55	1.52
7	J	615	NAG	C4-C3	2.02	1.57	1.52
4	A	605	MAN	C2-C3	2.03	1.55	1.52
4	H	605	MAN	C2-C3	2.03	1.55	1.52

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	610	NAG	C2-N2-C7	-3.24	118.88	123.04
6	J	610	NAG	C2-N2-C7	-3.23	118.89	123.04
6	K	610	NAG	C2-N2-C7	-3.23	118.89	123.04
6	L	610	NAG	C2-N2-C7	-3.22	118.91	123.04
6	D	610	NAG	C2-N2-C7	-3.20	118.93	123.04

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	616	NAG	O7-C7-N2-C2
7	E	616	NAG	O7-C7-N2-C2
7	D	616	NAG	O7-C7-N2-C2
7	K	616	NAG	O7-C7-N2-C2
7	A	616	NAG	O7-C7-N2-C2

There are no ring outliers.

74 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	1	0
4	A	602	NAG	4	0
6	A	609	NAG	3	0
6	A	610	NAG	2	0
7	A	616	NAG	1	0
7	A	617	BMA	1	0
4	B	601	NAG	1	0
4	B	602	NAG	5	0
6	B	609	NAG	3	0
6	B	610	NAG	2	0
7	B	616	NAG	1	0
7	B	617	BMA	1	0
4	C	601	NAG	1	0
4	C	602	NAG	1	0
6	C	609	NAG	4	0
6	C	610	NAG	8	0
7	C	616	NAG	1	0
7	C	617	BMA	1	0
4	D	601	NAG	1	0
4	D	602	NAG	4	0
6	D	609	NAG	3	0
6	D	610	NAG	6	0
7	D	616	NAG	1	0
7	D	617	BMA	1	0
4	E	601	NAG	1	0
4	E	602	NAG	2	0
6	E	609	NAG	3	0
6	E	610	NAG	2	0
7	E	616	NAG	1	0
7	E	617	BMA	1	0
4	F	601	NAG	1	0
4	F	602	NAG	2	0
6	F	609	NAG	3	0
6	F	610	NAG	8	0
6	F	611	BMA	2	0
7	F	616	NAG	1	0
7	F	617	BMA	1	0
4	G	601	NAG	1	0
4	G	602	NAG	2	0
6	G	609	NAG	3	0
6	G	610	NAG	2	0
7	G	615	NAG	1	0
7	G	616	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	617	BMA	1	0
4	H	601	NAG	1	0
4	H	602	NAG	2	0
6	H	609	NAG	3	0
6	H	610	NAG	2	0
7	H	616	NAG	1	0
7	H	617	BMA	1	0
4	I	601	NAG	1	0
4	I	602	NAG	1	0
6	I	609	NAG	3	0
6	I	610	NAG	3	0
7	I	616	NAG	1	0
7	I	617	BMA	1	0
4	J	601	NAG	1	0
4	J	602	NAG	4	0
6	J	609	NAG	3	0
6	J	610	NAG	2	0
7	J	616	NAG	1	0
7	J	617	BMA	1	0
4	K	601	NAG	1	0
4	K	602	NAG	7	0
6	K	609	NAG	3	0
6	K	610	NAG	2	0
7	K	616	NAG	1	0
7	K	617	BMA	1	0
4	L	601	NAG	1	0
4	L	602	NAG	5	0
6	L	609	NAG	3	0
6	L	610	NAG	3	0
7	L	616	NAG	1	0
7	L	617	BMA	1	0

5.6 Ligand geometry

24 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	608	1	14,14,15	0.61	0	15,19,21	0.73	1 (6%)
5	NAG	A	618	1	14,14,15	0.71	0	15,19,21	0.70	0
5	NAG	B	608	1	14,14,15	0.75	1 (7%)	15,19,21	0.73	1 (6%)
5	NAG	B	618	1	14,14,15	0.77	1 (7%)	15,19,21	0.69	0
5	NAG	C	608	1	14,14,15	0.68	0	15,19,21	0.73	1 (6%)
5	NAG	C	618	1	14,14,15	0.71	0	15,19,21	0.70	0
5	NAG	D	608	1	14,14,15	0.77	1 (7%)	15,19,21	0.72	1 (6%)
5	NAG	D	618	1	14,14,15	0.74	0	15,19,21	0.70	0
5	NAG	E	608	1	14,14,15	0.67	0	15,19,21	0.73	1 (6%)
5	NAG	E	618	1	14,14,15	0.71	0	15,19,21	0.69	0
5	NAG	F	608	1	14,14,15	0.65	0	15,19,21	0.72	1 (6%)
5	NAG	F	618	1	14,14,15	0.74	0	15,19,21	0.68	0
5	NAG	G	608	1	14,14,15	0.66	0	15,19,21	0.74	1 (6%)
5	NAG	G	618	1	14,14,15	0.70	0	15,19,21	0.69	0
5	NAG	H	608	1	14,14,15	0.76	1 (7%)	15,19,21	0.74	1 (6%)
5	NAG	H	618	1	14,14,15	1.08	1 (7%)	15,19,21	1.35	4 (26%)
5	NAG	I	608	1	14,14,15	0.68	0	15,19,21	0.73	1 (6%)
5	NAG	I	618	1	14,14,15	0.72	0	15,19,21	0.70	0
5	NAG	J	608	1	14,14,15	0.64	0	15,19,21	0.72	1 (6%)
5	NAG	J	618	1	14,14,15	0.72	0	15,19,21	0.66	0
5	NAG	K	608	1	14,14,15	0.69	0	15,19,21	0.74	1 (6%)
5	NAG	K	618	1	14,14,15	0.73	0	15,19,21	0.68	0
5	NAG	L	608	1	14,14,15	0.65	0	15,19,21	0.74	1 (6%)
5	NAG	L	618	1	14,14,15	0.70	0	15,19,21	0.69	0

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	608	1	-	0/6/23/26	0/1/1/1
5	NAG	A	618	1	-	0/6/23/26	0/1/1/1
5	NAG	B	608	1	-	0/6/23/26	0/1/1/1
5	NAG	B	618	1	-	0/6/23/26	0/1/1/1
5	NAG	C	608	1	-	0/6/23/26	0/1/1/1
5	NAG	C	618	1	-	0/6/23/26	0/1/1/1
5	NAG	D	608	1	-	0/6/23/26	0/1/1/1
5	NAG	D	618	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	608	1	-	0/6/23/26	0/1/1/1
5	NAG	E	618	1	-	0/6/23/26	0/1/1/1
5	NAG	F	608	1	-	0/6/23/26	0/1/1/1
5	NAG	F	618	1	-	0/6/23/26	0/1/1/1
5	NAG	G	608	1	-	0/6/23/26	0/1/1/1
5	NAG	G	618	1	-	0/6/23/26	0/1/1/1
5	NAG	H	608	1	-	0/6/23/26	0/1/1/1
5	NAG	H	618	1	-	0/6/23/26	0/1/1/1
5	NAG	I	608	1	-	0/6/23/26	0/1/1/1
5	NAG	I	618	1	-	0/6/23/26	0/1/1/1
5	NAG	J	608	1	-	0/6/23/26	0/1/1/1
5	NAG	J	618	1	-	0/6/23/26	0/1/1/1
5	NAG	K	608	1	-	0/6/23/26	0/1/1/1
5	NAG	K	618	1	-	0/6/23/26	0/1/1/1
5	NAG	L	608	1	-	0/6/23/26	0/1/1/1
5	NAG	L	618	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	618	NAG	C4-C3	2.01	1.57	1.52
5	B	608	NAG	C4-C3	2.10	1.57	1.52
5	H	608	NAG	C4-C3	2.17	1.58	1.52
5	D	608	NAG	C4-C3	2.19	1.58	1.52
5	H	618	NAG	O5-C5	2.26	1.48	1.43

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	608	NAG	C2-N2-C7	-2.33	120.04	123.04
5	H	608	NAG	C2-N2-C7	-2.33	120.04	123.04
5	G	608	NAG	C2-N2-C7	-2.32	120.06	123.04
5	B	608	NAG	C2-N2-C7	-2.32	120.06	123.04
5	D	608	NAG	C2-N2-C7	-2.30	120.08	123.04

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	493/493 (100%)	-0.28	4 (0%) 87 82	113, 184, 248, 333	0
1	B	493/493 (100%)	-0.32	3 (0%) 90 86	113, 184, 249, 332	0
1	C	493/493 (100%)	-0.21	6 (1%) 81 72	112, 184, 249, 333	0
1	D	493/493 (100%)	-0.16	10 (2%) 68 57	114, 184, 249, 333	0
1	E	493/493 (100%)	-0.14	10 (2%) 68 57	113, 184, 249, 333	0
1	F	493/493 (100%)	-0.21	3 (0%) 90 86	114, 184, 248, 333	0
1	G	493/493 (100%)	-0.25	7 (1%) 78 68	114, 184, 249, 333	0
1	H	493/493 (100%)	-0.20	4 (0%) 87 82	113, 184, 248, 333	0
1	I	493/493 (100%)	-0.29	3 (0%) 90 86	114, 184, 249, 333	0
1	J	493/493 (100%)	-0.27	9 (1%) 71 61	113, 184, 248, 333	0
1	K	493/493 (100%)	-0.24	5 (1%) 84 77	113, 184, 249, 333	0
1	L	493/493 (100%)	-0.16	14 (2%) 56 44	114, 184, 249, 333	0
2	1	226/226 (100%)	0.18	14 (6%) 24 16	125, 213, 300, 359	0
2	3	226/226 (100%)	0.34	17 (7%) 17 12	114, 213, 300, 359	0
2	5	226/226 (100%)	0.28	20 (8%) 12 9	134, 215, 300, 359	0
2	7	226/226 (100%)	0.05	9 (3%) 42 31	137, 212, 300, 359	0
2	9	226/226 (100%)	0.00	6 (2%) 58 46	131, 213, 300, 359	0
2	M	226/226 (100%)	0.19	13 (5%) 26 18	133, 213, 304, 359	0
2	O	226/226 (100%)	0.05	8 (3%) 48 37	136, 212, 306, 359	0
2	Q	226/226 (100%)	0.25	18 (7%) 15 11	140, 214, 306, 359	0
2	S	226/226 (100%)	0.42	25 (11%) 7 6	146, 214, 306, 359	0
2	U	226/226 (100%)	0.46	23 (10%) 9 7	145, 214, 306, 359	0
2	W	226/226 (100%)	0.42	26 (11%) 6 6	121, 213, 306, 359	0
2	Y	226/226 (100%)	0.24	19 (8%) 14 10	145, 214, 306, 359	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	0	212/220 (96%)	-0.12	0 100 100	146, 221, 284, 324	0
3	2	212/220 (96%)	-0.08	4 (1%) 70 59	146, 222, 284, 325	0
3	4	212/220 (96%)	0.08	4 (1%) 70 59	146, 221, 284, 325	0
3	6	212/220 (96%)	0.26	16 (7%) 17 12	146, 223, 284, 325	0
3	8	212/220 (96%)	0.03	3 (1%) 78 68	146, 223, 284, 324	0
3	N	212/220 (96%)	0.13	6 (2%) 56 44	146, 222, 284, 324	0
3	P	212/220 (96%)	0.06	4 (1%) 70 59	146, 222, 284, 324	0
3	R	212/220 (96%)	0.28	11 (5%) 31 23	146, 224, 284, 324	0
3	T	212/220 (96%)	0.36	15 (7%) 19 13	146, 224, 284, 324	0
3	V	212/220 (96%)	0.60	30 (14%) 4 4	146, 223, 284, 325	0
3	X	212/220 (96%)	0.36	18 (8%) 13 10	146, 222, 284, 325	0
3	Z	212/220 (96%)	0.24	11 (5%) 31 23	146, 223, 284, 325	0
All	All	11172/11268 (99%)	-0.02	398 (3%) 46 36	112, 200, 279, 359	0

The worst 5 of 398 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	3	139	PRO	8.9
2	U	174	SER	8.7
2	U	139	PRO	8.0
2	5	226	PRO	7.8
2	5	138	ALA	7.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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
4	NAG	G	601	14/15	0.86	0.27	0.27	168,168,168,168	0
4	NAG	E	601	14/15	0.94	0.32	0.07	169,169,169,169	0
6	NAG	D	609	14/15	0.88	0.23	-0.09	181,181,181,181	0
4	NAG	K	602	14/15	0.76	0.31	-0.16	199,199,199,199	0
4	NAG	A	601	14/15	0.90	0.23	-0.19	168,168,168,168	0
4	NAG	K	601	14/15	0.87	0.24	-0.25	168,168,168,168	0
4	NAG	H	601	14/15	0.90	0.24	-0.30	168,168,168,168	0
4	NAG	L	601	14/15	0.77	0.26	-0.33	169,169,169,169	0
4	NAG	I	601	14/15	0.93	0.22	-0.41	168,168,168,168	0
4	NAG	F	601	14/15	0.94	0.23	-0.54	169,169,169,169	0
4	NAG	B	601	14/15	0.86	0.23	-0.58	168,168,168,168	0
4	NAG	B	602	14/15	0.81	0.24	-0.72	198,198,198,198	0
4	NAG	J	602	14/15	0.86	0.26	-0.72	198,198,198,198	0
4	NAG	J	601	14/15	0.90	0.19	-0.73	169,169,169,169	0
6	NAG	F	609	14/15	0.89	0.16	-1.49	181,181,181,181	0
4	NAG	D	601	14/15	0.93	0.17	-1.84	168,168,168,168	0
4	MAN	B	604	11/12	0.96	0.10	-	235,235,235,235	0
6	NAG	B	609	14/15	0.87	0.24	-	181,181,181,181	0
4	MAN	C	607	11/12	0.80	0.45	-	244,244,244,244	0
6	BMA	G	611	11/12	0.94	0.23	-	224,224,224,224	0
6	BMA	L	611	11/12	0.85	0.11	-	223,223,223,223	0
4	MAN	L	605	11/12	0.83	0.36	-	235,235,235,235	0
4	BMA	G	603	11/12	0.84	0.22	-	212,212,212,212	0
4	MAN	A	607	11/12	0.84	0.36	-	244,244,244,244	0
7	NAG	K	615	14/15	0.77	0.33	-	251,251,251,251	0
4	NAG	C	602	14/15	0.81	0.35	-	199,199,199,199	0
6	MAN	E	614	11/12	0.78	0.13	-	253,253,253,253	0
4	BMA	J	603	11/12	0.88	0.25	-	212,212,212,212	0
4	MAN	K	606	11/12	0.86	0.28	-	222,222,222,222	0
6	MAN	L	614	11/12	0.84	0.17	-	254,254,254,254	0
4	MAN	L	607	11/12	0.84	0.55	-	245,245,245,245	0
6	NAG	I	609	14/15	0.88	0.22	-	181,181,181,181	0
4	MAN	G	607	11/12	0.88	0.35	-	244,244,244,244	0
6	MAN	F	614	11/12	0.85	0.14	-	253,253,253,253	0
6	BMA	H	611	11/12	0.83	0.17	-	223,223,223,223	0
4	MAN	K	604	11/12	0.85	0.17	-	236,236,236,236	0
4	MAN	E	606	11/12	0.66	0.33	-	222,222,222,222	0
7	NAG	J	615	14/15	0.89	0.23	-	251,251,251,251	0
6	MAN	K	613	11/12	0.75	0.46	-	294,294,294,294	0
4	BMA	F	603	11/12	0.84	0.36	-	212,212,212,212	0
4	MAN	G	605	11/12	0.83	0.29	-	235,235,235,235	0
7	BMA	A	617	11/12	0.46	0.54	-	301,301,301,301	0
4	MAN	J	606	11/12	0.64	0.36	-	222,222,222,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	I	602	14/15	0.89	0.23	-	199,199,199,199	0
6	BMA	F	611	11/12	0.73	0.19	-	224,224,224,224	0
4	MAN	H	607	11/12	0.79	0.37	-	245,245,245,245	0
6	BMA	C	611	11/12	0.87	0.10	-	223,223,223,223	0
4	NAG	G	602	14/15	0.93	0.30	-	198,198,198,198	0
6	MAN	B	614	11/12	0.79	0.18	-	254,254,254,254	0
4	MAN	K	607	11/12	0.77	0.35	-	244,244,244,244	0
7	NAG	I	616	14/15	0.78	0.33	-	270,270,270,270	0
4	MAN	J	605	11/12	0.69	0.29	-	235,235,235,235	0
7	BMA	B	617	11/12	0.11	0.46	-	301,301,301,301	0
6	MAN	I	614	11/12	0.79	0.19	-	254,254,254,254	0
4	MAN	B	607	11/12	0.57	0.54	-	245,245,245,245	0
6	NAG	G	609	14/15	0.84	0.23	-	181,181,181,181	0
6	NAG	A	610	14/15	0.91	0.27	-	201,201,201,201	0
6	NAG	J	610	14/15	0.86	0.21	-	202,202,202,202	0
7	BMA	I	617	11/12	0.44	0.41	-	301,301,301,301	0
6	MAN	G	614	11/12	0.79	0.24	-	254,254,254,254	0
4	MAN	B	605	11/12	0.80	0.35	-	235,235,235,235	0
4	MAN	F	606	11/12	0.71	0.30	-	222,222,222,222	0
6	MAN	B	612	11/12	0.72	0.20	-	271,271,271,271	0
4	MAN	C	606	11/12	0.45	0.50	-	223,223,223,223	0
6	NAG	I	610	14/15	0.85	0.30	-	202,202,202,202	0
4	BMA	A	603	11/12	0.94	0.23	-	212,212,212,212	0
4	MAN	F	607	11/12	0.87	0.19	-	244,244,244,244	0
4	MAN	D	607	11/12	0.69	0.35	-	244,244,244,244	0
6	BMA	D	611	11/12	0.61	0.21	-	224,224,224,224	0
6	MAN	H	614	11/12	0.79	0.23	-	253,253,253,253	0
6	MAN	L	613	11/12	0.47	0.40	-	294,294,294,294	0
4	MAN	A	604	11/12	0.79	0.20	-	236,236,236,236	0
4	MAN	I	605	11/12	0.85	0.12	-	235,235,235,235	0
6	NAG	H	609	14/15	0.94	0.14	-	181,181,181,181	0
6	BMA	I	611	11/12	0.85	0.21	-	224,224,224,224	0
6	MAN	D	612	11/12	0.59	0.31	-	271,271,271,271	0
6	MAN	F	612	11/12	0.75	0.32	-	271,271,271,271	0
7	NAG	G	616	14/15	0.82	0.36	-	270,270,270,270	0
4	MAN	E	604	11/12	0.90	0.12	-	236,236,236,236	0
6	NAG	L	610	14/15	0.80	0.25	-	202,202,202,202	0
4	MAN	K	605	11/12	0.73	0.24	-	235,235,235,235	0
6	BMA	J	611	11/12	0.86	0.20	-	223,223,223,223	0
4	BMA	L	603	11/12	0.85	0.21	-	212,212,212,212	0
6	BMA	K	611	11/12	0.85	0.15	-	224,224,224,224	0
6	NAG	C	609	14/15	0.92	0.20	-	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	B	610	14/15	0.90	0.21	-	202,202,202,202	0
6	NAG	A	609	14/15	0.87	0.24	-	180,180,180,180	0
7	BMA	F	617	11/12	0.68	0.42	-	301,301,301,301	0
7	NAG	L	615	14/15	0.74	0.29	-	251,251,251,251	0
6	BMA	B	611	11/12	0.89	0.21	-	223,223,223,223	0
6	MAN	H	613	11/12	0.61	0.54	-	294,294,294,294	0
6	BMA	E	611	11/12	0.87	0.12	-	223,223,223,223	0
6	MAN	C	612	11/12	0.84	0.14	-	271,271,271,271	0
7	BMA	L	617	11/12	0.69	0.38	-	301,301,301,301	0
4	MAN	H	604	11/12	0.92	0.11	-	235,235,235,235	0
4	MAN	J	604	11/12	0.87	0.22	-	236,236,236,236	0
6	MAN	J	614	11/12	0.35	0.33	-	254,254,254,254	0
4	BMA	E	603	11/12	0.94	0.22	-	212,212,212,212	0
7	BMA	K	617	11/12	0.37	0.44	-	301,301,301,301	0
4	BMA	C	603	11/12	0.66	0.28	-	212,212,212,212	0
4	NAG	D	602	14/15	0.84	0.36	-	199,199,199,199	0
6	BMA	A	611	11/12	0.70	0.29	-	223,223,223,223	0
4	MAN	J	607	11/12	0.81	0.38	-	244,244,244,244	0
4	MAN	L	604	11/12	0.83	0.15	-	236,236,236,236	0
4	MAN	I	604	11/12	0.72	0.26	-	235,235,235,235	0
7	NAG	L	616	14/15	0.89	0.37	-	270,270,270,270	0
4	MAN	I	607	11/12	0.86	0.27	-	245,245,245,245	0
6	MAN	K	614	11/12	0.79	0.27	-	254,254,254,254	0
4	MAN	L	606	11/12	0.63	0.52	-	222,222,222,222	0
4	MAN	I	606	11/12	0.74	0.35	-	222,222,222,222	0
4	MAN	D	604	11/12	0.90	0.39	-	236,236,236,236	0
4	MAN	D	606	11/12	0.63	0.39	-	223,223,223,223	0
6	MAN	K	612	11/12	0.87	0.20	-	271,271,271,271	0
6	MAN	I	612	11/12	0.72	0.22	-	271,271,271,271	0
6	NAG	C	610	14/15	0.91	0.17	-	201,201,201,201	0
6	MAN	E	612	11/12	0.71	0.17	-	271,271,271,271	0
4	BMA	D	603	11/12	0.87	0.28	-	212,212,212,212	0
6	NAG	J	609	14/15	0.88	0.16	-	181,181,181,181	0
4	MAN	A	606	11/12	0.72	0.41	-	222,222,222,222	0
6	MAN	J	612	11/12	0.71	0.21	-	271,271,271,271	0
7	NAG	J	616	14/15	0.91	0.39	-	270,270,270,270	0
7	BMA	H	617	11/12	0.48	0.47	-	301,301,301,301	0
4	MAN	C	605	11/12	0.78	0.38	-	235,235,235,235	0
6	MAN	E	613	11/12	0.74	0.24	-	293,293,293,293	0
4	BMA	H	603	11/12	0.88	0.15	-	212,212,212,212	0
4	MAN	F	605	11/12	0.77	0.21	-	235,235,235,235	0
6	NAG	G	610	14/15	0.84	0.26	-	202,202,202,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	602	14/15	0.90	0.20	-	198,198,198,198	0
6	NAG	L	609	14/15	0.92	0.18	-	181,181,181,181	0
6	MAN	A	613	11/12	0.68	0.44	-	293,293,293,293	0
4	MAN	H	605	11/12	0.90	0.20	-	235,235,235,235	0
4	MAN	B	606	11/12	0.38	0.47	-	222,222,222,222	0
6	NAG	F	610	14/15	0.87	0.21	-	202,202,202,202	0
7	NAG	H	615	14/15	0.62	0.35	-	251,251,251,251	0
6	NAG	D	610	14/15	0.84	0.27	-	202,202,202,202	0
7	NAG	H	616	14/15	0.85	0.45	-	270,270,270,270	0
6	MAN	A	614	11/12	0.59	0.33	-	253,253,253,253	0
6	NAG	E	609	14/15	0.87	0.25	-	180,180,180,180	0
4	MAN	G	606	11/12	0.75	0.30	-	222,222,222,222	0
4	NAG	C	601	14/15	0.84	0.34	-	168,168,168,168	0
6	MAN	G	612	11/12	0.55	0.25	-	271,271,271,271	0
4	NAG	L	602	14/15	0.77	0.42	-	199,199,199,199	0
7	BMA	E	617	11/12	0.60	0.31	-	301,301,301,301	0
7	NAG	B	616	14/15	0.88	0.27	-	270,270,270,270	0
7	NAG	E	616	14/15	0.84	0.28	-	270,270,270,270	0
4	MAN	G	604	11/12	0.90	0.18	-	236,236,236,236	0
7	NAG	E	615	14/15	0.86	0.22	-	251,251,251,251	0
7	NAG	D	615	14/15	0.91	0.15	-	250,250,250,250	0
6	MAN	D	613	11/12	0.44	0.35	-	294,294,294,294	0
6	MAN	B	613	11/12	0.56	0.34	-	294,294,294,294	0
4	BMA	I	603	11/12	0.76	0.24	-	212,212,212,212	0
6	MAN	C	613	11/12	0.59	0.25	-	294,294,294,294	0
6	MAN	I	613	11/12	0.51	0.59	-	294,294,294,294	0
6	NAG	K	610	14/15	0.94	0.14	-	202,202,202,202	0
7	NAG	C	616	14/15	0.84	0.30	-	270,270,270,270	0
7	NAG	A	616	14/15	0.81	0.32	-	271,271,271,271	0
7	NAG	C	615	14/15	0.90	0.19	-	251,251,251,251	0
4	NAG	F	602	14/15	0.86	0.40	-	198,198,198,198	0
4	MAN	F	604	11/12	0.83	0.20	-	236,236,236,236	0
4	MAN	C	604	11/12	0.73	0.24	-	236,236,236,236	0
6	MAN	L	612	11/12	0.39	0.29	-	271,271,271,271	0
6	NAG	E	610	14/15	0.92	0.18	-	201,201,201,201	0
7	BMA	J	617	11/12	0.33	0.40	-	301,301,301,301	0
4	NAG	E	602	14/15	0.95	0.32	-	198,198,198,198	0
4	NAG	H	602	14/15	0.83	0.25	-	199,199,199,199	0
6	MAN	H	612	11/12	0.72	0.26	-	271,271,271,271	0
6	MAN	J	613	11/12	0.68	0.44	-	294,294,294,294	0
4	BMA	B	603	11/12	0.92	0.17	-	212,212,212,212	0
6	NAG	K	609	14/15	0.91	0.20	-	181,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MAN	D	614	11/12	0.53	0.32	-	254,254,254,254	0
6	NAG	H	610	14/15	0.93	0.15	-	202,202,202,202	0
6	MAN	F	613	11/12	0.39	0.43	-	293,293,293,293	0
4	BMA	K	603	11/12	0.84	0.28	-	212,212,212,212	0
7	NAG	F	616	14/15	0.87	0.23	-	270,270,270,270	0
7	NAG	A	615	14/15	0.89	0.16	-	250,250,250,250	0
4	MAN	D	605	11/12	0.79	0.35	-	235,235,235,235	0
4	MAN	E	605	11/12	0.86	0.32	-	235,235,235,235	0
6	MAN	G	613	11/12	0.58	0.39	-	294,294,294,294	0
7	NAG	I	615	14/15	0.82	0.25	-	250,250,250,250	0
7	NAG	G	615	14/15	0.87	0.27	-	251,251,251,251	0
4	MAN	A	605	11/12	0.78	0.32	-	235,235,235,235	0
7	NAG	B	615	14/15	0.88	0.19	-	251,251,251,251	0
4	MAN	E	607	11/12	0.88	0.33	-	244,244,244,244	0
7	NAG	D	616	14/15	0.90	0.26	-	270,270,270,270	0
7	BMA	D	617	11/12	0.53	0.29	-	301,301,301,301	0
7	BMA	G	617	11/12	0.48	0.41	-	301,301,301,301	0
6	MAN	A	612	11/12	0.72	0.41	-	271,271,271,271	0
7	BMA	C	617	11/12	0.34	0.40	-	301,301,301,301	0
7	NAG	F	615	14/15	0.87	0.25	-	250,250,250,250	0
7	NAG	K	616	14/15	0.82	0.45	-	270,270,270,270	0
4	MAN	H	606	11/12	0.68	0.39	-	222,222,222,222	0
6	MAN	C	614	11/12	0.91	0.23	-	253,253,253,253	0

6.4 Ligands [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(\AA^2)	Q<0.9
5	NAG	H	608	14/15	0.19	0.80	8.60	238,238,238,238	0
5	NAG	H	618	14/15	0.71	0.45	1.16	291,291,291,291	0
5	NAG	C	618	14/15	0.75	0.32	-	290,290,290,290	0
5	NAG	A	608	14/15	0.73	0.27	-	238,238,238,238	0
5	NAG	J	618	14/15	0.72	0.48	-	291,291,291,291	0
5	NAG	C	608	14/15	0.76	0.40	-	238,238,238,238	0
5	NAG	D	618	14/15	0.61	0.49	-	291,291,291,291	0
5	NAG	E	608	14/15	0.61	0.33	-	238,238,238,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	F	608	14/15	0.80	0.27	-	238,238,238,238	0
5	NAG	F	618	14/15	0.62	0.37	-	291,291,291,291	0
5	NAG	L	608	14/15	0.68	0.33	-	238,238,238,238	0
5	NAG	I	618	14/15	0.70	0.25	-	290,290,290,290	0
5	NAG	A	618	14/15	0.63	0.29	-	291,291,291,291	0
5	NAG	G	618	14/15	0.73	0.49	-	291,291,291,291	0
5	NAG	D	608	14/15	0.67	0.30	-	238,238,238,238	0
5	NAG	G	608	14/15	0.77	0.20	-	238,238,238,238	0
5	NAG	J	608	14/15	0.79	0.19	-	238,238,238,238	0
5	NAG	K	608	14/15	0.72	0.29	-	238,238,238,238	0
5	NAG	I	608	14/15	0.74	0.23	-	238,238,238,238	0
5	NAG	B	608	14/15	0.73	0.33	-	238,238,238,238	0
5	NAG	L	618	14/15	0.67	0.52	-	291,291,291,291	0
5	NAG	B	618	14/15	0.60	0.54	-	291,291,291,291	0
5	NAG	K	618	14/15	0.64	0.55	-	291,291,291,291	0
5	NAG	E	618	14/15	0.81	0.41	-	291,291,291,291	0

6.5 Other polymers

There are no such residues in this entry.