



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:16 PM GMT

PDB ID : 4O5I  
Title : Crystal structure of broadly neutralizing antibody F045-092 in complex with A/Victoria/361/2011 (H3N2) influenza hemagglutinin  
Authors : Lee, P.S.; Wilson, I.A.  
Deposited on : 2013-12-19  
Resolution : 6.50 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](mailto: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.

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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

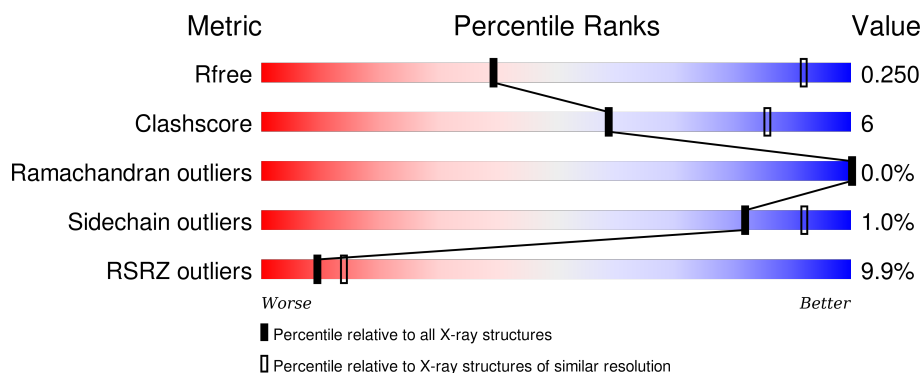
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)

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  $\geq 3$ , 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>6%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	323	<div> <div>6%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	E	323	<div> <div>7%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
1	G	323	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	I	323	<div> <div>11%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	323	
2	B	176	
2	D	176	
2	F	176	
2	H	176	
2	J	176	
2	L	176	
3	M	240	
3	O	240	
3	Q	240	
3	S	240	
3	U	240	
3	W	240	
4	N	216	
4	P	216	
4	R	216	
4	T	216	
4	V	216	
4	X	216	

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	C	420	-	-	-	X
5	NAG	E	421	-	-	-	X
6	NAG	A	415	-	-	-	X
6	NAG	K	401	-	-	-	X
7	NAG	A	408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	NAG	C	411	-	-	-	X
7	NAG	E	413	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44305 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	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	C	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	E	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	G	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	I	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			
1	K	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP R9U684
A	8	ASP	-	EXPRESSION TAG	UNP R9U684
A	9	PRO	-	EXPRESSION TAG	UNP R9U684
A	10	GLY	-	EXPRESSION TAG	UNP R9U684
C	7	ALA	-	EXPRESSION TAG	UNP R9U684
C	8	ASP	-	EXPRESSION TAG	UNP R9U684
C	9	PRO	-	EXPRESSION TAG	UNP R9U684
C	10	GLY	-	EXPRESSION TAG	UNP R9U684
E	7	ALA	-	EXPRESSION TAG	UNP R9U684
E	8	ASP	-	EXPRESSION TAG	UNP R9U684
E	9	PRO	-	EXPRESSION TAG	UNP R9U684
E	10	GLY	-	EXPRESSION TAG	UNP R9U684
G	7	ALA	-	EXPRESSION TAG	UNP R9U684
G	8	ASP	-	EXPRESSION TAG	UNP R9U684
G	9	PRO	-	EXPRESSION TAG	UNP R9U684
G	10	GLY	-	EXPRESSION TAG	UNP R9U684
I	7	ALA	-	EXPRESSION TAG	UNP R9U684

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Chain	Residue	Modelled	Actual	Comment	Reference
I	8	ASP	-	EXPRESSION TAG	UNP R9U684
I	9	PRO	-	EXPRESSION TAG	UNP R9U684
I	10	GLY	-	EXPRESSION TAG	UNP R9U684
K	7	ALA	-	EXPRESSION TAG	UNP R9U684
K	8	ASP	-	EXPRESSION TAG	UNP R9U684
K	9	PRO	-	EXPRESSION TAG	UNP R9U684
K	10	GLY	-	EXPRESSION TAG	UNP R9U684

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	D	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	F	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	H	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	J	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			
2	L	173	Total	C	N	O	S	0	0	0
			1396	869	246	275	6			

- Molecule 3 is a protein called Fab F045-092 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	O	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	Q	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	S	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	U	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			
3	W	226	Total	C	N	O	S	0	0	0
			1698	1076	279	335	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
M	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
M	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
M	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
M	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
M	222	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
O	222	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
Q	222	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
S	222	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
U	222	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
W	222	HIS	-	EXPRESSION TAG	UNP S6C4S0

- Molecule 4 is a protein called Fab F045-092 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	P	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	T	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	V	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			
4	X	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	C	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).



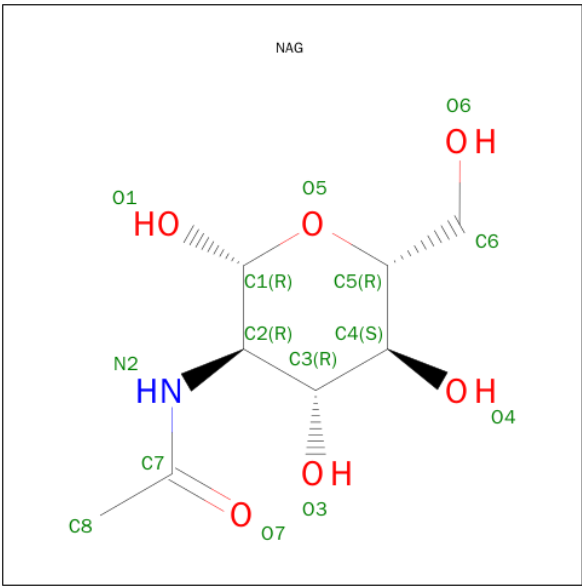
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	C	2	Total	C	N	O	0	0
			28	16	2	10		
6	E	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	I	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	5	Total	C	N	O	0	0
			61	34	2	25		
7	C	5	Total	C	N	O	0	0
			61	34	2	25		
7	E	5	Total	C	N	O	0	0
			61	34	2	25		
7	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

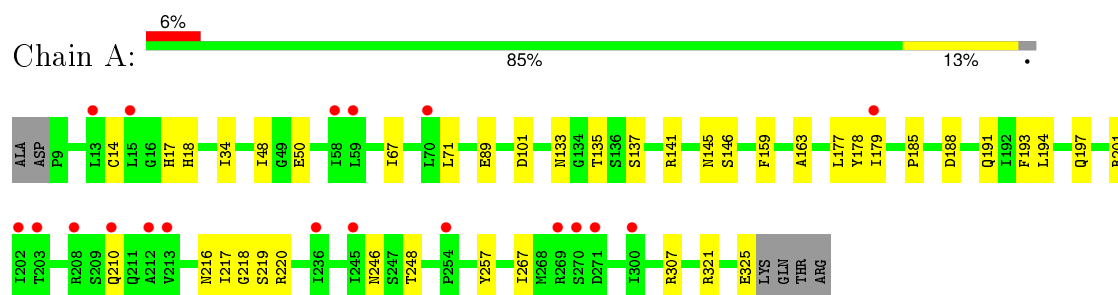
- Molecule 9 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	4	Total	C	N	O	0	0
			50	28	2	20		
9	C	4	Total	C	N	O	0	0
			50	28	2	20		
9	E	4	Total	C	N	O	0	0
			50	28	2	20		

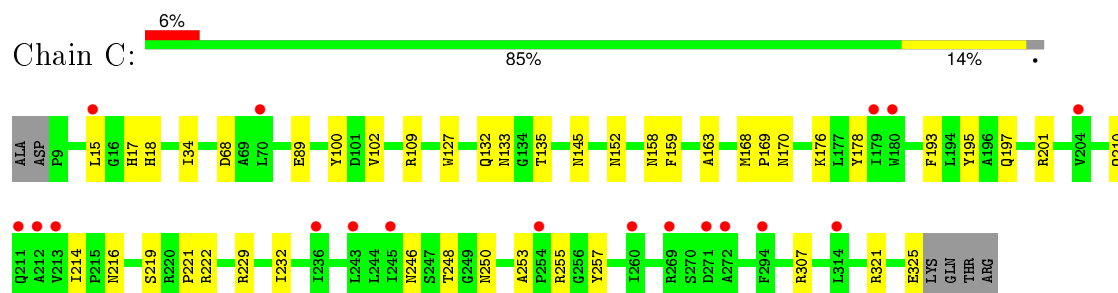
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $RSRZ > 2$ ). 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.

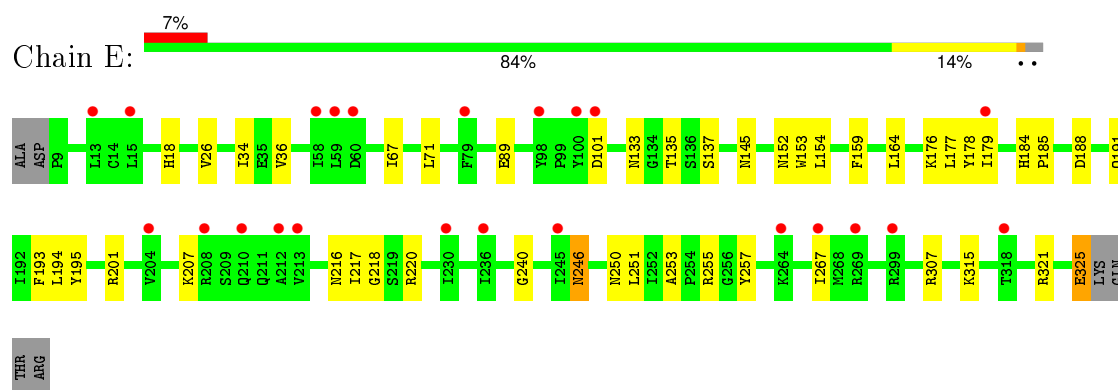
- Molecule 1: Hemagglutinin HA1 chain



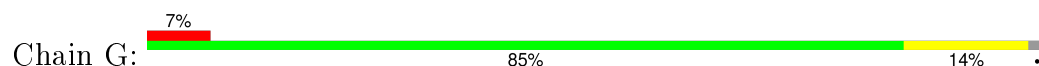
- Molecule 1: Hemagglutinin HA1 chain

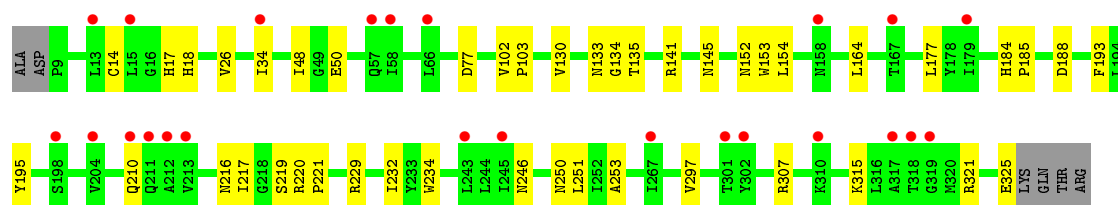


- Molecule 1: Hemagglutinin HA1 chain

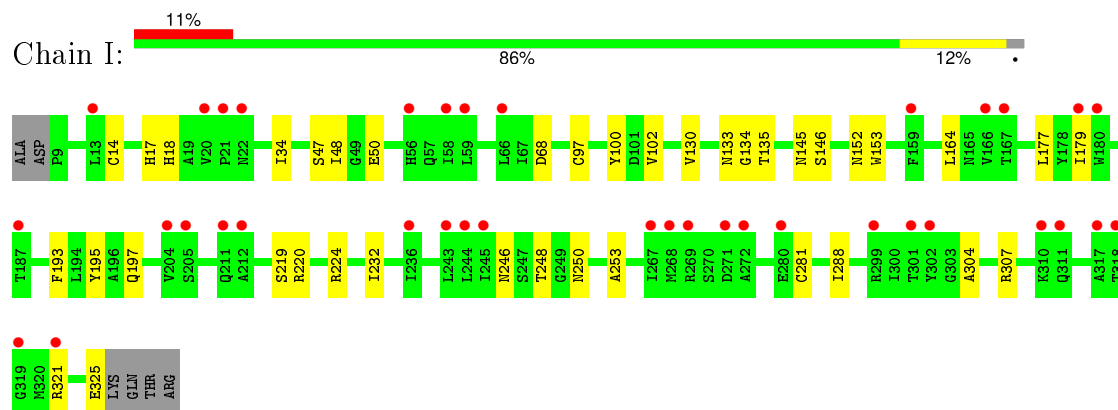


- Molecule 1: Hemagglutinin HA1 chain

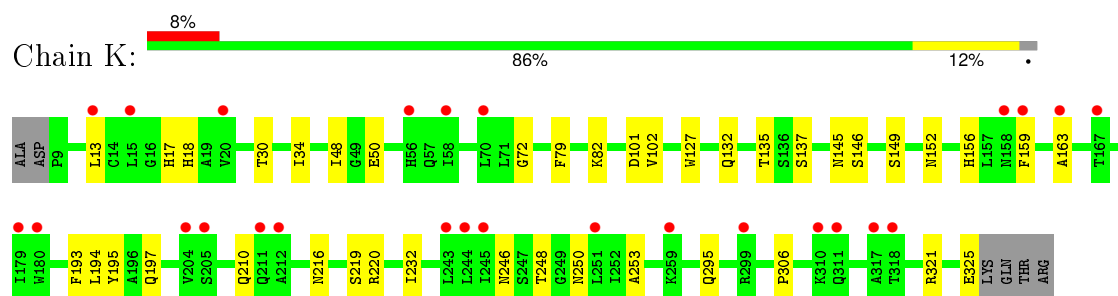




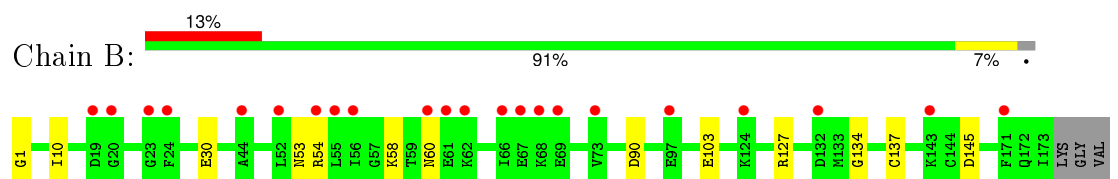
• Molecule 1: Hemagglutinin HA1 chain



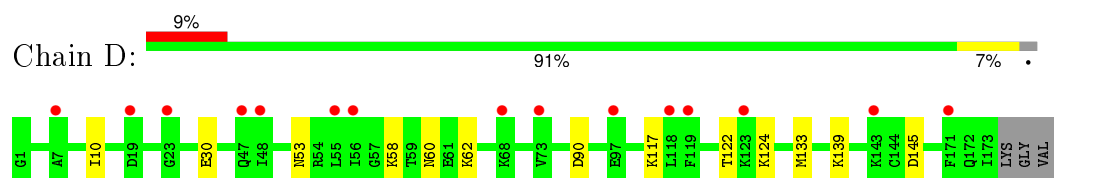
• Molecule 1: Hemagglutinin HA1 chain



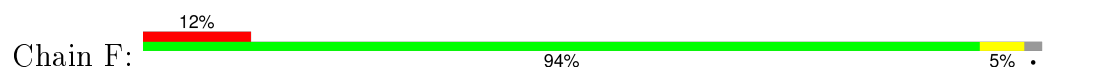
• Molecule 2: Hemagglutinin HA2 chain

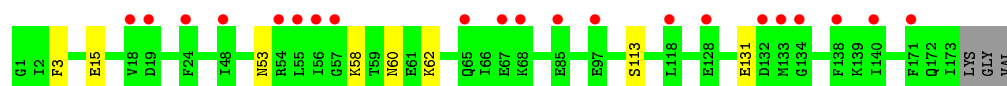


• Molecule 2: Hemagglutinin HA2 chain

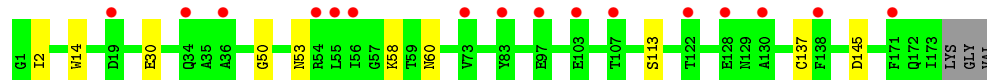


• Molecule 2: Hemagglutinin HA2 chain

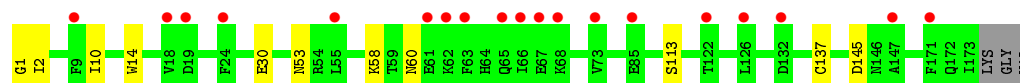
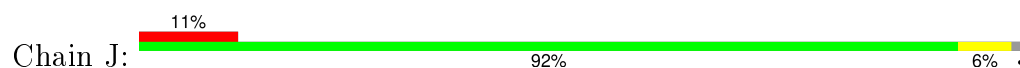




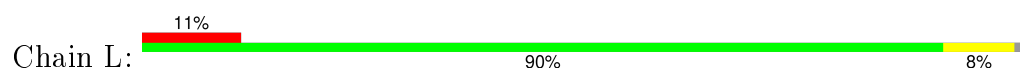
- Molecule 2: Hemagglutinin HA2 chain



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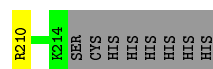
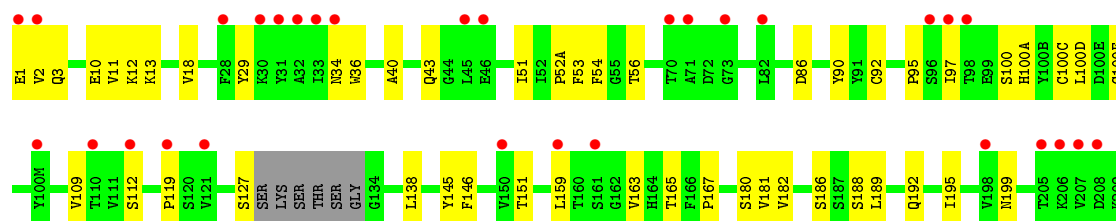
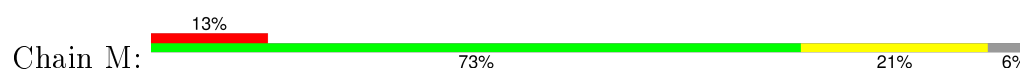


- Molecule 2: Hemagglutinin HA2 chain

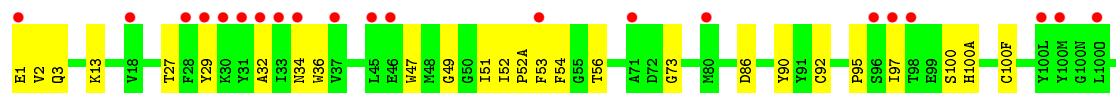
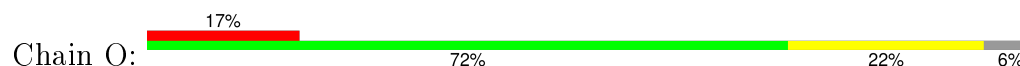


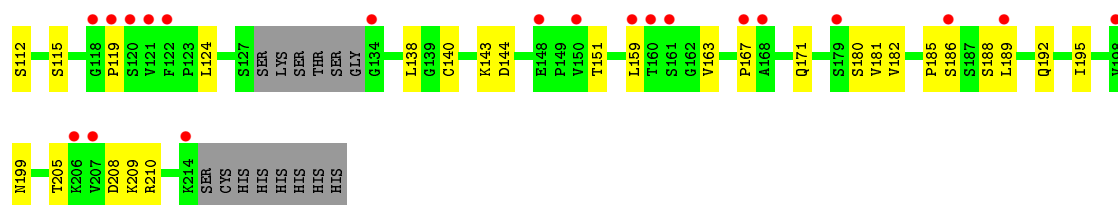
VAL

- Molecule 3: Fab F045-092 heavy chain

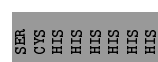
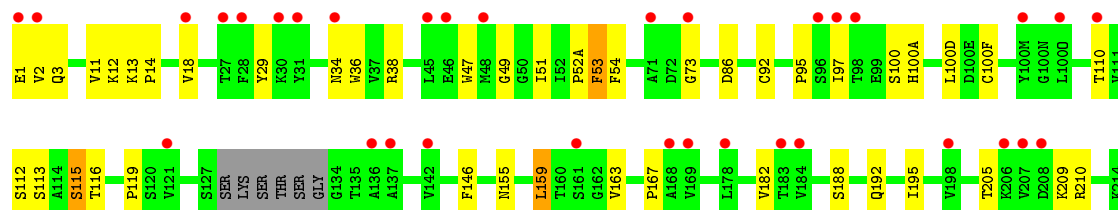
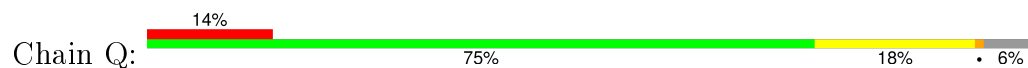


- Molecule 3: Fab F045-092 heavy chain

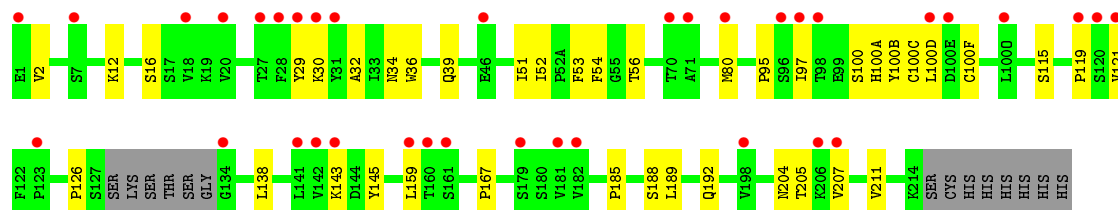
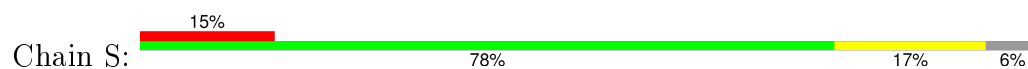




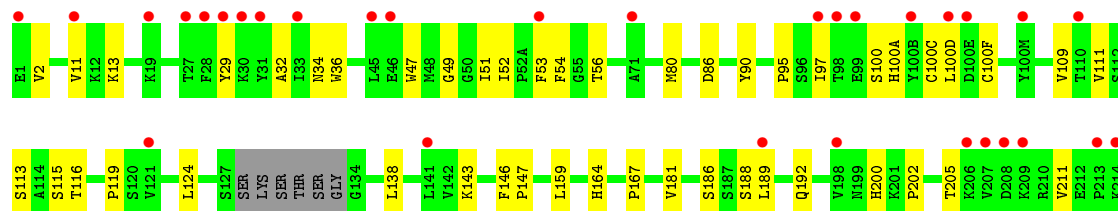
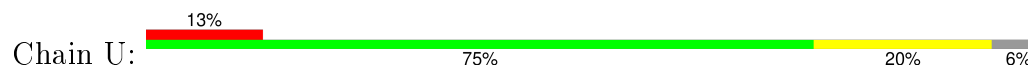
• Molecule 3: Fab F045-092 heavy chain



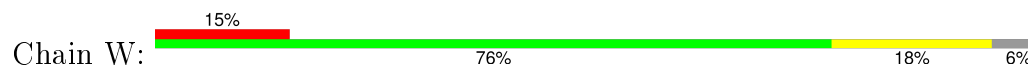
• Molecule 3: Fab F045-092 heavy chain

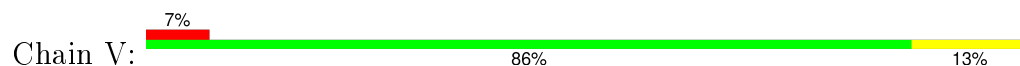


• Molecule 3: Fab F045-092 heavy chain

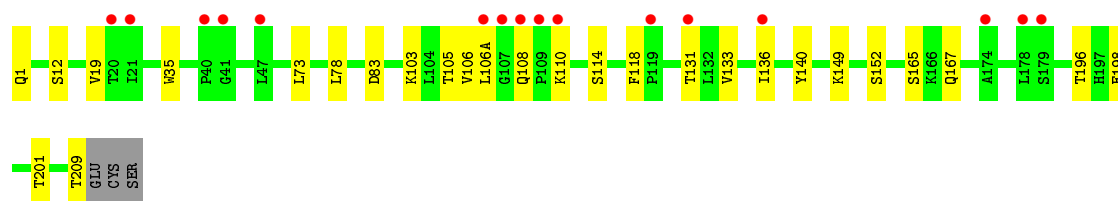


• Molecule 3: Fab F045-092 heavy chain



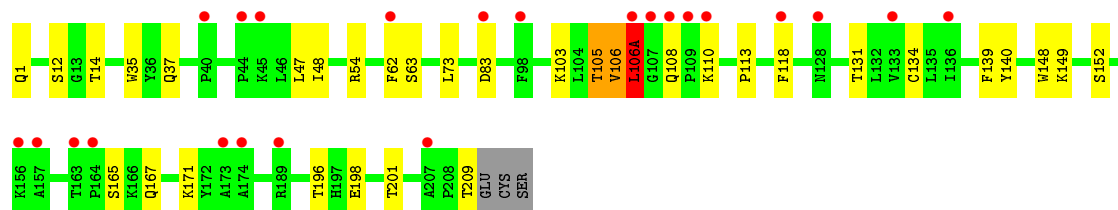






• Molecule 4: Fab F045-092 light chain

Chain X: 11% 83% 14% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	318.12Å 187.17Å 353.64Å 90.00° 90.47° 90.00°	Depositor
Resolution (Å)	49.00 – 6.50 49.00 – 6.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.00-6.50) 89.1 (49.00-6.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 6.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.201 , 0.248 0.204 , 0.250	Depositor DCC
$R_{free}$ test set	1924 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	209.5	Xtriage
Anisotropy	0.848	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.038 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.039 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.297 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.289 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.047 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 38224 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	44305	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.35	0/2532	0.59	0/3443
1	C	0.34	0/2532	0.57	0/3443
1	E	0.35	0/2532	0.58	0/3443
1	G	0.31	0/2532	0.57	0/3443
1	I	0.31	0/2532	0.57	0/3443
1	K	0.31	0/2532	0.58	0/3443
2	B	0.31	0/1420	0.57	0/1906
2	D	0.31	0/1420	0.55	0/1906
2	F	0.30	0/1420	0.55	0/1906
2	H	0.29	0/1420	0.54	0/1906
2	J	0.30	0/1420	0.54	0/1906
2	L	0.30	0/1420	0.54	0/1906
3	M	0.33	0/1740	0.63	0/2373
3	O	0.34	0/1740	0.64	0/2373
3	Q	0.33	0/1740	0.64	1/2373 (0.0%)
3	S	0.32	0/1740	0.64	0/2373
3	U	0.33	0/1740	0.66	1/2373 (0.0%)
3	W	0.31	0/1740	0.62	0/2373
4	N	0.34	0/1604	0.60	0/2190
4	P	0.30	0/1604	0.59	0/2190
4	R	0.30	0/1604	0.59	0/2190
4	T	0.30	0/1604	0.59	0/2190
4	V	0.31	0/1604	0.60	1/2190 (0.0%)
4	X	0.31	0/1604	0.65	3/2190 (0.1%)
All	All	0.32	0/43776	0.59	6/59472 (0.0%)

There are no bond length outliers.

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	105	THR	C-N-CA	6.21	137.22	121.70
4	V	106(A)	LEU	CA-CB-CG	5.87	128.80	115.30
4	X	106(A)	LEU	CA-CB-CG	5.73	128.47	115.30
4	X	105	THR	CA-C-N	5.50	129.29	117.20
3	U	29	TYR	CB-CG-CD1	-5.37	117.78	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2475	0	2423	38	0
1	C	2475	0	2422	43	0
1	E	2475	0	2422	42	0
1	G	2475	0	2422	40	0
1	I	2475	0	2422	39	0
1	K	2475	0	2422	36	0
2	B	1396	0	1327	10	0
2	D	1396	0	1327	10	0
2	F	1396	0	1327	6	0
2	H	1396	0	1327	10	0
2	J	1396	0	1327	11	0
2	L	1396	0	1327	10	0
3	M	1698	0	1649	43	0
3	O	1698	0	1649	47	0
3	Q	1698	0	1649	42	0
3	S	1698	0	1649	35	0
3	U	1698	0	1649	38	0
3	W	1698	0	1649	41	0
4	N	1567	0	1515	11	0
4	P	1567	0	1515	17	0
4	R	1567	0	1515	21	0
4	T	1567	0	1515	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	1567	0	1515	14	0
4	X	1567	0	1515	21	0
5	A	39	0	34	0	0
5	C	78	0	68	2	0
5	E	78	0	68	0	0
5	G	78	0	68	1	0
5	I	117	0	102	3	0
5	K	117	0	102	2	0
6	A	112	0	100	2	0
6	C	28	0	25	0	0
6	E	28	0	25	0	0
6	G	84	0	75	3	0
6	I	84	0	75	2	0
6	K	84	0	75	2	0
7	A	61	0	52	1	0
7	C	61	0	52	1	0
7	E	122	0	104	3	0
8	B	14	0	13	0	0
8	C	14	0	13	0	0
8	D	14	0	13	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
8	G	28	0	26	0	0
8	H	14	0	13	0	0
8	I	14	0	13	0	0
8	J	14	0	13	0	0
8	K	14	0	13	0	0
8	L	14	0	13	0	0
9	C	100	0	86	0	0
9	E	50	0	43	0	0
All	All	44305	0	42789	503	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 503 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:G:145:ASN:ND2	3:S:100(F):CYS:SG	2.44	0.90
1:C:145:ASN:ND2	3:O:100(F):CYS:SG	2.46	0.89
1:K:145:ASN:ND2	3:W:100(F):CYS:SG	2.48	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:195:ILE:HG12	3:O:210:ARG:HG2	1.54	0.86
3:Q:195:ILE:HG12	3:Q:210:ARG:HG2	1.62	0.82

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	C	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	E	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	G	315/323 (98%)	307 (98%)	8 (2%)	0	100	100
1	I	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
1	K	315/323 (98%)	306 (97%)	9 (3%)	0	100	100
2	B	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	D	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
2	F	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	H	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	J	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
2	L	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
3	M	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	O	222/240 (92%)	216 (97%)	6 (3%)	0	100	100
3	Q	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	S	222/240 (92%)	217 (98%)	5 (2%)	0	100	100
3	U	222/240 (92%)	219 (99%)	3 (1%)	0	100	100
3	W	222/240 (92%)	217 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	P	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
4	R	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	T	211/216 (98%)	207 (98%)	4 (2%)	0	100	100
4	V	211/216 (98%)	208 (99%)	3 (1%)	0	100	100
4	X	211/216 (98%)	205 (97%)	5 (2%)	1 (0%)	34	77
All	All	5514/5730 (96%)	5369 (97%)	144 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	106	VAL

### 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	280/285 (98%)	277 (99%)	3 (1%)	80	91
1	C	280/285 (98%)	277 (99%)	3 (1%)	80	91
1	E	280/285 (98%)	277 (99%)	3 (1%)	80	91
1	G	280/285 (98%)	277 (99%)	3 (1%)	80	91
1	I	280/285 (98%)	277 (99%)	3 (1%)	80	91
1	K	280/285 (98%)	277 (99%)	3 (1%)	80	91
2	B	146/148 (99%)	146 (100%)	0	100	100
2	D	146/148 (99%)	146 (100%)	0	100	100
2	F	146/148 (99%)	146 (100%)	0	100	100
2	H	146/148 (99%)	146 (100%)	0	100	100
2	J	146/148 (99%)	146 (100%)	0	100	100
2	L	146/148 (99%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	188/201 (94%)	186 (99%)	2 (1%)	80	91
3	O	188/201 (94%)	186 (99%)	2 (1%)	80	91
3	Q	188/201 (94%)	184 (98%)	4 (2%)	61	84
3	S	188/201 (94%)	186 (99%)	2 (1%)	80	91
3	U	188/201 (94%)	185 (98%)	3 (2%)	70	88
3	W	188/201 (94%)	186 (99%)	2 (1%)	80	91
4	N	178/181 (98%)	174 (98%)	4 (2%)	60	83
4	P	178/181 (98%)	176 (99%)	2 (1%)	80	91
4	R	178/181 (98%)	176 (99%)	2 (1%)	80	91
4	T	178/181 (98%)	176 (99%)	2 (1%)	80	91
4	V	178/181 (98%)	175 (98%)	3 (2%)	68	87
4	X	178/181 (98%)	175 (98%)	3 (2%)	68	87
All	All	4752/4890 (97%)	4703 (99%)	49 (1%)	82	92

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	110	LYS
4	P	209	THR
3	W	159	LEU
3	O	2	VAL
3	Q	2	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	60	ASN
1	K	145	ASN
3	W	34	ASN
1	K	17	HIS
3	M	34	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

101 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	$\# Z  > 2$
5	NAG	A	401	1,5	14,14,15	0.61	0	15,19,21	1.00	1 (6%)
5	NAG	A	402	5	14,14,15	0.60	0	15,19,21	1.55	1 (6%)
5	BMA	A	403	5	11,11,12	0.60	0	14,15,17	0.71	1 (7%)
6	NAG	A	404	1,6	14,14,15	0.49	0	15,19,21	0.71	0
6	NAG	A	405	6	14,14,15	0.54	0	15,19,21	0.81	0
6	NAG	A	406	1,6	14,14,15	0.61	0	15,19,21	0.98	2 (13%)
6	NAG	A	407	6	14,14,15	0.51	0	15,19,21	0.80	0
7	NAG	A	408	1,7	14,14,15	0.48	0	15,19,21	0.80	1 (6%)
7	NAG	A	409	7	14,14,15	0.54	0	15,19,21	0.92	0
7	BMA	A	410	7	11,11,12	0.57	0	14,15,17	1.17	2 (14%)
7	MAN	A	411	7	11,11,12	0.59	0	14,15,17	0.90	0
7	MAN	A	412	7	11,11,12	0.60	0	14,15,17	1.65	3 (21%)
6	NAG	A	413	1,6	14,14,15	0.47	0	15,19,21	0.78	0
6	NAG	A	414	6	14,14,15	0.47	0	15,19,21	0.75	0
6	NAG	A	415	1,6	14,14,15	0.45	0	15,19,21	1.10	1 (6%)
6	NAG	A	416	6	14,14,15	0.57	0	15,19,21	0.71	0
9	NAG	C	401	9,1	14,14,15	0.59	0	15,19,21	1.07	2 (13%)
9	NAG	C	402	9	14,14,15	0.59	0	15,19,21	0.74	0
9	BMA	C	403	9	11,11,12	0.61	0	14,15,17	0.86	0
9	MAN	C	404	9	11,11,12	0.58	0	14,15,17	0.90	0
6	NAG	C	405	1,6	14,14,15	0.50	0	15,19,21	0.71	0
6	NAG	C	406	6	14,14,15	0.55	0	15,19,21	0.60	0
9	NAG	C	407	9,1	14,14,15	0.57	0	15,19,21	0.81	1 (6%)
9	NAG	C	408	9	14,14,15	0.49	0	15,19,21	0.63	0
9	BMA	C	409	9	11,11,12	0.56	0	14,15,17	0.91	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	MAN	C	410	9	11,11,12	0.60	0	14,15,17	0.71	0
7	NAG	C	411	1,7	14,14,15	0.53	0	15,19,21	0.70	0
7	NAG	C	412	7	14,14,15	0.54	0	15,19,21	0.76	0
7	BMA	C	413	7	11,11,12	0.65	0	14,15,17	1.18	1 (7%)
7	MAN	C	414	7	11,11,12	0.54	0	14,15,17	1.07	1 (7%)
7	MAN	C	415	7	11,11,12	0.63	0	14,15,17	0.74	0
5	NAG	C	416	1,5	14,14,15	0.50	0	15,19,21	0.73	0
5	NAG	C	417	5	14,14,15	0.48	0	15,19,21	0.72	0
5	BMA	C	418	5	11,11,12	0.56	0	14,15,17	0.93	1 (7%)
5	NAG	C	420	1,5	14,14,15	0.44	0	15,19,21	1.06	1 (6%)
5	NAG	C	421	5	14,14,15	0.53	0	15,19,21	0.92	1 (6%)
5	BMA	C	422	5	11,11,12	0.59	0	14,15,17	1.01	2 (14%)
7	NAG	E	401	1,7	14,14,15	0.52	0	15,19,21	1.17	1 (6%)
7	NAG	E	402	7	14,14,15	0.56	0	15,19,21	0.75	0
7	BMA	E	403	7	11,11,12	0.57	0	14,15,17	0.80	0
7	MAN	E	404	7	11,11,12	0.57	0	14,15,17	0.77	0
7	MAN	E	405	7	11,11,12	0.68	0	14,15,17	0.95	1 (7%)
5	NAG	E	406	1,5	14,14,15	0.53	0	15,19,21	0.79	0
5	NAG	E	407	5	14,14,15	0.55	0	15,19,21	0.74	0
5	BMA	E	408	5	11,11,12	0.64	0	14,15,17	0.66	0
9	NAG	E	409	9,1	14,14,15	0.47	0	15,19,21	0.93	1 (6%)
9	NAG	E	410	9	14,14,15	0.48	0	15,19,21	0.79	0
9	BMA	E	411	9	11,11,12	0.53	0	14,15,17	1.16	2 (14%)
9	MAN	E	412	9	11,11,12	0.56	0	14,15,17	0.82	0
7	NAG	E	413	1,7	14,14,15	0.45	0	15,19,21	0.82	1 (6%)
7	NAG	E	414	7	14,14,15	0.53	0	15,19,21	0.89	1 (6%)
7	BMA	E	415	7	11,11,12	0.52	0	14,15,17	0.91	1 (7%)
7	MAN	E	416	7	11,11,12	0.54	0	14,15,17	1.04	1 (7%)
7	MAN	E	417	7	11,11,12	0.50	0	14,15,17	1.52	2 (14%)
6	NAG	E	418	1,6	14,14,15	0.48	0	15,19,21	0.60	0
6	NAG	E	419	6	14,14,15	0.51	0	15,19,21	0.63	0
5	NAG	E	421	1,5	14,14,15	0.45	0	15,19,21	1.07	1 (6%)
5	NAG	E	422	5	14,14,15	0.55	0	15,19,21	0.91	1 (6%)
5	BMA	E	423	5	11,11,12	0.60	0	14,15,17	1.05	1 (7%)
6	NAG	G	401	1,6	14,14,15	0.52	0	15,19,21	0.89	1 (6%)
6	NAG	G	402	6	14,14,15	0.52	0	15,19,21	0.71	0
6	NAG	G	404	1,6	14,14,15	0.45	0	15,19,21	0.73	0
6	NAG	G	405	6	14,14,15	0.51	0	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	G	406	1,6	14,14,15	0.47	0	15,19,21	0.63	0
6	NAG	G	407	6	14,14,15	0.57	0	15,19,21	0.98	0
5	NAG	G	408	1,5	14,14,15	0.42	0	15,19,21	0.56	0
5	NAG	G	409	5	14,14,15	0.48	0	15,19,21	0.72	0
5	BMA	G	410	5	11,11,12	0.58	0	14,15,17	0.74	1 (7%)
5	NAG	G	412	1,5	14,14,15	0.46	0	15,19,21	1.26	3 (20%)
5	NAG	G	413	5	14,14,15	0.53	0	15,19,21	0.87	1 (6%)
5	BMA	G	414	5	11,11,12	0.58	0	14,15,17	1.03	2 (14%)
6	NAG	I	401	1,6	14,14,15	0.52	0	15,19,21	0.93	1 (6%)
6	NAG	I	402	6	14,14,15	0.49	0	15,19,21	0.91	1 (6%)
6	NAG	I	403	1,6	14,14,15	0.65	0	15,19,21	0.90	0
6	NAG	I	404	6	14,14,15	0.51	0	15,19,21	0.72	0
6	NAG	I	405	1,6	14,14,15	0.53	0	15,19,21	0.76	1 (6%)
6	NAG	I	406	6	14,14,15	0.47	0	15,19,21	0.69	0
5	NAG	I	407	1,5	14,14,15	0.46	0	15,19,21	0.59	0
5	NAG	I	408	5	14,14,15	0.57	0	15,19,21	0.80	1 (6%)
5	BMA	I	409	5	11,11,12	0.62	0	14,15,17	1.02	2 (14%)
5	NAG	I	410	1,5	14,14,15	0.47	0	15,19,21	0.59	0
5	NAG	I	411	5	14,14,15	0.52	0	15,19,21	0.77	0
5	BMA	I	412	5	11,11,12	0.64	0	14,15,17	0.77	1 (7%)
5	NAG	I	414	1,5	14,14,15	0.53	0	15,19,21	1.05	1 (6%)
5	NAG	I	415	5	14,14,15	0.54	0	15,19,21	0.93	1 (6%)
5	BMA	I	416	5	11,11,12	0.62	0	14,15,17	1.03	1 (7%)
6	NAG	K	401	1,6	14,14,15	0.55	0	15,19,21	0.80	0
6	NAG	K	402	6	14,14,15	0.51	0	15,19,21	0.83	0
6	NAG	K	403	1,6	14,14,15	0.53	0	15,19,21	0.69	0
6	NAG	K	404	6	14,14,15	0.52	0	15,19,21	0.69	0
5	NAG	K	405	1,5	14,14,15	0.65	0	15,19,21	1.15	2 (13%)
5	NAG	K	406	5	14,14,15	0.51	0	15,19,21	0.71	0
5	BMA	K	407	5	11,11,12	0.60	0	14,15,17	0.74	0
6	NAG	K	408	1,6	14,14,15	0.52	0	15,19,21	0.59	0
6	NAG	K	409	6	14,14,15	0.57	0	15,19,21	0.83	0
5	NAG	K	410	1,5	14,14,15	0.43	0	15,19,21	0.80	1 (6%)
5	NAG	K	411	5	14,14,15	0.47	0	15,19,21	0.78	0
5	BMA	K	412	5	11,11,12	0.61	0	14,15,17	0.87	1 (7%)
5	NAG	K	414	1,5	14,14,15	1.32	3 (21%)	15,19,21	1.37	2 (13%)
5	NAG	K	415	5	14,14,15	0.60	0	15,19,21	1.07	2 (13%)
5	BMA	K	416	5	11,11,12	0.50	0	14,15,17	0.90	1 (7%)

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	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	402	5	-	0/6/23/26	0/1/1/1
5	BMA	A	403	5	-	0/2/19/22	0/1/1/1
6	NAG	A	404	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	405	6	-	0/6/23/26	0/1/1/1
6	NAG	A	406	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	407	6	-	0/6/23/26	0/1/1/1
7	NAG	A	408	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	409	7	-	0/6/23/26	0/1/1/1
7	BMA	A	410	7	-	0/2/19/22	0/1/1/1
7	MAN	A	411	7	-	0/2/19/22	0/1/1/1
7	MAN	A	412	7	-	0/2/19/22	0/1/1/1
6	NAG	A	413	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	414	6	-	0/6/23/26	0/1/1/1
6	NAG	A	415	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	416	6	-	0/6/23/26	0/1/1/1
9	NAG	C	401	9,1	-	0/6/23/26	0/1/1/1
9	NAG	C	402	9	-	0/6/23/26	0/1/1/1
9	BMA	C	403	9	-	0/2/19/22	0/1/1/1
9	MAN	C	404	9	-	0/2/19/22	0/1/1/1
6	NAG	C	405	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	406	6	-	0/6/23/26	0/1/1/1
9	NAG	C	407	9,1	-	0/6/23/26	0/1/1/1
9	NAG	C	408	9	-	0/6/23/26	0/1/1/1
9	BMA	C	409	9	-	0/2/19/22	0/1/1/1
9	MAN	C	410	9	-	0/2/19/22	0/1/1/1
7	NAG	C	411	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	412	7	-	0/6/23/26	0/1/1/1
7	BMA	C	413	7	-	0/2/19/22	0/1/1/1
7	MAN	C	414	7	-	0/2/19/22	0/1/1/1
7	MAN	C	415	7	-	0/2/19/22	0/1/1/1
5	NAG	C	416	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	417	5	-	0/6/23/26	0/1/1/1
5	BMA	C	418	5	-	0/2/19/22	0/1/1/1
5	NAG	C	420	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	421	5	-	0/6/23/26	0/1/1/1
5	BMA	C	422	5	-	0/2/19/22	0/1/1/1
7	NAG	E	401	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	402	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	E	403	7	-	0/2/19/22	0/1/1/1
7	MAN	E	404	7	-	0/2/19/22	0/1/1/1
7	MAN	E	405	7	-	0/2/19/22	0/1/1/1
5	NAG	E	406	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	407	5	-	0/6/23/26	0/1/1/1
5	BMA	E	408	5	-	0/2/19/22	0/1/1/1
9	NAG	E	409	9,1	-	0/6/23/26	0/1/1/1
9	NAG	E	410	9	-	0/6/23/26	0/1/1/1
9	BMA	E	411	9	-	0/2/19/22	0/1/1/1
9	MAN	E	412	9	-	0/2/19/22	0/1/1/1
7	NAG	E	413	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	414	7	-	0/6/23/26	0/1/1/1
7	BMA	E	415	7	-	0/2/19/22	0/1/1/1
7	MAN	E	416	7	-	0/2/19/22	0/1/1/1
7	MAN	E	417	7	-	0/2/19/22	1/1/1/1
6	NAG	E	418	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	419	6	-	0/6/23/26	0/1/1/1
5	NAG	E	421	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	422	5	-	0/6/23/26	0/1/1/1
5	BMA	E	423	5	-	0/2/19/22	0/1/1/1
6	NAG	G	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	402	6	-	0/6/23/26	0/1/1/1
6	NAG	G	404	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	405	6	-	0/6/23/26	0/1/1/1
6	NAG	G	406	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	407	6	-	0/6/23/26	0/1/1/1
5	NAG	G	408	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	409	5	-	0/6/23/26	0/1/1/1
5	BMA	G	410	5	-	0/2/19/22	0/1/1/1
5	NAG	G	412	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	413	5	-	0/6/23/26	0/1/1/1
5	BMA	G	414	5	-	0/2/19/22	0/1/1/1
6	NAG	I	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	402	6	-	0/6/23/26	0/1/1/1
6	NAG	I	403	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	404	6	-	0/6/23/26	0/1/1/1
6	NAG	I	405	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	406	6	-	0/6/23/26	0/1/1/1
5	NAG	I	407	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	408	5	-	0/6/23/26	0/1/1/1
5	BMA	I	409	5	-	0/2/19/22	0/1/1/1
5	NAG	I	410	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	411	5	-	0/6/23/26	0/1/1/1
5	BMA	I	412	5	-	0/2/19/22	0/1/1/1
5	NAG	I	414	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	415	5	-	0/6/23/26	0/1/1/1
5	BMA	I	416	5	-	0/2/19/22	0/1/1/1
6	NAG	K	401	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	402	6	-	0/6/23/26	0/1/1/1
6	NAG	K	403	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	404	6	-	0/6/23/26	0/1/1/1
5	NAG	K	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	406	5	-	0/6/23/26	0/1/1/1
5	BMA	K	407	5	-	0/2/19/22	0/1/1/1
6	NAG	K	408	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	409	6	-	0/6/23/26	0/1/1/1
5	NAG	K	410	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	411	5	-	0/6/23/26	0/1/1/1
5	BMA	K	412	5	-	0/2/19/22	0/1/1/1
5	NAG	K	414	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	415	5	-	0/6/23/26	0/1/1/1
5	BMA	K	416	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	414	NAG	O5-C1	-2.63	1.39	1.43
5	K	414	NAG	C2-N2	-2.55	1.41	1.46
5	K	414	NAG	C1-C2	-2.05	1.49	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	412	NAG	C3-C4-C5	-2.60	105.66	110.20
5	I	414	NAG	C3-C4-C5	-2.40	106.01	110.20
6	A	406	NAG	C2-N2-C7	-2.35	120.02	123.04
9	C	401	NAG	C2-N2-C7	-2.35	120.02	123.04
7	E	414	NAG	C2-N2-C7	-2.31	120.07	123.04

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	417	MAN	C1-C2-C3-C4-C5-O5

22 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	408	NAG	1	0
7	A	409	NAG	1	0
6	A	413	NAG	1	0
6	A	414	NAG	1	0
6	A	415	NAG	1	0
7	C	411	NAG	1	0
5	C	420	NAG	2	0
7	E	413	NAG	2	0
7	E	414	NAG	1	0
6	G	406	NAG	3	0
6	G	407	NAG	1	0
5	G	408	NAG	1	0
6	I	403	NAG	1	0
6	I	404	NAG	1	0
6	I	405	NAG	1	0
6	I	406	NAG	1	0
5	I	407	NAG	2	0
5	I	415	NAG	1	0
6	K	408	NAG	2	0
5	K	410	NAG	1	0
5	K	411	NAG	1	0
5	K	414	NAG	1	0

## 5.6 Ligand geometry ⓘ

12 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	$\# Z  > 2$
8	NAG	B	201	2	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
8	NAG	C	419	1	14,14,15	0.46	0	15,19,21	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	D	201	2	14,14,15	0.51	0	15,19,21	0.67	0
8	NAG	E	420	1	14,14,15	0.50	0	15,19,21	0.95	2 (13%)
8	NAG	F	201	2	14,14,15	0.56	0	15,19,21	0.89	0
8	NAG	G	403	1	14,14,15	0.45	0	15,19,21	0.63	0
8	NAG	G	411	1	14,14,15	0.48	0	15,19,21	0.77	0
8	NAG	H	201	2	14,14,15	0.45	0	15,19,21	0.71	0
8	NAG	I	413	1	14,14,15	0.46	0	15,19,21	0.83	1 (6%)
8	NAG	J	201	2	14,14,15	0.50	0	15,19,21	0.73	0
8	NAG	K	413	1	14,14,15	0.50	0	15,19,21	0.70	0
8	NAG	L	201	2	14,14,15	0.48	0	15,19,21	0.73	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
8	NAG	B	201	2	-	0/6/23/26	0/1/1/1
8	NAG	C	419	1	-	0/6/23/26	0/1/1/1
8	NAG	D	201	2	-	0/6/23/26	0/1/1/1
8	NAG	E	420	1	-	0/6/23/26	0/1/1/1
8	NAG	F	201	2	-	0/6/23/26	0/1/1/1
8	NAG	G	403	1	-	0/6/23/26	0/1/1/1
8	NAG	G	411	1	-	0/6/23/26	0/1/1/1
8	NAG	H	201	2	-	0/6/23/26	0/1/1/1
8	NAG	I	413	1	-	0/6/23/26	0/1/1/1
8	NAG	J	201	2	-	0/6/23/26	0/1/1/1
8	NAG	K	413	1	-	0/6/23/26	0/1/1/1
8	NAG	L	201	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	420	NAG	O5-C5-C6	2.06	111.81	107.35
8	I	413	NAG	C1-O5-C5	2.10	114.92	112.25
8	E	420	NAG	C1-O5-C5	2.24	115.09	112.25
8	B	201	NAG	C1-O5-C5	3.07	116.14	112.25

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	317/323 (98%)	0.46	19 (5%) 25 26	51, 102, 191, 323	0
1	C	317/323 (98%)	0.48	18 (5%) 27 28	48, 101, 201, 288	0
1	E	317/323 (98%)	0.46	23 (7%) 18 21	49, 99, 202, 331	0
1	G	317/323 (98%)	0.48	24 (7%) 17 19	65, 133, 251, 354	0
1	I	317/323 (98%)	0.53	37 (11%) 6 11	66, 131, 245, 350	0
1	K	317/323 (98%)	0.56	26 (8%) 14 18	62, 132, 248, 379	0
2	B	173/176 (98%)	0.77	22 (12%) 5 11	48, 99, 198, 361	0
2	D	173/176 (98%)	0.67	15 (8%) 13 17	47, 92, 202, 320	0
2	F	173/176 (98%)	0.78	21 (12%) 6 11	47, 95, 195, 276	0
2	H	173/176 (98%)	0.66	16 (9%) 11 16	57, 141, 306, 537	0
2	J	173/176 (98%)	0.71	19 (10%) 7 12	58, 142, 297, 584	0
2	L	173/176 (98%)	0.72	19 (10%) 7 12	56, 135, 263, 477	0
3	M	226/240 (94%)	0.71	30 (13%) 4 10	58, 130, 256, 349	0
3	O	226/240 (94%)	0.90	41 (18%) 2 7	65, 135, 302, 457	0
3	Q	226/240 (94%)	0.64	33 (14%) 3 9	68, 122, 232, 376	0
3	S	226/240 (94%)	0.74	36 (15%) 3 8	72, 166, 300, 444	0
3	U	226/240 (94%)	0.82	31 (13%) 4 9	106, 170, 303, 521	0
3	W	226/240 (94%)	0.77	36 (15%) 3 8	95, 168, 298, 474	0
4	N	213/216 (98%)	0.32	10 (4%) 35 35	48, 130, 258, 473	0
4	P	213/216 (98%)	0.29	10 (4%) 35 35	57, 122, 241, 435	0
4	R	213/216 (98%)	0.30	9 (4%) 40 38	60, 118, 243, 365	0
4	T	213/216 (98%)	0.53	18 (8%) 13 17	109, 182, 302, 468	0
4	V	213/216 (98%)	0.49	16 (7%) 17 20	118, 178, 337, 403	0
4	X	213/216 (98%)	0.50	23 (10%) 8 12	104, 181, 327, 448	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5574/5730 (97%)	0.58	552 (9%) 9 14	47, 135, 269, 584	0

The worst 5 of 552 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	207	VAL	12.0
4	V	108	GLN	8.1
2	F	132	ASP	7.9
3	S	207	VAL	7.8
3	Q	207	VAL	7.4

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	K	405	14/15	0.83	0.35	1.89	150,154,155,156	0
5	NAG	G	408	14/15	0.76	0.38	1.10	210,212,216,216	0
7	NAG	C	411	14/15	0.86	0.51	0.87	98,102,104,104	0
5	NAG	C	420	14/15	0.92	0.45	0.59	150,156,160,161	0
5	NAG	E	421	14/15	0.90	0.48	0.44	129,135,139,140	0
7	NAG	A	408	14/15	0.78	0.41	0.21	78,81,82,84	0
6	NAG	A	415	14/15	0.83	0.50	0.16	146,152,156,157	0
6	NAG	E	418	14/15	0.79	0.38	0.11	172,175,175,176	0
7	NAG	E	413	14/15	0.83	0.41	0.07	81,83,85,85	0
6	NAG	K	401	14/15	0.66	0.46	-0.03	122,129,130,131	0
9	NAG	C	401	14/15	0.72	0.38	-0.20	87,94,97,98	0
5	NAG	I	407	14/15	0.69	0.40	-0.26	141,147,150,151	0
6	NAG	G	401	14/15	0.73	0.34	-0.29	150,156,159,159	0
6	NAG	A	413	14/15	0.78	0.34	-0.29	175,178,181,182	0
5	NAG	I	414	14/15	0.87	0.30	-0.38	146,151,156,158	0
5	NAG	K	414	14/15	0.87	0.34	-0.39	124,133,141,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	G	406	14/15	0.62	0.38	-0.43	131,135,137,137	0
5	NAG	G	412	14/15	0.87	0.33	-0.52	117,121,127,129	0
6	NAG	K	408	14/15	0.65	0.36	-0.60	104,107,109,110	0
5	NAG	K	410	14/15	0.87	0.29	-	178,181,182,182	0
9	BMA	C	409	11/12	0.94	0.27	-	198,201,203,204	0
9	BMA	E	411	11/12	0.92	0.33	-	197,200,202,202	0
6	NAG	E	419	14/15	0.54	0.46	-	165,166,168,169	0
9	BMA	C	403	11/12	0.84	0.23	-	256,260,262,262	0
5	BMA	K	416	11/12	0.28	0.48	-	187,191,196,202	0
6	NAG	I	405	14/15	0.90	0.23	-	161,167,169,170	0
5	BMA	A	403	11/12	0.67	0.37	-	184,187,189,189	0
5	NAG	K	406	14/15	0.79	0.37	-	182,187,189,193	0
6	NAG	I	401	14/15	0.71	0.48	-	117,123,125,126	0
6	NAG	A	407	14/15	0.61	0.52	-	209,214,215,216	0
6	NAG	A	404	14/15	0.81	0.28	-	113,115,118,119	0
5	BMA	E	408	11/12	0.80	0.40	-	215,219,220,221	0
6	NAG	I	403	14/15	0.86	0.25	-	163,168,177,181	0
6	NAG	K	403	14/15	0.64	0.49	-	159,165,171,175	0
5	NAG	C	416	14/15	0.64	0.43	-	167,169,172,172	0
7	BMA	E	415	11/12	0.81	0.26	-	229,232,234,235	0
7	MAN	C	415	11/12	0.87	0.35	-	186,189,191,191	0
5	NAG	E	422	14/15	0.79	0.88	-	187,191,193,194	0
9	NAG	C	402	14/15	0.31	0.58	-	263,271,272,273	0
6	NAG	A	405	14/15	0.90	0.34	-	153,155,157,157	0
6	NAG	G	405	14/15	0.51	0.58	-	192,200,207,209	0
5	NAG	K	415	14/15	0.46	0.60	-	194,197,203,204	0
5	BMA	C	422	11/12	0.29	0.44	-	176,179,181,184	0
6	NAG	C	405	14/15	0.82	0.40	-	111,117,120,121	0
9	MAN	C	404	11/12	0.80	0.26	-	170,177,180,185	0
5	NAG	C	417	14/15	0.53	0.41	-	164,166,168,168	0
7	MAN	E	417	11/12	0.84	0.39	-	191,195,197,197	0
9	NAG	E	410	14/15	0.86	0.34	-	146,150,151,151	0
6	NAG	C	406	14/15	0.71	0.36	-	187,193,195,196	0
5	NAG	A	401	14/15	0.68	0.44	-	108,112,115,115	0
7	NAG	E	402	14/15	0.74	0.46	-	230,232,234,234	0
6	NAG	I	404	14/15	0.72	0.40	-	171,182,186,193	0
5	NAG	A	402	14/15	0.43	0.53	-	245,249,251,251	0
9	NAG	C	408	14/15	0.93	0.34	-	150,155,156,156	0
5	NAG	G	409	14/15	0.70	0.36	-	215,219,221,221	0
7	MAN	E	405	11/12	0.49	0.50	-	181,183,186,186	0
5	NAG	G	413	14/15	0.72	0.77	-	185,188,191,191	0
6	NAG	K	409	14/15	0.62	0.46	-	127,132,134,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	406	14/15	0.72	0.35	-	129,135,138,139	0
6	NAG	K	402	14/15	0.36	0.56	-	190,196,199,199	0
5	NAG	I	411	14/15	0.80	0.39	-	240,243,245,245	0
6	NAG	K	404	14/15	0.68	0.41	-	177,187,191,198	0
5	BMA	I	409	11/12	0.75	0.38	-	174,176,181,182	0
5	BMA	K	412	11/12	0.73	0.47	-	271,272,274,275	0
5	BMA	I	412	11/12	0.86	0.56	-	201,203,205,206	0
7	NAG	A	409	14/15	0.85	0.29	-	124,128,128,129	0
7	MAN	A	412	11/12	0.82	0.40	-	167,171,173,173	0
6	NAG	A	416	14/15	0.24	1.15	-	208,212,215,215	0
5	NAG	I	415	14/15	0.66	0.54	-	223,226,228,229	0
7	BMA	E	403	11/12	0.72	0.26	-	234,237,238,239	0
6	NAG	I	402	14/15	0.35	0.65	-	171,179,182,183	0
7	NAG	E	401	14/15	0.77	0.43	-	114,119,121,121	0
6	NAG	G	404	14/15	0.82	0.32	-	142,148,150,150	0
7	NAG	E	414	14/15	0.87	0.38	-	126,131,132,132	0
7	NAG	C	412	14/15	0.88	0.32	-	97,101,102,103	0
5	BMA	I	416	11/12	0.55	0.40	-	207,209,212,215	0
5	BMA	K	407	11/12	0.83	0.39	-	185,188,195,197	0
5	BMA	C	418	11/12	0.78	0.42	-	224,225,227,229	0
5	NAG	I	410	14/15	0.75	0.44	-	173,177,178,178	0
5	BMA	G	414	11/12	0.13	0.56	-	212,213,216,220	0
6	NAG	I	406	14/15	0.71	0.42	-	151,163,169,174	0
7	MAN	C	414	11/12	0.81	0.27	-	208,212,213,215	0
9	MAN	E	412	11/12	0.93	0.31	-	162,166,168,170	0
5	NAG	E	407	14/15	0.93	0.25	-	190,196,198,199	0
7	MAN	E	416	11/12	0.89	0.30	-	140,143,144,146	0
5	NAG	C	421	14/15	0.67	0.92	-	179,182,185,185	0
7	BMA	A	410	11/12	0.64	0.29	-	207,210,212,212	0
6	NAG	G	402	14/15	0.43	0.54	-	136,144,148,148	0
9	MAN	C	410	11/12	0.94	0.30	-	149,152,153,155	0
6	NAG	A	414	14/15	0.50	0.48	-	215,217,219,219	0
7	MAN	A	411	11/12	0.91	0.24	-	161,165,167,168	0
6	NAG	G	407	14/15	0.70	0.52	-	144,150,152,153	0
7	BMA	C	413	11/12	0.74	0.22	-	131,134,135,135	0
9	NAG	E	409	14/15	0.88	0.28	-	95,99,100,100	0
5	NAG	K	411	14/15	0.73	0.34	-	272,275,277,277	0
7	MAN	E	404	11/12	0.65	0.37	-	188,190,191,195	0
5	BMA	G	410	11/12	0.81	0.48	-	216,220,222,223	0
5	BMA	E	423	11/12	0.19	0.49	-	229,233,234,237	0
6	NAG	A	406	14/15	0.86	0.26	-	91,93,96,96	0
9	NAG	C	407	14/15	0.86	0.27	-	84,86,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	408	14/15	0.81	0.35	-	124,133,133,137	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	NAG	H	201	14/15	0.69	0.36	0.67	140,145,148,150	0
8	NAG	I	413	14/15	0.93	0.42	-	129,140,147,147	0
8	NAG	G	411	14/15	0.93	0.25	-	167,178,182,183	0
8	NAG	D	201	14/15	0.79	0.42	-	121,124,126,127	0
8	NAG	K	413	14/15	0.93	0.45	-	162,171,175,176	0
8	NAG	F	201	14/15	0.76	0.46	-	156,160,162,162	0
8	NAG	B	201	14/15	0.82	0.43	-	99,102,104,105	0
8	NAG	L	201	14/15	0.78	0.47	-	131,137,145,146	0
8	NAG	C	419	14/15	0.94	0.30	-	143,150,153,155	0
8	NAG	G	403	14/15	0.55	0.37	-	116,120,127,130	0
8	NAG	J	201	14/15	0.80	0.39	-	137,145,154,155	0
8	NAG	E	420	14/15	0.88	0.34	-	130,136,140,141	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.