



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 9, 2021 – 02:09 PM EST

PDB ID : 7L0N  
Title : Circulating SARS-CoV-2 spike N439K variants maintain fitness while evading antibody-mediated immunity  
Authors : Snell, G.; Czudnochowski, N.; Dillen, J.; Nix, J.C.; Croll, T.I.; Corti, D.  
Deposited on : 2020-12-11  
Resolution : 2.78 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17

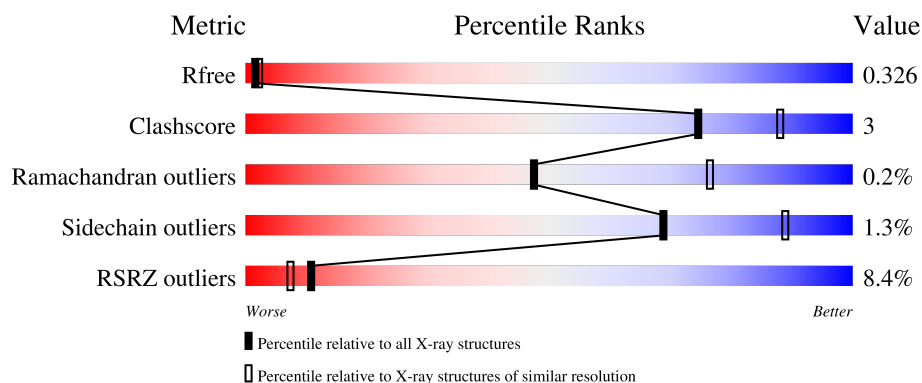
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	B	214	<div> <div>4%</div> <div>90%</div> <div>9%</div> </div>
1	D	214	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>
2	A	230	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	C	230	<div> <div>7%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
3	L	215	<div> <div>9%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	N	215	
4	H	223	
4	M	223	
5	E	597	
5	F	597	
6	R	204	
6	S	204	
7	G	6	
8	I	5	

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
15	NAG	E	702	-	-	-	X
7	MAN	G	5	X	-	-	-
8	MAN	I	4	-	-	-	X
9	CL	N	702	-	-	-	X

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 26468 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 Monoclonal antibody S309 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			
1	D	213	Total	C	N	O	S	0	0	0
			1624	1011	277	332	4			

- Molecule 2 is a protein called Monoclonal antibody S309 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	222	Total	C	N	O	S	0	0	0
			1674	1058	282	327	7			
2	C	224	Total	C	N	O	S	0	0	0
			1692	1069	286	330	7			

- Molecule 3 is a protein called Monoclonal antibody S304 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1627	1021	271	330	5			
3	N	213	Total	C	N	O	S	0	0	0
			1627	1021	271	330	5			

- Molecule 4 is a protein called Monoclonal antibody S304 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	212	Total	C	N	O	S	0	0	0
			1600	1016	263	315	6			
4	M	215	Total	C	N	O	S	0	0	0
			1619	1026	266	321	6			

- Molecule 5 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	579	Total	C	N	O	S	0	0	0
			4733	3031	784	891	27			
5	F	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			

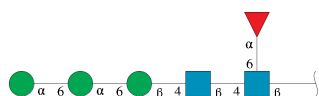
- Molecule 6 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	203	Total	C	N	O	S	0	0	0
			1609	1034	268	299	8			
6	S	201	Total	C	N	O	S	0	0	0
			1598	1027	268	295	8			

There are 2 discrepancies between the modelled and reference sequences:

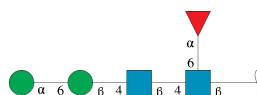
Chain	Residue	Modelled	Actual	Comment	Reference
R	439	LYS	ASN	variant	UNP P0DTC2
S	439	LYS	ASN	variant	UNP P0DTC2

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Cl 1	0	0
9	A	1	Total 1	Cl 1	0	0
9	D	1	Total 1	Cl 1	0	0
9	C	2	Total 2	Cl 2	0	0
9	H	3	Total 3	Cl 3	0	0
9	N	2	Total 2	Cl 2	0	0
9	M	5	Total 5	Cl 5	0	0
9	E	1	Total 1	Cl 1	0	0
9	F	6	Total 6	Cl 6	0	0
9	R	2	Total 2	Cl 2	0	0
9	S	3	Total 3	Cl 3	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

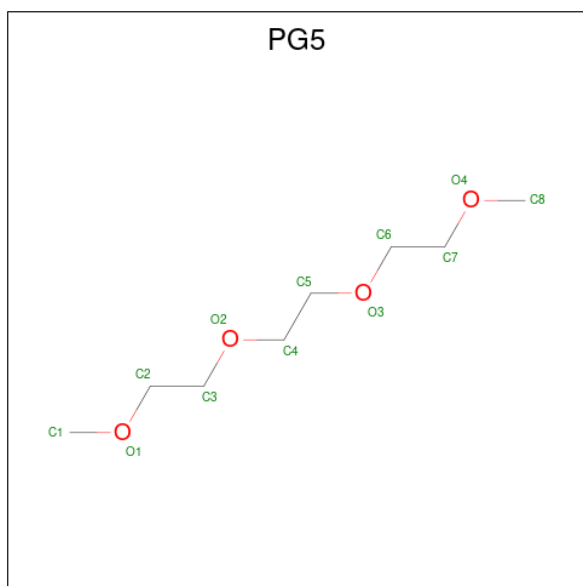


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	L	1	Total	O	S	0	0
			5	4	1		
10	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

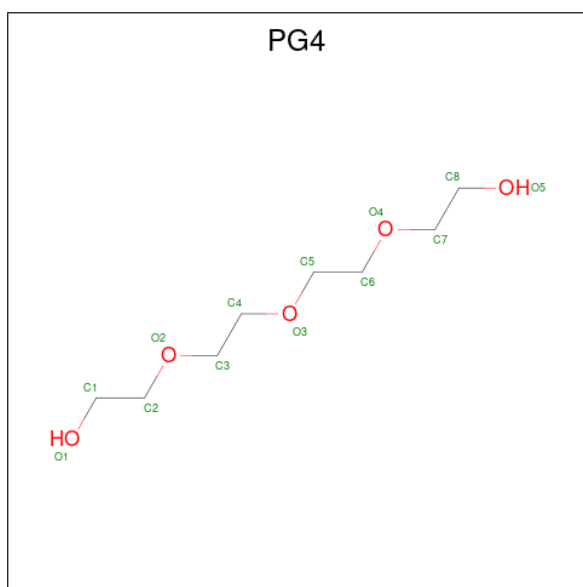
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	3	Total	Na	0	0
			3	3		
11	F	2	Total	Na	0	0
			2	2		
11	R	1	Total	Na	0	0
			1	1		

- Molecule 12 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	H	1	Total	C	O	0	0
			12	8	4		

- Molecule 13 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	N	1	Total	C	O	0	0
			13	8	5		

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	E	1	Total	Zn	0	0
			1	1		
14	F	1	Total	Zn	0	0
			1	1		

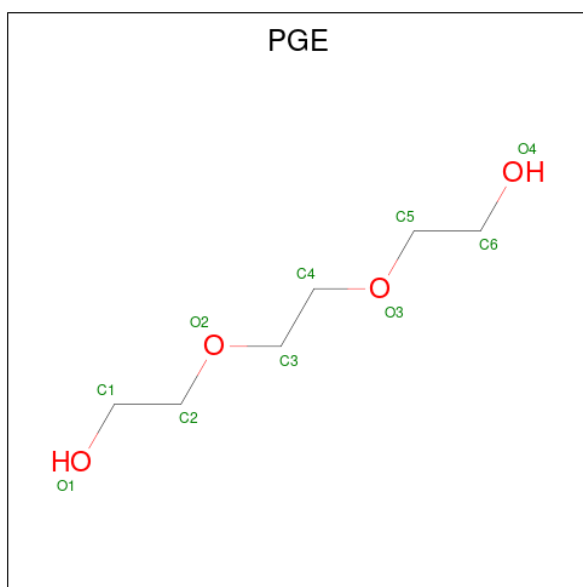
- Molecule 15 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).





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

- Molecule 16 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	C	O	0	0
			10	6	4		
16	S	1	Total	C	O	0	0
			10	6	4		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	B	32	Total	O	0	0
			32	32		
17	A	8	Total	O	0	0
			8	8		
17	D	19	Total	O	0	0
			19	19		
17	C	8	Total	O	0	0
			8	8		
17	L	22	Total	O	0	0
			22	22		
17	H	12	Total	O	0	0
			12	12		
17	N	11	Total	O	0	0
			11	11		
17	M	15	Total	O	0	0
			15	15		
17	E	15	Total	O	0	0
			15	15		
17	F	37	Total	O	0	0
			37	37		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	R	24	Total 24	O 24	0	0
17	S	29	Total 29	O 29	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

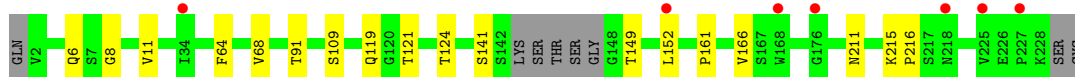
- Molecule 1: Monoclonal antibody S309 Fab light chain



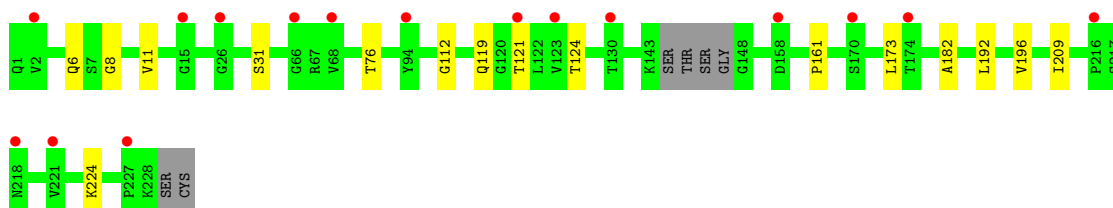
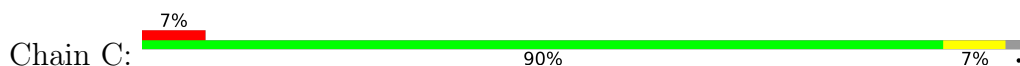
- Molecule 1: Monoclonal antibody S309 Fab light chain



- Molecule 2: Monoclonal antibody S309 Fab heavy chain

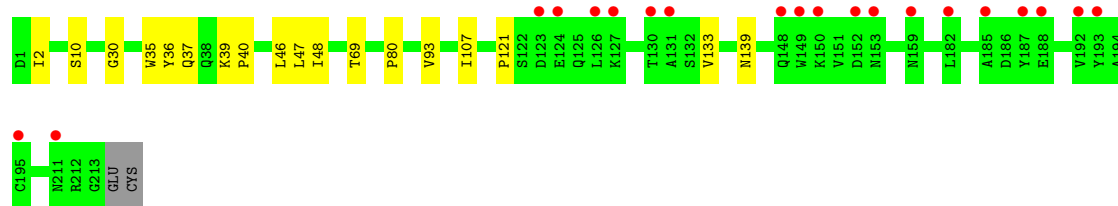


- Molecule 2: Monoclonal antibody S309 Fab heavy chain

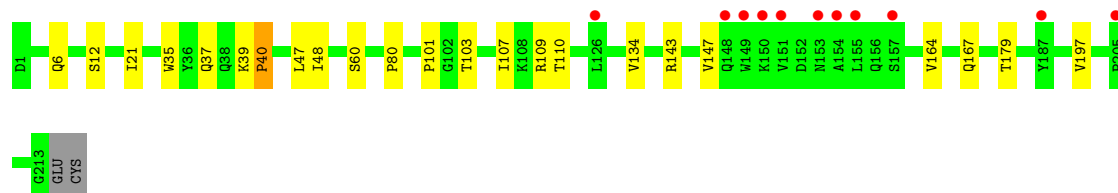
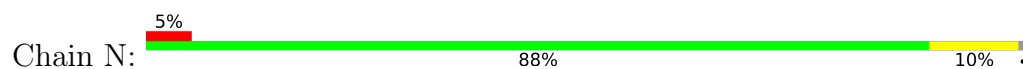


- Molecule 3: Monoclonal antibody S304 Fab light chain

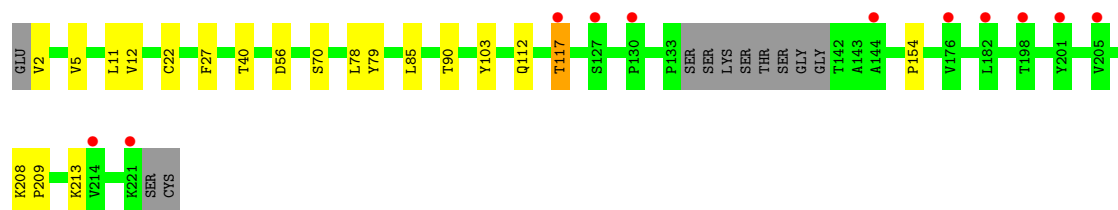
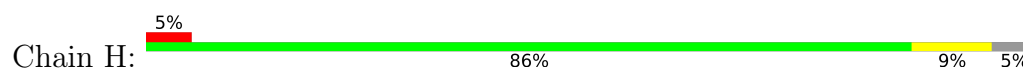




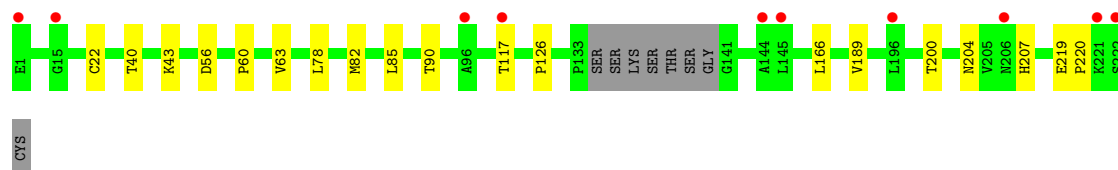
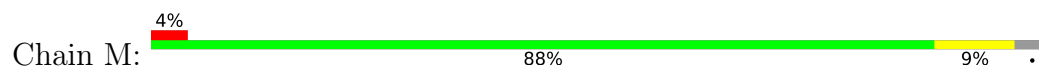
• Molecule 3: Monoclonal antibody S304 Fab light chain



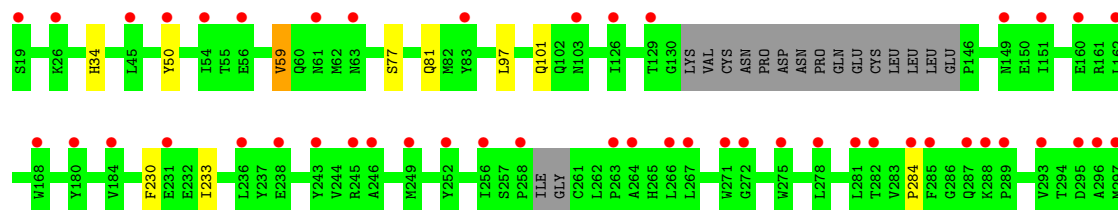
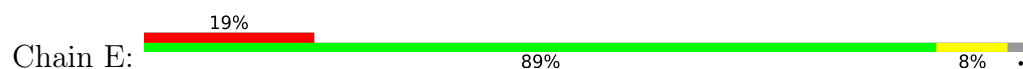
• Molecule 4: Monoclonal antibody S304 Fab heavy chain

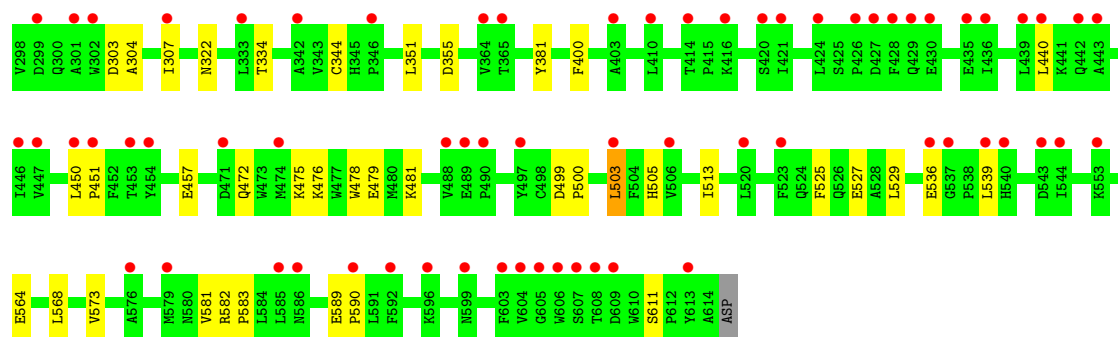


• Molecule 4: Monoclonal antibody S304 Fab heavy chain

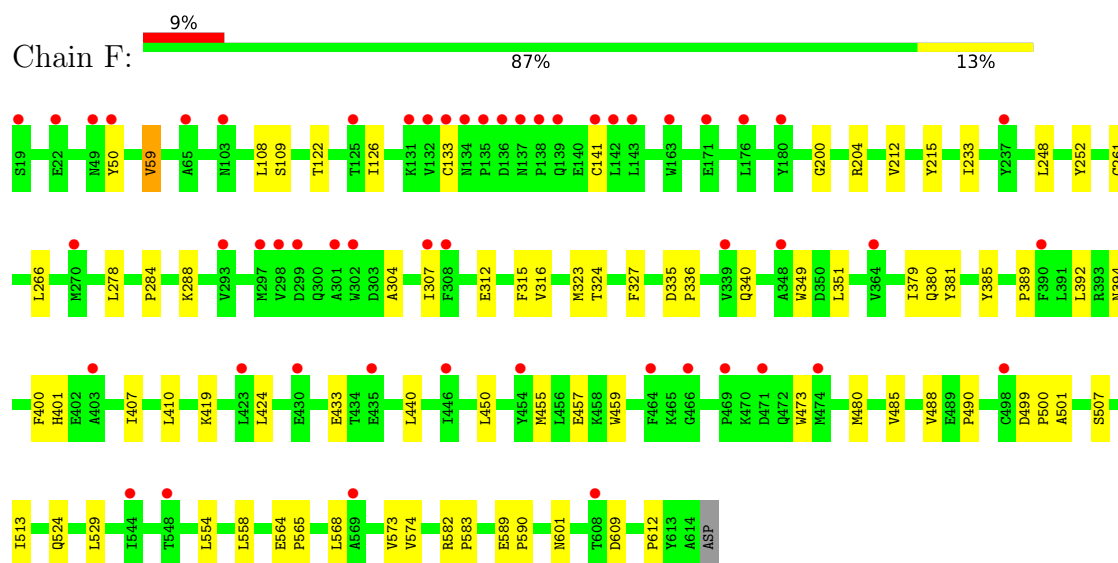


• Molecule 5: Angiotensin-converting enzyme 2

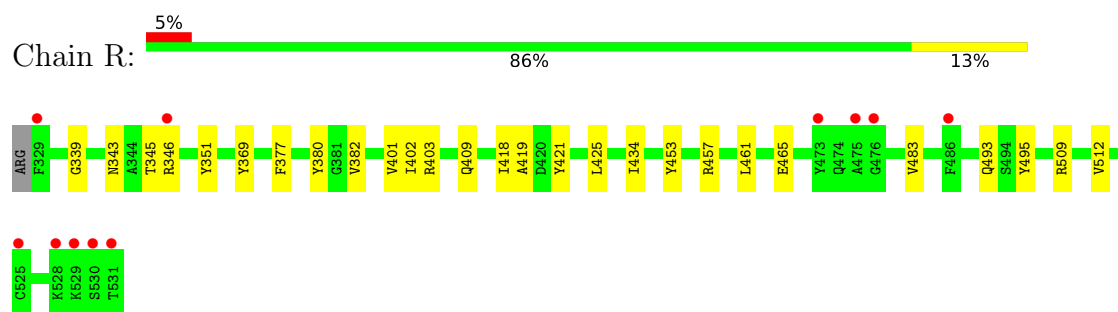




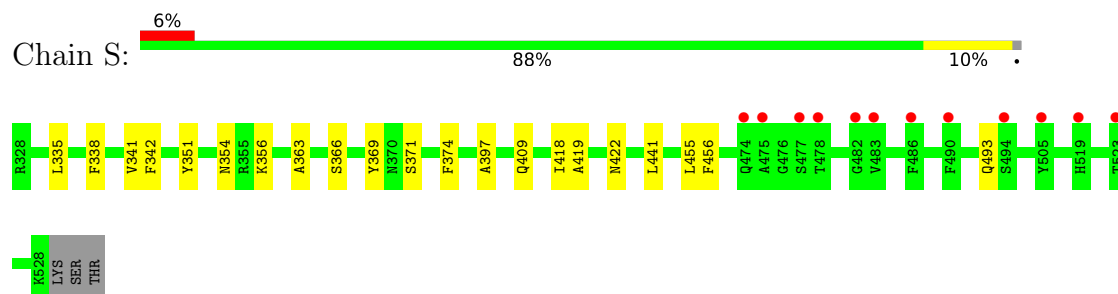
• Molecule 5: Angiotensin-converting enzyme 2



• Molecule 6: Spike protein S1

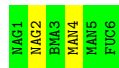


• Molecule 6: Spike protein S1




- Molecule 7:  $\alpha$ -D-mannopyranose-(1-6)- $\alpha$ -D-mannopyranose-(1-6)- $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-[ $\alpha$ -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain G:  67% 33%



- Molecule 8:  $\alpha$ -D-mannopyranose-(1-6)- $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-[ $\alpha$ -L-fucopyranose-(1-6)]2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain I:  80% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.98Å 186.58Å 194.52Å 90.00° 96.40° 90.00°	Depositor
Resolution (Å)	48.90 – 2.78 48.90 – 2.78	Depositor EDS
% Data completeness (in resolution range)	92.9 (48.90-2.78) 92.9 (48.90-2.78)	Depositor EDS
$R_{merge}$	0.51	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.290 , 0.325 0.291 , 0.326	Depositor DCC
$R_{free}$ test set	6375 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	26468	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.40 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7733e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, BMA, FUC, PG5, PGE, CL, NA, SO4, NAG, MAN, PG4

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	B	0.27	0/1657	0.52	0/2250
1	D	0.27	0/1657	0.51	0/2250
2	A	0.28	0/1716	0.52	0/2338
2	C	0.28	0/1734	0.54	0/2361
3	L	0.27	0/1663	0.52	0/2260
3	N	0.27	0/1663	0.53	0/2260
4	H	0.28	0/1641	0.52	0/2236
4	M	0.28	0/1660	0.51	0/2261
5	E	0.24	0/4866	0.47	0/6606
5	F	0.24	0/4999	0.48	0/6792
6	R	0.26	0/1655	0.51	0/2251
6	S	0.25	0/1644	0.51	0/2236
All	All	0.26	0/26555	0.50	0/36101

There are no bond length outliers.

There are no bond angle outliers.

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	B	1624	0	1582	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1624	0	1582	9	0
2	A	1674	0	1628	12	0
2	C	1692	0	1652	11	0
3	L	1627	0	1587	9	0
3	N	1627	0	1587	15	0
4	H	1600	0	1545	10	0
4	M	1619	0	1562	9	0
5	E	4733	0	4507	22	0
5	F	4862	0	4634	39	0
6	R	1609	0	1537	19	0
6	S	1598	0	1525	12	0
7	G	71	0	61	1	0
8	I	60	0	52	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	2	0	0	0	0
9	D	1	0	0	0	0
9	E	1	0	0	0	0
9	F	6	0	0	0	0
9	H	3	0	0	0	0
9	M	5	0	0	0	0
9	N	2	0	0	0	0
9	R	2	0	0	0	0
9	S	3	0	0	0	0
10	L	5	0	0	0	0
10	N	5	0	0	0	0
11	F	2	0	0	0	0
11	H	3	0	0	0	0
11	R	1	0	0	0	0
12	H	12	0	18	0	0
13	N	13	0	18	1	0
14	E	1	0	0	0	0
14	F	1	0	0	0	0
15	E	56	0	52	0	0
15	F	70	0	65	0	0
16	E	10	0	14	0	0
16	S	10	0	14	0	0
17	A	8	0	0	0	0
17	B	32	0	0	0	0
17	C	8	0	0	0	0
17	D	19	0	0	0	0
17	E	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	37	0	0	0	0
17	H	12	0	0	0	0
17	L	22	0	0	0	0
17	M	15	0	0	0	0
17	N	11	0	0	0	0
17	R	24	0	0	0	0
17	S	29	0	0	0	0
All	All	26468	0	25222	166	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 3.

The worst 5 of 166 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)
4:M:219:GLU:HG2	4:M:220:PRO:HD2	1.67	0.75
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.66	0.74
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.71	0.72
6:R:409:GLN:HB3	6:R:419:ALA:HB2	1.75	0.68
2:A:6:GLN:HB3	2:A:121:THR:HG23	1.77	0.65

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	B	211/214 (99%)	192 (91%)	17 (8%)	2 (1%)	17	44
1	D	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
2	A	218/230 (95%)	206 (94%)	11 (5%)	1 (0%)	29	58
2	C	220/230 (96%)	210 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	211/215 (98%)	197 (93%)	12 (6%)	2 (1%)	17	44
3	N	211/215 (98%)	198 (94%)	12 (6%)	1 (0%)	29	58
4	H	208/223 (93%)	196 (94%)	12 (6%)	0	100	100
4	M	211/223 (95%)	198 (94%)	13 (6%)	0	100	100
5	E	573/597 (96%)	547 (96%)	26 (4%)	0	100	100
5	F	594/597 (100%)	571 (96%)	23 (4%)	0	100	100
6	R	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
6	S	199/204 (98%)	187 (94%)	12 (6%)	0	100	100
All	All	3268/3366 (97%)	3095 (95%)	167 (5%)	6 (0%)	47	76

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ASP
3	L	30	GLY
1	B	138	ASN
2	A	141	SER
3	L	139	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	B	184/185 (100%)	182 (99%)	2 (1%)	73	90
1	D	184/185 (100%)	183 (100%)	1 (0%)	88	95
2	A	185/192 (96%)	183 (99%)	2 (1%)	73	90
2	C	187/192 (97%)	186 (100%)	1 (0%)	88	95
3	L	186/188 (99%)	185 (100%)	1 (0%)	88	95
3	N	186/188 (99%)	186 (100%)	0	100	100
4	H	177/186 (95%)	174 (98%)	3 (2%)	60	85
4	M	179/186 (96%)	177 (99%)	2 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	510/527 (97%)	499 (98%)	11 (2%)	52	80
5	F	526/527 (100%)	516 (98%)	10 (2%)	57	83
6	R	176/177 (99%)	174 (99%)	2 (1%)	73	90
6	S	174/177 (98%)	172 (99%)	2 (1%)	73	90
All	All	2854/2910 (98%)	2817 (99%)	37 (1%)	69	89

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	400	PHE
6	S	351	TYR
5	F	401	HIS
5	F	609	ASP
5	E	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	599	ASN
5	F	42	GLN
6	S	354	ASN
5	F	522	GLN
3	N	167	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 ⓘ

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	NAG	G	1	7,6	14,14,15	0.38	0	17,19,21	0.67	0
7	NAG	G	2	7	14,14,15	0.34	0	17,19,21	0.64	0
7	BMA	G	3	7	11,11,12	0.42	0	15,15,17	0.92	0
7	MAN	G	4	7	11,11,12	0.40	0	15,15,17	0.69	0
7	MAN	G	5	7	11,11,12	0.40	0	15,15,17	0.80	0
7	FUC	G	6	7	10,10,11	0.45	0	14,14,16	0.75	0
8	NAG	I	1	8,6	14,14,15	0.36	0	17,19,21	0.54	0
8	NAG	I	2	8	14,14,15	0.38	0	17,19,21	0.77	0
8	BMA	I	3	8	11,11,12	0.42	0	15,15,17	0.70	0
8	MAN	I	4	8	11,11,12	0.45	0	15,15,17	0.90	0
8	FUC	I	5	8	10,10,11	0.39	0	14,14,16	0.51	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
7	NAG	G	1	7,6	-	0/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	BMA	G	3	7	-	0/2/19/22	0/1/1/1
7	MAN	G	4	7	-	2/2/19/22	0/1/1/1
7	MAN	G	5	7	1/1/4/5	0/2/19/22	0/1/1/1
7	FUC	G	6	7	-	-	0/1/1/1
8	NAG	I	1	8,6	-	0/6/23/26	0/1/1/1
8	NAG	I	2	8	-	4/6/23/26	0/1/1/1
8	BMA	I	3	8	-	2/2/19/22	0/1/1/1
8	MAN	I	4	8	-	2/2/19/22	0/1/1/1
8	FUC	I	5	8	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	G	5	MAN	C1

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	2	NAG	O7-C7-N2-C2
8	I	2	NAG	C8-C7-N2-C2
7	G	4	MAN	O5-C5-C6-O6
8	I	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	NAG	1	0
7	G	2	NAG	1	0
7	G	4	MAN	1	0

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 35 are monoatomic - leaving 15 for Mogul analysis.

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	$\# Z  > 2$
16	PGE	E	706	-	9,9,9	0.15	0	8,8,8	0.10	0
16	PGE	S	602	-	9,9,9	0.17	0	8,8,8	0.11	0
10	SO4	L	700	-	4,4,4	0.39	0	6,6,6	0.05	0
15	NAG	F	705	5	14,14,15	0.34	0	17,19,21	0.87	1 (5%)
15	NAG	E	703	5	14,14,15	0.37	0	17,19,21	0.90	1 (5%)
10	SO4	N	700	-	4,4,4	0.39	0	6,6,6	0.05	0
15	NAG	E	704	5	14,14,15	0.47	0	17,19,21	1.02	1 (5%)
15	NAG	F	702	5	14,14,15	0.36	0	17,19,21	0.74	0
15	NAG	F	704	5	14,14,15	0.38	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	NAG	E	702	5	14,14,15	0.43	0	17,19,21	0.92	1 (5%)
15	NAG	E	705	5	14,14,15	0.41	0	17,19,21	1.30	1 (5%)
12	PG5	H	702	-	11,11,11	0.19	0	10,10,10	0.10	0
15	NAG	F	703	5	14,14,15	0.36	0	17,19,21	0.70	0
13	PG4	N	703	-	12,12,12	0.18	0	11,11,11	0.08	0
15	NAG	F	706	5	14,14,15	0.33	0	17,19,21	0.83	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
16	PGE	E	706	-	-	2/7/7/7	-
16	PGE	S	602	-	-	5/7/7/7	-
15	NAG	F	705	5	-	2/6/23/26	0/1/1/1
15	NAG	E	703	5	-	2/6/23/26	0/1/1/1
15	NAG	E	704	5	-	4/6/23/26	0/1/1/1
15	NAG	F	702	5	-	2/6/23/26	0/1/1/1
15	NAG	F	704	5	-	0/6/23/26	0/1/1/1
15	NAG	E	702	5	-	3/6/23/26	0/1/1/1
15	NAG	E	705	5	-	2/6/23/26	0/1/1/1
12	PG5	H	702	-	-	6/9/9/9	-
15	NAG	F	703	5	-	2/6/23/26	0/1/1/1
13	PG4	N	703	-	-	5/10/10/10	-
15	NAG	F	706	5	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	705	NAG	C1-O5-C5	4.58	118.40	112.19
15	F	705	NAG	C1-O5-C5	2.74	115.90	112.19
15	E	704	NAG	C4-C3-C2	2.71	115.00	111.02
15	E	702	NAG	C4-C3-C2	2.59	114.81	111.02
15	E	703	NAG	C4-C3-C2	2.40	114.54	111.02

There are no chirality outliers.



5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	702	NAG	C8-C7-N2-C2
15	E	702	NAG	O7-C7-N2-C2
15	E	703	NAG	C8-C7-N2-C2
15	E	703	NAG	O7-C7-N2-C2
15	E	704	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	N	703	PG4	1	0

## 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, 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	B	213/214 (99%)	0.52	9 (4%)	36 30	58, 74, 97, 109	0
1	D	213/214 (99%)	0.49	3 (1%)	75 73	55, 73, 92, 106	0
2	A	222/230 (96%)	0.56	7 (3%)	47 42	61, 78, 96, 114	0
2	C	224/230 (97%)	0.76	16 (7%)	16 11	61, 85, 101, 106	0
3	L	213/215 (99%)	0.79	20 (9%)	8 6	49, 68, 122, 133	0
3	N	213/215 (99%)	0.54	11 (5%)	27 22	45, 66, 108, 126	0
4	H	212/223 (95%)	0.65	11 (5%)	27 22	47, 83, 105, 126	0
4	M	215/223 (96%)	0.61	10 (4%)	31 25	45, 72, 94, 128	0
5	E	579/597 (96%)	1.15	114 (19%)	1 0	64, 116, 162, 189	0
5	F	596/597 (99%)	0.77	53 (8%)	9 6	55, 84, 111, 149	0
6	R	203/204 (99%)	0.72	11 (5%)	25 20	50, 73, 101, 125	0
6	S	201/204 (98%)	0.74	12 (5%)	21 16	47, 71, 99, 114	0
All	All	3304/3366 (98%)	0.75	277 (8%)	11 7	45, 80, 138, 189	0

The worst 5 of 277 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	266	LEU	9.5
5	F	135	PRO	8.6
5	F	430	GLU	7.4
5	F	136	ASP	7.2
1	B	63	PHE	7.1

### 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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
8	MAN	I	4	11/12	0.39	0.41	140,144,146,147	0
8	BMA	I	3	11/12	0.62	0.29	122,127,131,132	0
7	MAN	G	4	11/12	0.64	0.26	148,150,152,152	0
7	BMA	G	3	11/12	0.74	0.26	117,123,128,135	0
7	MAN	G	5	11/12	0.77	0.26	144,149,150,150	0
8	NAG	I	2	14/15	0.85	0.22	91,98,102,108	0
7	NAG	G	1	14/15	0.88	0.19	72,75,79,82	0
8	NAG	I	1	14/15	0.89	0.21	78,80,82,87	0
7	NAG	G	2	14/15	0.89	0.20	89,92,95,102	0
8	FUC	I	5	10/11	0.89	0.23	74,75,76,76	0
7	FUC	G	6	10/11	0.91	0.21	79,80,80,81	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
15	NAG	E	702	14/15	0.61	0.44	133,140,143,145	0
12	PG5	H	702	12/12	0.68	0.40	116,120,122,122	0
9	CL	M	303	1/1	0.68	0.13	113,113,113,113	0
16	PGE	S	602	10/10	0.71	0.28	97,103,109,110	0
11	NA	F	711	1/1	0.73	0.14	84,84,84,84	0
15	NAG	E	704	14/15	0.73	0.27	121,127,130,131	0
9	CL	N	702	1/1	0.73	0.54	114,114,114,114	0
13	PG4	N	703	13/13	0.79	0.26	84,94,96,96	0
15	NAG	F	706	14/15	0.80	0.16	135,137,137,138	0
15	NAG	F	704	14/15	0.83	0.19	94,97,99,100	0
9	CL	H	707	1/1	0.83	0.22	113,113,113,113	0
16	PGE	E	706	10/10	0.83	0.31	91,96,98,98	0
15	NAG	F	702	14/15	0.83	0.44	100,102,106,107	0
15	NAG	F	705	14/15	0.84	0.23	99,101,102,103	0
9	CL	C	701	1/1	0.84	0.12	105,105,105,105	0
9	CL	F	713	1/1	0.85	0.20	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	NAG	E	703	14/15	0.86	0.20	97,98,99,100	0
15	NAG	E	705	14/15	0.86	0.23	99,102,105,105	0
15	NAG	F	703	14/15	0.87	0.21	85,86,88,89	0
9	CL	A	301	1/1	0.87	0.18	98,98,98,98	0
9	CL	M	302	1/1	0.87	0.17	88,88,88,88	0
10	SO4	L	700	5/5	0.88	0.26	158,158,159,159	0
9	CL	F	709	1/1	0.88	0.26	101,101,101,101	0
9	CL	M	305	1/1	0.88	0.21	97,97,97,97	0
9	CL	R	602	1/1	0.89	0.26	105,105,105,105	0
11	NA	H	704	1/1	0.89	0.14	56,56,56,56	0
10	SO4	N	700	5/5	0.90	0.21	139,139,139,139	0
9	CL	S	604	1/1	0.90	0.29	103,103,103,103	0
9	CL	M	304	1/1	0.92	0.33	95,95,95,95	0
9	CL	N	701	1/1	0.93	0.15	75,75,75,75	0
9	CL	F	710	1/1	0.94	0.07	66,66,66,66	0
9	CL	F	712	1/1	0.94	0.13	91,91,91,91	0
9	CL	H	706	1/1	0.95	0.13	82,82,82,82	0
11	NA	H	701	1/1	0.95	0.28	38,38,38,38	0
9	CL	S	603	1/1	0.95	0.34	88,88,88,88	0
9	CL	C	700	1/1	0.95	0.15	76,76,76,76	0
11	NA	R	603	1/1	0.95	0.08	50,50,50,50	0
9	CL	R	601	1/1	0.95	0.27	95,95,95,95	0
9	CL	D	700	1/1	0.96	0.20	92,92,92,92	0
9	CL	E	707	1/1	0.96	0.07	77,77,77,77	0
9	CL	B	700	1/1	0.96	0.06	83,83,83,83	0
9	CL	F	714	1/1	0.96	0.13	76,76,76,76	0
11	NA	H	705	1/1	0.96	0.13	52,52,52,52	0
14	ZN	F	701	1/1	0.97	0.17	77,77,77,77	0
9	CL	M	301	1/1	0.97	0.11	67,67,67,67	0
9	CL	S	601	1/1	0.97	0.31	94,94,94,94	0
9	CL	F	707	1/1	0.97	0.18	64,64,64,64	0
11	NA	F	708	1/1	0.97	0.18	90,90,90,90	0
14	ZN	E	701	1/1	0.97	0.12	95,95,95,95	0
9	CL	H	703	1/1	0.98	0.13	81,81,81,81	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.