wwPDB X-ray Structure Validation Summary Report (i)

May 5, 2025 – 03:28 PM JST

PDB ID	:	8Z9L / pdb_00008z9l
Title	:	Crystal structure of SARS-CoV-2 RBD bound to Rhinolophus affinis ACE2
Authors	:	Lan, J.; Wang, C.H.
Deposited on	:	2024-04-23
Resolution	:	3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

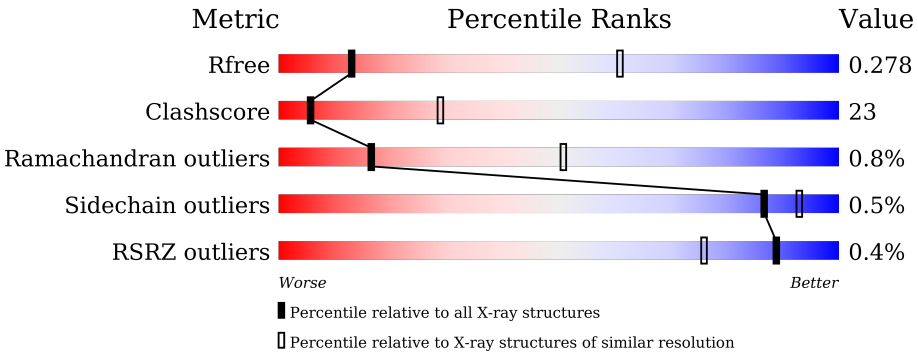
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	164625	1563 (3.70-3.50)
Clashscore	180529	1665 (3.70-3.50)
Ramachandran outliers	177936	1641 (3.70-3.50)
Sidechain outliers	177891	1640 (3.70-3.50)
RSRZ outliers	164620	1562 (3.70-3.50)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	598	68% 32%
1	I	598	59% 40%
1	O	598	% 58% 40%
1	U	598	59% 40%
2	F	197	% 59% 38%
2	L	197	% 58% 41%

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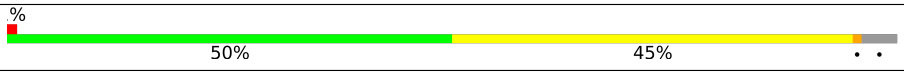
Mol	Chain	Length	Quality of chain
2	R	197	
2	X	197	
3	A	2	
3	C	2	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 25939 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 Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	598	Total	C	N	O	S	0	0	0
			4900	3131	818	921	30			
1	I	598	Total	C	N	O	S	0	0	0
			4900	3131	818	921	30			
1	O	598	Total	C	N	O	S	0	0	0
			4900	3131	818	921	30			
1	U	598	Total	C	N	O	S	0	0	0
			4900	3131	818	921	30			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	PRO	-	expression tag	UNP A0A7D7JS29
B	34	HIS	ARG	conflict	UNP A0A7D7JS29
B	38	ASP	GLU	conflict	UNP A0A7D7JS29
B	185	ALA	VAL	conflict	UNP A0A7D7JS29
B	300	GLN	HIS	conflict	UNP A0A7D7JS29
B	598	LYS	GLN	conflict	UNP A0A7D7JS29
B	614	ALA	SER	conflict	UNP A0A7D7JS29
I	18	PRO	-	expression tag	UNP A0A7D7JS29
I	34	HIS	ARG	conflict	UNP A0A7D7JS29
I	38	ASP	GLU	conflict	UNP A0A7D7JS29
I	185	ALA	VAL	conflict	UNP A0A7D7JS29
I	300	GLN	HIS	conflict	UNP A0A7D7JS29
I	598	LYS	GLN	conflict	UNP A0A7D7JS29
I	614	ALA	SER	conflict	UNP A0A7D7JS29
O	18	PRO	-	expression tag	UNP A0A7D7JS29
O	34	HIS	ARG	conflict	UNP A0A7D7JS29
O	38	ASP	GLU	conflict	UNP A0A7D7JS29
O	185	ALA	VAL	conflict	UNP A0A7D7JS29
O	300	GLN	HIS	conflict	UNP A0A7D7JS29
O	598	LYS	GLN	conflict	UNP A0A7D7JS29
O	614	ALA	SER	conflict	UNP A0A7D7JS29

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Chain	Residue	Modelled	Actual	Comment	Reference
U	18	PRO	-	expression tag	UNP A0A7D7JS29
U	34	HIS	ARG	conflict	UNP A0A7D7JS29
U	38	ASP	GLU	conflict	UNP A0A7D7JS29
U	185	ALA	VAL	conflict	UNP A0A7D7JS29
U	300	GLN	HIS	conflict	UNP A0A7D7JS29
U	598	LYS	GLN	conflict	UNP A0A7D7JS29
U	614	ALA	SER	conflict	UNP A0A7D7JS29

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	194	Total	C	N	O	S	0	0	0
			1539	987	256	288	8			
2	L	196	Total	C	N	O	S	0	0	0
			1553	995	260	290	8			
2	R	196	Total	C	N	O	S	0	0	0
			1553	995	260	290	8			
2	X	190	Total	C	N	O	S	0	0	0
			1509	968	251	282	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	332	PRO	-	expression tag	UNP P0DTC2
F	528	HIS	-	expression tag	UNP P0DTC2
L	332	PRO	-	expression tag	UNP P0DTC2
L	528	HIS	-	expression tag	UNP P0DTC2
R	332	PRO	-	expression tag	UNP P0DTC2
R	528	HIS	-	expression tag	UNP P0DTC2
X	332	PRO	-	expression tag	UNP P0DTC2
X	528	HIS	-	expression tag	UNP P0DTC2

- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	2	Total	C	N	O	0	0	0
			24	14	1	9			

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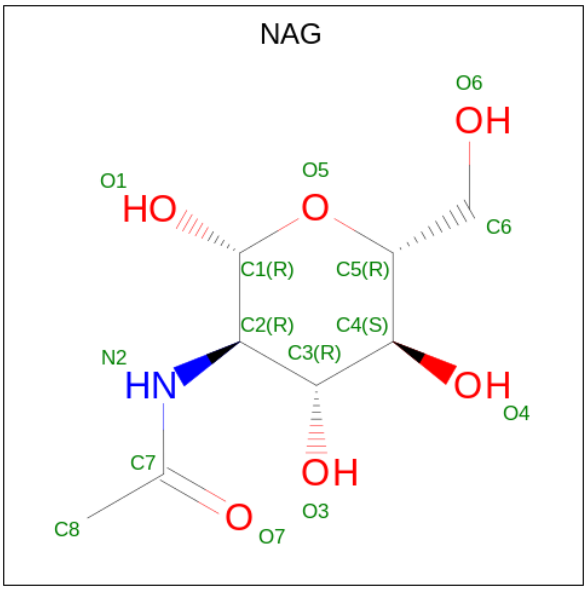
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	C	2	Total C N O 24 14 1 9	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



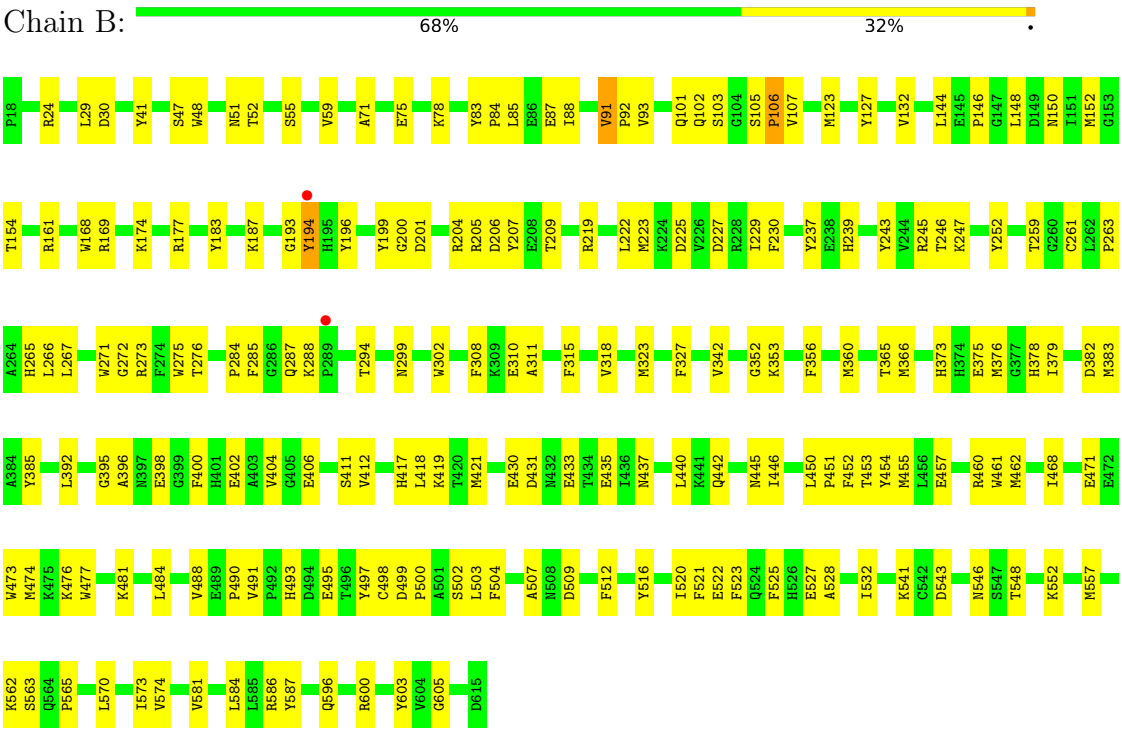
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 13 7 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 13 7 1 5	0	0
4	L	1	Total C N O 14 8 1 5	0	0
4	O	1	Total C N O 14 8 1 5	0	0
4	O	1	Total C N O 14 8 1 5	0	0
4	O	1	Total C N O 13 7 1 5	0	0
4	R	1	Total C N O 14 8 1 5	0	0
4	U	1	Total C N O 14 8 1 5	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.

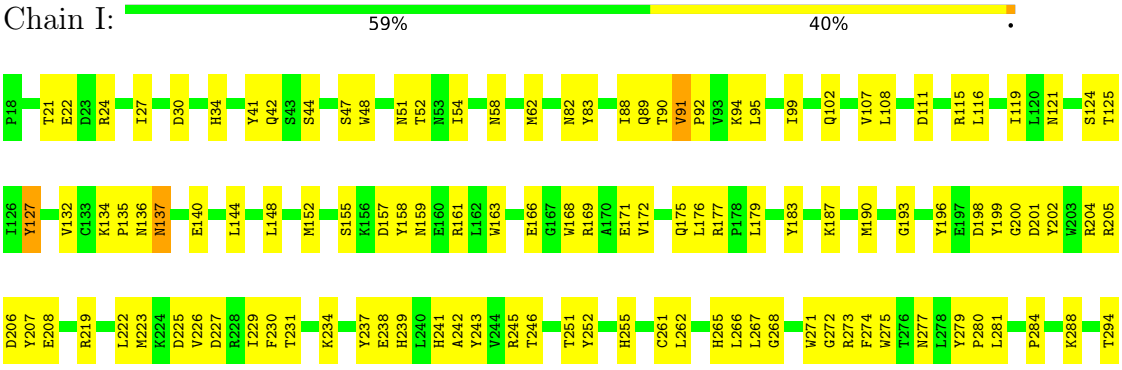
• Molecule 1: Angiotensin-converting enzyme

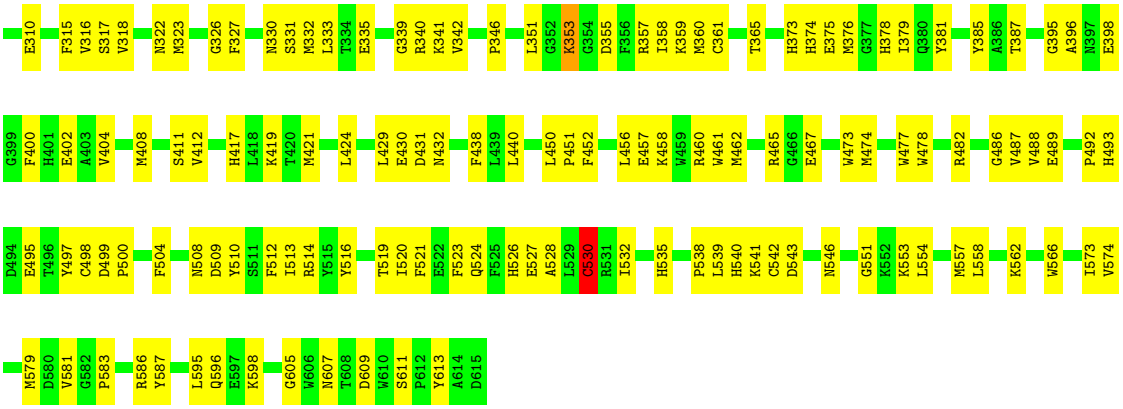
Chain B:



• Molecule 1: Angiotensin-converting enzyme

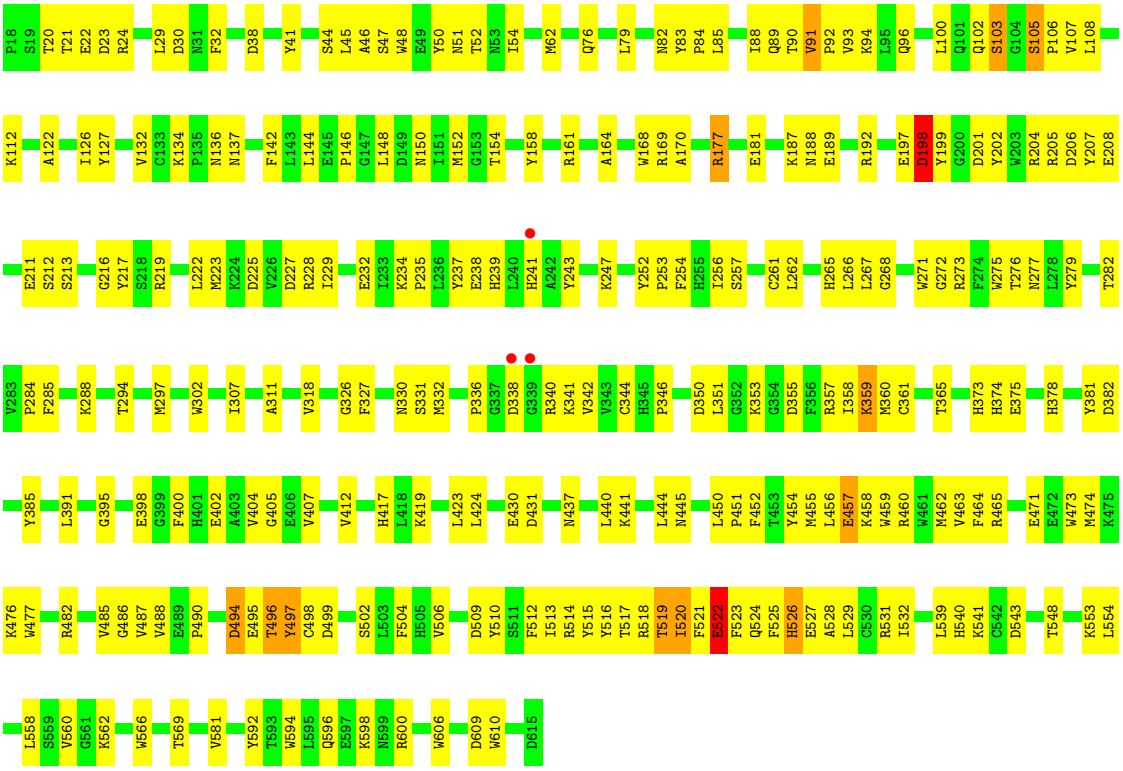
Chain I:





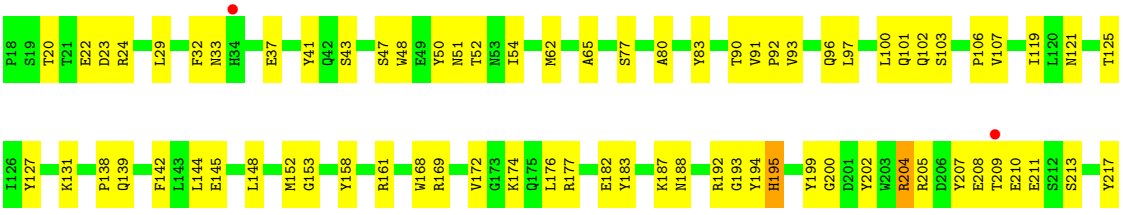
• Molecule 1: Angiotensin-converting enzyme

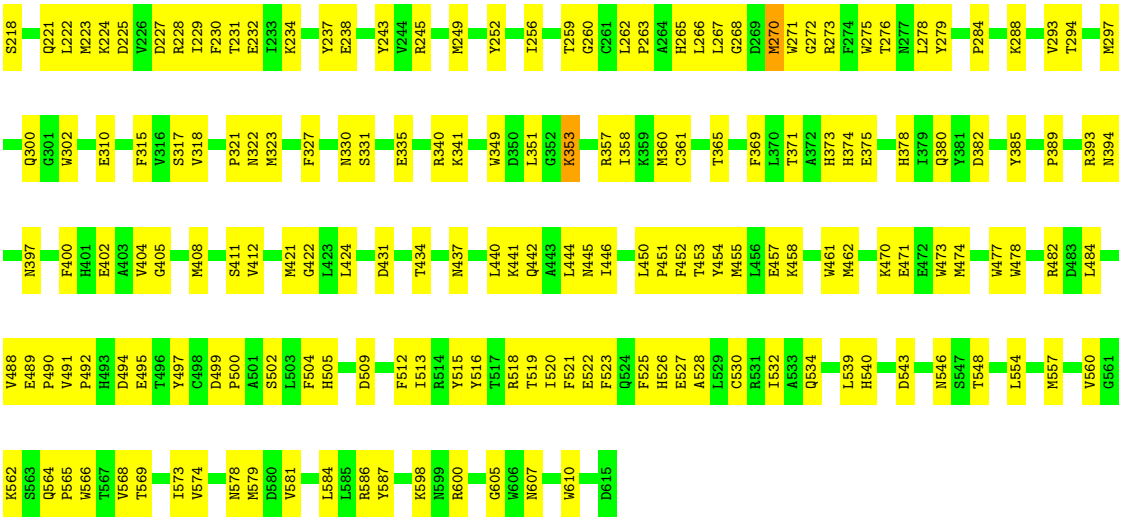
Chain O:



• Molecule 1: Angiotensin-converting enzyme

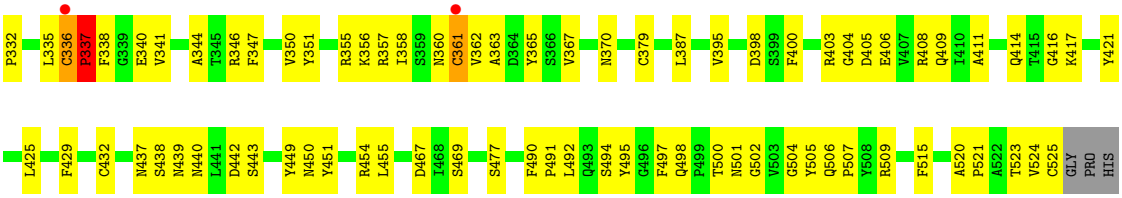
Chain U:





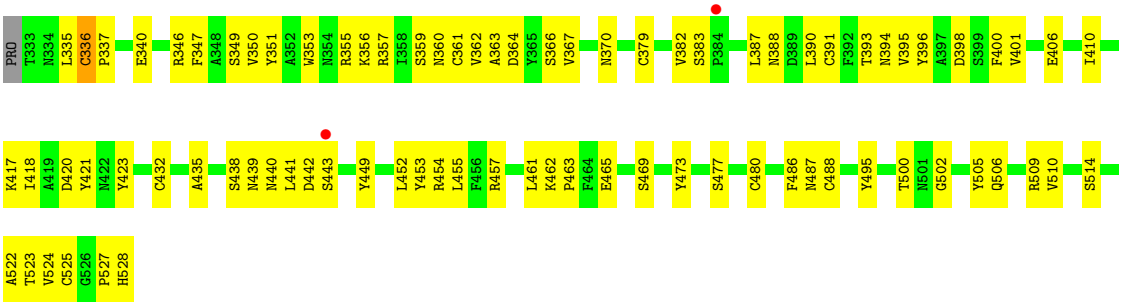
• Molecule 2: Spike protein S1

Chain F:



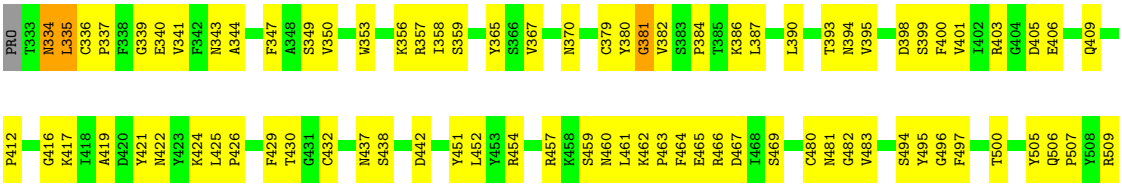
• Molecule 2: Spike protein S1

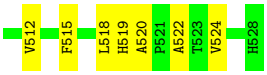
Chain L:



• Molecule 2: Spike protein S1

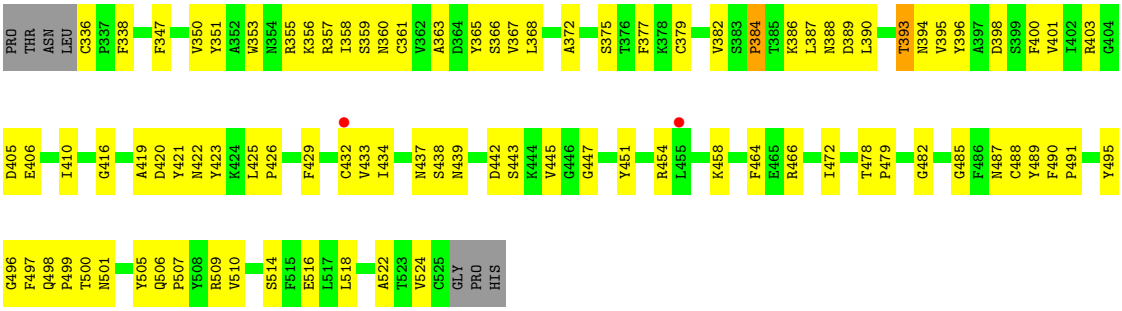
Chain R:





• Molecule 2: Spike protein S1

Chain X:

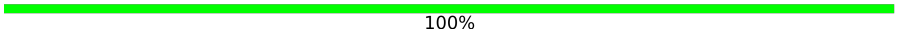


• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.74Å 129.48Å 563.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.01 – 3.60 38.01 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.01-3.60) 98.6 (38.01-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.56Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.242 , 0.277 0.244 , 0.278	Depositor DCC
R_{free} test set	2700 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25939	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.33	0/5043	0.63	1/6844 (0.0%)
1	I	0.34	2/5043 (0.0%)	0.65	2/6844 (0.0%)
1	O	0.44	3/5043 (0.1%)	0.75	12/6844 (0.2%)
1	U	0.37	3/5043 (0.1%)	0.70	6/6844 (0.1%)
2	F	0.33	0/1583	0.72	3/2155 (0.1%)
2	L	0.39	0/1598	0.70	1/2176 (0.0%)
2	R	0.32	0/1598	0.66	0/2176
2	X	0.31	0/1552	0.66	0/2112
All	All	0.36	8/26503 (0.0%)	0.68	25/35995 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	O	0	2
2	X	0	1
All	All	0	4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	177	ARG	CG-CD	6.56	1.72	1.52
1	O	177	ARG	CD-NE	6.31	1.55	1.46
1	U	204	ARG	CD-NE	-5.36	1.38	1.46
1	U	204	ARG	CB-CG	-5.28	1.36	1.52
1	O	177	ARG	NE-CZ	5.17	1.38	1.33

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	177	ARG	NE-CZ-NH2	12.00	130.00	119.20
1	U	204	ARG	NE-CZ-NH1	-10.56	110.94	121.50
1	U	204	ARG	CB-CG-CD	-8.64	91.44	111.30
1	O	177	ARG	CD-NE-CZ	8.42	136.19	124.40
1	O	177	ARG	NH1-CZ-NH2	-7.27	109.85	119.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	PRO	Peptide
1	O	338	ASP	Peptide
1	O	519	THR	Mainchain
2	X	393	THR	Peptide

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	4900	0	4684	171	1
1	I	4900	0	4685	236	1
1	O	4900	0	4682	248	2
1	U	4900	0	4682	231	3
2	F	1539	0	1458	66	2
2	L	1553	0	1468	69	2
2	R	1553	0	1468	75	0
2	X	1509	0	1428	88	1
3	A	24	0	20	2	0
3	C	24	0	22	0	0
4	B	27	0	25	5	0
4	I	27	0	22	3	0
4	L	14	0	13	0	0
4	O	41	0	34	3	0
4	R	14	0	13	1	0
4	U	14	0	13	0	0
All	All	25939	0	24717	1159	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 1159 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:R:518:LEU:HD23	2:R:519:HIS:N	1.68	1.07
1:O:177:ARG:NH1	1:O:474:MET:HG3	1.70	1.06
1:O:177:ARG:HH11	1:O:474:MET:HG3	0.93	1.06
2:L:438:SER:HB3	2:L:509:ARG:HG3	1.38	1.05
2:L:336:CYS:HA	2:L:361:CYS:HB2	1.41	1.02

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:351:TYR:OH	1:U:600:ARG:O[4_555]	2.11	0.09
2:L:346:ARG:NH1	1:U:238:GLU:OE1[4_555]	2.12	0.08
1:I:137:ASN:ND2	1:I:387:THR:OG1[1_455]	2.16	0.04
2:F:351:TYR:OH	1:O:600:ARG:O[3_555]	2.17	0.03
2:F:357:ARG:NH2	1:O:609:ASP:OD2[3_555]	2.17	0.03

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	596/598 (100%)	578 (97%)	14 (2%)	4 (1%)	19	53
1	I	596/598 (100%)	576 (97%)	18 (3%)	2 (0%)	37	67
1	O	596/598 (100%)	562 (94%)	26 (4%)	8 (1%)	10	41
1	U	596/598 (100%)	577 (97%)	16 (3%)	3 (0%)	25	59
2	F	192/197 (98%)	180 (94%)	11 (6%)	1 (0%)	25	59
2	L	194/197 (98%)	185 (95%)	8 (4%)	1 (0%)	25	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	R	194/197 (98%)	184 (95%)	9 (5%)	1 (0%)	25 59
2	X	188/197 (95%)	171 (91%)	13 (7%)	4 (2%)	5 33
All	All	3152/3180 (99%)	3013 (96%)	115 (4%)	24 (1%)	16 51

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	337	PRO
1	U	353	LYS
2	X	394	ASN
1	B	91	VAL
1	I	91	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	532/532 (100%)	532 (100%)	0	100 100
1	I	532/532 (100%)	531 (100%)	1 (0%)	92 96
1	O	532/532 (100%)	526 (99%)	6 (1%)	70 83
1	U	532/532 (100%)	532 (100%)	0	100 100
2	F	168/170 (99%)	165 (98%)	3 (2%)	54 74
2	L	169/170 (99%)	167 (99%)	2 (1%)	67 82
2	R	169/170 (99%)	166 (98%)	3 (2%)	54 74
2	X	164/170 (96%)	164 (100%)	0	100 100
All	All	2798/2808 (100%)	2783 (100%)	15 (0%)	86 93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	108	LEU
2	R	335	LEU

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Mol	Chain	Res	Type
1	O	198	ASP
2	R	336	CYS
1	O	526	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	175	GLN
2	R	481	ASN
1	U	556	GLN
1	O	300	GLN
2	R	394	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	$\#\|Z\| > 2$
3	NAG	A	1	3,1	14,14,15	0.62	0	17,19,21	1.20	1 (5%)
3	FUC	A	2	3	10,10,11	1.81	5 (50%)	14,14,16	1.26	2 (14%)
3	NAG	C	1	3,1	14,14,15	0.28	0	17,19,21	0.43	0
3	FUC	C	2	3	10,10,11	0.83	0	14,14,16	0.95	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
3	NAG	A	1	3,1	-	3/6/23/26	0/1/1/1
3	FUC	A	2	3	-	-	0/1/1/1
3	NAG	C	1	3,1	-	1/6/23/26	0/1/1/1
3	FUC	C	2	3	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	FUC	O3-C3	-3.15	1.35	1.43
3	A	2	FUC	C1-C2	-2.39	1.46	1.52
3	A	2	FUC	O5-C5	2.25	1.48	1.43
3	A	2	FUC	C2-C3	2.13	1.55	1.52
3	A	2	FUC	O2-C2	2.11	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1	NAG	C2-N2-C7	4.13	128.78	122.90
3	A	2	FUC	O3-C3-C4	-2.71	104.09	110.35
3	A	2	FUC	O5-C5-C6	2.61	112.95	107.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	NAG	C3-C2-N2-C7
3	A	1	NAG	C4-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

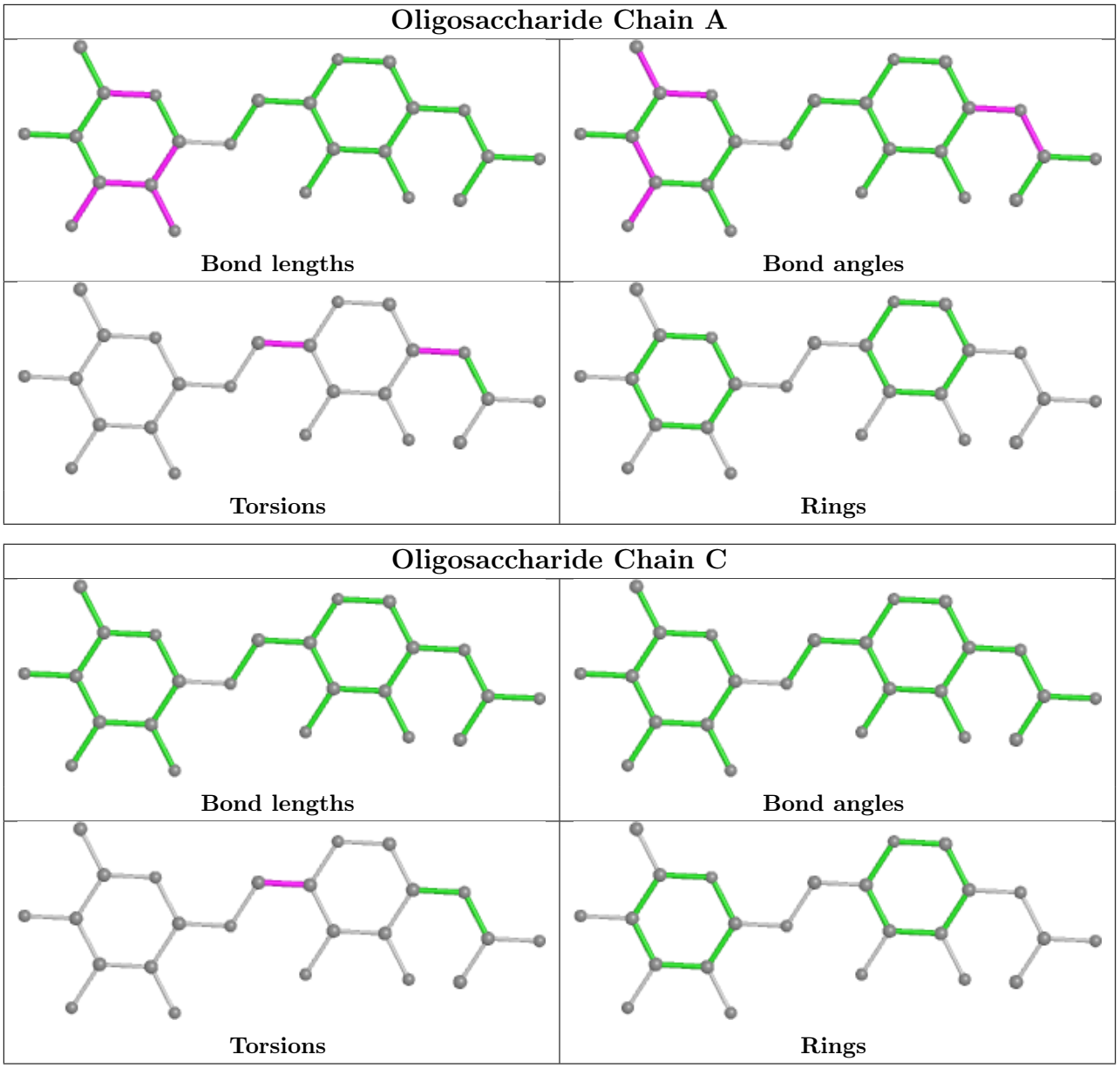
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

10 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	$\#\|Z\|>2$
4	NAG	I	703	-	11,11,15	0.38	0	11,12,21	0.82	0
4	NAG	O	702	1	14,14,15	0.63	1 (7%)	17,19,21	0.46	0
4	NAG	R	601	2	14,14,15	0.50	0	17,19,21	0.46	0
4	NAG	U	701	1	14,14,15	0.65	1 (7%)	17,19,21	0.62	0
4	NAG	O	704	1	11,11,15	0.40	0	12,12,21	0.41	0
4	NAG	B	701	1	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	I	701	-	14,14,15	0.20	0	17,19,21	0.50	0
4	NAG	L	601	2	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	O	701	1	14,14,15	0.19	0	17,19,21	0.35	0
4	NAG	B	703	-	12,12,15	0.21	0	15,15,21	0.57	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	I	703	-	-	3/10/10/26	-
4	NAG	O	702	1	-	1/6/23/26	0/1/1/1
4	NAG	R	601	2	-	2/6/23/26	0/1/1/1
4	NAG	U	701	1	-	0/6/23/26	0/1/1/1
4	NAG	O	704	1	-	3/11/11/26	-
4	NAG	B	701	1	-	1/6/23/26	0/1/1/1
4	NAG	I	701	-	-	1/6/23/26	0/1/1/1
4	NAG	L	601	2	-	2/6/23/26	0/1/1/1
4	NAG	O	701	1	-	2/6/23/26	0/1/1/1
4	NAG	B	703	-	-	2/15/15/26	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	702	NAG	O5-C1	2.26	1.47	1.43
4	U	701	NAG	O5-C1	2.10	1.47	1.43

There are no bond angle outliers.

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	O	704	NAG	C4-C5-C6-O6
4	O	704	NAG	O5-C5-C6-O6
4	R	601	NAG	C4-C5-C6-O6
4	R	601	NAG	O5-C5-C6-O6
4	O	701	NAG	O5-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	703	NAG	3	0
4	R	601	NAG	1	0
4	O	704	NAG	3	0
4	B	703	NAG	5	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	B	598/598 (100%)	-0.30	2 (0%) 90 79	49, 69, 105, 181	0
1	I	598/598 (100%)	-0.34	0 100 100	53, 72, 111, 169	0
1	O	598/598 (100%)	-0.23	3 (0%) 87 72	30, 86, 125, 193	0
1	U	598/598 (100%)	-0.28	2 (0%) 90 79	58, 82, 126, 190	0
2	F	194/197 (98%)	-0.11	2 (1%) 79 59	66, 94, 163, 212	0
2	L	196/197 (99%)	-0.13	2 (1%) 79 59	58, 80, 143, 177	0
2	R	196/197 (99%)	-0.28	0 100 100	48, 74, 138, 173	0
2	X	190/197 (96%)	0.03	2 (1%) 77 57	54, 88, 158, 223	0
All	All	3168/3180 (99%)	-0.25	13 (0%) 89 76	30, 79, 133, 223	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	384	PRO	4.0
1	O	339	GLY	3.0
2	X	432	CYS	2.5
1	U	34	HIS	2.5
1	O	241	HIS	2.5

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

SUGAR-RSR INFOmissingINFO

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	U	701	14/15	0.46	0.15	115,137,161,167	0
4	NAG	I	701	14/15	0.54	0.19	133,141,150,151	0
4	NAG	L	601	14/15	0.58	0.14	82,91,94,94	0
4	NAG	O	701	14/15	0.66	0.14	156,161,166,168	0
4	NAG	B	701	14/15	0.71	0.13	118,124,130,133	0
4	NAG	I	703	13/15	0.75	0.12	72,89,97,100	0
4	NAG	R	601	14/15	0.76	0.12	95,100,103,106	0
4	NAG	B	703	13/15	0.79	0.11	66,82,93,94	0
4	NAG	O	702	14/15	0.79	0.09	67,74,86,87	0
4	NAG	O	704	13/15	0.80	0.10	69,82,92,96	0

6.5 Other polymers (i)

There are no such residues in this entry.