Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 06:54 AM EDT

PDB ID	:	7MZH
Title	:	SARS-CoV-2 receptor binding domain bound to Fab WCSL 119
Authors	:	Pymm, P.; Tan, L.L.; Dietrich, M.H.; Chan, L.J.; Tham, W.H.
Deposited on	:	2021-05-24
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

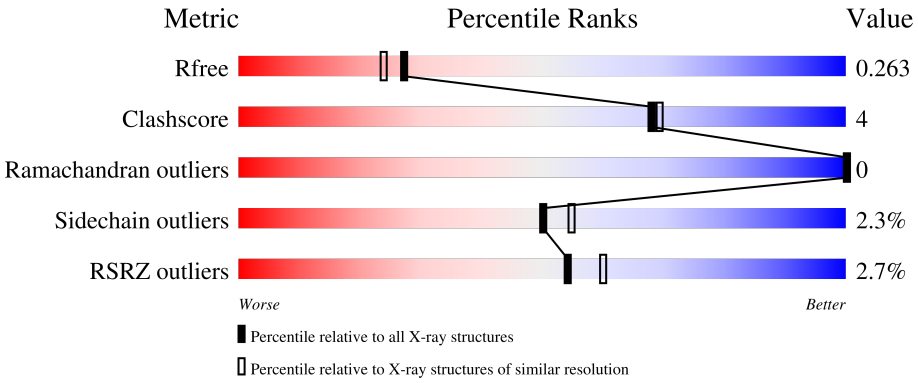
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	A	205	2% 84% 12% ·
1	E	205	7% 86% 9% ·
2	B	221	% 87% 10% · ·
2	H	221	3% 87% 10% ·
3	C	216	91% 8% ·

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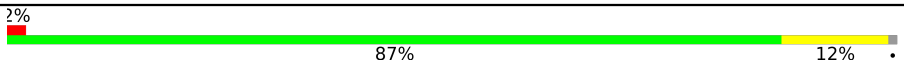
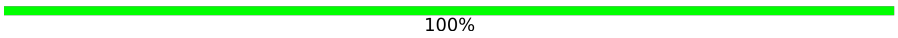
Mol	Chain	Length	Quality of chain
3	L	216	
4	D	3	
5	F	5	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9803 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	197	Total	C	N	O	S	0	0	0
			1522	978	247	289	8			
1	A	198	Total	C	N	O	S	0	0	0
			1536	981	256	291	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	528	GLY	-	expression tag	UNP P0DTC2
E	529	SER	-	expression tag	UNP P0DTC2
E	530	HIS	-	expression tag	UNP P0DTC2
E	531	HIS	-	expression tag	UNP P0DTC2
E	532	HIS	-	expression tag	UNP P0DTC2
E	533	HIS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
A	530	HIS	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2

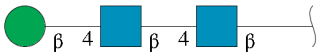
- Molecule 2 is a protein called WCSL 119 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	2	0
			1618	1018	274	315	11			
2	B	216	Total	C	N	O	S	0	2	0
			1615	1017	272	318	8			

- Molecule 3 is a protein called WCSL 119 light chain.

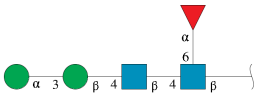
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	1	0
			1589	999	263	322	5			
3	C	216	Total	C	N	O	S	0	0	0
			1598	1002	266	325	5			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-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
5	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	23	Total	O	0	0
			23	23		
6	H	36	Total	O	0	0
			36	36		
6	L	26	Total	O	0	0
			26	26		
6	A	30	Total	O	0	0
			30	30		
6	B	56	Total	O	0	0
			56	56		

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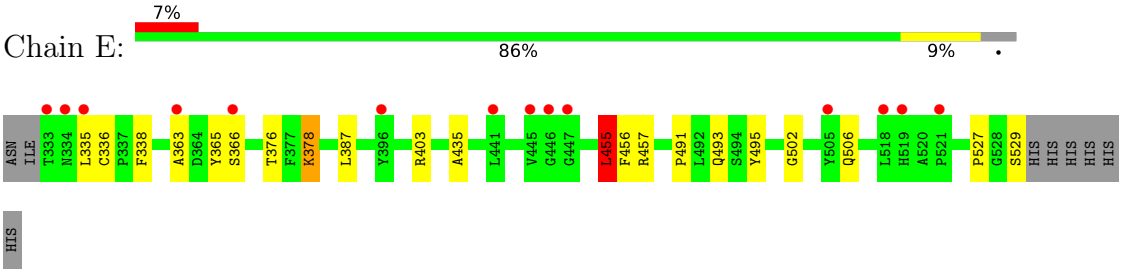
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	55	Total O 55 55	0	0

3 Residue-property plots

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.

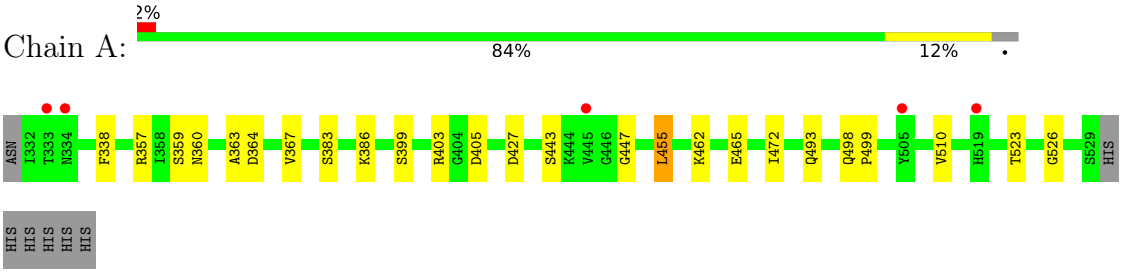
• Molecule 1: Spike protein S1

Chain E:



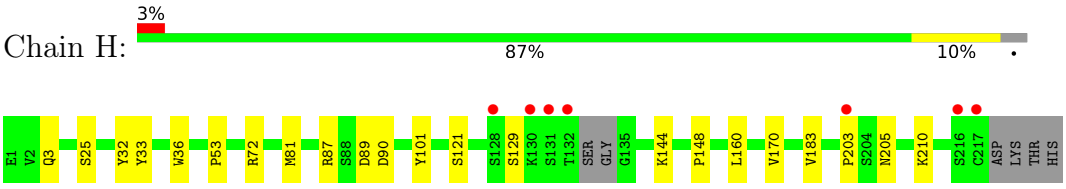
• Molecule 1: Spike protein S1

Chain A:



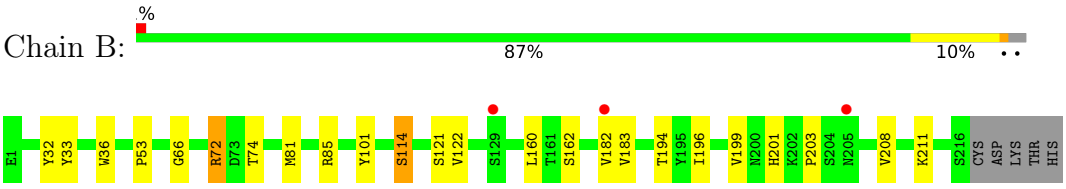
• Molecule 2: WCSL 119 heavy chain

Chain H:



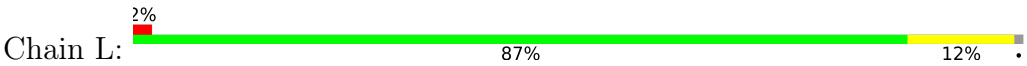
• Molecule 2: WCSL 119 heavy chain

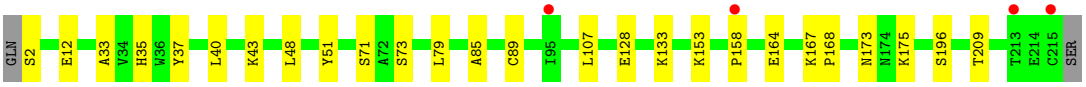
Chain B:



• Molecule 3: WCSL 119 light chain

Chain L:





• Molecule 3: WCSL 119 light chain

Chain C:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

• Molecule 5: alpha-D-mannopyranose-(1-3)-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 F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.70Å 72.83Å 103.99Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	45.70 – 2.10 46.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.70-2.10) 99.9 (46.85-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.220 , 0.265 0.218 , 0.263	Depositor DCC
R_{free} test set	3928 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.816	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9803	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.23% 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: BMA, FUC, 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	0.47	0/1579	0.64	1/2153 (0.0%)
1	E	0.44	0/1566	0.65	2/2138 (0.1%)
2	B	0.54	1/1658 (0.1%)	0.67	0/2262
2	H	0.46	0/1657	0.66	0/2259
3	C	0.48	0/1638	0.66	2/2241 (0.1%)
3	L	0.48	0/1632	0.67	2/2232 (0.1%)
All	All	0.48	1/9730 (0.0%)	0.66	7/13285 (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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	114	SER	CB-OG	7.57	1.52	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	455	LEU	CA-CB-CG	7.20	131.87	115.30
3	C	190	LYS	CB-CG-CD	6.58	128.71	111.60
3	C	139	LEU	CA-CB-CG	-5.78	102.01	115.30
1	A	455	LEU	CA-CB-CG	5.60	128.19	115.30
3	L	133	LYS	CD-CE-NZ	-5.54	98.97	111.70
3	L	2	SER	CA-C-N	5.40	129.09	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	378	LYS	CA-CB-CG	5.16	124.76	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	114	SER	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	A	1536	0	1422	13	0
1	E	1522	0	1408	11	0
2	B	1615	0	1560	15	0
2	H	1618	0	1551	12	0
3	C	1598	0	1530	13	0
3	L	1589	0	1528	14	0
4	D	39	0	34	0	0
5	F	60	0	52	0	0
6	A	30	0	0	1	0
6	B	56	0	0	1	0
6	C	55	0	0	2	0
6	E	23	0	0	2	1
6	H	36	0	0	1	1
6	L	26	0	0	0	0
All	All	9803	0	9085	70	1

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 4.

All (70) 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:H:144:LYS:NZ	3:L:128:GLU:OE2	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:SER:OG	6:C:301:HOH:O	1.95	0.84
1:A:360:ASN:HA	1:A:523:THR:HG22	1.61	0.83
3:C:186:PRO:O	3:C:190:LYS:HG3	1.79	0.83
3:C:160:LYS:O	6:C:302:HOH:O	2.02	0.77
2:H:205:ASN:OD1	6:H:301:HOH:O	2.05	0.74
2:H:170:VAL:HG11	3:L:164:GLU:HB3	1.72	0.72
3:C:33:ALA:HB1	3:C:51:TYR:HA	1.73	0.70
1:E:493:GLN:OE1	6:E:601:HOH:O	2.11	0.67
1:A:360:ASN:CA	1:A:523:THR:HG22	2.26	0.64
3:L:33:ALA:HB1	3:L:51:TYR:HA	1.80	0.63
2:B:182[B]:VAL:HG21	3:C:139:LEU:HD13	1.83	0.61
2:B:160:LEU:HD21	2:B:183:VAL:HG21	1.84	0.60
3:L:167:LYS:HD2	3:L:168:PRO:HD2	1.86	0.58
2:H:170:VAL:HG11	3:L:164:GLU:CB	2.35	0.56
2:B:182[B]:VAL:CG2	3:C:139:LEU:HD13	2.35	0.56
1:A:447:GLY:HA2	1:A:498:GLN:HG3	1.87	0.55
3:L:40:LEU:HD13	3:L:85:ALA:HB2	1.89	0.54
1:E:365:TYR:CD2	1:E:387:LEU:HB3	2.43	0.53
2:B:199:VAL:HB	2:B:208:VAL:HG13	1.89	0.53
2:B:194:THR:HG22	6:B:318:HOH:O	2.08	0.53
1:A:462:LYS:HG2	1:A:465:GLU:OE1	2.09	0.52
2:B:72:ARG:HD3	2:B:74:THR:OG1	2.10	0.51
3:L:153:LYS:HD3	3:L:158:PRO:HA	1.91	0.51
1:A:403:ARG:NH1	1:A:405:ASP:OD1	2.43	0.51
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.93	0.50
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.47	0.49
2:H:148:PRO:HD2	2:H:203:PRO:HB3	1.93	0.49
2:H:101:TYR:HB2	3:L:37:TYR:CE2	2.47	0.49
3:C:38:GLN:HB2	3:C:48:LEU:HD11	1.95	0.48
1:A:363:ALA:O	1:A:526:GLY:HA2	2.14	0.48
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.48	0.48
1:E:336:CYS:SG	1:E:363:ALA:HB2	2.54	0.47
1:A:443:SER:HB3	1:A:499:PRO:HD3	1.96	0.47
2:B:101:TYR:HB2	3:C:37:TYR:CE1	2.49	0.47
3:L:196:SER:HB2	3:L:209:THR:HG22	1.95	0.47
1:E:403:ARG:HG3	1:E:495:TYR:CE1	2.50	0.46
3:C:3:VAL:HB	3:C:100:VAL:HB	1.97	0.46
1:E:456:PHE:HD2	1:E:491:PRO:HA	1.81	0.46
2:B:182[A]:VAL:CG1	3:C:139:LEU:HD13	2.46	0.46
2:H:160:LEU:HD21	2:H:183:VAL:HG21	1.99	0.45
1:E:502:GLY:O	1:E:506:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:ASN:ND2	3:L:175:LYS:HD2	2.32	0.45
2:B:122:VAL:HG21	2:B:208:VAL:HG11	1.99	0.45
3:C:29:ILE:O	3:C:67:LYS:HE2	2.17	0.44
2:B:66:GLY:O	2:B:85:ARG:NH2	2.50	0.44
2:B:201:HIS:CD2	2:B:203:PRO:HD2	2.53	0.44
2:H:87:ARG:HG2	2:H:90:ASP:OD2	2.18	0.44
1:A:383:SER:HB3	1:A:386:LYS:HB2	1.99	0.43
3:C:196:SER:HB2	3:C:209:THR:HG22	2.00	0.43
1:E:378:LYS:HG3	6:E:611:HOH:O	2.18	0.43
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.82	0.43
1:A:364:ASP:O	1:A:367:VAL:HG22	2.17	0.43
1:E:338:PHE:HE2	1:E:363:ALA:HB1	1.82	0.43
1:E:376:THR:HB	1:E:435:ALA:HB3	2.01	0.43
2:H:3:GLN:HB2	2:H:25:SER:OG	2.18	0.43
3:L:79:LEU:HD11	3:L:107:LEU:HD21	2.01	0.43
1:A:399:SER:HA	1:A:510:VAL:O	2.19	0.43
2:H:87:ARG:HG3	2:H:89:ASP:OD1	2.19	0.42
1:E:363:ALA:O	1:E:527:PRO:HD3	2.20	0.42
2:B:72:ARG:O	2:B:72:ARG:HD2	2.20	0.42
2:H:32:TYR:O	2:H:53:PRO:HG3	2.20	0.41
2:B:196:ILE:HG12	2:B:211:LYS:HA	2.02	0.41
1:E:455:LEU:HD23	1:E:491:PRO:O	2.20	0.41
3:L:48:LEU:HD23	3:L:48:LEU:HA	1.89	0.41
2:B:32:TYR:O	2:B:53:PRO:HG3	2.20	0.41
1:A:472:ILE:HG12	6:A:619:HOH:O	2.21	0.40
3:L:35:HIS:O	3:L:89:CYS:HA	2.22	0.40
3:C:22:CYS:HB2	3:C:36:TRP:CH2	2.57	0.40
3:L:196:SER:CB	3:L:209:THR:HG22	2.51	0.40

All (1) 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)
6:E:621:HOH:O	6:H:330:HOH:O[2_545]	2.11	0.09

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	196/205 (96%)	188 (96%)	8 (4%)	0	100	100
1	E	195/205 (95%)	186 (95%)	9 (5%)	0	100	100
2	B	216/221 (98%)	205 (95%)	11 (5%)	0	100	100
2	H	213/221 (96%)	202 (95%)	11 (5%)	0	100	100
3	C	214/216 (99%)	210 (98%)	4 (2%)	0	100	100
3	L	213/216 (99%)	209 (98%)	4 (2%)	0	100	100
All	All	1247/1284 (97%)	1200 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	A	163/177 (92%)	160 (98%)	3 (2%)	59	65
1	E	162/177 (92%)	157 (97%)	5 (3%)	40	43
2	B	178/187 (95%)	174 (98%)	4 (2%)	52	57
2	H	177/187 (95%)	172 (97%)	5 (3%)	43	47
3	C	176/181 (97%)	173 (98%)	3 (2%)	60	67
3	L	176/181 (97%)	172 (98%)	4 (2%)	50	55
All	All	1032/1090 (95%)	1008 (98%)	24 (2%)	50	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	335	LEU
1	E	366	SER
1	E	455	LEU
1	E	457	ARG
1	E	529	SER
2	H	33	TYR
2	H	72	ARG
2	H	121	SER
2	H	129	SER
2	H	210	LYS
3	L	12	GLU
3	L	43	LYS
3	L	71	SER
3	L	73	SER
1	A	357	ARG
1	A	359	SER
1	A	427	ASP
2	B	33	TYR
2	B	72	ARG
2	B	121	SER
2	B	162	SER
3	C	12	GLU
3	C	51	TYR
3	C	71	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	172	GLN
3	L	198	GLN

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)

8 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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.30	0	17,19,21	0.53	0
4	NAG	D	2	4	14,14,15	0.28	0	17,19,21	0.43	0
4	BMA	D	3	4	11,11,12	0.72	0	15,15,17	0.83	0
5	NAG	F	1	1,5	14,14,15	0.40	0	17,19,21	0.53	0
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.51	0
5	BMA	F	3	5	11,11,12	0.81	0	15,15,17	0.93	0
5	MAN	F	4	5	11,11,12	1.19	1 (9%)	15,15,17	1.16	2 (13%)
5	FUC	F	5	5	10,10,11	1.22	0	14,14,16	1.00	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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	1/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
5	FUC	F	5	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	4	MAN	C2-C3	2.60	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4	MAN	C1-O5-C5	2.78	115.95	112.19
5	F	5	FUC	O2-C2-C1	2.31	113.88	109.15
5	F	4	MAN	O3-C3-C2	2.02	113.86	109.99

There are no chirality outliers.

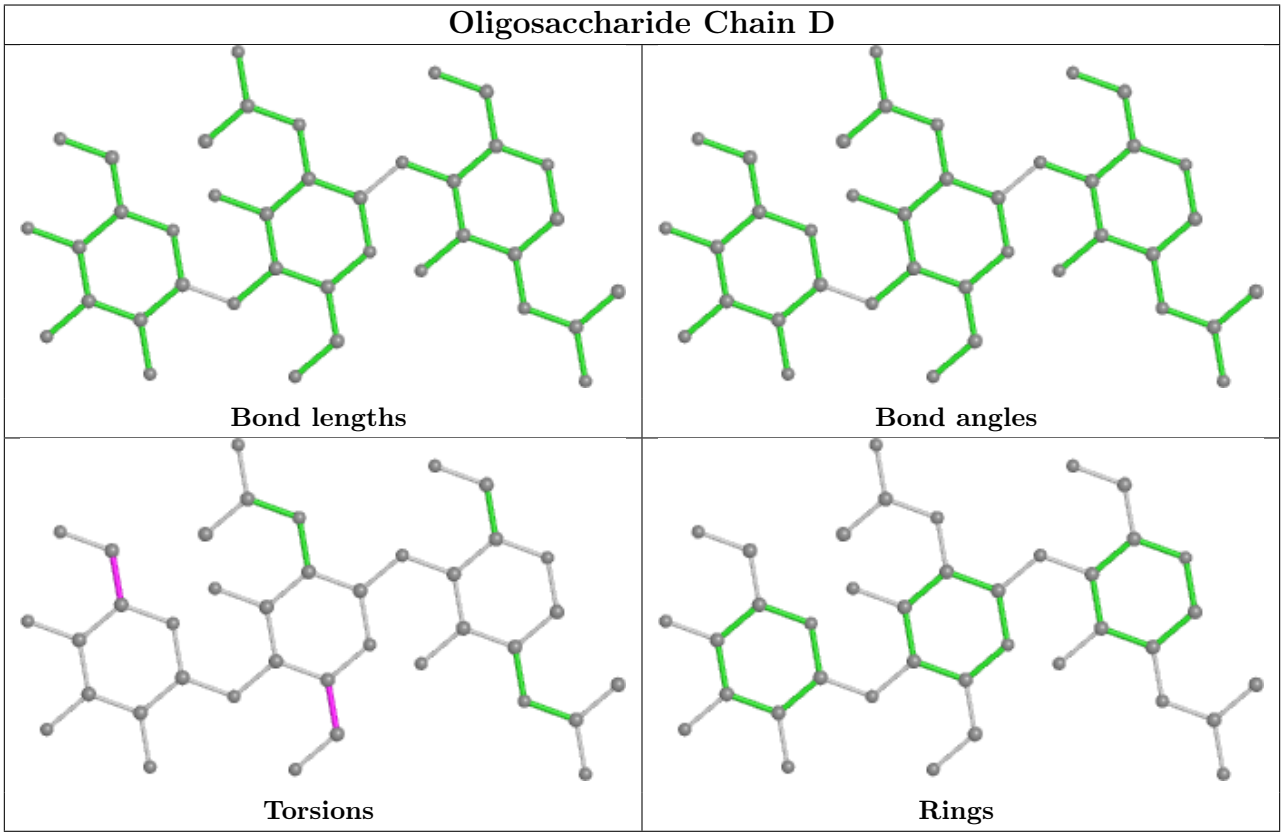
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	D	3	BMA	O5-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6

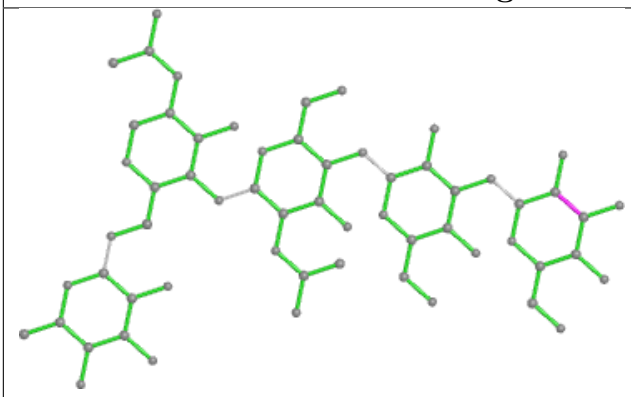
There are no ring outliers.

No monomer is involved in short contacts.

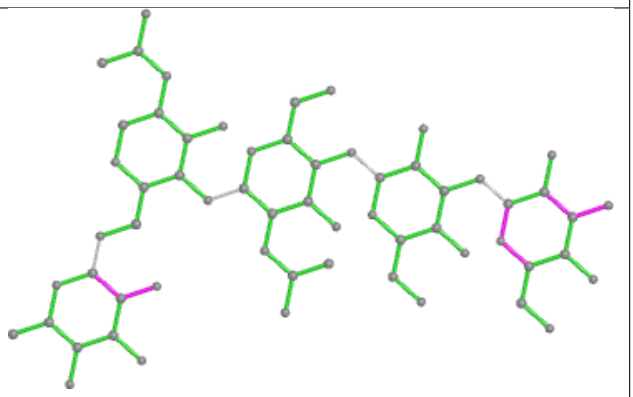
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



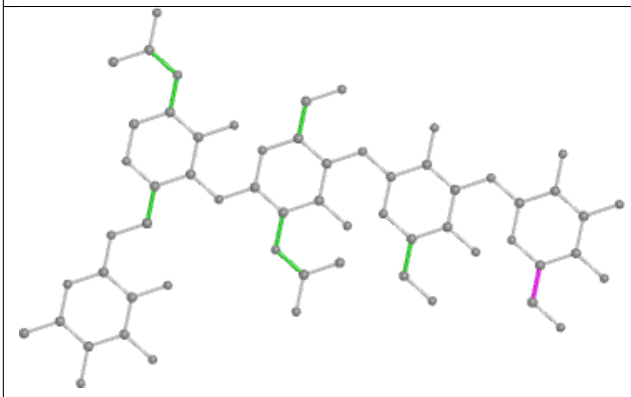
Oligosaccharide Chain F



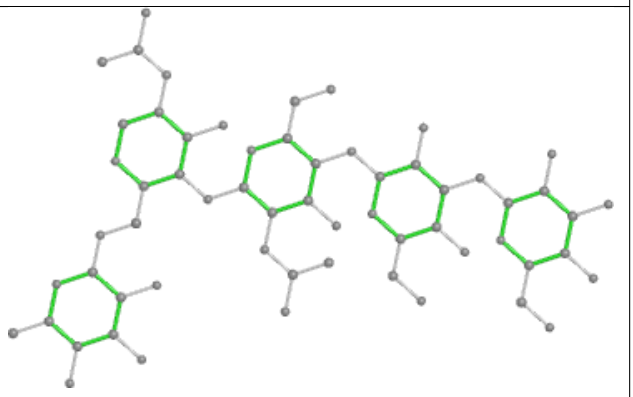
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

There are no ligands in this entry.

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^{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	A	198/205 (96%)	0.36	5 (2%) 57 62	37, 52, 72, 97	0
1	E	197/205 (96%)	0.48	14 (7%) 16 20	40, 52, 71, 87	0
2	B	216/221 (97%)	0.23	3 (1%) 75 78	33, 44, 65, 78	0
2	H	215/221 (97%)	0.33	7 (3%) 46 53	36, 47, 69, 107	0
3	C	216/216 (100%)	0.31	1 (0%) 91 92	35, 43, 59, 73	0
3	L	214/216 (99%)	0.36	4 (1%) 66 71	37, 47, 63, 98	0
All	All	1256/1284 (97%)	0.34	34 (2%) 54 60	33, 47, 68, 107	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	215	CYS	7.4
2	H	217	CYS	6.6
2	H	131	SER	6.5
1	E	334	ASN	4.3
1	A	445	VAL	4.1
1	E	519	HIS	3.6
2	B	129	SER	3.6
1	E	333	THR	3.4
1	E	518	LEU	3.4
1	E	446	GLY	3.1
1	E	445	VAL	3.0
1	E	505	TYR	2.9
1	E	335	LEU	2.9
2	B	205	ASN	2.9
3	C	1	GLN	2.8
1	E	447	GLY	2.8
1	A	333	THR	2.7
1	A	334	ASN	2.6
2	H	128	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	366	SER	2.5
2	H	132	THR	2.5
1	A	505	TYR	2.4
2	H	216	SER	2.4
3	L	158	PRO	2.3
1	E	396	TYR	2.3
1	E	363	ALA	2.3
2	H	130	LYS	2.2
3	L	95	ILE	2.2
1	E	521	PRO	2.2
1	A	519	HIS	2.2
2	H	203	PRO	2.1
3	L	213	THR	2.1
1	E	441	LEU	2.0
2	B	182[A]	VAL	2.0

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)

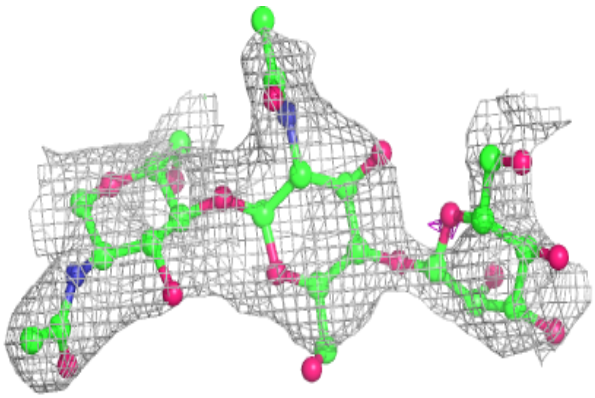
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

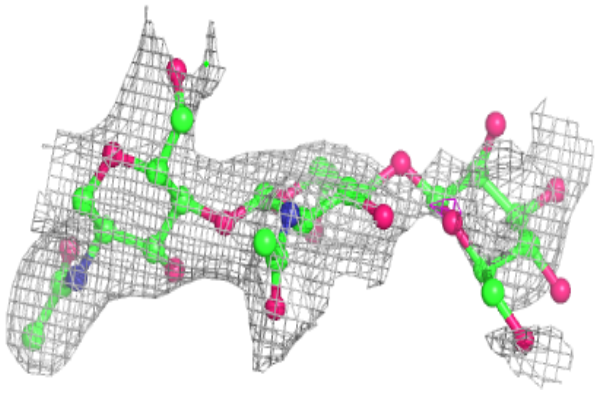
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BMA	D	3	11/12	0.51	0.38	102,105,107,109	0
4	NAG	D	2	14/15	0.76	0.32	90,93,99,103	0
5	NAG	F	2	14/15	0.76	0.24	71,74,78,79	0
4	NAG	D	1	14/15	0.79	0.21	67,82,85,88	0
5	BMA	F	3	11/12	0.80	0.21	75,76,78,79	0
5	MAN	F	4	11/12	0.83	0.19	69,73,78,79	0
5	FUC	F	5	10/11	0.83	0.32	72,78,81,83	0
5	NAG	F	1	14/15	0.84	0.13	55,66,75,77	0

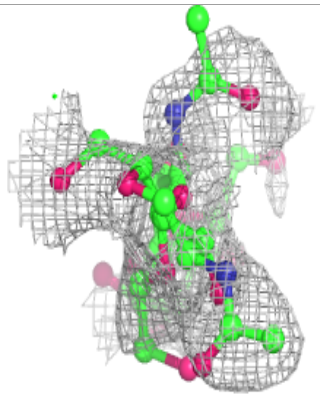
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

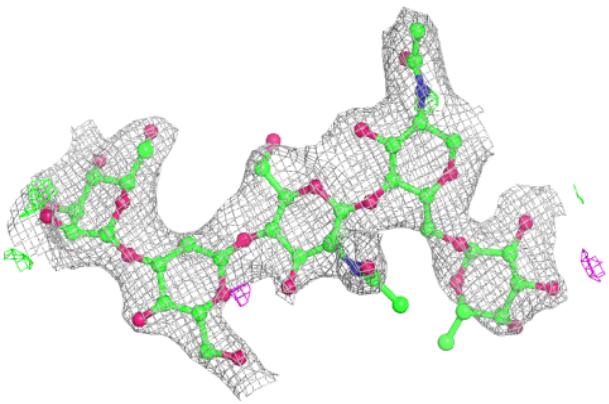


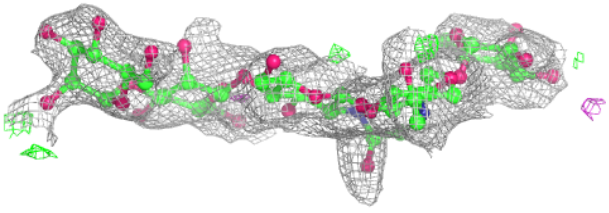


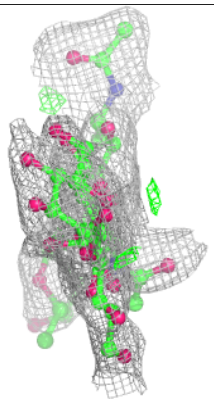


Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.