Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2021 – 12:12 pm GMT

PDB ID	:	7Q0H
Title	:	Crystal structure of the receptor binding domain of SARS-CoV-2 beta variant spike glycoprotein in complex with Beta-50 and Beta-54
Authors	:	Zhou, D.; Ren, J.; Stuart, D.I.
Deposited on	:	2021-10-14
Resolution	:	3.65 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 following versions of software and data (see references (i)) were used in the production of this report:

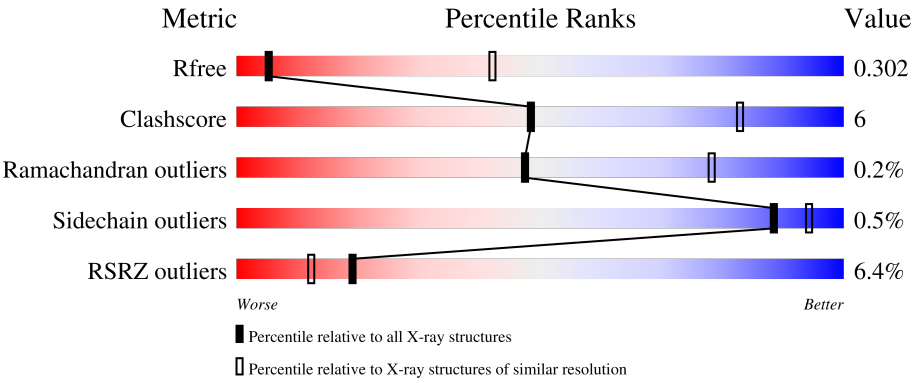
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 3.65 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.



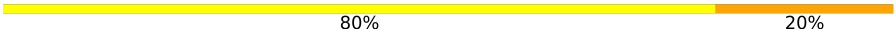
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	H	231	3% 88% 11% •
2	L	214	90% 9%
3	B	217	13% 84% 16%
4	A	223	12% 82% 12% • 5%
5	E	210	2% 77% 16% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	C	5	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8202 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 Beta-54 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	229	Total	C	N	O	S	0	0	0
			1706	1080	283	337	6			

- Molecule 2 is a protein called Beta-54 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1636	1028	272	331	5			

- Molecule 3 is a protein called Beta-50 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	216	Total	C	N	O	S	0	2	0
			1668	1045	282	334	7			

- Molecule 4 is a protein called Beta-50 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	212	Total	C	N	O	S	0	0	0
			1578	1002	258	311	7			

- Molecule 5 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1554	997	260	289	8			

There are 19 discrepancies between the modelled and reference sequences:

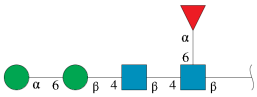
Chain	Residue	Modelled	Actual	Comment	Reference
E	319	MET	-	initiating methionine	UNP P0DTC2
E	320	GLY	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	321	CYS	-	expression tag	UNP P0DTC2
E	322	VAL	-	expression tag	UNP P0DTC2
E	323	ALA	-	expression tag	UNP P0DTC2
E	324	GLU	-	expression tag	UNP P0DTC2
E	325	THR	-	expression tag	UNP P0DTC2
E	326	GLY	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 6 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.



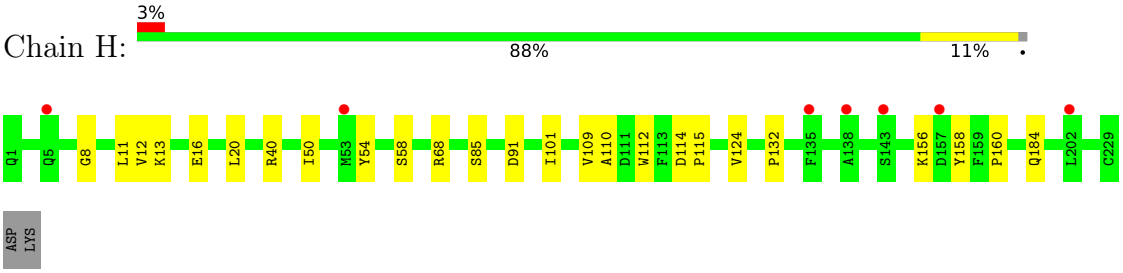
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	C	5	60	34	2	24	0	0	0

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.

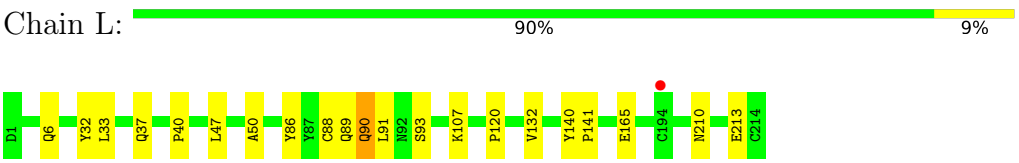
• Molecule 1: Beta-54 Fab heavy chain

Chain H:



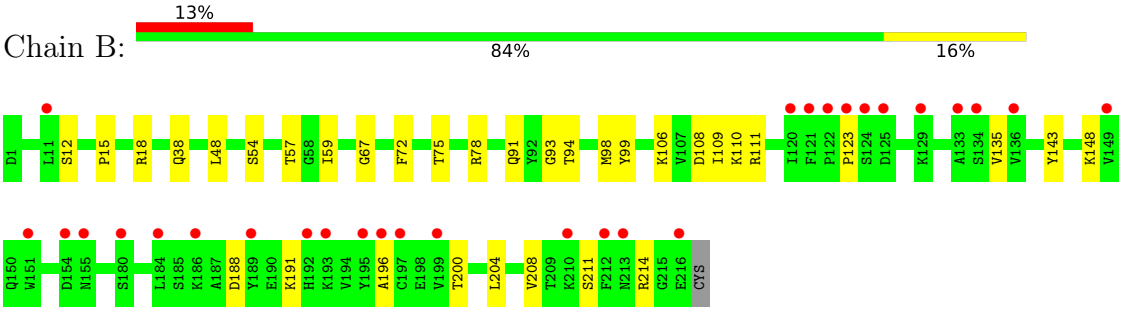
• Molecule 2: Beta-54 Fab light chain

Chain L:



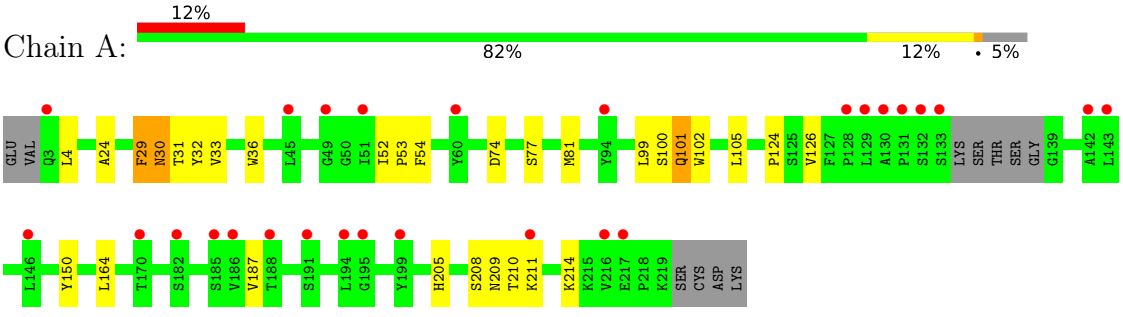
• Molecule 3: Beta-50 Fab light chain

Chain B:



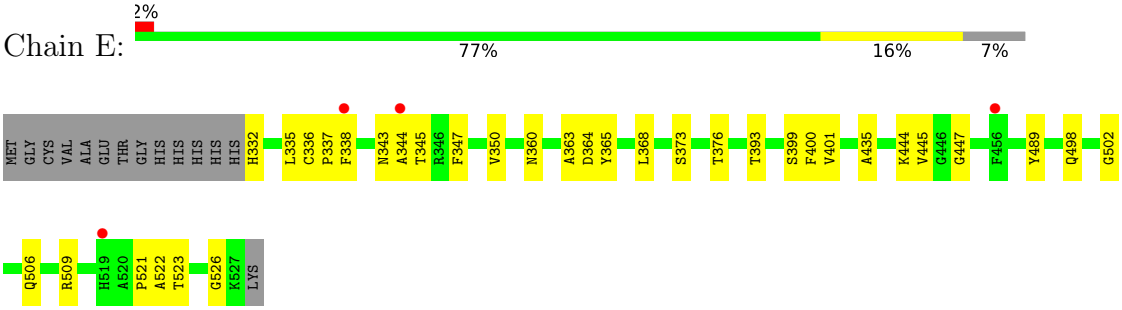
• Molecule 4: Beta-50 Fab heavy chain

Chain A:



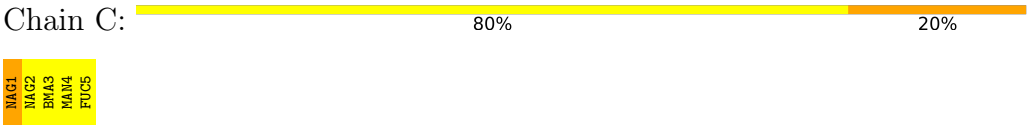
• Molecule 5: Spike protein S1

Chain E:



• Molecule 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 C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.21Å 42.47Å 138.41Å 90.00° 99.94° 90.00°	Depositor
Resolution (Å)	88.62 – 3.65 88.62 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.7 (88.62-3.65) 99.8 (88.62-3.65)	Depositor EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.255 , 0.303 0.257 , 0.302	Depositor DCC
R_{free} test set	706 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	97.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8202	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, MAN, FUC, BMA

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	H	0.25	0/1752	0.48	0/2399
2	L	0.25	0/1671	0.48	0/2269
3	B	0.26	0/1711	0.51	0/2323
4	A	0.27	0/1617	0.52	0/2208
5	E	0.31	0/1599	0.52	0/2177
All	All	0.27	0/8350	0.50	0/11376

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
5	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	489	TYR	Peptide

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	H	1706	0	1674	18	0
2	L	1636	0	1598	16	0
3	B	1668	0	1622	25	0
4	A	1578	0	1534	24	0
5	E	1554	0	1464	27	0
6	C	60	0	52	5	0
All	All	8202	0	7944	96	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.

All (96) 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)
3:B:54:SER:HB2	5:E:345:THR:HG22	1.65	0.78
2:L:90:GLN:HE21	2:L:93:SER:H	1.32	0.77
5:E:360:ASN:H	5:E:523:THR:HB	1.49	0.76
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.75	0.66
2:L:90:GLN:NE2	2:L:93:SER:O	2.29	0.66
4:A:126:VAL:O	4:A:214:LYS:NZ	2.29	0.65
3:B:38:GLN:HB2	3:B:48:LEU:HD11	1.79	0.65
5:E:393:THR:HA	5:E:522:ALA:HA	1.81	0.62
4:A:209:ASN:OD1	4:A:211:LYS:NZ	2.31	0.61
1:H:109:VAL:HG13	2:L:91:LEU:HD11	1.83	0.60
3:B:93:GLY:HA3	3:B:98:MET:HG3	1.83	0.60
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.83	0.59
3:B:188:ASP:HA	3:B:191:LYS:HD3	1.85	0.59
1:H:68:ARG:NH2	1:H:91:ASP:OD2	2.36	0.58
3:B:91:GLN:NE2	3:B:98:MET:O	2.37	0.58
4:A:24:ALA:N	4:A:77:SER:O	2.27	0.58
4:A:124:PRO:HB3	4:A:150:TYR:HB3	1.86	0.58
1:H:156:LYS:NZ	1:H:184:GLN:OE1	2.37	0.58
3:B:57:THR:HG21	6:C:2:NAG:H2	1.86	0.58
1:H:13:LYS:HB2	1:H:16:GLU:HG3	1.86	0.56
4:A:30:ASN:HB3	4:A:54:PHE:HB2	1.86	0.56
3:B:123:PRO:HD3	3:B:135:VAL:HG22	1.87	0.55
4:A:31:THR:HA	5:E:335:LEU:HD21	1.88	0.55
3:B:106:LYS:HE3	3:B:108:ASP:HB3	1.89	0.54
4:A:205:HIS:HB3	4:A:210:THR:HB	1.89	0.54
5:E:373:SER:OG	6:C:5:FUC:O3	2.17	0.53
5:E:363:ALA:O	5:E:526:GLY:HA3	2.08	0.53
3:B:67:GLY:HA3	3:B:72:PHE:HA	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:29:PHE:CD2	4:A:74:ASP:HA	2.45	0.52
4:A:124:PRO:HD2	4:A:210:THR:HG21	1.93	0.51
5:E:360:ASN:N	5:E:523:THR:HB	2.24	0.51
3:B:48:LEU:HD23	3:B:59:ILE:HD12	1.93	0.51
3:B:148:LYS:HB3	3:B:200:THR:HB	1.92	0.51
4:A:102:TRP:CZ3	5:E:368:LEU:HG	2.46	0.50
1:H:11:LEU:HB2	1:H:160:PRO:HG3	1.93	0.50
6:C:1:NAG:H61	6:C:2:NAG:HN2	1.76	0.50
3:B:110:LYS:HG2	3:B:111:ARG:H	1.78	0.49
4:A:32:TYR:O	4:A:53:PRO:HD2	2.13	0.49
3:B:15:PRO:HD3	3:B:109:ILE:HG23	1.95	0.49
1:H:85:SER:HB3	3:B:78:ARG:NH2	2.28	0.49
4:A:102:TRP:CE3	5:E:368:LEU:HG	2.48	0.49
3:B:18:ARG:HH21	3:B:75:THR:HG21	1.78	0.48
4:A:33:VAL:HG22	4:A:52:ILE:HG12	1.95	0.48
2:L:90:GLN:NE2	2:L:93:SER:H	2.06	0.48
2:L:107:LYS:HA	2:L:140:TYR:OH	2.14	0.47
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.96	0.47
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.96	0.47
5:E:336:CYS:O	5:E:338:PHE:N	2.45	0.47
3:B:196:ALA:HB2	3:B:211:SER:HB3	1.97	0.47
4:A:101:GLN:HB2	5:E:335:LEU:HD23	1.95	0.47
5:E:347:PHE:CE2	5:E:399:SER:HB2	2.50	0.47
5:E:364:ASP:OD1	5:E:365:TYR:N	2.48	0.47
4:A:101:GLN:NE2	5:E:364:ASP:H	2.13	0.47
5:E:344:ALA:HB3	5:E:347:PHE:CE1	2.50	0.47
5:E:401:VAL:HG22	5:E:509:ARG:HG2	1.96	0.46
2:L:6:GLN:NE2	2:L:86:TYR:O	2.49	0.46
4:A:24:ALA:HB3	4:A:77:SER:HB3	1.98	0.46
3:B:110:LYS:HA	3:B:143:TYR:OH	2.15	0.46
4:A:99:LEU:HG	4:A:100:SER:H	1.80	0.46
4:A:36:TRP:CE2	4:A:81:MET:HB2	2.51	0.46
2:L:32:TYR:HD1	2:L:91:LEU:HD12	1.80	0.46
5:E:368:LEU:HD23	5:E:368:LEU:HA	1.75	0.46
1:H:85:SER:HB3	3:B:78:ARG:HH22	1.81	0.45
3:B:12:SER:HB3	3:B:110:LYS:HG3	1.97	0.45
5:E:447:GLY:HA2	5:E:498:GLN:HG2	1.98	0.45
3:B:204:LEU:HD13	3:B:208:VAL:HG23	1.98	0.45
1:H:54:TYR:HB2	5:E:445:VAL:HG12	1.99	0.44
5:E:332:HIS:CE1	5:E:360:ASN:HD22	2.36	0.44
4:A:208:SER:OG	4:A:210:THR:OG1	2.27	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:210:ASN:HB2	2:L:213:GLU:HB2	2.00	0.44
4:A:105:LEU:CD2	6:C:2:NAG:H82	2.48	0.43
1:H:101:ILE:HG21	1:H:112:TRP:CE2	2.53	0.43
5:E:347:PHE:CD1	5:E:509:ARG:HD3	2.54	0.43
1:H:110:ALA:O	2:L:91:LEU:HD13	2.18	0.43
4:A:29:PHE:CE2	4:A:53:PRO:HB3	2.54	0.42
4:A:30:ASN:N	4:A:30:ASN:OD1	2.52	0.42
2:L:40:PRO:HB3	2:L:165:GLU:HG3	2.02	0.42
3:B:94:THR:HG21	5:E:337:PRO:HB3	2.01	0.42
2:L:140:TYR:CG	2:L:141:PRO:HA	2.55	0.42
1:H:132:PRO:HB3	1:H:158:TYR:HB3	2.01	0.42
1:H:114:ASP:HA	1:H:115:PRO:HA	1.93	0.42
2:L:33:LEU:HD12	2:L:89:GLN:O	2.20	0.41
4:A:4:LEU:HD23	4:A:24:ALA:HA	2.02	0.41
3:B:57:THR:CG2	6:C:2:NAG:H2	2.49	0.41
4:A:164:LEU:HD21	4:A:187:VAL:HG21	2.01	0.41
3:B:93:GLY:H	3:B:99:TYR:HE1	1.68	0.41
1:H:58:SER:OG	5:E:444:LYS:HA	2.20	0.41
1:H:40:ARG:HB3	1:H:50:ILE:HD11	2.03	0.41
1:H:109:VAL:HG11	2:L:50:ALA:HB2	2.02	0.41
5:E:350:VAL:HA	5:E:400:PHE:HB2	2.02	0.41
3:B:110:LYS:HG2	3:B:111:ARG:N	2.35	0.41
1:H:85:SER:H	3:B:78:ARG:HH12	1.69	0.41
1:H:12:VAL:O	1:H:124:VAL:HA	2.21	0.40
5:E:502:GLY:O	5:E:506:GLN:HG3	2.21	0.40
5:E:336:CYS:HB2	5:E:338:PHE:CE2	2.56	0.40
5:E:376:THR:HB	5:E:435:ALA:HB3	2.04	0.40

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	H	227/231 (98%)	216 (95%)	11 (5%)	0	100	100
2	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
3	B	216/217 (100%)	204 (94%)	11 (5%)	1 (0%)	29	66
4	A	208/223 (93%)	199 (96%)	9 (4%)	0	100	100
5	E	194/210 (92%)	175 (90%)	18 (9%)	1 (0%)	29	66
All	All	1057/1095 (96%)	999 (94%)	56 (5%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	214	ARG
5	E	521	PRO

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	H	197/200 (98%)	197 (100%)	0	100	100
2	L	186/186 (100%)	185 (100%)	1 (0%)	88	94
3	B	188/188 (100%)	188 (100%)	0	100	100
4	A	177/190 (93%)	174 (98%)	3 (2%)	60	79
5	E	168/180 (93%)	167 (99%)	1 (1%)	86	93
All	All	916/944 (97%)	911 (100%)	5 (0%)	88	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	90	GLN
4	A	29	PHE
4	A	30	ASN
4	A	101	GLN
5	E	343	ASN

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

Mol	Chain	Res	Type
5	E	332	HIS
5	E	360	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)

5 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	$\#\|Z\| > 2$
6	NAG	C	1	6,5	14,14,15	0.78	1 (7%)	17,19,21	0.62	0
6	NAG	C	2	6	14,14,15	0.53	0	17,19,21	0.66	0
6	BMA	C	3	6	11,11,12	0.72	0	15,15,17	0.84	1 (6%)
6	MAN	C	4	6	11,11,12	0.92	0	15,15,17	0.84	1 (6%)
6	FUC	C	5	6	10,10,11	0.79	0	14,14,16	0.76	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
6	NAG	C	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	C	2	6	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	C	3	6	-	2/2/19/22	0/1/1/1
6	MAN	C	4	6	-	2/2/19/22	0/1/1/1
6	FUC	C	5	6	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1	NAG	O5-C1	-2.81	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	4	MAN	O2-C2-C3	-2.25	105.64	110.14
6	C	3	BMA	O5-C5-C6	2.02	110.37	107.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	4	MAN	O5-C5-C6-O6
6	C	4	MAN	C4-C5-C6-O6
6	C	3	BMA	O5-C5-C6-O6
6	C	3	BMA	C4-C5-C6-O6
6	C	2	NAG	C1-C2-N2-C7
6	C	2	NAG	C3-C2-N2-C7

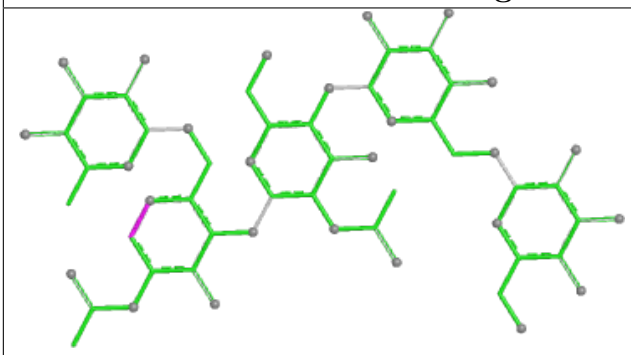
There are no ring outliers.

3 monomers are involved in 5 short contacts:

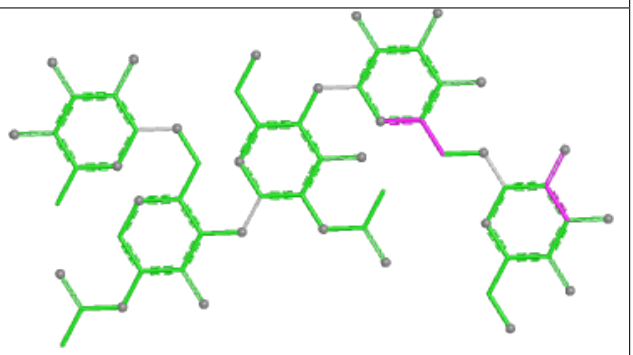
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	5	FUC	1	0
6	C	2	NAG	4	0
6	C	1	NAG	1	0

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

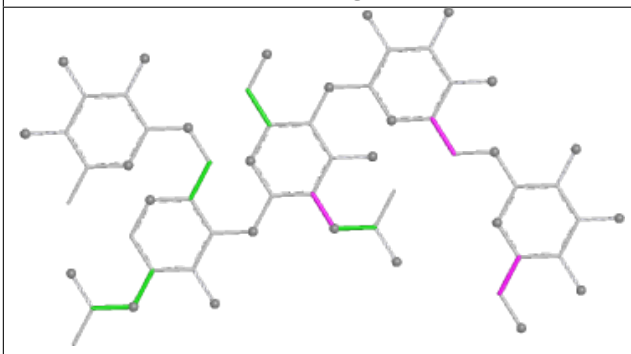
Oligosaccharide Chain C



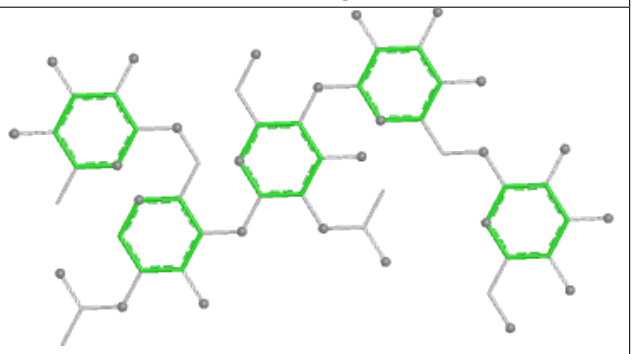
Bond lengths



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	H	229/231 (99%)	0.31	7 (3%) 49 35	65, 113, 172, 281	0
2	L	214/214 (100%)	0.19	1 (0%) 91 85	68, 119, 163, 197	0
3	B	216/217 (99%)	0.65	29 (13%) 3 2	74, 133, 241, 291	0
4	A	212/223 (95%)	0.78	27 (12%) 3 3	86, 142, 217, 296	0
5	E	196/210 (93%)	0.14	4 (2%) 65 52	53, 93, 170, 250	0
All	All	1067/1095 (97%)	0.42	68 (6%) 19 12	53, 119, 213, 296	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	131	PRO	9.6
4	A	132	SER	6.6
4	A	188	THR	5.3
4	A	143	LEU	5.0
3	B	134	SER	4.8
3	B	125	ASP	4.5
3	B	120	ILE	4.2
3	B	195	TYR	4.2
3	B	212	PHE	4.2
3	B	184	LEU	4.1
3	B	122	PRO	3.9
4	A	216	VAL	3.8
4	A	142	ALA	3.7
4	A	130	ALA	3.7
3	B	123	PRO	3.6
4	A	146	LEU	3.6
4	A	199	TYR	3.5
3	B	154	ASP	3.4
1	H	5	GLN	3.4
4	A	185	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	189	TYR	3.3
3	B	197[A]	CYS	3.3
3	B	186	LYS	3.2
4	A	186	VAL	3.1
4	A	128	PRO	3.1
4	A	170	THR	3.0
3	B	133	ALA	3.0
3	B	149	VAL	2.8
4	A	195	GLY	2.8
3	B	136	VAL	2.8
3	B	121	PHE	2.8
4	A	133	SER	2.7
3	B	216	GLU	2.7
3	B	193	LYS	2.7
1	H	202	LEU	2.7
5	E	519	HIS	2.6
3	B	155	ASN	2.6
3	B	129	LYS	2.6
4	A	60	TYR	2.5
4	A	94	TYR	2.5
3	B	124	SER	2.4
3	B	199	VAL	2.4
3	B	151	TRP	2.4
4	A	217	GLU	2.4
2	L	194	CYS	2.3
4	A	191	SER	2.3
4	A	49	GLY	2.3
1	H	143	SER	2.3
4	A	211	LYS	2.3
1	H	135	PHE	2.2
4	A	182	SER	2.2
3	B	210	LYS	2.2
5	E	338	PHE	2.2
4	A	45	LEU	2.2
5	E	344	ALA	2.1
3	B	213	ASN	2.1
5	E	456	PHE	2.1
3	B	11	LEU	2.1
4	A	51	ILE	2.1
4	A	194	LEU	2.1
1	H	53	MET	2.1
1	H	138	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	196	ALA	2.0
3	B	180	SER	2.0
4	A	129	LEU	2.0
4	A	3	GLN	2.0
1	H	157	ASP	2.0
3	B	192	HIS	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)

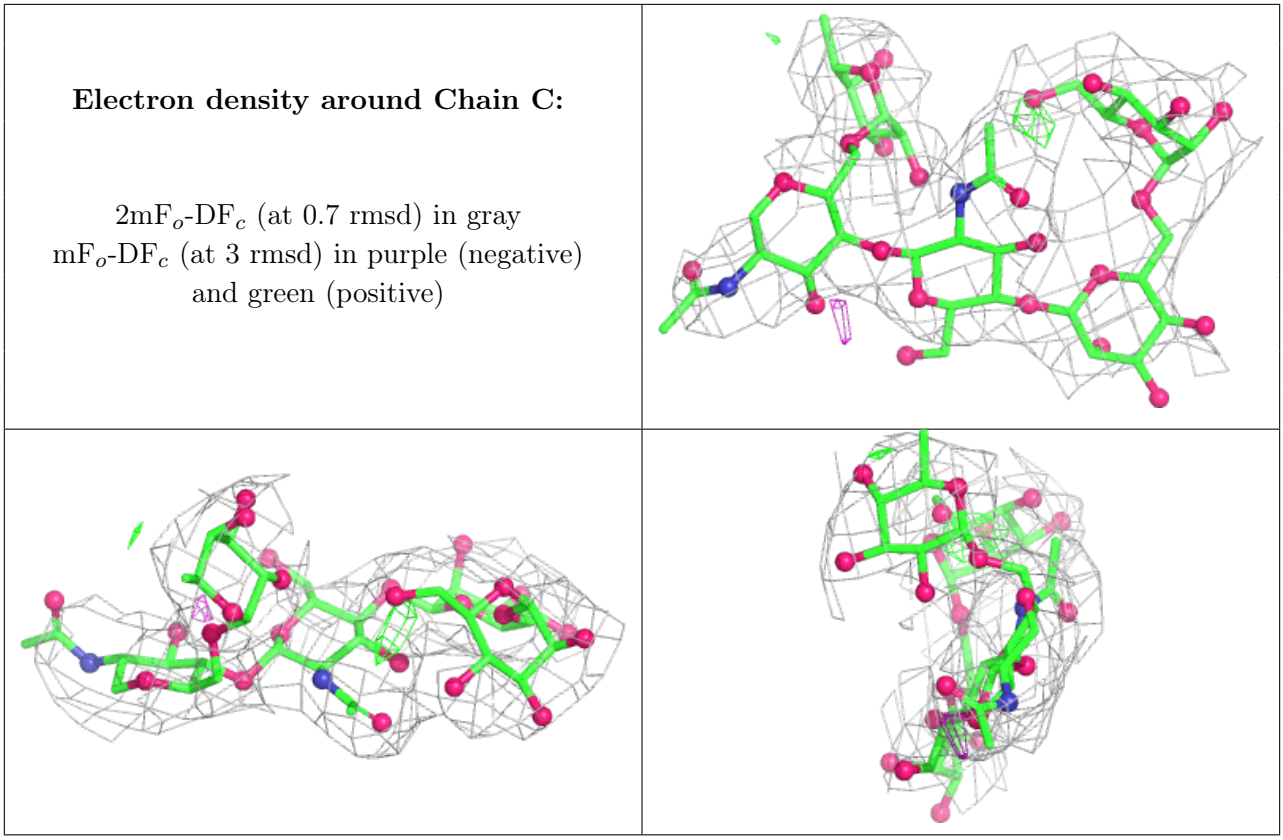
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	BMA	C	3	11/12	0.69	0.24	97,128,131,138	0
6	MAN	C	4	11/12	0.82	0.22	96,126,136,144	0
6	NAG	C	2	14/15	0.88	0.24	92,115,135,149	0
6	FUC	C	5	10/11	0.90	0.27	93,104,113,121	0
6	NAG	C	1	14/15	0.92	0.27	89,96,110,118	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 C:

$2mF_o$-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.