WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 09:34 AM EDT

PDB ID	:	7N4M
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing human antibody WRAIR-2151.
Authors	:	Sankhala, R.S.; Joyce, M.G.
Deposited on	:	2021-06-04
Resolution	:	3.79 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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 ⓘ

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

The reported resolution of this entry is 3.79 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	Percentile Ranks	Value
Rfree		0.328
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		3.3%
RSRZ outliers		14.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
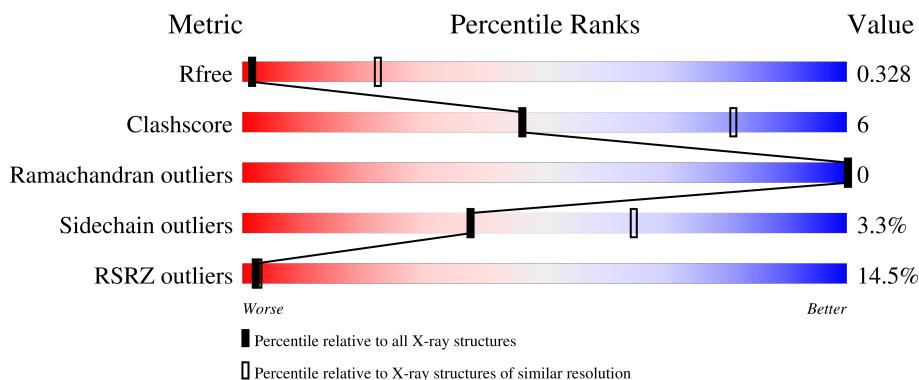
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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	225	6% / 37% 15% · 46%
2	A	205	7% / 84% 15% ·
3	L	216	23% / 87% 12% ·
4	B	2	50% 50%
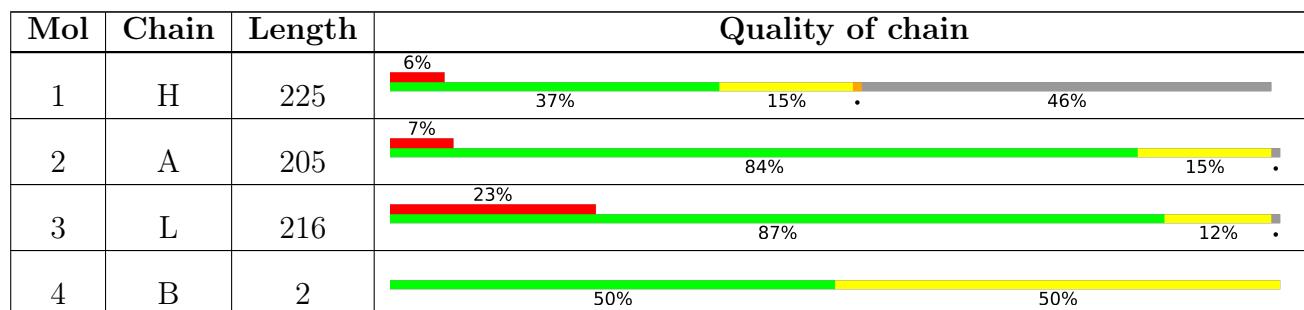
2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4170 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 WRAIR-2151 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	121	Total	C	N	O	S	0	0	0
			933	598	151	182	2			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	202	Total	C	N	O	S	0	0	0
			1597	1020	271	298	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 3 is a protein called WRAIR-2151 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1612	1003	269	335	5			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	2	28	16	2	10	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: WRAIR-2151 antibody Fab heavy chain
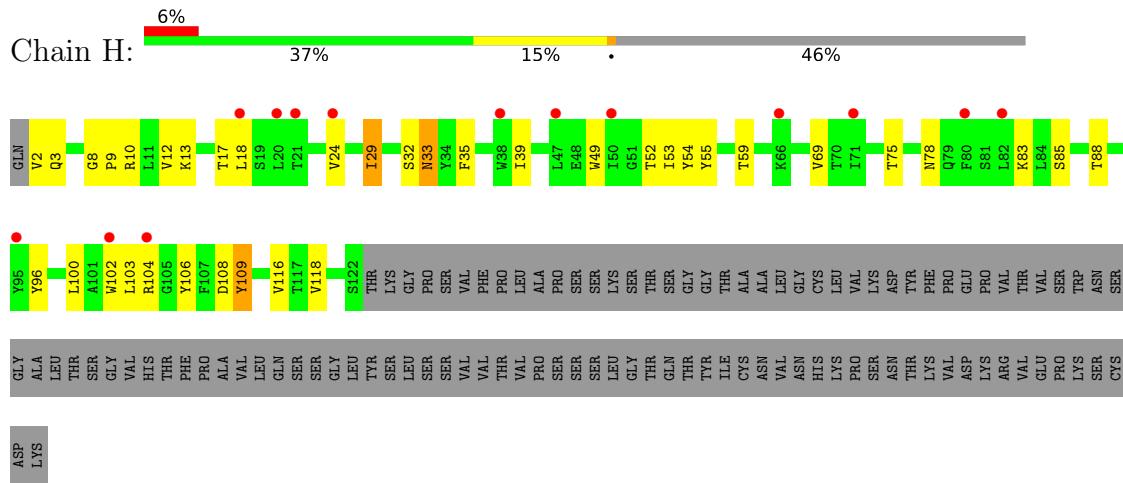
• Molecule 2: Spike protein S1
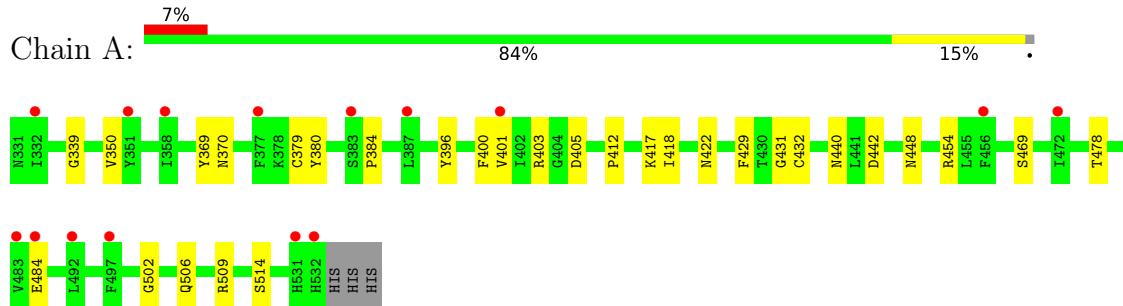
• Molecule 3: WRAIR-2151 antibody Fab light chain
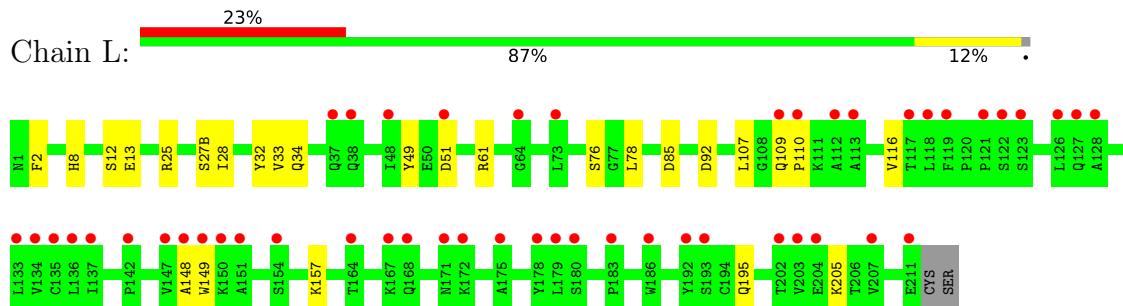
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.91Å 112.91Å 239.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.79 102.13 – 3.67	Depositor EDS
% Data completeness (in resolution range)	97.2 (19.99-3.79) 92.1 (102.13-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.258 , 0.317 0.266 , 0.328	Depositor DCC
R_{free} test set	808 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	155.3	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 172.9	EDS
L-test for twinning[2]	$< |L| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å^2)	200.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

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	0/959	0.47	0/1310
2	A	0.25	0/1644	0.42	0/2237
3	L	0.24	0/1651	0.44	0/2254
All	All	0.24	0/4254	0.44	0/5801

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 ⓘ

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	933	0	897	23	0
2	A	1597	0	1497	20	0
3	L	1612	0	1536	15	0
4	B	28	0	25	1	0
All	All	4170	0	3955	51	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 (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:LEU:HD12	2:A:369:TYR:HB2	1.70	0.73
1:H:35:PHE:HB2	1:H:100:LEU:HB3	1.73	0.69
1:H:102:TRP:O	2:A:370:ASN:ND2	2.24	0.68
1:H:49:TRP:HE1	1:H:52:THR:HG23	1.59	0.67
3:L:149:TRP:H	3:L:157:LYS:HD3	1.59	0.67
1:H:103:LEU:HD13	2:A:384:PRO:HB2	1.78	0.66
1:H:2:VAL:N	1:H:109:TYR:HH	1.95	0.65
3:L:149:TRP:HB2	3:L:157:LYS:HG2	1.78	0.64
1:H:24:VAL:O	1:H:78:ASN:ND2	2.31	0.64
2:A:379:CYS:HA	2:A:432:CYS:HA	1.81	0.62
2:A:339:GLY:HA2	4:B:1:NAG:H83	1.84	0.58
3:L:116:VAL:O	3:L:205:LYS:NZ	2.37	0.57
3:L:25:ARG:HB2	3:L:28:ILE:HD13	1.85	0.57
2:A:401:VAL:HG22	2:A:509:ARG:HG2	1.90	0.54
1:H:29:ILE:HG22	1:H:75:THR:HG22	1.91	0.52
2:A:417:LYS:O	2:A:422:ASN:ND2	2.40	0.52
2:A:440:ASN:OD1	2:A:440:ASN:N	2.41	0.51
2:A:412:PRO:HG3	2:A:429:PHE:HB3	1.93	0.51
3:L:33:VAL:N	3:L:51:ASP:OD1	2.31	0.50
1:H:53:ILE:HD13	1:H:59:THR:HG22	1.93	0.50
1:H:106:TYR:HB3	3:L:34:GLN:HG2	1.93	0.50
2:A:350:VAL:HA	2:A:400:PHE:HB2	1.93	0.50
1:H:8:GLY:N	1:H:9:PRO:HD3	2.27	0.49
2:A:454:ARG:NH2	2:A:469:SER:O	2.26	0.49
3:L:25:ARG:NH1	3:L:27(B):SER:O	2.46	0.49
1:H:17:THR:HG22	1:H:85:SER:HA	1.96	0.48
1:H:32:SER:HB3	1:H:55:TYR:HB3	1.95	0.47
3:L:12:SER:HB2	3:L:107:LEU:HD21	1.96	0.47
2:A:379:CYS:N	3:L:32:TYR:OH	2.47	0.47
2:A:418:ILE:HA	2:A:422:ASN:HB2	1.96	0.47
2:A:442:ASP:O	2:A:448:ASN:ND2	2.45	0.47
3:L:34:GLN:HG3	3:L:49:TYR:HA	1.97	0.47
3:L:61:ARG:HB3	3:L:76:SER:O	2.16	0.46
2:A:380:TYR:N	2:A:431:GLY:O	2.48	0.45
3:L:148:ALA:HB3	3:L:195:GLN:HB2	1.99	0.45
1:H:39:ILE:O	1:H:96:TYR:N	2.39	0.45
1:H:33:ASN:HB2	1:H:102:TRP:CZ2	2.52	0.44
2:A:417:LYS:HB2	2:A:417:LYS:HE2	1.77	0.44
2:A:502:GLY:O	2:A:506:GLN:HG3	2.17	0.44
1:H:12:VAL:HG21	1:H:18:LEU:HD12	2.00	0.44
1:H:32:SER:O	1:H:54:TYR:OH	2.22	0.43
1:H:106:TYR:CB	3:L:34:GLN:HG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:403:ARG:NH1	2:A:405:ASP:OD2	2.53	0.42
3:L:109:GLN:HA	3:L:110:PRO:HD3	1.92	0.42
2:A:396:TYR:HB2	2:A:514:SER:HB2	2.02	0.41
1:H:88:THR:O	1:H:118:VAL:HG21	2.21	0.41
1:H:102:TRP:HB3	2:A:369:TYR:HE1	1.85	0.41
3:L:25:ARG:NH2	3:L:92:ASP:OD2	2.53	0.41
1:H:24:VAL:HB	1:H:78:ASN:ND2	2.36	0.40
1:H:18:LEU:HD11	1:H:116:VAL:HG11	2.03	0.40
1:H:69:VAL:HA	1:H:83:LYS:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	119/225 (53%)	108 (91%)	11 (9%)	0	100	100
2	A	200/205 (98%)	193 (96%)	7 (4%)	0	100	100
3	L	210/216 (97%)	203 (97%)	7 (3%)	0	100	100
All	All	529/646 (82%)	504 (95%)	25 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	H	102/193 (53%)	94 (92%)	8 (8%)	12	42
2	A	174/177 (98%)	172 (99%)	2 (1%)	73	85
3	L	185/189 (98%)	180 (97%)	5 (3%)	44	69
All	All	461/559 (82%)	446 (97%)	15 (3%)	38	65

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	10	ARG
1	H	13	LYS
1	H	29	ILE
1	H	33	ASN
1	H	104	ARG
1	H	108	ASP
1	H	109	TYR
2	A	478	THR
2	A	484	GLU
3	L	2	PHE
3	L	8	HIS
3	L	13	GLU
3	L	78	LEU
3	L	85	ASP

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

Mol	Chain	Res	Type
1	H	41	GLN
3	L	38	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 ⓘ

2 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	B	1	2,4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	2	4	14,14,15	0.25	0	17,19,21	0.41	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	B	1	2,4	-	1/6/23/26	0/1/1/1
4	NAG	B	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	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 B
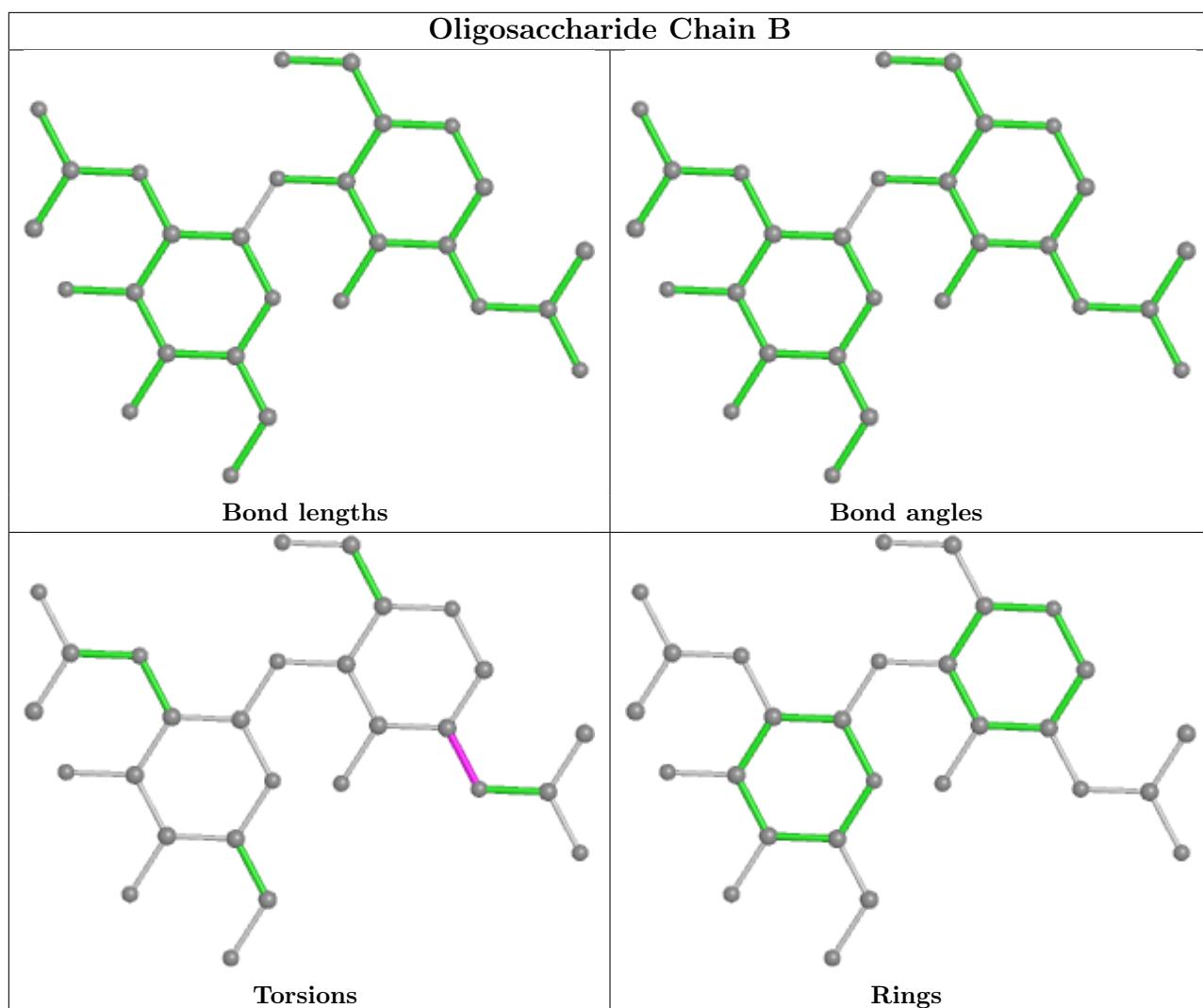
5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	108:GLY	C	109:GLN	N	3.11

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, 95th 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	121/225 (53%)	0.99	14 (11%)	4	5	110, 158, 215, 294	0
2	A	202/205 (98%)	0.82	15 (7%)	14	11	113, 159, 234, 321	0
3	L	214/216 (99%)	1.26	49 (22%)	0	0	134, 269, 372, 420	0
All	All	537/646 (83%)	1.04	78 (14%)	2	2	110, 175, 344, 420	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	134	VAL	8.0
3	L	126	LEU	7.8
3	L	178	TYR	7.2
3	L	171	ASN	6.8
3	L	175	ALA	6.7
1	H	102	TRP	6.3
3	L	118	LEU	6.0
3	L	119	PHE	6.0
3	L	147	VAL	5.0
3	L	123	SER	4.9
3	L	121	PRO	4.6
3	L	203	VAL	4.5
2	A	383	SER	4.3
3	L	112	ALA	4.3
3	L	137	ILE	4.2
3	L	151	ALA	4.2
3	L	127	GLN	4.1
3	L	179	LEU	4.1
3	L	122	SER	4.1
2	A	531	HIS	3.9
2	A	351	TYR	3.9
3	L	113	ALA	3.9
1	H	47	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	532	HIS	3.8
3	L	167	LYS	3.8
3	L	135	CYS	3.7
3	L	133	LEU	3.6
3	L	186	TRP	3.5
3	L	168	GLN	3.5
3	L	109	GLN	3.4
3	L	211	GLU	3.4
3	L	183	PRO	3.3
3	L	149	TRP	3.1
3	L	172	LYS	3.1
2	A	332	ILE	3.1
1	H	21	THR	3.1
2	A	497	PHE	3.0
2	A	483	VAL	3.0
1	H	20	LEU	3.0
1	H	18	LEU	2.8
1	H	50	ILE	2.7
3	L	192	TYR	2.7
3	L	202	THR	2.7
3	L	148	ALA	2.7
1	H	80	PHE	2.7
3	L	154	SER	2.7
3	L	110	PRO	2.6
3	L	180	SER	2.6
2	A	492	LEU	2.5
3	L	48	ILE	2.5
3	L	64	GLY	2.5
3	L	150	LYS	2.5
3	L	37	GLN	2.4
1	H	82	LEU	2.4
1	H	71	ILE	2.4
3	L	207	VAL	2.4
3	L	38	GLN	2.3
3	L	117	THR	2.3
2	A	456	PHE	2.3
3	L	142	PRO	2.2
2	A	387	LEU	2.2
2	A	401	VAL	2.2
2	A	472	ILE	2.2
2	A	358	ILE	2.2
2	A	377	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	193	SER	2.2
1	H	24	VAL	2.2
1	H	66	LYS	2.1
3	L	51	ASP	2.1
2	A	484	GLU	2.1
1	H	38	TRP	2.1
3	L	128	ALA	2.1
1	H	104	ARG	2.1
1	H	95	TYR	2.1
3	L	164	THR	2.1
3	L	136	LEU	2.1
3	L	73	LEU	2.1
3	L	204	GLU	2.0

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 ⓘ

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, 95th 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	B	2	14/15	0.85	0.34	325,330,336,337	0
4	NAG	B	1	14/15	0.90	0.22	243,261,305,314	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 B:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
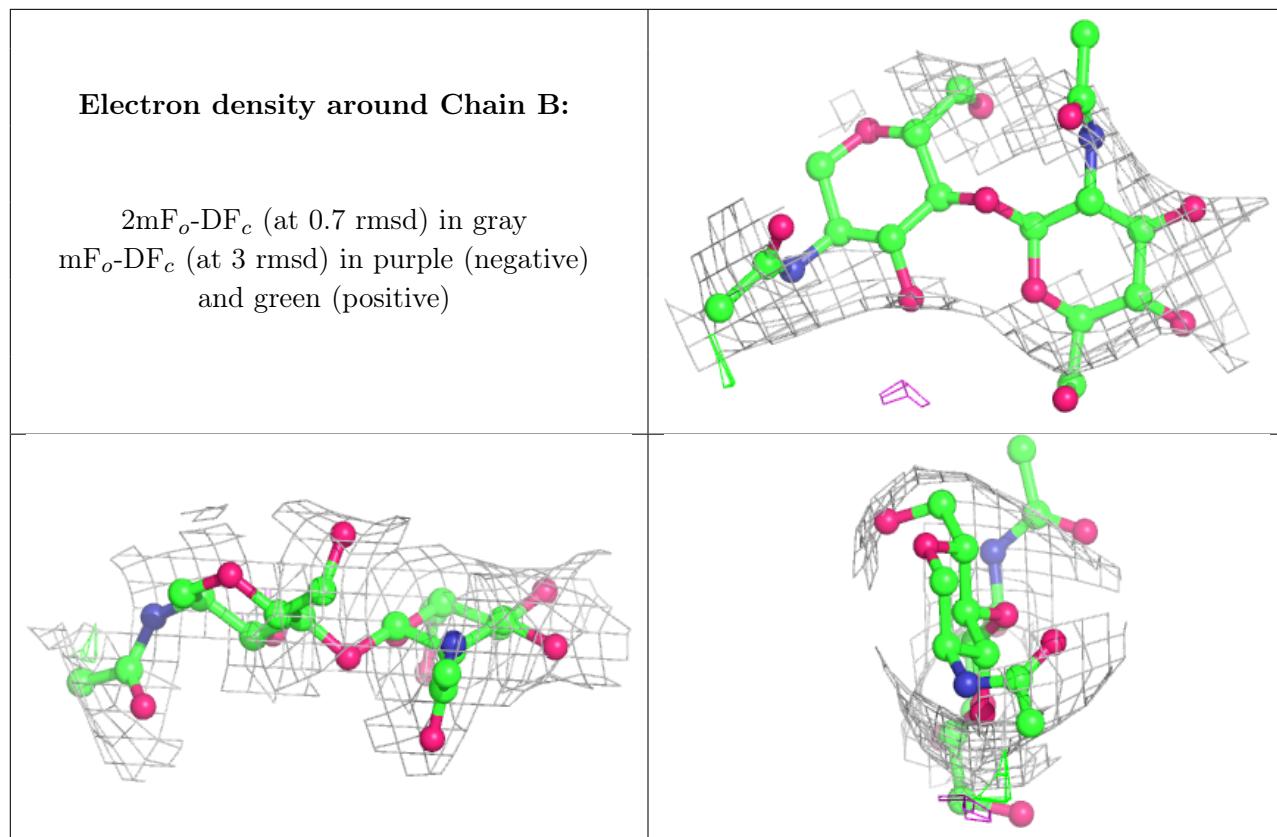
6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.