



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2022 – 04:06 PM EDT

PDB ID : 7TTY
Title : Crystal structure of potent neutralizing antibody 10-40 in complex with bat WIV1 receptor-binding domain
Authors : Reddem, E.R.; Shapiro, L.
Deposited on : 2022-02-02
Resolution : 3.11 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
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) : 2.28.1

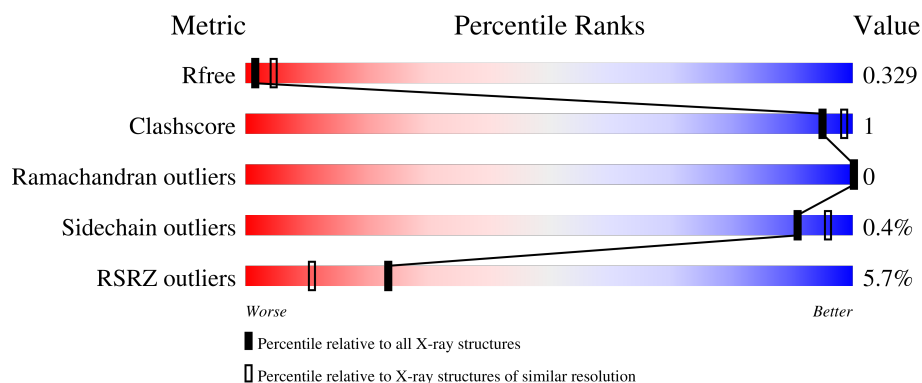
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	195	<div> <div>14%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>• •</div> </div> </div>
2	H	233	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
3	L	213	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>•</div> </div> </div>
4	B	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9600 atoms, of which 4705 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	A	190	Total	C	H	N	O	S	0	2	0
			2946	974	1431	251	282	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	LYS	-	expression tag	UNP U5WI05

- Molecule 2 is a protein called 1040 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	230	Total	C	H	N	O	S	0	4	0
			3436	1102	1701	284	343	6			

- Molecule 3 is a protein called 1040 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	213	Total	C	H	N	O	S	0	2	0
			3165	1004	1548	270	337	6			

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

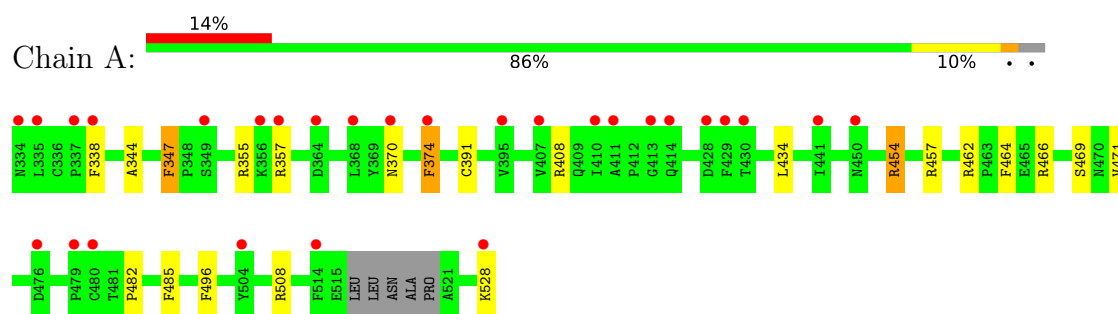


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	B	2	Total	C	H	N	O		0	0	0
			53	16	25	2	10				

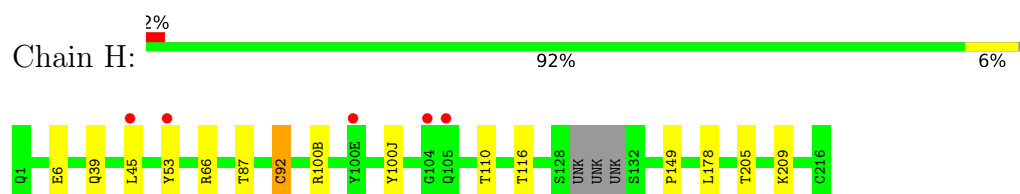
3 Residue-property plots

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.

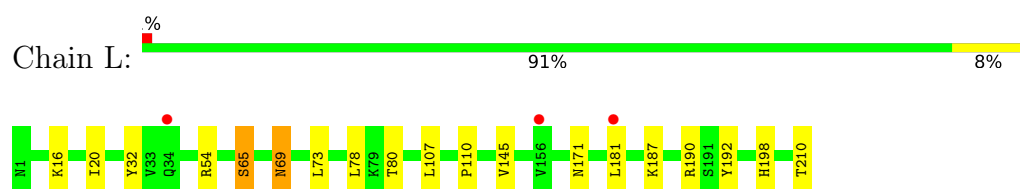
• Molecule 1: Spike protein S1



• Molecule 2: 1040 heavy chain



• Molecule 3: 1040 light chain



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.31Å 69.55Å 95.22Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	91.69 – 3.11 91.69 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.3 (91.69-3.11) 97.3 (91.69-3.11)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.235 , 0.329 0.235 , 0.329	Depositor DCC
R_{free} test set	1148 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	109.2	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 85.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.106 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9600	wwPDB-VP
Average B, all atoms (Å ²)	131.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	A	0.77	3/1561 (0.2%)	1.24	15/2128 (0.7%)
2	H	0.64	1/1787 (0.1%)	1.02	4/2440 (0.2%)
3	L	0.71	3/1665 (0.2%)	1.14	11/2271 (0.5%)
All	All	0.70	7/5013 (0.1%)	1.13	30/6839 (0.4%)

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	A	0	4
2	H	0	3
3	L	0	1
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	CYS	CB-SG	-9.80	1.65	1.82
3	L	192	TYR	CD1-CE1	-6.14	1.30	1.39
3	L	69	ASN	CG-OD1	-6.03	1.10	1.24
3	L	32	TYR	CD1-CE1	-6.00	1.30	1.39
2	H	209	LYS	CE-NZ	-5.38	1.35	1.49
1	A	485	PHE	CD1-CE1	-5.21	1.28	1.39
1	A	528	LYS	CD-CE	5.13	1.64	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	78	LEU	CB-CG-CD1	12.85	132.84	111.00
3	L	54	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	347	PHE	CB-CG-CD2	-10.92	113.16	120.80
2	H	66	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	A	485	PHE	CB-CG-CD1	10.21	127.94	120.80
1	A	347	PHE	CB-CG-CD1	9.55	127.49	120.80
1	A	338	PHE	CB-CG-CD1	9.31	127.32	120.80
1	A	466	ARG	NE-CZ-NH1	8.86	124.73	120.30
3	L	190	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	464	PHE	CB-CG-CD1	8.31	126.62	120.80
3	L	181	LEU	CA-CB-CG	8.02	133.73	115.30
1	A	457	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	408	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	454	ARG	NE-CZ-NH2	7.74	124.17	120.30
3	L	78	LEU	CA-CB-CG	7.74	133.10	115.30
3	L	16	LYS	CB-CG-CD	7.66	131.51	111.60
3	L	32	TYR	CB-CG-CD1	7.45	125.47	121.00
3	L	192	TYR	CB-CG-CD1	7.29	125.37	121.00
1	A	462	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	L	107	LEU	CA-CB-CG	6.74	130.80	115.30
1	A	434	LEU	CA-CB-CG	6.60	130.47	115.30
1	A	357	ARG	NE-CZ-NH1	6.53	123.57	120.30
3	L	16	LYS	CA-CB-CG	5.96	126.52	113.40
1	A	374	PHE	CB-CG-CD1	5.86	124.90	120.80
2	H	178	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	355	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	H	100(J)	TYR	CA-CB-CG	5.34	123.55	113.40
1	A	496	PHE	CB-CG-CD1	5.21	124.45	120.80
2	H	92	CYS	CA-CB-SG	5.16	123.30	114.00
3	L	110	PRO	CA-N-CD	-5.11	104.35	111.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	347	PHE	Sidechain
1	A	370	ASN	Peptide
1	A	471	VAL	Peptide
1	A	482	PRO	Peptide
2	H	149	PRO	Peptide
2	H	205	THR	Peptide
2	H	53	TYR	Peptide
3	L	69	ASN	Sidechain

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	A	1515	1431	1418	3	0
2	H	1735	1701	1694	4	0
3	L	1617	1548	1536	5	0
4	B	28	25	25	0	0
All	All	4895	4705	4673	11	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 1.

All (11) 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:A:454:ARG:NH1	1:A:469:SER:O	2.41	0.54
1:A:374:PHE:O	2:H:100(B):ARG:NH2	2.40	0.53
3:L:187:LYS:NZ	3:L:210:THR:O	2.46	0.48
1:A:344:ALA:O	1:A:508:ARG:NH1	2.46	0.48
2:H:87:THR:HG23	2:H:110:THR:HA	1.95	0.48
2:H:6:GLU:OE2	2:H:92:CYS:N	2.45	0.47
3:L:20:ILE:HD12	3:L:73:LEU:HD23	1.96	0.47
3:L:80:THR:O	3:L:171:ASN:ND2	2.49	0.45
3:L:145:VAL:HG12	3:L:198:HIS:HB2	1.98	0.45
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.00	0.44

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	A	186/195 (95%)	166 (89%)	20 (11%)	0	100	100
2	H	228/233 (98%)	209 (92%)	19 (8%)	0	100	100
3	L	213/213 (100%)	196 (92%)	17 (8%)	0	100	100
All	All	627/641 (98%)	571 (91%)	56 (9%)	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	A	166/170 (98%)	166 (100%)	0	100	100
2	H	200/198 (101%)	198 (99%)	2 (1%)	76	89
3	L	188/186 (101%)	186 (99%)	2 (1%)	73	88
All	All	554/554 (100%)	550 (99%)	4 (1%)	91	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	116[A]	THR
2	H	116[B]	THR
3	L	65[A]	SER
3	L	65[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	4,1	14,14,15	0.54	0	17,19,21	0.85	1 (5%)
4	NAG	B	2	4	14,14,15	0.54	0	17,19,21	0.62	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	4,1	-	2/6/23/26	0/1/1/1
4	NAG	B	2	4	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	NAG	C1-O5-C5	2.47	115.53	112.19

There are no chirality outliers.

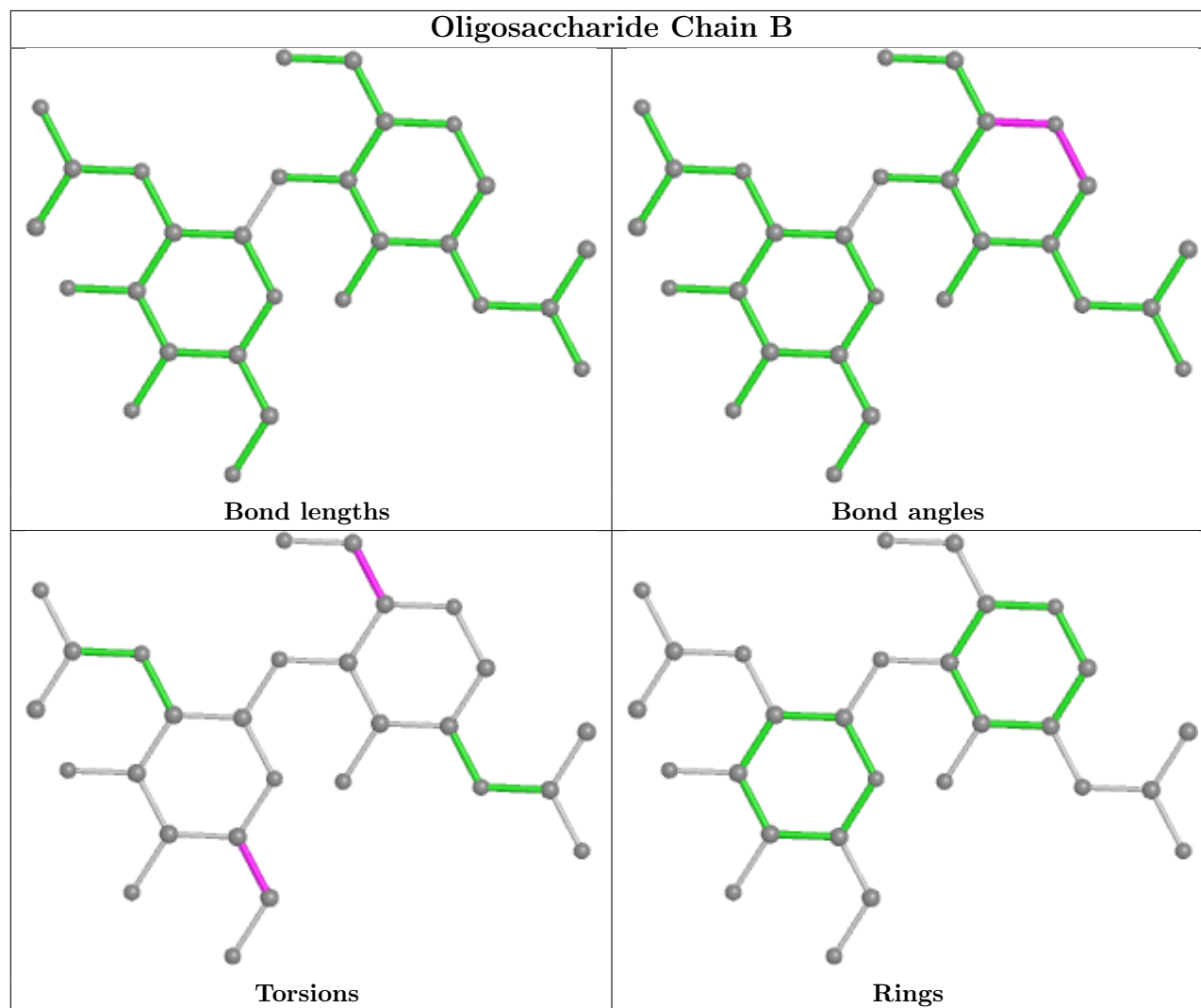
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1	NAG	O5-C5-C6-O6
4	B	2	NAG	O5-C5-C6-O6
4	B	1	NAG	C4-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.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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, 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	A	190/195 (97%)	0.72	28 (14%) 2 1	104, 139, 200, 238	0
2	H	230/233 (98%)	0.28	5 (2%) 62 41	74, 108, 142, 178	1 (0%)
3	L	213/213 (100%)	0.14	3 (1%) 75 58	75, 105, 144, 181	0
All	All	633/641 (98%)	0.36	36 (5%) 23 11	74, 115, 174, 238	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	ASP	5.0
1	A	368	LEU	4.8
1	A	429	PHE	4.6
1	A	338	PHE	4.1
1	A	407	VAL	3.8
1	A	337	PRO	3.8
3	L	34	GLN	3.6
3	L	181	LEU	3.4
2	H	53	TYR	3.2
1	A	514	PHE	3.2
1	A	370	ASN	3.2
1	A	413	GLY	3.2
1	A	410	ILE	3.0
1	A	414	GLN	3.0
1	A	395	VAL	2.9
1	A	476	ASP	2.9
1	A	479	PRO	2.9
1	A	335	LEU	2.8
1	A	411	ALA	2.8
2	H	45	LEU	2.8
3	L	156	VAL	2.8
1	A	528	LYS	2.8
1	A	504	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	480	CYS	2.6
1	A	349	SER	2.5
1	A	450	ASN	2.5
1	A	364	ASP	2.4
2	H	100(E)[A]	TYR	2.4
1	A	356	LYS	2.4
2	H	105	GLN	2.3
1	A	441	ILE	2.3
1	A	334	ASN	2.2
2	H	104	GLY	2.2
1	A	357	ARG	2.2
1	A	430	THR	2.1
1	A	374	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

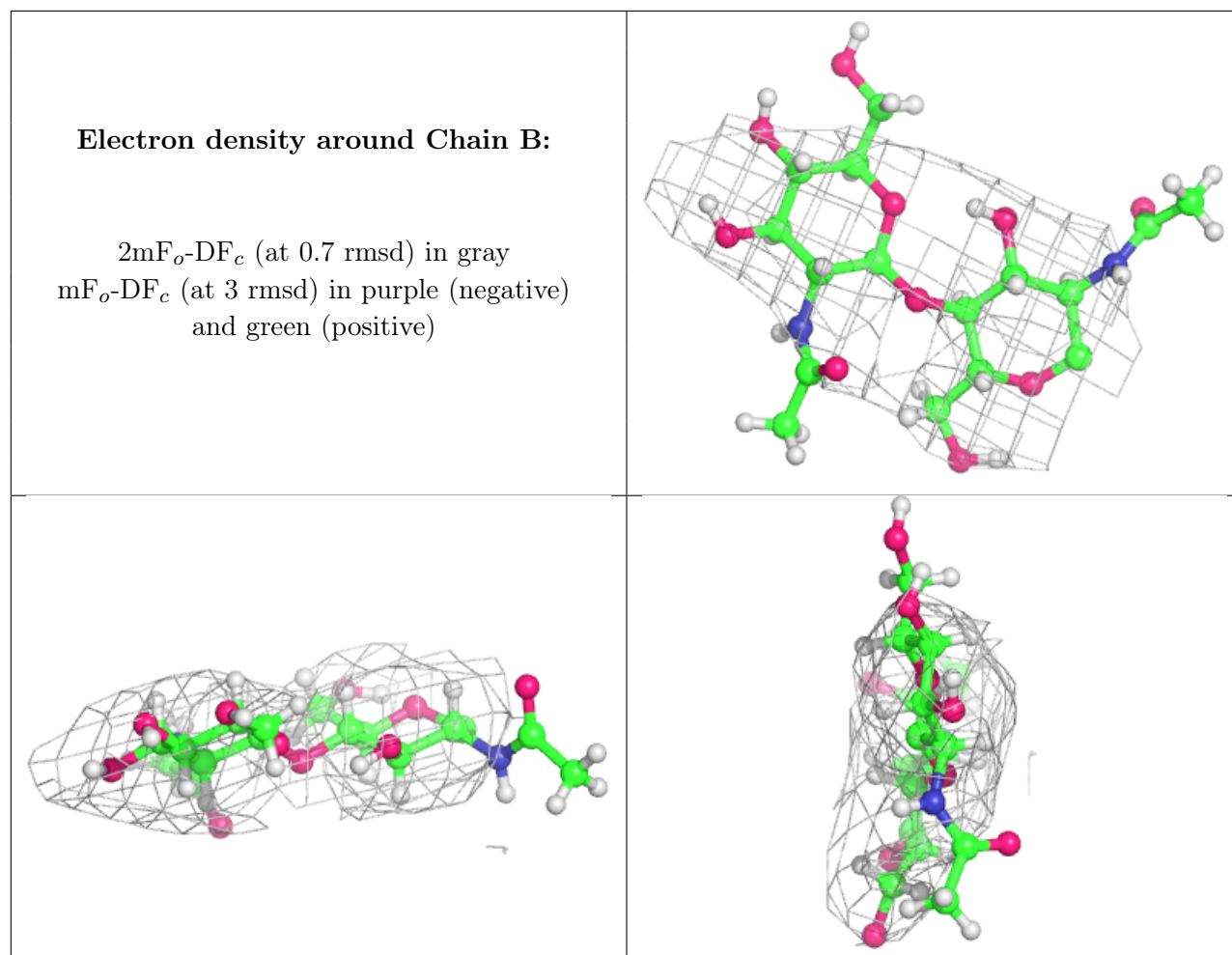
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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	0.74	0.28	137,169,203,208	0
4	NAG	B	1	14/15	0.84	0.22	135,167,185,207	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.



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.