



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 04:38 PM EST

PDB ID : 9BDH
Title : Crystal structure of HIV-1 MPER scaffold in complex with antibody Fab Ab45.1
Authors : Lee, C.C.D.; Wilson, I.A.
Deposited on : 2024-04-11
Resolution : 3.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

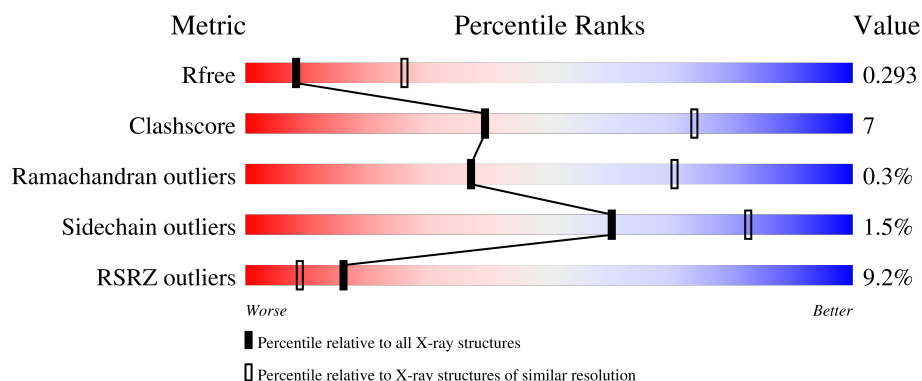
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	H	225	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
2	L	218	<div> <div>3%</div> <div>82%</div> <div>17%</div> </div>
3	C	153	<div> <div>18%</div> <div>73%</div> <div>25%</div> <div>.</div> </div>
4	A	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4639 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 Fab 45.1 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	225	Total	C	N	O	S	0	0	0
			1701	1075	280	339	7			

- Molecule 2 is a protein called Fab 45.1 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	218	Total	C	N	O	S	0	0	0
			1681	1053	284	337	7			

- Molecule 3 is a protein called GT10.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	153	Total	C	N	O	S	0	0	0
			1229	787	210	228	4			

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

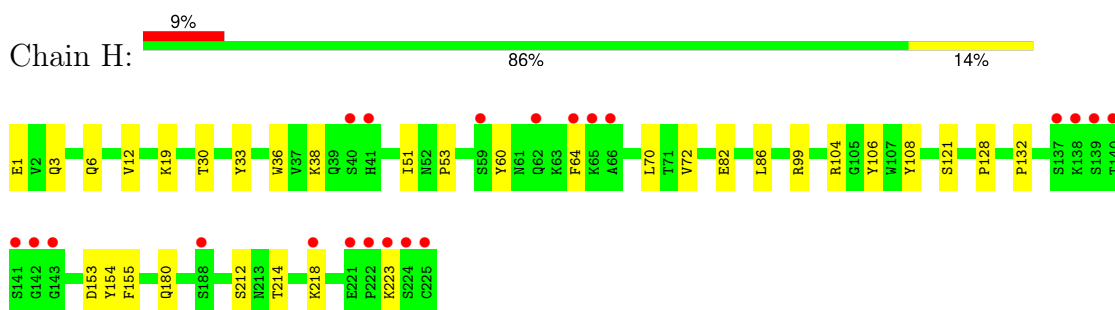


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	A	2	Total	C	N	O	0	0	0
			28	16	2	10			

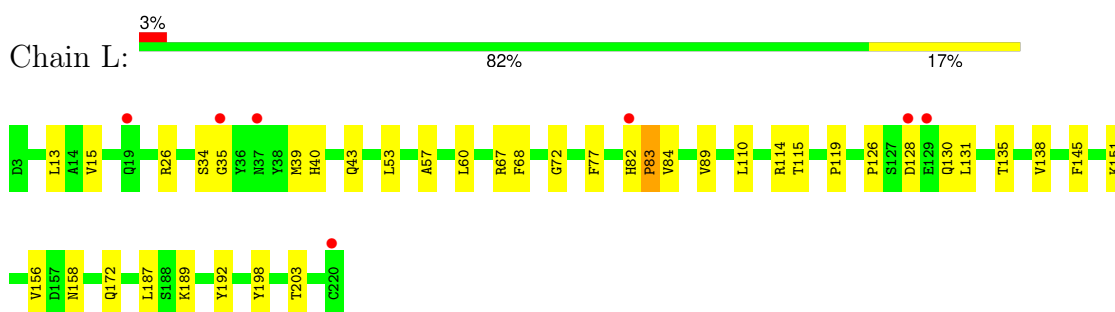
3 Residue-property plots

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.

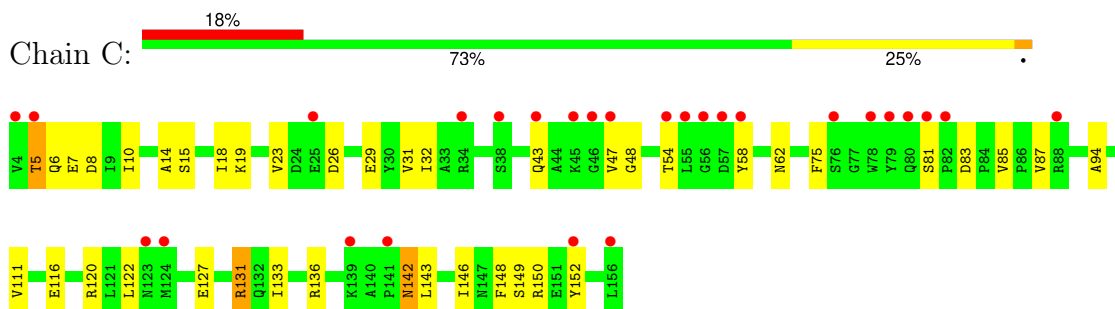
- Molecule 1: Fab 45.1 Heavy Chain



- Molecule 2: Fab 45.1 Light Chain



- Molecule 3: GT10.2



- 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 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.96Å 196.96Å 93.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.24 – 3.00 49.24 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (49.24-3.00) 96.7 (49.24-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.269 , 0.290 0.271 , 0.293	Depositor DCC
R_{free} test set	2122 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.007 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4639	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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 [i](#)

5.1 Standard geometry [i](#)

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	0/1744	0.47	0/2372
2	L	0.27	0/1719	0.49	0/2334
3	C	0.28	0/1255	0.51	0/1703
All	All	0.27	0/4718	0.49	0/6409

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 [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	H	1701	0	1662	17	0
2	L	1681	0	1630	20	0
3	C	1229	0	1234	25	0
4	A	28	0	25	0	0
All	All	4639	0	4551	61	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 7.

All (61) 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:C:31:VAL:HG12	3:C:54:THR:HB	1.71	0.73
1:H:128:PRO:HB3	1:H:154:TYR:HB3	1.73	0.70
2:L:192:TYR:O	2:L:198:TYR:OH	2.10	0.69
3:C:75:PHE:HB2	3:C:87:VAL:HG21	1.73	0.69
1:H:132:PRO:HD3	1:H:218:LYS:HE2	1.76	0.67
2:L:82:HIS:HB2	2:L:83:PRO:HD3	1.76	0.66
3:C:29:GLU:N	3:C:29:GLU:OE2	2.29	0.66
2:L:67:ARG:HB2	2:L:83:PRO:HD2	1.81	0.61
1:H:33:TYR:HB2	1:H:99:ARG:HD2	1.85	0.58
1:H:36:TRP:CD1	1:H:70:LEU:HD11	2.39	0.57
2:L:128:ASP:HA	2:L:131:LEU:HD23	1.87	0.57
2:L:34:SER:OG	2:L:35:GLY:N	2.39	0.56
2:L:39:MET:HB3	2:L:57:ALA:HB2	1.87	0.56
3:C:43:GLN:HG2	3:C:85:VAL:HG13	1.88	0.55
3:C:143:LEU:O	3:C:146:ILE:HG22	2.08	0.53
1:H:153:ASP:OD1	1:H:180:GLN:NE2	2.41	0.53
3:C:5:THR:OG1	3:C:6:GLN:N	2.42	0.52
2:L:130:GLN:HG2	2:L:135:THR:O	2.09	0.52
2:L:126:PRO:HD3	2:L:138:VAL:HG22	1.91	0.52
3:C:131:ARG:HH21	3:C:150:ARG:HH12	1.55	0.52
2:L:89:VAL:HG21	2:L:172:GLN:HB3	1.92	0.52
3:C:18:ILE:HG12	3:C:23:VAL:HG23	1.92	0.52
1:H:108:TYR:HB3	2:L:40:HIS:CE1	2.45	0.52
2:L:43:GLN:HB2	2:L:53:LEU:HD11	1.93	0.51
1:H:51:ILE:HD13	1:H:72:VAL:HG13	1.92	0.51
1:H:12:VAL:HG11	1:H:86:LEU:HD12	1.93	0.51
1:H:19:LYS:HG3	1:H:82:GLU:HB2	1.93	0.50
3:C:62:ASN:HB3	3:C:146:ILE:HD12	1.93	0.50
2:L:119:PRO:HB3	2:L:145:PHE:HB3	1.93	0.49
2:L:72:GLY:HA3	2:L:77:PHE:HA	1.93	0.49
2:L:131:LEU:HD12	2:L:189:LYS:HG3	1.95	0.49
3:C:7:GLU:N	3:C:7:GLU:OE2	2.45	0.49
3:C:48:GLY:HA3	3:C:87:VAL:HA	1.93	0.49
2:L:15:VAL:HG21	2:L:84:VAL:HG21	1.94	0.48
2:L:13:LEU:HD23	2:L:110:LEU:HD13	1.96	0.48
2:L:151:LYS:HB3	2:L:203:THR:HB	1.96	0.48
3:C:81:SER:O	3:C:83:ASP:N	2.42	0.46
1:H:104:ARG:HD3	1:H:106:TYR:CE2	2.50	0.46
1:H:212:SER:OG	1:H:214:THR:OG1	2.28	0.45
3:C:127:GLU:OE2	3:C:150:ARG:NH1	2.50	0.44
1:H:38:LYS:HD3	1:H:64:PHE:CZ	2.52	0.44
3:C:14:ALA:O	3:C:18:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:SER:C	3:C:83:ASP:H	2.21	0.43
1:H:1:GLU:OE1	1:H:3:GLN:NE2	2.49	0.43
2:L:60:LEU:HD11	2:L:68:PHE:O	2.19	0.42
3:C:5:THR:HG22	3:C:8:ASP:OD2	2.19	0.42
1:H:30:THR:HA	1:H:53:PRO:HB2	2.02	0.42
3:C:149:SER:H	3:C:152:TYR:HD2	1.66	0.41
2:L:156:VAL:HG22	2:L:198:TYR:HD1	1.85	0.41
3:C:142:ASN:HB3	3:C:143:LEU:H	1.71	0.41
3:C:15:SER:O	3:C:19:LYS:HD3	2.20	0.41
3:C:47:VAL:HG11	3:C:122:LEU:HD21	2.03	0.41
3:C:133:ILE:HB	3:C:148:PHE:CE2	2.55	0.41
3:C:62:ASN:HA	3:C:94:ALA:O	2.21	0.41
3:C:111:VAL:HA	3:C:136:ARG:HH12	1.84	0.41
1:H:223:LYS:HE3	1:H:223:LYS:HB2	1.93	0.41
3:C:116:GLU:O	3:C:120:ARG:HG3	2.21	0.41
1:H:121:SER:HG	1:H:155:PHE:HZ	1.69	0.40
1:H:60:TYR:HE1	1:H:70:LEU:HD23	1.86	0.40
2:L:114:ARG:NH1	2:L:115:THR:OG1	2.55	0.40
3:C:10:ILE:HG21	3:C:32:ILE:HG13	2.04	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	223/225 (99%)	209 (94%)	14 (6%)	0	100	100
2	L	216/218 (99%)	207 (96%)	8 (4%)	1 (0%)	25	61
3	C	151/153 (99%)	140 (93%)	10 (7%)	1 (1%)	19	54
All	All	590/596 (99%)	556 (94%)	32 (5%)	2 (0%)	37	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	142	ASN
2	L	83	PRO

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	194/194 (100%)	193 (100%)	1 (0%)	86	94
2	L	192/192 (100%)	189 (98%)	3 (2%)	58	82
3	C	135/135 (100%)	131 (97%)	4 (3%)	36	69
All	All	521/521 (100%)	513 (98%)	8 (2%)	60	83

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	6	GLN
2	L	26	ARG
2	L	158	ASN
2	L	187	LEU
3	C	5	THR
3	C	26	ASP
3	C	58	TYR
3	C	131	ARG

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	A	1	4,3	14,14,15	0.68	0	17,19,21	1.03	1 (5%)
4	NAG	A	2	4	14,14,15	0.71	0	17,19,21	0.91	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	A	1	4,3	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	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	A	1	NAG	O5-C1-C2	-2.22	107.85	111.29

There are no chirality outliers.

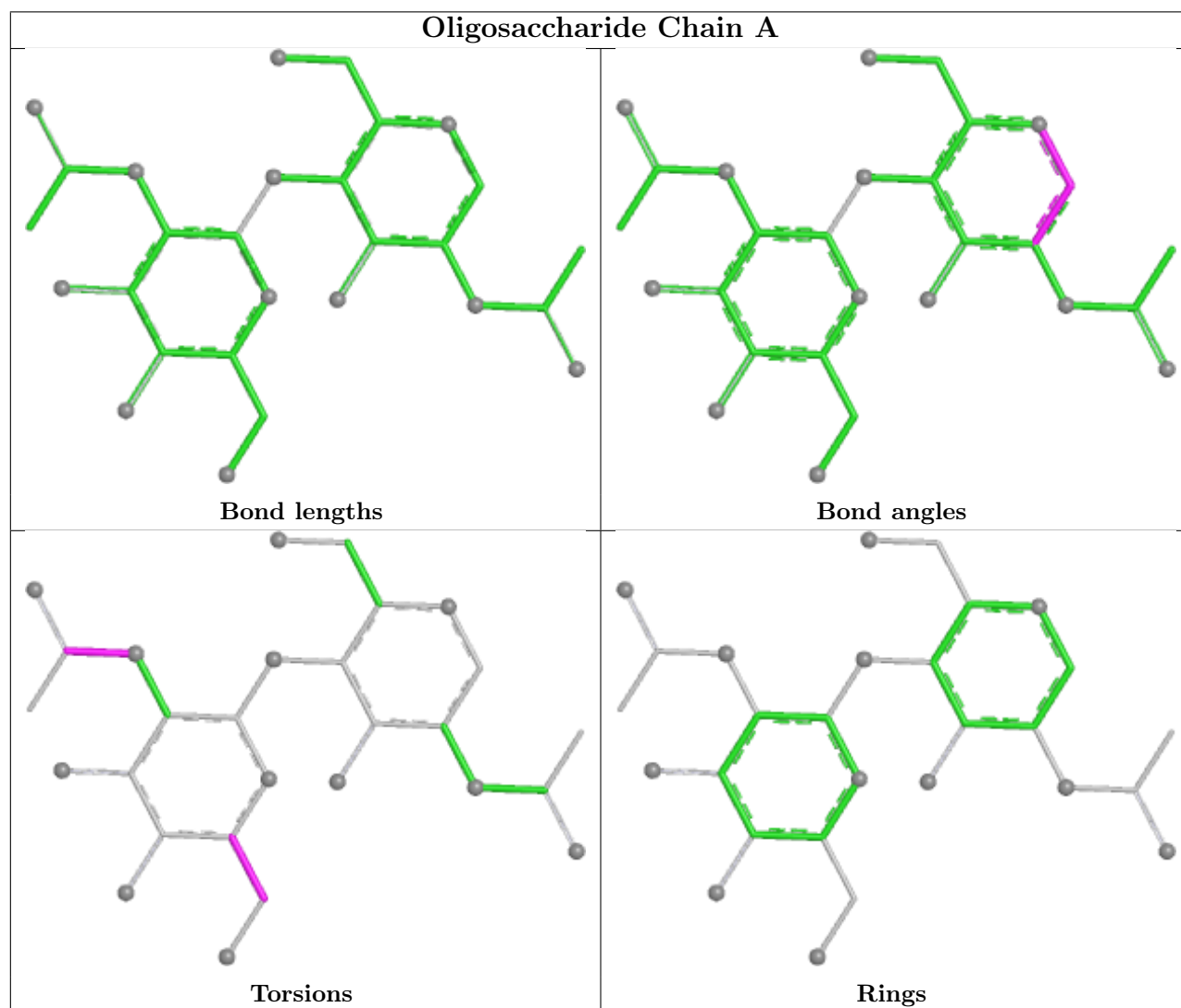
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
4	A	2	NAG	C4-C5-C6-O6
4	A	2	NAG	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.



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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	225/225 (100%)	0.36	21 (9%) 16 9	43, 66, 116, 164	0
2	L	218/218 (100%)	0.35	7 (3%) 50 30	47, 68, 89, 135	0
3	C	153/153 (100%)	1.07	27 (17%) 4 3	53, 84, 114, 142	0
All	All	596/596 (100%)	0.54	55 (9%) 16 9	43, 70, 110, 164	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	78	TRP	8.1
3	C	79	TYR	7.9
3	C	55	LEU	7.2
2	L	82	HIS	6.7
3	C	80	GLN	4.7
3	C	4	VAL	4.5
2	L	220	CYS	4.5
1	H	137	SER	4.1
3	C	45	LYS	4.1
3	C	43	GLN	3.9
1	H	141	SER	3.8
3	C	82	PRO	3.8
2	L	129	GLU	3.7
1	H	224	SER	3.6
1	H	41	HIS	3.5
3	C	54	THR	3.5
1	H	223	LYS	3.3
1	H	64	PHE	3.2
1	H	225	CYS	3.2
1	H	62	GLN	3.0
2	L	35	GLY	2.9
3	C	88	ARG	2.9
3	C	38	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	56	GLY	2.7
1	H	140	THR	2.7
1	H	142	GLY	2.6
3	C	47	VAL	2.6
3	C	57	ASP	2.6
2	L	37	ASN	2.5
3	C	123	ASN	2.5
3	C	25	GLU	2.5
3	C	141	PRO	2.5
3	C	76	SER	2.5
1	H	221	GLU	2.5
1	H	65	LYS	2.5
3	C	34	ARG	2.5
1	H	138	LYS	2.4
3	C	152	TYR	2.3
3	C	124	MET	2.3
3	C	46	GLY	2.3
1	H	188	SER	2.2
1	H	139	SER	2.2
2	L	128	ASP	2.2
1	H	143	GLY	2.2
1	H	40	SER	2.2
3	C	5	THR	2.2
2	L	19	GLN	2.2
3	C	139	LYS	2.1
3	C	156	LEU	2.1
3	C	58	TYR	2.1
1	H	222	PRO	2.1
1	H	66	ALA	2.1
1	H	59	SER	2.0
1	H	218	LYS	2.0
3	C	81	SER	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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.