



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:25 PM UTC

PDB ID : 8EE5 / pdb_00008ee5
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ119-D in complex with ZIKV E glycoprotein
Authors : Sankhala, R.S.; Joyce, M.G.
Deposited on : 2022-09-06
Resolution : 3.58 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

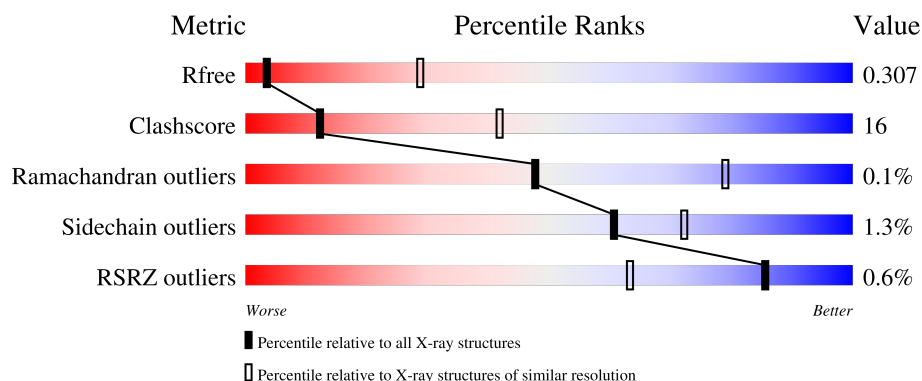
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

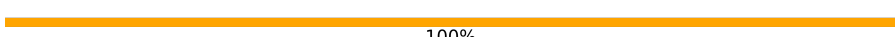
The reported resolution of this entry is 3.58 Å.

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}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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 $\leq 5\%$. 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	Z	405	 65% 32% .
2	H	218	 82% 17% .
3	L	212	 83% 17%
4	A	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6300 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Z	403	Total	C	N	O	S	0	0	0
			3079	1921	538	594	26			

- Molecule 2 is a protein called rhMZ119-D antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	215	Total	C	N	O	S	0	0	0
			1613	1016	267	324	6			

- Molecule 3 is a protein called rhMZ119-D antibody light chain.

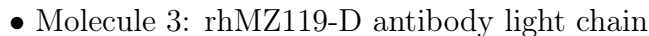
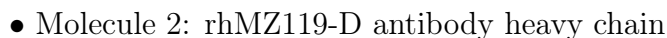
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1580	992	260	324	4			

- 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				

- Molecule 1: Envelope protein E



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

Chain A:

100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	51.68Å 103.67Å 196.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 3.58 14.99 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.6 (14.99-3.58) 89.9 (14.99-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.51 (at 3.55Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.249 , 0.296 0.275 , 0.307	Depositor DCC
R_{free} test set	654 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	91.6	Xtriage
Anisotropy	0.602	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6300	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	Z	0.41	1/3144 (0.0%)	0.71	7/4260 (0.2%)
2	H	0.11	0/1651	0.29	0/2249
3	L	0.17	0/1620	0.35	0/2209
All	All	0.31	1/6415 (0.0%)	0.54	7/8718 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	362	ASN	C-N	13.04	1.49	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	362	ASN	CA-C-N	14.88	135.52	119.90
1	Z	362	ASN	C-N-CA	14.88	135.52	119.90
1	Z	233	THR	CB-CA-C	8.49	118.39	111.00
1	Z	152	ILE	N-CA-C	-6.88	104.58	111.88
1	Z	150	GLY	CA-C-N	-5.49	114.09	122.21
1	Z	150	GLY	C-N-CA	-5.49	114.09	122.21
1	Z	176	ALA	N-CA-C	5.38	118.67	111.24

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	Z	3079	0	3007	140	0
2	H	1613	0	1580	24	0
3	L	1580	0	1522	25	0
4	A	28	0	25	15	0
All	All	6300	0	6134	193	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 16.

All (193) 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:Z:305:TYR:CE1	1:Z:338:PRO:HB2	1.38	1.53
1:Z:305:TYR:HE1	1:Z:338:PRO:CB	1.43	1.31
1:Z:151:MET:O	4:A:1:NAG:H82	1.43	1.18
3:L:109:GLN:HG2	3:L:110:PRO:HD2	1.21	1.16
1:Z:305:TYR:CE1	1:Z:338:PRO:CB	2.20	1.14
1:Z:27:HIS:NE2	1:Z:48:THR:CG2	2.16	1.08
1:Z:305:TYR:CD1	1:Z:338:PRO:HB2	1.87	1.08
4:A:1:NAG:H3	4:A:1:NAG:H83	1.32	1.07
1:Z:27:HIS:NE2	1:Z:48:THR:HG23	1.70	1.06
1:Z:152:ILE:HD13	4:A:1:NAG:H81	1.37	1.05
3:L:109:GLN:CG	3:L:110:PRO:HD2	1.86	1.05
1:Z:198:PHE:CE1	1:Z:284:LEU:HD21	1.92	1.04
1:Z:210:HIS:CE1	1:Z:277:MET:CG	2.47	0.97
1:Z:210:HIS:CE1	1:Z:277:MET:HG3	2.00	0.96
1:Z:152:ILE:CD1	4:A:1:NAG:H81	1.97	0.94
1:Z:302:GLY:HA2	1:Z:305:TYR:CD2	2.03	0.93
1:Z:198:PHE:CZ	1:Z:284:LEU:CD2	2.52	0.92
1:Z:148:HIS:O	1:Z:152:ILE:HD11	1.68	0.92
1:Z:1:ILE:HD11	1:Z:152:ILE:HB	1.52	0.91
1:Z:198:PHE:HZ	1:Z:284:LEU:CD2	1.85	0.89
1:Z:27:HIS:NE2	1:Z:48:THR:HG21	1.87	0.87
1:Z:198:PHE:HE1	1:Z:284:LEU:HD21	1.39	0.85
1:Z:198:PHE:CZ	1:Z:284:LEU:HD21	2.11	0.85
1:Z:210:HIS:ND1	1:Z:277:MET:HG2	1.91	0.85
3:L:170:ASN:H	3:L:171:ASN:HA	1.39	0.85
1:Z:27:HIS:CE1	1:Z:48:THR:HG23	2.12	0.83
3:L:109:GLN:HG2	3:L:110:PRO:CD	2.08	0.82
1:Z:210:HIS:CE1	1:Z:277:MET:HG2	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:148:HIS:CD2	1:Z:152:ILE:HD11	2.15	0.81
1:Z:148:HIS:O	1:Z:152:ILE:CD1	2.29	0.80
1:Z:158:HIS:CD2	1:Z:166:LYS:HE3	2.16	0.80
1:Z:151:MET:O	4:A:1:NAG:C8	2.28	0.80
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.65	0.78
1:Z:148:HIS:CD2	1:Z:152:ILE:CD1	2.67	0.78
1:Z:210:HIS:HE1	1:Z:277:MET:HG3	1.44	0.78
1:Z:148:HIS:O	1:Z:152:ILE:CG1	2.33	0.77
1:Z:302:GLY:HA2	1:Z:305:TYR:CE2	2.20	0.76
1:Z:144:HIS:HB3	1:Z:360:THR:HG23	1.66	0.76
1:Z:36:GLN:O	1:Z:38:LYS:N	2.20	0.74
1:Z:188:LEU:HD13	1:Z:293:LEU:HB3	1.69	0.72
4:A:1:NAG:H83	4:A:1:NAG:C3	2.15	0.72
1:Z:302:GLY:HA2	1:Z:305:TYR:HD2	1.56	0.71
4:A:1:NAG:H3	4:A:1:NAG:C8	2.15	0.70
1:Z:163:ASN:HB3	1:Z:183:PHE:HE1	1.57	0.70
1:Z:191:GLU:OE1	1:Z:292:ARG:NH1	2.24	0.69
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.74	0.69
1:Z:210:HIS:HE1	1:Z:277:MET:CG	2.00	0.69
1:Z:388:VAL:HG22	1:Z:397:THR:HG22	1.74	0.69
1:Z:7:SER:HA	1:Z:322:LEU:HD21	1.75	0.68
1:Z:16:SER:HA	1:Z:36:GLN:HB2	1.75	0.68
3:L:170:ASN:N	3:L:171:ASN:HA	2.09	0.67
4:A:1:NAG:H4	4:A:2:NAG:H82	1.76	0.66
1:Z:52:ASN:O	1:Z:134:ASN:ND2	2.29	0.66
1:Z:322:LEU:HD11	1:Z:323:HIS:CE1	2.31	0.66
1:Z:30:CYS:SG	1:Z:31:VAL:N	2.68	0.66
1:Z:148:HIS:O	1:Z:152:ILE:HG13	1.96	0.66
1:Z:147:GLN:NE2	1:Z:152:ILE:HG21	2.11	0.66
1:Z:335:THR:HG23	1:Z:369:THR:HG22	1.77	0.65
1:Z:70:SER:HB3	1:Z:113:LEU:HD11	1.78	0.64
1:Z:158:HIS:NE2	1:Z:166:LYS:HE3	2.12	0.63
1:Z:80:ALA:O	1:Z:94:ARG:NH1	2.31	0.63
1:Z:38:LYS:HB3	1:Z:298:LEU:HD23	1.80	0.62
1:Z:152:ILE:HD13	4:A:1:NAG:C8	2.22	0.62
1:Z:305:TYR:HE1	1:Z:338:PRO:CG	2.09	0.61
1:Z:322:LEU:HD11	1:Z:323:HIS:NE2	2.16	0.61
1:Z:153:VAL:HG12	1:Z:153:VAL:O	2.01	0.60
1:Z:350:GLN:O	1:Z:350:GLN:HG3	2.00	0.60
2:H:119:PRO:HB3	2:H:144:TYR:HB3	1.84	0.60
1:Z:62:GLU:HB3	1:Z:123:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:67:ASP:OD2	2:H:100:ARG:NH2	2.33	0.59
1:Z:135:LEU:C	1:Z:135:LEU:HD12	2.28	0.58
1:Z:198:PHE:HZ	1:Z:284:LEU:HD23	1.65	0.58
1:Z:364:VAL:HG12	1:Z:365:ILE:H	1.67	0.58
3:L:109:GLN:CG	3:L:110:PRO:CD	2.73	0.58
1:Z:149:SER:O	1:Z:375:MET:SD	2.62	0.57
1:Z:9:ARG:HH11	1:Z:11:PHE:HE1	1.53	0.56
4:A:1:NAG:C8	4:A:1:NAG:C3	2.79	0.56
1:Z:305:TYR:CE1	1:Z:338:PRO:HB3	2.34	0.56
1:Z:68:MET:HA	1:Z:116:CYS:O	2.05	0.56
2:H:20:ILE:HD11	2:H:80:LEU:HD23	1.88	0.56
1:Z:293:LEU:H	1:Z:293:LEU:HD23	1.71	0.56
1:Z:330:VAL:HG11	1:Z:389:ILE:HG21	1.88	0.55
1:Z:346:ALA:O	1:Z:386:TYR:HB2	2.06	0.55
1:Z:148:HIS:CD2	1:Z:152:ILE:HD12	2.40	0.55
3:L:109:GLN:HG3	3:L:110:PRO:HD2	1.82	0.55
1:Z:50:VAL:O	1:Z:281:LYS:HB3	2.07	0.55
2:H:199:HIS:CD2	2:H:201:PRO:HD2	2.42	0.54
1:Z:200:ASP:HB3	1:Z:215:LYS:HD3	1.88	0.54
1:Z:340:LYS:HD2	1:Z:362:ASN:OD1	2.06	0.54
1:Z:203:TYR:OH	1:Z:277:MET:HG2	2.07	0.54
1:Z:58:SER:HB2	1:Z:226:HIS:CE1	2.44	0.53
2:H:168:VAL:HB	3:L:163:THR:HG22	1.90	0.53
1:Z:152:ILE:HD12	4:A:1:NAG:H81	1.88	0.52
2:H:137:LEU:HB3	2:H:210:VAL:HG11	1.91	0.52
1:Z:196:LEU:HD13	1:Z:197:ASP:HB3	1.91	0.52
2:H:194:VAL:HG22	2:H:209:ARG:HA	1.90	0.52
1:Z:42:ASP:HB2	1:Z:142:SER:O	2.10	0.52
1:Z:61:TYR:HB2	1:Z:261:GLN:HB2	1.92	0.52
1:Z:154:ASN:OD1	1:Z:154:ASN:N	2.43	0.51
1:Z:305:TYR:HB3	1:Z:339:CYS:HA	1.93	0.51
3:L:184:ASP:O	3:L:188:SER:OG	2.21	0.51
1:Z:39:PRO:HD2	1:Z:298:LEU:HD21	1.93	0.51
1:Z:147:GLN:HB3	1:Z:152:ILE:HG21	1.93	0.51
3:L:146:GLU:HB2	3:L:197:THR:HB	1.92	0.51
1:Z:92:CYS:HA	1:Z:115:THR:O	2.10	0.50
1:Z:118:LYS:NZ	2:H:54:ASP:OD1	2.33	0.50
1:Z:43:ILE:HD13	1:Z:141:LEU:HB3	1.92	0.50
1:Z:171:PRO:HA	1:Z:192:PRO:HG2	1.94	0.50
2:H:144:TYR:OH	2:H:147:GLU:OE2	2.25	0.49
1:Z:358:LEU:HD22	1:Z:378:LEU:HD22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:305:TYR:HD1	1:Z:338:PRO:C	2.20	0.49
1:Z:158:HIS:HA	1:Z:164:ARG:HH21	1.78	0.48
4:A:1:NAG:H82	4:A:1:NAG:C1	2.43	0.48
1:Z:322:LEU:C	1:Z:322:LEU:HD12	2.38	0.48
1:Z:387:ILE:HG23	1:Z:398:HIS:HB3	1.95	0.48
1:Z:369:THR:HA	1:Z:370:GLU:HA	1.59	0.47
3:L:152:ASP:CG	3:L:189:HIS:HB3	2.38	0.47
1:Z:350:GLN:HA	1:Z:351:THR:CG2	2.44	0.47
2:H:51:ILE:HA	2:H:56:ASP:O	2.13	0.47
2:H:96:GLY:N	2:H:100(A):SER:O	2.47	0.47
3:L:33:ALA:N	3:L:51:ASP:OD1	2.33	0.47
1:Z:2:ARG:HG2	1:Z:142:SER:HB2	1.96	0.47
1:Z:50:VAL:HA	1:Z:135:LEU:HA	1.97	0.47
1:Z:162:GLU:OE2	1:Z:301:LYS:NZ	2.38	0.47
3:L:119:PHE:HB2	3:L:134:VAL:HB	1.96	0.47
1:Z:70:SER:HA	1:Z:114:VAL:O	2.15	0.46
1:Z:158:HIS:CE1	1:Z:166:LYS:HG3	2.50	0.46
2:H:6:GLN:HE21	2:H:6:GLN:HB3	1.60	0.46
2:H:35:SER:OG	2:H:95:GLU:OE2	2.32	0.46
4:A:1:NAG:C8	4:A:1:NAG:C1	2.94	0.46
1:Z:158:HIS:HB2	1:Z:164:ARG:HE	1.81	0.45
1:Z:22:ASP:OD1	1:Z:292:ARG:HG2	2.16	0.45
4:A:1:NAG:H4	4:A:2:NAG:C8	2.45	0.45
2:H:151:VAL:HA	2:H:196:ASN:O	2.16	0.45
1:Z:27:HIS:HD2	1:Z:287:GLY:HA3	1.80	0.45
1:Z:39:PRO:HD2	1:Z:298:LEU:CD2	2.46	0.45
1:Z:140:MET:HE2	1:Z:140:MET:HB3	1.77	0.45
1:Z:68:MET:HE3	2:H:97:ILE:HG22	1.99	0.45
1:Z:263:GLY:HA2	1:Z:266:HIS:HB2	1.99	0.45
2:H:90:TYR:O	2:H:106:GLY:HA2	2.17	0.45
1:Z:59:TYR:HD2	1:Z:223:LEU:HB2	1.82	0.44
1:Z:51:SER:HB3	1:Z:134:ASN:CG	2.42	0.44
1:Z:203:TYR:HH	1:Z:277:MET:HG2	1.82	0.44
2:H:33:TRP:CE2	2:H:52:ASP:HB2	2.52	0.44
1:Z:40:THR:HG23	1:Z:144:HIS:HB2	1.99	0.44
1:Z:347:VAL:HG12	1:Z:385:SER:HA	2.00	0.44
3:L:54:ARG:NH2	3:L:62:PHE:O	2.50	0.44
2:H:163:HIS:NE2	3:L:168:GLN:OE1	2.46	0.44
3:L:81:GLU:OE1	3:L:81:GLU:N	2.44	0.44
4:A:1:NAG:H4	4:A:2:NAG:C7	2.48	0.44
1:Z:198:PHE:CZ	1:Z:284:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:206:MET:SD	1:Z:262:GLU:HG3	2.59	0.43
3:L:4:LEU:HB2	3:L:99:GLY:HA2	2.00	0.43
1:Z:25:LEU:HD21	1:Z:43:ILE:HG22	2.01	0.43
1:Z:36:GLN:HG3	1:Z:37:ASP:H	1.83	0.43
1:Z:135:LEU:HD12	1:Z:135:LEU:O	2.19	0.43
1:Z:173:SER:O	1:Z:173:SER:OG	2.25	0.42
1:Z:331:GLN:CD	1:Z:371:ASN:HD21	2.26	0.42
2:H:144:TYR:O	2:H:175:TYR:N	2.49	0.42
1:Z:74:CYS:HB2	1:Z:77:GLN:HG3	2.02	0.42
1:Z:148:HIS:HA	1:Z:374:MET:HA	2.02	0.42
1:Z:10:ASP:HB3	1:Z:31:VAL:HG22	2.01	0.42
2:H:208:LYS:HD2	2:H:208:LYS:HA	1.81	0.42
1:Z:36:GLN:HA	1:Z:36:GLN:OE1	2.18	0.42
1:Z:347:VAL:HG22	1:Z:355:VAL:HG21	2.01	0.42
3:L:116:VAL:HA	3:L:136:LEU:O	2.20	0.42
3:L:135:CYS:HB2	3:L:149:TRP:CH2	2.54	0.41
1:Z:51:SER:H	1:Z:134:ASN:HB3	1.85	0.41
1:Z:56:VAL:HG11	1:Z:202:TYR:HE2	1.84	0.41
1:Z:142:SER:OG	1:Z:164:ARG:HG3	2.19	0.41
1:Z:196:LEU:HA	1:Z:197:ASP:HA	1.65	0.41
1:Z:332:TYR:O	1:Z:371:ASN:HA	2.20	0.41
3:L:193:SER:HA	3:L:205:LYS:O	2.20	0.41
1:Z:215:LYS:HG3	1:Z:219:HIS:CE1	2.55	0.41
1:Z:362:ASN:O	1:Z:362:ASN:ND2	2.54	0.41
1:Z:39:PRO:HG3	1:Z:300:LEU:HA	2.02	0.41
1:Z:310:ALA:HB3	1:Z:332:TYR:CZ	2.56	0.41
3:L:133:LEU:HD21	3:L:186:TRP:CZ3	2.56	0.41
1:Z:41:VAL:HG22	1:Z:143:VAL:HG22	2.02	0.41
1:Z:93:LYS:HB2	1:Z:245:PHE:CE2	2.56	0.41
2:H:93:ALA:HA	2:H:102:VAL:O	2.21	0.41
2:H:145:PHE:HA	2:H:146:PRO:HA	1.89	0.41
1:Z:143:VAL:HB	1:Z:163:ASN:HB2	2.01	0.41
1:Z:345:MET:HE2	1:Z:345:MET:HB3	1.93	0.41
3:L:181:LEU:HD23	3:L:181:LEU:HA	1.95	0.41
3:L:150:LYS:HD3	3:L:155:ALA:HA	2.03	0.40
1:Z:148:HIS:NE2	1:Z:152:ILE:CD1	2.84	0.40
1:Z:318:PRO:HB3	1:Z:328:VAL:HG22	2.03	0.40
1:Z:53:MET:HG2	1:Z:129:SER:O	2.22	0.40
2:H:85:SER:O	2:H:85:SER:OG	2.38	0.40
1:Z:148:HIS:NE2	1:Z:152:ILE:HD11	2.35	0.40
1:Z:322:LEU:CD1	1:Z:323:HIS:CD2	3.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:ARG:HA	2:H:58:ARG:HD2	1.90	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	Z	401/405 (99%)	369 (92%)	31 (8%)	1 (0%)	43	72
2	H	211/218 (97%)	204 (97%)	7 (3%)	0	100	100
3	L	209/212 (99%)	204 (98%)	5 (2%)	0	100	100
All	All	821/835 (98%)	777 (95%)	43 (5%)	1 (0%)	48	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	37	ASP

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	Z	337/338 (100%)	328 (97%)	9 (3%)	39	61
2	H	185/188 (98%)	185 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	175/176 (99%)	175 (100%)	0	100	100
All	All	697/702 (99%)	688 (99%)	9 (1%)	61	72

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	65	ILE
1	Z	141	LEU
1	Z	147	GLN
1	Z	148	HIS
1	Z	154	ASN
1	Z	158	HIS
1	Z	163	ASN
1	Z	235	HIS
1	Z	364	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	210	HIS
1	Z	344	GLN
1	Z	371	ASN
3	L	79	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	A	1	1,4	14,14,15	0.37	0	17,19,21	1.42	3 (17%)
4	NAG	A	2	4	14,14,15	0.48	0	17,19,21	1.26	3 (17%)

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	1,4	-	3/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2	NAG	C1-C2-N2	3.17	115.43	110.43
4	A	1	NAG	O4-C4-C3	3.15	117.81	110.38
4	A	1	NAG	O5-C1-C2	-2.67	107.16	111.29
4	A	2	NAG	C1-O5-C5	2.51	115.55	112.19
4	A	1	NAG	C1-O5-C5	2.38	115.38	112.19
4	A	2	NAG	O5-C1-C2	-2.25	107.81	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

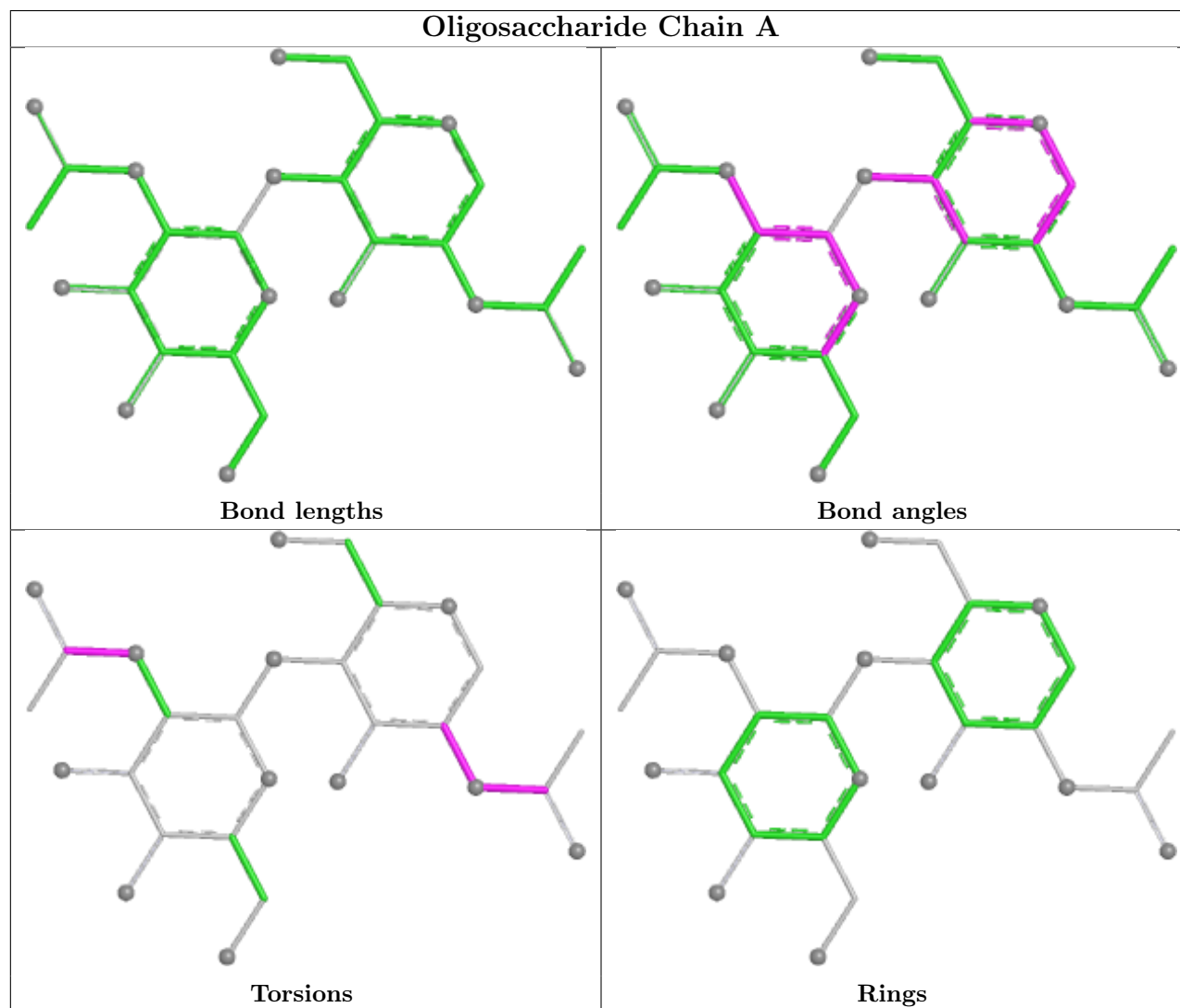
Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O7-C7-N2-C2
4	A	2	NAG	C8-C7-N2-C2
4	A	1	NAG	C8-C7-N2-C2
4	A	1	NAG	O7-C7-N2-C2
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2	NAG	3	0
4	A	1	NAG	15	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.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	Z	403/405 (99%)	0.04	2 (0%) 87 66	58, 101, 130, 165	0
2	H	215/218 (98%)	-0.05	3 (1%) 73 45	47, 105, 162, 188	0
3	L	211/212 (99%)	-0.05	0 100 100	70, 103, 133, 219	0
All	All	829/835 (99%)	-0.01	5 (0%) 85 63	47, 102, 139, 219	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1	GLU	2.5
1	Z	81	TYR	2.3
2	H	64	GLN	2.3
1	Z	176	ALA	2.3
2	H	211	GLU	2.1

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

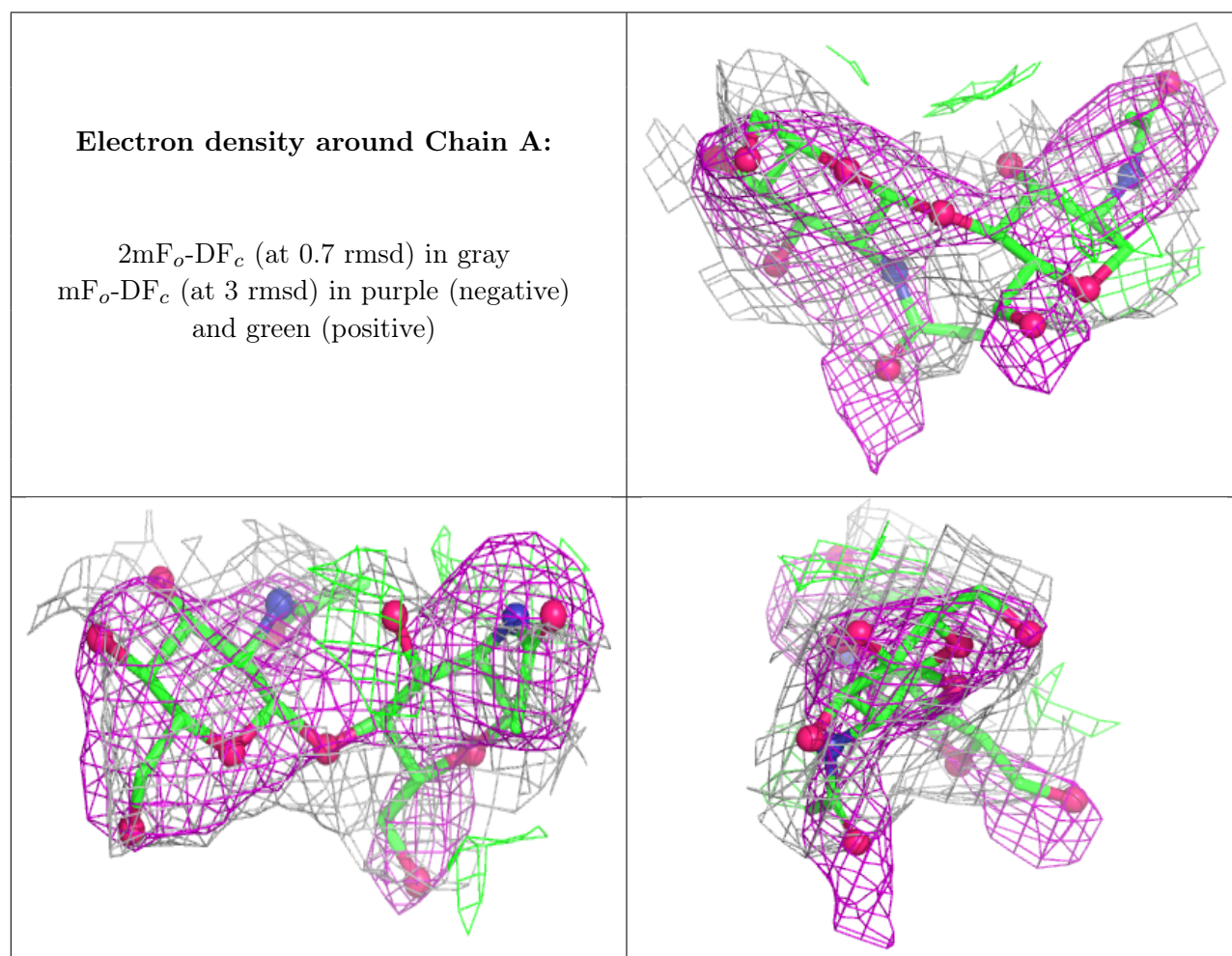
There are no non-standard protein/DNA/RNA residues in this entry.

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	A	1	14/15	-	-	30,30,30,30	0
4	NAG	A	2	14/15	-	-	30,30,30,30	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.