Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 01:03 AM EST

PDB ID	:	9AZT
Title	:	CH67 Fab bound to A/Massachusetts/1/1990 influenza hemagglutinin head with a G189E mutation (1)
Authors	:	Maurer, D.P.; Schmidt, A.G.
Deposited on	:	2024-03-11
Resolution	:	2.94 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:

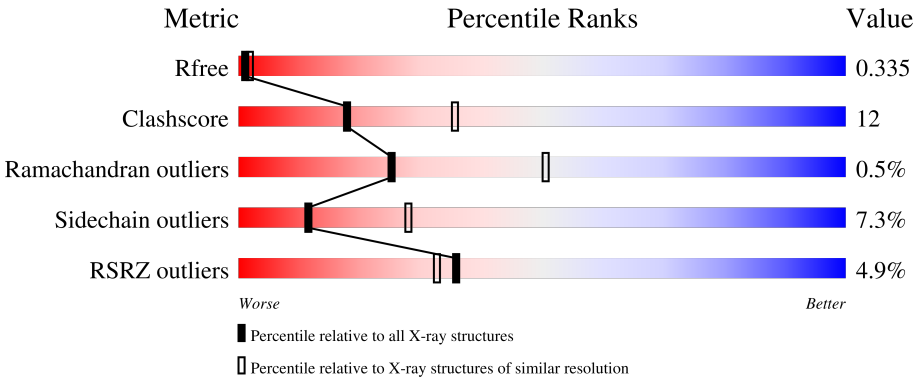
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.94 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	1067 (2.96-2.92)
Clashscore	180529	1122 (2.96-2.92)
Ramachandran outliers	177936	1075 (2.96-2.92)
Sidechain outliers	177891	1075 (2.96-2.92)
RSRZ outliers	164620	1067 (2.96-2.92)

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	E	224	4% 69% 24% • 5%
2	H	250	5% 60% 26% • 10%
3	L	214	4% 71% 21% • 7%
4	A	2	100%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4977 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	213	Total	C	N	O	S	0	0	0
			1724	1100	292	328	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	189	GLU	GLY	engineered mutation	UNP Q07775
E	264	GLY	-	expression tag	UNP Q07775
E	265	ALA	-	expression tag	UNP Q07775
E	266	GLY	-	expression tag	UNP Q07775
E	267	SER	-	expression tag	UNP Q07775
E	268	SER	-	expression tag	UNP Q07775
E	269	LEU	-	expression tag	UNP Q07775
E	270	GLU	-	expression tag	UNP Q07775
E	271	VAL	-	expression tag	UNP Q07775
E	272	LEU	-	expression tag	UNP Q07775
E	273	PHE	-	expression tag	UNP Q07775
E	274	GLN	-	expression tag	UNP Q07775

- Molecule 2 is a protein called CH67 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1711	1081	290	333	7			

- Molecule 3 is a protein called CH67 Fab light chain.

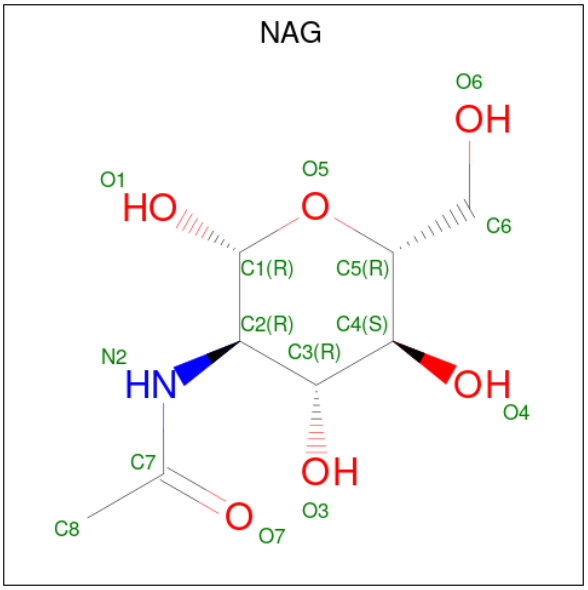
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	200	Total	C	N	O	S	0	0	0
			1500	938	253	305	4			

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

cetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



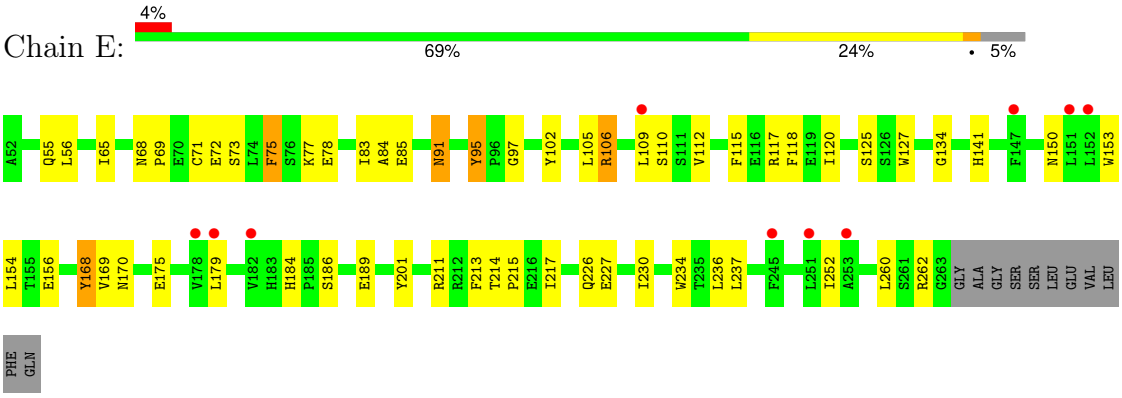
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	E	1	14	8	1	5	0	0

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.

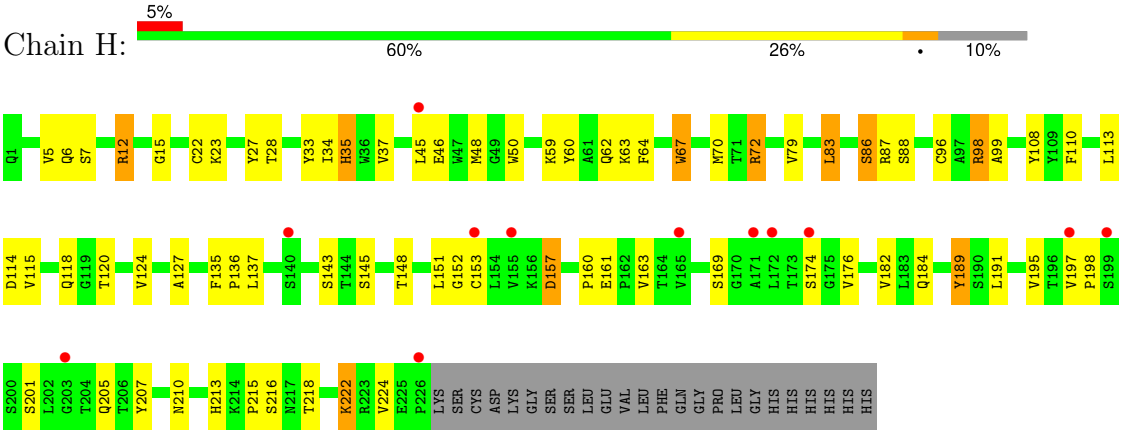
• Molecule 1: Hemagglutinin HA1 chain

Chain E:



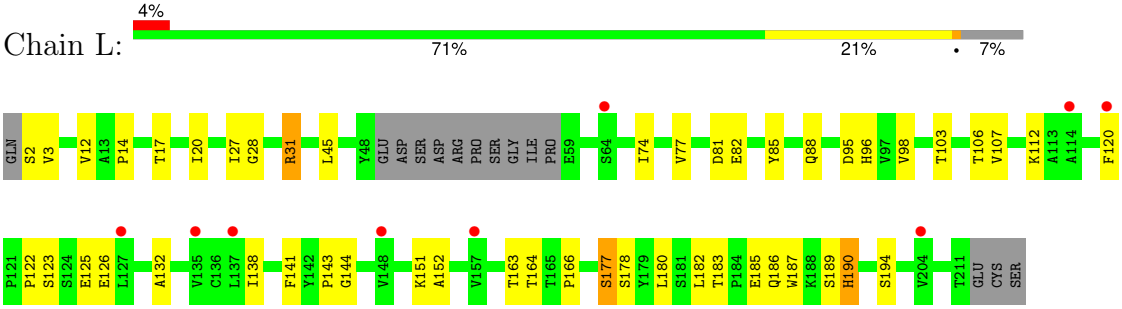
• Molecule 2: CH67 Fab heavy chain

Chain H:

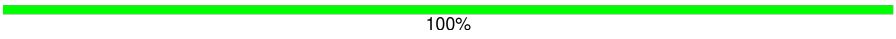


• Molecule 3: CH67 Fab light chain

Chain L:



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

Chain A: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	80.75Å 91.70Å 110.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.20 – 2.94 47.20 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.20-2.94) 99.1 (47.20-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.294 , 0.338 0.295 , 0.335	Depositor DCC
R_{free} test set	16132 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	107.9	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 98.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4977	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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	E	0.27	0/1777	0.57	1/2419 (0.0%)
2	H	0.28	0/1757	0.55	0/2398
3	L	0.29	0/1535	0.55	0/2099
All	All	0.28	0/5069	0.56	1/6916 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	109	LEU	CA-CB-CG	5.27	127.41	115.30

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	E	1724	0	1627	39	0
2	H	1711	0	1660	52	0
3	L	1500	0	1451	36	0
4	A	28	0	25	0	0
5	E	14	0	13	0	0
All	All	4977	0	4776	118	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 12.

All (118) 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:L:106:THR:HG21	3:L:143:PRO:HB3	1.65	0.76
2:H:34:ILE:HG21	2:H:79:VAL:HG11	1.66	0.76
1:E:211:ARG:HH21	1:E:213:PHE:HA	1.53	0.72
3:L:163:THR:HG23	3:L:178:SER:HB2	1.74	0.70
1:E:189:GLU:OE1	1:E:189:GLU:N	2.22	0.67
2:H:176:VAL:HG22	2:H:195:VAL:HG12	1.77	0.67
3:L:183:THR:HG23	3:L:185:GLU:H	1.60	0.66
2:H:6:GLN:HE22	2:H:96:CYS:H	1.41	0.66
2:H:136:PRO:HG3	2:H:222:LYS:HG3	1.78	0.66
2:H:222:LYS:HA	2:H:222:LYS:HE2	1.78	0.66
1:E:120:ILE:HG13	1:E:168:TYR:HD2	1.60	0.65
1:E:95:TYR:HD1	1:E:230:ILE:HG13	1.60	0.65
1:E:83:ILE:HD12	1:E:85:GLU:H	1.63	0.63
2:H:35:HIS:CD2	2:H:113:LEU:HD21	2.34	0.63
2:H:136:PRO:HA	2:H:153:CYS:HA	1.81	0.62
3:L:20:ILE:HD12	3:L:103:THR:HG21	1.80	0.62
3:L:125:GLU:H	3:L:125:GLU:CD	2.02	0.62
2:H:6:GLN:NE2	2:H:96:CYS:SG	2.72	0.62
2:H:108:TYR:HD2	3:L:31:ARG:H	1.47	0.62
1:E:120:ILE:HG13	1:E:168:TYR:CD2	2.36	0.61
1:E:175:GLU:OE1	1:E:262:ARG:NH1	2.21	0.61
2:H:33:TYR:HB2	2:H:99:ALA:HB3	1.84	0.60
1:E:95:TYR:CD1	1:E:230:ILE:HG13	2.37	0.60
2:H:6:GLN:NE2	2:H:96:CYS:H	2.01	0.59
3:L:2:SER:HA	3:L:98:VAL:HG21	1.85	0.59
3:L:81:ASP:O	3:L:85:TYR:OH	2.19	0.58
2:H:60:TYR:HE2	2:H:70:MET:HG3	1.67	0.58
2:H:148:THR:HA	2:H:198:PRO:HA	1.86	0.57
1:E:168:TYR:HD1	1:E:169:VAL:N	2.03	0.57
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.87	0.57
3:L:82:GLU:HB2	3:L:107:VAL:HG23	1.88	0.55
3:L:125:GLU:OE2	3:L:125:GLU:N	2.36	0.55
3:L:12:VAL:HG21	3:L:77:VAL:HG11	1.87	0.55
2:H:12:ARG:HG2	2:H:12:ARG:HH11	1.73	0.54
1:E:117:ARG:NH1	1:E:150:ASN:OD1	2.40	0.54
1:E:230:ILE:HD13	1:E:252:ILE:HG13	1.90	0.54
2:H:88:SER:HA	2:H:124:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:HB3	2:H:79:VAL:HG12	1.90	0.53
1:E:102:TYR:O	1:E:106:ARG:HD3	2.09	0.53
2:H:15:GLY:N	2:H:86:SER:O	2.42	0.53
1:E:234:TRP:HZ3	1:E:236:LEU:HD13	1.73	0.52
2:H:197:VAL:HG11	2:H:207:TYR:OH	2.09	0.52
3:L:82:GLU:OE2	3:L:106:THR:HA	2.09	0.52
3:L:152:ALA:HB1	3:L:190:HIS:HD2	1.74	0.52
1:E:69:PRO:HB2	1:E:141:HIS:HB2	1.91	0.52
2:H:62:GLN:HB2	3:L:96:HIS:HE1	1.74	0.52
3:L:151:LYS:HB2	3:L:194:SER:HB2	1.91	0.51
2:H:110:PHE:O	3:L:31:ARG:NH2	2.44	0.51
2:H:114:ASP:OD1	2:H:115:VAL:N	2.44	0.51
1:E:112:VAL:HG12	1:E:262:ARG:HG3	1.94	0.50
2:H:5:VAL:HG22	2:H:23:LYS:HB3	1.93	0.50
2:H:169:SER:O	2:H:169:SER:OG	2.22	0.49
1:E:170:ASN:HB2	1:E:237:LEU:HD23	1.93	0.49
3:L:141:PHE:HZ	3:L:166:PRO:HB3	1.76	0.49
2:H:114:ASP:HA	3:L:45:LEU:HD12	1.94	0.49
2:H:108:TYR:CE1	2:H:110:PHE:HB3	2.47	0.49
2:H:135:PHE:HB3	3:L:123:SER:OG	2.13	0.48
1:E:68:ASN:HB3	1:E:71:CYS:HB2	1.96	0.48
2:H:216:SER:OG	2:H:218:THR:OG1	2.26	0.48
2:H:201:SER:HB2	2:H:205:GLN:HB3	1.95	0.48
3:L:3:VAL:HG13	3:L:3:VAL:O	2.14	0.48
1:E:186:SER:HB3	1:E:227:GLU:HB3	1.95	0.47
2:H:64:PHE:HA	2:H:67:TRP:NE1	2.28	0.47
2:H:50:TRP:CZ2	2:H:59:LYS:HD2	2.49	0.47
2:H:6:GLN:H	2:H:118:GLN:NE2	2.13	0.47
2:H:136:PRO:HB3	2:H:224:VAL:HG22	1.96	0.47
3:L:164:THR:HG22	3:L:177:SER:H	1.81	0.46
3:L:132:ALA:HB3	3:L:182:LEU:HB2	1.97	0.46
3:L:141:PHE:CE2	3:L:144:GLY:HA2	2.51	0.46
1:E:71:CYS:O	1:E:73:SER:N	2.49	0.45
1:E:71:CYS:SG	1:E:91:ASN:HB3	2.56	0.45
3:L:12:VAL:HG23	3:L:77:VAL:HG21	1.98	0.45
1:E:83:ILE:HD12	1:E:85:GLU:N	2.28	0.45
2:H:48:MET:HB2	2:H:48:MET:HE2	1.60	0.45
1:E:95:TYR:CE2	1:E:226:GLN:HG2	2.52	0.45
1:E:175:GLU:OE1	1:E:236:LEU:HD23	2.17	0.45
3:L:14:PRO:HA	3:L:77:VAL:HG23	1.98	0.45
1:E:56:LEU:HD12	1:E:85:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:SER:O	2:H:120:THR:OG1	2.33	0.44
2:H:137:LEU:HB3	3:L:120:PHE:CG	2.52	0.44
2:H:182:VAL:HG12	3:L:164:THR:HB	1.98	0.44
3:L:183:THR:HG22	3:L:186:GLN:HG3	2.00	0.44
3:L:152:ALA:HB1	3:L:190:HIS:CD2	2.52	0.44
2:H:135:PHE:CG	3:L:126:GLU:HB2	2.52	0.44
2:H:205:GLN:HG2	2:H:207:TYR:CZ	2.53	0.44
1:E:112:VAL:HA	1:E:262:ARG:HA	2.00	0.44
2:H:161:GLU:HG2	2:H:189:TYR:CE1	2.53	0.43
1:E:55:GLN:H	1:E:84:ALA:HB3	1.82	0.43
2:H:160:PRO:HD2	2:H:215:PRO:HB2	2.01	0.43
1:E:65:ILE:HG13	1:E:179:LEU:HD11	2.00	0.43
2:H:98:ARG:HG2	2:H:115:VAL:HG12	2.01	0.43
2:H:12:ARG:HG2	2:H:12:ARG:NH1	2.34	0.43
1:E:214:THR:O	1:E:214:THR:OG1	2.31	0.43
2:H:137:LEU:N	2:H:152:GLY:O	2.50	0.43
3:L:183:THR:HG23	3:L:185:GLU:N	2.30	0.43
2:H:137:LEU:H	2:H:153:CYS:HA	1.84	0.43
2:H:213:HIS:CE1	2:H:216:SER:H	2.37	0.43
1:E:184:HIS:CE1	1:E:215:PRO:HA	2.53	0.42
1:E:118:PHE:HE2	1:E:168:TYR:HE2	1.67	0.42
2:H:145:SER:O	2:H:145:SER:OG	2.36	0.42
1:E:97:GLY:HA3	1:E:230:ILE:O	2.19	0.42
1:E:127:TRP:CD1	1:E:154:LEU:HD21	2.54	0.42
2:H:46:GLU:OE2	2:H:63:LYS:NZ	2.52	0.42
1:E:217:ILE:HD12	1:E:217:ILE:O	2.19	0.42
3:L:12:VAL:O	3:L:107:VAL:HA	2.20	0.41
2:H:163:VAL:HG13	2:H:191:LEU:HD21	2.02	0.41
1:E:77:LYS:HG3	1:E:78:GLU:N	2.35	0.41
2:H:67:TRP:CZ3	2:H:83:LEU:HD21	2.55	0.41
2:H:72:ARG:HD2	2:H:72:ARG:C	2.41	0.41
2:H:136:PRO:HD2	3:L:125:GLU:OE1	2.20	0.41
3:L:74:ILE:HG22	3:L:77:VAL:HG12	2.03	0.41
1:E:105:LEU:HD23	1:E:234:TRP:CE3	2.55	0.40
1:E:56:LEU:HA	1:E:75:PHE:HE1	1.85	0.40
3:L:122:PRO:HD2	3:L:187:TRP:CZ2	2.56	0.40
1:E:78:GLU:HA	1:E:115:PHE:HB3	2.02	0.40
1:E:118:PHE:HE2	1:E:168:TYR:CE2	2.39	0.40
2:H:37:VAL:HA	2:H:48:MET:HG3	2.04	0.40
3:L:27:ILE:H	3:L:27:ILE:HG13	1.72	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	E	211/224 (94%)	198 (94%)	13 (6%)	0	100 100
2	H	224/250 (90%)	214 (96%)	8 (4%)	2 (1%)	14 35
3	L	196/214 (92%)	186 (95%)	9 (5%)	1 (0%)	25 50
All	All	631/688 (92%)	598 (95%)	30 (5%)	3 (0%)	25 50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	28	GLY
2	H	127	ALA
2	H	157	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	E	188/196 (96%)	177 (94%)	11 (6%)	16 36
2	H	189/210 (90%)	170 (90%)	19 (10%)	6 16
3	L	169/182 (93%)	159 (94%)	10 (6%)	16 36
All	All	546/588 (93%)	506 (93%)	40 (7%)	11 28

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	72	GLU
1	E	75	PHE
1	E	91	ASN
1	E	95	TYR
1	E	106	ARG
1	E	110	SER
1	E	125	SER
1	E	156	GLU
1	E	168	TYR
1	E	201	TYR
1	E	260	LEU
2	H	12	ARG
2	H	27	TYR
2	H	28	THR
2	H	35	HIS
2	H	45	LEU
2	H	67	TRP
2	H	72	ARG
2	H	83	LEU
2	H	86	SER
2	H	87	ARG
2	H	98	ARG
2	H	143	SER
2	H	151	LEU
2	H	157	ASP
2	H	174	SER
2	H	184	GLN
2	H	189	TYR
2	H	210	ASN
2	H	222	LYS
3	L	17	THR
3	L	31	ARG
3	L	88	GLN
3	L	95	ASP
3	L	112	LYS
3	L	138	ILE
3	L	177	SER
3	L	180	LEU
3	L	189	SER
3	L	190	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	141	HIS
1	E	142	ASN
1	E	170	ASN
2	H	6	GLN
3	L	96	HIS

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)

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	0.29	0	17,19,21	0.54	0
4	NAG	A	2	4	14,14,15	0.30	0	17,19,21	0.58	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	1,4	-	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.

There are no bond angle outliers.

There are no chirality outliers.

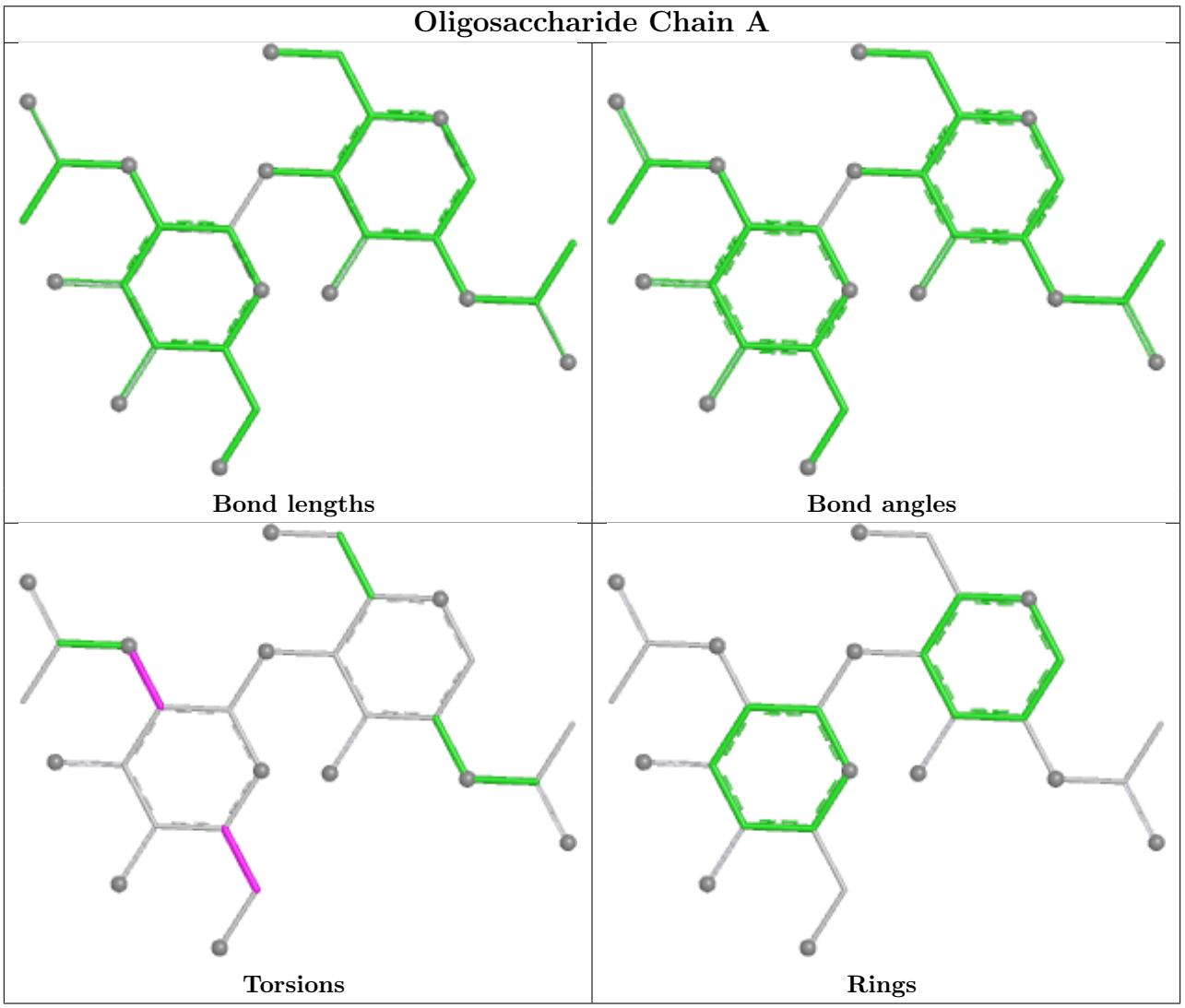
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	O5-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
4	A	2	NAG	C1-C2-N2-C7
4	A	2	NAG	C3-C2-N2-C7

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)

1 ligand is 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	$\#\|Z\| > 2$
5	NAG	E	301	1	14,14,15	0.28	0	17,19,21	0.55	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
5	NAG	E	301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	301	NAG	C1-C2-N2-C7
5	E	301	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	E	213/224 (95%)	0.31	10 (4%)	37	34	85, 123, 194, 208	0
2	H	226/250 (90%)	0.48	12 (5%)	33	30	77, 121, 201, 223	0
3	L	200/214 (93%)	0.63	9 (4%)	39	36	75, 142, 241, 252	0
All	All	639/688 (92%)	0.47	31 (4%)	36	33	75, 129, 215, 252	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	251	LEU	4.0
3	L	114	ALA	4.0
3	L	148	VAL	3.9
2	H	155	VAL	3.4
2	H	165	VAL	3.4
3	L	120	PHE	3.2
1	E	179	LEU	3.0
1	E	245	PHE	2.9
2	H	171	ALA	2.9
1	E	253	ALA	2.7
1	E	182	VAL	2.7
3	L	137	LEU	2.7
2	H	140	SER	2.6
1	E	109	LEU	2.6
2	H	174	SER	2.4
1	E	151	LEU	2.4
1	E	147	PHE	2.4
1	E	178	VAL	2.4
2	H	172	LEU	2.3
3	L	135	VAL	2.3
2	H	153	CYS	2.3
3	L	204	VAL	2.3
3	L	127	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	152	LEU	2.2
2	H	197	VAL	2.2
3	L	64	SER	2.2
3	L	157	VAL	2.1
2	H	203	GLY	2.1
2	H	45	LEU	2.1
2	H	226	PRO	2.1
2	H	199	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)

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
5	NAG	E	301	14/15	0.65	0.11	141,145,151,152	0

6.5 Other polymers (i)

There are no such residues in this entry.