



Full wwPDB EM Validation Report ⓘ

Nov 26, 2025 – 12:07 PM EST

PDB ID : 9N5Y / pdb_00009n5y
EMDB ID : EMD-49043
Title : Hemagglutinin CA09 homotrimer bound to AEL31302/AEL31311 Fab
Authors : Fernandez-Quintero, M.L.; Turner, H.L.
Deposited on : 2025-02-04
Resolution : 4.10 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis	: FAILED
Mogul	: 2022.3.0, CSD as543be (2022)
MolProbity	: 4-5-2 with Phenix2.0
Percentile statistics	: 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	: NOT EXECUTED
MapQ	: FAILED
Ideal geometry (proteins)	: Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	: 2.46

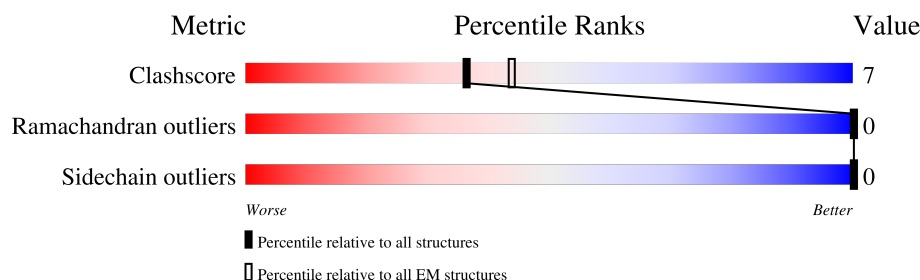
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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.




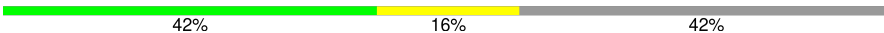

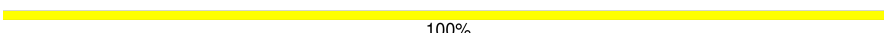
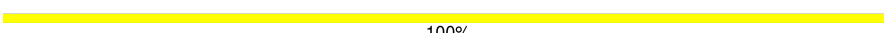
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	L	237	
1	M	237	
1	O	237	
2	I	251	
2	J	251	
2	P	251	
3	A	554	
3	B	554	
3	C	554	

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Mol	Chain	Length	Quality of chain
3	D	554	 25% 5% 69%
3	E	554	 42% 16% 42%
3	F	554	 27% • 69%
4	G	2	 100%
4	H	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17643 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 light chain antibody AEL31302.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	111	Total	C	N	O	S	0	0
			855	535	147	170	3		
1	O	111	Total	C	N	O	S	0	0
			855	535	147	170	3		
1	M	111	Total	C	N	O	S	0	0
			855	535	147	170	3		

- Molecule 2 is a protein called Fab heavy antibody AEL31311.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	129	Total	C	N	O	S	0	0
			1020	646	177	193	4		
2	P	129	Total	C	N	O	S	0	0
			1020	646	177	193	4		
2	J	129	Total	C	N	O	S	0	0
			1020	646	177	193	4		

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	324	Total	C	N	O	S	0	0
			2529	1599	436	483	11		
3	C	323	Total	C	N	O	S	0	0
			2523	1596	435	481	11		
3	E	324	Total	C	N	O	S	0	0
			2529	1599	436	483	11		
3	B	175	Total	C	N	O	S	0	0
			1411	885	239	281	6		
3	D	171	Total	C	N	O	S	0	0
			1380	867	235	272	6		
3	F	171	Total	C	N	O	S	0	0
			1380	867	235	272	6		

There are 324 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	expression tag	UNP A0A3S7XTA4
A	376	LYS	GLU	conflict	UNP A0A3S7XTA4
A	504	SER	-	expression tag	UNP A0A3S7XTA4
A	505	GLY	-	expression tag	UNP A0A3S7XTA4
A	506	TYR	-	expression tag	UNP A0A3S7XTA4
A	507	ILE	-	expression tag	UNP A0A3S7XTA4
A	508	PRO	-	expression tag	UNP A0A3S7XTA4
A	509	GLU	-	expression tag	UNP A0A3S7XTA4
A	510	ALA	-	expression tag	UNP A0A3S7XTA4
A	511	PRO	-	expression tag	UNP A0A3S7XTA4
A	512	ARG	-	expression tag	UNP A0A3S7XTA4
A	513	ASP	-	expression tag	UNP A0A3S7XTA4
A	514	GLY	-	expression tag	UNP A0A3S7XTA4
A	515	GLN	-	expression tag	UNP A0A3S7XTA4
A	516	ALA	-	expression tag	UNP A0A3S7XTA4
A	517	TYR	-	expression tag	UNP A0A3S7XTA4
A	518	VAL	-	expression tag	UNP A0A3S7XTA4
A	519	ARG	-	expression tag	UNP A0A3S7XTA4
A	520	LYS	-	expression tag	UNP A0A3S7XTA4
A	521	ASP	-	expression tag	UNP A0A3S7XTA4
A	522	GLY	-	expression tag	UNP A0A3S7XTA4
A	523	GLU	-	expression tag	UNP A0A3S7XTA4
A	524	TRP	-	expression tag	UNP A0A3S7XTA4
A	525	VAL	-	expression tag	UNP A0A3S7XTA4
A	526	LEU	-	expression tag	UNP A0A3S7XTA4
A	527	LEU	-	expression tag	UNP A0A3S7XTA4
A	528	SER	-	expression tag	UNP A0A3S7XTA4
A	529	THR	-	expression tag	UNP A0A3S7XTA4
A	530	PHE	-	expression tag	UNP A0A3S7XTA4
A	531	LEU	-	expression tag	UNP A0A3S7XTA4
A	532	GLY	-	expression tag	UNP A0A3S7XTA4
A	533	SER	-	expression tag	UNP A0A3S7XTA4
A	534	GLY	-	expression tag	UNP A0A3S7XTA4
A	535	LEU	-	expression tag	UNP A0A3S7XTA4
A	536	ASN	-	expression tag	UNP A0A3S7XTA4
A	537	ASP	-	expression tag	UNP A0A3S7XTA4
A	538	ILE	-	expression tag	UNP A0A3S7XTA4
A	539	PHE	-	expression tag	UNP A0A3S7XTA4
A	540	GLU	-	expression tag	UNP A0A3S7XTA4
A	541	ALA	-	expression tag	UNP A0A3S7XTA4
A	542	GLN	-	expression tag	UNP A0A3S7XTA4
A	543	LYS	-	expression tag	UNP A0A3S7XTA4
A	544	ILE	-	expression tag	UNP A0A3S7XTA4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	545	GLU	-	expression tag	UNP A0A3S7XTA4
A	546	TRP	-	expression tag	UNP A0A3S7XTA4
A	547	HIS	-	expression tag	UNP A0A3S7XTA4
A	548	GLU	-	expression tag	UNP A0A3S7XTA4
A	549	GLY	-	expression tag	UNP A0A3S7XTA4
A	550	HIS	-	expression tag	UNP A0A3S7XTA4
A	551	HIS	-	expression tag	UNP A0A3S7XTA4
A	552	HIS	-	expression tag	UNP A0A3S7XTA4
A	553	HIS	-	expression tag	UNP A0A3S7XTA4
A	554	HIS	-	expression tag	UNP A0A3S7XTA4
A	555	HIS	-	expression tag	UNP A0A3S7XTA4
C	10	GLY	-	expression tag	UNP A0A3S7XTA4
C	376	LYS	GLU	conflict	UNP A0A3S7XTA4
C	504	SER	-	expression tag	UNP A0A3S7XTA4
C	505	GLY	-	expression tag	UNP A0A3S7XTA4
C	506	TYR	-	expression tag	UNP A0A3S7XTA4
C	507	ILE	-	expression tag	UNP A0A3S7XTA4
C	508	PRO	-	expression tag	UNP A0A3S7XTA4
C	509	GLU	-	expression tag	UNP A0A3S7XTA4
C	510	ALA	-	expression tag	UNP A0A3S7XTA4
C	511	PRO	-	expression tag	UNP A0A3S7XTA4
C	512	ARG	-	expression tag	UNP A0A3S7XTA4
C	513	ASP	-	expression tag	UNP A0A3S7XTA4
C	514	GLY	-	expression tag	UNP A0A3S7XTA4
C	515	GLN	-	expression tag	UNP A0A3S7XTA4
C	516	ALA	-	expression tag	UNP A0A3S7XTA4
C	517	TYR	-	expression tag	UNP A0A3S7XTA4
C	518	VAL	-	expression tag	UNP A0A3S7XTA4
C	519	ARG	-	expression tag	UNP A0A3S7XTA4
C	520	LYS	-	expression tag	UNP A0A3S7XTA4
C	521	ASP	-	expression tag	UNP A0A3S7XTA4
C	522	GLY	-	expression tag	UNP A0A3S7XTA4
C	523	GLU	-	expression tag	UNP A0A3S7XTA4
C	524	TRP	-	expression tag	UNP A0A3S7XTA4
C	525	VAL	-	expression tag	UNP A0A3S7XTA4
C	526	LEU	-	expression tag	UNP A0A3S7XTA4
C	527	LEU	-	expression tag	UNP A0A3S7XTA4
C	528	SER	-	expression tag	UNP A0A3S7XTA4
C	529	THR	-	expression tag	UNP A0A3S7XTA4
C	530	PHE	-	expression tag	UNP A0A3S7XTA4
C	531	LEU	-	expression tag	UNP A0A3S7XTA4
C	532	GLY	-	expression tag	UNP A0A3S7XTA4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	533	SER	-	expression tag	UNP A0A3S7XTA4
C	534	GLY	-	expression tag	UNP A0A3S7XTA4
C	535	LEU	-	expression tag	UNP A0A3S7XTA4
C	536	ASN	-	expression tag	UNP A0A3S7XTA4
C	537	ASP	-	expression tag	UNP A0A3S7XTA4
C	538	ILE	-	expression tag	UNP A0A3S7XTA4
C	539	PHE	-	expression tag	UNP A0A3S7XTA4
C	540	GLU	-	expression tag	UNP A0A3S7XTA4
C	541	ALA	-	expression tag	UNP A0A3S7XTA4
C	542	GLN	-	expression tag	UNP A0A3S7XTA4
C	543	LYS	-	expression tag	UNP A0A3S7XTA4
C	544	ILE	-	expression tag	UNP A0A3S7XTA4
C	545	GLU	-	expression tag	UNP A0A3S7XTA4
C	546	TRP	-	expression tag	UNP A0A3S7XTA4
C	547	HIS	-	expression tag	UNP A0A3S7XTA4
C	548	GLU	-	expression tag	UNP A0A3S7XTA4
C	549	GLY	-	expression tag	UNP A0A3S7XTA4
C	550	HIS	-	expression tag	UNP A0A3S7XTA4
C	551	HIS	-	expression tag	UNP A0A3S7XTA4
C	552	HIS	-	expression tag	UNP A0A3S7XTA4
C	553	HIS	-	expression tag	UNP A0A3S7XTA4
C	554	HIS	-	expression tag	UNP A0A3S7XTA4
C	555	HIS	-	expression tag	UNP A0A3S7XTA4
E	10	GLY	-	expression tag	UNP A0A3S7XTA4
E	376	LYS	GLU	conflict	UNP A0A3S7XTA4
E	504	SER	-	expression tag	UNP A0A3S7XTA4
E	505	GLY	-	expression tag	UNP A0A3S7XTA4
E	506	TYR	-	expression tag	UNP A0A3S7XTA4
E	507	ILE	-	expression tag	UNP A0A3S7XTA4
E	508	PRO	-	expression tag	UNP A0A3S7XTA4
E	509	GLU	-	expression tag	UNP A0A3S7XTA4
E	510	ALA	-	expression tag	UNP A0A3S7XTA4
E	511	PRO	-	expression tag	UNP A0A3S7XTA4
E	512	ARG	-	expression tag	UNP A0A3S7XTA4
E	513	ASP	-	expression tag	UNP A0A3S7XTA4
E	514	GLY	-	expression tag	UNP A0A3S7XTA4
E	515	GLN	-	expression tag	UNP A0A3S7XTA4
E	516	ALA	-	expression tag	UNP A0A3S7XTA4
E	517	TYR	-	expression tag	UNP A0A3S7XTA4
E	518	VAL	-	expression tag	UNP A0A3S7XTA4
E	519	ARG	-	expression tag	UNP A0A3S7XTA4
E	520	LYS	-	expression tag	UNP A0A3S7XTA4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	521	ASP	-	expression tag	UNP A0A3S7XTA4
E	522	GLY	-	expression tag	UNP A0A3S7XTA4
E	523	GLU	-	expression tag	UNP A0A3S7XTA4
E	524	TRP	-	expression tag	UNP A0A3S7XTA4
E	525	VAL	-	expression tag	UNP A0A3S7XTA4
E	526	LEU	-	expression tag	UNP A0A3S7XTA4
E	527	LEU	-	expression tag	UNP A0A3S7XTA4
E	528	SER	-	expression tag	UNP A0A3S7XTA4
E	529	THR	-	expression tag	UNP A0A3S7XTA4
E	530	PHE	-	expression tag	UNP A0A3S7XTA4
E	531	LEU	-	expression tag	UNP A0A3S7XTA4
E	532	GLY	-	expression tag	UNP A0A3S7XTA4
E	533	SER	-	expression tag	UNP A0A3S7XTA4
E	534	GLY	-	expression tag	UNP A0A3S7XTA4
E	535	LEU	-	expression tag	UNP A0A3S7XTA4
E	536	ASN	-	expression tag	UNP A0A3S7XTA4
E	537	ASP	-	expression tag	UNP A0A3S7XTA4
E	538	ILE	-	expression tag	UNP A0A3S7XTA4
E	539	PHE	-	expression tag	UNP A0A3S7XTA4
E	540	GLU	-	expression tag	UNP A0A3S7XTA4
E	541	ALA	-	expression tag	UNP A0A3S7XTA4
E	542	GLN	-	expression tag	UNP A0A3S7XTA4
E	543	LYS	-	expression tag	UNP A0A3S7XTA4
E	544	ILE	-	expression tag	UNP A0A3S7XTA4
E	545	GLU	-	expression tag	UNP A0A3S7XTA4
E	546	TRP	-	expression tag	UNP A0A3S7XTA4
E	547	HIS	-	expression tag	UNP A0A3S7XTA4
E	548	GLU	-	expression tag	UNP A0A3S7XTA4
E	549	GLY	-	expression tag	UNP A0A3S7XTA4
E	550	HIS	-	expression tag	UNP A0A3S7XTA4
E	551	HIS	-	expression tag	UNP A0A3S7XTA4
E	552	HIS	-	expression tag	UNP A0A3S7XTA4
E	553	HIS	-	expression tag	UNP A0A3S7XTA4
E	554	HIS	-	expression tag	UNP A0A3S7XTA4
E	555	HIS	-	expression tag	UNP A0A3S7XTA4
B	-327	GLY	-	expression tag	UNP A0A3S7XTA4
B	47	LYS	GLU	conflict	UNP A0A3S7XTA4
B	175	SER	-	expression tag	UNP A0A3S7XTA4
B	176	GLY	-	expression tag	UNP A0A3S7XTA4
B	177	TYR	-	expression tag	UNP A0A3S7XTA4
B	178	ILE	-	expression tag	UNP A0A3S7XTA4
B	179	PRO	-	expression tag	UNP A0A3S7XTA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	GLU	-	expression tag	UNP A0A3S7XTA4
B	181	ALA	-	expression tag	UNP A0A3S7XTA4
B	182	PRO	-	expression tag	UNP A0A3S7XTA4
B	183	ARG	-	expression tag	UNP A0A3S7XTA4
B	184	ASP	-	expression tag	UNP A0A3S7XTA4
B	185	GLY	-	expression tag	UNP A0A3S7XTA4
B	186	GLN	-	expression tag	UNP A0A3S7XTA4
B	187	ALA	-	expression tag	UNP A0A3S7XTA4
B	188	TYR	-	expression tag	UNP A0A3S7XTA4
B	189	VAL	-	expression tag	UNP A0A3S7XTA4
B	190	ARG	-	expression tag	UNP A0A3S7XTA4
B	191	LYS	-	expression tag	UNP A0A3S7XTA4
B	192	ASP	-	expression tag	UNP A0A3S7XTA4
B	193	GLY	-	expression tag	UNP A0A3S7XTA4
B	194	GLU	-	expression tag	UNP A0A3S7XTA4
B	195	TRP	-	expression tag	UNP A0A3S7XTA4
B	196	VAL	-	expression tag	UNP A0A3S7XTA4
B	197	LEU	-	expression tag	UNP A0A3S7XTA4
B	198	LEU	-	expression tag	UNP A0A3S7XTA4
B	199	SER	-	expression tag	UNP A0A3S7XTA4
B	200	THR	-	expression tag	UNP A0A3S7XTA4
B	201	PHE	-	expression tag	UNP A0A3S7XTA4
B	202	LEU	-	expression tag	UNP A0A3S7XTA4
B	203	GLY	-	expression tag	UNP A0A3S7XTA4
B	204	SER	-	expression tag	UNP A0A3S7XTA4
B	205	GLY	-	expression tag	UNP A0A3S7XTA4
B	206	LEU	-	expression tag	UNP A0A3S7XTA4
B	207	ASN	-	expression tag	UNP A0A3S7XTA4
B	208	ASP	-	expression tag	UNP A0A3S7XTA4
B	209	ILE	-	expression tag	UNP A0A3S7XTA4
B	210	PHE	-	expression tag	UNP A0A3S7XTA4
B	211	GLU	-	expression tag	UNP A0A3S7XTA4
B	212	ALA	-	expression tag	UNP A0A3S7XTA4
B	213	GLN	-	expression tag	UNP A0A3S7XTA4
B	214	LYS	-	expression tag	UNP A0A3S7XTA4
B	215	ILE	-	expression tag	UNP A0A3S7XTA4
B	216	GLU	-	expression tag	UNP A0A3S7XTA4
B	217	TRP	-	expression tag	UNP A0A3S7XTA4
B	218	HIS	-	expression tag	UNP A0A3S7XTA4
B	219	GLU	-	expression tag	UNP A0A3S7XTA4
B	220	GLY	-	expression tag	UNP A0A3S7XTA4
B	221	HIS	-	expression tag	UNP A0A3S7XTA4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	222	HIS	-	expression tag	UNP A0A3S7XTA4
B	223	HIS	-	expression tag	UNP A0A3S7XTA4
B	224	HIS	-	expression tag	UNP A0A3S7XTA4
B	225	HIS	-	expression tag	UNP A0A3S7XTA4
B	226	HIS	-	expression tag	UNP A0A3S7XTA4
D	-327	GLY	-	expression tag	UNP A0A3S7XTA4
D	47	LYS	GLU	conflict	UNP A0A3S7XTA4
D	175	SER	-	expression tag	UNP A0A3S7XTA4
D	176	GLY	-	expression tag	UNP A0A3S7XTA4
D	177	TYR	-	expression tag	UNP A0A3S7XTA4
D	178	ILE	-	expression tag	UNP A0A3S7XTA4
D	179	PRO	-	expression tag	UNP A0A3S7XTA4
D	180	GLU	-	expression tag	UNP A0A3S7XTA4
D	181	ALA	-	expression tag	UNP A0A3S7XTA4
D	182	PRO	-	expression tag	UNP A0A3S7XTA4
D	183	ARG	-	expression tag	UNP A0A3S7XTA4
D	184	ASP	-	expression tag	UNP A0A3S7XTA4
D	185	GLY	-	expression tag	UNP A0A3S7XTA4
D	186	GLN	-	expression tag	UNP A0A3S7XTA4
D	187	ALA	-	expression tag	UNP A0A3S7XTA4
D	188	TYR	-	expression tag	UNP A0A3S7XTA4
D	189	VAL	-	expression tag	UNP A0A3S7XTA4
D	190	ARG	-	expression tag	UNP A0A3S7XTA4
D	191	LYS	-	expression tag	UNP A0A3S7XTA4
D	192	ASP	-	expression tag	UNP A0A3S7XTA4
D	193	GLY	-	expression tag	UNP A0A3S7XTA4
D	194	GLU	-	expression tag	UNP A0A3S7XTA4
D	195	TRP	-	expression tag	UNP A0A3S7XTA4
D	196	VAL	-	expression tag	UNP A0A3S7XTA4
D	197	LEU	-	expression tag	UNP A0A3S7XTA4
D	198	LEU	-	expression tag	UNP A0A3S7XTA4
D	199	SER	-	expression tag	UNP A0A3S7XTA4
D	200	THR	-	expression tag	UNP A0A3S7XTA4
D	201	PHE	-	expression tag	UNP A0A3S7XTA4
D	202	LEU	-	expression tag	UNP A0A3S7XTA4
D	203	GLY	-	expression tag	UNP A0A3S7XTA4
D	204	SER	-	expression tag	UNP A0A3S7XTA4
D	205	GLY	-	expression tag	UNP A0A3S7XTA4
D	206	LEU	-	expression tag	UNP A0A3S7XTA4
D	207	ASN	-	expression tag	UNP A0A3S7XTA4
D	208	ASP	-	expression tag	UNP A0A3S7XTA4
D	209	ILE	-	expression tag	UNP A0A3S7XTA4

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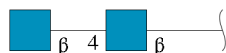
Chain	Residue	Modelled	Actual	Comment	Reference
D	210	PHE	-	expression tag	UNP A0A3S7XTA4
D	211	GLU	-	expression tag	UNP A0A3S7XTA4
D	212	ALA	-	expression tag	UNP A0A3S7XTA4
D	213	GLN	-	expression tag	UNP A0A3S7XTA4
D	214	LYS	-	expression tag	UNP A0A3S7XTA4
D	215	ILE	-	expression tag	UNP A0A3S7XTA4
D	216	GLU	-	expression tag	UNP A0A3S7XTA4
D	217	TRP	-	expression tag	UNP A0A3S7XTA4
D	218	HIS	-	expression tag	UNP A0A3S7XTA4
D	219	GLU	-	expression tag	UNP A0A3S7XTA4
D	220	GLY	-	expression tag	UNP A0A3S7XTA4
D	221	HIS	-	expression tag	UNP A0A3S7XTA4
D	222	HIS	-	expression tag	UNP A0A3S7XTA4
D	223	HIS	-	expression tag	UNP A0A3S7XTA4
D	224	HIS	-	expression tag	UNP A0A3S7XTA4
D	225	HIS	-	expression tag	UNP A0A3S7XTA4
D	226	HIS	-	expression tag	UNP A0A3S7XTA4
F	-327	GLY	-	expression tag	UNP A0A3S7XTA4
F	47	LYS	GLU	conflict	UNP A0A3S7XTA4
F	175	SER	-	expression tag	UNP A0A3S7XTA4
F	176	GLY	-	expression tag	UNP A0A3S7XTA4
F	177	TYR	-	expression tag	UNP A0A3S7XTA4
F	178	ILE	-	expression tag	UNP A0A3S7XTA4
F	179	PRO	-	expression tag	UNP A0A3S7XTA4
F	180	GLU	-	expression tag	UNP A0A3S7XTA4
F	181	ALA	-	expression tag	UNP A0A3S7XTA4
F	182	PRO	-	expression tag	UNP A0A3S7XTA4
F	183	ARG	-	expression tag	UNP A0A3S7XTA4
F	184	ASP	-	expression tag	UNP A0A3S7XTA4
F	185	GLY	-	expression tag	UNP A0A3S7XTA4
F	186	GLN	-	expression tag	UNP A0A3S7XTA4
F	187	ALA	-	expression tag	UNP A0A3S7XTA4
F	188	TYR	-	expression tag	UNP A0A3S7XTA4
F	189	VAL	-	expression tag	UNP A0A3S7XTA4
F	190	ARG	-	expression tag	UNP A0A3S7XTA4
F	191	LYS	-	expression tag	UNP A0A3S7XTA4
F	192	ASP	-	expression tag	UNP A0A3S7XTA4
F	193	GLY	-	expression tag	UNP A0A3S7XTA4
F	194	GLU	-	expression tag	UNP A0A3S7XTA4
F	195	TRP	-	expression tag	UNP A0A3S7XTA4
F	196	VAL	-	expression tag	UNP A0A3S7XTA4
F	197	LEU	-	expression tag	UNP A0A3S7XTA4

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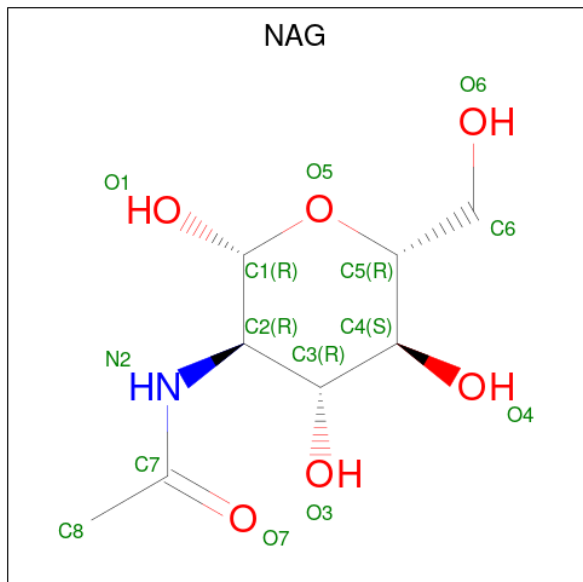
Chain	Residue	Modelled	Actual	Comment	Reference
F	198	LEU	-	expression tag	UNP A0A3S7XTA4
F	199	SER	-	expression tag	UNP A0A3S7XTA4
F	200	THR	-	expression tag	UNP A0A3S7XTA4
F	201	PHE	-	expression tag	UNP A0A3S7XTA4
F	202	LEU	-	expression tag	UNP A0A3S7XTA4
F	203	GLY	-	expression tag	UNP A0A3S7XTA4
F	204	SER	-	expression tag	UNP A0A3S7XTA4
F	205	GLY	-	expression tag	UNP A0A3S7XTA4
F	206	LEU	-	expression tag	UNP A0A3S7XTA4
F	207	ASN	-	expression tag	UNP A0A3S7XTA4
F	208	ASP	-	expression tag	UNP A0A3S7XTA4
F	209	ILE	-	expression tag	UNP A0A3S7XTA4
F	210	PHE	-	expression tag	UNP A0A3S7XTA4
F	211	GLU	-	expression tag	UNP A0A3S7XTA4
F	212	ALA	-	expression tag	UNP A0A3S7XTA4
F	213	GLN	-	expression tag	UNP A0A3S7XTA4
F	214	LYS	-	expression tag	UNP A0A3S7XTA4
F	215	ILE	-	expression tag	UNP A0A3S7XTA4
F	216	GLU	-	expression tag	UNP A0A3S7XTA4
F	217	TRP	-	expression tag	UNP A0A3S7XTA4
F	218	HIS	-	expression tag	UNP A0A3S7XTA4
F	219	GLU	-	expression tag	UNP A0A3S7XTA4
F	220	GLY	-	expression tag	UNP A0A3S7XTA4
F	221	HIS	-	expression tag	UNP A0A3S7XTA4
F	222	HIS	-	expression tag	UNP A0A3S7XTA4
F	223	HIS	-	expression tag	UNP A0A3S7XTA4
F	224	HIS	-	expression tag	UNP A0A3S7XTA4
F	225	HIS	-	expression tag	UNP A0A3S7XTA4
F	226	HIS	-	expression tag	UNP A0A3S7XTA4

- 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				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		

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

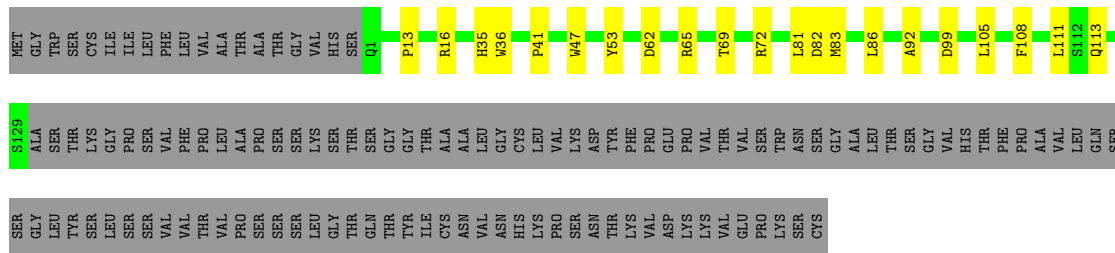


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5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

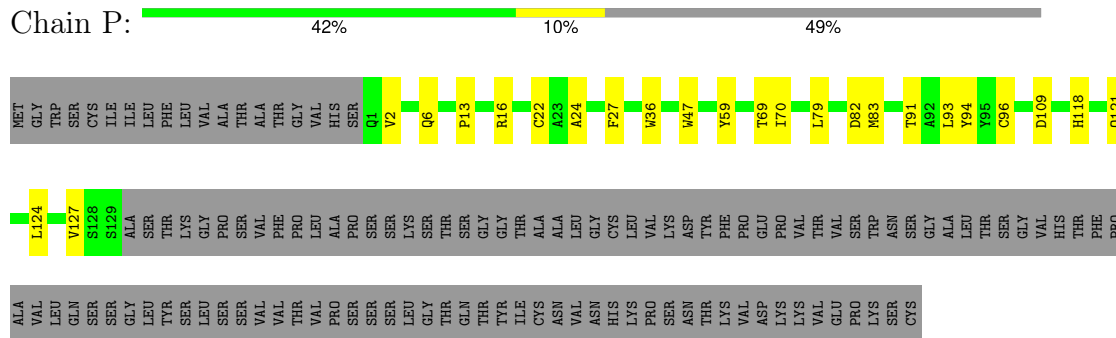
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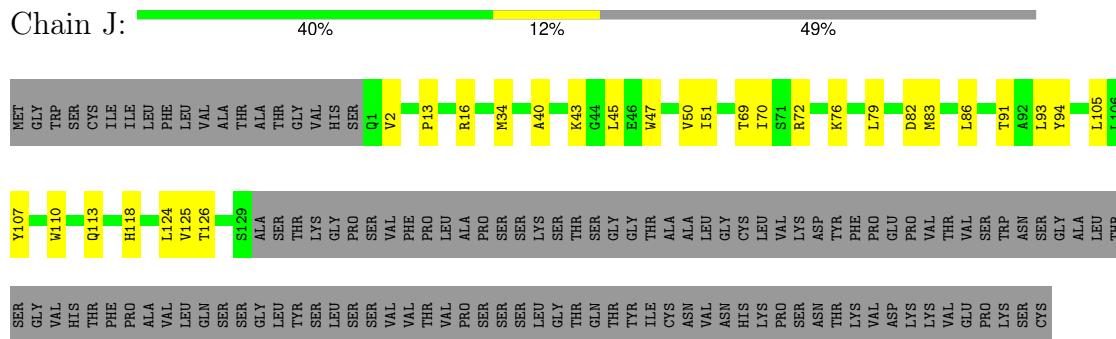
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	



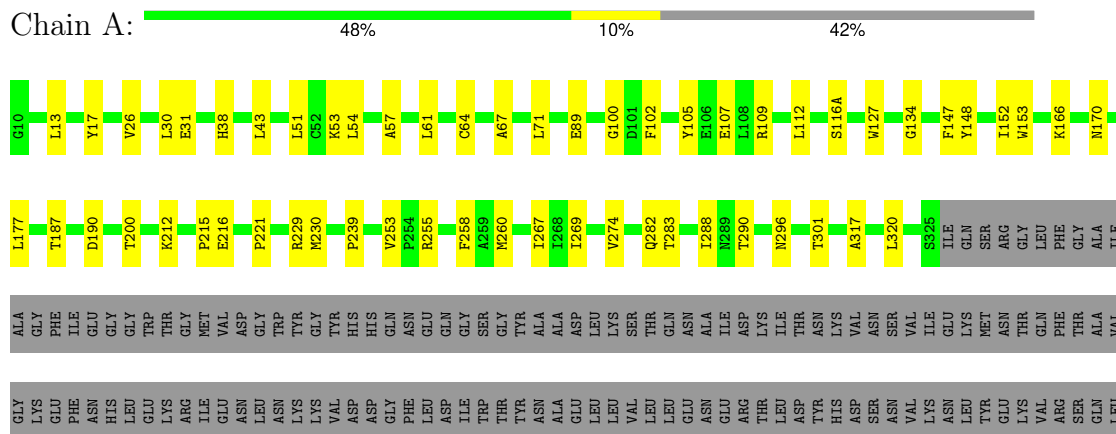
• Molecule 2: Fab heavy antibody AEL31311



• Molecule 2: Fab heavy antibody AEL31311



• Molecule 3: Hemagglutinin



68%

[illegible]

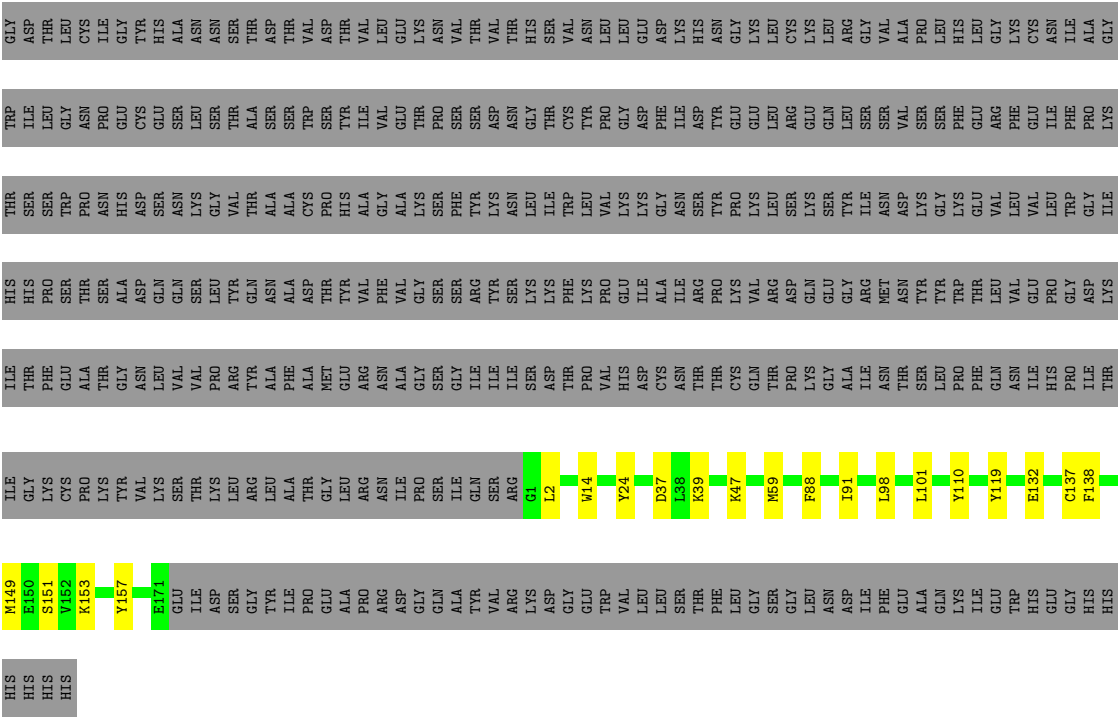
- Molecule 3: Hemagglutinin

69%

ASN	A96	H11	D112	S113	L118	N135	F140	T147	C148	M149	E150	S151	N154	K167	R170	E171	GLU	ILE	ASP	SER	GLY	TVR	ILE	PNO	GLU	ALA	ALA	ARG	ASP	GLY	GLN	ALA	VAL	THR	ARG	LYS	ASP	GLY	GLU	TRP	VAL	LEU	LEU	SER	THR	PHE	LEU	GLY	SER	GLY	LEU	LEU
-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 3: Hemagglutinin

69%



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

Chain G: 100%

MAG1
MAG2

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

Chain H: 100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	190000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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	L	0.16	0/875	0.42	0/1189
1	M	0.19	0/875	0.48	0/1189
1	O	0.18	0/875	0.50	0/1189
2	I	0.15	0/1046	0.34	0/1419
2	J	0.16	0/1046	0.36	0/1419
2	P	0.16	0/1046	0.38	0/1419
3	A	0.15	0/2593	0.37	0/3524
3	B	0.20	0/1439	0.46	0/1938
3	C	0.16	0/2587	0.36	0/3516
3	D	0.19	0/1408	0.42	0/1896
3	E	0.18	0/2593	0.43	0/3524
3	F	0.17	0/1408	0.39	0/1896
All	All	0.17	0/17791	0.40	0/24118

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	L	855	0	825	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	855	0	825	14	0
1	O	855	0	825	17	0
2	I	1020	0	975	14	0
2	J	1020	0	975	18	0
2	P	1020	0	975	14	0
3	A	2529	0	2475	38	0
3	B	1411	0	1334	12	0
3	C	2523	0	2469	46	0
3	D	1380	0	1308	30	0
3	E	2529	0	2475	62	0
3	F	1380	0	1310	17	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
5	A	42	0	39	0	0
5	B	28	0	26	0	0
5	C	70	0	65	0	0
5	D	28	0	26	1	0
5	E	42	0	39	0	0
All	All	17643	0	17016	259	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 (259) 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)
2:J:83:MET:HB3	2:J:86:LEU:HD11	1.61	0.81
2:P:6:GLN:HB3	2:P:22:CYS:HB3	1.61	0.81
3:D:150:GLU:O	3:D:154:ASN:HB2	1.85	0.75
2:J:50:VAL:HG11	2:J:113:GLN:HE22	1.51	0.75
3:D:147:THR:O	3:D:151:SER:HB2	1.86	0.75
3:D:24:TYR:HE1	3:D:118:LEU:HD21	1.53	0.72
3:C:293:PRO:HD3	3:D:56:ILE:HG23	1.71	0.72
2:P:59:TYR:HE2	2:P:109:ASP:HA	1.54	0.72
2:P:13:PRO:HG2	2:P:16:ARG:HE	1.55	0.71
2:J:69:THR:HB	2:J:82:ASP:HB2	1.72	0.71
3:E:260:MET:HE1	3:E:262:ARG:HD3	1.73	0.70
3:D:167:LYS:HD3	3:D:170:ARG:HH22	1.55	0.70
3:B:131:LYS:HB2	3:B:141:TYR:HE1	1.57	0.69
3:E:288:ILE:HG22	3:E:290:THR:H	1.57	0.69
3:C:279:THR:HG21	3:C:287:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:PRO:HD2	2:I:16:ARG:HH12	1.59	0.68
3:E:202:VAL:HB	3:E:213:PHE:HB2	1.76	0.67
3:D:150:GLU:O	3:D:154:ASN:CB	2.43	0.66
3:D:17:MET:HE3	3:D:23:GLY:HA3	1.77	0.66
3:C:220:ARG:HD3	3:C:229:ARG:HG2	1.78	0.66
3:A:51:LEU:HA	3:A:282:GLN:HE22	1.62	0.65
3:A:216:GLU:HB2	3:E:212:LYS:HD2	1.78	0.64
3:C:123:LYS:HD2	3:C:255:ARG:HD2	1.79	0.64
3:E:122:PRO:HD2	3:E:126:SER:HB3	1.78	0.64
3:C:42:LEU:HA	3:C:292:LEU:HD12	1.79	0.64
3:B:128:ASN:HB2	3:B:170:ARG:HH12	1.63	0.62
3:C:70:ILE:HG22	3:C:179:LEU:HD11	1.81	0.62
3:E:43:LEU:HD11	3:E:296:ASN:HB2	1.81	0.62
1:L:98:THR:O	1:L:100:PRO:HD3	2.01	0.61
3:E:44:GLU:HG2	3:E:288:ILE:HG23	1.83	0.61
3:E:152:ILE:HD11	3:E:255:ARG:HE	1.66	0.60
3:A:170:ASN:HD22	3:A:239:PRO:HA	1.66	0.60
1:M:4:MET:HE1	1:M:92:CYS:HB3	1.83	0.60
2:P:83:MET:HE1	2:P:94:TYR:CE2	2.36	0.60
3:E:220:ARG:HG2	3:E:229:ARG:HG2	1.83	0.60
2:J:2:VAL:HG11	2:J:118:HIS:CG	2.37	0.59
3:A:283:THR:HG22	3:A:301:THR:HG22	1.84	0.59
1:M:41:GLN:HB2	1:M:51:LEU:HD22	1.85	0.58
3:B:3:PHE:HB3	3:B:116:LYS:HD2	1.85	0.58
1:O:14:SER:HB3	1:O:111:LYS:HB3	1.86	0.58
1:M:102:PHE:HD2	2:J:45:LEU:HB2	1.68	0.57
3:F:24:TYR:HE1	3:F:37:ASP:HB2	1.69	0.57
3:E:290:THR:HG22	3:E:306:PRO:HD3	1.86	0.57
3:E:127:TRP:H	3:E:166:LYS:HZ2	1.53	0.57
3:C:318:THR:HG23	3:D:48:ILE:HG21	1.86	0.57
2:P:91:THR:HG22	2:P:127:VAL:H	1.69	0.57
1:M:53:TYR:HD2	1:M:54:TRP:CD1	2.23	0.56
3:D:24:TYR:CE1	3:D:118:LEU:HD21	2.37	0.56
3:A:152:ILE:HG13	3:A:255:ARG:HB2	1.87	0.56
2:I:83:MET:HE3	2:I:86:LEU:HD11	1.88	0.56
3:D:30:GLN:HG3	5:D:302:NAG:H3	1.86	0.56
2:J:91:THR:HG23	2:J:126:THR:HA	1.87	0.56
3:A:200:THR:HG23	3:A:215:PRO:HG2	1.87	0.56
1:L:93:GLN:HE22	1:L:95:HIS:HB3	1.69	0.56
1:M:93:GLN:HG2	1:M:102:PHE:CE1	2.42	0.55
3:E:102:PHE:CD1	3:E:232:TYR:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:GLY:HA3	3:D:14:TRP:HE1	1.71	0.55
3:C:71:LEU:HD23	3:C:179:LEU:HD13	1.87	0.55
3:C:320:LEU:HD23	3:D:111:HIS:HB3	1.89	0.55
3:D:140:PHE:HE2	3:D:149:MET:HE1	1.71	0.55
3:F:47:LYS:HD2	3:F:110:TYR:OH	2.06	0.55
1:O:8:PRO:HB2	1:O:11:LEU:HD23	1.88	0.55
3:E:74:PRO:HB3	3:E:141:HIS:HB2	1.89	0.54
3:E:115:VAL:HG11	3:E:116(B):PHE:HD1	1.70	0.54
3:C:202:VAL:HG13	3:C:251:LEU:HD12	1.89	0.54
3:E:98:TYR:CE1	3:E:226:GLN:HG2	2.43	0.54
1:O:10:SER:HA	1:O:107:LYS:HB2	1.87	0.54
2:I:69:THR:HB	2:I:82:ASP:HB2	1.90	0.54
3:A:61:LEU:HD12	3:A:64:CYS:HB2	1.89	0.54
3:B:51:LYS:HZ1	3:B:103:GLU:HB3	1.72	0.54
2:P:83:MET:HE1	2:P:94:TYR:HE2	1.73	0.53
3:E:88:VAL:HG23	3:E:268:ILE:HG23	1.91	0.53
2:I:35:HIS:HE1	2:I:99:ASP:HB3	1.73	0.53
3:C:182:ILE:HD11	3:C:202:VAL:HG11	1.90	0.53
3:A:288:ILE:HG22	3:A:290:THR:H	1.74	0.53
3:D:147:THR:O	3:D:151:SER:CB	2.57	0.52
3:E:122:PRO:HG2	3:E:125:SER:HB3	1.90	0.52
1:L:93:GLN:HE21	1:L:100:PRO:HB3	1.74	0.52
3:C:14:CYS:HB2	3:D:25:HIS:HB3	1.91	0.52
3:E:50:LYS:HB3	3:E:275:HIS:HB2	1.90	0.52
2:J:105:LEU:HB3	2:J:107:TYR:CE2	2.44	0.52
3:E:42:LEU:HD11	3:E:316:LEU:HD12	1.92	0.52
3:E:116(C):GLU:HB2	3:E:259:ALA:HB3	1.92	0.51
3:F:88:PHE:HD1	3:F:91:ILE:HD11	1.75	0.51
2:P:2:VAL:HG11	2:P:118:HIS:ND1	2.25	0.51
3:A:89:GLU:HB2	3:A:269:ILE:HG12	1.93	0.51
3:E:288:ILE:HD11	3:E:297:ILE:HD12	1.91	0.51
3:A:134:GLY:HA3	3:A:153:TRP:HB3	1.93	0.51
1:M:102:PHE:CD2	2:J:45:LEU:HB2	2.45	0.51
3:F:151:SER:HB3	3:F:157:TYR:HA	1.92	0.51
3:A:100:GLY:HA2	3:A:229:ARG:HD3	1.93	0.51
3:C:123:LYS:HA	3:C:127:TRP:HZ3	1.75	0.51
3:E:104:ASP:HB3	3:E:107:GLU:HB2	1.92	0.51
3:E:87:ILE:HG23	3:E:267:ILE:HG13	1.93	0.50
1:L:98:THR:HG23	2:I:111:LEU:N	2.26	0.50
1:M:21:ILE:HG21	1:M:106:THR:HG21	1.93	0.50
3:A:54:LEU:HD11	3:A:282:GLN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:GLN:H	2:P:121:GLN:HE22	1.60	0.50
3:C:268:ILE:HG23	3:C:284:PRO:HG3	1.94	0.49
1:O:13:VAL:HG21	1:O:19:ALA:HB2	1.94	0.49
3:A:212:LYS:HB3	3:C:216:GLU:HG2	1.94	0.49
3:C:180:TRP:HE1	3:C:213:PHE:HE2	1.60	0.49
2:J:70:ILE:HD11	2:J:79:LEU:HD11	1.95	0.49
3:C:17:TYR:HD2	3:C:320:LEU:HD13	1.78	0.48
3:C:288:ILE:HD11	3:C:305:CYS:HB2	1.95	0.48
3:A:51:LEU:HB2	3:A:274:VAL:HG22	1.94	0.48
3:A:53:LYS:HG2	3:A:57:ALA:HA	1.93	0.48
1:O:98:THR:O	1:O:100:PRO:HD3	2.12	0.48
3:E:66:ILE:HD13	3:E:109:ARG:HG2	1.96	0.48
3:E:184:HIS:ND1	3:E:216:GLU:HB2	2.27	0.48
3:C:152:ILE:HG12	3:C:255:ARG:HB2	1.96	0.48
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.96	0.48
2:I:41:PRO:HD3	2:I:92:ALA:HA	1.95	0.48
3:C:16:GLY:HA3	3:D:14:TRP:NE1	2.29	0.48
3:E:108:LEU:HD12	3:E:234:TRP:CG	2.49	0.47
3:E:220:ARG:HD3	3:E:228:GLY:HA2	1.96	0.47
1:L:70:GLY:HA3	1:L:75:PHE:HA	1.96	0.47
3:E:13:LEU:HD11	3:F:24:TYR:HD2	1.79	0.47
3:B:47:LYS:HD2	3:B:110:TYR:OH	2.14	0.47
3:C:107:GLU:O	3:C:111:GLN:HB2	2.14	0.47
1:M:2:ILE:HD12	1:M:27:GLN:HB3	1.96	0.47
1:O:37:LEU:HD22	1:O:75:PHE:CD2	2.50	0.47
2:J:47:TRP:CH2	2:J:50:VAL:HB	2.50	0.47
1:O:39:TRP:CD2	1:O:77:LEU:HD22	2.50	0.47
1:O:89:VAL:HG22	1:O:107:LYS:HG2	1.95	0.47
2:J:34:MET:HB3	2:J:79:LEU:HD22	1.96	0.47
1:O:100:PRO:HD2	2:P:47:TRP:CG	2.50	0.47
3:E:61:LEU:HD21	3:E:87:ILE:HD11	1.96	0.47
2:J:51:ILE:HG12	2:J:72:ARG:HD2	1.97	0.46
3:C:314:LEU:HD21	3:D:96:ALA:HB1	1.97	0.46
1:L:66:PHE:HE1	1:L:79:ILE:HG12	1.80	0.46
1:O:107:LYS:HB3	1:O:107:LYS:HE2	1.82	0.46
3:E:156:LYS:HD3	3:E:159:ASN:HA	1.97	0.46
3:D:84:VAL:O	3:D:88:PHE:HD2	1.98	0.46
1:M:14:SER:HB3	1:M:111:LYS:HB3	1.97	0.46
3:A:107:GLU:CD	3:D:76:ARG:HE	2.24	0.46
1:O:37:LEU:HB3	1:O:55:ALA:HB2	1.98	0.46
3:C:268:ILE:HG13	3:C:302:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:99:PRO:HA	2:I:47:TRP:CE3	2.51	0.46
3:A:53:LYS:HE2	3:A:57:ALA:HB2	1.97	0.46
3:C:102:PHE:CD1	3:C:232:TYR:HB2	2.51	0.46
2:J:93:LEU:HD13	2:J:124:LEU:HD13	1.99	0.45
3:E:16:GLY:HA3	3:F:14:TRP:HE1	1.80	0.45
3:F:98:LEU:HD23	3:F:101:LEU:HD12	1.98	0.45
3:F:132:GLU:HG2	3:F:138:PHE:HE1	1.81	0.45
1:L:29:VAL:HG23	1:L:96:TYR:HB2	1.99	0.45
3:A:109:ARG:HH21	3:A:267:ILE:HG21	1.81	0.45
1:O:51:LEU:HD11	1:O:66:PHE:HE2	1.81	0.45
3:F:149:MET:O	3:F:153:LYS:HG3	2.16	0.45
1:O:38:ALA:HB3	1:O:93:GLN:NE2	2.32	0.45
3:E:187:THR:HG23	3:E:190:ASP:H	1.81	0.45
3:E:160:SER:HA	3:E:196:GLN:HG2	1.99	0.45
3:A:320:LEU:HD23	3:A:320:LEU:H	1.81	0.45
3:C:42:LEU:HD11	3:D:56:ILE:HD11	1.99	0.45
1:M:98:THR:HG23	2:J:110:TRP:C	2.42	0.45
1:L:14:SER:HA	1:L:110:ILE:HD12	1.97	0.45
3:A:26:VAL:HG11	3:A:317:ALA:HB2	1.98	0.45
3:C:156:LYS:HA	3:C:161:TYR:HD2	1.81	0.45
3:C:223:VAL:HG12	3:C:224:ARG:HG2	1.99	0.45
2:I:105:LEU:HD11	3:B:52:VAL:HG11	1.99	0.44
3:C:234:TRP:HZ3	3:C:236:LEU:HG	1.82	0.44
3:E:26:VAL:HG11	3:E:317:ALA:HB2	1.99	0.44
2:J:13:PRO:HG2	2:J:16:ARG:HE	1.81	0.44
2:I:35:HIS:CE1	2:I:99:ASP:HB3	2.51	0.44
3:E:180:TRP:CZ2	3:E:204:VAL:HG11	2.52	0.44
3:A:112:LEU:HD23	3:A:112:LEU:HA	1.83	0.44
3:C:26:VAL:HG21	3:C:317:ALA:HB2	1.98	0.44
3:C:236:LEU:HD13	3:C:262:ARG:HH22	1.82	0.44
3:E:201:TYR:HB2	3:E:212:LYS:HE2	1.99	0.44
1:M:34:LYS:HD2	1:M:34:LYS:HA	1.88	0.44
1:L:65:ARG:HB2	1:L:80:SER:O	2.18	0.44
2:P:70:ILE:HD11	2:P:79:LEU:HD11	1.99	0.44
2:I:108:PHE:HD2	2:I:111:LEU:HD11	1.83	0.44
3:A:166:LYS:HA	3:A:166:LYS:HD2	1.80	0.44
3:A:187:THR:HG23	3:A:190:ASP:H	1.82	0.44
1:M:37:LEU:HB3	1:M:55:ALA:HB2	1.99	0.44
3:D:17:MET:HE1	3:D:20:GLY:H	1.83	0.44
3:D:52:VAL:HG13	3:D:56:ILE:HD13	1.99	0.44
3:A:17:TYR:HB2	3:A:320:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:42:LEU:HA	3:E:292:LEU:HD12	1.99	0.43
3:A:177:LEU:HD21	3:A:258:PHE:HB2	2.00	0.43
3:C:293:PRO:HA	3:C:306:PRO:HG3	2.00	0.43
3:E:299:PRO:HG3	3:E:308:TYR:CE2	2.53	0.43
3:E:314:LEU:HD23	3:E:314:LEU:HA	1.83	0.43
3:E:116(A):SER:O	3:E:260:MET:HA	2.18	0.43
3:E:234:TRP:HZ3	3:E:236:LEU:HD12	1.82	0.43
3:A:43:LEU:HD11	3:A:296:ASN:CG	2.42	0.43
1:M:32:ASN:N	1:M:32:ASN:HD22	2.17	0.43
3:E:16:GLY:HA3	3:F:14:TRP:NE1	2.33	0.43
3:A:100:GLY:HA3	3:A:230:MET:O	2.19	0.43
3:E:52:CYS:HB3	3:E:277:CYS:HB2	1.37	0.43
3:E:86:TYR:CZ	3:E:282:GLN:HG2	2.53	0.43
3:A:127:TRP:HZ2	3:A:253:VAL:HG11	1.82	0.43
3:E:184:HIS:CG	3:E:216:GLU:HB2	2.54	0.43
3:D:3:PHE:HD2	3:D:113:SER:HA	1.84	0.43
3:A:221:PRO:HG2	3:E:206:SER:HA	2.01	0.43
2:P:93:LEU:HD13	2:P:124:LEU:HD13	2.01	0.43
1:O:39:TRP:HD1	1:O:52:ILE:HB	1.84	0.43
1:L:66:PHE:CE1	1:L:79:ILE:HG12	2.54	0.42
1:O:4:MET:HE3	1:O:4:MET:HA	2.00	0.42
3:C:176:VAL:HA	3:C:259:ALA:HA	2.01	0.42
3:C:184:HIS:CE1	3:C:216:GLU:H	2.37	0.42
3:C:108:LEU:HD23	3:C:108:LEU:HA	1.85	0.42
1:M:98:THR:O	1:M:100:PRO:HD3	2.19	0.42
3:E:293:PRO:HA	3:F:59:MET:HG3	2.00	0.42
3:D:9:PHE:O	3:D:135:ASN:HA	2.19	0.42
3:E:172:LYS:O	3:E:174:LYS:HG2	2.19	0.42
3:D:3:PHE:CE2	3:D:113:SER:HB2	2.54	0.42
1:L:51:LEU:HD11	1:L:66:PHE:CD2	2.54	0.42
1:L:98:THR:HA	2:I:113:GLN:OE1	2.19	0.42
3:C:66:ILE:HG13	3:C:109:ARG:HG2	2.01	0.42
3:E:216:GLU:HB3	3:E:220:ARG:NH2	2.34	0.42
3:D:140:PHE:CE2	3:D:149:MET:HE1	2.52	0.42
3:A:30:LEU:HD22	3:F:47:LYS:HB3	2.00	0.42
3:A:38:HIS:CE1	3:B:21:TRP:HE1	2.37	0.42
3:A:147:PHE:CE1	3:A:148:TYR:HD2	2.37	0.42
1:O:79:ILE:HG21	1:O:82:LEU:HD12	2.02	0.42
3:B:87:GLY:O	3:B:91:ILE:HG12	2.20	0.42
3:C:175:GLU:OE2	3:C:236:LEU:HB3	2.19	0.42
2:J:76:LYS:HE2	2:J:76:LYS:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:23:GLY:HA2	3:B:37:ASP:H	1.83	0.42
3:A:31:GLU:OE2	3:F:47:LYS:HE2	2.19	0.42
3:C:67:ALA:O	3:C:71:LEU:HB2	2.19	0.42
3:E:116:SER:HB2	3:E:263:ASN:ND2	2.35	0.42
2:I:36:TRP:NE1	2:I:81:LEU:HB2	2.34	0.41
2:J:94:TYR:CE2	2:J:125:VAL:HG11	2.55	0.41
3:E:74:PRO:HG2	3:E:139:CYS:HB3	2.02	0.41
3:C:105:TYR:CE2	3:C:109:ARG:HD2	2.56	0.41
3:C:129:ASN:HB3	3:C:162:PRO:HG2	2.02	0.41
3:C:237:VAL:HG13	3:C:241:ASP:HB3	2.01	0.41
3:E:66:ILE:HD12	3:E:66:ILE:H	1.84	0.41
3:B:51:LYS:NZ	3:B:103:GLU:HB3	2.35	0.41
3:A:67:ALA:HB2	3:A:105:TYR:CE1	2.54	0.41
3:A:71:LEU:HD11	3:A:102:PHE:HE2	1.86	0.41
3:E:135:VAL:HG23	3:E:145:LYS:HE2	2.02	0.41
2:P:36:TRP:CZ3	2:P:96:CYS:HB3	2.55	0.41
3:D:3:PHE:CE2	3:F:2:LEU:HB3	2.56	0.41
3:F:39:LYS:HB2	3:F:39:LYS:HE2	1.80	0.41
3:C:102:PHE:HD2	3:C:105:TYR:HB2	1.84	0.41
3:E:281:CYS:HB2	3:E:290:THR:CG2	2.51	0.41
3:E:15:ILE:HD12	3:F:119:TYR:HD1	1.86	0.41
3:C:116(A):SER:O	3:C:260:MET:HA	2.20	0.41
3:C:207:SER:HA	3:E:229:ARG:HH12	1.85	0.41
3:C:307:LYS:HG3	3:D:92:TRP:CE2	2.56	0.41
3:E:14:CYS:HA	3:F:137:CYS:HA	2.03	0.41
2:I:53:TYR:HA	2:I:72:ARG:HH12	1.85	0.41
3:A:13:LEU:HD21	3:B:152:VAL:HG11	2.02	0.41
3:A:317:ALA:O	3:B:107:THR:HG21	2.21	0.41
2:P:24:ALA:HB1	2:P:27:PHE:CE1	2.55	0.41
3:E:102:PHE:HD2	3:E:105:TYR:CD2	2.39	0.41
3:E:185:PRO:HB3	3:E:190:ASP:HB3	2.02	0.41
1:O:47:PRO:HA	1:O:48:PRO:HD3	2.00	0.40
2:P:69:THR:HB	2:P:82:ASP:HB2	2.02	0.40
3:E:30:LEU:O	3:D:47:LYS:HG2	2.22	0.40
3:A:116(A):SER:O	3:A:260:MET:HA	2.21	0.40
3:C:201:TYR:HB2	3:C:212:LYS:HE3	2.02	0.40
3:E:30:LEU:HB3	3:D:47:LYS:HG2	2.04	0.40
2:I:62:ASP:HA	2:I:65:ARG:HH12	1.86	0.40
3:E:47:HIS:HB2	3:E:286:GLY:HA3	2.03	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 PDB entries followed by that with respect to all EM entries.

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	L	109/237 (46%)	99 (91%)	10 (9%)	0	100	100
1	M	109/237 (46%)	101 (93%)	8 (7%)	0	100	100
1	O	109/237 (46%)	99 (91%)	10 (9%)	0	100	100
2	I	127/251 (51%)	122 (96%)	5 (4%)	0	100	100
2	J	127/251 (51%)	122 (96%)	5 (4%)	0	100	100
2	P	127/251 (51%)	121 (95%)	6 (5%)	0	100	100
3	A	322/554 (58%)	314 (98%)	8 (2%)	0	100	100
3	B	173/554 (31%)	162 (94%)	11 (6%)	0	100	100
3	C	321/554 (58%)	310 (97%)	11 (3%)	0	100	100
3	D	169/554 (30%)	164 (97%)	5 (3%)	0	100	100
3	E	322/554 (58%)	304 (94%)	18 (6%)	0	100	100
3	F	169/554 (30%)	159 (94%)	10 (6%)	0	100	100
All	All	2184/4788 (46%)	2077 (95%)	107 (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 PDB entries followed by that with respect to all EM entries.

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	L	95/206 (46%)	95 (100%)	0	100	100
1	M	95/206 (46%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	95/206 (46%)	95 (100%)	0	100	100
2	I	109/213 (51%)	109 (100%)	0	100	100
2	J	109/213 (51%)	109 (100%)	0	100	100
2	P	109/213 (51%)	109 (100%)	0	100	100
3	A	284/481 (59%)	284 (100%)	0	100	100
3	B	151/481 (31%)	151 (100%)	0	100	100
3	C	283/481 (59%)	283 (100%)	0	100	100
3	D	147/481 (31%)	147 (100%)	0	100	100
3	E	284/481 (59%)	284 (100%)	0	100	100
3	F	147/481 (31%)	147 (100%)	0	100	100
All	All	1908/4143 (46%)	1908 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	6	GLN
1	L	93	GLN
3	A	18	HIS
3	A	111	GLN
3	A	282	GLN
1	M	32	ASN
2	J	6	GLN
2	J	113	GLN
3	D	114	ASN
3	D	125	GLN
3	D	135	ASN
3	F	43	ASN
3	F	169	ASN

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 ⓘ

4 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	G	1	3,4	14,14,15	0.76	0	17,19,21	1.52	2 (11%)
4	NAG	G	2	4	14,14,15	0.75	0	17,19,21	1.10	1 (5%)
4	NAG	H	1	3,4	14,14,15	0.75	0	17,19,21	1.38	2 (11%)
4	NAG	H	2	4	14,14,15	0.72	0	17,19,21	1.04	1 (5%)

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	G	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	1/6/23/26	0/1/1/1
4	NAG	H	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	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	G	1	NAG	C1-O5-C5	4.38	118.06	112.19
4	H	1	NAG	C1-O5-C5	4.14	117.73	112.19
4	G	2	NAG	C1-O5-C5	3.13	116.38	112.19
4	G	1	NAG	O4-C4-C5	3.10	116.96	109.32
4	H	2	NAG	C1-O5-C5	2.80	115.94	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	NAG	O4-C4-C5	2.52	115.53	109.32

There are no chirality outliers.

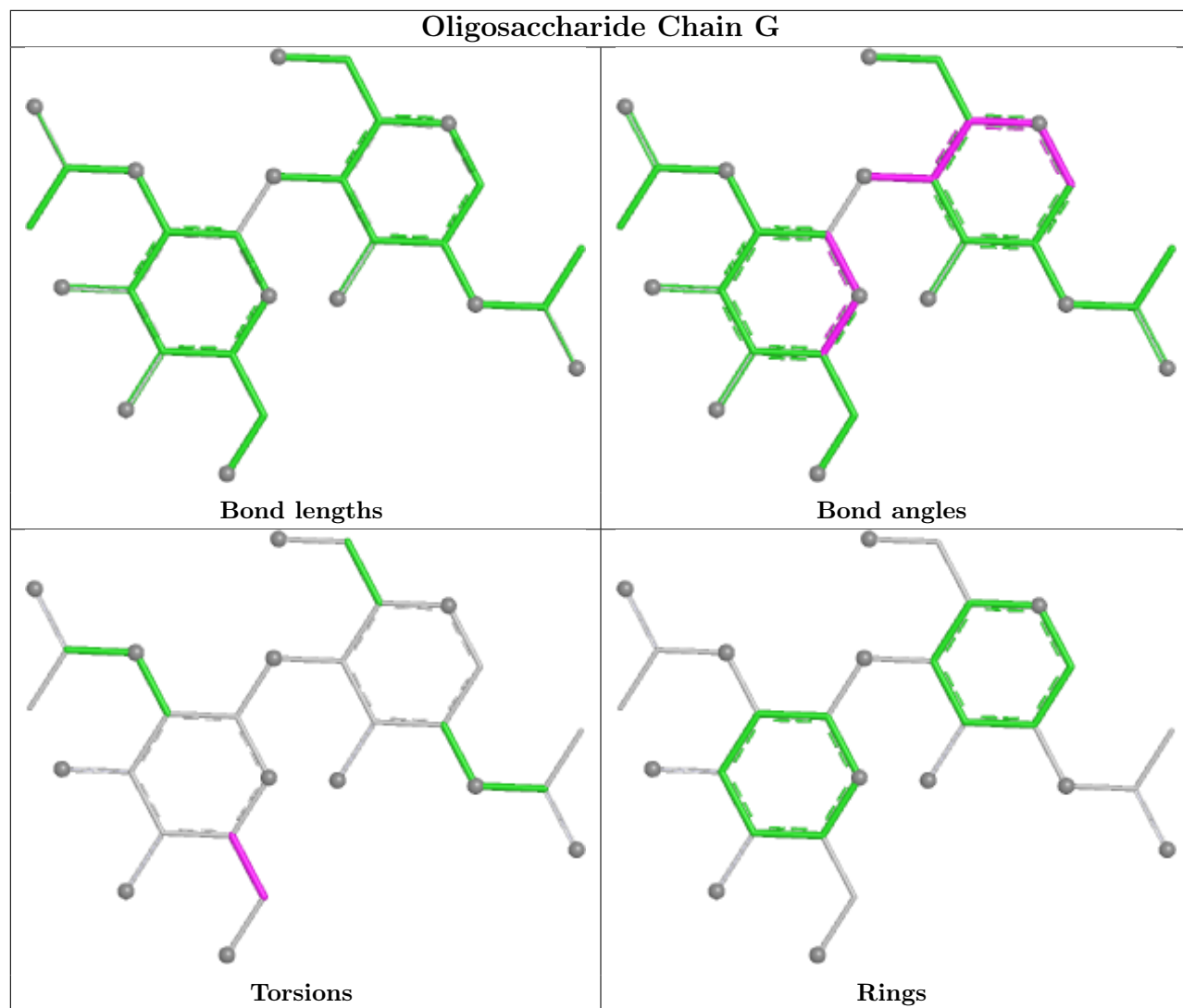
All (4) torsion outliers are listed below:

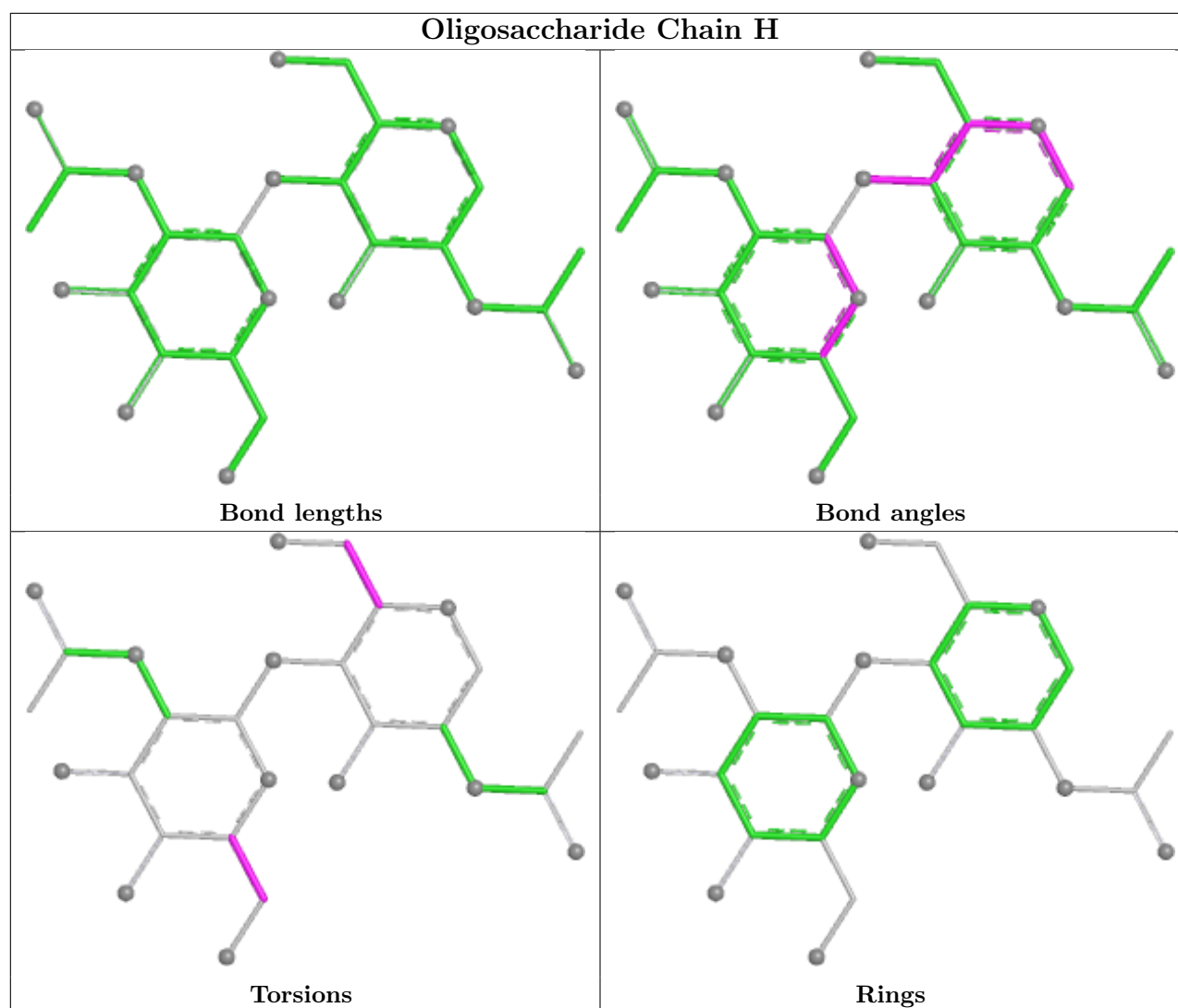
Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6

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](#)

15 ligands 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	$\# Z > 2$
5	NAG	B	301	3	14,14,15	0.72	0	17,19,21	0.82	0
5	NAG	C	601	3	14,14,15	0.70	0	17,19,21	0.85	0
5	NAG	C	604	3	14,14,15	0.77	0	17,19,21	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	603	3	14,14,15	0.70	0	17,19,21	1.34	1 (5%)
5	NAG	A	601	3	14,14,15	0.72	0	17,19,21	0.90	0
5	NAG	C	602	3	14,14,15	0.79	0	17,19,21	1.01	1 (5%)
5	NAG	A	602	3	14,14,15	0.72	0	17,19,21	0.81	0
5	NAG	E	601	3	14,14,15	0.75	0	17,19,21	2.04	3 (17%)
5	NAG	C	605	3	14,14,15	0.71	0	17,19,21	0.75	0
5	NAG	D	301	3	14,14,15	0.77	0	17,19,21	1.43	2 (11%)
5	NAG	E	602	3	14,14,15	0.69	0	17,19,21	0.90	0
5	NAG	A	603	3	14,14,15	0.74	0	17,19,21	0.79	0
5	NAG	C	603	3	14,14,15	0.74	0	17,19,21	0.85	0
5	NAG	B	302	3	14,14,15	0.82	1 (7%)	17,19,21	1.57	3 (17%)
5	NAG	D	302	3	14,14,15	0.77	0	17,19,21	2.05	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
5	NAG	B	301	3	-	0/6/23/26	0/1/1/1
5	NAG	C	601	3	-	1/6/23/26	0/1/1/1
5	NAG	C	604	3	-	1/6/23/26	0/1/1/1
5	NAG	E	603	3	-	3/6/23/26	0/1/1/1
5	NAG	A	601	3	-	2/6/23/26	0/1/1/1
5	NAG	C	602	3	-	0/6/23/26	0/1/1/1
5	NAG	A	602	3	-	1/6/23/26	0/1/1/1
5	NAG	E	601	3	-	0/6/23/26	0/1/1/1
5	NAG	C	605	3	-	1/6/23/26	0/1/1/1
5	NAG	D	301	3	-	3/6/23/26	0/1/1/1
5	NAG	E	602	3	-	1/6/23/26	0/1/1/1
5	NAG	A	603	3	-	0/6/23/26	0/1/1/1
5	NAG	C	603	3	-	0/6/23/26	0/1/1/1
5	NAG	B	302	3	-	0/6/23/26	0/1/1/1
5	NAG	D	302	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	302	NAG	O5-C1	-2.02	1.40	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	601	NAG	C1-O5-C5	6.14	120.42	112.19
5	D	302	NAG	C1-O5-C5	6.12	120.39	112.19
5	D	302	NAG	O5-C1-C2	4.28	117.92	111.29
5	D	301	NAG	C2-N2-C7	4.17	128.49	122.90
5	E	603	NAG	C2-N2-C7	3.99	128.25	122.90
5	E	601	NAG	C2-N2-C7	3.86	128.08	122.90
5	B	302	NAG	C1-O5-C5	-3.70	107.22	112.19
5	B	302	NAG	C2-N2-C7	2.97	126.88	122.90
5	C	602	NAG	C2-N2-C7	2.82	126.68	122.90
5	D	302	NAG	C3-C4-C5	-2.50	105.70	110.23
5	B	302	NAG	C4-C3-C2	2.28	114.36	111.02
5	D	301	NAG	C1-C2-N2	2.12	113.77	110.43
5	E	601	NAG	C8-C7-N2	-2.03	112.75	116.12

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	302	NAG	O5-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6
5	E	603	NAG	O5-C5-C6-O6
5	A	602	NAG	O5-C5-C6-O6
5	E	602	NAG	O5-C5-C6-O6
5	C	601	NAG	O5-C5-C6-O6
5	C	604	NAG	O5-C5-C6-O6
5	E	603	NAG	C1-C2-N2-C7
5	D	301	NAG	C3-C2-N2-C7
5	D	302	NAG	C4-C5-C6-O6
5	A	601	NAG	C1-C2-N2-C7
5	C	605	NAG	C1-C2-N2-C7
5	D	301	NAG	C1-C2-N2-C7
5	E	603	NAG	C3-C2-N2-C7
5	D	301	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	302	NAG	1	0

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.