



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 11:29 PM UTC

PDB ID : 6P3S / pdb_00006p3s
Title : Crystal structure of human Fab H5.28 in complex with influenza A H5N1
Vietnam hemagglutinin head domain
Authors : Dong, J.; Crowe, J.E.
Deposited on : 2019-05-24
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

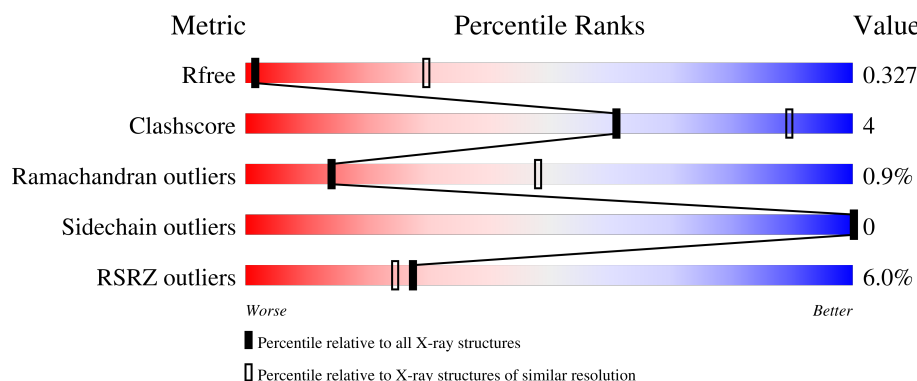
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	3% 86% 12% .
1	C	230	11% 87% 7% 5%
1	F	230	4% 87% 10% .
1	I	230	8% 87% 7% 6%
1	M	230	3% 92% 6% .

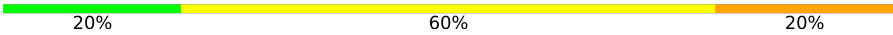
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Mol	Chain	Length	Quality of chain
1	P	230	
1	S	230	
1	V	230	
2	B	215	
2	D	215	
2	G	215	
2	J	215	
2	N	215	
2	Q	215	
2	T	215	
2	W	215	
3	E	219	
3	H	219	
3	K	219	
3	L	219	
3	O	219	
3	R	219	
3	U	219	
3	X	219	
4	Y	7	
5	Z	7	
6	a	6	
7	b	7	
8	c	5	
9	d	7	

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Mol	Chain	Length	Quality of chain
10	e	5	 20% 60% 20%
11	f	7	 29% 29% 43%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 32097 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 Human Fab H5.28 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1472	932	258	275	7			
1	C	218	Total	C	N	O	S	0	0	0
			1301	803	237	257	4			
1	F	223	Total	C	N	O	S	0	0	0
			1436	902	258	269	7			
1	I	217	Total	C	N	O	S	0	0	0
			1364	850	248	260	6			
1	M	225	Total	C	N	O	S	0	0	0
			1432	908	260	257	7			
1	P	220	Total	C	N	O	S	0	0	0
			1313	820	241	246	6			
1	S	224	Total	C	N	O	S	0	0	0
			1393	875	256	255	7			
1	V	208	Total	C	N	O	S	0	0	0
			1236	773	225	232	6			

- Molecule 2 is a protein called Human Fab H5.28 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	215	Total	C	N	O	S	0	0	0
			1477	932	254	285	6			
2	D	203	Total	C	N	O	S	0	0	0
			1211	741	228	238	4			
2	G	214	Total	C	N	O	S	0	0	0
			1363	853	243	261	6			
2	J	187	Total	C	N	O	S	0	0	0
			1097	677	201	215	4			
2	N	214	Total	C	N	O	S	0	0	0
			1295	812	233	244	6			
2	Q	202	Total	C	N	O	S	0	0	0
			1179	731	224	219	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	214	Total	C	N	O	S	0	0	0
			1280	797	240	238	5			
2	W	198	Total	C	N	O	S	0	0	0
			1121	694	212	212	3			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	196	Total	C	N	O	S	0	0	0
			1221	777	216	223	5			
3	H	202	Total	C	N	O	S	0	0	0
			1337	849	243	240	5			
3	K	206	Total	C	N	O	S	0	0	0
			1397	883	245	264	5			
3	L	185	Total	C	N	O	S	0	0	0
			1219	772	218	226	3			
3	O	209	Total	C	N	O	S	0	0	0
			1414	895	252	262	5			
3	R	194	Total	C	N	O	S	0	0	0
			1258	792	230	231	5			
3	U	196	Total	C	N	O	S	0	0	0
			1285	811	233	236	5			
3	X	196	Total	C	N	O	S	0	0	0
			1236	778	224	229	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	269	ALA	-	expression tag	UNP Q1KHK2
E	270	ALA	-	expression tag	UNP Q1KHK2
E	271	HIS	-	expression tag	UNP Q1KHK2
E	272	HIS	-	expression tag	UNP Q1KHK2
E	273	HIS	-	expression tag	UNP Q1KHK2
E	274	HIS	-	expression tag	UNP Q1KHK2
E	275	HIS	-	expression tag	UNP Q1KHK2
E	276	HIS	-	expression tag	UNP Q1KHK2
H	269	ALA	-	expression tag	UNP Q1KHK2
H	270	ALA	-	expression tag	UNP Q1KHK2
H	271	HIS	-	expression tag	UNP Q1KHK2
H	272	HIS	-	expression tag	UNP Q1KHK2
H	273	HIS	-	expression tag	UNP Q1KHK2
H	274	HIS	-	expression tag	UNP Q1KHK2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	275	HIS	-	expression tag	UNP Q1KHK2
H	276	HIS	-	expression tag	UNP Q1KHK2
K	269	ALA	-	expression tag	UNP Q1KHK2
K	270	ALA	-	expression tag	UNP Q1KHK2
K	271	HIS	-	expression tag	UNP Q1KHK2
K	272	HIS	-	expression tag	UNP Q1KHK2
K	273	HIS	-	expression tag	UNP Q1KHK2
K	274	HIS	-	expression tag	UNP Q1KHK2
K	275	HIS	-	expression tag	UNP Q1KHK2
K	276	HIS	-	expression tag	UNP Q1KHK2
L	269	ALA	-	expression tag	UNP Q1KHK2
L	270	ALA	-	expression tag	UNP Q1KHK2
L	271	HIS	-	expression tag	UNP Q1KHK2
L	272	HIS	-	expression tag	UNP Q1KHK2
L	273	HIS	-	expression tag	UNP Q1KHK2
L	274	HIS	-	expression tag	UNP Q1KHK2
L	275	HIS	-	expression tag	UNP Q1KHK2
L	276	HIS	-	expression tag	UNP Q1KHK2
O	269	ALA	-	expression tag	UNP Q1KHK2
O	270	ALA	-	expression tag	UNP Q1KHK2
O	271	HIS	-	expression tag	UNP Q1KHK2
O	272	HIS	-	expression tag	UNP Q1KHK2
O	273	HIS	-	expression tag	UNP Q1KHK2
O	274	HIS	-	expression tag	UNP Q1KHK2
O	275	HIS	-	expression tag	UNP Q1KHK2
O	276	HIS	-	expression tag	UNP Q1KHK2
R	269	ALA	-	expression tag	UNP Q1KHK2
R	270	ALA	-	expression tag	UNP Q1KHK2
R	271	HIS	-	expression tag	UNP Q1KHK2
R	272	HIS	-	expression tag	UNP Q1KHK2
R	273	HIS	-	expression tag	UNP Q1KHK2
R	274	HIS	-	expression tag	UNP Q1KHK2
R	275	HIS	-	expression tag	UNP Q1KHK2
R	276	HIS	-	expression tag	UNP Q1KHK2
U	269	ALA	-	expression tag	UNP Q1KHK2
U	270	ALA	-	expression tag	UNP Q1KHK2
U	271	HIS	-	expression tag	UNP Q1KHK2
U	272	HIS	-	expression tag	UNP Q1KHK2
U	273	HIS	-	expression tag	UNP Q1KHK2
U	274	HIS	-	expression tag	UNP Q1KHK2
U	275	HIS	-	expression tag	UNP Q1KHK2
U	276	HIS	-	expression tag	UNP Q1KHK2

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Chain	Residue	Modelled	Actual	Comment	Reference
X	269	ALA	-	expression tag	UNP Q1KHK2
X	270	ALA	-	expression tag	UNP Q1KHK2
X	271	HIS	-	expression tag	UNP Q1KHK2
X	272	HIS	-	expression tag	UNP Q1KHK2
X	273	HIS	-	expression tag	UNP Q1KHK2
X	274	HIS	-	expression tag	UNP Q1KHK2
X	275	HIS	-	expression tag	UNP Q1KHK2
X	276	HIS	-	expression tag	UNP Q1KHK2

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 5 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



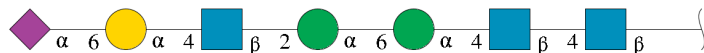
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Z	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 6 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



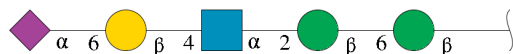
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	a	6	Total	C	N	O	0	0	0
			81	45	3	33			

- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	b	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 8 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose.



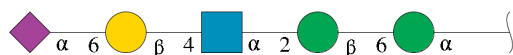
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	c	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 9 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	d	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 10 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose.



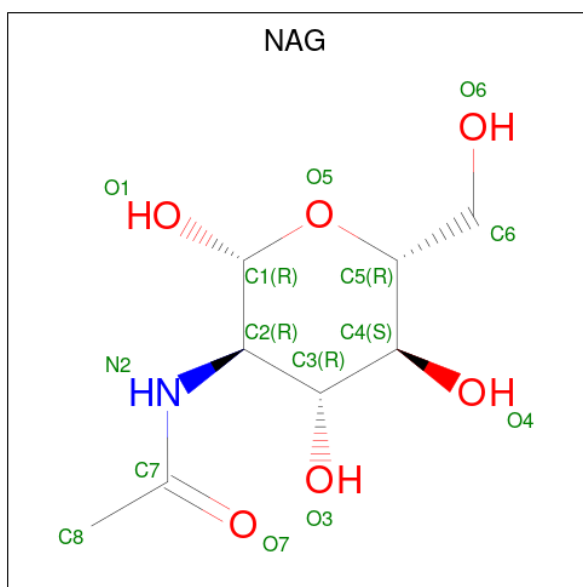
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	e	5	Total	C	N	O	0	0	0
			67	37	2	28			

- Molecule 11 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	f	7	Total	C	N	O	0	0	0
			95	53	4	38			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

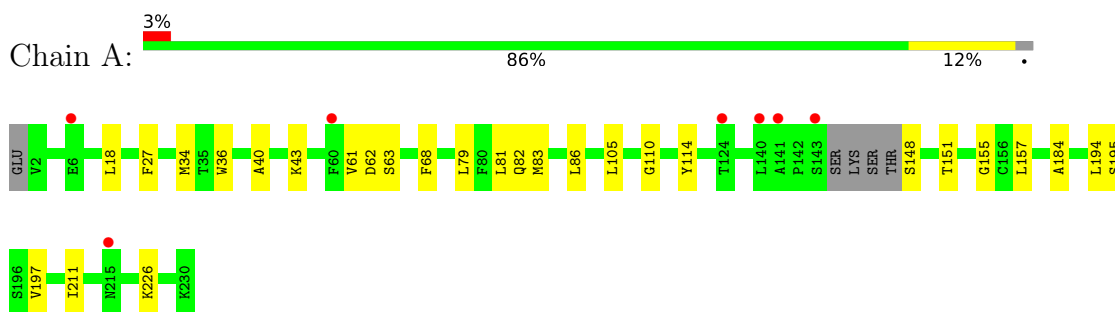


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			14	8	1	5		
12	O	1	Total	C	N	O	0	0
			14	8	1	5		
12	R	1	Total	C	N	O	0	0
			14	8	1	5		
12	U	1	Total	C	N	O	0	0
			14	8	1	5		
12	X	1	Total	C	N	O	0	0
			14	8	1	5		

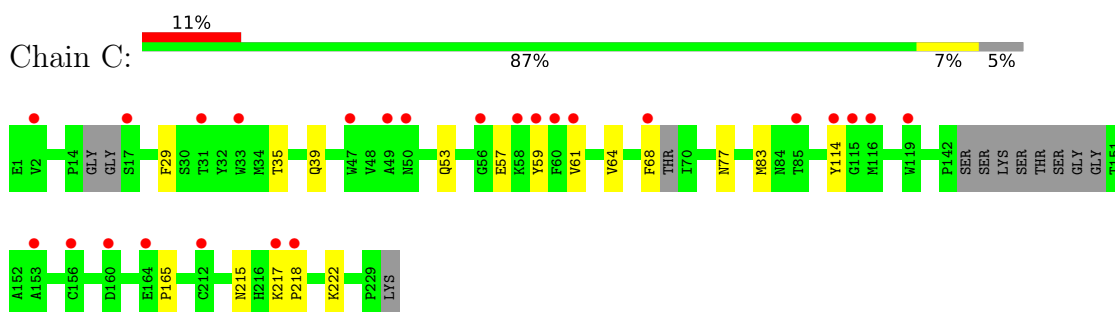
3 Residue-property plots [i](#)

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.

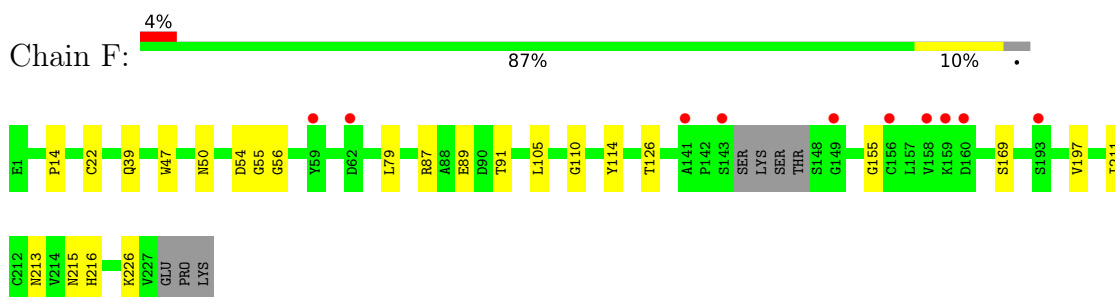
- Molecule 1: Human Fab H5.28 heavy chain



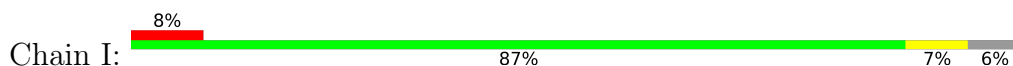
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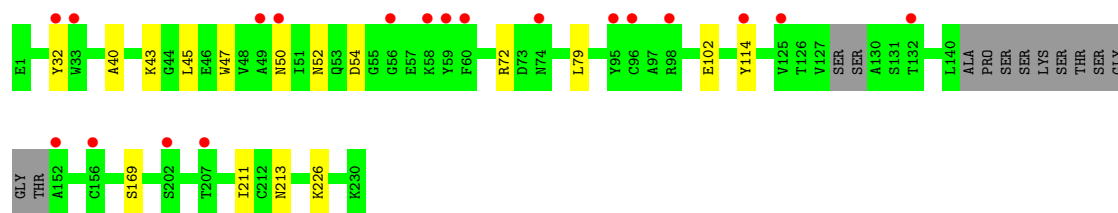


- Molecule 1: Human Fab H5.28 heavy chain

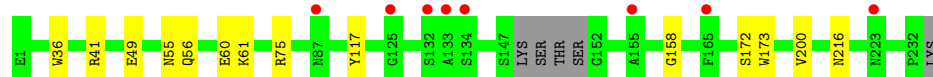


- Molecule 1: Human Fab H5.28 heavy chain

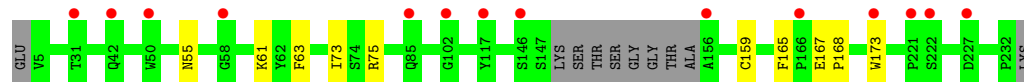
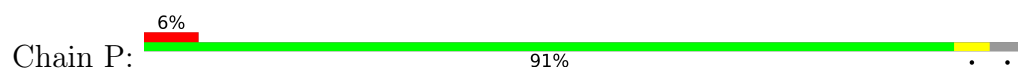




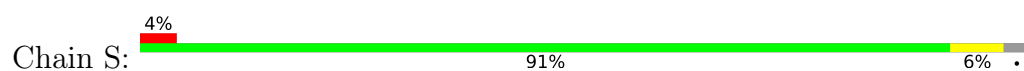
- Molecule 1: Human Fab H5.28 heavy chain



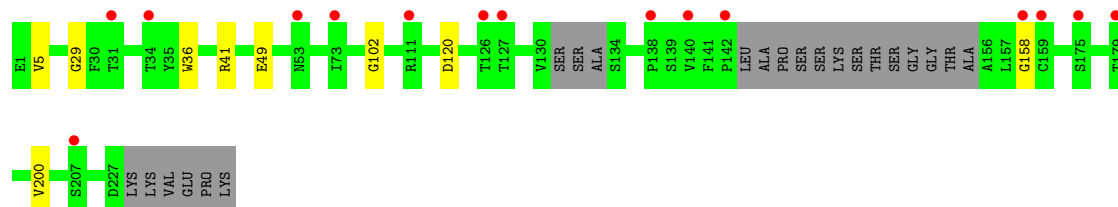
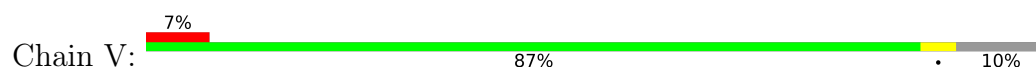
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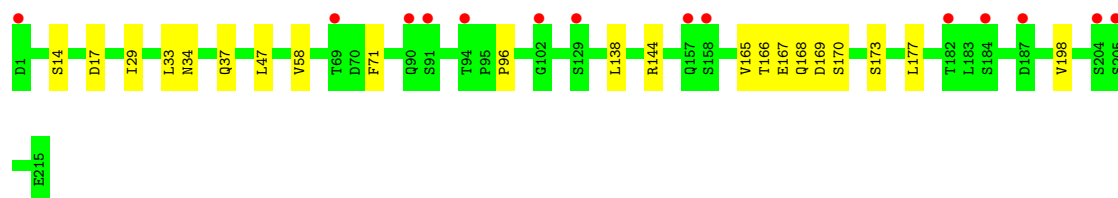
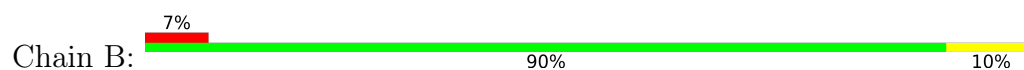
- Molecule 1: Human Fab H5.28 heavy chain



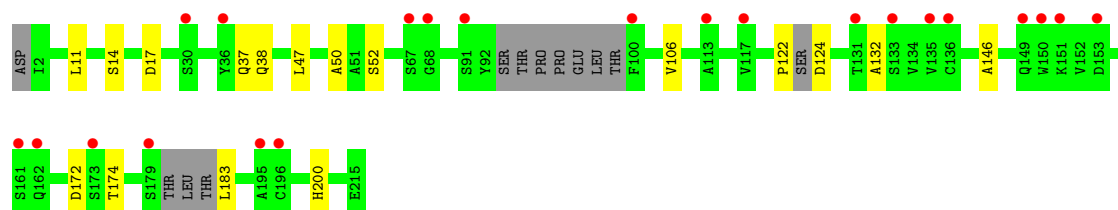
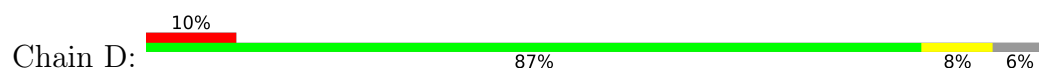
- Molecule 1: Human Fab H5.28 heavy chain



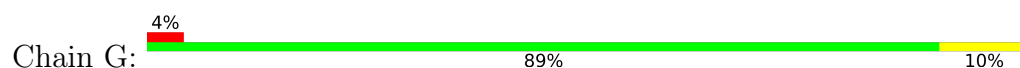
- Molecule 2: Human Fab H5.28 light chain



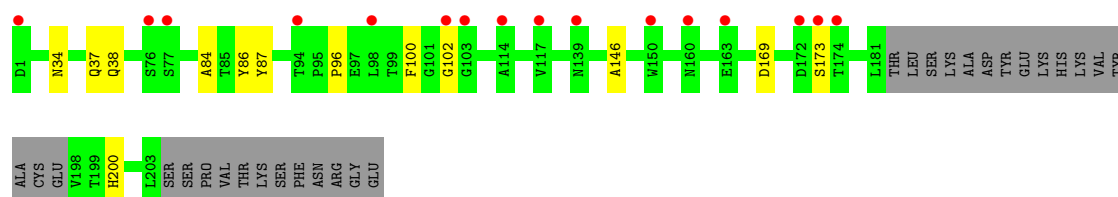
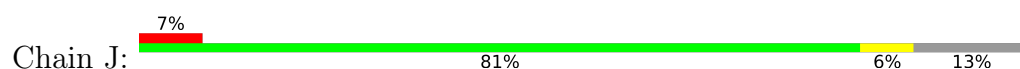
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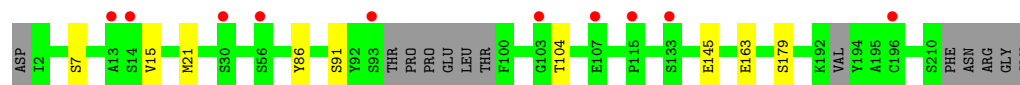
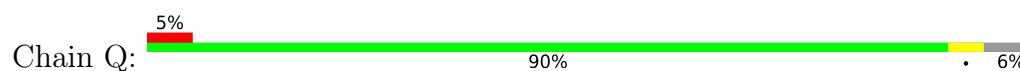
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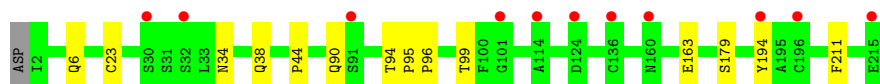


- Molecule 2: Human Fab H5.28 light chain

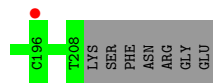
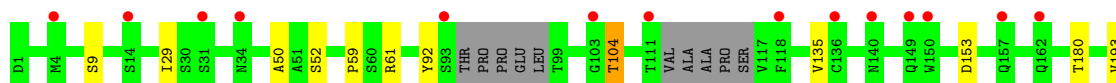
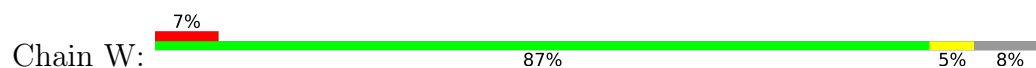


- Molecule 2: Human Fab H5.28 light chain

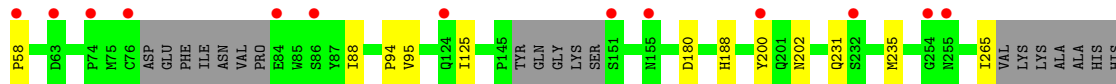
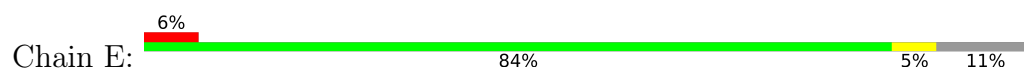




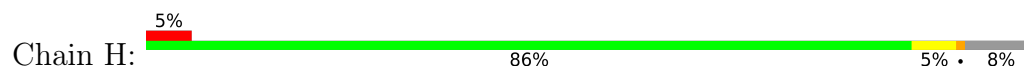
- Molecule 2: Human Fab H5.28 light chain



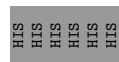
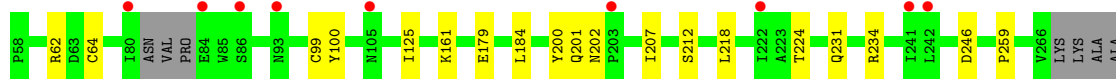
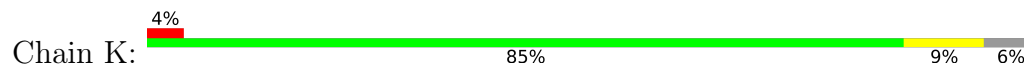
- Molecule 3: Hemagglutinin



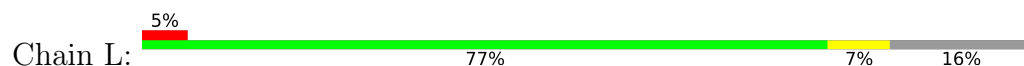
- Molecule 3: Hemagglutinin

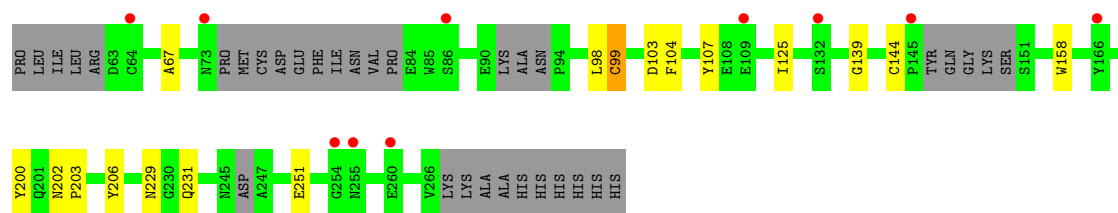


- Molecule 3: Hemagglutinin

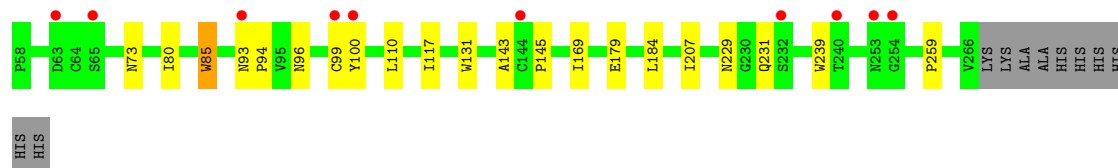
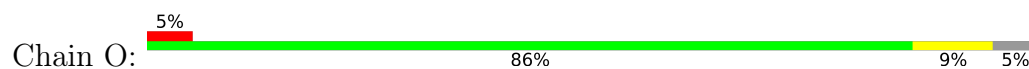


- Molecule 3: Hemagglutinin

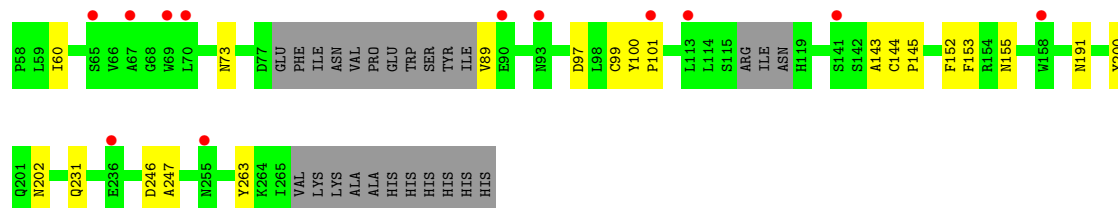




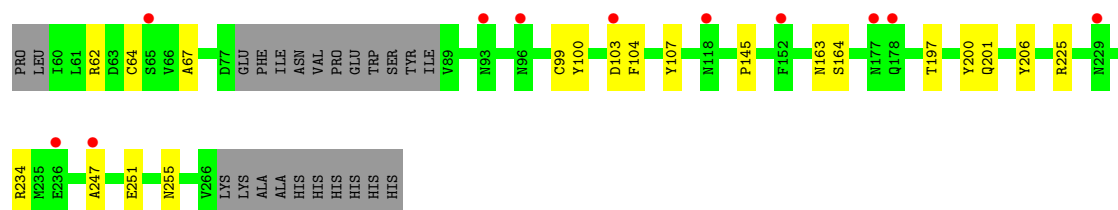
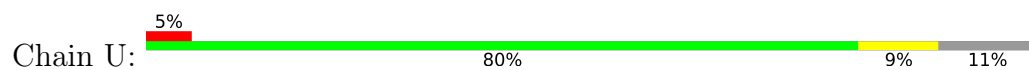
• Molecule 3: Hemagglutinin



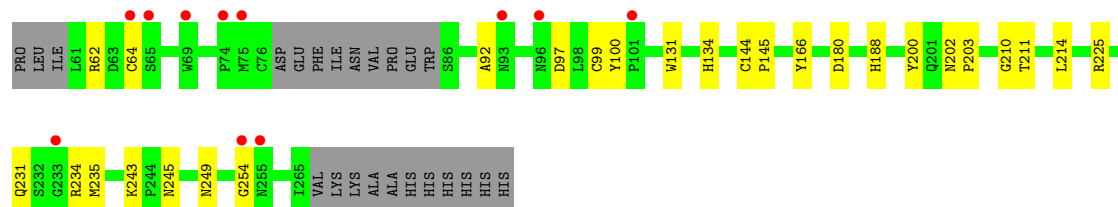
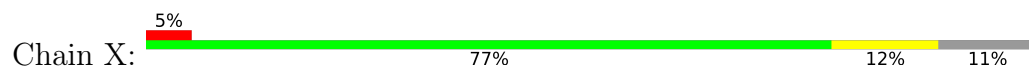
• Molecule 3: Hemagglutinin



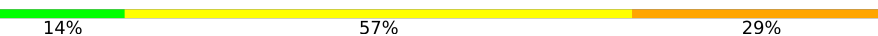
• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin



- Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  14% 57% 29%



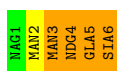
- Molecule 5: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  71% 29%



- Molecule 6: N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:  17% 17% 67%



- Molecule 7: N-acetyl-alpha-neuraminic acid-(2-6)-alpha-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:  29% 29% 43%

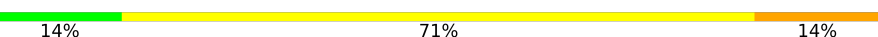


- Molecule 8: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-beta-D-mannopyranose

Chain c:  20% 40% 40%

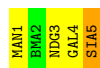


- Molecule 9: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

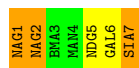
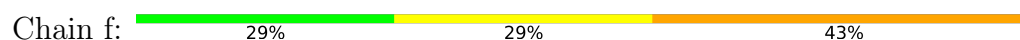
Chain d:  14% 71% 14%



- Molecule 10: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-beta-D-mannopyranose-(1-6)-alpha-D-mannopyranose



- Molecule 11: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	135.48 Å 187.22 Å 342.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.46 – 4.00 49.46 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.46-4.00) 99.9 (49.46-4.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 4.00 Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.281 , 0.326 0.284 , 0.327	Depositor DCC
R_{free} test set	3660 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 196.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	32097	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, MAN, BMA, SIA, GLA, NAG, NDG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/1506	0.26	0/2064
1	C	0.07	0/1325	0.28	0/1826
1	F	0.08	0/1471	0.24	0/2020
1	I	0.08	0/1395	0.23	0/1916
1	M	0.07	0/1472	0.23	0/2019
1	P	0.07	0/1344	0.28	0/1851
1	S	0.07	0/1429	0.22	0/1963
1	V	0.08	0/1267	0.22	0/1746
2	B	0.08	0/1509	0.28	0/2065
2	D	0.07	0/1230	0.23	0/1694
2	G	0.08	0/1395	0.25	0/1919
2	J	0.07	0/1118	0.29	0/1547
2	N	0.08	0/1324	0.25	0/1826
2	Q	0.09	0/1201	0.31	0/1657
2	T	0.09	0/1308	0.25	0/1807
2	W	0.07	0/1139	0.24	0/1574
3	E	0.08	0/1255	0.24	0/1736
3	H	0.09	0/1373	0.25	0/1891
3	K	0.07	0/1432	0.22	0/1968
3	L	0.08	0/1247	0.25	0/1711
3	O	0.09	0/1453	0.27	0/2004
3	R	0.10	0/1291	0.26	0/1779
3	U	0.09	0/1321	0.26	0/1818
3	X	0.10	0/1270	0.27	0/1754
All	All	0.08	0/32075	0.25	0/44155

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 ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1472	0	1144	18	0
1	C	1301	0	860	9	0
1	F	1436	0	1090	12	0
1	I	1364	0	956	11	0
1	M	1432	0	1020	10	0
1	P	1313	0	811	4	0
1	S	1393	0	957	10	0
1	V	1236	0	750	5	0
2	B	1477	0	1244	12	0
2	D	1211	0	797	9	0
2	G	1363	0	954	12	0
2	J	1097	0	671	7	0
2	N	1295	0	826	8	0
2	Q	1179	0	718	2	0
2	T	1280	0	805	8	0
2	W	1121	0	650	9	0
3	E	1221	0	769	4	1
3	H	1337	0	963	8	0
3	K	1397	0	1099	10	2
3	L	1219	0	844	8	4
3	O	1414	0	1027	9	2
3	R	1258	0	835	9	1
3	U	1285	0	862	11	0
3	X	1236	0	763	13	4
4	Y	95	0	79	4	4
5	Z	95	0	80	2	0
6	a	81	0	64	7	0
7	b	95	0	80	2	1
8	c	67	0	55	1	2
9	d	95	0	79	2	4
10	e	67	0	55	1	2
11	f	95	0	79	3	1
12	L	14	0	13	0	0
12	O	14	0	13	0	0
12	R	14	0	13	1	0
12	U	14	0	13	2	0
12	X	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32097	0	22051	225	14

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 4.

All (225) 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:S:105:GLU:OE2	3:U:234:ARG:NE	2.08	0.87
1:C:217:LYS:HG3	1:C:218:PRO:HD3	1.71	0.72
3:R:152:PHE:HD1	3:R:153:PHE:H	1.36	0.71
3:H:99:CYS:SG	3:H:100:TYR:N	2.63	0.71
3:H:199:LEU:HD11	6:a:6:SIA:H7	1.71	0.70
1:A:155:GLY:HA3	1:A:197:VAL:HA	1.76	0.67
1:M:117:TYR:O	2:N:34:ASN:ND2	2.26	0.67
3:U:103:ASP:OD1	3:U:104:PHE:N	2.27	0.67
1:I:45:LEU:HD21	2:J:38:GLN:HE22	1.60	0.67
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.77	0.66
1:A:157:LEU:HD12	1:A:195:SER:HB3	1.78	0.66
3:L:103:ASP:OD1	3:L:104:PHE:N	2.29	0.65
3:U:99:CYS:SG	3:U:100:TYR:N	2.70	0.64
1:A:61:VAL:O	1:A:63:SER:N	2.31	0.63
1:I:102:GLU:OE2	3:K:234:ARG:NE	2.29	0.63
1:P:61:LYS:HD3	1:P:63:PHE:HE1	1.63	0.62
3:X:99:CYS:HB2	3:X:144:CYS:HA	1.82	0.62
1:P:55:ASN:O	1:P:75:ARG:NH1	2.33	0.62
1:M:55:ASN:O	1:M:75:ARG:NH1	2.33	0.61
3:O:179:GLU:N	3:O:179:GLU:OE2	2.33	0.61
1:A:184:ALA:HA	1:A:194:LEU:HB3	1.81	0.61
2:T:194:TYR:HB2	2:T:211:PHE:HE1	1.65	0.60
3:U:197:THR:HA	3:U:201:GLN:HA	1.83	0.59
7:b:6:GLA:O6	7:b:6:GLA:O4	2.09	0.59
1:I:40:ALA:HB3	1:I:43:LYS:HB2	1.85	0.59
1:I:169:SER:O	1:I:213:ASN:N	2.34	0.59
3:K:161:LYS:NZ	3:K:201:GLN:OE1	2.35	0.59
2:D:172:ASP:OD2	2:D:174:THR:OG1	2.17	0.58
2:B:14:SER:OG	2:B:17:ASP:OD2	2.20	0.58
2:W:29:ILE:HA	2:W:92:TYR:CE1	2.37	0.58
1:S:50:TRP:NE1	1:S:53:ASN:OD1	2.36	0.58
9:d:1:NAG:H4	9:d:2:NAG:H83	1.85	0.58
1:A:211:ILE:HA	1:A:226:LYS:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.86	0.58
2:G:110:ARG:NH1	2:G:172:ASP:O	2.37	0.58
2:B:169:ASP:OD1	2:B:170:SER:N	2.37	0.58
3:X:99:CYS:SG	3:X:100:TYR:N	2.76	0.58
3:K:99:CYS:SG	3:K:100:TYR:N	2.78	0.57
6:a:5:GLA:O4	6:a:6:SIA:O1B	2.21	0.57
1:A:34:MET:HB3	1:A:79:LEU:HD22	1.86	0.57
4:Y:6:GAL:O4	4:Y:6:GAL:O6	2.14	0.57
1:V:158:GLY:HA3	1:V:200:VAL:HA	1.87	0.56
3:O:99:CYS:SG	3:O:100:TYR:N	2.79	0.56
1:F:47:TRP:NE1	1:F:50:ASN:OD1	2.37	0.56
3:X:97:ASP:N	3:X:97:ASP:OD1	2.39	0.55
1:A:68:PHE:HB3	1:A:83:MET:HA	1.89	0.55
1:C:35:THR:OG1	1:C:114:TYR:OH	2.24	0.55
3:H:200:TYR:O	3:H:202:ASN:N	2.39	0.54
2:T:90:GLN:HB3	2:T:99:THR:H	1.70	0.54
1:A:148:SER:N	1:A:151:THR:O	2.41	0.54
1:F:211:ILE:HA	1:F:226:LYS:HA	1.90	0.54
3:H:144:CYS:HB3	3:H:151:SER:O	2.08	0.54
3:U:225:ARG:HD3	3:U:234:ARG:HD2	1.89	0.54
1:S:55:ASN:O	1:S:75:ARG:NH1	2.40	0.54
2:D:146:ALA:HB2	2:D:200:HIS:HD2	1.73	0.54
1:C:61:VAL:HG13	1:C:64:VAL:H	1.73	0.54
6:a:4:NDG:H4	6:a:5:GLA:H4	1.91	0.53
1:I:114:TYR:O	2:J:34:ASN:ND2	2.41	0.53
2:D:11:LEU:HB3	2:D:106:VAL:HG22	1.89	0.52
3:R:73:ASN:ND2	3:R:97:ASP:O	2.43	0.52
2:T:6:GLN:HA	2:T:23:CYS:HA	1.90	0.52
1:P:61:LYS:NZ	1:P:73:ILE:O	2.43	0.52
2:G:88:CYS:O	2:G:101:GLY:N	2.43	0.52
1:F:54:ASP:O	1:F:56:GLY:N	2.41	0.52
2:G:33:LEU:HD11	2:G:88:CYS:HB2	1.92	0.52
3:E:200:TYR:O	3:E:202:ASN:N	2.41	0.51
2:N:66:GLY:HA3	2:N:71:PHE:HA	1.91	0.51
2:B:138:LEU:HB2	2:B:177:LEU:HD23	1.93	0.51
1:F:22:CYS:HB3	1:F:79:LEU:HB3	1.91	0.51
3:L:200:TYR:O	3:L:202:ASN:N	2.40	0.51
1:F:105:LEU:HA	1:F:110:GLY:HA3	1.93	0.51
3:X:180:ASP:OD2	3:X:243:LYS:NZ	2.30	0.51
3:K:200:TYR:O	3:K:202:ASN:N	2.39	0.51
3:L:67:ALA:HB2	3:L:107:TYR:HE1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:9:SER:HA	2:W:104:THR:H	1.76	0.51
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.93	0.50
1:P:159:CYS:HB2	1:P:173:TRP:CZ2	2.46	0.50
3:E:180:ASP:O	3:E:265:ILE:N	2.42	0.50
3:H:199:LEU:HD21	6:a:6:SIA:H5	1.92	0.50
2:D:50:ALA:O	2:D:52:SER:N	2.42	0.50
3:U:206:TYR:OH	3:U:251:GLU:OE2	2.30	0.49
1:A:68:PHE:HB2	1:A:82:GLN:O	2.12	0.49
3:L:206:TYR:OH	3:L:251:GLU:OE2	2.25	0.49
1:F:91:THR:HG23	1:F:126:THR:HA	1.93	0.49
12:U:301:NAG:O7	12:U:301:NAG:O3	2.29	0.49
1:C:29:PHE:HD2	1:C:77:ASN:HA	1.78	0.49
1:A:114:TYR:O	2:B:34:ASN:ND2	2.33	0.48
1:I:72:ARG:HA	1:I:79:LEU:HA	1.95	0.48
3:K:62:ARG:O	3:K:64:CYS:N	2.44	0.48
3:L:229:ASN:O	3:L:229:ASN:ND2	2.46	0.48
1:M:158:GLY:HA2	1:M:173:TRP:HZ2	1.78	0.48
1:C:215:ASN:HA	1:C:222:LYS:HA	1.95	0.48
2:W:29:ILE:C	2:W:92:TYR:HE1	2.22	0.48
3:X:225:ARG:HD3	3:X:234:ARG:HG2	1.95	0.48
1:S:37:MET:HB3	1:S:82:LEU:HD22	1.96	0.48
10:e:5:SIA:O9	10:e:5:SIA:O7	2.24	0.48
2:D:14:SER:OG	2:D:17:ASP:OD2	2.32	0.47
6:a:6:SIA:O6	6:a:6:SIA:O8	2.31	0.47
2:W:135:VAL:HA	2:W:180:THR:HA	1.95	0.47
1:V:120:ASP:OD1	1:V:120:ASP:N	2.47	0.47
3:K:212:SER:OG	3:K:246:ASP:OD2	2.23	0.47
3:O:131:TRP:HZ3	3:O:169:ILE:HG21	1.79	0.47
1:V:5:VAL:HA	1:V:29:GLY:HA3	1.97	0.47
2:B:144:ARG:HD2	2:B:165:VAL:HG11	1.96	0.47
3:E:58:PRO:HA	3:E:88:ILE:HG12	1.96	0.47
1:F:155:GLY:HA3	1:F:197:VAL:HA	1.96	0.47
2:N:78:LEU:H	2:N:78:LEU:HD23	1.80	0.47
4:Y:7:SIA:O6	4:Y:7:SIA:O8	2.22	0.47
1:C:39:GLN:OE1	2:D:38:GLN:NE2	2.36	0.47
3:X:131:TRP:HB3	3:X:134:HIS:HB2	1.97	0.47
2:G:165:VAL:HA	2:G:177:LEU:HA	1.97	0.47
1:I:47:TRP:NE1	1:I:50:ASN:OD1	2.33	0.47
1:A:27:PHE:HD1	1:A:27:PHE:H	1.63	0.47
1:F:39:GLN:NE2	2:G:38:GLN:OE1	2.45	0.47
1:F:169:SER:O	1:F:213:ASN:N	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:LEU:HD21	2:B:198:VAL:HG11	1.97	0.46
2:G:85:THR:HA	2:G:105:LYS:HA	1.96	0.46
2:N:33:LEU:HD22	2:N:71:PHE:CG	2.50	0.46
2:W:29:ILE:C	2:W:92:TYR:CE1	2.94	0.46
11:f:5:NDG:H2	11:f:5:NDG:H8C1	1.56	0.46
3:L:99:CYS:HB3	3:L:144:CYS:HB2	1.72	0.46
1:M:36:TRP:NE1	1:M:56:GLN:OE1	2.49	0.46
2:W:50:ALA:O	2:W:52:SER:N	2.46	0.46
2:J:146:ALA:HB2	2:J:200:HIS:HD2	1.79	0.46
2:G:6:GLN:HA	2:G:23:CYS:HA	1.97	0.46
3:R:155:ASN:ND2	3:R:263:TYR:OH	2.49	0.46
1:S:25:CYS:HB3	1:S:82:LEU:HB3	1.97	0.46
2:G:37:GLN:HB3	2:G:47:LEU:HD11	1.97	0.46
3:H:71:LEU:O	3:H:153:PHE:HB3	2.16	0.46
1:M:41:ARG:O	1:M:49:GLU:N	2.43	0.46
1:A:68:PHE:CB	1:A:83:MET:HA	2.46	0.45
2:D:132:ALA:O	2:D:183:LEU:N	2.49	0.45
2:B:33:LEU:HD13	2:B:71:PHE:CD1	2.52	0.45
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.45
1:I:211:ILE:HA	1:I:226:LYS:HA	1.98	0.45
1:I:32:TYR:OH	3:K:224:THR:N	2.37	0.45
2:Q:21:MET:HE1	2:Q:86:TYR:HD2	1.80	0.45
2:W:29:ILE:HA	2:W:92:TYR:CD1	2.51	0.45
3:X:166:TYR:HE2	3:X:254:GLY:HA2	1.81	0.45
2:N:33:LEU:HD11	2:N:88:CYS:SG	2.57	0.45
2:T:38:GLN:HB2	2:T:44:PRO:HB3	1.97	0.45
3:O:143:ALA:O	3:O:145:PRO:HD3	2.16	0.45
9:d:7:SIA:O6	9:d:7:SIA:O8	2.32	0.45
3:O:85:TRP:HA	3:O:117:ILE:HG23	1.98	0.44
3:R:246:ASP:OD1	3:R:247:ALA:N	2.39	0.44
3:E:188:HIS:HA	3:E:235:MET:HG2	1.98	0.44
3:O:110:LEU:HD12	3:O:239:TRP:CD1	2.52	0.44
3:X:211:THR:N	3:X:214:LEU:O	2.47	0.44
3:O:73:ASN:HD21	3:O:99:CYS:HB3	1.82	0.44
3:X:62:ARG:O	3:X:64:CYS:N	2.45	0.44
2:B:168:GLN:HE21	2:B:173:SER:HB3	1.82	0.44
12:R:301:NAG:O7	12:R:301:NAG:O3	2.30	0.44
2:G:21:MET:HE3	2:G:73:LEU:HD23	1.98	0.44
3:H:231:GLN:NE2	6:a:5:GLA:H62	2.32	0.44
1:S:155:ALA:N	1:S:203:VAL:O	2.48	0.44
1:M:172:SER:O	1:M:216:ASN:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:122:PRO:O	2:D:124:ASP:N	2.51	0.44
3:L:139:GLY:HA3	3:L:158:TRP:HB3	2.00	0.44
3:X:188:HIS:HB2	3:X:235:MET:HE3	2.00	0.44
2:J:87:TYR:CE2	2:J:102:GLY:HA2	2.53	0.43
2:N:33:LEU:HB3	2:N:51:ALA:HB2	2.00	0.43
2:T:163:GLU:HA	2:T:179:SER:HA	2.00	0.43
3:U:67:ALA:HB2	3:U:107:TYR:CZ	2.54	0.43
3:U:163:ASN:HB3	3:U:164:SER:H	1.69	0.43
4:Y:6:GAL:H61	4:Y:7:SIA:H32	1.59	0.43
1:A:18:LEU:O	1:A:83:MET:N	2.50	0.43
1:F:87:ARG:HB2	1:F:89:GLU:HG2	2.00	0.43
3:K:184:LEU:O	3:K:259:PRO:HB3	2.19	0.43
3:R:200:TYR:O	3:R:202:ASN:N	2.43	0.43
3:X:200:TYR:C	3:X:202:ASN:H	2.26	0.43
2:B:166:THR:HG22	2:B:167:GLU:N	2.33	0.43
3:X:245:ASN:O	12:X:301:NAG:H82	2.19	0.43
4:Y:1:NAG:H61	4:Y:2:NAG:H83	2.01	0.43
3:U:62:ARG:O	3:U:64:CYS:N	2.45	0.43
1:A:18:LEU:O	1:A:82:GLN:NE2	2.51	0.42
2:B:29:ILE:HD11	2:B:71:PHE:HE1	1.84	0.42
3:U:247:ALA:HB3	12:U:301:NAG:H82	2.00	0.42
7:b:2:NAG:H4	7:b:3:MAN:H2	1.89	0.42
1:F:215:ASN:HD22	1:F:216:HIS:N	2.16	0.42
2:W:153:ASP:N	2:W:193:VAL:O	2.52	0.42
1:I:52:ASN:O	1:I:72:ARG:NH2	2.33	0.42
1:S:117:TYR:O	2:T:34:ASN:ND2	2.47	0.42
1:V:41:ARG:O	1:V:49:GLU:N	2.39	0.42
3:K:207:ILE:HB	3:K:218:LEU:HB2	2.01	0.42
3:R:143:ALA:HB2	3:R:231:GLN:H	1.84	0.42
1:S:42:GLN:OE1	2:T:38:GLN:NE2	2.46	0.42
2:J:84:ALA:HB3	2:J:86:TYR:HE1	1.84	0.42
11:f:7:SIA:O6	11:f:7:SIA:O8	2.28	0.42
1:I:54:ASP:OD1	1:I:54:ASP:N	2.49	0.42
2:J:37:GLN:HB2	2:J:86:TYR:CE1	2.55	0.42
8:c:3:NDG:H2	8:c:3:NDG:H8C1	1.58	0.42
3:R:60:ILE:HA	3:R:89:VAL:O	2.20	0.41
6:a:3:MAN:O6	6:a:4:NDG:O7	2.35	0.41
1:A:36:TRP:CG	1:A:81:LEU:HD22	2.55	0.41
1:M:61:LYS:HE2	1:M:61:LYS:HB3	1.96	0.41
3:R:99:CYS:HB3	3:R:144:CYS:HB2	1.69	0.41
2:G:135:VAL:HA	2:G:180:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:36:TRP:HB2	1:V:102:GLY:O	2.21	0.41
5:Z:2:NAG:H3	5:Z:4:BMA:H62	2.02	0.41
1:F:114:TYR:O	2:G:34:ASN:ND2	2.41	0.41
2:J:169:ASP:HB3	2:J:173:SER:N	2.35	0.41
3:R:100:TYR:CD1	3:R:101:PRO:HD2	2.56	0.41
2:B:47:LEU:HA	2:B:58:VAL:HG21	2.02	0.41
1:C:57:GLU:OE2	1:C:59:TYR:OH	2.38	0.41
3:H:131:TRP:CD1	3:H:131:TRP:H	2.38	0.41
2:Q:163:GLU:HA	2:Q:179:SER:HA	2.03	0.41
1:S:165:PHE:HA	1:S:166:PRO:HA	1.81	0.41
1:M:158:GLY:HA2	1:M:173:TRP:CZ2	2.55	0.41
1:A:105:LEU:HA	1:A:110:GLY:HA3	2.02	0.41
1:M:158:GLY:HA3	1:M:200:VAL:HA	2.02	0.41
11:f:1:NAG:H83	11:f:2:NAG:H61	2.03	0.41
2:N:53:ASN:HB3	3:O:229:ASN:H	1.85	0.41
1:C:53:GLN:CD	1:C:53:GLN:H	2.30	0.40
3:K:179:GLU:OE2	3:K:179:GLU:N	2.53	0.40
1:M:55:ASN:ND2	1:M:60:GLU:H	2.19	0.40
2:N:21:MET:HE1	2:N:86:TYR:CG	2.56	0.40
3:U:200:TYR:CE2	3:U:255:ASN:HA	2.56	0.40
2:W:59:PRO:HB2	2:W:61:ARG:HG2	2.02	0.40
5:Z:1:NAG:H61	5:Z:2:NAG:H83	2.03	0.40
3:O:184:LEU:O	3:O:259:PRO:HB3	2.21	0.40
3:X:210:GLY:N	3:X:249:ASN:O	2.51	0.40
2:G:169:ASP:HB3	2:G:173:SER:N	2.36	0.40
1:C:68:PHE:HA	1:C:83:MET:HA	2.04	0.40
3:L:229:ASN:HD22	3:L:229:ASN:C	2.28	0.40
1:S:42:GLN:CD	2:T:38:GLN:HE22	2.28	0.40

All (14) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:231:GLN:NE2	4:Y:6:GAL:O6[4_455]	1.13	1.07
3:E:231:GLN:NE2	11:f:7:SIA:O1A[4_454]	1.30	0.90
3:K:231:GLN:NE2	10:e:5:SIA:O1B[2_555]	1.30	0.90
3:O:231:GLN:NE2	8:c:5:SIA:O1B[3_554]	1.30	0.90
3:R:191:ASN:ND2	7:b:7:SIA:O9[2_555]	1.30	0.90
3:L:231:GLN:NE2	9:d:7:SIA:C1[3_544]	1.43	0.77
3:X:231:GLN:NE2	4:Y:7:SIA:C2[4_455]	1.44	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:231:GLN:NE2	9:d:7:SIA:O1B[3_544]	1.49	0.71
3:L:231:GLN:NE2	9:d:7:SIA:O1A[3_544]	1.64	0.56
3:O:231:GLN:NE2	8:c:5:SIA:C1[3_554]	1.71	0.49
3:X:231:GLN:NE2	4:Y:7:SIA:C1[4_455]	1.85	0.35
3:L:231:GLN:OE1	9:d:7:SIA:O8[3_544]	2.01	0.19
3:X:231:GLN:NE2	4:Y:7:SIA:O6[4_455]	2.16	0.04
3:K:100:TYR:OH	10:e:5:SIA:O9[2_555]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/230 (96%)	202 (91%)	18 (8%)	1 (0%)	24	60
1	C	210/230 (91%)	197 (94%)	12 (6%)	1 (0%)	24	60
1	F	219/230 (95%)	201 (92%)	16 (7%)	2 (1%)	14	48
1	I	211/230 (92%)	192 (91%)	19 (9%)	0	100	100
1	M	221/230 (96%)	209 (95%)	12 (5%)	0	100	100
1	P	216/230 (94%)	200 (93%)	13 (6%)	3 (1%)	9	39
1	S	220/230 (96%)	208 (94%)	12 (6%)	0	100	100
1	V	202/230 (88%)	185 (92%)	17 (8%)	0	100	100
2	B	213/215 (99%)	198 (93%)	14 (7%)	1 (0%)	24	60
2	D	195/215 (91%)	182 (93%)	13 (7%)	0	100	100
2	G	212/215 (99%)	195 (92%)	16 (8%)	1 (0%)	24	60
2	J	183/215 (85%)	167 (91%)	14 (8%)	2 (1%)	11	44
2	N	212/215 (99%)	198 (93%)	11 (5%)	3 (1%)	9	39
2	Q	196/215 (91%)	175 (89%)	16 (8%)	5 (3%)	4	29
2	T	212/215 (99%)	189 (89%)	20 (9%)	3 (1%)	9	39
2	W	192/215 (89%)	180 (94%)	11 (6%)	1 (0%)	24	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	190/219 (87%)	172 (90%)	15 (8%)	3 (2%)	7	37
3	H	198/219 (90%)	172 (87%)	22 (11%)	4 (2%)	6	33
3	K	202/219 (92%)	185 (92%)	16 (8%)	1 (0%)	24	60
3	L	175/219 (80%)	160 (91%)	11 (6%)	4 (2%)	5	31
3	O	207/219 (94%)	186 (90%)	15 (7%)	6 (3%)	3	26
3	R	188/219 (86%)	171 (91%)	16 (8%)	1 (0%)	24	60
3	U	192/219 (88%)	175 (91%)	16 (8%)	1 (0%)	24	60
3	X	192/219 (88%)	170 (88%)	19 (10%)	3 (2%)	7	37
All	All	4879/5312 (92%)	4469 (92%)	364 (8%)	46 (1%)	14	48

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	94	PRO
2	J	96	PRO
3	K	125	ILE
2	N	96	PRO
3	O	80	ILE
3	O	93	ASN
3	O	94	PRO
1	P	167	GLU
1	P	168	PRO
2	Q	7	SER
3	R	145	PRO
2	T	94	THR
2	T	96	PRO
3	U	145	PRO
3	X	145	PRO
2	B	96	PRO
3	E	95	VAL
3	E	125	ILE
1	F	55	GLY
2	G	96	PRO
3	H	125	ILE
2	N	99	THR
2	Q	91	SER
2	Q	145	GLU
3	H	131	TRP
3	L	99	CYS

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Mol	Chain	Res	Type
3	O	96	ASN
2	Q	104	THR
1	C	165	PRO
2	J	100	PHE
3	L	125	ILE
2	Q	15	VAL
1	A	62	ASP
3	H	63	ASP
3	L	98	LEU
3	O	85	TRP
3	X	92	ALA
2	W	104	THR
1	P	165	PHE
3	X	203	PRO
3	H	144	CYS
2	T	95	PRO
3	L	203	PRO
2	N	142	TYR
1	F	14	PRO
3	O	207	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/190 (54%)	103 (100%)	0	100	100
1	C	64/190 (34%)	64 (100%)	0	100	100
1	F	93/190 (49%)	93 (100%)	0	100	100
1	I	76/190 (40%)	76 (100%)	0	100	100
1	M	77/190 (40%)	77 (100%)	0	100	100
1	P	53/190 (28%)	53 (100%)	0	100	100
1	S	71/190 (37%)	71 (100%)	0	100	100
1	V	48/190 (25%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	125/189 (66%)	125 (100%)	0	100	100
2	D	61/189 (32%)	61 (100%)	0	100	100
2	G	81/189 (43%)	81 (100%)	0	100	100
2	J	46/189 (24%)	46 (100%)	0	100	100
2	N	58/189 (31%)	58 (100%)	0	100	100
2	Q	42/189 (22%)	42 (100%)	0	100	100
2	T	54/189 (29%)	54 (100%)	0	100	100
2	W	33/189 (18%)	33 (100%)	0	100	100
3	E	58/197 (29%)	58 (100%)	0	100	100
3	H	83/197 (42%)	83 (100%)	0	100	100
3	K	109/197 (55%)	109 (100%)	0	100	100
3	L	72/197 (36%)	72 (100%)	0	100	100
3	O	94/197 (48%)	94 (100%)	0	100	100
3	R	69/197 (35%)	69 (100%)	0	100	100
3	U	73/197 (37%)	73 (100%)	0	100	100
3	X	58/197 (29%)	58 (100%)	0	100	100
All	All	1701/4608 (37%)	1701 (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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
2	D	37	GLN
1	F	82	GLN
1	F	208	GLN
2	G	140	ASN
3	L	245	ASN
2	N	38	GLN
3	O	124	GLN
3	O	216	GLN
1	P	219	HIS
3	R	191	ASN
3	R	196	GLN
2	T	37	GLN

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Mol	Chain	Res	Type
1	V	80	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 ⓘ

51 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	Y	1	4,3	14,14,15	0.31	0	17,19,21	0.59	0
4	NAG	Y	2	4	14,14,15	0.30	0	17,19,21	1.27	2 (11%)
4	MAN	Y	3	4	11,11,12	0.23	0	15,15,17	0.59	0
4	MAN	Y	4	4	11,11,12	0.65	0	15,15,17	1.47	1 (6%)
4	NDG	Y	5	4	14,14,15	0.38	0	17,19,21	1.91	4 (23%)
4	GAL	Y	6	4	11,11,12	0.30	0	15,15,17	0.67	0
4	SIA	Y	7	4	20,20,21	0.55	0	21,28,31	1.32	3 (14%)
5	NAG	Z	1	5,3	14,14,15	0.33	0	17,19,21	0.57	0
5	NAG	Z	2	5	14,14,15	0.28	0	17,19,21	1.24	1 (5%)
5	BMA	Z	3	5	11,11,12	0.30	0	15,15,17	1.02	1 (6%)
5	BMA	Z	4	5	11,11,12	0.34	0	15,15,17	1.53	2 (13%)
5	NAG	Z	5	5	14,14,15	0.32	0	17,19,21	1.20	2 (11%)
5	GAL	Z	6	5	11,11,12	0.36	0	15,15,17	1.35	2 (13%)
5	SIA	Z	7	5	20,20,21	0.57	0	21,28,31	0.92	2 (9%)
6	NAG	a	1	6	14,14,15	0.35	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MAN	a	2	6	11,11,12	0.28	0	15,15,17	0.87	1 (6%)
6	MAN	a	3	6	11,11,12	0.49	0	15,15,17	1.66	2 (13%)
6	NDG	a	4	6	14,14,15	0.37	0	17,19,21	1.14	2 (11%)
6	GLA	a	5	6	11,11,12	0.56	0	15,15,17	2.49	4 (26%)
6	SIA	a	6	6	20,20,21	0.58	0	21,28,31	0.82	1 (4%)
7	NAG	b	1	7,3	14,14,15	0.31	0	17,19,21	0.90	0
7	NAG	b	2	7	14,14,15	0.49	0	17,19,21	1.65	2 (11%)
7	MAN	b	3	7	11,11,12	0.35	0	15,15,17	0.93	1 (6%)
7	MAN	b	4	7	11,11,12	0.25	0	15,15,17	0.89	1 (6%)
7	NAG	b	5	7	14,14,15	0.26	0	17,19,21	0.72	0
7	GLA	b	6	7	11,11,12	0.24	0	15,15,17	0.63	0
7	SIA	b	7	7	20,20,21	0.59	0	21,28,31	1.16	3 (14%)
8	BMA	c	1	8	11,11,12	0.24	0	15,15,17	0.54	0
8	BMA	c	2	8	11,11,12	0.37	0	15,15,17	1.53	2 (13%)
8	NDG	c	3	8	14,14,15	0.41	0	17,19,21	1.55	3 (17%)
8	GAL	c	4	8	11,11,12	0.40	0	15,15,17	1.68	2 (13%)
8	SIA	c	5	8	20,20,21	0.52	0	21,28,31	0.79	1 (4%)
9	NAG	d	1	9	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
9	NAG	d	2	9	14,14,15	0.27	0	17,19,21	0.49	0
9	MAN	d	3	9	11,11,12	0.33	0	15,15,17	1.36	1 (6%)
9	BMA	d	4	9	11,11,12	0.26	0	15,15,17	0.56	0
9	NDG	d	5	9	14,14,15	0.29	0	17,19,21	0.87	1 (5%)
9	GAL	d	6	9	11,11,12	0.28	0	15,15,17	1.22	1 (6%)
9	SIA	d	7	9	20,20,21	0.58	0	21,28,31	0.81	0
10	MAN	e	1	10	11,11,12	0.31	0	15,15,17	1.05	2 (13%)
10	BMA	e	2	10	11,11,12	0.29	0	15,15,17	0.57	0
10	NDG	e	3	10	14,14,15	0.40	0	17,19,21	0.94	1 (5%)
10	GAL	e	4	10	11,11,12	0.37	0	15,15,17	1.11	2 (13%)
10	SIA	e	5	10	20,20,21	0.59	0	21,28,31	1.18	4 (19%)
11	NAG	f	1	11	14,14,15	0.41	0	17,19,21	0.91	1 (5%)
11	NAG	f	2	11	14,14,15	0.39	0	17,19,21	0.81	1 (5%)
11	BMA	f	3	11	11,11,12	0.27	0	15,15,17	0.72	0
11	MAN	f	4	11	11,11,12	0.24	0	15,15,17	0.68	0
11	NDG	f	5	11	14,14,15	0.33	0	17,19,21	0.83	0
11	GAL	f	6	11	11,11,12	0.30	0	15,15,17	1.49	2 (13%)
11	SIA	f	7	11	20,20,21	0.55	0	21,28,31	0.81	2 (9%)

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	Y	1	4,3	-	2/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	MAN	Y	3	4	-	2/2/19/22	0/1/1/1
4	MAN	Y	4	4	-	1/2/19/22	0/1/1/1
4	NDG	Y	5	4	-	3/6/23/26	0/1/1/1
4	GAL	Y	6	4	-	2/2/19/22	0/1/1/1
4	SIA	Y	7	4	-	9/18/34/38	0/1/1/1
5	NAG	Z	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	3/6/23/26	0/1/1/1
5	BMA	Z	3	5	-	1/2/19/22	1/1/1/1
5	BMA	Z	4	5	-	0/2/19/22	0/1/1/1
5	NAG	Z	5	5	-	3/6/23/26	0/1/1/1
5	GAL	Z	6	5	-	2/2/19/22	0/1/1/1
5	SIA	Z	7	5	-	8/18/34/38	0/1/1/1
6	NAG	a	1	6	-	2/6/23/26	0/1/1/1
6	MAN	a	2	6	-	0/2/19/22	1/1/1/1
6	MAN	a	3	6	-	0/2/19/22	0/1/1/1
6	NDG	a	4	6	-	1/6/23/26	0/1/1/1
6	GLA	a	5	6	-	2/2/19/22	0/1/1/1
6	SIA	a	6	6	-	8/18/34/38	0/1/1/1
7	NAG	b	1	7,3	-	2/6/23/26	0/1/1/1
7	NAG	b	2	7	-	1/6/23/26	0/1/1/1
7	MAN	b	3	7	-	1/2/19/22	0/1/1/1
7	MAN	b	4	7	-	1/2/19/22	1/1/1/1
7	NAG	b	5	7	-	4/6/23/26	0/1/1/1
7	GLA	b	6	7	-	2/2/19/22	0/1/1/1
7	SIA	b	7	7	-	10/18/34/38	0/1/1/1
8	BMA	c	1	8	-	2/2/19/22	0/1/1/1
8	BMA	c	2	8	-	0/2/19/22	1/1/1/1
8	NDG	c	3	8	-	4/6/23/26	0/1/1/1
8	GAL	c	4	8	-	1/2/19/22	0/1/1/1
8	SIA	c	5	8	-	2/18/34/38	0/1/1/1
9	NAG	d	1	9	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	d	3	9	-	2/2/19/22	0/1/1/1
9	BMA	d	4	9	-	1/2/19/22	0/1/1/1
9	NDG	d	5	9	-	4/6/23/26	0/1/1/1
9	GAL	d	6	9	-	1/2/19/22	0/1/1/1
9	SIA	d	7	9	-	7/18/34/38	0/1/1/1
10	MAN	e	1	10	-	2/2/19/22	1/1/1/1
10	BMA	e	2	10	-	0/2/19/22	0/1/1/1
10	NDG	e	3	10	-	0/6/23/26	0/1/1/1
10	GAL	e	4	10	-	0/2/19/22	0/1/1/1
10	SIA	e	5	10	-	7/18/34/38	0/1/1/1
11	NAG	f	1	11	-	0/6/23/26	0/1/1/1
11	NAG	f	2	11	-	4/6/23/26	0/1/1/1
11	BMA	f	3	11	-	0/2/19/22	0/1/1/1
11	MAN	f	4	11	-	0/2/19/22	1/1/1/1
11	NDG	f	5	11	-	2/6/23/26	0/1/1/1
11	GAL	f	6	11	-	1/2/19/22	0/1/1/1
11	SIA	f	7	11	-	3/18/34/38	0/1/1/1

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	5	GLA	C1-O5-C5	6.64	121.09	112.19
7	b	2	NAG	C1-O5-C5	6.03	120.26	112.19
6	a	5	GLA	C1-C2-C3	5.38	117.47	109.64
8	c	4	GAL	C1-O5-C5	5.10	119.02	112.19
8	c	2	BMA	C1-O5-C5	4.93	118.80	112.19
4	Y	4	MAN	O2-C2-C3	4.87	120.23	110.15
5	Z	4	BMA	C1-O5-C5	4.85	118.69	112.19
6	a	3	MAN	C1-O5-C5	4.70	118.48	112.19
4	Y	2	NAG	C1-O5-C5	4.26	117.90	112.19
5	Z	2	NAG	C1-O5-C5	4.19	117.81	112.19
4	Y	5	NDG	C2-N2-C7	4.07	128.35	122.90
5	Z	6	GAL	C1-O5-C5	3.99	117.54	112.19
4	Y	5	NDG	C1-C2-N2	3.92	116.61	110.43
8	c	3	NDG	O5-C1-C2	-3.89	105.27	111.29
9	d	3	MAN	C1-O5-C5	3.84	117.33	112.19
4	Y	5	NDG	C1-O5-C5	3.82	117.30	112.19
8	c	3	NDG	C3-C4-C5	3.76	117.04	110.23
6	a	4	NDG	O5-C1-C2	-3.55	105.80	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	7	SIA	O1B-C1-C2	3.47	121.74	112.71
11	f	6	GAL	C1-O5-C5	3.37	116.71	112.19
5	Z	3	BMA	C1-O5-C5	3.27	116.57	112.19
4	Y	7	SIA	O6-C2-C1	3.17	113.71	107.72
8	c	4	GAL	C1-C2-C3	3.15	114.22	109.64
7	b	3	MAN	O5-C5-C6	2.86	113.24	107.66
6	a	5	GLA	O5-C1-C2	2.84	117.56	110.79
4	Y	7	SIA	O1A-C1-C2	-2.82	116.77	122.85
6	a	5	GLA	O5-C5-C6	2.78	113.08	107.66
6	a	3	MAN	C3-C4-C5	2.67	115.08	110.23
5	Z	6	GAL	C1-C2-C3	2.67	113.53	109.64
9	d	6	GAL	O5-C5-C6	2.64	112.81	107.66
10	e	1	MAN	C1-O5-C5	2.63	115.71	112.19
7	b	4	MAN	C1-O5-C5	2.62	115.70	112.19
10	e	4	GAL	O5-C5-C6	2.59	112.70	107.66
7	b	7	SIA	O6-C2-C3	2.58	114.03	110.56
5	Z	4	BMA	O5-C5-C6	2.55	112.63	107.66
6	a	2	MAN	C1-O5-C5	2.54	115.59	112.19
5	Z	5	NAG	O5-C1-C2	-2.53	107.38	111.29
4	Y	5	NDG	C3-C4-C5	2.44	114.65	110.23
10	e	5	SIA	C8-C7-C6	2.42	117.61	113.05
10	e	5	SIA	O1B-C1-C2	2.42	119.00	112.71
11	f	7	SIA	O1B-C1-C2	2.40	118.96	112.71
10	e	3	NDG	C1-O5-C5	2.40	115.41	112.19
4	Y	2	NAG	O5-C5-C6	2.39	112.31	107.66
7	b	7	SIA	C8-C7-C6	2.37	117.51	113.05
10	e	5	SIA	C4-C5-N5	-2.34	105.83	110.44
10	e	1	MAN	O5-C5-C6	2.31	112.17	107.66
8	c	2	BMA	O5-C5-C6	2.30	112.13	107.66
7	b	7	SIA	O1B-C1-C2	2.29	118.67	112.71
5	Z	7	SIA	O1B-C1-C2	2.29	118.66	112.71
8	c	5	SIA	O1B-C1-C2	2.26	118.59	112.71
6	a	4	NDG	C3-C4-C5	2.23	114.27	110.23
11	f	1	NAG	C4-C3-C2	2.21	114.26	111.02
6	a	6	SIA	O1B-C1-C2	2.18	118.39	112.71
11	f	7	SIA	O1A-C1-C2	-2.17	118.17	122.85
5	Z	7	SIA	O1A-C1-C2	-2.14	118.22	122.85
5	Z	5	NAG	C2-N2-C7	2.14	125.77	122.90
10	e	4	GAL	C1-C2-C3	2.14	112.76	109.64
9	d	1	NAG	O5-C1-C2	-2.13	108.00	111.29
11	f	2	NAG	C4-C3-C2	2.09	114.09	111.02
7	b	2	NAG	C4-C3-C2	2.09	114.08	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	f	6	GAL	O5-C1-C2	-2.03	105.94	110.79
8	c	3	NDG	C4-C3-C2	2.01	113.97	111.02
9	d	5	NDG	O5-C1-C2	-2.01	108.18	111.29
10	e	5	SIA	O1A-C1-C2	-2.00	118.53	122.85

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Y	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Y	5	NDG	C1-C2-N2-C7
4	Y	5	NDG	C8-C7-N2-C2
4	Y	5	NDG	O7-C7-N2-C2
4	Y	7	SIA	C5-C6-C7-C8
4	Y	7	SIA	C5-C6-C7-O7
4	Y	7	SIA	O6-C6-C7-C8
4	Y	7	SIA	O6-C6-C7-O7
5	Z	2	NAG	C1-C2-N2-C7
5	Z	7	SIA	O6-C6-C7-O7
6	a	6	SIA	C6-C7-C8-O8
6	a	6	SIA	O7-C7-C8-O8
6	a	6	SIA	C11-C10-N5-C5
6	a	6	SIA	O10-C10-N5-C5
7	b	7	SIA	O1A-C1-C2-O6
7	b	7	SIA	C5-C6-C7-C8
7	b	7	SIA	C5-C6-C7-O7
7	b	7	SIA	O6-C6-C7-C8
7	b	7	SIA	O6-C6-C7-O7
7	b	7	SIA	C6-C7-C8-C9
7	b	7	SIA	C6-C7-C8-O8
7	b	7	SIA	O7-C7-C8-C9
7	b	7	SIA	O7-C7-C8-O8
9	d	5	NDG	C3-C2-N2-C7
9	d	5	NDG	C8-C7-N2-C2
9	d	5	NDG	O7-C7-N2-C2
9	d	7	SIA	C6-C5-N5-C10
9	d	7	SIA	C5-C6-C7-C8
9	d	7	SIA	C5-C6-C7-O7
9	d	7	SIA	O6-C6-C7-C8
9	d	7	SIA	C11-C10-N5-C5
9	d	7	SIA	O10-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
10	e	5	SIA	C5-C6-C7-C8
10	e	5	SIA	C5-C6-C7-O7
10	e	5	SIA	O6-C6-C7-C8
11	f	2	NAG	C3-C2-N2-C7
11	f	2	NAG	C8-C7-N2-C2
11	f	2	NAG	O7-C7-N2-C2
11	f	7	SIA	C11-C10-N5-C5
11	f	7	SIA	O10-C10-N5-C5
5	Z	6	GAL	C4-C5-C6-O6
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
4	Y	6	GAL	C4-C5-C6-O6
10	e	1	MAN	O5-C5-C6-O6
7	b	6	GLA	C4-C5-C6-O6
8	c	3	NDG	C4-C5-C6-O6
6	a	6	SIA	O7-C7-C8-C9
6	a	6	SIA	C6-C7-C8-C9
5	Z	6	GAL	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
10	e	1	MAN	C4-C5-C6-O6
4	Y	2	NAG	C8-C7-N2-C2
8	c	1	BMA	O5-C5-C6-O6
8	c	3	NDG	O5-C5-C6-O6
4	Y	6	GAL	O5-C5-C6-O6
6	a	5	GLA	O5-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
7	b	6	GLA	O5-C5-C6-O6
4	Y	3	MAN	C4-C5-C6-O6
4	Y	2	NAG	O7-C7-N2-C2
9	d	2	NAG	C8-C7-N2-C2
9	d	2	NAG	O7-C7-N2-C2
6	a	1	NAG	C4-C5-C6-O6
9	d	2	NAG	C4-C5-C6-O6
6	a	5	GLA	C4-C5-C6-O6
8	c	1	BMA	C4-C5-C6-O6
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	7	SIA	C11-C10-N5-C5
8	c	3	NDG	C8-C7-N2-C2
8	c	3	NDG	O7-C7-N2-C2
8	c	5	SIA	C11-C10-N5-C5
8	c	5	SIA	O10-C10-N5-C5

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Mol	Chain	Res	Type	Atoms
9	d	1	NAG	C8-C7-N2-C2
9	d	1	NAG	O7-C7-N2-C2
11	f	5	NDG	C8-C7-N2-C2
11	f	5	NDG	O7-C7-N2-C2
4	Y	3	MAN	O5-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
9	d	4	BMA	O5-C5-C6-O6
9	d	6	GAL	O5-C5-C6-O6
6	a	4	NDG	O5-C5-C6-O6
4	Y	7	SIA	C11-C10-N5-C5
5	Z	7	SIA	O10-C10-N5-C5
7	b	5	NAG	C8-C7-N2-C2
9	d	3	MAN	O5-C5-C6-O6
7	b	5	NAG	O7-C7-N2-C2
5	Z	5	NAG	O5-C5-C6-O6
4	Y	7	SIA	O10-C10-N5-C5
8	c	4	GAL	O5-C5-C6-O6
4	Y	4	MAN	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
5	Z	3	BMA	O5-C5-C6-O6
7	b	3	MAN	O5-C5-C6-O6
7	b	4	MAN	O5-C5-C6-O6
7	b	5	NAG	O5-C5-C6-O6
7	b	2	NAG	O5-C5-C6-O6
7	b	5	NAG	C3-C2-N2-C7
11	f	2	NAG	O5-C5-C6-O6
5	Z	7	SIA	O1A-C1-C2-O6
10	e	5	SIA	O7-C7-C8-C9
10	e	5	SIA	O7-C7-C8-O8
9	d	3	MAN	C4-C5-C6-O6
5	Z	5	NAG	C1-C2-N2-C7
5	Z	7	SIA	C5-C6-C7-O7
9	d	7	SIA	O6-C6-C7-O7
4	Y	7	SIA	O7-C7-C8-C9
11	f	6	GAL	C4-C5-C6-O6
5	Z	7	SIA	O6-C6-C7-C8
5	Z	5	NAG	C3-C2-N2-C7
5	Z	7	SIA	C5-C6-C7-C8
11	f	7	SIA	O1A-C1-C2-O6
6	a	6	SIA	C6-C5-N5-C10
4	Y	7	SIA	C6-C7-C8-C9
6	a	6	SIA	C4-C5-N5-C10

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Mol	Chain	Res	Type	Atoms
7	b	7	SIA	O1B-C1-C2-O6
4	Y	7	SIA	O7-C7-C8-O8
9	d	5	NDG	C1-C2-N2-C7
10	e	5	SIA	C6-C7-C8-O8
10	e	5	SIA	O1A-C1-C2-O6
5	Z	7	SIA	C4-C5-N5-C10

All (6) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	3	BMA	C1-C2-C3-C4-C5-O5
11	f	4	MAN	C1-C2-C3-C4-C5-O5
8	c	2	BMA	C1-C2-C3-C4-C5-O5
10	e	1	MAN	C1-C2-C3-C4-C5-O5
6	a	2	MAN	C1-C2-C3-C4-C5-O5
7	b	4	MAN	C1-C2-C3-C4-C5-O5

25 monomers are involved in 36 short contacts:

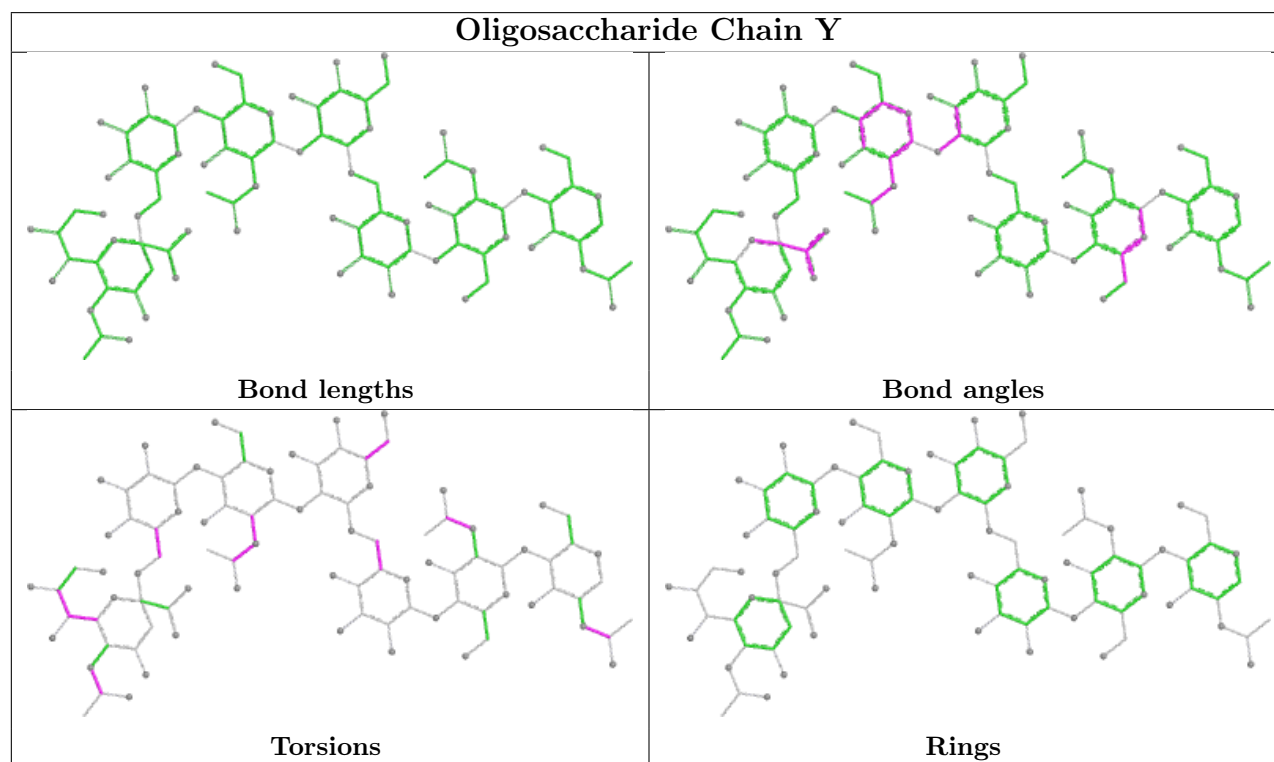
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	f	2	NAG	1	0
5	Z	1	NAG	1	0
9	d	7	SIA	1	4
9	d	1	NAG	1	0
4	Y	6	GAL	2	1
11	f	7	SIA	1	1
6	a	5	GLA	3	0
6	a	4	NDG	2	0
7	b	6	GLA	1	0
8	c	3	NDG	1	0
5	Z	2	NAG	2	0
6	a	3	MAN	1	0
7	b	3	MAN	1	0
4	Y	1	NAG	1	0
9	d	2	NAG	1	0
11	f	5	NDG	1	0
7	b	2	NAG	1	0
4	Y	7	SIA	2	3
8	c	5	SIA	0	2
4	Y	2	NAG	1	0
10	e	5	SIA	1	2
11	f	1	NAG	1	0

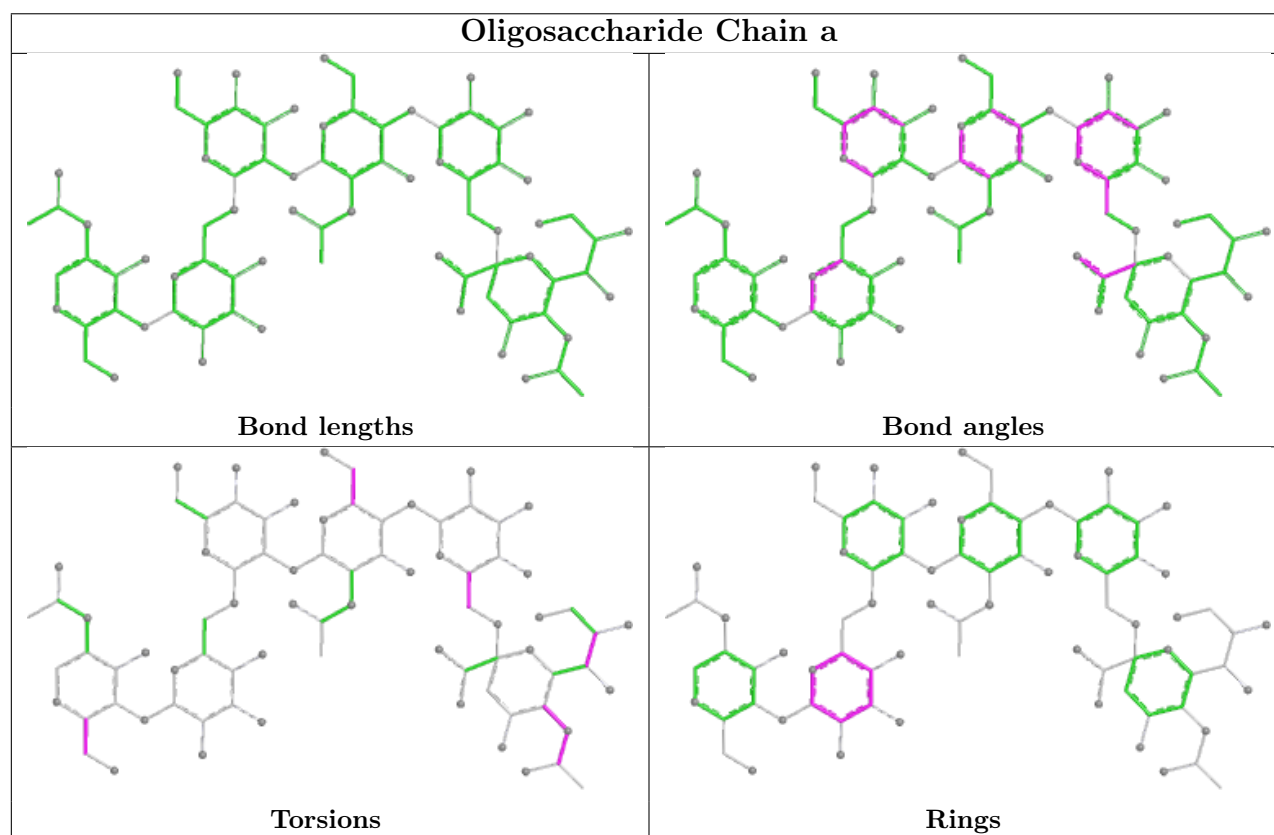
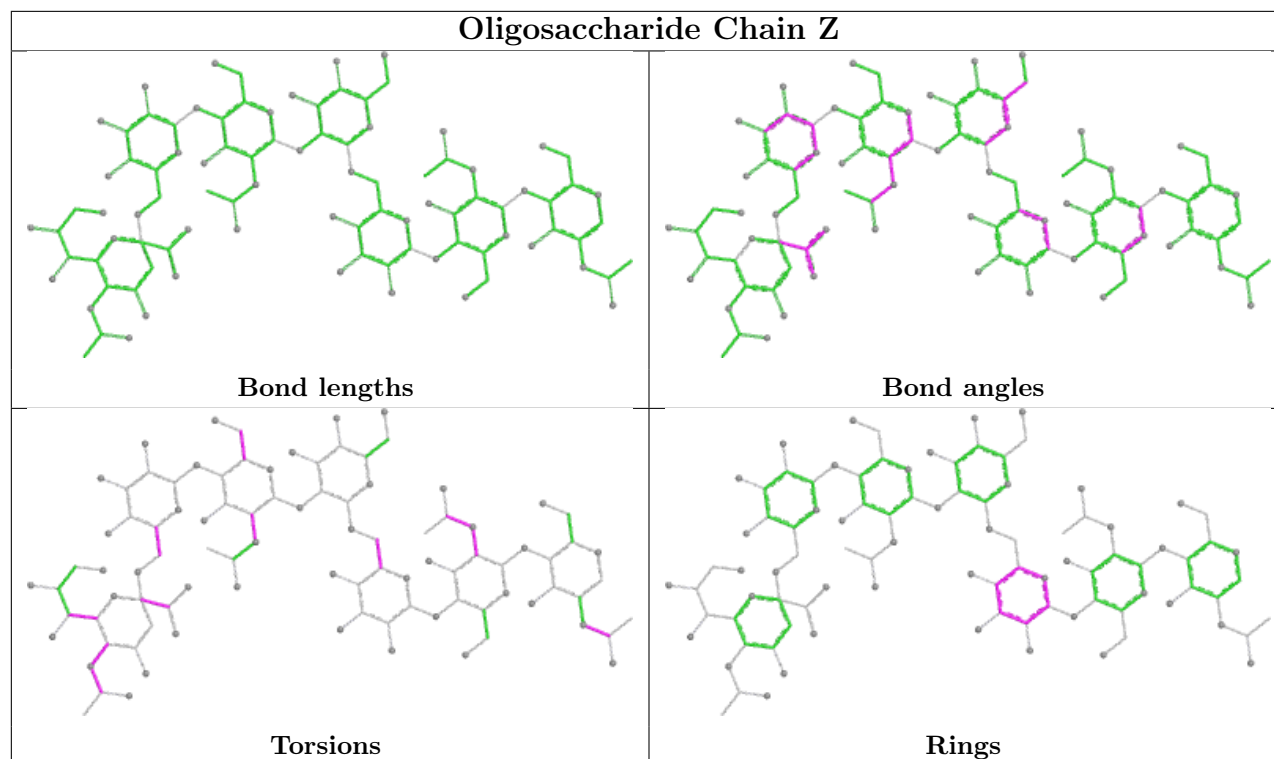
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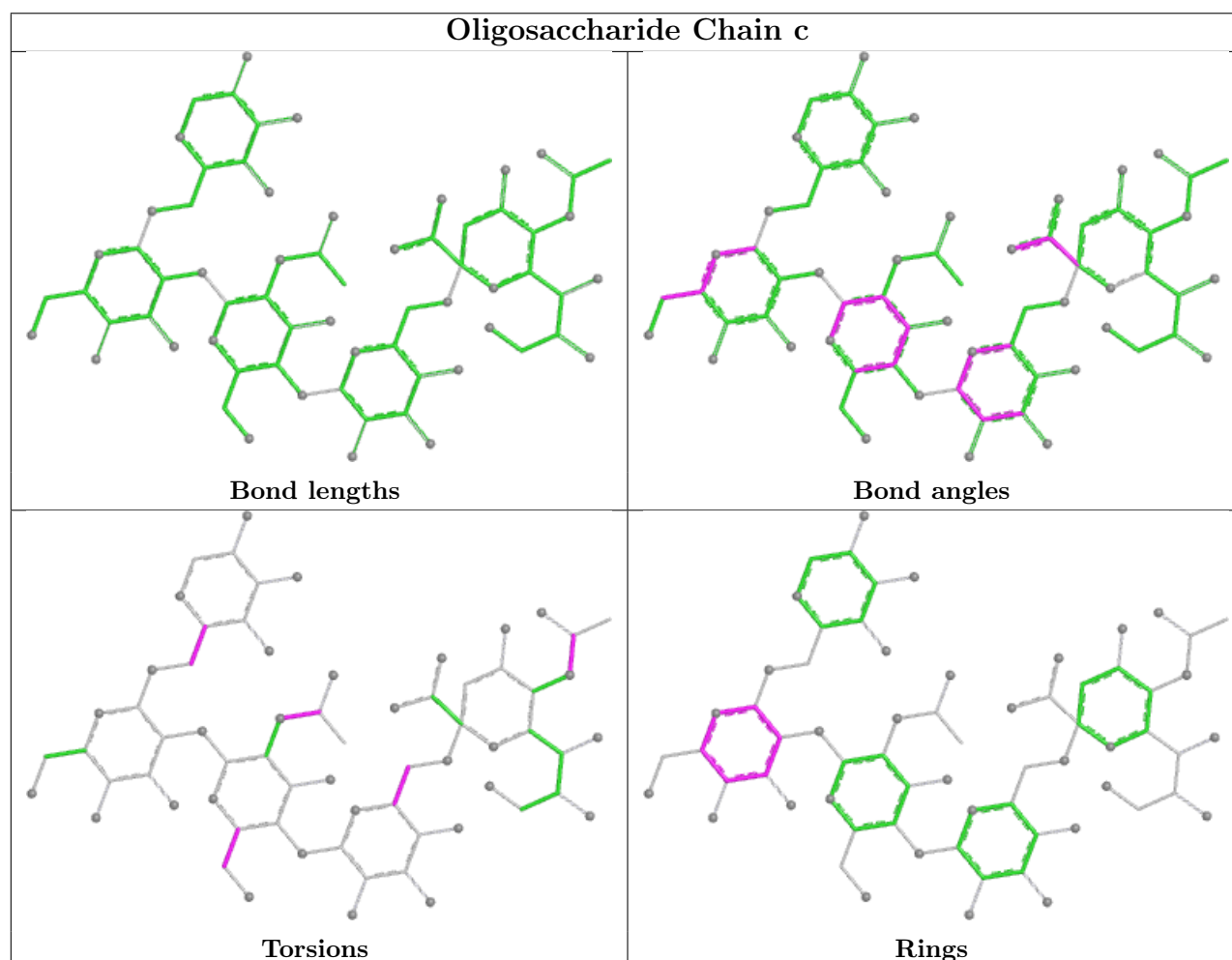
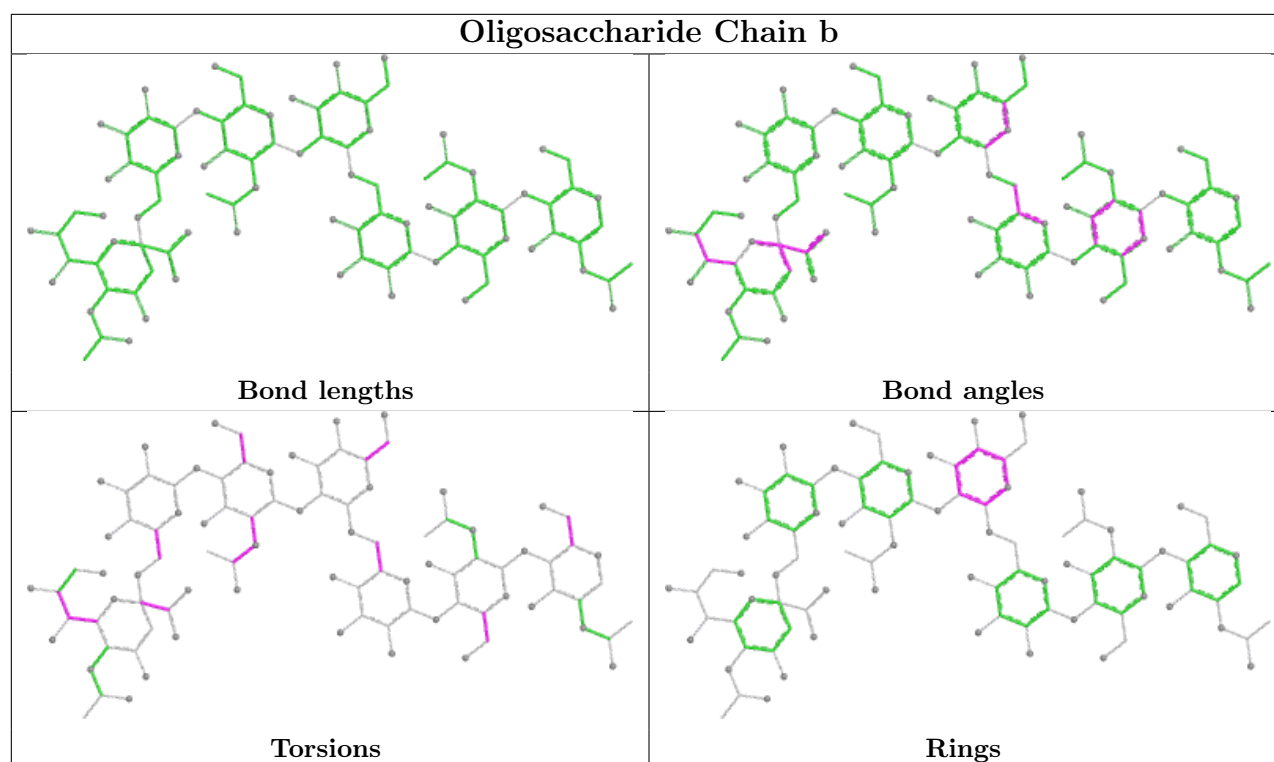
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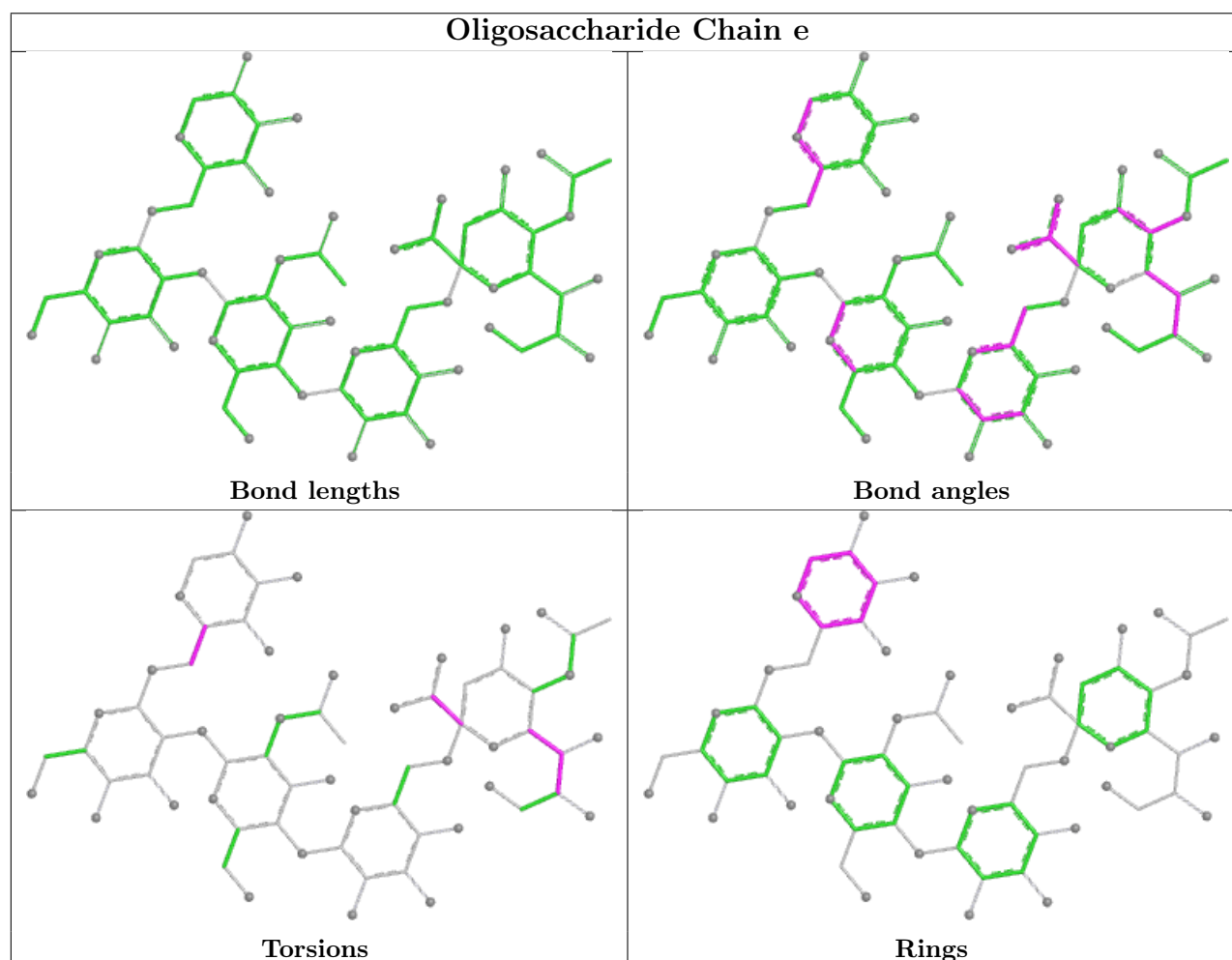
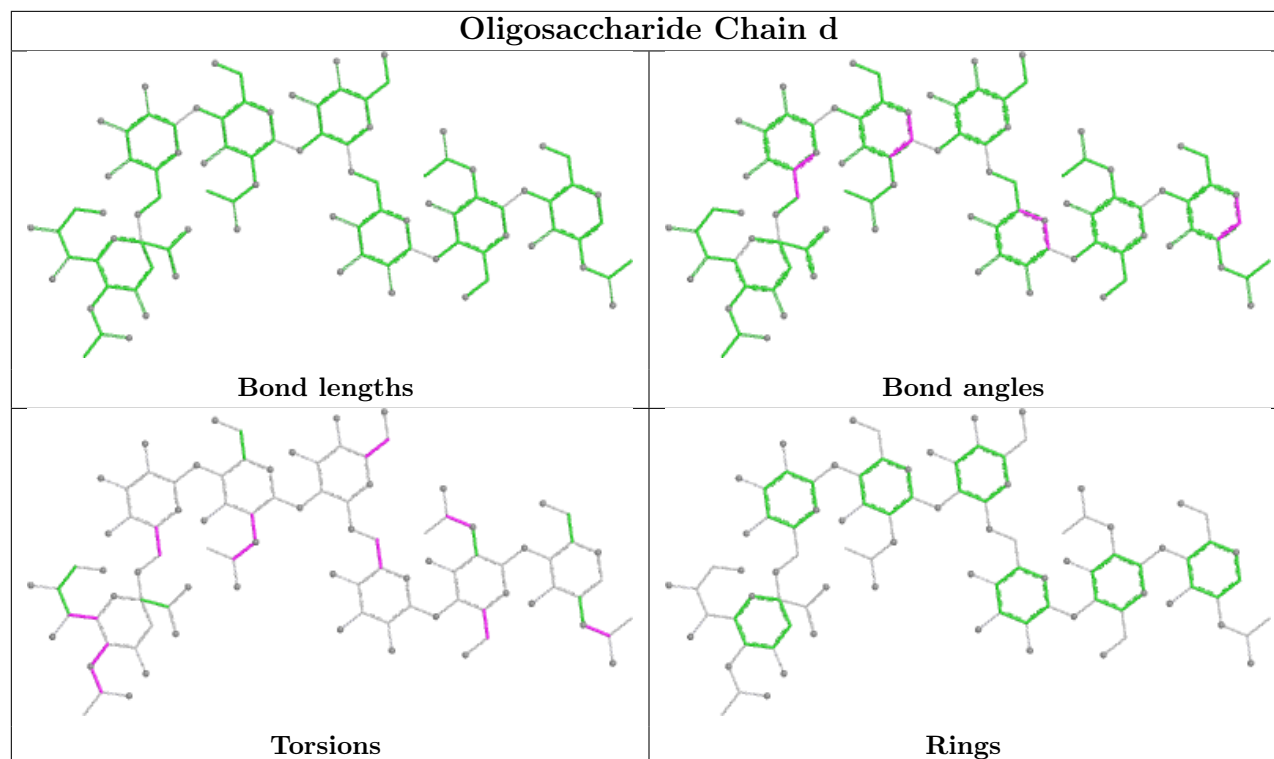
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	6	SIA	4	0
7	b	7	SIA	0	1
5	Z	4	BMA	1	0

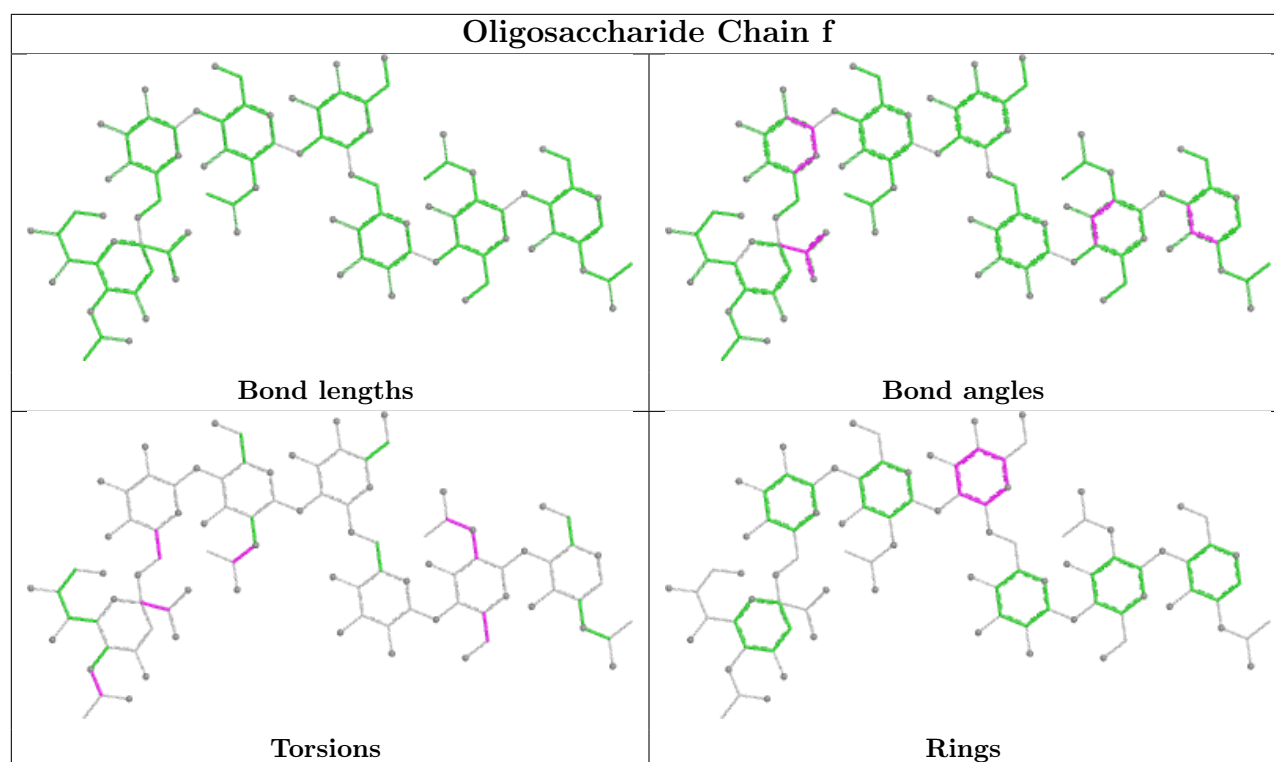
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

5 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$
12	NAG	O	301	3	14,14,15	0.32	0	17,19,21	0.59	0
12	NAG	X	301	3	14,14,15	0.23	0	17,19,21	0.46	0
12	NAG	R	301	3	14,14,15	0.37	0	17,19,21	0.46	0
12	NAG	L	306	-	14,14,15	0.26	0	17,19,21	0.97	0
12	NAG	U	301	3	14,14,15	0.42	0	17,19,21	0.44	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
12	NAG	O	301	3	-	0/6/23/26	0/1/1/1
12	NAG	X	301	3	-	2/6/23/26	0/1/1/1
12	NAG	R	301	3	-	3/6/23/26	0/1/1/1
12	NAG	L	306	-	-	0/6/23/26	0/1/1/1
12	NAG	U	301	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	U	301	NAG	C4-C5-C6-O6
12	U	301	NAG	O5-C5-C6-O6
12	R	301	NAG	O5-C5-C6-O6
12	X	301	NAG	O5-C5-C6-O6
12	R	301	NAG	C4-C5-C6-O6
12	R	301	NAG	C3-C2-N2-C7
12	U	301	NAG	C3-C2-N2-C7
12	X	301	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	X	301	NAG	1	0
12	R	301	NAG	1	0
12	U	301	NAG	2	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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	225/230 (97%)	0.52	7 (3%)	51	37	36, 61, 122, 163	0
1	C	218/230 (94%)	0.89	25 (11%)	9	13	59, 120, 178, 200	0
1	F	223/230 (96%)	0.48	10 (4%)	38	30	36, 70, 143, 176	0
1	I	217/230 (94%)	0.82	19 (8%)	15	17	46, 113, 161, 179	0
1	M	225/230 (97%)	0.50	8 (3%)	46	35	43, 82, 128, 151	0
1	P	220/230 (95%)	0.66	14 (6%)	25	23	64, 109, 149, 172	0
1	S	224/230 (97%)	0.62	10 (4%)	38	30	46, 92, 150, 182	0
1	V	208/230 (90%)	0.78	15 (7%)	21	20	57, 108, 158, 201	0
2	B	215/215 (100%)	0.58	14 (6%)	25	23	39, 64, 126, 159	0
2	D	203/215 (94%)	0.84	22 (10%)	11	13	59, 107, 178, 210	0
2	G	214/215 (99%)	0.57	9 (4%)	40	31	38, 64, 136, 183	0
2	J	187/215 (86%)	0.72	16 (8%)	16	17	50, 90, 160, 187	0
2	N	214/215 (99%)	0.57	9 (4%)	40	31	39, 84, 135, 158	0
2	Q	202/215 (93%)	0.73	10 (4%)	34	28	56, 103, 151, 185	0
2	T	214/215 (99%)	0.58	11 (5%)	33	27	54, 87, 144, 177	0
2	W	198/215 (92%)	0.80	15 (7%)	20	20	63, 104, 164, 189	0
3	E	196/219 (89%)	0.69	13 (6%)	24	22	57, 95, 138, 167	0
3	H	202/219 (92%)	0.66	10 (4%)	34	28	37, 79, 122, 147	0
3	K	206/219 (94%)	0.64	9 (4%)	39	31	47, 81, 132, 152	0
3	L	185/219 (84%)	0.66	10 (5%)	31	27	51, 85, 137, 160	0
3	O	209/219 (95%)	0.56	10 (4%)	35	29	35, 60, 118, 143	0
3	R	194/219 (88%)	0.66	12 (6%)	26	24	68, 92, 136, 156	0
3	U	196/219 (89%)	0.65	11 (5%)	30	26	40, 70, 125, 175	0
3	X	196/219 (89%)	0.86	11 (5%)	30	26	65, 96, 147, 174	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	4991/5312 (93%)	0.67	300 (6%)	27	24	35, 89, 150, 210	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	132	SER	7.5
1	C	56	GLY	7.5
2	D	195	ALA	4.8
1	C	60	PHE	4.8
1	S	125	GLY	4.7
3	X	255	ASN	4.6
1	M	133	ALA	4.5
3	E	84	GLU	4.4
3	O	253	ASN	4.3
3	L	255	ASN	4.3
3	X	74	PRO	4.3
1	I	56	GLY	4.2
3	K	86	SER	4.2
3	X	96	ASN	4.0
3	R	141	SER	3.9
1	A	60	PHE	3.9
3	X	64	CYS	3.9
1	M	134	SER	3.8
2	W	93	SER	3.8
1	P	221	PRO	3.8
2	W	118	PHE	3.8
1	F	141	ALA	3.7
3	R	69	TRP	3.7
1	C	59	TYR	3.7
3	R	255	ASN	3.7
1	F	160	ASP	3.7
3	E	200	TYR	3.6
2	B	90	GLN	3.6
3	K	242	LEU	3.6
2	W	34	ASN	3.5
3	X	69	TRP	3.5
3	E	74	PRO	3.4
2	J	77	SER	3.4
3	O	93	ASN	3.4
1	V	126	THR	3.4
2	N	196	CYS	3.4
1	C	47	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	150	TRP	3.3
2	G	194	TYR	3.3
3	X	75	MET	3.3
3	L	109	GLU	3.3
2	G	211	PHE	3.3
2	J	172	ASP	3.3
3	H	255	ASN	3.3
1	C	49	ALA	3.3
2	G	133	SER	3.3
2	J	94	THR	3.2
3	K	84	GLU	3.2
2	D	151	LYS	3.2
1	I	50	ASN	3.2
2	N	189	GLU	3.2
2	Q	115	PRO	3.2
1	S	133	ALA	3.2
1	P	227	ASP	3.1
2	Q	93	SER	3.1
1	F	59	TYR	3.1
3	H	253	ASN	3.1
2	D	161	SER	3.1
3	L	73	ASN	3.1
1	M	155	ALA	3.1
1	I	202	SER	3.1
3	L	132	SER	3.1
3	X	254	GLY	3.1
2	J	139	ASN	3.0
1	I	59	TYR	3.0
2	N	1	ASP	3.0
3	H	86	SER	3.0
1	V	159	CYS	3.0
3	U	236	GLU	3.0
1	F	62	ASP	3.0
3	U	65	SER	3.0
2	W	4	MET	3.0
3	E	151	SER	3.0
2	T	91	SER	2.9
2	D	36	TYR	2.9
2	Q	103	GLY	2.9
1	I	96	CYS	2.9
3	H	84	GLU	2.9
3	O	99	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	P	146	SER	2.9
2	D	136	CYS	2.9
1	P	31	THR	2.9
1	V	158	GLY	2.9
2	D	196	CYS	2.8
1	A	215	ASN	2.8
1	I	114	TYR	2.8
2	Q	13	ALA	2.8
3	E	58	PRO	2.8
3	E	254	GLY	2.8
1	C	58	LYS	2.8
1	V	142	PRO	2.8
1	S	57	ASP	2.8
1	I	152	ALA	2.8
2	G	195	ALA	2.8
3	R	67	ALA	2.8
1	C	50	ASN	2.8
1	I	125	VAL	2.8
3	X	233	GLY	2.8
2	D	162	GLN	2.8
2	G	212	ASN	2.7
1	I	60	PHE	2.7
2	D	173	SER	2.7
3	U	96	ASN	2.7
2	N	124	ASP	2.7
1	I	95	TYR	2.7
3	O	254	GLY	2.7
3	L	166	TYR	2.7
1	I	58	LYS	2.7
3	U	118	ASN	2.7
2	Q	107	GLU	2.7
3	U	103	ASP	2.6
1	I	74	ASN	2.6
3	R	93	ASN	2.6
2	T	215	GLU	2.6
2	W	136	CYS	2.6
3	O	63	ASP	2.6
2	J	163	GLU	2.6
2	B	102	GLY	2.6
1	I	132	THR	2.6
3	K	80	ILE	2.6
1	V	207	SER	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	145	PRO	2.6
2	W	150	TRP	2.6
3	H	76	CYS	2.6
1	A	141	ALA	2.6
3	R	65	SER	2.6
3	X	101	PRO	2.6
2	J	150	TRP	2.6
3	R	158	TRP	2.6
3	U	229	ASN	2.6
2	W	162	GLN	2.5
1	F	158	VAL	2.5
2	J	1	ASP	2.5
2	W	149	GLN	2.5
1	F	156	CYS	2.5
1	C	116	MET	2.5
2	D	100	PHE	2.5
1	F	193	SER	2.5
2	T	32	SER	2.5
2	J	160	ASN	2.5
1	I	49	ALA	2.5
1	V	175	SER	2.5
2	Q	133	SER	2.5
2	J	114	ALA	2.5
1	C	217	LYS	2.4
2	W	196	CYS	2.4
3	L	260	GLU	2.4
1	C	114	TYR	2.4
3	O	65	SER	2.4
1	P	222	SER	2.4
2	T	30	SER	2.4
1	P	102	GLY	2.4
2	B	204	SER	2.4
3	U	152	PHE	2.4
2	N	151	LYS	2.4
3	H	118	ASN	2.4
1	C	85	THR	2.4
3	H	254	GLY	2.4
2	D	133	SER	2.4
2	Q	30	SER	2.4
2	W	14	SER	2.4
3	O	232	SER	2.4
2	B	1	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	68	PHE	2.3
2	N	68	GLY	2.3
1	C	153	ALA	2.3
1	V	34	THR	2.3
2	T	124	ASP	2.3
1	V	138	PRO	2.3
2	T	101	GLY	2.3
1	F	159	LYS	2.3
2	D	149	GLN	2.3
1	V	31	THR	2.3
1	V	111	ARG	2.3
1	S	192	SER	2.3
3	X	65	SER	2.3
2	D	153	ASP	2.3
1	V	53	ASN	2.3
1	I	98	ARG	2.3
2	W	111	THR	2.3
1	P	50	TRP	2.3
1	I	32	TYR	2.3
2	T	194	TYR	2.3
3	E	232	SER	2.3
2	B	187	ASP	2.3
2	J	103	GLY	2.3
3	E	63	ASP	2.3
3	E	124	GLN	2.3
1	F	149	GLY	2.3
2	W	103	GLY	2.3
3	U	247	ALA	2.3
1	I	33	TRP	2.3
3	O	100	TYR	2.3
1	M	165	PHE	2.3
1	V	127	THR	2.3
2	D	131	THR	2.3
2	G	129	SER	2.3
2	J	173	SER	2.3
1	S	144	ALA	2.3
2	B	157	GLN	2.3
2	W	157	GLN	2.3
1	A	143	SER	2.2
1	C	17	SER	2.2
2	B	205	SER	2.2
3	X	93	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	94	THR	2.2
2	B	182	THR	2.2
3	H	102	GLY	2.2
1	P	117	TYR	2.2
1	C	61	VAL	2.2
1	P	166	PRO	2.2
2	J	174	THR	2.2
2	J	76	SER	2.2
1	V	73	ILE	2.2
3	R	90	GLU	2.2
2	J	117	VAL	2.2
2	G	196	CYS	2.2
3	L	64	CYS	2.2
1	S	6	GLN	2.2
3	R	113	LEU	2.2
1	I	207	THR	2.2
2	B	69	THR	2.2
1	S	141	PHE	2.2
2	B	184	SER	2.2
3	E	76	CYS	2.2
2	J	102	GLY	2.2
1	C	218	PRO	2.2
1	S	145	PRO	2.2
3	E	155	ASN	2.2
2	W	31	SER	2.2
1	P	42	GLN	2.2
1	C	160	ASP	2.1
3	L	254	GLY	2.1
3	U	93	ASN	2.1
1	C	31	THR	2.1
1	C	2	VAL	2.1
2	B	129	SER	2.1
2	Q	56	SER	2.1
3	R	236	GLU	2.1
1	I	156	CYS	2.1
3	K	93	ASN	2.1
3	K	105	ASN	2.1
1	V	179	THR	2.1
2	B	158	SER	2.1
2	D	67	SER	2.1
2	D	91	SER	2.1
1	S	156	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	203	PRO	2.1
3	H	104	PHE	2.1
2	D	135	VAL	2.1
2	T	160	ASN	2.1
3	H	96	ASN	2.1
3	E	86	SER	2.1
3	L	86	SER	2.1
1	A	6	GLU	2.1
1	P	58	GLY	2.1
2	D	68	GLY	2.1
1	C	156	CYS	2.1
2	Q	196	CYS	2.1
2	N	15	VAL	2.1
1	C	115	GLY	2.1
2	D	113	ALA	2.1
1	C	119	TRP	2.1
1	C	164	GLU	2.1
2	N	100	PHE	2.1
2	T	136	CYS	2.1
2	G	188	TYR	2.1
1	M	223	ASN	2.1
1	F	143	SER	2.1
2	B	91	SER	2.1
2	D	179	SER	2.1
1	V	140	VAL	2.1
1	M	125	GLY	2.1
3	K	222	ILE	2.1
1	C	33	TRP	2.1
1	P	173	TRP	2.1
2	D	30	SER	2.1
3	K	241	ILE	2.0
2	T	196	CYS	2.0
3	O	144	CYS	2.0
1	M	87	ASN	2.0
1	P	156	ALA	2.0
2	G	186	ALA	2.0
2	T	114	ALA	2.0
1	A	124	THR	2.0
1	P	85	GLN	2.0
2	W	140	ASN	2.0
3	E	255	ASN	2.0
3	R	101	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
3	O	240	THR	2.0
3	U	177	ASN	2.0
3	U	178	GLN	2.0
1	A	140	LEU	2.0
2	J	98	LEU	2.0
2	Q	14	SER	2.0
3	R	70	LEU	2.0
2	N	103	GLY	2.0
1	S	112	GLN	2.0
2	D	117	VAL	2.0
1	C	212	CYS	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](#)

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
5	BMA	Z	3	11/12	0.34	0.14	153,157,159,161	0
5	NAG	Z	2	14/15	0.35	0.16	104,141,148,153	0
4	MAN	Y	3	11/12	0.46	0.17	140,153,163,163	0
4	NAG	Y	1	14/15	0.51	0.15	135,146,152,152	0
4	MAN	Y	4	11/12	0.53	0.13	130,141,147,151	0
4	NAG	Y	2	14/15	0.54	0.12	115,141,152,155	0
5	GAL	Z	6	11/12	0.56	0.21	90,109,117,123	0
5	BMA	Z	4	11/12	0.59	0.12	141,155,158,159	0
4	NDG	Y	5	14/15	0.59	0.15	143,145,157,161	0
5	NAG	Z	1	14/15	0.60	0.17	152,162,176,177	0
4	GAL	Y	6	11/12	0.71	0.15	141,146,156,161	0
5	SIA	Z	7	20/21	0.78	0.18	61,75,105,105	0
5	NAG	Z	5	14/15	0.84	0.17	113,128,152,155	0
4	SIA	Y	7	20/21	0.86	0.17	110,144,159,159	0
6	NAG	a	1	14/15	-	-	129,139,148,148	0
6	MAN	a	2	11/12	-	-	119,122,125,129	0
6	MAN	a	3	11/12	-	-	135,142,147,148	0

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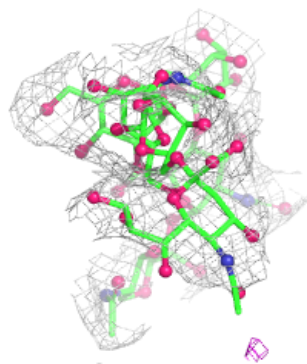
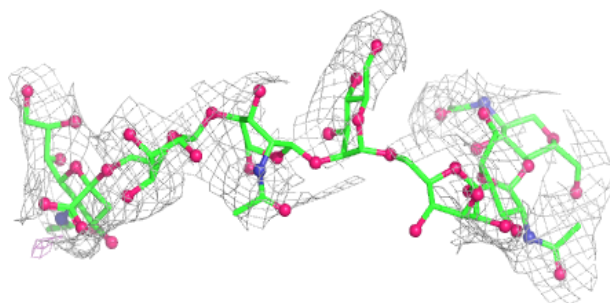
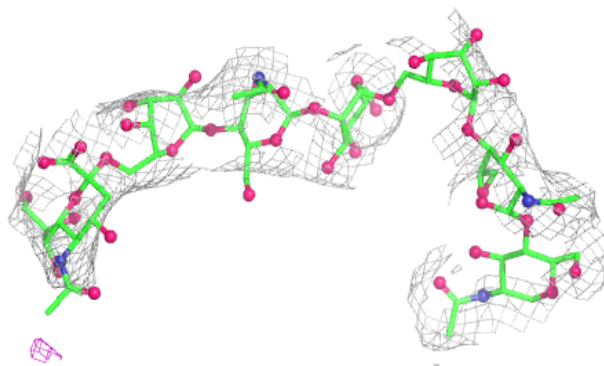
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NDG	a	4	14/15	-	-	118,129,137,139	0
6	GLA	a	5	11/12	-	-	109,128,145,150	0
6	SIA	a	6	20/21	-	-	85,101,111,124	0
7	NAG	b	1	14/15	-	-	142,156,163,167	0
7	NAG	b	2	14/15	-	-	163,172,178,182	0
7	MAN	b	3	11/12	-	-	169,183,186,187	0
7	MAN	b	4	11/12	-	-	151,167,171,172	0
7	NAG	b	5	14/15	-	-	90,128,136,140	0
7	GLA	b	6	11/12	-	-	103,118,127,129	0
7	SIA	b	7	20/21	-	-	115,135,147,155	0
8	BMA	c	1	11/12	-	-	129,155,160,162	0
8	BMA	c	2	11/12	-	-	127,136,139,139	0
8	NDG	c	3	14/15	-	-	111,128,136,141	0
8	GAL	c	4	11/12	-	-	99,112,121,124	0
8	SIA	c	5	20/21	-	-	55,109,134,136	0
9	NAG	d	1	14/15	-	-	138,149,158,160	0
9	NAG	d	2	14/15	-	-	120,145,156,157	0
9	MAN	d	3	11/12	-	-	128,148,153,154	0
9	BMA	d	4	11/12	-	-	103,113,120,122	0
9	NDG	d	5	14/15	-	-	113,124,128,133	0
9	GAL	d	6	11/12	-	-	94,100,112,115	0
9	SIA	d	7	20/21	-	-	45,99,124,125	0
10	MAN	e	1	11/12	-	-	150,153,161,164	0
10	BMA	e	2	11/12	-	-	141,155,158,160	0
10	NDG	e	3	14/15	-	-	107,130,149,150	0
10	GAL	e	4	11/12	-	-	101,115,136,136	0
10	SIA	e	5	20/21	-	-	64,75,107,108	0
11	NAG	f	1	14/15	-	-	114,124,133,135	0
11	NAG	f	2	14/15	-	-	119,141,149,150	0
11	BMA	f	3	11/12	-	-	134,146,151,154	0
11	MAN	f	4	11/12	-	-	149,154,158,159	0
11	NDG	f	5	14/15	-	-	119,144,156,158	0
11	GAL	f	6	11/12	-	-	105,112,114,117	0
11	SIA	f	7	20/21	-	-	86,103,124,126	0

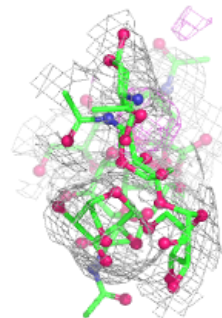
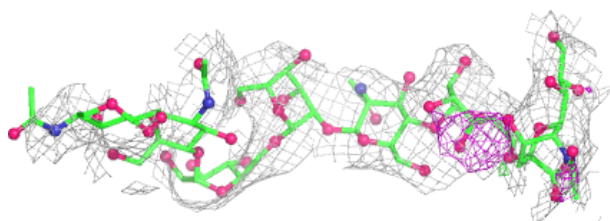
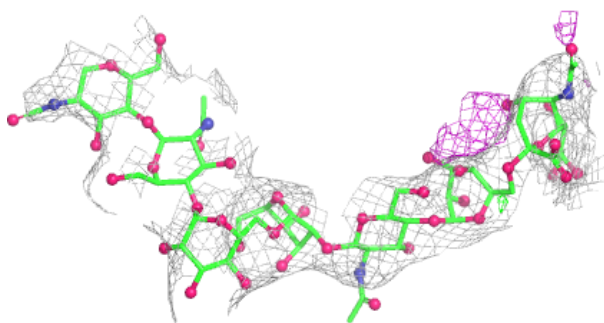
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

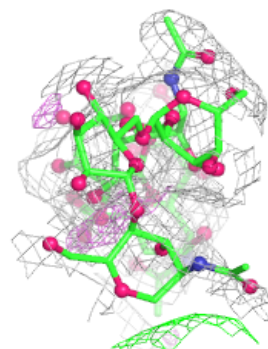
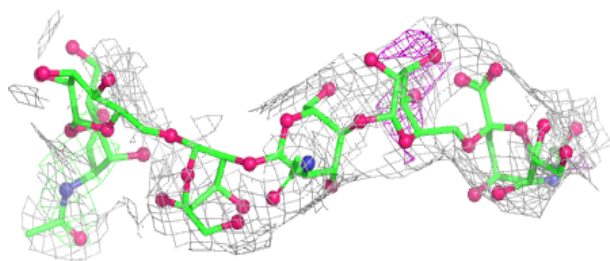
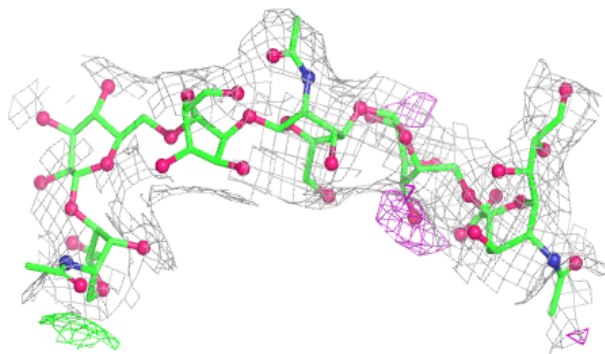
**Electron density around Chain Z:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

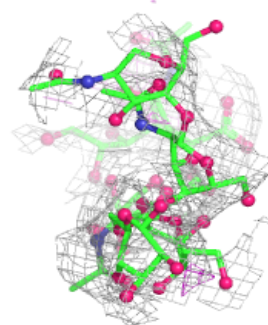
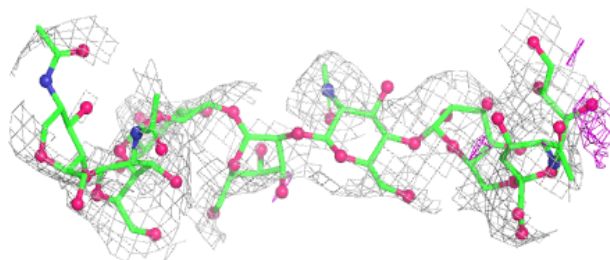
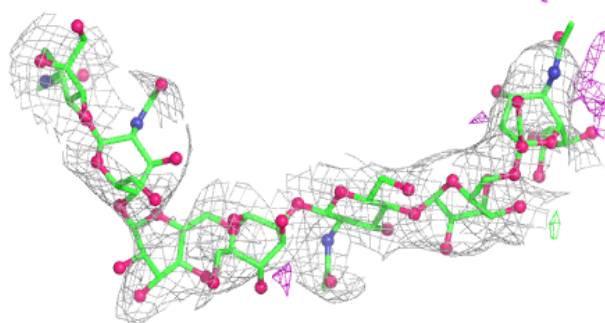


Electron density around Chain a:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

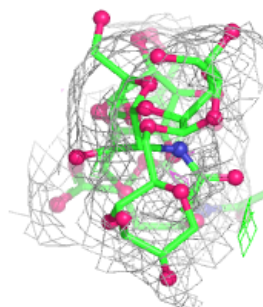
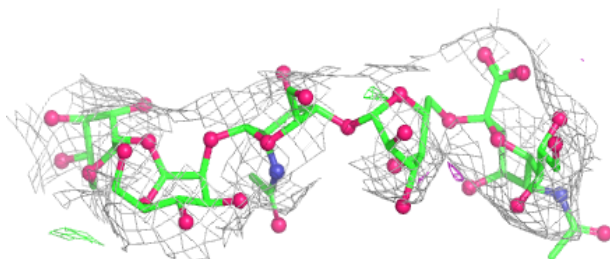
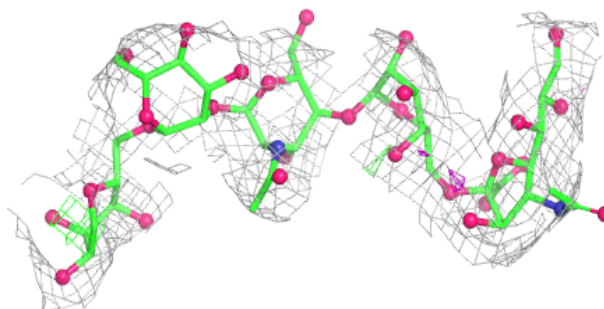
**Electron density around Chain b:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

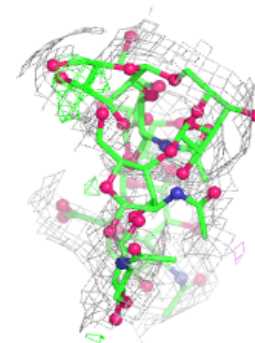
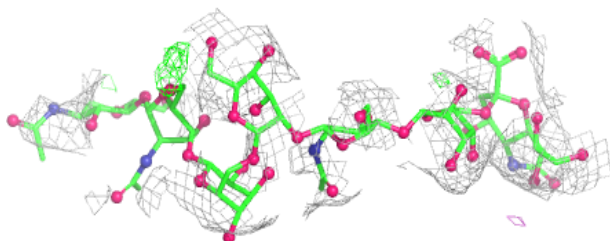
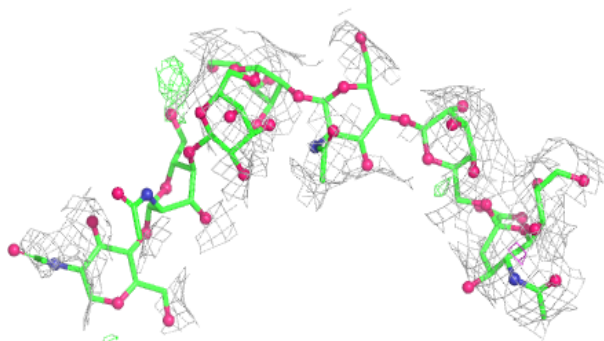


Electron density around Chain c:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

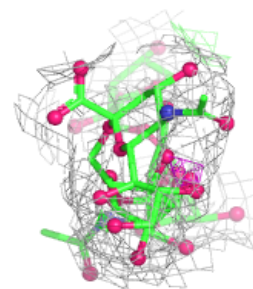
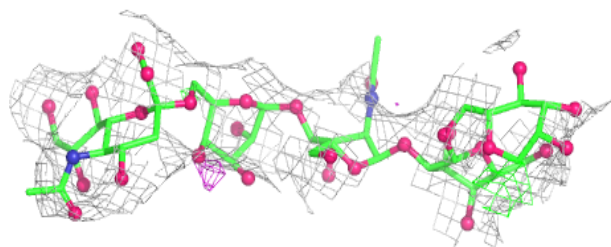
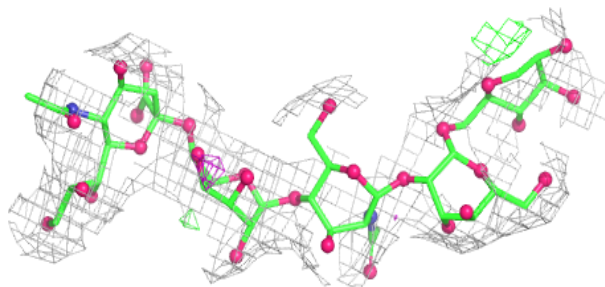
**Electron density around Chain d:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

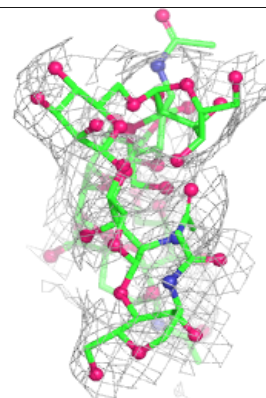
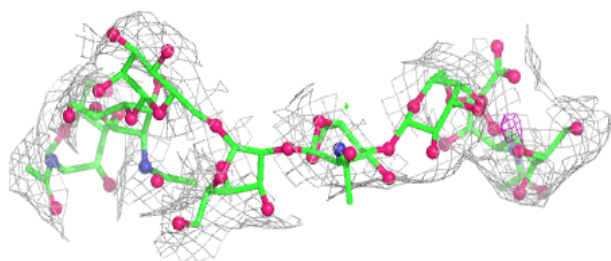
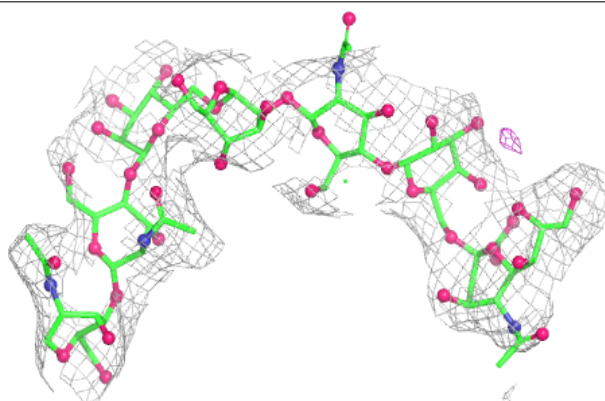


Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain f:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands

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
12	NAG	L	306	14/15	0.59	0.22	148,153,160,161	0
12	NAG	O	301	14/15	0.59	0.19	34,65,73,75	0
12	NAG	R	301	14/15	0.70	0.15	80,114,118,121	0
12	NAG	U	301	14/15	0.72	0.22	92,108,117,126	0
12	NAG	X	301	14/15	0.79	0.11	88,114,119,124	0

6.5 Other polymers

There are no such residues in this entry.