Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2026 – 07:20 PM UTC

PDB ID	:	3UBN / pdb_00003ubn
Title	:	Influenza hemagglutinin from the 2009 pandemic in complex with ligand 6SLN
Authors	:	Xu, R.; Wilson, I.A.
Deposited on	:	2011-10-24
Resolution	:	2.51 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 (i) 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 (1)) were used in the production of this report:

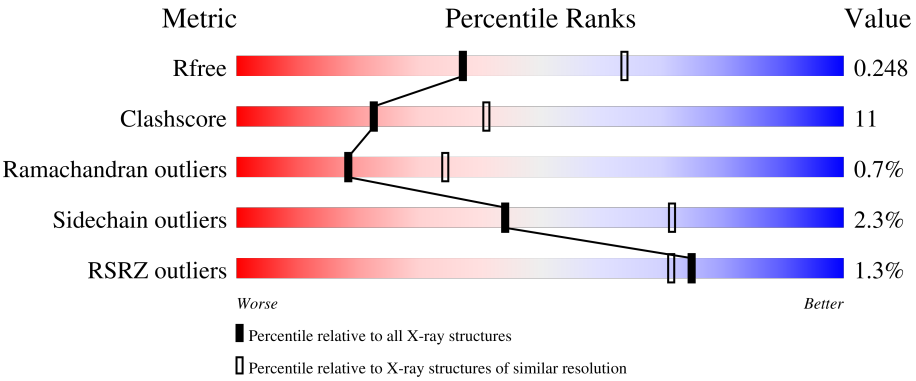
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	329	77% 19%
1	C	329	% 72% 23%
1	E	329	% 71% 25%
1	G	329	73% 24%
1	I	329	% 73% 22%

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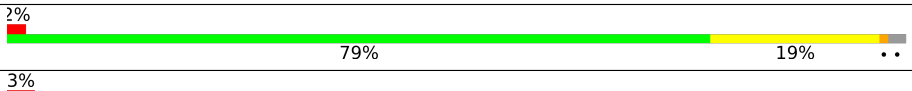
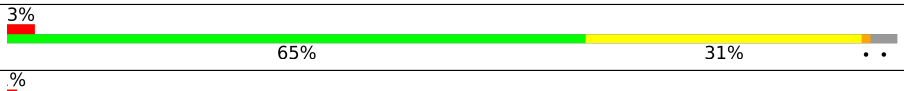
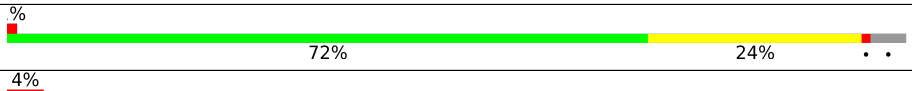
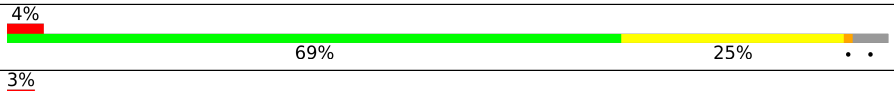
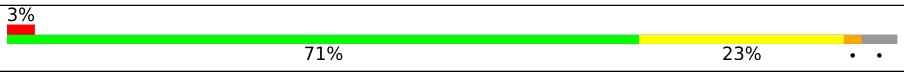
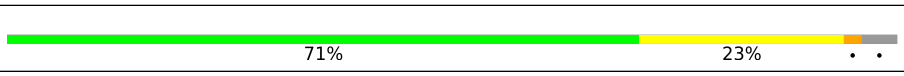
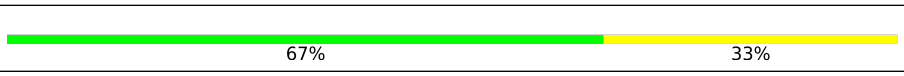
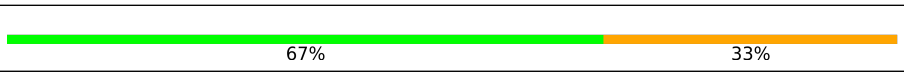
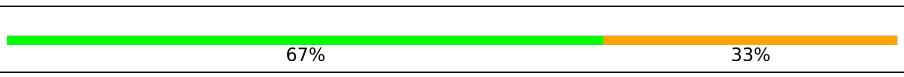
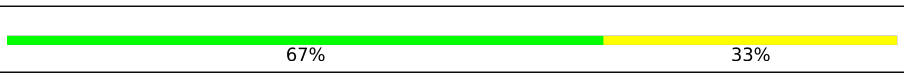
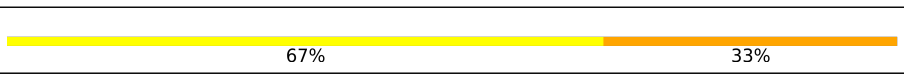
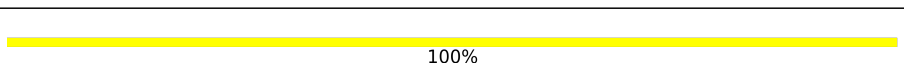
Mol	Chain	Length	Quality of chain
1	K	329	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	
3	M	3	
3	N	3	
3	O	3	
3	R	3	
3	S	3	
4	P	2	
5	Q	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 24203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	C	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	E	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	G	321	Total	C	N	O	S	0	0	0
			2508	1586	430	479	13			
1	I	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	K	319	Total	C	N	O	S	0	0	0
			2492	1578	428	473	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP C3W5S1
A	10	GLY	-	expression tag	UNP C3W5S1
A	205	CYS	GLY	engineered mutation	UNP C3W5S1
A	220	CYS	ARG	engineered mutation	UNP C3W5S1
C	9	PRO	-	expression tag	UNP C3W5S1
C	10	GLY	-	expression tag	UNP C3W5S1
C	205	CYS	GLY	engineered mutation	UNP C3W5S1
C	220	CYS	ARG	engineered mutation	UNP C3W5S1
E	9	PRO	-	expression tag	UNP C3W5S1
E	10	GLY	-	expression tag	UNP C3W5S1
E	205	CYS	GLY	engineered mutation	UNP C3W5S1
E	220	CYS	ARG	engineered mutation	UNP C3W5S1
G	9	PRO	-	expression tag	UNP C3W5S1
G	10	GLY	-	expression tag	UNP C3W5S1
G	205	CYS	GLY	engineered mutation	UNP C3W5S1
G	220	CYS	ARG	engineered mutation	UNP C3W5S1
I	9	PRO	-	expression tag	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	10	GLY	-	expression tag	UNP C3W5S1
I	205	CYS	GLY	engineered mutation	UNP C3W5S1
I	220	CYS	ARG	engineered mutation	UNP C3W5S1
K	9	PRO	-	expression tag	UNP C3W5S1
K	10	GLY	-	expression tag	UNP C3W5S1
K	205	CYS	GLY	engineered mutation	UNP C3W5S1
K	220	CYS	ARG	engineered mutation	UNP C3W5S1

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	174	Total	C	N	O	S	0	0	0
			1405	881	237	281	6			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	234	274	6			
2	F	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	H	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	J	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	L	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP C3W5S1
B	176	GLY	-	expression tag	UNP C3W5S1
B	177	ARG	-	expression tag	UNP C3W5S1
D	175	SER	-	expression tag	UNP C3W5S1
D	176	GLY	-	expression tag	UNP C3W5S1
D	177	ARG	-	expression tag	UNP C3W5S1
F	175	SER	-	expression tag	UNP C3W5S1
F	176	GLY	-	expression tag	UNP C3W5S1
F	177	ARG	-	expression tag	UNP C3W5S1
H	175	SER	-	expression tag	UNP C3W5S1
H	176	GLY	-	expression tag	UNP C3W5S1
H	177	ARG	-	expression tag	UNP C3W5S1
J	175	SER	-	expression tag	UNP C3W5S1
J	176	GLY	-	expression tag	UNP C3W5S1
J	177	ARG	-	expression tag	UNP C3W5S1

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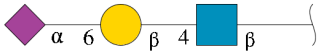
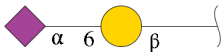
Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	expression tag	UNP C3W5S1
L	176	GLY	-	expression tag	UNP C3W5S1
L	177	ARG	-	expression tag	UNP C3W5S1

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	N	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	O	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	R	3	Total	C	N	O	0	0	0
			46	25	2	19			
3	S	3	Total	C	N	O	0	0	0
			46	25	2	19			

- Molecule 4 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galacto pyranose.



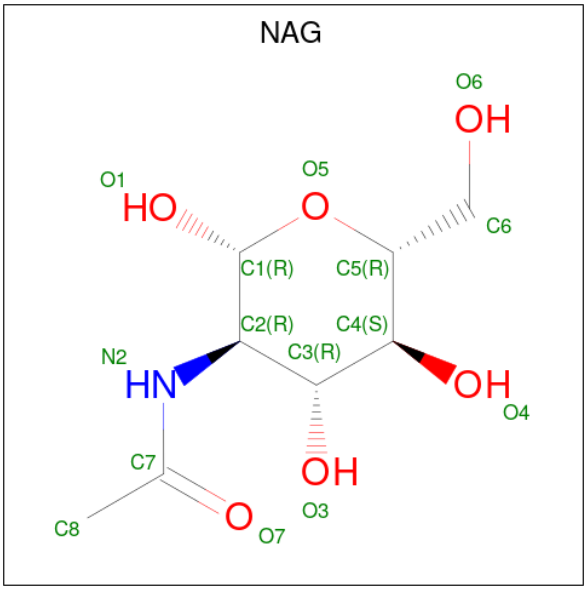
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	2	Total	C	N	O	0	0	0
			31	17	1	13			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is water.

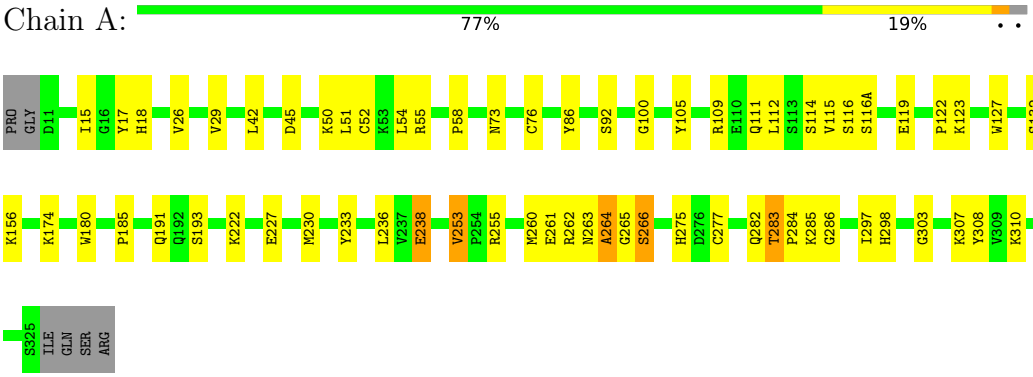
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	55	Total O 55 55	0	0
7	B	28	Total O 28 28	0	0
7	C	60	Total O 60 60	0	0
7	D	31	Total O 31 31	0	0
7	E	33	Total O 33 33	0	0
7	F	22	Total O 22 22	0	0
7	G	63	Total O 63 63	0	0
7	H	27	Total O 27 27	0	0
7	I	44	Total O 44 44	0	0
7	J	36	Total O 36 36	0	0
7	K	51	Total O 51 51	0	0
7	L	35	Total O 35 35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

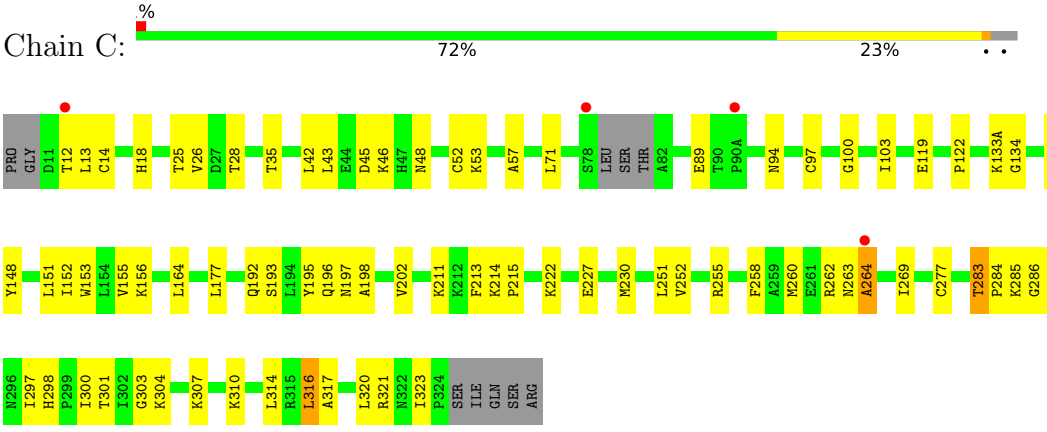
• Molecule 1: Hemagglutinin HA1

Chain A:



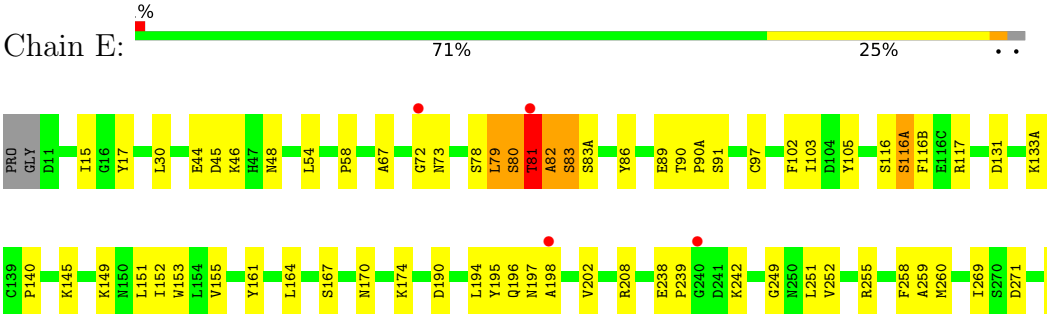
• Molecule 1: Hemagglutinin HA1

Chain C:



• Molecule 1: Hemagglutinin HA1

Chain E:

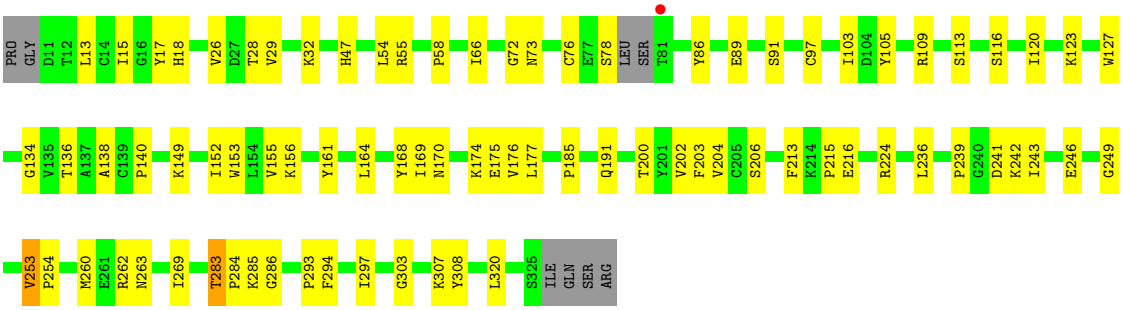




• Molecule 1: Hemagglutinin HA1

Chain G:

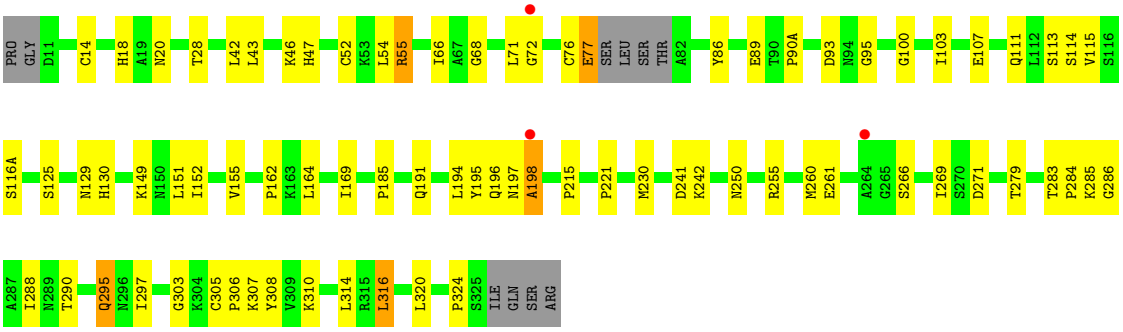




• Molecule 1: Hemagglutinin HA1

Chain I:

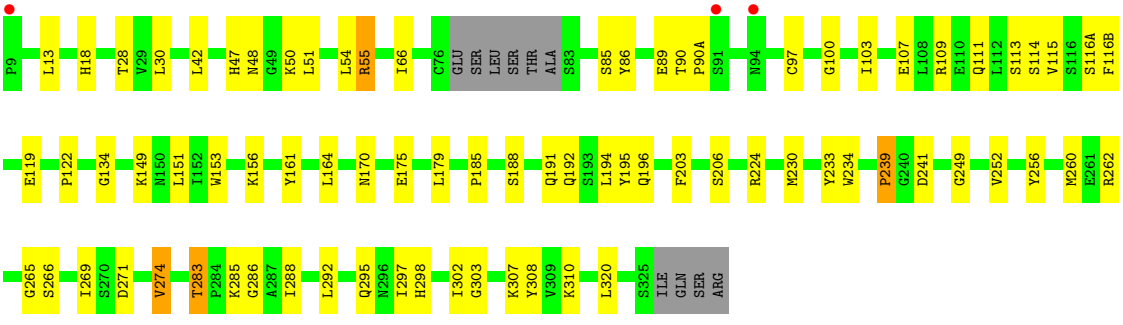




• Molecule 1: Hemagglutinin HA1

Chain K:

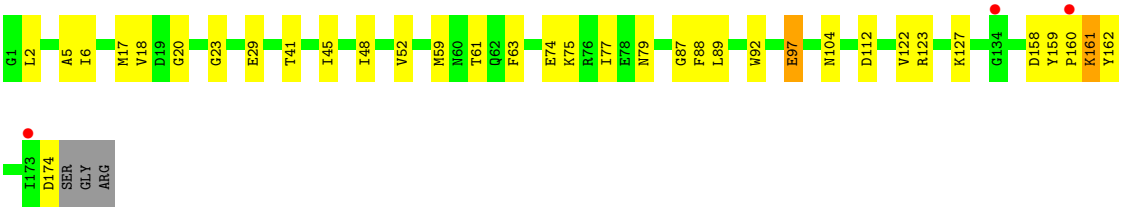




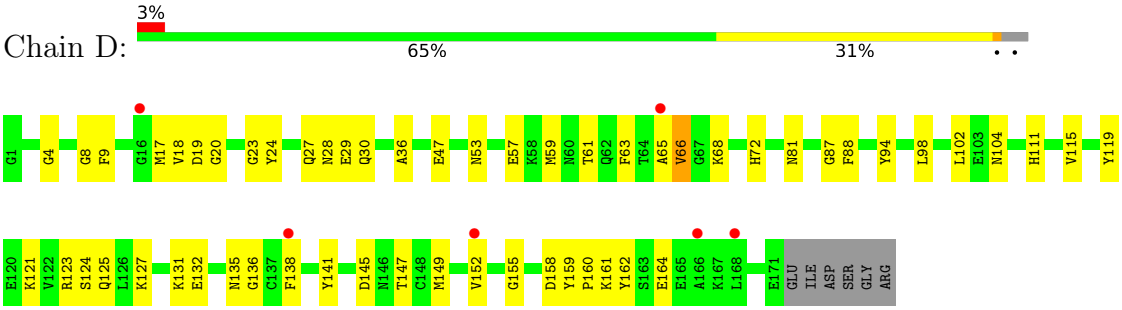
• Molecule 2: Hemagglutinin HA2

Chain B:

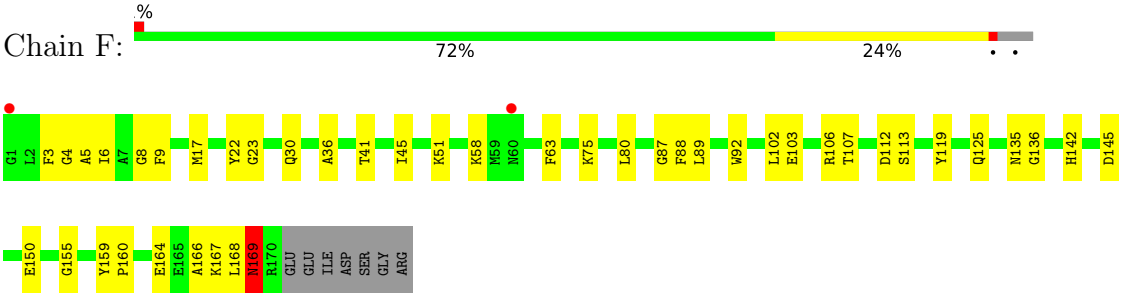




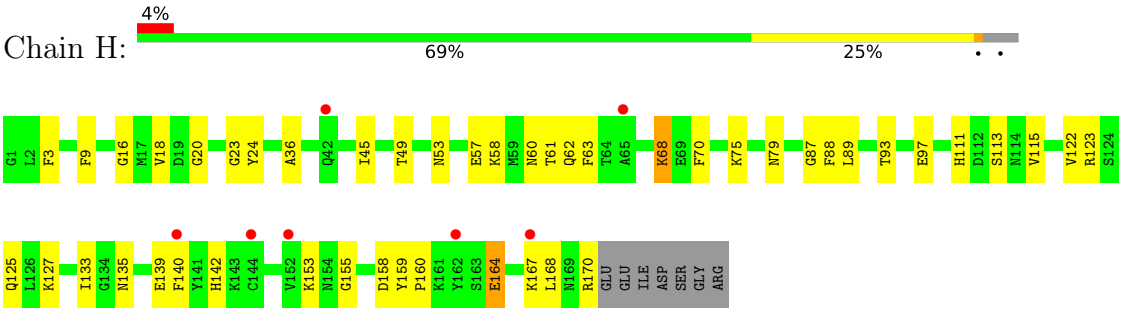
• Molecule 2: Hemagglutinin HA2



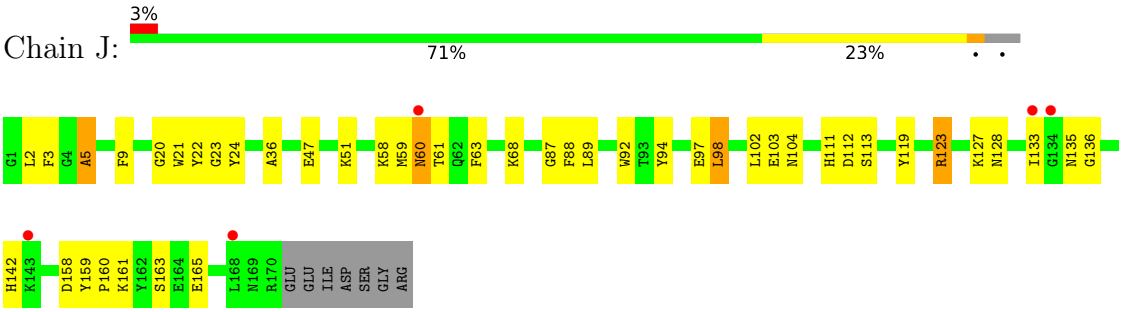
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

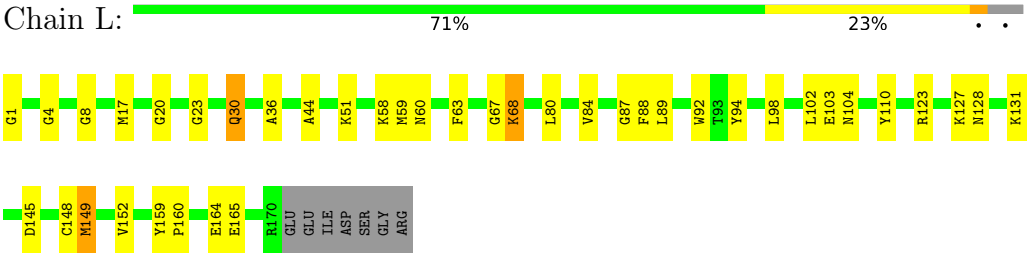


• Molecule 2: Hemagglutinin HA2



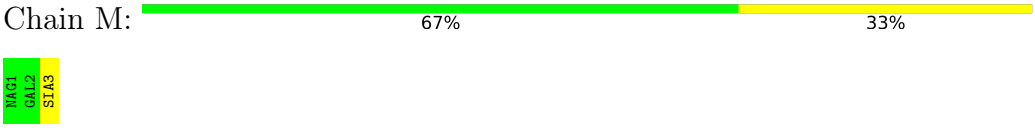
• Molecule 2: Hemagglutinin HA2

Chain L:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



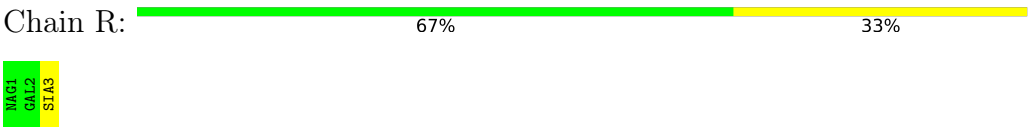
• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 4: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose

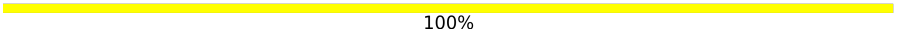
Chain P:





• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.00Å 116.71Å 119.66Å 60.61° 77.05° 80.38°	Depositor
Resolution (Å)	49.68 – 2.51 49.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.68-2.51) 94.2 (49.68-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.6.2_432	Depositor
R, R_{free}	0.205 , 0.253 0.202 , 0.248	Depositor DCC
R_{free} test set	4909 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	24203	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.26	0/2586	0.70	0/3516
1	C	0.26	0/2558	0.69	0/3476
1	E	0.26	0/2586	0.73	2/3516 (0.1%)
1	G	0.27	0/2571	0.70	0/3494
1	I	0.27	0/2558	0.72	1/3476 (0.0%)
1	K	0.26	0/2556	0.71	0/3473
2	B	0.26	0/1433	0.64	0/1931
2	D	0.26	0/1408	0.63	0/1897
2	F	0.27	0/1399	0.64	0/1885
2	H	0.26	0/1399	0.65	1/1885 (0.1%)
2	J	0.27	0/1399	0.66	0/1885
2	L	0.27	0/1399	0.66	0/1885
All	All	0.26	0/23852	0.69	4/32319 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	20	ASN	N-CA-C	6.17	116.74	108.23
2	H	127	LYS	CB-CA-C	-5.70	110.02	116.63
1	E	82	ALA	CA-C-N	5.28	131.21	121.70
1	E	82	ALA	C-N-CA	5.28	131.21	121.70

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	A	2522	0	2464	52	0
1	C	2495	0	2437	53	0
1	E	2522	0	2467	76	0
1	G	2508	0	2450	57	0
1	I	2495	0	2439	55	0
1	K	2492	0	2438	55	0
2	B	1405	0	1324	30	0
2	D	1380	0	1303	46	0
2	F	1371	0	1297	33	0
2	H	1371	0	1297	39	0
2	J	1371	0	1296	37	0
2	L	1371	0	1297	33	0
3	M	46	0	40	0	0
3	N	46	0	40	1	0
3	O	46	0	40	2	0
3	R	46	0	40	0	0
3	S	46	0	40	1	0
4	P	31	0	26	0	0
5	Q	28	0	25	2	0
6	A	56	0	52	0	0
6	C	28	0	26	1	0
6	E	14	0	13	1	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
7	A	55	0	0	1	0
7	B	28	0	0	0	0
7	C	60	0	0	1	0
7	D	31	0	0	0	0
7	E	33	0	0	0	0
7	F	22	0	0	1	0
7	G	63	0	0	0	0
7	H	27	0	0	0	0
7	I	44	0	0	0	0
7	J	36	0	0	1	0
7	K	51	0	0	0	0
7	L	35	0	0	1	0
All	All	24203	0	22877	491	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 11.

All (491) 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:E:79:LEU:HA	1:E:80:SER:CB	1.81	1.10
1:E:79:LEU:HA	1:E:80:SER:HB3	1.26	1.10
2:J:59:MET:HA	2:J:60:ASN:HB3	1.03	1.03
1:E:82:ALA:HB3	1:E:83:SER:HB2	1.41	1.00
2:J:59:MET:HA	2:J:60:ASN:CB	1.91	0.97
2:J:59:MET:CA	2:J:60:ASN:HB3	1.94	0.96
1:E:79:LEU:CA	1:E:80:SER:HB3	2.02	0.89
1:E:82:ALA:CB	1:E:83:SER:HB2	2.02	0.88
1:E:283:THR:HG22	1:E:285:LYS:H	1.37	0.87
2:H:97:GLU:HG2	2:L:58:LYS:HD2	1.57	0.87
1:I:283:THR:HG22	1:I:285:LYS:H	1.38	0.87
1:G:283:THR:HG22	1:G:285:LYS:H	1.41	0.85
1:C:283:THR:HG22	1:C:285:LYS:H	1.42	0.84
2:H:58:LYS:HD2	2:J:97:GLU:HG2	1.58	0.83
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.62	0.81
2:F:164:GLU:O	2:F:167:LYS:HG2	1.82	0.79
1:E:298:HIS:HD2	1:E:300:ILE:H	1.30	0.79
1:A:283:THR:HG22	1:A:285:LYS:H	1.45	0.79
1:E:72:GLY:HA3	1:E:149:LYS:H	1.48	0.77
1:A:283:THR:HB	1:A:286:GLY:O	1.87	0.75
2:H:62:GLN:HE21	1:I:310:LYS:HZ3	1.32	0.75
1:I:283:THR:HB	1:I:286:GLY:O	1.87	0.74
2:H:24:TYR:CE1	2:H:153:LYS:HG3	2.22	0.74
1:C:260:MET:HE2	1:C:262:ARG:HG2	1.71	0.72
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.73	0.71
1:E:190:ASP:O	1:E:194:LEU:HB2	1.92	0.69
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.74	0.69
1:K:114:SER:HB2	1:K:266:SER:HB2	1.75	0.69
2:H:167:LYS:HG3	2:H:170:ARG:HH12	1.59	0.68
1:K:283:THR:HG23	1:K:285:LYS:H	1.59	0.67
1:C:25:THR:HG22	1:C:35:THR:HG22	1.77	0.67
2:H:167:LYS:HG3	2:H:170:ARG:NH1	2.10	0.67
1:G:283:THR:HB	1:G:286:GLY:O	1.94	0.66
1:I:303:GLY:HA2	2:J:63:PHE:CE1	2.30	0.66
1:K:13:LEU:HB2	2:L:149:MET:HE1	1.76	0.66
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.75	0.66
2:L:131:LYS:NZ	2:L:133:ILE:HG22	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.78	0.66
1:E:298:HIS:CD2	1:E:300:ILE:H	2.12	0.65
2:H:62:GLN:NE2	1:I:310:LYS:HZ3	1.95	0.65
1:E:72:GLY:HA3	1:E:149:LYS:N	2.12	0.65
2:J:9:PHE:O	2:J:135:ASN:HA	1.96	0.65
1:K:307:LYS:HG3	2:L:92:TRP:CE2	2.32	0.64
1:E:174:LYS:HE3	1:E:259:ALA:HB1	1.79	0.64
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.33	0.64
1:I:89:GLU:O	1:I:269:ILE:HA	1.98	0.64
2:H:53:ASN:O	2:H:57:GLU:HG2	1.97	0.64
2:D:161:LYS:HD2	2:D:162:TYR:CZ	2.34	0.63
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.64	0.63
1:E:283:THR:HB	1:E:286:GLY:O	1.99	0.62
1:K:114:SER:HB2	1:K:266:SER:CB	2.29	0.62
2:B:75:LYS:NZ	2:B:79:ASN:HD21	1.98	0.61
1:I:28:THR:HG22	2:J:104:ASN:HB3	1.80	0.61
1:K:170:ASN:HB3	1:K:239:PRO:O	2.00	0.61
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.83	0.61
1:E:82:ALA:CB	1:E:83:SER:CB	2.78	0.61
1:I:169:ILE:HD13	1:I:242:LYS:HB2	1.83	0.60
1:C:222:LYS:HZ3	1:C:227:GLU:HG3	1.67	0.60
1:E:80:SER:O	1:E:81:THR:HG23	2.01	0.60
1:I:54:LEU:C	1:I:55:ARG:HG3	2.25	0.60
1:C:303:GLY:HA2	2:D:63:PHE:CE1	2.36	0.60
1:E:310:LYS:HG2	2:F:89:LEU:HD11	1.83	0.60
1:C:283:THR:HB	1:C:286:GLY:O	2.02	0.59
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.83	0.59
2:H:9:PHE:O	2:H:135:ASN:HA	2.02	0.59
1:G:97:CYS:O	1:G:224:ARG:HD3	2.02	0.59
1:G:253:VAL:HG22	1:G:254:PRO:HD2	1.85	0.59
2:H:123:ARG:HH12	2:J:123:ARG:HH21	1.50	0.59
1:A:236:LEU:HD13	1:A:262:ARG:NH1	2.18	0.58
2:B:41:THR:O	2:B:45:ILE:HG13	2.02	0.58
2:D:149:MET:O	2:D:152:VAL:HG22	2.04	0.58
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.86	0.58
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.39	0.58
1:E:167:SER:OG	1:E:242:LYS:HE2	2.04	0.58
2:B:123:ARG:NH1	2:D:123:ARG:HH22	2.02	0.58
2:D:65:ALA:O	2:D:66:VAL:HG12	2.04	0.57
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.86	0.57
2:D:9:PHE:O	2:D:135:ASN:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:THR:HG23	1:G:284:PRO:HD2	1.85	0.57
1:A:174:LYS:HD2	1:A:261:GLU:HG3	1.87	0.57
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.86	0.57
1:I:115:VAL:HG12	1:I:116(A):SER:H	1.70	0.57
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.70	0.57
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.69	0.57
1:A:116:SER:HB3	1:A:263:ASN:HD21	1.70	0.56
1:E:44:GLU:OE2	1:E:46:LYS:HG2	2.06	0.56
2:J:160:PRO:HA	2:J:163:SER:OG	2.06	0.56
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.41	0.56
2:D:53:ASN:O	2:D:57:GLU:HG2	2.05	0.56
1:G:307:LYS:HE2	2:H:61:THR:HG22	1.87	0.56
2:H:123:ARG:HH12	2:J:123:ARG:NH2	2.03	0.56
1:K:303:GLY:HA2	2:L:63:PHE:CE1	2.41	0.56
1:C:214:LYS:HG3	1:C:215:PRO:HD2	1.87	0.56
1:E:151:LEU:HB3	1:E:252:VAL:HG12	1.87	0.56
1:G:13:LEU:HD11	2:H:24:TYR:HB3	1.87	0.56
1:G:127:TRP:CH2	1:G:253:VAL:HG21	2.41	0.56
1:A:260:MET:HE2	1:A:262:ARG:HG2	1.86	0.56
1:K:206:SER:HB2	1:K:241:ASP:OD2	2.06	0.56
1:E:79:LEU:HA	1:E:80:SER:OG	2.04	0.55
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.41	0.55
1:C:140:PRO:HD2	6:C:333:NAG:H83	1.89	0.55
1:I:52:CYS:HB2	1:I:279:THR:HG22	1.88	0.55
1:C:300:ILE:HA	2:D:66:VAL:HG11	1.88	0.55
2:H:164:GLU:H	2:H:164:GLU:CD	2.14	0.55
1:G:303:GLY:HA2	2:H:63:PHE:CE1	2.41	0.55
1:K:115:VAL:HG11	1:K:116(B):PHE:HB2	1.88	0.55
1:G:200:THR:OG1	1:G:215:PRO:HG3	2.07	0.55
1:K:283:THR:HG22	1:K:286:GLY:H	1.72	0.55
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.41	0.55
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.42	0.54
1:G:170:ASN:HB3	1:G:239:PRO:O	2.07	0.54
1:C:288:ILE:HD13	1:C:295:GLN:HG3	1.90	0.54
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.89	0.54
2:L:4:GLY:O	2:L:8:GLY:HA3	2.06	0.54
1:A:111:GLN:O	1:A:262:ARG:HD2	2.07	0.54
1:I:290:THR:HG23	1:I:306:PRO:HD3	1.89	0.54
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.87	0.54
1:I:197:ASN:O	1:I:198:ALA:HB3	2.07	0.54
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:119:GLU:CD	1:K:122:PRO:HA	2.33	0.54
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.08	0.54
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.90	0.54
1:K:18:HIS:HB2	2:L:20:GLY:O	2.08	0.54
1:E:208:ARG:NH2	1:E:238:GLU:H	2.06	0.53
2:L:30:GLN:OE1	2:L:145:ASP:HB2	2.08	0.53
2:D:124:SER:O	2:D:127:LYS:HE3	2.08	0.53
1:K:107:GLU:O	1:K:111:GLN:HG3	2.08	0.53
1:E:140:PRO:HD2	6:E:333:NAG:H83	1.90	0.53
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.44	0.53
1:C:152:ILE:HD11	1:C:255:ARG:HD2	1.90	0.53
1:G:72:GLY:O	1:G:149:LYS:HG2	2.08	0.53
2:H:88:PHE:CZ	2:J:87:GLY:HA3	2.44	0.53
2:H:159:TYR:HB3	2:H:160:PRO:HD3	1.89	0.53
1:E:82:ALA:HB1	1:E:83:SER:CA	2.39	0.53
1:G:203:PHE:HD1	1:G:204:VAL:N	2.07	0.53
1:A:310:LYS:HE3	2:B:89:LEU:HD21	1.90	0.53
1:C:18:HIS:HB2	2:D:20:GLY:O	2.08	0.53
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.08	0.53
1:A:112:LEU:HD23	1:A:260:MET:HE1	1.91	0.52
1:C:301:THR:H	2:D:66:VAL:HG11	1.74	0.52
2:L:1:GLY:HA3	7:L:280:HOH:O	2.09	0.52
2:B:74:GLU:HB3	2:B:77:ILE:HD11	1.91	0.52
1:C:13:LEU:HD22	2:D:152:VAL:HG21	1.91	0.52
1:E:283:THR:HG22	1:E:285:LYS:N	2.16	0.52
2:D:17:MET:C	2:D:19:ASP:H	2.16	0.52
2:B:161:LYS:HE3	2:B:162:TYR:CE1	2.43	0.52
1:E:90(A):PRO:HD2	1:E:271:ASP:OD1	2.09	0.52
1:E:116(A):SER:O	1:E:260:MET:HA	2.09	0.52
1:A:152:ILE:HG13	1:A:255:ARG:HB2	1.90	0.52
2:D:131:LYS:HE3	2:D:141:TYR:OH	2.10	0.52
1:G:283:THR:CG2	1:G:285:LYS:HG2	2.39	0.52
1:G:47:HIS:HB3	1:G:297:ILE:HD13	1.92	0.51
1:I:76:CYS:O	1:I:77:GLU:C	2.54	0.51
1:E:72:GLY:CA	1:E:149:LYS:H	2.21	0.51
1:E:103:ILE:HD12	1:E:103:ILE:N	2.25	0.51
1:E:303:GLY:HA2	2:F:63:PHE:CE1	2.45	0.51
1:I:116(A):SER:HB3	1:I:261:GLU:HG2	1.92	0.51
1:E:164:LEU:HD12	1:E:164:LEU:C	2.36	0.51
2:H:123:ARG:HH22	2:J:123:ARG:HH22	1.58	0.51
1:A:155:VAL:HG12	1:A:156:LYS:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:PHE:CZ	2:D:87:GLY:HA3	2.46	0.51
1:C:52:CYS:HB3	1:C:277:CYS:O	2.10	0.51
2:J:47:GLU:HB3	1:K:30:LEU:HG	1.93	0.51
2:L:131:LYS:HZ2	2:L:133:ILE:HG22	1.74	0.51
1:E:195:TYR:O	1:E:196:GLN:HB3	2.11	0.51
1:K:164:LEU:C	1:K:164:LEU:HD12	2.36	0.51
1:A:116(A):SER:O	1:A:260:MET:HA	2.11	0.51
2:L:127:LYS:HG3	2:L:128:ASN:H	1.75	0.51
1:E:170:ASN:HB3	1:E:239:PRO:O	2.11	0.51
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.46	0.51
1:I:164:LEU:HD12	1:I:164:LEU:C	2.36	0.51
2:J:58:LYS:O	2:L:94:TYR:HD1	1.94	0.51
2:L:44:ALA:HA	2:L:110:TYR:OH	2.11	0.51
1:C:45:ASP:C	1:C:297:ILE:HD11	2.36	0.50
1:E:308:TYR:CD2	2:F:89:LEU:HD13	2.45	0.50
1:A:307:LYS:HE2	2:B:61:THR:HG22	1.93	0.50
2:D:59:MET:HG3	2:D:61:THR:HG23	1.93	0.50
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.46	0.50
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.92	0.50
1:A:50:LYS:HG2	1:A:275:HIS:ND1	2.27	0.50
1:C:26:VAL:HG21	1:C:317:ALA:HB2	1.94	0.50
1:E:295:GLN:O	1:E:308:TYR:HA	2.12	0.50
1:K:116(A):SER:O	1:K:260:MET:HA	2.12	0.50
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.46	0.50
1:C:28:THR:HG22	2:D:104:ASN:HB3	1.94	0.49
1:C:89:GLU:O	1:C:269:ILE:HA	2.12	0.49
1:C:164:LEU:C	1:C:164:LEU:HD12	2.37	0.49
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.76	0.49
1:G:89:GLU:O	1:G:269:ILE:HA	2.12	0.49
2:B:59:MET:HE1	2:B:92:TRP:CH2	2.47	0.49
1:E:117:ARG:HD3	1:E:258:PHE:CE1	2.47	0.49
1:I:114:SER:HB2	1:I:266:SER:HB2	1.94	0.49
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.93	0.49
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.13	0.49
1:E:131:ASP:HB3	1:E:155:VAL:HG23	1.95	0.49
2:J:158:ASP:CG	2:J:161:LYS:HB2	2.38	0.49
1:C:304:LYS:HE2	2:D:61:THR:O	2.12	0.49
1:E:82:ALA:HB1	1:E:83:SER:HA	1.94	0.49
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.94	0.49
1:K:47:HIS:HB3	1:K:297:ILE:HD13	1.94	0.49
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:LEU:N	1:E:320:LEU:HD23	2.27	0.49
1:K:86:TYR:HA	1:K:113:SER:O	2.12	0.49
1:C:283:THR:HG23	1:C:284:PRO:HD2	1.93	0.49
1:I:42:LEU:HD11	1:I:316:LEU:HG	1.95	0.49
1:K:66:ILE:HD12	1:K:109:ARG:HG2	1.95	0.49
2:H:87:GLY:HA3	2:L:88:PHE:CZ	2.48	0.48
1:E:152:ILE:HG13	1:E:255:ARG:HB2	1.96	0.48
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.48	0.48
1:A:265:GLY:O	1:A:266:SER:HB3	2.12	0.48
1:C:103:ILE:N	1:C:103:ILE:HD12	2.28	0.48
2:D:94:TYR:CZ	2:D:98:LEU:HD11	2.49	0.48
1:E:152:ILE:HD11	1:E:255:ARG:HD2	1.94	0.48
2:F:17:MET:SD	2:F:23:GLY:HA3	2.53	0.48
2:F:125:GLN:NE2	2:F:155:GLY:HA2	2.28	0.48
2:F:169:ASN:OD1	2:F:169:ASN:N	2.43	0.48
1:K:28:THR:HG22	2:L:104:ASN:HB3	1.96	0.48
2:D:125:GLN:CD	2:D:155:GLY:HA2	2.39	0.48
1:E:82:ALA:CB	1:E:83:SER:CA	2.91	0.48
1:E:103:ILE:HD12	1:E:103:ILE:H	1.77	0.48
1:I:307:LYS:HE2	2:J:61:THR:HG22	1.96	0.48
1:K:156:LYS:HD2	1:K:196:GLN:HE21	1.79	0.48
5:Q:1:NAG:H62	5:Q:2:NAG:H82	1.96	0.48
2:B:75:LYS:HZ2	2:B:79:ASN:HD21	1.61	0.48
2:F:6:ILE:HG13	2:F:112:ASP:HA	1.95	0.48
1:I:130:HIS:CE1	1:I:164:LEU:HB3	2.49	0.48
2:B:17:MET:SD	2:B:23:GLY:HA3	2.54	0.48
1:E:137:ALA:O	1:E:140:PRO:HD3	2.14	0.48
1:C:45:ASP:O	1:C:46:LYS:HD2	2.14	0.48
1:E:283:THR:CG2	1:E:285:LYS:H	2.19	0.48
1:G:105:TYR:CZ	1:G:109:ARG:HD2	2.49	0.47
2:H:75:LYS:HE3	2:H:79:ASN:HD21	1.79	0.47
1:I:68:GLY:HA3	1:I:95:GLY:HA2	1.95	0.47
2:F:159:TYR:N	2:F:160:PRO:HD2	2.29	0.47
1:G:103:ILE:HD12	1:G:103:ILE:N	2.28	0.47
2:H:45:ILE:O	2:H:49:THR:HG23	2.14	0.47
1:I:18:HIS:HB2	2:J:20:GLY:O	2.14	0.47
1:I:71:LEU:HD22	1:I:151:LEU:HD11	1.96	0.47
1:K:48:ASN:O	1:K:50:LYS:HG3	2.14	0.47
1:A:105:TYR:CE2	1:A:109:ARG:HD2	2.50	0.47
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.48	0.47
1:G:293:PRO:HG2	1:G:294:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:GLY:HA3	1:I:230:MET:O	2.14	0.47
1:G:18:HIS:HB2	2:H:20:GLY:O	2.14	0.47
1:G:202:VAL:HB	1:G:213:PHE:HB2	1.96	0.47
1:I:130:HIS:CE1	1:I:162:PRO:HG2	2.49	0.47
1:A:73:ASN:HB3	1:A:76:CYS:SG	2.55	0.47
1:G:164:LEU:C	1:G:164:LEU:HD23	2.39	0.47
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.29	0.47
1:E:82:ALA:HB1	1:E:83:SER:CB	2.44	0.47
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.14	0.47
1:C:156:LYS:HE2	1:C:193:SER:O	2.15	0.47
1:G:78:SER:HB2	1:G:149:LYS:NZ	2.29	0.47
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.14	0.47
1:I:68:GLY:CA	1:I:95:GLY:HA2	2.44	0.47
2:J:94:TYR:O	2:J:98:LEU:HB2	2.15	0.47
2:H:133:ILE:HD13	2:H:139:GLU:HB2	1.97	0.47
1:C:316:LEU:HD22	7:C:335:HOH:O	2.14	0.47
1:I:129:ASN:HB3	1:I:162:PRO:HG3	1.97	0.47
1:C:100:GLY:HA3	1:C:230:MET:O	2.15	0.47
1:I:66:ILE:HG13	1:I:89:GLU:OE2	2.14	0.47
1:K:66:ILE:HG13	1:K:89:GLU:OE2	2.15	0.47
1:C:151:LEU:HB3	1:C:252:VAL:HG12	1.98	0.46
1:C:202:VAL:HB	1:C:213:PHE:HB2	1.95	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.95	0.46
1:I:107:GLU:O	1:I:111:GLN:HG3	2.16	0.46
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.50	0.46
1:K:54:LEU:HB3	1:K:85:SER:HB2	1.95	0.46
2:B:161:LYS:HE3	2:B:162:TYR:CZ	2.50	0.46
2:F:106:ARG:HD3	7:F:427:HOH:O	2.15	0.46
1:G:164:LEU:O	1:G:246:GLU:HA	2.15	0.46
1:I:288:ILE:HG21	1:I:297:ILE:HD12	1.97	0.46
1:A:54:LEU:O	1:A:55:ARG:HB2	2.14	0.46
2:J:5:ALA:HB3	2:J:112:ASP:OD2	2.16	0.46
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.97	0.46
1:E:89:GLU:O	1:E:269:ILE:HA	2.15	0.46
1:G:216:GLU:HB3	1:K:203:PHE:HE2	1.79	0.46
1:G:308:TYR:CD2	2:H:89:LEU:HD13	2.51	0.46
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.51	0.46
2:D:145:ASP:OD2	2:D:147:THR:HG22	2.16	0.46
1:C:195:TYR:O	1:C:196:GLN:HB3	2.14	0.46
1:G:175:GLU:OE1	1:G:236:LEU:HD13	2.16	0.46
2:H:125:GLN:OE1	2:H:155:GLY:HA2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.51	0.46
2:D:164:GLU:CD	2:D:164:GLU:H	2.24	0.46
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.46
1:A:320:LEU:HD23	1:A:320:LEU:H	1.81	0.46
2:F:9:PHE:O	2:F:135:ASN:HA	2.16	0.46
1:C:298:HIS:CE1	1:C:300:ILE:HB	2.51	0.45
1:K:185:PRO:HG2	1:K:191:GLN:OE1	2.16	0.45
1:A:123:LYS:HE2	1:A:132:SER:O	2.16	0.45
1:C:12:THR:OG1	2:D:27:GLN:HG2	2.16	0.45
1:G:73:ASN:HB3	1:G:76:CYS:SG	2.56	0.45
1:I:47:HIS:HB3	1:I:288:ILE:HG22	1.98	0.45
2:B:97:GLU:HG2	2:F:58:LYS:CD	2.42	0.45
1:E:317:ALA:O	2:F:107:THR:HG21	2.15	0.45
2:H:168:LEU:HD23	2:H:168:LEU:O	2.16	0.45
1:E:197:ASN:O	1:E:198:ALA:HB3	2.17	0.45
2:F:30:GLN:NE2	2:F:145:ASP:HB2	2.30	0.45
1:E:46:LYS:N	1:E:297:ILE:HD11	2.31	0.45
2:L:148:CYS:O	2:L:152:VAL:HG23	2.17	0.45
1:A:238:GLU:H	1:A:238:GLU:HG2	1.54	0.45
1:C:71:LEU:O	1:C:148:TYR:HB3	2.16	0.45
2:D:30:GLN:CD	2:D:30:GLN:C	2.84	0.45
1:E:164:LEU:HD12	1:E:164:LEU:O	2.17	0.45
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.97	0.45
1:G:320:LEU:HB3	2:H:111:HIS:CG	2.52	0.45
2:L:159:TYR:N	2:L:160:PRO:HD2	2.30	0.45
1:A:18:HIS:HB2	2:B:20:GLY:O	2.16	0.45
2:J:159:TYR:N	2:J:160:PRO:HD2	2.32	0.45
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.98	0.45
1:C:177:LEU:HB3	1:C:258:PHE:HB2	1.99	0.45
1:I:86:TYR:HA	1:I:113:SER:O	2.17	0.45
1:K:51:LEU:HB2	1:K:274:VAL:HA	1.99	0.45
2:L:149:MET:HE2	2:L:149:MET:HA	1.99	0.45
1:A:180:TRP:CE2	1:A:233:TYR:HB2	2.51	0.45
1:C:53:LYS:HG2	1:C:57:ALA:HA	1.98	0.45
2:J:127:LYS:HG2	2:J:128:ASN:N	2.32	0.45
2:D:125:GLN:NE2	2:D:155:GLY:HA2	2.32	0.45
1:G:116:SER:HB3	1:G:263:ASN:OD1	2.16	0.45
2:L:51:LYS:HE3	2:L:103:GLU:OE2	2.17	0.45
1:C:45:ASP:C	1:C:46:LYS:HD2	2.42	0.44
1:E:45:ASP:C	1:E:297:ILE:HD11	2.41	0.44
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:LYS:HE2	1:K:256:TYR:HE1	1.82	0.44
1:A:238:GLU:HG2	7:A:352:HOH:O	2.17	0.44
1:G:66:ILE:HG13	1:G:89:GLU:OE2	2.17	0.44
1:I:195:TYR:O	1:I:196:GLN:HB3	2.18	0.44
1:K:151:LEU:HB3	1:K:252:VAL:HG12	1.99	0.44
1:A:45:ASP:C	1:A:297:ILE:HD11	2.42	0.44
1:E:320:LEU:HD23	1:E:320:LEU:H	1.82	0.44
1:G:97:CYS:HB2	1:G:138:ALA:O	2.16	0.44
2:J:59:MET:CA	2:J:60:ASN:CB	2.69	0.44
1:I:114:SER:HB2	1:I:266:SER:CB	2.47	0.44
1:K:103:ILE:HG12	1:K:233:TYR:CE2	2.52	0.44
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.53	0.44
2:L:127:LYS:HG3	2:L:128:ASN:N	2.33	0.44
1:C:43:LEU:HB2	1:C:314:LEU:HB2	2.00	0.44
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.53	0.44
1:G:169:ILE:N	1:G:169:ILE:HD12	2.33	0.44
2:L:67:GLY:O	2:L:68:LYS:HE3	2.18	0.44
1:A:156:LYS:HE2	1:A:193:SER:O	2.17	0.44
1:C:119:GLU:CD	1:C:122:PRO:HA	2.43	0.44
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.47	0.44
2:H:123:ARG:HH22	2:J:123:ARG:NH2	2.15	0.44
1:I:316:LEU:HD22	7:J:189:HOH:O	2.17	0.44
1:A:51:LEU:HA	1:A:282:GLN:NE2	2.32	0.44
1:A:114:SER:HB2	1:A:266:SER:CB	2.48	0.44
2:H:3:PHE:CZ	2:J:2:LEU:HG	2.53	0.44
1:E:288:ILE:HD11	1:E:306:PRO:HD2	1.99	0.44
1:I:116(A):SER:HB3	1:I:261:GLU:CG	2.48	0.44
2:L:133:ILE:HD13	2:L:139:GLU:HB2	2.00	0.44
2:D:18:VAL:O	2:D:18:VAL:HG22	2.18	0.43
1:K:54:LEU:O	1:K:55:ARG:HG3	2.18	0.43
1:K:97:CYS:O	1:K:224:ARG:HD3	2.19	0.43
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.54	0.43
1:A:114:SER:OG	1:A:263:ASN:HB2	2.19	0.43
1:E:145:LYS:NZ	3:O:3:SIA:H31	2.32	0.43
1:I:185:PRO:HG2	1:I:191:GLN:OE1	2.19	0.43
1:I:305:CYS:O	2:J:61:THR:HG21	2.18	0.43
1:K:175:GLU:OE1	1:K:262:ARG:NH1	2.48	0.43
1:E:15:ILE:HD12	1:E:15:ILE:N	2.32	0.43
1:E:67:ALA:HB2	1:E:105:TYR:CE1	2.53	0.43
1:G:54:LEU:O	1:G:55:ARG:HB2	2.17	0.43
2:H:68:LYS:HB3	2:H:70:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:LYS:O	2:D:125:GLN:HG3	2.18	0.43
1:E:102:PHE:O	1:E:105:TYR:HB2	2.18	0.43
1:A:308:TYR:CD2	2:B:89:LEU:HD13	2.54	0.43
1:C:263:ASN:O	1:C:264:ALA:C	2.61	0.43
2:D:81:ASN:OD1	2:F:80:LEU:HD13	2.19	0.43
1:E:133(A):LYS:O	3:O:3:SIA:H113	2.19	0.43
2:J:51:LYS:HE3	2:J:103:GLU:OE2	2.19	0.43
1:A:26:VAL:HB	2:B:104:ASN:ND2	2.34	0.43
1:A:255:ARG:HH22	1:G:91:SER:HG	1.66	0.43
2:B:127:LYS:HB2	2:B:159:TYR:CE1	2.53	0.43
2:D:4:GLY:O	2:D:8:GLY:HA3	2.19	0.43
2:F:3:PHE:CE1	2:F:113:SER:HB2	2.53	0.43
1:K:179:LEU:HD23	1:K:234:TRP:HB3	2.01	0.43
1:K:283:THR:OG1	1:K:298:HIS:HB3	2.18	0.43
1:G:120:ILE:HG13	1:G:168:TYR:CD1	2.53	0.43
1:G:206:SER:HA	1:I:221:PRO:HG2	2.01	0.43
1:K:89:GLU:O	1:K:269:ILE:HA	2.18	0.43
1:K:283:THR:HG22	1:K:286:GLY:O	2.19	0.43
1:E:90:THR:C	1:E:91:SER:H	2.27	0.43
2:H:93:THR:O	2:H:97:GLU:HB2	2.19	0.43
2:J:3:PHE:CE2	2:J:113:SER:HB2	2.53	0.43
1:K:54:LEU:HD21	1:K:302:ILE:HG22	2.01	0.43
2:D:131:LYS:HB3	2:D:141:TYR:CZ	2.54	0.42
2:F:75:LYS:HD3	2:F:75:LYS:HA	1.79	0.42
1:I:241:ASP:OD1	1:I:242:LYS:N	2.50	0.42
1:A:52:CYS:HB3	1:A:277:CYS:O	2.18	0.42
1:A:263:ASN:O	1:A:264:ALA:C	2.61	0.42
1:G:155:VAL:HG12	1:G:156:LYS:N	2.34	0.42
2:H:16:GLY:O	2:H:18:VAL:HG23	2.20	0.42
1:I:308:TYR:CD2	2:J:89:LEU:HD13	2.54	0.42
1:K:288:ILE:O	1:K:288:ILE:HG13	2.18	0.42
1:A:127:TRP:CZ2	1:A:253:VAL:HG11	2.54	0.42
1:C:14:CYS:O	2:D:24:TYR:HA	2.19	0.42
1:C:307:LYS:HE2	2:D:61:THR:HG22	2.00	0.42
2:F:41:THR:O	2:F:45:ILE:HG13	2.19	0.42
1:G:253:VAL:HA	1:G:254:PRO:HD3	1.93	0.42
1:I:72:GLY:HA3	1:I:149:LYS:H	1.85	0.42
1:I:116(A):SER:O	1:I:260:MET:HA	2.20	0.42
1:K:100:GLY:HA3	1:K:230:MET:O	2.19	0.42
1:K:288:ILE:HG21	1:K:297:ILE:HD12	2.00	0.42
1:I:14:CYS:O	2:J:24:TYR:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:HG22	2:B:18:VAL:O	2.19	0.42
1:C:197:ASN:O	1:C:198:ALA:HB3	2.18	0.42
1:G:86:TYR:HA	1:G:113:SER:O	2.18	0.42
1:G:262:ARG:HG2	1:G:262:ARG:NH1	2.32	0.42
2:H:140:PHE:C	2:H:142:HIS:H	2.28	0.42
1:K:149:LYS:HE2	1:K:256:TYR:CE1	2.55	0.42
1:K:194:LEU:HD11	3:S:3:SIA:H91	2.00	0.42
1:C:321:ARG:HD2	1:C:323:ILE:HD11	2.01	0.42
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.19	0.42
2:L:164:GLU:CD	2:L:165:GLU:H	2.27	0.42
1:K:188:SER:O	1:K:192:GLN:HG2	2.20	0.42
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.55	0.42
1:E:17:TYR:HB2	1:E:320:LEU:HD11	2.02	0.42
1:G:170:ASN:HD21	1:G:176:VAL:HG23	1.85	0.42
2:H:53:ASN:C	2:H:57:GLU:HG2	2.44	0.42
1:I:46:LYS:N	1:I:297:ILE:HD11	2.35	0.42
2:B:48:ILE:O	2:B:52:VAL:HG23	2.20	0.42
1:G:242:LYS:HG2	1:G:243:ILE:N	2.35	0.42
1:I:155:VAL:HG13	1:I:194:LEU:O	2.20	0.42
2:J:60:ASN:O	2:J:60:ASN:CG	2.63	0.42
2:L:17:MET:SD	2:L:23:GLY:HA3	2.60	0.42
1:A:42:LEU:HD11	1:A:316:LEU:HD22	2.01	0.41
2:D:27:GLN:O	2:D:27:GLN:HG3	2.20	0.41
1:K:42:LEU:O	1:K:292:LEU:HB3	2.20	0.41
2:D:28:ASN:C	2:D:30:GLN:H	2.28	0.41
2:F:51:LYS:HE3	2:F:103:GLU:OE2	2.20	0.41
1:G:241:ASP:CG	1:G:242:LYS:H	2.28	0.41
1:I:72:GLY:C	1:I:149:LYS:H	2.28	0.41
1:I:152:ILE:HG13	1:I:255:ARG:HB2	2.02	0.41
1:K:103:ILE:N	1:K:103:ILE:HD12	2.35	0.41
1:K:195:TYR:O	1:K:196:GLN:HB3	2.20	0.41
2:L:131:LYS:HZ1	2:L:133:ILE:HG22	1.86	0.41
1:I:43:LEU:HB2	1:I:314:LEU:HB2	2.02	0.41
1:I:90(A):PRO:HD2	1:I:271:ASP:CG	2.46	0.41
1:K:283:THR:CG2	1:K:285:LYS:H	2.31	0.41
2:D:111:HIS:O	2:D:115:VAL:HG23	2.20	0.41
1:E:83(A):SER:CB	1:E:116:SER:HA	2.50	0.41
1:G:29:VAL:CG2	2:L:51:LYS:HG3	2.51	0.41
1:A:222:LYS:HE2	1:A:227:GLU:HG3	2.03	0.41
1:E:310:LYS:HD3	2:F:89:LEU:HD21	2.03	0.41
2:F:5:ALA:HB3	2:F:112:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:140:PRO:HD2	5:Q:1:NAG:H83	2.02	0.41
1:C:164:LEU:HD12	1:C:164:LEU:O	2.20	0.41
1:E:116(B):PHE:CE1	1:E:260:MET:HE2	2.56	0.41
1:G:17:TYR:HB3	2:H:115:VAL:HG21	2.02	0.41
1:G:155:VAL:CG1	1:G:156:LYS:N	2.83	0.41
1:I:215:PRO:HB3	1:I:250:ASN:ND2	2.35	0.41
1:C:211:LYS:HD3	1:C:213:PHE:CZ	2.55	0.41
2:F:142:HIS:HD2	2:F:166:ALA:HB2	1.85	0.41
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.03	0.41
1:E:97:CYS:HB2	1:E:138:ALA:O	2.21	0.41
2:F:167:LYS:HG3	2:F:168:LEU:HD12	2.02	0.41
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.56	0.41
1:K:47:HIS:HB3	1:K:288:ILE:HG22	2.03	0.41
1:A:119:GLU:CD	1:A:122:PRO:HA	2.46	0.41
1:A:265:GLY:O	1:A:266:SER:CB	2.69	0.41
2:B:158:ASP:CG	2:B:161:LYS:HB3	2.46	0.41
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.36	0.41
2:D:72:HIS:H	2:D:72:HIS:CD2	2.39	0.41
1:E:72:GLY:O	1:E:73:ASN:C	2.63	0.41
1:G:26:VAL:O	1:G:32:LYS:O	2.38	0.41
1:G:177:LEU:HB2	1:G:260:MET:HE3	2.03	0.41
2:J:21:TRP:CE3	2:J:111:HIS:HE1	2.39	0.41
1:K:310:LYS:O	1:K:310:LYS:HG2	2.21	0.41
1:C:97:CYS:HB2	1:C:138:ALA:O	2.22	0.41
1:I:295:GLN:HE21	1:I:295:GLN:HB3	1.73	0.41
1:A:284:PRO:HG2	1:A:298:HIS:CE1	2.56	0.40
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.84	0.40
2:D:125:GLN:O	2:D:127:LYS:HD2	2.21	0.40
1:G:123:LYS:HB2	1:G:152:ILE:HD11	2.03	0.40
2:L:80:LEU:O	2:L:84:VAL:HG23	2.20	0.40
1:K:134:GLY:HA3	1:K:153:TRP:HB3	2.04	0.40
1:A:29:VAL:CG2	2:F:51:LYS:HG3	2.52	0.40
1:A:100:GLY:HA3	1:A:230:MET:O	2.20	0.40
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.74	0.40
2:H:3:PHE:CE1	2:H:113:SER:HB2	2.57	0.40
2:J:142:HIS:HB2	2:J:165:GLU:CD	2.47	0.40
2:L:123:ARG:HB2	2:L:138:PHE:HZ	1.86	0.40
1:I:103:ILE:HD12	1:I:103:ILE:N	2.37	0.40
1:K:90:THR:HA	1:K:90(A):PRO:HD3	1.97	0.40
1:K:90(A):PRO:HD2	1:K:271:ASP:OD1	2.21	0.40
2:L:149:MET:HA	2:L:149:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:VAL:HG21	1:A:317:ALA:HB2	2.03	0.40
1:C:133(A):LYS:O	3:N:3:SIA:H113	2.21	0.40
1:E:298:HIS:CG	1:E:299:PRO:HD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	321/329 (98%)	300 (94%)	18 (6%)	3 (1%)	14 27
1	C	315/329 (96%)	300 (95%)	13 (4%)	2 (1%)	21 38
1	E	321/329 (98%)	294 (92%)	22 (7%)	5 (2%)	7 14
1	G	317/329 (96%)	301 (95%)	16 (5%)	0	100 100
1	I	315/329 (96%)	291 (92%)	21 (7%)	3 (1%)	12 24
1	K	315/329 (96%)	297 (94%)	16 (5%)	2 (1%)	21 38
2	B	172/177 (97%)	167 (97%)	5 (3%)	0	100 100
2	D	169/177 (96%)	156 (92%)	13 (8%)	0	100 100
2	F	168/177 (95%)	157 (94%)	10 (6%)	1 (1%)	21 38
2	H	168/177 (95%)	159 (95%)	9 (5%)	0	100 100
2	J	168/177 (95%)	158 (94%)	8 (5%)	2 (1%)	10 20
2	L	168/177 (95%)	161 (96%)	5 (3%)	2 (1%)	10 20
All	All	2917/3036 (96%)	2741 (94%)	156 (5%)	20 (1%)	18 34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	60	ASN

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Mol	Chain	Res	Type
1	C	264	ALA
1	E	80	SER
1	I	93	ASP
1	K	265	GLY
1	A	266	SER
1	C	94	ASN
1	E	78	SER
1	E	83	SER
1	E	116(A)	SER
1	I	198	ALA
2	J	5	ALA
1	A	92	SER
1	A	264	ALA
2	F	169	ASN
1	I	324	PRO
1	K	239	PRO
2	L	60	ASN
1	E	81	THR
2	L	59	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/290 (98%)	280 (98%)	5 (2%)	51	77
1	C	281/290 (97%)	275 (98%)	6 (2%)	47	74
1	E	285/290 (98%)	278 (98%)	7 (2%)	42	69
1	G	283/290 (98%)	278 (98%)	5 (2%)	51	77
1	I	281/290 (97%)	275 (98%)	6 (2%)	47	74
1	K	281/290 (97%)	276 (98%)	5 (2%)	51	77
2	B	150/152 (99%)	146 (97%)	4 (3%)	39	67
2	D	147/152 (97%)	143 (97%)	4 (3%)	39	67
2	F	146/152 (96%)	142 (97%)	4 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	H	146/152 (96%)	143 (98%)	3 (2%)	47 74
2	J	146/152 (96%)	140 (96%)	6 (4%)	27 53
2	L	146/152 (96%)	141 (97%)	5 (3%)	32 60
All	All	2577/2652 (97%)	2517 (98%)	60 (2%)	44 72

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	A	238	GLU
1	A	253	VAL
1	A	283	THR
1	A	320	LEU
2	B	29	GLU
2	B	97	GLU
2	B	161	LYS
2	B	174	ASP
1	C	155	VAL
1	C	192	GLN
1	C	283	THR
1	C	295	GLN
1	C	316	LEU
1	C	320	LEU
2	D	29	GLU
2	D	66	VAL
2	D	68	LYS
2	D	102	LEU
1	E	54	LEU
1	E	79	LEU
1	E	81	THR
1	E	274	VAL
1	E	280	THR
1	E	283	THR
1	E	320	LEU
2	F	22	TYR
2	F	102	LEU
2	F	150	GLU
2	F	169	ASN
1	G	28	THR
1	G	136	THR
1	G	174	LYS

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Mol	Chain	Res	Type
1	G	253	VAL
1	G	283	THR
2	H	60	ASN
2	H	68	LYS
2	H	164	GLU
1	I	55	ARG
1	I	77	GLU
1	I	125	SER
1	I	295	GLN
1	I	316	LEU
1	I	320	LEU
2	J	22	TYR
2	J	68	LYS
2	J	98	LEU
2	J	102	LEU
2	J	123	ARG
2	J	133	ILE
1	K	55	ARG
1	K	274	VAL
1	K	283	THR
1	K	295	GLN
1	K	320	LEU
2	L	30	GLN
2	L	68	LYS
2	L	98	LEU
2	L	102	LEU
2	L	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	A	263	ASN
1	A	298	HIS
2	B	25	HIS
2	B	26	HIS
2	B	43	ASN
2	B	79	ASN
2	D	25	HIS
1	E	150	ASN
1	E	278	ASN
1	E	298	HIS

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Mol	Chain	Res	Type
2	F	30	GLN
2	F	60	ASN
2	F	142	HIS
1	G	159	ASN
2	H	43	ASN
2	H	60	ASN
2	H	62	GLN
2	H	128	ASN
2	H	142	HIS
1	I	21	ASN
1	I	130	HIS
1	I	275	HIS
1	I	278	ASN
1	I	289	ASN
2	J	30	GLN
2	J	95	ASN
2	J	117	ASN
1	K	159	ASN
1	K	196	GLN
2	L	62	GLN
2	L	95	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

19 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	$\#\|Z\|>2$
3	NAG	M	1	3	15,15,15	0.44	0	21,21,21	0.58	0
3	GAL	M	2	3	11,11,12	0.70	0	15,15,17	0.69	0
3	SIA	M	3	3	20,20,21	0.61	0	21,28,31	1.01	1 (4%)
3	NAG	N	1	3	15,15,15	0.49	0	21,21,21	0.60	0
3	GAL	N	2	3	11,11,12	0.67	0	15,15,17	0.69	0
3	SIA	N	3	3	20,20,21	0.60	0	21,28,31	0.99	3 (14%)
3	NAG	O	1	3	15,15,15	0.46	0	21,21,21	0.73	0
3	GAL	O	2	3	11,11,12	0.62	0	15,15,17	0.57	0
3	SIA	O	3	3	20,20,21	0.58	0	21,28,31	0.95	3 (14%)
4	GAL	P	1	4	11,11,12	0.62	0	15,15,17	0.45	0
4	SIA	P	2	4	20,20,21	0.57	0	21,28,31	0.98	3 (14%)
5	NAG	Q	1	1,5	14,14,15	0.57	0	17,19,21	0.71	0
5	NAG	Q	2	5	14,14,15	0.56	0	17,19,21	0.68	0
3	NAG	R	1	3	15,15,15	0.50	0	21,21,21	0.67	0
3	GAL	R	2	3	11,11,12	0.64	0	15,15,17	0.58	0
3	SIA	R	3	3	20,20,21	0.62	0	21,28,31	1.03	2 (9%)
3	NAG	S	1	3	15,15,15	0.46	0	21,21,21	0.99	1 (4%)
3	GAL	S	2	3	11,11,12	0.66	0	15,15,17	0.75	1 (6%)
3	SIA	S	3	3	20,20,21	0.63	0	21,28,31	1.05	3 (14%)

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
3	NAG	M	1	3	-	0/6/26/26	0/1/1/1
3	GAL	M	2	3	-	0/2/19/22	0/1/1/1
3	SIA	M	3	3	-	0/18/34/38	0/1/1/1
3	NAG	N	1	3	-	0/6/26/26	0/1/1/1
3	GAL	N	2	3	-	0/2/19/22	0/1/1/1
3	SIA	N	3	3	-	0/18/34/38	0/1/1/1
3	NAG	O	1	3	-	0/6/26/26	0/1/1/1
3	GAL	O	2	3	-	0/2/19/22	0/1/1/1
3	SIA	O	3	3	-	0/18/34/38	0/1/1/1
4	GAL	P	1	4	-	0/2/19/22	0/1/1/1
4	SIA	P	2	4	-	0/18/34/38	0/1/1/1
5	NAG	Q	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GAL	R	2	3	-	0/2/19/22	0/1/1/1
3	SIA	R	3	3	-	0/18/34/38	0/1/1/1
3	NAG	S	1	3	-	0/6/26/26	0/1/1/1
3	GAL	S	2	3	-	1/2/19/22	0/1/1/1
3	SIA	S	3	3	-	0/18/34/38	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	1	NAG	O5-C1-C2	2.75	112.28	109.52
3	R	3	SIA	O6-C2-C3	2.68	114.17	110.56
3	M	3	SIA	O1B-C1-C2	2.39	118.94	112.71
3	N	3	SIA	O1B-C1-C2	2.38	118.91	112.71
3	R	3	SIA	O1B-C1-C2	2.36	118.84	112.71
4	P	2	SIA	O1B-C1-C2	2.35	118.83	112.71
3	S	3	SIA	O1B-C1-C2	2.34	118.79	112.71
3	O	3	SIA	O1B-C1-C2	2.26	118.58	112.71
3	S	3	SIA	O1A-C1-C2	-2.24	118.00	122.85
3	N	3	SIA	O6-C2-C3	2.15	113.45	110.56
3	O	3	SIA	O6-C2-C3	2.12	113.40	110.56
4	P	2	SIA	O6-C2-C3	2.12	113.40	110.56
3	O	3	SIA	O1A-C1-C2	-2.10	118.31	122.85
4	P	2	SIA	O1A-C1-C2	-2.04	118.45	122.85
3	S	2	GAL	C1-O5-C5	-2.03	109.47	112.19
3	S	3	SIA	O6-C2-C3	2.02	113.28	110.56
3	N	3	SIA	O1A-C1-C2	-2.01	118.51	122.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	Q	2	NAG	C8-C7-N2-C2
5	Q	2	NAG	O7-C7-N2-C2
3	S	2	GAL	C4-C5-C6-O6

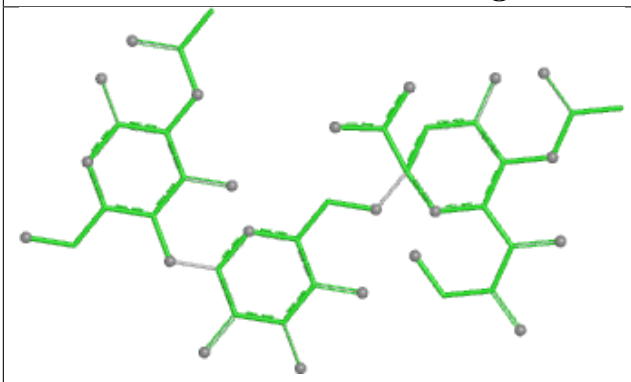
There are no ring outliers.

5 monomers are involved in 6 short contacts:

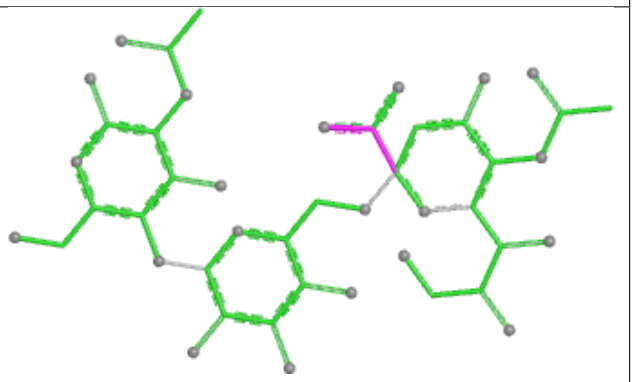
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Q	2	NAG	1	0
3	N	3	SIA	1	0
3	S	3	SIA	1	0
5	Q	1	NAG	2	0
3	O	3	SIA	2	0

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

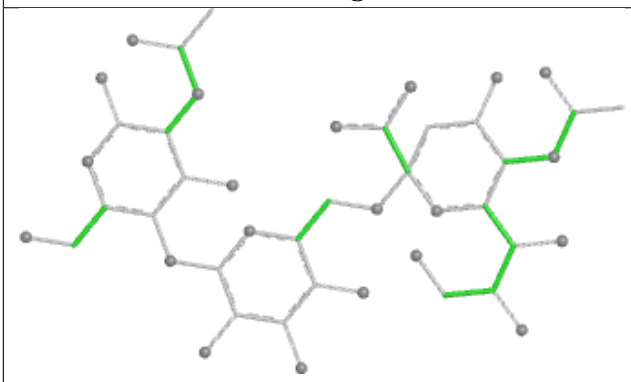
Oligosaccharide Chain M



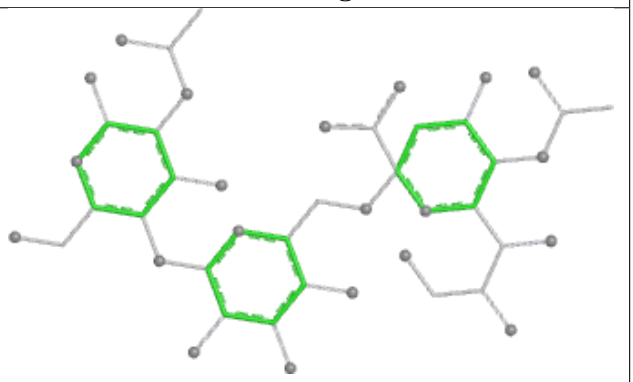
Bond lengths



Bond angles

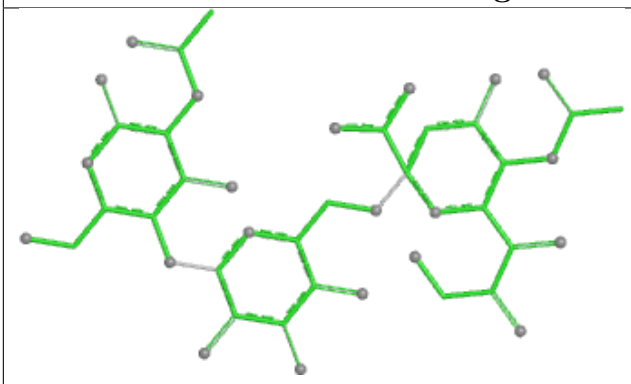


Torsions

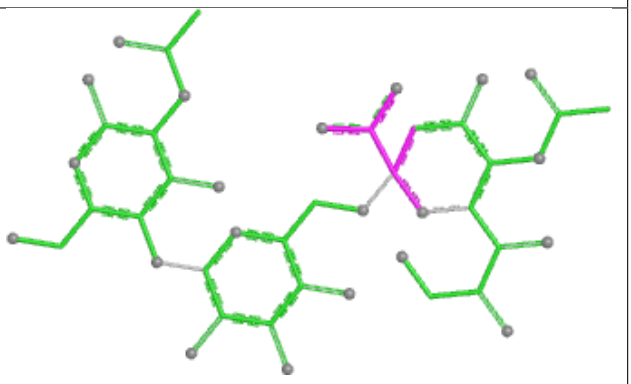


Rings

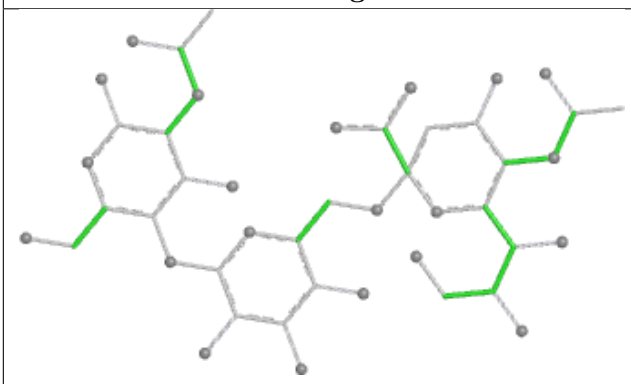
Oligosaccharide Chain N



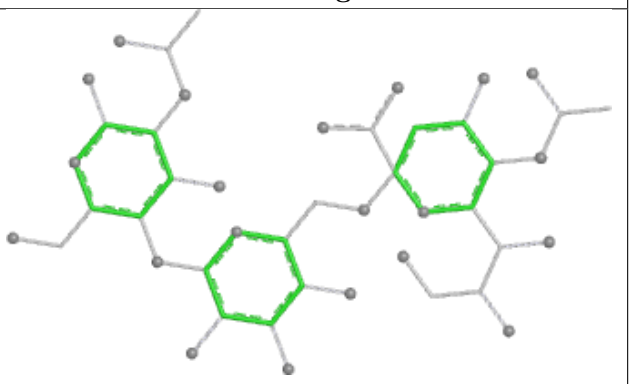
Bond lengths



Bond angles

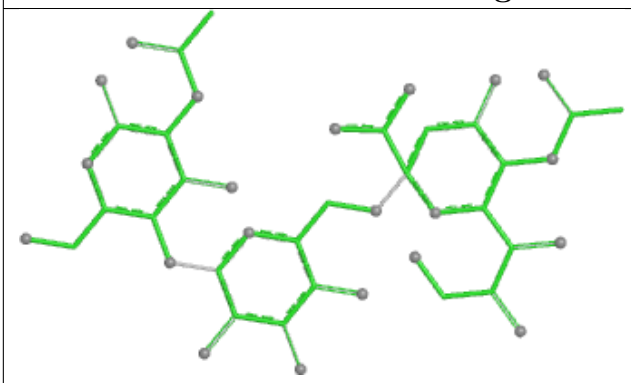


Torsions

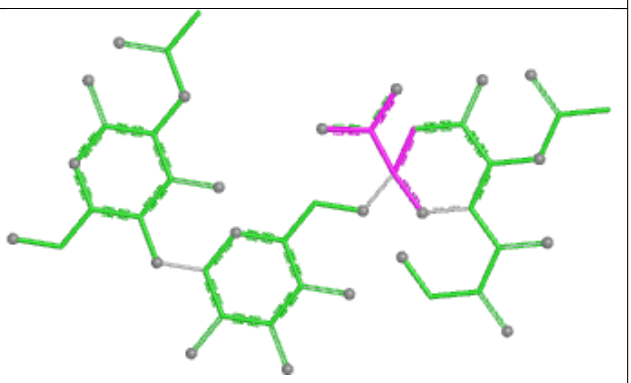


Rings

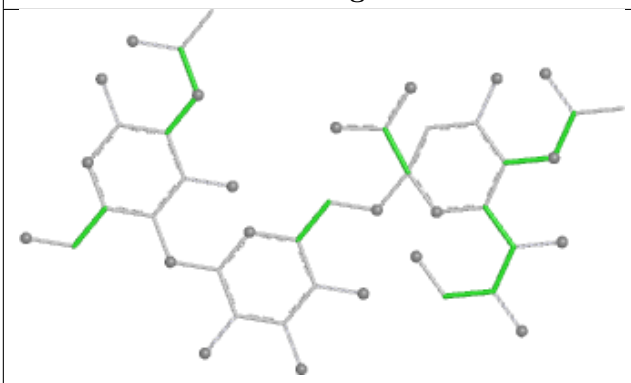
Oligosaccharide Chain O



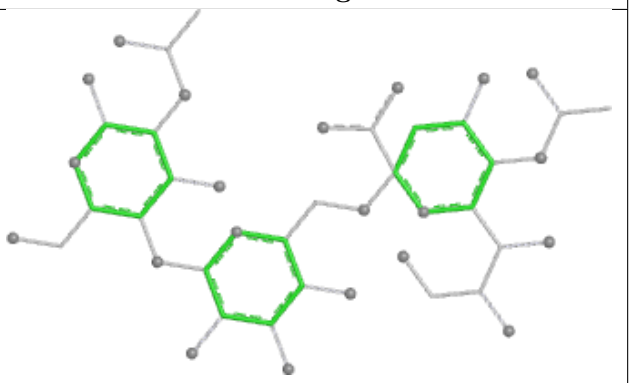
Bond lengths



Bond angles

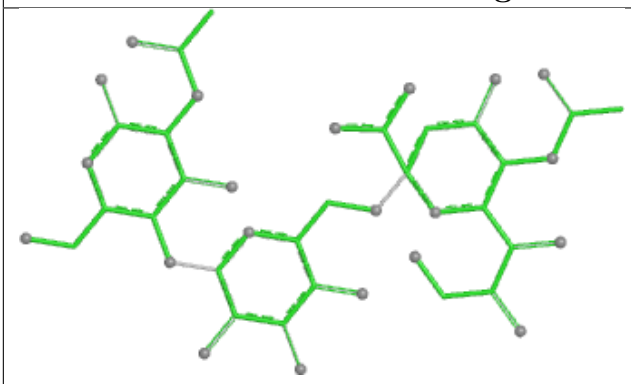


Torsions

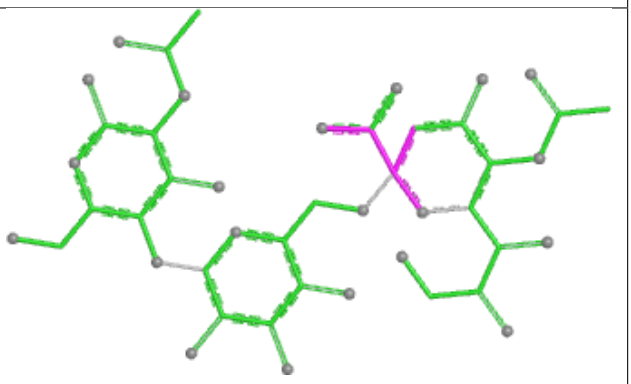


Rings

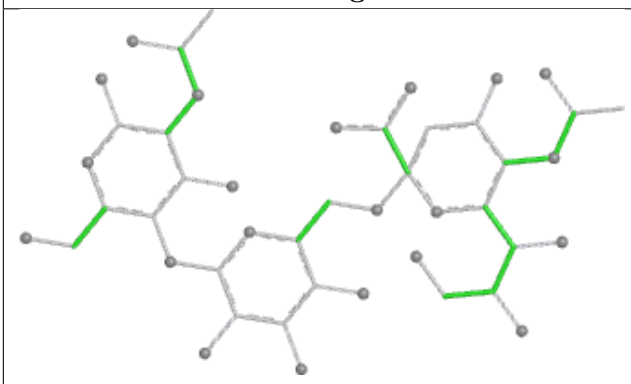
Oligosaccharide Chain R



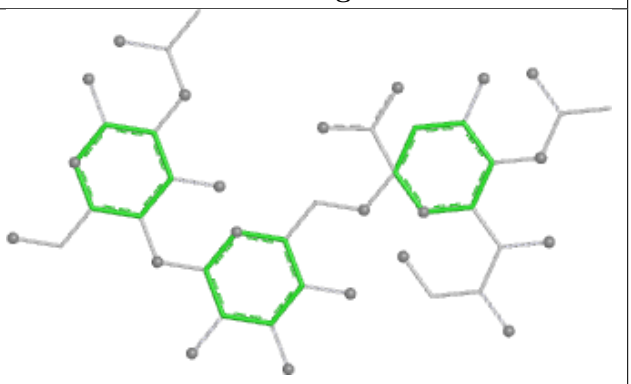
Bond lengths



Bond angles

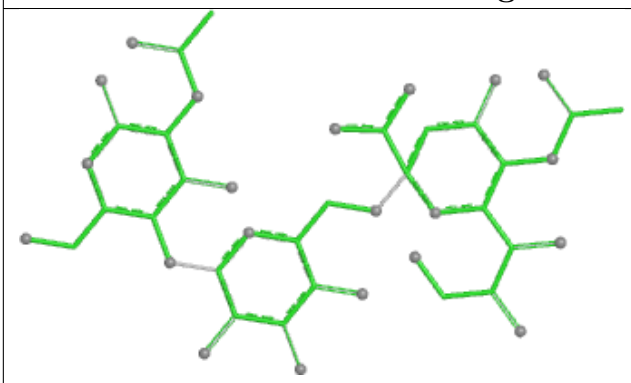


Torsions

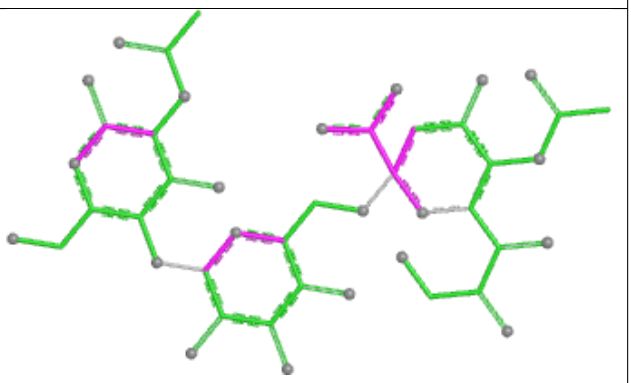


Rings

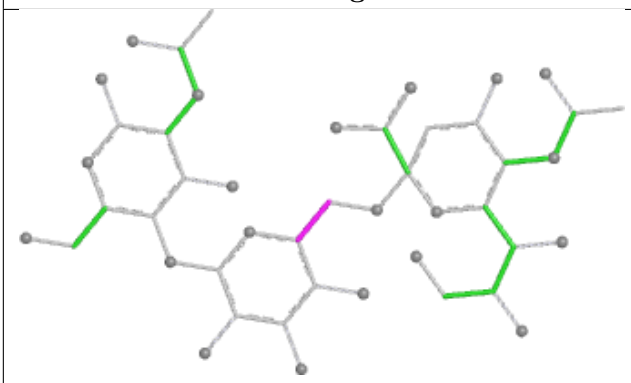
Oligosaccharide Chain S



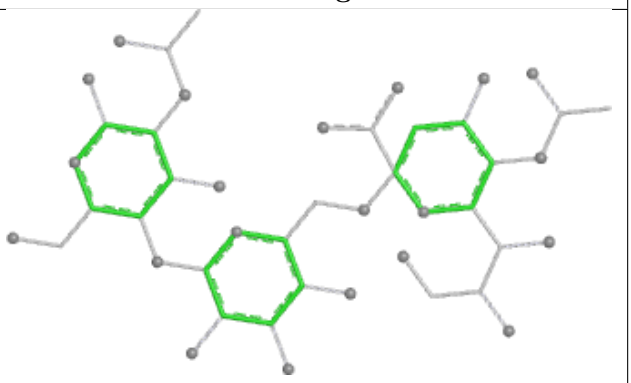
Bond lengths



Bond angles

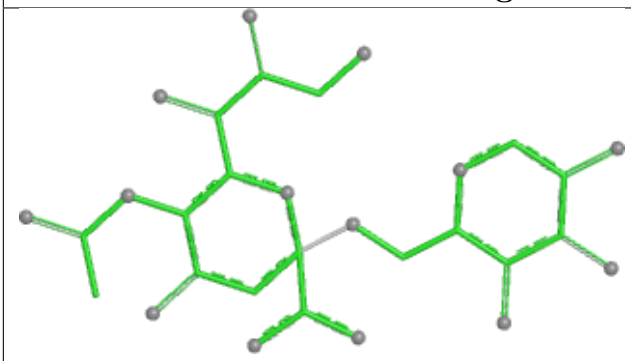


Torsions

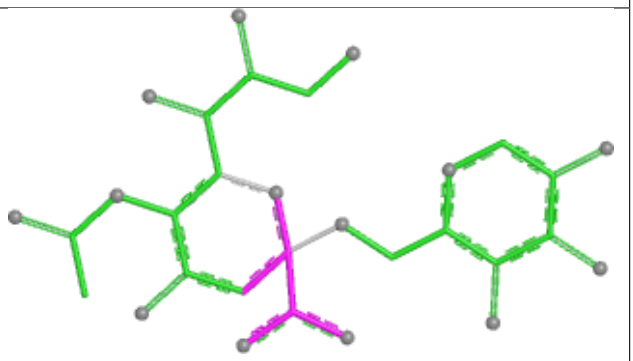


Rings

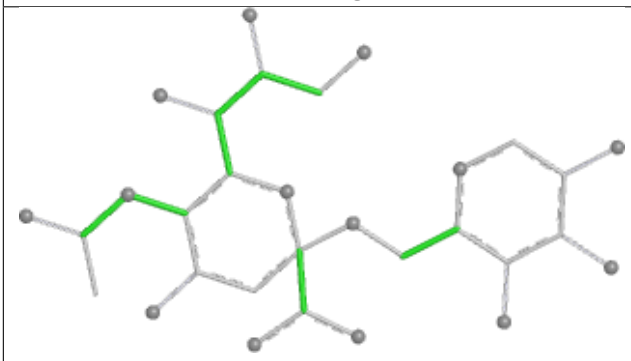
Oligosaccharide Chain P



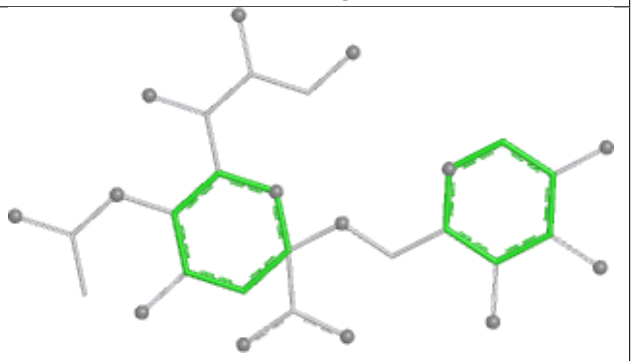
Bond lengths



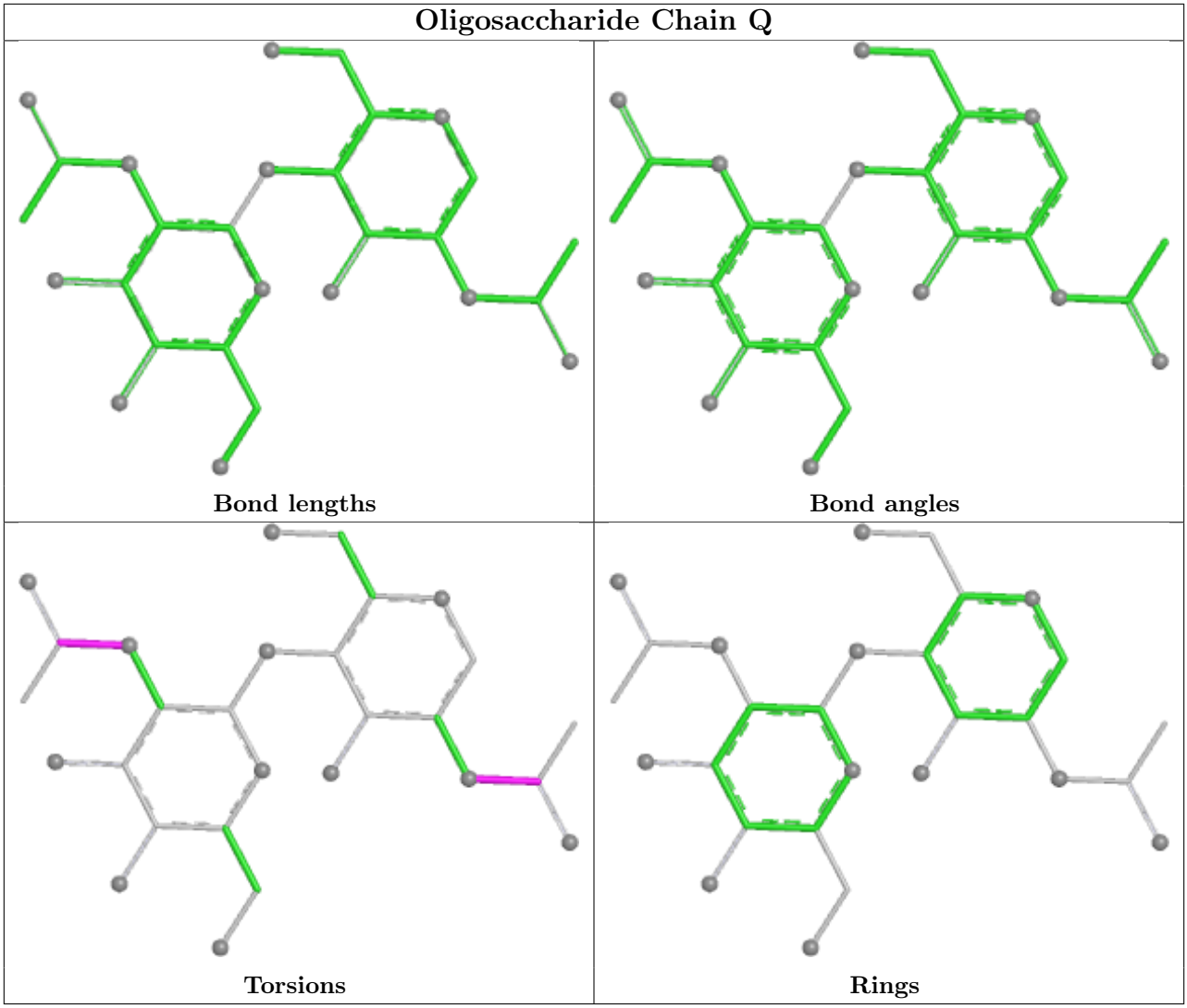
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
6	NAG	C	334	1	14,14,15	0.51	0	17,19,21	0.66	0
6	NAG	A	333	1	14,14,15	0.53	0	17,19,21	0.80	0
6	NAG	E	333	1	14,14,15	0.53	0	17,19,21	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	A	334	1	14,14,15	0.50	0	17,19,21	0.69	0
6	NAG	K	641	1	14,14,15	0.49	0	17,19,21	0.94	1 (5%)
6	NAG	A	335	1	14,14,15	0.49	0	17,19,21	0.80	0
6	NAG	A	336	1	14,14,15	0.48	0	17,19,21	0.99	1 (5%)
6	NAG	C	333	1	14,14,15	0.49	0	17,19,21	0.77	0
6	NAG	J	561	2	14,14,15	0.50	0	17,19,21	0.60	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
6	NAG	C	334	1	-	0/6/23/26	0/1/1/1
6	NAG	A	333	1	-	4/6/23/26	0/1/1/1
6	NAG	E	333	1	-	2/6/23/26	0/1/1/1
6	NAG	A	334	1	-	5/6/23/26	0/1/1/1
6	NAG	K	641	1	-	0/6/23/26	0/1/1/1
6	NAG	A	335	1	-	0/6/23/26	0/1/1/1
6	NAG	A	336	1	-	5/6/23/26	0/1/1/1
6	NAG	C	333	1	-	1/6/23/26	0/1/1/1
6	NAG	J	561	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	336	NAG	C1-O5-C5	2.09	114.99	112.19
6	K	641	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	334	NAG	C3-C2-N2-C7
6	A	334	NAG	C8-C7-N2-C2
6	A	334	NAG	O7-C7-N2-C2
6	A	333	NAG	C8-C7-N2-C2
6	A	336	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	333	NAG	O7-C7-N2-C2
6	A	336	NAG	C8-C7-N2-C2
6	J	561	NAG	C8-C7-N2-C2
6	A	336	NAG	O7-C7-N2-C2
6	J	561	NAG	O7-C7-N2-C2
6	E	333	NAG	C8-C7-N2-C2
6	C	333	NAG	O5-C5-C6-O6
6	E	333	NAG	O7-C7-N2-C2
6	A	333	NAG	C4-C5-C6-O6
6	A	336	NAG	C4-C5-C6-O6
6	A	334	NAG	C4-C5-C6-O6
6	A	333	NAG	O5-C5-C6-O6
6	A	334	NAG	O5-C5-C6-O6
6	A	336	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	333	NAG	1	0
6	C	333	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.

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	323/329 (98%)	0.08	0 100 100	30, 44, 60, 79	0
1	C	319/329 (96%)	-0.00	4 (1%) 75 71	30, 41, 60, 85	0
1	E	323/329 (98%)	0.25	4 (1%) 76 73	35, 49, 67, 88	0
1	G	321/329 (97%)	0.02	1 (0%) 90 87	28, 41, 61, 83	0
1	I	319/329 (96%)	0.16	3 (0%) 81 78	32, 46, 62, 81	0
1	K	319/329 (96%)	0.07	3 (0%) 81 78	28, 42, 60, 85	0
2	B	174/177 (98%)	0.36	3 (1%) 69 65	34, 58, 80, 95	0
2	D	171/177 (96%)	0.46	6 (3%) 47 42	30, 57, 90, 103	0
2	F	170/177 (96%)	0.40	2 (1%) 76 73	32, 55, 94, 105	0
2	H	170/177 (96%)	0.48	7 (4%) 41 37	31, 51, 88, 98	0
2	J	170/177 (96%)	0.27	5 (2%) 53 49	31, 49, 69, 81	0
2	L	170/177 (96%)	0.09	0 100 100	30, 46, 62, 69	0
All	All	2949/3036 (97%)	0.18	38 (1%) 75 71	28, 46, 79, 105	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	9	PRO	4.2
1	I	198	ALA	3.4
2	B	173	ILE	3.3
2	H	144	CYS	3.2
1	K	94	ASN	3.1
1	I	72	GLY	3.0
2	J	134	GLY	2.8
1	E	240	GLY	2.7
2	D	152	VAL	2.7
2	D	16	GLY	2.7
1	E	81	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	152	VAL	2.6
2	H	65	ALA	2.6
1	C	78	SER	2.5
2	J	143	LYS	2.5
2	J	168	LEU	2.5
1	I	264	ALA	2.4
2	F	60	ASN	2.4
2	H	167	LYS	2.4
2	J	133	ILE	2.4
1	C	264	ALA	2.4
2	H	42	GLN	2.3
2	B	160	PRO	2.3
2	H	140	PHE	2.2
1	G	81	THR	2.2
1	E	198	ALA	2.2
1	C	12	THR	2.2
1	E	72	GLY	2.2
2	B	134	GLY	2.2
2	D	168	LEU	2.2
1	K	91	SER	2.1
2	D	166	ALA	2.1
2	J	60	ASN	2.1
2	D	65	ALA	2.1
2	F	1	GLY	2.0
1	C	90(A)	PRO	2.0
2	D	138	PHE	2.0
2	H	162	TYR	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
3	NAG	S	1	15/15	0.70	0.12	58,77,81,85	0

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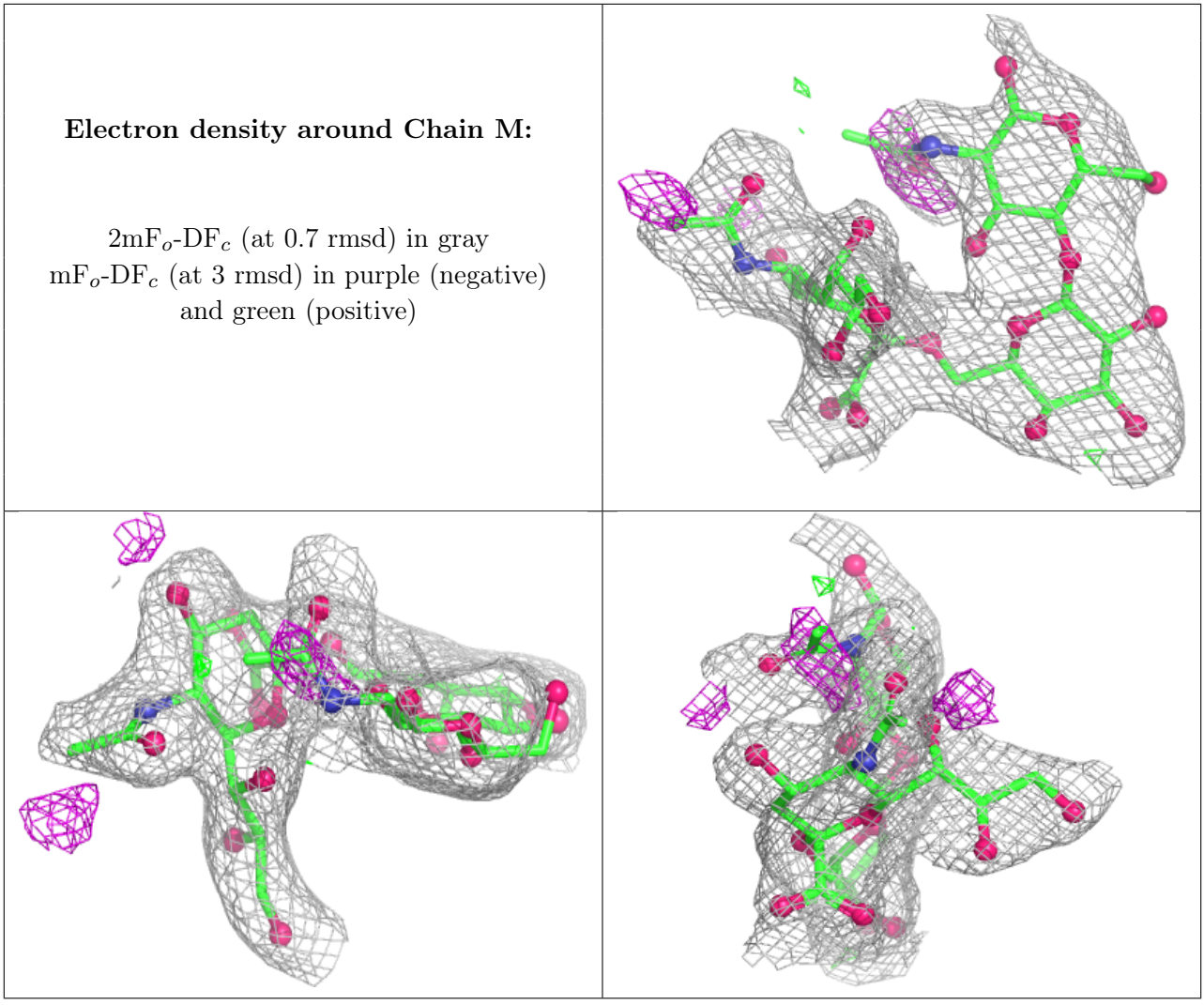
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	M	1	15/15	0.74	0.15	57,69,76,78	0
3	GAL	S	2	11/12	0.75	0.12	64,73,82,85	0
4	GAL	P	1	11/12	0.80	0.12	55,67,74,76	0
5	NAG	Q	2	14/15	0.82	0.11	48,57,64,68	0
3	NAG	N	1	15/15	0.83	0.11	47,53,64,65	0
3	NAG	O	1	15/15	0.84	0.11	55,63,66,68	0
3	GAL	M	2	11/12	0.85	0.10	49,59,66,73	0
3	NAG	R	1	15/15	0.85	0.11	45,54,65,66	0
3	GAL	R	2	11/12	0.86	0.09	48,51,56,58	0
3	GAL	N	2	11/12	0.87	0.09	44,51,54,58	0
3	GAL	O	2	11/12	0.89	0.09	51,58,61,61	0
3	SIA	S	3	20/21	0.89	0.10	47,59,66,68	0
3	SIA	O	3	20/21	0.90	0.10	49,55,62,66	0
5	NAG	Q	1	14/15	0.91	0.09	38,50,56,56	0
3	SIA	R	3	20/21	0.92	0.08	31,46,52,52	0
3	SIA	M	3	20/21	0.93	0.08	36,43,50,52	0
3	SIA	N	3	20/21	0.94	0.07	33,39,43,47	0
4	SIA	P	2	20/21	0.94	0.07	35,45,51,52	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.

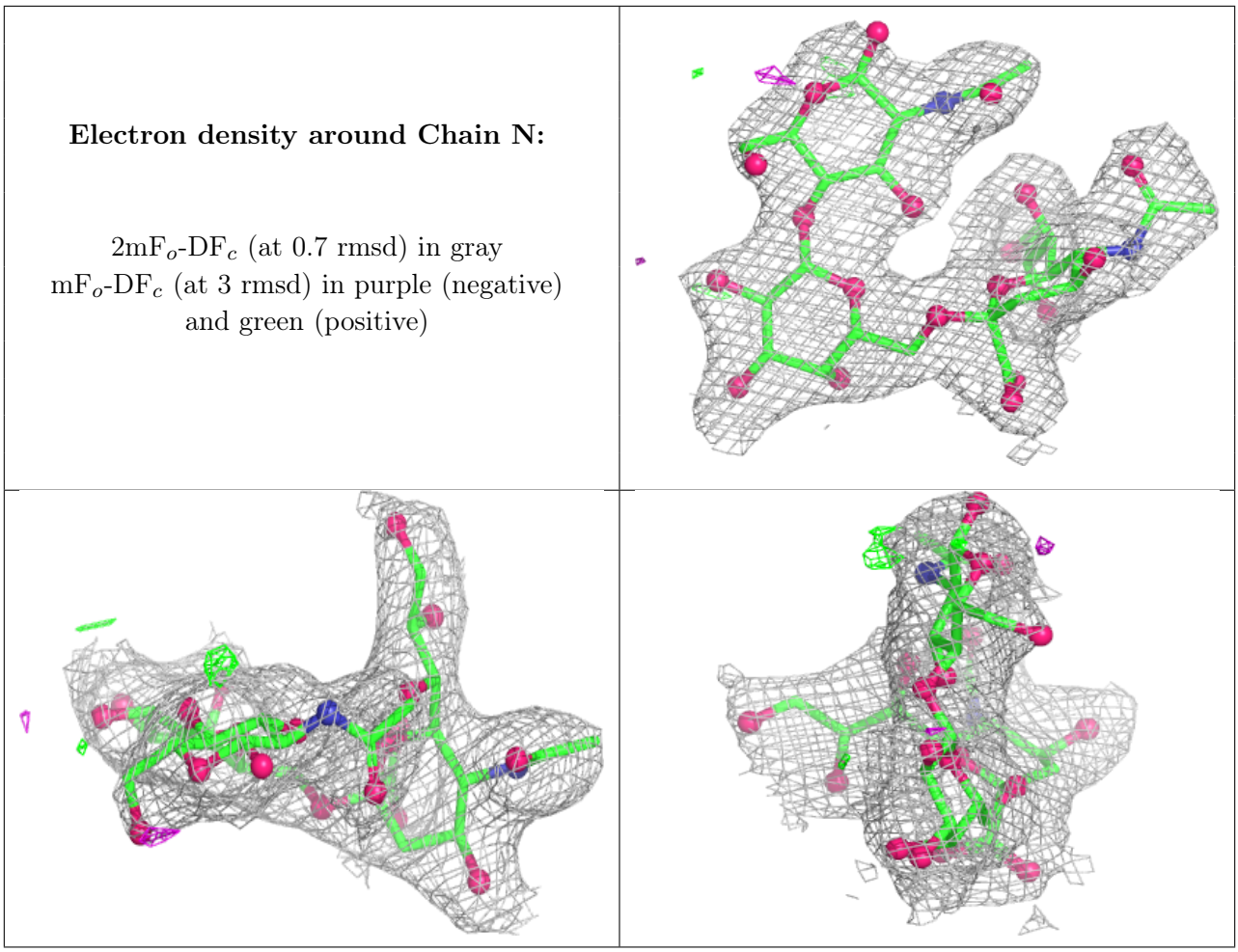
Electron density around Chain M:

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



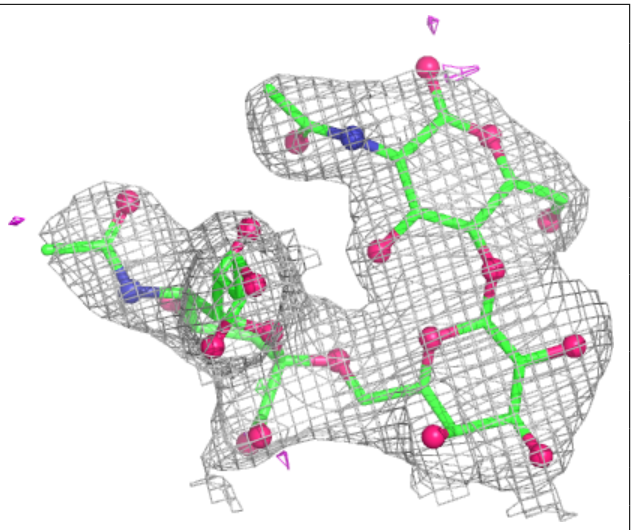
Electron density around Chain N:

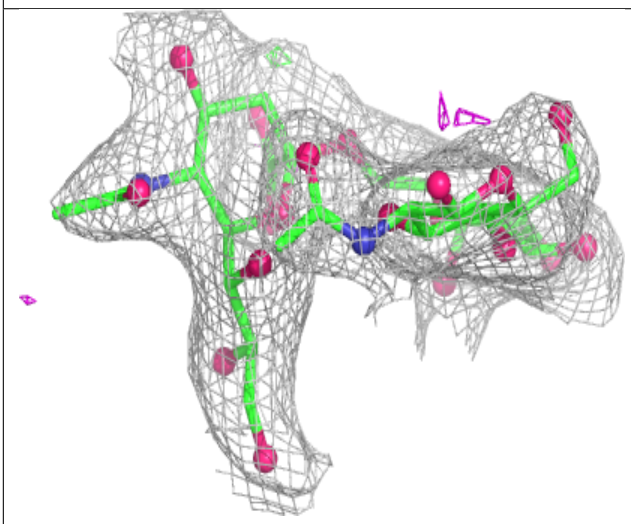
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

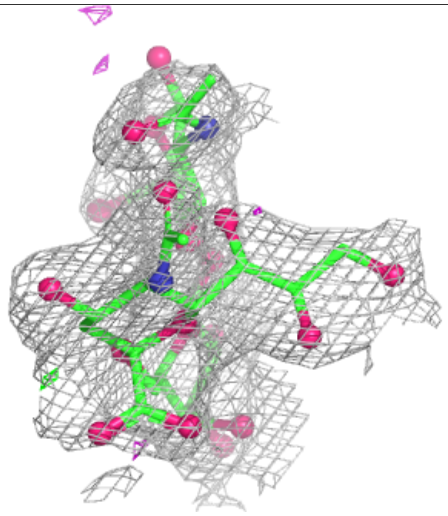


Electron density around Chain O:

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

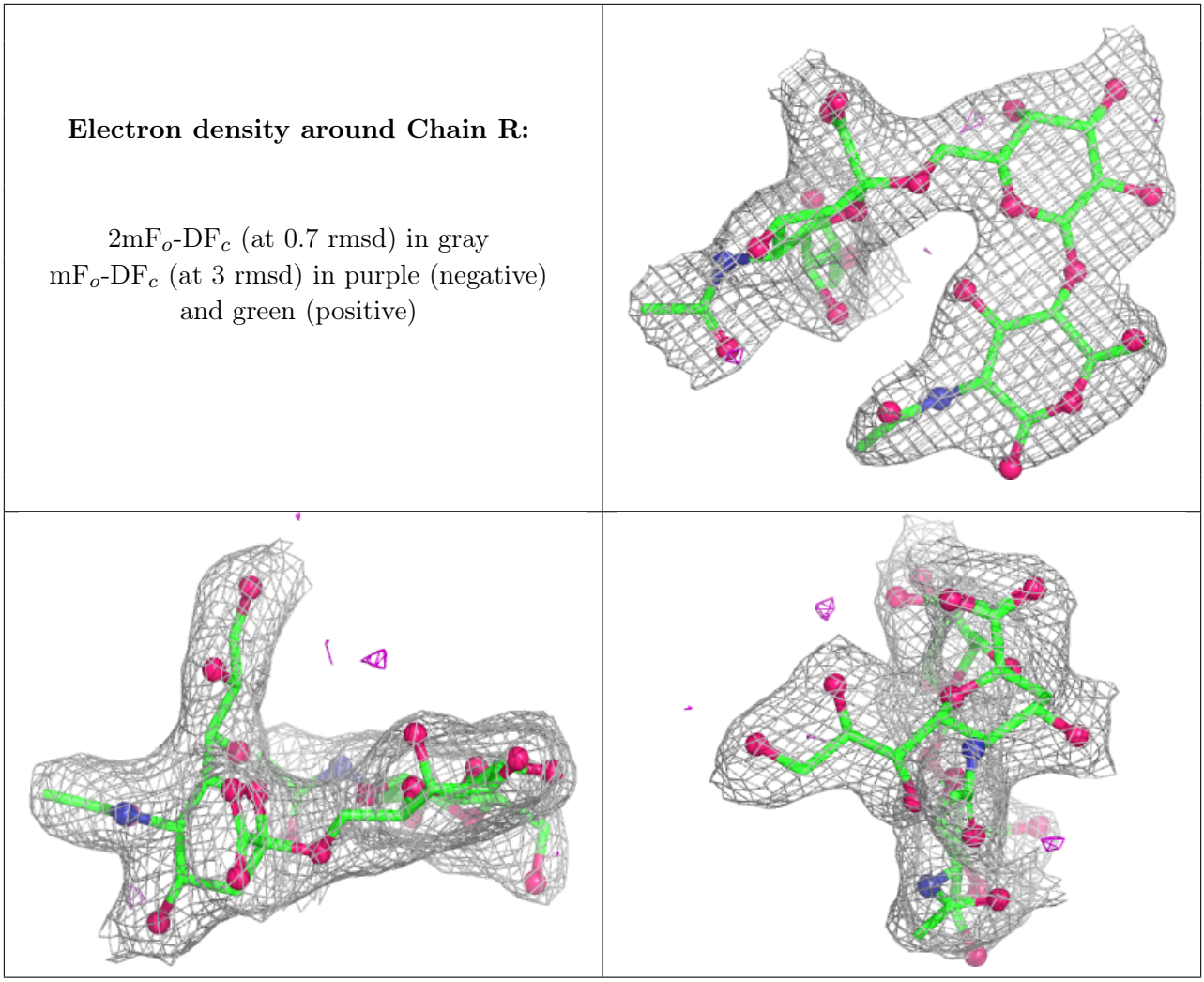






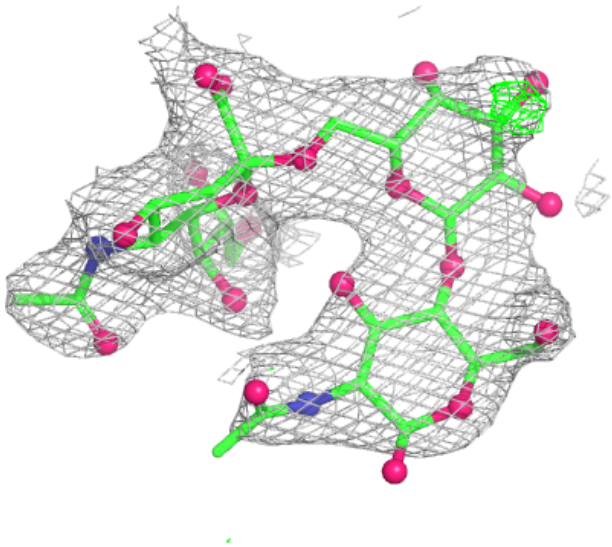
Electron density around Chain R:

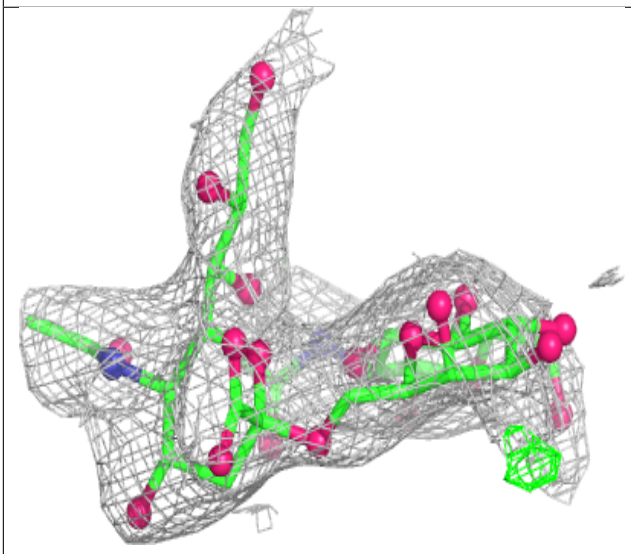
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

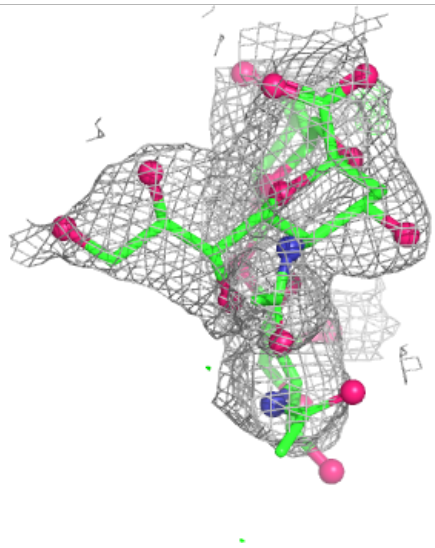


Electron density around Chain S:

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

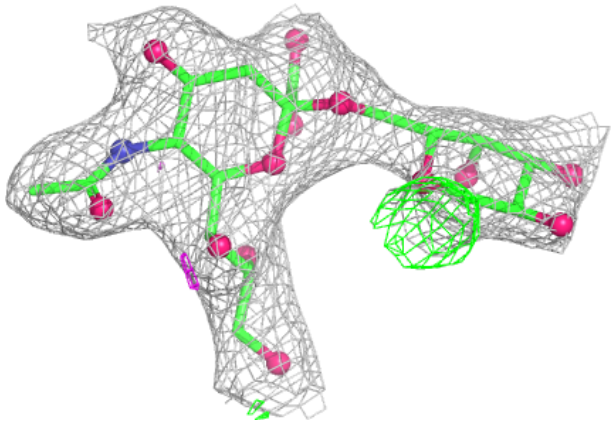


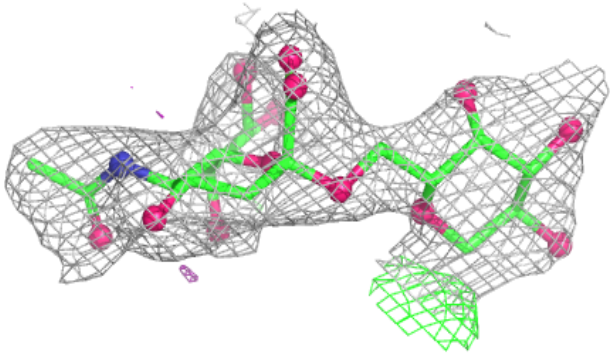


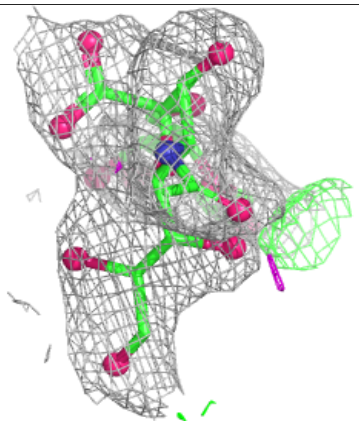


Electron density around Chain P:

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

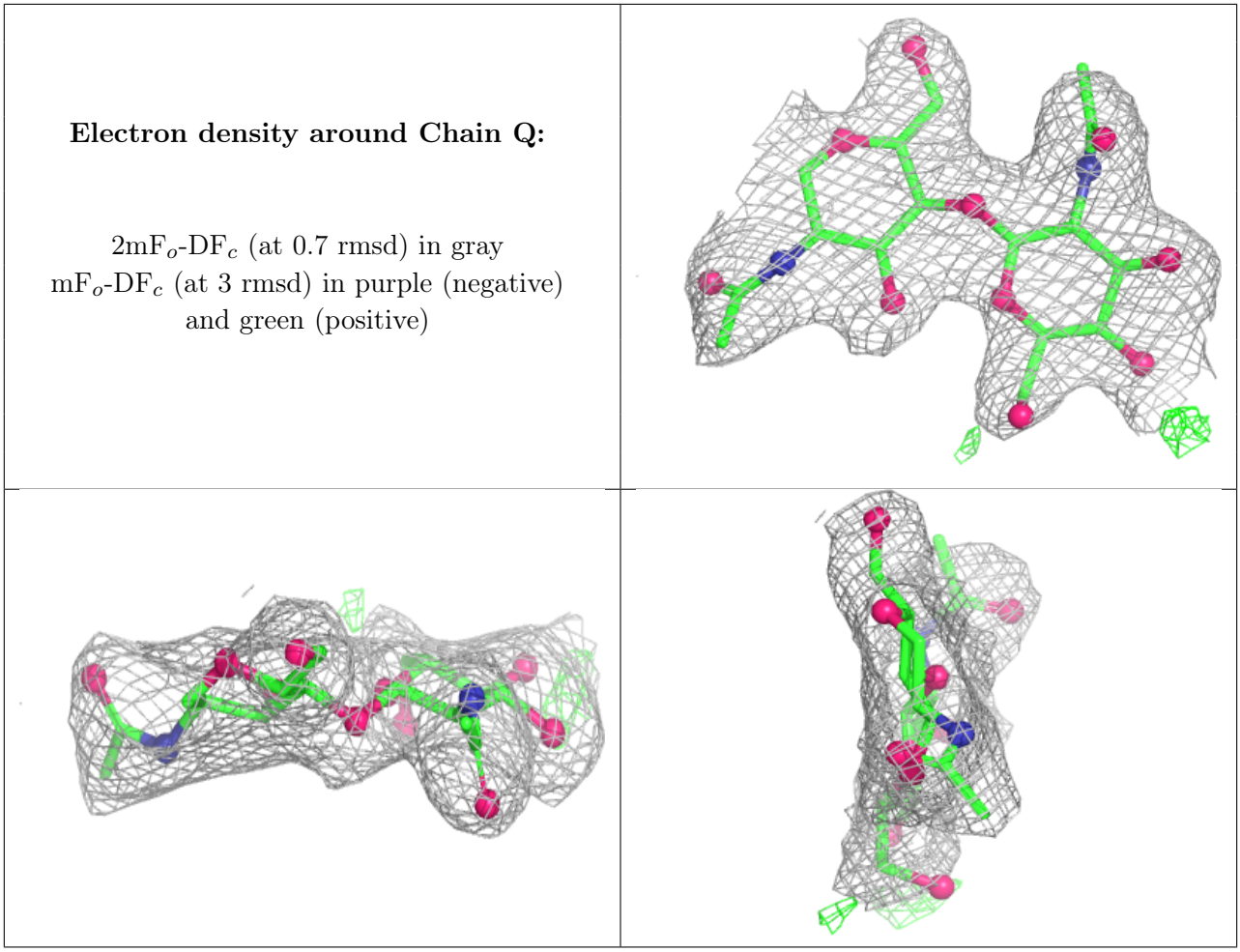






Electron density around Chain Q:

$2mF_o$-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
6	NAG	A	333	14/15	0.62	0.13	70,84,86,87	0
6	NAG	A	334	14/15	0.63	0.17	65,74,89,90	0
6	NAG	C	334	14/15	0.67	0.12	62,76,83,84	0
6	NAG	J	561	14/15	0.68	0.14	76,78,83,84	0
6	NAG	A	336	14/15	0.71	0.14	71,76,80,83	0
6	NAG	K	641	14/15	0.74	0.14	71,81,89,91	0
6	NAG	A	335	14/15	0.85	0.11	48,52,58,61	0
6	NAG	C	333	14/15	0.87	0.10	47,56,67,69	0
6	NAG	E	333	14/15	0.87	0.10	48,56,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.