



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 11:46 PM EDT

PDB ID : 3UBE  
Title : Influenza hemagglutinin from the 2009 pandemic in complex with ligand LSTc  
Authors : Xu, R.; Wilson, I.A.  
Deposited on : 2011-10-24  
Resolution : 2.15 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

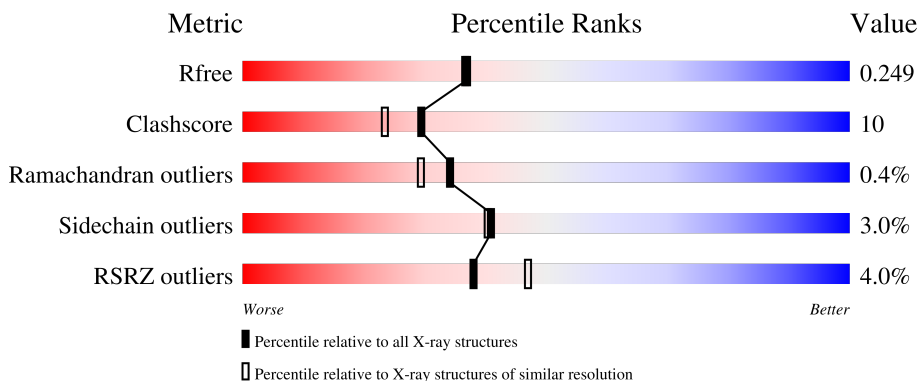
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	329	 81% 16% ..
1	C	329	 83% 13% ..
1	E	329	 76% 21% ..
1	G	329	 76% 21% ..
1	I	329	 73% 21% ..

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Mol	Chain	Length	Quality of chain
1	K	329	 2% 77% 18% ..
2	B	177	 3% 78% 19% ..
2	D	177	 15% 68% 26% ..
2	F	177	 11% 73% 22% ..
2	H	177	 15% 69% 27% ..
2	J	177	 3% 67% 26% . 5%
2	L	177	 2% 80% 16% ..
3	M	4	 25% 50% 25%
3	N	4	 50% 50%
3	R	4	 50% 50%
4	O	3	 67% 33%
4	Q	3	 67% 33%
5	P	2	 50% 50%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 24588 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
			Total	C	N	O	S			
1	A	323	2522	1595	432	482	13	0	0	0
1	C	320	2501	1582	429	477	13	0	0	0
1	E	323	2522	1595	432	482	13	0	0	0
1	G	321	2508	1586	430	479	13	0	0	0
1	I	319	2495	1579	428	475	13	0	0	0
1	K	320	2497	1581	429	474	13	0	0	0

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
			Total	C	N	O	S			
2	B	174	1405	881	237	281	6	0	0	0
2	D	171	1380	866	234	274	6	0	0	0
2	F	170	1371	861	233	271	6	0	0	0
2	H	170	1371	861	233	271	6	0	0	0
2	J	169	1360	855	229	270	6	0	0	0
2	L	170	1371	861	233	271	6	0	0	0

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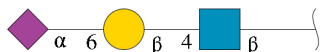
Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	expression tag	UNP C3W5S1
L	176	GLY	-	expression tag	UNP C3W5S1
L	177	ARG	-	expression tag	UNP C3W5S1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	M	4	57	31	2	24	0	0	0
3	N	4	57	31	2	24	0	0	0
3	R	4	57	31	2	24	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	O	3	45	25	2	18	0	0	0
4	Q	3	45	25	2	18	0	0	0

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



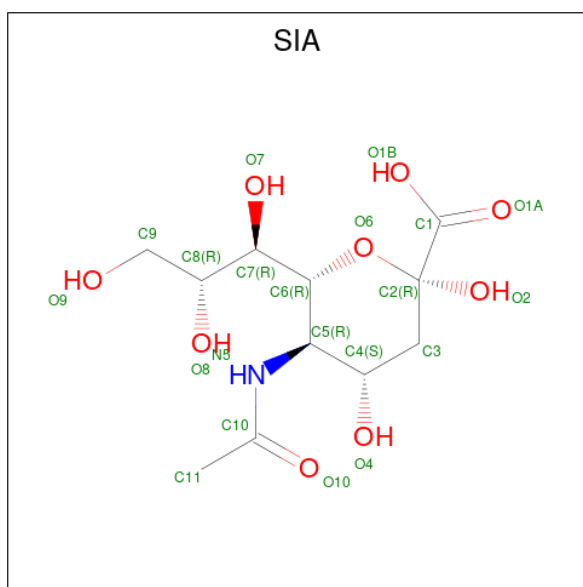
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	P	2	28	16	2	10	0	0	0

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



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

- Molecule 7 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula:  $C_{11}H_{19}NO_9$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	G	1	20	11	1	8	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	99	Total	O	0	0
			99	99		
8	B	54	Total	O	0	0
			54	54		
8	C	124	Total	O	0	0
			124	124		
8	D	48	Total	O	0	0
			48	48		
8	E	85	Total	O	0	0
			85	85		
8	F	49	Total	O	0	0
			49	49		
8	G	105	Total	O	0	0
			105	105		
8	H	45	Total	O	0	0
			45	45		
8	I	90	Total	O	0	0
			90	90		
8	J	50	Total	O	0	0
			50	50		
8	K	71	Total	O	0	0
			71	71		

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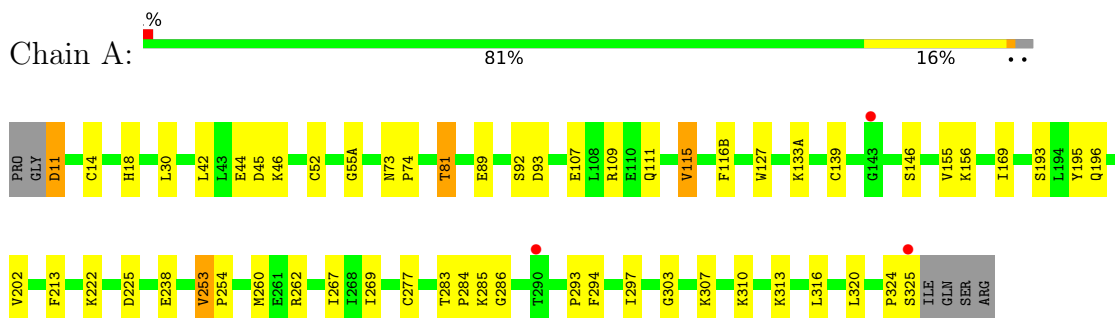
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
8	L	58	Total	O	0	0
			58	58		

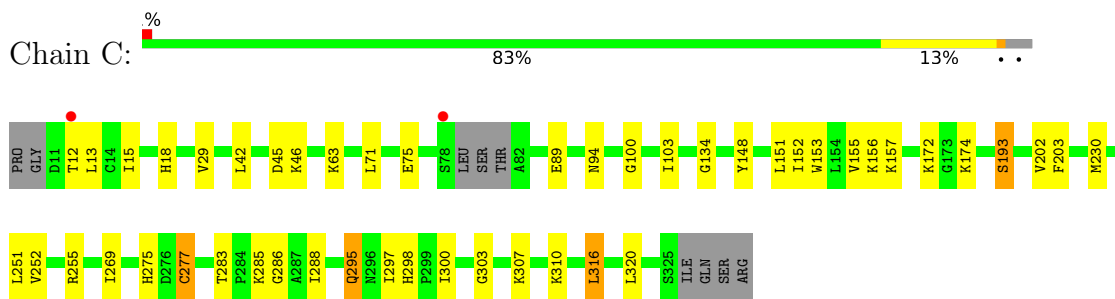
### 3 Residue-property plots [i](#)

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.

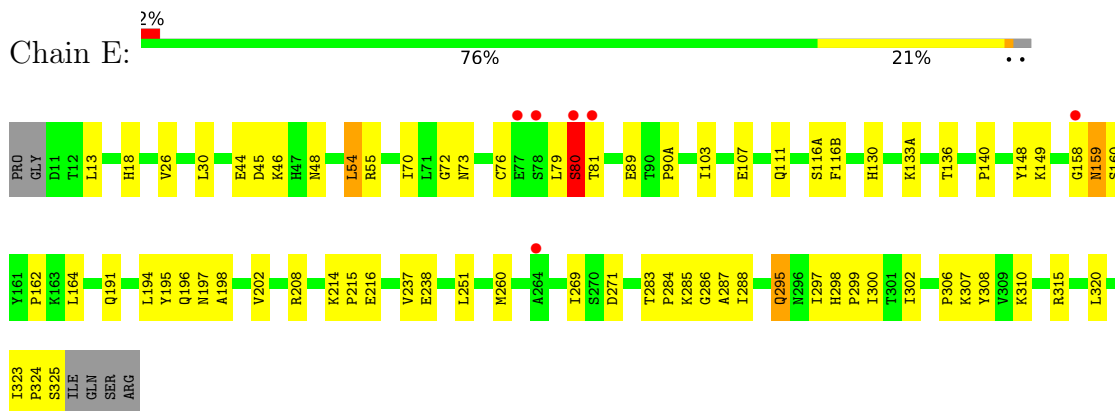
- Molecule 1: Hemagglutinin HA1



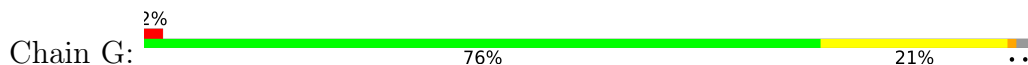
- Molecule 1: Hemagglutinin HA1

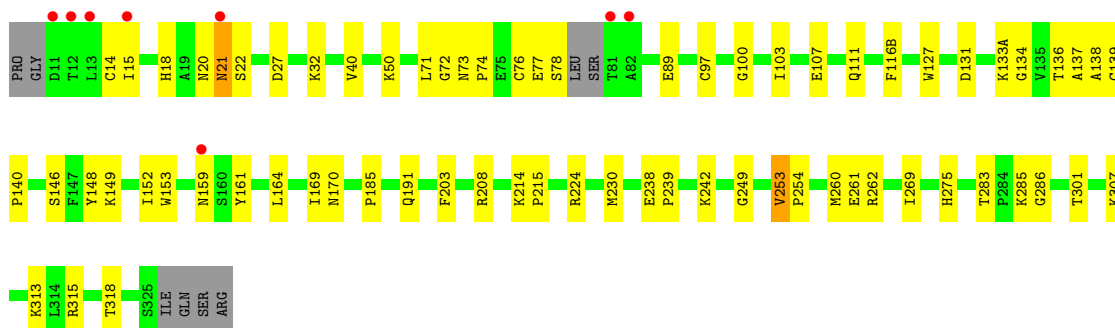


- Molecule 1: Hemagglutinin HA1

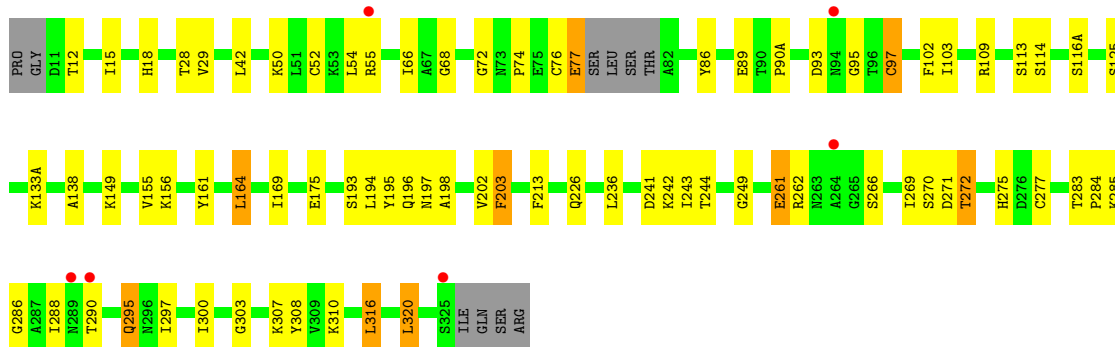


- Molecule 1: Hemagglutinin HA1

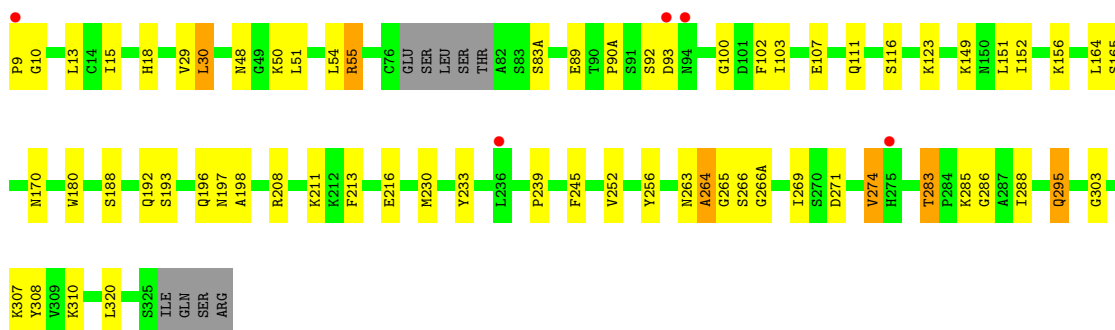
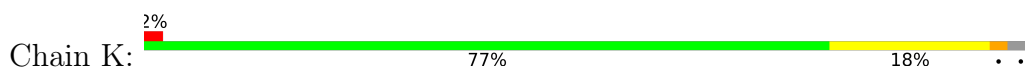




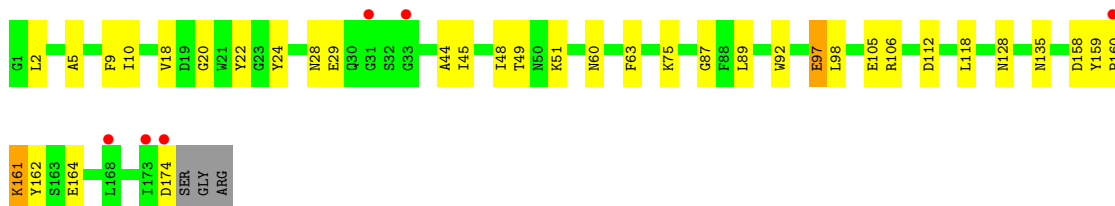
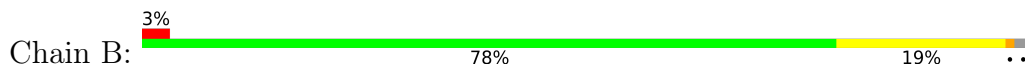
• Molecule 1: Hemagglutinin HA1



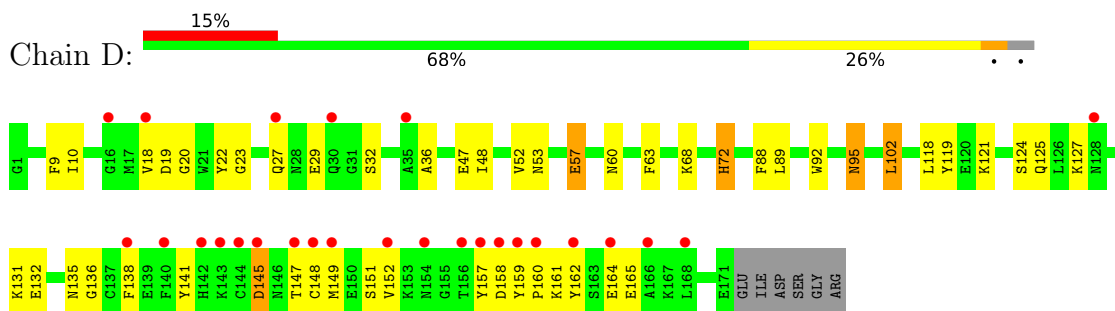
• Molecule 1: Hemagglutinin HA1



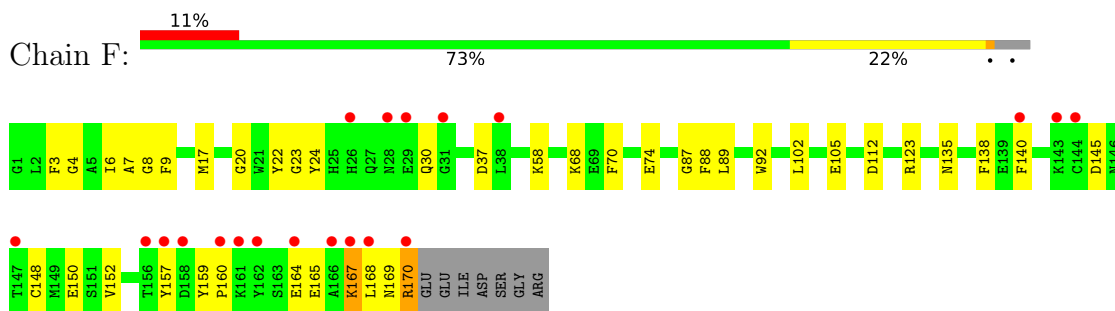
• Molecule 2: Hemagglutinin HA2



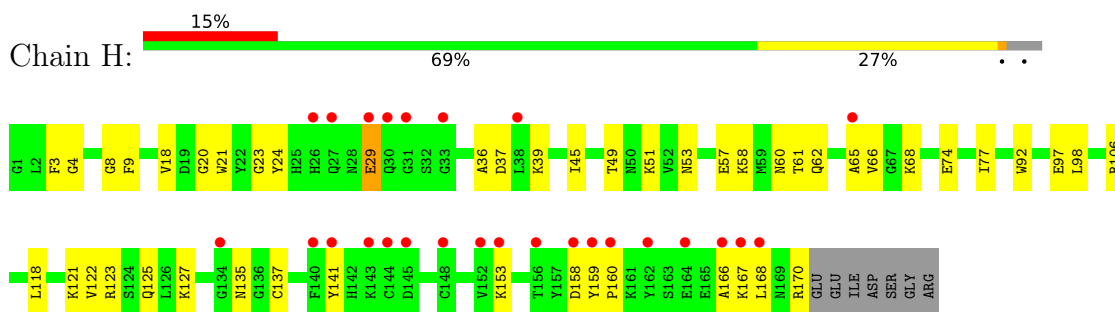
• Molecule 2: Hemagglutinin HA2



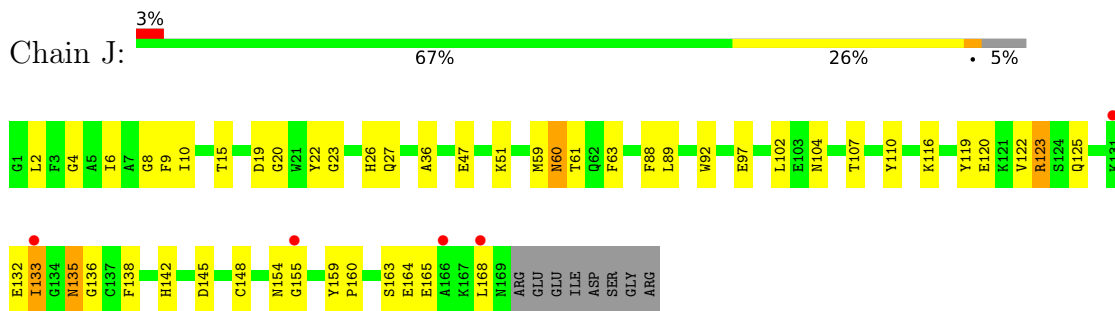
• Molecule 2: Hemagglutinin HA2



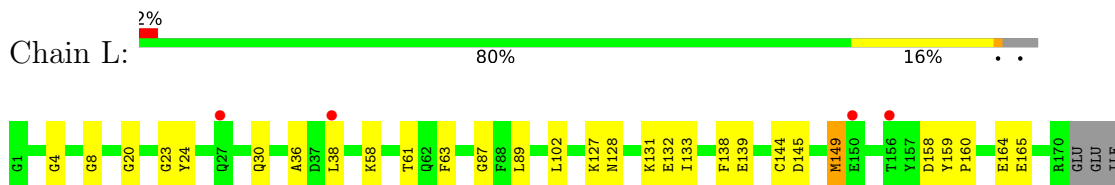
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

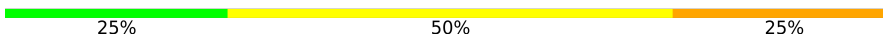


• Molecule 2: Hemagglutinin HA2



ASP  
SER  
GLY  
ARG

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

Chain M:  25% 50% 25%

GAL1  
NAG2  
GAL3  
SIA4

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

Chain N:  50% 50%

GAL1  
NAG2  
GAL3  
SIA4

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

Chain R:  50% 50%

GAL1  
NAG2  
GAL3  
SIA4

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

Chain O:  67% 33%

NAG1  
GAL2  
SIA3

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

Chain Q:  67% 33%

NAG1  
GAL2  
SIA3

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

Chain P:  50% 50%

NAG1  
NAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.78Å 116.59Å 118.72Å 60.86° 77.29° 80.71°	Depositor
Resolution (Å)	49.54 – 2.15 49.54 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.4 (49.54-2.15) 92.3 (49.54-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.14Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, $R_{free}$	0.193 , 0.252 0.190 , 0.249	Depositor DCC
$R_{free}$ test set	7691 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtrriage
Anisotropy	0.169	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	24588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.27	0/2586	0.46	0/3516
1	C	0.26	0/2564	0.46	0/3484
1	E	0.26	0/2586	0.47	0/3516
1	G	0.26	0/2571	0.45	0/3494
1	I	0.25	0/2558	0.46	0/3476
1	K	0.26	0/2561	0.47	0/3480
2	B	0.25	0/1433	0.40	0/1931
2	D	0.26	0/1408	0.41	0/1897
2	F	0.25	0/1399	0.40	0/1885
2	H	0.25	0/1399	0.41	0/1885
2	J	0.25	0/1388	0.42	0/1871
2	L	0.26	0/1399	0.40	0/1885
All	All	0.26	0/23852	0.44	0/32320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2465	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2501	0	2443	32	0
1	E	2522	0	2467	63	0
1	G	2508	0	2450	49	0
1	I	2495	0	2439	67	0
1	K	2497	0	2443	50	0
2	B	1405	0	1324	28	0
2	D	1380	0	1303	40	0
2	F	1371	0	1297	28	0
2	H	1371	0	1297	50	0
2	J	1360	0	1283	42	0
2	L	1371	0	1297	23	0
3	M	57	0	49	1	0
3	N	57	0	49	0	0
3	R	57	0	49	0	0
4	O	45	0	38	1	0
4	Q	45	0	38	0	0
5	P	28	0	25	0	0
6	A	42	0	39	1	0
6	C	14	0	13	1	0
6	E	14	0	13	1	0
6	J	14	0	13	0	0
6	K	14	0	13	0	0
7	G	20	0	17	0	0
8	A	99	0	0	2	0
8	B	54	0	0	3	0
8	C	124	0	0	2	0
8	D	48	0	0	0	0
8	E	85	0	0	1	0
8	F	49	0	0	0	0
8	G	105	0	0	0	0
8	H	45	0	0	1	0
8	I	90	0	0	0	0
8	J	50	0	0	1	0
8	K	71	0	0	3	0
8	L	58	0	0	1	0
All	All	24588	0	22864	443	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 10.

All (443) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:MET:HA	2:J:60:ASN:CB	1.77	1.11
2:J:59:MET:CA	2:J:60:ASN:HB2	1.82	1.09
1:E:79:LEU:HA	1:E:80:SER:HB3	1.13	1.08
1:E:79:LEU:CA	1:E:80:SER:HB3	1.88	1.03
1:C:283:THR:HG22	1:C:285:LYS:H	1.27	0.99
1:I:283:THR:HG22	1:I:285:LYS:H	1.29	0.95
1:E:79:LEU:HA	1:E:80:SER:CB	1.99	0.93
2:H:58:LYS:HD2	2:J:97:GLU:HG2	1.52	0.92
1:E:298:HIS:HD2	1:E:300:ILE:H	1.13	0.89
2:H:53:ASN:O	2:H:57:GLU:HG2	1.71	0.89
1:G:283:THR:HG22	1:G:285:LYS:H	1.38	0.87
2:B:97:GLU:HG2	2:F:58:LYS:HD2	1.56	0.86
1:E:283:THR:HG22	1:E:285:LYS:H	1.40	0.85
1:I:270:SER:OG	1:I:272:THR:HG23	1.77	0.83
2:H:45:ILE:O	2:H:49:THR:HG23	1.80	0.82
1:G:283:THR:HB	1:G:286:GLY:O	1.81	0.81
1:C:283:THR:HB	1:C:286:GLY:O	1.79	0.81
1:E:283:THR:HB	1:E:286:GLY:O	1.80	0.81
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.62	0.80
1:E:72:GLY:HA3	1:E:149:LYS:H	1.44	0.80
1:A:283:THR:HB	1:A:286:GLY:O	1.81	0.80
2:H:97:GLU:HG2	2:L:58:LYS:HD2	1.65	0.79
2:J:59:MET:HA	2:J:60:ASN:HB2	0.87	0.77
2:H:62:GLN:HE21	1:I:310:LYS:NZ	1.81	0.77
1:A:283:THR:HG22	1:A:285:LYS:H	1.49	0.76
2:L:30:GLN:OE1	2:L:145:ASP:HB2	1.85	0.76
1:I:283:THR:HB	1:I:286:GLY:O	1.86	0.75
2:J:9:PHE:O	2:J:135:ASN:HA	1.87	0.74
1:K:211:LYS:HD3	1:K:213:PHE:CZ	2.23	0.73
2:D:149:MET:O	2:D:152:VAL:HG22	1.90	0.72
1:E:208:ARG:NH2	1:E:238:GLU:H	1.87	0.72
1:K:283:THR:CG2	1:K:285:LYS:H	2.03	0.71
1:E:160:SER:O	1:E:162:PRO:HD3	1.91	0.71
2:H:62:GLN:HE21	1:I:310:LYS:HZ3	1.40	0.68
1:C:12:THR:OG1	2:D:27:GLN:HG2	1.94	0.68
1:I:236:LEU:HD13	1:I:262:ARG:NH1	2.08	0.68
1:E:310:LYS:HG2	2:F:89:LEU:HD11	1.76	0.67
1:I:303:GLY:HA2	2:J:63:PHE:CE1	2.29	0.67
1:K:283:THR:HG22	1:K:285:LYS:H	1.58	0.67
2:L:127:LYS:HG3	2:L:128:ASN:H	1.60	0.67
2:H:123:ARG:HH12	2:J:123:ARG:HH21	1.43	0.67
1:E:158:GLY:O	1:E:159:ASN:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:VAL:HG11	1:E:251:LEU:HD13	1.79	0.65
2:L:144:CYS:SG	2:L:149:MET:HE3	2.37	0.65
2:J:47:GLU:HB3	1:K:30:LEU:HG	1.79	0.64
1:E:298:HIS:CD2	1:E:300:ILE:H	2.05	0.64
1:E:283:THR:HG22	1:E:285:LYS:N	2.13	0.63
1:K:211:LYS:HD3	1:K:213:PHE:CE1	2.34	0.63
1:E:26:VAL:HG12	1:E:315:ARG:HG3	1.80	0.62
2:B:60:ASN:HB3	8:B:749:HOH:O	1.98	0.62
1:I:116(A):SER:HB3	1:I:261:GLU:HG2	1.80	0.62
2:D:47:GLU:HB3	1:E:30:LEU:HG	1.80	0.62
2:D:27:GLN:HA	2:D:32:SER:HB3	1.81	0.62
1:G:77:GLU:O	1:G:78:SER:HB3	2.00	0.62
1:K:48:ASN:O	1:K:50:LYS:HG3	2.00	0.61
2:B:45:ILE:O	2:B:49:THR:HG23	2.00	0.61
1:K:288:ILE:HD12	1:K:295:GLN:HG3	1.82	0.61
1:I:18:HIS:HB2	2:J:20:GLY:O	2.00	0.61
1:E:72:GLY:HA3	1:E:149:LYS:N	2.16	0.61
2:H:167:LYS:HG3	2:H:170:ARG:NH1	2.15	0.61
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.81	0.61
1:E:208:ARG:HH22	1:E:238:GLU:H	1.49	0.61
1:A:222:LYS:HD3	1:A:225:ASP:HA	1.83	0.60
1:A:310:LYS:HG3	2:B:89:LEU:HD11	1.82	0.60
2:H:167:LYS:HG3	2:H:170:ARG:HH12	1.66	0.60
2:D:158:ASP:OD2	2:D:160:PRO:HD2	2.01	0.60
1:C:18:HIS:HB2	2:D:20:GLY:O	2.01	0.60
1:I:74:PRO:HB3	1:I:149:LYS:HE3	1.83	0.60
2:B:161:LYS:HE3	2:B:162:TYR:CZ	2.37	0.60
1:C:13:LEU:HD22	2:D:152:VAL:HG21	1.84	0.59
1:C:42:LEU:HD11	1:C:316:LEU:HG	1.83	0.59
1:A:55(A):GLY:HA3	6:A:336:NAG:H83	1.85	0.59
1:E:140:PRO:HD2	6:E:333:NAG:H83	1.83	0.59
2:H:123:ARG:HH12	2:J:123:ARG:NH2	2.00	0.58
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.69	0.58
2:H:123:ARG:HH22	2:J:123:ARG:NH2	1.99	0.58
1:E:90(A):PRO:HD2	1:E:271:ASP:OD1	2.02	0.58
1:C:134:GLY:HA3	1:C:153:TRP:HB3	1.86	0.58
2:D:158:ASP:OD1	2:D:161:LYS:HB2	2.02	0.58
1:I:42:LEU:HD11	1:I:316:LEU:HG	1.86	0.58
1:I:28:THR:HG22	2:J:104:ASN:HB3	1.86	0.58
2:H:3:PHE:CZ	2:J:2:LEU:HG	2.39	0.58
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)
2:H:125:GLN:O	2:H:127:LYS:HG3	2.04	0.57
1:G:283:THR:CG2	1:G:285:LYS:HG2	2.33	0.57
1:G:262:ARG:HG2	1:G:262:ARG:HH11	1.69	0.57
1:A:42:LEU:HD11	1:A:316:LEU:HD22	1.87	0.57
1:C:275:HIS:HB3	8:C:819:HOH:O	2.04	0.57
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.87	0.57
1:K:283:THR:HG22	1:K:285:LYS:N	2.20	0.57
1:A:155:VAL:HG12	1:A:156:LYS:N	2.18	0.57
1:I:97:CYS:HB2	1:I:138:ALA:O	2.05	0.57
2:L:4:GLY:O	2:L:8:GLY:HA3	2.05	0.57
1:E:44:GLU:OE2	1:E:46:LYS:HG2	2.05	0.57
1:K:18:HIS:HB2	2:L:20:GLY:O	2.04	0.57
1:I:307:LYS:HE2	2:J:61:THR:HG22	1.87	0.56
1:E:208:ARG:HH22	1:E:237:VAL:HA	1.69	0.56
2:F:169:ASN:O	2:F:170:ARG:HB2	2.04	0.56
1:G:116(B):PHE:HE1	1:G:260:MET:HE1	1.71	0.56
1:I:116(A):SER:HB3	1:I:261:GLU:CG	2.35	0.56
1:I:288:ILE:HG21	1:I:297:ILE:HD13	1.86	0.56
1:I:89:GLU:O	1:I:269:ILE:HA	2.05	0.56
1:A:253:VAL:HG13	1:A:254:PRO:O	2.06	0.56
2:F:165:GLU:O	2:F:168:LEU:HB2	2.06	0.56
1:G:127:TRP:CH2	1:G:253:VAL:HG21	2.41	0.56
2:J:160:PRO:HA	2:J:163:SER:OG	2.06	0.56
1:A:18:HIS:HB2	2:B:20:GLY:O	2.06	0.56
1:A:283:THR:HG23	1:A:284:PRO:HD2	1.88	0.55
1:I:283:THR:HG22	1:I:285:LYS:N	2.11	0.55
1:G:253:VAL:HG22	1:G:254:PRO:HD2	1.88	0.55
2:L:149:MET:HE2	2:L:149:MET:HA	1.87	0.55
1:C:63:LYS:NZ	1:C:75:GLU:HB3	2.21	0.55
2:F:9:PHE:O	2:F:135:ASN:HA	2.07	0.55
1:E:288:ILE:CD1	1:E:295:GLN:HG3	2.37	0.55
2:H:62:GLN:NE2	1:I:310:LYS:NZ	2.53	0.55
2:L:132:GLU:HG2	2:L:138:PHE:CE2	2.40	0.55
1:C:288:ILE:HD13	1:C:295:GLN:HG3	1.88	0.54
1:K:170:ASN:O	1:K:239:PRO:O	2.25	0.54
1:A:238:GLU:HG2	8:A:362:HOH:O	2.06	0.54
2:H:153:LYS:HG2	2:H:153:LYS:O	2.07	0.54
1:G:169:ILE:HG13	1:G:242:LYS:HG3	1.90	0.54
2:H:4:GLY:O	2:H:8:GLY:HA3	2.08	0.54
2:H:24:TYR:CE1	2:H:153:LYS:HG3	2.43	0.54
1:K:54:LEU:O	1:K:55:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:30:GLN:NE2	2:F:145:ASP:HB2	2.21	0.54
1:G:18:HIS:HB2	2:H:20:GLY:O	2.08	0.54
2:D:23:GLY:HA3	2:D:36:ALA:HA	1.90	0.53
2:J:19:ASP:OD2	2:J:36:ALA:HB3	2.08	0.53
1:G:214:LYS:HG3	1:G:215:PRO:HD2	1.88	0.53
2:D:119:TYR:CE1	2:D:136:GLY:HA2	2.43	0.53
2:D:132:GLU:HG2	2:D:138:PHE:CE2	2.43	0.53
2:H:24:TYR:CE1	2:H:37:ASP:HB2	2.44	0.53
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.08	0.53
2:B:87:GLY:HA3	2:F:88:PHE:CZ	2.44	0.53
2:D:53:ASN:O	2:D:57:GLU:CG	2.57	0.53
1:G:131:ASP:OD1	1:G:133(A):LYS:HE2	2.08	0.53
2:D:161:LYS:HD2	2:D:162:TYR:CZ	2.43	0.53
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.09	0.53
1:C:310:LYS:HE3	2:D:89:LEU:HD21	1.90	0.52
1:C:151:LEU:HB3	1:C:252:VAL:HG12	1.90	0.52
2:J:164:GLU:O	2:J:168:LEU:HG	2.09	0.52
2:B:75:LYS:HE3	8:E:562:HOH:O	2.09	0.52
1:K:310:LYS:O	1:K:310:LYS:HG2	2.09	0.52
2:F:164:GLU:O	2:F:168:LEU:HD13	2.09	0.52
1:K:307:LYS:HE2	2:L:61:THR:HG22	1.91	0.52
2:D:53:ASN:O	2:D:57:GLU:HG2	2.10	0.52
1:G:27:ASP:HA	1:G:32:LYS:O	2.10	0.51
1:I:284:PRO:HD3	1:I:300:ILE:O	2.11	0.51
2:H:51:LYS:HG3	1:I:29:VAL:HG22	1.92	0.51
1:K:89:GLU:O	1:K:269:ILE:HA	2.09	0.51
1:I:12:THR:OG1	2:J:27:GLN:HB3	2.10	0.51
1:I:72:GLY:O	1:I:149:LYS:HG2	2.10	0.51
1:I:290:THR:HG22	1:I:290:THR:O	2.09	0.51
1:K:156:LYS:HD2	1:K:196:GLN:HE21	1.76	0.51
1:A:81:THR:HG21	8:A:827:HOH:O	2.10	0.51
1:I:52:CYS:HB3	1:I:277:CYS:O	2.10	0.51
1:A:127:TRP:CZ2	1:A:253:VAL:HG11	2.45	0.51
1:E:107:GLU:O	1:E:111:GLN:HG3	2.11	0.51
2:H:62:GLN:HE21	1:I:310:LYS:HZ2	1.57	0.51
1:K:164:LEU:C	1:K:164:LEU:HD12	2.31	0.51
2:L:149:MET:HA	2:L:149:MET:CE	2.41	0.51
1:I:242:LYS:HG2	1:I:243:ILE:N	2.25	0.51
1:K:93:ASP:N	8:K:682:HOH:O	2.44	0.51
2:D:151:SER:OG	2:D:157:TYR:HA	2.12	0.50
1:C:45:ASP:C	1:C:46:LYS:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:LYS:HG3	1:E:215:PRO:HD2	1.92	0.50
2:D:19:ASP:HB3	2:D:36:ALA:HB2	1.94	0.50
2:D:124:SER:O	2:D:127:LYS:HE3	2.12	0.50
1:A:155:VAL:CG1	1:A:156:LYS:N	2.75	0.50
2:L:23:GLY:HA3	2:L:36:ALA:HA	1.94	0.50
2:H:23:GLY:HA3	2:H:36:ALA:HA	1.94	0.50
2:L:127:LYS:HG3	2:L:128:ASN:N	2.27	0.50
1:I:133(A):LYS:HG3	1:I:133(A):LYS:O	2.12	0.50
2:B:9:PHE:O	2:B:135:ASN:HA	2.12	0.50
1:G:134:GLY:HA3	1:G:153:TRP:HB3	1.92	0.49
1:K:263:ASN:O	1:K:264:ALA:C	2.49	0.49
1:C:156:LYS:HE2	1:C:193:SER:O	2.11	0.49
2:F:17:MET:SD	2:F:23:GLY:HA3	2.52	0.49
1:G:97:CYS:O	1:G:224:ARG:HD3	2.11	0.49
1:I:155:VAL:HG13	1:I:194:LEU:O	2.12	0.49
1:I:236:LEU:HD13	1:I:262:ARG:HH11	1.75	0.49
2:B:106:ARG:HD3	8:B:190:HOH:O	2.11	0.49
1:G:137:ALA:O	1:G:140:PRO:HD3	2.11	0.49
1:K:54:LEU:C	1:K:55:ARG:HG3	2.33	0.49
2:B:2:LEU:HG	2:F:3:PHE:CZ	2.47	0.49
1:K:197:ASN:O	1:K:198:ALA:HB3	2.13	0.49
2:F:70:PHE:HB3	2:F:74:GLU:HB2	1.94	0.49
1:K:151:LEU:HB3	1:K:252:VAL:HG12	1.95	0.49
1:G:283:THR:HG22	1:G:285:LYS:N	2.18	0.49
2:H:65:ALA:O	2:H:66:VAL:HB	2.13	0.49
2:H:168:LEU:HD23	2:H:168:LEU:O	2.11	0.49
1:G:103:ILE:HD12	1:G:103:ILE:N	2.28	0.49
1:I:169:ILE:HD13	1:I:242:LYS:HB2	1.93	0.49
1:A:109:ARG:HB3	1:A:267:ILE:CD1	2.43	0.49
1:G:127:TRP:CZ2	1:G:253:VAL:HG21	2.47	0.49
1:K:303:GLY:HA2	2:L:63:PHE:CE1	2.48	0.49
2:F:148:CYS:O	2:F:152:VAL:HG23	2.13	0.49
1:I:164:LEU:HD12	1:I:164:LEU:C	2.33	0.49
1:K:308:TYR:CD2	2:L:89:LEU:HD13	2.48	0.49
2:H:9:PHE:O	2:H:135:ASN:HA	2.12	0.49
1:E:72:GLY:O	1:E:73:ASN:C	2.52	0.48
1:G:89:GLU:O	1:G:269:ILE:HA	2.13	0.48
1:K:149:LYS:HE2	1:K:256:TYR:CE1	2.48	0.48
1:C:295:GLN:OE1	1:C:297:ILE:N	2.46	0.48
1:E:89:GLU:O	1:E:269:ILE:HA	2.13	0.48
1:A:89:GLU:O	1:A:269:ILE:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:HIS:HB2	2:F:20:GLY:O	2.13	0.48
1:G:208:ARG:HG3	1:G:238:GLU:OE2	2.14	0.48
1:E:54:LEU:C	1:E:55:ARG:HG2	2.34	0.48
2:H:123:ARG:HG2	2:H:123:ARG:HH11	1.77	0.48
2:J:119:TYR:CE1	2:J:136:GLY:HA2	2.48	0.48
1:E:79:LEU:CB	1:E:80:SER:HB3	2.44	0.48
2:F:4:GLY:O	2:F:8:GLY:HA3	2.14	0.48
1:C:203:PHE:HE2	1:E:216:GLU:HB3	1.79	0.48
1:G:73:ASN:HB3	1:G:76:CYS:SG	2.54	0.48
2:D:95:ASN:N	2:D:95:ASN:HD22	2.10	0.48
2:F:167:LYS:HG2	2:F:168:LEU:N	2.28	0.47
1:I:114:SER:HB2	1:I:266:SER:HB2	1.95	0.47
2:J:88:PHE:CZ	2:L:87:GLY:HA3	2.49	0.47
1:E:116(B):PHE:CE1	1:E:260:MET:HE2	2.50	0.47
1:E:208:ARG:NH1	1:E:238:GLU:HG3	2.28	0.47
2:J:4:GLY:O	2:J:8:GLY:HA3	2.13	0.47
1:K:50:LYS:O	1:K:286:GLY:HA2	2.14	0.47
2:L:159:TYR:N	2:L:160:PRO:HD2	2.30	0.47
2:D:131:LYS:HE3	2:D:141:TYR:OH	2.14	0.47
1:A:115:VAL:HG11	1:A:116(B):PHE:HB2	1.96	0.47
1:C:298:HIS:CE1	1:C:300:ILE:HB	2.50	0.47
1:E:164:LEU:HD12	1:E:164:LEU:C	2.35	0.47
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.96	0.47
1:G:107:GLU:O	1:G:111:GLN:HG3	2.15	0.47
2:J:132:GLU:HG2	2:J:138:PHE:CE2	2.50	0.47
2:J:15:THR:HG23	8:J:202:HOH:O	2.15	0.47
1:K:283:THR:HG22	1:K:286:GLY:H	1.80	0.47
1:C:307:LYS:HG3	2:D:92:TRP:CE2	2.50	0.47
1:E:54:LEU:O	1:E:55:ARG:HG2	2.15	0.47
1:E:195:TYR:O	1:E:196:GLN:HB3	2.14	0.47
1:E:164:LEU:HD12	1:E:164:LEU:O	2.15	0.46
1:A:109:ARG:HB3	1:A:267:ILE:HD11	1.97	0.46
1:E:324:PRO:O	1:E:325:SER:C	2.54	0.46
1:G:71:LEU:O	1:G:148:TYR:HB3	2.15	0.46
1:G:97:CYS:HB2	1:G:138:ALA:O	2.14	0.46
1:C:152:ILE:HD11	1:C:255:ARG:HD2	1.98	0.46
1:E:197:ASN:O	1:E:198:ALA:HB3	2.14	0.46
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.97	0.46
1:K:283:THR:HB	1:K:286:GLY:O	2.15	0.46
1:E:30:LEU:HB2	2:F:105:GLU:OE1	2.16	0.46
1:E:72:GLY:H	1:E:148:TYR:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:270:SER:HG	1:I:272:THR:HG23	1.79	0.46
1:A:52:CYS:HB3	1:A:277:CYS:O	2.15	0.46
1:A:202:VAL:HB	1:A:213:PHE:HB2	1.98	0.46
1:C:277:CYS:HA	6:C:334:NAG:H82	1.98	0.46
2:F:152:VAL:HA	2:F:157:TYR:HB2	1.96	0.46
2:D:121:LYS:O	2:D:125:GLN:HG3	2.15	0.46
1:K:92:SER:HA	8:K:682:HOH:O	2.15	0.46
1:I:68:GLY:HA3	1:I:95:GLY:HA2	1.97	0.46
1:K:165:SER:HA	1:K:245:PHE:O	2.16	0.46
1:G:77:GLU:HA	1:G:77:GLU:OE1	2.14	0.46
1:G:283:THR:CG2	1:G:285:LYS:H	2.18	0.46
1:I:310:LYS:HG2	2:J:89:LEU:HD11	1.98	0.46
1:K:90(A):PRO:HD2	1:K:271:ASP:OD1	2.15	0.46
2:J:51:LYS:HG3	1:K:29:VAL:CG2	2.46	0.46
2:L:164:GLU:CD	2:L:165:GLU:H	2.19	0.46
1:C:89:GLU:O	1:C:269:ILE:HA	2.16	0.45
1:I:138:ALA:HB2	1:I:226:GLN:HE21	1.81	0.45
2:B:158:ASP:OD2	2:B:160:PRO:HD2	2.17	0.45
1:I:288:ILE:CG2	1:I:297:ILE:HD13	2.46	0.45
1:K:107:GLU:O	1:K:111:GLN:HG3	2.16	0.45
1:A:30:LEU:HD12	2:B:105:GLU:OE2	2.17	0.45
2:H:74:GLU:HB3	2:H:77:ILE:HD11	1.99	0.45
1:K:266:SER:OG	1:K:266(A):GLY:N	2.48	0.45
1:A:195:TYR:O	1:A:196:GLN:HB3	2.16	0.45
1:I:15:ILE:N	1:I:15:ILE:HD12	2.32	0.45
1:A:324:PRO:O	1:A:325:SER:HB3	2.17	0.45
1:C:103:ILE:N	1:C:103:ILE:HD12	2.32	0.45
2:D:29:GLU:HA	2:D:29:GLU:OE1	2.16	0.45
1:I:295:GLN:O	1:I:308:TYR:HA	2.16	0.45
2:D:132:GLU:HG2	2:D:138:PHE:HE2	1.82	0.45
2:D:164:GLU:HG2	2:D:165:GLU:N	2.32	0.45
1:G:100:GLY:HA3	1:G:230:MET:O	2.17	0.45
1:K:13:LEU:HD11	2:L:24:TYR:HB3	1.99	0.45
1:A:260:MET:HE2	1:A:262:ARG:HG2	1.98	0.45
1:I:241:ASP:OD1	1:I:242:LYS:N	2.49	0.45
2:J:142:HIS:HB2	2:J:165:GLU:CD	2.37	0.45
2:H:51:LYS:HG3	1:I:29:VAL:CG2	2.47	0.44
1:E:54:LEU:HD11	1:E:302:ILE:HG22	1.98	0.44
1:E:103:ILE:HD12	1:E:103:ILE:N	2.33	0.44
2:H:62:GLN:NE2	1:I:310:LYS:HZ2	2.15	0.44
1:I:202:VAL:HB	1:I:213:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.16	0.44
2:B:51:LYS:HG3	1:C:29:VAL:CG2	2.47	0.44
1:I:15:ILE:HD11	2:J:122:VAL:HG21	2.00	0.44
1:I:161:TYR:CZ	1:I:249:GLY:HA2	2.53	0.44
1:G:170:ASN:HB3	1:G:239:PRO:O	2.18	0.44
1:I:90(A):PRO:HD2	1:I:271:ASP:CG	2.37	0.44
2:J:125:GLN:OE1	2:J:155:GLY:HA2	2.18	0.44
1:K:103:ILE:N	1:K:103:ILE:HD12	2.32	0.44
1:K:9:PRO:HB2	1:K:10:GLY:H	1.64	0.44
2:D:72:HIS:H	2:D:72:HIS:CD2	2.36	0.44
1:K:123:LYS:HG3	1:K:152:ILE:HD13	2.00	0.44
2:L:131:LYS:NZ	2:L:133:ILE:HG22	2.33	0.44
1:E:295:GLN:O	1:E:308:TYR:HA	2.17	0.43
1:G:40:VAL:HG13	1:G:318:THR:HG21	2.00	0.43
2:H:141:TYR:CE1	2:H:170:ARG:HG3	2.53	0.43
1:A:107:GLU:O	1:A:111:GLN:HG3	2.18	0.43
1:A:293:PRO:HG2	1:A:294:PHE:CD2	2.53	0.43
1:E:133(A):LYS:O	4:O:3:SIA:H113	2.18	0.43
2:H:29:GLU:CD	2:H:29:GLU:H	2.22	0.43
2:H:39:LYS:HD2	2:H:39:LYS:HA	1.73	0.43
1:I:203:PHE:HE2	1:K:216:GLU:HB3	1.83	0.43
1:I:320:LEU:HD13	2:J:6:ILE:HD13	1.99	0.43
2:H:58:LYS:HD2	2:J:97:GLU:CG	2.37	0.43
1:I:68:GLY:CA	1:I:95:GLY:HA2	2.48	0.43
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.53	0.43
1:G:14:CYS:HA	2:H:137:CYS:HA	1.99	0.43
2:H:167:LYS:HE2	2:H:170:ARG:HH12	1.82	0.43
2:J:107:THR:O	2:J:110:TYR:HB3	2.18	0.43
2:L:158:ASP:HB2	8:L:714:HOH:O	2.18	0.43
2:F:123:ARG:HB2	2:F:138:PHE:HZ	1.84	0.43
1:A:156:LYS:HE2	1:A:193:SER:O	2.19	0.43
2:H:21:TRP:CH2	2:H:45:ILE:HD13	2.54	0.43
1:K:51:LEU:HB2	1:K:274:VAL:HA	2.01	0.43
2:B:105:GLU:OE1	2:B:105:GLU:HA	2.18	0.43
1:K:83(A):SER:HB3	1:K:116:SER:O	2.19	0.43
1:K:123:LYS:HG3	1:K:152:ILE:CD1	2.49	0.43
2:L:133:ILE:HD13	2:L:139:GLU:HB2	2.01	0.43
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.87	0.43
2:D:164:GLU:CD	2:D:164:GLU:H	2.22	0.43
1:G:21:ASN:OD1	1:G:21:ASN:N	2.50	0.43
1:G:152:ILE:HB	1:G:253:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:VAL:CG1	1:I:156:LYS:N	2.82	0.43
1:A:73:ASN:HA	1:A:74:PRO:HD3	1.94	0.43
2:H:106:ARG:HD3	8:H:388:HOH:O	2.18	0.43
1:I:50:LYS:NZ	1:I:275:HIS:CG	2.87	0.43
1:I:66:ILE:HD12	1:I:109:ARG:HG2	2.00	0.43
1:A:139:CYS:O	1:A:146:SER:HB3	2.19	0.43
1:C:310:LYS:HB3	1:C:310:LYS:HE2	1.62	0.43
2:D:148:CYS:O	2:D:151:SER:HB3	2.19	0.43
2:H:118:LEU:O	2:H:121:LYS:HB3	2.19	0.43
1:G:20:ASN:OD1	1:G:22:SER:HB3	2.19	0.42
1:G:50:LYS:HD2	1:G:275:HIS:CE1	2.54	0.42
1:G:50:LYS:HD2	1:G:275:HIS:ND1	2.33	0.42
2:H:123:ARG:HG2	2:H:123:ARG:NH1	2.34	0.42
1:I:203:PHE:CE2	1:K:216:GLU:HB3	2.54	0.42
1:K:100:GLY:HA3	1:K:230:MET:O	2.19	0.42
2:B:5:ALA:HB3	2:B:112:ASP:OD2	2.19	0.42
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.54	0.42
1:I:76:CYS:O	1:I:77:GLU:C	2.58	0.42
1:I:103:ILE:HD12	1:I:103:ILE:N	2.34	0.42
2:B:159:TYR:HB3	2:B:160:PRO:HD3	2.00	0.42
1:E:191:GLN:HG2	1:E:198:ALA:HA	2.01	0.42
1:I:197:ASN:O	1:I:198:ALA:HB3	2.19	0.42
1:A:283:THR:HG22	1:A:285:LYS:HG2	2.01	0.42
2:F:68:LYS:HD3	2:F:68:LYS:HA	1.89	0.42
1:G:116(B):PHE:CE1	1:G:260:MET:HE1	2.51	0.42
2:H:18:VAL:HG12	2:H:18:VAL:O	2.20	0.42
1:I:175:GLU:OE1	1:I:262:ARG:NH1	2.53	0.42
1:K:283:THR:HG23	1:K:285:LYS:H	1.81	0.42
1:G:72:GLY:O	1:G:149:LYS:HG2	2.19	0.42
2:H:53:ASN:C	2:H:57:GLU:HG2	2.38	0.42
1:C:15:ILE:N	1:C:15:ILE:HD12	2.34	0.42
1:E:79:LEU:HD23	1:E:79:LEU:H	1.84	0.42
1:G:301:THR:O	2:H:65:ALA:O	2.37	0.42
1:I:303:GLY:HA2	2:J:63:PHE:CD1	2.55	0.42
1:E:45:ASP:C	1:E:297:ILE:HD11	2.39	0.42
2:F:24:TYR:CE1	2:F:37:ASP:HB2	2.55	0.42
1:G:283:THR:HG21	1:G:285:LYS:HG2	2.01	0.42
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.55	0.42
2:B:49:THR:HG22	8:B:684:HOH:O	2.20	0.42
2:D:145:ASP:OD2	2:D:147:THR:HG22	2.19	0.42
1:G:164:LEU:C	1:G:164:LEU:HD23	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:313:LYS:HE2	1:G:313:LYS:HB3	1.82	0.42
2:H:123:ARG:HH22	2:J:123:ARG:HH22	1.63	0.42
2:H:141:TYR:O	2:H:166:ALA:HA	2.20	0.42
1:K:188:SER:O	1:K:192:GLN:HG2	2.20	0.42
1:A:313:LYS:HE3	1:A:313:LYS:HB2	1.88	0.42
1:E:130:HIS:CE1	1:E:162:PRO:HD2	2.55	0.42
2:F:6:ILE:HG13	2:F:112:ASP:HA	2.02	0.42
2:F:159:TYR:N	2:F:160:PRO:HD2	2.34	0.42
1:G:307:LYS:HG3	2:H:92:TRP:CE2	2.55	0.42
1:E:13:LEU:HB2	2:F:140:PHE:HE1	1.85	0.41
2:J:119:TYR:HE1	2:J:136:GLY:HA2	1.84	0.41
1:K:15:ILE:N	1:K:15:ILE:HD12	2.35	0.41
1:C:63:LYS:HZ2	1:C:75:GLU:HB3	1.83	0.41
2:D:131:LYS:HE3	2:D:141:TYR:CZ	2.55	0.41
1:K:180:TRP:CE2	1:K:233:TYR:HB2	2.55	0.41
2:B:44:ALA:O	2:B:48:ILE:HG12	2.20	0.41
2:B:118:LEU:HD12	2:B:118:LEU:HA	1.92	0.41
1:C:303:GLY:HA2	2:D:63:PHE:CE1	2.55	0.41
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.55	0.41
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.85	0.41
1:E:73:ASN:HB3	1:E:76:CYS:SG	2.61	0.41
1:E:307:LYS:HG3	2:F:92:TRP:CE2	2.55	0.41
1:I:307:LYS:HG3	2:J:92:TRP:CE2	2.55	0.41
2:J:116:LYS:O	2:J:120:GLU:HG3	2.20	0.41
2:J:133:ILE:O	2:J:133:ILE:HD12	2.19	0.41
2:J:159:TYR:N	2:J:160:PRO:HD2	2.35	0.41
1:K:208:ARG:HG3	8:K:357:HOH:O	2.20	0.41
1:A:14:CYS:O	2:B:24:TYR:HA	2.20	0.41
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.84	0.41
2:D:88:PHE:CZ	2:F:87:GLY:HA3	2.55	0.41
1:E:54:LEU:O	1:E:55:ARG:CG	2.68	0.41
1:E:158:GLY:O	1:E:159:ASN:CB	2.65	0.41
1:E:295:GLN:HB2	1:E:306:PRO:HB2	2.02	0.41
1:G:73:ASN:HA	1:G:74:PRO:HD3	1.92	0.41
1:K:149:LYS:HE2	1:K:256:TYR:HE1	1.86	0.41
1:C:202:VAL:HG11	1:C:251:LEU:HD13	2.03	0.41
1:C:100:GLY:HA3	1:C:230:MET:O	2.21	0.41
2:D:48:ILE:O	2:D:52:VAL:HG23	2.20	0.41
1:I:169:ILE:HD13	1:I:242:LYS:HG3	2.03	0.41
1:K:156:LYS:HE2	1:K:193:SER:O	2.21	0.41
2:B:18:VAL:HG22	2:B:18:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:HIS:CD2	1:E:299:PRO:HD2	2.56	0.41
1:A:307:LYS:HG3	2:B:92:TRP:CE2	2.55	0.41
1:C:157:LYS:HA	8:C:704:HOH:O	2.21	0.41
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.56	0.41
2:J:145:ASP:O	2:J:148:CYS:HB3	2.20	0.41
1:A:169:ILE:HD12	1:A:169:ILE:N	2.35	0.41
1:E:72:GLY:CA	1:E:149:LYS:H	2.24	0.41
1:G:139:CYS:O	1:G:146:SER:HB3	2.21	0.41
1:G:307:LYS:HE2	2:H:61:THR:HG22	2.03	0.41
1:I:156:LYS:HE2	1:I:193:SER:O	2.20	0.41
2:L:158:ASP:OD2	2:L:160:PRO:HD2	2.20	0.41
1:A:44:GLU:OE1	1:A:46:LYS:HG2	2.21	0.41
1:A:303:GLY:HA2	2:B:63:PHE:CE1	2.56	0.41
2:H:159:TYR:HB3	2:H:160:PRO:HD3	2.03	0.41
1:I:114:SER:HB2	1:I:266:SER:CB	2.50	0.41
1:I:195:TYR:O	1:I:196:GLN:HB3	2.21	0.41
1:I:308:TYR:CD2	2:J:89:LEU:HD13	2.56	0.41
2:D:18:VAL:O	2:D:18:VAL:HG22	2.21	0.40
1:E:323:ILE:HD11	2:F:7:ALA:HB2	2.02	0.40
1:I:86:TYR:HA	1:I:113:SER:O	2.21	0.40
1:A:133(A):LYS:O	3:M:4:SIA:H113	2.21	0.40
2:B:9:PHE:CD1	2:B:10:ILE:HG13	2.57	0.40
1:E:72:GLY:O	1:E:149:LYS:HG3	2.21	0.40
2:H:98:LEU:HD23	2:H:98:LEU:HA	1.90	0.40
2:L:127:LYS:CG	2:L:128:ASN:N	2.84	0.40
1:C:172:LYS:C	1:C:174:LYS:H	2.24	0.40
1:E:130:HIS:NE2	1:E:162:PRO:HD2	2.37	0.40
2:F:152:VAL:HG22	2:F:157:TYR:CD1	2.56	0.40
1:A:45:ASP:C	1:A:297:ILE:HD11	2.41	0.40
2:D:102:LEU:HD12	2:D:102:LEU:HA	1.95	0.40
1:C:71:LEU:O	1:C:148:TYR:HB3	2.21	0.40
1:E:70:ILE:HD12	1:E:70:ILE:HA	1.92	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%)	303 (94%)	17 (5%)	1 (0%)	41	37
1	C	316/329 (96%)	304 (96%)	11 (4%)	1 (0%)	41	37
1	E	321/329 (98%)	303 (94%)	15 (5%)	3 (1%)	17	11
1	G	317/329 (96%)	299 (94%)	18 (6%)	0	100	100
1	I	315/329 (96%)	297 (94%)	17 (5%)	1 (0%)	41	37
1	K	316/329 (96%)	304 (96%)	10 (3%)	2 (1%)	25	18
2	B	172/177 (97%)	168 (98%)	4 (2%)	0	100	100
2	D	169/177 (96%)	159 (94%)	8 (5%)	2 (1%)	13	7
2	F	168/177 (95%)	155 (92%)	13 (8%)	0	100	100
2	H	168/177 (95%)	155 (92%)	13 (8%)	0	100	100
2	J	167/177 (94%)	157 (94%)	8 (5%)	2 (1%)	13	7
2	L	168/177 (95%)	163 (97%)	5 (3%)	0	100	100
All	All	2918/3036 (96%)	2767 (95%)	139 (5%)	12 (0%)	34	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	116(A)	SER
1	E	159	ASN
1	A	92	SER
1	E	80	SER
1	I	93	ASP
2	J	60	ASN
1	K	265	GLY
2	D	60	ASN
2	J	135	ASN
1	K	264	ALA
1	C	94	ASN
2	D	145	ASP

### 5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/290 (98%)	279 (98%)	6 (2%)	53	57
1	C	282/290 (97%)	276 (98%)	6 (2%)	53	57
1	E	285/290 (98%)	278 (98%)	7 (2%)	47	49
1	G	283/290 (98%)	276 (98%)	7 (2%)	47	49
1	I	281/290 (97%)	267 (95%)	14 (5%)	24	21
1	K	281/290 (97%)	274 (98%)	7 (2%)	47	49
2	B	150/152 (99%)	143 (95%)	7 (5%)	26	23
2	D	147/152 (97%)	141 (96%)	6 (4%)	30	29
2	F	146/152 (96%)	141 (97%)	5 (3%)	37	35
2	H	146/152 (96%)	143 (98%)	3 (2%)	53	57
2	J	145/152 (95%)	139 (96%)	6 (4%)	30	29
2	L	146/152 (96%)	143 (98%)	3 (2%)	53	57
All	All	2577/2652 (97%)	2500 (97%)	77 (3%)	41	40

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	81	THR
1	A	93	ASP
1	A	115	VAL
1	A	253	VAL
1	A	320	LEU
2	B	22	TYR
2	B	29	GLU
2	B	97	GLU
2	B	128	ASN
2	B	161	LYS
2	B	164	GLU
2	B	174	ASP
1	C	155	VAL
1	C	193	SER
1	C	277	CYS
1	C	295	GLN
1	C	316	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	320	LEU
2	D	22	TYR
2	D	57	GLU
2	D	68	LYS
2	D	72	HIS
2	D	95	ASN
2	D	102	LEU
1	E	54	LEU
1	E	80	SER
1	E	81	THR
1	E	136	THR
1	E	194	LEU
1	E	295	GLN
1	E	320	LEU
2	F	22	TYR
2	F	102	LEU
2	F	150	GLU
2	F	167	LYS
2	F	170	ARG
1	G	21	ASN
1	G	136	THR
1	G	159	ASN
1	G	203	PHE
1	G	253	VAL
1	G	261	GLU
1	G	315	ARG
2	H	29	GLU
2	H	60	ASN
2	H	68	LYS
1	I	54	LEU
1	I	55	ARG
1	I	77	GLU
1	I	97	CYS
1	I	102	PHE
1	I	125	SER
1	I	164	LEU
1	I	203	PHE
1	I	244	THR
1	I	261	GLU
1	I	272	THR
1	I	295	GLN
1	I	316	LEU

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Mol	Chain	Res	Type
1	I	320	LEU
2	J	22	TYR
2	J	26	HIS
2	J	102	LEU
2	J	123	ARG
2	J	133	ILE
2	J	154	ASN
1	K	30	LEU
1	K	55	ARG
1	K	102	PHE
1	K	274	VAL
1	K	283	THR
1	K	295	GLN
1	K	320	LEU
2	L	38	LEU
2	L	102	LEU
2	L	149	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	79	ASN
2	B	95	ASN
1	C	263	ASN
2	D	43	ASN
2	D	72	HIS
2	D	95	ASN
1	E	298	HIS
2	F	30	GLN
1	G	159	ASN
2	H	43	ASN
2	H	60	ASN
2	H	62	GLN
2	H	142	HIS
1	I	289	ASN
2	J	95	ASN
1	K	196	GLN
1	K	263	ASN
2	L	62	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

20 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	GAL	M	1	3	12,12,12	0.54	0	17,17,17	0.49	0
3	NAG	M	2	3	14,14,15	0.57	0	17,19,21	1.06	1 (5%)
3	GAL	M	3	3	11,11,12	0.63	0	15,15,17	0.77	1 (6%)
3	SIA	M	4	3	20,20,21	0.56	0	24,28,31	0.99	1 (4%)
3	GAL	N	1	3	12,12,12	0.58	0	17,17,17	0.59	0
3	NAG	N	2	3	14,14,15	0.62	0	17,19,21	0.90	1 (5%)
3	GAL	N	3	3	11,11,12	0.68	0	15,15,17	0.74	0
3	SIA	N	4	3	20,20,21	0.59	0	24,28,31	1.20	3 (12%)
4	NAG	O	1	4	14,14,15	0.57	0	17,19,21	0.80	0
4	GAL	O	2	4	11,11,12	0.60	0	15,15,17	0.85	0
4	SIA	O	3	4	20,20,21	0.53	0	24,28,31	0.99	2 (8%)
5	NAG	P	1	1,5	14,14,15	0.55	0	17,19,21	0.92	0
5	NAG	P	2	5	14,14,15	0.65	0	17,19,21	1.36	3 (17%)
4	NAG	Q	1	4	14,14,15	0.57	0	17,19,21	0.72	0
4	GAL	Q	2	4	11,11,12	0.67	0	15,15,17	0.74	0
4	SIA	Q	3	4	20,20,21	0.57	0	24,28,31	1.07	2 (8%)
3	GAL	R	1	3	12,12,12	0.53	0	17,17,17	0.59	0
3	NAG	R	2	3	14,14,15	0.67	0	17,19,21	1.00	1 (5%)
3	GAL	R	3	3	11,11,12	0.67	0	15,15,17	0.71	0
3	SIA	R	4	3	20,20,21	0.64	0	24,28,31	1.12	1 (4%)



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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2	NAG	C1-O5-C5	3.36	116.74	112.19
5	P	2	NAG	C4-C3-C2	2.99	115.39	111.02
4	Q	3	SIA	C6-O6-C2	2.92	117.58	111.34
5	P	2	NAG	C2-N2-C7	-2.67	119.11	122.90
3	N	2	NAG	C1-O5-C5	2.60	115.72	112.19
5	P	2	NAG	C3-C4-C5	2.47	114.64	110.24
3	R	4	SIA	C6-O6-C2	2.43	116.54	111.34
3	N	4	SIA	O6-C2-C3	2.35	113.69	110.46
4	O	3	SIA	C6-O6-C2	2.33	116.32	111.34
4	O	3	SIA	O1B-C1-C2	2.19	119.27	113.03
3	M	4	SIA	O1B-C1-C2	2.17	119.22	113.03
3	M	3	GAL	O5-C1-C2	-2.09	107.54	110.77
3	R	2	NAG	O5-C1-C2	2.06	114.54	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Q	3	SIA	O1B-C1-C2	2.03	118.83	113.03
3	N	4	SIA	O1B-C1-C2	2.02	118.81	113.03
3	N	4	SIA	O1A-C1-C2	-2.01	117.82	122.57

There are no chirality outliers.

All (11) torsion outliers are listed below:

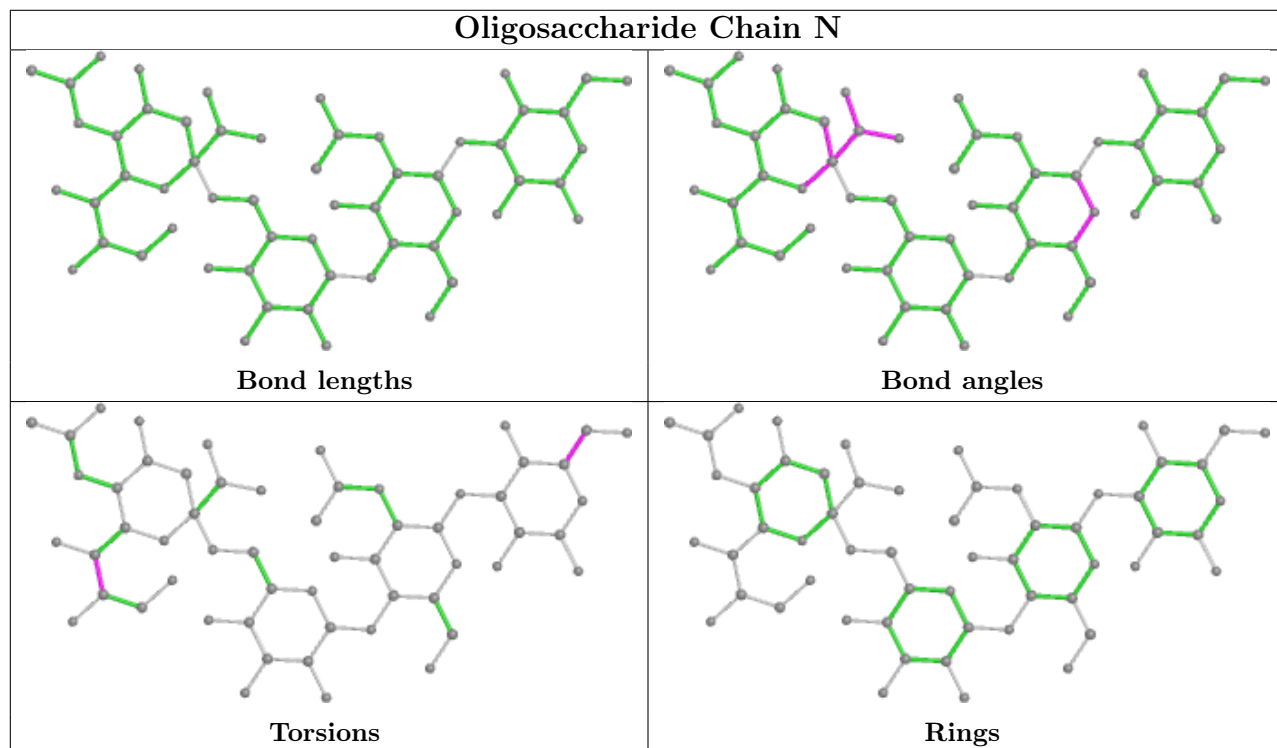
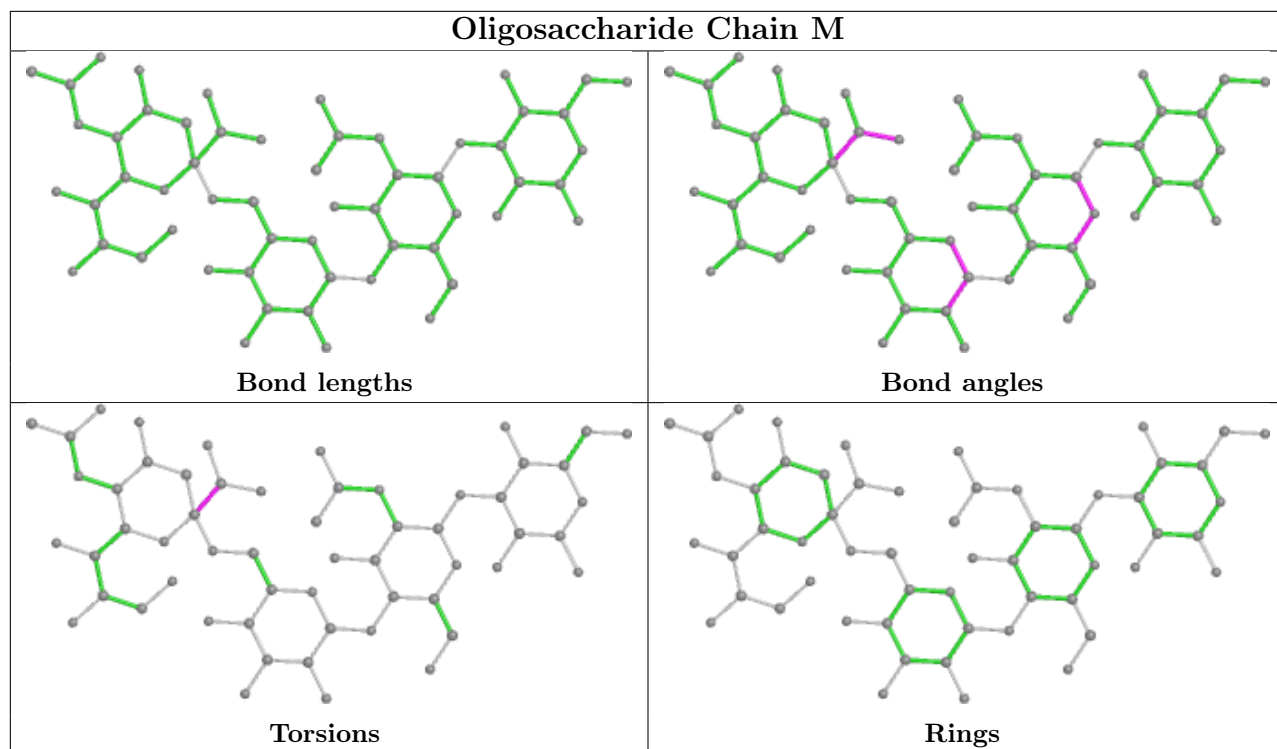
Mol	Chain	Res	Type	Atoms
3	N	1	GAL	O5-C5-C6-O6
3	N	1	GAL	C4-C5-C6-O6
3	R	1	GAL	O5-C5-C6-O6
5	P	1	NAG	C8-C7-N2-C2
3	N	4	SIA	C6-C7-C8-O8
5	P	1	NAG	O7-C7-N2-C2
3	M	4	SIA	O1B-C1-C2-O6
3	R	4	SIA	O1B-C1-C2-O6
4	Q	3	SIA	O1B-C1-C2-O6
3	N	4	SIA	O7-C7-C8-O8
3	N	4	SIA	O7-C7-C8-C9

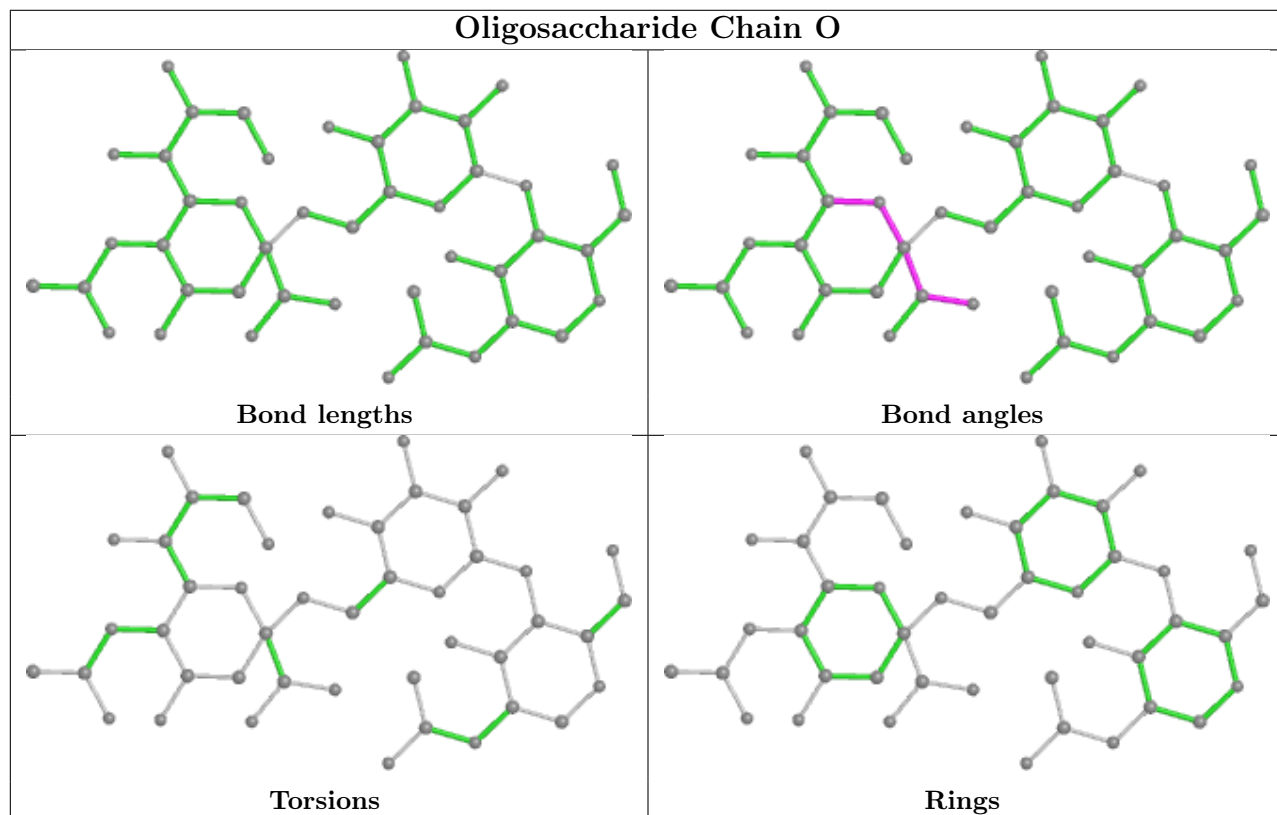
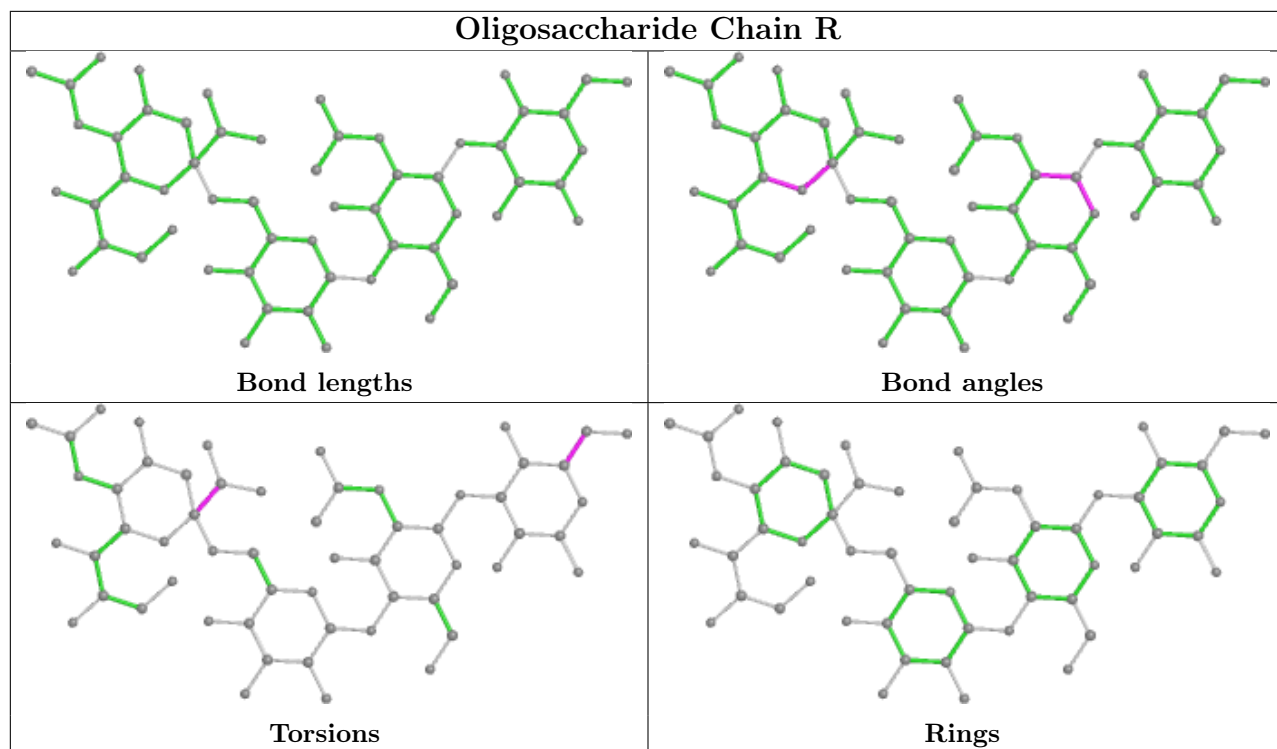
There are no ring outliers.

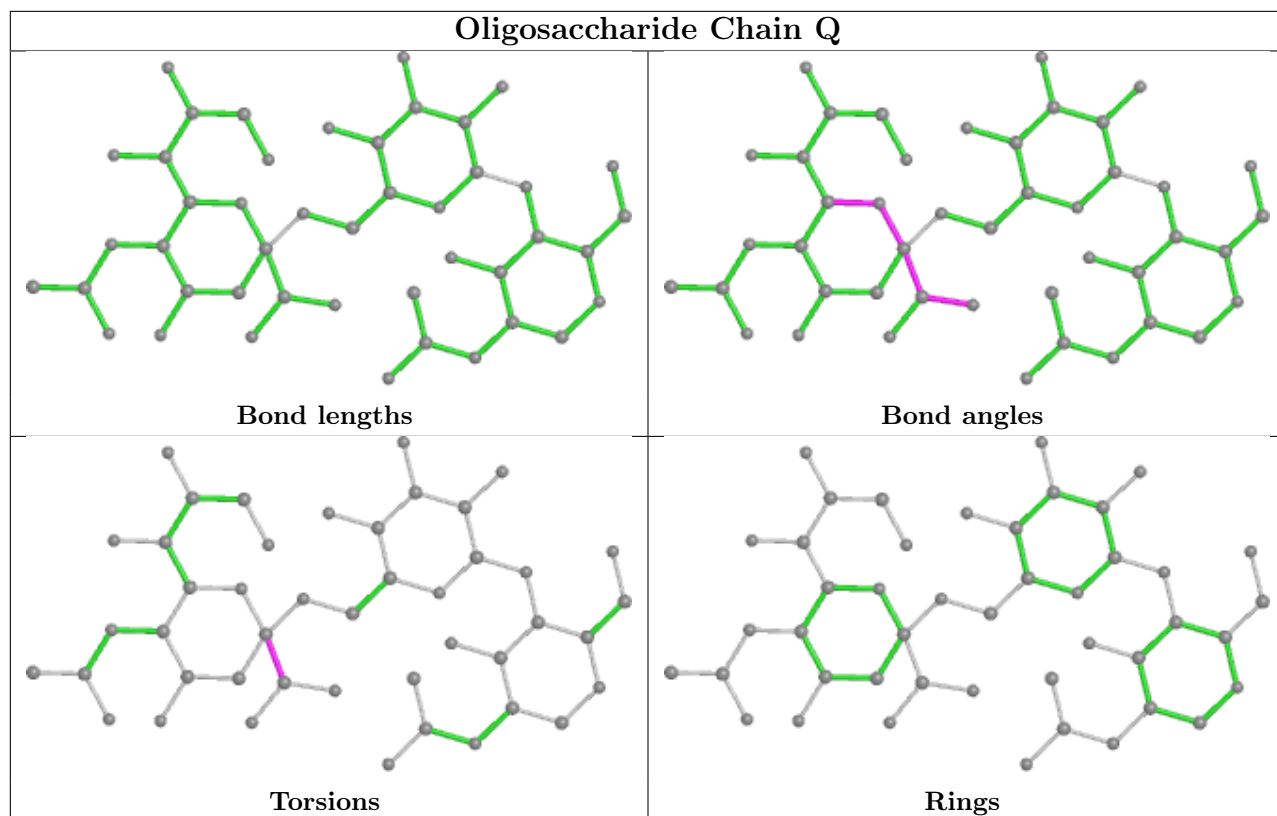
2 monomers are involved in 2 short contacts:

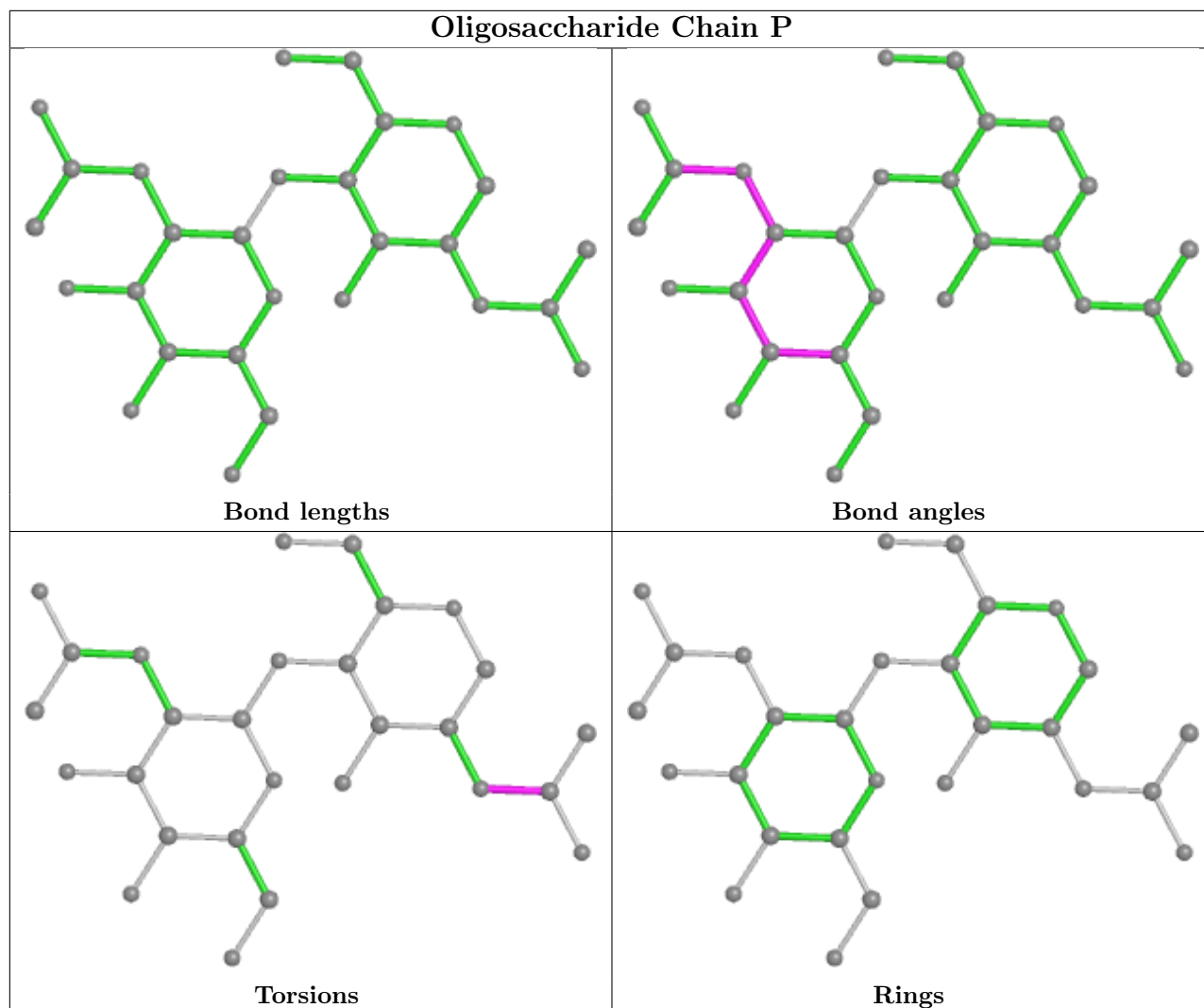
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	4	SIA	1	0
4	O	3	SIA	1	0

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](#)

8 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	K	641	1	14,14,15	0.43	0	17,19,21	1.51	3 (17%)
6	NAG	C	334	1	14,14,15	0.50	0	17,19,21	0.80	0
6	NAG	A	336	1	14,14,15	0.61	0	17,19,21	1.37	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	A	335	1	14,14,15	0.43	0	17,19,21	1.07	1 (5%)
6	NAG	A	334	1	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
7	SIA	G	401	-	20,20,21	0.60	0	24,28,31	0.99	2 (8%)
6	NAG	E	333	1	14,14,15	0.49	0	17,19,21	0.87	0
6	NAG	J	561	2	14,14,15	0.49	0	17,19,21	0.86	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	K	641	1	-	0/6/23/26	0/1/1/1
6	NAG	C	334	1	-	0/6/23/26	0/1/1/1
6	NAG	A	336	1	-	4/6/23/26	0/1/1/1
6	NAG	A	335	1	-	0/6/23/26	0/1/1/1
6	NAG	A	334	1	-	2/6/23/26	0/1/1/1
7	SIA	G	401	-	-	0/18/34/38	0/1/1/1
6	NAG	E	333	1	-	0/6/23/26	0/1/1/1
6	NAG	J	561	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	336	NAG	O5-C1-C2	-4.32	104.47	111.29
6	K	641	NAG	C1-O5-C5	3.77	117.30	112.19
6	K	641	NAG	C4-C3-C2	-2.88	106.80	111.02
6	A	335	NAG	C1-O5-C5	2.57	115.68	112.19
6	K	641	NAG	C2-N2-C7	-2.40	119.49	122.90
6	A	334	NAG	O5-C5-C6	2.17	110.61	107.20
7	G	401	SIA	O1B-C1-C2	2.09	118.99	113.03
7	G	401	SIA	C6-O6-C2	2.08	115.78	111.34

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	336	NAG	C8-C7-N2-C2
6	J	561	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	336	NAG	O7-C7-N2-C2
6	J	561	NAG	O7-C7-N2-C2
6	A	334	NAG	C4-C5-C6-O6
6	A	336	NAG	O5-C5-C6-O6
6	A	334	NAG	O5-C5-C6-O6
6	A	336	NAG	C1-C2-N2-C7

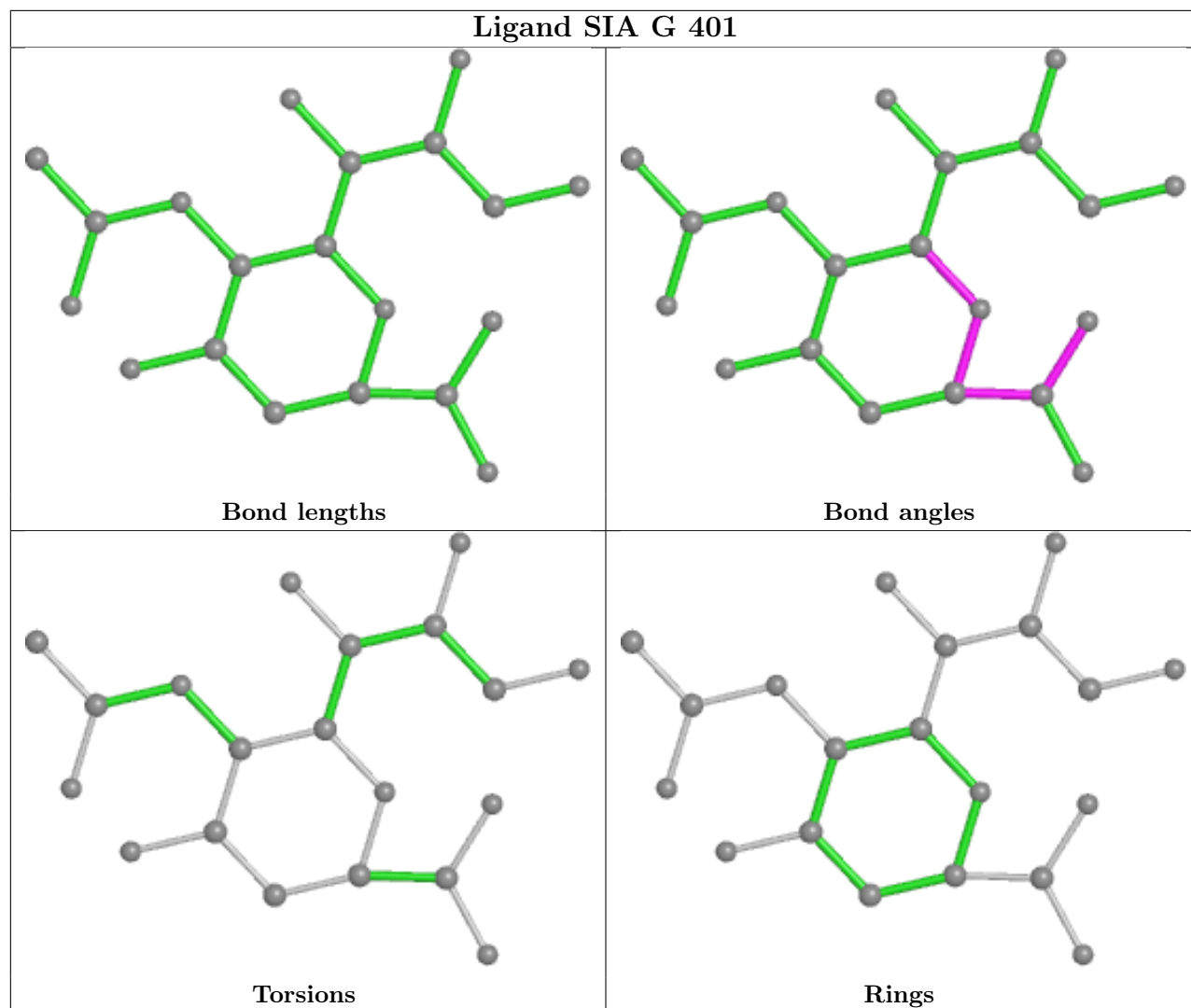
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	334	NAG	1	0
6	A	336	NAG	1	0
6	E	333	NAG	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	323/329 (98%)	-0.01	3 (0%) 84 88	21, 34, 52, 71	0
1	C	320/329 (97%)	-0.24	2 (0%) 89 91	20, 33, 51, 76	0
1	E	323/329 (98%)	-0.01	6 (1%) 66 74	24, 38, 58, 80	0
1	G	321/329 (97%)	-0.04	8 (2%) 57 65	22, 35, 56, 71	0
1	I	319/329 (96%)	-0.08	6 (1%) 66 74	28, 41, 57, 77	0
1	K	320/329 (97%)	-0.02	5 (1%) 72 77	22, 35, 53, 71	0
2	B	174/177 (98%)	0.11	6 (3%) 45 53	24, 43, 66, 82	0
2	D	171/177 (96%)	0.59	26 (15%) 2 2	23, 43, 76, 96	0
2	F	170/177 (96%)	0.60	20 (11%) 4 6	22, 44, 80, 95	0
2	H	170/177 (96%)	0.76	26 (15%) 2 2	23, 47, 84, 95	0
2	J	169/177 (95%)	0.23	5 (2%) 50 59	22, 46, 68, 77	0
2	L	170/177 (96%)	0.16	4 (2%) 59 67	22, 41, 61, 69	0
All	All	2950/3036 (97%)	0.10	117 (3%) 38 47	20, 38, 68, 96	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	LEU	7.3
2	H	144	CYS	6.0
2	D	160	PRO	5.6
2	D	152	VAL	5.1
2	H	29	GLU	5.0
2	H	143	LYS	4.9
2	H	164	GLU	4.8
2	D	147	THR	4.6
1	I	290	THR	4.6
2	D	166	ALA	4.5
2	H	168	LEU	4.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	29	GLU	4.4
2	H	159	TYR	4.2
1	K	94	ASN	4.2
2	H	160	PRO	4.2
1	I	264	ALA	4.1
2	D	156	THR	4.1
1	G	12	THR	4.1
2	D	144	CYS	3.9
2	J	166	ALA	3.9
2	F	156	THR	3.9
2	H	140	PHE	3.9
2	B	173	ILE	3.9
2	D	158	ASP	3.9
2	D	143	LYS	3.9
1	G	81	THR	3.8
2	F	144	CYS	3.8
2	F	161	LYS	3.7
2	F	162	TYR	3.6
2	F	31	GLY	3.6
2	F	160	PRO	3.4
2	J	168	LEU	3.4
2	H	33	GLY	3.4
2	H	141	TYR	3.3
2	H	167	LYS	3.3
2	H	166	ALA	3.2
2	F	166	ALA	3.2
2	D	168	LEU	3.2
1	I	55	ARG	3.1
2	F	147	THR	3.1
2	D	159	TYR	3.1
2	F	140	PHE	3.1
1	E	80	SER	3.1
1	G	13	LEU	3.0
2	F	158	ASP	3.0
2	D	162	TYR	3.0
2	H	158	ASP	3.0
1	K	93	ASP	3.0
1	A	325	SER	3.0
1	I	325	SER	3.0
2	D	157	TYR	3.0
1	E	78	SER	2.9
2	D	148	CYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	164	GLU	2.9
1	K	9	PRO	2.9
2	D	138	PHE	2.9
2	D	140	PHE	2.9
2	F	143	LYS	2.9
2	D	16	GLY	2.8
2	D	145	ASP	2.8
2	J	133	ILE	2.8
2	D	128	ASN	2.8
2	H	31	GLY	2.7
2	H	38	LEU	2.7
2	F	28	ASN	2.7
1	C	78	SER	2.7
2	F	26	HIS	2.7
1	G	21	ASN	2.6
1	C	12	THR	2.6
1	E	81	THR	2.6
1	A	143	GLY	2.6
2	H	156	THR	2.6
2	B	174	ASP	2.6
1	I	289	ASN	2.6
2	H	152	VAL	2.5
2	D	154	ASN	2.5
2	H	162	TYR	2.5
2	D	142	HIS	2.5
2	F	167	LYS	2.5
2	B	168	LEU	2.4
2	D	27	GLN	2.4
2	F	170	ARG	2.4
1	I	94	ASN	2.4
2	F	38	LEU	2.4
2	H	30	GLN	2.4
2	H	148	CYS	2.4
1	A	290	THR	2.4
1	E	158	GLY	2.4
2	D	30	GLN	2.3
2	B	31	GLY	2.3
2	J	155	GLY	2.3
1	E	77	GLU	2.3
2	L	156	THR	2.3
1	G	159	ASN	2.3
2	B	33	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	38	LEU	2.2
2	B	160	PRO	2.2
2	H	27	GLN	2.2
2	L	150	GLU	2.2
1	G	15	ILE	2.2
2	D	35	ALA	2.2
2	F	164	GLU	2.2
2	L	27	GLN	2.2
2	H	65	ALA	2.2
1	K	275	HIS	2.1
2	H	145	ASP	2.1
2	H	153	LYS	2.1
2	J	131	LYS	2.1
2	F	157	TYR	2.1
1	G	11	ASP	2.1
2	H	26	HIS	2.1
2	H	134	GLY	2.1
1	E	264	ALA	2.1
1	G	82	ALA	2.1
2	D	149	MET	2.0
1	K	236	LEU	2.0
2	D	18	VAL	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, 95<sup>th</sup> 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.

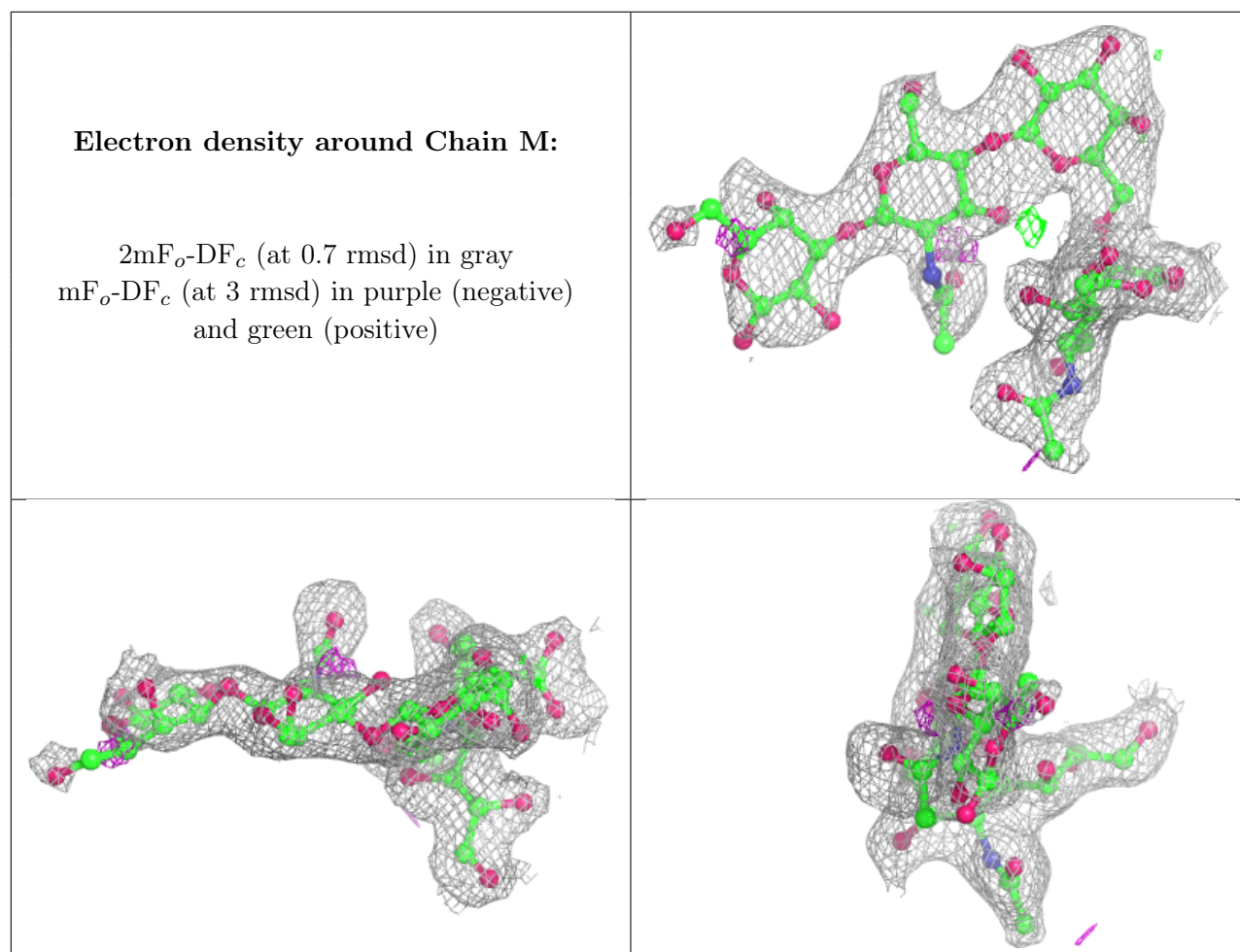
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GAL	N	1	12/12	0.79	0.21	55,70,76,89	0
3	NAG	R	2	14/15	0.79	0.18	46,62,67,67	0
5	NAG	P	2	14/15	0.80	0.24	48,55,66,75	0
3	GAL	R	1	12/12	0.82	0.22	67,76,84,88	0
3	GAL	M	1	12/12	0.85	0.33	63,71,82,83	0
3	NAG	M	2	14/15	0.85	0.20	49,60,65,65	0

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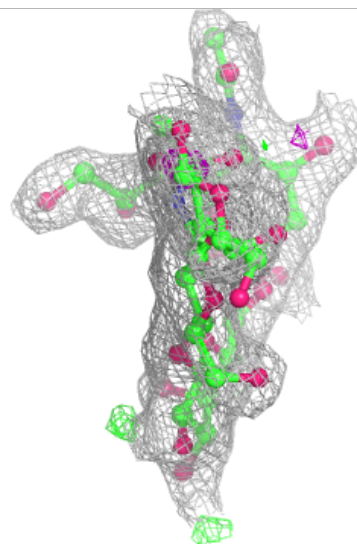
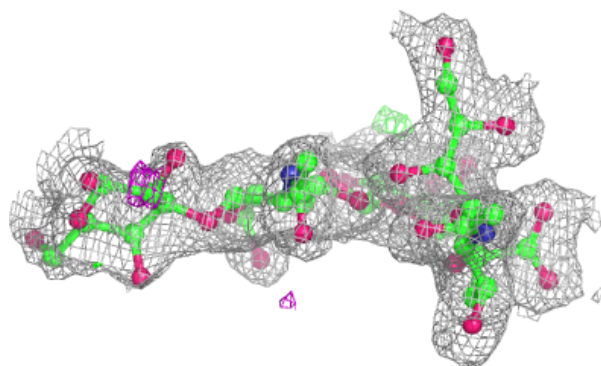
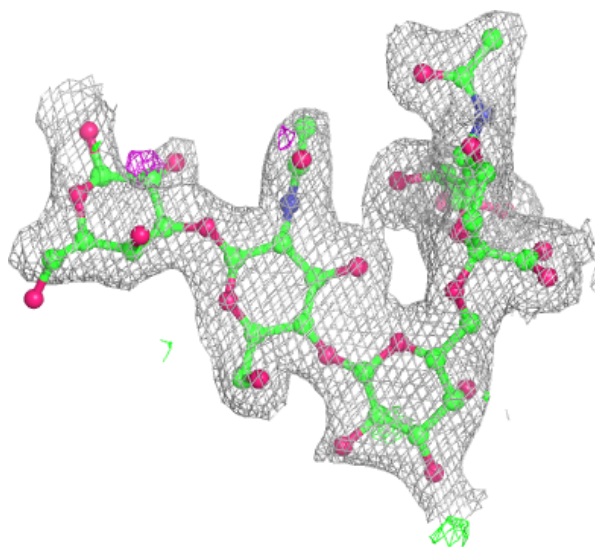
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	O	1	14/15	0.88	0.15	47,51,56,60	0
4	NAG	Q	1	14/15	0.89	0.10	35,44,51,51	0
3	GAL	R	3	11/12	0.90	0.16	40,56,61,69	0
4	GAL	O	2	11/12	0.91	0.10	41,50,54,62	0
3	NAG	N	2	14/15	0.93	0.12	39,49,55,57	0
3	GAL	M	3	11/12	0.93	0.13	39,52,58,62	0
4	SIA	O	3	20/21	0.94	0.10	32,45,50,53	0
3	SIA	M	4	20/21	0.95	0.11	31,37,42,46	0
4	GAL	Q	2	11/12	0.95	0.09	38,43,48,54	0
5	NAG	P	1	14/15	0.95	0.10	32,39,46,46	0
3	GAL	N	3	11/12	0.95	0.12	39,44,53,59	0
3	SIA	R	4	20/21	0.96	0.11	33,40,45,46	0
4	SIA	Q	3	20/21	0.96	0.10	29,38,42,42	0
3	SIA	N	4	20/21	0.97	0.08	27,33,39,42	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.



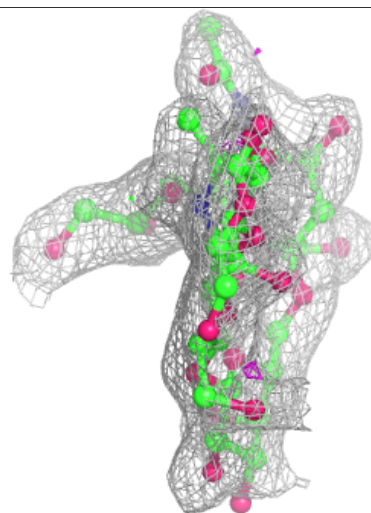
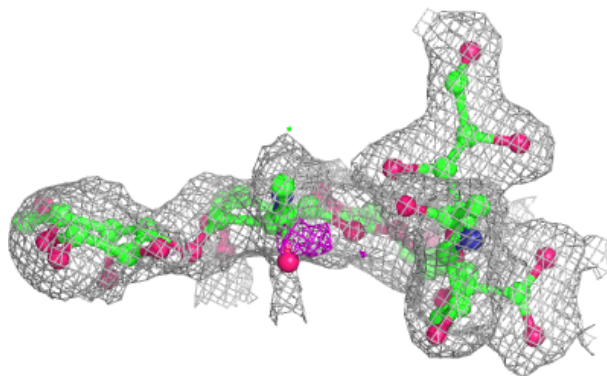
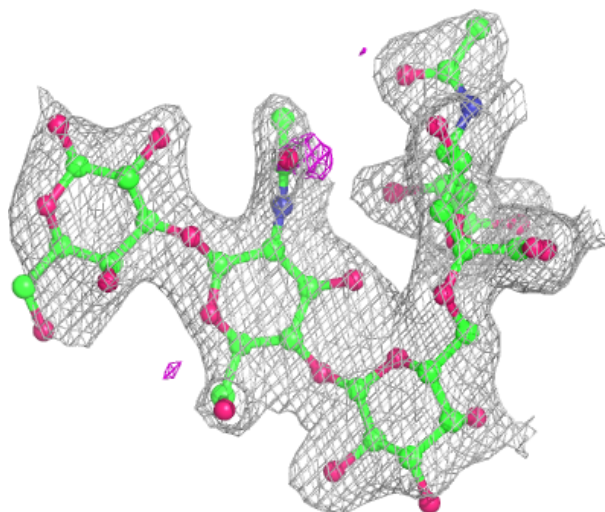
**Electron density around Chain N:**

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



**Electron density around Chain R:**

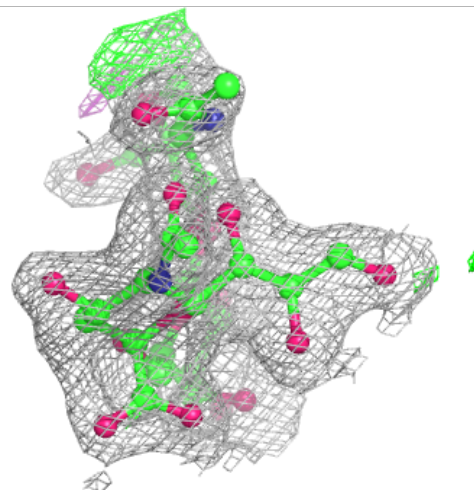
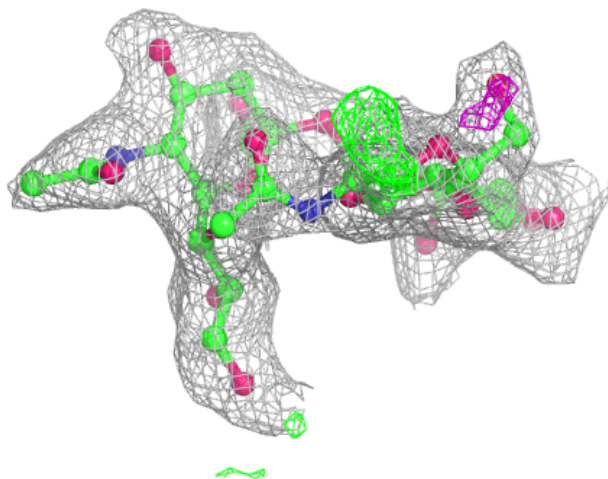
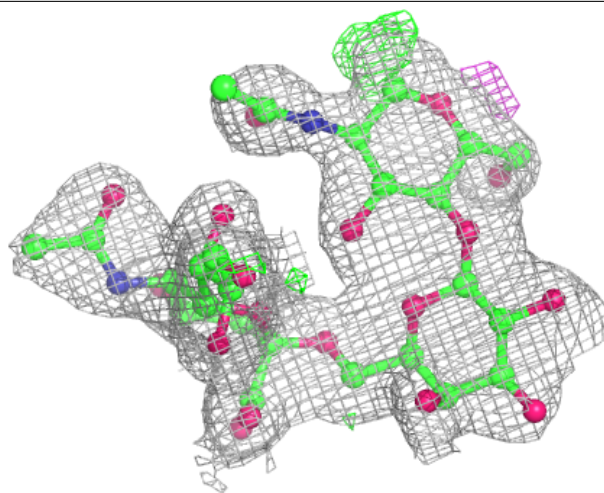
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





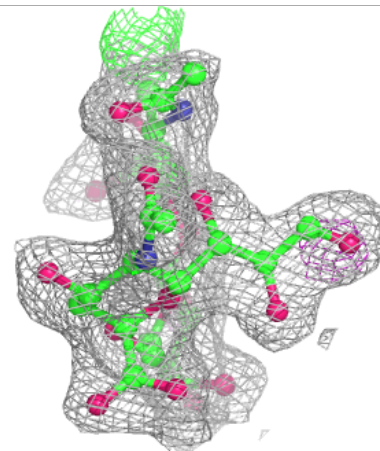
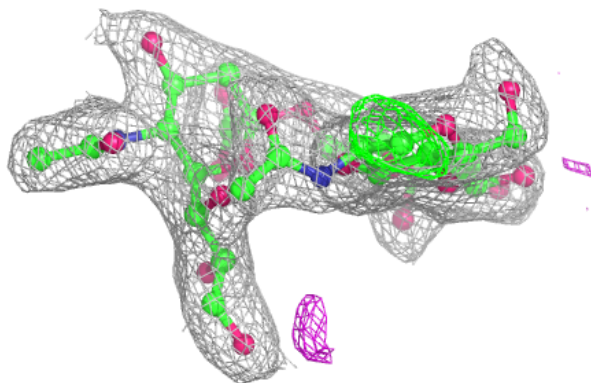
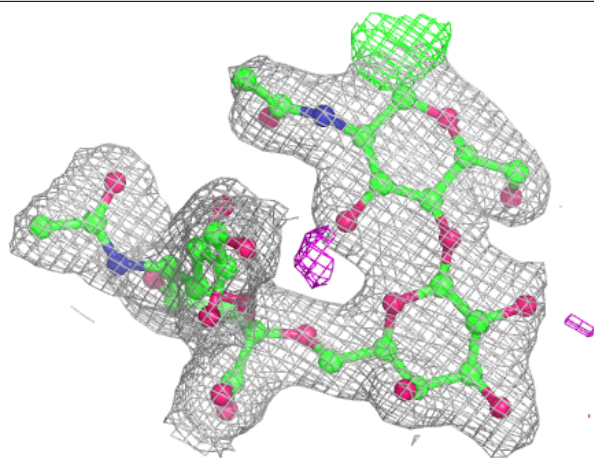
**Electron density around Chain O:**

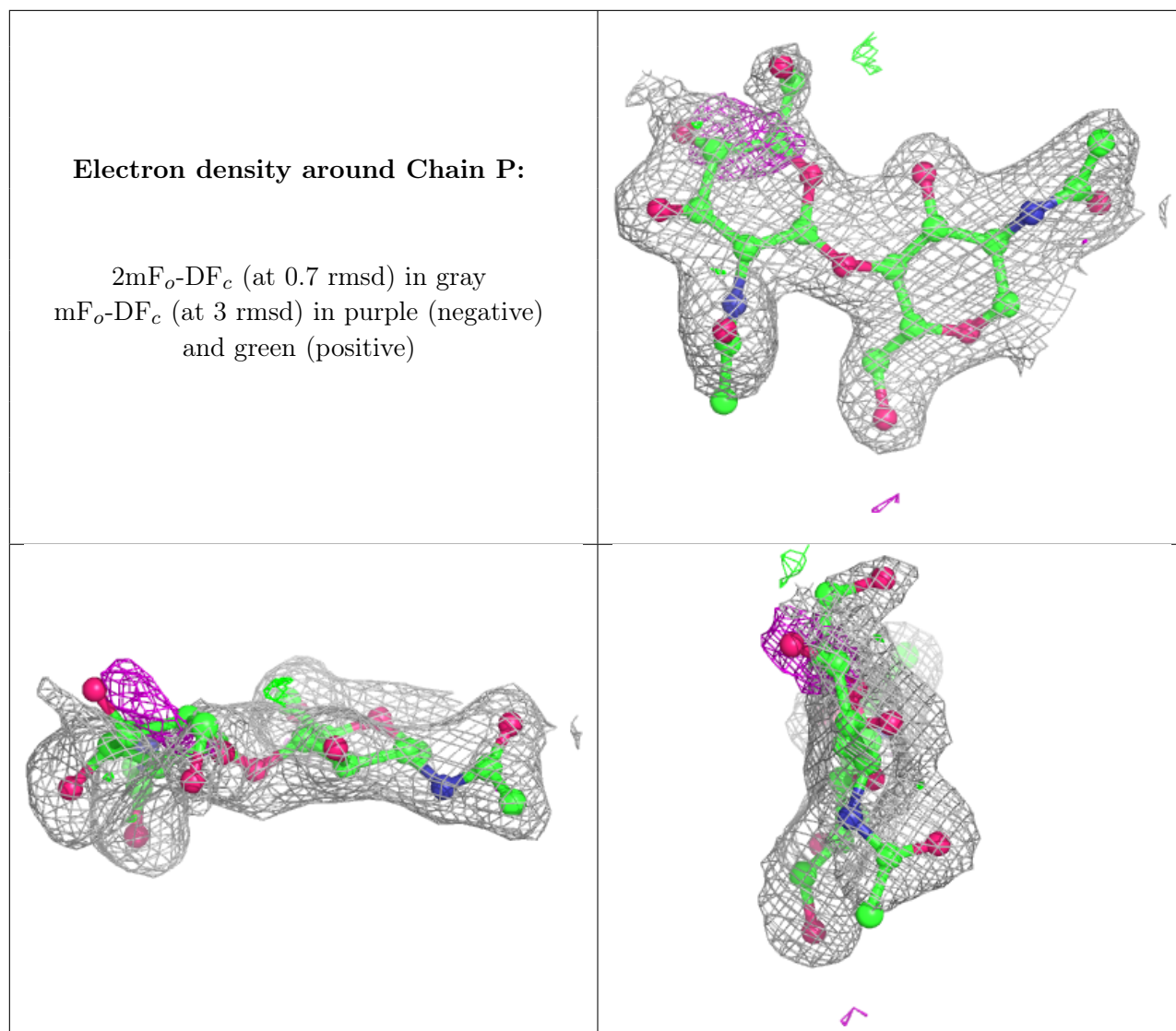
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

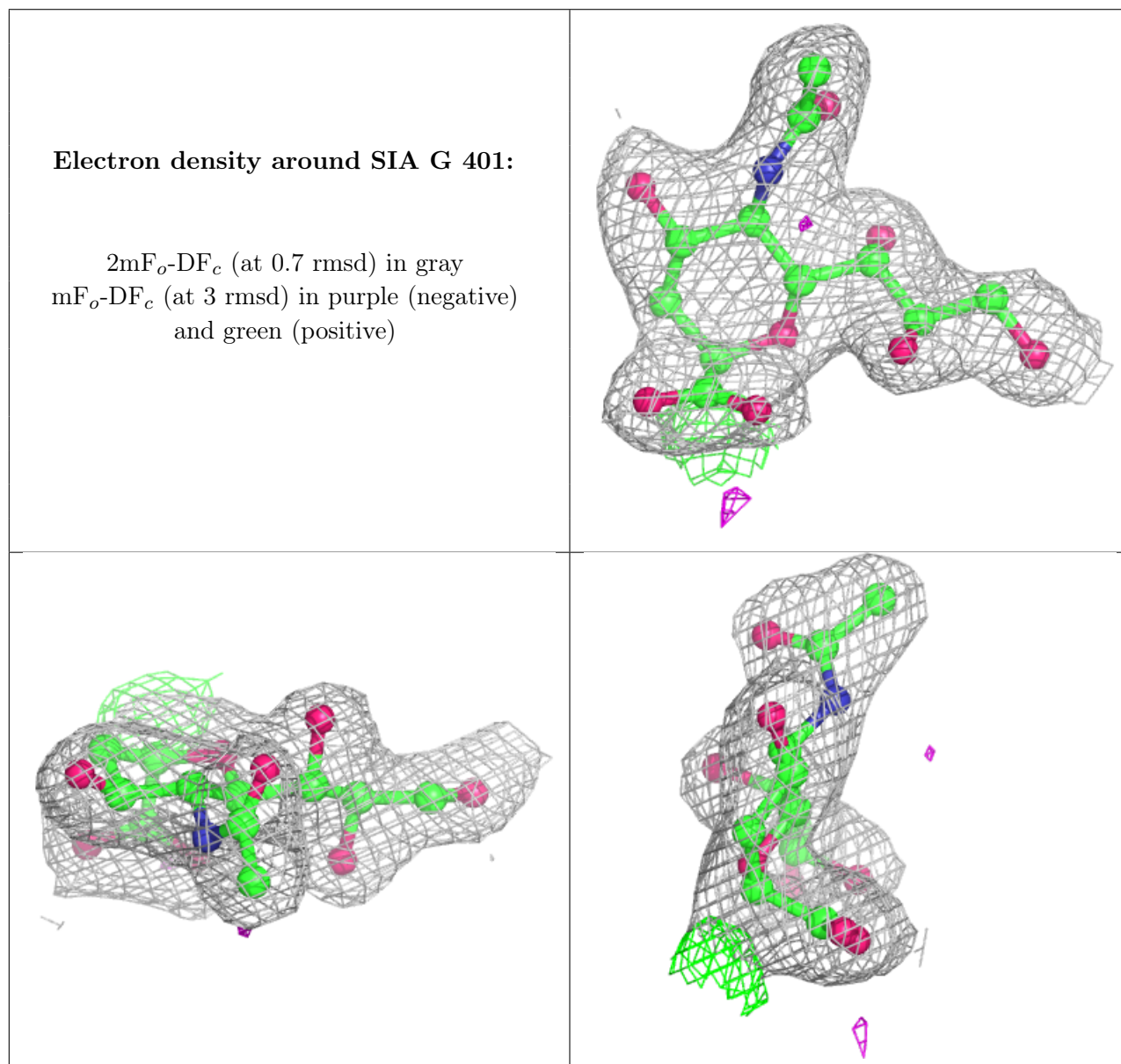
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NAG	A	334	14/15	0.71	0.38	78,80,93,93	0
6	NAG	A	336	14/15	0.77	0.30	62,69,71,76	0
6	NAG	C	334	14/15	0.84	0.16	50,63,74,75	0
6	NAG	J	561	14/15	0.86	0.15	62,69,76,78	0
6	NAG	K	641	14/15	0.88	0.27	65,75,84,88	0
6	NAG	A	335	14/15	0.89	0.13	34,46,56,58	0
6	NAG	E	333	14/15	0.90	0.11	44,51,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SIA	G	401	20/21	0.93	0.11	29,38,45,46	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.